Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 09:26 PM EDT

PDB ID	:	1XXH
Title	:	ATPgS Bound E. Coli Clamp Loader Complex
Authors	:	Kazmirski, S.L.; Podobnik, M.; Weitze, T.F.; O'Donnell, M.; Kuriyan, J.
Deposited on	:	2004-11-05
Resolution	:	3.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

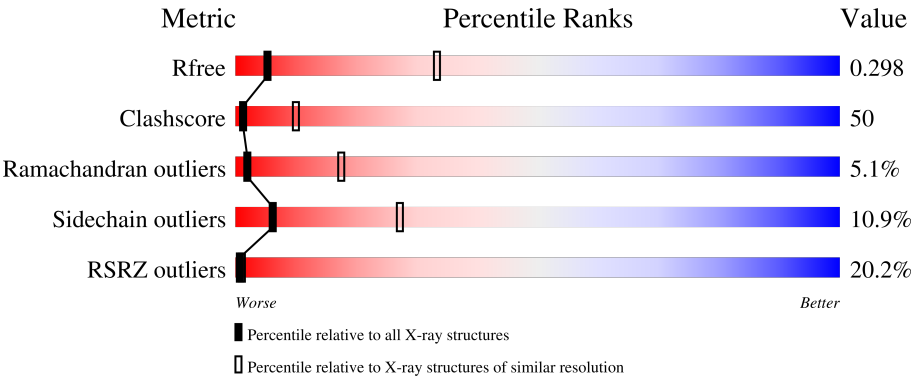
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	12% 28% 53% 16%
1	F	343	21% 35% 54% 8%
2	B	373	13% 38% 48% 12%
2	C	373	8% 29% 56% 13%
2	D	373	7% 32% 54% 11%

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Mol	Chain	Length	Quality of chain
2	G	373	36% 42% 48% 7%
2	H	373	36% 38% 54% 6%
2	I	373	36% 52% 40% 6%
3	E	334	3% 28% 55% 15%
3	J	334	23% 39% 53% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AGS	I	803	-	-	X	-
6	PO4	C	1300	-	-	X	-
6	PO4	H	1400	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 27736 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	Se	0	0	0
			2687	1702	488	487	5	5			
1	F	338	Total	C	N	O	S	Se	0	0	0
			2687	1702	488	487	5	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P28630
A	71	MSE	MET	MODIFIED RESIDUE	UNP P28630
A	223	MSE	MET	MODIFIED RESIDUE	UNP P28630
A	285	MSE	MET	MODIFIED RESIDUE	UNP P28630
A	286	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	1	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	71	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	223	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	285	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	286	MSE	MET	MODIFIED RESIDUE	UNP P28630

- Molecule 2 is a protein called DNA polymerase III subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	C	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
2	D	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	G	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	H	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			

- Molecule 3 is a protein called DNA polymerase III, delta prime subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	Se	0	0	0
			2602	1655	468	466	7	6			
3	J	334	Total	C	N	O	S	Se	0	0	0
			2602	1655	468	466	7	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	35	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	68	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	182	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	253	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	301	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	1	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	35	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	68	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	182	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	253	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	301	MSE	MET	MODIFIED RESIDUE	UNP P28631

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	G	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		

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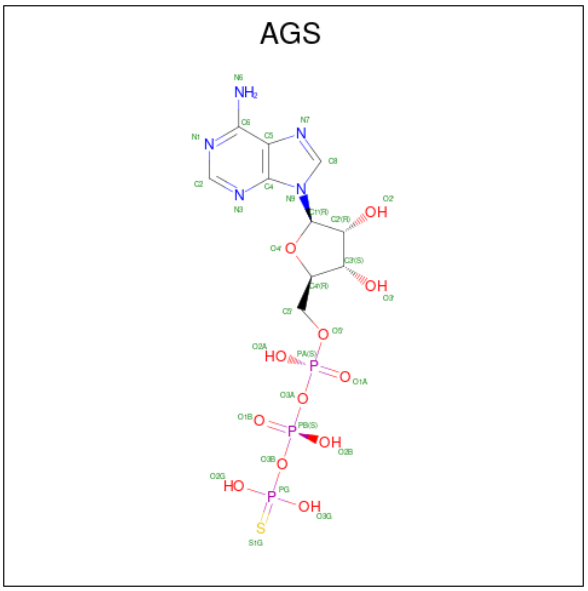
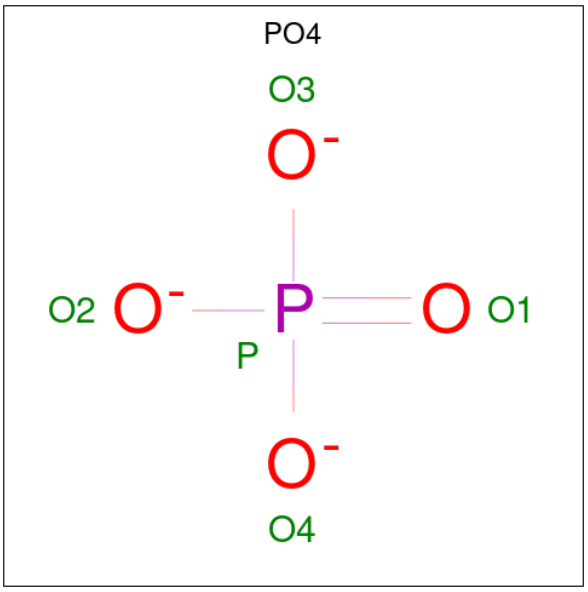
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total Zn 1 1	0	0
4	J	1	Total Zn 1 1	0	0

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O P S 31 10 5 12 3 1	0	0
5	D	1	Total C N O P S 31 10 5 12 3 1	0	0
5	G	1	Total C N O P S 31 10 5 12 3 1	0	0
5	I	1	Total C N O P S 31 10 5 12 3 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



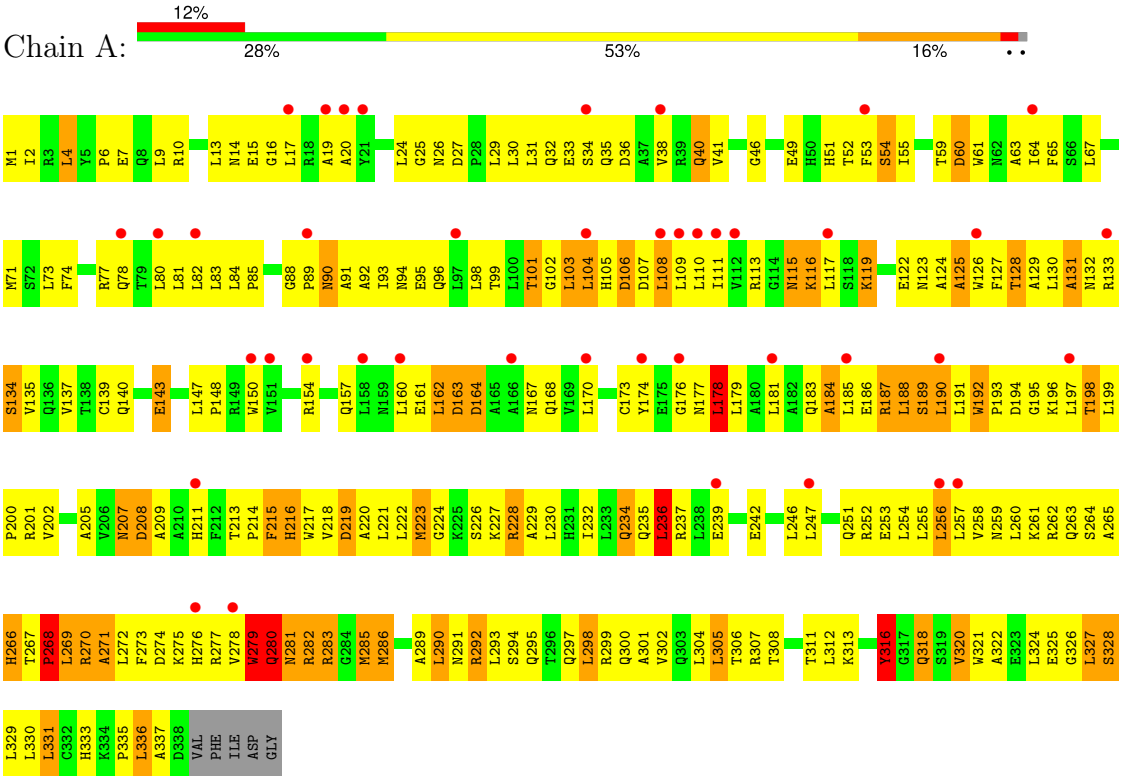
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 5 4 1	0	0
6	H	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

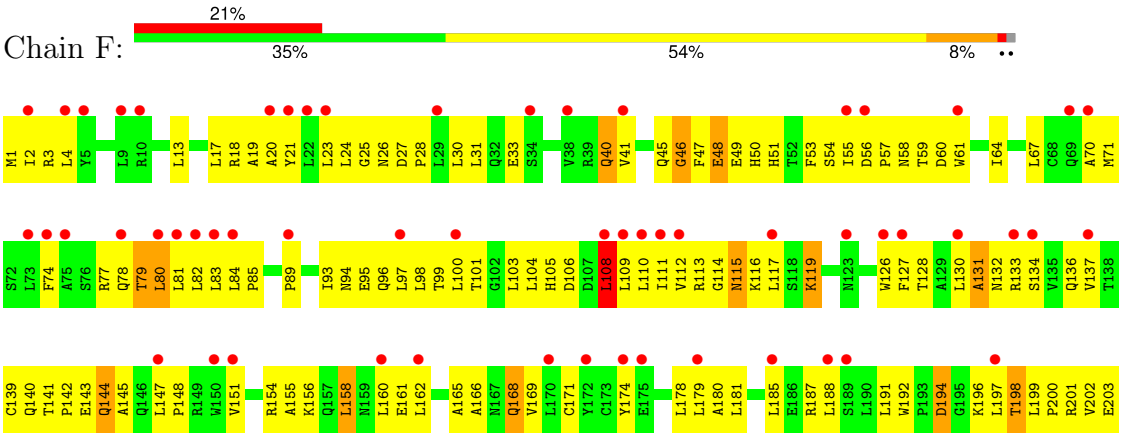
• Molecule 1: DNA polymerase III, delta subunit

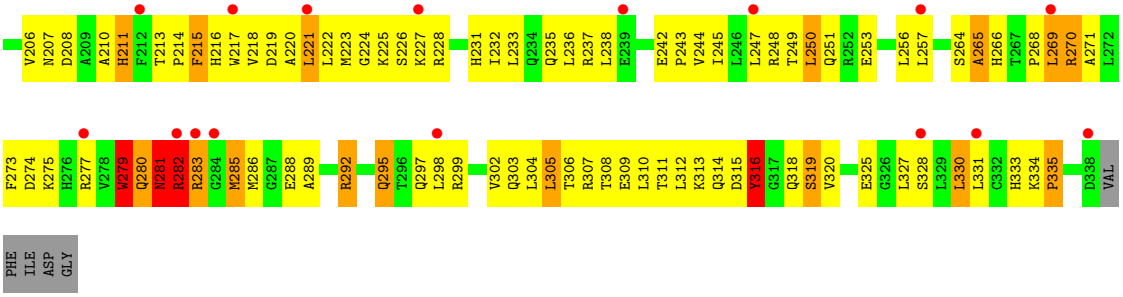
Chain A:



• Molecule 1: DNA polymerase III, delta subunit

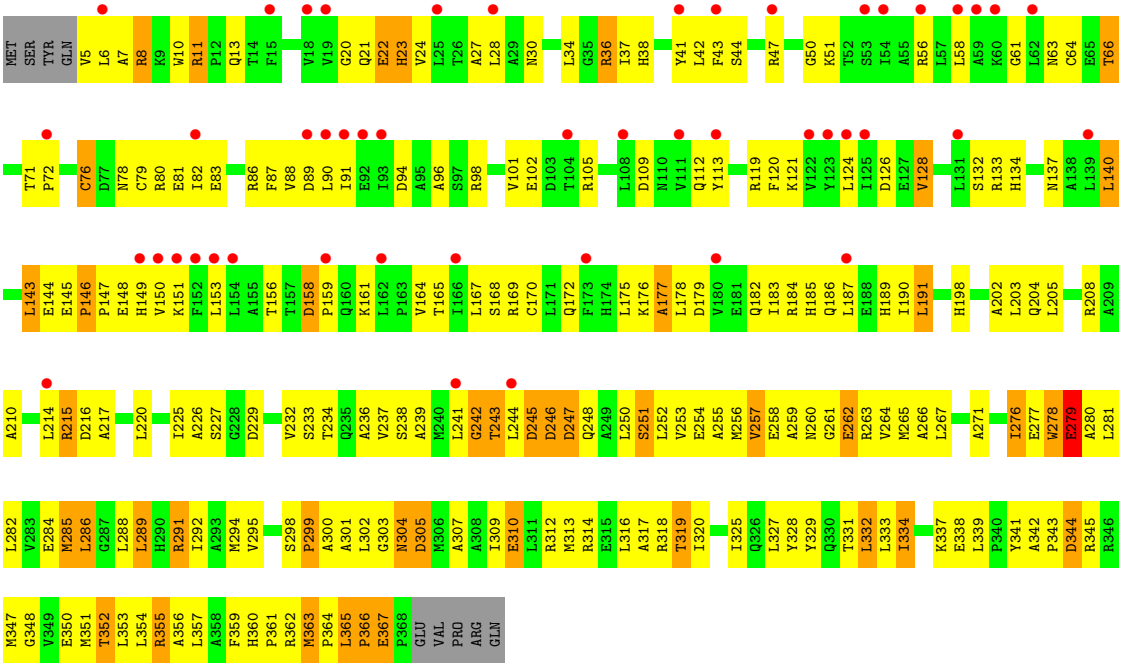
Chain F:





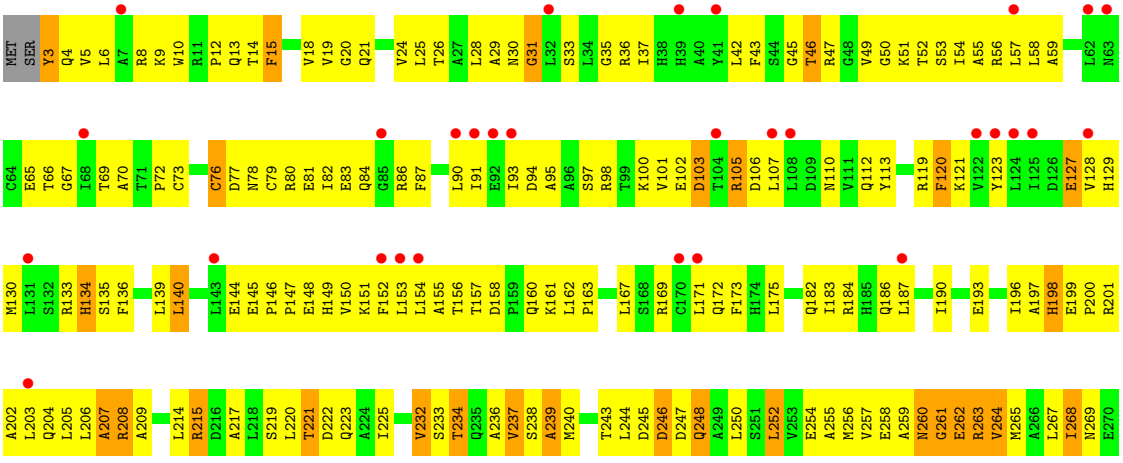
• Molecule 2: DNA polymerase III subunit gamma

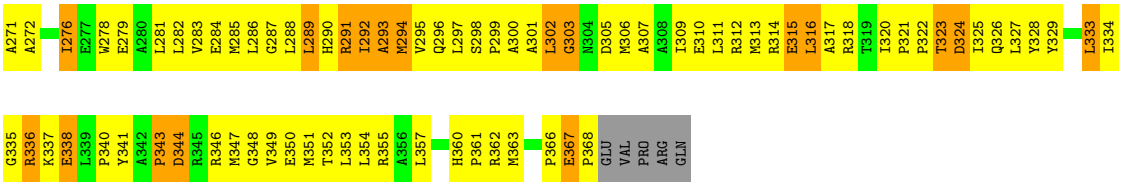
Chain B:



• Molecule 2: DNA polymerase III subunit gamma

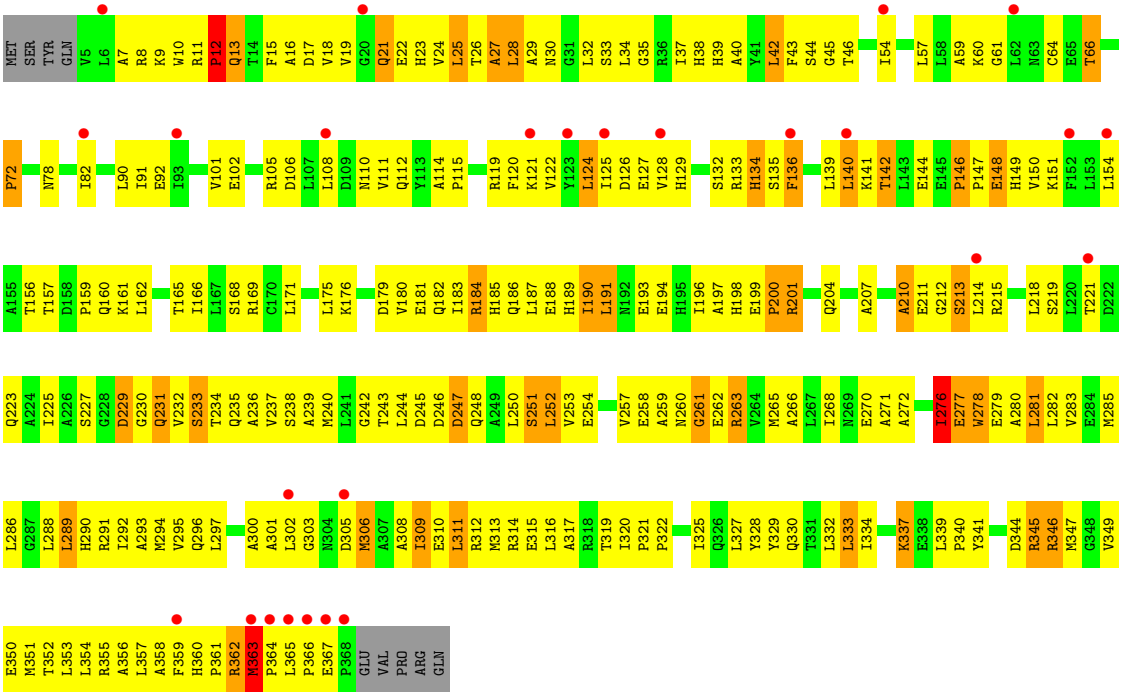
Chain C:





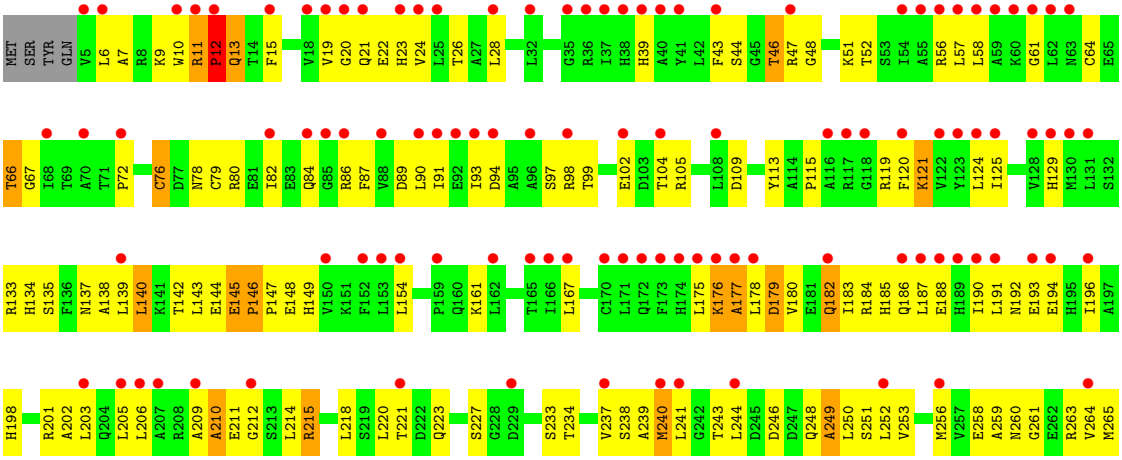
• Molecule 2: DNA polymerase III subunit gamma

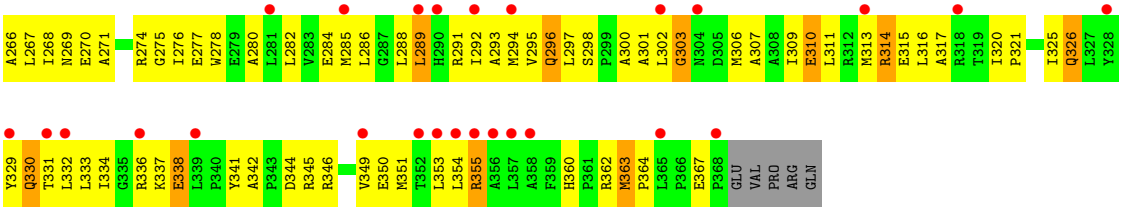
Chain D:



• Molecule 2: DNA polymerase III subunit gamma

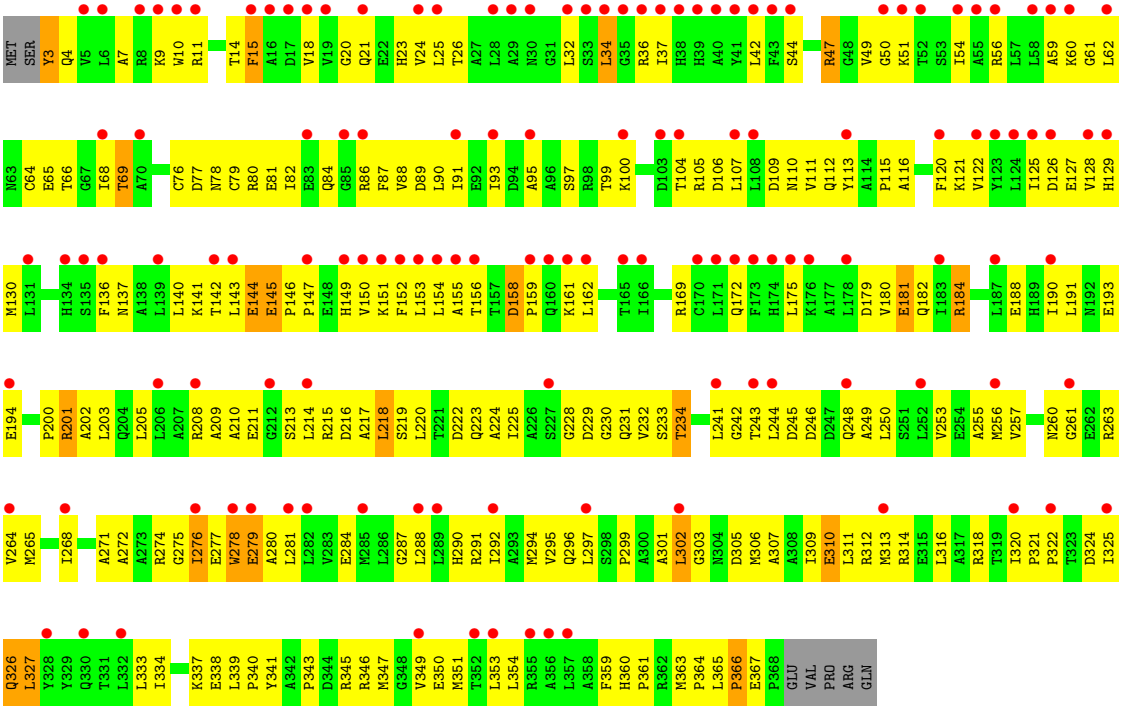
Chain G:





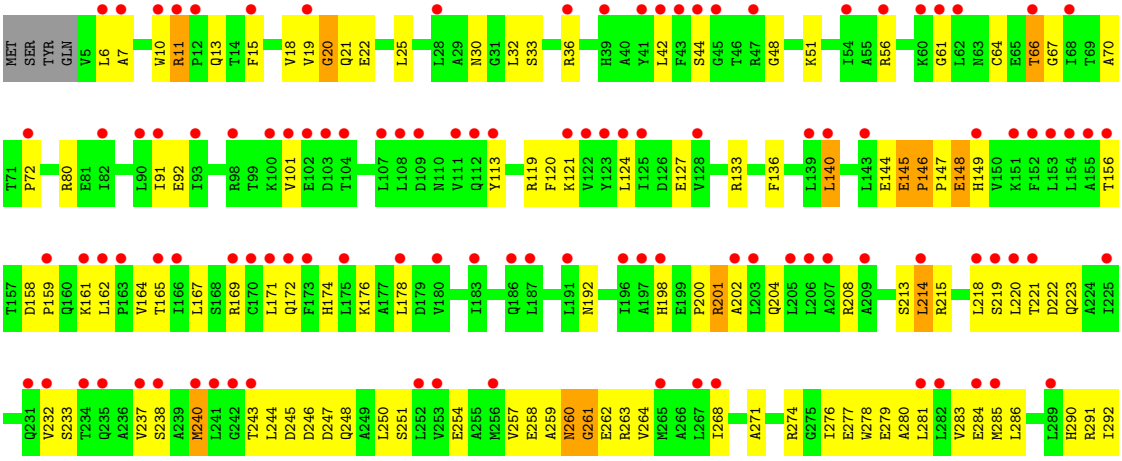
• Molecule 2: DNA polymerase III subunit gamma

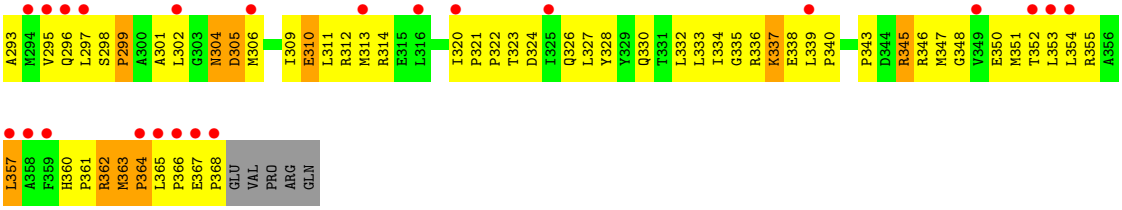
Chain H:



• Molecule 2: DNA polymerase III subunit gamma

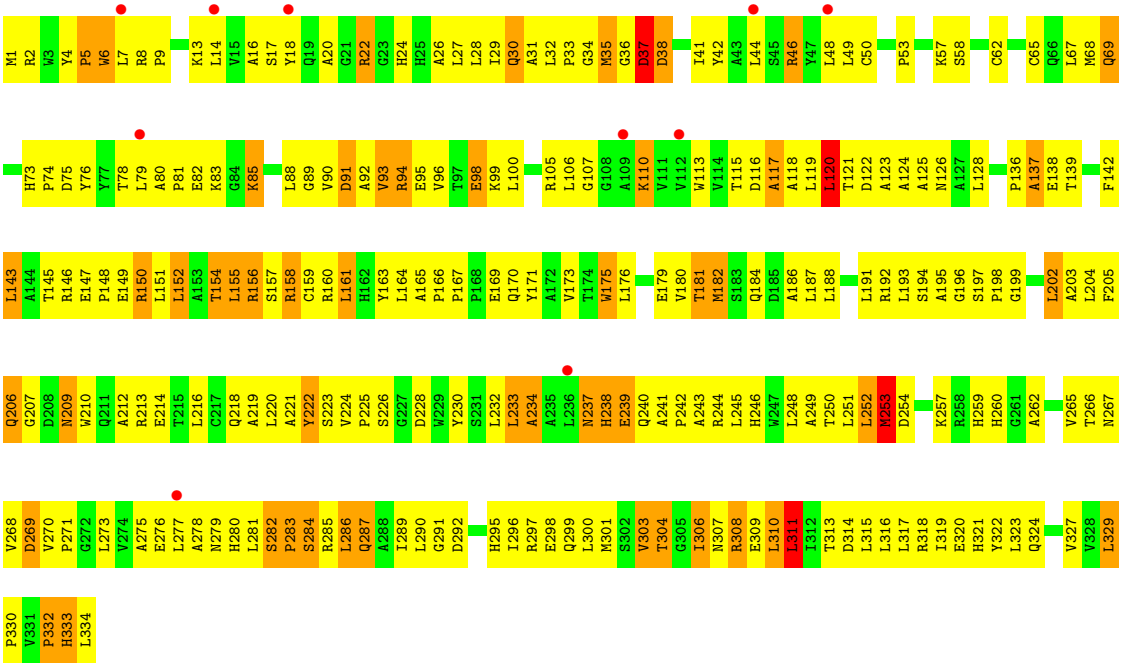
Chain I:





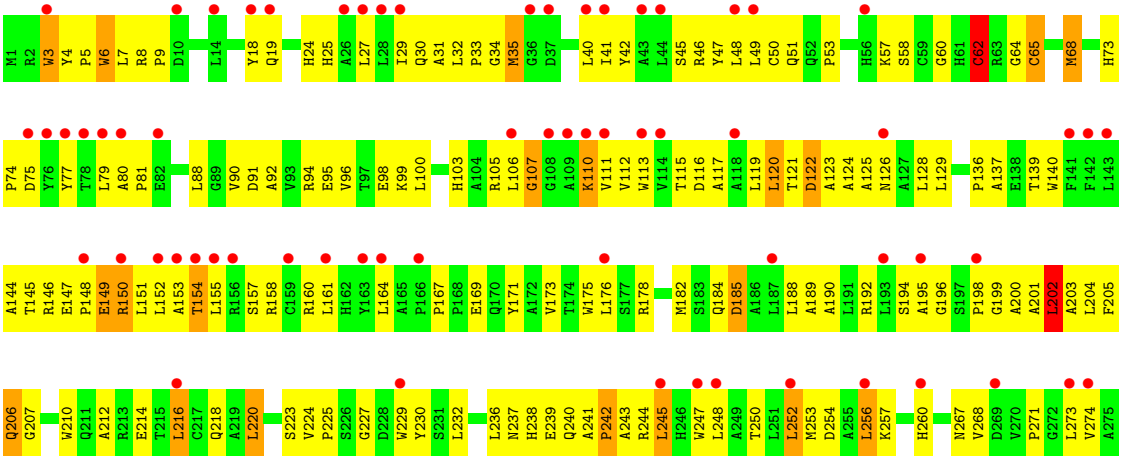
• Molecule 3: DNA polymerase III, delta prime subunit

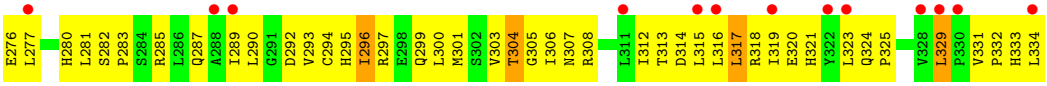
Chain E:



• Molecule 3: DNA polymerase III, delta prime subunit

Chain J:




E276
L277
H280
L281
S282
P283
S284
R285
L286
Q287
A288
I289
L290
G291
D292
V293
C294
H295
I296
R297
E298
Q299
L300
M301
S302
V303
T304
G305
I306
N307
R308
L311
I312
T313
D314
L315
L316
L317
R318
I319
E320
H321
Y322
L323
Q324
P325
V328
L329
P330
V331
P332
H333
L334

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.45Å 106.46Å 535.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.45 98.93 – 3.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-3.45) 97.7 (98.93-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.315 , 0.350 0.256 , 0.298	Depositor DCC
R_{free} test set	7449 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å^2)	106.7	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 116.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	27736	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, ZN, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.60	3/2731 (0.1%)	0.88	6/3704 (0.2%)
1	F	0.55	2/2731 (0.1%)	0.73	4/3704 (0.1%)
2	B	0.52	1/2876 (0.0%)	0.81	1/3900 (0.0%)
2	C	0.61	0/2898	0.84	0/3930
2	D	0.63	0/2876	0.93	3/3900 (0.1%)
2	G	0.38	0/2876	0.66	1/3900 (0.0%)
2	H	0.29	0/2898	0.58	0/3930
2	I	0.34	0/2876	0.63	1/3900 (0.0%)
3	E	0.54	2/2662 (0.1%)	0.77	4/3624 (0.1%)
3	J	0.37	0/2662	0.56	1/3624 (0.0%)
All	All	0.50	8/28086 (0.0%)	0.75	21/38116 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	285	MSE	SE-CE	16.36	2.92	1.95
1	A	286	MSE	C-N	11.64	1.54	1.33
1	F	285	MSE	CG-SE	8.13	2.23	1.95
1	A	286	MSE	CG-SE	-8.08	1.68	1.95
3	E	253	MSE	CG-SE	-6.37	1.73	1.95
1	A	285	MSE	SE-CE	5.65	2.28	1.95
3	E	35	MSE	CG-SE	-5.33	1.77	1.95
2	B	285	MET	SD-CE	5.06	2.06	1.77

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	285	MSE	CG-SE-CE	-15.68	64.40	98.90
1	A	268	PRO	CA-N-CD	-13.61	92.44	111.50
1	F	283	ARG	CA-C-N	-8.30	99.59	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	12	PRO	CA-N-CD	-8.17	100.06	111.50
2	G	12	PRO	CA-N-CD	-7.64	100.81	111.50
1	A	283	ARG	CA-C-N	-7.62	100.95	116.20
2	D	191	LEU	CA-CB-CG	-7.10	98.96	115.30
3	J	202	LEU	CA-CB-CG	6.75	130.81	115.30
3	E	333	HIS	N-CA-C	6.29	127.97	111.00
1	A	285	MSE	CG-SE-CE	-6.12	85.43	98.90
1	F	280	GLN	C-N-CA	6.04	136.81	121.70
2	D	303	GLY	N-CA-C	5.87	127.77	113.10
3	E	286	LEU	N-CA-C	-5.83	95.27	111.00
2	B	363	MET	N-CA-C	5.57	126.04	111.00
1	A	280	GLN	CB-CA-C	-5.41	99.57	110.40
1	A	337	ALA	N-CA-C	5.34	125.42	111.00
2	I	171	LEU	N-CA-C	-5.31	96.67	111.00
3	E	120	LEU	CA-CB-CG	5.24	127.35	115.30
3	E	329	LEU	N-CA-C	5.16	124.92	111.00
1	A	283	ARG	C-N-CA	5.07	132.94	122.30
1	F	281	ASN	N-CA-CB	5.03	119.66	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2687	0	2743	371	0
1	F	2687	0	2737	337	6
2	B	2829	0	2881	302	0
2	C	2850	0	2897	334	0
2	D	2829	0	2879	361	0
2	G	2829	0	2881	274	0
2	H	2850	0	2898	276	0
2	I	2829	0	2877	267	6
3	E	2602	0	2605	304	0
3	J	2602	0	2605	238	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	4	0
5	D	31	0	12	4	0
5	G	31	0	12	2	0
5	I	31	0	12	27	0
6	C	5	0	0	3	0
6	H	5	0	0	4	0
All	All	27736	0	28051	2798	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (2798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:MSE:SE	1:F:228:ARG:HA	1.53	1.56
2:H:100:LYS:NZ	2:I:133:ARG:CG	1.68	1.54
2:G:10:TRP:CZ2	2:G:193:GLU:HB3	1.47	1.48
1:A:74:PHE:CZ	1:F:206:VAL:HB	1.49	1.47
2:I:223:GLN:NE2	2:I:240:MET:HE1	1.29	1.46
2:B:285:MET:CE	2:B:285:MET:SD	2.06	1.43
2:G:10:TRP:HZ2	2:G:193:GLU:CB	1.28	1.43
1:A:74:PHE:CD1	1:F:203:GLU:HG3	1.53	1.41
2:I:215:ARG:HD3	5:I:803:AGS:C4'	1.48	1.41
2:I:215:ARG:CD	5:I:803:AGS:H4'	1.52	1.39
2:I:21:GLN:HE22	2:I:176:LYS:N	1.17	1.36
1:A:73:LEU:HB2	1:F:207:ASN:OD1	1.24	1.36
2:I:21:GLN:NE2	2:I:176:LYS:H	1.18	1.35
1:F:285:MSE:SE	1:F:285:MSE:CG	2.23	1.35
2:I:6:LEU:HG	2:I:222:ASP:CG	1.42	1.33
2:I:215:ARG:NH1	5:I:803:AGS:H5'2	1.40	1.33
1:A:285:MSE:CE	1:A:285:MSE:SE	2.28	1.31
2:I:215:ARG:HB2	5:I:803:AGS:C4'	1.59	1.30
1:A:71:MSE:CE	1:F:231:HIS:HB2	1.61	1.29
1:F:45:GLN:OE1	1:F:77:ARG:HD3	1.18	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:TRP:CZ2	2:G:193:GLU:CB	2.12	1.25
1:A:269:LEU:HG	1:A:273:PHE:CE1	1.76	1.21
1:A:74:PHE:CD1	1:F:203:GLU:CG	2.23	1.20
1:F:273:PHE:CD1	1:F:283:ARG:HG3	1.76	1.20
2:I:215:ARG:CZ	5:I:803:AGS:H5'2	1.69	1.20
2:I:200:PRO:CB	2:I:305:ASP:HB2	1.72	1.20
2:G:6:LEU:HB3	2:G:190:ILE:CG2	1.71	1.19
2:D:184:ARG:HH11	2:D:184:ARG:HG3	1.07	1.19
2:G:20:GLY:HA2	2:G:22:GLU:OE2	1.41	1.19
2:I:215:ARG:CB	5:I:803:AGS:O4'	1.91	1.19
1:A:74:PHE:HZ	1:F:206:VAL:CB	1.55	1.18
2:I:215:ARG:HB2	5:I:803:AGS:O4'	1.02	1.18
2:H:326:GLN:HA	2:H:326:GLN:HE21	1.10	1.17
1:F:273:PHE:CE1	1:F:283:ARG:HG3	1.80	1.16
2:I:200:PRO:HB2	2:I:305:ASP:CB	1.75	1.15
2:B:276:ILE:HD11	2:B:281:LEU:HB2	1.29	1.15
1:A:71:MSE:SE	1:F:228:ARG:CA	2.45	1.15
1:F:47:PHE:HD2	1:F:78:GLN:O	1.29	1.15
2:I:355:ARG:HH21	3:J:332:PRO:HD3	1.09	1.14
2:H:100:LYS:HG2	2:I:133:ARG:HB2	1.20	1.14
2:I:215:ARG:CZ	5:I:803:AGS:C5'	2.26	1.14
2:B:76:CYS:SG	2:B:78:ASN:HB2	1.88	1.13
1:F:244:VAL:HG22	1:F:312:LEU:HD21	1.27	1.12
2:H:229:ASP:OD2	2:I:30:ASN:ND2	1.83	1.11
1:A:105:HIS:CE1	1:A:108:LEU:HB2	1.85	1.10
2:G:6:LEU:HB3	2:G:190:ILE:HG21	1.17	1.10
2:B:360:HIS:CD2	2:B:361:PRO:HD2	1.86	1.09
2:B:360:HIS:HD2	2:B:361:PRO:HD2	1.06	1.09
1:F:223:MSE:HG3	1:F:289:ALA:HA	1.26	1.09
1:A:71:MSE:HE1	1:F:231:HIS:CB	1.83	1.09
3:J:303:VAL:HB	3:J:306:ILE:HD11	1.33	1.09
1:A:336:LEU:H	1:A:336:LEU:HD22	1.17	1.08
2:G:248:GLN:O	2:G:250:LEU:N	1.86	1.08
2:D:265:MET:HE1	2:D:354:LEU:HD21	1.35	1.07
2:H:100:LYS:NZ	2:I:133:ARG:HG3	0.75	1.07
1:A:74:PHE:CZ	1:F:206:VAL:CB	2.32	1.07
1:F:47:PHE:CD2	1:F:78:GLN:O	2.07	1.07
2:I:19:VAL:HG12	2:I:178:LEU:HD22	1.35	1.07
2:G:11:ARG:HH22	2:G:52:THR:HG22	1.16	1.06
1:A:74:PHE:HE2	1:F:206:VAL:HG11	1.20	1.06
1:A:119:LYS:HD3	1:A:119:LYS:H	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PHE:CE1	1:F:203:GLU:O	2.09	1.05
2:G:7:ALA:CB	2:G:218:LEU:HD13	1.86	1.05
2:G:295:VAL:HG22	2:G:301:ALA:HB3	1.38	1.05
2:D:10:TRP:CE2	2:D:190:ILE:HD12	1.90	1.05
2:G:46:THR:HG22	2:G:47:ARG:H	1.20	1.04
2:C:360:HIS:HD2	2:C:361:PRO:HD2	1.17	1.04
2:C:14:THR:HG22	2:C:15:PHE:H	1.22	1.04
2:H:229:ASP:OD2	2:I:30:ASN:CG	1.96	1.03
1:F:45:GLN:OE1	1:F:77:ARG:CD	2.07	1.02
2:I:215:ARG:NE	5:I:803:AGS:H5'1	1.72	1.02
1:F:166:ALA:HB1	1:F:202:VAL:HG21	1.41	1.02
2:C:254:GLU:O	2:C:258:GLU:HG3	1.58	1.02
2:I:6:LEU:HG	2:I:222:ASP:OD2	1.60	1.01
2:B:360:HIS:HD2	2:B:361:PRO:CD	1.73	1.01
2:D:285:MET:HE3	2:D:353:LEU:HD21	1.40	1.00
1:A:71:MSE:CE	1:F:231:HIS:CB	2.38	1.00
2:H:128:VAL:HG11	2:H:154:LEU:HD22	1.42	1.00
2:G:6:LEU:HD11	2:G:191:LEU:HD21	1.43	1.00
1:A:193:PRO:HG3	2:B:36:ARG:HH22	1.27	1.00
1:F:270:ARG:HG2	1:F:283:ARG:NH2	1.77	1.00
2:B:260:ASN:HD22	2:B:263:ARG:HB2	1.24	0.99
3:J:30:GLN:HG3	3:J:148:PRO:HD3	1.40	0.99
1:F:217:TRP:HE1	1:F:233:LEU:HB2	1.28	0.99
2:I:223:GLN:NE2	2:I:240:MET:CE	2.23	0.99
2:B:36:ARG:CB	2:B:36:ARG:HH11	1.76	0.99
2:I:11:ARG:HH21	2:I:56:ARG:HH21	1.07	0.98
2:G:11:ARG:NH2	2:G:52:THR:HG22	1.77	0.98
2:I:215:ARG:CB	5:I:803:AGS:C4'	2.41	0.98
2:H:360:HIS:HD2	2:H:363:MET:H	1.01	0.97
2:I:271:ALA:HB1	2:I:276:ILE:HD12	1.42	0.97
1:F:24:LEU:HD12	1:F:136:GLN:NE2	1.80	0.97
2:G:7:ALA:HB2	2:G:218:LEU:HD13	1.45	0.97
2:B:260:ASN:ND2	2:B:263:ARG:HB2	1.79	0.97
2:G:11:ARG:HH22	2:G:52:THR:CG2	1.77	0.97
2:I:215:ARG:NE	5:I:803:AGS:C5'	2.28	0.97
2:C:245:ASP:O	2:C:247:ASP:N	1.98	0.96
1:A:73:LEU:CB	1:F:207:ASN:OD1	2.13	0.96
2:G:274:ARG:HE	2:G:276:ILE:HD11	1.30	0.96
2:C:128:VAL:HG11	2:C:154:LEU:HD22	1.46	0.96
1:F:304:LEU:HB3	1:F:327:LEU:HD21	1.47	0.95
1:A:74:PHE:CG	1:F:203:GLU:HG3	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:LEU:O	1:F:101:THR:HG22	1.67	0.95
2:H:80:ARG:O	2:H:84:GLN:HG3	1.66	0.95
1:F:282:ARG:HG3	1:F:285:MSE:CE	1.96	0.95
2:C:360:HIS:CD2	2:C:361:PRO:HD2	2.02	0.94
2:D:363:MET:HB3	2:D:364:PRO:HD2	1.49	0.94
2:G:248:GLN:O	2:G:251:SER:N	2.00	0.94
2:D:265:MET:CE	2:D:354:LEU:HD21	1.97	0.94
2:I:223:GLN:CD	2:I:240:MET:HE1	1.87	0.94
1:A:183:GLN:HE21	2:B:172:GLN:H	1.05	0.94
2:B:309:ILE:HG22	2:B:313:MET:HG2	1.50	0.94
2:I:215:ARG:HD3	5:I:803:AGS:C5'	1.97	0.94
3:J:117:ALA:O	3:J:120:LEU:HD22	1.66	0.94
1:A:251:GLN:HE21	1:A:255:LEU:HD11	1.33	0.94
2:H:100:LYS:HZ1	2:I:133:ARG:HG3	1.23	0.94
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.49	0.94
1:A:74:PHE:CE2	1:F:206:VAL:CG1	2.50	0.93
1:A:253:GLU:OE1	1:A:286:MSE:HE1	1.68	0.93
1:F:119:LYS:HD3	1:F:119:LYS:H	1.30	0.93
1:A:74:PHE:CE2	1:F:206:VAL:HG11	2.03	0.93
1:F:299:ARG:HG3	3:J:317:LEU:HD11	1.48	0.93
3:J:253:MSE:HG3	3:J:257:LYS:HE3	1.50	0.93
1:F:270:ARG:HG2	1:F:283:ARG:HH21	1.32	0.93
2:I:215:ARG:CD	5:I:803:AGS:C5'	2.46	0.93
3:J:49:LEU:HD23	3:J:68:MSE:SE	2.20	0.92
3:E:74:PRO:HB3	3:E:105:ARG:HD3	1.51	0.92
1:F:222:LEU:CD1	1:F:285:MSE:HE3	1.99	0.92
1:A:93:ILE:HG12	1:A:96:GLN:OE1	1.69	0.92
2:C:263:ARG:O	2:C:267:LEU:HG	1.70	0.92
2:D:10:TRP:NE1	2:D:190:ILE:HG23	1.84	0.91
1:F:71:MSE:SE	1:F:80:LEU:HD12	2.20	0.91
3:J:46:ARG:CZ	3:J:68:MSE:HG3	2.01	0.91
2:C:243:THR:HG22	2:C:244:LEU:N	1.83	0.91
2:C:343:PRO:O	2:C:344:ASP:HB2	1.68	0.91
2:G:10:TRP:HZ2	2:G:193:GLU:HB3	0.75	0.91
2:I:363:MET:HB3	2:I:364:PRO:HD2	1.53	0.91
3:J:296:ILE:HG21	3:J:315:LEU:HD12	1.53	0.91
2:G:248:GLN:HA	2:G:251:SER:OG	1.69	0.91
2:B:343:PRO:HG2	2:B:347:MET:SD	2.11	0.90
2:G:291:ARG:NH2	2:G:303:GLY:H	1.67	0.90
3:J:4:TYR:H	3:J:7:LEU:HD12	1.33	0.90
1:F:24:LEU:HD12	1:F:136:GLN:HE21	1.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:ARG:HD3	2:D:185:HIS:N	1.85	0.90
1:F:80:LEU:HD13	1:F:80:LEU:H	1.37	0.90
1:F:48:GLU:OE2	1:F:74:PHE:HZ	1.53	0.90
1:F:71:MSE:HB3	1:F:108:LEU:HD13	1.54	0.90
2:G:6:LEU:HD21	2:G:196:ILE:HD12	1.54	0.90
3:E:296:ILE:HA	3:E:299:GLN:HG3	1.53	0.90
2:I:6:LEU:CG	2:I:222:ASP:CG	2.37	0.89
1:A:150:TRP:CH2	1:A:178:LEU:HD11	2.08	0.89
2:B:351:MET:HE3	2:C:290:HIS:HA	1.54	0.89
2:C:243:THR:CG2	2:C:244:LEU:N	2.33	0.89
2:D:357:LEU:HA	2:D:363:MET:HE3	1.51	0.89
2:I:354:LEU:HD12	3:J:253:MSE:HE1	1.53	0.89
2:C:316:LEU:HD22	2:C:320:ILE:HD11	1.53	0.89
2:D:10:TRP:CD2	2:D:190:ILE:HD12	2.07	0.89
1:A:336:LEU:HD22	1:A:336:LEU:N	1.86	0.89
1:A:125:ALA:O	1:A:128:THR:HG23	1.71	0.88
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.55	0.88
3:E:79:LEU:HD11	3:E:96:VAL:HG11	1.54	0.88
3:E:121:THR:HG22	3:E:123:ALA:H	1.39	0.88
2:G:11:ARG:HH21	2:G:56:ARG:NH2	1.72	0.88
2:G:10:TRP:HZ2	2:G:193:GLU:HB2	1.34	0.88
1:A:73:LEU:HB2	1:F:207:ASN:CG	1.92	0.88
2:D:108:LEU:O	2:D:111:VAL:HG23	1.73	0.88
1:F:295:GLN:CD	1:F:295:GLN:H	1.75	0.87
2:C:156:THR:HG22	2:C:158:ASP:H	1.37	0.87
2:G:11:ARG:NH2	2:G:56:ARG:NH2	2.23	0.87
2:D:184:ARG:HH11	2:D:184:ARG:CG	1.88	0.87
1:F:48:GLU:HG2	1:F:49:GLU:N	1.88	0.87
2:I:215:ARG:CD	5:I:803:AGS:C4'	2.27	0.87
2:B:44:SER:CB	2:B:159:PRO:HG2	2.05	0.87
1:F:27:ASP:OD2	1:F:30:LEU:HG	1.75	0.87
1:A:281:ASN:O	1:A:283:ARG:N	2.08	0.86
3:E:58:SER:HB3	3:E:65:CYS:SG	2.16	0.86
2:H:261:GLY:HA3	2:I:297:LEU:HD11	1.58	0.86
1:A:74:PHE:CE1	1:F:203:GLU:HG3	2.09	0.86
1:A:74:PHE:HE1	1:F:203:GLU:O	1.58	0.86
2:G:268:ILE:HD11	2:G:353:LEU:HD12	1.56	0.86
2:I:244:LEU:HD11	2:I:276:ILE:HD13	1.58	0.86
2:C:243:THR:CG2	2:C:244:LEU:H	1.88	0.85
2:B:257:VAL:HG11	2:B:320:ILE:HD13	1.58	0.85
2:I:20:GLY:HA2	2:I:22:GLU:OE2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:LYS:HZ2	2:I:133:ARG:HG3	1.10	0.85
2:B:198:HIS:CD2	2:B:203:LEU:HD11	2.11	0.85
3:J:31:ALA:HB2	3:J:164:LEU:HB3	1.59	0.85
1:A:71:MSE:HE1	1:F:231:HIS:HB2	0.89	0.85
1:A:269:LEU:HG	1:A:273:PHE:HE1	1.42	0.85
3:E:186:ALA:HA	3:E:269:ASP:OD1	1.77	0.85
2:H:326:GLN:HA	2:H:326:GLN:NE2	1.91	0.85
2:H:291:ARG:HA	2:H:294:MET:HB2	1.58	0.85
2:C:198:HIS:HB2	2:C:232:VAL:HG22	1.57	0.85
1:A:1:MSE:HE1	1:A:127:PHE:CZ	2.11	0.85
2:I:248:GLN:HG3	2:I:274:ARG:HH22	1.39	0.85
2:H:88:VAL:HG11	2:H:116:ALA:HB3	1.58	0.84
2:D:363:MET:CB	2:D:364:PRO:HD2	2.05	0.84
1:A:183:GLN:NE2	2:B:172:GLN:H	1.76	0.84
2:G:10:TRP:CZ2	2:G:193:GLU:HB2	2.07	0.84
2:C:259:ALA:HB2	2:C:360:HIS:CE1	2.12	0.84
2:I:215:ARG:CG	5:I:803:AGS:H4'	2.07	0.84
1:A:74:PHE:CD1	1:F:207:ASN:OD1	2.07	0.84
2:H:367:GLU:HG3	2:I:321:PRO:HA	1.58	0.84
2:B:165:THR:O	2:B:168:SER:HB3	1.77	0.84
2:D:354:LEU:HD13	3:E:253:MSE:HE1	1.59	0.84
2:H:201:ARG:HD2	2:H:246:ASP:OD2	1.77	0.84
2:I:11:ARG:HH21	2:I:56:ARG:NH2	1.75	0.84
1:F:273:PHE:CE1	1:F:283:ARG:CG	2.61	0.84
1:A:133:ARG:HH21	2:G:300:ALA:CB	1.90	0.83
2:C:200:PRO:HG2	2:C:305:ASP:OD2	1.77	0.83
2:H:360:HIS:CD2	2:H:363:MET:H	1.93	0.83
2:B:351:MET:SD	2:C:326:GLN:NE2	2.49	0.83
2:I:355:ARG:NH2	3:J:332:PRO:HD3	1.93	0.83
1:A:214:PRO:HA	1:A:236:LEU:HD11	1.60	0.83
2:D:306:MET:HG2	2:D:309:ILE:HD11	1.61	0.83
2:D:184:ARG:HG3	2:D:184:ARG:NH1	1.83	0.83
2:H:24:VAL:HG11	2:H:175:LEU:HD21	1.60	0.83
3:E:333:HIS:O	3:E:334:LEU:HB2	1.78	0.83
3:J:317:LEU:HD13	3:J:318:ARG:N	1.93	0.83
3:J:68:MSE:HA	3:J:68:MSE:HE3	1.60	0.83
3:J:230:TYR:HE1	3:J:313:THR:HG23	1.42	0.83
2:D:223:GLN:HB3	2:D:240:MET:HE1	1.60	0.83
2:D:257:VAL:HG11	2:D:320:ILE:HG12	1.60	0.83
3:E:30:GLN:CG	3:E:163:TYR:HD1	1.93	0.82
2:H:100:LYS:NZ	2:I:133:ARG:CB	2.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:215:ARG:CZ	5:I:803:AGS:H5'1	2.02	0.82
1:F:282:ARG:HG3	1:F:285:MSE:HE1	1.59	0.82
2:H:339:LEU:HB3	2:H:340:PRO:HD3	1.59	0.82
3:E:30:GLN:HG2	3:E:163:TYR:HD1	1.44	0.82
2:B:261:GLY:HA3	2:C:297:LEU:HD11	1.61	0.82
2:D:223:GLN:HB3	2:D:240:MET:CE	2.10	0.82
2:G:19:VAL:HG21	2:G:186:GLN:OE1	1.80	0.82
3:E:169:GLU:O	3:E:173:VAL:HG23	1.78	0.82
2:H:84:GLN:O	2:I:144:GLU:OE2	1.98	0.81
2:C:197:ALA:O	2:C:198:HIS:HB3	1.80	0.81
2:I:244:LEU:HD21	2:I:276:ILE:HG12	1.61	0.81
1:A:74:PHE:HZ	1:F:206:VAL:HB	0.75	0.81
1:A:262:ARG:NH2	3:E:320:GLU:OE2	2.13	0.81
2:C:119:ARG:HB2	2:C:120:PHE:CD2	2.15	0.81
2:D:358:ALA:O	2:D:360:HIS:N	2.10	0.81
1:A:193:PRO:HD3	2:B:30:ASN:HD21	1.45	0.81
1:F:304:LEU:HD13	1:F:327:LEU:HD22	1.61	0.81
2:G:6:LEU:HD11	2:G:191:LEU:CD2	2.10	0.81
2:G:250:LEU:HD23	2:G:288:LEU:HD13	1.61	0.81
2:C:268:ILE:HD11	2:C:353:LEU:HD12	1.63	0.81
2:D:42:LEU:HD23	2:D:154:LEU:HB2	1.62	0.81
1:F:282:ARG:CG	1:F:285:MSE:CE	2.58	0.81
1:F:253:GLU:O	1:F:256:LEU:HB3	1.81	0.81
2:G:291:ARG:HH21	2:G:303:GLY:H	1.27	0.81
2:I:6:LEU:CG	2:I:222:ASP:OD2	2.22	0.81
1:A:150:TRP:CZ2	1:A:178:LEU:HD11	2.16	0.80
2:G:20:GLY:CA	2:G:22:GLU:OE2	2.28	0.80
2:D:229:ASP:O	2:D:231:GLN:N	2.12	0.80
2:I:246:ASP:HB3	2:I:248:GLN:HG2	1.63	0.80
1:A:208:ASP:O	2:B:176:LYS:HE2	1.80	0.80
2:G:98:ARG:HH11	2:H:140:LEU:HD22	1.46	0.80
1:A:25:GLY:HA3	1:A:139:CYS:O	1.82	0.80
3:J:35:MSE:HE3	3:J:198:PRO:HD2	1.64	0.80
2:B:302:LEU:HD12	2:B:314:ARG:HH21	1.47	0.80
2:C:128:VAL:HG23	2:C:162:LEU:HD21	1.63	0.80
2:D:10:TRP:CD2	2:D:190:ILE:CD1	2.65	0.80
2:I:223:GLN:CD	2:I:240:MET:CE	2.49	0.80
2:C:236:ALA:O	2:C:239:ALA:HB3	1.81	0.80
2:G:248:GLN:O	2:G:249:ALA:C	2.18	0.80
2:C:14:THR:HG22	2:C:15:PHE:N	1.98	0.79
2:G:271:ALA:HB1	2:G:276:ILE:HD12	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:ALA:HB2	2:B:360:HIS:CE1	2.17	0.79
1:F:223:MSE:HG3	1:F:289:ALA:CA	2.12	0.79
1:F:223:MSE:HE1	1:F:292:ARG:HB2	1.65	0.79
1:A:234:GLN:HA	1:A:237:ARG:HE	1.48	0.79
2:B:248:GLN:HA	2:B:251:SER:HB2	1.64	0.79
1:F:119:LYS:HD3	1:F:119:LYS:N	1.97	0.79
1:A:71:MSE:HE3	1:F:231:HIS:CG	2.17	0.79
2:B:351:MET:CE	2:C:290:HIS:HA	2.12	0.79
3:E:161:LEU:HD12	3:E:161:LEU:H	1.45	0.79
2:H:295:VAL:HG22	2:H:301:ALA:HB3	1.65	0.79
1:A:74:PHE:CZ	1:F:203:GLU:O	2.35	0.79
1:F:142:PRO:HD2	1:F:178:LEU:HD11	1.63	0.79
2:I:215:ARG:NH1	5:I:803:AGS:C5'	2.34	0.79
1:A:105:HIS:HB3	1:F:227:LYS:HD3	1.65	0.79
2:H:42:LEU:HD23	2:H:172:GLN:HG2	1.63	0.79
2:I:223:GLN:HE21	2:I:240:MET:HE1	1.48	0.79
2:B:61:GLY:HA2	2:B:72:PRO:HG3	1.65	0.79
2:G:98:ARG:HD3	2:H:140:LEU:HB3	1.65	0.79
1:A:59:THR:HG22	1:A:60:ASP:N	1.98	0.79
1:A:219:ASP:O	1:A:222:LEU:HB2	1.83	0.79
2:B:140:LEU:HA	2:B:143:LEU:HD22	1.65	0.79
1:A:91:ALA:HA	1:A:94:ASN:ND2	1.98	0.78
2:H:341:TYR:CE2	2:I:337:LYS:HB2	2.18	0.78
3:J:58:SER:HB3	3:J:65:CYS:SG	2.24	0.78
2:G:11:ARG:HH21	2:G:56:ARG:CZ	1.96	0.78
1:F:144:GLN:HG3	1:F:280:GLN:CD	2.04	0.78
2:G:271:ALA:O	2:G:274:ARG:HG2	1.83	0.78
2:B:215:ARG:HD3	5:B:802:AGS:H5'1	1.66	0.78
2:G:239:ALA:HB1	2:H:23:HIS:NE2	1.98	0.78
2:B:42:LEU:HB2	2:B:170:CYS:SG	2.23	0.78
1:F:48:GLU:OE2	1:F:74:PHE:CZ	2.36	0.78
1:F:104:LEU:HB3	1:F:133:ARG:NH1	1.99	0.78
2:G:248:GLN:HA	2:G:251:SER:CB	2.14	0.78
3:E:218:GLN:O	3:E:221:ALA:HB3	1.84	0.78
2:H:100:LYS:CG	2:I:133:ARG:HB2	2.06	0.78
1:F:198:THR:HB	1:F:200:PRO:HD2	1.66	0.78
2:H:113:TYR:HA	2:H:149:HIS:CE1	2.19	0.78
1:F:222:LEU:HD12	1:F:285:MSE:HE3	1.66	0.78
1:F:187:ARG:O	1:F:191:LEU:HD23	1.84	0.77
1:F:282:ARG:HG3	1:F:285:MSE:HE2	1.64	0.77
2:I:6:LEU:HG	2:I:222:ASP:OD1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:SER:OG	2:C:100:LYS:HD2	1.84	0.77
2:H:137:ASN:HA	2:H:140:LEU:HD12	1.66	0.77
2:I:355:ARG:HH21	3:J:332:PRO:CD	1.96	0.77
2:B:156:THR:HG23	2:B:159:PRO:HG3	1.65	0.77
1:A:193:PRO:CD	2:B:30:ASN:HD21	1.98	0.77
2:B:344:ASP:OD2	2:B:344:ASP:C	2.20	0.77
2:G:341:TYR:O	2:H:333:LEU:HD11	1.85	0.77
2:I:363:MET:CB	2:I:364:PRO:HD2	2.15	0.77
2:B:263:ARG:HG2	2:B:267:LEU:HD13	1.65	0.77
1:F:242:GLU:O	1:F:245:ILE:HG22	1.84	0.77
2:C:287:GLY:O	2:C:290:HIS:HB3	1.83	0.77
2:G:98:ARG:HD3	2:H:140:LEU:HD13	1.67	0.77
2:D:197:ALA:HB3	2:D:231:GLN:HG2	1.67	0.76
2:I:61:GLY:HA2	2:I:72:PRO:HG3	1.66	0.76
3:E:283:PRO:HG2	3:E:284:SER:H	1.50	0.76
1:F:1:MSE:HE1	1:F:127:PHE:CZ	2.20	0.76
2:I:215:ARG:HH11	5:I:803:AGS:H5'2	1.44	0.76
1:A:63:ALA:O	1:A:67:LEU:HG	1.85	0.76
1:A:74:PHE:CE1	1:F:203:GLU:CG	2.66	0.76
1:F:213:THR:H	1:F:216:HIS:HD2	1.33	0.76
2:D:10:TRP:CE2	2:D:190:ILE:HG23	2.21	0.76
2:H:100:LYS:HG2	2:I:133:ARG:CB	2.09	0.76
3:E:158:ARG:HH11	3:E:158:ARG:HG3	1.49	0.76
2:H:11:ARG:HH12	2:I:169:ARG:HH12	1.28	0.76
2:H:136:PHE:O	2:H:140:LEU:HG	1.84	0.76
2:I:348:GLY:O	2:I:351:MET:HB2	1.86	0.76
2:B:36:ARG:HH11	2:B:36:ARG:HB3	1.49	0.76
2:G:46:THR:HG22	2:G:47:ARG:N	2.00	0.76
2:H:179:ASP:HB3	2:H:182:GLN:HB2	1.67	0.76
1:A:74:PHE:CD1	1:F:203:GLU:HG2	2.20	0.75
2:H:359:PHE:CE1	2:I:323:THR:HG23	2.20	0.75
2:H:11:ARG:HH12	2:I:169:ARG:NH1	1.85	0.75
1:A:74:PHE:CZ	1:F:206:VAL:CG1	2.66	0.75
2:C:95:ALA:HB3	2:C:127:GLU:O	1.87	0.75
1:F:304:LEU:HB2	1:F:327:LEU:HD11	1.68	0.75
2:I:201:ARG:NH2	2:I:284:GLU:OE2	2.19	0.75
2:C:37:ILE:HD13	2:C:120:PHE:CE1	2.20	0.75
2:D:259:ALA:CB	2:D:363:MET:HG2	2.15	0.75
1:F:310:LEU:HB3	1:F:314:GLN:NE2	2.01	0.75
2:I:248:GLN:HG3	2:I:274:ARG:NH2	2.01	0.75
1:F:248:ARG:HH21	1:F:309:GLU:CD	1.89	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:HB	1:A:200:PRO:HD2	1.69	0.75
1:F:80:LEU:HD13	1:F:80:LEU:N	2.01	0.75
1:A:71:MSE:CE	1:F:231:HIS:CG	2.69	0.75
1:A:133:ARG:HH21	2:G:300:ALA:HB2	1.51	0.75
1:A:190:LEU:HD21	2:B:38:HIS:CE1	2.21	0.75
1:A:281:ASN:C	1:A:283:ARG:H	1.89	0.75
2:B:76:CYS:SG	2:B:78:ASN:CB	2.73	0.75
3:E:246:HIS:O	3:E:250:THR:HG23	1.86	0.75
2:B:81:GLU:HB2	2:B:87:PHE:HD1	1.50	0.74
2:G:6:LEU:HB3	2:G:190:ILE:HG22	1.68	0.74
2:I:257:VAL:O	2:I:360:HIS:HE1	1.70	0.74
1:A:279:TRP:CG	1:A:279:TRP:O	2.40	0.74
3:J:57:LYS:HG3	3:J:58:SER:H	1.52	0.74
3:J:303:VAL:HB	3:J:306:ILE:CD1	2.14	0.74
2:C:147:PRO:HG2	2:C:150:VAL:HB	1.69	0.74
2:G:11:ARG:NH2	2:G:56:ARG:HH21	1.84	0.74
2:D:78:ASN:O	2:D:82:ILE:HG13	1.85	0.74
2:D:354:LEU:CD1	3:E:253:MSE:HE1	2.17	0.74
2:C:42:LEU:HD12	2:C:154:LEU:HB2	1.69	0.74
2:C:119:ARG:HB2	2:C:120:PHE:HD2	1.51	0.74
2:D:119:ARG:HG3	2:D:120:PHE:CD2	2.21	0.74
1:F:13:LEU:HD23	1:F:41:VAL:HG21	1.68	0.74
2:H:202:ALA:HB2	2:H:234:THR:HG23	1.70	0.74
1:F:53:PHE:HZ	1:F:67:LEU:HD13	1.52	0.74
1:F:188:LEU:HD23	1:F:197:LEU:HD13	1.70	0.74
2:H:271:ALA:O	2:H:274:ARG:HG2	1.88	0.74
1:A:52:THR:HG22	1:A:81:LEU:HB3	1.69	0.74
1:A:55:ILE:O	1:A:85:PRO:HG3	1.88	0.74
3:E:292:ASP:OD2	3:E:318:ARG:NH1	2.19	0.74
2:G:274:ARG:NE	2:G:276:ILE:HD11	2.01	0.74
1:A:263:GLN:HB2	1:A:272:LEU:HD21	1.70	0.73
1:F:213:THR:H	1:F:216:HIS:CD2	2.05	0.73
2:B:304:ASN:OD1	2:B:305:ASP:N	2.21	0.73
2:G:67:GLY:HA2	2:G:119:ARG:NH2	2.03	0.73
2:I:148:GLU:CD	2:I:149:HIS:H	1.90	0.73
1:A:260:LEU:HB3	1:A:290:LEU:HD11	1.70	0.73
1:A:272:LEU:O	1:A:275:LYS:HB2	1.88	0.73
1:A:269:LEU:HD11	1:A:273:PHE:CZ	2.23	0.73
2:D:10:TRP:CE2	2:D:190:ILE:CD1	2.70	0.73
1:F:217:TRP:NE1	1:F:233:LEU:HB2	2.00	0.73
1:F:310:LEU:O	1:F:314:GLN:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:LEU:O	2:B:245:ASP:HB3	1.86	0.73
2:C:343:PRO:O	2:C:344:ASP:CB	2.36	0.73
1:F:281:ASN:O	1:F:283:ARG:N	2.22	0.73
2:G:214:LEU:HD23	5:G:804:AGS:N9	2.03	0.73
1:A:184:ALA:HA	1:A:187:ARG:HD2	1.71	0.73
2:D:363:MET:HB3	2:D:364:PRO:CD	2.18	0.73
2:I:248:GLN:HE21	2:I:248:GLN:HA	1.52	0.73
1:F:279:TRP:CG	1:F:279:TRP:O	2.42	0.73
1:A:251:GLN:NE2	1:A:255:LEU:HD11	2.04	0.73
1:F:282:ARG:CG	1:F:285:MSE:HE2	2.17	0.73
2:G:243:THR:HG21	2:G:274:ARG:HD2	1.69	0.73
2:D:246:ASP:HB3	2:D:248:GLN:HE21	1.54	0.73
2:B:156:THR:CG2	2:B:159:PRO:HG3	2.19	0.72
2:I:215:ARG:HD3	5:I:803:AGS:H4'	0.74	0.72
2:D:248:GLN:O	2:D:252:LEU:HB2	1.90	0.72
2:D:357:LEU:HA	2:D:363:MET:CE	2.18	0.72
2:H:271:ALA:HA	2:H:274:ARG:NE	2.04	0.72
2:I:354:LEU:CD1	3:J:253:MSE:HE1	2.18	0.72
1:A:164:ASP:O	1:A:168:GLN:HG3	1.89	0.72
1:A:269:LEU:HG	1:A:273:PHE:CZ	2.24	0.72
3:E:222:TYR:O	3:E:225:PRO:HD2	1.89	0.72
2:I:7:ALA:HB1	2:I:215:ARG:HG3	1.70	0.72
3:J:121:THR:HG22	3:J:123:ALA:H	1.54	0.72
2:D:315:GLU:O	2:D:319:THR:HG23	1.89	0.72
2:I:6:LEU:HB3	2:I:218:LEU:HB3	1.72	0.72
2:D:276:ILE:HG22	2:D:277:GLU:N	2.05	0.72
2:H:327:LEU:HD21	2:H:361:PRO:HD3	1.70	0.72
1:A:27:ASP:OD1	1:A:29:LEU:HD23	1.90	0.72
2:D:295:VAL:HA	2:D:301:ALA:HB3	1.71	0.72
1:F:80:LEU:HD11	1:F:108:LEU:HD12	1.71	0.72
3:J:230:TYR:CE1	3:J:313:THR:HG23	2.24	0.72
2:G:6:LEU:HD21	2:G:191:LEU:HD23	1.72	0.71
2:H:100:LYS:HE2	2:I:133:ARG:HA	1.72	0.71
1:A:269:LEU:CG	1:A:273:PHE:CE1	2.67	0.71
2:C:243:THR:HG23	2:C:244:LEU:H	1.53	0.71
2:D:9:LYS:NZ	2:D:194:GLU:OE2	2.22	0.71
2:G:10:TRP:CD1	2:G:190:ILE:HG23	2.25	0.71
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.55	0.71
3:E:253:MSE:HA	3:E:253:MSE:HE3	1.72	0.71
2:I:354:LEU:HD13	3:J:256:LEU:HD22	1.73	0.71
3:J:116:ASP:HA	3:J:144:ALA:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:TRP:O	2:B:281:LEU:N	2.24	0.71
2:B:328:TYR:O	2:B:329:TYR:C	2.27	0.71
2:D:25:LEU:HD21	2:D:54:ILE:CD1	2.20	0.71
2:D:150:VAL:O	2:D:151:LYS:HD3	1.90	0.71
2:B:36:ARG:HH11	2:B:36:ARG:HB2	1.55	0.71
2:C:86:ARG:HH12	2:D:141:LYS:HG3	1.55	0.71
2:C:133:ARG:HD3	2:C:133:ARG:N	2.05	0.71
3:E:233:LEU:HD12	3:E:237:ASN:HB2	1.72	0.71
1:F:165:ALA:O	1:F:169:VAL:HG23	1.91	0.71
2:H:213:SER:OG	2:H:216:ASP:HB2	1.91	0.71
1:A:34:SER:O	1:A:38:VAL:HG23	1.90	0.71
2:C:259:ALA:HB2	2:C:360:HIS:ND1	2.05	0.71
2:I:292:ILE:O	2:I:296:GLN:HG3	1.90	0.71
2:G:355:ARG:HD2	2:G:355:ARG:C	2.12	0.70
1:A:181:LEU:O	1:A:185:LEU:HG	1.91	0.70
2:D:10:TRP:NE1	2:D:190:ILE:HD12	2.06	0.70
3:E:237:ASN:O	3:E:238:HIS:HB2	1.91	0.70
1:F:299:ARG:HG3	3:J:317:LEU:CD1	2.20	0.70
3:E:181:THR:O	3:E:182:MSE:HG2	1.91	0.70
2:D:32:LEU:O	2:D:34:LEU:N	2.24	0.70
1:A:308:THR:HG23	1:A:320:VAL:HG22	1.73	0.70
2:I:6:LEU:HD12	2:I:218:LEU:O	1.90	0.70
3:J:41:ILE:HG21	3:J:113:TRP:CD1	2.26	0.70
1:A:140:GLN:OE1	1:A:140:GLN:HA	1.91	0.70
2:C:261:GLY:HA3	2:D:297:LEU:HD21	1.71	0.70
2:C:323:THR:HG22	2:C:324:ASP:N	2.06	0.70
1:F:281:ASN:C	1:F:283:ARG:H	1.95	0.70
2:G:302:LEU:HD13	2:G:310:GLU:HG2	1.73	0.70
3:J:273:LEU:O	3:J:277:LEU:HB2	1.91	0.70
1:A:71:MSE:SE	1:F:231:HIS:CB	2.90	0.70
3:E:163:TYR:CD2	3:E:165:ALA:HB2	2.26	0.70
1:F:48:GLU:HG2	1:F:49:GLU:H	1.56	0.70
1:F:84:LEU:HG	1:F:89:PRO:HG3	1.74	0.70
2:G:9:LYS:HD3	2:G:194:GLU:CD	2.12	0.70
1:A:221:LEU:HD21	1:A:328:SER:CB	2.22	0.70
1:F:25:GLY:HA2	1:F:140:GLN:NE2	2.07	0.70
3:J:252:LEU:HD23	3:J:290:LEU:HA	1.74	0.70
2:C:361:PRO:O	2:C:362:ARG:HD3	1.92	0.70
1:A:281:ASN:C	1:A:283:ARG:N	2.45	0.69
3:E:74:PRO:HB3	3:E:105:ARG:CD	2.19	0.69
3:E:26:ALA:HB1	3:E:159:CYS:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:200:PRO:HG2	2:H:305:ASP:OD2	1.92	0.69
3:J:117:ALA:HB3	3:J:145:THR:OG1	1.92	0.69
1:A:270:ARG:HG2	1:A:283:ARG:NH2	2.07	0.69
2:B:354:LEU:HD11	2:C:294:MET:HG2	1.75	0.69
2:C:186:GLN:OE1	2:C:186:GLN:HA	1.91	0.69
2:I:6:LEU:HD12	2:I:221:THR:HB	1.73	0.69
2:B:333:LEU:HD11	2:B:337:LYS:HE3	1.75	0.69
2:C:360:HIS:HD2	2:C:361:PRO:CD	1.98	0.69
1:F:299:ARG:CG	3:J:317:LEU:HD11	2.21	0.69
2:C:186:GLN:HG3	2:C:190:ILE:HD11	1.73	0.69
2:D:148:GLU:CD	2:D:149:HIS:H	1.95	0.69
3:E:238:HIS:ND1	3:E:239:GLU:N	2.41	0.69
2:I:144:GLU:C	2:I:146:PRO:HD3	2.13	0.69
3:J:51:GLN:HG2	3:J:62:CYS:SG	2.32	0.69
2:B:78:ASN:HA	2:B:87:PHE:CE1	2.28	0.69
2:C:28:LEU:HD21	2:C:173:PHE:CE2	2.28	0.69
3:E:29:ILE:HD13	3:E:41:ILE:HD11	1.73	0.69
2:I:113:TYR:HD2	2:I:147:PRO:HB3	1.56	0.69
2:B:44:SER:HB2	2:B:159:PRO:HG2	1.74	0.69
1:F:218:VAL:O	1:F:222:LEU:HG	1.92	0.69
2:G:220:LEU:HD23	2:G:223:GLN:HE21	1.58	0.69
2:H:287:GLY:O	2:H:290:HIS:HB3	1.92	0.69
1:A:183:GLN:HE21	2:B:172:GLN:N	1.87	0.69
2:D:183:ILE:HG23	2:D:214:LEU:HD12	1.72	0.69
1:F:25:GLY:O	1:F:115:ASN:HA	1.91	0.69
1:F:144:GLN:HG3	1:F:280:GLN:OE1	1.92	0.69
1:F:247:LEU:HD21	1:F:308:THR:HG21	1.75	0.69
2:G:248:GLN:C	2:G:250:LEU:N	2.44	0.69
2:H:112:GLN:HB2	2:H:121:LYS:NZ	2.07	0.69
1:A:253:GLU:OE1	1:A:286:MSE:CE	2.39	0.69
2:D:366:PRO:HB3	3:E:282:SER:HB2	1.74	0.69
1:F:80:LEU:HD11	1:F:108:LEU:CD1	2.23	0.68
2:G:277:GLU:HG3	2:G:280:ALA:H	1.57	0.68
2:I:10:TRP:HB2	2:I:218:LEU:HD13	1.74	0.68
3:J:45:SER:O	3:J:49:LEU:HB2	1.93	0.68
2:B:360:HIS:CD2	2:B:361:PRO:CD	2.62	0.68
3:E:74:PRO:HD2	3:E:106:LEU:HD11	1.75	0.68
3:E:225:PRO:HA	3:E:280:HIS:ND1	2.08	0.68
2:H:142:THR:O	2:H:146:PRO:HB3	1.92	0.68
1:A:55:ILE:HD12	1:A:84:LEU:HD12	1.75	0.68
2:H:88:VAL:CG1	2:H:116:ALA:HB3	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:242:GLY:HA3	2:H:277:GLU:HG2	1.74	0.68
1:A:193:PRO:HD3	2:B:30:ASN:ND2	2.07	0.68
3:E:179:GLU:O	3:E:180:VAL:HG23	1.94	0.68
2:C:327:LEU:HD12	2:C:327:LEU:O	1.94	0.68
2:G:220:LEU:HD23	2:G:223:GLN:NE2	2.08	0.68
3:J:256:LEU:HD11	3:J:287:GLN:HG2	1.74	0.68
1:A:154:ARG:O	1:A:157:GLN:HG2	1.94	0.68
1:F:285:MSE:SE	1:F:285:MSE:CE	2.92	0.68
2:C:14:THR:CG2	2:C:15:PHE:H	2.04	0.68
1:F:54:SER:O	1:F:57:PRO:HD2	1.94	0.68
2:G:178:LEU:HD22	2:G:182:GLN:HE21	1.59	0.68
2:D:184:ARG:CG	2:D:184:ARG:NH1	2.48	0.68
2:D:196:ILE:HG22	2:D:197:ALA:N	2.09	0.68
2:D:296:GLN:HE22	2:D:322:PRO:HA	1.57	0.68
3:E:289:ILE:HG23	3:E:319:ILE:HD13	1.75	0.68
1:F:158:LEU:O	1:F:160:LEU:HD13	1.93	0.68
2:G:7:ALA:HB2	2:G:218:LEU:CD1	2.23	0.68
1:F:225:LYS:HG3	1:F:227:LYS:H	1.59	0.68
2:G:9:LYS:CD	2:G:194:GLU:OE1	2.42	0.68
2:G:278:TRP:HE3	2:G:349:VAL:HG21	1.58	0.68
2:G:291:ARG:NH2	2:G:303:GLY:N	2.40	0.68
2:I:208:ARG:NH2	2:I:283:VAL:HG11	2.08	0.68
1:A:214:PRO:HB3	1:A:246:LEU:HD22	1.75	0.67
2:C:198:HIS:CB	2:C:232:VAL:HG22	2.24	0.67
2:C:291:ARG:O	2:C:295:VAL:HG23	1.94	0.67
2:C:329:TYR:CE2	2:C:333:LEU:HD12	2.30	0.67
1:A:17:LEU:HD21	1:A:109:LEU:HD12	1.76	0.67
2:B:61:GLY:CA	2:B:72:PRO:HG3	2.24	0.67
3:J:297:ARG:NH1	3:J:301:MSE:SE	2.78	0.67
1:A:25:GLY:O	1:A:115:ASN:HA	1.94	0.67
2:D:24:VAL:O	2:D:26:THR:N	2.27	0.67
3:E:125:ALA:O	3:E:128:LEU:N	2.26	0.67
2:H:249:ALA:O	2:H:253:VAL:HG23	1.94	0.67
2:I:260:ASN:O	2:I:262:GLU:N	2.28	0.67
1:A:234:GLN:HB3	1:A:237:ARG:HH21	1.58	0.67
1:A:263:GLN:OE1	1:A:272:LEU:HD11	1.93	0.67
2:B:302:LEU:HD12	2:B:314:ARG:NH2	2.09	0.67
2:C:184:ARG:HG2	2:C:184:ARG:HH11	1.59	0.67
2:D:285:MET:CE	2:D:353:LEU:HD21	2.21	0.67
3:E:277:LEU:C	3:E:279:ASN:H	1.98	0.67
3:E:277:LEU:CD2	3:E:281:LEU:HD12	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:282:SER:HB2	3:E:283:PRO:HD2	1.77	0.67
2:G:295:VAL:HG22	2:G:301:ALA:CB	2.21	0.67
2:I:278:TRP:HD1	2:I:345:ARG:HD3	1.59	0.67
2:C:21:GLN:OE1	2:C:175:LEU:HD22	1.94	0.67
2:G:291:ARG:HH21	2:G:303:GLY:N	1.92	0.67
2:I:19:VAL:HG21	2:I:214:LEU:HD21	1.77	0.67
2:C:208:ARG:HG2	2:C:209:ALA:N	2.10	0.67
2:C:261:GLY:O	2:C:264:VAL:N	2.28	0.67
2:D:337:LYS:O	2:D:340:PRO:HD2	1.95	0.67
2:G:238:SER:HA	2:G:241:LEU:O	1.95	0.67
2:H:24:VAL:HG11	2:H:175:LEU:CD2	2.25	0.67
2:I:113:TYR:CD2	2:I:147:PRO:HB3	2.30	0.67
3:E:242:PRO:HG2	3:E:243:ALA:H	1.60	0.67
2:B:264:VAL:CG1	2:B:353:LEU:HD13	2.25	0.67
2:C:65:GLU:HA	2:C:119:ARG:HH21	1.58	0.67
2:C:152:PHE:O	2:C:153:LEU:HD23	1.95	0.67
2:D:277:GLU:HB2	2:D:280:ALA:HB3	1.76	0.67
2:D:292:ILE:HG22	2:D:293:ALA:N	2.08	0.67
1:F:119:LYS:H	1:F:119:LYS:CD	1.95	0.67
2:G:10:TRP:CE2	2:G:193:GLU:HB3	2.23	0.67
1:A:269:LEU:CD1	1:A:273:PHE:CZ	2.78	0.67
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.09	0.67
2:C:264:VAL:HG12	2:C:265:MET:N	2.09	0.67
2:H:292:ILE:O	2:H:296:GLN:HG3	1.95	0.67
1:A:190:LEU:HD21	2:B:38:HIS:HE1	1.57	0.66
2:C:271:ALA:CB	2:C:276:ILE:HD11	2.25	0.66
3:J:145:THR:HG22	3:J:147:GLU:H	1.60	0.66
2:B:216:ASP:O	2:B:220:LEU:HG	1.96	0.66
3:E:80:ALA:HB1	3:E:81:PRO:HD2	1.77	0.66
2:D:260:ASN:O	2:D:262:GLU:N	2.27	0.66
2:H:149:HIS:ND1	2:H:150:VAL:HG23	2.09	0.66
3:J:241:ALA:N	3:J:242:PRO:HD2	2.09	0.66
2:C:43:PHE:O	2:C:155:ALA:HA	1.96	0.66
2:C:144:GLU:HA	2:C:144:GLU:OE1	1.96	0.66
3:J:201:ALA:HA	3:J:204:LEU:HD22	1.77	0.66
2:B:44:SER:HB3	2:B:159:PRO:HG2	1.77	0.66
2:I:238:SER:HB2	2:I:243:THR:HB	1.75	0.66
1:A:234:GLN:HA	1:A:237:ARG:NE	2.11	0.66
2:B:298:SER:O	2:B:300:ALA:N	2.29	0.66
2:D:10:TRP:CD1	2:D:190:ILE:HD12	2.30	0.66
2:D:15:PHE:HE2	2:D:57:LEU:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:116:ASP:O	3:E:118:ALA:N	2.29	0.66
2:G:220:LEU:HD22	2:G:241:LEU:HD11	1.76	0.66
1:A:74:PHE:CE2	1:F:206:VAL:HB	2.25	0.66
2:D:254:GLU:OE2	2:D:312:ARG:HD3	1.96	0.66
3:E:193:LEU:HD23	3:E:266:THR:HG21	1.78	0.66
2:B:21:GLN:HE22	2:B:175:LEU:HA	1.61	0.66
2:D:221:THR:O	2:D:225:ILE:HG13	1.95	0.66
3:E:50:CYS:SG	3:E:53:PRO:HA	2.36	0.66
2:I:21:GLN:OE1	2:I:176:LYS:O	2.13	0.66
1:A:267:THR:CG2	1:A:271:ALA:HB3	2.25	0.66
2:D:42:LEU:HD22	2:D:43:PHE:N	2.11	0.66
2:D:268:ILE:O	2:D:271:ALA:HB3	1.96	0.66
3:E:238:HIS:H	3:E:308:ARG:HD3	1.61	0.66
2:G:285:MET:HB2	2:G:332:LEU:HD21	1.77	0.66
2:H:91:ILE:HG21	2:H:107:LEU:HD13	1.78	0.66
1:A:291:ASN:O	1:A:292:ARG:HD2	1.95	0.65
2:D:254:GLU:OE2	2:D:312:ARG:CD	2.44	0.65
2:D:259:ALA:HB2	2:D:363:MET:HG2	1.77	0.65
1:F:166:ALA:CB	1:F:202:VAL:HG21	2.22	0.65
1:F:203:GLU:HG2	1:F:207:ASN:ND2	2.11	0.65
1:F:225:LYS:HD3	1:F:226:SER:N	2.11	0.65
2:I:277:GLU:HB2	2:I:280:ALA:HB3	1.75	0.65
2:C:198:HIS:CD2	2:C:203:LEU:HD11	2.31	0.65
2:C:243:THR:HG23	2:C:284:GLU:HG3	1.78	0.65
3:E:306:ILE:HG21	3:E:311:LEU:HD21	1.77	0.65
2:H:326:GLN:HE21	2:H:326:GLN:CA	1.96	0.65
1:A:223:MSE:HE2	1:A:292:ARG:HB2	1.77	0.65
1:A:261:LYS:HE3	1:A:293:LEU:O	1.95	0.65
2:D:353:LEU:O	2:D:357:LEU:HD13	1.96	0.65
1:F:222:LEU:HD13	1:F:285:MSE:HE3	1.78	0.65
2:H:271:ALA:C	2:H:276:ILE:HD11	2.16	0.65
2:I:243:THR:HG22	2:I:245:ASP:H	1.60	0.65
2:C:260:ASN:HD21	2:C:263:ARG:H	1.43	0.65
3:E:158:ARG:HG3	3:E:158:ARG:NH1	2.12	0.65
2:G:82:ILE:HG23	2:G:90:LEU:HD22	1.79	0.65
2:I:215:ARG:CG	5:I:803:AGS:C4'	2.73	0.65
2:I:363:MET:HB3	2:I:364:PRO:CD	2.24	0.65
1:A:221:LEU:HD21	1:A:328:SER:HB3	1.79	0.65
2:B:202:ALA:HB1	2:B:237:VAL:HG21	1.79	0.65
2:B:243:THR:HG22	2:B:246:ASP:HB2	1.76	0.65
3:E:145:THR:HG22	3:E:146:ARG:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:ASN:HA	2:H:140:LEU:CD1	2.26	0.65
2:C:198:HIS:HB2	2:C:232:VAL:CG2	2.26	0.65
2:C:265:MET:CE	2:D:294:MET:SD	2.85	0.65
2:G:9:LYS:HD3	2:G:194:GLU:OE1	1.97	0.65
2:I:148:GLU:HA	2:I:148:GLU:OE1	1.97	0.65
1:A:1:MSE:HE1	1:A:127:PHE:CE1	2.31	0.65
1:A:59:THR:CG2	1:A:60:ASP:N	2.60	0.65
2:C:367:GLU:OE2	2:C:368:PRO:N	2.29	0.65
1:F:274:ASP:HA	1:F:279:TRP:CE3	2.31	0.65
1:F:309:GLU:O	1:F:312:LEU:HB3	1.96	0.65
3:J:200:ALA:O	3:J:204:LEU:HD13	1.97	0.65
1:A:124:ALA:O	1:A:126:TRP:N	2.30	0.65
2:B:271:ALA:HB1	2:B:276:ILE:HG21	1.78	0.65
2:G:6:LEU:HD22	2:G:190:ILE:HG22	1.79	0.65
2:I:351:MET:SD	3:J:290:LEU:HD22	2.36	0.65
3:E:14:LEU:HD13	3:E:44:LEU:HD11	1.78	0.65
1:F:281:ASN:C	1:F:283:ARG:N	2.50	0.65
3:E:95:GLU:O	3:E:99:LYS:HB2	1.97	0.65
3:E:307:ASN:O	3:E:309:GLU:N	2.30	0.65
2:H:201:ARG:HE	2:H:205:LEU:HD21	1.61	0.65
2:H:271:ALA:HA	2:H:274:ARG:HE	1.61	0.65
2:C:221:THR:O	2:C:225:ILE:HG13	1.97	0.64
1:F:53:PHE:CZ	1:F:67:LEU:HD22	2.32	0.64
2:I:6:LEU:CD1	2:I:221:THR:HB	2.27	0.64
1:A:74:PHE:CE2	1:F:206:VAL:CB	2.78	0.64
2:B:158:ASP:O	2:B:158:ASP:CG	2.36	0.64
2:D:42:LEU:HD23	2:D:154:LEU:CB	2.26	0.64
2:G:61:GLY:HA2	2:G:72:PRO:HG3	1.79	0.64
2:H:250:LEU:HD22	2:H:309:ILE:HD12	1.79	0.64
2:I:19:VAL:HG12	2:I:178:LEU:CD2	2.21	0.64
2:I:283:VAL:HG22	2:I:336:ARG:NH1	2.13	0.64
2:B:367:GLU:N	2:B:367:GLU:OE2	2.30	0.64
2:C:232:VAL:CG2	2:C:232:VAL:O	2.45	0.64
2:H:279:GLU:HG2	2:H:339:LEU:CD2	2.28	0.64
2:I:268:ILE:HD11	2:I:353:LEU:HD12	1.78	0.64
3:J:238:HIS:ND1	3:J:239:GLU:N	2.45	0.64
1:A:214:PRO:O	1:A:218:VAL:HG23	1.98	0.64
1:A:222:LEU:O	1:A:224:GLY:N	2.31	0.64
2:I:19:VAL:CG1	2:I:178:LEU:HD22	2.22	0.64
2:B:186:GLN:HE21	2:B:190:ILE:HD11	1.63	0.64
3:E:31:ALA:HB2	3:E:164:LEU:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:GLY:HA3	1:F:139:CYS:O	1.97	0.64
2:D:38:HIS:CD2	2:D:40:ALA:H	2.15	0.64
3:E:136:PRO:O	3:E:137:ALA:O	2.15	0.64
1:F:64:ILE:HG12	1:F:96:GLN:HE21	1.61	0.64
2:G:250:LEU:CD2	2:G:288:LEU:HD13	2.28	0.64
2:H:7:ALA:HA	2:H:218:LEU:HD23	1.79	0.64
2:H:93:ILE:HG12	2:I:133:ARG:HH12	1.63	0.64
2:H:279:GLU:HG2	2:H:339:LEU:HD23	1.80	0.64
2:B:260:ASN:HD22	2:B:263:ARG:CB	2.06	0.64
2:B:343:PRO:CG	2:B:347:MET:SD	2.86	0.64
2:G:76:CYS:SG	2:G:78:ASN:HB2	2.38	0.64
2:H:215:ARG:NH1	6:H:1400:PO4:O1	2.30	0.64
2:B:58:LEU:HD23	2:B:153:LEU:HD22	1.79	0.64
2:D:345:ARG:CZ	3:E:150:ARG:HE	2.10	0.64
1:F:295:GLN:H	1:F:295:GLN:NE2	1.96	0.64
2:G:6:LEU:CB	2:G:190:ILE:CG2	2.64	0.64
2:I:246:ASP:CB	2:I:248:GLN:HG2	2.27	0.64
2:B:347:MET:HG3	2:C:290:HIS:CE1	2.33	0.63
3:J:161:LEU:HD12	3:J:161:LEU:H	1.63	0.63
1:A:269:LEU:CG	1:A:273:PHE:CZ	2.81	0.63
2:D:259:ALA:HA	2:D:363:MET:CE	2.28	0.63
2:D:360:HIS:CD2	2:D:363:MET:HG3	2.33	0.63
1:F:225:LYS:HD3	1:F:226:SER:H	1.63	0.63
2:H:128:VAL:HG23	2:H:162:LEU:HD21	1.80	0.63
1:A:71:MSE:SE	1:F:231:HIS:HB2	2.47	0.63
2:D:24:VAL:O	2:D:25:LEU:C	2.36	0.63
3:E:254:ASP:CG	3:E:265:VAL:HG13	2.18	0.63
3:E:289:ILE:HG23	3:E:319:ILE:CD1	2.28	0.63
1:F:61:TRP:HA	1:F:64:ILE:HD13	1.81	0.63
2:H:93:ILE:HG12	2:I:133:ARG:NH1	2.13	0.63
2:H:351:MET:CE	2:I:326:GLN:HE22	2.11	0.63
2:I:279:GLU:HB3	3:J:149:GLU:OE2	1.97	0.63
2:C:293:ALA:HA	2:C:296:GLN:HG3	1.80	0.63
3:E:151:LEU:HD11	3:E:155:LEU:HD12	1.79	0.63
2:B:179:ASP:HB2	2:B:182:GLN:NE2	2.13	0.63
2:C:65:GLU:HA	2:C:119:ARG:NH2	2.13	0.63
2:C:86:ARG:NH1	2:D:141:LYS:HG3	2.12	0.63
3:E:68:MSE:HE3	3:E:73:HIS:CB	2.28	0.63
2:B:350:GLU:OE1	2:C:294:MET:CE	2.47	0.63
2:C:35:GLY:O	2:C:37:ILE:N	2.31	0.63
2:D:27:ALA:O	2:D:28:LEU:C	2.37	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:THR:HG23	1:F:320:VAL:HG13	1.81	0.63
2:G:316:LEU:HD22	2:G:320:ILE:HD11	1.80	0.63
2:B:13:GLN:NE2	2:B:83:GLU:OE2	2.31	0.63
2:B:304:ASN:CG	2:B:305:ASP:H	2.01	0.63
2:D:263:ARG:O	2:D:266:ALA:HB3	1.99	0.63
1:F:330:LEU:O	1:F:330:LEU:HD13	1.97	0.63
2:D:184:ARG:HD3	2:D:184:ARG:C	2.19	0.63
3:E:145:THR:HG22	3:E:147:GLU:H	1.64	0.63
2:I:271:ALA:O	2:I:276:ILE:HG13	1.99	0.63
1:A:268:PRO:O	1:A:270:ARG:N	2.30	0.63
2:B:333:LEU:HD13	2:B:333:LEU:C	2.19	0.63
2:I:6:LEU:CB	2:I:218:LEU:HB3	2.29	0.63
2:B:165:THR:HB	2:B:169:ARG:HH12	1.64	0.62
2:D:15:PHE:HD2	2:D:57:LEU:HD13	1.62	0.62
2:G:278:TRP:CE3	2:G:349:VAL:HG21	2.34	0.62
2:C:147:PRO:HB2	2:C:149:HIS:CE1	2.34	0.62
3:E:36:GLY:O	3:E:37:ASP:C	2.38	0.62
3:E:253:MSE:O	3:E:257:LYS:HG3	1.99	0.62
1:F:26:ASN:O	1:F:28:PRO:HD3	1.99	0.62
2:G:6:LEU:CD2	2:G:194:GLU:HG3	2.29	0.62
1:A:331:LEU:N	1:A:331:LEU:HD23	2.14	0.62
1:F:99:THR:O	1:F:103:LEU:HD13	1.99	0.62
2:H:215:ARG:CZ	6:H:1400:PO4:O1	2.47	0.62
2:I:215:ARG:HB2	5:I:803:AGS:C5'	2.28	0.62
2:D:360:HIS:HD2	2:D:363:MET:N	1.97	0.62
3:E:297:ARG:HG2	3:E:298:GLU:N	2.14	0.62
1:A:263:GLN:HG2	1:A:266:HIS:HD2	1.64	0.62
2:C:49:VAL:HG11	2:C:175:LEU:HB3	1.80	0.62
2:C:260:ASN:ND2	2:C:263:ARG:H	1.97	0.62
2:D:260:ASN:OD1	2:D:263:ARG:HB2	1.99	0.62
1:F:299:ARG:O	1:F:302:VAL:HB	1.98	0.62
2:H:257:VAL:HG11	2:H:320:ILE:CD1	2.30	0.62
2:I:295:VAL:HG11	2:I:314:ARG:HG2	1.81	0.62
3:J:30:GLN:CG	3:J:148:PRO:HD3	2.22	0.62
3:J:110:LYS:HB2	3:J:139:THR:HG23	1.82	0.62
1:A:278:VAL:O	1:A:280:GLN:OE1	2.18	0.62
3:E:220:LEU:HD21	3:E:248:LEU:HD13	1.82	0.62
3:J:244:ARG:HG2	3:J:247:TRP:CZ3	2.34	0.62
3:E:30:GLN:CG	3:E:163:TYR:CD1	2.81	0.62
1:F:46:GLY:O	1:F:77:ARG:HB2	1.99	0.62
2:G:288:LEU:O	2:G:292:ILE:HG13	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:LYS:HE2	2:I:136:PHE:HD2	1.64	0.62
2:C:97:SER:CB	2:C:100:LYS:HD2	2.30	0.62
1:F:162:LEU:HD11	1:F:185:LEU:HD21	1.82	0.62
2:G:102:GLU:HG3	2:G:105:ARG:NH2	2.14	0.62
2:H:350:GLU:O	2:H:354:LEU:HD12	2.00	0.62
2:B:309:ILE:CG2	2:B:313:MET:HG2	2.28	0.62
1:A:154:ARG:HH11	1:A:157:GLN:HE21	1.46	0.62
2:C:341:TYR:HB2	2:D:333:LEU:HD11	1.81	0.62
2:D:366:PRO:O	2:D:367:GLU:HG3	2.00	0.62
3:E:303:VAL:HB	3:E:306:ILE:CD1	2.26	0.62
2:H:229:ASP:OD2	2:I:30:ASN:OD1	2.18	0.62
3:J:64:GLY:O	3:J:68:MSE:HB2	2.00	0.62
2:C:100:LYS:HD3	2:D:133:ARG:HE	1.65	0.61
2:D:10:TRP:CG	2:D:190:ILE:HD12	2.34	0.61
2:D:129:HIS:HB2	2:D:161:LYS:HB2	1.82	0.61
1:F:93:ILE:HG23	1:F:97:LEU:HD13	1.82	0.61
2:G:248:GLN:O	2:G:250:LEU:C	2.37	0.61
2:H:343:PRO:HB3	2:I:283:VAL:HG13	1.80	0.61
2:B:5:VAL:HG23	2:B:7:ALA:HB3	1.81	0.61
2:C:77:ASP:O	2:C:81:GLU:HG3	2.00	0.61
2:D:285:MET:O	2:D:286:LEU:C	2.39	0.61
1:F:199:LEU:HB3	1:F:200:PRO:HD3	1.82	0.61
1:F:303:GLN:O	1:F:306:THR:HB	2.00	0.61
2:G:316:LEU:HB3	2:G:320:ILE:HD12	1.82	0.61
3:J:90:VAL:HG22	3:J:124:ALA:N	2.15	0.61
2:C:184:ARG:HG2	2:C:184:ARG:NH1	2.15	0.61
2:D:277:GLU:HB2	2:D:280:ALA:CB	2.29	0.61
2:I:363:MET:SD	2:I:364:PRO:HD2	2.40	0.61
2:G:15:PHE:CE2	2:G:57:LEU:HB3	2.36	0.61
2:H:201:ARG:HH21	2:H:205:LEU:HD23	1.64	0.61
2:C:202:ALA:HB2	2:C:234:THR:HA	1.82	0.61
2:B:205:LEU:HD11	2:B:234:THR:HG23	1.82	0.61
2:C:120:PHE:CD2	2:C:120:PHE:N	2.69	0.61
2:C:271:ALA:HB1	2:C:276:ILE:HD11	1.81	0.61
2:D:360:HIS:HD2	2:D:363:MET:H	1.48	0.61
2:G:98:ARG:CG	2:H:169:ARG:HH22	2.13	0.61
2:I:215:ARG:CA	5:I:803:AGS:O4'	2.48	0.61
2:B:44:SER:CB	2:B:159:PRO:CG	2.78	0.61
2:C:15:PHE:CE1	2:C:57:LEU:HB3	2.35	0.61
2:C:58:LEU:HD23	2:C:153:LEU:CD2	2.31	0.61
2:I:11:ARG:NH2	2:I:56:ARG:NH2	2.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG11	1:A:111:ILE:HD11	1.82	0.61
2:C:259:ALA:HB2	2:C:360:HIS:HD1	1.64	0.61
2:C:265:MET:HE3	2:D:294:MET:SD	2.40	0.61
2:D:180:VAL:O	2:D:181:GLU:C	2.39	0.61
2:D:259:ALA:HB2	2:D:363:MET:CG	2.30	0.61
2:G:186:GLN:O	2:G:190:ILE:HG13	2.01	0.61
3:J:126:ASN:HA	3:J:129:LEU:HD13	1.82	0.61
1:F:47:PHE:HA	1:F:77:ARG:O	1.99	0.61
1:F:202:VAL:O	1:F:206:VAL:HG23	2.01	0.61
2:G:6:LEU:CB	2:G:190:ILE:HG21	2.11	0.61
2:B:76:CYS:O	2:B:80:ARG:HG3	2.01	0.61
1:A:74:PHE:CE1	1:F:203:GLU:C	2.74	0.60
1:A:264:SER:O	1:A:265:ALA:HB3	2.01	0.60
1:A:275:LYS:HA	1:A:275:LYS:HE2	1.83	0.60
2:C:354:LEU:O	2:C:357:LEU:N	2.34	0.60
2:H:21:GLN:OE1	2:H:175:LEU:HB3	2.01	0.60
2:I:56:ARG:HH11	2:I:56:ARG:HG3	1.64	0.60
1:A:222:LEU:CD1	1:A:285:MSE:HE3	2.31	0.60
2:C:278:TRP:CZ2	2:C:346:ARG:HD2	2.36	0.60
2:D:355:ARG:HH21	3:E:332:PRO:HD3	1.66	0.60
1:F:27:ASP:OD2	1:F:178:LEU:HD12	2.01	0.60
2:G:341:TYR:CZ	2:H:337:LYS:HG2	2.36	0.60
2:B:44:SER:HB3	2:B:159:PRO:CG	2.32	0.60
2:B:64:CYS:SG	2:B:66:THR:HB	2.41	0.60
1:F:13:LEU:HD23	1:F:41:VAL:CG2	2.31	0.60
1:F:304:LEU:CB	1:F:327:LEU:HD11	2.32	0.60
3:J:188:LEU:HD23	3:J:268:VAL:HG21	1.84	0.60
3:J:320:GLU:HA	3:J:323:LEU:HD12	1.83	0.60
2:B:226:ALA:O	2:C:26:THR:HG22	2.01	0.60
2:G:274:ARG:HE	2:G:276:ILE:CD1	2.09	0.60
1:A:213:THR:HG22	1:A:215:PHE:H	1.65	0.60
2:C:347:MET:HG2	2:D:290:HIS:CE1	2.36	0.60
2:D:355:ARG:NH1	3:E:287:GLN:HB3	2.16	0.60
3:E:50:CYS:SG	3:E:53:PRO:CA	2.89	0.60
2:H:112:GLN:HB2	2:H:121:LYS:HZ3	1.66	0.60
1:A:130:LEU:O	1:A:132:ASN:N	2.35	0.60
2:C:112:GLN:CD	2:C:121:LYS:HE2	2.22	0.60
2:C:140:LEU:HD13	2:C:169:ARG:NH1	2.17	0.60
2:D:277:GLU:HB3	3:E:149:GLU:HB2	1.84	0.60
3:E:41:ILE:HD12	3:E:142:PHE:HB3	1.83	0.60
1:F:188:LEU:HG	1:F:197:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:316:LEU:HA	3:J:319:ILE:HD12	1.84	0.60
2:D:332:LEU:CD2	2:D:352:THR:HG22	2.32	0.60
2:D:357:LEU:HG	2:D:363:MET:HE1	1.84	0.60
2:G:6:LEU:HD23	2:G:194:GLU:HG3	1.82	0.60
2:I:277:GLU:HB3	3:J:149:GLU:HG3	1.82	0.60
3:J:79:LEU:HD13	3:J:112:VAL:HG13	1.84	0.60
1:A:333:HIS:HB3	2:B:298:SER:OG	2.01	0.60
2:H:64:CYS:SG	2:H:66:THR:HB	2.41	0.60
2:H:191:LEU:HD12	2:H:203:LEU:HD21	1.84	0.60
2:H:302:LEU:HD12	2:H:314:ARG:HE	1.65	0.60
2:I:200:PRO:HB2	2:I:305:ASP:HB2	0.80	0.60
3:J:214:GLU:HG2	3:J:218:GLN:HE21	1.66	0.60
2:H:89:ASP:HB3	2:H:121:LYS:HA	1.83	0.60
2:I:198:HIS:HA	2:I:232:VAL:O	2.02	0.60
2:B:243:THR:CG2	2:B:246:ASP:HB2	2.31	0.60
2:D:60:LYS:HA	2:D:82:ILE:HD12	1.83	0.60
1:F:165:ALA:HB1	1:F:199:LEU:HD13	1.84	0.60
2:I:7:ALA:CB	2:I:215:ARG:HG3	2.31	0.60
2:I:158:ASP:CG	2:I:161:LYS:HG2	2.22	0.60
2:I:244:LEU:HD21	2:I:276:ILE:CG1	2.31	0.60
3:J:111:VAL:HA	3:J:140:TRP:O	2.01	0.60
3:J:212:ALA:HB1	3:J:244:ARG:NH2	2.16	0.60
1:A:20:ALA:HB2	1:A:110:LEU:HB3	1.84	0.59
2:B:347:MET:HG3	2:C:290:HIS:ND1	2.17	0.59
2:C:52:THR:O	2:C:55:ALA:HB3	2.02	0.59
2:D:329:TYR:C	2:D:329:TYR:CD2	2.75	0.59
2:G:263:ARG:O	2:G:267:LEU:HG	2.00	0.59
3:J:220:LEU:HA	3:J:232:LEU:HD21	1.83	0.59
1:A:19:ALA:HB3	1:A:133:ARG:HB3	1.85	0.59
2:B:278:TRP:O	2:B:280:ALA:N	2.35	0.59
2:C:18:VAL:HG11	2:C:54:ILE:HD11	1.84	0.59
2:C:59:ALA:O	2:C:82:ILE:HD13	2.00	0.59
2:C:257:VAL:O	2:C:360:HIS:CE1	2.55	0.59
2:C:300:ALA:O	2:C:302:LEU:N	2.35	0.59
2:D:247:ASP:O	2:D:251:SER:HB2	2.02	0.59
2:D:360:HIS:CG	2:D:361:PRO:N	2.70	0.59
3:E:232:LEU:O	3:E:233:LEU:C	2.39	0.59
1:F:130:LEU:HB3	1:F:134:SER:OG	2.02	0.59
1:F:264:SER:O	1:F:265:ALA:HB3	2.01	0.59
1:F:316:TYR:CG	1:F:316:TYR:O	2.55	0.59
2:H:95:ALA:HB3	2:H:127:GLU:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:HIS:HD2	2:H:161:LYS:HD2	1.66	0.59
1:A:119:LYS:O	1:A:123:ASN:ND2	2.35	0.59
1:A:128:THR:O	1:A:131:ALA:HB3	2.02	0.59
3:E:163:TYR:CE2	3:E:165:ALA:HB2	2.36	0.59
2:G:179:ASP:HB3	2:G:182:GLN:HB2	1.84	0.59
2:G:286:LEU:HG	2:G:332:LEU:HD23	1.83	0.59
2:H:21:GLN:HE22	2:H:49:VAL:CG1	2.15	0.59
2:H:152:PHE:O	2:H:153:LEU:HD23	2.02	0.59
1:A:73:LEU:HB2	1:F:207:ASN:CB	2.31	0.59
2:C:186:GLN:HG3	2:C:190:ILE:CD1	2.32	0.59
2:D:302:LEU:HD13	2:D:310:GLU:OE2	2.03	0.59
2:D:345:ARG:NH2	3:E:150:ARG:HE	2.00	0.59
2:I:18:VAL:CG1	2:I:25:LEU:HD11	2.32	0.59
2:D:111:VAL:CG1	2:D:112:GLN:N	2.65	0.59
2:D:363:MET:CB	2:D:364:PRO:CD	2.79	0.59
1:F:223:MSE:HE1	1:F:292:ARG:CB	2.32	0.59
1:F:251:GLN:HE22	3:J:307:ASN:ND2	2.00	0.59
2:H:21:GLN:OE1	2:H:175:LEU:HD22	2.02	0.59
2:H:78:ASN:O	2:H:82:ILE:HG13	2.01	0.59
3:J:229:TRP:CE3	3:J:319:ILE:HG21	2.37	0.59
1:A:193:PRO:CG	2:B:36:ARG:HH22	2.11	0.59
2:B:81:GLU:HB2	2:B:87:PHE:CD1	2.35	0.59
2:C:120:PHE:HB3	2:C:149:HIS:O	2.01	0.59
3:E:5:PRO:O	3:E:7:LEU:N	2.35	0.59
1:F:174:TYR:HB2	1:F:181:LEU:CD2	2.33	0.59
2:H:272:ALA:HB2	2:H:278:TRP:HH2	1.68	0.59
3:J:4:TYR:HB3	3:J:5:PRO:HD2	1.83	0.59
3:J:253:MSE:O	3:J:253:MSE:HE3	2.02	0.59
1:F:310:LEU:C	1:F:314:GLN:HG3	2.23	0.59
3:J:18:TYR:HB3	3:J:48:LEU:HD21	1.85	0.59
2:B:245:ASP:O	2:B:246:ASP:C	2.40	0.59
2:B:276:ILE:CD1	2:B:281:LEU:HB2	2.20	0.59
2:C:264:VAL:HG13	2:C:353:LEU:HD13	1.84	0.59
2:D:124:LEU:HD22	2:D:124:LEU:C	2.22	0.59
2:D:357:LEU:O	2:D:360:HIS:HB3	2.01	0.59
3:E:20:ALA:HB3	3:E:22:ARG:HD3	1.84	0.59
2:G:144:GLU:C	2:G:146:PRO:HD3	2.23	0.59
2:H:21:GLN:HE22	2:H:49:VAL:HG13	1.68	0.59
2:I:250:LEU:HD21	2:I:312:ARG:HD2	1.84	0.59
2:D:253:VAL:O	2:D:254:GLU:C	2.41	0.59
1:F:279:TRP:O	1:F:279:TRP:CD2	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:111:VAL:CG1	2:H:150:VAL:HG21	2.33	0.59
3:E:281:LEU:HD21	3:E:323:LEU:HD21	1.84	0.59
1:F:57:PRO:C	1:F:59:THR:H	2.06	0.59
1:F:264:SER:O	1:F:265:ALA:CB	2.51	0.59
2:G:240:MET:HG3	2:G:241:LEU:H	1.68	0.59
2:B:263:ARG:HG2	2:B:267:LEU:CD1	2.32	0.58
2:C:281:LEU:O	2:C:285:MET:HG3	2.02	0.58
2:C:360:HIS:CD2	2:C:361:PRO:CD	2.80	0.58
1:F:211:HIS:CG	1:F:211:HIS:O	2.56	0.58
2:G:295:VAL:HA	2:G:298:SER:O	2.03	0.58
2:H:11:ARG:HH22	2:I:165:THR:HG22	1.68	0.58
2:H:316:LEU:HB3	2:H:320:ILE:HD12	1.85	0.58
2:I:248:GLN:CG	2:I:274:ARG:HH22	2.13	0.58
3:J:92:ALA:O	3:J:96:VAL:HG23	2.03	0.58
1:A:130:LEU:HB3	1:A:134:SER:OG	2.02	0.58
1:A:213:THR:CG2	1:A:215:PHE:HB2	2.33	0.58
2:D:355:ARG:NH2	3:E:332:PRO:HD3	2.17	0.58
3:E:314:ASP:OD2	3:E:318:ARG:NH2	2.37	0.58
1:F:285:MSE:CG	1:F:285:MSE:CE	2.80	0.58
1:F:299:ARG:HG3	3:J:317:LEU:HD21	1.86	0.58
2:G:355:ARG:HD2	2:G:355:ARG:O	2.02	0.58
3:J:29:ILE:HD12	3:J:29:ILE:N	2.17	0.58
2:C:133:ARG:HD3	2:C:133:ARG:H	1.66	0.58
2:C:324:ASP:O	2:C:327:LEU:HB3	2.03	0.58
3:E:220:LEU:HA	3:E:223:SER:HB2	1.85	0.58
1:F:59:THR:O	1:F:60:ASP:HB2	2.02	0.58
2:G:210:ALA:HB2	2:G:220:LEU:HD12	1.85	0.58
2:H:51:LYS:HE2	6:H:1400:PO4:O2	2.03	0.58
1:A:85:PRO:HB2	1:A:88:GLY:H	1.68	0.58
1:A:285:MSE:CE	1:A:285:MSE:CG	2.80	0.58
2:D:360:HIS:CG	2:D:363:MET:HG3	2.38	0.58
3:E:209:ASN:O	3:E:212:ALA:HB3	2.04	0.58
2:G:43:PHE:O	2:G:51:LYS:HD2	2.02	0.58
2:G:252:LEU:O	2:G:252:LEU:HD23	2.03	0.58
2:G:277:GLU:HG2	2:G:280:ALA:HB2	1.84	0.58
3:J:8:ARG:CG	3:J:9:PRO:HD3	2.33	0.58
1:A:54:SER:HA	1:A:83:LEU:HB2	1.86	0.58
1:A:269:LEU:O	1:A:273:PHE:CD1	2.57	0.58
2:B:41:TYR:C	2:B:170:CYS:SG	2.81	0.58
2:B:76:CYS:SG	2:B:78:ASN:N	2.75	0.58
2:C:201:ARG:HG3	2:C:234:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:ASP:HB3	2:D:248:GLN:NE2	2.18	0.58
3:E:214:GLU:O	3:E:218:GLN:HG3	2.04	0.58
1:F:71:MSE:HA	1:F:78:GLN:HE22	1.69	0.58
1:F:247:LEU:HD21	1:F:308:THR:CG2	2.33	0.58
2:I:254:GLU:O	2:I:258:GLU:HG2	2.04	0.58
2:I:261:GLY:HA2	2:I:357:LEU:HD21	1.86	0.58
3:J:188:LEU:HD11	3:J:192:ARG:HE	1.68	0.58
2:B:362:ARG:O	2:B:364:PRO:HD3	2.03	0.58
2:C:49:VAL:HG11	2:C:175:LEU:CB	2.32	0.58
2:D:260:ASN:OD1	2:D:263:ARG:CB	2.51	0.58
1:F:250:LEU:N	1:F:250:LEU:HD23	2.18	0.58
2:C:204:GLN:O	2:C:207:ALA:HB3	2.04	0.58
2:C:367:GLU:CG	2:D:321:PRO:HA	2.34	0.58
2:D:278:TRP:CE2	2:D:346:ARG:HB2	2.39	0.58
3:E:204:LEU:O	3:E:209:ASN:HB2	2.03	0.58
1:F:304:LEU:HD13	1:F:327:LEU:CD2	2.32	0.58
2:G:253:VAL:O	2:G:256:MET:HB3	2.04	0.58
1:A:17:LEU:HD21	1:A:109:LEU:CD1	2.34	0.58
1:A:232:ILE:O	1:A:236:LEU:HB2	2.04	0.58
1:A:293:LEU:HB3	1:A:298:LEU:HD11	1.85	0.58
2:B:63:ASN:O	2:B:78:ASN:ND2	2.25	0.58
2:D:15:PHE:CE2	2:D:57:LEU:HB3	2.38	0.58
2:G:61:GLY:CA	2:G:72:PRO:HG3	2.32	0.58
2:G:239:ALA:HB1	2:H:23:HIS:CD2	2.39	0.58
2:I:6:LEU:HB2	2:I:218:LEU:O	2.04	0.58
2:D:306:MET:C	2:D:308:ALA:H	2.07	0.58
3:E:194:SER:O	3:E:195:ALA:HB3	2.03	0.58
2:G:177:ALA:HB1	2:G:212:GLY:O	2.03	0.58
2:G:191:LEU:HD22	2:G:196:ILE:HB	1.86	0.58
1:A:196:LYS:H	1:A:201:ARG:NH1	2.01	0.58
2:D:91:ILE:HD11	2:D:121:LYS:HE3	1.86	0.58
2:D:148:GLU:HA	2:D:148:GLU:OE1	2.04	0.58
2:D:236:ALA:O	2:D:239:ALA:HB3	2.04	0.58
2:G:362:ARG:O	2:G:363:MET:HB2	2.02	0.58
1:A:119:LYS:HD3	1:A:119:LYS:N	2.04	0.57
2:C:292:ILE:HG12	2:C:313:MET:HE3	1.85	0.57
2:D:144:GLU:C	2:D:146:PRO:HD3	2.24	0.57
2:D:289:LEU:HD12	2:D:329:TYR:HA	1.86	0.57
3:J:111:VAL:HG12	3:J:140:TRP:HB2	1.84	0.57
1:A:273:PHE:HB3	1:A:279:TRP:CB	2.34	0.57
2:C:244:LEU:HD22	2:C:248:GLN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:314:ARG:HG2	2:C:314:ARG:HH11	1.69	0.57
2:D:19:VAL:HG21	2:D:186:GLN:HG3	1.85	0.57
2:D:185:HIS:ND1	2:D:185:HIS:O	2.37	0.57
2:D:276:ILE:CG2	2:D:277:GLU:N	2.67	0.57
3:E:42:TYR:HE2	3:E:46:ARG:HH12	1.51	0.57
3:E:220:LEU:O	3:E:224:VAL:HG23	2.03	0.57
3:E:321:HIS:CE1	3:E:327:VAL:HG22	2.39	0.57
2:H:21:GLN:O	2:H:25:LEU:HG	2.03	0.57
2:I:309:ILE:HG22	2:I:313:MET:HG2	1.85	0.57
2:B:42:LEU:HD23	2:B:42:LEU:C	2.24	0.57
2:C:80:ARG:O	2:C:84:GLN:HG3	2.04	0.57
3:E:57:LYS:HG3	3:E:58:SER:H	1.68	0.57
1:F:166:ALA:HB1	1:F:202:VAL:CG2	2.25	0.57
3:J:253:MSE:O	3:J:257:LYS:HG3	2.04	0.57
1:A:90:ASN:OD1	1:A:93:ILE:HG13	2.03	0.57
1:A:106:ASP:OD2	1:F:225:LYS:HB2	2.03	0.57
2:B:10:TRP:CE2	2:B:190:ILE:HG23	2.39	0.57
2:B:143:LEU:HD23	2:B:144:GLU:N	2.20	0.57
2:B:251:SER:HB3	2:B:267:LEU:HD21	1.86	0.57
2:C:102:GLU:HA	2:C:105:ARG:HD3	1.87	0.57
2:D:259:ALA:HB1	2:D:363:MET:HG2	1.84	0.57
2:D:363:MET:CG	2:D:364:PRO:HD2	2.34	0.57
2:H:100:LYS:CE	2:I:133:ARG:HA	2.34	0.57
2:I:61:GLY:CA	2:I:72:PRO:HG3	2.34	0.57
1:A:187:ARG:HG2	1:A:188:LEU:N	2.19	0.57
3:E:152:LEU:HD22	3:E:154:THR:CG2	2.34	0.57
3:E:209:ASN:O	3:E:212:ALA:N	2.37	0.57
3:E:270:VAL:HG23	3:E:270:VAL:O	2.03	0.57
1:F:295:GLN:NE2	1:F:295:GLN:N	2.53	0.57
2:G:6:LEU:CD2	2:G:191:LEU:HD23	2.34	0.57
1:A:24:LEU:HD13	1:A:117:LEU:HG	1.86	0.57
1:A:279:TRP:O	1:A:279:TRP:CD2	2.58	0.57
1:A:293:LEU:HB3	1:A:298:LEU:CD1	2.35	0.57
2:C:30:ASN:O	2:C:33:SER:N	2.38	0.57
2:C:232:VAL:O	2:C:232:VAL:HG23	2.05	0.57
2:D:25:LEU:HD21	2:D:54:ILE:HD11	1.86	0.57
3:E:17:SER:HB2	3:E:22:ARG:O	2.04	0.57
3:E:216:LEU:O	3:E:219:ALA:HB3	2.04	0.57
2:H:360:HIS:HD2	2:H:363:MET:N	1.86	0.57
2:I:10:TRP:HB2	2:I:218:LEU:CD1	2.35	0.57
3:E:149:GLU:C	3:E:151:LEU:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:VAL:HG12	2:G:178:LEU:CD1	2.35	0.57
3:J:202:LEU:C	3:J:202:LEU:HD22	2.25	0.57
2:B:36:ARG:CB	2:B:36:ARG:NH1	2.58	0.57
2:B:286:LEU:O	2:B:289:LEU:HB2	2.05	0.57
2:C:271:ALA:HB1	2:C:276:ILE:CD1	2.35	0.57
2:C:309:ILE:HG13	2:C:313:MET:HG2	1.87	0.57
3:E:75:ASP:HB3	3:E:110:LYS:HA	1.87	0.57
2:G:64:CYS:SG	2:G:66:THR:HB	2.45	0.57
2:G:82:ILE:HG23	2:G:90:LEU:CD2	2.35	0.57
2:G:214:LEU:HD23	5:G:804:AGS:C8	2.34	0.57
2:H:209:ALA:HB2	2:H:241:LEU:HD11	1.86	0.57
1:A:2:ILE:HB	1:A:135:VAL:HG22	1.87	0.57
2:C:333:LEU:O	2:C:335:GLY:N	2.38	0.57
3:E:90:VAL:HG22	3:E:124:ALA:N	2.19	0.57
3:E:90:VAL:O	3:E:94:ARG:HG3	2.05	0.57
1:F:222:LEU:O	1:F:223:MSE:HB2	2.04	0.57
2:H:302:LEU:HD13	2:H:310:GLU:HG3	1.86	0.57
2:I:286:LEU:HD23	2:I:332:LEU:HD23	1.85	0.57
2:B:242:GLY:O	2:B:244:LEU:HG	2.05	0.57
2:B:253:VAL:O	2:B:256:MET:HB3	2.05	0.57
2:B:362:ARG:O	2:B:364:PRO:CD	2.53	0.57
2:C:271:ALA:C	2:C:276:ILE:HD11	2.25	0.57
2:D:199:GLU:OE1	2:D:233:SER:HB2	2.05	0.57
2:G:10:TRP:HD1	2:G:190:ILE:HG23	1.69	0.57
2:G:98:ARG:CD	2:H:140:LEU:HD13	2.34	0.57
2:G:198:HIS:CD2	2:G:203:LEU:HD11	2.40	0.57
3:J:214:GLU:HG2	3:J:218:GLN:NE2	2.20	0.57
2:B:165:THR:HB	2:B:169:ARG:NH1	2.20	0.56
2:C:296:GLN:OE1	2:C:322:PRO:HB3	2.04	0.56
1:A:6:PRO:HG2	1:A:30:LEU:HD13	1.87	0.56
1:A:222:LEU:HD12	1:A:285:MSE:HE3	1.88	0.56
2:B:238:SER:HA	2:B:241:LEU:O	2.05	0.56
1:F:218:VAL:HG11	1:F:253:GLU:HG3	1.87	0.56
2:G:250:LEU:HD11	2:G:309:ILE:HD13	1.87	0.56
2:H:143:LEU:O	2:H:146:PRO:HD3	2.04	0.56
3:J:296:ILE:CG2	3:J:315:LEU:HD12	2.31	0.56
2:B:184:ARG:HG3	2:B:204:GLN:OE1	2.05	0.56
2:B:259:ALA:HB2	2:B:360:HIS:HE1	1.68	0.56
2:C:234:THR:O	2:C:238:SER:OG	2.17	0.56
2:D:25:LEU:CD2	2:D:54:ILE:HD13	2.35	0.56
2:D:364:PRO:HG3	3:E:260:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LEU:HD21	1:F:109:LEU:HD12	1.86	0.56
1:F:24:LEU:HD13	1:F:117:LEU:HG	1.87	0.56
1:F:251:GLN:HE22	3:J:307:ASN:HD21	1.52	0.56
2:H:9:LYS:NZ	2:H:194:GLU:OE1	2.39	0.56
2:H:216:ASP:O	2:H:220:LEU:HG	2.05	0.56
2:I:264:VAL:O	2:I:268:ILE:HG13	2.05	0.56
3:J:32:LEU:HB2	3:J:35:MSE:HG3	1.87	0.56
1:A:27:ASP:O	1:A:31:LEU:HG	2.06	0.56
1:A:259:ASN:O	1:A:262:ARG:HB2	2.04	0.56
1:A:270:ARG:HG2	1:A:283:ARG:HH21	1.67	0.56
2:B:210:ALA:CB	2:B:217:ALA:HB2	2.34	0.56
2:B:359:PHE:HE2	2:C:323:THR:HG1	1.52	0.56
2:D:201:ARG:O	2:D:204:GLN:N	2.39	0.56
3:E:20:ALA:CB	3:E:22:ARG:HD3	2.36	0.56
1:A:59:THR:CG2	1:A:60:ASP:H	2.18	0.56
2:B:252:LEU:CD2	2:B:281:LEU:HD21	2.36	0.56
3:E:68:MSE:HE1	3:E:76:TYR:CB	2.36	0.56
1:A:27:ASP:OD2	1:A:30:LEU:HG	2.06	0.56
1:A:115:ASN:O	1:A:116:LYS:O	2.24	0.56
1:A:260:LEU:CB	1:A:290:LEU:HD11	2.36	0.56
2:D:361:PRO:O	2:D:362:ARG:HB2	2.06	0.56
1:F:64:ILE:CG1	1:F:96:GLN:HE21	2.17	0.56
2:G:28:LEU:HD22	2:G:58:LEU:HD13	1.87	0.56
2:G:258:GLU:HB3	2:G:260:ASN:ND2	2.21	0.56
2:H:50:GLY:O	2:H:54:ILE:HG13	2.06	0.56
2:H:84:GLN:HB3	2:I:144:GLU:OE2	2.06	0.56
3:J:280:HIS:O	3:J:281:LEU:HD23	2.06	0.56
1:A:117:LEU:HB2	1:A:122:GLU:HG3	1.88	0.56
2:B:262:GLU:HG3	2:B:263:ARG:N	2.21	0.56
2:C:285:MET:O	2:C:286:LEU:C	2.43	0.56
2:G:21:GLN:O	2:G:24:VAL:HB	2.05	0.56
2:H:10:TRP:NE1	2:H:190:ILE:HG23	2.21	0.56
2:B:140:LEU:O	2:B:143:LEU:HD23	2.05	0.56
2:D:259:ALA:CB	2:D:363:MET:CG	2.84	0.56
3:E:254:ASP:OD1	3:E:265:VAL:HG13	2.05	0.56
2:G:184:ARG:HG3	2:G:185:HIS:N	2.20	0.56
2:H:223:GLN:HE22	2:I:174:HIS:CE1	2.24	0.56
2:I:140:LEU:HD22	2:I:144:GLU:HG3	1.87	0.56
1:F:156:LYS:O	1:F:156:LYS:HD3	2.06	0.56
2:G:341:TYR:CE2	2:H:337:LYS:HA	2.41	0.56
2:H:32:LEU:HD13	2:H:69:THR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:220:LEU:HD21	3:J:157:SER:OG	2.06	0.56
1:A:71:MSE:SE	1:F:228:ARG:CB	3.04	0.56
2:B:250:LEU:HD23	2:B:312:ARG:CZ	2.35	0.56
2:D:45:GLY:O	2:D:157:THR:HA	2.06	0.56
2:G:261:GLY:HA3	2:H:297:LEU:HD21	1.88	0.56
3:J:8:ARG:HG2	3:J:9:PRO:HD3	1.88	0.56
2:B:277:GLU:O	2:B:278:TRP:C	2.45	0.55
3:E:214:GLU:HG2	3:E:218:GLN:HE21	1.70	0.55
2:G:326:GLN:O	2:G:330:GLN:HB3	2.07	0.55
2:I:251:SER:HB3	2:I:263:ARG:NH2	2.21	0.55
2:I:360:HIS:CG	2:I:363:MET:HG3	2.41	0.55
2:D:272:ALA:HB2	2:D:346:ARG:HH11	1.71	0.55
3:E:296:ILE:O	3:E:297:ARG:C	2.44	0.55
1:F:25:GLY:HA2	1:F:140:GLN:HE21	1.69	0.55
2:G:341:TYR:C	2:H:333:LEU:HD11	2.26	0.55
2:H:284:GLU:OE1	2:H:284:GLU:HA	2.06	0.55
2:I:248:GLN:HA	2:I:248:GLN:NE2	2.20	0.55
2:I:361:PRO:O	2:I:362:ARG:HB2	2.07	0.55
3:J:220:LEU:O	3:J:220:LEU:HD22	2.05	0.55
3:E:313:THR:O	3:E:313:THR:HG22	2.06	0.55
1:F:24:LEU:HB3	1:F:116:LYS:HA	1.88	0.55
1:F:56:ASP:OD1	1:F:85:PRO:HA	2.06	0.55
1:F:282:ARG:HG2	1:F:285:MSE:CE	2.37	0.55
2:G:10:TRP:CH2	2:G:193:GLU:CD	2.79	0.55
2:G:11:ARG:HH21	2:G:56:ARG:NE	2.04	0.55
2:G:333:LEU:CD1	2:G:337:LYS:HE3	2.37	0.55
2:I:291:ARG:HD2	2:I:306:MET:SD	2.45	0.55
2:D:27:ALA:O	2:D:30:ASN:N	2.40	0.55
3:E:280:HIS:O	3:E:281:LEU:HD23	2.07	0.55
1:F:46:GLY:C	1:F:77:ARG:HB2	2.27	0.55
2:H:307:ALA:HA	2:H:310:GLU:HB2	1.87	0.55
2:B:119:ARG:HG3	2:B:120:PHE:CD2	2.42	0.55
2:C:18:VAL:HB	2:C:25:LEU:HD11	1.88	0.55
2:C:245:ASP:O	2:C:246:ASP:C	2.43	0.55
2:G:98:ARG:HD3	2:H:140:LEU:CB	2.35	0.55
2:H:147:PRO:HG2	2:H:150:VAL:HB	1.87	0.55
2:I:56:ARG:HG3	2:I:56:ARG:NH1	2.21	0.55
2:I:80:ARG:HG2	2:I:80:ARG:HH11	1.71	0.55
1:A:274:ASP:HA	1:A:279:TRP:CE3	2.41	0.55
2:B:51:LYS:NZ	5:B:802:AGS:S1G	2.71	0.55
2:B:76:CYS:SG	2:B:79:CYS:N	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:24:VAL:O	2:C:24:VAL:HG12	2.07	0.55
3:E:151:LEU:HD11	3:E:155:LEU:CD1	2.36	0.55
2:G:7:ALA:CA	2:G:218:LEU:HD13	2.36	0.55
2:G:306:MET:O	2:G:310:GLU:HG3	2.06	0.55
2:H:291:ARG:CA	2:H:294:MET:HB2	2.34	0.55
2:I:113:TYR:HE2	2:I:147:PRO:HG3	1.71	0.55
2:B:178:LEU:HD22	2:B:178:LEU:N	2.22	0.55
2:C:261:GLY:O	2:C:262:GLU:C	2.44	0.55
2:C:263:ARG:NH1	2:C:263:ARG:HG3	2.21	0.55
2:D:144:GLU:OE1	2:D:144:GLU:HA	2.07	0.55
2:D:354:LEU:CD1	3:E:253:MSE:CE	2.85	0.55
2:G:12:PRO:O	2:G:57:LEU:HD21	2.06	0.55
2:H:115:PRO:HG3	2:H:121:LYS:HB2	1.89	0.55
2:H:250:LEU:CD2	2:H:309:ILE:HB	2.37	0.55
2:I:238:SER:CB	2:I:243:THR:HB	2.37	0.55
3:J:35:MSE:HE3	3:J:198:PRO:CD	2.33	0.55
1:A:73:LEU:HD13	1:F:206:VAL:O	2.06	0.55
2:C:215:ARG:NH2	6:C:1300:PO4:O1	2.40	0.55
2:C:316:LEU:HD22	2:C:320:ILE:CD1	2.31	0.55
3:E:241:ALA:N	3:E:242:PRO:HD2	2.21	0.55
3:E:276:GLU:O	3:E:279:ASN:HB2	2.07	0.55
1:F:194:ASP:CB	1:F:201:ARG:HH12	2.19	0.55
2:G:9:LYS:HD2	2:G:194:GLU:OE1	2.06	0.55
2:B:158:ASP:OD2	2:B:161:LYS:HG2	2.06	0.55
2:C:201:ARG:HG3	2:C:234:THR:CG2	2.37	0.55
2:D:306:MET:C	2:D:308:ALA:N	2.60	0.55
1:F:310:LEU:HB3	1:F:314:GLN:CD	2.27	0.55
2:H:11:ARG:NH2	2:I:165:THR:HG22	2.22	0.55
2:H:156:THR:HG22	2:H:158:ASP:H	1.72	0.55
3:J:161:LEU:HD12	3:J:161:LEU:N	2.21	0.55
1:A:102:GLY:HA3	2:G:310:GLU:OE1	2.06	0.55
1:F:270:ARG:CG	1:F:283:ARG:NH2	2.63	0.55
2:G:113:TYR:CD2	2:G:147:PRO:HB3	2.42	0.55
2:H:77:ASP:O	2:H:81:GLU:HG3	2.06	0.55
2:I:215:ARG:CD	5:I:803:AGS:H5'1	2.25	0.55
2:I:347:MET:O	2:I:351:MET:HG2	2.07	0.55
2:D:119:ARG:HG3	2:D:120:PHE:HD2	1.67	0.54
1:F:47:PHE:HD2	1:F:78:GLN:C	2.05	0.54
1:F:315:ASP:O	1:F:316:TYR:C	2.44	0.54
2:G:263:ARG:NE	2:G:267:LEU:HD21	2.22	0.54
2:B:353:LEU:O	2:B:354:LEU:C	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:PRO:HG2	2:C:305:ASP:CG	2.27	0.54
2:C:258:GLU:O	2:C:259:ALA:HB3	2.05	0.54
1:F:217:TRP:CZ3	1:F:250:LEU:HD22	2.42	0.54
2:H:34:LEU:HD13	2:H:36:ARG:NE	2.22	0.54
2:I:240:MET:SD	3:J:157:SER:HA	2.46	0.54
1:A:234:GLN:HA	1:A:237:ARG:HG3	1.89	0.54
2:C:100:LYS:HB3	2:D:133:ARG:NE	2.22	0.54
2:C:217:ALA:O	2:C:221:THR:OG1	2.21	0.54
2:D:124:LEU:HD22	2:D:125:ILE:N	2.21	0.54
3:E:285:ARG:HD3	3:E:323:LEU:HD23	1.90	0.54
1:F:247:LEU:HD12	1:F:312:LEU:HD22	1.89	0.54
2:G:248:GLN:HA	2:G:251:SER:HB2	1.88	0.54
2:H:87:PHE:HB3	2:H:90:LEU:HB3	1.90	0.54
1:A:161:GLU:OE1	1:A:196:LYS:HE2	2.07	0.54
2:D:238:SER:HB2	2:D:243:THR:HB	1.88	0.54
2:D:290:HIS:NE2	2:D:294:MET:HE1	2.22	0.54
3:E:210:TRP:CH2	3:E:213:ARG:NH1	2.76	0.54
1:F:174:TYR:HB2	1:F:181:LEU:HD23	1.89	0.54
1:F:250:LEU:HD23	1:F:250:LEU:H	1.73	0.54
2:G:23:HIS:CE1	2:G:176:LYS:HE3	2.42	0.54
1:A:52:THR:HG22	1:A:81:LEU:HD23	1.90	0.54
2:B:233:SER:O	2:B:237:VAL:HG23	2.07	0.54
2:C:42:LEU:HB3	2:C:172:GLN:HA	1.90	0.54
3:E:296:ILE:CA	3:E:299:GLN:HG3	2.34	0.54
2:G:148:GLU:OE1	2:G:148:GLU:HA	2.06	0.54
2:G:248:GLN:O	2:G:250:LEU:CA	2.56	0.54
2:H:91:ILE:CG2	2:H:107:LEU:HD13	2.37	0.54
2:H:93:ILE:HG21	2:H:104:THR:HG23	1.89	0.54
2:C:15:PHE:HE1	2:C:57:LEU:HB3	1.71	0.54
2:D:82:ILE:HG23	2:D:90:LEU:HD22	1.90	0.54
3:E:199:GLY:O	3:E:202:LEU:HB3	2.08	0.54
3:E:205:PHE:O	3:E:207:GLY:N	2.34	0.54
1:F:299:ARG:HG3	3:J:317:LEU:CG	2.37	0.54
2:G:284:GLU:O	2:G:288:LEU:HG	2.08	0.54
2:H:97:SER:HB3	2:H:100:LYS:HB2	1.89	0.54
3:J:46:ARG:NH1	3:J:68:MSE:HG3	2.22	0.54
2:C:314:ARG:O	2:C:315:GLU:O	2.25	0.54
3:E:13:LYS:O	3:E:16:ALA:HB3	2.06	0.54
3:E:49:LEU:HD23	3:E:68:MSE:SE	2.58	0.54
3:E:202:LEU:HD13	3:E:203:ALA:N	2.23	0.54
2:H:257:VAL:HG11	2:H:320:ILE:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:212:ALA:HB1	3:J:244:ARG:HH21	1.73	0.54
1:A:187:ARG:O	1:A:190:LEU:HB2	2.07	0.54
1:A:197:LEU:HB3	1:A:202:VAL:CG2	2.38	0.54
2:C:24:VAL:HG13	2:C:173:PHE:CD1	2.42	0.54
2:C:199:GLU:OE2	2:C:201:ARG:NH2	2.39	0.54
2:D:279:GLU:HB3	3:E:149:GLU:OE2	2.08	0.54
3:E:237:ASN:HD22	3:E:238:HIS:N	2.06	0.54
2:G:6:LEU:CD1	2:G:191:LEU:CD2	2.85	0.54
2:G:227:SER:HA	2:H:26:THR:HG22	1.90	0.54
2:G:354:LEU:HD11	2:H:294:MET:SD	2.47	0.54
2:H:201:ARG:HH21	2:H:205:LEU:CD2	2.21	0.54
2:I:51:LYS:NZ	5:I:803:AGS:S1G	2.80	0.54
2:B:245:ASP:OD1	2:B:246:ASP:N	2.41	0.54
2:B:299:PRO:C	2:B:301:ALA:H	2.11	0.54
2:B:339:LEU:HG	2:B:345:ARG:HD3	1.90	0.54
2:C:49:VAL:CG1	2:C:175:LEU:HB3	2.38	0.54
2:D:198:HIS:HA	2:D:232:VAL:O	2.08	0.54
3:E:4:TYR:HB3	3:E:5:PRO:HD2	1.89	0.54
1:F:311:THR:HA	1:F:314:GLN:OE1	2.08	0.54
2:G:338:GLU:HB3	2:H:333:LEU:CD2	2.38	0.54
2:H:100:LYS:CE	2:I:136:PHE:HD2	2.20	0.54
3:J:90:VAL:HG21	3:J:123:ALA:HB3	1.90	0.54
3:J:139:THR:HG22	3:J:140:TRP:N	2.23	0.54
1:A:316:TYR:N	1:A:316:TYR:CD1	2.76	0.54
2:D:60:LYS:HA	2:D:82:ILE:CD1	2.38	0.54
2:D:259:ALA:HA	2:D:363:MET:HE1	1.90	0.54
2:G:188:GLU:O	2:G:192:ASN:ND2	2.41	0.54
2:H:316:LEU:HD22	2:H:320:ILE:HD11	1.90	0.54
2:I:244:LEU:CD1	2:I:276:ILE:HD13	2.34	0.54
3:J:203:ALA:O	3:J:206:GLN:HG2	2.07	0.54
1:A:32:GLN:O	1:A:35:GLN:HB3	2.08	0.53
2:B:285:MET:O	2:B:286:LEU:C	2.47	0.53
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.41	0.53
2:H:295:VAL:CG2	2:H:301:ALA:HB3	2.36	0.53
2:I:277:GLU:HB2	2:I:280:ALA:CB	2.38	0.53
3:J:304:THR:HG22	3:J:305:GLY:N	2.24	0.53
1:A:82:LEU:HD13	1:A:110:LEU:HD11	1.90	0.53
2:D:38:HIS:HD2	2:D:40:ALA:H	1.54	0.53
2:D:61:GLY:CA	2:D:72:PRO:HG3	2.38	0.53
3:E:233:LEU:CD1	3:E:237:ASN:HB2	2.37	0.53
3:E:321:HIS:O	3:E:327:VAL:HG21	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ALA:HB2	1:F:133:ARG:HD3	1.90	0.53
1:F:217:TRP:HZ2	1:F:328:SER:HG	1.55	0.53
2:G:269:ASN:HA	2:G:346:ARG:HH21	1.71	0.53
3:J:331:VAL:HG13	3:J:332:PRO:HD2	1.90	0.53
2:B:198:HIS:HD2	2:B:203:LEU:HD11	1.66	0.53
2:B:236:ALA:O	2:B:239:ALA:HB3	2.08	0.53
2:C:101:VAL:HG23	2:C:102:GLU:OE2	2.08	0.53
2:D:22:GLU:C	2:D:24:VAL:N	2.62	0.53
2:H:111:VAL:HG11	2:H:150:VAL:HG21	1.90	0.53
2:I:214:LEU:HB3	5:I:803:AGS:C4	2.38	0.53
2:C:98:ARG:O	2:C:101:VAL:HG22	2.07	0.53
2:D:102:GLU:HG2	2:D:106:ASP:OD2	2.07	0.53
2:D:215:ARG:NH1	5:D:801:AGS:O2G	2.41	0.53
3:E:6:TRP:O	3:E:9:PRO:HD2	2.08	0.53
1:F:299:ARG:CG	3:J:317:LEU:HD21	2.39	0.53
2:I:258:GLU:O	2:I:259:ALA:HB3	2.09	0.53
3:J:4:TYR:N	3:J:7:LEU:HD12	2.14	0.53
3:J:51:GLN:HB2	3:J:62:CYS:HB2	1.90	0.53
2:C:302:LEU:O	2:C:303:GLY:O	2.26	0.53
2:C:350:GLU:OE1	2:D:294:MET:HE1	2.09	0.53
3:E:214:GLU:HG2	3:E:218:GLN:NE2	2.23	0.53
3:J:153:ALA:O	3:J:157:SER:OG	2.25	0.53
1:A:262:ARG:NH1	3:E:230:TYR:HB3	2.24	0.53
2:C:263:ARG:HG3	2:C:263:ARG:HH11	1.73	0.53
3:E:203:ALA:HA	3:E:206:GLN:HB2	1.91	0.53
3:E:251:LEU:O	3:E:254:ASP:N	2.39	0.53
1:F:147:LEU:HB3	1:F:148:PRO:HD3	1.90	0.53
1:F:249:THR:HB	1:F:250:LEU:HD23	1.90	0.53
2:G:119:ARG:HG3	2:G:120:PHE:CD2	2.44	0.53
2:I:159:PRO:O	2:I:162:LEU:HB2	2.08	0.53
1:A:103:LEU:C	1:A:103:LEU:HD12	2.28	0.53
2:D:25:LEU:HD21	2:D:54:ILE:HD13	1.89	0.53
2:D:61:GLY:HA2	2:D:72:PRO:HG3	1.91	0.53
3:E:74:PRO:HD2	3:E:106:LEU:CD1	2.38	0.53
3:E:88:LEU:HD23	3:E:89:GLY:N	2.23	0.53
3:E:251:LEU:O	3:E:252:LEU:C	2.46	0.53
3:E:296:ILE:O	3:E:300:LEU:HD12	2.09	0.53
1:F:1:MSE:HE1	1:F:127:PHE:CE1	2.44	0.53
1:F:96:GLN:OE1	1:F:96:GLN:HA	2.08	0.53
1:F:188:LEU:HD21	1:F:202:VAL:HG22	1.91	0.53
1:F:299:ARG:NH1	3:J:321:HIS:ND1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:48:GLY:HA3	2:G:215:ARG:H	1.74	0.53
3:J:315:LEU:O	3:J:319:ILE:HG13	2.09	0.53
1:A:213:THR:C	1:A:215:PHE:N	2.62	0.53
1:A:237:ARG:HG2	1:A:321:TRP:CZ3	2.43	0.53
2:B:21:GLN:OE1	2:B:175:LEU:HB3	2.09	0.53
2:B:133:ARG:O	2:B:137:ASN:ND2	2.42	0.53
2:B:191:LEU:HD11	2:B:232:VAL:HG21	1.90	0.53
2:G:309:ILE:HG22	2:G:313:MET:HG2	1.91	0.53
1:A:32:GLN:HE21	1:A:113:ARG:HH22	1.56	0.53
2:B:47:ARG:HD2	5:B:802:AGS:O2G	2.09	0.53
3:E:92:ALA:O	3:E:96:VAL:HG23	2.09	0.53
3:E:279:ASN:C	3:E:281:LEU:H	2.11	0.53
2:H:276:ILE:HD12	2:H:278:TRP:CZ3	2.44	0.53
2:H:295:VAL:HG13	2:H:299:PRO:HA	1.91	0.53
3:J:232:LEU:O	3:J:236:LEU:HG	2.09	0.53
3:J:333:HIS:O	3:J:334:LEU:OXT	2.27	0.53
1:A:6:PRO:HB2	1:A:7:GLU:OE2	2.08	0.53
2:B:210:ALA:HB2	2:B:217:ALA:HB2	1.90	0.53
2:B:316:LEU:O	2:B:317:ALA:C	2.46	0.53
2:D:292:ILE:HG13	2:D:313:MET:CE	2.39	0.53
2:G:341:TYR:O	2:H:333:LEU:CD1	2.56	0.53
2:I:257:VAL:HG11	2:I:320:ILE:HD13	1.91	0.53
2:C:307:ALA:HA	2:C:310:GLU:HB2	1.91	0.52
3:E:277:LEU:HD23	3:E:281:LEU:HD12	1.91	0.52
1:F:55:ILE:HG22	1:F:55:ILE:O	2.09	0.52
2:G:11:ARG:HH21	2:G:56:ARG:HH21	1.47	0.52
2:G:94:ASP:OD2	2:G:97:SER:HB2	2.08	0.52
2:H:60:LYS:HG2	2:H:79:CYS:SG	2.49	0.52
3:J:50:CYS:SG	3:J:53:PRO:HA	2.49	0.52
1:A:59:THR:HG22	1:A:60:ASP:H	1.72	0.52
2:I:271:ALA:HB1	2:I:276:ILE:CD1	2.28	0.52
2:I:357:LEU:HA	2:I:363:MET:CE	2.39	0.52
2:I:364:PRO:HG3	3:J:260:HIS:CE1	2.43	0.52
1:A:71:MSE:SE	1:F:231:HIS:HB3	2.59	0.52
2:C:220:LEU:O	2:C:222:ASP:N	2.42	0.52
2:D:254:GLU:OE2	2:D:312:ARG:HD2	2.08	0.52
1:F:2:ILE:HD11	1:F:18:ARG:HH21	1.73	0.52
3:J:94:ARG:O	3:J:98:GLU:HG2	2.09	0.52
1:A:24:LEU:HB3	1:A:116:LYS:HA	1.91	0.52
3:E:118:ALA:HB2	3:E:145:THR:HG23	1.90	0.52
1:F:19:ALA:CB	1:F:133:ARG:HD3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:GLN:CD	1:F:77:ARG:HD3	2.03	0.52
1:F:57:PRO:C	1:F:59:THR:N	2.63	0.52
3:J:147:GLU:OE2	3:J:150:ARG:HG3	2.08	0.52
1:A:102:GLY:HA3	2:G:310:GLU:CD	2.30	0.52
1:A:289:ALA:C	1:A:291:ASN:H	2.13	0.52
2:D:214:LEU:HD23	5:D:801:AGS:N3	2.23	0.52
2:I:148:GLU:CD	2:I:149:HIS:N	2.62	0.52
2:I:291:ARG:O	2:I:295:VAL:HG23	2.09	0.52
2:C:84:GLN:NE2	2:D:144:GLU:OE2	2.43	0.52
2:C:350:GLU:O	2:C:351:MET:C	2.47	0.52
2:D:268:ILE:HG23	2:D:278:TRP:CH2	2.45	0.52
3:E:145:THR:HG22	3:E:147:GLU:N	2.24	0.52
2:H:219:SER:HA	2:H:222:ASP:OD2	2.09	0.52
2:I:309:ILE:CG2	2:I:313:MET:HG2	2.39	0.52
3:J:50:CYS:SG	3:J:53:PRO:CA	2.97	0.52
3:J:317:LEU:HD22	3:J:317:LEU:C	2.30	0.52
1:F:145:ALA:O	1:F:148:PRO:HD2	2.08	0.52
1:F:221:LEU:HD13	1:F:331:LEU:HD12	1.92	0.52
2:I:21:GLN:NE2	2:I:176:LYS:N	2.00	0.52
2:B:255:ALA:HB2	2:B:263:ARG:HD3	1.92	0.52
2:C:367:GLU:HG3	2:D:321:PRO:HA	1.91	0.52
3:E:155:LEU:C	3:E:157:SER:H	2.13	0.52
1:F:269:LEU:HG	1:F:273:PHE:CE1	2.44	0.52
2:G:7:ALA:CB	2:G:218:LEU:CD1	2.76	0.52
3:J:31:ALA:CB	3:J:164:LEU:HB3	2.35	0.52
1:A:213:THR:O	1:A:216:HIS:HB2	2.10	0.52
1:A:222:LEU:C	1:A:224:GLY:H	2.12	0.52
2:B:44:SER:HB2	2:B:159:PRO:CG	2.40	0.52
2:B:360:HIS:HD2	2:B:361:PRO:N	2.08	0.52
2:C:5:VAL:O	2:C:5:VAL:HG23	2.10	0.52
2:D:268:ILE:HD11	2:D:353:LEU:HD12	1.92	0.52
2:D:292:ILE:HD11	2:D:316:LEU:HD12	1.92	0.52
2:G:139:LEU:O	2:G:143:LEU:HG	2.09	0.52
2:H:268:ILE:HD11	2:H:353:LEU:HD12	1.91	0.52
2:I:145:GLU:N	2:I:146:PRO:HD3	2.25	0.52
2:C:254:GLU:O	2:C:258:GLU:CG	2.47	0.52
2:D:218:LEU:O	2:D:221:THR:N	2.42	0.52
3:E:239:GLU:HA	3:E:308:ARG:NH2	2.25	0.52
1:F:24:LEU:HA	1:F:114:GLY:O	2.10	0.52
2:G:10:TRP:CH2	2:G:193:GLU:OE1	2.63	0.52
2:H:181:GLU:OE1	2:H:184:ARG:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD23	1:A:324:LEU:HD21	1.92	0.51
2:B:316:LEU:HD22	2:B:320:ILE:CD1	2.40	0.51
2:D:32:LEU:HD23	2:D:37:ILE:HD11	1.92	0.51
2:D:265:MET:HE3	2:D:354:LEU:HD21	1.90	0.51
2:D:363:MET:SD	2:D:364:PRO:HD2	2.50	0.51
2:I:339:LEU:N	2:I:340:PRO:HD2	2.25	0.51
1:A:105:HIS:CD2	1:A:107:ASP:HB2	2.46	0.51
1:A:105:HIS:ND1	1:A:108:LEU:HB2	2.22	0.51
2:B:318:ARG:CG	2:B:319:THR:N	2.72	0.51
2:C:10:TRP:CE2	2:C:190:ILE:HG23	2.45	0.51
2:C:37:ILE:HD13	2:C:120:PHE:HE1	1.73	0.51
2:C:100:LYS:HB3	2:D:133:ARG:HE	1.75	0.51
2:D:290:HIS:CE1	2:D:294:MET:CE	2.93	0.51
3:E:110:LYS:HD3	3:E:139:THR:OG1	2.09	0.51
3:J:220:LEU:HD23	3:J:232:LEU:HD11	1.92	0.51
3:J:253:MSE:HE2	3:J:257:LYS:HG3	1.93	0.51
3:J:303:VAL:CB	3:J:306:ILE:HD11	2.23	0.51
1:A:223:MSE:HE2	1:A:292:ARG:CB	2.39	0.51
2:B:262:GLU:O	2:B:266:ALA:HB2	2.10	0.51
2:D:244:LEU:HD21	2:D:276:ILE:HD13	1.92	0.51
2:D:265:MET:HG2	3:E:262:ALA:HB2	1.92	0.51
2:D:333:LEU:C	2:D:333:LEU:CD1	2.79	0.51
1:F:50:HIS:ND1	1:F:79:THR:CG2	2.74	0.51
2:H:253:VAL:O	2:H:256:MET:HB3	2.10	0.51
2:I:346:ARG:O	2:I:350:GLU:HG3	2.11	0.51
3:J:149:GLU:C	3:J:151:LEU:H	2.14	0.51
1:A:4:LEU:CD1	1:A:137:VAL:HG22	2.40	0.51
2:D:32:LEU:O	2:D:35:GLY:N	2.41	0.51
2:D:238:SER:O	2:D:242:GLY:N	2.43	0.51
2:D:355:ARG:HH12	3:E:287:GLN:HB3	1.74	0.51
2:G:10:TRP:CZ2	2:G:193:GLU:CD	2.83	0.51
2:H:11:ARG:NH1	2:I:169:ARG:NH1	2.56	0.51
2:I:360:HIS:CD2	2:I:360:HIS:C	2.84	0.51
3:J:225:PRO:HB3	3:J:276:GLU:OE2	2.10	0.51
1:A:74:PHE:CZ	1:F:207:ASN:N	2.79	0.51
1:A:133:ARG:HH21	2:G:300:ALA:HB1	1.73	0.51
1:A:154:ARG:HH11	1:A:157:GLN:NE2	2.08	0.51
2:B:28:LEU:HD11	2:B:43:PHE:HE1	1.75	0.51
2:D:44:SER:HA	2:D:156:THR:O	2.11	0.51
2:D:211:GLU:O	2:D:213:SER:N	2.44	0.51
3:E:220:LEU:HD21	3:E:248:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:201:ARG:HA	2:I:204:GLN:HE21	1.76	0.51
2:I:281:LEU:O	2:I:284:GLU:HB2	2.11	0.51
3:J:293:VAL:HA	3:J:315:LEU:HD11	1.92	0.51
2:B:140:LEU:HA	2:B:143:LEU:CD2	2.35	0.51
2:B:232:VAL:O	2:B:232:VAL:HG12	2.10	0.51
2:B:318:ARG:HG3	2:B:319:THR:N	2.25	0.51
2:C:19:VAL:O	2:C:21:GLN:N	2.44	0.51
3:E:92:ALA:O	3:E:95:GLU:HG2	2.10	0.51
3:E:268:VAL:O	3:E:271:PRO:HD3	2.11	0.51
1:F:82:LEU:HB2	1:F:112:VAL:HG22	1.93	0.51
1:F:217:TRP:HZ3	1:F:250:LEU:HD13	1.75	0.51
1:F:304:LEU:HB3	1:F:327:LEU:CD2	2.31	0.51
2:G:98:ARG:NH1	2:H:140:LEU:HD22	2.21	0.51
1:A:20:ALA:CB	1:A:110:LEU:HB3	2.40	0.51
1:A:80:LEU:HG	1:A:82:LEU:HD12	1.93	0.51
2:C:254:GLU:OE1	2:C:312:ARG:NH2	2.41	0.51
3:E:318:ARG:O	3:E:321:HIS:HB3	2.11	0.51
1:F:237:ARG:O	1:F:237:ARG:HG2	2.11	0.51
2:H:44:SER:HB2	2:H:159:PRO:HG3	1.91	0.51
2:H:149:HIS:CE1	2:H:150:VAL:HG23	2.46	0.51
3:J:19:GLN:HB2	3:J:47:TYR:OH	2.11	0.51
1:A:29:LEU:O	1:A:33:GLU:HG3	2.11	0.51
1:A:105:HIS:HE1	1:A:108:LEU:HB2	1.63	0.51
1:A:300:GLN:OE1	1:A:335:PRO:HB2	2.11	0.51
2:B:158:ASP:N	2:B:159:PRO:HD3	2.26	0.51
2:C:14:THR:O	2:C:57:LEU:HD13	2.11	0.51
2:C:28:LEU:HD13	2:C:58:LEU:HD13	1.92	0.51
2:C:367:GLU:OE2	2:C:367:GLU:C	2.49	0.51
3:E:277:LEU:O	3:E:279:ASN:N	2.43	0.51
3:E:286:LEU:O	3:E:289:ILE:N	2.43	0.51
2:G:291:ARG:HH22	2:G:303:GLY:HA3	1.74	0.51
2:I:21:GLN:HE22	2:I:176:LYS:CA	2.13	0.51
1:A:98:LEU:O	1:A:101:THR:HG22	2.11	0.51
2:C:279:GLU:HG3	2:C:336:ARG:HD2	1.93	0.51
2:D:366:PRO:HB3	3:E:282:SER:CB	2.41	0.51
3:E:117:ALA:O	3:E:120:LEU:HD23	2.10	0.51
3:E:317:LEU:O	3:E:320:GLU:HB2	2.10	0.51
2:H:156:THR:HG22	2:H:158:ASP:N	2.26	0.51
3:J:253:MSE:CG	3:J:257:LYS:HE3	2.32	0.51
1:A:298:LEU:CD1	1:A:298:LEU:N	2.73	0.51
1:A:299:ARG:O	1:A:302:VAL:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ILE:HG13	2:B:277:GLU:N	2.26	0.51
2:C:296:GLN:HE21	2:C:317:ALA:HA	1.76	0.51
2:D:128:VAL:HG13	2:D:162:LEU:HD21	1.91	0.51
3:E:298:GLU:HA	3:E:301:MSE:HG3	1.92	0.51
1:F:93:ILE:CG2	1:F:97:LEU:HD13	2.41	0.51
2:G:98:ARG:HD3	2:H:140:LEU:CD1	2.39	0.51
2:G:205:LEU:CD1	2:G:234:THR:HG23	2.40	0.51
2:G:205:LEU:HD11	2:G:234:THR:HG23	1.91	0.51
3:J:320:GLU:O	3:J:323:LEU:HB2	2.11	0.51
1:A:103:LEU:HD12	1:A:103:LEU:O	2.10	0.50
2:B:357:LEU:HB3	2:B:365:LEU:HD21	1.92	0.50
2:C:220:LEU:O	2:C:223:GLN:N	2.44	0.50
2:C:236:ALA:O	2:C:239:ALA:CB	2.57	0.50
2:C:263:ARG:HH11	2:C:263:ARG:CG	2.25	0.50
2:D:229:ASP:OD1	2:D:229:ASP:N	2.45	0.50
3:E:35:MSE:CE	3:E:166:PRO:HA	2.41	0.50
3:E:303:VAL:CG1	3:E:306:ILE:HG12	2.41	0.50
2:G:178:LEU:HD22	2:G:182:GLN:NE2	2.24	0.50
2:G:227:SER:O	2:H:26:THR:HG21	2.11	0.50
2:H:37:ILE:HD13	2:H:151:LYS:HE3	1.93	0.50
2:H:93:ILE:HD13	2:H:104:THR:HG23	1.92	0.50
2:H:224:ALA:O	2:H:228:GLY:N	2.43	0.50
2:I:250:LEU:CD2	2:I:312:ARG:HD2	2.41	0.50
1:A:74:PHE:CG	1:F:207:ASN:OD1	2.60	0.50
1:A:193:PRO:HB2	2:B:34:LEU:HD12	1.91	0.50
1:A:254:LEU:HD23	1:A:305:LEU:HD12	1.93	0.50
3:E:143:LEU:HD22	3:E:143:LEU:N	2.26	0.50
3:E:175:TRP:CD1	3:E:176:LEU:HD23	2.46	0.50
2:G:9:LYS:HB3	2:G:194:GLU:OE2	2.11	0.50
2:G:48:GLY:O	2:G:214:LEU:HB3	2.11	0.50
2:G:98:ARG:CZ	2:H:140:LEU:HD13	2.42	0.50
2:H:327:LEU:HD12	2:H:327:LEU:O	2.10	0.50
1:A:119:LYS:H	1:A:119:LYS:CD	2.01	0.50
2:B:191:LEU:CD2	2:B:198:HIS:HB3	2.41	0.50
2:D:332:LEU:HD23	2:D:352:THR:HG22	1.93	0.50
3:E:249:ALA:O	3:E:250:THR:C	2.50	0.50
1:F:162:LEU:HD11	1:F:185:LEU:CD2	2.40	0.50
2:G:46:THR:CG2	2:G:47:ARG:H	2.01	0.50
2:G:309:ILE:CG2	2:G:313:MET:HG2	2.41	0.50
1:A:289:ALA:O	1:A:291:ASN:N	2.44	0.50
2:D:244:LEU:CD2	2:D:276:ILE:HD13	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:125:ALA:O	3:E:128:LEU:HB3	2.12	0.50
1:F:154:ARG:O	1:F:154:ARG:HD2	2.10	0.50
1:F:188:LEU:CD2	1:F:197:LEU:HD13	2.39	0.50
1:F:217:TRP:CZ3	1:F:250:LEU:HD13	2.45	0.50
2:H:225:ILE:HG23	2:H:230:GLY:HA2	1.94	0.50
1:A:74:PHE:CE1	1:F:203:GLU:HG2	2.44	0.50
1:A:177:ASN:OD1	1:A:179:LEU:HB3	2.12	0.50
1:A:262:ARG:NH2	3:E:230:TYR:HB2	2.26	0.50
1:A:271:ALA:O	1:A:275:LYS:HG2	2.12	0.50
2:B:147:PRO:O	2:B:150:VAL:HB	2.11	0.50
2:B:360:HIS:CD2	2:B:361:PRO:N	2.80	0.50
2:C:282:LEU:O	2:C:283:VAL:C	2.49	0.50
2:D:111:VAL:HG13	2:D:112:GLN:N	2.27	0.50
2:D:196:ILE:HG22	2:D:197:ALA:H	1.75	0.50
2:D:346:ARG:O	2:D:347:MET:C	2.47	0.50
3:E:303:VAL:O	3:E:303:VAL:HG12	2.12	0.50
2:G:93:ILE:CG2	2:G:104:THR:HG23	2.42	0.50
2:G:99:THR:HG21	2:H:145:GLU:CB	2.41	0.50
2:I:244:LEU:C	2:I:246:ASP:N	2.65	0.50
2:I:324:ASP:O	2:I:327:LEU:HB3	2.12	0.50
2:B:256:MET:HE1	2:B:328:TYR:HB3	1.94	0.50
2:C:140:LEU:O	2:C:169:ARG:NH1	2.45	0.50
2:C:338:GLU:C	2:C:340:PRO:HD2	2.32	0.50
2:D:42:LEU:HD22	2:D:42:LEU:C	2.30	0.50
3:E:216:LEU:HD23	3:E:216:LEU:C	2.32	0.50
1:F:71:MSE:HA	1:F:78:GLN:NE2	2.26	0.50
1:F:273:PHE:CD1	1:F:283:ARG:CG	2.70	0.50
1:F:285:MSE:HE2	1:F:285:MSE:HB3	1.93	0.50
1:F:295:GLN:CD	1:F:295:GLN:N	2.54	0.50
2:H:245:ASP:HB2	2:H:248:GLN:HG3	1.93	0.50
2:H:277:GLU:O	2:H:279:GLU:N	2.45	0.50
2:B:148:GLU:HG3	2:B:149:HIS:CE1	2.46	0.50
2:B:252:LEU:HD23	2:B:285:MET:SD	2.52	0.50
2:B:354:LEU:O	2:B:355:ARG:C	2.49	0.50
2:C:112:GLN:HB2	2:C:121:LYS:HE2	1.92	0.50
2:C:250:LEU:HB2	2:C:288:LEU:HD13	1.94	0.50
2:C:293:ALA:HB2	2:C:325:ILE:HG21	1.93	0.50
3:E:8:ARG:N	3:E:9:PRO:CD	2.74	0.50
3:E:237:ASN:ND2	3:E:308:ARG:HD2	2.27	0.50
3:E:249:ALA:O	3:E:252:LEU:N	2.45	0.50
1:F:179:LEU:HD21	2:G:167:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:91:ILE:HD11	2:I:121:LYS:HE3	1.94	0.50
3:J:282:SER:HB3	3:J:283:PRO:HD2	1.92	0.50
1:A:93:ILE:HG22	1:A:93:ILE:O	2.10	0.50
1:A:192:TRP:HB3	1:A:195:GLY:HA3	1.94	0.50
1:A:268:PRO:C	1:A:270:ARG:N	2.65	0.50
2:B:183:ILE:HG12	2:B:214:LEU:HD13	1.94	0.50
2:B:191:LEU:HD21	2:B:198:HIS:HB3	1.94	0.50
2:B:295:VAL:HA	2:B:301:ALA:HB3	1.92	0.50
2:B:341:TYR:CD1	2:C:337:LYS:HG3	2.47	0.50
2:C:333:LEU:C	2:C:335:GLY:N	2.63	0.50
3:E:32:LEU:HB3	3:E:33:PRO:HD2	1.94	0.50
1:F:104:LEU:HB3	1:F:133:ARG:HH11	1.74	0.50
1:F:144:GLN:OE1	1:F:280:GLN:HG3	2.12	0.50
1:F:161:GLU:HB2	1:F:196:LYS:HA	1.94	0.50
1:F:168:GLN:HA	1:F:171:CYS:SG	2.52	0.50
2:H:210:ALA:HB1	2:H:213:SER:HG	1.77	0.50
3:J:116:ASP:HB3	3:J:119:LEU:HD12	1.93	0.50
3:J:154:THR:O	3:J:157:SER:HB2	2.11	0.50
3:J:196:GLY:O	3:J:198:PRO:HD3	2.10	0.50
1:A:38:VAL:CG1	1:A:111:ILE:HD11	2.42	0.50
1:A:329:LEU:CD1	2:B:291:ARG:HH21	2.25	0.50
2:C:3:TYR:CD2	2:C:3:TYR:N	2.80	0.50
2:C:91:ILE:HD12	2:C:123:TYR:CZ	2.47	0.50
2:D:360:HIS:ND1	2:D:361:PRO:HD2	2.27	0.50
1:F:128:THR:O	1:F:131:ALA:HB3	2.12	0.50
2:H:112:GLN:HB2	2:H:121:LYS:HZ2	1.77	0.50
2:H:191:LEU:CD1	2:H:203:LEU:HD21	2.41	0.50
2:H:351:MET:HE1	2:I:326:GLN:HE22	1.76	0.50
2:I:233:SER:O	2:I:237:VAL:HG23	2.11	0.50
1:A:196:LYS:H	1:A:201:ARG:HH12	1.60	0.49
1:A:295:GLN:CD	1:A:295:GLN:H	2.15	0.49
2:B:164:VAL:HG23	2:B:165:THR:N	2.26	0.49
2:C:58:LEU:HD23	2:C:153:LEU:HD21	1.93	0.49
2:C:65:GLU:C	2:C:67:GLY:H	2.16	0.49
2:C:206:LEU:HD13	2:C:221:THR:HA	1.94	0.49
2:C:343:PRO:HG2	2:C:347:MET:SD	2.52	0.49
2:D:32:LEU:HD23	2:D:37:ILE:CD1	2.42	0.49
2:D:38:HIS:CD2	2:D:39:HIS:H	2.30	0.49
2:D:309:ILE:O	2:D:310:GLU:C	2.48	0.49
2:G:202:ALA:HB1	2:G:237:VAL:HG21	1.94	0.49
2:H:184:ARG:HH12	2:H:203:LEU:CD1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:321:PRO:HB2	2:H:324:ASP:OD1	2.12	0.49
1:A:92:ALA:O	1:A:96:GLN:HG3	2.12	0.49
1:A:188:LEU:HD12	1:A:197:LEU:HD21	1.93	0.49
2:C:354:LEU:O	2:C:355:ARG:C	2.50	0.49
1:F:330:LEU:O	1:F:330:LEU:CD1	2.61	0.49
2:I:334:ILE:HG21	3:J:332:PRO:CB	2.42	0.49
2:I:357:LEU:HA	2:I:363:MET:HE1	1.94	0.49
3:J:77:TYR:HE2	3:J:100:LEU:HD21	1.76	0.49
1:A:81:LEU:HD12	1:A:111:ILE:O	2.12	0.49
1:A:101:THR:OG1	1:A:129:ALA:HB3	2.13	0.49
1:A:105:HIS:HE1	1:A:108:LEU:HD12	1.77	0.49
2:B:11:ARG:HH21	2:B:56:ARG:HH21	1.60	0.49
2:C:248:GLN:O	2:C:252:LEU:HD12	2.12	0.49
1:F:257:LEU:HD21	1:F:286:MSE:SE	2.63	0.49
2:I:158:ASP:OD2	2:I:161:LYS:HG2	2.11	0.49
2:I:244:LEU:C	2:I:246:ASP:H	2.15	0.49
2:C:13:GLN:OE1	2:C:83:GLU:OE1	2.30	0.49
2:C:306:MET:O	2:C:309:ILE:HG12	2.12	0.49
2:D:277:GLU:O	2:D:279:GLU:N	2.46	0.49
3:E:118:ALA:HB2	3:E:145:THR:CG2	2.42	0.49
3:E:169:GLU:CD	3:E:192:ARG:HH21	2.16	0.49
2:H:311:LEU:HD13	2:H:312:ARG:N	2.27	0.49
2:I:219:SER:OG	3:J:158:ARG:NH2	2.45	0.49
3:J:7:LEU:HD22	3:J:40:LEU:HB2	1.94	0.49
3:J:297:ARG:HH12	3:J:301:MSE:SE	2.44	0.49
1:A:293:LEU:CB	1:A:298:LEU:HD11	2.42	0.49
1:A:298:LEU:O	1:A:301:ALA:HB3	2.13	0.49
1:A:311:THR:CG2	1:A:318:GLN:HG2	2.42	0.49
2:C:37:ILE:HD11	2:C:151:LYS:HG3	1.93	0.49
2:C:102:GLU:HB3	2:C:105:ARG:NH1	2.27	0.49
2:D:136:PHE:HD1	2:D:166:ILE:HD11	1.77	0.49
3:E:192:ARG:C	3:E:194:SER:H	2.16	0.49
2:G:252:LEU:HD21	2:G:353:LEU:CD1	2.43	0.49
1:A:247:LEU:CD2	1:A:324:LEU:HD21	2.42	0.49
2:C:367:GLU:HG2	2:D:321:PRO:HA	1.95	0.49
2:D:244:LEU:CD1	2:D:276:ILE:HD13	2.42	0.49
2:H:250:LEU:HD21	2:H:312:ARG:HB2	1.95	0.49
2:H:296:GLN:OE1	2:H:322:PRO:HB3	2.11	0.49
1:A:262:ARG:NH1	3:E:228:ASP:OD2	2.46	0.49
1:A:298:LEU:N	1:A:298:LEU:HD13	2.28	0.49
2:C:59:ALA:O	2:C:82:ILE:CD1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:GLY:CA	2:C:357:LEU:HD21	2.43	0.49
2:C:347:MET:O	2:C:348:GLY:C	2.51	0.49
2:D:10:TRP:HE1	2:D:190:ILE:HG23	1.71	0.49
2:G:10:TRP:CZ2	2:G:193:GLU:CG	2.90	0.49
2:G:179:ASP:OD1	2:G:180:VAL:N	2.46	0.49
2:H:264:VAL:O	2:H:268:ILE:HG13	2.13	0.49
3:J:106:LEU:O	3:J:107:GLY:C	2.50	0.49
1:A:49:GLU:HB2	1:A:77:ARG:O	2.11	0.49
1:A:143:GLU:O	1:A:147:LEU:HB2	2.13	0.49
1:A:259:ASN:O	1:A:262:ARG:N	2.45	0.49
2:D:38:HIS:CG	2:D:39:HIS:H	2.31	0.49
2:D:223:GLN:HB3	2:D:240:MET:HE3	1.91	0.49
2:D:257:VAL:CG1	2:D:320:ILE:HG12	2.36	0.49
3:E:24:HIS:HB2	3:E:160:ARG:CZ	2.43	0.49
3:E:193:LEU:HD23	3:E:266:THR:CG2	2.43	0.49
1:F:31:LEU:HD23	1:F:139:CYS:SG	2.53	0.49
2:G:7:ALA:HB2	2:G:218:LEU:HB3	1.95	0.49
2:G:7:ALA:HB1	2:G:218:LEU:HD13	1.86	0.49
2:G:293:ALA:HB2	2:G:325:ILE:HG21	1.94	0.49
2:H:81:GLU:HB3	2:H:86:ARG:O	2.12	0.49
2:I:309:ILE:O	2:I:311:LEU:N	2.45	0.49
3:J:223:SER:O	3:J:227:GLY:N	2.41	0.49
1:A:170:LEU:HD21	1:A:202:VAL:CG1	2.43	0.49
1:A:264:SER:O	1:A:265:ALA:CB	2.61	0.49
3:E:237:ASN:O	3:E:238:HIS:CB	2.55	0.49
2:G:252:LEU:HD21	2:G:353:LEU:HD11	1.95	0.49
2:G:334:ILE:O	2:G:337:LYS:HB2	2.11	0.49
2:H:65:GLU:HG3	2:H:78:ASN:ND2	2.28	0.49
2:H:277:GLU:O	2:H:280:ALA:N	2.46	0.49
2:H:351:MET:HE3	2:H:354:LEU:HD22	1.94	0.49
1:A:164:ASP:O	1:A:167:ASN:HB3	2.13	0.49
1:A:213:THR:H	1:A:216:HIS:CG	2.31	0.49
2:B:36:ARG:HB2	2:B:36:ARG:NH1	2.27	0.49
2:B:362:ARG:C	2:B:364:PRO:CD	2.81	0.49
2:C:51:LYS:HB2	6:C:1300:PO4:O4	2.13	0.49
2:C:58:LEU:HD23	2:C:153:LEU:HD22	1.94	0.49
2:C:134:HIS:ND1	2:C:135:SER:N	2.61	0.49
2:C:255:ALA:HB2	2:C:263:ARG:NH1	2.28	0.49
2:C:269:ASN:O	2:C:272:ALA:N	2.46	0.49
2:D:82:ILE:O	2:D:82:ILE:HG22	2.13	0.49
2:D:357:LEU:C	2:D:363:MET:SD	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:196:GLY:O	3:E:198:PRO:HD3	2.12	0.49
1:F:2:ILE:HD11	1:F:18:ARG:NH2	2.28	0.49
1:F:213:THR:C	1:F:215:PHE:H	2.15	0.49
2:H:215:ARG:NH1	2:I:164:VAL:HG11	2.28	0.49
2:H:351:MET:HE2	2:I:326:GLN:HE22	1.78	0.49
2:I:285:MET:HB2	2:I:332:LEU:HD21	1.94	0.49
1:A:55:ILE:CG2	1:A:93:ILE:HD13	2.43	0.48
1:A:267:THR:HG22	1:A:271:ALA:HB3	1.95	0.48
2:C:6:LEU:N	2:C:6:LEU:HD23	2.27	0.48
2:C:202:ALA:HB2	2:C:234:THR:CA	2.42	0.48
1:F:53:PHE:CZ	1:F:67:LEU:HD13	2.41	0.48
2:H:281:LEU:HD23	2:H:281:LEU:C	2.32	0.48
3:J:3:TRP:HH2	3:J:8:ARG:HB3	1.78	0.48
1:A:255:LEU:O	1:A:258:VAL:N	2.43	0.48
2:B:265:MET:HG3	2:C:297:LEU:HD21	1.94	0.48
2:C:78:ASN:O	2:C:82:ILE:HG13	2.11	0.48
2:C:327:LEU:HD12	2:C:327:LEU:C	2.32	0.48
2:D:37:ILE:HG22	2:D:38:HIS:N	2.28	0.48
2:D:139:LEU:O	2:D:142:THR:N	2.44	0.48
3:E:18:TYR:HB3	3:E:48:LEU:HD21	1.96	0.48
2:H:51:LYS:HB2	6:H:1400:PO4:O4	2.13	0.48
2:H:281:LEU:HD22	2:H:349:VAL:HG11	1.95	0.48
2:I:64:CYS:SG	2:I:66:THR:HB	2.53	0.48
2:I:257:VAL:HG13	2:I:328:TYR:OH	2.13	0.48
1:A:298:LEU:HD13	1:A:298:LEU:H	1.78	0.48
2:B:250:LEU:HD12	2:B:288:LEU:HD13	1.95	0.48
2:D:7:ALA:HA	2:D:218:LEU:HD13	1.95	0.48
2:D:244:LEU:HD11	2:D:276:ILE:HD13	1.95	0.48
2:D:276:ILE:HG22	2:D:277:GLU:H	1.77	0.48
2:D:344:ASP:HB3	2:D:347:MET:HB2	1.94	0.48
3:E:74:PRO:HB2	3:E:105:ARG:HB2	1.94	0.48
3:E:230:TYR:CD1	3:E:230:TYR:O	2.65	0.48
3:E:307:ASN:O	3:E:308:ARG:C	2.51	0.48
3:J:314:ASP:OD2	3:J:318:ARG:NH2	2.46	0.48
1:A:318:GLN:CG	1:A:318:GLN:O	2.61	0.48
1:A:318:GLN:O	1:A:318:GLN:HG3	2.13	0.48
2:B:352:THR:O	2:B:355:ARG:HB3	2.13	0.48
2:C:257:VAL:O	2:C:360:HIS:HE1	1.95	0.48
2:C:269:ASN:C	2:C:271:ALA:N	2.65	0.48
2:D:142:THR:HG22	2:D:147:PRO:HD3	1.96	0.48
3:E:161:LEU:HD12	3:E:161:LEU:N	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:THR:O	1:F:104:LEU:HG	2.13	0.48
1:F:318:GLN:O	1:F:319:SER:C	2.52	0.48
2:G:125:ILE:HD12	2:G:154:LEU:CD2	2.44	0.48
2:H:144:GLU:OE2	2:H:169:ARG:HD3	2.13	0.48
2:H:278:TRP:HB3	2:H:349:VAL:HG21	1.94	0.48
3:J:90:VAL:HG13	3:J:124:ALA:HA	1.95	0.48
3:J:169:GLU:O	3:J:173:VAL:HG23	2.14	0.48
1:A:36:ASP:O	1:A:40:GLN:HB2	2.13	0.48
2:B:179:ASP:HB3	2:B:182:GLN:HB2	1.95	0.48
2:B:246:ASP:C	2:B:248:GLN:H	2.16	0.48
2:D:12:PRO:C	2:D:13:GLN:HE21	2.17	0.48
2:D:196:ILE:CG2	2:D:197:ALA:N	2.77	0.48
2:D:268:ILE:HD12	2:D:350:GLU:HG2	1.94	0.48
1:F:191:LEU:HD13	2:G:26:THR:CG2	2.43	0.48
2:G:310:GLU:O	2:G:314:ARG:HG2	2.14	0.48
1:A:186:GLU:O	1:A:190:LEU:HD23	2.14	0.48
2:B:28:LEU:HD11	2:B:43:PHE:CE1	2.48	0.48
2:B:145:GLU:O	2:B:147:PRO:HD3	2.13	0.48
2:B:205:LEU:CD1	2:B:234:THR:HG23	2.44	0.48
2:B:225:ILE:O	2:B:229:ASP:N	2.47	0.48
2:C:321:PRO:O	2:C:324:ASP:HB2	2.13	0.48
1:F:222:LEU:HD12	1:F:285:MSE:CE	2.42	0.48
2:I:286:LEU:CD2	2:I:332:LEU:HD23	2.43	0.48
3:J:120:LEU:O	3:J:120:LEU:HD23	2.14	0.48
3:J:241:ALA:O	3:J:244:ARG:N	2.47	0.48
2:B:82:ILE:HG23	2:B:90:LEU:HD22	1.96	0.48
2:C:341:TYR:HB2	2:D:333:LEU:CD1	2.42	0.48
3:E:117:ALA:C	3:E:119:LEU:H	2.17	0.48
1:F:285:MSE:CE	1:F:285:MSE:HG2	2.44	0.48
2:G:99:THR:HG21	2:H:145:GLU:HB3	1.94	0.48
2:G:289:LEU:HD13	2:G:329:TYR:HA	1.96	0.48
2:H:181:GLU:CD	2:H:184:ARG:HD2	2.33	0.48
3:J:295:HIS:O	3:J:299:GLN:HG3	2.14	0.48
1:A:301:ALA:CB	1:A:331:LEU:HD21	2.44	0.48
3:E:285:ARG:O	3:E:289:ILE:HG13	2.14	0.48
1:F:3:ARG:NE	1:F:136:GLN:OE1	2.47	0.48
1:F:98:LEU:HD22	1:F:101:THR:CG2	2.44	0.48
2:G:9:LYS:CD	2:G:194:GLU:CD	2.78	0.48
2:C:37:ILE:O	2:C:37:ILE:HG23	2.14	0.48
2:C:45:GLY:C	2:C:46:THR:O	2.51	0.48
2:C:157:THR:HG22	2:C:157:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:346:ARG:O	2:C:347:MET:C	2.52	0.48
2:D:140:LEU:HD11	2:D:165:THR:OG1	2.14	0.48
2:D:250:LEU:HD23	2:D:309:ILE:HG21	1.94	0.48
2:D:260:ASN:O	2:D:260:ASN:OD1	2.32	0.48
2:D:276:ILE:CG2	2:D:277:GLU:H	2.25	0.48
2:G:113:TYR:HD2	2:G:147:PRO:HB3	1.76	0.48
1:A:26:ASN:ND2	1:A:140:GLN:HE22	2.12	0.48
1:A:52:THR:CG2	1:A:81:LEU:HD23	2.44	0.48
1:A:134:SER:O	1:A:135:VAL:HG23	2.14	0.48
1:A:247:LEU:HD21	1:A:308:THR:HG21	1.95	0.48
2:D:24:VAL:O	2:D:27:ALA:N	2.47	0.48
2:D:156:THR:HG21	2:D:159:PRO:HA	1.96	0.48
2:D:290:HIS:NE2	2:D:294:MET:CE	2.77	0.48
3:E:318:ARG:HD2	3:E:322:TYR:HH	1.79	0.48
1:F:304:LEU:HD12	1:F:327:LEU:HD13	1.95	0.48
2:I:257:VAL:O	2:I:257:VAL:HG12	2.14	0.48
1:A:14:ASN:O	1:A:16:GLY:N	2.47	0.47
2:B:128:VAL:O	2:B:128:VAL:HG22	2.14	0.47
2:C:128:VAL:CG1	2:C:154:LEU:HD22	2.32	0.47
2:D:189:HIS:O	2:D:190:ILE:C	2.50	0.47
2:D:262:GLU:O	2:D:266:ALA:HB2	2.13	0.47
3:E:251:LEU:O	3:E:254:ASP:HB2	2.13	0.47
2:H:250:LEU:HD22	2:H:309:ILE:HB	1.95	0.47
2:I:19:VAL:HG21	2:I:214:LEU:CD2	2.44	0.47
3:J:5:PRO:C	3:J:7:LEU:H	2.17	0.47
3:J:268:VAL:O	3:J:271:PRO:HD3	2.14	0.47
1:A:19:ALA:CB	1:A:133:ARG:HD3	2.44	0.47
2:C:245:ASP:O	2:C:248:GLN:N	2.47	0.47
2:D:127:GLU:OE1	2:D:157:THR:HG23	2.14	0.47
3:E:58:SER:CB	3:E:65:CYS:SG	2.97	0.47
2:H:14:THR:HG22	2:H:15:PHE:N	2.28	0.47
1:A:274:ASP:O	1:A:277:ARG:N	2.48	0.47
2:C:136:PHE:CZ	2:C:163:PRO:HG2	2.49	0.47
2:C:260:ASN:OD1	2:C:263:ARG:HB2	2.14	0.47
2:D:237:VAL:O	2:D:239:ALA:N	2.47	0.47
3:E:167:PRO:HB2	3:E:171:TYR:HD1	1.79	0.47
3:E:202:LEU:HD13	3:E:202:LEU:C	2.35	0.47
3:J:155:LEU:C	3:J:157:SER:H	2.17	0.47
2:B:21:GLN:NE2	2:B:175:LEU:HA	2.27	0.47
2:B:227:SER:HA	2:C:26:THR:CG2	2.45	0.47
2:B:242:GLY:O	2:B:244:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:245:ASP:C	2:C:247:ASP:N	2.66	0.47
2:C:268:ILE:O	2:C:271:ALA:HB3	2.13	0.47
3:E:145:THR:CG2	3:E:146:ARG:N	2.76	0.47
2:I:364:PRO:HG3	3:J:260:HIS:HE1	1.79	0.47
3:J:73:HIS:HE1	3:J:106:LEU:HD22	1.80	0.47
3:J:296:ILE:HA	3:J:299:GLN:HG3	1.97	0.47
1:A:199:LEU:N	1:A:200:PRO:CD	2.78	0.47
1:A:205:ALA:O	1:A:209:ALA:HB2	2.15	0.47
3:E:42:TYR:CE2	3:E:46:ARG:NH1	2.82	0.47
3:E:82:GLU:OE1	3:E:85:LYS:HD3	2.15	0.47
3:E:152:LEU:HD22	3:E:154:THR:HG23	1.97	0.47
3:E:249:ALA:O	3:E:252:LEU:HB2	2.14	0.47
2:G:350:GLU:O	2:G:354:LEU:HG	2.15	0.47
2:I:44:SER:HA	2:I:156:THR:O	2.14	0.47
3:J:5:PRO:O	3:J:7:LEU:N	2.48	0.47
2:C:243:THR:HG23	2:C:284:GLU:CG	2.44	0.47
2:C:362:ARG:C	2:C:363:MET:HG3	2.35	0.47
2:D:18:VAL:HB	2:D:25:LEU:HD11	1.96	0.47
2:D:214:LEU:HD23	5:D:801:AGS:C4	2.45	0.47
2:D:347:MET:O	2:D:351:MET:HG3	2.14	0.47
2:G:243:THR:HG22	2:G:243:THR:O	2.14	0.47
2:G:248:GLN:C	2:G:250:LEU:H	2.18	0.47
2:G:282:LEU:HD13	2:G:336:ARG:HA	1.96	0.47
2:G:342:ALA:C	2:G:344:ASP:H	2.17	0.47
2:H:295:VAL:O	2:H:295:VAL:HG12	2.14	0.47
3:J:3:TRP:CH2	3:J:8:ARG:HB3	2.50	0.47
1:A:179:LEU:HD21	2:B:167:LEU:HD22	1.96	0.47
2:B:5:VAL:C	2:B:7:ALA:N	2.67	0.47
2:B:208:ARG:O	2:B:210:ALA:O	2.33	0.47
2:B:299:PRO:O	2:B:301:ALA:N	2.43	0.47
2:C:244:LEU:HD11	2:C:281:LEU:HD12	1.97	0.47
2:C:344:ASP:HB3	2:C:347:MET:HB2	1.96	0.47
2:D:32:LEU:C	2:D:34:LEU:H	2.16	0.47
2:D:160:GLN:C	2:D:162:LEU:H	2.18	0.47
3:E:225:PRO:HA	3:E:280:HIS:CE1	2.49	0.47
3:E:277:LEU:C	3:E:279:ASN:N	2.64	0.47
1:F:13:LEU:HD12	1:F:21:TYR:OH	2.14	0.47
1:F:71:MSE:O	1:F:105:HIS:HE1	1.97	0.47
2:G:148:GLU:O	2:G:149:HIS:HB2	2.15	0.47
2:H:56:ARG:O	2:H:60:LYS:HB2	2.14	0.47
3:J:32:LEU:HB3	3:J:33:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:73:HIS:CD2	3:J:75:ASP:H	2.31	0.47
3:J:171:TYR:CD2	3:J:171:TYR:N	2.81	0.47
1:A:59:THR:HG21	1:A:64:ILE:HD11	1.97	0.47
1:A:95:GLU:O	1:A:98:LEU:N	2.47	0.47
2:C:120:PHE:HD2	2:C:120:PHE:N	2.12	0.47
2:C:220:LEU:O	2:C:221:THR:C	2.51	0.47
3:E:122:ASP:O	3:E:126:ASN:OD1	2.33	0.47
2:H:360:HIS:O	2:H:364:PRO:HG3	2.14	0.47
1:A:150:TRP:CH2	1:A:178:LEU:CD1	2.90	0.47
1:A:252:ARG:O	1:A:256:LEU:HB2	2.15	0.47
2:B:179:ASP:HB3	2:B:182:GLN:CB	2.45	0.47
2:B:332:LEU:HD13	2:B:332:LEU:HA	1.73	0.47
2:C:265:MET:HG3	2:D:297:LEU:HD23	1.97	0.47
2:D:22:GLU:O	2:D:24:VAL:N	2.48	0.47
2:D:184:ARG:HD3	2:D:185:HIS:CA	2.45	0.47
2:D:291:ARG:HD2	2:D:306:MET:SD	2.55	0.47
2:H:100:LYS:NZ	2:I:133:ARG:HA	2.30	0.47
2:H:202:ALA:HB2	2:H:234:THR:CG2	2.42	0.47
2:H:346:ARG:O	2:H:350:GLU:HG3	2.15	0.47
1:A:31:LEU:HB3	1:A:113:ARG:HD2	1.97	0.47
2:B:140:LEU:O	2:B:143:LEU:CD2	2.62	0.47
2:B:254:GLU:HA	2:B:257:VAL:HG23	1.95	0.47
2:B:294:MET:HE2	2:B:294:MET:HA	1.97	0.47
2:C:233:SER:O	2:C:234:THR:C	2.52	0.47
2:D:288:LEU:O	2:D:290:HIS:N	2.47	0.47
3:E:24:HIS:HB2	3:E:160:ARG:NH2	2.30	0.47
3:E:323:LEU:O	3:E:324:GLN:C	2.51	0.47
1:F:67:LEU:CD1	1:F:71:MSE:HE3	2.46	0.47
1:F:223:MSE:SE	1:F:292:ARG:HB3	2.65	0.47
2:G:253:VAL:HA	2:G:256:MET:HE3	1.97	0.47
2:H:47:ARG:O	2:H:47:ARG:HG3	2.14	0.47
2:H:327:LEU:CD2	2:H:361:PRO:HD3	2.43	0.47
3:J:155:LEU:C	3:J:155:LEU:HD13	2.35	0.47
1:A:6:PRO:O	1:A:9:LEU:HB3	2.15	0.46
1:A:59:THR:HB	1:A:61:TRP:NE1	2.29	0.46
2:B:42:LEU:HD23	2:B:43:PHE:N	2.30	0.46
2:B:259:ALA:HB2	2:B:360:HIS:ND1	2.30	0.46
2:B:265:MET:HA	2:B:265:MET:HE3	1.98	0.46
2:B:286:LEU:HD21	2:B:333:LEU:HA	1.97	0.46
2:B:342:ALA:O	2:B:343:PRO:C	2.51	0.46
2:C:51:LYS:HB2	2:C:51:LYS:HE3	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:GLN:NE2	2:C:240:MET:HE3	2.30	0.46
2:D:238:SER:CB	2:D:243:THR:HB	2.45	0.46
2:D:355:ARG:HH21	3:E:332:PRO:CD	2.26	0.46
3:E:32:LEU:CD1	3:E:166:PRO:HG2	2.45	0.46
3:E:32:LEU:HD22	3:E:195:ALA:CB	2.45	0.46
2:G:133:ARG:O	2:G:137:ASN:ND2	2.48	0.46
2:G:259:ALA:HB2	2:G:360:HIS:CE1	2.50	0.46
2:G:291:ARG:O	2:G:295:VAL:HG23	2.16	0.46
2:G:313:MET:O	2:G:314:ARG:C	2.53	0.46
2:H:62:LEU:HB3	2:H:120:PHE:CD2	2.51	0.46
2:I:259:ALA:HA	2:I:363:MET:SD	2.55	0.46
3:J:129:LEU:CD1	3:J:129:LEU:H	2.28	0.46
3:J:254:ASP:HA	3:J:257:LYS:HD2	1.97	0.46
1:A:13:LEU:HD12	1:A:13:LEU:HA	1.74	0.46
1:A:190:LEU:HD22	2:B:36:ARG:CZ	2.45	0.46
1:A:226:SER:O	1:A:229:ALA:HB3	2.15	0.46
1:A:306:THR:O	1:A:307:ARG:C	2.54	0.46
1:A:321:TRP:O	1:A:322:ALA:C	2.54	0.46
2:B:98:ARG:O	2:B:101:VAL:HG13	2.14	0.46
2:C:47:ARG:O	2:C:47:ARG:HG3	2.15	0.46
2:C:292:ILE:HG12	2:C:313:MET:CE	2.46	0.46
2:D:105:ARG:HG3	2:D:134:HIS:NE2	2.30	0.46
2:D:288:LEU:C	2:D:290:HIS:N	2.68	0.46
2:D:357:LEU:O	2:D:358:ALA:C	2.53	0.46
3:E:28:LEU:HA	3:E:143:LEU:O	2.15	0.46
1:F:80:LEU:CD1	1:F:108:LEU:HD12	2.44	0.46
2:G:98:ARG:HG3	2:H:169:ARG:HH22	1.79	0.46
2:G:227:SER:HA	2:H:26:THR:CG2	2.45	0.46
2:I:32:LEU:HD13	2:I:70:ALA:HA	1.97	0.46
2:I:259:ALA:CB	2:I:363:MET:SD	3.04	0.46
2:I:361:PRO:O	2:I:362:ARG:CB	2.63	0.46
1:A:213:THR:HB	1:A:216:HIS:ND1	2.30	0.46
1:A:223:MSE:HG3	1:A:289:ALA:HA	1.97	0.46
1:A:226:SER:O	1:A:227:LYS:C	2.54	0.46
2:B:56:ARG:HH11	2:B:56:ARG:CG	2.23	0.46
2:B:113:TYR:CD2	2:B:147:PRO:HB3	2.50	0.46
2:B:226:ALA:HA	2:C:30:ASN:ND2	2.30	0.46
2:D:92:GLU:HG2	2:D:124:LEU:HD12	1.97	0.46
3:E:34:GLY:O	3:E:197:SER:OG	2.34	0.46
3:E:319:ILE:HA	3:E:322:TYR:CD2	2.49	0.46
2:G:140:LEU:HD22	2:G:144:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:354:LEU:HD22	2:I:293:ALA:HB1	1.97	0.46
3:J:31:ALA:HB2	3:J:164:LEU:CB	2.40	0.46
1:A:102:GLY:HA3	2:G:310:GLU:OE2	2.15	0.46
1:A:129:ALA:C	1:A:131:ALA:N	2.68	0.46
2:B:81:GLU:CB	2:B:87:PHE:HD1	2.23	0.46
2:D:334:ILE:HG21	3:E:332:PRO:HB2	1.97	0.46
3:E:73:HIS:CE1	3:E:106:LEU:HD22	2.50	0.46
1:F:155:ALA:CB	1:F:162:LEU:HD12	2.46	0.46
1:F:199:LEU:N	1:F:200:PRO:CD	2.78	0.46
2:G:209:ALA:CB	2:G:241:LEU:HD13	2.46	0.46
2:H:56:ARG:HG2	2:H:56:ARG:HH11	1.81	0.46
2:I:260:ASN:HB3	2:I:263:ARG:HB3	1.98	0.46
3:J:4:TYR:O	3:J:7:LEU:HB2	2.15	0.46
3:J:80:ALA:HB1	3:J:81:PRO:HD2	1.97	0.46
3:J:240:GLN:O	3:J:244:ARG:HG3	2.15	0.46
3:J:308:ARG:O	3:J:312:ILE:HG13	2.15	0.46
2:B:5:VAL:O	2:B:7:ALA:N	2.48	0.46
2:B:255:ALA:CB	2:B:263:ARG:HD3	2.45	0.46
2:C:5:VAL:O	2:C:6:LEU:C	2.53	0.46
2:C:37:ILE:CD1	2:C:151:LYS:HE3	2.46	0.46
2:C:289:LEU:H	2:C:289:LEU:CD2	2.28	0.46
2:D:10:TRP:CG	2:D:190:ILE:CD1	2.97	0.46
2:D:64:CYS:SG	2:D:66:THR:HB	2.55	0.46
2:D:341:TYR:CD2	3:E:295:HIS:CE1	3.04	0.46
2:G:309:ILE:O	2:G:311:LEU:N	2.48	0.46
2:I:360:HIS:HD2	2:I:361:PRO:N	2.13	0.46
3:J:317:LEU:HD22	3:J:317:LEU:O	2.15	0.46
1:A:276:HIS:O	1:A:277:ARG:HB2	2.16	0.46
2:B:260:ASN:O	2:B:261:GLY:C	2.52	0.46
2:C:6:LEU:O	2:C:8:ARG:N	2.48	0.46
2:D:129:HIS:HD2	2:D:161:LYS:HG3	1.81	0.46
3:E:13:LYS:O	3:E:16:ALA:N	2.48	0.46
3:E:78:THR:O	3:E:78:THR:HG22	2.14	0.46
3:E:281:LEU:CD2	3:E:323:LEU:HD21	2.45	0.46
1:F:273:PHE:HB3	1:F:279:TRP:CB	2.46	0.46
2:I:357:LEU:HD12	2:I:363:MET:HE1	1.97	0.46
1:A:126:TRP:CG	1:A:127:PHE:N	2.83	0.46
1:A:269:LEU:HD11	1:A:273:PHE:HZ	1.79	0.46
2:B:140:LEU:CA	2:B:143:LEU:HD22	2.42	0.46
2:B:299:PRO:C	2:B:301:ALA:N	2.69	0.46
2:C:292:ILE:O	2:C:294:MET:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:302:LEU:CD1	2:C:310:GLU:HG3	2.46	0.46
2:D:10:TRP:NE1	2:D:190:ILE:CG2	2.69	0.46
2:D:11:ARG:O	2:D:13:GLN:NE2	2.48	0.46
3:E:32:LEU:HD12	3:E:166:PRO:CG	2.45	0.46
3:E:281:LEU:O	3:E:282:SER:O	2.33	0.46
1:F:20:ALA:HB2	1:F:110:LEU:HB3	1.96	0.46
1:F:299:ARG:CD	3:J:317:LEU:HD21	2.46	0.46
2:H:184:ARG:HH12	2:H:203:LEU:HD12	1.80	0.46
2:I:334:ILE:HG21	3:J:332:PRO:HB2	1.98	0.46
3:J:50:CYS:SG	3:J:53:PRO:N	2.88	0.46
3:J:185:ASP:OD2	3:J:185:ASP:N	2.49	0.46
3:J:225:PRO:HA	3:J:280:HIS:ND1	2.30	0.46
1:A:221:LEU:HD21	1:A:328:SER:HB2	1.94	0.46
1:A:256:LEU:O	1:A:260:LEU:HG	2.16	0.46
2:B:276:ILE:CD1	2:B:281:LEU:HD13	2.45	0.46
2:B:333:LEU:HD11	2:B:337:LYS:CE	2.45	0.46
2:D:13:GLN:HE21	2:D:13:GLN:N	2.14	0.46
2:D:21:GLN:HE21	2:D:21:GLN:HA	1.81	0.46
2:D:292:ILE:O	2:D:296:GLN:HG3	2.16	0.46
3:E:292:ASP:OD2	3:E:322:TYR:OH	2.33	0.46
2:G:98:ARG:CD	2:H:140:LEU:HB3	2.43	0.46
2:G:330:GLN:HG3	2:G:331:THR:N	2.31	0.46
2:H:223:GLN:NE2	2:I:174:HIS:CE1	2.84	0.46
1:A:106:ASP:OD2	1:F:225:LYS:HE2	2.15	0.46
2:C:30:ASN:O	2:C:31:GLY:C	2.53	0.46
2:D:142:THR:HG22	2:D:147:PRO:CD	2.46	0.46
2:D:237:VAL:C	2:D:239:ALA:N	2.69	0.46
3:E:1:MSE:HE1	3:E:42:TYR:CG	2.51	0.46
3:E:283:PRO:CG	3:E:284:SER:H	2.25	0.46
1:F:45:GLN:CD	1:F:77:ARG:CD	2.66	0.46
1:F:181:LEU:O	1:F:185:LEU:HG	2.15	0.46
1:F:223:MSE:CE	1:F:292:ARG:HB2	2.43	0.46
2:H:18:VAL:HB	2:H:25:LEU:HD11	1.97	0.46
2:H:314:ARG:O	2:H:318:ARG:HG2	2.15	0.46
3:J:182:MSE:HG3	3:J:205:PHE:CE1	2.50	0.46
3:J:205:PHE:O	3:J:207:GLY:N	2.48	0.46
1:A:154:ARG:NH1	1:A:157:GLN:HE21	2.12	0.46
1:A:234:GLN:HB3	1:A:237:ARG:NH2	2.28	0.46
2:B:140:LEU:HD22	2:B:144:GLU:OE1	2.16	0.46
2:B:179:ASP:HB3	2:B:182:GLN:HG3	1.97	0.46
2:C:106:ASP:O	2:C:110:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:259:ALA:CB	2:C:360:HIS:HD1	2.27	0.46
2:C:302:LEU:CD2	2:C:306:MET:HG3	2.45	0.46
2:D:197:ALA:CB	2:D:231:GLN:HG2	2.44	0.46
2:D:328:TYR:O	2:D:329:TYR:C	2.53	0.46
2:D:339:LEU:HD11	2:D:345:ARG:HG3	1.97	0.46
1:F:147:LEU:N	1:F:148:PRO:CD	2.79	0.46
2:I:354:LEU:HD23	2:I:357:LEU:HD22	1.98	0.46
2:C:42:LEU:HD23	2:C:172:GLN:HG3	1.98	0.45
2:C:310:GLU:O	2:C:311:LEU:C	2.53	0.45
3:E:182:MSE:HA	3:E:182:MSE:HE3	1.98	0.45
1:F:242:GLU:O	1:F:245:ILE:CG2	2.60	0.45
2:H:351:MET:SD	2:I:290:HIS:HA	2.56	0.45
2:I:248:GLN:HE21	2:I:248:GLN:CA	2.20	0.45
2:I:286:LEU:HD21	2:I:332:LEU:HB3	1.98	0.45
1:A:20:ALA:HA	1:A:110:LEU:O	2.16	0.45
1:A:254:LEU:O	1:A:258:VAL:HG23	2.15	0.45
1:A:336:LEU:H	1:A:336:LEU:CD2	2.06	0.45
2:D:21:GLN:HE22	2:D:176:LYS:H	1.65	0.45
2:H:184:ARG:NH1	2:H:188:GLU:HB2	2.31	0.45
3:J:316:LEU:HA	3:J:319:ILE:CD1	2.45	0.45
1:A:19:ALA:CB	1:A:133:ARG:HB3	2.46	0.45
2:C:73:CYS:SG	2:C:76:CYS:HB3	2.56	0.45
3:E:120:LEU:HD12	3:E:125:ALA:N	2.31	0.45
1:F:80:LEU:N	1:F:80:LEU:CD1	2.73	0.45
1:F:271:ALA:O	1:F:275:LYS:HG2	2.15	0.45
2:H:100:LYS:HE2	2:I:136:PHE:CD2	2.48	0.45
2:I:337:LYS:HD2	2:I:337:LYS:O	2.16	0.45
3:J:129:LEU:H	3:J:129:LEU:HD12	1.80	0.45
3:J:202:LEU:C	3:J:202:LEU:CD2	2.84	0.45
1:A:105:HIS:CE1	1:A:108:LEU:HD12	2.51	0.45
2:B:105:ARG:O	2:B:109:ASP:OD2	2.34	0.45
2:B:247:ASP:HB2	2:B:312:ARG:HH12	1.82	0.45
2:B:347:MET:HG3	2:C:290:HIS:CG	2.51	0.45
2:C:136:PHE:HZ	2:C:163:PRO:HG2	1.80	0.45
2:D:257:VAL:HG11	2:D:320:ILE:CG1	2.39	0.45
2:D:332:LEU:HD23	2:D:332:LEU:HA	1.68	0.45
3:E:316:LEU:HD23	3:E:316:LEU:HA	1.68	0.45
1:F:250:LEU:H	1:F:250:LEU:CD2	2.28	0.45
2:G:268:ILE:HD11	2:G:353:LEU:CD1	2.35	0.45
2:H:214:LEU:HD12	2:H:217:ALA:HB3	1.99	0.45
2:I:127:GLU:OE1	2:I:127:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:220:LEU:CD2	3:J:157:SER:OG	2.64	0.45
3:J:35:MSE:SE	3:J:167:PRO:HD3	2.66	0.45
2:B:10:TRP:CH2	2:B:190:ILE:HA	2.52	0.45
2:B:50:GLY:HA2	5:B:802:AGS:O1A	2.16	0.45
2:B:356:ALA:O	2:B:360:HIS:N	2.49	0.45
2:C:367:GLU:OE2	2:C:368:PRO:CD	2.65	0.45
1:F:56:ASP:N	1:F:57:PRO:CD	2.79	0.45
2:I:15:PHE:O	2:I:18:VAL:HB	2.16	0.45
2:I:248:GLN:NE2	2:I:248:GLN:CA	2.79	0.45
3:J:190:ALA:HB2	3:J:210:TRP:CZ3	2.52	0.45
3:J:271:PRO:O	3:J:274:VAL:HG22	2.16	0.45
1:A:280:GLN:H	1:A:280:GLN:HG2	1.43	0.45
2:B:245:ASP:O	2:B:246:ASP:O	2.35	0.45
2:D:15:PHE:O	2:D:17:ASP:N	2.49	0.45
2:D:115:PRO:HG3	2:D:121:LYS:HB2	1.99	0.45
2:D:201:ARG:HB2	2:D:305:ASP:OD2	2.17	0.45
1:F:299:ARG:HG3	3:J:317:LEU:CD2	2.47	0.45
2:I:309:ILE:O	2:I:310:GLU:C	2.55	0.45
2:I:330:GLN:O	2:I:334:ILE:HG13	2.15	0.45
3:J:27:LEU:HG	3:J:29:ILE:HD11	1.98	0.45
1:A:117:LEU:CB	1:A:122:GLU:HG3	2.46	0.45
2:B:124:LEU:HA	2:B:153:LEU:O	2.17	0.45
2:B:307:ALA:HA	2:B:310:GLU:HG3	1.99	0.45
3:E:91:ASP:O	3:E:92:ALA:C	2.54	0.45
2:G:148:GLU:OE1	2:G:148:GLU:CA	2.65	0.45
2:H:61:GLY:O	2:H:68:ILE:HA	2.17	0.45
2:H:351:MET:HA	2:H:354:LEU:HD13	1.99	0.45
2:B:42:LEU:C	2:B:42:LEU:CD2	2.85	0.45
2:B:94:ASP:OD1	2:B:96:ALA:HB3	2.16	0.45
2:B:304:ASN:CG	2:B:305:ASP:N	2.68	0.45
2:D:13:GLN:C	2:D:57:LEU:HD21	2.37	0.45
2:D:27:ALA:O	2:D:29:ALA:N	2.50	0.45
2:D:179:ASP:O	2:D:182:GLN:HB2	2.16	0.45
2:D:290:HIS:C	2:D:292:ILE:N	2.68	0.45
2:D:292:ILE:HG13	2:D:313:MET:HE1	1.99	0.45
3:E:6:TRP:CH2	3:E:198:PRO:HB2	2.52	0.45
3:E:81:PRO:O	3:E:82:GLU:C	2.55	0.45
3:E:222:TYR:CE1	3:E:226:SER:HB3	2.51	0.45
3:E:333:HIS:ND1	3:E:333:HIS:N	2.65	0.45
1:F:214:PRO:HA	1:F:236:LEU:HD11	1.99	0.45
2:G:44:SER:O	2:G:175:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:76:CYS:O	2:G:80:ARG:HG3	2.17	0.45
2:G:93:ILE:HG21	2:G:104:THR:HG23	1.99	0.45
2:I:367:GLU:HB3	2:I:368:PRO:HD2	1.99	0.45
1:A:80:LEU:HG	1:A:82:LEU:CD1	2.47	0.45
1:A:207:ASN:HD22	1:A:207:ASN:C	2.20	0.45
2:B:286:LEU:HD21	2:B:333:LEU:CA	2.47	0.45
2:B:307:ALA:HA	2:B:310:GLU:CD	2.37	0.45
2:B:314:ARG:O	2:B:317:ALA:HB3	2.17	0.45
2:C:18:VAL:HG12	2:C:19:VAL:N	2.32	0.45
2:D:288:LEU:C	2:D:290:HIS:H	2.19	0.45
2:D:328:TYR:HD1	2:D:356:ALA:HB1	1.81	0.45
2:D:352:THR:O	2:D:355:ARG:HB3	2.17	0.45
1:F:168:GLN:HE21	1:F:168:GLN:HB2	1.49	0.45
1:F:220:ALA:C	1:F:222:LEU:H	2.20	0.45
2:H:208:ARG:O	2:H:209:ALA:C	2.55	0.45
2:I:119:ARG:HG3	2:I:120:PHE:CD2	2.52	0.45
1:A:228:ARG:H	1:A:228:ARG:HG2	1.42	0.45
2:B:10:TRP:CZ2	2:B:190:ILE:HG23	2.51	0.45
2:B:177:ALA:C	2:B:178:LEU:HD22	2.38	0.45
2:C:15:PHE:CE1	2:C:57:LEU:O	2.70	0.45
2:C:163:PRO:O	2:C:167:LEU:HG	2.17	0.45
2:C:276:ILE:H	2:C:276:ILE:HG13	1.52	0.45
2:D:10:TRP:O	2:D:12:PRO:HD3	2.16	0.45
2:D:134:HIS:CG	2:D:135:SER:N	2.84	0.45
1:F:97:LEU:HD23	1:F:126:TRP:CE3	2.50	0.45
2:G:98:ARG:HD2	2:H:169:ARG:NH2	2.32	0.45
2:G:295:VAL:CG2	2:G:301:ALA:HB3	2.27	0.45
2:H:129:HIS:CD2	2:H:161:LYS:HD2	2.50	0.45
3:J:121:THR:HG22	3:J:122:ASP:N	2.32	0.45
1:A:220:ALA:O	1:A:224:GLY:N	2.50	0.44
2:B:285:MET:HE1	2:B:332:LEU:HD21	1.98	0.44
2:C:6:LEU:C	2:C:8:ARG:N	2.69	0.44
2:C:268:ILE:O	2:C:272:ALA:N	2.45	0.44
2:D:128:VAL:HG13	2:D:129:HIS:N	2.33	0.44
2:D:191:LEU:HD23	2:D:191:LEU:HA	1.68	0.44
2:D:258:GLU:O	2:D:259:ALA:HB3	2.17	0.44
2:D:329:TYR:HD2	2:D:330:GLN:N	2.15	0.44
3:E:98:GLU:H	3:E:98:GLU:HG2	1.61	0.44
1:F:318:GLN:O	1:F:318:GLN:HG3	2.17	0.44
2:H:62:LEU:HB3	2:H:120:PHE:HD2	1.81	0.44
2:H:359:PHE:CZ	2:I:323:THR:HG23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:60:GLY:N	3:J:65:CYS:SG	2.89	0.44
3:J:245:LEU:O	3:J:248:LEU:HB3	2.16	0.44
1:A:99:THR:C	1:A:101:THR:H	2.20	0.44
1:A:191:LEU:HD23	2:B:27:ALA:HA	1.99	0.44
1:A:223:MSE:CE	1:A:292:ARG:CB	2.96	0.44
2:B:5:VAL:C	2:B:7:ALA:H	2.19	0.44
2:D:302:LEU:HD23	2:D:302:LEU:HA	1.79	0.44
3:E:57:LYS:HD2	3:E:57:LYS:HA	1.79	0.44
3:E:155:LEU:C	3:E:157:SER:N	2.70	0.44
3:E:270:VAL:HG23	3:E:273:LEU:HB3	1.99	0.44
1:F:67:LEU:O	1:F:70:ALA:N	2.50	0.44
1:F:147:LEU:O	1:F:151:VAL:HG23	2.17	0.44
2:G:145:GLU:N	2:G:146:PRO:HD3	2.32	0.44
2:G:309:ILE:O	2:G:310:GLU:C	2.56	0.44
2:H:365:LEU:HB2	2:I:322:PRO:HG3	1.98	0.44
3:J:35:MSE:HA	3:J:35:MSE:HE2	2.00	0.44
3:J:290:LEU:HD23	3:J:294:CYS:HG	1.83	0.44
3:J:317:LEU:HD13	3:J:317:LEU:C	2.36	0.44
2:B:333:LEU:HD13	2:B:334:ILE:N	2.32	0.44
2:C:113:TYR:HD2	2:C:147:PRO:HB3	1.82	0.44
2:C:324:ASP:OD1	2:C:362:ARG:NH2	2.46	0.44
2:D:22:GLU:C	2:D:24:VAL:H	2.21	0.44
2:D:354:LEU:HD13	3:E:253:MSE:CE	2.38	0.44
3:E:68:MSE:HE2	3:E:68:MSE:HA	2.00	0.44
3:E:275:ALA:O	3:E:279:ASN:ND2	2.49	0.44
2:G:313:MET:O	2:G:316:LEU:N	2.50	0.44
2:I:299:PRO:O	2:I:314:ARG:NH2	2.49	0.44
2:I:345:ARG:NH2	3:J:146:ARG:O	2.50	0.44
3:J:241:ALA:HB3	3:J:242:PRO:CD	2.48	0.44
1:A:308:THR:O	1:A:312:LEU:N	2.49	0.44
2:B:8:ARG:HD2	2:B:8:ARG:O	2.17	0.44
2:B:148:GLU:CD	2:B:149:HIS:H	2.21	0.44
2:B:291:ARG:O	2:B:294:MET:HB3	2.17	0.44
2:B:328:TYR:O	2:B:329:TYR:O	2.36	0.44
2:C:100:LYS:HG2	2:D:133:ARG:HG3	1.99	0.44
2:C:171:LEU:HD12	2:C:171:LEU:HA	1.87	0.44
2:C:261:GLY:O	2:C:263:ARG:N	2.51	0.44
2:D:268:ILE:O	2:D:271:ALA:N	2.48	0.44
2:D:295:VAL:HG21	2:D:302:LEU:HG	2.00	0.44
3:E:90:VAL:HA	3:E:124:ALA:HA	2.00	0.44
1:F:237:ARG:O	1:F:238:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:ASP:HA	2:H:155:ALA:HB3	1.98	0.44
2:H:142:THR:O	2:H:142:THR:HG22	2.17	0.44
2:H:265:MET:SD	2:I:297:LEU:HD23	2.56	0.44
3:J:77:TYR:HE1	3:J:99:LYS:HE2	1.82	0.44
3:J:194:SER:O	3:J:195:ALA:HB3	2.18	0.44
1:A:74:PHE:HD1	1:F:203:GLU:CG	2.17	0.44
1:A:274:ASP:HA	1:A:279:TRP:CZ3	2.52	0.44
2:B:316:LEU:HD23	2:B:316:LEU:HA	1.85	0.44
2:D:132:SER:O	2:D:133:ARG:C	2.54	0.44
2:D:278:TRP:CZ2	2:D:346:ARG:HB2	2.52	0.44
3:E:120:LEU:CD1	3:E:125:ALA:HA	2.47	0.44
1:F:310:LEU:O	1:F:313:LYS:N	2.47	0.44
2:I:202:ALA:HB1	2:I:237:VAL:HG21	2.00	0.44
2:I:365:LEU:HB3	2:I:366:PRO:HD2	2.00	0.44
3:J:94:ARG:HA	3:J:94:ARG:HD3	1.81	0.44
3:J:95:GLU:O	3:J:99:LYS:HB2	2.18	0.44
3:J:155:LEU:C	3:J:157:SER:N	2.70	0.44
2:B:156:THR:HG21	2:B:159:PRO:HG3	2.00	0.44
2:B:158:ASP:O	2:B:158:ASP:OD1	2.36	0.44
2:B:248:GLN:HA	2:B:251:SER:CB	2.42	0.44
2:C:252:LEU:O	2:C:256:MET:N	2.49	0.44
2:C:295:VAL:HG12	2:C:299:PRO:HA	2.00	0.44
2:D:136:PHE:HD1	2:D:166:ILE:CD1	2.31	0.44
1:F:174:TYR:HB2	1:F:181:LEU:HD21	1.98	0.44
2:G:307:ALA:HA	2:G:310:GLU:HG3	1.99	0.44
2:H:100:LYS:NZ	2:I:133:ARG:CA	2.80	0.44
2:I:48:GLY:O	2:I:213:SER:HA	2.16	0.44
3:J:317:LEU:HD13	3:J:318:ARG:CA	2.48	0.44
1:A:221:LEU:HD11	1:A:328:SER:HB3	1.98	0.44
1:A:320:VAL:HG12	1:A:321:TRP:N	2.33	0.44
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.73	0.44
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.67	0.44
2:D:13:GLN:HE21	2:D:13:GLN:CA	2.30	0.44
2:D:250:LEU:C	2:D:252:LEU:N	2.69	0.44
2:D:268:ILE:HG23	2:D:278:TRP:HH2	1.82	0.44
3:E:7:LEU:HD21	3:E:36:GLY:HA3	2.00	0.44
2:H:91:ILE:HD13	2:H:107:LEU:HD22	1.99	0.44
2:I:167:LEU:HD21	2:I:172:GLN:OE1	2.17	0.44
1:A:53:PHE:CD2	1:A:64:ILE:HG12	2.52	0.44
1:A:130:LEU:C	1:A:132:ASN:H	2.21	0.44
1:A:177:ASN:O	1:A:179:LEU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:O	1:A:223:MSE:N	2.50	0.44
2:B:227:SER:HA	2:C:26:THR:HG21	1.99	0.44
2:C:52:THR:OG1	2:C:53:SER:N	2.51	0.44
2:C:240:MET:HA	2:D:23:HIS:CB	2.48	0.44
2:C:333:LEU:C	2:C:335:GLY:H	2.21	0.44
2:D:149:HIS:C	2:D:150:VAL:HG23	2.37	0.44
1:F:219:ASP:O	1:F:222:LEU:HB2	2.17	0.44
2:G:289:LEU:CD2	2:G:325:ILE:HG23	2.47	0.44
2:H:3:TYR:CD2	2:H:3:TYR:N	2.86	0.44
2:H:44:SER:CB	2:H:159:PRO:HG3	2.48	0.44
2:I:295:VAL:HG22	2:I:301:ALA:HB3	2.00	0.44
3:J:5:PRO:HG2	3:J:6:TRP:H	1.81	0.44
3:J:125:ALA:O	3:J:128:LEU:HB3	2.17	0.44
3:J:253:MSE:CE	3:J:257:LYS:HG3	2.48	0.44
1:A:105:HIS:HB3	1:F:227:LYS:CD	2.42	0.44
2:B:132:SER:C	2:B:134:HIS:N	2.69	0.44
2:B:179:ASP:O	2:B:183:ILE:HG13	2.18	0.44
2:C:66:THR:O	2:C:66:THR:HG22	2.18	0.44
2:C:328:TYR:O	2:C:329:TYR:C	2.56	0.44
2:C:346:ARG:O	2:C:349:VAL:N	2.51	0.44
2:D:215:ARG:HD2	5:D:801:AGS:H5'1	2.00	0.44
1:F:297:GLN:HG2	1:F:335:PRO:HD3	2.00	0.44
2:G:345:ARG:O	2:G:349:VAL:HG23	2.18	0.44
2:H:279:GLU:HG3	2:H:345:ARG:HH12	1.82	0.44
2:I:277:GLU:O	2:I:280:ALA:N	2.51	0.44
2:I:337:LYS:HE3	2:I:338:GLU:HG2	2.00	0.44
3:J:173:VAL:HG11	3:J:184:GLN:HG3	2.00	0.44
1:A:192:TRP:CH2	1:A:201:ARG:HB3	2.53	0.43
1:A:304:LEU:O	1:A:305:LEU:C	2.57	0.43
2:C:367:GLU:HG3	2:D:321:PRO:CA	2.48	0.43
2:D:260:ASN:CG	2:D:263:ARG:HB2	2.39	0.43
3:E:68:MSE:CE	3:E:73:HIS:HB2	2.48	0.43
3:E:137:ALA:O	3:E:138:GLU:C	2.57	0.43
3:E:295:HIS:O	3:E:296:ILE:C	2.55	0.43
3:E:318:ARG:HD2	3:E:322:TYR:OH	2.18	0.43
1:F:81:LEU:HD13	1:F:111:ILE:HG22	2.00	0.43
1:F:192:TRP:C	1:F:194:ASP:N	2.71	0.43
2:G:124:LEU:O	2:G:124:LEU:HD13	2.18	0.43
2:G:129:HIS:HB2	2:G:161:LYS:HB2	2.00	0.43
2:H:60:LYS:O	2:H:64:CYS:HB2	2.18	0.43
3:J:315:LEU:HD22	3:J:319:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:C	1:A:162:LEU:CD2	2.87	0.43
1:A:170:LEU:O	1:A:173:CYS:O	2.36	0.43
1:A:217:TRP:NE1	1:A:221:LEU:HD11	2.33	0.43
2:B:102:GLU:HG3	2:B:105:ARG:NH2	2.33	0.43
2:B:124:LEU:HD13	2:B:124:LEU:C	2.39	0.43
2:C:351:MET:HA	2:C:354:LEU:HD12	2.00	0.43
2:D:257:VAL:O	2:D:257:VAL:HG12	2.17	0.43
2:D:321:PRO:O	2:D:322:PRO:C	2.57	0.43
3:E:1:MSE:HA	3:E:38:ASP:OD2	2.18	0.43
1:F:48:GLU:CG	1:F:49:GLU:N	2.71	0.43
1:F:55:ILE:HB	1:F:83:LEU:O	2.18	0.43
1:F:299:ARG:HH12	3:J:321:HIS:CE1	2.35	0.43
2:G:250:LEU:HD11	2:G:309:ILE:CD1	2.48	0.43
2:H:303:GLY:O	2:H:306:MET:HB2	2.18	0.43
2:I:215:ARG:NH1	5:I:803:AGS:O2A	2.51	0.43
2:B:278:TRP:O	2:B:279:GLU:C	2.56	0.43
2:D:278:TRP:CE3	2:D:349:VAL:HG21	2.53	0.43
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.54	0.43
3:E:67:LEU:HD23	3:E:67:LEU:HA	1.87	0.43
3:E:333:HIS:HB2	3:E:334:LEU:H	1.54	0.43
1:F:4:LEU:CD1	1:F:137:VAL:HG22	2.48	0.43
1:F:23:LEU:HB2	1:F:113:ARG:HB2	2.00	0.43
1:F:94:ASN:HA	1:F:126:TRP:CD1	2.54	0.43
1:F:274:ASP:HA	1:F:279:TRP:CZ3	2.52	0.43
2:H:339:LEU:HB3	2:H:340:PRO:CD	2.39	0.43
2:I:140:LEU:HD22	2:I:144:GLU:CG	2.47	0.43
3:J:5:PRO:C	3:J:7:LEU:N	2.71	0.43
1:A:176:GLY:O	1:A:178:LEU:N	2.50	0.43
1:A:188:LEU:O	1:A:189:SER:C	2.56	0.43
2:B:124:LEU:HD22	2:B:153:LEU:O	2.18	0.43
2:B:179:ASP:HB3	2:B:182:GLN:H	1.83	0.43
2:B:292:ILE:HD13	2:B:316:LEU:HB2	2.00	0.43
2:C:197:ALA:O	2:C:198:HIS:CB	2.54	0.43
2:C:214:LEU:O	2:C:215:ARG:C	2.54	0.43
2:C:314:ARG:O	2:C:315:GLU:C	2.55	0.43
3:E:149:GLU:C	3:E:151:LEU:N	2.72	0.43
3:E:163:TYR:CE2	3:E:165:ALA:CB	3.00	0.43
1:F:192:TRP:C	1:F:194:ASP:H	2.22	0.43
2:G:48:GLY:HA3	2:G:215:ARG:HB2	2.00	0.43
2:H:295:VAL:HG21	2:H:302:LEU:HG	2.01	0.43
3:J:24:HIS:HD2	3:J:160:ARG:CZ	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:145:THR:HG22	3:J:147:GLU:N	2.31	0.43
1:A:235:GLN:C	1:A:237:ARG:H	2.22	0.43
1:A:255:LEU:O	1:A:256:LEU:C	2.56	0.43
1:A:255:LEU:HD13	3:E:309:GLU:OE2	2.18	0.43
2:B:357:LEU:HD12	2:B:357:LEU:N	2.33	0.43
2:C:250:LEU:O	2:C:254:GLU:HB2	2.17	0.43
2:C:265:MET:HE1	2:D:294:MET:HE2	2.00	0.43
2:D:260:ASN:CG	2:D:263:ARG:CB	2.87	0.43
3:E:4:TYR:CD2	3:E:6:TRP:CZ2	3.06	0.43
3:E:32:LEU:HD12	3:E:166:PRO:HG2	2.01	0.43
3:E:68:MSE:HE3	3:E:73:HIS:HB2	2.01	0.43
3:E:89:GLY:O	3:E:93:VAL:HG23	2.18	0.43
3:E:125:ALA:O	3:E:126:ASN:C	2.56	0.43
3:E:224:VAL:HB	3:E:225:PRO:HD3	2.01	0.43
3:E:296:ILE:HG21	3:E:315:LEU:HD12	2.01	0.43
1:F:248:ARG:CZ	3:J:307:ASN:HB2	2.49	0.43
2:G:56:ARG:HH11	2:G:56:ARG:HG3	1.84	0.43
2:G:206:LEU:HD13	2:G:221:THR:OG1	2.18	0.43
2:H:93:ILE:HB	2:H:125:ILE:HG12	2.01	0.43
2:H:250:LEU:HD13	2:H:313:MET:SD	2.58	0.43
2:H:281:LEU:HD23	2:H:281:LEU:O	2.18	0.43
1:A:329:LEU:HD11	2:B:291:ARG:HH21	1.83	0.43
2:B:298:SER:HA	2:B:299:PRO:HD2	1.71	0.43
2:B:318:ARG:CG	2:B:319:THR:H	2.31	0.43
2:C:133:ARG:H	2:C:133:ARG:CD	2.25	0.43
2:D:210:ALA:O	2:D:211:GLU:C	2.56	0.43
2:D:244:LEU:HD11	2:D:276:ILE:HG23	2.01	0.43
3:E:49:LEU:CD2	3:E:68:MSE:SE	3.16	0.43
1:F:19:ALA:HB3	1:F:133:ARG:HB3	2.00	0.43
1:F:215:PHE:HD2	1:F:215:PHE:HA	1.68	0.43
1:F:273:PHE:HB3	1:F:279:TRP:CG	2.53	0.43
1:F:312:LEU:O	1:F:316:TYR:HA	2.18	0.43
2:G:91:ILE:HD11	2:G:121:LYS:HE3	2.00	0.43
2:G:233:SER:O	2:G:237:VAL:HG23	2.18	0.43
2:G:286:LEU:HD21	2:G:332:LEU:HB3	2.00	0.43
2:H:242:GLY:O	2:H:276:ILE:HG22	2.18	0.43
2:I:243:THR:HG22	2:I:244:LEU:N	2.33	0.43
3:J:151:LEU:O	3:J:152:LEU:C	2.57	0.43
2:B:23:HIS:CE1	2:B:176:LYS:NZ	2.86	0.43
2:B:37:ILE:HG21	2:B:151:LYS:HE3	2.01	0.43
2:B:350:GLU:HB2	2:C:290:HIS:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:338:GLU:C	2:C:340:PRO:CD	2.87	0.43
2:D:38:HIS:CG	2:D:39:HIS:N	2.87	0.43
2:D:159:PRO:O	2:D:162:LEU:HB2	2.18	0.43
2:D:265:MET:HE3	2:D:354:LEU:HD11	1.99	0.43
2:D:282:LEU:O	2:D:283:VAL:C	2.56	0.43
2:D:320:ILE:HG22	2:D:325:ILE:HG13	2.00	0.43
3:E:30:GLN:HB2	3:E:148:PRO:HD3	2.01	0.43
3:E:68:MSE:CE	3:E:73:HIS:CB	2.95	0.43
1:F:64:ILE:HD12	1:F:64:ILE:N	2.34	0.43
1:F:221:LEU:HD11	1:F:328:SER:HA	2.01	0.43
2:G:244:LEU:HD23	2:G:244:LEU:HA	1.71	0.43
2:H:291:ARG:O	2:H:294:MET:HB2	2.18	0.43
2:H:354:LEU:HD22	2:I:293:ALA:CB	2.48	0.43
2:I:304:ASN:C	2:I:306:MET:H	2.21	0.43
2:I:332:LEU:HA	2:I:352:THR:HG21	1.99	0.43
2:I:366:PRO:O	2:I:367:GLU:HG3	2.18	0.43
1:A:74:PHE:CZ	1:F:203:GLU:HA	2.54	0.43
1:A:150:TRP:CE2	1:A:154:ARG:HG3	2.54	0.43
1:A:213:THR:O	1:A:216:HIS:N	2.44	0.43
2:C:46:THR:HG22	2:C:47:ARG:H	1.83	0.43
2:D:235:GLN:HG2	2:D:236:ALA:N	2.31	0.43
3:E:121:THR:O	3:E:124:ALA:N	2.52	0.43
1:F:78:GLN:O	1:F:79:THR:HB	2.19	0.43
2:G:142:THR:HG23	2:G:147:PRO:HG2	2.01	0.43
2:G:314:ARG:O	2:G:317:ALA:HB3	2.18	0.43
2:H:288:LEU:C	2:H:290:HIS:H	2.22	0.43
2:I:309:ILE:O	2:I:312:ARG:N	2.50	0.43
3:J:303:VAL:HB	3:J:306:ILE:CG1	2.49	0.43
1:A:80:LEU:CD2	1:A:82:LEU:HD11	2.49	0.43
1:A:255:LEU:HD22	3:E:313:THR:HG21	2.01	0.43
2:C:65:GLU:C	2:C:67:GLY:N	2.72	0.43
2:C:70:ALA:C	2:C:72:PRO:HD3	2.39	0.43
2:C:139:LEU:O	2:C:140:LEU:C	2.58	0.43
2:C:237:VAL:O	2:C:238:SER:C	2.56	0.43
2:C:347:MET:HG2	2:D:290:HIS:ND1	2.33	0.43
2:D:114:ALA:HA	2:D:115:PRO:HD3	1.83	0.43
2:D:120:PHE:CE1	2:D:151:LYS:HE2	2.54	0.43
2:D:184:ARG:HB2	2:D:207:ALA:HB2	2.00	0.43
2:G:326:GLN:O	2:G:326:GLN:HG2	2.17	0.43
2:H:351:MET:HE2	2:H:354:LEU:HB2	2.01	0.43
2:I:263:ARG:HH11	2:I:263:ARG:HG3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:CD2	1:A:282:ARG:NH2	2.86	0.43
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.33	0.43
2:C:285:MET:O	2:C:288:LEU:N	2.51	0.43
2:C:333:LEU:C	2:C:333:LEU:HD23	2.38	0.43
3:E:143:LEU:N	3:E:143:LEU:CD2	2.81	0.43
2:H:265:MET:HA	2:H:268:ILE:HD12	2.01	0.43
2:H:271:ALA:CB	2:H:276:ILE:HD11	2.48	0.43
2:H:343:PRO:HG2	2:H:347:MET:SD	2.59	0.43
3:J:57:LYS:CG	3:J:58:SER:H	2.28	0.43
3:J:252:LEU:HD23	3:J:290:LEU:CA	2.46	0.43
3:J:296:ILE:HD12	3:J:299:GLN:HE21	1.84	0.43
1:A:230:LEU:HD22	2:B:303:GLY:HA3	2.01	0.42
2:B:176:LYS:C	2:B:177:ALA:O	2.56	0.42
2:B:254:GLU:O	2:B:257:VAL:HG23	2.19	0.42
2:D:281:LEU:O	2:D:281:LEU:HD13	2.18	0.42
2:D:321:PRO:HA	2:D:322:PRO:HD2	1.89	0.42
1:F:47:PHE:CD2	1:F:78:GLN:N	2.86	0.42
2:G:140:LEU:HD22	2:G:144:GLU:CD	2.39	0.42
2:H:179:ASP:CG	2:H:180:VAL:N	2.71	0.42
2:I:201:ARG:NH2	2:I:284:GLU:CD	2.72	0.42
3:J:27:LEU:HD12	3:J:160:ARG:O	2.19	0.42
3:J:41:ILE:HG21	3:J:113:TRP:CG	2.54	0.42
3:J:90:VAL:HG12	3:J:90:VAL:O	2.18	0.42
3:J:289:ILE:O	3:J:293:VAL:HG23	2.19	0.42
3:J:316:LEU:O	3:J:319:ILE:HB	2.19	0.42
1:A:4:LEU:HD11	1:A:137:VAL:HG22	2.01	0.42
2:B:351:MET:HG2	2:C:329:TYR:CE1	2.53	0.42
2:C:285:MET:O	2:C:287:GLY:N	2.52	0.42
2:D:171:LEU:HD12	2:D:171:LEU:HA	1.83	0.42
2:D:188:GLU:O	2:D:189:HIS:C	2.57	0.42
3:E:155:LEU:O	3:E:157:SER:N	2.52	0.42
2:G:313:MET:O	2:G:315:GLU:N	2.52	0.42
2:H:60:LYS:HA	2:H:82:ILE:HD13	2.00	0.42
2:H:260:ASN:CG	2:H:260:ASN:O	2.57	0.42
2:I:158:ASP:CG	2:I:161:LYS:CG	2.87	0.42
2:I:347:MET:SD	3:J:253:MSE:HG2	2.59	0.42
3:J:6:TRP:O	3:J:9:PRO:HD2	2.19	0.42
1:A:65:PHE:CE1	1:A:99:THR:CG2	3.02	0.42
1:A:105:HIS:O	1:A:107:ASP:N	2.53	0.42
1:A:207:ASN:C	1:A:207:ASN:ND2	2.73	0.42
1:A:336:LEU:HD11	2:B:294:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:ASP:HB3	2:B:182:GLN:CG	2.49	0.42
2:B:241:LEU:O	2:B:242:GLY:O	2.37	0.42
2:B:254:GLU:C	2:B:256:MET:N	2.73	0.42
2:B:304:ASN:OD1	2:B:305:ASP:HB2	2.19	0.42
2:D:132:SER:O	2:D:134:HIS:N	2.52	0.42
2:D:339:LEU:HD11	2:D:345:ARG:CG	2.48	0.42
2:G:13:GLN:HA	2:G:13:GLN:HE21	1.83	0.42
2:G:115:PRO:HD3	2:G:149:HIS:HB3	2.01	0.42
2:G:261:GLY:O	2:G:265:MET:HG2	2.19	0.42
2:I:113:TYR:HE2	2:I:147:PRO:CG	2.32	0.42
2:I:345:ARG:H	2:I:345:ARG:HG3	1.41	0.42
3:J:24:HIS:CD2	3:J:160:ARG:NE	2.88	0.42
1:A:98:LEU:HD22	1:A:101:THR:HG21	2.01	0.42
1:A:173:CYS:SG	1:A:211:HIS:HE1	2.42	0.42
1:A:333:HIS:CB	2:B:298:SER:OG	2.66	0.42
2:C:206:LEU:O	2:C:209:ALA:HB3	2.19	0.42
2:C:260:ASN:HD21	2:C:263:ARG:HB2	1.84	0.42
2:C:264:VAL:CG1	2:C:353:LEU:HD13	2.47	0.42
2:C:325:ILE:HA	2:C:328:TYR:HD2	1.84	0.42
2:D:126:ASP:OD1	2:D:127:GLU:HG2	2.20	0.42
2:D:280:ALA:N	3:E:149:GLU:OE2	2.50	0.42
3:E:238:HIS:HB3	3:E:244:ARG:NH1	2.34	0.42
1:F:231:HIS:O	1:F:235:GLN:HG2	2.20	0.42
1:F:248:ARG:HD2	1:F:251:GLN:OE1	2.20	0.42
1:F:282:ARG:CG	1:F:285:MSE:HE1	2.33	0.42
2:G:316:LEU:HB3	2:G:320:ILE:CD1	2.48	0.42
2:I:343:PRO:HB3	3:J:297:ARG:HE	1.85	0.42
3:J:58:SER:CB	3:J:65:CYS:SG	3.03	0.42
3:J:250:THR:CB	3:J:267:ASN:HD21	2.33	0.42
1:A:27:ASP:OD2	1:A:30:LEU:CB	2.67	0.42
1:A:147:LEU:HB3	1:A:148:PRO:CD	2.38	0.42
1:A:285:MSE:HB3	1:A:285:MSE:HE2	2.01	0.42
1:A:305:LEU:O	1:A:308:THR:HB	2.18	0.42
2:B:91:ILE:HD11	2:B:112:GLN:NE2	2.34	0.42
2:C:160:GLN:C	2:C:162:LEU:H	2.23	0.42
2:C:351:MET:SD	2:D:329:TYR:CD1	3.13	0.42
3:E:121:THR:C	3:E:123:ALA:N	2.72	0.42
3:E:283:PRO:HG2	3:E:284:SER:N	2.27	0.42
1:F:57:PRO:O	1:F:58:ASN:HB2	2.19	0.42
1:F:108:LEU:O	1:F:108:LEU:HG	2.19	0.42
2:G:148:GLU:O	2:G:149:HIS:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:SER:HB2	2:H:159:PRO:CG	2.50	0.42
2:H:122:VAL:HG13	2:H:153:LEU:HG	2.02	0.42
2:H:243:THR:HG22	2:H:244:LEU:N	2.34	0.42
2:H:276:ILE:HG22	2:H:277:GLU:H	1.84	0.42
2:H:353:LEU:HD23	2:H:353:LEU:HA	1.90	0.42
3:J:25:HIS:ND1	3:J:25:HIS:N	2.62	0.42
3:J:88:LEU:HB3	3:J:120:LEU:HA	2.01	0.42
3:J:329:LEU:N	3:J:329:LEU:HD23	2.34	0.42
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.82	0.42
2:B:37:ILE:CG2	2:B:151:LYS:HE3	2.49	0.42
2:B:132:SER:O	2:B:134:HIS:N	2.52	0.42
2:B:244:LEU:O	2:B:245:ASP:CB	2.59	0.42
2:B:258:GLU:O	2:B:259:ALA:HB3	2.20	0.42
2:D:102:GLU:HG3	2:D:105:ARG:NH2	2.34	0.42
2:D:112:GLN:OE1	2:D:112:GLN:HA	2.19	0.42
2:D:250:LEU:O	2:D:252:LEU:N	2.53	0.42
2:D:320:ILE:HA	2:D:321:PRO:HD3	1.91	0.42
3:E:73:HIS:CE1	3:E:106:LEU:CD2	3.02	0.42
3:E:289:ILE:CG2	3:E:319:ILE:HD13	2.46	0.42
2:H:34:LEU:HD13	2:H:36:ARG:CZ	2.50	0.42
1:A:209:ALA:O	2:B:176:LYS:HE3	2.19	0.42
1:A:326:GLY:O	1:A:327:LEU:C	2.57	0.42
2:C:269:ASN:O	2:C:271:ALA:N	2.52	0.42
2:D:285:MET:HE3	2:D:353:LEU:CD2	2.30	0.42
3:E:68:MSE:SE	3:E:76:TYR:CD2	3.23	0.42
1:F:26:ASN:O	1:F:26:ASN:OD1	2.38	0.42
1:F:217:TRP:HZ3	1:F:250:LEU:HD22	1.83	0.42
2:I:140:LEU:O	2:I:144:GLU:HG3	2.18	0.42
2:I:192:ASN:OD1	2:I:198:HIS:HE1	2.03	0.42
3:J:42:TYR:O	3:J:46:ARG:HG2	2.19	0.42
1:A:51:HIS:HB3	1:A:53:PHE:HE1	1.85	0.42
1:A:134:SER:HB2	1:A:135:VAL:H	1.68	0.42
1:A:213:THR:HG22	1:A:215:PHE:HB2	2.02	0.42
2:B:264:VAL:HG11	2:B:353:LEU:HD13	2.01	0.42
3:E:50:CYS:SG	3:E:53:PRO:N	2.93	0.42
3:E:74:PRO:CD	3:E:106:LEU:HD11	2.47	0.42
3:E:117:ALA:HA	3:E:120:LEU:HD23	2.01	0.42
3:E:187:LEU:HA	3:E:187:LEU:HD23	1.80	0.42
3:E:238:HIS:CB	3:E:244:ARG:NH1	2.83	0.42
1:F:27:ASP:HB2	1:F:141:THR:OG1	2.20	0.42
1:F:268:PRO:O	1:F:270:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:TRP:O	2:G:12:PRO:HD3	2.20	0.42
2:G:264:VAL:CG1	2:G:353:LEU:HD13	2.50	0.42
2:H:137:ASN:O	2:H:141:LYS:HG3	2.20	0.42
2:H:260:ASN:ND2	2:H:263:ARG:HB3	2.35	0.42
3:J:220:LEU:HD22	3:J:224:VAL:HG23	2.01	0.42
3:J:225:PRO:HA	3:J:280:HIS:CE1	2.54	0.42
1:A:262:ARG:NH2	3:E:320:GLU:CD	2.73	0.42
1:A:301:ALA:HB2	1:A:331:LEU:HD21	2.02	0.42
2:B:42:LEU:HD21	2:B:156:THR:HG22	2.01	0.42
2:B:187:LEU:C	2:B:189:HIS:N	2.71	0.42
2:B:309:ILE:O	2:B:312:ARG:N	2.50	0.42
2:D:136:PHE:O	2:D:140:LEU:HB2	2.20	0.42
2:D:353:LEU:C	2:D:355:ARG:N	2.73	0.42
3:E:158:ARG:HA	3:E:158:ARG:HD2	1.81	0.42
3:E:188:LEU:O	3:E:191:LEU:HB3	2.20	0.42
3:E:334:LEU:HD13	3:E:334:LEU:HA	1.78	0.42
1:F:303:GLN:OE1	3:J:314:ASP:OD1	2.38	0.42
2:G:98:ARG:NE	2:H:140:LEU:HD13	2.35	0.42
2:G:209:ALA:O	2:G:211:GLU:N	2.52	0.42
2:G:266:ALA:O	2:G:270:GLU:HB2	2.20	0.42
2:H:231:GLN:C	2:H:233:SER:H	2.23	0.42
2:I:92:GLU:HG2	2:I:124:LEU:HD12	2.02	0.42
2:I:276:ILE:HG22	2:I:277:GLU:N	2.32	0.42
2:I:352:THR:O	2:I:355:ARG:HB3	2.20	0.42
3:J:189:ALA:HB3	3:J:210:TRP:HH2	1.84	0.42
2:B:76:CYS:SG	2:B:78:ASN:CA	3.08	0.42
2:B:164:VAL:CG2	2:B:165:THR:N	2.83	0.42
2:B:185:HIS:O	2:B:185:HIS:ND1	2.50	0.42
2:B:285:MET:CE	2:B:332:LEU:HD21	2.49	0.42
2:B:334:ILE:O	2:B:338:GLU:HG3	2.19	0.42
2:C:320:ILE:HA	2:C:321:PRO:HD3	1.94	0.42
2:D:184:ARG:C	2:D:184:ARG:CD	2.83	0.42
3:E:192:ARG:C	3:E:194:SER:N	2.74	0.42
1:F:40:GLN:HE21	1:F:40:GLN:HB3	1.60	0.42
1:F:174:TYR:CD2	1:F:180:ALA:HB1	2.55	0.42
1:F:334:LYS:H	1:F:334:LYS:HG3	1.66	0.42
2:G:19:VAL:HG12	2:G:178:LEU:HD13	2.01	0.42
2:H:106:ASP:O	2:H:110:ASN:ND2	2.52	0.42
2:I:11:ARG:HH12	5:I:803:AGS:PA	2.42	0.42
2:I:302:LEU:HD13	2:I:310:GLU:HA	2.01	0.42
3:J:176:LEU:C	3:J:178:ARG:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:H	1:A:143:GLU:CD	2.19	0.41
1:A:213:THR:C	1:A:215:PHE:H	2.23	0.41
2:B:88:VAL:HG13	2:B:89:ASP:N	2.35	0.41
2:B:178:LEU:HD13	2:B:178:LEU:HA	1.69	0.41
2:B:179:ASP:HB2	2:B:182:GLN:HE21	1.81	0.41
2:B:359:PHE:HE2	2:C:323:THR:OG1	2.03	0.41
2:C:51:LYS:HE2	6:C:1300:PO4:O3	2.20	0.41
2:D:128:VAL:CG1	2:D:129:HIS:N	2.83	0.41
2:D:132:SER:O	2:D:135:SER:N	2.53	0.41
2:D:290:HIS:CE1	2:D:294:MET:HE3	2.54	0.41
2:D:314:ARG:O	2:D:317:ALA:HB3	2.20	0.41
2:D:332:LEU:HD23	2:D:352:THR:CG2	2.50	0.41
2:D:361:PRO:O	2:D:362:ARG:CB	2.68	0.41
3:E:42:TYR:HE2	3:E:46:ARG:NH1	2.17	0.41
3:E:250:THR:O	3:E:251:LEU:C	2.58	0.41
3:E:292:ASP:CG	3:E:322:TYR:HH	2.22	0.41
3:E:318:ARG:O	3:E:319:ILE:C	2.57	0.41
1:F:191:LEU:HD13	2:G:26:THR:HG21	2.00	0.41
1:F:220:ALA:O	1:F:222:LEU:N	2.53	0.41
2:I:113:TYR:CE2	2:I:147:PRO:CG	3.03	0.41
3:J:158:ARG:CG	3:J:158:ARG:HH11	2.33	0.41
1:A:221:LEU:HA	1:A:221:LEU:HD23	1.63	0.41
2:B:41:TYR:N	2:B:41:TYR:CD1	2.88	0.41
2:C:56:ARG:HG2	2:C:56:ARG:HH11	1.85	0.41
2:C:65:GLU:CA	2:C:119:ARG:HH21	2.30	0.41
2:C:102:GLU:HB3	2:C:105:ARG:HH11	1.84	0.41
2:C:323:THR:CG2	2:C:324:ASP:N	2.74	0.41
2:D:243:THR:HG22	2:D:244:LEU:N	2.36	0.41
2:D:259:ALA:CB	2:D:363:MET:SD	3.08	0.41
2:D:316:LEU:HA	2:D:316:LEU:HD23	1.67	0.41
3:E:279:ASN:C	3:E:281:LEU:N	2.73	0.41
1:F:81:LEU:HA	1:F:111:ILE:O	2.20	0.41
2:G:99:THR:HB	2:H:145:GLU:HB2	2.02	0.41
2:G:201:ARG:HB2	2:G:234:THR:OG1	2.20	0.41
2:G:277:GLU:CG	2:G:280:ALA:HB2	2.49	0.41
2:I:343:PRO:HA	3:J:297:ARG:HH21	1.85	0.41
3:J:116:ASP:HB3	3:J:119:LEU:CD1	2.50	0.41
3:J:324:GLN:HA	3:J:325:PRO:HD3	1.93	0.41
1:A:27:ASP:OD1	1:A:27:ASP:C	2.58	0.41
1:A:74:PHE:CZ	1:F:206:VAL:HG12	2.54	0.41
1:A:98:LEU:HG	1:A:125:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:HIS:O	1:F:81:LEU:N	2.53	0.41
1:F:55:ILE:HD11	1:F:82:LEU:HG	2.02	0.41
1:F:225:LYS:HZ3	1:F:333:HIS:HE1	1.68	0.41
3:J:73:HIS:HA	3:J:74:PRO:HD3	1.82	0.41
3:J:216:LEU:HD11	3:J:236:LEU:HD21	2.03	0.41
1:A:143:GLU:O	1:A:147:LEU:N	2.50	0.41
2:B:365:LEU:HA	2:B:366:PRO:HD3	1.81	0.41
2:C:245:ASP:HB3	2:C:248:GLN:CG	2.50	0.41
2:C:305:ASP:C	2:C:307:ALA:N	2.72	0.41
2:D:24:VAL:C	2:D:26:THR:N	2.72	0.41
2:D:290:HIS:O	2:D:291:ARG:C	2.59	0.41
3:E:88:LEU:HD23	3:E:88:LEU:C	2.40	0.41
3:E:88:LEU:HD21	3:E:93:VAL:HG22	2.02	0.41
1:F:4:LEU:O	1:F:137:VAL:HA	2.20	0.41
2:G:98:ARG:CB	2:H:169:ARG:HH22	2.33	0.41
2:G:285:MET:CB	2:G:332:LEU:HD21	2.47	0.41
2:H:59:ALA:CB	2:H:122:VAL:HG21	2.51	0.41
1:A:128:THR:O	1:A:131:ALA:CB	2.67	0.41
1:A:220:ALA:C	1:A:222:LEU:N	2.72	0.41
2:B:186:GLN:O	2:B:190:ILE:HG13	2.20	0.41
2:C:187:LEU:HD22	2:C:221:THR:OG1	2.20	0.41
3:E:69:GLN:HE21	3:E:69:GLN:C	2.24	0.41
3:E:161:LEU:H	3:E:161:LEU:CD1	2.23	0.41
3:E:233:LEU:O	3:E:234:ALA:C	2.58	0.41
3:E:307:ASN:O	3:E:310:LEU:N	2.51	0.41
2:G:87:PHE:CE2	2:G:89:ASP:HB2	2.55	0.41
2:G:278:TRP:CH2	2:G:346:ARG:HG3	2.55	0.41
2:I:148:GLU:O	2:I:149:HIS:HB2	2.21	0.41
2:B:22:GLU:O	2:B:24:VAL:N	2.53	0.41
2:B:247:ASP:OD2	2:B:312:ARG:NH1	2.44	0.41
2:C:183:ILE:HD13	2:C:217:ALA:HB2	2.01	0.41
2:C:240:MET:HE3	2:C:240:MET:HB3	1.77	0.41
2:C:351:MET:HG2	2:D:329:TYR:CE1	2.56	0.41
3:E:31:ALA:CB	3:E:164:LEU:HB3	2.49	0.41
2:G:7:ALA:HA	2:G:218:LEU:HD13	2.02	0.41
2:G:183:ILE:O	2:G:187:LEU:HG	2.20	0.41
2:H:272:ALA:N	2:H:276:ILE:HD11	2.35	0.41
2:I:333:LEU:C	2:I:333:LEU:HD13	2.41	0.41
3:J:297:ARG:O	3:J:300:LEU:HB2	2.21	0.41
1:A:105:HIS:CB	1:F:227:LYS:HD3	2.41	0.41
2:C:144:GLU:OE1	2:C:144:GLU:CA	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:ALA:HB2	2:C:234:THR:N	2.35	0.41
2:C:205:LEU:O	2:C:206:LEU:C	2.59	0.41
2:C:288:LEU:O	2:C:289:LEU:C	2.59	0.41
2:D:357:LEU:HG	2:D:363:MET:CE	2.49	0.41
1:F:50:HIS:ND1	1:F:79:THR:HG23	2.36	0.41
1:F:275:LYS:HA	1:F:275:LYS:HD3	1.91	0.41
1:A:162:LEU:HD21	1:A:167:ASN:N	2.35	0.41
2:B:71:THR:O	2:B:72:PRO:C	2.59	0.41
2:B:179:ASP:CB	2:B:182:GLN:HB2	2.50	0.41
2:B:253:VAL:O	2:B:257:VAL:HG22	2.21	0.41
2:C:93:ILE:HG23	2:D:133:ARG:HH22	1.84	0.41
2:C:103:ASP:O	2:C:107:LEU:HG	2.21	0.41
2:C:196:ILE:C	2:C:197:ALA:O	2.54	0.41
2:D:59:ALA:HB2	2:D:122:VAL:HG11	2.01	0.41
3:E:27:LEU:HB3	3:E:142:PHE:CD1	2.56	0.41
3:E:37:ASP:CG	3:E:38:ASP:N	2.73	0.41
3:E:136:PRO:O	3:E:137:ALA:C	2.58	0.41
3:E:142:PHE:C	3:E:143:LEU:HD22	2.41	0.41
3:E:242:PRO:CG	3:E:243:ALA:H	2.31	0.41
1:F:70:ALA:C	1:F:71:MSE:HE2	2.40	0.41
1:F:174:TYR:O	1:F:181:LEU:HD21	2.20	0.41
1:F:247:LEU:HD22	1:F:305:LEU:CD2	2.51	0.41
2:G:10:TRP:CH2	2:G:193:GLU:HB2	2.52	0.41
2:G:246:ASP:O	2:G:246:ASP:CG	2.57	0.41
3:J:254:ASP:O	3:J:257:LYS:HB2	2.21	0.41
3:J:296:ILE:HD12	3:J:299:GLN:NE2	2.36	0.41
1:A:41:VAL:O	1:A:41:VAL:HG12	2.19	0.41
2:B:286:LEU:HD21	2:B:333:LEU:N	2.36	0.41
2:C:87:PHE:HB3	2:C:90:LEU:HB3	2.03	0.41
2:C:94:ASP:HB3	2:C:97:SER:HB2	2.02	0.41
2:C:129:HIS:ND1	2:C:156:THR:HG23	2.36	0.41
2:C:220:LEU:C	2:C:222:ASP:N	2.73	0.41
2:C:302:LEU:HD23	2:C:302:LEU:HA	1.73	0.41
2:C:367:GLU:HG2	2:D:322:PRO:HD2	2.03	0.41
2:D:234:THR:HG22	2:D:245:ASP:OD1	2.20	0.41
2:D:272:ALA:CB	2:D:346:ARG:HH11	2.34	0.41
2:D:316:LEU:HD22	2:D:320:ILE:CD1	2.51	0.41
3:E:98:GLU:C	3:E:100:LEU:H	2.24	0.41
3:E:218:GLN:O	3:E:221:ALA:CB	2.61	0.41
3:E:329:LEU:HA	3:E:330:PRO:HD3	1.71	0.41
1:F:93:ILE:C	1:F:95:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:LEU:HD23	1:F:110:LEU:N	2.36	0.41
1:F:223:MSE:HE2	1:F:288:GLU:O	2.21	0.41
2:G:285:MET:O	2:G:289:LEU:HB2	2.21	0.41
2:G:333:LEU:HD11	2:G:337:LYS:HE3	2.03	0.41
2:H:93:ILE:HG21	2:H:104:THR:CG2	2.51	0.41
2:H:93:ILE:HG23	2:H:104:THR:OG1	2.20	0.41
2:H:288:LEU:O	2:H:292:ILE:HG13	2.21	0.41
2:H:292:ILE:HG22	2:H:325:ILE:CD1	2.51	0.41
2:I:240:MET:SD	3:J:157:SER:CA	3.09	0.41
2:I:298:SER:HA	2:I:299:PRO:HD2	1.84	0.41
2:I:335:GLY:O	2:I:338:GLU:N	2.53	0.41
3:J:34:GLY:O	3:J:199:GLY:HA3	2.21	0.41
3:J:41:ILE:HG21	3:J:113:TRP:NE1	2.36	0.41
3:J:77:TYR:CE1	3:J:99:LYS:HE2	2.56	0.41
3:J:90:VAL:HG21	3:J:123:ALA:CB	2.51	0.41
3:J:242:PRO:HG2	3:J:243:ALA:H	1.86	0.41
1:A:322:ALA:O	1:A:325:GLU:HB3	2.20	0.41
2:B:347:MET:O	2:B:348:GLY:C	2.59	0.41
2:C:261:GLY:CA	2:D:297:LEU:HD21	2.44	0.41
2:C:315:GLU:O	2:C:316:LEU:C	2.59	0.41
2:D:32:LEU:C	2:D:34:LEU:N	2.74	0.41
2:D:134:HIS:ND1	2:D:135:SER:N	2.68	0.41
2:D:148:GLU:O	2:D:149:HIS:HB2	2.21	0.41
2:D:235:GLN:O	2:D:236:ALA:C	2.59	0.41
3:E:169:GLU:OE1	3:E:192:ARG:NE	2.49	0.41
3:E:173:VAL:CG1	3:E:184:GLN:HE21	2.34	0.41
1:F:188:LEU:HG	1:F:197:LEU:CD2	2.49	0.41
1:F:233:LEU:HD23	1:F:325:GLU:HG3	2.02	0.41
2:G:243:THR:HG21	2:G:274:ARG:CD	2.44	0.41
3:J:236:LEU:O	3:J:237:ASN:C	2.58	0.41
2:C:15:PHE:CD1	2:C:57:LEU:HB3	2.55	0.40
2:C:29:ALA:O	2:C:33:SER:OG	2.27	0.40
2:C:302:LEU:HD13	2:C:310:GLU:HG3	2.02	0.40
2:D:160:GLN:C	2:D:162:LEU:N	2.74	0.40
2:D:297:LEU:O	2:D:297:LEU:HG	2.20	0.40
2:D:365:LEU:HB3	2:D:366:PRO:HD2	2.02	0.40
3:E:80:ALA:HA	3:E:115:THR:OG1	2.21	0.40
3:E:94:ARG:HH11	3:E:94:ARG:CB	2.33	0.40
3:E:230:TYR:O	3:E:230:TYR:HD1	2.04	0.40
2:G:11:ARG:O	2:G:12:PRO:C	2.59	0.40
2:H:213:SER:HG	2:H:216:ASP:HB2	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:309:ILE:O	2:H:311:LEU:N	2.54	0.40
1:A:55:ILE:HD11	1:A:82:LEU:HD23	2.02	0.40
1:A:163:ASP:O	1:A:167:ASN:N	2.54	0.40
1:A:297:GLN:HG2	1:A:335:PRO:HG3	2.02	0.40
2:B:338:GLU:O	2:B:339:LEU:C	2.60	0.40
2:C:43:PHE:CD1	2:C:173:PHE:HB2	2.56	0.40
2:C:100:LYS:CB	2:D:133:ARG:HE	2.33	0.40
2:D:15:PHE:CD2	2:D:57:LEU:HD13	2.48	0.40
2:D:21:GLN:CD	2:D:175:LEU:HG	2.41	0.40
2:D:310:GLU:O	2:D:311:LEU:C	2.58	0.40
3:E:73:HIS:HE1	3:E:106:LEU:CD2	2.34	0.40
1:F:232:ILE:O	1:F:236:LEU:N	2.50	0.40
2:G:6:LEU:CB	2:G:190:ILE:HG22	2.45	0.40
2:G:125:ILE:HD12	2:G:154:LEU:HD21	2.04	0.40
2:H:37:ILE:HG23	2:H:37:ILE:O	2.21	0.40
2:H:334:ILE:O	2:H:338:GLU:HG3	2.22	0.40
2:I:178:LEU:HD13	2:I:214:LEU:HD22	2.02	0.40
3:J:57:LYS:HD2	3:J:57:LYS:HA	1.91	0.40
3:J:158:ARG:HH11	3:J:158:ARG:HG3	1.86	0.40
1:A:91:ALA:HA	1:A:94:ASN:HD21	1.83	0.40
1:A:124:ALA:O	1:A:125:ALA:C	2.60	0.40
1:A:273:PHE:HB3	1:A:279:TRP:HB2	2.04	0.40
1:A:295:GLN:HA	1:A:298:LEU:HD22	2.04	0.40
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.88	0.40
2:B:144:GLU:C	2:B:146:PRO:HD3	2.42	0.40
2:B:257:VAL:C	2:B:259:ALA:N	2.74	0.40
2:C:9:LYS:HG2	2:C:9:LYS:O	2.21	0.40
2:C:73:CYS:O	2:C:79:CYS:SG	2.78	0.40
2:D:261:GLY:O	2:D:265:MET:HB2	2.21	0.40
2:D:332:LEU:O	2:D:333:LEU:C	2.58	0.40
3:E:8:ARG:H	3:E:9:PRO:CD	2.35	0.40
3:E:68:MSE:HE3	3:E:73:HIS:CG	2.55	0.40
1:F:105:HIS:CE1	1:F:108:LEU:HB3	2.56	0.40
1:F:211:HIS:O	1:F:211:HIS:ND1	2.55	0.40
2:G:135:SER:O	2:G:138:ALA:HB3	2.21	0.40
2:G:363:MET:N	2:G:364:PRO:CD	2.85	0.40
2:H:243:THR:CG2	2:H:284:GLU:HG3	2.50	0.40
3:J:35:MSE:HE1	3:J:167:PRO:CD	2.51	0.40
1:A:237:ARG:C	1:A:239:GLU:H	2.23	0.40
1:A:292:ARG:HD2	1:A:292:ARG:HA	1.66	0.40
1:A:318:GLN:O	1:A:318:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:THR:HG23	2:B:355:ARG:HG2	2.02	0.40
2:C:15:PHE:HE1	2:C:57:LEU:O	2.05	0.40
2:C:291:ARG:CG	2:C:291:ARG:HH11	2.34	0.40
2:D:186:GLN:O	2:D:187:LEU:C	2.59	0.40
2:D:237:VAL:O	2:D:238:SER:C	2.60	0.40
2:D:268:ILE:O	2:D:272:ALA:N	2.51	0.40
3:E:94:ARG:HH11	3:E:94:ARG:HB3	1.87	0.40
3:E:156:ARG:HE	3:E:156:ARG:HB3	1.46	0.40
3:E:222:TYR:CE1	3:E:226:SER:CB	3.04	0.40
3:E:237:ASN:HD22	3:E:237:ASN:C	2.25	0.40
3:E:238:HIS:CG	3:E:239:GLU:N	2.88	0.40
1:F:243:PRO:HG2	1:F:244:VAL:H	1.85	0.40
2:G:193:GLU:O	2:G:193:GLU:HG2	2.21	0.40
2:G:294:MET:C	2:G:296:GLN:N	2.74	0.40
2:G:320:ILE:HA	2:G:321:PRO:HD3	1.90	0.40
2:H:15:PHE:HD1	2:H:15:PHE:HA	1.76	0.40
2:H:88:VAL:HG11	2:H:116:ALA:CB	2.41	0.40
2:H:105:ARG:O	2:H:109:ASP:OD2	2.40	0.40
2:H:145:GLU:N	2:H:146:PRO:CD	2.84	0.40
2:H:255:ALA:CB	2:H:264:VAL:HG22	2.51	0.40
2:I:80:ARG:HG2	2:I:80:ARG:NH1	2.36	0.40
3:J:29:ILE:N	3:J:29:ILE:CD1	2.84	0.40
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.85	0.40
1:A:294:SER:O	1:A:295:GLN:C	2.60	0.40
2:B:143:LEU:CD1	2:B:169:ARG:HB2	2.51	0.40
2:B:265:MET:HG3	2:C:297:LEU:CD2	2.51	0.40
2:G:51:LYS:HG2	2:G:175:LEU:HD22	2.02	0.40
2:G:99:THR:CG2	2:H:145:GLU:HB2	2.51	0.40
2:G:234:THR:O	2:G:234:THR:HG22	2.22	0.40
2:H:261:GLY:O	2:H:264:VAL:N	2.51	0.40
2:H:366:PRO:O	2:H:367:GLU:HG2	2.22	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ASP:OD2	2:I:33:SER:O[1_455]	1.82	0.38
1:F:277:ARG:NH2	2:I:67:GLY:CA[1_455]	1.82	0.38
1:F:277:ARG:NE	2:I:66:THR:O[1_455]	1.87	0.33
1:F:277:ARG:CZ	2:I:67:GLY:CA[1_455]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:ARG:NH2	2:I:67:GLY:C[1_455]	2.10	0.10
1:F:277:ARG:NH2	2:I:67:GLY:N[1_455]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	336/343 (98%)	244 (73%)	70 (21%)	22 (6%)	1 12
1	F	336/343 (98%)	270 (80%)	47 (14%)	19 (6%)	1 15
2	B	362/373 (97%)	278 (77%)	62 (17%)	22 (6%)	1 13
2	C	364/373 (98%)	283 (78%)	54 (15%)	27 (7%)	1 10
2	D	362/373 (97%)	261 (72%)	77 (21%)	24 (7%)	1 12
2	G	362/373 (97%)	312 (86%)	39 (11%)	11 (3%)	4 29
2	H	364/373 (98%)	312 (86%)	44 (12%)	8 (2%)	6 35
2	I	362/373 (97%)	335 (92%)	18 (5%)	9 (2%)	5 32
3	E	332/334 (99%)	237 (71%)	68 (20%)	27 (8%)	1 9
3	J	332/334 (99%)	271 (82%)	50 (15%)	11 (3%)	4 27
All	All	3512/3592 (98%)	2803 (80%)	529 (15%)	180 (5%)	2 17

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
1	A	116	LYS
1	A	125	ALA
1	A	131	ALA
1	A	223	MSE
1	A	269	LEU
1	A	270	ARG

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Mol	Chain	Res	Type
1	A	279	TRP
1	A	282	ARG
1	A	290	LEU
1	A	316	TYR
2	B	245	ASP
2	B	246	ASP
2	B	278	TRP
2	B	279	GLU
2	B	299	PRO
2	B	304	ASN
2	B	310	GLU
2	B	363	MET
2	C	36	ARG
2	C	198	HIS
2	C	246	ASP
2	C	262	GLU
2	C	301	ALA
2	C	303	GLY
2	C	315	GLU
2	C	344	ASP
2	D	27	ALA
2	D	33	SER
2	D	261	GLY
2	D	278	TRP
2	D	359	PHE
3	E	62	CYS
3	E	117	ALA
3	E	137	ALA
3	E	206	GLN
3	E	303	VAL
3	E	304	THR
3	E	308	ARG
1	F	279	TRP
1	F	281	ASN
2	G	179	ASP
2	G	249	ALA
2	G	310	GLU
2	H	278	TRP
2	H	302	LEU
2	I	261	GLY
2	I	310	GLU
2	I	362	ARG

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Mol	Chain	Res	Type
3	J	62	CYS
3	J	137	ALA
3	J	304	THR
1	A	15	GLU
1	A	134	SER
1	A	178	LEU
1	A	236	LEU
2	B	20	GLY
2	B	242	GLY
2	B	243	THR
2	B	319	THR
2	C	4	GLN
2	C	20	GLY
2	C	50	GLY
2	C	207	ALA
2	C	237	VAL
2	C	316	LEU
2	D	25	LEU
2	D	28	LEU
2	D	190	ILE
2	D	212	GLY
2	D	227	SER
2	D	230	GLY
3	E	2	ARG
3	E	6	TRP
3	E	85	LYS
3	E	107	GLY
3	E	156	ARG
3	E	238	HIS
3	E	278	ALA
3	E	284	SER
1	F	132	ASN
1	F	210	ALA
1	F	269	LEU
1	F	282	ARG
1	F	316	TYR
1	F	335	PRO
2	G	275	GLY
2	H	275	GLY
3	J	103	HIS
3	J	107	GLY
3	J	206	GLN

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Mol	Chain	Res	Type
1	A	106	ASP
1	A	184	ALA
1	A	281	ASN
2	B	6	LEU
2	B	23	HIS
2	B	366	PRO
2	C	221	THR
2	C	261	GLY
2	C	293	ALA
2	C	333	LEU
2	D	16	ALA
2	D	46	THR
2	D	247	ASP
3	E	37	ASP
3	E	83	LYS
3	E	150	ARG
3	E	287	GLN
1	F	46	GLY
1	F	79	THR
1	F	108	LEU
1	F	131	ALA
1	F	143	GLU
1	F	221	LEU
1	F	270	ARG
2	G	46	THR
2	G	177	ALA
2	G	303	GLY
2	H	211	GLU
2	H	310	GLU
2	I	146	PRO
2	I	299	PRO
2	I	304	ASN
2	I	305	ASP
2	I	364	PRO
3	J	6	TRP
3	J	115	THR
1	A	46	GLY
1	A	90	ASN
2	B	22	GLU
2	B	247	ASP
2	B	286	LEU
2	C	127	GLU

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Mol	Chain	Res	Type
2	C	334	ILE
2	D	306	MET
3	E	38	ASP
1	F	319	SER
2	G	146	PRO
2	G	210	ALA
2	G	314	ARG
3	J	150	ARG
1	A	271	ALA
2	B	146	PRO
2	B	177	ALA
2	B	355	ARG
2	C	46	THR
2	C	239	ALA
2	C	264	VAL
2	C	292	ILE
2	C	343	PRO
2	D	276	ILE
2	D	289	LEU
2	D	300	ALA
2	D	362	ARG
2	D	363	MET
3	E	209	ASN
3	E	291	GLY
3	E	311	LEU
1	F	106	ASP
2	H	232	VAL
1	A	89	PRO
2	C	161	LYS
2	D	210	ALA
3	E	234	ALA
1	F	265	ALA
2	G	363	MET
2	H	20	GLY
2	D	101	VAL
2	H	366	PRO
3	J	136	PRO
2	D	146	PRO
3	E	282	SER
3	J	242	PRO
2	D	200	PRO
3	E	5	PRO

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Mol	Chain	Res	Type
3	E	283	PRO
1	F	224	GLY
2	B	128	VAL
2	C	31	GLY
2	I	20	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	287/286 (100%)	234 (82%)	53 (18%)	1 7
1	F	287/286 (100%)	260 (91%)	27 (9%)	8 33
2	B	301/310 (97%)	271 (90%)	30 (10%)	7 31
2	C	303/310 (98%)	263 (87%)	40 (13%)	4 19
2	D	301/310 (97%)	261 (87%)	40 (13%)	4 19
2	G	301/310 (97%)	274 (91%)	27 (9%)	9 35
2	H	303/310 (98%)	281 (93%)	22 (7%)	14 45
2	I	301/310 (97%)	283 (94%)	18 (6%)	19 51
3	E	270/264 (102%)	232 (86%)	38 (14%)	3 17
3	J	270/264 (102%)	245 (91%)	25 (9%)	9 34
All	All	2924/2960 (99%)	2604 (89%)	320 (11%)	6 27

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	10	ARG
1	A	40	GLN
1	A	54	SER
1	A	60	ASP
1	A	78	GLN
1	A	101	THR
1	A	103	LEU

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Mol	Chain	Res	Type
1	A	104	LEU
1	A	108	LEU
1	A	115	ASN
1	A	119	LYS
1	A	128	THR
1	A	143	GLU
1	A	160	LEU
1	A	162	LEU
1	A	163	ASP
1	A	164	ASP
1	A	174	TYR
1	A	178	LEU
1	A	187	ARG
1	A	188	LEU
1	A	189	SER
1	A	190	LEU
1	A	192	TRP
1	A	194	ASP
1	A	198	THR
1	A	207	ASN
1	A	208	ASP
1	A	215	PHE
1	A	216	HIS
1	A	219	ASP
1	A	228	ARG
1	A	234	GLN
1	A	236	LEU
1	A	242	GLU
1	A	256	LEU
1	A	266	HIS
1	A	268	PRO
1	A	279	TRP
1	A	280	GLN
1	A	292	ARG
1	A	298	LEU
1	A	305	LEU
1	A	313	LYS
1	A	316	TYR
1	A	318	GLN
1	A	320	VAL
1	A	327	LEU
1	A	328	SER

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Mol	Chain	Res	Type
1	A	330	LEU
1	A	331	LEU
1	A	336	LEU
2	B	8	ARG
2	B	11	ARG
2	B	36	ARG
2	B	66	THR
2	B	76	CYS
2	B	86	ARG
2	B	121	LYS
2	B	126	ASP
2	B	140	LEU
2	B	143	LEU
2	B	158	ASP
2	B	191	LEU
2	B	215	ARG
2	B	251	SER
2	B	257	VAL
2	B	262	GLU
2	B	276	ILE
2	B	279	GLU
2	B	284	GLU
2	B	289	LEU
2	B	291	ARG
2	B	305	ASP
2	B	325	ILE
2	B	327	LEU
2	B	332	LEU
2	B	334	ILE
2	B	344	ASP
2	B	352	THR
2	B	365	LEU
2	B	367	GLU
2	C	3	TYR
2	C	12	PRO
2	C	15	PHE
2	C	69	THR
2	C	76	CYS
2	C	103	ASP
2	C	105	ARG
2	C	120	PHE
2	C	130	MET

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Mol	Chain	Res	Type
2	C	134	HIS
2	C	140	LEU
2	C	145	GLU
2	C	146	PRO
2	C	148	GLU
2	C	182	GLN
2	C	193	GLU
2	C	208	ARG
2	C	215	ARG
2	C	219	SER
2	C	232	VAL
2	C	234	THR
2	C	248	GLN
2	C	252	LEU
2	C	260	ASN
2	C	263	ARG
2	C	268	ILE
2	C	276	ILE
2	C	289	LEU
2	C	291	ARG
2	C	294	MET
2	C	298	SER
2	C	302	LEU
2	C	318	ARG
2	C	323	THR
2	C	324	ASP
2	C	336	ARG
2	C	338	GLU
2	C	352	THR
2	C	366	PRO
2	C	367	GLU
2	D	8	ARG
2	D	12	PRO
2	D	13	GLN
2	D	21	GLN
2	D	42	LEU
2	D	66	THR
2	D	72	PRO
2	D	110	ASN
2	D	124	LEU
2	D	134	HIS
2	D	136	PHE

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Mol	Chain	Res	Type
2	D	140	LEU
2	D	142	THR
2	D	148	GLU
2	D	168	SER
2	D	169	ARG
2	D	184	ARG
2	D	193	GLU
2	D	200	PRO
2	D	201	ARG
2	D	213	SER
2	D	219	SER
2	D	229	ASP
2	D	231	GLN
2	D	233	SER
2	D	251	SER
2	D	252	LEU
2	D	263	ARG
2	D	270	GLU
2	D	276	ILE
2	D	277	GLU
2	D	281	LEU
2	D	309	ILE
2	D	311	LEU
2	D	327	LEU
2	D	333	LEU
2	D	337	LYS
2	D	345	ARG
2	D	346	ARG
2	D	363	MET
3	E	22	ARG
3	E	30	GLN
3	E	37	ASP
3	E	46	ARG
3	E	69	GLN
3	E	91	ASP
3	E	93	VAL
3	E	94	ARG
3	E	98	GLU
3	E	110	LYS
3	E	120	LEU
3	E	143	LEU
3	E	152	LEU

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Mol	Chain	Res	Type
3	E	154	THR
3	E	155	LEU
3	E	158	ARG
3	E	161	LEU
3	E	170	GLN
3	E	175	TRP
3	E	181	THR
3	E	182	MSE
3	E	202	LEU
3	E	222	TYR
3	E	233	LEU
3	E	237	ASN
3	E	239	GLU
3	E	240	GLN
3	E	245	LEU
3	E	252	LEU
3	E	253	MSE
3	E	259	HIS
3	E	269	ASP
3	E	290	LEU
3	E	304	THR
3	E	306	ILE
3	E	310	LEU
3	E	311	LEU
3	E	332	PRO
1	F	33	GLU
1	F	40	GLN
1	F	48	GLU
1	F	80	LEU
1	F	100	LEU
1	F	108	LEU
1	F	115	ASN
1	F	119	LYS
1	F	144	GLN
1	F	158	LEU
1	F	168	GLN
1	F	194	ASP
1	F	198	THR
1	F	208	ASP
1	F	211	HIS
1	F	215	PHE
1	F	250	LEU

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Mol	Chain	Res	Type
1	F	266	HIS
1	F	279	TRP
1	F	282	ARG
1	F	292	ARG
1	F	295	GLN
1	F	298	LEU
1	F	305	LEU
1	F	307	ARG
1	F	316	TYR
1	F	330	LEU
2	G	11	ARG
2	G	12	PRO
2	G	13	GLN
2	G	39	HIS
2	G	66	THR
2	G	76	CYS
2	G	79	CYS
2	G	84	GLN
2	G	86	ARG
2	G	109	ASP
2	G	121	LYS
2	G	134	HIS
2	G	140	LEU
2	G	145	GLU
2	G	176	LYS
2	G	182	GLN
2	G	215	ARG
2	G	240	MET
2	G	289	LEU
2	G	296	GLN
2	G	297	LEU
2	G	326	GLN
2	G	330	GLN
2	G	338	GLU
2	G	351	MET
2	G	355	ARG
2	G	367	GLU
2	H	3	TYR
2	H	4	GLN
2	H	15	PHE
2	H	34	LEU
2	H	47	ARG

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Mol	Chain	Res	Type
2	H	69	THR
2	H	76	CYS
2	H	99	THR
2	H	130	MET
2	H	144	GLU
2	H	145	GLU
2	H	158	ASP
2	H	181	GLU
2	H	184	ARG
2	H	193	GLU
2	H	201	ARG
2	H	218	LEU
2	H	234	THR
2	H	276	ILE
2	H	279	GLU
2	H	326	GLN
2	H	327	LEU
2	I	11	ARG
2	I	13	GLN
2	I	36	ARG
2	I	42	LEU
2	I	66	THR
2	I	101	VAL
2	I	140	LEU
2	I	145	GLU
2	I	148	GLU
2	I	201	ARG
2	I	214	LEU
2	I	240	MET
2	I	247	ASP
2	I	260	ASN
2	I	337	LYS
2	I	345	ARG
2	I	357	LEU
2	I	363	MET
3	J	3	TRP
3	J	35	MSE
3	J	62	CYS
3	J	65	CYS
3	J	68	MSE
3	J	91	ASP
3	J	105	ARG

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Mol	Chain	Res	Type
3	J	110	LYS
3	J	120	LEU
3	J	122	ASP
3	J	149	GLU
3	J	154	THR
3	J	175	TRP
3	J	185	ASP
3	J	202	LEU
3	J	216	LEU
3	J	220	LEU
3	J	245	LEU
3	J	252	LEU
3	J	256	LEU
3	J	285	ARG
3	J	292	ASP
3	J	296	ILE
3	J	317	LEU
3	J	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	58	ASN
1	A	105	HIS
1	A	157	GLN
1	A	183	GLN
1	A	207	ASN
1	A	211	HIS
1	A	251	GLN
1	A	266	HIS
1	A	297	GLN
2	B	13	GLN
2	B	30	ASN
2	B	38	HIS
2	B	112	GLN
2	B	160	GLN
2	B	172	GLN
2	B	182	GLN
2	B	186	GLN
2	B	198	HIS
2	B	260	ASN

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Mol	Chain	Res	Type
2	B	326	GLN
2	B	360	HIS
2	C	84	GLN
2	C	198	HIS
2	C	223	GLN
2	C	235	GLN
2	C	260	ASN
2	C	304	ASN
2	C	360	HIS
2	D	13	GLN
2	D	21	GLN
2	D	30	ASN
2	D	38	HIS
2	D	110	ASN
2	D	129	HIS
2	D	198	HIS
2	D	231	GLN
2	D	248	GLN
2	D	296	GLN
2	D	360	HIS
3	E	19	GLN
3	E	24	HIS
3	E	69	GLN
3	E	101	ASN
3	E	184	GLN
3	E	209	ASN
3	E	218	GLN
3	E	237	ASN
3	E	307	ASN
3	E	321	HIS
1	F	40	GLN
1	F	51	HIS
1	F	96	GLN
1	F	105	HIS
1	F	140	GLN
1	F	168	GLN
1	F	183	GLN
1	F	216	HIS
1	F	231	HIS
1	F	235	GLN
1	F	333	HIS
2	G	13	GLN

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Mol	Chain	Res	Type
2	G	21	GLN
2	G	30	ASN
2	G	137	ASN
2	G	172	GLN
2	G	182	GLN
2	G	192	ASN
2	G	198	HIS
2	G	223	GLN
2	G	260	ASN
2	G	326	GLN
2	G	360	HIS
2	H	110	ASN
2	H	129	HIS
2	H	174	HIS
2	H	182	GLN
2	H	192	ASN
2	H	198	HIS
2	H	204	GLN
2	H	223	GLN
2	H	326	GLN
2	H	360	HIS
2	I	21	GLN
2	I	160	GLN
2	I	198	HIS
2	I	204	GLN
2	I	223	GLN
2	I	326	GLN
2	I	360	HIS
3	J	19	GLN
3	J	24	HIS
3	J	73	HIS
3	J	101	ASN
3	J	218	GLN
3	J	260	HIS
3	J	299	GLN
3	J	307	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PO4	C	1300	-	4,4,4	1.42	1 (25%)	6,6,6	0.90	0
6	PO4	H	1400	-	4,4,4	0.40	0	6,6,6	0.38	0
5	AGS	I	803	-	28,33,33	2.02	4 (14%)	31,52,52	1.28	2 (6%)
5	AGS	D	801	-	28,33,33	2.01	4 (14%)	31,52,52	1.28	2 (6%)
5	AGS	G	804	-	28,33,33	2.02	4 (14%)	31,52,52	1.28	2 (6%)
5	AGS	B	802	-	28,33,33	2.01	4 (14%)	31,52,52	1.28	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	G	804	-	-	5/17/38/38	0/3/3/3
5	AGS	B	802	-	-	5/17/38/38	0/3/3/3
5	AGS	D	801	-	-	5/17/38/38	0/3/3/3
5	AGS	I	803	-	-	5/17/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	803	AGS	PG-S1G	-8.39	1.72	1.90
5	D	801	AGS	PG-S1G	-8.39	1.72	1.90
5	G	804	AGS	PG-S1G	-8.39	1.72	1.90
5	B	802	AGS	PG-S1G	-8.36	1.72	1.90
5	G	804	AGS	C2-N3	3.27	1.37	1.32
5	D	801	AGS	C2-N3	3.26	1.37	1.32
5	I	803	AGS	C2-N3	3.24	1.37	1.32
5	B	802	AGS	C2-N3	3.22	1.37	1.32
5	I	803	AGS	O4'-C1'	2.98	1.44	1.40
5	D	801	AGS	O4'-C1'	2.97	1.44	1.40
5	G	804	AGS	O4'-C1'	2.96	1.44	1.40
5	B	802	AGS	O4'-C1'	2.92	1.44	1.40
6	C	1300	PO4	P-O1	2.45	1.56	1.50
5	D	801	AGS	C2-N1	2.28	1.38	1.33
5	B	802	AGS	C2-N1	2.27	1.38	1.33
5	G	804	AGS	C2-N1	2.27	1.38	1.33
5	I	803	AGS	C2-N1	2.21	1.37	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	803	AGS	C1'-N9-C4	4.67	134.84	126.64
5	G	804	AGS	C1'-N9-C4	4.65	134.82	126.64
5	B	802	AGS	C1'-N9-C4	4.64	134.80	126.64
5	D	801	AGS	C1'-N9-C4	4.63	134.78	126.64
5	B	802	AGS	O3G-PG-O3B	2.34	112.46	104.64
5	I	803	AGS	O3G-PG-O3B	2.33	112.42	104.64
5	D	801	AGS	O3G-PG-O3B	2.33	112.42	104.64
5	G	804	AGS	O3G-PG-O3B	2.32	112.39	104.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	802	AGS	C5'-O5'-PA-O2A
5	B	802	AGS	C5'-O5'-PA-O3A
5	D	801	AGS	C5'-O5'-PA-O2A
5	D	801	AGS	C5'-O5'-PA-O3A
5	G	804	AGS	C5'-O5'-PA-O2A
5	G	804	AGS	C5'-O5'-PA-O3A
5	I	803	AGS	C5'-O5'-PA-O2A
5	I	803	AGS	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	B	802	AGS	PA-O3A-PB-O2B
5	D	801	AGS	PA-O3A-PB-O2B
5	G	804	AGS	PA-O3A-PB-O2B
5	I	803	AGS	PA-O3A-PB-O2B
5	B	802	AGS	C5'-O5'-PA-O1A
5	D	801	AGS	C5'-O5'-PA-O1A
5	G	804	AGS	C5'-O5'-PA-O1A
5	I	803	AGS	C5'-O5'-PA-O1A
5	B	802	AGS	PA-O3A-PB-O1B
5	D	801	AGS	PA-O3A-PB-O1B
5	G	804	AGS	PA-O3A-PB-O1B
5	I	803	AGS	PA-O3A-PB-O1B

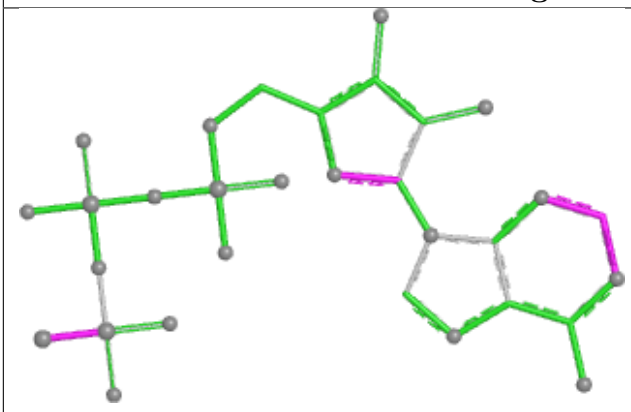
There are no ring outliers.

6 monomers are involved in 44 short contacts:

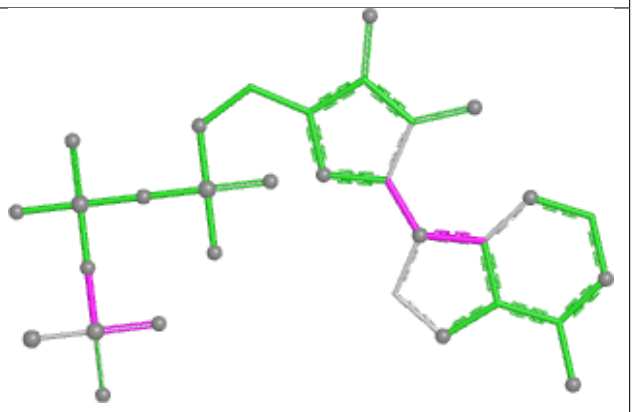
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1300	PO4	3	0
6	H	1400	PO4	4	0
5	I	803	AGS	27	0
5	D	801	AGS	4	0
5	G	804	AGS	2	0
5	B	802	AGS	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

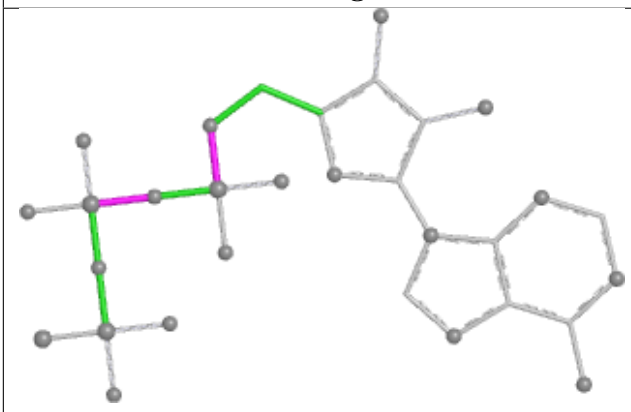
Ligand AGS I 803



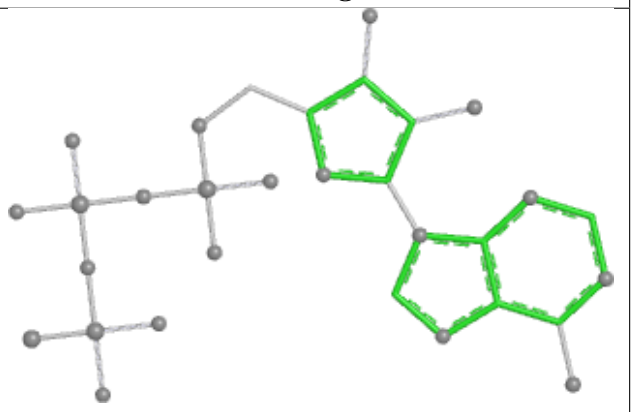
Bond lengths



Bond angles

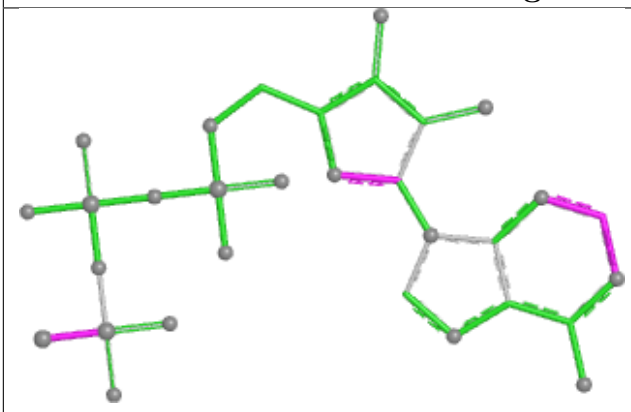


Torsions

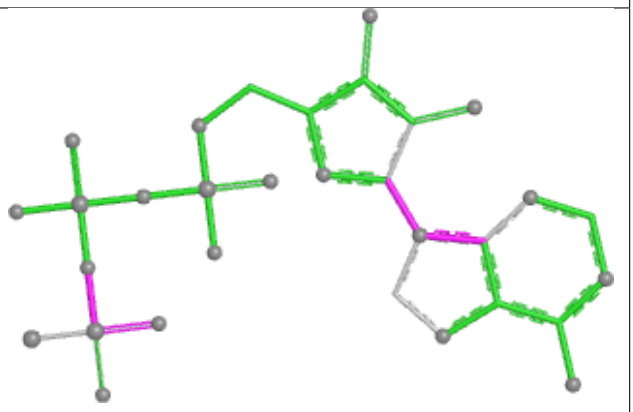


Rings

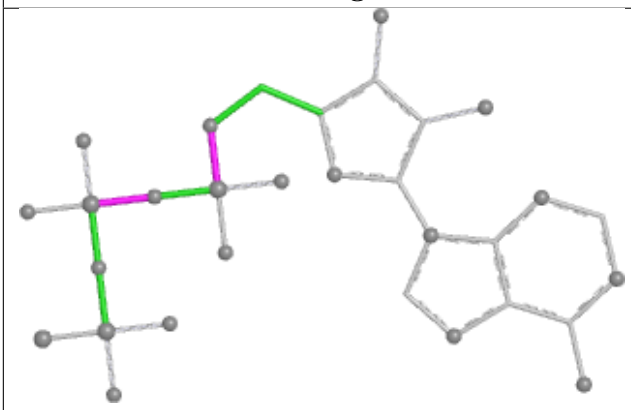
Ligand AGS D 801



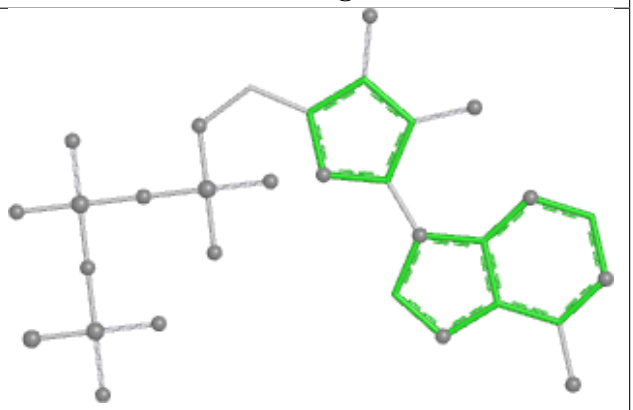
Bond lengths



Bond angles

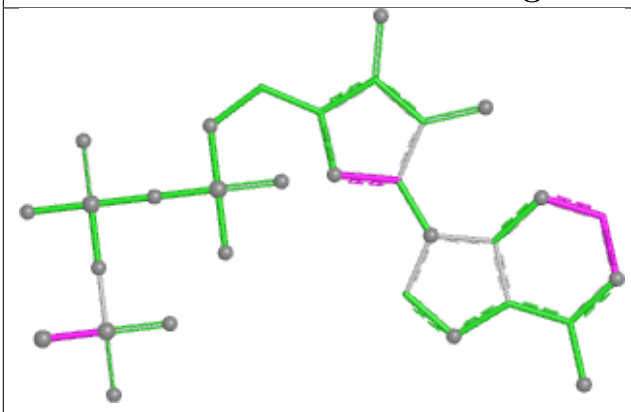


Torsions

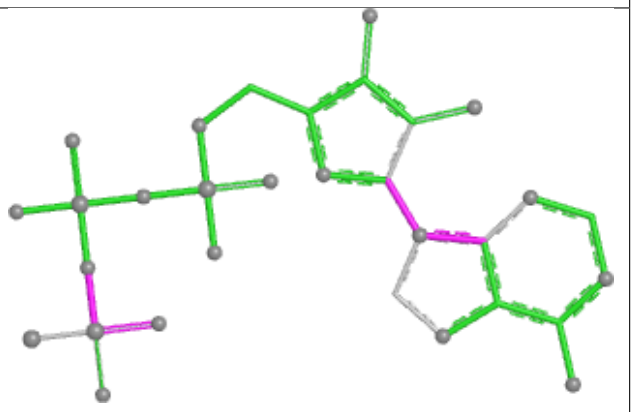


Rings

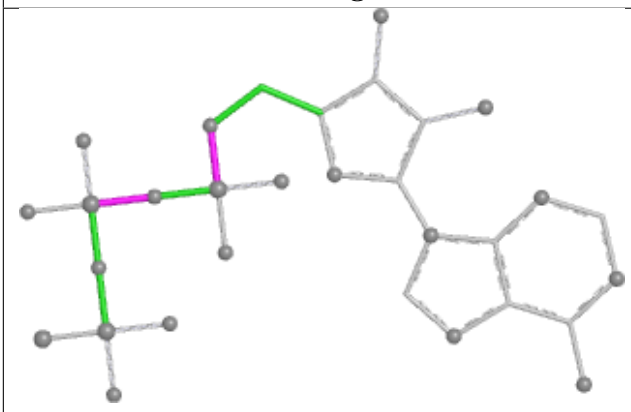
Ligand AGS G 804



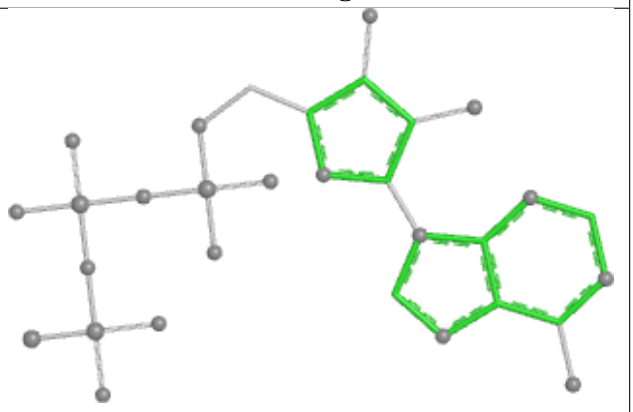
Bond lengths



Bond angles

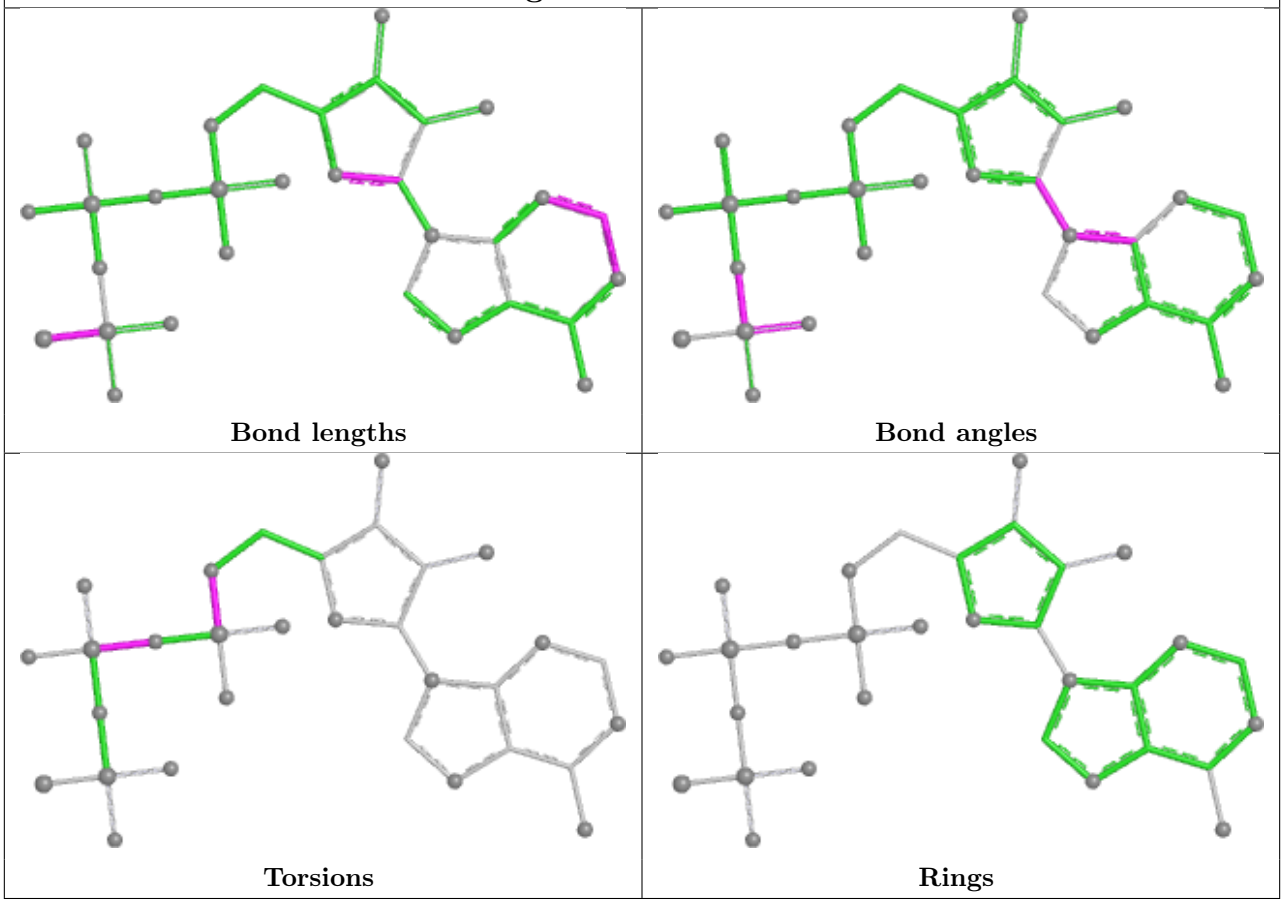


Torsions



Rings

Ligand AGS B 802



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	285:MSE	C	286:MSE	N	1.06

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	333/343 (97%)	0.73	42 (12%) 3 5	25, 164, 218, 268	0
1	F	333/343 (97%)	0.94	73 (21%) 0 1	107, 191, 234, 262	0
2	B	364/373 (97%)	0.78	48 (13%) 3 5	21, 146, 212, 262	0
2	C	366/373 (98%)	0.60	30 (8%) 11 14	15, 78, 194, 216	0
2	D	364/373 (97%)	0.74	26 (7%) 16 18	27, 71, 187, 248	0
2	G	364/373 (97%)	1.90	134 (36%) 0 0	131, 213, 247, 284	0
2	H	366/373 (98%)	1.67	134 (36%) 0 0	142, 205, 246, 278	0
2	I	364/373 (97%)	1.73	133 (36%) 0 0	121, 210, 286, 390	0
3	E	328/334 (98%)	0.45	10 (3%) 50 48	39, 90, 175, 206	0
3	J	328/334 (98%)	1.03	78 (23%) 0 0	121, 190, 229, 269	0
All	All	3510/3592 (97%)	1.07	708 (20%) 1 1	15, 174, 240, 390	0

All (708) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	366	PRO	22.0
2	H	152	PHE	18.7
2	D	368	PRO	16.9
2	H	41	TYR	13.4
2	D	366	PRO	12.0
2	G	59	ALA	11.9
2	G	15	PHE	10.9
2	G	28	LEU	10.9
2	G	124	LEU	10.6
3	J	76	TYR	10.6
2	I	367	GLU	10.5
2	G	92	GLU	10.4
2	I	108	LEU	10.1

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Mol	Chain	Res	Type	RSRZ
2	G	57	LEU	10.0
2	G	58	LEU	10.0
2	G	152	PHE	9.7
2	G	62	LEU	9.7
2	H	15	PHE	9.7
2	G	6	LEU	9.6
2	I	241	LEU	9.5
3	J	18	TYR	9.1
2	G	56	ARG	9.0
2	I	365	LEU	9.0
2	G	177	ALA	8.9
2	H	28	LEU	8.9
2	I	43	PHE	8.9
2	G	206	LEU	8.8
2	H	40	ALA	8.8
2	H	55	ALA	8.8
2	G	41	TYR	8.6
2	H	131	LEU	8.6
2	I	41	TYR	8.3
2	G	153	LEU	8.2
2	I	128	VAL	8.0
2	B	152	PHE	7.8
2	I	154	LEU	7.7
2	G	37	ILE	7.7
2	G	54	ILE	7.6
2	G	55	ALA	7.6
2	G	186	GLN	7.6
2	B	90	LEU	7.6
2	G	19	VAL	7.6
3	J	79	LEU	7.6
2	H	123	TYR	7.5
2	I	7	ALA	7.4
2	G	85	GLY	7.4
2	G	357	LEU	7.4
2	I	171	LEU	7.4
2	B	151	LYS	7.3
2	H	43	PHE	7.3
3	J	142	PHE	7.3
2	H	124	LEU	7.3
2	G	203	LEU	7.3
2	H	54	ILE	7.3
2	H	153	LEU	7.2

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Mol	Chain	Res	Type	RSRZ
2	G	93	ILE	7.1
2	H	128	VAL	7.0
3	J	109	ALA	7.0
2	H	58	LEU	7.0
2	G	166	ILE	6.9
2	I	100	LYS	6.9
2	I	19	VAL	6.8
2	H	104	THR	6.8
2	B	108	LEU	6.8
2	D	367	GLU	6.8
2	H	175	LEU	6.7
2	I	28	LEU	6.7
2	G	24	VAL	6.6
2	G	154	LEU	6.6
2	H	159	PRO	6.6
2	G	173	PHE	6.6
2	I	153	LEU	6.5
2	H	10	TRP	6.5
2	I	183	ILE	6.5
2	I	232	VAL	6.4
2	B	104	THR	6.4
2	G	178	LEU	6.3
2	H	154	LEU	6.3
2	I	364	PRO	6.3
3	J	143	LEU	6.2
2	G	104	THR	6.2
2	H	37	ILE	6.2
1	F	109	LEU	6.1
2	I	359	PHE	6.1
2	H	39	HIS	6.1
2	I	180	VAL	6.1
2	C	152	PHE	6.1
2	G	21	GLN	6.0
2	I	113	TYR	6.0
2	G	125	ILE	6.0
1	F	89	PRO	6.0
2	I	93	ILE	6.0
2	I	178	LEU	5.8
3	J	334	LEU	5.8
2	H	108	LEU	5.8
2	H	34	LEU	5.7
2	G	128	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
2	H	172	GLN	5.7
2	H	171	LEU	5.7
1	A	82	LEU	5.7
3	J	164	LEU	5.6
1	A	78	GLN	5.5
2	B	122	VAL	5.5
2	D	364	PRO	5.5
2	G	194	GLU	5.5
2	G	304	ASN	5.5
2	G	187	LEU	5.5
2	I	221	THR	5.5
2	I	313	MET	5.5
2	I	112	GLN	5.4
1	A	174	TYR	5.4
2	I	218	LEU	5.4
1	F	126	TRP	5.4
2	G	229	ASP	5.4
2	I	173	PHE	5.4
3	J	154	THR	5.3
3	J	106	LEU	5.3
2	G	96	ALA	5.2
2	H	125	ILE	5.2
1	F	117	LEU	5.2
1	A	80	LEU	5.2
2	G	25	LEU	5.2
2	G	47	ARG	5.2
2	H	42	LEU	5.2
1	F	188	LEU	5.2
2	H	161	LYS	5.1
1	A	109	LEU	5.1
2	B	41	TYR	5.1
2	B	62	LEU	5.1
2	G	70	ALA	5.1
2	H	151	LYS	5.0
2	I	187	LEU	5.0
2	H	107	LEU	5.0
2	I	72	PRO	5.0
2	I	252	LEU	5.0
2	G	108	LEU	5.0
1	F	74	PHE	4.9
2	G	237	VAL	4.9
2	H	21	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
3	J	27	LEU	4.9
2	H	187	LEU	4.9
2	H	18	VAL	4.9
1	A	150	TRP	4.9
2	I	159	PRO	4.9
2	H	52	THR	4.8
2	G	190	ILE	4.8
2	G	212	GLY	4.8
2	I	124	LEU	4.8
2	I	44	SER	4.8
2	H	173	PHE	4.8
2	I	12	PRO	4.8
1	F	130	LEU	4.8
2	G	130	MET	4.8
2	G	18	VAL	4.8
2	I	161	LYS	4.7
2	B	82	ILE	4.7
2	H	25	LEU	4.7
1	F	110	LEU	4.7
2	B	123	TYR	4.7
2	I	289	LEU	4.6
2	B	54	ILE	4.6
2	G	209	ALA	4.6
2	I	155	ALA	4.6
2	B	124	LEU	4.6
3	J	113	TRP	4.6
2	I	297	LEU	4.6
2	G	175	LEU	4.6
2	H	356	ALA	4.5
2	I	368	PRO	4.5
2	G	328	TYR	4.5
2	B	93	ILE	4.5
2	B	60	LYS	4.5
2	H	139	LEU	4.5
1	F	22	LEU	4.5
2	I	91	ILE	4.5
2	G	10	TRP	4.5
1	A	17	LEU	4.5
2	G	294	MET	4.4
2	G	244	LEU	4.4
3	J	111	VAL	4.4
2	B	43	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
2	H	93	ILE	4.4
3	J	14	LEU	4.4
2	I	156	THR	4.4
1	A	110	LEU	4.4
2	I	42	LEU	4.4
3	J	80	ALA	4.4
2	G	86	ARG	4.3
2	C	62	LEU	4.3
1	F	111	ILE	4.3
2	I	203	LEU	4.3
2	I	302	LEU	4.3
3	J	26	ALA	4.3
2	H	100	LYS	4.3
2	H	313	MET	4.3
2	C	123	TYR	4.3
2	H	143	LEU	4.3
2	H	59	ALA	4.3
2	C	41	TYR	4.2
2	G	82	ILE	4.2
2	H	35	GLY	4.2
2	G	241	LEU	4.2
2	B	150	VAL	4.2
2	H	297	LEU	4.2
2	H	122	VAL	4.2
2	H	86	ARG	4.2
1	F	84	LEU	4.2
2	G	353	LEU	4.2
3	J	193	LEU	4.2
1	F	239	GLU	4.2
1	A	108	LEU	4.1
2	I	358	ALA	4.1
2	H	349	VAL	4.1
1	F	82	LEU	4.1
2	I	162	LEU	4.1
2	H	170	CYS	4.1
2	G	88	VAL	4.1
2	H	6	LEU	4.1
3	J	141	PHE	4.1
2	G	32	LEU	4.1
2	G	40	ALA	4.1
3	J	40	LEU	4.1
2	H	165	THR	4.1

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Mol	Chain	Res	Type	RSRZ
2	C	124	LEU	4.1
2	G	302	LEU	4.1
3	J	41	ILE	4.1
2	H	32	LEU	4.0
2	C	122	VAL	4.0
2	C	32	LEU	4.0
3	J	161	LEU	4.0
1	F	2	ILE	4.0
2	H	16	ALA	4.0
2	I	6	LEU	4.0
2	H	24	VAL	4.0
2	B	58	LEU	4.0
1	F	137	VAL	4.0
1	F	217	TRP	4.0
1	A	158	LEU	4.0
2	I	149	HIS	4.0
2	H	174	HIS	4.0
2	I	243	THR	4.0
2	G	98	ARG	3.9
2	G	170	CYS	3.9
1	A	89	PRO	3.9
2	G	171	LEU	3.9
2	H	178	LEU	3.9
2	I	111	VAL	3.9
1	F	185	LEU	3.9
2	G	91	ILE	3.9
2	I	152	PHE	3.9
1	A	166	ALA	3.9
3	J	311	LEU	3.9
1	A	160	LEU	3.9
2	G	123	TYR	3.9
2	G	39	HIS	3.9
2	C	90	LEU	3.8
2	H	162	LEU	3.8
2	G	20	GLY	3.8
2	H	214	LEU	3.8
2	G	165	THR	3.8
2	I	82	ILE	3.8
2	I	101	VAL	3.8
2	G	84	GLN	3.8
3	J	256	LEU	3.8
2	H	150	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	133	ARG	3.8
2	I	214	LEU	3.8
2	D	152	PHE	3.8
3	J	126	ASN	3.8
2	G	118	GLY	3.7
2	I	61	GLY	3.7
2	I	166	ILE	3.7
2	H	29	ALA	3.7
2	I	186	GLN	3.7
3	J	48	LEU	3.7
2	C	92	GLU	3.7
2	B	89	ASP	3.7
3	J	37	ASP	3.7
2	B	244	LEU	3.7
1	A	64	ILE	3.7
1	A	112	VAL	3.7
2	H	56	ARG	3.7
3	J	155	LEU	3.7
3	J	252	LEU	3.7
2	G	292	ILE	3.7
2	I	225	ILE	3.7
1	F	283	ARG	3.7
1	A	151	VAL	3.7
2	B	113	TYR	3.7
2	I	242	GLY	3.6
2	G	368	PRO	3.6
2	D	123	TYR	3.6
2	H	206	LEU	3.6
2	C	91	ILE	3.6
2	I	15	PHE	3.6
2	C	170	CYS	3.6
2	G	349	VAL	3.6
2	I	197	ALA	3.6
3	E	109	ALA	3.6
2	B	154	LEU	3.6
2	H	120	PHE	3.6
2	G	90	LEU	3.6
2	G	189	HIS	3.6
1	F	147	LEU	3.6
2	H	243	THR	3.6
1	F	34	SER	3.6
2	D	154	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	I	237	VAL	3.6
2	G	354	LEU	3.5
3	J	118	ALA	3.5
3	J	75	ASP	3.5
1	F	108	LEU	3.5
2	G	43	PHE	3.5
2	B	56	ARG	3.5
2	B	159	PRO	3.5
2	H	244	LEU	3.5
2	H	256	MET	3.5
3	E	14	LEU	3.5
2	I	220	LEU	3.5
2	I	125	ILE	3.5
2	I	238	SER	3.5
2	G	139	LEU	3.5
2	I	47	ARG	3.5
3	J	56	HIS	3.5
2	H	136	PHE	3.5
2	H	227	SER	3.5
2	I	10	TRP	3.5
2	B	125	ILE	3.5
2	B	92	GLU	3.5
3	J	44	LEU	3.5
1	A	53	PHE	3.5
2	H	357	LEU	3.4
2	I	316	LEU	3.4
2	H	62	LEU	3.4
2	I	165	THR	3.4
2	G	60	LYS	3.4
3	J	322	TYR	3.4
2	B	153	LEU	3.4
2	C	63	ASN	3.4
2	G	63	ASN	3.4
1	A	97	LEU	3.4
2	I	219	SER	3.4
2	D	136	PHE	3.4
1	F	284	GLY	3.4
2	H	95	ALA	3.4
2	I	206	LEU	3.3
3	J	248	LEU	3.3
2	I	209	ALA	3.3
2	G	285	MET	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	353	LEU	3.3
2	I	151	LYS	3.3
1	F	331	LEU	3.3
2	G	131	LEU	3.3
2	H	183	ILE	3.3
3	J	29	ILE	3.3
2	G	240	MET	3.3
2	D	359	PHE	3.3
2	H	83	GLU	3.3
1	F	150	TRP	3.3
1	F	21	TYR	3.3
2	G	205	LEU	3.3
2	I	139	LEU	3.3
2	B	131	LEU	3.3
2	H	44	SER	3.2
2	G	12	PRO	3.2
2	I	231	GLN	3.2
2	G	120	PHE	3.2
2	H	68	ILE	3.2
1	F	23	LEU	3.2
2	G	174	HIS	3.2
2	H	292	ILE	3.2
2	I	353	LEU	3.2
1	A	278	VAL	3.2
2	B	173	PHE	3.2
2	I	60	LYS	3.2
2	G	193	GLU	3.2
2	I	256	MET	3.2
1	F	80	LEU	3.2
2	B	15	PHE	3.2
3	J	163	TYR	3.2
3	J	216	LEU	3.2
2	G	256	MET	3.2
2	H	289	LEU	3.1
1	F	257	LEU	3.1
1	F	269	LEU	3.1
2	H	160	GLN	3.1
2	H	149	HIS	3.1
2	I	143	LEU	3.1
1	F	69	GLN	3.1
2	I	175	LEU	3.1
2	D	6	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	62	LEU	3.1
2	C	93	ILE	3.1
2	I	56	ARG	3.1
2	G	289	LEU	3.1
2	I	102	GLU	3.1
2	G	332	LEU	3.1
2	G	196	ILE	3.1
2	I	68	ILE	3.1
2	H	103	ASP	3.1
2	G	365	LEU	3.1
3	J	159	CYS	3.1
2	I	170	CYS	3.1
3	J	3	TRP	3.1
1	F	112	VAL	3.0
1	A	170	LEU	3.0
1	A	126	TRP	3.0
1	F	170	LEU	3.0
2	B	166	ILE	3.0
3	J	289	ILE	3.0
1	A	21	TYR	3.0
2	C	85	GLY	3.0
2	G	117	ARG	3.0
1	F	221	LEU	3.0
3	J	78	THR	3.0
3	J	82	GLU	3.0
1	F	133	ARG	3.0
1	F	338	ASP	3.0
2	C	154	LEU	3.0
1	F	277	ARG	3.0
2	D	93	ILE	3.0
2	C	128	VAL	3.0
2	H	268	ILE	3.0
1	A	211	HIS	2.9
2	H	51	LYS	2.9
2	I	39	HIS	2.9
2	C	108	LEU	2.9
2	I	169	ARG	2.9
2	G	150	VAL	2.9
2	H	134	HIS	2.9
2	H	135	SER	2.9
2	H	276	ILE	2.9
2	I	109	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
3	J	330	PRO	2.9
2	G	167	LEU	2.9
2	H	129	HIS	2.9
2	C	153	LEU	2.9
2	I	253	VAL	2.9
2	H	328	TYR	2.9
2	D	82	ILE	2.9
2	I	196	ILE	2.9
2	I	234	THR	2.9
1	A	181	LEU	2.9
1	F	247	LEU	2.9
2	C	125	ILE	2.8
2	G	313	MET	2.8
2	H	212	GLY	2.8
2	H	325	ILE	2.8
2	C	171	LEU	2.8
2	B	139	LEU	2.8
2	B	91	ILE	2.8
2	I	205	LEU	2.8
2	H	85	GLY	2.8
2	B	59	ALA	2.8
2	G	356	ALA	2.8
2	H	155	ALA	2.8
3	J	195	ALA	2.8
2	G	352	THR	2.8
1	F	100	LEU	2.8
1	F	29	LEU	2.8
2	I	163	PRO	2.8
1	A	197	LEU	2.7
2	D	302	LEU	2.7
2	I	202	ALA	2.7
2	H	60	LYS	2.7
1	F	298	LEU	2.7
2	H	70	ALA	2.7
2	H	320	ILE	2.7
1	F	97	LEU	2.7
3	J	187	LEU	2.7
2	G	329	TYR	2.7
3	J	114	VAL	2.7
2	D	140	LEU	2.7
2	H	281	LEU	2.7
3	E	7	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	147	PRO	2.7
2	I	306	MET	2.7
3	J	108	GLY	2.7
1	A	247	LEU	2.7
2	I	265	MET	2.7
1	F	189	SER	2.7
2	I	123	TYR	2.7
2	H	36	ARG	2.7
2	I	36	ARG	2.7
2	C	7	ALA	2.7
3	J	43	ALA	2.7
3	J	10	ASP	2.6
2	H	352	THR	2.6
2	B	180	VAL	2.6
2	G	176	LYS	2.6
2	G	207	ALA	2.6
2	I	90	LEU	2.6
2	I	268	ILE	2.6
1	F	38	VAL	2.6
2	B	111	VAL	2.6
2	I	66	THR	2.6
1	F	20	ALA	2.6
1	F	70	ALA	2.6
3	J	49	LEU	2.6
1	A	239	GLU	2.6
2	H	208	ARG	2.6
2	C	104	THR	2.6
2	H	38	HIS	2.6
2	G	172	GLN	2.6
1	F	78	GLN	2.6
2	I	172	GLN	2.6
2	H	241	LEU	2.6
1	F	127	PHE	2.6
2	H	50	GLY	2.6
1	A	111	ILE	2.6
2	I	354	LEU	2.6
3	J	329	LEU	2.6
1	A	34	SER	2.6
2	H	126	ASP	2.6
3	J	36	GLY	2.6
1	F	197	LEU	2.6
2	H	278	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	128	VAL	2.5
2	G	252	LEU	2.5
3	J	110	LYS	2.5
2	G	122	VAL	2.5
2	D	121	LYS	2.5
2	I	267	LEU	2.5
2	G	72	PRO	2.5
2	H	322	PRO	2.5
3	J	156	ARG	2.5
2	G	188	GLU	2.5
3	J	153	ALA	2.5
2	I	325	ILE	2.5
3	J	150	ARG	2.5
2	C	39	HIS	2.5
2	G	331	THR	2.5
3	J	274	VAL	2.5
2	I	62	LEU	2.5
1	F	73	LEU	2.5
3	J	260	HIS	2.5
2	I	140	LEU	2.5
2	H	166	ILE	2.5
2	I	349	VAL	2.5
1	F	179	LEU	2.5
2	I	107	LEU	2.5
2	G	61	GLY	2.5
2	H	252	LEU	2.5
1	F	55	ILE	2.5
2	G	102	GLU	2.5
2	H	279	GLU	2.5
2	H	142	THR	2.5
3	J	148	PRO	2.5
2	B	53	SER	2.5
2	I	198	HIS	2.5
1	F	282	ARG	2.5
2	H	5	VAL	2.5
1	F	9	LEU	2.4
2	I	339	LEU	2.4
2	H	17	ASP	2.4
2	I	191	LEU	2.4
3	J	152	LEU	2.4
1	F	212	PHE	2.4
3	J	166	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	187	LEU	2.4
1	F	151	VAL	2.4
1	F	162	LEU	2.4
2	C	131	LEU	2.4
2	I	240	MET	2.4
2	I	281	LEU	2.4
2	G	355	ARG	2.4
2	G	159	PRO	2.4
2	H	285	MET	2.4
2	I	121	LYS	2.4
2	D	108	LEU	2.4
2	H	11	ARG	2.4
2	G	5	VAL	2.4
2	I	122	VAL	2.4
1	F	75	ALA	2.4
2	G	290	HIS	2.4
3	E	18	TYR	2.4
2	B	162	LEU	2.4
3	J	28	LEU	2.4
2	G	23	HIS	2.4
2	C	57	LEU	2.4
2	I	282	LEU	2.4
2	G	182	GLN	2.4
3	J	328	VAL	2.4
2	B	72	PRO	2.4
3	J	315	LEU	2.4
1	A	185	LEU	2.4
2	I	103	ASP	2.4
2	G	129	HIS	2.4
3	E	44	LEU	2.4
1	A	19	ALA	2.3
2	I	54	ILE	2.3
2	H	8	ARG	2.3
2	G	35	GLY	2.3
2	I	320	ILE	2.3
1	F	4	LEU	2.3
2	I	357	LEU	2.3
3	J	19	GLN	2.3
2	H	302	LEU	2.3
3	J	277	LEU	2.3
2	G	11	ARG	2.3
2	B	214	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	91	ILE	2.3
2	I	295	VAL	2.3
1	A	104	LEU	2.3
2	G	191	LEU	2.3
3	J	176	LEU	2.3
3	J	273	LEU	2.3
1	F	83	LEU	2.3
3	J	288	ALA	2.3
2	H	261	GLY	2.3
2	D	214	LEU	2.3
1	F	61	TRP	2.3
2	G	116	ALA	2.3
2	H	9	LYS	2.3
3	J	198	PRO	2.3
2	B	241	LEU	2.3
1	F	41	VAL	2.3
2	I	98	ARG	2.3
1	F	123	ASN	2.3
2	D	54	ILE	2.3
2	I	11	ARG	2.3
1	F	328	SER	2.3
2	G	336	ARG	2.2
2	H	156	THR	2.2
3	J	323	LEU	2.2
2	B	25	LEU	2.2
2	H	282	LEU	2.2
2	D	221	THR	2.2
2	I	104	THR	2.2
2	G	264	VAL	2.2
1	A	20	ALA	2.2
2	I	296	GLN	2.2
2	B	28	LEU	2.2
2	D	363	MET	2.2
2	D	125	ILE	2.2
2	H	194	GLU	2.2
2	I	207	ALA	2.2
3	E	79	LEU	2.2
2	D	20	GLY	2.2
2	C	107	LEU	2.2
3	J	319	ILE	2.2
1	F	160	LEU	2.2
2	H	30	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	355	ARG	2.2
2	B	18	VAL	2.2
2	C	68	ILE	2.2
2	C	187	LEU	2.2
2	D	365	LEU	2.2
2	I	45	GLY	2.2
2	B	6	LEU	2.1
1	F	227	LYS	2.1
2	G	94	ASP	2.1
2	G	68	ILE	2.1
2	H	19	VAL	2.1
2	H	33	SER	2.1
1	F	81	LEU	2.1
2	C	143	LEU	2.1
2	C	203	LEU	2.1
2	G	162	LEU	2.1
1	A	38	VAL	2.1
3	E	277	LEU	2.1
2	G	339	LEU	2.1
1	F	5	TYR	2.1
2	G	38	HIS	2.1
2	G	281	LEU	2.1
3	E	236	LEU	2.1
1	F	10	ARG	2.1
2	G	36	ARG	2.1
2	G	358	ALA	2.1
3	J	269	ASP	2.1
3	J	229	TRP	2.1
2	H	176	LYS	2.1
2	I	285	MET	2.1
1	A	190	LEU	2.1
1	A	257	LEU	2.1
2	H	288	LEU	2.1
3	J	245	LEU	2.1
2	B	47	ARG	2.1
2	B	149	HIS	2.1
3	J	316	LEU	2.1
2	H	264	VAL	2.1
1	F	172	TYR	2.0
1	F	174	TYR	2.0
1	A	276	HIS	2.0
2	G	318	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	248	GLN	2.0
2	I	284	GLU	2.0
2	H	113	TYR	2.0
1	A	256	LEU	2.0
1	F	134	SER	2.0
2	H	190	ILE	2.0
2	H	332	LEU	2.0
1	A	154	ARG	2.0
2	I	352	THR	2.0
2	I	294	MET	2.0
2	I	235	GLN	2.0
1	F	56	ASP	2.0
2	B	19	VAL	2.0
2	G	221	THR	2.0
1	F	175	GLU	2.0
1	A	117	LEU	2.0
2	D	305	ASP	2.0
3	J	247	TRP	2.0
3	E	48	LEU	2.0
1	A	176	GLY	2.0
2	H	330	GLN	2.0
3	E	112	VAL	2.0
3	J	77	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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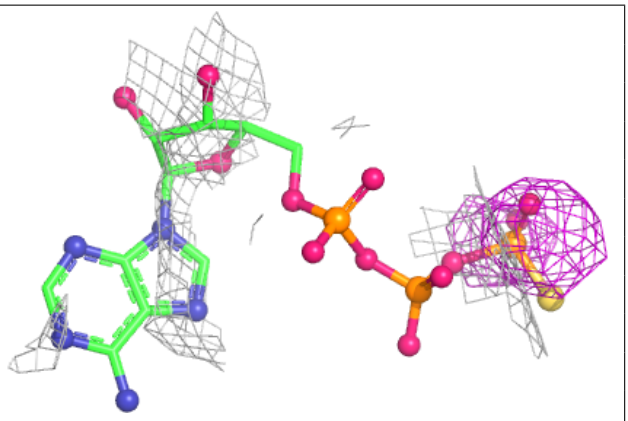
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

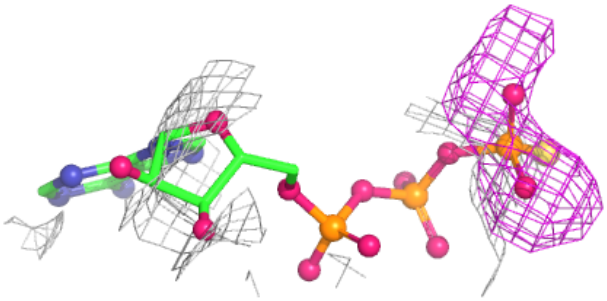
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	H	405	1/1	0.76	0.04	224,224,224,224	0
5	AGS	G	804	31/31	0.77	0.30	263,263,263,263	0
4	ZN	E	404	1/1	0.81	0.28	175,175,175,175	0
4	ZN	G	407	1/1	0.83	0.12	200,200,200,200	0
5	AGS	I	803	31/31	0.83	0.45	265,265,265,265	0
5	AGS	B	802	31/31	0.84	0.35	165,165,165,165	0
4	ZN	I	406	1/1	0.86	0.17	160,160,160,160	0
5	AGS	D	801	31/31	0.86	0.35	132,132,132,132	0
6	PO4	C	1300	5/5	0.88	0.25	116,116,116,116	0
6	PO4	H	1400	5/5	0.92	0.10	180,180,180,180	0
4	ZN	J	408	1/1	0.94	0.23	169,169,169,169	0
4	ZN	D	402	1/1	0.95	0.26	94,94,94,94	0
4	ZN	B	403	1/1	0.95	0.18	173,173,173,173	0
4	ZN	C	401	1/1	0.97	0.27	144,144,144,144	0

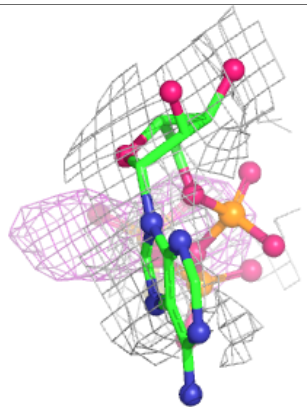
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS G 804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

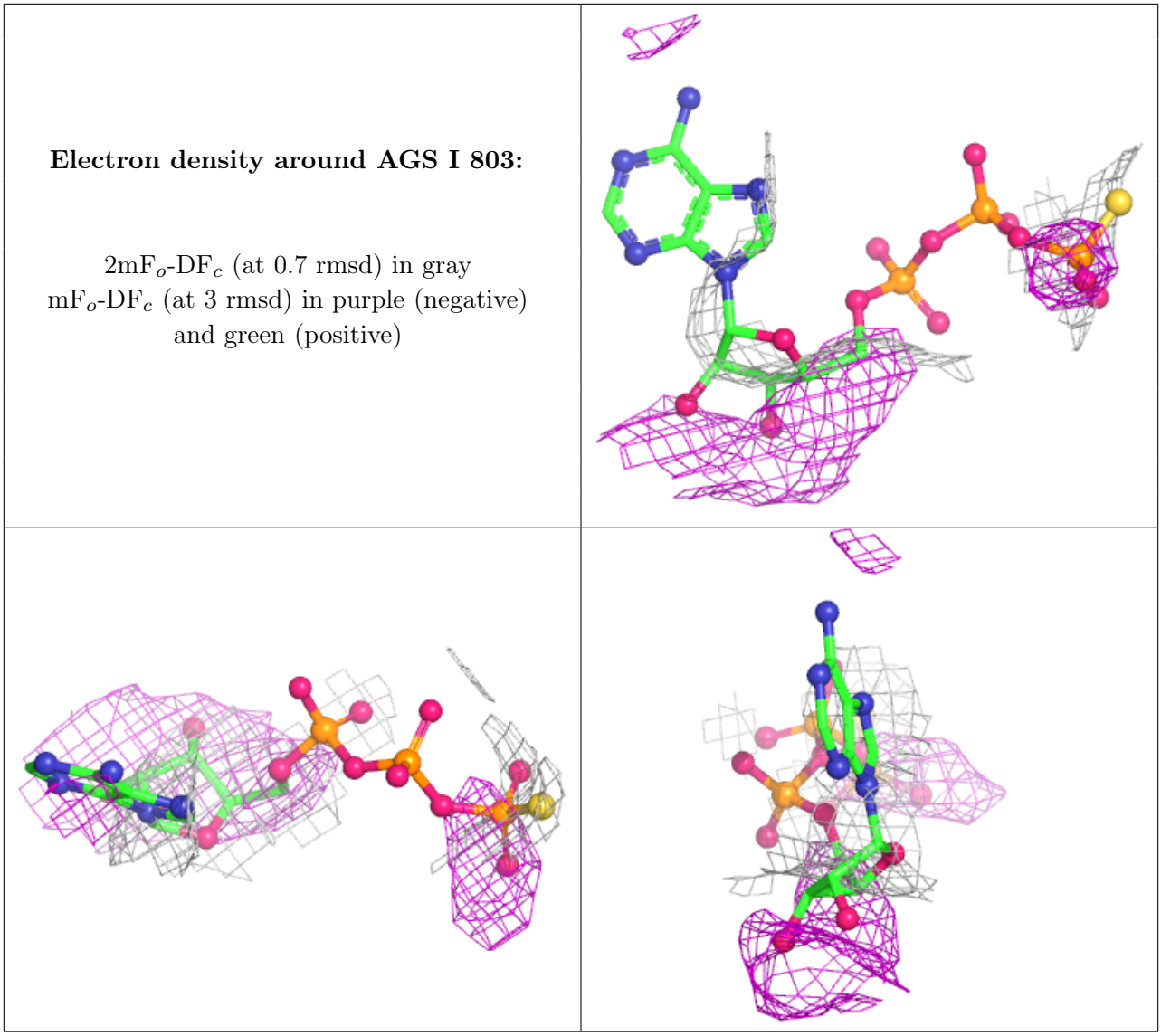






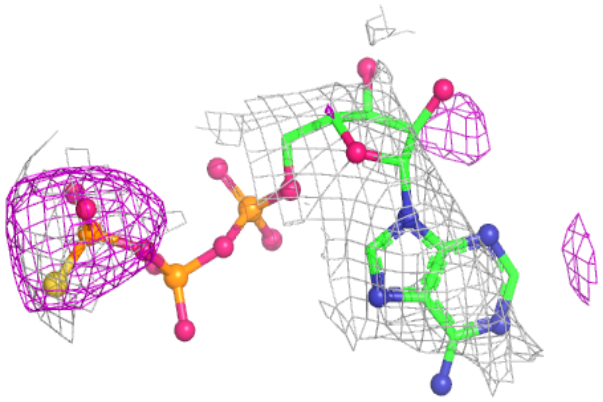
Electron density around AGS I 803:

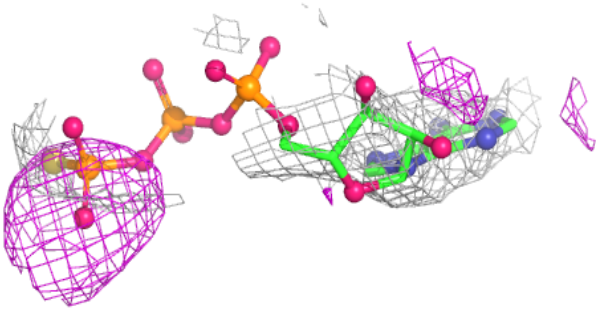
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

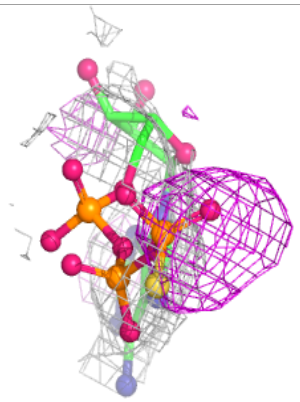


Electron density around AGS B 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

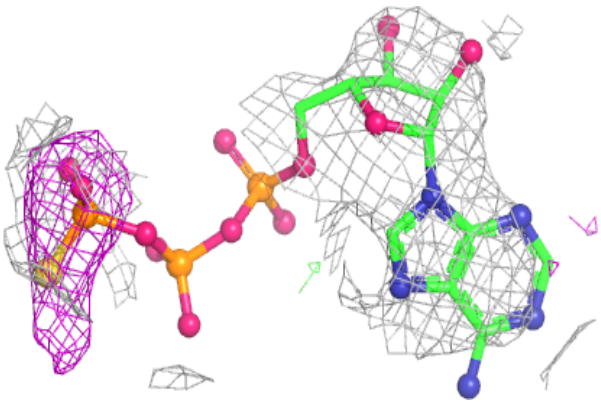


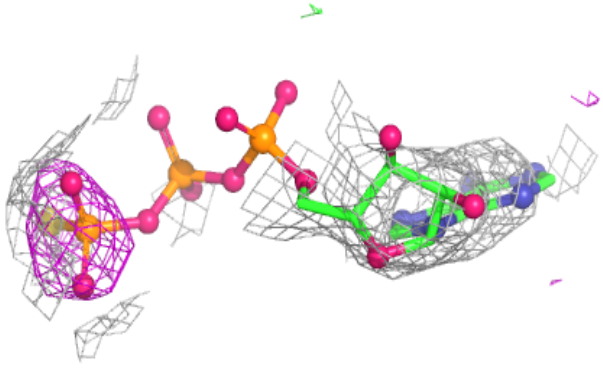


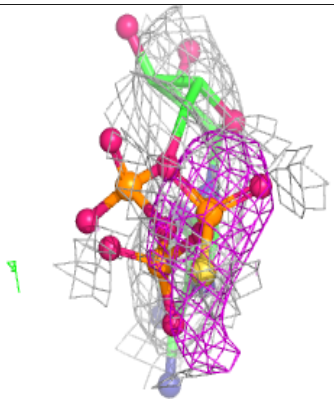


Electron density around AGS D 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.