



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 03:07 PM EDT

PDB ID : 1WE5
Title : Crystal Structure of Alpha-Xylosidase from Escherichia coli
Authors : Ose, T.; Kitamura, M.; Okuyama, M.; Mori, H.; Kimura, A.; Watanabe, N.; Yao, M.; Tanaka, I.
Deposited on : 2004-05-24
Resolution : 2.40 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
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

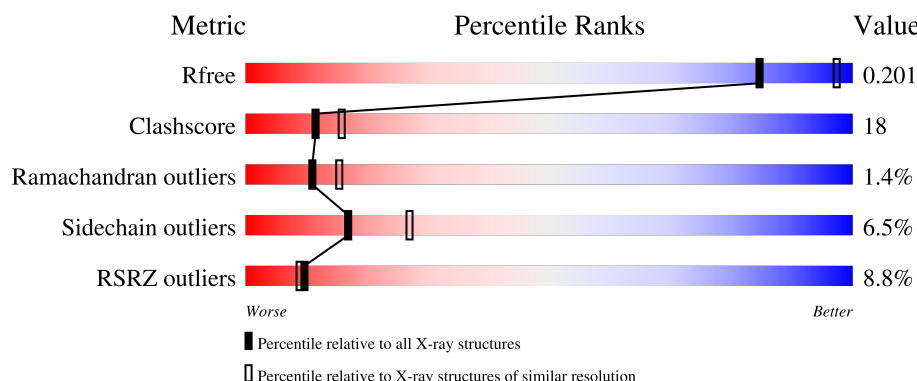
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	772	<div> <div>10%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
1	B	772	<div> <div>8%</div> <div>65%</div> <div>29%</div> <div>...</div> </div>
1	C	772	<div> <div>6%</div> <div>65%</div> <div>28%</div> <div>5%</div> <div>.</div> </div>
1	D	772	<div> <div>8%</div> <div>66%</div> <div>28%</div> <div>..</div> </div>
1	E	772	<div> <div>9%</div> <div>64%</div> <div>30%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	772	<div><div></div><div>10%</div><div>68%</div><div>27%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37302 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	Se	0	0	0
			6222	3975	1068	1147	13	19			
1	B	760	Total	C	N	O	S	Se	0	0	0
			6121	3909	1051	1129	13	19			
1	C	756	Total	C	N	O	S	Se	0	0	0
			6093	3891	1047	1123	13	19			
1	D	757	Total	C	N	O	S	Se	0	0	0
			6096	3892	1047	1125	13	19			
1	E	755	Total	C	N	O	S	Se	0	0	0
			6086	3887	1045	1122	13	19			
1	F	757	Total	C	N	O	S	Se	0	0	0
			6094	3891	1047	1124	13	19			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	593	MSE	MET	MODIFIED RESIDUE	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
A	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
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C	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	32	MSE	MET	MODIFIED RESIDUE	UNP P31434

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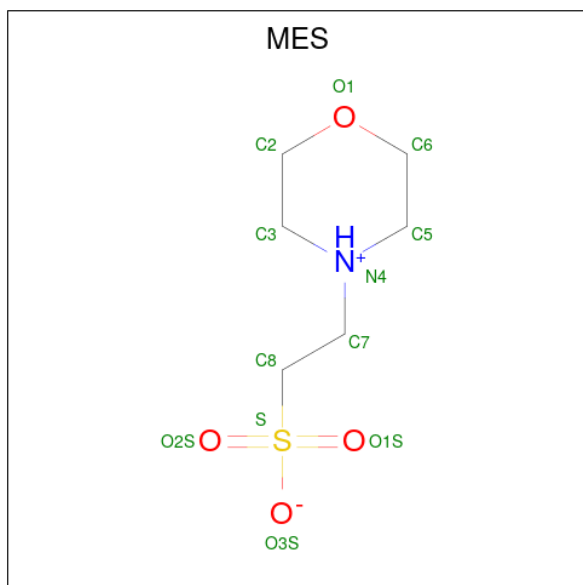
Chain	Residue	Modelled	Actual	Comment	Reference
D	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	310	MSE	MET	MODIFIED RESIDUE	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
F	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	615	MSE	MET	MODIFIED RESIDUE	UNP P31434

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

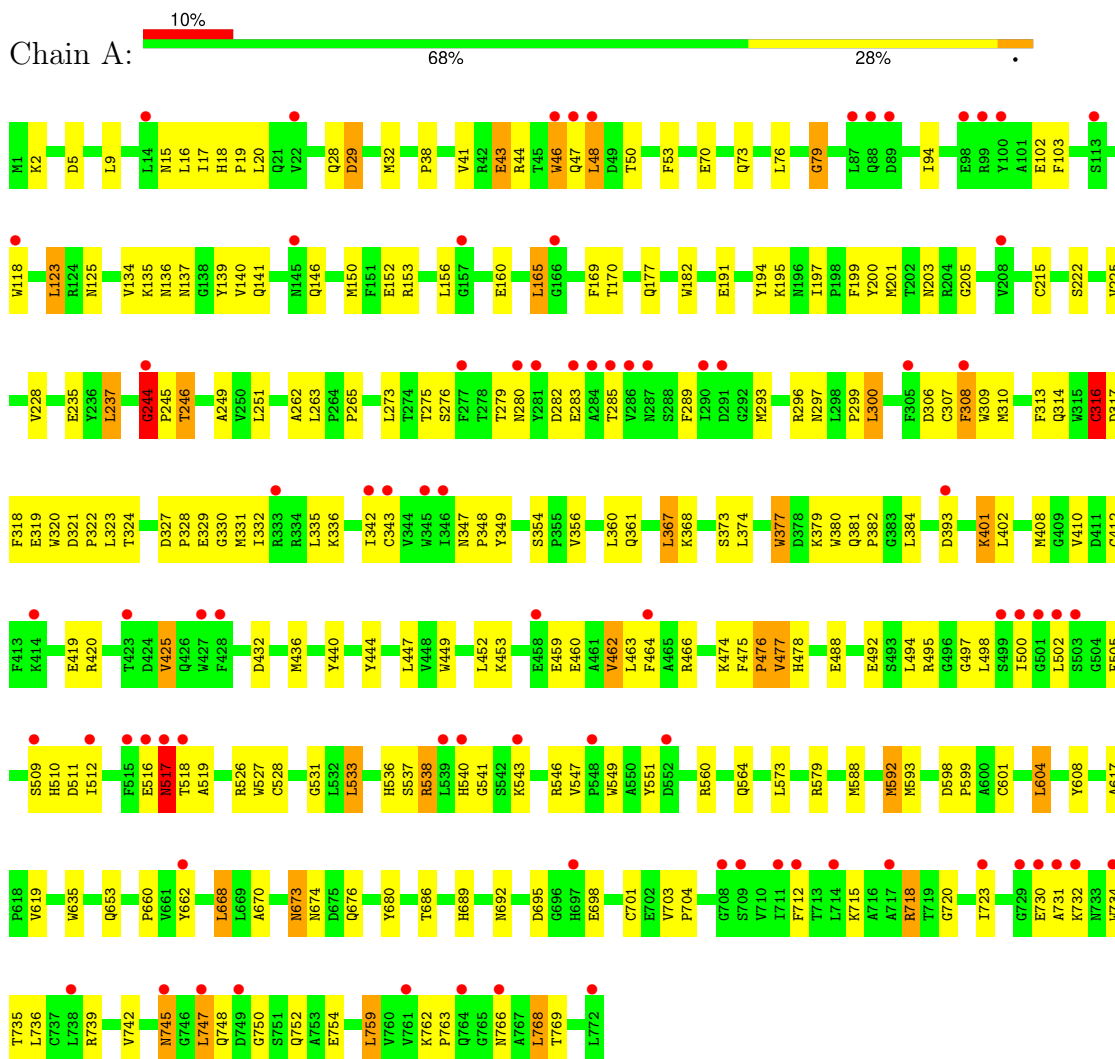
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	80	Total	O	0	0
			80	80		
3	C	108	Total	O	0	0
			108	108		
3	D	110	Total	O	0	0
			110	110		
3	E	61	Total	O	0	0
			61	61		
3	F	73	Total	O	0	0
			73	73		

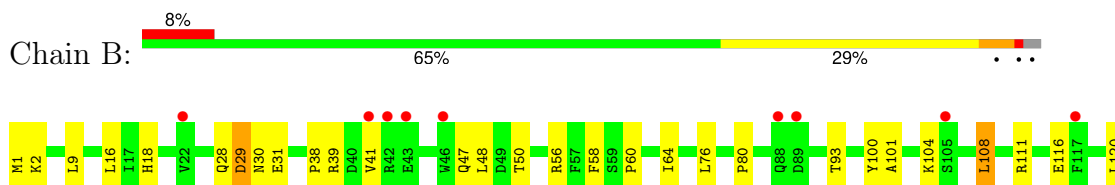
3 Residue-property plots [i](#)

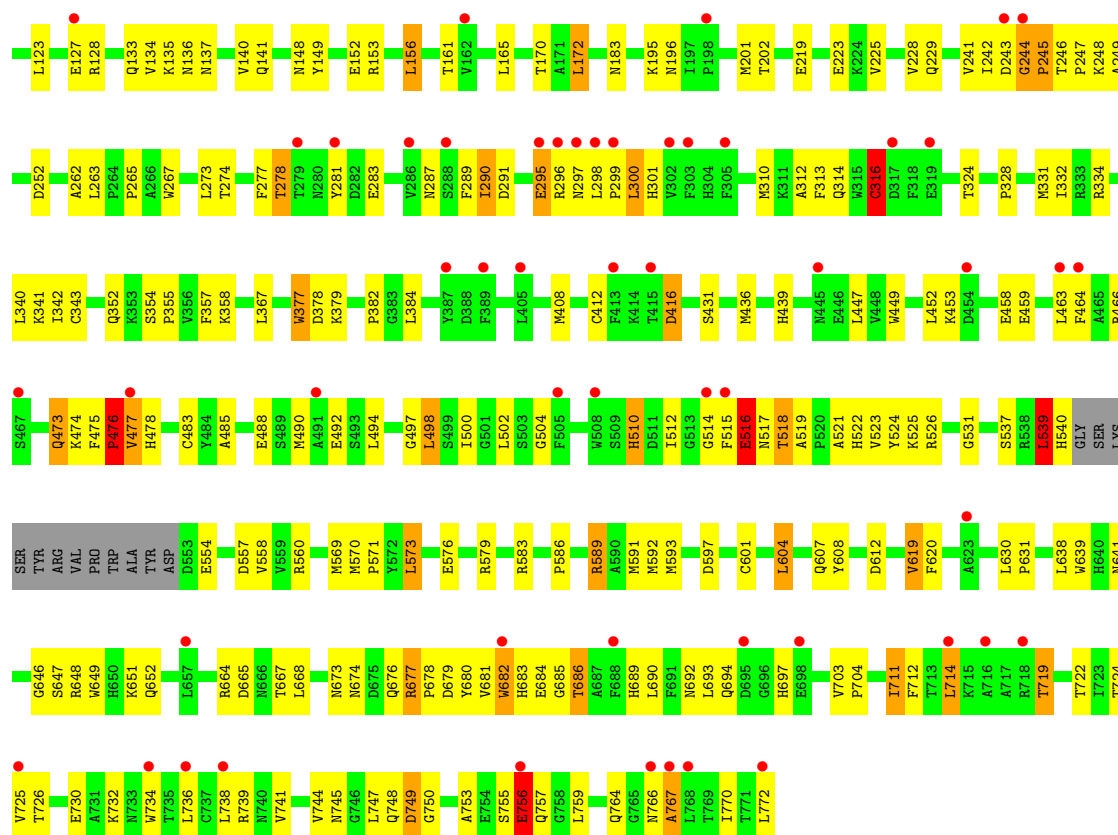
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative family 31 glucosidase yicI

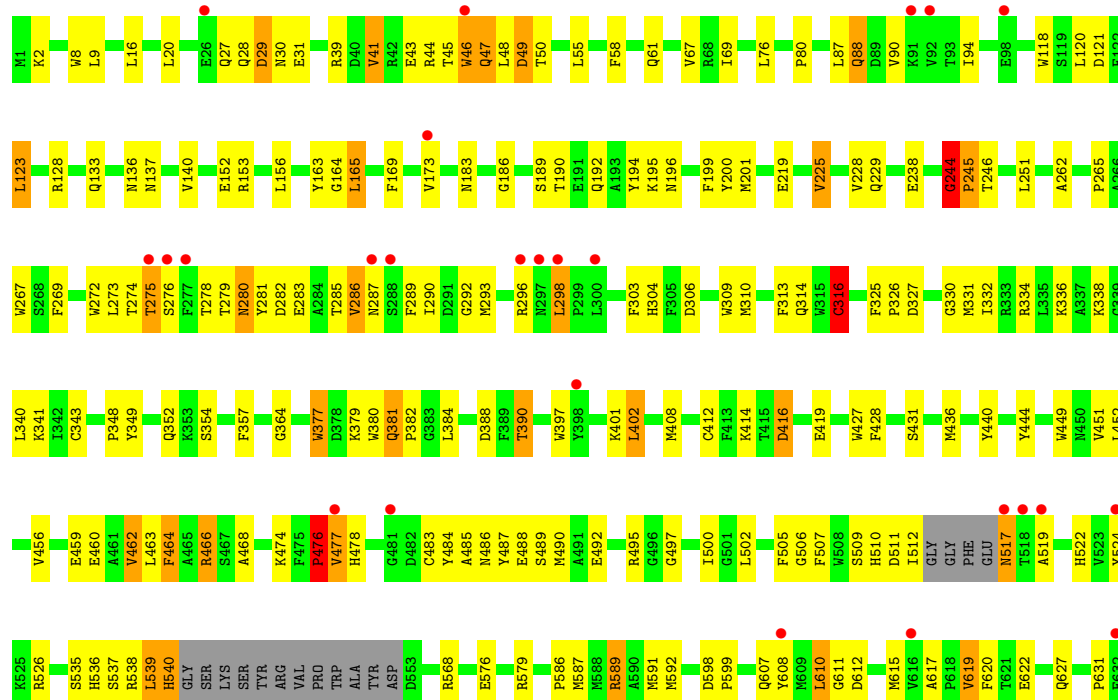


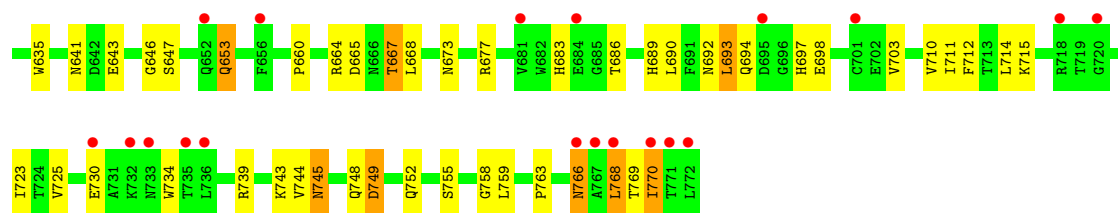
• Molecule 1: Putative family 31 glucosidase yicI





● Molecule 1: Putative family 31 glucosidase yicI

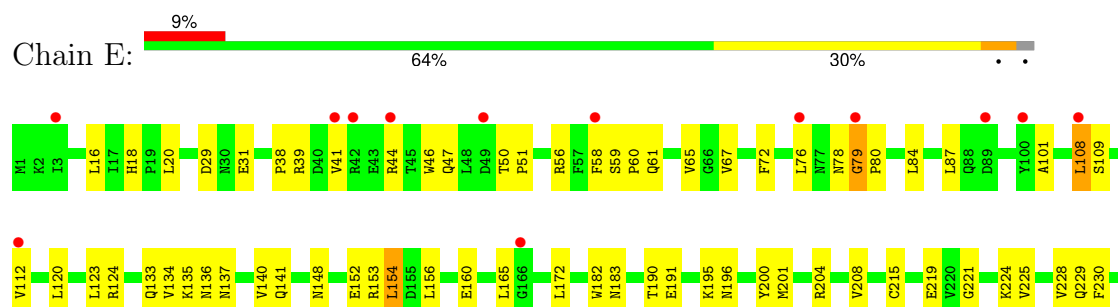


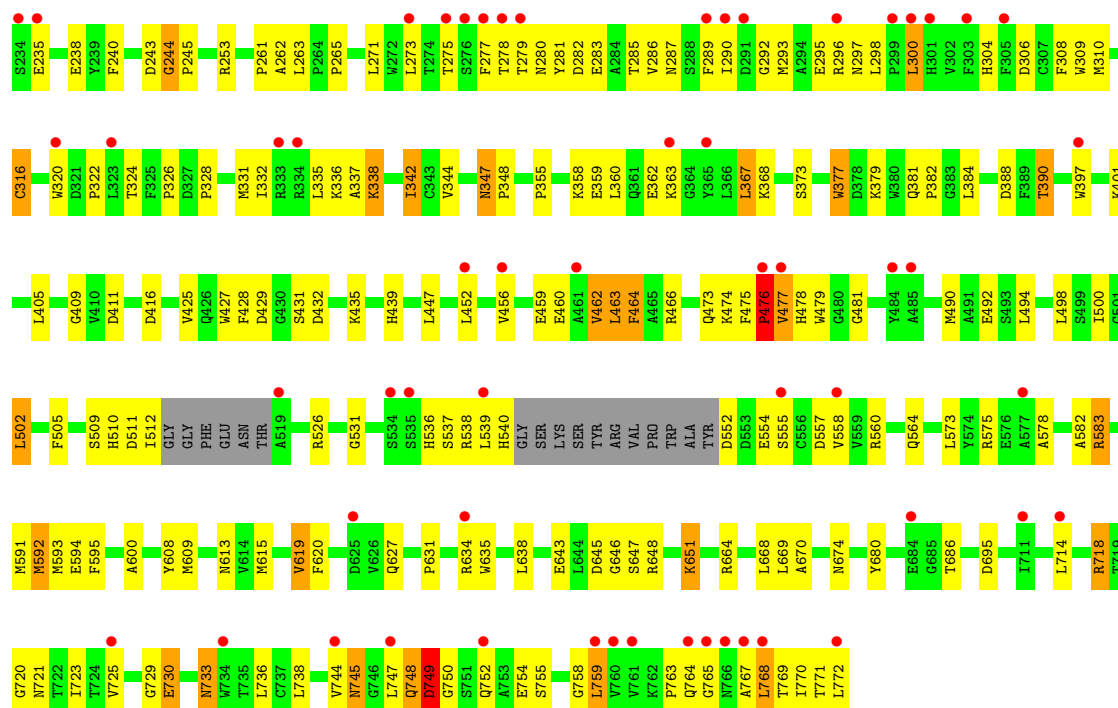


• Molecule 1: Putative family 31 glucosidase yicI

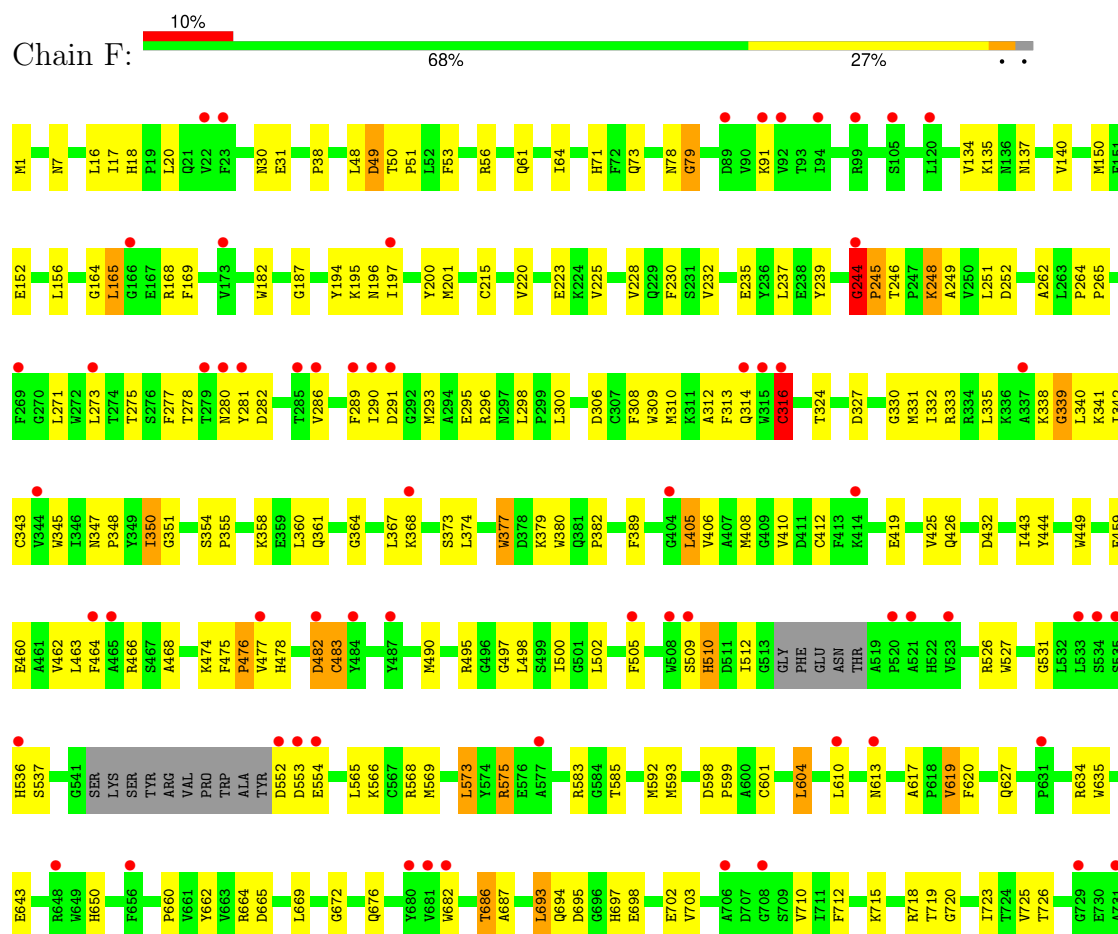


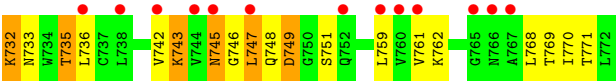
• Molecule 1: Putative family 31 glucosidase yicI





- Molecule 1: Putative family 31 glucosidase yicI





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	161.34Å 174.79Å 209.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 39.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.40) 99.2 (39.61-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.247 0.210 , 0.201	Depositor DCC
R_{free} test set	20756 reflections (9.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	37302	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES

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	0.38	0/6387	0.66	2/8650 (0.0%)
1	B	0.38	0/6280	0.66	4/8502 (0.0%)
1	C	0.40	0/6250	0.66	3/8461 (0.0%)
1	D	0.38	0/6253	0.66	3/8464 (0.0%)
1	E	0.38	0/6243	0.64	1/8451 (0.0%)
1	F	0.37	0/6251	0.64	1/8461 (0.0%)
All	All	0.38	0/37664	0.65	14/50989 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	CYS	CA-CB-SG	-6.30	102.66	114.00
1	C	316	CYS	CA-CB-SG	-6.12	102.99	114.00
1	C	416	ASP	N-CA-C	6.06	127.36	111.00
1	D	316	CYS	CA-CB-SG	-5.73	103.69	114.00
1	B	416	ASP	N-CA-C	5.69	126.36	111.00
1	F	244	GLY	N-CA-C	-5.51	99.34	113.10
1	D	279	THR	N-CA-C	5.44	125.69	111.00
1	A	244	GLY	N-CA-C	-5.41	99.58	113.10
1	D	613	ASN	N-CA-C	5.32	125.36	111.00
1	E	244	GLY	N-CA-C	-5.27	99.93	113.10
1	B	244	GLY	N-CA-C	-5.14	100.24	113.10
1	C	244	GLY	N-CA-C	-5.04	100.49	113.10
1	B	101	ALA	N-CA-C	-5.04	97.40	111.00
1	A	48	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	6222	0	5932	236	0
1	B	6121	0	5839	225	0
1	C	6093	0	5817	231	0
1	D	6096	0	5816	202	0
1	E	6086	0	5808	230	0
1	F	6094	0	5814	192	0
2	A	12	0	13	1	0
2	B	12	0	13	0	0
2	C	12	0	13	2	0
2	D	12	0	13	0	0
2	E	12	0	13	1	0
2	F	12	0	13	0	0
3	A	86	0	0	1	0
3	B	80	0	0	3	0
3	C	108	0	0	3	0
3	D	110	0	0	2	0
3	E	61	0	0	1	0
3	F	73	0	0	1	0
All	All	37302	0	35104	1268	0

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 18.

All (1268) 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:E:591:MSE:SE	1:E:609:MSE:HE3	1.99	1.12
1:B:485:ALA:HB1	1:B:519:ALA:HB2	1.21	1.11
1:B:591:MSE:HE3	1:B:607:GLN:HG3	1.32	1.11
1:D:591:MSE:HE3	1:D:607:GLN:HG3	1.34	1.10
1:A:310:MSE:HE1	1:A:317:ASP:H	1.08	1.09
1:E:283:GLU:HA	1:E:331:MSE:HE3	1.33	1.07
1:A:32:MSE:HE2	1:A:94:ILE:HG23	1.21	1.07
1:B:358:LYS:H	1:B:358:LYS:HD2	1.08	1.06
1:B:690:LEU:HD11	1:B:693:LEU:HB2	1.31	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:CYS:HA	1:A:604:LEU:HD22	1.41	1.03
1:E:609:MSE:HE1	1:E:615:MSE:HG2	1.38	1.01
1:A:502:LEU:HD11	1:A:592:MSE:HE2	1.42	1.00
1:C:668:LEU:HD21	1:C:714:LEU:HD12	1.44	0.98
1:D:591:MSE:SE	1:D:609:MSE:HE2	2.15	0.96
1:B:379:LYS:HA	1:B:379:LYS:HE2	1.46	0.96
1:C:76:LEU:HD22	1:E:373:SER:HB3	1.49	0.94
1:A:246:THR:HG22	1:A:249:ALA:H	1.33	0.94
1:D:332:ILE:HD12	1:D:408:MSE:HE2	1.51	0.92
1:B:526:ARG:HD2	1:B:619:VAL:HG22	1.52	0.92
1:A:592:MSE:HE3	1:A:593:MSE:HB2	1.51	0.91
1:A:273:LEU:HB2	1:A:300:LEU:HD21	1.53	0.90
1:A:310:MSE:HE1	1:A:317:ASP:N	1.85	0.90
1:F:265:PRO:HD2	1:F:462:VAL:HG22	1.52	0.90
1:C:28:GLN:HA	1:C:28:GLN:HE21	1.36	0.90
1:B:358:LYS:HD2	1:B:358:LYS:N	1.86	0.89
1:E:609:MSE:HE1	1:E:615:MSE:CG	2.02	0.89
1:C:591:MSE:HE1	1:C:615:MSE:HG2	1.53	0.89
1:D:690:LEU:HD11	1:D:693:LEU:HB2	1.53	0.89
1:D:591:MSE:CE	1:D:607:GLN:HG3	2.05	0.87
1:B:589:ARG:HG2	1:B:593:MSE:CE	2.05	0.87
1:C:591:MSE:HE3	1:C:607:GLN:HE21	1.36	0.87
1:F:565:LEU:HG	1:F:569:MSE:HE2	1.54	0.87
1:B:485:ALA:CB	1:B:519:ALA:HB2	2.05	0.86
1:B:31:GLU:HG2	1:B:58:PHE:HB3	1.56	0.86
1:D:570:MSE:CE	1:D:573:LEU:HD23	2.06	0.85
1:F:443:ILE:HD12	1:F:444:TYR:N	1.92	0.85
1:F:332:ILE:HD12	1:F:408:MSE:HE2	1.58	0.84
1:F:526:ARG:HD2	1:F:619:VAL:HG22	1.58	0.84
1:D:283:GLU:HG3	1:D:331:MSE:HE3	1.58	0.84
1:B:358:LYS:H	1:B:358:LYS:CD	1.89	0.84
1:C:274:THR:HG22	1:C:304:HIS:HB3	1.57	0.84
1:B:641:ASN:ND2	1:B:757:GLN:HG3	1.93	0.83
1:A:275:THR:HG21	1:A:280:ASN:ND2	1.93	0.83
1:D:79:GLY:HA2	1:D:432:ASP:H	1.42	0.83
1:A:373:SER:HB3	1:E:76:LEU:HD22	1.60	0.83
1:D:519:ALA:HB3	1:D:520:PRO:HD3	1.61	0.83
1:A:332:ILE:HD12	1:A:408:MSE:HE2	1.59	0.83
1:B:668:LEU:HD13	1:B:690:LEU:HD23	1.60	0.83
1:A:488:GLU:O	1:A:492:GLU:HG3	1.78	0.82
1:D:246:THR:HG22	1:D:249:ALA:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:GLU:HA	1:E:331:MSE:CE	2.10	0.82
1:C:743:LYS:HA	1:C:759:LEU:HD12	1.62	0.82
1:D:11:GLN:HB2	1:D:14:LEU:HD22	1.59	0.81
1:B:589:ARG:HG2	1:B:593:MSE:HE1	1.60	0.81
1:D:388:ASP:OD1	1:D:390:THR:HG22	1.81	0.80
1:E:609:MSE:CE	1:E:615:MSE:HG2	2.11	0.80
1:E:526:ARG:HD2	1:E:619:VAL:HG22	1.62	0.80
1:E:609:MSE:HE1	1:E:615:MSE:CB	2.11	0.80
1:C:273:LEU:HD11	1:C:289:PHE:HE2	1.45	0.80
1:E:502:LEU:HD11	1:E:592:MSE:HE2	1.64	0.80
1:D:18:HIS:O	1:D:20:LEU:HD12	1.82	0.79
1:C:31:GLU:HG2	1:C:58:PHE:HB3	1.64	0.79
1:D:595:PHE:CE1	1:D:609:MSE:HE3	2.17	0.79
1:E:609:MSE:CE	1:E:615:MSE:HA	2.13	0.79
1:E:286:VAL:HG21	1:E:331:MSE:HE2	1.64	0.79
1:B:277:PHE:O	1:B:278:THR:HB	1.82	0.78
1:A:763:PRO:HB3	1:A:768:LEU:HD12	1.66	0.77
1:D:748:GLN:HB2	1:D:769:THR:HG22	1.66	0.77
1:A:32:MSE:HE2	1:A:94:ILE:CG2	2.10	0.77
1:A:44:ARG:HH21	1:C:278:THR:HA	1.47	0.77
1:B:300:LEU:HD13	1:B:340:LEU:HD21	1.66	0.77
1:E:282:ASP:O	1:E:285:THR:HG22	1.83	0.77
1:F:368:LYS:O	1:F:425:VAL:HG13	1.85	0.77
1:B:28:GLN:HG3	1:B:56:ARG:HH12	1.48	0.77
1:A:314:GLN:HB2	1:A:354:SER:HB2	1.66	0.77
1:D:595:PHE:HE1	1:D:609:MSE:HE3	1.49	0.77
1:B:591:MSE:CE	1:B:607:GLN:HG3	2.12	0.77
1:F:703:VAL:HG22	1:F:712:PHE:HB3	1.66	0.76
1:E:79:GLY:CA	1:E:432:ASP:H	1.99	0.76
1:E:755:SER:HB3	1:E:758:GLY:O	1.86	0.76
1:B:310:MSE:SE	1:B:316:CYS:HA	2.36	0.76
1:A:275:THR:HG21	1:A:280:ASN:HD21	1.49	0.76
1:A:518:THR:HG22	1:A:519:ALA:H	1.51	0.76
1:C:44:ARG:O	1:C:47:GLN:HB2	1.86	0.76
1:E:342:ILE:H	1:E:342:ILE:HD13	1.51	0.76
1:F:314:GLN:HB2	1:F:354:SER:HB2	1.67	0.76
1:E:767:ALA:O	1:E:768:LEU:HB2	1.84	0.75
1:E:695:ASP:HA	1:E:718:ARG:HD2	1.69	0.75
1:B:678:PRO:O	1:B:682:TRP:HZ3	1.70	0.75
1:B:287:ASN:HA	1:B:290:ILE:HG22	1.68	0.75
1:B:485:ALA:HB1	1:B:519:ALA:CB	2.10	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:GLU:HG2	1:E:58:PHE:HB3	1.67	0.75
1:A:170:THR:HG21	1:A:177:GLN:OE1	1.87	0.75
1:B:201:MSE:HE2	1:B:502:LEU:O	1.86	0.75
1:D:586:PRO:O	1:D:589:ARG:HD2	1.86	0.75
1:E:79:GLY:HA2	1:E:432:ASP:H	1.52	0.74
1:E:265:PRO:HG3	1:E:459:GLU:O	1.87	0.74
1:A:32:MSE:HE1	1:A:102:GLU:O	1.87	0.74
1:B:711:ILE:H	1:B:711:ILE:HD13	1.52	0.74
1:E:733:ASN:N	1:E:733:ASN:HD22	1.86	0.74
1:E:668:LEU:HD21	1:E:714:LEU:HD22	1.68	0.73
1:F:732:LYS:HE2	1:F:732:LYS:HA	1.68	0.73
1:B:474:LYS:C	1:B:476:PRO:HD3	2.08	0.73
1:D:262:ALA:HB3	1:D:476:PRO:HG2	1.69	0.73
1:C:269:PHE:HE2	1:C:587:MSE:HE1	1.54	0.73
1:F:195:LYS:HE2	1:F:478:HIS:HB3	1.69	0.73
1:A:313:PHE:HZ	1:E:41:VAL:HG21	1.54	0.73
1:B:677:ARG:HD3	1:B:679:ASP:O	1.89	0.73
1:C:310:MSE:SE	1:C:316:CYS:HA	2.39	0.73
1:A:283:GLU:HG3	1:A:331:MSE:HG3	1.72	0.72
1:C:332:ILE:HD12	1:C:408:MSE:HE2	1.70	0.72
1:F:300:LEU:HD22	1:F:340:LEU:HD21	1.69	0.72
1:E:310:MSE:SE	1:E:316:CYS:HA	2.40	0.72
1:D:79:GLY:CA	1:D:432:ASP:H	2.02	0.71
1:F:566:LYS:HA	1:F:569:MSE:HE3	1.71	0.71
1:C:539:LEU:O	1:C:540:HIS:HB2	1.90	0.71
1:A:262:ALA:HB3	1:A:476:PRO:HG2	1.72	0.71
1:E:108:LEU:HD23	1:E:109:SER:N	2.05	0.71
1:B:586:PRO:O	1:B:589:ARG:HD2	1.90	0.71
1:E:367:LEU:HD22	1:E:425:VAL:CG2	2.20	0.71
1:A:79:GLY:HA2	1:A:432:ASP:H	1.54	0.71
1:B:741:VAL:O	1:B:759:LEU:HB2	1.91	0.71
1:E:714:LEU:HD21	1:E:725:VAL:HG13	1.72	0.71
1:B:283:GLU:HG3	1:B:331:MSE:HG3	1.73	0.71
1:E:613:ASN:HB3	1:E:664:ARG:HG2	1.72	0.71
1:C:28:GLN:HA	1:C:28:GLN:NE2	2.06	0.71
1:A:703:VAL:HG22	1:A:712:PHE:HB3	1.73	0.70
1:B:689:HIS:CD2	1:B:739:ARG:HH11	2.09	0.70
1:D:368:LYS:O	1:D:425:VAL:HG22	1.91	0.70
1:D:570:MSE:HE2	1:D:573:LEU:HD23	1.72	0.70
1:B:772:LEU:H	1:B:772:LEU:HD22	1.57	0.70
1:C:703:VAL:CG1	1:C:712:PHE:HB3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLN:HB2	1:B:354:SER:HB2	1.73	0.69
1:D:390:THR:HG23	1:D:428:PHE:HB3	1.73	0.69
1:A:273:LEU:HD21	1:A:289:PHE:HE1	1.57	0.69
1:C:591:MSE:HE3	1:C:607:GLN:NE2	2.06	0.69
1:D:367:LEU:HG	1:D:425:VAL:HG21	1.73	0.69
1:C:61:GLN:HB3	1:C:87:LEU:HD23	1.74	0.69
1:E:347:ASN:C	1:E:347:ASN:HD22	1.96	0.69
1:F:262:ALA:HB3	1:F:476:PRO:HG2	1.73	0.69
1:F:310:MSE:SE	1:F:316:CYS:HA	2.43	0.69
1:F:474:LYS:O	1:F:476:PRO:HD3	1.92	0.69
1:A:310:MSE:SE	1:A:316:CYS:HA	2.43	0.69
1:B:262:ALA:HB3	1:B:476:PRO:HG2	1.74	0.69
1:C:88:GLN:CD	1:C:88:GLN:H	1.95	0.69
1:C:755:SER:HB3	1:C:758:GLY:O	1.93	0.69
1:F:474:LYS:C	1:F:476:PRO:HD3	2.12	0.69
1:C:46:TRP:HA	1:C:46:TRP:CE3	2.27	0.69
1:A:516:GLU:CD	1:A:516:GLU:H	1.97	0.68
1:A:592:MSE:HE3	1:A:593:MSE:CB	2.22	0.68
1:D:526:ARG:HD2	1:D:619:VAL:HG22	1.75	0.68
1:E:295:GLU:O	1:E:296:ARG:HB2	1.93	0.68
1:C:262:ALA:HB3	1:C:476:PRO:HG2	1.75	0.68
1:A:279:THR:HG23	1:A:546:ARG:NH1	2.07	0.68
1:A:331:MSE:O	1:A:335:LEU:HD13	1.94	0.68
1:F:747:LEU:HD22	1:F:770:ILE:HG22	1.76	0.68
1:E:744:VAL:HG23	1:E:772:LEU:HA	1.75	0.68
1:B:100:TYR:CD2	1:B:111:ARG:HD3	2.29	0.68
1:D:291:ASP:O	1:D:295:GLU:HG3	1.94	0.68
1:D:512:ILE:CD1	1:D:531:GLY:HA3	2.24	0.68
1:F:725:VAL:HG13	1:F:768:LEU:HB3	1.76	0.68
1:C:414:LYS:HD2	1:C:464:PHE:HB3	1.75	0.68
1:C:509:SER:HB3	1:C:536:HIS:HB2	1.74	0.68
1:E:609:MSE:HE2	1:E:615:MSE:HA	1.76	0.68
1:E:750:GLY:N	1:E:764:GLN:HG2	2.08	0.68
1:B:703:VAL:O	1:B:711:ILE:HD13	1.93	0.68
1:D:698:GLU:OE2	1:D:715:LYS:HD3	1.93	0.68
1:F:425:VAL:CG1	1:F:426:GLN:N	2.57	0.68
1:F:265:PRO:HG3	1:F:459:GLU:O	1.94	0.68
1:B:571:PRO:HG3	1:B:682:TRP:HB2	1.76	0.67
1:C:88:GLN:H	1:C:88:GLN:NE2	1.92	0.67
1:C:690:LEU:HD11	1:C:693:LEU:HB2	1.75	0.67
1:E:44:ARG:HA	1:E:47:GLN:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ASN:HD22	1:B:757:GLN:HG3	1.59	0.67
1:E:511:ASP:OD2	1:E:538:ARG:HD3	1.93	0.67
1:C:502:LEU:HD21	1:C:592:MSE:HE1	1.77	0.67
1:E:474:LYS:C	1:E:476:PRO:HD3	2.15	0.67
1:F:425:VAL:HG12	1:F:426:GLN:N	2.09	0.67
1:D:310:MSE:SE	1:D:316:CYS:HA	2.44	0.67
1:E:41:VAL:HG22	1:E:47:GLN:HG2	1.76	0.67
1:E:645:ASP:HB2	1:E:648:ARG:HH21	1.59	0.67
1:A:194:TYR:CD2	1:A:466:ARG:HD3	2.30	0.66
1:F:168:ARG:NH2	1:F:196:ASN:OD1	2.27	0.66
1:F:367:LEU:HD11	1:F:425:VAL:HG11	1.76	0.66
1:D:601:CYS:HA	1:D:604:LEU:HD22	1.78	0.66
1:E:627:GLN:HG2	1:E:651:LYS:HG2	1.77	0.66
1:F:20:LEU:HD12	1:F:38:PRO:O	1.94	0.66
1:B:690:LEU:CD1	1:B:693:LEU:HB2	2.20	0.66
1:D:474:LYS:C	1:D:476:PRO:HD3	2.15	0.66
1:B:474:LYS:O	1:B:476:PRO:HD3	1.95	0.66
1:C:169:PHE:O	1:F:225:VAL:HG11	1.96	0.66
1:D:195:LYS:HE2	1:D:478:HIS:HB3	1.77	0.66
1:D:748:GLN:CB	1:D:769:THR:HG22	2.25	0.66
1:D:591:MSE:HE1	1:D:608:TYR:N	2.11	0.66
1:A:512:ILE:HD11	1:A:531:GLY:HA3	1.78	0.66
1:C:27:GLN:HG3	1:C:94:ILE:HD12	1.78	0.66
1:D:694:GLN:HB2	1:D:697:HIS:CD2	2.30	0.66
1:A:79:GLY:CA	1:A:432:ASP:H	2.10	0.65
1:E:367:LEU:HD22	1:E:425:VAL:HG21	1.78	0.65
1:A:276:SER:HB3	1:A:279:THR:OG1	1.95	0.65
1:E:16:LEU:HD22	1:E:140:VAL:HG22	1.76	0.65
1:C:664:ARG:O	1:C:667:THR:HG23	1.96	0.65
1:C:698:GLU:OE2	1:C:715:LYS:HD3	1.96	0.65
1:D:747:LEU:HD12	1:D:748:GLN:H	1.60	0.65
1:B:281:TYR:O	1:B:324:THR:HG23	1.96	0.65
1:B:591:MSE:HE3	1:B:607:GLN:CG	2.19	0.65
1:F:761:VAL:HG11	1:F:768:LEU:HD21	1.79	0.65
1:A:768:LEU:HD13	1:A:768:LEU:H	1.61	0.65
1:F:367:LEU:CG	1:F:425:VAL:HG11	2.27	0.65
1:B:576:GLU:OE2	1:B:579:ARG:HD2	1.97	0.65
1:F:194:TYR:CD2	1:F:466:ARG:HD3	2.31	0.65
1:E:124:ARG:HD3	1:E:243:ASP:OD1	1.97	0.64
1:C:591:MSE:HE2	1:C:608:TYR:CA	2.26	0.64
1:E:608:TYR:O	1:E:609:MSE:HE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:PRO:HG3	1:B:682:TRP:CB	2.28	0.64
1:F:327:ASP:OD2	1:F:330:GLY:HA3	1.96	0.64
1:A:32:MSE:CE	1:A:94:ILE:HG23	2.12	0.64
1:F:137:ASN:HB3	1:F:152:GLU:OE1	1.95	0.64
1:B:463:LEU:O	1:B:477:VAL:HB	1.98	0.64
1:B:382:PRO:HG3	1:D:50:THR:O	1.97	0.64
1:B:591:MSE:HE1	1:B:608:TYR:N	2.13	0.64
1:C:388:ASP:OD1	1:C:390:THR:HG22	1.98	0.64
1:E:750:GLY:CA	1:E:764:GLN:HG2	2.28	0.64
1:E:331:MSE:O	1:E:335:LEU:HD23	1.97	0.64
1:B:29:ASP:CG	1:B:30:ASN:H	2.01	0.64
1:C:46:TRP:HA	1:C:46:TRP:HE3	1.63	0.64
1:A:474:LYS:C	1:A:476:PRO:HD3	2.18	0.63
1:D:483:CYS:HB3	1:D:489:SER:OG	1.98	0.63
1:D:137:ASN:HB3	1:D:152:GLU:OE1	1.97	0.63
1:A:310:MSE:CE	1:A:317:ASP:H	1.99	0.63
1:F:79:GLY:HA2	1:F:432:ASP:H	1.63	0.63
1:E:744:VAL:HG22	1:E:771:THR:O	1.99	0.63
1:E:592:MSE:HE3	1:E:593:MSE:HB2	1.80	0.63
1:A:463:LEU:O	1:A:477:VAL:HB	1.99	0.62
1:C:16:LEU:HD22	1:C:140:VAL:HG22	1.81	0.62
1:A:361:GLN:HG3	1:A:374:LEU:HD11	1.81	0.62
1:F:702:GLU:HB3	1:F:710:VAL:HG13	1.80	0.62
1:C:522:HIS:CD2	1:C:622:GLU:HB2	2.35	0.62
1:E:763:PRO:HB2	1:E:765:GLY:O	1.98	0.62
1:F:278:THR:HG22	1:F:308:PHE:CE1	2.34	0.62
1:A:310:MSE:CE	1:A:317:ASP:OD1	2.47	0.62
1:C:502:LEU:CD2	1:C:592:MSE:HE1	2.30	0.62
1:C:201:MSE:HE2	1:C:502:LEU:O	1.99	0.62
1:D:300:LEU:HD12	1:D:340:LEU:CD2	2.28	0.62
1:E:509:SER:HB3	1:E:536:HIS:HB2	1.82	0.62
1:B:16:LEU:HD22	1:B:140:VAL:HG22	1.81	0.62
1:A:201:MSE:CE	1:A:502:LEU:O	2.48	0.62
1:F:634:ARG:HD3	1:F:643:GLU:OE1	2.00	0.62
1:C:27:GLN:HG3	1:C:94:ILE:CD1	2.30	0.61
1:D:20:LEU:HD11	3:D:1129:HOH:O	1.99	0.61
1:B:377:TRP:CE2	1:B:379:LYS:HB2	2.35	0.61
1:C:273:LEU:HD11	1:C:289:PHE:CE2	2.30	0.61
1:D:474:LYS:O	1:D:476:PRO:HD3	1.99	0.61
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.00	0.61
1:E:609:MSE:HE1	1:E:615:MSE:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASN:C	1:B:299:PRO:HD3	2.20	0.61
1:F:693:LEU:HD13	1:F:718:ARG:HB2	1.81	0.61
1:A:509:SER:HB3	1:A:536:HIS:HB2	1.83	0.61
1:F:746:GLY:HA3	1:F:771:THR:OG1	2.00	0.61
1:D:511:ASP:OD1	1:D:538:ARG:HD2	2.00	0.61
1:F:48:LEU:HD12	1:F:49:ASP:HB2	1.81	0.61
1:F:150:MSE:HE3	1:F:235:GLU:C	2.20	0.61
1:F:296:ARG:O	1:F:298:LEU:HD13	2.01	0.61
1:C:586:PRO:O	1:C:589:ARG:HD2	2.00	0.61
1:C:507:PHE:HD2	1:C:587:MSE:HE2	1.65	0.61
1:D:354:SER:OG	1:D:356:VAL:HG12	2.00	0.61
1:E:560:ARG:O	1:E:564:GLN:HG3	2.01	0.61
1:A:16:LEU:HD22	1:A:140:VAL:HG22	1.82	0.61
1:C:456:VAL:HG12	1:C:460:GLU:CB	2.30	0.61
1:E:328:PRO:O	1:E:332:ILE:HD13	2.00	0.61
1:B:711:ILE:HG12	1:B:712:PHE:N	2.15	0.61
1:C:282:ASP:H	1:C:285:THR:CG2	2.13	0.61
1:E:733:ASN:N	1:E:733:ASN:ND2	2.49	0.61
1:C:41:VAL:HG22	1:C:47:GLN:HG3	1.81	0.60
1:C:484:TYR:HD2	1:C:486:ASN:ND2	1.99	0.60
1:C:507:PHE:CD2	1:C:587:MSE:HE2	2.36	0.60
1:E:368:LYS:O	1:E:425:VAL:HG22	2.01	0.60
1:B:539:LEU:O	1:B:540:HIS:HB3	2.01	0.60
1:C:269:PHE:CE2	1:C:587:MSE:HE1	2.36	0.60
1:B:41:VAL:HG12	1:B:47:GLN:HG2	1.83	0.60
1:B:290:ILE:HG13	1:B:340:LEU:HD11	1.83	0.60
1:E:390:THR:CG2	1:E:429:ASP:H	2.14	0.60
1:F:703:VAL:CG2	1:F:712:PHE:HB3	2.30	0.60
1:B:638:LEU:HD12	1:B:639:TRP:HE3	1.66	0.60
1:C:474:LYS:C	1:C:476:PRO:HD3	2.22	0.60
1:D:246:THR:CG2	1:D:249:ALA:H	2.14	0.60
1:A:32:MSE:HE1	1:A:102:GLU:C	2.22	0.60
1:B:641:ASN:HD22	1:B:757:GLN:CG	2.15	0.60
1:C:283:GLU:HA	1:C:331:MSE:CE	2.30	0.60
1:D:273:LEU:HD11	1:D:289:PHE:CE2	2.36	0.60
1:E:18:HIS:O	1:E:38:PRO:HA	2.01	0.60
1:E:609:MSE:HE2	1:E:609:MSE:HA	1.82	0.60
1:F:248:LYS:HD2	1:F:585:THR:HG23	1.82	0.60
1:F:698:GLU:OE1	1:F:715:LYS:HD3	2.02	0.60
1:B:497:GLY:O	1:B:500:ILE:HG22	2.02	0.60
1:C:61:GLN:HA	1:C:90:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.37	0.60
1:D:512:ILE:HD11	1:D:531:GLY:HA3	1.84	0.60
1:A:41:VAL:HG22	1:A:47:GLN:HG2	1.83	0.60
1:A:205:GLY:O	1:A:244:GLY:O	2.20	0.60
1:B:1:MSE:HE1	1:B:149:TYR:CZ	2.37	0.60
1:C:485:ALA:HB1	1:C:519:ALA:CB	2.32	0.60
1:E:342:ILE:HD11	1:E:409:GLY:O	2.02	0.60
1:A:32:MSE:HE3	1:A:103:PHE:HB2	1.83	0.59
1:A:511:ASP:OD1	1:A:540:HIS:HD2	1.85	0.59
1:B:744:VAL:HG13	1:B:772:LEU:HA	1.84	0.59
1:E:738:LEU:H	1:E:738:LEU:HD22	1.66	0.59
1:A:246:THR:HG22	1:A:249:ALA:N	2.12	0.59
1:B:300:LEU:CD1	1:B:340:LEU:HD21	2.32	0.59
1:E:72:PHE:H	1:E:235:GLU:HG3	1.66	0.59
1:C:123:LEU:N	1:C:123:LEU:HD22	2.16	0.59
1:F:361:GLN:HG3	1:F:374:LEU:HD11	1.83	0.59
1:A:150:MSE:HE3	1:A:235:GLU:C	2.22	0.59
1:D:274:THR:O	1:D:541:GLY:N	2.35	0.59
1:D:342:ILE:HD11	1:D:410:VAL:HG22	1.85	0.59
1:C:591:MSE:HE2	1:C:608:TYR:N	2.17	0.59
1:C:698:GLU:CD	1:C:715:LYS:HD3	2.23	0.59
1:E:273:LEU:HD22	1:E:300:LEU:HD21	1.84	0.59
1:E:750:GLY:HA2	1:E:764:GLN:HG2	1.83	0.59
1:A:689:HIS:CD2	1:A:739:ARG:HH11	2.21	0.59
1:A:731:ALA:C	1:A:732:LYS:HD2	2.22	0.59
1:C:244:GLY:O	1:C:245:PRO:C	2.40	0.59
1:C:485:ALA:HB1	1:C:519:ALA:HB2	1.84	0.59
1:D:591:MSE:HE3	1:D:607:GLN:CG	2.21	0.59
1:B:591:MSE:HE1	1:B:608:TYR:CA	2.33	0.59
1:C:743:LYS:NZ	1:C:743:LYS:HB3	2.18	0.59
1:F:350:ILE:HD13	1:F:351:GLY:O	2.02	0.59
1:F:509:SER:HB3	1:F:536:HIS:HB2	1.85	0.59
1:A:297:ASN:O	1:A:299:PRO:HD3	2.02	0.59
1:E:283:GLU:CA	1:E:331:MSE:HE3	2.19	0.59
1:A:518:THR:HG22	1:A:519:ALA:N	2.17	0.59
1:B:328:PRO:CB	1:B:408:MSE:HE1	2.33	0.59
1:B:601:CYS:HA	1:B:604:LEU:HD22	1.85	0.59
1:C:290:ILE:HD11	1:C:338:LYS:HD2	1.84	0.59
1:C:744:VAL:HG11	1:C:770:ILE:HD11	1.83	0.59
1:F:265:PRO:CD	1:F:462:VAL:HG22	2.30	0.59
1:A:225:VAL:HG13	1:D:495:ARG:NH2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:PRO:O	1:C:646:GLY:HA3	2.02	0.58
1:E:748:GLN:HG3	1:E:769:THR:HB	1.84	0.58
1:F:367:LEU:CD1	1:F:425:VAL:HG11	2.32	0.58
1:F:500:ILE:HG12	1:F:505:PHE:HB2	1.85	0.58
1:B:111:ARG:HD2	3:B:1450:HOH:O	2.02	0.58
1:C:332:ILE:CD1	1:C:408:MSE:HE2	2.32	0.58
1:E:609:MSE:HE1	1:E:615:MSE:CA	2.33	0.58
1:F:79:GLY:CA	1:F:432:ASP:H	2.15	0.58
1:F:296:ARG:HH12	1:F:553:ASP:CG	2.07	0.58
1:A:169:PHE:O	1:D:225:VAL:HG11	2.04	0.58
1:A:244:GLY:O	1:A:245:PRO:C	2.42	0.58
1:A:273:LEU:CB	1:A:300:LEU:HD21	2.30	0.58
1:B:290:ILE:HD13	1:B:290:ILE:O	2.03	0.58
1:B:576:GLU:HA	1:B:579:ARG:HG3	1.86	0.58
1:D:749:ASP:O	1:D:764:GLN:HG3	2.03	0.58
1:B:674:ASN:HB3	1:B:680:TYR:CE1	2.37	0.58
1:C:283:GLU:O	1:C:287:ASN:HB2	2.03	0.58
1:F:350:ILE:HD11	1:F:354:SER:HB3	1.85	0.58
1:A:718:ARG:HB2	1:A:723:ILE:HG12	1.85	0.58
1:B:41:VAL:HG12	1:B:41:VAL:O	2.03	0.58
1:F:497:GLY:O	1:F:500:ILE:HG22	2.03	0.58
1:B:517:ASN:O	1:B:518:THR:HG23	2.04	0.58
1:E:72:PHE:HB2	1:E:235:GLU:CG	2.33	0.58
1:C:589:ARG:NH2	1:C:612:ASP:OD2	2.33	0.58
1:E:464:PHE:HE2	1:E:538:ARG:HD2	1.69	0.58
1:F:18:HIS:O	1:F:38:PRO:HA	2.02	0.58
1:A:419:GLU:OE2	1:A:466:ARG:HD2	2.04	0.57
1:B:750:GLY:N	1:B:764:GLN:HG2	2.19	0.57
1:C:495:ARG:NH2	1:F:225:VAL:CG1	2.66	0.57
1:A:293:MSE:HE2	1:A:549:TRP:CH2	2.39	0.57
1:A:332:ILE:HD12	1:A:408:MSE:CE	2.31	0.57
1:A:732:LYS:HD2	1:A:732:LYS:N	2.19	0.57
1:C:380:TRP:CH2	2:C:803:MES:H21	2.39	0.57
1:C:766:ASN:C	1:C:766:ASN:HD22	2.08	0.57
1:D:153:ARG:HG2	1:D:229:GLN:HB2	1.86	0.57
1:D:358:LYS:O	1:D:362:GLU:HG3	2.05	0.57
1:E:244:GLY:HA2	1:E:253:ARG:HH12	1.69	0.57
1:F:732:LYS:CE	1:F:733:ASN:H	2.16	0.57
1:A:43:GLU:HG2	1:A:46:TRP:HB2	1.86	0.57
1:A:601:CYS:HA	1:A:604:LEU:CD2	2.26	0.57
1:B:631:PRO:O	1:B:646:GLY:HA3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:PRO:CD	1:C:462:VAL:HG22	2.34	0.57
1:D:752:GLN:HG3	1:D:759:LEU:HD11	1.86	0.57
1:D:763:PRO:HB3	1:D:768:LEU:HD11	1.86	0.57
1:D:300:LEU:HD12	1:D:340:LEU:HD22	1.86	0.57
1:E:613:ASN:HD22	1:E:664:ARG:HD3	1.69	0.57
1:F:273:LEU:HD11	1:F:289:PHE:CE1	2.39	0.57
1:B:352:GLN:NE2	1:D:73:GLN:HG3	2.19	0.57
1:A:273:LEU:HD21	1:A:289:PHE:CE1	2.39	0.57
1:A:730:GLU:OE2	1:A:732:LYS:HE3	2.03	0.57
1:C:275:THR:HG21	1:C:280:ASN:HB3	1.86	0.57
1:E:347:ASN:C	1:E:347:ASN:ND2	2.58	0.57
1:F:237:LEU:CD1	1:F:239:TYR:HD2	2.17	0.57
1:A:474:LYS:O	1:A:476:PRO:HD3	2.05	0.57
1:E:265:PRO:HD2	1:E:462:VAL:HG22	1.85	0.57
1:E:273:LEU:HB3	1:E:300:LEU:HD11	1.86	0.57
1:E:463:LEU:O	1:E:477:VAL:HB	2.05	0.57
1:B:379:LYS:HA	1:B:379:LYS:CE	2.29	0.57
1:A:123:LEU:N	1:A:123:LEU:HD22	2.19	0.57
1:A:698:GLU:CD	1:A:715:LYS:HE2	2.25	0.57
1:C:495:ARG:HH21	1:F:225:VAL:CG1	2.18	0.57
1:C:535:SER:HA	1:C:587:MSE:HE3	1.86	0.57
1:E:123:LEU:N	1:E:123:LEU:HD22	2.20	0.57
1:E:243:ASP:CG	1:E:244:GLY:H	2.07	0.57
1:E:324:THR:O	1:E:326:PRO:HD3	2.05	0.57
1:A:516:GLU:HB3	1:A:543:LYS:NZ	2.20	0.57
1:E:72:PHE:HB2	1:E:235:GLU:HG2	1.85	0.57
1:D:509:SER:HB3	1:D:536:HIS:HB2	1.86	0.56
1:A:150:MSE:HG2	1:A:237:LEU:HB2	1.88	0.56
1:A:343:CYS:HB2	1:A:412:CYS:SG	2.45	0.56
1:A:494:LEU:HD12	1:A:588:MSE:HE3	1.87	0.56
1:B:265:PRO:HG3	1:B:459:GLU:O	2.05	0.56
1:C:48:LEU:HD12	1:C:49:ASP:HB2	1.86	0.56
1:C:748:GLN:HB3	1:C:769:THR:CG2	2.35	0.56
1:E:367:LEU:HD22	1:E:425:VAL:HG22	1.86	0.56
1:E:747:LEU:HD23	1:E:748:GLN:N	2.21	0.56
1:F:768:LEU:HD12	1:F:769:THR:H	1.69	0.56
1:B:554:GLU:O	1:B:558:VAL:HG23	2.06	0.56
1:D:28:GLN:HG3	1:D:56:ARG:HH12	1.69	0.56
1:B:301:HIS:HE2	1:B:677:ARG:HA	1.70	0.56
1:D:347:ASN:C	1:D:347:ASN:HD22	2.08	0.56
1:F:348:PRO:HD3	1:F:444:TYR:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:531:GLY:O	1:F:537:SER:HB3	2.05	0.56
1:C:8:TRP:C	1:C:9:LEU:HD12	2.26	0.56
1:D:571:PRO:HB2	1:D:670:ALA:O	2.06	0.56
1:E:195:LYS:HE2	1:E:478:HIS:HB3	1.87	0.56
1:F:347:ASN:HB2	1:F:348:PRO:HD2	1.88	0.56
1:F:443:ILE:HD12	1:F:444:TYR:H	1.70	0.56
1:A:46:TRP:HE3	1:A:46:TRP:HA	1.71	0.56
1:A:265:PRO:CD	1:A:462:VAL:HG22	2.36	0.56
1:A:689:HIS:HD2	1:A:739:ARG:HD3	1.71	0.56
1:B:195:LYS:HE2	1:B:478:HIS:HB3	1.87	0.56
1:D:690:LEU:HD11	1:D:693:LEU:CB	2.33	0.56
1:E:287:ASN:O	1:E:290:ILE:HG12	2.06	0.56
1:E:368:LYS:O	1:E:425:VAL:CG2	2.54	0.56
1:B:447:LEU:HD23	1:B:447:LEU:C	2.26	0.55
1:D:329:GLU:N	1:D:408:MSE:HE3	2.22	0.55
1:D:282:ASP:OD1	1:D:285:THR:HG23	2.06	0.55
1:E:512:ILE:CD1	1:E:531:GLY:HA3	2.35	0.55
1:F:482:ASP:O	1:F:483:CYS:HB2	2.06	0.55
1:A:16:LEU:CD2	1:A:140:VAL:HG22	2.36	0.55
1:A:367:LEU:HD21	1:A:425:VAL:CG1	2.36	0.55
1:D:265:PRO:HG3	1:D:460:GLU:HA	1.87	0.55
1:A:367:LEU:HD22	1:A:425:VAL:HG22	1.89	0.55
1:B:352:GLN:HA	1:B:357:PHE:CD1	2.42	0.55
1:C:526:ARG:HD2	1:C:619:VAL:HG22	1.89	0.55
1:E:295:GLU:C	1:E:297:ASN:H	2.08	0.55
1:E:381:GLN:HB2	1:E:384:LEU:HD12	1.88	0.55
1:A:367:LEU:HD22	1:A:425:VAL:CG2	2.37	0.55
1:C:279:THR:O	1:C:281:TYR:N	2.39	0.55
1:F:715:LYS:O	1:F:725:VAL:HA	2.07	0.55
1:A:41:VAL:HG21	1:C:313:PHE:HZ	1.72	0.55
1:A:146:GLN:HE21	1:A:146:GLN:HA	1.71	0.55
1:A:592:MSE:HE3	1:A:593:MSE:CA	2.37	0.55
1:A:698:GLU:OE2	1:A:715:LYS:HE2	2.06	0.55
1:D:133:GLN:O	1:D:136:ASN:HB2	2.06	0.55
1:D:485:ALA:HB1	1:D:519:ALA:N	2.21	0.55
1:C:703:VAL:HG12	1:C:712:PHE:HB3	1.87	0.55
1:B:244:GLY:O	1:B:246:THR:N	2.40	0.55
1:E:200:TYR:CE2	1:E:228:VAL:HG11	2.42	0.55
1:E:342:ILE:HD13	1:E:342:ILE:N	2.20	0.55
1:A:46:TRP:HA	1:A:46:TRP:CE3	2.41	0.55
1:A:195:LYS:NZ	1:A:478:HIS:HB3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:MSE:CE	1:C:607:GLN:HE21	2.16	0.55
1:D:165:LEU:HD13	1:D:200:TYR:HB3	1.88	0.55
1:D:273:LEU:HD11	1:D:289:PHE:HE2	1.71	0.55
1:E:134:VAL:O	1:E:135:LYS:HB2	2.06	0.55
1:E:265:PRO:CD	1:E:462:VAL:HG22	2.37	0.55
1:A:246:THR:HG23	3:A:1042:HOH:O	2.07	0.54
1:B:136:ASN:HB3	1:B:153:ARG:HB2	1.90	0.54
1:B:248:LYS:HG3	1:B:593:MSE:HE3	1.89	0.54
1:B:328:PRO:HB3	1:B:408:MSE:HE1	1.89	0.54
1:E:342:ILE:HD13	1:E:411:ASP:OD1	2.07	0.54
1:A:170:THR:CG2	1:A:177:GLN:OE1	2.56	0.54
1:C:67:VAL:O	1:C:238:GLU:HA	2.07	0.54
1:A:18:HIS:O	1:A:38:PRO:HA	2.08	0.54
1:B:28:GLN:HG3	1:B:56:ARG:NH1	2.22	0.54
1:B:108:LEU:HG	1:B:243:ASP:HB2	1.90	0.54
1:B:591:MSE:HG2	1:B:604:LEU:HD23	1.90	0.54
1:D:168:ARG:HB2	1:D:174:ARG:NH1	2.23	0.54
1:E:39:ARG:HH22	1:E:46:TRP:HB3	1.72	0.54
1:E:286:VAL:CG2	1:E:331:MSE:HE2	2.36	0.54
1:B:483:CYS:O	1:B:514:GLY:HA2	2.08	0.54
1:D:71:HIS:HD2	1:D:235:GLU:OE1	1.91	0.54
1:D:591:MSE:HE1	1:D:608:TYR:CA	2.37	0.54
1:E:464:PHE:CE2	1:E:538:ARG:HD2	2.43	0.54
1:A:617:ALA:HB3	1:A:660:PRO:HB2	1.89	0.54
1:D:742:VAL:HG23	1:D:743:LYS:H	1.73	0.54
1:F:379:LYS:HE2	1:F:379:LYS:HA	1.90	0.54
1:A:265:PRO:HG3	1:A:460:GLU:HA	1.90	0.54
1:A:377:TRP:CE2	1:A:379:LYS:HB2	2.43	0.54
1:C:745:ASN:C	1:C:745:ASN:HD22	2.11	0.54
1:D:390:THR:CG2	1:D:428:PHE:HB3	2.37	0.54
1:E:152:GLU:HB3	1:E:230:PHE:CE1	2.43	0.54
1:E:320:TRP:O	1:E:322:PRO:HD3	2.08	0.54
1:F:306:ASP:O	1:F:309:TRP:HD1	1.91	0.54
1:A:495:ARG:NH2	1:D:225:VAL:CG1	2.71	0.54
1:A:748:GLN:O	1:A:768:LEU:HB2	2.07	0.54
1:B:50:THR:O	1:F:382:PRO:HG3	2.07	0.54
1:B:287:ASN:HA	1:B:290:ILE:CG2	2.38	0.54
1:B:512:ILE:HD12	1:B:539:LEU:HA	1.90	0.54
1:A:146:GLN:HA	1:A:146:GLN:NE2	2.23	0.53
1:B:343:CYS:HB2	1:B:412:CYS:SG	2.48	0.53
1:F:367:LEU:HG	1:F:425:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:ASP:OD1	1:C:538:ARG:HD2	2.08	0.53
1:D:61:GLN:HB2	1:D:64:ILE:HD12	1.90	0.53
1:E:38:PRO:HG3	1:E:51:PRO:HD2	1.90	0.53
1:E:490:MSE:HE2	1:E:620:PHE:CE2	2.43	0.53
1:F:291:ASP:O	1:F:295:GLU:HG3	2.09	0.53
1:F:575:ARG:HG3	1:F:702:GLU:O	2.09	0.53
1:A:279:THR:HG22	1:A:279:THR:O	2.08	0.53
1:C:456:VAL:HG12	1:C:460:GLU:HB2	1.91	0.53
1:D:20:LEU:HD13	1:D:38:PRO:C	2.28	0.53
1:A:327:ASP:OD2	1:A:330:GLY:HA3	2.07	0.53
1:A:516:GLU:HB3	1:A:543:LYS:HZ2	1.72	0.53
1:C:41:VAL:O	1:C:41:VAL:HG13	2.07	0.53
1:D:723:ILE:HB	1:D:770:ILE:HB	1.90	0.53
1:E:273:LEU:HD21	1:E:289:PHE:CE1	2.44	0.53
1:E:752:GLN:HB2	1:E:759:LEU:HD11	1.89	0.53
1:E:768:LEU:HD23	1:E:769:THR:N	2.24	0.53
1:F:389:PHE:HB2	1:F:443:ILE:HD13	1.90	0.53
1:A:222:SER:O	1:D:191:GLU:HG2	2.08	0.53
1:A:283:GLU:HG3	1:A:331:MSE:CG	2.39	0.53
1:B:283:GLU:HG3	1:B:331:MSE:CG	2.39	0.53
1:B:473:GLN:HG2	1:B:504:GLY:O	2.09	0.53
1:D:265:PRO:HD2	1:D:462:VAL:HG22	1.90	0.53
1:F:601:CYS:HA	1:F:604:LEU:HD22	1.90	0.53
1:F:694:GLN:HB2	1:F:697:HIS:CD2	2.44	0.53
1:D:715:LYS:HB3	1:D:726:THR:HG22	1.89	0.53
1:C:282:ASP:H	1:C:285:THR:HG22	1.72	0.53
1:E:390:THR:HG21	1:E:427:TRP:HB3	1.89	0.53
1:E:390:THR:HG22	1:E:428:PHE:HB3	1.91	0.53
1:F:723:ILE:HB	1:F:770:ILE:HG13	1.90	0.53
1:A:668:LEU:HB3	1:A:701:CYS:HB2	1.91	0.53
1:F:31:GLU:OE2	1:F:56:ARG:HD3	2.09	0.53
1:F:246:THR:HG23	1:F:249:ALA:H	1.73	0.53
1:F:244:GLY:O	1:F:246:THR:N	2.42	0.53
1:A:20:LEU:HD22	1:A:134:VAL:HG22	1.90	0.53
1:A:511:ASP:OD2	1:A:538:ARG:HD2	2.09	0.53
1:B:246:THR:HG23	1:B:249:ALA:H	1.73	0.53
1:D:497:GLY:O	1:D:500:ILE:HG22	2.09	0.53
1:D:566:LYS:HG2	1:D:570:MSE:HE3	1.91	0.53
1:B:719:THR:O	1:B:722:THR:HG22	2.09	0.52
1:C:743:LYS:HA	1:C:759:LEU:CD1	2.38	0.52
1:D:617:ALA:O	1:D:660:PRO:HD2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:VAL:HG12	1:B:745:ASN:N	2.24	0.52
1:C:397:TRP:CZ2	1:C:401:LYS:HE3	2.43	0.52
1:E:201:MSE:HE2	1:E:502:LEU:O	2.08	0.52
1:D:332:ILE:O	1:D:336:LYS:HG3	2.10	0.52
1:B:714:LEU:HD21	1:B:725:VAL:CG1	2.40	0.52
1:F:187:GLY:HA2	1:F:482:ASP:OD2	2.09	0.52
1:E:730:GLU:HG3	1:E:730:GLU:O	2.09	0.52
1:F:310:MSE:SE	1:F:316:CYS:H	2.42	0.52
1:F:748:GLN:O	1:F:749:ASP:HB2	2.09	0.52
1:B:244:GLY:O	1:B:245:PRO:C	2.46	0.52
1:B:747:LEU:HD13	1:B:770:ILE:HG12	1.91	0.52
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.91	0.52
1:D:763:PRO:HB3	1:D:768:LEU:CD1	2.40	0.52
1:C:352:GLN:HA	1:C:357:PHE:CD1	2.45	0.52
1:D:283:GLU:HA	1:D:331:MSE:CE	2.40	0.52
1:E:359:GLU:O	1:E:363:LYS:HG2	2.08	0.52
1:E:594:GLU:HG3	1:E:609:MSE:HG3	1.90	0.52
1:E:595:PHE:CE1	1:E:631:PRO:HG2	2.45	0.52
1:A:150:MSE:CG	1:A:237:LEU:HB2	2.40	0.52
1:B:449:TRP:CH2	1:B:476:PRO:HD2	2.45	0.52
1:C:283:GLU:HA	1:C:331:MSE:HE3	1.91	0.52
1:D:160:GLU:HG3	1:D:204:ARG:HG2	1.92	0.52
1:D:348:PRO:HD3	1:D:444:TYR:CZ	2.45	0.52
1:B:80:PRO:HD3	1:B:436:MSE:HE2	1.91	0.52
1:C:195:LYS:HE2	1:C:478:HIS:HB3	1.92	0.52
1:A:310:MSE:SE	1:A:316:CYS:H	2.42	0.51
1:B:133:GLN:HB2	1:B:136:ASN:HD22	1.75	0.51
1:B:589:ARG:NH2	1:B:612:ASP:OD1	2.41	0.51
1:B:673:ASN:ND2	1:B:684:GLU:O	2.43	0.51
1:B:689:HIS:HD2	1:B:739:ARG:HD3	1.75	0.51
1:C:377:TRP:CE2	1:C:379:LYS:HB2	2.44	0.51
1:F:343:CYS:HB2	1:F:412:CYS:SG	2.50	0.51
1:C:190:THR:HA	1:F:223:GLU:O	2.10	0.51
1:C:225:VAL:CG1	1:F:495:ARG:NH2	2.74	0.51
1:C:390:THR:CG2	1:C:428:PHE:HB3	2.41	0.51
1:E:502:LEU:HD11	1:E:592:MSE:CE	2.37	0.51
1:C:50:THR:O	1:E:382:PRO:HG3	2.10	0.51
1:D:651:LYS:HD3	1:D:651:LYS:C	2.30	0.51
1:A:560:ARG:O	1:A:564:GLN:HG3	2.09	0.51
1:B:267:TRP:CE3	1:B:341:LYS:HG3	2.45	0.51
1:C:539:LEU:O	1:C:540:HIS:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:ILE:HG12	1:C:711:ILE:O	2.11	0.51
1:D:201:MSE:CE	1:D:502:LEU:O	2.59	0.51
1:D:569:MSE:HB3	1:D:573:LEU:HD22	1.91	0.51
1:F:338:LYS:HD3	1:F:339:GLY:N	2.26	0.51
1:A:265:PRO:HD2	1:A:462:VAL:HG22	1.93	0.51
1:D:352:GLN:HA	1:D:357:PHE:CD1	2.45	0.51
1:A:70:GLU:OE2	1:A:73:GLN:NE2	2.31	0.51
1:B:170:THR:HG22	1:E:225:VAL:HG12	1.92	0.51
1:B:225:VAL:HG11	1:E:492:GLU:HG2	1.92	0.51
1:C:535:SER:CB	1:C:587:MSE:HE3	2.40	0.51
1:E:20:LEU:HD12	1:E:38:PRO:O	2.11	0.51
1:A:382:PRO:HG3	1:E:50:THR:O	2.11	0.51
1:B:299:PRO:HG2	1:B:676:GLN:OE1	2.11	0.51
1:E:401:LYS:O	1:E:405:LEU:HD13	2.11	0.51
1:F:71:HIS:HD2	1:F:235:GLU:OE1	1.94	0.51
1:F:617:ALA:HB3	1:F:660:PRO:HB2	1.92	0.51
1:B:522:HIS:CE1	1:B:523:VAL:HG23	2.46	0.51
1:B:526:ARG:HD2	1:B:619:VAL:CG2	2.33	0.51
1:E:645:ASP:HB2	1:E:648:ARG:NH2	2.25	0.51
1:F:195:LYS:HB3	1:F:468:ALA:HB3	1.91	0.51
1:A:526:ARG:HD2	1:A:619:VAL:HB	1.93	0.51
1:B:724:THR:HG22	1:B:726:THR:HG23	1.93	0.51
1:C:269:PHE:HE2	1:C:587:MSE:CE	2.21	0.51
1:C:497:GLY:O	1:C:500:ILE:HG22	2.11	0.51
1:E:133:GLN:HB2	1:E:136:ASN:HD22	1.75	0.51
1:E:201:MSE:CE	1:E:502:LEU:O	2.59	0.51
1:E:512:ILE:HG12	1:E:538:ARG:O	2.10	0.51
1:C:194:TYR:CD2	1:C:466:ARG:HD3	2.46	0.51
1:E:44:ARG:HG3	1:E:44:ARG:HH11	1.75	0.51
1:F:244:GLY:O	1:F:245:PRO:C	2.49	0.51
1:F:332:ILE:HD12	1:F:408:MSE:CE	2.36	0.51
1:C:262:ALA:HB3	1:C:476:PRO:CG	2.39	0.50
1:D:20:LEU:HD13	1:D:38:PRO:O	2.11	0.50
1:D:742:VAL:HG23	1:D:743:LYS:N	2.26	0.50
1:A:329:GLU:N	1:A:408:MSE:HE3	2.26	0.50
1:C:436:MSE:CE	1:C:440:TYR:HA	2.41	0.50
1:F:273:LEU:HD13	1:F:273:LEU:C	2.31	0.50
1:B:291:ASP:O	1:B:295:GLU:HG3	2.11	0.50
1:D:347:ASN:HA	1:D:444:TYR:OH	2.11	0.50
1:E:282:ASP:OD1	1:E:285:THR:HB	2.11	0.50
1:F:293:MSE:HG3	1:F:300:LEU:HD12	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:GLN:O	1:B:749:ASP:C	2.50	0.50
1:E:390:THR:HG23	1:E:429:ASP:H	1.76	0.50
1:D:347:ASN:C	1:D:347:ASN:ND2	2.64	0.50
1:E:745:ASN:C	1:E:745:ASN:HD22	2.15	0.50
1:A:449:TRP:CH2	1:A:476:PRO:HD2	2.47	0.50
1:A:754:GLU:HG2	1:A:759:LEU:CD2	2.42	0.50
1:B:738:LEU:N	1:B:738:LEU:HD22	2.27	0.50
1:C:748:GLN:HB3	1:C:769:THR:HG23	1.94	0.50
1:D:18:HIS:O	1:D:38:PRO:HA	2.11	0.50
1:F:282:ASP:O	1:F:286:VAL:HG23	2.11	0.50
1:B:296:ARG:O	1:B:560:ARG:NH1	2.45	0.50
1:C:343:CYS:HB2	1:C:412:CYS:SG	2.51	0.50
1:C:664:ARG:O	1:C:667:THR:CG2	2.59	0.50
1:D:745:ASN:C	1:D:745:ASN:HD22	2.14	0.50
1:F:281:TYR:O	1:F:324:THR:HG23	2.11	0.50
1:F:695:ASP:OD1	1:F:720:GLY:N	2.45	0.50
1:A:73:GLN:HG3	1:C:352:GLN:NE2	2.26	0.50
1:A:244:GLY:C	1:A:246:THR:N	2.65	0.50
1:C:485:ALA:CB	1:C:519:ALA:HB2	2.40	0.50
1:E:344:VAL:HG21	1:E:405:LEU:HD23	1.94	0.50
1:E:456:VAL:HG12	1:E:460:GLU:CB	2.41	0.50
1:E:61:GLN:NE2	1:E:87:LEU:CD2	2.75	0.50
1:E:456:VAL:HG12	1:E:460:GLU:HB2	1.94	0.50
1:F:405:LEU:C	1:F:410:VAL:HG22	2.33	0.50
1:A:44:ARG:HH21	1:C:278:THR:CA	2.22	0.49
1:D:265:PRO:CD	1:D:462:VAL:HG22	2.41	0.49
1:F:742:VAL:HG13	1:F:743:LYS:HG3	1.94	0.49
1:A:308:PHE:CD1	1:A:308:PHE:C	2.86	0.49
1:A:718:ARG:O	1:A:718:ARG:HG3	2.10	0.49
1:A:745:ASN:C	1:A:745:ASN:HD22	2.14	0.49
1:A:768:LEU:HD13	1:A:768:LEU:N	2.25	0.49
1:B:277:PHE:O	1:B:278:THR:CB	2.57	0.49
1:C:273:LEU:HD13	1:C:273:LEU:C	2.32	0.49
1:B:379:LYS:HE2	1:B:379:LYS:CA	2.31	0.49
1:C:416:ASP:O	1:C:416:ASP:OD2	2.30	0.49
1:E:416:ASP:OD1	1:E:466:ARG:HD3	2.12	0.49
1:E:439:HIS:HD2	3:E:1490:HOH:O	1.94	0.49
1:B:108:LEU:HD11	1:B:241:VAL:HG12	1.94	0.49
1:B:134:VAL:O	1:B:135:LYS:HB2	2.12	0.49
1:C:591:MSE:CE	1:C:615:MSE:HG2	2.36	0.49
1:C:646:GLY:O	1:C:647:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:VAL:HG23	1:D:108:LEU:HD13	1.94	0.49
1:E:278:THR:HG22	1:E:308:PHE:CE2	2.47	0.49
1:F:201:MSE:CE	1:F:502:LEU:O	2.60	0.49
1:F:201:MSE:HE2	1:F:502:LEU:O	2.12	0.49
1:A:512:ILE:HD13	1:A:528:CYS:HA	1.95	0.49
1:B:273:LEU:HD13	1:B:274:THR:N	2.28	0.49
1:B:665:ASP:O	1:B:667:THR:HG23	2.13	0.49
1:B:686:THR:HG23	1:B:734:TRP:HB3	1.94	0.49
1:C:725:VAL:HB	1:C:768:LEU:HD13	1.94	0.49
1:D:195:LYS:CE	1:D:478:HIS:HB3	2.43	0.49
1:E:474:LYS:O	1:E:476:PRO:HD3	2.12	0.49
1:E:738:LEU:HD22	1:E:738:LEU:N	2.28	0.49
1:F:747:LEU:HD22	1:F:770:ILE:CG2	2.42	0.49
1:C:568:ARG:HG2	1:C:568:ARG:HH11	1.77	0.49
1:D:447:LEU:HD13	1:D:447:LEU:C	2.32	0.49
1:D:617:ALA:HB3	1:D:660:PRO:HB2	1.95	0.49
1:E:265:PRO:HG3	1:E:460:GLU:HA	1.95	0.49
1:C:332:ILE:O	1:C:336:LYS:HG3	2.13	0.49
1:D:262:ALA:HB3	1:D:476:PRO:CG	2.39	0.49
1:B:31:GLU:HG2	1:B:58:PHE:CB	2.37	0.49
1:B:100:TYR:CG	1:B:111:ARG:HD3	2.48	0.49
1:B:689:HIS:CD2	1:B:739:ARG:NH1	2.79	0.49
1:C:137:ASN:HB3	1:C:152:GLU:OE1	2.13	0.49
1:D:571:PRO:HG2	1:D:672:GLY:N	2.28	0.49
1:A:368:LYS:O	1:A:425:VAL:HG22	2.13	0.49
1:A:373:SER:HB3	1:E:76:LEU:CD2	2.38	0.49
1:C:244:GLY:O	1:C:246:THR:N	2.46	0.49
1:C:689:HIS:CE1	1:C:739:ARG:HH21	2.31	0.49
1:D:43:GLU:HB3	1:D:46:TRP:HD1	1.77	0.49
1:E:141:GLN:HA	1:E:148:ASN:HD22	1.78	0.49
1:A:134:VAL:O	1:A:135:LYS:HB2	2.13	0.48
1:C:275:THR:HG23	1:C:303:PHE:HZ	1.77	0.48
1:C:474:LYS:O	1:C:476:PRO:HD3	2.12	0.48
1:D:635:TRP:HB3	1:D:662:TYR:HB3	1.94	0.48
1:B:694:GLN:HB2	1:B:697:HIS:CD2	2.48	0.48
1:D:368:LYS:O	1:D:425:VAL:CG2	2.61	0.48
1:A:225:VAL:CG1	1:D:495:ARG:NH2	2.76	0.48
1:A:332:ILE:O	1:A:336:LYS:HG3	2.13	0.48
1:A:703:VAL:CG2	1:A:712:PHE:HB3	2.40	0.48
1:D:526:ARG:CD	1:D:619:VAL:HG22	2.43	0.48
1:E:65:VAL:HG21	1:E:108:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ALA:HB3	1:E:476:PRO:HG2	1.93	0.48
1:B:295:GLU:OE2	1:B:296:ARG:HG3	2.13	0.48
1:B:298:LEU:N	1:B:299:PRO:HD3	2.28	0.48
1:C:163:TYR:HB3	1:C:502:LEU:HD13	1.95	0.48
1:C:276:SER:HB2	1:C:279:THR:OG1	2.12	0.48
1:C:635:TRP:O	1:C:643:GLU:HA	2.14	0.48
1:A:41:VAL:HG22	1:A:47:GLN:CG	2.43	0.48
1:B:416:ASP:OD2	1:B:466:ARG:HD3	2.13	0.48
1:D:500:ILE:HG12	1:D:505:PHE:HB2	1.96	0.48
1:D:644:LEU:HG	1:D:650:HIS:CE1	2.48	0.48
1:D:744:VAL:HG22	1:D:759:LEU:CD2	2.43	0.48
1:E:44:ARG:HA	1:E:47:GLN:CG	2.44	0.48
1:E:261:PRO:HA	1:E:473:GLN:O	2.12	0.48
1:E:279:THR:O	1:E:279:THR:HG22	2.13	0.48
1:F:16:LEU:HD22	1:F:140:VAL:HG22	1.94	0.48
1:A:308:PHE:CD1	1:A:309:TRP:N	2.81	0.48
1:A:546:ARG:HG3	1:A:547:VAL:HG13	1.96	0.48
1:B:488:GLU:O	1:B:492:GLU:HG3	2.14	0.48
1:D:38:PRO:HG3	1:D:51:PRO:HD2	1.96	0.48
1:E:304:HIS:CD2	1:E:538:ARG:HH21	2.32	0.48
1:A:401:LYS:HB2	1:A:401:LYS:NZ	2.28	0.48
1:B:39:ARG:O	1:B:41:VAL:HG23	2.14	0.48
1:B:515:PHE:O	1:B:516:GLU:HB2	2.14	0.48
1:B:41:VAL:CG1	1:B:47:GLN:HG2	2.43	0.48
1:D:501:GLY:HA2	1:D:505:PHE:O	2.14	0.48
1:D:570:MSE:HE1	1:D:573:LEU:HD23	1.92	0.48
1:E:355:PRO:O	1:E:358:LYS:HE2	2.13	0.48
1:F:687:ALA:HA	1:F:735:THR:HG23	1.96	0.48
1:B:141:GLN:HA	1:B:148:ASN:HD22	1.78	0.48
1:C:536:HIS:HA	3:C:1154:HOH:O	2.13	0.48
1:F:405:LEU:O	1:F:410:VAL:HG22	2.13	0.48
1:B:651:LYS:HD3	1:B:652:GLN:N	2.29	0.48
1:C:265:PRO:HG3	1:C:459:GLU:O	2.13	0.48
1:F:425:VAL:CG1	1:F:426:GLN:H	2.26	0.48
1:B:156:LEU:HD11	1:B:228:VAL:HG23	1.95	0.47
1:C:517:ASN:HD22	1:C:517:ASN:HA	1.53	0.47
1:D:28:GLN:HE21	1:D:28:GLN:HA	1.79	0.47
1:D:201:MSE:HE2	1:D:251:LEU:HD21	1.94	0.47
1:E:512:ILE:HD11	1:E:531:GLY:HA3	1.95	0.47
1:F:38:PRO:HG3	1:F:51:PRO:HD2	1.95	0.47
1:A:262:ALA:HB3	1:A:476:PRO:CG	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASP:OD2	1:A:306:ASP:C	2.52	0.47
1:A:321:ASP:HB3	1:A:324:THR:OG1	2.13	0.47
1:D:200:TYR:CE2	1:D:228:VAL:HG11	2.49	0.47
1:D:591:MSE:HE1	1:D:607:GLN:C	2.34	0.47
1:E:290:ILE:HD11	1:E:338:LYS:NZ	2.28	0.47
1:E:733:ASN:HD22	1:E:733:ASN:H	1.59	0.47
1:F:406:VAL:HA	1:F:410:VAL:HG22	1.95	0.47
1:B:273:LEU:HD13	1:B:273:LEU:C	2.33	0.47
1:C:768:LEU:C	1:C:768:LEU:HD22	2.35	0.47
1:D:273:LEU:HD13	1:D:274:THR:N	2.29	0.47
1:E:78:ASN:O	1:E:435:LYS:HE3	2.14	0.47
1:F:262:ALA:HB3	1:F:476:PRO:CG	2.43	0.47
1:B:290:ILE:HD13	1:B:290:ILE:C	2.35	0.47
1:C:576:GLU:O	1:C:579:ARG:HB2	2.14	0.47
1:D:439:HIS:HD2	3:D:1125:HOH:O	1.96	0.47
1:D:712:PHE:HB2	1:D:730:GLU:O	2.13	0.47
1:E:526:ARG:CZ	1:E:619:VAL:HG21	2.45	0.47
1:A:280:ASN:HB2	1:A:308:PHE:CE2	2.50	0.47
1:A:502:LEU:CD1	1:A:592:MSE:HE2	2.29	0.47
1:A:695:ASP:HA	1:A:718:ARG:CG	2.44	0.47
1:C:186:GLY:HA3	1:C:192:GLN:HE21	1.79	0.47
1:C:200:TYR:CE2	1:C:228:VAL:HG11	2.49	0.47
1:D:377:TRP:CE2	1:D:379:LYS:HB2	2.49	0.47
1:D:684:GLU:CD	1:D:732:LYS:HD2	2.34	0.47
1:E:447:LEU:C	1:E:447:LEU:HD13	2.35	0.47
1:A:279:THR:CG2	1:A:546:ARG:NH1	2.75	0.47
1:A:453:LYS:NZ	1:A:453:LYS:HB3	2.29	0.47
1:B:123:LEU:HD23	1:B:128:ARG:HA	1.96	0.47
1:B:730:GLU:HG2	1:B:732:LYS:HE2	1.96	0.47
1:D:335:LEU:O	1:D:338:LYS:HB2	2.14	0.47
1:D:591:MSE:HE1	1:D:608:TYR:HA	1.95	0.47
1:E:41:VAL:HG22	1:E:41:VAL:O	2.14	0.47
1:E:101:ALA:HB3	1:E:112:VAL:CG1	2.45	0.47
1:F:275:THR:HG21	1:F:280:ASN:OD1	2.13	0.47
1:F:331:MSE:O	1:F:335:LEU:HG	2.14	0.47
1:A:310:MSE:CE	1:A:316:CYS:H	2.28	0.47
1:B:156:LEU:CD1	1:B:228:VAL:HG23	2.44	0.47
1:B:262:ALA:HB3	1:B:476:PRO:CG	2.43	0.47
1:C:283:GLU:HA	1:C:331:MSE:HE1	1.96	0.47
1:C:292:GLY:O	1:C:296:ARG:NH1	2.46	0.47
1:C:487:TYR:OH	1:C:522:HIS:HD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ILE:HG12	1:C:505:PHE:HB2	1.97	0.47
1:D:273:LEU:HD23	1:D:539:LEU:HB3	1.96	0.47
1:F:377:TRP:CE2	1:F:379:LYS:HB2	2.50	0.47
1:A:41:VAL:O	1:A:41:VAL:HG13	2.14	0.47
1:B:439:HIS:HD2	3:B:1268:HOH:O	1.98	0.47
1:C:29:ASP:O	1:C:30:ASN:HB2	2.15	0.47
1:C:279:THR:HA	1:C:281:TYR:CZ	2.50	0.47
1:D:668:LEU:HD13	1:D:690:LEU:HD23	1.97	0.47
1:E:80:PRO:HD3	1:E:431:SER:HB3	1.96	0.47
1:F:694:GLN:O	1:F:697:HIS:HB2	2.13	0.47
1:F:745:ASN:H	1:F:745:ASN:HD22	1.63	0.47
1:A:222:SER:O	1:D:191:GLU:CG	2.62	0.47
1:A:279:THR:O	1:A:279:THR:CG2	2.63	0.47
1:A:310:MSE:HE1	1:A:316:CYS:CA	2.44	0.47
1:E:243:ASP:CG	1:E:244:GLY:N	2.68	0.47
1:B:133:GLN:HB2	1:B:136:ASN:ND2	2.30	0.47
1:C:290:ILE:CD1	1:C:338:LYS:HD2	2.45	0.47
1:E:275:THR:OG1	1:E:280:ASN:ND2	2.48	0.47
1:F:364:GLY:HA2	3:F:1136:HOH:O	2.14	0.47
1:A:500:ILE:HG12	1:A:505:PHE:HB2	1.98	0.46
1:B:296:ARG:O	1:B:298:LEU:HG	2.14	0.46
1:D:419:GLU:HG3	1:D:467:SER:OG	2.15	0.46
1:F:345:TRP:CH2	1:F:347:ASN:ND2	2.83	0.46
1:B:651:LYS:HD3	1:B:651:LYS:C	2.36	0.46
1:C:183:ASN:HA	1:C:196:ASN:ND2	2.30	0.46
1:C:225:VAL:HG11	1:F:169:PHE:O	2.15	0.46
1:D:396:LYS:HB2	1:D:396:LYS:NZ	2.30	0.46
1:D:436:MSE:HE1	1:D:443:ILE:HD12	1.96	0.46
1:E:281:TYR:O	1:E:282:ASP:HB3	2.14	0.46
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.46	0.46
1:F:759:LEU:C	1:F:759:LEU:HD23	2.35	0.46
1:A:280:ASN:HB2	1:A:308:PHE:CZ	2.50	0.46
1:B:298:LEU:CD2	1:B:560:ARG:HB2	2.46	0.46
1:C:48:LEU:HD12	1:C:48:LEU:C	2.36	0.46
1:D:382:PRO:HG3	1:F:50:THR:O	2.16	0.46
1:D:738:LEU:N	1:D:738:LEU:HD22	2.29	0.46
1:F:165:LEU:HA	1:F:197:ILE:O	2.16	0.46
1:A:244:GLY:O	1:A:246:THR:N	2.49	0.46
1:A:735:THR:HG22	1:A:762:LYS:HG2	1.98	0.46
1:B:569:MSE:HB2	1:B:573:LEU:HD22	1.97	0.46
1:B:766:ASN:O	1:B:767:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ARG:HG2	1:C:229:GLN:HB2	1.96	0.46
1:D:390:THR:HG21	1:D:427:TRP:HB3	1.96	0.46
1:F:732:LYS:HE2	1:F:733:ASN:H	1.80	0.46
1:A:15:ASN:HB2	1:A:141:GLN:HE21	1.79	0.46
1:A:635:TRP:HB3	1:A:662:TYR:HB3	1.98	0.46
1:C:752:GLN:HB2	1:C:759:LEU:HD21	1.98	0.46
1:E:292:GLY:O	1:E:296:ARG:HD3	2.16	0.46
1:F:252:ASP:HA	1:F:583:ARG:O	2.14	0.46
1:F:526:ARG:CD	1:F:619:VAL:HG22	2.36	0.46
1:A:367:LEU:HD21	1:A:425:VAL:HG13	1.96	0.46
1:A:747:LEU:HD21	1:A:750:GLY:O	2.14	0.46
1:B:273:LEU:HD23	1:B:539:LEU:HB3	1.96	0.46
1:C:225:VAL:HG13	1:F:495:ARG:NH2	2.30	0.46
1:C:273:LEU:HD13	1:C:274:THR:N	2.31	0.46
1:C:488:GLU:O	1:C:492:GLU:HG3	2.15	0.46
1:F:552:ASP:OD1	1:F:554:GLU:N	2.48	0.46
1:B:80:PRO:HD3	1:B:431:SER:HB3	1.98	0.46
1:B:248:LYS:CG	1:B:593:MSE:HE3	2.46	0.46
1:B:591:MSE:HE1	1:B:608:TYR:HA	1.98	0.46
1:C:314:GLN:HB3	1:C:354:SER:HB2	1.97	0.46
1:C:331:MSE:HA	1:C:334:ARG:HH11	1.79	0.46
1:D:163:TYR:HB3	1:D:502:LEU:HD13	1.96	0.46
1:D:384:LEU:C	1:D:384:LEU:HD23	2.36	0.46
1:E:502:LEU:HD13	1:E:593:MSE:HE2	1.97	0.46
1:F:419:GLU:OE2	1:F:466:ARG:HD2	2.16	0.46
1:B:223:GLU:O	1:E:190:THR:HA	2.16	0.46
1:B:278:THR:HG23	1:D:44:ARG:CD	2.45	0.46
1:B:664:ARG:HG3	1:B:665:ASP:N	2.30	0.46
1:B:714:LEU:HD21	1:B:725:VAL:HG13	1.98	0.46
1:C:195:LYS:HB3	1:C:468:ALA:HB3	1.97	0.46
1:E:646:GLY:O	1:E:647:SER:HB2	2.16	0.46
1:A:734:TRP:CZ2	1:A:763:PRO:HG3	2.51	0.46
1:B:332:ILE:HG23	1:B:342:ILE:HG13	1.97	0.46
1:C:76:LEU:CD2	1:E:373:SER:HB3	2.33	0.46
1:C:296:ARG:HG3	1:C:296:ARG:HH11	1.79	0.46
1:C:402:LEU:HB3	1:C:451:VAL:HG11	1.98	0.46
1:D:41:VAL:HG22	1:D:47:GLN:HG2	1.98	0.46
1:D:512:ILE:HG21	1:D:528:CYS:SG	2.55	0.46
1:F:512:ILE:HD12	1:F:512:ILE:N	2.31	0.46
1:A:319:GLU:OE2	1:A:356:VAL:HG23	2.15	0.46
1:C:296:ARG:O	1:C:298:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:635:TRP:CH2	1:E:664:ARG:HB3	2.51	0.46
1:F:736:LEU:HD13	1:F:736:LEU:C	2.36	0.46
1:A:199:PHE:HE2	1:A:201:MSE:HE2	1.81	0.45
1:D:273:LEU:HD13	1:D:273:LEU:C	2.37	0.45
1:D:329:GLU:CA	1:D:408:MSE:HE3	2.46	0.45
1:E:65:VAL:CG2	1:E:108:LEU:HD22	2.46	0.45
1:E:137:ASN:HB3	1:E:152:GLU:OE2	2.16	0.45
1:E:160:GLU:HG3	1:E:204:ARG:HG2	1.98	0.45
1:E:183:ASN:HA	1:E:196:ASN:ND2	2.31	0.45
1:E:310:MSE:SE	1:E:316:CYS:H	2.48	0.45
1:C:463:LEU:O	1:C:477:VAL:HB	2.15	0.45
1:C:734:TRP:CH2	1:C:763:PRO:HG2	2.51	0.45
1:D:246:THR:HG22	1:D:249:ALA:N	2.21	0.45
1:D:310:MSE:SE	1:D:316:CYS:H	2.49	0.45
1:D:494:LEU:HD22	1:D:498:LEU:HG	1.98	0.45
1:E:397:TRP:CZ2	1:E:401:LYS:HE2	2.52	0.45
1:A:736:LEU:HD13	1:A:736:LEU:C	2.37	0.45
1:B:490:MSE:HE2	1:B:620:PHE:CE2	2.50	0.45
1:B:638:LEU:HD12	1:B:639:TRP:CE3	2.50	0.45
1:D:732:LYS:O	1:D:733:ASN:HB2	2.16	0.45
1:E:278:THR:HG22	1:E:308:PHE:CD2	2.50	0.45
1:F:367:LEU:HD11	1:F:425:VAL:CG1	2.44	0.45
1:A:191:GLU:HB3	1:D:222:SER:O	2.17	0.45
1:B:498:LEU:HD11	1:B:608:TYR:HB3	1.98	0.45
1:B:630:LEU:O	1:B:647:SER:N	2.49	0.45
1:D:408:MSE:HE2	1:D:408:MSE:HB3	1.81	0.45
1:F:719:THR:O	1:F:719:THR:HG23	2.16	0.45
1:A:273:LEU:HB3	1:A:300:LEU:HD11	1.96	0.45
1:B:591:MSE:HE3	1:B:607:GLN:HE21	1.81	0.45
1:C:133:GLN:O	1:C:136:ASN:HB2	2.17	0.45
1:D:753:ALA:O	1:D:759:LEU:HD12	2.17	0.45
1:E:182:TRP:CE3	1:E:215:CYS:HB2	2.52	0.45
1:C:390:THR:HG21	1:C:427:TRP:HB3	1.98	0.45
1:C:748:GLN:O	1:C:749:ASP:HB2	2.17	0.45
1:A:768:LEU:C	1:A:768:LEU:HD22	2.37	0.45
1:C:283:GLU:CD	1:C:326:PRO:HD2	2.37	0.45
1:C:449:TRP:CH2	1:C:476:PRO:HD2	2.52	0.45
1:D:718:ARG:HG3	1:D:723:ILE:HD13	1.99	0.45
1:D:725:VAL:HB	1:D:768:LEU:HB2	1.97	0.45
1:F:164:GLY:O	1:F:165:LEU:HB2	2.16	0.45
1:A:436:MSE:HE3	1:A:440:TYR:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ALA:HB2	1:A:701:CYS:SG	2.57	0.45
1:B:195:LYS:CE	1:B:478:HIS:HB3	2.46	0.45
1:B:252:ASP:HA	1:B:583:ARG:O	2.16	0.45
1:C:568:ARG:HG2	1:C:568:ARG:NH1	2.32	0.45
1:E:265:PRO:CG	1:E:460:GLU:HA	2.46	0.45
1:F:61:GLN:HB2	1:F:64:ILE:HD12	1.99	0.45
1:A:306:ASP:OD2	1:A:308:PHE:CD2	2.69	0.45
1:B:127:GLU:OE2	1:B:127:GLU:HA	2.16	0.45
1:B:287:ASN:CA	1:B:290:ILE:HG22	2.42	0.45
1:B:689:HIS:HD2	1:B:739:ARG:HH11	1.63	0.45
1:C:348:PRO:HG2	1:C:349:TYR:CE1	2.52	0.45
1:C:766:ASN:C	1:C:766:ASN:ND2	2.70	0.45
1:D:134:VAL:HG22	1:D:135:LYS:HG2	1.98	0.45
1:E:335:LEU:HD13	1:E:335:LEU:HA	1.86	0.45
1:F:490:MSE:HE2	1:F:620:PHE:CD2	2.52	0.45
1:B:524:TYR:OH	1:B:539:LEU:HD21	2.17	0.45
1:C:653:GLN:HE21	1:C:653:GLN:HB3	1.51	0.45
1:E:335:LEU:O	1:E:338:LYS:HB3	2.17	0.45
1:F:682:TRP:O	1:F:686:THR:HB	2.17	0.45
1:A:195:LYS:HZ2	1:A:478:HIS:HB3	1.81	0.44
1:A:276:SER:HA	1:A:541:GLY:O	2.17	0.44
1:B:673:ASN:HD22	1:B:685:GLY:HA3	1.82	0.44
1:B:674:ASN:HB3	1:B:680:TYR:CD1	2.52	0.44
1:E:265:PRO:HD2	1:E:462:VAL:CG2	2.46	0.44
1:E:290:ILE:O	1:E:293:MSE:HB2	2.17	0.44
1:F:78:ASN:HB3	1:F:79:GLY:H	1.41	0.44
1:F:568:ARG:NH1	1:F:672:GLY:O	2.50	0.44
1:F:695:ASP:HA	1:F:718:ARG:HD3	1.99	0.44
1:B:464:PHE:CE2	1:B:477:VAL:HG11	2.52	0.44
1:C:164:GLY:O	1:C:165:LEU:HB2	2.18	0.44
1:C:576:GLU:HG3	1:C:611:GLY:HA3	1.98	0.44
1:D:196:ASN:O	1:D:197:ILE:HD13	2.17	0.44
1:D:512:ILE:HD12	1:D:531:GLY:HA3	1.99	0.44
1:E:59:SER:HA	1:E:60:PRO:HD3	1.84	0.44
1:C:483:CYS:HB3	1:C:489:SER:OG	2.16	0.44
1:F:405:LEU:HB3	1:F:410:VAL:HG21	1.99	0.44
1:A:182:TRP:CE3	1:A:215:CYS:HB2	2.53	0.44
1:C:419:GLU:OE2	1:C:466:ARG:HD3	2.17	0.44
1:E:510:HIS:N	1:E:510:HIS:CD2	2.86	0.44
1:E:554:GLU:O	1:E:558:VAL:HG23	2.17	0.44
1:A:18:HIS:HB2	1:A:20:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:PRO:HB2	1:B:408:MSE:HE1	1.99	0.44
1:C:502:LEU:HD21	1:C:592:MSE:CE	2.45	0.44
1:D:25:VAL:HG21	1:D:114:LYS:HE2	1.99	0.44
1:E:67:VAL:O	1:E:238:GLU:HA	2.17	0.44
1:A:5:ASP:HB3	1:A:9:LEU:HB2	2.00	0.44
1:A:50:THR:O	1:C:382:PRO:HG3	2.18	0.44
1:A:194:TYR:CE2	1:A:466:ARG:HD3	2.53	0.44
1:B:93:THR:HG23	1:B:104:LYS:HB3	2.00	0.44
1:B:310:MSE:SE	1:B:316:CYS:H	2.51	0.44
1:B:453:LYS:NZ	1:B:458:GLU:HG3	2.32	0.44
1:B:755:SER:O	1:B:757:GLN:N	2.50	0.44
1:C:189:SER:OG	1:F:7:ASN:ND2	2.38	0.44
1:C:436:MSE:HE3	1:C:440:TYR:N	2.32	0.44
1:C:591:MSE:HE3	1:C:607:GLN:HG3	1.99	0.44
1:F:230:PHE:HE1	1:F:237:LEU:HD11	1.83	0.44
1:F:265:PRO:HG3	1:F:460:GLU:HA	1.99	0.44
1:C:276:SER:HB2	1:C:279:THR:CG2	2.48	0.44
1:D:80:PRO:HD3	1:D:431:SER:HB3	1.99	0.44
1:F:300:LEU:HD22	1:F:340:LEU:CD2	2.43	0.44
1:F:751:SER:HB3	1:F:762:LYS:HB3	2.00	0.44
1:C:278:THR:O	1:C:279:THR:HG23	2.17	0.44
1:D:402:LEU:HB3	1:D:451:VAL:HG11	2.00	0.44
1:E:388:ASP:C	1:E:390:THR:H	2.21	0.44
1:E:575:ARG:O	1:E:578:ALA:HB3	2.18	0.44
1:E:635:TRP:O	1:E:643:GLU:HA	2.18	0.44
1:F:725:VAL:CG1	1:F:768:LEU:HB3	2.46	0.44
1:A:160:GLU:HA	1:A:203:ASN:OD1	2.18	0.44
1:A:279:THR:HG23	1:A:546:ARG:HH12	1.81	0.44
1:A:517:ASN:CG	1:A:518:THR:H	2.22	0.44
1:C:309:TRP:HA	1:C:325:PHE:CE1	2.53	0.44
1:C:683:HIS:CD2	1:C:711:ILE:HD13	2.53	0.44
1:D:591:MSE:CE	1:D:608:TYR:HA	2.48	0.44
1:E:674:ASN:HB3	1:E:680:TYR:CE1	2.53	0.44
1:F:747:LEU:HD21	1:F:761:VAL:CG1	2.48	0.44
1:B:648:ARG:HG3	1:B:648:ARG:HH11	1.83	0.43
1:E:539:LEU:HD23	1:E:540:HIS:N	2.33	0.43
1:E:557:ASP:OD1	1:E:560:ARG:NH2	2.51	0.43
1:E:718:ARG:HD3	1:E:720:GLY:O	2.18	0.43
1:F:502:LEU:HD13	1:F:593:MSE:CE	2.48	0.43
1:A:598:ASP:HA	1:A:599:PRO:HD3	1.84	0.43
1:F:200:TYR:CE2	1:F:228:VAL:HG11	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:747:LEU:HD21	1:F:761:VAL:HG13	2.00	0.43
1:B:137:ASN:HB3	1:B:152:GLU:OE1	2.18	0.43
1:C:495:ARG:HH21	1:F:225:VAL:HG11	1.81	0.43
1:D:300:LEU:HD12	1:D:340:LEU:HD21	1.97	0.43
1:D:734:TRP:CH2	1:D:763:PRO:HG3	2.53	0.43
1:E:154:LEU:HD12	1:E:154:LEU:HA	1.84	0.43
1:E:748:GLN:HE21	1:E:748:GLN:HB3	1.60	0.43
1:F:598:ASP:HA	1:F:599:PRO:HD3	1.89	0.43
1:B:531:GLY:O	1:B:537:SER:HB3	2.18	0.43
1:C:617:ALA:O	1:C:660:PRO:HD2	2.18	0.43
1:E:16:LEU:CD2	1:E:140:VAL:HG22	2.45	0.43
1:E:191:GLU:OE2	1:E:191:GLU:N	2.44	0.43
1:E:475:PHE:N	1:E:476:PRO:HD3	2.32	0.43
1:F:134:VAL:O	1:F:135:LYS:HB2	2.18	0.43
1:A:137:ASN:HB3	1:A:152:GLU:OE1	2.18	0.43
1:C:723:ILE:HB	1:C:770:ILE:HG23	1.99	0.43
1:C:744:VAL:HG11	1:C:770:ILE:CD1	2.48	0.43
1:D:488:GLU:O	1:D:492:GLU:HG3	2.18	0.43
1:E:526:ARG:HD2	1:E:619:VAL:CG2	2.40	0.43
1:E:723:ILE:HB	1:E:770:ILE:HB	2.01	0.43
1:F:265:PRO:HD2	1:F:462:VAL:CG2	2.38	0.43
1:F:449:TRP:CH2	1:F:476:PRO:HD2	2.54	0.43
1:F:568:ARG:HG2	1:F:568:ARG:HH11	1.84	0.43
1:A:348:PRO:HD3	1:A:444:TYR:CZ	2.53	0.43
1:A:695:ASP:HA	1:A:718:ARG:HG3	2.00	0.43
1:A:754:GLU:HG2	1:A:759:LEU:HD21	2.01	0.43
1:B:18:HIS:O	1:B:38:PRO:HA	2.18	0.43
1:B:354:SER:HA	1:B:355:PRO:HD3	1.92	0.43
1:C:219:GLU:HB2	1:C:229:GLN:HB3	2.00	0.43
1:C:290:ILE:O	1:C:293:MSE:HB2	2.18	0.43
1:C:768:LEU:HD13	1:C:768:LEU:H	1.83	0.43
1:D:104:LYS:HE2	1:D:106:GLY:O	2.19	0.43
1:D:668:LEU:O	1:D:701:CYS:HB2	2.18	0.43
1:D:735:THR:OG1	1:D:760:VAL:HG13	2.19	0.43
1:D:744:VAL:HG22	1:D:759:LEU:HD21	2.00	0.43
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.54	0.43
1:F:743:LYS:HA	1:F:759:LEU:HD12	1.99	0.43
1:A:673:ASN:N	1:A:673:ASN:HD22	2.14	0.43
1:A:745:ASN:C	1:A:745:ASN:ND2	2.72	0.43
1:B:510:HIS:N	1:B:510:HIS:CD2	2.87	0.43
1:A:136:ASN:HB3	1:A:153:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LEU:HD13	1:A:447:LEU:C	2.39	0.43
1:A:498:LEU:O	1:A:502:LEU:HD23	2.19	0.43
1:A:734:TRP:CH2	1:A:763:PRO:HG3	2.53	0.43
1:B:755:SER:O	1:B:756:GLU:C	2.57	0.43
1:C:730:GLU:HA	1:C:730:GLU:OE2	2.19	0.43
1:D:401:LYS:HA	1:D:401:LYS:HD3	1.81	0.43
1:E:244:GLY:CA	1:E:253:ARG:HH12	2.31	0.43
1:E:479:TRP:CZ3	1:E:481:GLY:HA2	2.53	0.43
1:E:500:ILE:HG12	1:E:505:PHE:HB2	1.99	0.43
1:E:745:ASN:O	1:E:745:ASN:ND2	2.52	0.43
1:A:251:LEU:HD11	1:A:593:MSE:HE2	2.00	0.43
1:B:246:THR:OG1	1:B:247:PRO:HD2	2.19	0.43
1:B:313:PHE:HZ	1:D:41:VAL:HG21	1.84	0.43
1:B:557:ASP:OD2	1:B:560:ARG:NH2	2.52	0.43
1:C:282:ASP:H	1:C:285:THR:HG21	1.81	0.43
1:E:336:LYS:O	1:E:337:ALA:C	2.54	0.43
1:A:165:LEU:HA	1:A:197:ILE:O	2.19	0.43
1:A:320:TRP:O	1:A:322:PRO:HD3	2.19	0.43
1:B:29:ASP:CG	1:B:30:ASN:N	2.71	0.43
1:C:286:VAL:HG11	1:C:331:MSE:HE1	2.01	0.43
1:C:768:LEU:H	1:C:768:LEU:CD1	2.31	0.43
1:D:246:THR:HG22	1:D:249:ALA:CB	2.49	0.43
1:D:283:GLU:HA	1:D:331:MSE:HE3	2.01	0.43
1:E:367:LEU:HD13	1:E:425:VAL:HG21	2.01	0.43
1:F:475:PHE:N	1:F:476:PRO:HD3	2.33	0.43
1:A:28:GLN:O	1:A:29:ASP:HB2	2.19	0.42
1:A:377:TRP:HH2	1:A:420:ARG:HD3	1.82	0.42
1:E:498:LEU:O	1:E:502:LEU:HD22	2.19	0.42
1:F:635:TRP:HB3	1:F:662:TYR:HB3	2.00	0.42
1:A:200:TYR:CE2	1:A:228:VAL:HG11	2.53	0.42
1:A:306:ASP:O	1:A:309:TRP:HD1	2.03	0.42
1:A:348:PRO:HG2	1:A:349:TYR:CE2	2.54	0.42
1:B:384:LEU:C	1:B:384:LEU:HD23	2.40	0.42
1:C:641:ASN:OD1	1:C:739:ARG:HD2	2.18	0.42
1:D:152:GLU:HB3	1:D:230:PHE:CE1	2.54	0.42
1:D:745:ASN:H	1:D:745:ASN:ND2	2.17	0.42
1:E:720:GLY:C	1:E:721:ASN:HD22	2.22	0.42
1:F:379:LYS:O	1:F:380:TRP:HB3	2.19	0.42
1:A:2:LYS:HD3	1:A:2:LYS:HA	1.74	0.42
1:A:342:ILE:CG1	1:A:410:VAL:HA	2.49	0.42
1:B:172:LEU:HD22	3:B:1047:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:THR:HG23	1:C:303:PHE:CZ	2.53	0.42
1:C:390:THR:HG22	1:C:428:PHE:HB3	2.01	0.42
1:C:627:GLN:NE2	1:F:599:PRO:HG3	2.34	0.42
1:D:264:PRO:HG3	1:D:476:PRO:HB3	2.01	0.42
1:D:356:VAL:HG23	1:D:359:GLU:OE2	2.19	0.42
1:E:219:GLU:HB2	1:E:229:GLN:HB3	2.01	0.42
1:E:244:GLY:O	1:E:245:PRO:C	2.57	0.42
1:F:290:ILE:HD13	1:F:340:LEU:CD1	2.50	0.42
1:F:312:ALA:O	1:F:313:PHE:HB2	2.19	0.42
1:A:139:TYR:CD1	1:A:150:MSE:HE1	2.55	0.42
1:B:2:LYS:HA	1:B:223:GLU:OE2	2.18	0.42
1:B:41:VAL:HG11	1:F:313:PHE:HZ	1.84	0.42
1:B:750:GLY:HA2	1:B:764:GLN:H	1.83	0.42
1:C:16:LEU:CD2	1:C:140:VAL:HG22	2.47	0.42
1:C:87:LEU:HD22	1:C:87:LEU:N	2.35	0.42
1:C:617:ALA:HB3	1:C:660:PRO:HB2	2.01	0.42
1:D:378:ASP:OD2	1:F:71:HIS:HE1	2.02	0.42
1:D:479:TRP:CZ3	1:D:481:GLY:HA2	2.54	0.42
1:B:641:ASN:ND2	1:B:757:GLN:CG	2.71	0.42
1:F:627:GLN:HA	1:F:650:HIS:O	2.20	0.42
1:B:76:LEU:HG	1:F:373:SER:HB3	2.02	0.42
1:C:225:VAL:CG1	1:F:495:ARG:HH21	2.33	0.42
1:C:490:MSE:HE2	1:C:620:PHE:CE2	2.55	0.42
1:C:591:MSE:HE2	1:C:608:TYR:HA	2.00	0.42
1:D:320:TRP:O	1:D:322:PRO:HD3	2.20	0.42
1:F:237:LEU:HD13	1:F:237:LEU:C	2.40	0.42
1:A:310:MSE:CE	1:A:318:PHE:H	2.32	0.42
1:A:310:MSE:HE2	1:A:310:MSE:HB3	1.89	0.42
1:B:570:MSE:HG3	1:B:678:PRO:HA	2.02	0.42
1:C:348:PRO:HD3	1:C:444:TYR:CZ	2.55	0.42
1:E:306:ASP:HA	2:E:805:MES:O2S	2.19	0.42
1:A:299:PRO:HB3	1:A:676:GLN:O	2.20	0.42
1:A:588:MSE:HG3	1:A:608:TYR:CD2	2.54	0.42
1:B:64:ILE:CD1	1:B:242:ILE:HD12	2.50	0.42
1:B:273:LEU:HD11	1:B:289:PHE:CE1	2.55	0.42
1:D:685:GLY:HA2	1:D:733:ASN:O	2.20	0.42
1:E:277:PHE:C	1:E:278:THR:HG23	2.40	0.42
1:E:582:ALA:O	1:E:583:ARG:HD2	2.20	0.42
1:A:310:MSE:HE1	1:A:318:PHE:H	1.85	0.42
1:A:342:ILE:HG13	1:A:410:VAL:HA	2.01	0.42
1:B:219:GLU:HB2	1:B:229:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:CG1	1:E:492:GLU:HG2	2.49	0.42
1:B:521:ALA:O	1:B:525:LYS:HG3	2.20	0.42
1:C:123:LEU:HD13	1:C:128:ARG:HA	2.02	0.42
1:C:364:GLY:HA2	3:C:1069:HOH:O	2.19	0.42
1:D:1:MSE:HE1	1:D:149:TYR:CZ	2.55	0.42
1:D:715:LYS:HG2	1:D:716:ALA:N	2.34	0.42
1:A:282:ASP:OD2	1:A:285:THR:HG23	2.20	0.42
1:B:539:LEU:HB3	1:B:540:HIS:H	1.73	0.42
1:C:43:GLU:O	1:C:45:THR:O	2.38	0.42
1:C:225:VAL:HG13	1:F:495:ARG:HH21	1.84	0.42
1:E:41:VAL:CG2	1:E:47:GLN:HA	2.50	0.42
1:E:208:VAL:HA	1:E:240:PHE:O	2.20	0.42
1:A:718:ARG:HD2	1:A:720:GLY:O	2.19	0.41
1:B:416:ASP:OD2	1:B:416:ASP:O	2.38	0.41
1:B:591:MSE:HE1	1:B:607:GLN:C	2.40	0.41
1:C:380:TRP:HH2	2:C:803:MES:H21	1.83	0.41
1:D:71:HIS:CD2	1:D:235:GLU:OE1	2.72	0.41
1:D:519:ALA:HB3	1:D:520:PRO:CD	2.41	0.41
1:D:589:ARG:HG2	1:D:593:MSE:SE	2.70	0.41
1:E:273:LEU:HD21	1:E:289:PHE:HE1	1.82	0.41
1:E:296:ARG:HB3	1:E:298:LEU:HD23	2.01	0.41
1:E:377:TRP:CE2	1:E:379:LYS:HB2	2.55	0.41
1:A:300:LEU:HD22	1:A:300:LEU:HA	1.90	0.41
1:A:308:PHE:C	1:A:308:PHE:HD1	2.23	0.41
1:A:323:LEU:HD22	1:A:323:LEU:N	2.35	0.41
1:A:742:VAL:O	1:A:759:LEU:HD23	2.21	0.41
1:B:331:MSE:HA	1:B:334:ARG:NH1	2.35	0.41
1:C:55:LEU:HG	1:C:69:ILE:HG12	2.02	0.41
1:C:296:ARG:NH1	1:C:296:ARG:HG3	2.35	0.41
1:D:641:ASN:HD21	1:D:757:GLN:HG2	1.85	0.41
1:E:136:ASN:HB3	1:E:153:ARG:HB2	2.01	0.41
1:E:295:GLU:C	1:E:297:ASN:N	2.74	0.41
1:F:566:LYS:HA	1:F:569:MSE:CE	2.45	0.41
1:A:20:LEU:O	1:A:118:TRP:HB2	2.21	0.41
1:B:539:LEU:O	1:B:540:HIS:CB	2.68	0.41
1:C:384:LEU:C	1:C:384:LEU:HD23	2.41	0.41
1:D:570:MSE:HG3	1:D:678:PRO:HA	2.02	0.41
1:F:137:ASN:HB3	1:F:152:GLU:CD	2.41	0.41
1:F:220:VAL:HG13	1:F:228:VAL:HG22	2.00	0.41
1:B:463:LEU:O	1:B:464:PHE:HD2	2.03	0.41
1:C:524:TYR:OH	1:C:539:LEU:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:SER:CA	1:C:587:MSE:HE3	2.49	0.41
1:D:76:LEU:HD12	1:D:76:LEU:HA	1.82	0.41
1:D:352:GLN:NE2	1:F:73:GLN:HG3	2.35	0.41
1:E:388:ASP:OD1	1:E:390:THR:HB	2.20	0.41
1:E:552:ASP:N	1:E:555:SER:HG	2.18	0.41
1:F:669:LEU:HD23	1:F:669:LEU:HA	1.92	0.41
1:A:689:HIS:CD2	1:A:739:ARG:HD3	2.52	0.41
1:A:752:GLN:HB2	1:A:759:LEU:CD1	2.51	0.41
1:C:20:LEU:O	1:C:118:TRP:HB2	2.21	0.41
1:C:272:TRP:HB2	1:C:538:ARG:HA	2.01	0.41
1:C:665:ASP:O	1:C:667:THR:HG22	2.21	0.41
1:E:358:LYS:O	1:E:362:GLU:HG3	2.21	0.41
1:F:425:VAL:HG13	1:F:426:GLN:H	1.86	0.41
1:A:306:ASP:OD2	1:A:307:CYS:N	2.54	0.41
1:A:342:ILE:HD11	1:A:410:VAL:HG12	2.03	0.41
1:B:378:ASP:OD1	1:D:71:HIS:HE1	2.04	0.41
1:C:80:PRO:HD3	1:C:431:SER:HB3	2.02	0.41
1:C:610:LEU:HD23	1:C:610:LEU:HA	1.94	0.41
1:D:749:ASP:O	1:D:763:PRO:HA	2.21	0.41
1:F:345:TRP:HH2	1:F:347:ASN:ND2	2.18	0.41
1:A:265:PRO:HG3	1:A:459:GLU:O	2.20	0.41
1:A:318:PHE:HB2	1:A:401:LYS:HG2	2.02	0.41
1:B:475:PHE:N	1:B:476:PRO:HD3	2.34	0.41
1:B:649:TRP:CD1	1:E:600:ALA:HB2	2.55	0.41
1:C:121:ASP:OD1	1:C:128:ARG:HD2	2.20	0.41
1:C:173:VAL:HB	3:C:1086:HOH:O	2.20	0.41
1:C:281:TYR:N	1:C:285:THR:HG21	2.35	0.41
1:D:82:TYR:CE2	1:D:470:VAL:HB	2.55	0.41
1:D:309:TRP:CE2	1:D:310:MSE:HE2	2.55	0.41
1:E:290:ILE:HD11	1:E:338:LYS:HZ2	1.85	0.41
1:F:182:TRP:CE3	1:F:215:CYS:HB2	2.55	0.41
1:F:232:VAL:HG12	1:F:237:LEU:HD23	2.03	0.41
1:F:246:THR:HG23	1:F:249:ALA:CB	2.50	0.41
1:F:262:ALA:O	1:F:264:PRO:HD3	2.21	0.41
1:F:358:LYS:HE2	1:F:358:LYS:HB3	1.91	0.41
1:A:380:TRP:CH2	2:A:801:MES:H21	2.55	0.41
1:A:518:THR:CG2	1:A:519:ALA:H	2.28	0.41
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.85	0.41
1:B:591:MSE:CE	1:B:608:TYR:HA	2.51	0.41
1:C:262:ALA:HB3	1:C:476:PRO:CD	2.51	0.41
1:C:327:ASP:OD2	1:C:330:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:GLY:HA2	1:C:586:PRO:HA	2.02	0.41
1:D:275:THR:HA	1:D:541:GLY:HA3	2.02	0.41
1:E:286:VAL:O	1:E:290:ILE:HG23	2.21	0.41
1:F:569:MSE:HB2	1:F:573:LEU:HD22	2.02	0.41
1:F:664:ARG:HG2	1:F:665:ASP:N	2.36	0.41
1:F:723:ILE:HB	1:F:770:ILE:CG1	2.50	0.41
1:A:296:ARG:HD2	1:A:549:TRP:CZ3	2.56	0.41
1:B:41:VAL:HG12	1:B:47:GLN:CG	2.50	0.41
1:B:161:THR:O	1:B:202:THR:HA	2.20	0.41
1:B:273:LEU:HD23	1:B:539:LEU:HD13	2.03	0.41
1:B:764:GLN:O	1:B:764:GLN:HG3	2.19	0.41
1:D:354:SER:HA	1:D:355:PRO:HD3	1.86	0.41
1:F:17:ILE:HG13	1:F:53:PHE:HZ	1.85	0.41
1:F:354:SER:HA	1:F:355:PRO:HD3	1.90	0.41
1:F:510:HIS:CD2	1:F:510:HIS:N	2.89	0.41
1:A:519:ALA:O	1:A:551:TYR:HE2	2.04	0.41
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.21	0.41
1:B:243:ASP:CG	1:B:244:GLY:H	2.25	0.41
1:C:267:TRP:CE3	1:C:341:LYS:HG3	2.56	0.41
1:D:273:LEU:HD22	1:D:274:THR:H	1.86	0.41
1:D:283:GLU:HA	1:D:331:MSE:HE1	2.02	0.41
1:F:341:LYS:O	1:F:342:ILE:HD12	2.21	0.41
1:F:745:ASN:HD22	1:F:745:ASN:C	2.24	0.41
1:F:745:ASN:HD22	1:F:745:ASN:N	2.19	0.41
1:B:377:TRP:NE1	1:B:379:LYS:HB2	2.36	0.40
1:B:569:MSE:CB	1:B:573:LEU:HD22	2.51	0.40
1:B:744:VAL:HG11	1:B:770:ILE:CG2	2.51	0.40
1:B:772:LEU:H	1:B:772:LEU:CD2	2.31	0.40
1:C:199:PHE:CE2	1:C:201:MSE:HG3	2.56	0.40
1:C:306:ASP:O	1:C:309:TRP:HD1	2.04	0.40
1:C:381:GLN:CA	1:C:381:GLN:HE21	2.34	0.40
1:C:408:MSE:HE2	1:C:408:MSE:HB3	1.96	0.40
1:C:512:ILE:HD12	1:C:539:LEU:HD22	2.02	0.40
1:E:609:MSE:HE2	1:E:609:MSE:CA	2.49	0.40
1:E:749:ASP:C	1:E:764:GLN:HG2	2.42	0.40
1:F:78:ASN:HD22	1:F:78:ASN:HA	1.70	0.40
1:A:20:LEU:HD22	1:A:134:VAL:CG2	2.50	0.40
1:A:79:GLY:HA3	1:A:432:ASP:HB3	2.03	0.40
1:A:306:ASP:CG	1:A:308:PHE:CD2	2.95	0.40
1:D:156:LEU:HD13	1:D:228:VAL:HG23	2.03	0.40
1:E:221:GLY:HA2	1:E:224:LYS:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLN:HB2	1:A:354:SER:CB	2.44	0.40
1:A:495:ARG:HH21	1:D:225:VAL:CG1	2.33	0.40
1:A:579:ARG:HH21	1:A:579:ARG:HG2	1.87	0.40
1:B:183:ASN:HA	1:B:196:ASN:ND2	2.36	0.40
1:E:271:LEU:O	1:E:271:LEU:HD13	2.22	0.40
1:E:309:TRP:CE2	1:E:310:MSE:HE2	2.57	0.40
1:F:408:MSE:HE2	1:F:408:MSE:HB3	1.92	0.40
1:A:19:PRO:HD2	1:A:137:ASN:OD1	2.22	0.40
1:A:275:THR:O	1:A:276:SER:C	2.59	0.40
1:A:381:GLN:HB2	1:A:384:LEU:HD12	2.03	0.40
1:A:475:PHE:N	1:A:476:PRO:HD3	2.36	0.40
1:A:497:GLY:C	1:A:588:MSE:HE2	2.41	0.40
1:A:674:ASN:HB3	1:A:680:TYR:CZ	2.57	0.40
1:B:312:ALA:O	1:B:313:PHE:HB2	2.22	0.40
1:C:39:ARG:NH2	1:C:50:THR:HB	2.37	0.40
1:C:748:GLN:HB3	1:C:769:THR:HG22	2.03	0.40
1:D:754:GLU:OE2	1:D:759:LEU:HD13	2.21	0.40
1:E:326:PRO:O	1:E:328:PRO:HD3	2.21	0.40
1:E:347:ASN:HB2	1:E:348:PRO:HD2	2.03	0.40
1:E:669:LEU:HD13	1:E:670:ALA:N	2.37	0.40
1:F:195:LYS:CE	1:F:478:HIS:HB3	2.45	0.40
1:F:264:PRO:HA	1:F:265:PRO:HD3	1.83	0.40
1:A:17:ILE:HG13	1:A:53:PHE:HZ	1.86	0.40
1:A:43:GLU:CD	1:A:46:TRP:HD1	2.25	0.40
1:A:43:GLU:CG	1:A:46:TRP:CD1	3.05	0.40
1:B:153:ARG:HG2	1:B:229:GLN:HB2	2.04	0.40
1:C:598:ASP:HA	1:C:599:PRO:HD3	1.86	0.40
1:D:749:ASP:HB3	1:D:764:GLN:HG3	2.03	0.40
1:E:293:MSE:HE2	1:E:296:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	770/772 (100%)	722 (94%)	39 (5%)	9 (1%)	13	19
1	B	756/772 (98%)	702 (93%)	40 (5%)	14 (2%)	8	10
1	C	750/772 (97%)	695 (93%)	46 (6%)	9 (1%)	13	19
1	D	751/772 (97%)	700 (93%)	39 (5%)	12 (2%)	9	13
1	E	749/772 (97%)	696 (93%)	45 (6%)	8 (1%)	14	20
1	F	751/772 (97%)	703 (94%)	38 (5%)	10 (1%)	12	17
All	All	4527/4632 (98%)	4218 (93%)	247 (6%)	62 (1%)	11	15

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ASP
1	B	539	LEU
1	B	749	ASP
1	B	767	ALA
1	C	29	ASP
1	D	29	ASP
1	D	277	PHE
1	D	748	GLN
1	F	482	ASP
1	A	316	CYS
1	A	517	ASN
1	A	766	ASN
1	B	516	GLU
1	C	280	ASN
1	C	476	PRO
1	D	476	PRO
1	D	541	GLY
1	E	29	ASP
1	E	79	GLY
1	E	476	PRO
1	E	729	GLY
1	E	768	LEU
1	F	339	GLY
1	B	476	PRO
1	B	518	THR
1	B	756	GLU
1	F	79	GLY
1	B	278	THR
1	B	316	CYS
1	B	692	ASN

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Mol	Chain	Res	Type
1	B	753	ALA
1	C	316	CYS
1	D	78	ASN
1	D	731	ALA
1	D	751	SER
1	E	338	LYS
1	F	476	PRO
1	F	749	ASP
1	A	477	VAL
1	A	692	ASN
1	B	477	VAL
1	C	692	ASN
1	D	477	VAL
1	E	477	VAL
1	E	749	ASP
1	F	316	CYS
1	F	477	VAL
1	C	244	GLY
1	C	477	VAL
1	D	79	GLY
1	F	483	CYS
1	A	79	GLY
1	B	245	PRO
1	F	245	PRO
1	A	328	PRO
1	A	476	PRO
1	F	244	GLY
1	C	245	PRO
1	D	681	VAL
1	D	765	GLY
1	A	244	GLY
1	C	225	VAL

5.3.2 Protein sidechains ⓘ

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	659/640 (103%)	613 (93%)	46 (7%)	15	24
1	B	649/640 (101%)	608 (94%)	41 (6%)	18	28
1	C	647/640 (101%)	602 (93%)	45 (7%)	15	24
1	D	647/640 (101%)	602 (93%)	45 (7%)	15	24
1	E	646/640 (101%)	605 (94%)	41 (6%)	18	28
1	F	646/640 (101%)	610 (94%)	36 (6%)	21	34
All	All	3894/3840 (101%)	3640 (94%)	254 (6%)	17	27

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	43	GLU
1	A	46	TRP
1	A	48	LEU
1	A	76	LEU
1	A	123	LEU
1	A	125	ASN
1	A	156	LEU
1	A	165	LEU
1	A	237	LEU
1	A	246	THR
1	A	263	LEU
1	A	300	LEU
1	A	308	PHE
1	A	316	CYS
1	A	347	ASN
1	A	360	LEU
1	A	367	LEU
1	A	377	TRP
1	A	393	ASP
1	A	401	LYS
1	A	402	LEU
1	A	425	VAL
1	A	452	LEU
1	A	462	VAL
1	A	464	PHE
1	A	510	HIS
1	A	517	ASN
1	A	527	TRP
1	A	533	LEU

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Mol	Chain	Res	Type
1	A	537	SER
1	A	538	ARG
1	A	573	LEU
1	A	592	MSE
1	A	604	LEU
1	A	653	GLN
1	A	668	LEU
1	A	673	ASN
1	A	686	THR
1	A	704	PRO
1	A	718	ARG
1	A	745	ASN
1	A	747	LEU
1	A	759	LEU
1	A	768	LEU
1	A	769	THR
1	B	9	LEU
1	B	48	LEU
1	B	60	PRO
1	B	108	LEU
1	B	116	GLU
1	B	120	LEU
1	B	156	LEU
1	B	165	LEU
1	B	172	LEU
1	B	263	LEU
1	B	290	ILE
1	B	295	GLU
1	B	300	LEU
1	B	316	CYS
1	B	367	LEU
1	B	377	TRP
1	B	452	LEU
1	B	473	GLN
1	B	476	PRO
1	B	494	LEU
1	B	498	LEU
1	B	510	HIS
1	B	516	GLU
1	B	539	LEU
1	B	573	LEU
1	B	589	ARG

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Mol	Chain	Res	Type
1	B	592	MSE
1	B	597	ASP
1	B	604	LEU
1	B	619	VAL
1	B	677	ARG
1	B	681	VAL
1	B	682	TRP
1	B	683	HIS
1	B	686	THR
1	B	704	PRO
1	B	711	ILE
1	B	714	LEU
1	B	719	THR
1	B	736	LEU
1	B	756	GLU
1	C	2	LYS
1	C	41	VAL
1	C	46	TRP
1	C	47	GLN
1	C	49	ASP
1	C	88	GLN
1	C	120	LEU
1	C	123	LEU
1	C	156	LEU
1	C	165	LEU
1	C	251	LEU
1	C	275	THR
1	C	286	VAL
1	C	298	LEU
1	C	316	CYS
1	C	340	LEU
1	C	377	TRP
1	C	381	GLN
1	C	390	THR
1	C	402	LEU
1	C	452	LEU
1	C	462	VAL
1	C	464	PHE
1	C	466	ARG
1	C	476	PRO
1	C	510	HIS
1	C	517	ASN

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Mol	Chain	Res	Type
1	C	537	SER
1	C	539	LEU
1	C	540	HIS
1	C	589	ARG
1	C	610	LEU
1	C	619	VAL
1	C	653	GLN
1	C	667	THR
1	C	673	ASN
1	C	677	ARG
1	C	686	THR
1	C	693	LEU
1	C	710	VAL
1	C	745	ASN
1	C	749	ASP
1	C	766	ASN
1	C	768	LEU
1	C	770	ILE
1	D	43	GLU
1	D	76	LEU
1	D	108	LEU
1	D	120	LEU
1	D	123	LEU
1	D	156	LEU
1	D	165	LEU
1	D	191	GLU
1	D	246	THR
1	D	278	THR
1	D	300	LEU
1	D	316	CYS
1	D	342	ILE
1	D	347	ASN
1	D	377	TRP
1	D	390	THR
1	D	402	LEU
1	D	458	GLU
1	D	459	GLU
1	D	462	VAL
1	D	463	LEU
1	D	464	PHE
1	D	467	SER
1	D	476	PRO

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Mol	Chain	Res	Type
1	D	494	LEU
1	D	537	SER
1	D	539	LEU
1	D	540	HIS
1	D	552	ASP
1	D	553	ASP
1	D	573	LEU
1	D	592	MSE
1	D	604	LEU
1	D	630	LEU
1	D	638	LEU
1	D	644	LEU
1	D	684	GLU
1	D	686	THR
1	D	704	PRO
1	D	732	LYS
1	D	735	THR
1	D	743	LYS
1	D	745	ASN
1	D	747	LEU
1	D	764	GLN
1	E	84	LEU
1	E	108	LEU
1	E	120	LEU
1	E	154	LEU
1	E	156	LEU
1	E	165	LEU
1	E	172	LEU
1	E	263	LEU
1	E	300	LEU
1	E	316	CYS
1	E	342	ILE
1	E	347	ASN
1	E	360	LEU
1	E	367	LEU
1	E	377	TRP
1	E	390	THR
1	E	452	LEU
1	E	462	VAL
1	E	463	LEU
1	E	464	PHE
1	E	476	PRO

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Mol	Chain	Res	Type
1	E	494	LEU
1	E	502	LEU
1	E	537	SER
1	E	573	LEU
1	E	583	ARG
1	E	592	MSE
1	E	619	VAL
1	E	634	ARG
1	E	638	LEU
1	E	651	LYS
1	E	686	THR
1	E	718	ARG
1	E	730	GLU
1	E	733	ASN
1	E	736	LEU
1	E	745	ASN
1	E	748	GLN
1	E	749	ASP
1	E	754	GLU
1	E	759	LEU
1	F	1	MSE
1	F	30	ASN
1	F	49	ASP
1	F	91	LYS
1	F	156	LEU
1	F	165	LEU
1	F	248	LYS
1	F	251	LEU
1	F	271	LEU
1	F	316	CYS
1	F	333	ARG
1	F	350	ILE
1	F	360	LEU
1	F	377	TRP
1	F	405	LEU
1	F	463	LEU
1	F	464	PHE
1	F	498	LEU
1	F	510	HIS
1	F	527	TRP
1	F	573	LEU
1	F	575	ARG

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Mol	Chain	Res	Type
1	F	592	MSE
1	F	604	LEU
1	F	610	LEU
1	F	613	ASN
1	F	619	VAL
1	F	676	GLN
1	F	686	THR
1	F	693	LEU
1	F	726	THR
1	F	732	LYS
1	F	735	THR
1	F	743	LYS
1	F	745	ASN
1	F	747	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	18	HIS
1	A	27	GLN
1	A	28	GLN
1	A	88	GLN
1	A	107	ASN
1	A	125	ASN
1	A	141	GLN
1	A	146	GLN
1	A	192	GLN
1	A	280	ASN
1	A	287	ASN
1	A	439	HIS
1	A	450	ASN
1	A	517	ASN
1	A	540	HIS
1	A	613	ASN
1	A	653	GLN
1	A	673	ASN
1	A	689	HIS
1	A	721	ASN
1	A	733	ASN
1	A	745	ASN
1	B	15	ASN

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Mol	Chain	Res	Type
1	B	27	GLN
1	B	28	GLN
1	B	73	GLN
1	B	78	ASN
1	B	107	ASN
1	B	125	ASN
1	B	141	GLN
1	B	148	ASN
1	B	192	GLN
1	B	361	GLN
1	B	439	HIS
1	B	450	ASN
1	B	564	GLN
1	B	613	ASN
1	B	689	HIS
1	B	697	HIS
1	B	748	GLN
1	C	15	ASN
1	C	28	GLN
1	C	73	GLN
1	C	77	ASN
1	C	107	ASN
1	C	125	ASN
1	C	141	GLN
1	C	146	GLN
1	C	192	GLN
1	C	445	ASN
1	C	450	ASN
1	C	517	ASN
1	C	522	HIS
1	C	627	GLN
1	C	653	GLN
1	C	673	ASN
1	C	697	HIS
1	C	733	ASN
1	C	745	ASN
1	C	766	ASN
1	D	28	GLN
1	D	71	HIS
1	D	88	GLN
1	D	192	GLN
1	D	347	ASN

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Mol	Chain	Res	Type
1	D	434	GLN
1	D	439	HIS
1	D	445	ASN
1	D	564	GLN
1	D	627	GLN
1	D	697	HIS
1	D	733	ASN
1	D	745	ASN
1	D	752	GLN
1	D	757	GLN
1	E	11	GLN
1	E	27	GLN
1	E	28	GLN
1	E	73	GLN
1	E	78	ASN
1	E	88	GLN
1	E	146	GLN
1	E	148	ASN
1	E	280	ASN
1	E	347	ASN
1	E	361	GLN
1	E	613	ASN
1	E	721	ASN
1	E	733	ASN
1	E	745	ASN
1	E	748	GLN
1	F	7	ASN
1	F	18	HIS
1	F	71	HIS
1	F	77	ASN
1	F	78	ASN
1	F	107	ASN
1	F	125	ASN
1	F	564	GLN
1	F	627	GLN
1	F	676	GLN
1	F	697	HIS
1	F	745	ASN
1	F	748	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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	$\# Z > 2$
2	MES	A	801	-	12,12,12	0.61	0	15,16,16	0.80	0
2	MES	B	802	-	12,12,12	0.52	0	15,16,16	0.70	0
2	MES	E	805	-	12,12,12	0.51	0	15,16,16	0.65	0
2	MES	C	803	-	12,12,12	0.50	0	15,16,16	0.71	0
2	MES	F	806	-	12,12,12	0.44	0	15,16,16	0.91	1 (6%)
2	MES	D	804	-	12,12,12	0.52	0	15,16,16	0.76	0

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
2	MES	A	801	-	-	3/6/14/14	0/1/1/1
2	MES	B	802	-	-	3/6/14/14	0/1/1/1
2	MES	E	805	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	C	803	-	-	3/6/14/14	0/1/1/1
2	MES	F	806	-	-	5/6/14/14	0/1/1/1
2	MES	D	804	-	-	6/6/14/14	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	806	MES	O1S-S-C8	-2.06	103.61	106.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	802	MES	C7-C8-S-O2S
2	B	802	MES	C7-C8-S-O3S
2	C	803	MES	C7-C8-S-O2S
2	C	803	MES	C7-C8-S-O3S
2	D	804	MES	N4-C7-C8-S
2	D	804	MES	C7-C8-S-O1S
2	D	804	MES	C7-C8-S-O3S
2	E	805	MES	C8-C7-N4-C3
2	E	805	MES	C8-C7-N4-C5
2	F	806	MES	C7-C8-S-O1S
2	F	806	MES	C7-C8-S-O2S
2	A	801	MES	C7-C8-S-O3S
2	D	804	MES	C8-C7-N4-C3
2	F	806	MES	C8-C7-N4-C5
2	F	806	MES	C7-C8-S-O3S
2	A	801	MES	C7-C8-S-O1S
2	A	801	MES	C7-C8-S-O2S
2	B	802	MES	C7-C8-S-O1S
2	C	803	MES	C7-C8-S-O1S
2	D	804	MES	C7-C8-S-O2S
2	D	804	MES	C8-C7-N4-C5
2	F	806	MES	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	MES	1	0
2	E	805	MES	1	0
2	C	803	MES	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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, 95th 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	753/772 (97%)	0.29	80 (10%) 6 5	29, 45, 79, 101	0
1	B	741/772 (95%)	0.33	62 (8%) 11 10	31, 45, 86, 102	0
1	C	737/772 (95%)	0.18	44 (5%) 21 20	30, 43, 75, 95	0
1	D	738/772 (95%)	0.19	59 (7%) 12 11	29, 42, 75, 100	0
1	E	736/772 (95%)	0.33	70 (9%) 8 7	31, 47, 79, 99	0
1	F	738/772 (95%)	0.39	76 (10%) 6 6	32, 48, 82, 100	0
All	All	4443/4632 (95%)	0.29	391 (8%) 10 9	29, 45, 79, 102	0

All (391) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	772	LEU	17.3
1	A	516	GLU	11.1
1	B	768	LEU	10.6
1	C	287	ASN	10.1
1	F	766	ASN	10.0
1	B	772	LEU	9.5
1	C	518	THR	9.4
1	F	767	ALA	9.4
1	F	765	GLY	9.2
1	D	765	GLY	9.2
1	F	552	ASP	8.6
1	B	89	ASP	8.5
1	E	484	TYR	8.3
1	B	298	LEU	7.9
1	F	281	TYR	7.7
1	B	389	PHE	7.2
1	C	300	LEU	7.2
1	B	41	VAL	7.1
1	A	517	ASN	7.1

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Mol	Chain	Res	Type	RSRZ
1	D	290	ILE	7.1
1	E	765	GLY	6.7
1	A	731	ALA	6.7
1	E	452	LEU	6.6
1	A	280	ASN	6.4
1	B	88	GLN	6.2
1	F	759	LEU	6.1
1	E	519	ALA	6.0
1	B	767	ALA	5.8
1	B	296	ARG	5.7
1	A	712	PHE	5.6
1	A	286	VAL	5.6
1	F	656	PHE	5.6
1	D	319	GLU	5.5
1	E	766	ASN	5.5
1	B	286	VAL	5.4
1	A	518	THR	5.4
1	C	297	ASN	5.4
1	F	553	ASP	5.4
1	A	772	LEU	5.3
1	F	744	VAL	5.2
1	A	284	ALA	5.1
1	E	276	SER	5.0
1	D	719	THR	5.0
1	B	302	VAL	5.0
1	A	745	ASN	5.0
1	F	289	PHE	5.0
1	E	42	ARG	4.9
1	F	314	GLN	4.8
1	A	89	ASP	4.8
1	E	767	ALA	4.8
1	B	295	GLU	4.7
1	F	745	ASN	4.7
1	C	770	ILE	4.7
1	F	706	ALA	4.6
1	C	519	ALA	4.6
1	C	276	SER	4.6
1	D	14	LEU	4.6
1	E	734	TRP	4.5
1	B	46	TRP	4.5
1	A	749	ASP	4.4
1	A	14	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	305	PHE	4.4
1	C	720	GLY	4.3
1	E	289	PHE	4.3
1	A	98	GLU	4.3
1	D	286	VAL	4.3
1	F	738	LEU	4.2
1	B	725	VAL	4.2
1	F	23	PHE	4.2
1	F	94	ILE	4.2
1	A	48	LEU	4.2
1	E	300	LEU	4.2
1	D	724	THR	4.2
1	F	521	ALA	4.2
1	C	767	ALA	4.1
1	A	543	LYS	4.1
1	E	768	LEU	4.1
1	E	485	ALA	4.1
1	E	290	ILE	4.1
1	D	91	LYS	4.1
1	E	108	LEU	4.0
1	E	89	ASP	4.0
1	F	535	SER	4.0
1	C	681	VAL	4.0
1	E	278	THR	4.0
1	E	764	GLN	3.9
1	D	484	TYR	3.9
1	D	552	ASP	3.9
1	E	461	ALA	3.9
1	E	320	TRP	3.9
1	B	718	ARG	3.9
1	E	772	LEU	3.9
1	C	733	ASN	3.9
1	E	759	LEU	3.8
1	F	404	GLY	3.8
1	A	291	ASP	3.8
1	B	297	ASN	3.8
1	C	772	LEU	3.7
1	F	315	TRP	3.7
1	A	305	PHE	3.7
1	D	721	ASN	3.7
1	D	690	LEU	3.7
1	D	46	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	553	ASP	3.6
1	E	234	SER	3.6
1	D	729	GLY	3.6
1	C	768	LEU	3.6
1	A	281	TYR	3.6
1	A	500	ILE	3.6
1	A	711	ILE	3.6
1	D	300	LEU	3.6
1	D	281	TYR	3.6
1	A	766	ASN	3.5
1	F	286	VAL	3.5
1	B	695	ASP	3.5
1	D	282	ASP	3.5
1	D	696	GLY	3.5
1	F	736	LEU	3.5
1	F	316	CYS	3.5
1	C	735	THR	3.5
1	B	734	TRP	3.5
1	C	275	THR	3.5
1	E	323	LEU	3.4
1	F	742	VAL	3.4
1	D	534	SER	3.4
1	C	517	ASN	3.4
1	D	738	LEU	3.4
1	B	736	LEU	3.4
1	D	659	LEU	3.3
1	B	477	VAL	3.3
1	A	393	ASP	3.3
1	C	91	LYS	3.3
1	B	657	LEU	3.3
1	A	734	TRP	3.3
1	B	288	SER	3.3
1	F	509	SER	3.3
1	D	477	VAL	3.3
1	A	732	LYS	3.3
1	E	725	VAL	3.3
1	B	714	LEU	3.2
1	C	296	ARG	3.2
1	E	112	VAL	3.2
1	A	501	GLY	3.2
1	A	290	ILE	3.2
1	C	277	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	771	THR	3.2
1	E	279	THR	3.2
1	D	764	GLN	3.2
1	E	44	ARG	3.2
1	F	273	LEU	3.2
1	D	27	GLN	3.2
1	D	394	ALA	3.2
1	C	656	PHE	3.2
1	F	290	ILE	3.2
1	A	87	LEU	3.2
1	E	76	LEU	3.2
1	B	682	TRP	3.2
1	D	718	ARG	3.2
1	A	285	THR	3.1
1	B	117	PHE	3.1
1	B	688	PHE	3.1
1	B	22	VAL	3.1
1	C	736	LEU	3.1
1	E	539	LEU	3.1
1	D	289	PHE	3.1
1	A	46	TRP	3.1
1	F	482	ASP	3.1
1	A	747	LEU	3.1
1	C	298	LEU	3.1
1	E	744	VAL	3.1
1	A	464	PHE	3.1
1	E	277	PHE	3.1
1	C	732	LYS	3.1
1	C	46	TRP	3.1
1	F	534	SER	3.1
1	E	714	LEU	3.1
1	A	22	VAL	3.1
1	F	464	PHE	3.1
1	D	695	ASP	3.1
1	A	515	PHE	3.0
1	D	634	ARG	3.0
1	A	244	GLY	3.0
1	D	292	GLY	3.0
1	B	738	LEU	3.0
1	F	279	THR	3.0
1	B	317	ASP	3.0
1	A	277	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	387	TYR	3.0
1	E	291	ASP	3.0
1	D	112	VAL	3.0
1	D	535	SER	3.0
1	A	539	LEU	3.0
1	E	577	ALA	3.0
1	A	308	PHE	2.9
1	F	729	GLY	2.9
1	C	616	VAL	2.9
1	F	465	ALA	2.9
1	B	105	SER	2.9
1	C	684	GLU	2.9
1	E	711	ILE	2.9
1	C	608	TYR	2.9
1	B	515	PHE	2.9
1	E	296	ARG	2.9
1	C	652	GLN	2.9
1	E	752	GLN	2.9
1	E	747	LEU	2.9
1	E	456	VAL	2.8
1	B	415	THR	2.8
1	D	26	GLU	2.8
1	D	116	GLU	2.8
1	F	280	ASN	2.8
1	A	333	ARG	2.8
1	F	487	TYR	2.8
1	D	53	PHE	2.8
1	A	717	ALA	2.8
1	F	89	ASP	2.8
1	F	760	VAL	2.8
1	B	766	ASN	2.8
1	F	681	VAL	2.7
1	D	464	PHE	2.7
1	D	374	LEU	2.7
1	F	761	VAL	2.7
1	B	623	ALA	2.7
1	D	386	ILE	2.7
1	B	43	GLU	2.7
1	B	127	GLU	2.7
1	A	730	GLU	2.7
1	C	524	TYR	2.7
1	D	454	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	275	THR	2.7
1	E	555	SER	2.7
1	E	100	TYR	2.7
1	D	497	GLY	2.7
1	A	512	ILE	2.7
1	F	244	GLY	2.7
1	F	631	PRO	2.7
1	B	305	PHE	2.6
1	F	484	TYR	2.6
1	B	319	GLU	2.6
1	E	535	SER	2.6
1	A	764	GLN	2.6
1	A	88	GLN	2.6
1	B	162	VAL	2.6
1	F	682	TRP	2.6
1	B	198	PRO	2.6
1	F	197	ILE	2.6
1	A	502	LEU	2.6
1	F	120	LEU	2.6
1	B	303	PHE	2.6
1	C	730	GLU	2.6
1	C	481	GLY	2.6
1	F	680	TYR	2.6
1	D	476	PRO	2.5
1	A	709	SER	2.5
1	B	244	GLY	2.5
1	F	708	GLY	2.5
1	A	458	GLU	2.5
1	F	648	ARG	2.5
1	A	145	ASN	2.5
1	B	243	ASP	2.5
1	F	554	GLU	2.5
1	F	91	LYS	2.5
1	E	79	GLY	2.5
1	E	634	ARG	2.5
1	F	523	VAL	2.5
1	E	476	PRO	2.5
1	A	113	SER	2.5
1	F	99	ARG	2.5
1	C	632	GLU	2.5
1	F	536	HIS	2.4
1	D	143	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	337	ALA	2.4
1	B	514	GLY	2.4
1	B	491	ALA	2.4
1	D	52	LEU	2.4
1	B	42	ARG	2.4
1	B	716	ALA	2.4
1	E	235	GLU	2.4
1	E	558	VAL	2.4
1	E	760	VAL	2.4
1	F	173	VAL	2.4
1	D	728	ALA	2.4
1	A	708	GLY	2.4
1	C	398	TYR	2.4
1	D	767	ALA	2.4
1	B	279	THR	2.4
1	A	287	ASN	2.4
1	C	477	VAL	2.4
1	F	92	VAL	2.4
1	F	731	ALA	2.4
1	A	509	SER	2.4
1	E	397	TRP	2.4
1	A	414	LYS	2.3
1	F	414	LYS	2.3
1	F	508	TRP	2.3
1	E	301	HIS	2.3
1	B	299	PRO	2.3
1	F	520	PRO	2.3
1	E	303	PHE	2.3
1	F	610	LEU	2.3
1	D	89	ASP	2.3
1	E	477	VAL	2.3
1	F	22	VAL	2.3
1	A	503	SER	2.3
1	C	288	SER	2.3
1	C	98	GLU	2.3
1	E	333	ARG	2.3
1	A	118	TRP	2.3
1	D	770	ILE	2.3
1	F	505	PHE	2.3
1	D	633	GLY	2.3
1	A	697	HIS	2.3
1	F	613	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	729	GLY	2.3
1	A	662	TYR	2.3
1	D	524	TYR	2.3
1	A	738	LEU	2.3
1	E	273	LEU	2.3
1	F	477	VAL	2.3
1	F	368	LYS	2.3
1	D	536	HIS	2.3
1	E	334	ARG	2.2
1	C	173	VAL	2.2
1	E	3	ILE	2.2
1	A	345	TRP	2.2
1	E	299	PRO	2.2
1	C	92	VAL	2.2
1	D	703	VAL	2.2
1	B	508	TRP	2.2
1	F	533	LEU	2.2
1	F	747	LEU	2.2
1	A	283	GLU	2.2
1	E	684	GLU	2.2
1	A	723	ILE	2.2
1	C	766	ASN	2.2
1	F	752	GLN	2.2
1	C	695	ASP	2.2
1	E	363	LYS	2.2
1	D	617	ALA	2.2
1	D	723	ILE	2.2
1	A	343	CYS	2.2
1	F	166	GLY	2.2
1	A	346	ILE	2.2
1	B	698	GLU	2.2
1	A	47	GLN	2.1
1	F	291	ASP	2.1
1	B	756	GLU	2.1
1	E	58	PHE	2.1
1	A	208	VAL	2.1
1	D	648	ARG	2.1
1	B	413	PHE	2.1
1	B	505	PHE	2.1
1	B	454	ASP	2.1
1	E	761	VAL	2.1
1	F	344	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	682	TRP	2.1
1	F	269	PHE	2.1
1	A	99	ARG	2.1
1	C	26	GLU	2.1
1	B	445	ASN	2.1
1	A	166	GLY	2.1
1	E	365	TYR	2.1
1	A	548	PRO	2.1
1	A	342	ILE	2.1
1	B	464	PHE	2.1
1	E	625	ASP	2.1
1	E	166	GLY	2.1
1	F	285	THR	2.1
1	E	49	ASP	2.1
1	B	467	SER	2.1
1	A	157	GLY	2.1
1	F	577	ALA	2.1
1	A	428	PHE	2.1
1	E	534	SER	2.1
1	D	635	TRP	2.1
1	B	405	LEU	2.0
1	D	366	LEU	2.0
1	C	718	ARG	2.0
1	A	540	HIS	2.0
1	A	761	VAL	2.0
1	F	105	SER	2.0
1	A	100	TYR	2.0
1	A	552	ASP	2.0
1	A	427	TRP	2.0
1	A	423	THR	2.0
1	C	701	CYS	2.0
1	A	499	SER	2.0
1	E	41	VAL	2.0
1	A	714	LEU	2.0
1	B	463	LEU	2.0
1	B	281	TYR	2.0

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

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, 95th 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MES	C	803	12/12	0.84	0.23	54,59,60,62	0
2	MES	A	801	12/12	0.85	0.30	81,82,83,83	0
2	MES	E	805	12/12	0.85	0.24	79,80,81,81	0
2	MES	B	802	12/12	0.91	0.27	81,85,86,87	0
2	MES	F	806	12/12	0.92	0.24	67,73,76,76	0
2	MES	D	804	12/12	0.97	0.10	56,64,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.