Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2024 – 02:14 PM JST

PDB ID	:	8IOF
Title	:	Crystal structure of N-methyl-Cis-4-hydroxy-D-proline dehydratase in Clostridium sp. FS41
Authors	:	Jiang, L.; Zhang, Y.
Deposited on	:	2023-03-11
Resolution	:	2.33 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:

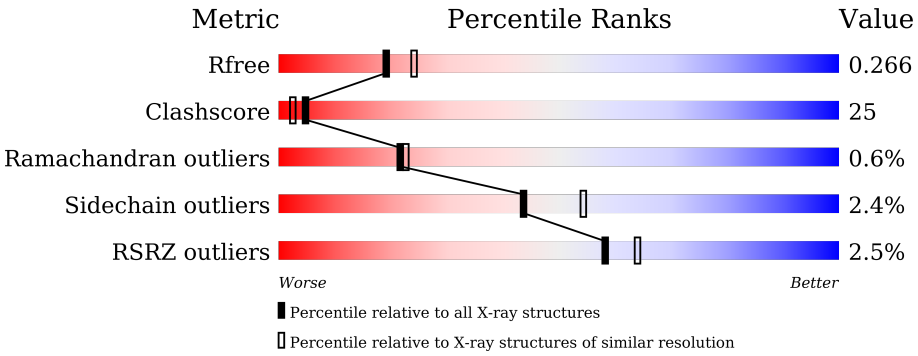
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.33 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}	164625	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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

Mol	Chain	Length	Quality of chain
1	A	793	3% 61% 36%
1	B	793	2% 58% 39%
1	C	793	2% 63% 35%
1	D	793	3% 56% 42%

2 Entry composition

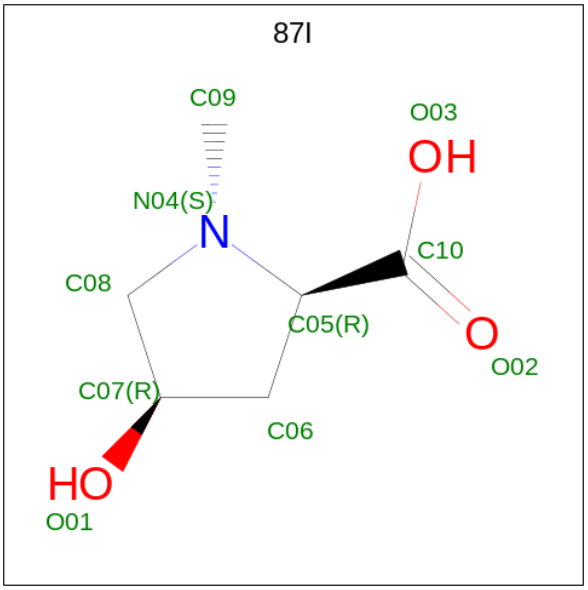
There are 3 unique types of molecules in this entry. The entry contains 26256 atoms, of which 40 are hydrogens and 0 are deuteriums.

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 Benzylsuccinate synthase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6224	3924	1049	1200	51			
1	B	791	Total	C	N	O	S	0	0	0
			6224	3924	1049	1200	51			
1	C	792	Total	C	N	O	S	0	0	0
			6230	3927	1050	1202	51			
1	D	791	Total	C	N	O	S	0	0	0
			6224	3924	1049	1200	51			

- Molecule 2 is (2R,4R)-1-methyl-4-hydroxyl-pyrrolidine-2-carboxylic acid (three-letter code: 87I) (formula: $C_6H_{11}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			20	6	10	1	3		
2	B	1	Total	C	H	N	O	0	0
			20	6	10	1	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			20	6	10	1	3		
2	D	1	Total	C	H	N	O	0	0
			20	6	10	1	3		

- Molecule 3 is water.

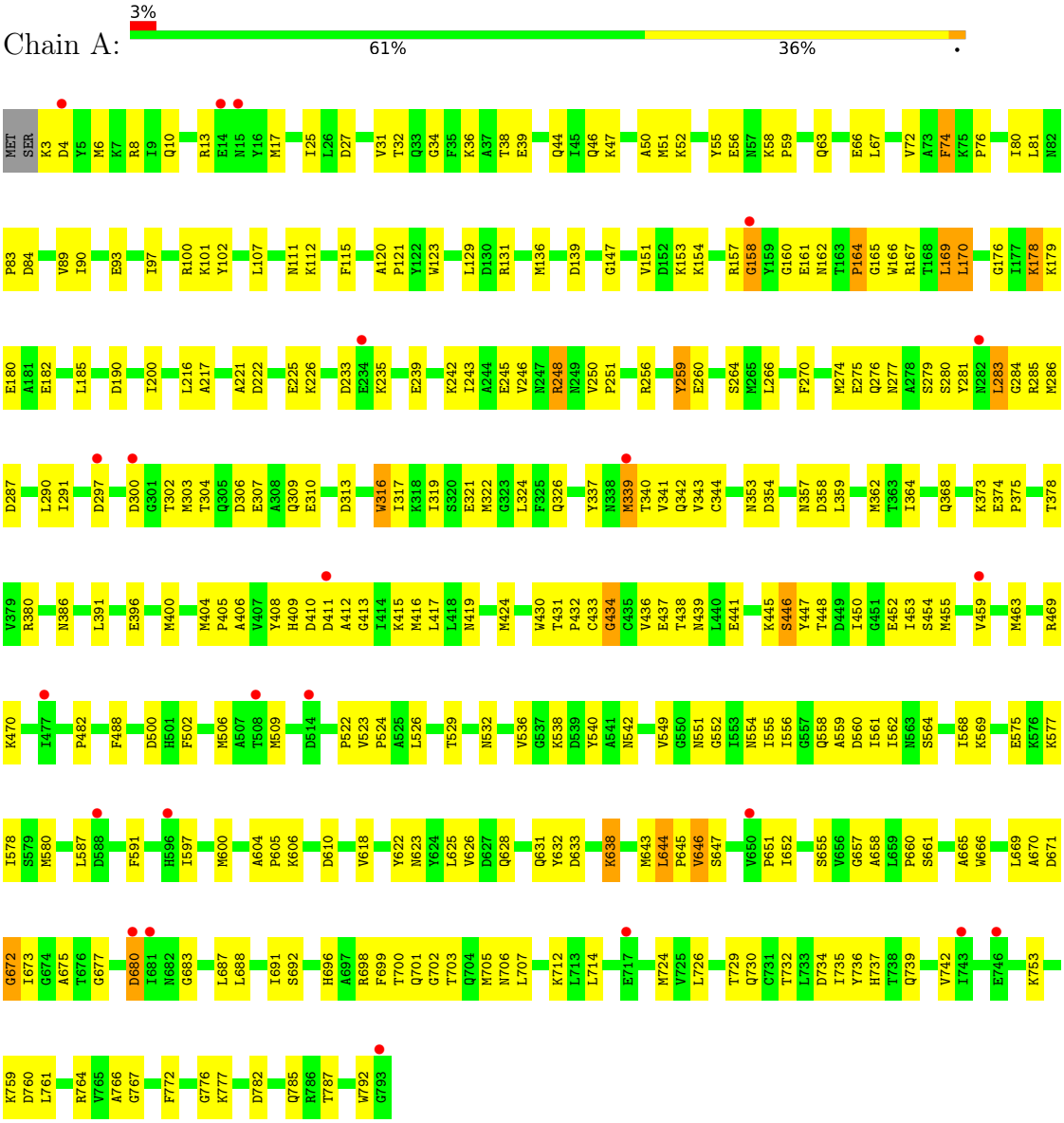
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	345	Total	O	0	0
			345	345		
3	B	319	Total	O	0	0
			319	319		
3	C	315	Total	O	0	0
			315	315		
3	D	295	Total	O	0	0
			295	295		

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.

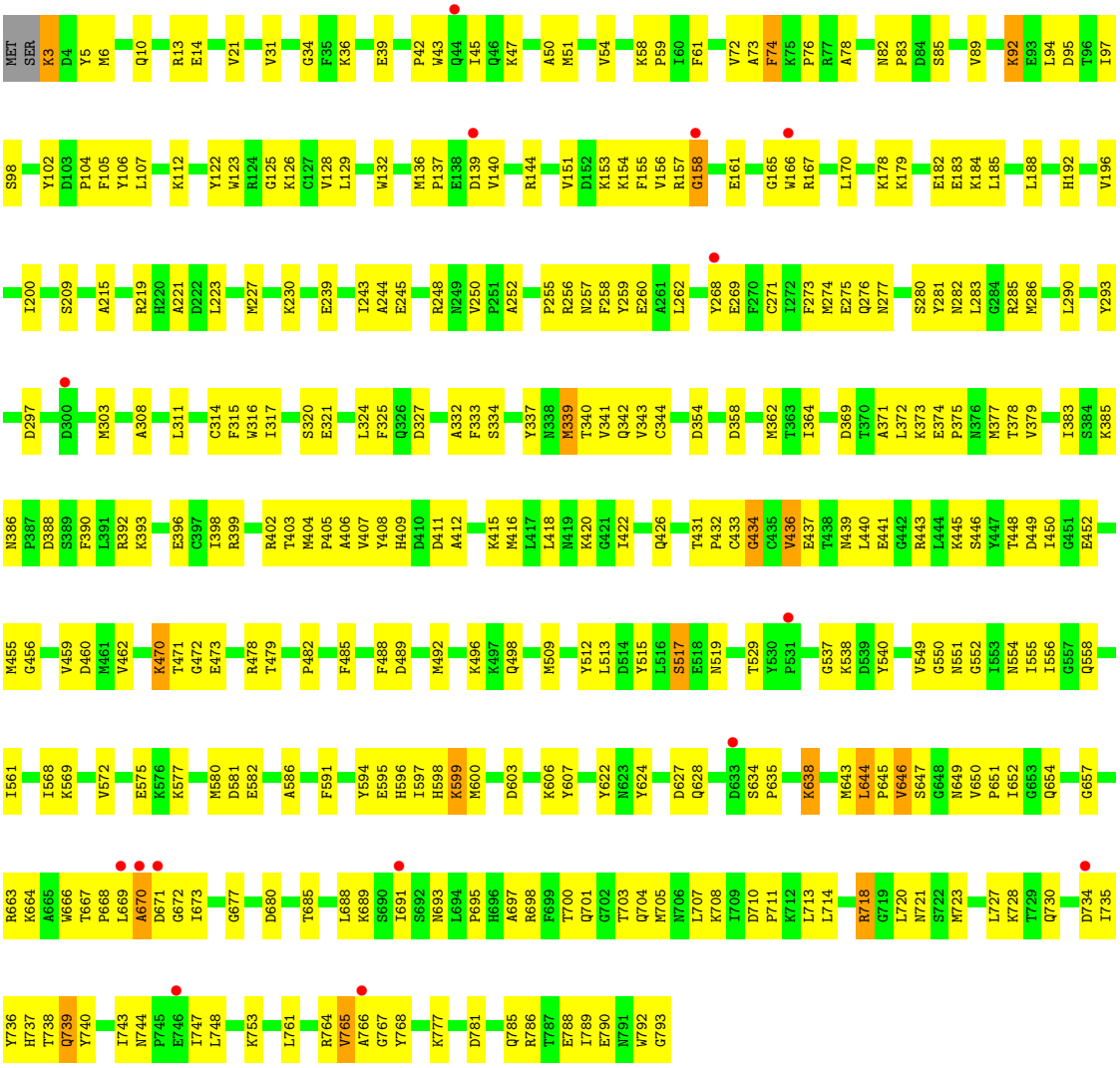
• Molecule 1: Benzylsuccinate synthase alpha subunit

Chain A:



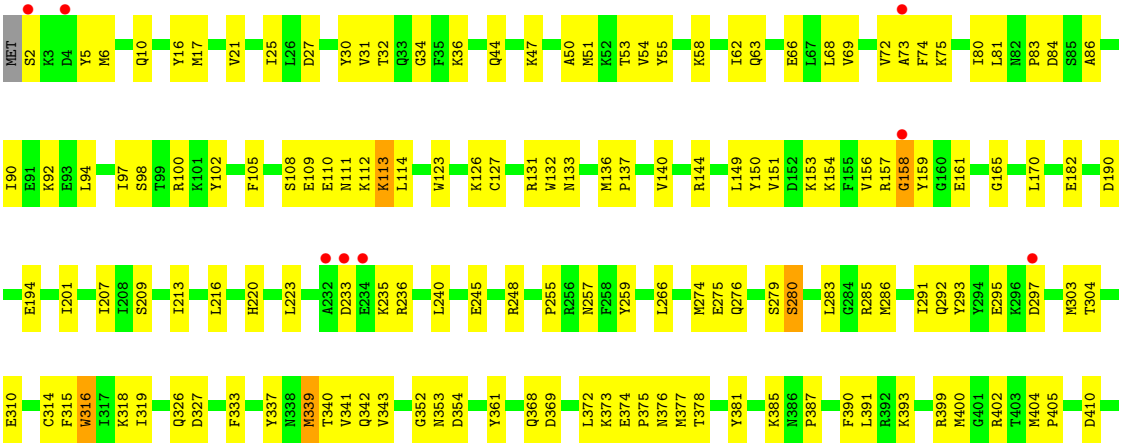
• Molecule 1: Benzylsuccinate synthase alpha subunit

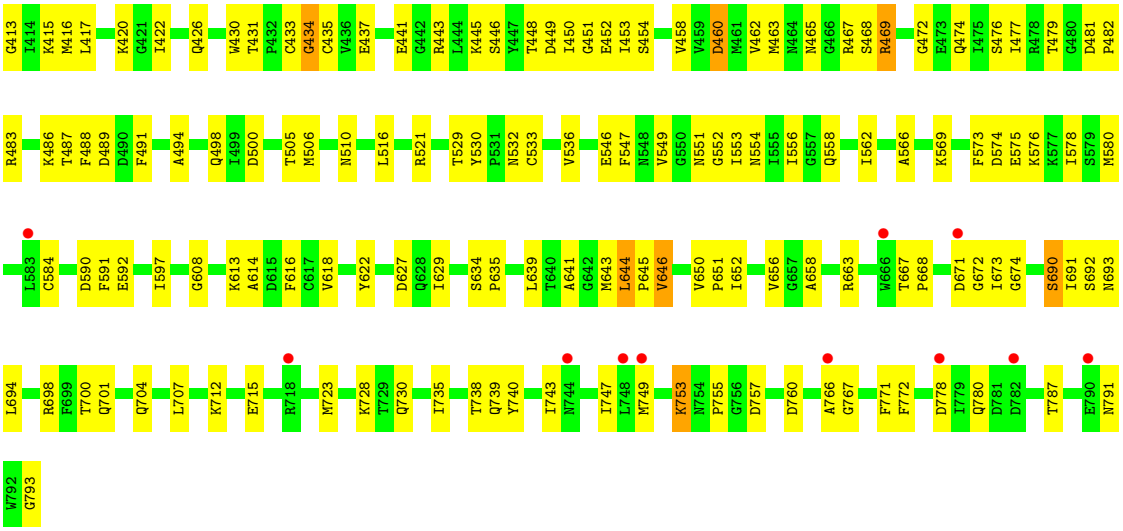
Chain B:



• Molecule 1: Benzylsuccinate synthase alpha subunit

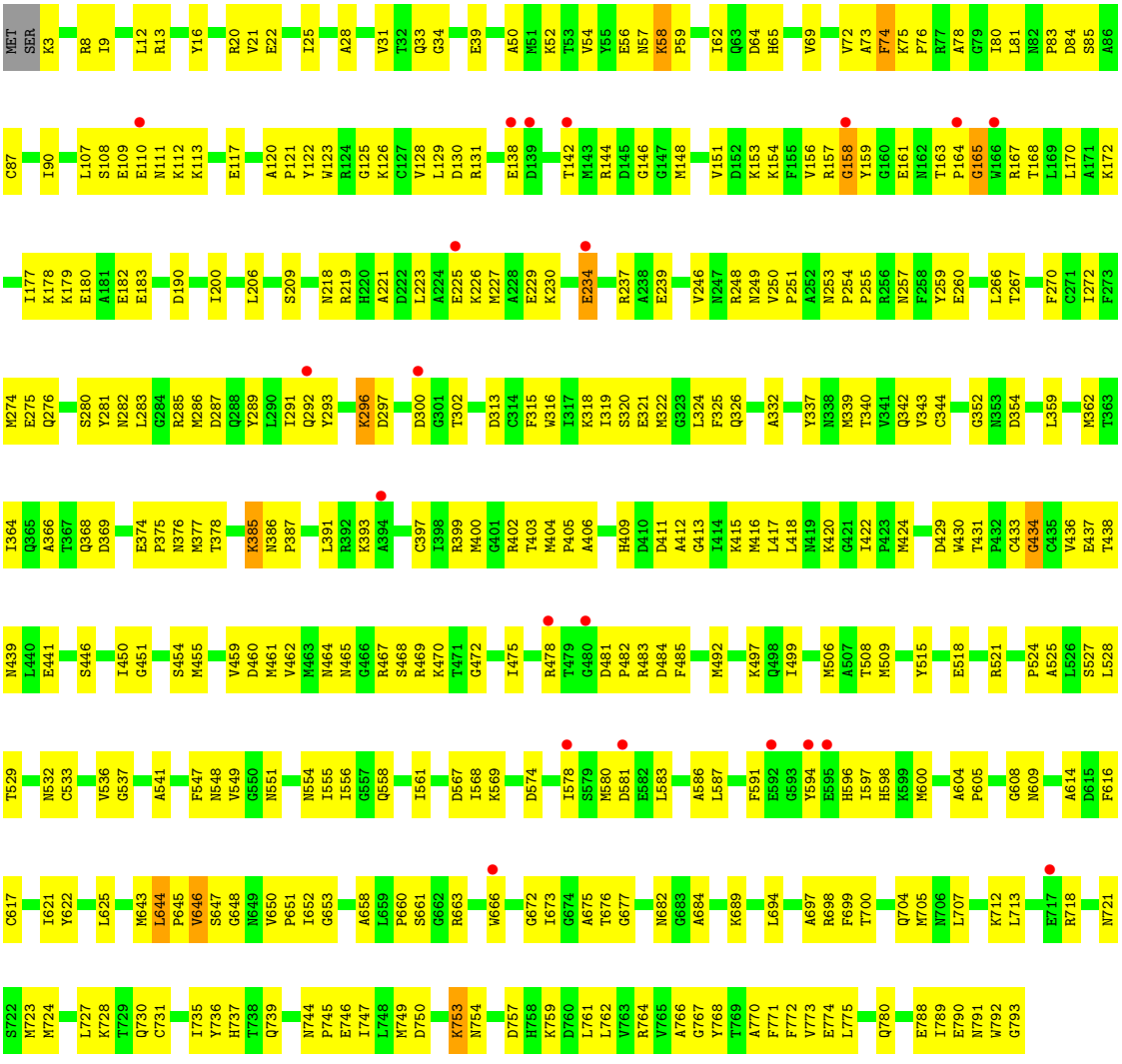
Chain C:





• Molecule 1: Benzylsuccinate synthase alpha subunit

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.97Å 103.60Å 114.25Å 83.13° 75.71° 79.84°	Depositor
Resolution (Å)	39.43 – 2.33 39.43 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.43-2.33) 96.3 (39.43-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.14_3247: ???)	Depositor
R, R_{free}	0.190 , 0.266 0.191 , 0.266	Depositor DCC
R_{free} test set	142895 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å^2)	9.2	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	26256	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 87I

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	0.54	3/6346 (0.0%)	0.62	3/8571 (0.0%)
1	B	0.66	11/6346 (0.2%)	0.64	2/8571 (0.0%)
1	C	0.45	0/6352	0.58	0/8579
1	D	0.51	1/6346 (0.0%)	0.60	1/8571 (0.0%)
All	All	0.55	15/25390 (0.1%)	0.61	6/34292 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	GLU	CD-OE2	-8.72	1.16	1.25
1	B	268	TYR	CZ-OH	-6.90	1.26	1.37
1	B	43	TRP	CE3-CZ3	-6.58	1.27	1.38
1	B	269	GLU	CD-OE1	-6.39	1.18	1.25
1	D	165	GLY	C-O	-6.19	1.13	1.23
1	B	472	GLY	C-O	-5.98	1.14	1.23
1	B	252	ALA	C-O	-5.94	1.12	1.23
1	B	43	TRP	C-O	-5.74	1.12	1.23
1	B	166	TRP	CE3-CZ3	-5.47	1.29	1.38
1	A	281	TYR	C-O	-5.46	1.12	1.23
1	A	792	TRP	CD1-NE1	-5.25	1.29	1.38
1	B	166	TRP	CD1-NE1	-5.25	1.29	1.38
1	B	167	ARG	CZ-NH2	-5.07	1.26	1.33
1	A	683	GLY	C-O	-5.04	1.15	1.23
1	B	471	THR	C-O	-5.03	1.13	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	ARG	NE-CZ-NH1	14.46	127.53	120.30
1	A	680	ASP	O-C-N	10.35	139.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	680	ASP	CA-C-N	-8.07	99.44	117.20
1	D	287	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	680	ASP	C-N-CA	5.28	134.91	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6224	0	6107	286	0
1	B	6224	0	6107	328	0
1	C	6230	0	6112	278	0
1	D	6224	0	6107	349	0
2	A	10	10	0	2	0
2	B	10	10	0	0	0
2	C	10	10	0	1	0
2	D	10	10	0	2	0
3	A	345	0	0	25	1
3	B	319	0	0	51	0
3	C	315	0	0	43	1
3	D	295	0	0	54	0
All	All	26216	40	24433	1234	1

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 25.

All (1234) 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:D:342:GLN:HE21	1:D:378:THR:HG21	1.06	1.10
1:B:459:VAL:CG2	1:B:561:ILE:HD12	1.84	1.08
1:C:274:MET:SD	3:C:1193:HOH:O	2.13	1.06
2:D:801:87I:O02	3:D:902:HOH:O	1.74	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:ASP:OD1	3:D:903:HOH:O	1.75	1.05
1:B:327:ASP:OD2	3:B:901:HOH:O	1.77	1.01
1:B:3:LYS:N	3:B:904:HOH:O	1.94	1.00
1:B:183:GLU:OE1	3:B:902:HOH:O	1.81	0.98
1:C:793:GLY:O	3:C:902:HOH:O	1.82	0.97
1:A:279:SER:HB2	1:A:340:THR:HG22	1.44	0.97
1:A:222:ASP:OD1	1:A:248:ARG:NH2	1.98	0.96
1:B:188:LEU:HD12	1:B:196:VAL:HG13	1.44	0.95
1:C:279:SER:HB2	3:C:901:HOH:O	1.67	0.94
1:C:437:GLU:HG2	1:C:448:THR:HB	1.49	0.94
1:A:558:GLN:NE2	3:A:903:HOH:O	2.02	0.93
1:D:397:CYS:HA	1:D:400:MET:HE2	1.50	0.93
1:A:568:ILE:HD11	1:A:660:PRO:HG3	1.51	0.92
1:C:420:LYS:HD2	1:C:700:THR:HB	1.50	0.92
1:D:713:LEU:HG	1:D:792:TRP:NE1	1.82	0.92
1:A:275:GLU:OE2	3:A:901:HOH:O	1.88	0.92
1:D:180:GLU:O	1:D:183:GLU:HG2	1.69	0.91
1:A:673:ILE:HD13	1:A:703:THR:CG2	1.99	0.91
1:C:487:THR:HG22	1:C:489:ASP:H	1.36	0.91
1:A:753:LYS:NZ	3:A:902:HOH:O	1.99	0.91
1:B:39:GLU:OE1	1:B:122:TYR:OH	1.87	0.91
1:A:739:GLN:HE22	1:A:767:GLY:H	1.02	0.90
1:B:744:ASN:HB3	1:B:747:ILE:HG12	1.52	0.90
1:C:157:ARG:O	3:C:905:HOH:O	1.90	0.90
1:A:633:ASP:OD1	1:A:638:LYS:HD2	1.72	0.90
1:C:460:ASP:OD1	3:C:904:HOH:O	1.88	0.89
1:D:3:LYS:N	3:D:904:HOH:O	2.05	0.89
1:D:342:GLN:NE2	1:D:378:THR:HG21	1.88	0.88
1:C:739:GLN:HE22	1:C:767:GLY:H	1.16	0.88
2:C:801:87I:O03	3:C:906:HOH:O	1.92	0.88
1:C:154:LYS:NZ	1:C:449:ASP:O	2.06	0.87
1:B:14:GLU:OE1	3:B:903:HOH:O	1.91	0.86
1:B:342:GLN:HE21	1:B:378:THR:HG21	1.40	0.86
1:B:685:THR:HG23	1:B:792:TRP:O	1.75	0.86
1:D:369:ASP:OD2	3:D:901:HOH:O	1.94	0.86
1:B:153:LYS:N	3:B:910:HOH:O	2.08	0.86
1:D:3:LYS:N	3:D:910:HOH:O	2.09	0.86
1:B:738:THR:HG23	1:B:740:TYR:HE1	1.42	0.85
1:B:459:VAL:HG23	1:B:561:ILE:HD12	1.59	0.84
1:A:417:LEU:HD22	1:A:430:TRP:HB3	1.58	0.84
1:A:8:ARG:NH2	1:A:310:GLU:OE2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:ARG:NH1	1:C:667:THR:O	2.10	0.83
1:A:578:ILE:HG23	1:A:600:MET:HE1	1.59	0.83
1:B:646:VAL:HG12	1:B:647:SER:H	1.44	0.83
1:C:58:LYS:HD2	1:C:274:MET:HE1	1.61	0.83
1:D:157:ARG:HE	1:D:324:LEU:HD21	1.43	0.83
1:B:320:SER:O	3:B:905:HOH:O	1.96	0.83
1:B:128:VAL:HG12	3:B:917:HOH:O	1.79	0.82
1:B:339:MET:HE3	1:B:339:MET:H	1.45	0.81
1:C:161:GLU:HG2	1:C:448:THR:OG1	1.81	0.81
1:D:467:ARG:NH2	1:D:472:GLY:O	2.13	0.81
1:A:373:LYS:HG3	1:A:374:GLU:HG2	1.63	0.81
1:C:532:ASN:O	1:C:536:VAL:HG22	1.81	0.80
1:A:562:ILE:HD13	1:A:618:VAL:HG22	1.64	0.80
1:B:10:GLN:OE1	3:B:903:HOH:O	2.00	0.80
1:D:558:GLN:CG	1:D:643:MET:HE1	2.12	0.80
1:A:587:LEU:HD11	1:A:660:PRO:HD3	1.63	0.80
1:B:738:THR:HG23	1:B:740:TYR:CE1	2.17	0.79
1:D:723:MET:HE2	1:D:727:LEU:HD11	1.63	0.79
1:A:279:SER:HB2	1:A:340:THR:CG2	2.13	0.79
1:A:705:MET:H	1:A:737:HIS:HD2	1.28	0.79
1:C:154:LYS:HA	3:C:905:HOH:O	1.82	0.78
1:A:739:GLN:NE2	1:A:767:GLY:H	1.81	0.78
1:B:392:ARG:NH1	1:B:721:ASN:OD1	2.16	0.78
1:B:441:GLU:O	1:B:443:ARG:HD3	1.82	0.77
1:D:142:THR:HG21	3:D:1160:HOH:O	1.85	0.77
1:D:33:GLN:HG2	3:D:923:HOH:O	1.84	0.77
1:D:344:CYS:HA	1:D:378:THR:O	1.83	0.77
1:A:239:GLU:O	1:A:243:ILE:HG13	1.84	0.76
1:C:102:TYR:OH	1:C:778:ASP:OD2	2.03	0.76
1:D:168:THR:HG22	1:D:177:ILE:HD11	1.66	0.76
1:D:739:GLN:HE22	1:D:767:GLY:CA	1.98	0.76
1:B:459:VAL:HG22	1:B:561:ILE:HD12	1.64	0.76
1:D:705:MET:H	1:D:737:HIS:HD2	1.33	0.76
1:A:564:SER:O	1:A:568:ILE:HG13	1.86	0.76
1:A:161:GLU:H	1:A:280:SER:HB2	1.51	0.76
1:A:233:ASP:OD1	3:A:904:HOH:O	2.04	0.76
1:A:673:ILE:HD13	1:A:703:THR:HG23	1.67	0.75
1:D:57:ASN:ND2	3:D:918:HOH:O	2.18	0.75
1:B:140:VAL:HG13	3:B:1206:HOH:O	1.85	0.75
1:B:509:MET:HG3	3:B:913:HOH:O	1.86	0.75
1:C:369:ASP:OD1	3:C:908:HOH:O	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:LEU:HD22	1:D:430:TRP:HB3	1.67	0.75
1:B:364:ILE:HG21	1:B:393:LYS:HG2	1.69	0.74
1:A:286:MET:HG3	1:A:343:VAL:HG23	1.67	0.74
1:B:286:MET:HE3	1:B:343:VAL:HG21	1.69	0.74
1:D:558:GLN:HG3	1:D:643:MET:HE1	1.68	0.74
1:C:257:ASN:HB2	1:C:297:ASP:OD2	1.88	0.74
1:C:578:ILE:HD12	1:C:597:ILE:HD12	1.70	0.74
1:D:234:GLU:HG2	1:D:237:ARG:NH2	2.01	0.74
1:D:578:ILE:HD11	1:D:597:ILE:HG23	1.67	0.74
1:C:738:THR:HG23	1:C:740:TYR:CE1	2.22	0.74
1:D:764:ARG:HD2	1:D:768:TYR:O	1.87	0.73
1:D:157:ARG:NH2	3:D:913:HOH:O	2.12	0.73
1:D:791:ASN:ND2	3:D:907:HOH:O	2.07	0.73
1:D:713:LEU:HG	1:D:792:TRP:CE2	2.23	0.73
1:D:548:ASN:O	3:D:906:HOH:O	2.06	0.72
1:C:368:GLN:OE1	1:C:393:LYS:HE3	1.90	0.72
1:A:182:GLU:OE1	3:A:905:HOH:O	2.07	0.72
1:C:154:LYS:HE2	3:C:964:HOH:O	1.88	0.72
1:B:153:LYS:NZ	3:B:920:HOH:O	2.22	0.72
1:D:429:ASP:OD1	3:D:905:HOH:O	2.06	0.72
1:A:304:THR:CG2	1:A:307:GLU:H	2.03	0.71
1:B:170:LEU:HD22	1:B:255:PRO:HG3	1.71	0.71
1:C:131:ARG:HG2	3:C:959:HOH:O	1.89	0.71
1:C:297:ASP:OD2	3:C:909:HOH:O	2.06	0.71
1:A:696:HIS:CD2	1:A:703:THR:HG21	2.26	0.71
1:B:479:THR:HG23	3:B:931:HOH:O	1.89	0.71
1:B:446:SER:HB3	1:B:549:VAL:HG23	1.71	0.71
1:D:285:ARG:HD2	3:D:905:HOH:O	1.90	0.71
1:D:109:GLU:OE2	3:D:908:HOH:O	2.08	0.71
1:D:750:ASP:OD1	1:D:754:ASN:ND2	2.23	0.71
1:A:153:LYS:HD3	2:A:801:87I:O03	1.90	0.71
1:A:417:LEU:HD22	1:A:430:TRP:CB	2.20	0.71
1:B:688:LEU:HD22	1:B:735:ILE:HD13	1.73	0.71
1:B:250:VAL:HG11	1:B:260:GLU:HB3	1.71	0.71
1:D:39:GLU:OE1	1:D:39:GLU:HA	1.91	0.71
1:B:392:ARG:NH2	3:B:907:HOH:O	2.02	0.70
1:D:168:THR:CG2	1:D:177:ILE:HD11	2.21	0.70
1:D:578:ILE:CD1	1:D:597:ILE:HG23	2.20	0.70
1:C:454:SER:HB2	1:C:652:ILE:HG12	1.73	0.70
1:B:36:LYS:O	3:B:911:HOH:O	2.08	0.70
1:C:553:ILE:HB	1:C:629:ILE:HD13	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:GLN:HE22	1:B:767:GLY:HA2	1.57	0.70
1:B:582:GLU:OE1	3:B:912:HOH:O	2.08	0.70
1:D:677:GLY:O	3:D:911:HOH:O	2.09	0.70
1:B:140:VAL:CG1	3:B:1206:HOH:O	2.40	0.70
1:B:184:LYS:O	1:B:188:LEU:HD23	1.92	0.70
1:A:342:GLN:NE2	1:A:408:TYR:OH	2.21	0.69
1:B:743:ILE:HG21	1:B:748:LEU:HD11	1.74	0.69
1:D:161:GLU:HA	1:D:280:SER:HB2	1.74	0.69
1:B:581:ASP:OD1	3:B:914:HOH:O	2.10	0.69
1:D:793:GLY:O	3:D:909:HOH:O	2.09	0.69
1:B:13:ARG:HD3	3:B:903:HOH:O	1.92	0.69
1:A:17:MET:CE	1:A:759:LYS:HG2	2.22	0.69
1:D:85:SER:HB2	1:D:521:ARG:HH21	1.57	0.69
1:B:185:LEU:HD11	1:B:200:ILE:HG23	1.75	0.69
1:A:246:VAL:HG13	1:A:260:GLU:HG2	1.76	0.68
1:B:591:PHE:O	3:B:915:HOH:O	2.11	0.68
1:B:151:VAL:O	3:B:913:HOH:O	2.10	0.68
1:A:705:MET:H	1:A:737:HIS:CD2	2.11	0.68
1:B:72:VAL:HG11	1:B:273:PHE:CD2	2.29	0.68
1:D:352:GLY:O	1:D:385:LYS:HE3	1.92	0.68
1:B:693:ASN:ND2	3:B:923:HOH:O	2.26	0.68
1:B:156:VAL:HG21	1:B:327:ASP:OD1	1.94	0.68
1:A:701:GLN:OE1	1:A:701:GLN:HA	1.94	0.67
1:C:452:GLU:HG2	1:C:556:ILE:HD11	1.75	0.67
1:C:739:GLN:HE22	1:C:767:GLY:N	1.90	0.67
1:A:622:TYR:O	1:A:626:VAL:HG23	1.95	0.67
1:B:470:LYS:CA	1:B:470:LYS:HE2	2.24	0.67
1:B:470:LYS:HE2	1:B:470:LYS:HA	1.76	0.67
1:A:396:GLU:O	1:A:400:MET:HG3	1.94	0.67
1:C:674:GLY:HA3	3:C:1120:HOH:O	1.93	0.67
1:D:556:ILE:HG12	1:D:645:PRO:HB3	1.77	0.67
1:D:737:HIS:CE1	1:D:739:GLN:HG3	2.29	0.67
1:B:188:LEU:CD1	1:B:196:VAL:HG13	2.20	0.67
1:D:286:MET:HG3	1:D:343:VAL:HG23	1.76	0.67
1:B:47:LYS:HE3	1:B:51:MET:HE3	1.77	0.66
1:A:739:GLN:HE22	1:A:767:GLY:N	1.85	0.66
1:B:178:LYS:HE2	1:B:182:GLU:OE1	1.95	0.66
1:B:245:GLU:OE2	1:B:256:ARG:NH2	2.27	0.66
1:D:417:LEU:HD22	1:D:430:TRP:CB	2.25	0.66
1:C:469:ARG:HD2	3:C:904:HOH:O	1.95	0.66
1:A:169:LEU:HD23	1:A:170:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:MET:SD	3:C:926:HOH:O	2.53	0.66
1:D:285:ARG:CD	3:D:905:HOH:O	2.44	0.66
1:C:165:GLY:HA3	1:C:529:THR:O	1.95	0.66
1:A:157:ARG:NE	3:A:915:HOH:O	2.29	0.66
1:A:378:THR:HG22	1:A:406:ALA:HB3	1.78	0.66
1:B:456:GLY:HA3	1:B:669:LEU:HD11	1.78	0.65
1:D:644:LEU:HD11	3:D:1033:HOH:O	1.95	0.65
1:D:248:ARG:NE	3:D:915:HOH:O	2.25	0.65
1:A:63:GLN:NE2	1:A:66:GLU:OE2	2.29	0.65
1:A:450:ILE:HD12	1:A:509:MET:HE1	1.79	0.65
1:C:339:MET:HE2	1:C:374:GLU:HB3	1.77	0.65
1:B:743:ILE:CD1	1:B:761:LEU:HD11	2.26	0.65
1:D:712:LYS:HG2	3:D:1053:HOH:O	1.95	0.65
1:D:462:VAL:O	3:D:914:HOH:O	2.12	0.65
1:D:605:PRO:HB2	1:D:614:ALA:HB2	1.78	0.65
1:A:340:THR:HG23	1:A:340:THR:O	1.97	0.65
1:D:342:GLN:HE21	1:D:378:THR:CG2	1.98	0.65
1:A:222:ASP:OD2	3:A:906:HOH:O	2.14	0.65
1:D:749:MET:O	1:D:753:LYS:HD2	1.96	0.65
1:A:286:MET:HG3	1:A:343:VAL:CG2	2.26	0.65
1:A:558:GLN:HA	1:A:622:TYR:OH	1.96	0.65
1:A:101:LYS:HE3	1:A:102:TYR:CE2	2.32	0.64
1:B:739:GLN:HG2	1:B:764:ARG:HG2	1.79	0.64
1:D:587:LEU:HD11	1:D:660:PRO:HD3	1.79	0.64
1:C:463:MET:HE1	1:C:491:PHE:HE1	1.62	0.64
1:C:757:ASP:OD2	3:C:910:HOH:O	2.14	0.64
1:B:82:ASN:OD1	1:B:277:ASN:HB3	1.97	0.64
1:B:151:VAL:HG21	3:B:1206:HOH:O	1.97	0.64
1:C:487:THR:HG22	1:C:489:ASP:N	2.11	0.64
1:B:743:ILE:HD11	1:B:761:LEU:HD11	1.80	0.64
1:D:157:ARG:HD3	1:D:326:GLN:HB3	1.78	0.64
1:D:454:SER:HB2	1:D:652:ILE:HG12	1.80	0.64
1:B:669:LEU:O	1:B:670:ALA:HB3	1.98	0.64
1:D:170:LEU:O	1:D:255:PRO:HD2	1.98	0.64
1:D:249:ASN:HB2	3:D:972:HOH:O	1.97	0.64
1:C:291:ILE:HG13	1:C:295:GLU:OE1	1.97	0.64
1:C:404:MET:HB3	1:C:405:PRO:HA	1.79	0.64
1:D:234:GLU:HG2	1:D:237:ARG:CZ	2.27	0.64
1:B:657:GLY:O	1:B:663:ARG:NH2	2.31	0.63
1:D:412:ALA:O	1:D:416:MET:HG3	1.98	0.63
1:B:426:GLN:HB3	1:B:443:ARG:HH21	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:SER:OG	1:D:110:GLU:HG2	1.98	0.63
1:D:153:LYS:HD3	3:D:902:HOH:O	1.97	0.63
1:B:94:LEU:HG	1:B:112:LYS:HD3	1.81	0.63
1:B:730:GLN:HG3	1:B:735:ILE:HB	1.80	0.63
1:C:62:ILE:HG12	1:C:69:VAL:HG21	1.81	0.63
1:A:326:GLN:NE2	3:A:924:HOH:O	2.31	0.63
1:B:404:MET:HB3	1:B:405:PRO:HA	1.80	0.63
1:C:157:ARG:O	1:C:158:GLY:O	2.17	0.63
1:C:381:TYR:CZ	1:C:391:LEU:HD22	2.33	0.63
1:C:433:CYS:HB3	1:C:437:GLU:HB2	1.79	0.63
1:C:74:PHE:CE2	1:C:75:LYS:HE2	2.34	0.63
1:D:107:LEU:HG	1:D:112:LYS:HG2	1.80	0.63
1:D:368:GLN:HG2	1:D:400:MET:HE1	1.79	0.63
1:B:155:PHE:HB3	3:B:917:HOH:O	1.98	0.63
1:C:236:ARG:HG3	1:C:240:LEU:HD11	1.81	0.63
1:C:558:GLN:HA	1:C:622:TYR:OH	1.98	0.63
1:A:417:LEU:CD1	1:A:438:THR:HB	2.28	0.63
1:B:705:MET:H	1:B:737:HIS:HD2	1.44	0.63
1:C:627:ASP:OD1	1:C:698:ARG:NH2	2.29	0.63
1:D:138:GLU:O	1:D:142:THR:HG23	1.99	0.63
1:D:368:GLN:HG2	1:D:397:CYS:SG	2.38	0.63
1:A:452:GLU:HG2	1:A:556:ILE:HD11	1.80	0.62
1:B:793:GLY:O	3:B:916:HOH:O	2.16	0.62
1:D:368:GLN:HE21	1:D:400:MET:HE1	1.65	0.62
1:C:374:GLU:HB3	1:C:375:PRO:HA	1.82	0.62
1:C:462:VAL:HG12	1:C:463:MET:CE	2.29	0.62
1:D:604:ALA:HB1	1:D:605:PRO:HD2	1.82	0.62
1:B:607:TYR:OH	1:B:691:ILE:HG22	1.99	0.62
1:B:627:ASP:OD1	1:B:698:ARG:NH2	2.29	0.62
1:C:339:MET:HE1	1:C:341:VAL:HB	1.82	0.62
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.65	0.62
1:D:470:LYS:HE3	3:D:926:HOH:O	1.99	0.62
1:D:648:GLY:C	1:D:651:PRO:HD2	2.20	0.62
1:A:309:GLN:OE1	1:A:362:MET:HB3	1.99	0.62
1:B:239:GLU:HG3	3:B:922:HOH:O	1.99	0.61
1:A:706:ASN:ND2	1:A:739:GLN:HE21	1.97	0.61
1:B:556:ILE:HD12	1:B:652:ILE:CD1	2.30	0.61
1:C:420:LYS:HB3	1:C:549:VAL:HG11	1.81	0.61
1:D:28:ALA:CB	1:D:81:LEU:HD12	2.30	0.61
1:A:17:MET:HE3	1:A:759:LYS:HG2	1.82	0.61
1:A:500:ASP:HB2	3:A:921:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLN:HG3	3:A:1110:HOH:O	1.99	0.61
1:A:469:ARG:HD2	1:A:657:GLY:HA3	1.81	0.61
1:D:374:GLU:HB3	1:D:375:PRO:HA	1.82	0.61
1:A:304:THR:HG23	1:A:307:GLU:H	1.65	0.61
1:C:109:GLU:O	1:C:113:LYS:HE2	2.01	0.61
1:D:85:SER:HB2	1:D:521:ARG:NH2	2.16	0.61
1:B:342:GLN:HE21	1:B:378:THR:CG2	2.13	0.60
1:B:743:ILE:CG2	1:B:748:LEU:HD11	2.31	0.60
1:C:772:PHE:CZ	1:C:780:GLN:HB3	2.36	0.60
1:A:604:ALA:HB1	1:A:605:PRO:HD2	1.82	0.60
1:D:455:MET:HE3	1:D:561:ILE:CD1	2.32	0.60
1:A:162:ASN:HA	1:A:439:ASN:OD1	2.02	0.60
1:A:404:MET:HB3	1:A:405:PRO:HA	1.83	0.60
1:B:34:GLY:HA3	1:B:50:ALA:HA	1.83	0.60
1:B:446:SER:CB	1:B:549:VAL:HG23	2.31	0.60
1:C:72:VAL:O	1:C:80:ILE:HG21	2.01	0.60
1:A:25:ILE:HG13	1:A:111:ASN:HB3	1.83	0.60
1:B:739:GLN:CD	1:B:764:ARG:HE	2.05	0.60
1:D:597:ILE:HA	1:D:600:MET:HE3	1.83	0.60
1:A:31:VAL:HA	1:A:50:ALA:HB1	1.83	0.60
1:A:157:ARG:O	1:A:158:GLY:O	2.20	0.60
1:A:416:MET:HG2	1:A:700:THR:HA	1.83	0.60
1:C:62:ILE:HG13	1:C:223:LEU:HD23	1.82	0.60
1:D:739:GLN:NE2	1:D:764:ARG:HE	1.99	0.60
1:A:578:ILE:HG21	1:A:597:ILE:HD13	1.83	0.60
1:B:651:PRO:HA	1:B:654:GLN:NE2	2.17	0.60
1:D:451:GLY:HA3	1:D:506:MET:HE1	1.82	0.60
1:A:52:LYS:O	1:A:56:GLU:HG3	2.01	0.60
1:A:587:LEU:CD1	1:A:660:PRO:HD3	2.30	0.60
1:B:701:GLN:HA	1:B:701:GLN:OE1	2.01	0.60
1:C:730:GLN:HG3	1:C:735:ILE:HB	1.84	0.60
1:D:229:GLU:OE1	1:D:229:GLU:HA	2.01	0.60
1:A:157:ARG:CD	1:A:324:LEU:HD21	2.32	0.60
1:A:235:LYS:O	1:A:239:GLU:HG2	2.01	0.60
1:B:151:VAL:HB	3:B:913:HOH:O	2.00	0.60
1:C:34:GLY:HA3	1:C:50:ALA:HA	1.84	0.60
1:C:280:SER:HB2	1:C:434:GLY:CA	2.31	0.60
1:A:115:PHE:CE2	1:A:120:ALA:HB2	2.37	0.59
1:B:132:TRP:CZ2	1:B:136:MET:HG3	2.37	0.59
1:B:688:LEU:HD22	1:B:735:ILE:CD1	2.31	0.59
1:B:708:LYS:O	1:B:789:ILE:HG13	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:MET:HE3	1:B:727:LEU:HD21	1.84	0.59
1:C:132:TRP:CZ2	1:C:136:MET:HG3	2.37	0.59
1:B:42:PRO:HG2	1:B:45:ILE:HG12	1.84	0.59
1:A:157:ARG:NE	1:A:324:LEU:HD21	2.17	0.59
1:A:575:GLU:HB3	1:A:577:LYS:HG3	1.84	0.59
1:D:737:HIS:NE2	1:D:739:GLN:HG3	2.17	0.59
1:B:634:SER:HB2	1:B:635:PRO:HD2	1.84	0.59
1:A:628:GLN:O	1:A:631:GLN:HG2	2.02	0.59
1:B:47:LYS:HE3	1:B:51:MET:CE	2.33	0.59
1:C:521:ARG:HA	3:C:1074:HOH:O	2.02	0.59
1:A:161:GLU:N	1:A:280:SER:HB2	2.16	0.59
1:B:538:LYS:CE	1:B:538:LYS:HA	2.33	0.59
1:C:445:LYS:O	1:C:446:SER:HB3	2.02	0.59
1:D:402:ARG:HD3	3:D:1104:HOH:O	2.02	0.59
1:B:482:PRO:O	1:B:580:MET:HG2	2.02	0.59
1:D:157:ARG:NE	1:D:324:LEU:HD21	2.14	0.59
1:D:368:GLN:HE21	1:D:400:MET:CE	2.15	0.59
1:C:339:MET:HE3	1:C:341:VAL:H	1.68	0.59
1:C:573:PHE:O	1:C:576:LYS:HE3	2.03	0.59
1:D:157:ARG:O	1:D:158:GLY:O	2.21	0.59
1:D:762:LEU:O	3:D:916:HOH:O	2.16	0.59
1:A:358:ASP:O	1:A:362:MET:HG3	2.03	0.58
1:B:558:GLN:HA	1:B:622:TYR:OH	2.03	0.58
1:C:462:VAL:HA	1:C:479:THR:HG21	1.85	0.58
1:A:270:PHE:O	1:A:274:MET:HG3	2.03	0.58
1:C:634:SER:HB2	1:C:635:PRO:HD2	1.85	0.58
1:A:304:THR:HG22	1:A:307:GLU:CG	2.33	0.58
1:B:358:ASP:O	1:B:362:MET:HG3	2.04	0.58
1:D:128:VAL:HG21	1:D:521:ARG:NH2	2.18	0.58
1:A:688:LEU:HD12	1:A:726:LEU:HD11	1.85	0.58
1:B:378:THR:HG23	1:B:408:TYR:CE1	2.38	0.58
1:C:479:THR:HA	3:C:919:HOH:O	2.02	0.58
1:C:743:ILE:HD11	1:C:747:ILE:HG21	1.84	0.58
1:A:578:ILE:HG23	1:A:600:MET:CE	2.31	0.58
1:D:464:ASN:ND2	1:D:469:ARG:HG2	2.17	0.58
1:C:58:LYS:HE3	1:C:274:MET:HE3	1.86	0.58
1:C:467:ARG:HD2	3:C:1177:HOH:O	2.03	0.58
1:C:738:THR:HG23	1:C:740:TYR:HE1	1.65	0.58
1:A:165:GLY:HA3	1:A:529:THR:O	2.04	0.58
1:A:342:GLN:NE2	1:A:432:PRO:HB2	2.19	0.58
1:B:285:ARG:HG3	1:B:431:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LEU:HG	1:C:112:LYS:HG2	1.86	0.58
1:C:376:ASN:ND2	1:C:434:GLY:O	2.37	0.58
1:D:481:ASP:HB3	1:D:484:ASP:OD2	2.04	0.58
1:B:104:PRO:O	1:B:337:TYR:OH	2.17	0.58
1:B:596:HIS:O	1:B:600:MET:HG3	2.03	0.58
1:C:5:TYR:HB2	1:C:310:GLU:HB2	1.84	0.58
1:A:732:THR:HG22	3:A:919:HOH:O	2.03	0.57
1:C:280:SER:HB2	1:C:434:GLY:HA3	1.86	0.57
1:D:608:GLY:HA3	1:D:675:ALA:HB2	1.86	0.57
1:A:632:TYR:HB3	3:B:1090:HOH:O	2.03	0.57
1:A:245:GLU:HA	1:A:245:GLU:OE1	2.04	0.57
1:A:245:GLU:OE2	1:A:256:ARG:NH2	2.33	0.57
1:D:85:SER:HA	1:D:128:VAL:HG22	1.84	0.57
1:A:470:LYS:HG2	1:A:666:TRP:CH2	2.40	0.57
1:B:739:GLN:NE2	1:B:764:ARG:HE	2.03	0.57
1:D:153:LYS:HE2	3:D:913:HOH:O	2.04	0.57
1:D:455:MET:HE3	1:D:561:ILE:HD13	1.87	0.57
1:D:569:LYS:HD3	1:D:574:ASP:OD2	2.04	0.57
1:D:226:LYS:HE3	1:D:226:LYS:HA	1.86	0.57
1:D:292:GLN:OE1	1:D:292:GLN:HA	2.04	0.57
1:B:374:GLU:HB3	1:B:375:PRO:HA	1.84	0.57
1:B:470:LYS:HG2	1:B:666:TRP:CH2	2.39	0.57
1:C:391:LEU:CD2	1:C:728:LYS:HZ3	2.18	0.57
1:D:617:CYS:HB2	1:D:621:ILE:HD12	1.87	0.57
1:A:72:VAL:HG11	1:A:322:MET:HG2	1.87	0.57
1:A:178:LYS:HE3	3:A:1220:HOH:O	2.04	0.57
1:B:50:ALA:O	1:B:54:VAL:HG23	2.04	0.57
1:B:285:ARG:HG3	1:B:344:CYS:SG	2.45	0.57
1:A:285:ARG:HG3	1:A:431:THR:CG2	2.35	0.57
1:B:161:GLU:HA	1:B:280:SER:HB2	1.87	0.57
1:C:86:ALA:HB2	1:C:156:VAL:O	2.04	0.57
1:C:482:PRO:O	1:C:580:MET:HG2	2.05	0.57
1:A:378:THR:CG2	1:A:406:ALA:HB3	2.35	0.57
1:D:159:TYR:CE2	1:D:521:ARG:HG2	2.40	0.57
1:A:523:VAL:HG23	1:A:523:VAL:O	2.04	0.56
1:D:368:GLN:CG	1:D:400:MET:HE1	2.35	0.56
1:D:497:LYS:HE3	3:D:1021:HOH:O	2.05	0.56
1:A:27:ASP:HB2	3:A:1081:HOH:O	2.06	0.56
1:A:687:LEU:HD21	1:A:705:MET:CE	2.35	0.56
1:C:98:SER:HA	1:C:105:PHE:O	2.06	0.56
1:C:646:VAL:O	1:C:766:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LYS:O	1:D:117:GLU:HG3	2.05	0.56
1:A:185:LEU:HD11	1:A:200:ILE:HG23	1.88	0.56
1:A:279:SER:CB	1:A:340:THR:HG22	2.28	0.56
1:A:578:ILE:HD13	1:A:600:MET:HE2	1.86	0.56
1:A:714:LEU:CD1	1:A:742:VAL:HG11	2.35	0.56
1:D:459:VAL:HG23	1:D:561:ILE:HG13	1.87	0.56
1:B:459:VAL:HG23	1:B:561:ILE:CD1	2.34	0.56
1:B:492:MET:CE	1:B:496:LYS:HE3	2.35	0.56
1:D:646:VAL:O	1:D:766:ALA:HB3	2.05	0.56
1:D:730:GLN:HG3	1:D:735:ILE:HB	1.86	0.56
1:D:773:VAL:HG22	3:D:1074:HOH:O	2.05	0.56
1:B:283:LEU:HD13	1:B:315:PHE:HE2	1.70	0.56
1:B:646:VAL:HG12	1:B:647:SER:N	2.16	0.56
1:C:194:GLU:HG3	1:D:515:TYR:HB2	1.87	0.56
1:C:402:ARG:HD3	3:C:1142:HOH:O	2.06	0.56
1:B:83:PRO:HB2	1:B:123:TRP:CD1	2.40	0.56
1:B:378:THR:CG2	1:B:408:TYR:CE1	2.89	0.56
1:A:374:GLU:HB3	1:A:375:PRO:HA	1.88	0.56
1:C:233:ASP:OD1	1:C:235:LYS:HB2	2.06	0.56
1:D:52:LYS:O	1:D:56:GLU:HG3	2.05	0.56
1:D:172:LYS:NZ	1:D:180:GLU:OE2	2.24	0.56
1:D:555:ILE:HD13	1:D:625:LEU:CD2	2.36	0.56
1:A:470:LYS:HE3	1:A:666:TRP:CE3	2.41	0.55
1:B:31:VAL:CG2	1:B:51:MET:HE1	2.35	0.55
1:B:165:GLY:HA3	1:B:529:THR:O	2.06	0.55
1:D:397:CYS:HA	1:D:400:MET:CE	2.30	0.55
1:D:87:CYS:SG	1:D:123:TRP:HB2	2.46	0.55
1:D:218:ASN:ND2	3:D:915:HOH:O	2.15	0.55
1:A:286:MET:HE3	1:A:290:LEU:HD11	1.89	0.55
1:A:559:ALA:HB3	1:A:670:ALA:CB	2.35	0.55
1:D:296:LYS:HD2	3:D:1076:HOH:O	2.05	0.55
1:C:381:TYR:OH	1:C:728:LYS:NZ	2.38	0.55
1:D:417:LEU:CD1	1:D:438:THR:HB	2.36	0.55
1:D:788:GLU:O	1:D:790:GLU:HG3	2.06	0.55
1:B:106:TYR:N	3:B:918:HOH:O	2.40	0.55
1:B:161:GLU:HB3	1:B:448:THR:HG23	1.89	0.55
1:B:334:SER:HB2	3:B:908:HOH:O	2.06	0.55
1:B:342:GLN:NE2	1:B:378:THR:HG21	2.15	0.55
1:C:144:ARG:HG3	1:C:151:VAL:HG22	1.88	0.55
1:B:317:ILE:HD13	1:B:372:LEU:HD12	1.89	0.55
1:B:650:VAL:HB	1:B:651:PRO:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:LYS:HE2	1:D:666:TRP:CE2	2.41	0.55
1:A:447:TYR:HB2	1:A:551:ASN:OD1	2.07	0.55
1:B:407:VAL:HB	1:B:738:THR:HG22	1.89	0.55
1:C:463:MET:HA	1:C:463:MET:HE2	1.88	0.55
1:C:319:ILE:HG21	1:C:375:PRO:HB3	1.87	0.55
1:B:73:ALA:CB	1:B:78:ALA:HB3	2.37	0.55
1:B:450:ILE:CG2	1:B:551:ASN:HB3	2.35	0.55
1:D:266:LEU:HD11	1:D:270:PHE:CZ	2.42	0.55
1:A:317:ILE:O	1:A:321:GLU:HG3	2.07	0.54
1:C:454:SER:HB2	1:C:652:ILE:CG1	2.37	0.54
1:B:286:MET:HG2	1:B:290:LEU:HD22	1.87	0.54
1:B:738:THR:CG2	1:B:740:TYR:HE1	2.18	0.54
1:C:27:ASP:HB3	3:C:921:HOH:O	2.06	0.54
1:C:156:VAL:HG21	1:C:327:ASP:OD2	2.07	0.54
1:B:89:VAL:CG2	1:B:327:ASP:HB3	2.37	0.54
1:B:437:GLU:OE1	1:B:644:LEU:HD13	2.08	0.54
1:A:562:ILE:CD1	1:A:618:VAL:HG22	2.36	0.54
1:B:314:CYS:HB3	3:B:1141:HOH:O	2.06	0.54
1:C:63:GLN:HB2	1:C:66:GLU:CD	2.27	0.54
1:C:280:SER:HA	1:C:340:THR:O	2.08	0.54
1:C:452:GLU:CG	1:C:556:ILE:HD11	2.37	0.54
1:D:157:ARG:NH1	1:D:157:ARG:HG3	2.21	0.54
1:D:286:MET:HG3	1:D:343:VAL:CG2	2.36	0.54
1:A:411:ASP:OD1	1:D:415:LYS:HE2	2.07	0.54
1:D:617:CYS:HB2	1:D:621:ILE:CD1	2.38	0.54
1:A:680:ASP:O	1:A:787:THR:HG21	2.07	0.54
1:A:761:LEU:HD23	1:A:772:PHE:HB3	1.90	0.54
1:B:340:THR:HG22	1:B:768:TYR:CB	2.38	0.54
1:C:159:TYR:HB2	3:C:1022:HOH:O	2.06	0.54
1:D:157:ARG:HG3	1:D:157:ARG:HH11	1.73	0.54
1:D:658:ALA:HA	1:D:663:ARG:O	2.07	0.54
1:A:450:ILE:CD1	1:A:509:MET:HE1	2.38	0.54
1:A:688:LEU:HD22	1:A:735:ILE:HD13	1.90	0.54
1:C:54:VAL:HG12	1:C:274:MET:CE	2.37	0.54
1:D:747:ILE:HG22	1:D:761:LEU:CD2	2.38	0.54
1:A:266:LEU:HD11	1:A:270:PHE:CZ	2.43	0.53
1:A:555:ILE:HD13	1:A:699:PHE:HE2	1.74	0.53
1:A:568:ILE:HD11	1:A:660:PRO:CG	2.30	0.53
1:D:578:ILE:HD11	1:D:597:ILE:CG2	2.35	0.53
1:C:158:GLY:HA2	1:C:521:ARG:HD3	1.89	0.53
1:C:673:ILE:HD11	1:C:691:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ARG:HB2	3:D:1143:HOH:O	2.08	0.53
1:B:6:MET:HE1	1:B:369:ASP:HB3	1.90	0.53
1:B:317:ILE:HD13	1:B:372:LEU:CD1	2.38	0.53
1:B:333:PHE:CE2	1:B:652:ILE:HG13	2.42	0.53
1:B:406:ALA:HB1	1:B:737:HIS:CE1	2.43	0.53
1:A:158:GLY:HA3	1:A:276:GLN:HB3	1.90	0.53
1:A:706:ASN:O	1:A:707:LEU:HD12	2.08	0.53
1:B:239:GLU:O	1:B:243:ILE:HG13	2.09	0.53
1:B:255:PRO:HG2	1:B:293:TYR:CE1	2.44	0.53
1:C:58:LYS:HD2	1:C:274:MET:CE	2.35	0.53
1:C:280:SER:O	1:C:280:SER:OG	2.16	0.53
1:C:629:ILE:HD12	1:C:641:ALA:HB2	1.91	0.53
1:D:157:ARG:HD3	1:D:325:PHE:O	2.07	0.53
1:A:291:ILE:HD13	1:A:357:ASN:CG	2.29	0.53
1:C:30:TYR:HB3	1:C:53:THR:HG22	1.90	0.53
1:D:16:TYR:CE2	1:D:320:SER:HB3	2.44	0.53
1:A:319:ILE:HG21	1:A:375:PRO:HB3	1.91	0.53
1:A:380:ARG:NE	1:A:410:ASP:OD1	2.41	0.53
1:A:552:GLY:HA3	1:A:701:GLN:HG3	1.91	0.53
1:B:324:LEU:HB2	1:B:339:MET:HB3	1.91	0.53
1:C:47:LYS:HD2	1:C:51:MET:HE3	1.91	0.53
1:D:459:VAL:CG2	1:D:561:ILE:HG13	2.38	0.53
1:D:497:LYS:CE	3:D:1021:HOH:O	2.57	0.53
1:B:285:ARG:HG2	3:B:1028:HOH:O	2.09	0.53
1:B:452:GLU:HB3	1:B:556:ILE:HD12	1.90	0.53
1:C:352:GLY:O	1:C:385:LYS:HE3	2.08	0.53
1:D:21:VAL:HG11	1:D:337:TYR:CE1	2.44	0.53
1:D:622:TYR:CE1	1:D:643:MET:CE	2.92	0.53
1:D:645:PRO:HG3	1:D:672:GLY:N	2.24	0.53
1:B:422:ILE:HG21	1:B:440:LEU:HD22	1.91	0.52
1:C:92:LYS:NZ	3:C:946:HOH:O	2.42	0.52
1:A:406:ALA:HB2	1:A:764:ARG:HH21	1.74	0.52
1:A:417:LEU:HD11	1:A:438:THR:HB	1.92	0.52
1:B:445:LYS:HG2	1:B:540:TYR:CZ	2.44	0.52
1:D:157:ARG:NE	3:D:946:HOH:O	2.40	0.52
1:D:404:MET:HB3	1:D:405:PRO:HA	1.91	0.52
1:A:101:LYS:NZ	3:A:944:HOH:O	2.43	0.52
1:A:777:LYS:NZ	3:A:902:HOH:O	2.30	0.52
1:B:282:ASN:ND2	1:B:433:CYS:HA	2.23	0.52
1:B:285:ARG:HG2	1:B:285:ARG:HH11	1.75	0.52
1:B:462:VAL:HG23	1:B:498:GLN:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LYS:HA	1:B:538:LYS:HE2	1.90	0.52
1:C:73:ALA:HB2	1:C:80:ILE:CG2	2.38	0.52
1:C:433:CYS:N	1:C:437:GLU:O	2.41	0.52
1:D:433:CYS:HB2	1:D:439:ASN:CG	2.29	0.52
1:B:449:ASP:OD1	1:B:554:ASN:HB2	2.09	0.52
1:C:158:GLY:HA3	1:C:276:GLN:HB3	1.91	0.52
1:C:454:SER:HB2	1:C:652:ILE:CD1	2.38	0.52
1:D:594:TYR:HD2	1:D:597:ILE:HD12	1.75	0.52
1:A:696:HIS:NE2	1:A:703:THR:HG21	2.25	0.52
1:C:450:ILE:CG2	1:C:551:ASN:HB3	2.40	0.52
1:D:125:GLY:N	1:D:130:ASP:OD2	2.40	0.52
1:B:412:ALA:HB2	1:B:734:ASP:OD1	2.10	0.52
1:A:89:VAL:HG23	1:A:129:LEU:CD2	2.40	0.52
1:A:646:VAL:HG12	1:A:647:SER:H	1.75	0.52
1:C:83:PRO:O	1:C:127:CYS:HB3	2.10	0.52
1:D:319:ILE:O	1:D:339:MET:HE1	2.10	0.52
1:D:429:ASP:C	3:D:905:HOH:O	2.48	0.52
1:A:297:ASP:HB3	1:A:303:MET:HB3	1.92	0.52
1:A:455:MET:HG2	1:A:555:ILE:HG23	1.91	0.52
1:B:713:LEU:HD11	1:B:790:GLU:O	2.10	0.52
1:C:592:GLU:HA	1:C:592:GLU:OE2	2.09	0.52
1:C:656:VAL:O	1:C:663:ARG:NH2	2.40	0.52
1:C:760:ASP:HA	1:C:771:PHE:CD1	2.45	0.52
1:D:180:GLU:HA	1:D:183:GLU:CD	2.31	0.52
1:B:61:PHE:CZ	1:B:76:PRO:HD3	2.44	0.51
1:B:339:MET:HE3	1:B:339:MET:N	2.19	0.51
1:B:436:VAL:O	1:B:736:TYR:HE2	1.93	0.51
1:C:650:VAL:HB	1:C:651:PRO:CD	2.40	0.51
1:D:246:VAL:O	1:D:250:VAL:HG22	2.09	0.51
1:A:250:VAL:HB	1:A:251:PRO:HA	1.91	0.51
1:C:292:GLN:HG3	1:C:293:TYR:N	2.25	0.51
1:C:342:GLN:HG2	1:C:376:ASN:HB3	1.91	0.51
1:C:650:VAL:HA	1:C:668:PRO:HB3	1.91	0.51
1:B:650:VAL:HB	1:B:651:PRO:HD3	1.91	0.51
1:C:32:THR:HG22	1:C:36:LYS:HD2	1.92	0.51
1:D:718:ARG:HE	1:D:721:ASN:HD22	1.56	0.51
1:A:242:LYS:HE2	1:A:259:TYR:CD2	2.46	0.51
1:D:190:ASP:HB3	1:D:200:ILE:CD1	2.41	0.51
1:D:429:ASP:O	3:D:905:HOH:O	2.19	0.51
1:A:256:ARG:HB2	1:A:260:GLU:OE1	2.10	0.51
1:A:368:GLN:HB3	1:A:400:MET:HE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:MET:HB3	1:A:561:ILE:HB	1.92	0.51
1:B:89:VAL:HG22	1:B:327:ASP:HB3	1.91	0.51
1:B:286:MET:HE3	1:B:343:VAL:CG2	2.38	0.51
1:D:400:MET:HE3	1:D:402:ARG:HG2	1.91	0.51
1:D:518:GLU:HG2	1:D:541:ALA:O	2.11	0.51
1:B:739:GLN:HE22	1:B:767:GLY:CA	2.23	0.51
1:C:108:SER:OG	1:C:110:GLU:HG2	2.11	0.51
1:A:450:ILE:CG2	1:A:551:ASN:HB3	2.41	0.51
1:B:552:GLY:HA3	1:B:701:GLN:HG3	1.93	0.51
1:C:73:ALA:HB2	1:C:80:ILE:HG22	1.92	0.51
1:D:617:CYS:O	1:D:621:ILE:HD12	2.09	0.51
1:B:708:LYS:HE3	1:B:786:ARG:O	2.11	0.51
1:D:62:ILE:HB	1:D:227:MET:SD	2.50	0.51
1:A:74:PHE:HD1	1:A:74:PHE:H	1.59	0.51
1:B:97:ILE:HD11	1:B:325:PHE:HE1	1.76	0.51
1:C:415:LYS:NZ	3:C:925:HOH:O	2.29	0.51
1:C:416:MET:HG2	1:C:700:THR:HA	1.92	0.51
1:C:437:GLU:HG2	1:C:448:THR:CB	2.33	0.51
1:D:391:LEU:HG	1:D:724:MET:HG2	1.91	0.51
1:D:739:GLN:NE2	1:D:767:GLY:HA2	2.26	0.51
1:A:364:ILE:O	1:A:368:GLN:HG3	2.10	0.51
1:B:333:PHE:CE1	1:B:651:PRO:HB2	2.46	0.51
1:B:385:LYS:NZ	1:C:692:SER:O	2.38	0.51
1:B:378:THR:HG21	1:B:432:PRO:HG3	1.94	0.50
1:C:481:ASP:OD1	1:C:482:PRO:HD2	2.11	0.50
1:C:482:PRO:HG2	1:C:584:CYS:SG	2.51	0.50
1:C:658:ALA:HA	1:C:663:ARG:O	2.11	0.50
1:A:304:THR:HG22	1:A:307:GLU:H	1.76	0.50
1:A:730:GLN:HG3	1:A:735:ILE:HB	1.93	0.50
1:B:276:GLN:HA	1:B:276:GLN:OE1	2.09	0.50
1:A:447:TYR:HB2	1:A:551:ASN:CG	2.31	0.50
1:A:559:ALA:HB3	1:A:670:ALA:HB2	1.93	0.50
1:B:420:LYS:NZ	3:B:929:HOH:O	2.29	0.50
1:C:6:MET:O	1:C:10:GLN:HG2	2.11	0.50
1:C:216:LEU:HD11	1:C:220:HIS:HE1	1.75	0.50
1:A:665:ALA:HB1	1:A:666:TRP:CE2	2.47	0.50
1:B:710:ASP:HA	1:B:788:GLU:OE2	2.10	0.50
1:A:562:ILE:HD13	1:A:618:VAL:CG2	2.40	0.50
1:B:669:LEU:O	1:B:670:ALA:CB	2.59	0.50
1:C:31:VAL:HA	1:C:50:ALA:HB1	1.93	0.50
1:C:553:ILE:HD11	1:C:639:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ARG:NH1	1:D:144:ARG:HG2	2.27	0.50
1:B:257:ASN:HB2	1:B:297:ASP:OD2	2.11	0.50
1:C:137:PRO:HG2	1:C:140:VAL:CG2	2.42	0.50
1:D:144:ARG:HG2	1:D:144:ARG:HH11	1.77	0.50
1:D:206:LEU:HD22	1:D:528:LEU:HD23	1.92	0.50
1:D:567:ASP:OD2	1:D:661:SER:HA	2.10	0.50
1:A:344:CYS:HA	1:A:378:THR:O	2.11	0.50
1:B:47:LYS:CE	1:B:51:MET:HE3	2.41	0.50
1:B:161:GLU:H	1:B:280:SER:HB2	1.76	0.50
1:B:286:MET:CG	1:B:290:LEU:HD22	2.41	0.50
1:B:667:THR:HB	1:B:668:PRO:HD2	1.94	0.50
1:D:34:GLY:HA3	1:D:50:ALA:HA	1.93	0.50
1:A:157:ARG:HD2	1:A:324:LEU:HD21	1.93	0.50
1:A:610:ASP:HB3	3:A:908:HOH:O	2.11	0.50
1:C:54:VAL:CG1	1:C:274:MET:HE2	2.42	0.50
1:D:33:GLN:NE2	3:D:923:HOH:O	2.21	0.50
1:B:399:ARG:NH2	1:B:720:LEU:HD11	2.27	0.50
1:C:2:SER:N	3:C:922:HOH:O	2.44	0.50
1:C:723:MET:HE3	1:C:740:TYR:CZ	2.47	0.50
1:D:555:ILE:HD12	1:D:699:PHE:HE2	1.77	0.50
1:A:353:ASN:ND2	3:A:922:HOH:O	2.30	0.49
1:A:454:SER:HB2	1:A:652:ILE:CD1	2.41	0.49
1:A:706:ASN:HD21	1:A:739:GLN:HE21	1.59	0.49
1:D:81:LEU:HD13	1:D:83:PRO:N	2.27	0.49
1:D:225:GLU:CD	1:D:248:ARG:HH12	2.15	0.49
1:D:364:ILE:O	1:D:368:GLN:HG3	2.12	0.49
1:A:459:VAL:O	1:A:463:MET:HG2	2.12	0.49
1:B:415:LYS:HA	1:B:418:LEU:HD12	1.94	0.49
1:B:426:GLN:HB3	1:B:443:ARG:NH2	2.27	0.49
1:C:16:TYR:CE2	1:C:372:LEU:HD13	2.47	0.49
1:C:487:THR:HG21	3:C:1176:HOH:O	2.11	0.49
1:C:488:PHE:O	1:C:491:PHE:HB3	2.12	0.49
1:D:209:SER:OG	1:D:524:PRO:HB2	2.10	0.49
1:D:532:ASN:O	1:D:536:VAL:HG22	2.13	0.49
1:D:622:TYR:CD1	1:D:643:MET:HE3	2.47	0.49
1:D:705:MET:H	1:D:737:HIS:CD2	2.22	0.49
1:D:761:LEU:HD12	1:D:762:LEU:N	2.26	0.49
1:A:413:GLY:HA3	1:A:430:TRP:CZ2	2.47	0.49
1:B:452:GLU:CG	1:B:556:ILE:HD11	2.42	0.49
1:A:83:PRO:HB2	1:A:123:TRP:CD1	2.46	0.49
1:A:102:TYR:CE1	1:A:776:GLY:HA3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:NZ	1:A:734:ASP:OD1	2.41	0.49
1:B:488:PHE:CD1	1:B:569:LYS:HB2	2.47	0.49
1:D:25:ILE:HG13	1:D:111:ASN:HB3	1.95	0.49
1:D:59:PRO:HB2	3:D:1172:HOH:O	2.12	0.49
1:D:266:LEU:HB2	1:D:315:PHE:CE2	2.47	0.49
1:D:689:LYS:HD3	3:D:1140:HOH:O	2.12	0.49
1:A:416:MET:HE2	1:A:702:GLY:HA2	1.95	0.49
1:A:644:LEU:HG	1:A:644:LEU:O	2.13	0.49
1:A:714:LEU:HD13	1:A:742:VAL:HG11	1.94	0.49
1:B:139:ASP:OD1	1:B:140:VAL:N	2.45	0.49
1:B:537:GLY:O	1:B:538:LYS:HE3	2.12	0.49
1:D:739:GLN:HB3	1:D:764:ARG:HG2	1.94	0.49
1:A:161:GLU:HA	1:A:280:SER:HB2	1.94	0.49
1:C:83:PRO:HB2	1:C:123:TRP:CD1	2.48	0.49
1:D:455:MET:CE	1:D:561:ILE:HD13	2.42	0.49
1:D:554:ASN:HB2	3:D:1155:HOH:O	2.12	0.49
1:A:304:THR:HG22	1:A:307:GLU:HG3	1.94	0.49
1:A:558:GLN:NE2	1:A:672:GLY:O	2.46	0.49
1:B:5:TYR:CE1	1:B:6:MET:CE	2.96	0.49
1:B:155:PHE:O	3:B:917:HOH:O	2.20	0.49
1:B:340:THR:HG22	1:B:768:TYR:HB2	1.95	0.49
1:B:437:GLU:HA	1:B:701:GLN:O	2.13	0.49
1:C:314:CYS:HB3	3:C:1158:HOH:O	2.12	0.49
1:D:58:LYS:HZ1	1:D:72:VAL:C	2.16	0.49
1:D:313:ASP:OD1	1:D:366:ALA:HA	2.13	0.49
1:D:648:GLY:O	1:D:651:PRO:HD2	2.12	0.49
1:A:453:ILE:HG23	1:A:502:PHE:HD2	1.78	0.49
1:B:95:ASP:OD1	1:B:112:LYS:HE3	2.12	0.49
1:B:271:CYS:HA	1:B:274:MET:HE3	1.93	0.49
1:D:754:ASN:HB3	1:D:757:ASP:OD2	2.12	0.49
1:B:371:ALA:HB2	1:B:402:ARG:NE	2.27	0.49
1:B:227:MET:HA	1:B:230:LYS:HE2	1.94	0.49
1:C:137:PRO:HG2	1:C:140:VAL:HG23	1.94	0.49
1:C:434:GLY:HA3	3:C:903:HOH:O	2.13	0.49
1:D:793:GLY:HA3	3:D:1079:HOH:O	2.12	0.49
1:B:72:VAL:HG11	1:B:273:PHE:HD2	1.75	0.48
1:B:244:ALA:O	1:B:248:ARG:HG3	2.13	0.48
1:B:339:MET:H	1:B:339:MET:CE	2.20	0.48
1:B:445:LYS:O	1:B:446:SER:HB3	2.13	0.48
1:C:236:ARG:HG3	1:C:240:LEU:CD1	2.43	0.48
1:D:568:ILE:HD13	1:D:583:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ILE:HD13	1:A:625:LEU:HD21	1.95	0.48
1:A:564:SER:HB3	1:A:660:PRO:HG2	1.95	0.48
1:B:97:ILE:CD1	1:B:325:PHE:HE1	2.26	0.48
1:B:433:CYS:HB2	1:B:439:ASN:CG	2.32	0.48
1:C:68:LEU:HB3	1:C:266:LEU:CD2	2.43	0.48
1:C:450:ILE:HG23	1:C:551:ASN:HB3	1.95	0.48
1:C:650:VAL:HB	1:C:651:PRO:HD3	1.95	0.48
1:A:179:LYS:HA	1:A:182:GLU:OE2	2.12	0.48
1:A:575:GLU:CB	1:A:577:LYS:HG3	2.43	0.48
1:A:766:ALA:HB1	3:A:935:HOH:O	2.13	0.48
1:B:5:TYR:CE1	1:B:6:MET:HE3	2.48	0.48
1:B:393:LYS:HA	1:B:396:GLU:OE2	2.13	0.48
1:B:437:GLU:HG2	1:B:448:THR:HB	1.94	0.48
1:D:704:GLN:OE1	1:D:766:ALA:HB1	2.13	0.48
1:A:47:LYS:HE3	1:A:275:GLU:HG3	1.95	0.48
1:A:316:TRP:CD1	1:A:375:PRO:HD2	2.48	0.48
1:B:92:LYS:NZ	3:B:930:HOH:O	2.30	0.48
1:B:192:HIS:HB2	1:B:196:VAL:HG21	1.96	0.48
1:C:569:LYS:HD2	1:C:616:PHE:CZ	2.49	0.48
1:D:465:ASN:ND2	1:D:478:ARG:NH1	2.62	0.48
1:A:147:GLY:HA3	1:A:655:SER:OG	2.13	0.48
1:A:157:ARG:CZ	1:A:324:LEU:HD21	2.44	0.48
1:B:420:LYS:HB3	1:B:549:VAL:HG11	1.94	0.48
1:C:62:ILE:HG13	1:C:223:LEU:CD2	2.43	0.48
1:D:31:VAL:HG23	1:D:54:VAL:HG21	1.94	0.48
1:D:62:ILE:HD13	1:D:69:VAL:HG11	1.96	0.48
1:D:257:ASN:OD1	1:D:260:GLU:HG3	2.13	0.48
1:A:84:ASP:OD2	1:A:276:GLN:NE2	2.47	0.48
1:A:313:ASP:O	1:A:317:ILE:HG13	2.12	0.48
1:C:730:GLN:OE1	1:C:738:THR:CG2	2.62	0.48
1:D:739:GLN:HE22	1:D:767:GLY:HA2	1.74	0.48
1:B:373:LYS:HD3	3:B:1059:HOH:O	2.14	0.48
1:B:470:LYS:HG2	1:B:666:TRP:CZ3	2.47	0.48
1:B:479:THR:CG2	1:B:498:GLN:HE21	2.26	0.48
1:C:339:MET:CE	1:C:341:VAL:HB	2.43	0.48
1:C:479:THR:HB	1:C:498:GLN:HE21	1.79	0.48
1:D:12:LEU:HD13	3:D:1132:HOH:O	2.13	0.48
1:D:122:TYR:CE2	1:D:126:LYS:HE2	2.49	0.48
1:D:413:GLY:HA3	1:D:430:TRP:CE2	2.48	0.48
1:D:415:LYS:NZ	1:D:697:ALA:HB2	2.29	0.48
1:D:597:ILE:HA	1:D:600:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:PHE:O	3:D:921:HOH:O	2.20	0.48
1:A:688:LEU:CD1	1:A:726:LEU:HD11	2.44	0.48
1:B:285:ARG:HG2	1:B:285:ARG:NH1	2.28	0.48
1:C:303:MET:HG2	1:C:304:THR:N	2.28	0.48
1:C:613:LYS:O	3:C:913:HOH:O	2.20	0.48
1:D:72:VAL:O	1:D:80:ILE:HG21	2.14	0.48
1:D:403:THR:HB	1:D:764:ARG:HB2	1.95	0.48
1:A:644:LEU:N	1:A:644:LEU:HD23	2.29	0.48
1:C:54:VAL:HG11	1:C:274:MET:HE2	1.96	0.48
1:C:558:GLN:HA	1:C:622:TYR:HH	1.77	0.48
1:C:645:PRO:CG	1:C:672:GLY:H	2.27	0.48
1:A:38:THR:OG1	1:A:46:GLN:HG2	2.14	0.48
1:B:5:TYR:HE1	1:B:6:MET:HE3	1.78	0.48
1:B:513:LEU:O	1:B:517:SER:HB2	2.14	0.48
1:D:272:ILE:HG13	1:D:281:TYR:CD1	2.49	0.48
1:D:404:MET:CB	1:D:405:PRO:HA	2.42	0.48
1:A:97:ILE:HA	1:A:100:ARG:HD3	1.96	0.47
1:A:161:GLU:CA	1:A:280:SER:HB2	2.45	0.47
1:A:688:LEU:HA	1:A:691:ILE:HG12	1.95	0.47
1:C:644:LEU:HG	1:C:644:LEU:O	2.13	0.47
1:D:622:TYR:CE1	1:D:643:MET:HE3	2.48	0.47
1:C:449:ASP:OD1	1:C:554:ASN:HB2	2.14	0.47
1:D:28:ALA:HB2	1:D:81:LEU:HD12	1.97	0.47
1:D:257:ASN:HB2	1:D:297:ASP:OD2	2.14	0.47
1:A:304:THR:HG22	1:A:307:GLU:CB	2.43	0.47
1:C:413:GLY:HA3	1:C:430:TRP:CZ2	2.49	0.47
1:A:63:GLN:OE1	1:A:76:PRO:HG2	2.14	0.47
1:A:284:GLY:HA2	3:A:1152:HOH:O	2.13	0.47
1:A:445:LYS:HG2	1:A:540:TYR:CZ	2.50	0.47
1:B:129:LEU:N	3:B:917:HOH:O	2.46	0.47
1:B:459:VAL:CG2	1:B:561:ILE:CD1	2.75	0.47
1:B:670:ALA:HA	3:B:983:HOH:O	2.15	0.47
1:D:165:GLY:HA3	1:D:529:THR:O	2.14	0.47
1:D:492:MET:HE2	1:D:492:MET:HA	1.95	0.47
1:A:169:LEU:HD21	1:A:264:SER:OG	2.14	0.47
1:A:488:PHE:CE1	1:A:569:LYS:HB2	2.49	0.47
1:A:647:SER:O	1:A:651:PRO:HD2	2.13	0.47
1:B:320:SER:OG	1:B:374:GLU:O	2.33	0.47
1:D:450:ILE:CG2	1:D:551:ASN:HB3	2.45	0.47
1:D:718:ARG:O	1:D:721:ASN:HB2	2.15	0.47
1:A:131:ARG:HG2	1:A:131:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:GLU:HG2	1:A:448:THR:HB	1.96	0.47
1:A:671:ASP:OD1	1:A:671:ASP:N	2.47	0.47
1:B:652:ILE:HG22	1:B:669:LEU:HD22	1.96	0.47
1:B:680:ASP:OD1	1:B:680:ASP:N	2.42	0.47
1:C:47:LYS:NZ	1:C:275:GLU:O	2.27	0.47
1:C:54:VAL:CG1	1:C:274:MET:CE	2.92	0.47
1:C:58:LYS:HE3	1:C:274:MET:CE	2.44	0.47
1:D:83:PRO:HB2	1:D:123:TRP:CD1	2.49	0.47
1:D:713:LEU:CG	1:D:792:TRP:NE1	2.68	0.47
1:A:44:GLN:HG2	1:A:522:PRO:CB	2.45	0.47
1:A:692:SER:HA	3:A:1116:HOH:O	2.14	0.47
1:B:21:VAL:O	3:B:918:HOH:O	2.20	0.47
1:B:126:LYS:HG3	3:B:1057:HOH:O	2.14	0.47
1:B:698:ARG:HG3	1:B:698:ARG:HH11	1.80	0.47
1:C:68:LEU:HB3	1:C:266:LEU:HD22	1.97	0.47
1:C:378:THR:HA	1:C:405:PRO:HB2	1.97	0.47
1:C:453:ILE:HG13	1:C:506:MET:HG3	1.96	0.47
1:D:81:LEU:HG	1:D:90:ILE:HG13	1.97	0.47
1:D:158:GLY:HA3	1:D:276:GLN:HB3	1.95	0.47
1:D:283:LEU:O	1:D:289:TYR:HE2	1.98	0.47
1:D:482:PRO:HA	1:D:485:PHE:CE2	2.49	0.47
1:D:483:ARG:HG3	1:D:483:ARG:HH11	1.80	0.47
1:D:772:PHE:CZ	1:D:780:GLN:HB3	2.50	0.47
1:A:139:ASP:OD1	1:A:139:ASP:N	2.48	0.47
1:B:144:ARG:HD2	3:B:1176:HOH:O	2.15	0.47
1:B:595:GLU:HG2	3:B:915:HOH:O	2.14	0.47
1:A:13:ARG:HH22	1:A:760:ASP:HB2	1.80	0.47
1:A:153:LYS:HD3	2:A:801:87I:C10	2.44	0.47
1:B:280:SER:OG	1:B:434:GLY:HA3	2.15	0.47
1:C:84:ASP:OD1	1:C:84:ASP:N	2.47	0.47
1:C:413:GLY:HA3	1:C:430:TRP:CE2	2.50	0.47
1:D:429:ASP:CA	3:D:905:HOH:O	2.63	0.47
1:A:626:VAL:HG11	1:A:698:ARG:HB3	1.97	0.47
1:D:465:ASN:HD21	1:D:478:ARG:CZ	2.27	0.47
1:B:403:THR:HA	3:B:1009:HOH:O	2.15	0.46
1:C:31:VAL:HG22	1:C:51:MET:HE2	1.97	0.46
1:C:55:TYR:HB3	1:C:216:LEU:HB2	1.97	0.46
1:C:437:GLU:HA	1:C:701:GLN:O	2.14	0.46
1:D:324:LEU:HD23	1:D:326:GLN:HE22	1.79	0.46
1:B:283:LEU:HB3	1:B:286:MET:HE2	1.95	0.46
1:B:575:GLU:OE2	1:B:575:GLU:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:MET:SD	1:D:405:PRO:HB3	2.54	0.46
1:B:556:ILE:HG12	1:B:645:PRO:HA	1.97	0.46
1:B:738:THR:CG2	1:B:740:TYR:CE1	2.93	0.46
1:B:777:LYS:HE3	1:B:781:ASP:OD2	2.16	0.46
1:D:739:GLN:NE2	1:D:764:ARG:NE	2.62	0.46
1:A:34:GLY:HA3	1:A:50:ALA:HA	1.96	0.46
1:B:258:PHE:HE1	1:B:290:LEU:HB3	1.81	0.46
1:C:158:GLY:HA2	1:C:521:ARG:NE	2.30	0.46
1:C:158:GLY:HA2	1:C:521:ARG:CD	2.45	0.46
1:C:361:TYR:HE1	1:C:390:PHE:HA	1.79	0.46
1:D:462:VAL:HA	3:D:914:HOH:O	2.16	0.46
1:A:32:THR:O	1:A:36:LYS:HG3	2.16	0.46
1:A:523:VAL:HG21	1:A:526:LEU:HD23	1.98	0.46
1:C:133:ASN:ND2	3:C:912:HOH:O	2.20	0.46
1:C:451:GLY:O	1:C:554:ASN:HB3	2.15	0.46
1:C:479:THR:CB	3:C:919:HOH:O	2.63	0.46
1:D:647:SER:O	1:D:651:PRO:HD3	2.15	0.46
1:A:712:LYS:HD2	1:A:712:LYS:HA	1.72	0.46
1:B:154:LYS:N	3:B:910:HOH:O	2.16	0.46
1:B:568:ILE:O	1:B:572:VAL:HG22	2.16	0.46
1:D:469:ARG:HG2	1:D:469:ARG:NH1	2.31	0.46
1:B:445:LYS:HD3	1:B:445:LYS:C	2.35	0.46
1:C:156:VAL:HB	3:C:1026:HOH:O	2.15	0.46
1:C:216:LEU:HD11	1:C:220:HIS:CE1	2.51	0.46
1:D:285:ARG:HG3	1:D:431:THR:CG2	2.46	0.46
1:D:568:ILE:HD13	1:D:583:LEU:HD21	1.96	0.46
1:A:154:LYS:HD2	1:A:447:TYR:HD1	1.81	0.46
1:A:286:MET:HE3	1:A:290:LEU:CD1	2.45	0.46
1:A:482:PRO:O	1:A:580:MET:HG2	2.16	0.46
1:B:31:VAL:HG21	1:B:51:MET:HE1	1.97	0.46
1:C:84:ASP:HA	1:C:123:TRP:CZ3	2.50	0.46
1:C:435:CYS:HB3	1:C:767:GLY:HA3	1.98	0.46
1:C:479:THR:OG1	1:C:494:ALA:HB1	2.16	0.46
1:C:646:VAL:O	1:C:766:ALA:CB	2.63	0.46
1:D:131:ARG:HG2	1:D:131:ARG:NH1	2.29	0.46
1:D:234:GLU:HG2	1:D:237:ARG:HH22	1.80	0.46
1:A:538:LYS:HE3	1:A:542:ASN:O	2.16	0.46
1:C:354:ASP:OD2	1:C:387:PRO:HD3	2.16	0.46
1:C:377:MET:CE	1:C:405:PRO:HB3	2.46	0.46
1:C:488:PHE:CE1	1:C:569:LYS:HB2	2.50	0.46
1:A:166:TRP:O	1:A:170:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:VAL:HG13	1:B:390:PHE:CE2	2.51	0.45
1:C:62:ILE:HG12	1:C:69:VAL:CG2	2.44	0.45
1:C:377:MET:SD	1:C:405:PRO:HB3	2.56	0.45
1:C:712:LYS:O	1:C:715:GLU:HG3	2.16	0.45
1:C:791:ASN:ND2	1:C:793:GLY:H	2.14	0.45
1:D:406:ALA:HB1	1:D:737:HIS:CE1	2.51	0.45
1:A:154:LYS:HD2	1:A:447:TYR:CD1	2.51	0.45
1:A:374:GLU:HA	1:A:375:PRO:C	2.36	0.45
1:B:420:LYS:HG3	1:B:700:THR:HB	1.97	0.45
1:C:190:ASP:CG	1:D:508:THR:HG23	2.37	0.45
1:C:339:MET:HE2	1:C:374:GLU:CB	2.45	0.45
1:C:787:THR:HB	3:C:986:HOH:O	2.16	0.45
1:B:739:GLN:HE21	1:B:764:ARG:HH11	1.65	0.45
1:C:170:LEU:O	1:C:255:PRO:HD2	2.16	0.45
1:C:286:MET:HG3	1:C:343:VAL:HG23	1.98	0.45
1:C:316:TRP:CD1	1:C:375:PRO:HD2	2.51	0.45
1:D:167:ARG:HD2	1:D:441:GLU:OE1	2.16	0.45
1:A:8:ARG:NH1	1:A:67:LEU:HD21	2.31	0.45
1:A:279:SER:HA	1:A:339:MET:O	2.16	0.45
1:A:450:ILE:CG1	1:A:509:MET:HE1	2.46	0.45
1:B:663:ARG:NH1	1:B:667:THR:O	2.50	0.45
1:C:10:GLN:OE1	1:C:10:GLN:HA	2.17	0.45
1:C:21:VAL:HG11	1:C:337:TYR:CE1	2.52	0.45
1:A:283:LEU:HD22	1:A:341:VAL:CG1	2.46	0.45
1:B:129:LEU:CA	3:B:917:HOH:O	2.64	0.45
1:B:599:LYS:HD2	1:B:603:ASP:OD2	2.16	0.45
1:C:673:ILE:CD1	1:C:691:ILE:HD12	2.46	0.45
1:C:753:LYS:C	1:C:755:PRO:HD3	2.37	0.45
1:D:682:ASN:ND2	3:D:968:HOH:O	2.46	0.45
1:B:74:PHE:H	1:B:74:PHE:HD1	1.64	0.45
1:B:342:GLN:NE2	1:B:432:PRO:HB2	2.31	0.45
1:B:409:HIS:HD2	1:B:734:ASP:OD1	1.99	0.45
1:B:765:VAL:HG11	1:B:768:TYR:OH	2.16	0.45
1:C:157:ARG:HG3	3:C:905:HOH:O	2.16	0.45
1:D:280:SER:HB3	1:D:434:GLY:CA	2.47	0.45
1:D:483:ARG:HE	1:D:581:ASP:CG	2.19	0.45
1:A:151:VAL:HB	1:A:509:MET:HG3	1.98	0.45
1:A:176:GLY:O	1:A:180:GLU:HG3	2.17	0.45
1:B:378:THR:HG23	1:B:408:TYR:CD1	2.51	0.45
1:B:558:GLN:HG2	1:B:673:ILE:HA	1.97	0.45
1:C:373:LYS:HG3	1:C:374:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:MET:CE	1:D:461:MET:CE	2.95	0.45
1:D:280:SER:HB3	1:D:434:GLY:H	1.82	0.45
1:D:558:GLN:HG2	1:D:643:MET:HE1	1.95	0.45
1:C:556:ILE:HG23	1:C:645:PRO:HB3	1.98	0.45
1:C:575:GLU:OE1	1:C:575:GLU:HA	2.16	0.45
1:D:739:GLN:HE22	1:D:767:GLY:C	2.19	0.45
1:A:162:ASN:CA	1:A:439:ASN:OD1	2.65	0.45
1:C:5:TYR:HB2	1:C:310:GLU:OE2	2.17	0.45
1:C:17:MET:CE	1:C:760:ASP:HB3	2.47	0.45
1:C:590:ASP:O	1:C:591:PHE:HB2	2.17	0.45
1:D:146:GLY:HA2	3:D:1161:HOH:O	2.16	0.45
1:D:255:PRO:HG2	1:D:293:TYR:CZ	2.51	0.45
1:D:468:SER:HB2	1:D:475:ILE:HD13	1.99	0.45
1:A:121:PRO:HG2	3:A:965:HOH:O	2.17	0.45
1:B:342:GLN:NE2	1:B:378:THR:OG1	2.49	0.45
1:D:144:ARG:HD2	1:D:151:VAL:CG2	2.47	0.45
1:D:322:MET:HB2	1:D:339:MET:SD	2.57	0.45
1:A:55:TYR:HB3	1:A:216:LEU:HB2	1.98	0.44
1:A:555:ILE:CD1	1:A:625:LEU:HD21	2.47	0.44
1:B:129:LEU:HA	3:B:917:HOH:O	2.16	0.44
1:B:262:LEU:CD1	1:B:311:LEU:HB3	2.47	0.44
1:B:334:SER:HA	1:B:646:VAL:HG11	1.99	0.44
1:C:361:TYR:CE1	1:C:390:PHE:HA	2.52	0.44
1:D:28:ALA:HB1	1:D:81:LEU:HD12	1.99	0.44
1:D:31:VAL:HG23	1:D:54:VAL:CG2	2.48	0.44
1:D:157:ARG:NH2	2:D:801:87I:O02	2.50	0.44
1:D:170:LEU:HD22	1:D:255:PRO:HG3	1.99	0.44
1:A:391:LEU:HG	1:A:724:MET:HG2	1.99	0.44
1:B:107:LEU:HG	1:B:112:LYS:HG2	1.98	0.44
1:B:250:VAL:CG1	1:B:260:GLU:HB3	2.44	0.44
1:B:698:ARG:HG3	1:B:698:ARG:NH1	2.32	0.44
1:B:723:MET:O	1:B:727:LEU:HG	2.17	0.44
1:D:84:ASP:OD1	1:D:84:ASP:N	2.49	0.44
1:D:492:MET:HE3	1:D:492:MET:HB2	1.72	0.44
1:B:436:VAL:O	1:B:736:TYR:CE2	2.70	0.44
1:B:478:ARG:HG3	3:B:977:HOH:O	2.17	0.44
1:C:417:LEU:HD22	1:C:422:ILE:HD13	1.98	0.44
1:C:435:CYS:N	3:C:903:HOH:O	1.86	0.44
1:D:653:GLY:O	1:D:666:TRP:HA	2.16	0.44
1:A:44:GLN:HG2	1:A:522:PRO:HB3	1.99	0.44
1:B:378:THR:CG2	1:B:408:TYR:HE1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:GLN:OE1	1:B:766:ALA:HB1	2.18	0.44
1:D:58:LYS:NZ	1:D:274:MET:SD	2.85	0.44
1:D:280:SER:HA	1:D:340:THR:O	2.17	0.44
1:B:179:LYS:HD2	1:B:182:GLU:OE2	2.18	0.44
1:B:337:TYR:O	1:B:339:MET:HE3	2.18	0.44
1:C:486:LYS:HB2	1:C:486:LYS:HE3	1.53	0.44
1:C:500:ASP:HB2	3:C:948:HOH:O	2.17	0.44
1:D:555:ILE:HD13	1:D:625:LEU:HD21	1.97	0.44
1:A:58:LYS:HG3	1:A:59:PRO:O	2.18	0.44
1:A:154:LYS:NZ	1:A:161:GLU:OE2	2.46	0.44
1:B:157:ARG:O	1:B:158:GLY:O	2.35	0.44
1:C:97:ILE:HD12	1:C:100:ARG:NH1	2.33	0.44
1:C:510:ASN:OD1	1:C:551:ASN:HB2	2.18	0.44
1:D:154:LYS:HD3	1:D:154:LYS:HA	1.80	0.44
1:B:286:MET:CE	1:B:343:VAL:HG21	2.44	0.44
1:D:387:PRO:HG3	3:D:920:HOH:O	2.17	0.44
1:D:650:VAL:HB	1:D:651:PRO:HD3	2.00	0.44
1:A:285:ARG:HG3	1:A:431:THR:HG22	2.00	0.44
1:A:705:MET:HE3	1:A:706:ASN:O	2.18	0.44
1:A:705:MET:O	1:A:739:GLN:HG2	2.18	0.44
1:B:399:ARG:HD2	1:B:714:LEU:O	2.18	0.44
1:B:450:ILE:HG23	1:B:551:ASN:HB3	1.99	0.44
1:C:44:GLN:NE2	1:C:201:ILE:HG22	2.33	0.44
1:D:8:ARG:NH2	1:D:239:GLU:OE2	2.33	0.44
1:D:74:PHE:CZ	1:D:75:LYS:HD2	2.53	0.44
1:D:206:LEU:HD21	1:D:527:SER:HB2	2.00	0.44
1:A:3:LYS:O	1:A:6:MET:HB2	2.18	0.43
1:A:80:ILE:HD12	1:A:274:MET:HA	2.00	0.43
1:A:81:LEU:HD22	1:A:90:ILE:HG13	1.99	0.43
1:A:453:ILE:HG23	1:A:502:PHE:HB3	2.00	0.43
1:D:31:VAL:HA	1:D:50:ALA:HB1	1.99	0.43
1:D:275:GLU:OE1	1:D:525:ALA:HB3	2.18	0.43
1:D:429:ASP:HA	3:D:905:HOH:O	2.18	0.43
1:D:744:ASN:ND2	1:D:746:GLU:HB2	2.33	0.43
1:A:259:TYR:HB2	3:A:1108:HOH:O	2.18	0.43
1:B:6:MET:HE3	1:B:369:ASP:OD2	2.18	0.43
1:B:283:LEU:CD1	1:B:315:PHE:HE2	2.30	0.43
1:C:749:MET:O	1:C:753:LYS:HE2	2.18	0.43
1:D:253:ASN:HB3	1:D:254:PRO:HD2	2.00	0.43
1:A:339:MET:CE	1:A:374:GLU:HG3	2.48	0.43
1:A:424:MET:CG	1:D:698:ARG:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:SER:HB3	1:B:156:VAL:O	2.19	0.43
1:B:455:MET:HG2	1:B:555:ILE:HG23	1.99	0.43
1:C:266:LEU:HD21	1:C:318:LYS:HG3	2.00	0.43
1:D:178:LYS:HE2	1:D:182:GLU:OE2	2.19	0.43
1:D:180:GLU:HA	1:D:183:GLU:OE2	2.18	0.43
1:D:280:SER:OG	1:D:434:GLY:HA3	2.18	0.43
1:D:409:HIS:CE1	1:D:731:CYS:HB3	2.53	0.43
1:D:558:GLN:HA	1:D:622:TYR:OH	2.19	0.43
1:A:532:ASN:O	1:A:536:VAL:HG22	2.19	0.43
1:B:31:VAL:HA	1:B:50:ALA:HB1	1.99	0.43
1:B:275:GLU:O	1:B:276:GLN:HG2	2.19	0.43
1:B:416:MET:HG2	1:B:700:THR:HA	2.00	0.43
1:B:488:PHE:CE1	1:B:569:LYS:HB2	2.53	0.43
1:B:624:TYR:O	1:B:628:GLN:HG2	2.18	0.43
1:C:417:LEU:HD12	1:C:430:TRP:HB3	1.99	0.43
1:C:608:GLY:HA2	1:C:690:SER:CB	2.48	0.43
1:D:22:GLU:O	1:D:78:ALA:HA	2.18	0.43
1:D:285:ARG:HD3	3:D:905:HOH:O	2.15	0.43
1:D:609:ASN:HB3	1:D:682:ASN:OD1	2.18	0.43
1:D:673:ILE:HB	1:D:694:LEU:CD1	2.48	0.43
1:A:340:THR:CG2	1:A:340:THR:O	2.65	0.43
1:A:446:SER:HB2	1:A:549:VAL:HG23	2.01	0.43
1:B:398:ILE:CG2	1:B:740:TYR:HB2	2.49	0.43
1:C:342:GLN:HG3	1:C:434:GLY:O	2.18	0.43
1:C:465:ASN:OD1	1:C:479:THR:N	2.52	0.43
1:D:73:ALA:HB2	1:D:80:ILE:HG22	2.00	0.43
1:D:455:MET:HE3	1:D:561:ILE:HD12	2.00	0.43
1:D:747:ILE:HG22	1:D:761:LEU:HD21	2.01	0.43
1:A:285:ARG:HG2	1:A:344:CYS:SG	2.58	0.43
1:A:459:VAL:HG23	1:A:561:ILE:HD13	2.00	0.43
1:B:151:VAL:CB	3:B:1206:HOH:O	2.66	0.43
1:C:154:LYS:HG3	1:C:450:ILE:HA	2.00	0.43
1:C:285:ARG:HG3	1:C:431:THR:CG2	2.49	0.43
1:C:377:MET:O	1:C:405:PRO:HA	2.19	0.43
1:C:574:ASP:O	1:C:576:LYS:HD2	2.18	0.43
1:A:453:ILE:CG1	1:A:506:MET:HG3	2.48	0.43
1:B:170:LEU:CD2	1:B:255:PRO:HG3	2.46	0.43
1:B:649:ASN:OD1	1:B:649:ASN:N	2.52	0.43
1:B:718:ARG:HH11	1:B:721:ASN:CB	2.32	0.43
1:C:404:MET:CB	1:C:405:PRO:HA	2.42	0.43
1:D:251:PRO:HD3	1:D:267:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:724:MET:O	1:D:728:LYS:HG3	2.19	0.43
1:D:179:LYS:HE2	1:D:179:LYS:HB2	1.61	0.43
1:D:446:SER:HB3	1:D:549:VAL:HG22	2.01	0.43
1:B:5:TYR:HE1	1:B:6:MET:CE	2.31	0.43
1:C:546:GLU:HG2	1:C:547:PHE:CD2	2.54	0.43
1:D:163:THR:HA	1:D:164:PRO:HD2	1.94	0.43
1:D:285:ARG:HG3	1:D:431:THR:HG22	2.00	0.43
1:D:451:GLY:O	1:D:554:ASN:HB3	2.19	0.43
1:D:707:LEU:HD23	1:D:789:ILE:HD13	2.00	0.43
1:A:688:LEU:HD12	1:A:726:LEU:CD1	2.48	0.43
1:A:688:LEU:HA	1:A:688:LEU:HD23	1.71	0.43
1:C:81:LEU:HD22	1:C:90:ILE:HG13	2.00	0.43
1:C:566:ALA:HB1	1:C:614:ALA:HA	2.01	0.43
1:D:9:ILE:O	1:D:13:ARG:HB2	2.18	0.43
1:D:129:LEU:HD22	1:D:156:VAL:HG22	2.01	0.43
1:D:148:MET:HE2	1:D:461:MET:SD	2.59	0.43
1:D:163:THR:OG1	1:D:282:ASN:HB2	2.19	0.43
1:D:399:ARG:O	3:D:922:HOH:O	2.21	0.43
1:D:416:MET:HB3	1:D:700:THR:HA	2.00	0.43
1:D:499:ILE:HG23	1:D:625:LEU:HD13	2.01	0.43
1:D:676:THR:HG22	3:D:911:HOH:O	2.19	0.43
1:B:184:LYS:HE2	3:B:1130:HOH:O	2.19	0.42
1:B:550:GLY:HA3	1:B:638:LYS:O	2.19	0.42
1:B:677:GLY:HA3	1:B:785:GLN:NE2	2.33	0.42
1:C:182:GLU:HG3	1:C:207:ILE:HD12	2.01	0.42
1:D:318:LYS:NZ	1:D:321:GLU:OE1	2.48	0.42
1:A:136:MET:HE2	1:A:136:MET:HB2	1.88	0.42
1:A:340:THR:HG23	1:A:434:GLY:HA2	2.01	0.42
1:B:83:PRO:HB2	1:B:123:TRP:NE1	2.34	0.42
1:B:250:VAL:HG21	1:B:260:GLU:O	2.19	0.42
1:B:671:ASP:OD1	1:B:671:ASP:N	2.42	0.42
1:C:410:ASP:OD2	3:C:914:HOH:O	2.21	0.42
1:C:562:ILE:HD13	1:C:618:VAL:HG22	2.01	0.42
1:D:433:CYS:HB2	1:D:439:ASN:OD1	2.19	0.42
1:D:515:TYR:OH	3:D:919:HOH:O	2.19	0.42
1:A:436:VAL:O	1:A:736:TYR:HE2	2.02	0.42
1:A:782:ASP:O	1:A:785:GLN:HG3	2.18	0.42
1:B:31:VAL:HG22	1:B:51:MET:HE1	2.00	0.42
1:D:359:LEU:HD23	1:D:362:MET:SD	2.59	0.42
1:D:422:ILE:CD1	1:D:547:PHE:CG	3.03	0.42
1:A:419:ASN:ND2	1:D:424:MET:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LEU:HD21	1:A:705:MET:HE1	2.01	0.42
1:B:281:TYR:O	1:B:341:VAL:HG13	2.19	0.42
1:B:664:LYS:HB2	3:B:1205:HOH:O	2.19	0.42
1:C:463:MET:HE1	1:C:491:PHE:CE1	2.48	0.42
1:C:643:MET:HE1	1:C:694:LEU:HD13	2.01	0.42
1:C:747:ILE:HD13	1:C:747:ILE:HA	1.84	0.42
1:D:291:ILE:HG23	1:D:292:GLN:NE2	2.34	0.42
1:D:354:ASP:OD1	1:D:386:ASN:ND2	2.45	0.42
1:A:645:PRO:HD3	3:A:903:HOH:O	2.18	0.42
1:B:415:LYS:HE2	1:B:697:ALA:HB2	2.01	0.42
1:C:420:LYS:CD	1:C:700:THR:HB	2.34	0.42
1:C:673:ILE:HG12	1:C:704:GLN:O	2.18	0.42
1:C:690:SER:O	1:C:693:ASN:ND2	2.38	0.42
1:D:368:GLN:NE2	1:D:400:MET:HE1	2.33	0.42
1:D:433:CYS:HB3	1:D:437:GLU:HB2	2.02	0.42
1:D:464:ASN:HD22	1:D:469:ARG:HG2	1.83	0.42
1:D:465:ASN:HD21	1:D:478:ARG:NH1	2.16	0.42
1:D:556:ILE:HG12	1:D:645:PRO:CB	2.48	0.42
1:D:718:ARG:HE	1:D:721:ASN:ND2	2.17	0.42
1:A:89:VAL:O	1:A:93:GLU:HG2	2.20	0.42
1:A:606:LYS:HD3	1:A:606:LYS:HA	1.88	0.42
1:A:675:ALA:HB3	1:A:680:ASP:OD1	2.20	0.42
1:C:149:LEU:HD11	1:C:505:THR:HB	2.02	0.42
1:C:530:TYR:O	1:C:533:CYS:HB2	2.19	0.42
1:D:332:ALA:HB1	1:D:651:PRO:HG3	2.02	0.42
1:D:413:GLY:HA3	1:D:430:TRP:CZ2	2.55	0.42
1:D:739:GLN:HE22	1:D:767:GLY:N	2.17	0.42
1:A:277:ASN:OD1	1:A:324:LEU:HD12	2.19	0.42
1:B:283:LEU:HD13	1:B:286:MET:HE1	2.01	0.42
1:B:685:THR:O	1:B:689:LYS:HG3	2.20	0.42
1:C:339:MET:HE2	1:C:374:GLU:OE1	2.19	0.42
1:D:221:ALA:CB	1:D:248:ARG:HG2	2.50	0.42
1:D:280:SER:HB3	1:D:434:GLY:N	2.34	0.42
1:A:39:GLU:HG3	1:B:125:GLY:HA3	2.01	0.42
1:A:221:ALA:CB	1:A:248:ARG:HG2	2.50	0.42
1:B:258:PHE:CE2	1:B:262:LEU:HD11	2.55	0.42
1:B:334:SER:HA	1:B:646:VAL:CG1	2.49	0.42
1:B:598:HIS:CD2	1:B:664:LYS:HE3	2.53	0.42
1:B:643:MET:HE3	1:B:673:ILE:HG21	2.01	0.42
1:C:58:LYS:HB2	1:C:58:LYS:HE2	1.87	0.42
1:C:190:ASP:OD1	1:D:508:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:723:MET:HE2	1:D:727:LEU:CD1	2.44	0.42
1:D:770:ALA:CB	1:D:775:LEU:HD21	2.49	0.42
1:A:606:LYS:HE3	1:A:661:SER:O	2.19	0.42
1:B:354:ASP:OD1	1:B:386:ASN:ND2	2.52	0.42
1:B:482:PRO:HA	1:B:485:PHE:CD2	2.55	0.42
1:C:643:MET:CE	1:C:694:LEU:HD13	2.49	0.42
1:D:190:ASP:HB3	1:D:200:ILE:HD12	2.02	0.42
1:D:368:GLN:OE1	1:D:393:LYS:HE2	2.20	0.42
1:A:300:ASP:HB3	1:A:302:THR:HG23	2.01	0.42
1:A:409:HIS:HD2	1:A:412:ALA:HB2	1.84	0.42
1:A:433:CYS:HB3	1:A:437:GLU:HB2	2.01	0.42
1:A:558:GLN:HE21	1:A:673:ILE:HA	1.85	0.42
1:B:378:THR:HG21	1:B:408:TYR:CE1	2.54	0.42
1:B:383:ILE:HD12	1:B:728:LYS:HG2	2.02	0.42
1:B:402:ARG:C	1:B:403:THR:HG23	2.41	0.42
1:B:586:ALA:CB	1:B:597:ILE:HG21	2.50	0.42
1:B:688:LEU:HD23	1:B:688:LEU:HA	1.77	0.42
1:B:695:PRO:O	1:B:698:ARG:HB2	2.20	0.42
1:C:25:ILE:HG22	1:C:114:LEU:HD23	2.02	0.42
1:C:483:ARG:HG3	1:C:483:ARG:HH11	1.84	0.42
1:C:645:PRO:HG3	1:C:672:GLY:H	1.85	0.42
1:D:120:ALA:HB3	1:D:121:PRO:HD3	2.02	0.42
1:D:420:LYS:HG3	1:D:700:THR:HB	2.02	0.42
1:D:645:PRO:CD	1:D:672:GLY:HA2	2.50	0.42
1:D:684:ALA:HB2	1:D:789:ILE:HG21	2.01	0.42
1:B:161:GLU:CA	1:B:280:SER:HB2	2.49	0.41
1:B:554:ASN:O	1:B:555:ILE:HG13	2.20	0.41
1:B:764:ARG:HD2	1:B:768:TYR:O	2.20	0.41
1:D:223:LEU:HD12	1:D:223:LEU:O	2.20	0.41
1:D:342:GLN:HA	1:D:376:ASN:O	2.20	0.41
1:D:645:PRO:CG	1:D:672:GLY:H	2.33	0.41
1:A:164:PRO:O	1:A:441:GLU:HG2	2.19	0.41
1:A:368:GLN:HB3	1:A:400:MET:CE	2.50	0.41
1:C:126:LYS:HE2	3:C:1139:HOH:O	2.18	0.41
1:C:283:LEU:HG	1:C:341:VAL:CG1	2.50	0.41
1:C:368:GLN:HB3	1:C:400:MET:HE1	2.01	0.41
1:A:80:ILE:CD1	1:A:274:MET:HA	2.49	0.41
1:A:107:LEU:HG	1:A:112:LYS:HG3	2.02	0.41
1:A:160:GLY:HA3	1:A:279:SER:O	2.20	0.41
1:A:275:GLU:OE1	1:A:524:PRO:HD2	2.20	0.41
1:A:453:ILE:CG2	1:A:502:PHE:HD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:HG2	1:B:74:PHE:CB	2.51	0.41
1:B:137:PRO:HD3	1:B:512:TYR:CZ	2.56	0.41
1:B:215:ALA:O	1:B:219:ARG:HG3	2.20	0.41
1:B:378:THR:HG23	1:B:408:TYR:HE1	1.83	0.41
1:B:707:LEU:HD23	1:B:789:ILE:HD12	2.02	0.41
1:B:711:PRO:HD2	1:B:788:GLU:OE2	2.20	0.41
1:B:730:GLN:CG	1:B:735:ILE:HB	2.49	0.41
1:C:150:TYR:CE2	1:C:153:LYS:HG3	2.55	0.41
1:C:668:PRO:O	3:C:915:HOH:O	2.22	0.41
1:D:646:VAL:O	1:D:766:ALA:CB	2.67	0.41
1:A:450:ILE:HD12	1:A:509:MET:CE	2.49	0.41
1:A:538:LYS:HB2	1:A:538:LYS:HE2	1.88	0.41
1:A:677:GLY:HA3	1:A:785:GLN:OE1	2.21	0.41
1:B:223:LEU:HD12	1:B:223:LEU:O	2.20	0.41
1:B:377:MET:SD	1:B:405:PRO:HB3	2.60	0.41
1:B:708:LYS:HE2	1:B:786:ARG:HB2	2.03	0.41
1:C:80:ILE:CD1	1:C:274:MET:HA	2.51	0.41
1:C:333:PHE:O	1:C:646:VAL:HB	2.20	0.41
1:D:285:ARG:CG	1:D:431:THR:HG22	2.50	0.41
1:D:744:ASN:OD1	1:D:745:PRO:HD2	2.19	0.41
1:A:131:ARG:HG2	1:A:131:ARG:NH1	2.35	0.41
1:A:304:THR:HG23	1:A:306:ASP:N	2.35	0.41
1:A:354:ASP:OD1	1:A:386:ASN:ND2	2.53	0.41
1:A:726:LEU:O	1:A:729:THR:HB	2.21	0.41
1:C:707:LEU:O	1:C:740:TYR:HA	2.21	0.41
1:D:159:TYR:HE2	1:D:521:ARG:O	2.04	0.41
1:D:219:ARG:HG3	3:D:944:HOH:O	2.20	0.41
1:D:415:LYS:HZ2	1:D:697:ALA:HB2	1.84	0.41
1:A:404:MET:CB	1:A:405:PRO:HA	2.48	0.41
1:B:98:SER:HA	1:B:105:PHE:O	2.21	0.41
1:B:154:LYS:HD3	1:B:154:LYS:HA	1.85	0.41
1:B:221:ALA:CB	1:B:248:ARG:HG2	2.51	0.41
1:B:538:LYS:HE2	3:B:1038:HOH:O	2.21	0.41
1:C:333:PHE:HB3	3:C:1112:HOH:O	2.21	0.41
1:C:476:SER:OG	1:C:477:ILE:N	2.52	0.41
1:C:591:PHE:CE2	1:C:658:ALA:HB1	2.55	0.41
1:C:644:LEU:N	1:C:644:LEU:HD23	2.36	0.41
1:D:74:PHE:CE2	1:D:75:LYS:HE3	2.55	0.41
1:D:81:LEU:O	1:D:83:PRO:HD3	2.20	0.41
1:D:144:ARG:HD2	1:D:151:VAL:HG22	2.01	0.41
1:D:586:ALA:HB2	1:D:594:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MET:SD	1:A:275:GLU:HA	2.61	0.41
1:A:217:ALA:HB2	1:A:251:PRO:HD2	2.02	0.41
1:B:420:LYS:HE3	1:B:700:THR:O	2.20	0.41
1:C:453:ILE:HD12	1:C:553:ILE:CG2	2.50	0.41
1:C:463:MET:CE	1:C:463:MET:HA	2.50	0.41
1:D:482:PRO:O	1:D:580:MET:HG2	2.21	0.41
1:A:287:ASP:HA	1:A:359:LEU:HB3	2.03	0.41
1:A:560:ASP:CG	1:A:669:LEU:HD22	2.41	0.41
1:A:591:PHE:CE2	1:A:658:ALA:HB1	2.55	0.41
1:C:108:SER:OG	1:C:111:ASN:HB2	2.20	0.41
1:C:399:ARG:HB3	3:C:939:HOH:O	2.21	0.41
1:C:458:VAL:O	1:C:462:VAL:HG23	2.21	0.41
1:C:566:ALA:CB	1:C:614:ALA:HA	2.50	0.41
1:D:416:MET:HE3	1:D:736:TYR:CD1	2.56	0.41
1:D:533:CYS:O	1:D:537:GLY:N	2.53	0.41
1:D:591:PHE:CD1	1:D:598:HIS:HB2	2.55	0.41
1:A:153:LYS:HD3	1:A:157:ARG:HH22	1.85	0.41
1:A:154:LYS:HG3	1:A:450:ILE:HA	2.02	0.41
1:A:226:LYS:HA	1:A:226:LYS:HD2	1.83	0.41
1:A:554:ASN:ND2	1:A:644:LEU:HG	2.35	0.41
1:A:623:ASN:OD1	1:A:698:ARG:NH1	2.54	0.41
1:A:673:ILE:HG21	1:A:703:THR:HG23	2.03	0.41
1:B:283:LEU:HG	1:B:341:VAL:CG1	2.51	0.41
1:B:303:MET:CE	1:B:308:ALA:HB2	2.49	0.41
1:B:317:ILE:O	1:B:321:GLU:HG3	2.21	0.41
1:B:342:GLN:HE21	1:B:378:THR:CB	2.33	0.41
1:B:606:LYS:HD3	1:B:606:LYS:HA	1.79	0.41
1:C:245:GLU:HA	1:C:248:ARG:NH2	2.36	0.41
1:C:426:GLN:OE1	1:C:443:ARG:HD2	2.21	0.41
1:C:468:SER:O	1:C:472:GLY:HA2	2.21	0.41
1:D:151:VAL:HB	1:D:509:MET:HG3	2.02	0.41
1:D:622:TYR:CE1	1:D:643:MET:HE2	2.56	0.41
1:D:739:GLN:HE21	1:D:764:ARG:HH21	1.68	0.41
1:A:167:ARG:NE	3:A:957:HOH:O	2.45	0.41
1:A:753:LYS:N	1:A:753:LYS:HD3	2.35	0.41
1:B:102:TYR:CD2	1:B:332:ALA:HB2	2.55	0.41
1:B:703:THR:O	1:B:737:HIS:HB3	2.21	0.41
1:C:209:SER:O	1:C:213:ILE:HG13	2.21	0.41
1:C:462:VAL:HG12	1:C:463:MET:HE2	2.03	0.41
1:C:553:ILE:HB	1:C:629:ILE:CD1	2.47	0.41
1:D:74:PHE:C	1:D:75:LYS:HG3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LEU:HD12	1:D:129:LEU:HA	1.78	0.41
1:D:578:ILE:HD12	1:D:600:MET:HE3	2.02	0.41
1:D:771:PHE:HB2	1:D:774:GLU:HG3	2.03	0.41
1:B:452:GLU:N	1:B:452:GLU:CD	2.74	0.40
1:D:28:ALA:HB2	1:D:81:LEU:HB3	2.02	0.40
1:D:374:GLU:HA	1:D:375:PRO:C	2.42	0.40
1:D:450:ILE:HG21	1:D:551:ASN:HB3	2.01	0.40
1:D:648:GLY:CA	1:D:651:PRO:HD2	2.51	0.40
1:A:324:LEU:HD12	1:A:324:LEU:HA	1.75	0.40
1:A:703:THR:O	1:A:737:HIS:HB3	2.20	0.40
1:B:47:LYS:HE2	1:B:275:GLU:HG3	2.03	0.40
1:B:179:LYS:HD2	1:B:179:LYS:HA	1.85	0.40
1:B:409:HIS:CD2	1:B:734:ASP:HA	2.55	0.40
1:B:515:TYR:O	1:B:519:ASN:ND2	2.55	0.40
1:B:594:TYR:HD2	1:B:597:ILE:HG13	1.87	0.40
1:B:718:ARG:HH11	1:B:721:ASN:HB2	1.86	0.40
1:C:102:TYR:HH	1:C:778:ASP:CG	2.23	0.40
1:C:353:ASN:HB2	3:C:1013:HOH:O	2.22	0.40
1:B:151:VAL:CG2	3:B:1206:HOH:O	2.63	0.40
1:B:645:PRO:HG2	1:B:672:GLY:N	2.36	0.40
1:B:718:ARG:NH1	1:B:721:ASN:HD22	2.19	0.40
1:D:300:ASP:CB	1:D:302:THR:HG23	2.51	0.40
1:A:153:LYS:HG3	3:A:915:HOH:O	2.22	0.40
1:A:339:MET:O	1:A:340:THR:HG22	2.21	0.40
1:B:144:ARG:HE	1:B:144:ARG:HB3	1.74	0.40
1:B:418:LEU:CD1	1:C:415:LYS:HG2	2.52	0.40
1:C:280:SER:HB2	1:C:434:GLY:HA2	2.04	0.40
1:C:479:THR:CA	3:C:919:HOH:O	2.66	0.40
1:C:516:LEU:HD23	1:C:516:LEU:HA	1.76	0.40
1:C:552:GLY:HA3	1:C:701:GLN:HG3	2.03	0.40
1:D:322:MET:HB2	1:D:339:MET:CE	2.50	0.40
1:D:417:LEU:HD13	1:D:438:THR:HB	2.03	0.40
1:D:418:LEU:HD23	1:D:422:ILE:O	2.21	0.40
1:A:643:MET:HE1	1:A:699:PHE:CE1	2.57	0.40
1:B:161:GLU:N	1:B:280:SER:HB2	2.36	0.40
1:C:157:ARG:HG3	3:C:976:HOH:O	2.21	0.40
1:C:283:LEU:HD13	1:C:315:PHE:HE1	1.86	0.40
1:C:318:LYS:HA	1:C:318:LYS:HD2	1.93	0.40
1:D:64:ASP:O	1:D:65:HIS:HB2	2.21	0.40
1:D:76:PRO:HB3	1:D:321:GLU:HG2	2.04	0.40
1:D:759:LYS:HA	1:D:773:VAL:HG21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1122:HOH:O	3:C:1184:HOH:O[1_556]	2.04	0.16

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/793 (100%)	753 (95%)	31 (4%)	5 (1%)	22	23
1	B	789/793 (100%)	749 (95%)	34 (4%)	6 (1%)	16	16
1	C	790/793 (100%)	743 (94%)	42 (5%)	5 (1%)	22	23
1	D	789/793 (100%)	737 (93%)	48 (6%)	4 (0%)	25	27
All	All	3157/3172 (100%)	2982 (94%)	155 (5%)	20 (1%)	22	23

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	GLY
1	B	158	GLY
1	C	158	GLY
1	C	434	GLY
1	C	474	GLN
1	D	158	GLY
1	D	434	GLY
1	A	646	VAL
1	B	646	VAL
1	C	441	GLU
1	D	436	VAL
1	A	672	GLY
1	B	670	ALA
1	B	765	VAL
1	C	646	VAL

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Mol	Chain	Res	Type
1	D	646	VAL
1	B	436	VAL
1	A	164	PRO
1	B	434	GLY
1	A	434	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	665/667 (100%)	648 (97%)	17 (3%)	41	51
1	B	665/667 (100%)	643 (97%)	22 (3%)	33	41
1	C	666/667 (100%)	654 (98%)	12 (2%)	54	66
1	D	665/667 (100%)	652 (98%)	13 (2%)	50	62
All	All	2661/2668 (100%)	2597 (98%)	64 (2%)	44	54

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	10	GLN
1	A	74	PHE
1	A	169	LEU
1	A	170	LEU
1	A	178	LYS
1	A	190	ASP
1	A	225	GLU
1	A	248	ARG
1	A	259	TYR
1	A	283	LEU
1	A	316	TRP
1	A	337	TYR
1	A	339	MET
1	A	446	SER
1	A	638	LYS

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Mol	Chain	Res	Type
1	A	644	LEU
1	B	3	LYS
1	B	58	LYS
1	B	74	PHE
1	B	92	LYS
1	B	209	SER
1	B	259	TYR
1	B	316	TRP
1	B	339	MET
1	B	388	ASP
1	B	411	ASP
1	B	460	ASP
1	B	470	LYS
1	B	473	GLU
1	B	489	ASP
1	B	517	SER
1	B	577	LYS
1	B	599	LYS
1	B	638	LYS
1	B	644	LEU
1	B	718	ARG
1	B	739	GLN
1	B	753	LYS
1	C	113	LYS
1	C	259	TYR
1	C	280	SER
1	C	316	TRP
1	C	326	GLN
1	C	339	MET
1	C	460	ASP
1	C	469	ARG
1	C	644	LEU
1	C	671	ASP
1	C	690	SER
1	C	753	LYS
1	D	20	ARG
1	D	58	LYS
1	D	74	PHE
1	D	230	LYS
1	D	234	GLU
1	D	259	TYR
1	D	296	LYS

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Mol	Chain	Res	Type
1	D	316	TRP
1	D	385	LYS
1	D	460	ASP
1	D	596	HIS
1	D	644	LEU
1	D	753	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	GLN
1	A	558	GLN
1	A	706	ASN
1	A	737	HIS
1	B	220	HIS
1	B	342	GLN
1	B	654	GLN
1	B	739	GLN
1	D	342	GLN
1	D	368	GLN
1	D	532	ASN
1	D	704	GLN
1	D	737	HIS
1	D	739	GLN
1	D	744	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	87I	A	801	-	9,10,10	6.40	4 (44%)	12,14,14	0.99	0
2	87I	B	801	-	9,10,10	6.54	4 (44%)	12,14,14	1.34	2 (16%)
2	87I	D	801	-	9,10,10	6.17	3 (33%)	12,14,14	1.65	2 (16%)
2	87I	C	801	-	9,10,10	6.16	4 (44%)	12,14,14	1.38	2 (16%)

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	87I	A	801	-	-	4/4/16/16	0/1/1/1
2	87I	B	801	-	-	4/4/16/16	0/1/1/1
2	87I	D	801	-	-	2/4/16/16	0/1/1/1
2	87I	C	801	-	-	0/4/16/16	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	87I	C08-N04	13.97	1.66	1.47
2	A	801	87I	C08-N04	13.74	1.65	1.47
2	D	801	87I	C08-N04	13.01	1.64	1.47
2	C	801	87I	C08-N04	12.92	1.64	1.47
2	B	801	87I	C08-C07	-12.91	1.33	1.52
2	D	801	87I	C08-C07	-12.53	1.34	1.52
2	C	801	87I	C08-C07	-12.48	1.34	1.52
2	A	801	87I	C08-C07	-12.37	1.34	1.52
2	A	801	87I	C06-C07	2.93	1.58	1.52
2	B	801	87I	C06-C05	2.84	1.59	1.53
2	A	801	87I	C06-C05	2.81	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	87I	C06-C07	2.65	1.57	1.52
2	C	801	87I	C06-C07	2.59	1.57	1.52
2	B	801	87I	C06-C07	2.58	1.57	1.52
2	C	801	87I	C06-C05	2.01	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	87I	C06-C07-C08	4.01	108.24	103.31
2	D	801	87I	C07-C06-C05	-2.93	100.22	103.97
2	C	801	87I	C06-C07-C08	2.62	106.53	103.31
2	C	801	87I	C09-N04-C08	-2.50	109.06	112.45
2	B	801	87I	C06-C07-C08	-2.14	100.67	103.31
2	B	801	87I	O03-C10-C05	2.14	120.79	113.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	87I	N04-C05-C10-O02
2	B	801	87I	N04-C05-C10-O03
2	A	801	87I	N04-C05-C10-O02
2	A	801	87I	N04-C05-C10-O03
2	B	801	87I	C06-C05-C10-O03
2	B	801	87I	C06-C05-C10-O02
2	A	801	87I	C06-C05-C10-O02
2	A	801	87I	C06-C05-C10-O03
2	D	801	87I	C06-C05-C10-O02
2	D	801	87I	C06-C05-C10-O03

There are no ring outliers.

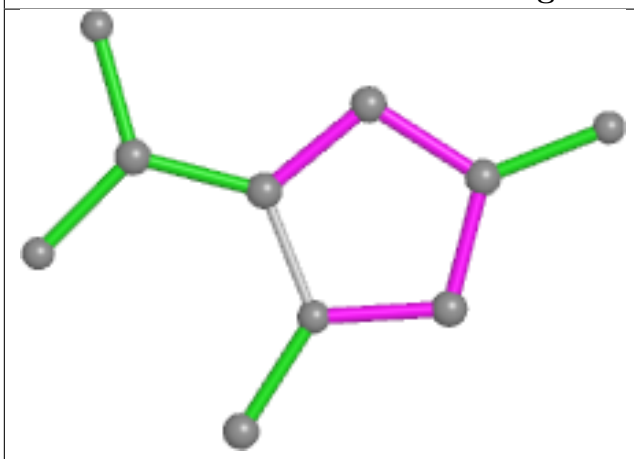
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	87I	2	0
2	D	801	87I	2	0
2	C	801	87I	1	0

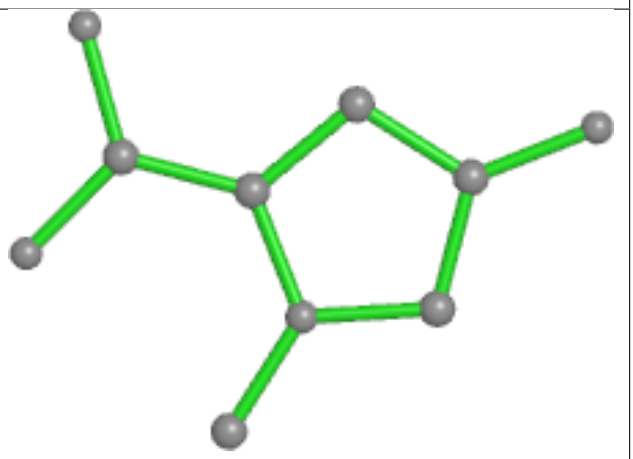
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

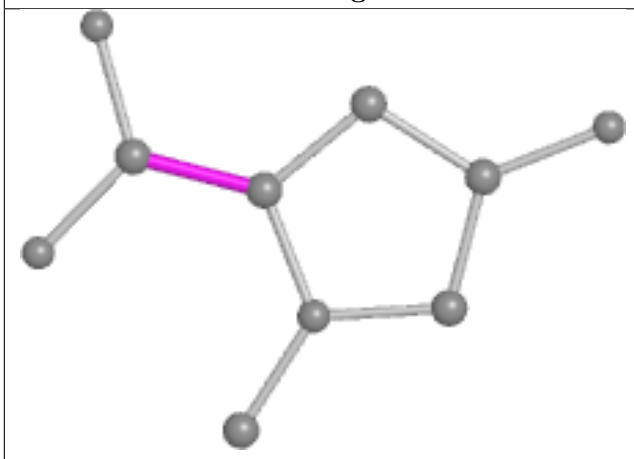
Ligand 87I A 801



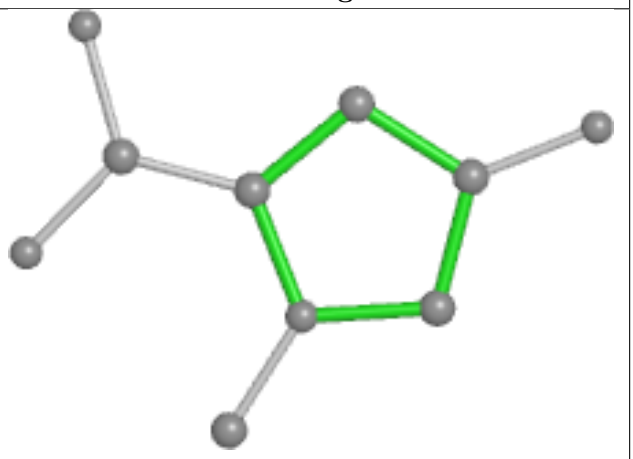
Bond lengths



Bond angles

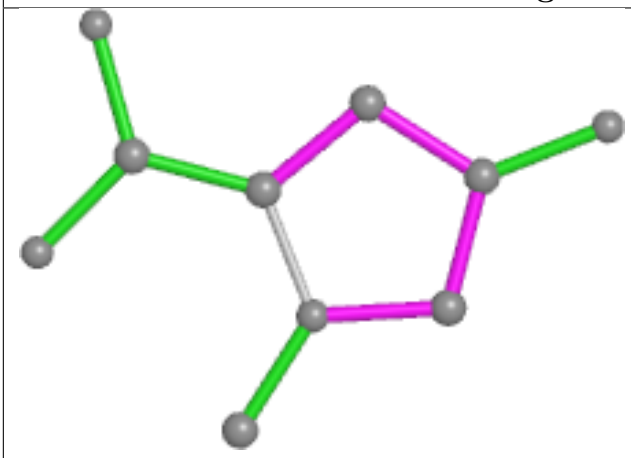


Torsions

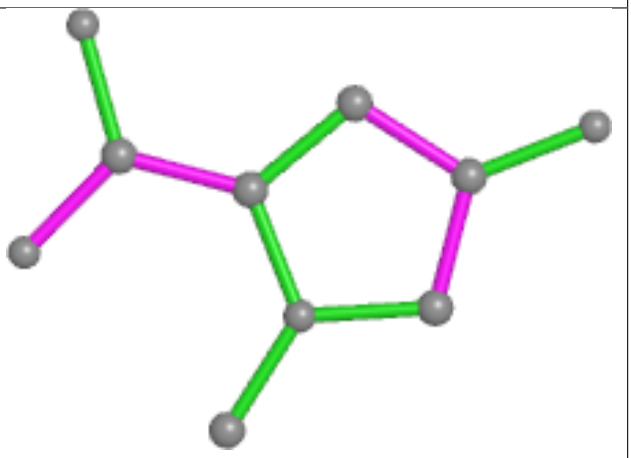


Rings

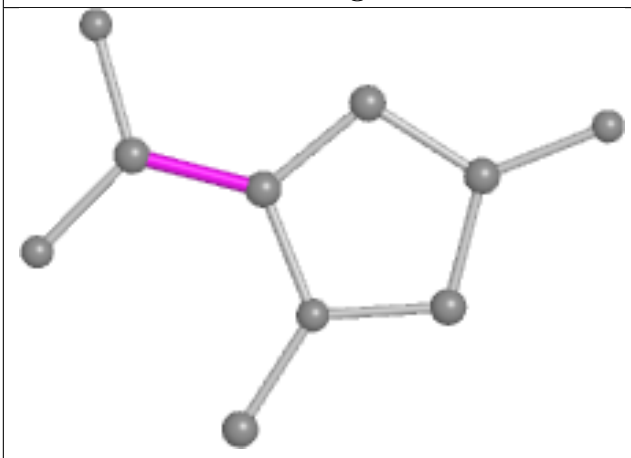
Ligand 87I B 801



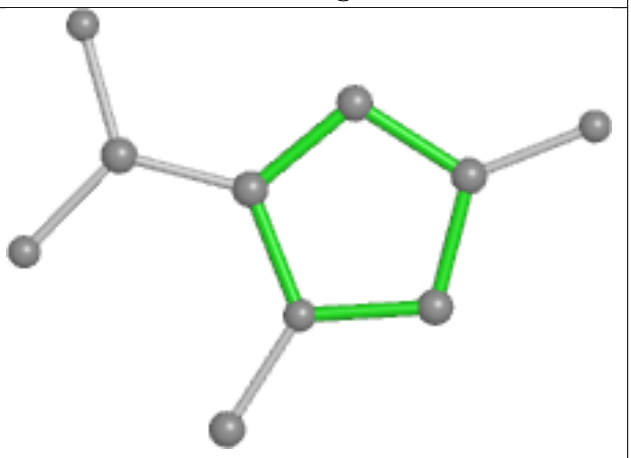
Bond lengths



Bond angles

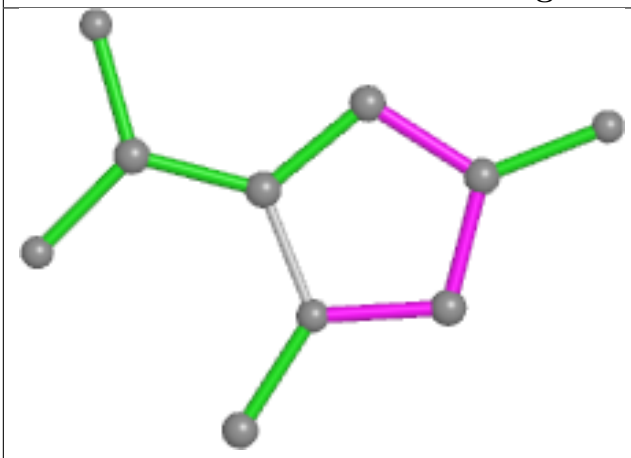


Torsions

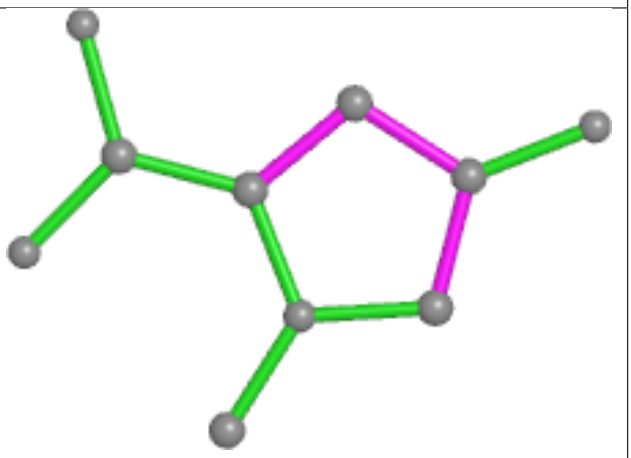


Rings

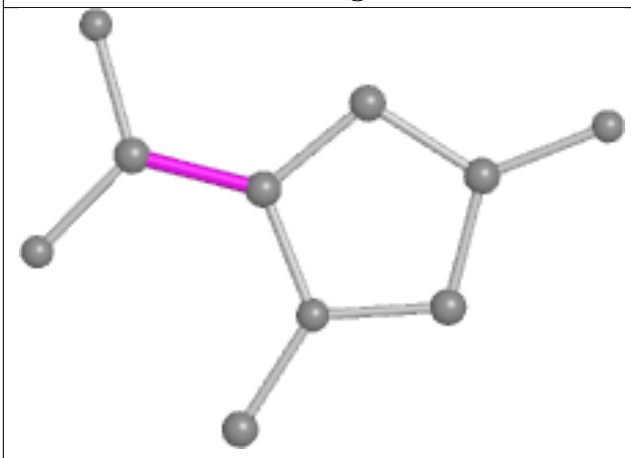
Ligand 87I D 801



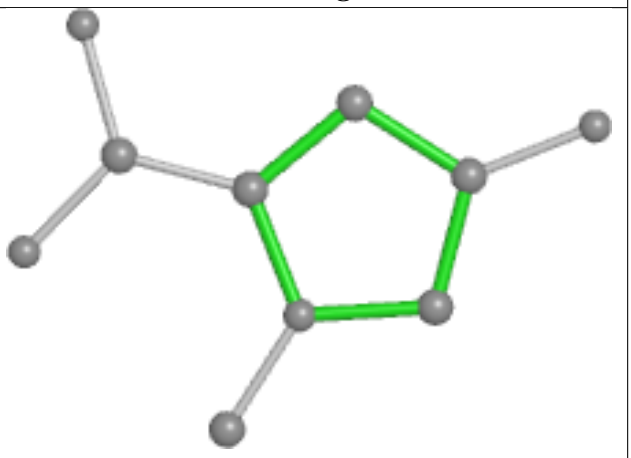
Bond lengths



Bond angles

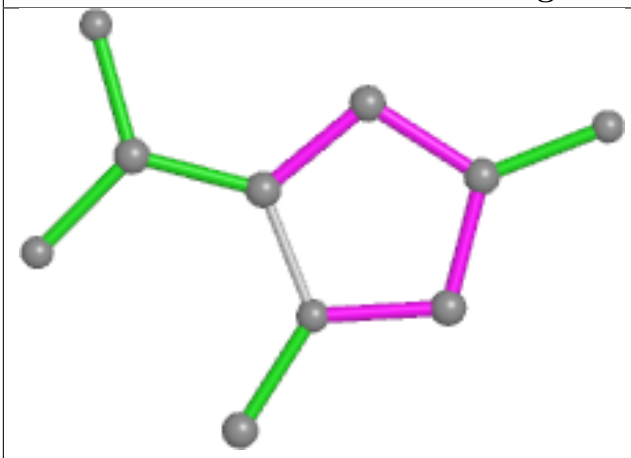


Torsions

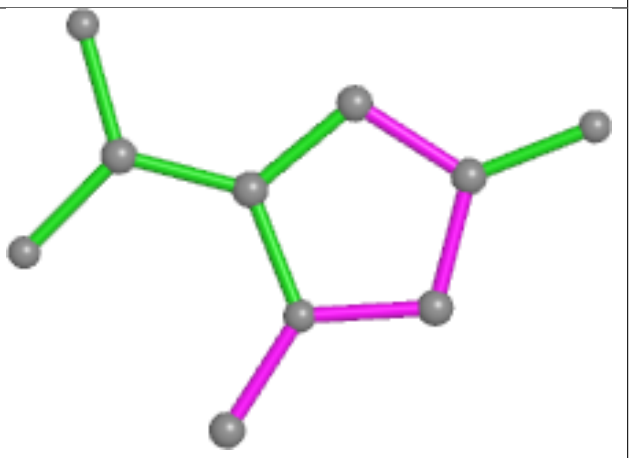


Rings

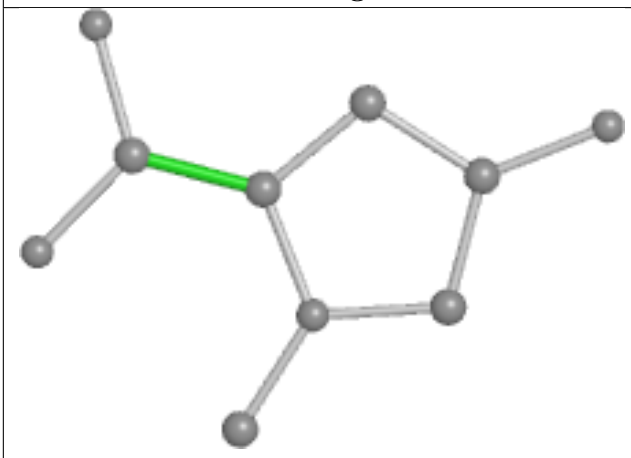
Ligand 87I C 801



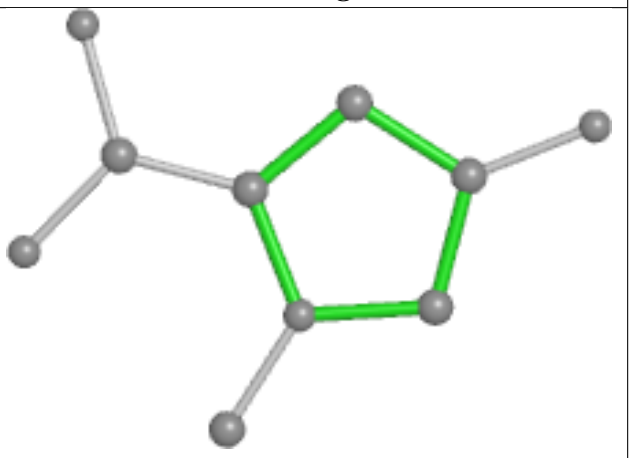
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	791/793 (99%)	0.48	23 (2%)	54	60	3, 10, 25, 43	0
1	B	791/793 (99%)	0.45	15 (1%)	66	71	3, 11, 24, 37	0
1	C	792/793 (99%)	0.53	19 (2%)	59	65	4, 12, 25, 44	0
1	D	791/793 (99%)	0.51	21 (2%)	56	62	4, 12, 28, 41	0
All	All	3165/3172 (99%)	0.49	78 (2%)	58	64	3, 11, 26, 44	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	GLY	5.4
1	A	681	ILE	5.0
1	C	2	SER	4.8
1	C	232	ALA	4.6
1	B	166	TRP	4.1
1	A	793	GLY	3.8
1	D	166	TRP	3.7
1	D	164	PRO	3.7
1	B	268	TYR	3.6
1	D	158	GLY	3.5
1	A	680	ASP	3.4
1	A	508	THR	3.4
1	D	138	GLU	3.4
1	D	139	ASP	3.2
1	B	671	ASP	3.1
1	A	596	HIS	3.0
1	D	666	TRP	2.9
1	B	531	PRO	2.9
1	A	339	MET	2.9
1	A	282	ASN	2.8
1	C	766	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	2.7
1	A	411	ASP	2.7
1	A	300	ASP	2.6
1	D	300	ASP	2.6
1	C	790	GLU	2.6
1	A	158	GLY	2.6
1	B	670	ALA	2.6
1	A	588	ASP	2.6
1	B	734	ASP	2.6
1	B	158	GLY	2.5
1	C	73	ALA	2.5
1	D	142	THR	2.5
1	A	4	ASP	2.5
1	B	746	GLU	2.5
1	B	669	LEU	2.5
1	D	234	GLU	2.4
1	A	14	GLU	2.4
1	B	766	ALA	2.4
1	C	4	ASP	2.4
1	A	717	GLU	2.4
1	A	746	GLU	2.4
1	A	743	ILE	2.4
1	C	671	ASP	2.3
1	C	583	LEU	2.3
1	C	744	ASN	2.3
1	A	234	GLU	2.3
1	A	459	VAL	2.3
1	D	578	ILE	2.3
1	C	666	TRP	2.3
1	D	478	ARG	2.2
1	B	300	ASP	2.2
1	D	595	GLU	2.2
1	D	717	GLU	2.2
1	A	15	ASN	2.2
1	D	594	TYR	2.2
1	B	44	GLN	2.2
1	D	292	GLN	2.2
1	C	233	ASP	2.2
1	C	778	ASP	2.2
1	D	592	GLU	2.2
1	B	691	ILE	2.1
1	C	234	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	718	ARG	2.1
1	C	297	ASP	2.1
1	C	748	LEU	2.1
1	D	394	ALA	2.1
1	A	297	ASP	2.0
1	B	633	ASP	2.0
1	C	782	ASP	2.0
1	D	480	GLY	2.0
1	A	477	ILE	2.0
1	C	749	MET	2.0
1	D	110	GLU	2.0
1	D	225	GLU	2.0
1	A	650	VAL	2.0
1	A	514	ASP	2.0
1	D	581	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

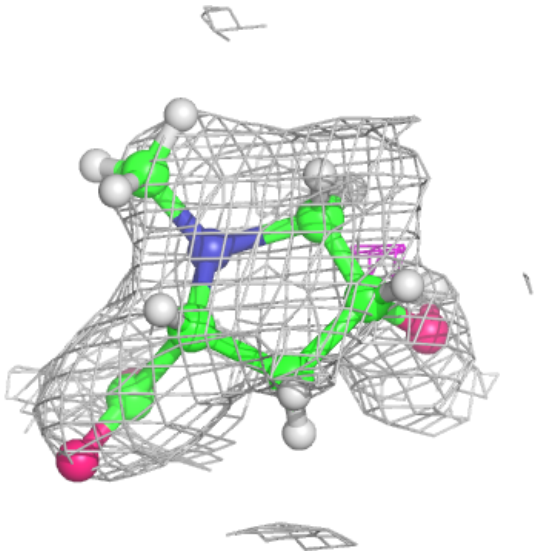
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

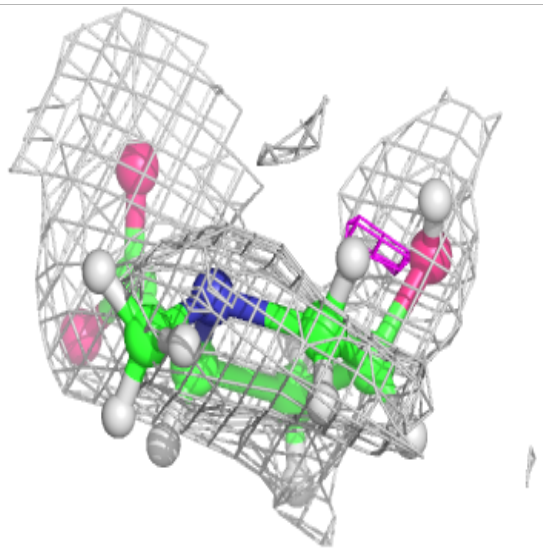
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	87I	C	801	10/10	0.82	0.20	18,28,36,40	0
2	87I	D	801	10/10	0.83	0.20	23,35,42,44	0
2	87I	A	801	10/10	0.85	0.15	15,22,28,28	0
2	87I	B	801	10/10	0.86	0.17	22,26,34,34	0

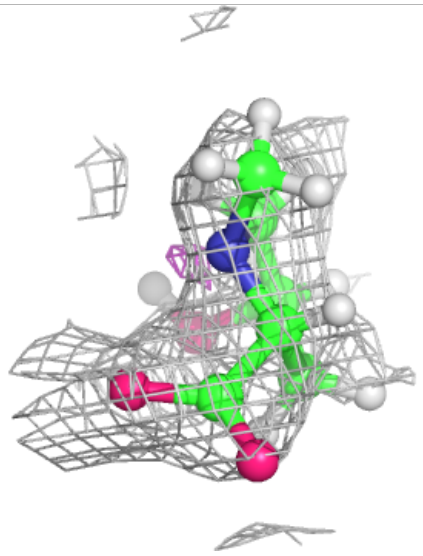
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 87I C 801:

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

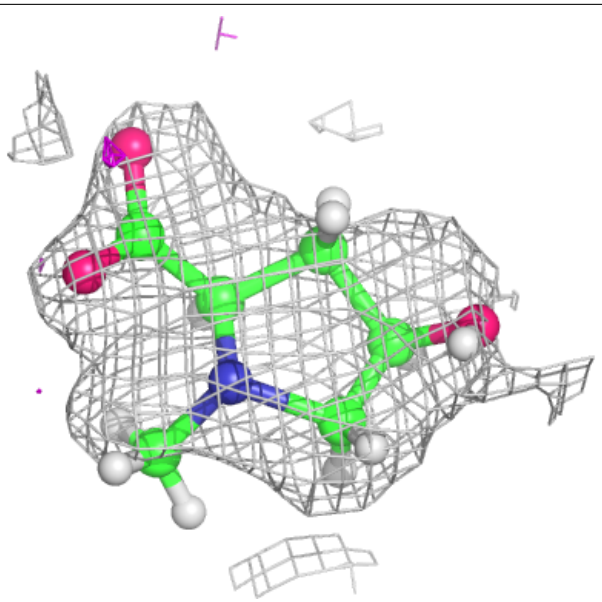


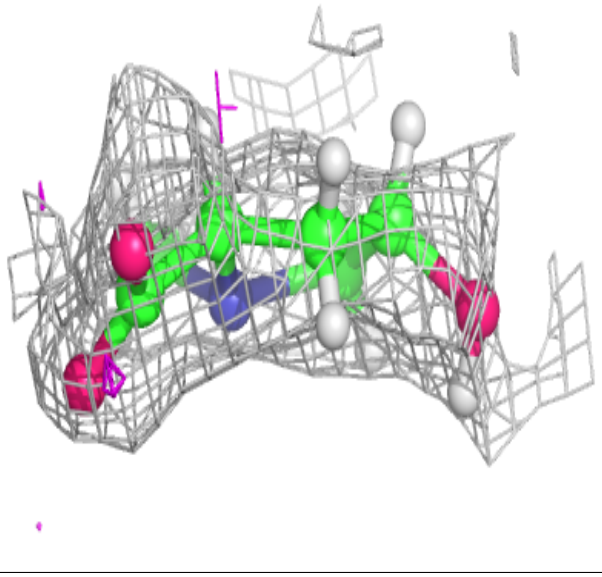


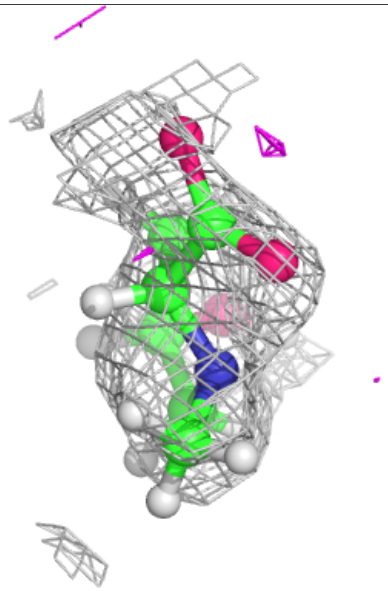


Electron density around 87I D 801:

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

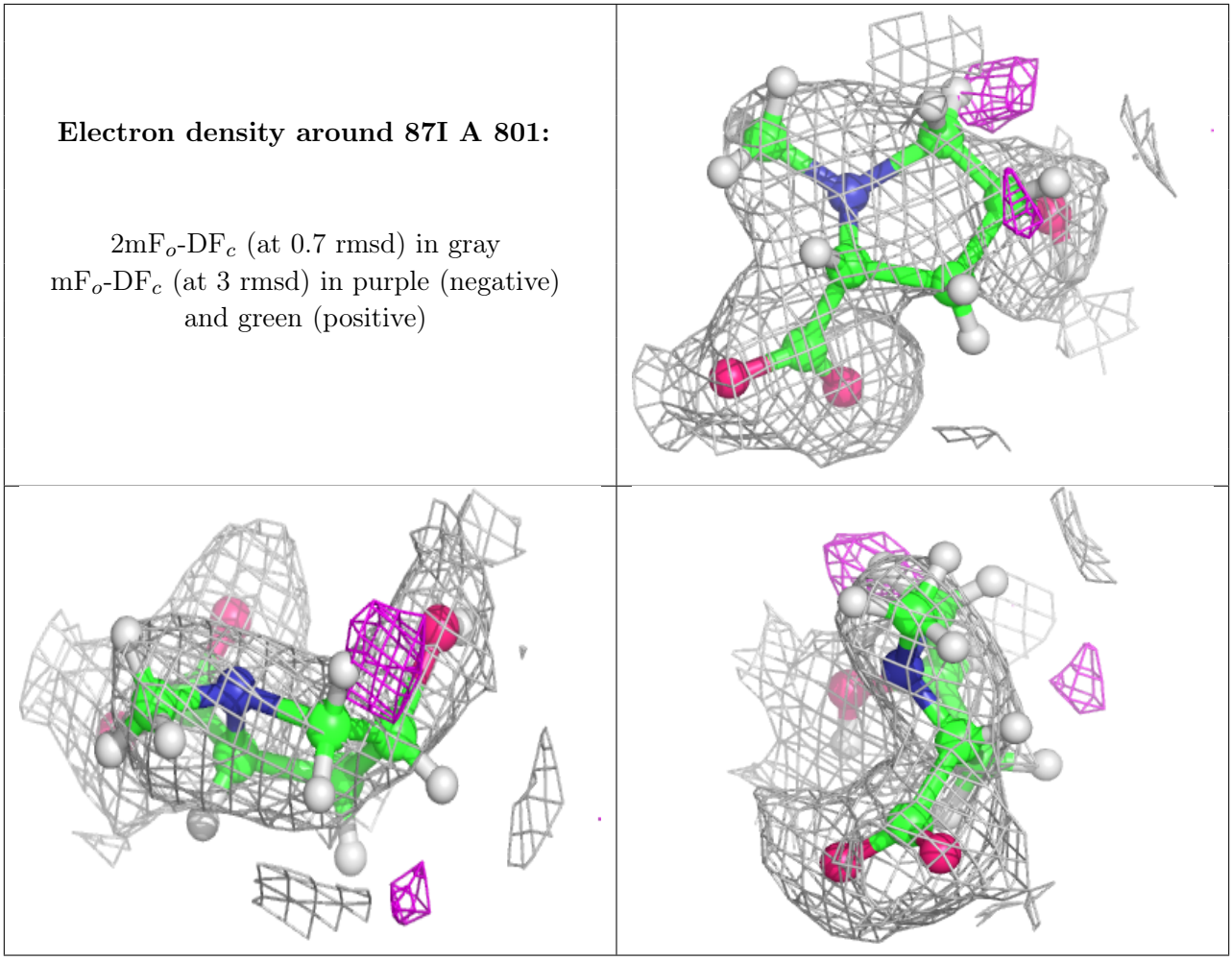






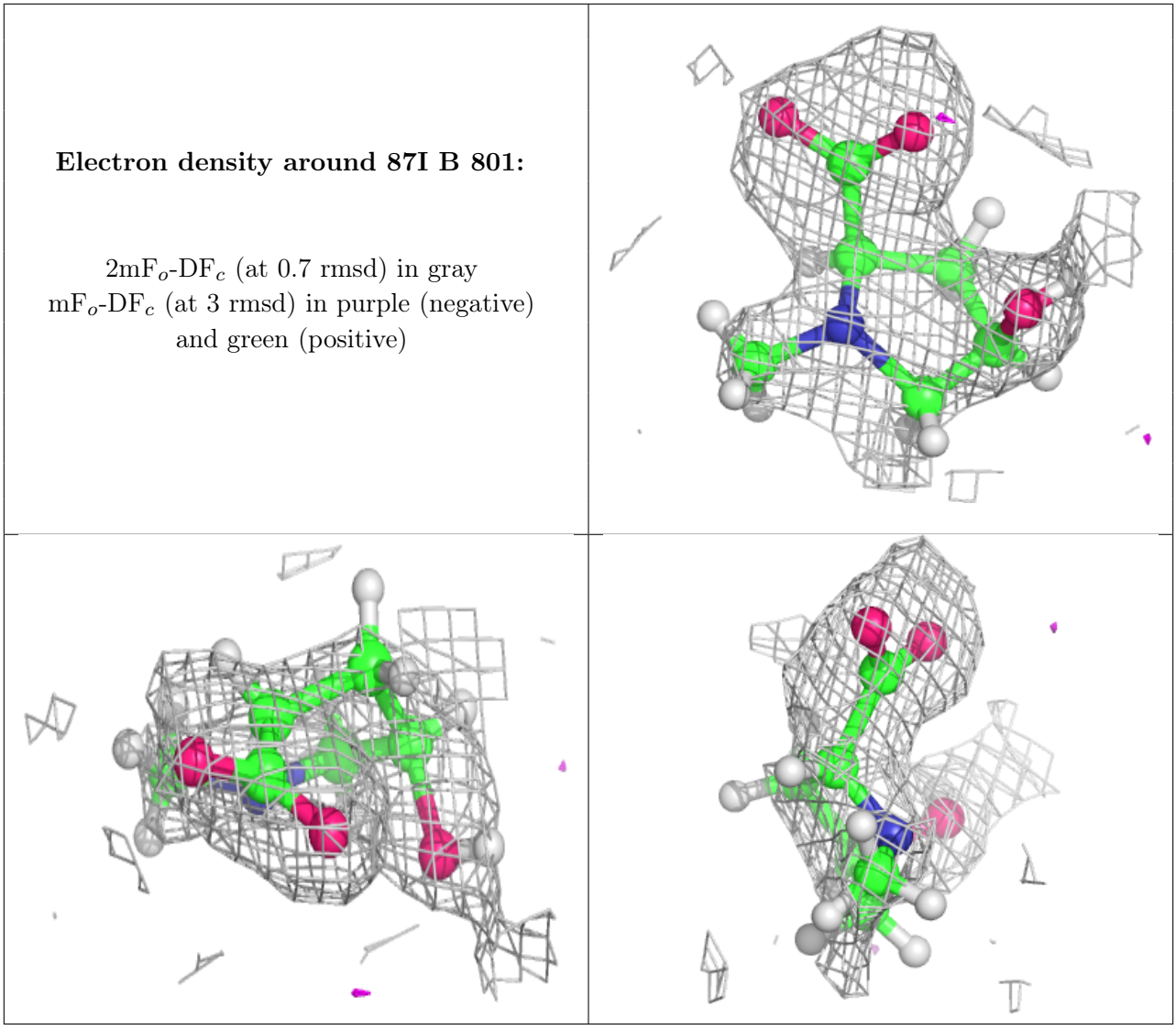
Electron density around 87I A 801:

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



Electron density around 87I B 801:

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



6.5 Other polymers

There are no such residues in this entry.