



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:39 AM UTC

PDB ID : 6JRS / pdb_00006jrs
EMDB ID : EMD-9880
Title : Structure of RyR2 (*F/A/C/L-Ca2+/Ca2+-CaM dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-04-05
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

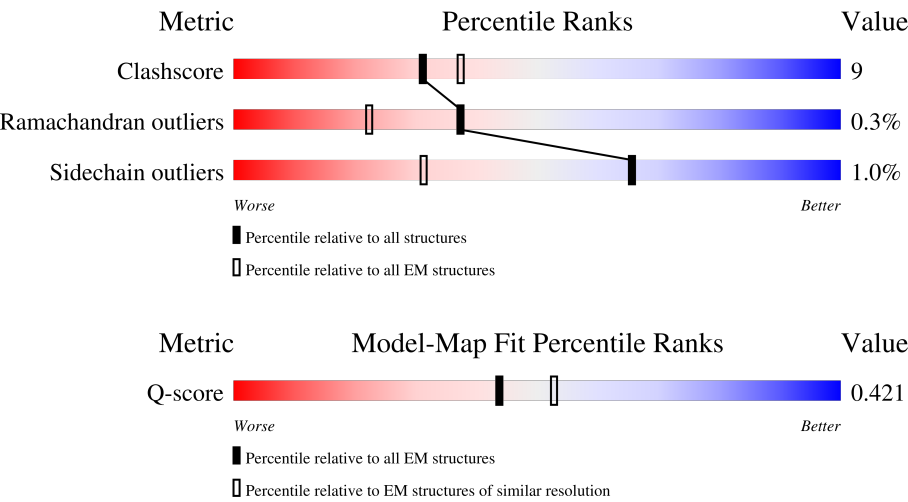
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4968	
1	D	4968	
1	G	4968	
1	J	4968	

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Mol	Chain	Length	Quality of chain
2	B	108	 82% 17%
2	E	108	 82% 17%
2	H	108	 82% 17%
2	K	108	 82% 17%
3	C	149	 40% 37% 9% 54%
3	F	149	 40% 37% 9% 54%
3	I	149	 40% 37% 9% 54%
3	L	149	 40% 37% 9% 54%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CFF	A	6003	-	X	-	-
7	CFF	D	6003	-	X	-	-
7	CFF	G	6003	-	X	-	-
7	CFF	J	6003	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 112168 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3488	Total	C	N	O	S	0	0
			26650	16980	4570	4941	159		
1	D	3488	Total	C	N	O	S	0	0
			26650	16980	4570	4941	159		
1	G	3488	Total	C	N	O	S	0	0
			26650	16980	4570	4941	159		
1	J	3488	Total	C	N	O	S	0	0
			26650	16980	4570	4941	159		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	K	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	F	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	I	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	L	68	Total	C	N	O	S	0	0
			524	326	83	110	5		

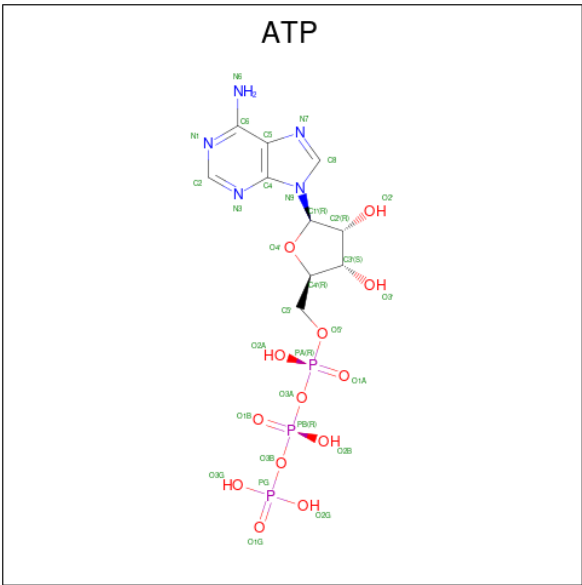
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	J	1	Total 1	Zn 1	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

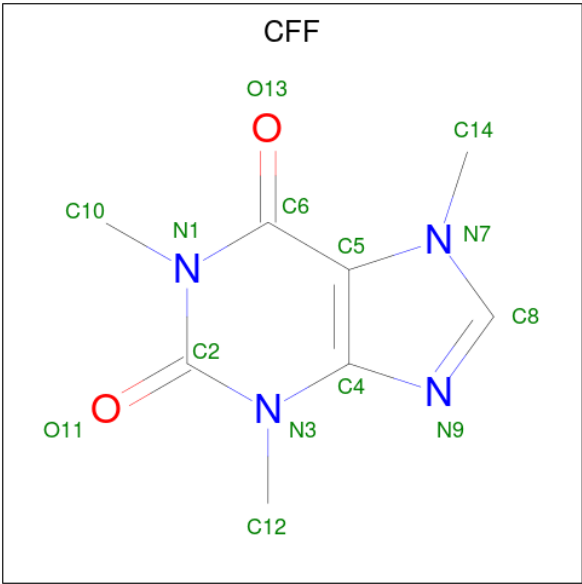
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	C	2	Total 2	Ca 2	0
5	D	1	Total 1	Ca 1	0
5	F	2	Total 2	Ca 2	0
5	G	1	Total 1	Ca 1	0
5	I	2	Total 2	Ca 2	0
5	J	1	Total 1	Ca 1	0
5	L	2	Total 2	Ca 2	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 4	O 2	0
7	D	1	Total 14	C 8	N 4	O 2	0
7	G	1	Total 14	C 8	N 4	O 2	0
7	J	1	Total 14	C 8	N 4	O 2	0



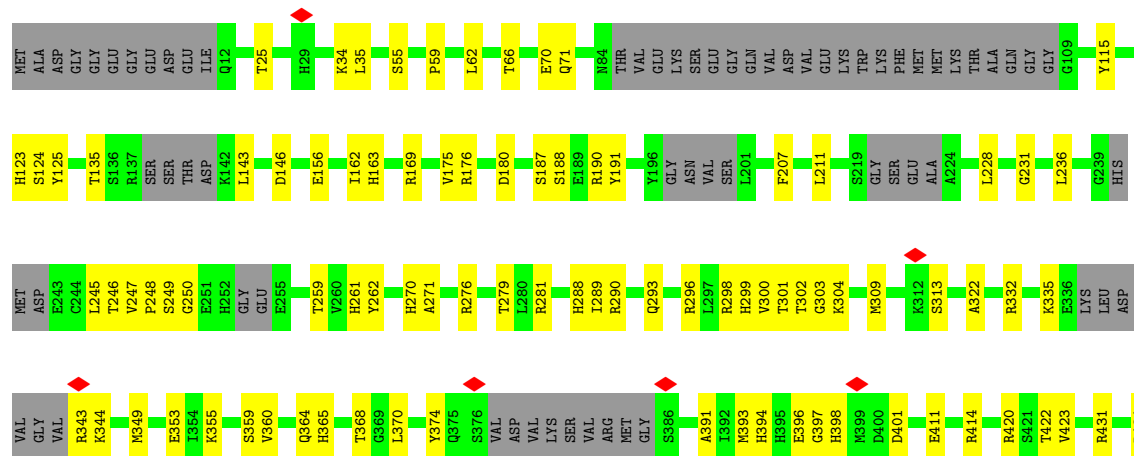














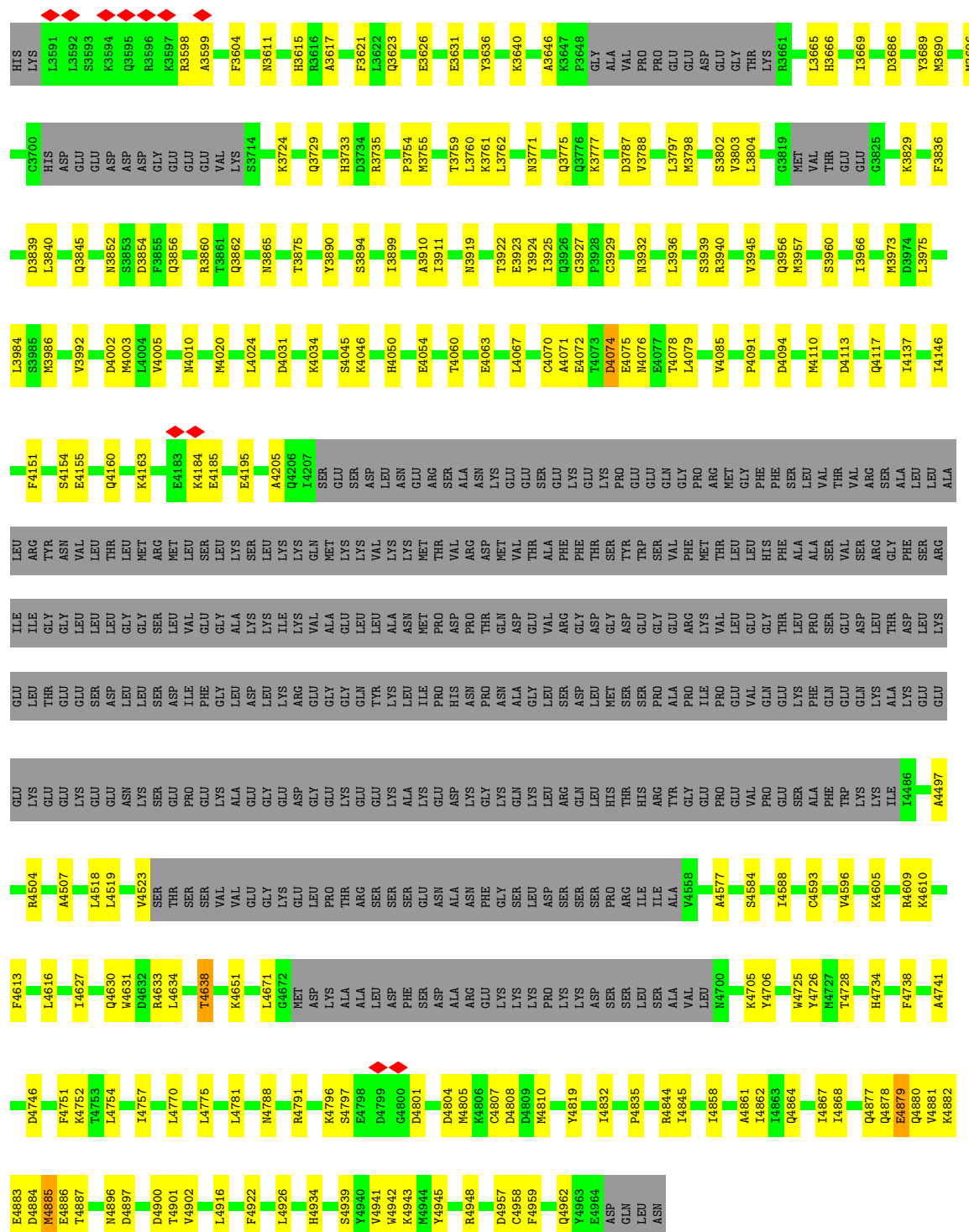












Chain E:  82% 17%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:  82% 17%



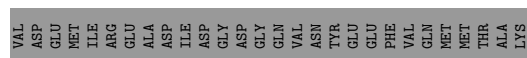
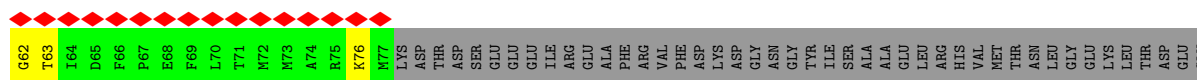
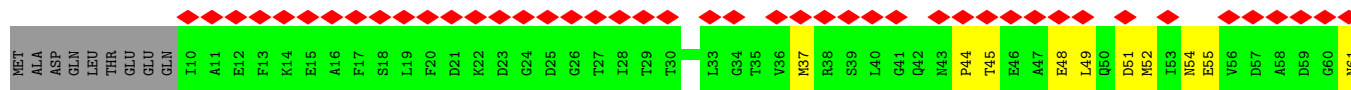
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:  82% 17%



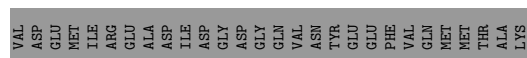
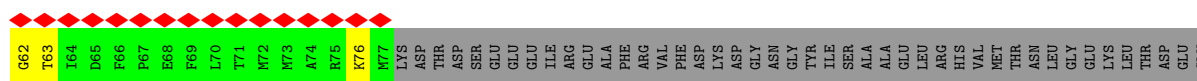
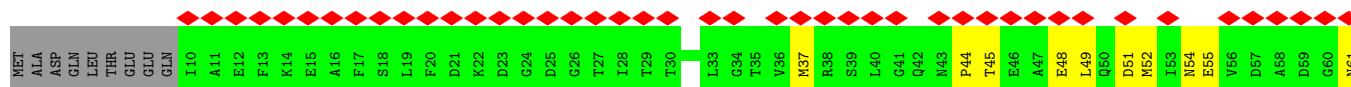
- Molecule 3: Calmodulin-1

Chain C:  40% 37% 9% 54%



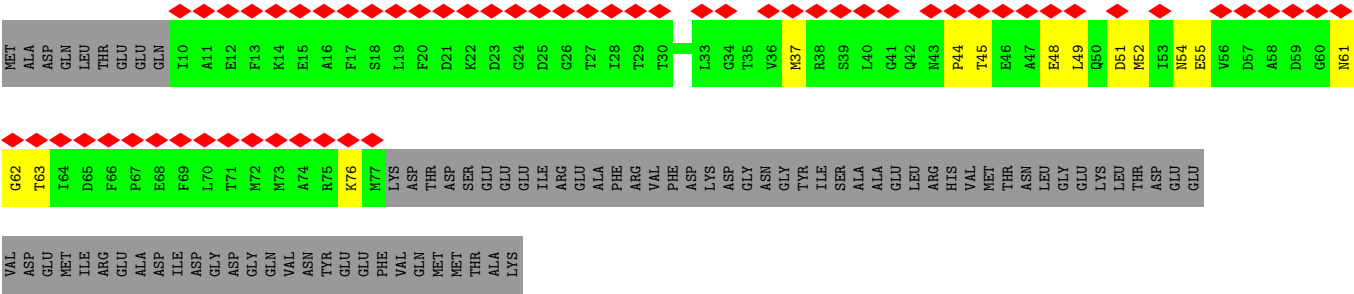
- Molecule 3: Calmodulin-1

Chain F:  40% 37% 9% 54%

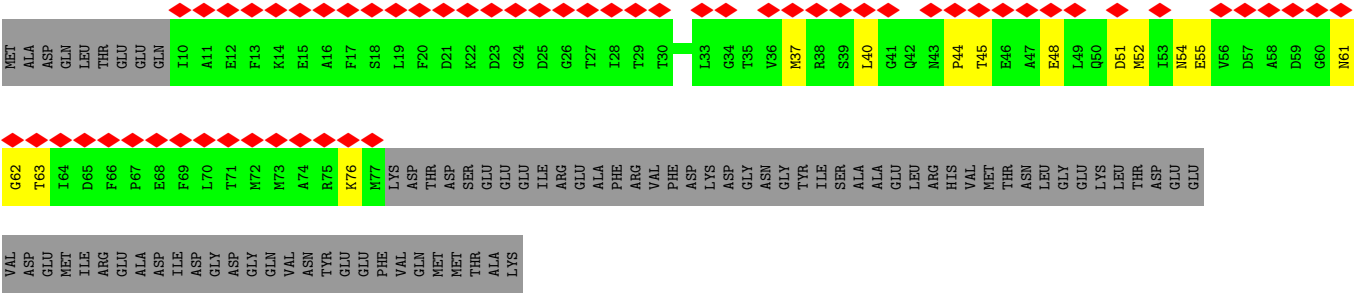
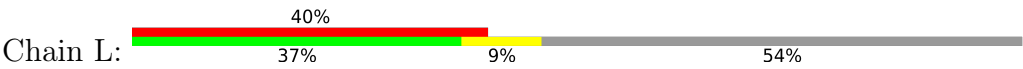


- Molecule 3: Calmodulin-1

Chain I:  40% 37% 9% 54%



• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	154111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.021	Depositor
Map size ($\text{\AA}$)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, CA, ATP, ZN

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	0.42	1/27151 (0.0%)	0.61	4/36715 (0.0%)
1	D	0.42	1/27151 (0.0%)	0.61	4/36715 (0.0%)
1	G	0.42	1/27151 (0.0%)	0.61	4/36715 (0.0%)
1	J	0.42	1/27151 (0.0%)	0.61	4/36715 (0.0%)
2	B	0.33	0/835	0.54	0/1123
2	E	0.33	0/835	0.54	0/1123
2	H	0.33	0/835	0.54	0/1123
2	K	0.33	0/835	0.54	0/1123
3	C	0.23	0/530	0.51	0/711
3	F	0.23	0/530	0.51	0/711
3	I	0.23	0/530	0.51	0/711
3	L	0.23	0/530	0.51	0/711
All	All	0.42	4/114064 (0.0%)	0.61	16/154196 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	D	0	17
1	G	0	17
1	J	0	17
All	All	0	68

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1305	SER	C-N	-5.06	1.23	1.33
1	D	1305	SER	C-N	-5.06	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1305	SER	C-N	-5.06	1.23	1.33
1	J	1305	SER	C-N	-5.06	1.23	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	2321	VAL	N-CA-C	6.25	122.33	109.34
1	A	2321	VAL	N-CA-C	6.24	122.31	109.34
1	D	2321	VAL	N-CA-C	6.24	122.31	109.34
1	J	2321	VAL	N-CA-C	6.22	122.28	109.34
1	J	2294	VAL	N-CA-C	-6.16	107.50	113.53
1	A	2294	VAL	N-CA-C	-6.12	107.53	113.53
1	G	2294	VAL	N-CA-C	-6.12	107.53	113.53
1	D	2294	VAL	N-CA-C	-6.10	107.56	113.53
1	A	2156	PHE	N-CA-C	-5.99	107.20	114.75
1	D	2156	PHE	N-CA-C	-5.99	107.20	114.75
1	G	2156	PHE	N-CA-C	-5.99	107.20	114.75
1	J	2156	PHE	N-CA-C	-5.99	107.20	114.75
1	A	839	GLU	N-CA-C	5.14	118.42	111.17
1	G	839	GLU	N-CA-C	5.14	118.42	111.17
1	J	839	GLU	N-CA-C	5.14	118.42	111.17
1	D	839	GLU	N-CA-C	5.13	118.41	111.17

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1570	LEU	Peptide
1	A	1579	VAL	Peptide
1	A	1808	ASP	Peptide
1	A	1847	GLU	Peptide
1	A	2248	VAL	Peptide
1	A	2320	VAL	Peptide
1	A	3802	SER	Peptide
1	A	3829	LYS	Peptide
1	A	3925	ILE	Peptide
1	A	4074	ASP	Peptide
1	A	4091	PRO	Peptide
1	A	4163	LYS	Peptide
1	A	729	GLY	Peptide
1	A	739	ARG	Peptide
1	A	816	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	819	TYR	Peptide
1	A	838	ARG	Peptide
1	D	1570	LEU	Peptide
1	D	1579	VAL	Peptide
1	D	1808	ASP	Peptide
1	D	1847	GLU	Peptide
1	D	2248	VAL	Peptide
1	D	2320	VAL	Peptide
1	D	3802	SER	Peptide
1	D	3829	LYS	Peptide
1	D	3925	ILE	Peptide
1	D	4074	ASP	Peptide
1	D	4091	PRO	Peptide
1	D	4163	LYS	Peptide
1	D	729	GLY	Peptide
1	D	739	ARG	Peptide
1	D	816	PRO	Peptide
1	D	819	TYR	Peptide
1	D	838	ARG	Peptide
1	G	1570	LEU	Peptide
1	G	1579	VAL	Peptide
1	G	1808	ASP	Peptide
1	G	1847	GLU	Peptide
1	G	2248	VAL	Peptide
1	G	2320	VAL	Peptide
1	G	3802	SER	Peptide
1	G	3829	LYS	Peptide
1	G	3925	ILE	Peptide
1	G	4074	ASP	Peptide
1	G	4091	PRO	Peptide
1	G	4163	LYS	Peptide
1	G	729	GLY	Peptide
1	G	739	ARG	Peptide
1	G	816	PRO	Peptide
1	G	819	TYR	Peptide
1	G	838	ARG	Peptide
1	J	1570	LEU	Peptide
1	J	1579	VAL	Peptide
1	J	1808	ASP	Peptide
1	J	1847	GLU	Peptide
1	J	2248	VAL	Peptide
1	J	2320	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	J	3802	SER	Peptide
1	J	3829	LYS	Peptide
1	J	3925	ILE	Peptide
1	J	4074	ASP	Peptide
1	J	4091	PRO	Peptide
1	J	4163	LYS	Peptide
1	J	729	GLY	Peptide
1	J	739	ARG	Peptide
1	J	816	PRO	Peptide
1	J	819	TYR	Peptide
1	J	838	ARG	Peptide

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	26650	0	25168	502	0
1	D	26650	0	25168	513	0
1	G	26650	0	25168	499	0
1	J	26650	0	25168	511	0
2	B	819	0	824	13	0
2	E	819	0	824	12	0
2	H	819	0	824	13	0
2	K	819	0	824	13	0
3	C	524	0	503	8	0
3	F	524	0	503	8	0
3	I	524	0	503	8	0
3	L	524	0	503	8	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	1	0	0	0	0
5	L	2	0	0	0	0
6	A	31	0	12	1	0
6	D	31	0	12	0	0
6	G	31	0	12	1	0
6	J	31	0	12	1	0
7	A	14	0	10	1	0
7	D	14	0	10	1	0
7	G	14	0	10	1	0
7	J	14	0	10	1	0
All	All	112168	0	106068	1920	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 9.

All (1920) 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:G:143:LEU:HD22	1:J:2427:LEU:CB	1.57	1.34
1:A:2427:LEU:CB	1:J:143:LEU:HD22	1.56	1.33
1:A:143:LEU:HD22	1:D:2427:LEU:CB	1.58	1.33
1:D:143:LEU:HD22	1:G:2427:LEU:CB	1.55	1.33
1:A:2427:LEU:HB3	1:J:143:LEU:CD2	1.60	1.29
1:D:143:LEU:CD2	1:G:2427:LEU:HB3	1.60	1.29
1:A:143:LEU:CD2	1:D:2427:LEU:HB3	1.62	1.28
1:G:143:LEU:CD2	1:J:2427:LEU:HB3	1.61	1.27
1:D:4788:ASN:ND2	1:G:4738:PHE:HD2	1.42	1.17
1:A:4738:PHE:HD2	1:J:4788:ASN:ND2	1.44	1.14
1:G:4788:ASN:ND2	1:J:4738:PHE:HD2	1.45	1.13
1:A:207:PHE:HD1	1:D:2326:ILE:HD13	1.10	1.11
1:A:2326:ILE:HD13	1:J:207:PHE:HD1	1.11	1.10
1:D:207:PHE:HD1	1:G:2326:ILE:HD13	1.12	1.08
1:G:207:PHE:HD1	1:J:2326:ILE:HD13	1.11	1.08
1:D:4788:ASN:ND2	1:G:4738:PHE:CD2	2.22	1.00
1:D:207:PHE:CD1	1:G:2326:ILE:HB	1.96	1.00
1:A:2326:ILE:HB	1:J:207:PHE:CD1	1.96	1.00
1:A:207:PHE:CD1	1:D:2326:ILE:HB	1.98	0.99
1:G:207:PHE:CD1	1:J:2326:ILE:HB	1.97	0.98
1:A:207:PHE:CD1	1:D:2326:ILE:HD13	1.97	0.98
1:G:207:PHE:CD1	1:J:2326:ILE:HD13	1.97	0.98
1:A:2326:ILE:HD13	1:J:207:PHE:CD1	1.98	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4862:ILE:HG22	1:D:4868:ILE:HD12	1.46	0.98
1:D:207:PHE:CD1	1:G:2326:ILE:HD13	1.99	0.97
1:G:4862:ILE:HG22	1:J:4868:ILE:HD12	1.47	0.97
1:A:4868:ILE:HD12	1:J:4862:ILE:HG22	1.48	0.95
1:A:4788:ASN:HD21	1:D:4738:PHE:HE2	1.04	0.93
1:A:2427:LEU:HD12	1:A:2428:ILE:HG22	1.52	0.92
1:A:4738:PHE:CD2	1:J:4788:ASN:ND2	2.25	0.92
1:D:4862:ILE:HG22	1:G:4868:ILE:HD12	1.50	0.92
1:J:2427:LEU:HD12	1:J:2428:ILE:HG22	1.52	0.92
1:D:2427:LEU:HD12	1:D:2428:ILE:HG22	1.52	0.91
1:J:2427:LEU:CD1	1:J:2428:ILE:HG22	2.01	0.90
1:A:2427:LEU:CD1	1:A:2428:ILE:HG22	2.01	0.90
1:G:2427:LEU:HD12	1:G:2428:ILE:HG22	1.52	0.90
1:G:2427:LEU:CD1	1:G:2428:ILE:HG22	2.01	0.89
1:G:4788:ASN:ND2	1:J:4738:PHE:CD2	2.26	0.89
1:D:2427:LEU:CD1	1:D:2428:ILE:HG22	2.01	0.89
1:J:2423:ILE:O	1:J:2427:LEU:HG	1.73	0.88
1:D:2423:ILE:O	1:D:2427:LEU:HG	1.73	0.88
1:G:4770:LEU:O	1:J:4754:LEU:HD21	1.74	0.87
1:A:4770:LEU:O	1:D:4754:LEU:HD21	1.74	0.87
1:G:2423:ILE:O	1:G:2427:LEU:HG	1.73	0.87
1:A:2423:ILE:O	1:A:2427:LEU:HG	1.73	0.86
1:A:4754:LEU:HD21	1:J:4770:LEU:O	1.75	0.86
1:D:4770:LEU:O	1:G:4754:LEU:HD21	1.76	0.85
1:G:4184:LYS:HG3	1:G:4185:GLU:OE1	1.78	0.84
1:D:4184:LYS:HG3	1:D:4185:GLU:OE1	1.78	0.84
1:J:4184:LYS:HG3	1:J:4185:GLU:OE1	1.78	0.83
1:A:4788:ASN:ND2	1:D:4738:PHE:CE2	2.45	0.83
1:A:4184:LYS:HG3	1:A:4185:GLU:OE1	1.78	0.82
1:G:2326:ILE:HD12	1:G:2327:ARG:HG3	1.61	0.82
1:A:2326:ILE:CD1	1:A:2327:ARG:HG3	2.10	0.82
1:A:2326:ILE:HD12	1:A:2327:ARG:HG3	1.60	0.82
1:A:2423:ILE:HG22	1:A:2427:LEU:HD23	1.62	0.82
1:D:2326:ILE:CD1	1:D:2327:ARG:HG3	2.09	0.82
1:D:2326:ILE:HD12	1:D:2327:ARG:HG3	1.60	0.82
1:J:2326:ILE:HD12	1:J:2327:ARG:HG3	1.60	0.81
1:J:2326:ILE:CD1	1:J:2327:ARG:HG3	2.10	0.81
1:G:2423:ILE:HG22	1:G:2427:LEU:HD23	1.62	0.81
1:G:2326:ILE:CD1	1:G:2327:ARG:HG3	2.10	0.81
1:J:2423:ILE:HG22	1:J:2427:LEU:HD23	1.62	0.81
1:D:2423:ILE:HG22	1:D:2427:LEU:HD23	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2423:ILE:CG2	1:A:2427:LEU:HD23	2.12	0.79
1:J:2423:ILE:CG2	1:J:2427:LEU:HD23	2.12	0.79
1:G:2423:ILE:CG2	1:G:2427:LEU:HD23	2.12	0.79
1:D:2423:ILE:CG2	1:D:2427:LEU:HD23	2.12	0.78
1:D:143:LEU:HD13	1:G:2426:SER:C	2.12	0.75
1:A:2426:SER:C	1:J:143:LEU:HD13	2.13	0.73
1:G:143:LEU:HD13	1:J:2426:SER:C	2.14	0.73
1:A:143:LEU:HD13	1:D:2426:SER:C	2.15	0.72
1:A:2326:ILE:CD1	1:J:207:PHE:HD1	1.99	0.71
1:A:4862:ILE:HG22	1:D:4868:ILE:CD1	2.19	0.70
1:A:207:PHE:CD1	1:D:2326:ILE:CD1	2.75	0.70
1:G:4862:ILE:HG22	1:J:4868:ILE:CD1	2.20	0.70
1:G:4796:LYS:NZ	1:G:4807:CYS:SG	2.65	0.69
1:J:4796:LYS:NZ	1:J:4807:CYS:SG	2.65	0.69
1:A:207:PHE:CG	1:D:2326:ILE:HB	2.28	0.69
1:A:4796:LYS:NZ	1:A:4807:CYS:SG	2.65	0.69
1:D:207:PHE:CG	1:G:2326:ILE:HB	2.27	0.69
1:G:1763:PHE:HB3	1:G:1781:GLU:HB3	1.75	0.69
1:D:4796:LYS:NZ	1:D:4807:CYS:SG	2.65	0.69
1:A:207:PHE:HD1	1:D:2326:ILE:CD1	1.99	0.69
1:A:2326:ILE:HB	1:J:207:PHE:CG	2.27	0.69
1:J:1763:PHE:HB3	1:J:1781:GLU:HB3	1.75	0.68
1:G:207:PHE:CD1	1:J:2326:ILE:CB	2.76	0.68
1:G:207:PHE:CD1	1:J:2326:ILE:CD1	2.75	0.68
1:A:4868:ILE:CD1	1:J:4862:ILE:HG22	2.21	0.68
1:G:207:PHE:CG	1:J:2326:ILE:HB	2.27	0.68
1:A:1763:PHE:HB3	1:A:1781:GLU:HB3	1.75	0.67
1:D:207:PHE:CD1	1:G:2326:ILE:CD1	2.76	0.67
1:D:4862:ILE:HG22	1:G:4868:ILE:CD1	2.23	0.67
1:D:190:ARG:NE	1:D:207:PHE:CE2	2.62	0.67
1:G:190:ARG:NE	1:G:207:PHE:CE2	2.62	0.67
1:D:1763:PHE:HB3	1:D:1781:GLU:HB3	1.75	0.67
1:G:4883:GLU:O	1:G:4887:THR:HG22	1.95	0.67
1:A:2326:ILE:CD1	1:J:207:PHE:CD1	2.75	0.66
1:D:143:LEU:HB2	1:G:2427:LEU:HA	1.78	0.66
1:A:2326:ILE:CB	1:J:207:PHE:CD1	2.76	0.66
1:J:4883:GLU:O	1:J:4887:THR:HG22	1.96	0.66
1:A:190:ARG:NE	1:A:207:PHE:CE2	2.62	0.66
1:J:190:ARG:NE	1:J:207:PHE:CE2	2.62	0.66
1:D:207:PHE:CD1	1:G:2326:ILE:CB	2.76	0.66
1:A:4883:GLU:O	1:A:4887:THR:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:HD13	1:G:2427:LEU:N	2.11	0.66
1:D:4879:GLU:OE1	1:D:4879:GLU:HA	1.96	0.65
1:G:4862:ILE:CG2	1:J:4868:ILE:HD12	2.25	0.65
1:A:2427:LEU:HA	1:J:143:LEU:HB2	1.78	0.65
1:A:4879:GLU:OE1	1:A:4879:GLU:HA	1.96	0.65
1:D:4883:GLU:O	1:D:4887:THR:HG22	1.96	0.65
1:D:2706:PRO:HB3	1:D:2855:LYS:HG3	1.79	0.65
1:G:2706:PRO:HB3	1:G:2855:LYS:HG3	1.79	0.65
1:G:2769:LYS:HG3	1:G:2773:ARG:HB2	1.79	0.65
1:J:2769:LYS:HG3	1:J:2773:ARG:HB2	1.79	0.64
1:G:143:LEU:HB2	1:J:2427:LEU:HA	1.79	0.64
1:A:143:LEU:HB2	1:D:2427:LEU:HA	1.79	0.64
1:A:2769:LYS:HG3	1:A:2773:ARG:HB2	1.79	0.64
1:A:4788:ASN:ND2	1:D:4738:PHE:HE2	1.87	0.64
1:D:2423:ILE:HG22	1:D:2427:LEU:CD2	2.28	0.64
1:D:4638:THR:HG21	1:D:4706:TYR:HB2	1.80	0.64
1:A:2427:LEU:N	1:J:143:LEU:HD13	2.11	0.64
1:J:2706:PRO:HB3	1:J:2855:LYS:HG3	1.79	0.64
1:D:2436:VAL:HG23	1:D:2437:ILE:HG13	1.80	0.64
1:G:1219:LYS:H	1:G:1240:ALA:HB2	1.63	0.64
1:G:2436:VAL:HG23	1:G:2437:ILE:HG13	1.80	0.64
1:J:4879:GLU:OE1	1:J:4879:GLU:HA	1.96	0.64
2:H:17:LYS:HE2	2:H:20:GLN:HE22	1.63	0.64
1:D:4781:LEU:HD11	1:G:4741:ALA:O	1.98	0.64
2:E:17:LYS:HE2	2:E:20:GLN:HE22	1.63	0.64
1:G:143:LEU:HD13	1:J:2427:LEU:N	2.12	0.64
1:J:2436:VAL:HG23	1:J:2437:ILE:HG13	1.80	0.64
1:A:143:LEU:HD13	1:D:2427:LEU:N	2.12	0.64
2:K:17:LYS:HE2	2:K:20:GLN:HE22	1.63	0.64
1:A:4741:ALA:O	1:J:4781:LEU:HD11	1.98	0.64
2:B:17:LYS:HE2	2:B:20:GLN:HE22	1.63	0.63
1:G:3775:GLN:OE1	1:G:3852:ASN:ND2	2.29	0.63
1:G:4781:LEU:HD11	1:J:4741:ALA:O	1.98	0.63
1:A:207:PHE:CD1	1:D:2326:ILE:CB	2.77	0.63
1:G:143:LEU:HG	1:G:143:LEU:O	1.98	0.63
1:J:143:LEU:HG	1:J:143:LEU:O	1.98	0.63
1:D:1682:GLU:HG3	1:D:1782:PHE:HB2	1.81	0.63
1:D:191:TYR:OH	1:G:2327:ARG:HD3	1.98	0.63
1:A:2423:ILE:HG22	1:A:2427:LEU:CD2	2.28	0.63
1:A:2706:PRO:HB3	1:A:2855:LYS:HG3	1.79	0.63
1:J:1682:GLU:HG3	1:J:1782:PHE:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2423:ILE:HG22	1:J:2427:LEU:CD2	2.28	0.63
1:A:2327:ARG:HD3	1:J:191:TYR:OH	1.99	0.63
1:A:2436:VAL:HG23	1:A:2437:ILE:HG13	1.80	0.63
1:A:4638:THR:HG21	1:A:4706:TYR:HB2	1.80	0.63
1:A:4862:ILE:CG2	1:D:4868:ILE:CD1	2.76	0.63
1:A:1102:TYR:HB2	1:A:1165:MET:HG2	1.81	0.63
1:A:1682:GLU:HG3	1:A:1782:PHE:HB2	1.81	0.63
1:A:3729:GLN:OE1	1:A:3771:ASN:ND2	2.32	0.63
1:D:1219:LYS:H	1:D:1240:ALA:HB2	1.63	0.63
1:D:2769:LYS:HG3	1:D:2773:ARG:HB2	1.79	0.63
1:A:143:LEU:HG	1:A:143:LEU:O	1.98	0.63
1:D:143:LEU:HD22	1:G:2427:LEU:CA	2.28	0.63
1:D:1102:TYR:HB2	1:D:1165:MET:HG2	1.81	0.63
1:G:2423:ILE:HG22	1:G:2427:LEU:CD2	2.28	0.63
1:J:1102:TYR:HB2	1:J:1165:MET:HG2	1.81	0.63
1:A:4868:ILE:HD12	1:J:4862:ILE:CG2	2.26	0.63
1:G:1682:GLU:HG3	1:G:1782:PHE:HB2	1.81	0.63
1:J:1219:LYS:H	1:J:1240:ALA:HB2	1.63	0.63
1:D:143:LEU:HG	1:D:143:LEU:O	1.98	0.62
1:A:4070:CYS:SG	1:A:4071:ALA:N	2.72	0.62
1:A:4862:ILE:CG2	1:D:4868:ILE:HD12	2.23	0.62
1:G:191:TYR:OH	1:J:2327:ARG:HD3	2.00	0.62
1:G:1102:TYR:HB2	1:G:1165:MET:HG2	1.81	0.62
1:G:4862:ILE:CG2	1:J:4868:ILE:CD1	2.77	0.62
1:J:4638:THR:HG21	1:J:4706:TYR:HB2	1.80	0.62
1:A:1219:LYS:H	1:A:1240:ALA:HB2	1.63	0.62
1:D:4070:CYS:SG	1:D:4071:ALA:N	2.72	0.62
1:J:3729:GLN:OE1	1:J:3771:ASN:ND2	2.32	0.62
1:J:3775:GLN:OE1	1:J:3852:ASN:ND2	2.29	0.62
1:D:4791:ARG:NH2	1:G:4523:VAL:HG21	2.14	0.62
1:G:4070:CYS:SG	1:G:4071:ALA:N	2.72	0.62
1:J:810:GLU:OE1	1:J:812:LYS:NZ	2.33	0.62
1:A:2427:LEU:CA	1:J:143:LEU:HD22	2.29	0.62
1:J:4070:CYS:SG	1:J:4071:ALA:N	2.72	0.62
1:D:810:GLU:OE1	1:D:812:LYS:NZ	2.33	0.62
1:A:3854:ASP:OD1	1:A:3854:ASP:N	2.33	0.61
1:A:4788:ASN:ND2	1:D:4738:PHE:CD2	2.68	0.61
1:G:810:GLU:OE1	1:G:812:LYS:NZ	2.33	0.61
1:J:3939:SER:OG	1:J:3940:ARG:N	2.33	0.61
1:D:3729:GLN:OE1	1:D:3771:ASN:ND2	2.32	0.61
1:D:3775:GLN:OE1	1:D:3852:ASN:ND2	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:335:LYS:NZ	1:J:398:HIS:O	2.33	0.61
1:G:3729:GLN:OE1	1:G:3771:ASN:ND2	2.32	0.61
1:G:4638:THR:HG21	1:G:4706:TYR:HB2	1.80	0.61
1:A:4781:LEU:HD11	1:D:4741:ALA:O	2.00	0.61
1:A:4868:ILE:CD1	1:J:4862:ILE:CG2	2.78	0.61
1:A:810:GLU:OE1	1:A:812:LYS:NZ	2.33	0.61
1:D:335:LYS:NZ	1:D:398:HIS:O	2.33	0.61
1:D:4862:ILE:CG2	1:G:4868:ILE:HD12	2.27	0.61
1:G:954:ASP:HB2	1:G:1061:GLY:HA3	1.83	0.61
1:G:4858:ILE:HD12	1:J:4867:ILE:HG21	1.82	0.61
1:A:3939:SER:OG	1:A:3940:ARG:N	2.33	0.61
1:A:4523:VAL:HG21	1:J:4791:ARG:NH2	2.16	0.61
1:G:1425:THR:N	1:G:1510:VAL:O	2.34	0.61
1:J:1425:THR:N	1:J:1510:VAL:O	2.34	0.61
1:A:143:LEU:HD22	1:D:2427:LEU:HB3	0.71	0.61
1:A:335:LYS:NZ	1:A:398:HIS:O	2.33	0.61
1:D:4788:ASN:OD1	1:G:4738:PHE:CE2	2.54	0.61
1:D:4862:ILE:CG2	1:G:4868:ILE:CD1	2.79	0.60
1:A:954:ASP:HB2	1:A:1061:GLY:HA3	1.83	0.60
1:G:618:CYS:HB2	1:G:629:GLN:HG2	1.84	0.60
1:G:1272:ARG:HH11	1:G:1586:LEU:HD21	1.67	0.60
2:H:62:GLY:HA3	2:H:74:LEU:HD21	1.82	0.60
1:A:3775:GLN:OE1	1:A:3852:ASN:ND2	2.29	0.60
2:E:62:GLY:HA3	2:E:74:LEU:HD21	1.82	0.60
1:J:954:ASP:HB2	1:J:1061:GLY:HA3	1.83	0.60
1:A:191:TYR:OH	1:D:2327:ARG:HD3	2.01	0.60
1:D:954:ASP:HB2	1:D:1061:GLY:HA3	1.83	0.60
1:D:1792:ILE:HG23	1:D:1842:ILE:HD13	1.84	0.60
1:G:881:ILE:HA	1:G:884:LYS:HD2	1.84	0.60
1:G:2427:LEU:HD11	1:G:2428:ILE:HG22	1.84	0.60
1:G:3939:SER:OG	1:G:3940:ARG:N	2.33	0.60
1:G:4791:ARG:NH2	1:J:4523:VAL:HG21	2.17	0.60
1:A:697:TRP:NE1	1:A:757:CYS:SG	2.75	0.60
1:A:1792:ILE:HG23	1:A:1842:ILE:HD13	1.84	0.60
1:D:1425:THR:N	1:D:1510:VAL:O	2.34	0.60
1:G:697:TRP:NE1	1:G:757:CYS:SG	2.75	0.60
1:J:1205:CYS:SG	1:J:1206:SER:N	2.75	0.60
1:D:2425:ARG:NH2	1:D:2476:VAL:O	2.35	0.60
1:A:1205:CYS:SG	1:A:1206:SER:N	2.75	0.59
1:A:4738:PHE:CE2	1:J:4788:ASN:OD1	2.55	0.59
1:D:2838:LEU:HD12	1:D:2904:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2838:LEU:HD12	1:G:2904:VAL:HG11	1.84	0.59
1:J:881:ILE:HA	1:J:884:LYS:HD2	1.84	0.59
1:J:2425:ARG:NH2	1:J:2476:VAL:O	2.35	0.59
1:A:1425:THR:N	1:A:1510:VAL:O	2.34	0.59
1:D:143:LEU:HD22	1:G:2427:LEU:HB3	0.69	0.59
1:G:2782:THR:OG1	1:G:2848:ASN:ND2	2.36	0.59
1:J:2782:THR:OG1	1:J:2848:ASN:ND2	2.36	0.59
2:K:62:GLY:HA3	2:K:74:LEU:HD21	1.82	0.59
1:A:207:PHE:O	1:D:2327:ARG:HG2	2.03	0.59
1:A:881:ILE:HA	1:A:884:LYS:HD2	1.84	0.59
2:B:62:GLY:HA3	2:B:74:LEU:HD21	1.82	0.59
1:G:2425:ARG:NH2	1:G:2476:VAL:O	2.35	0.59
1:J:618:CYS:HB2	1:J:629:GLN:HG2	1.84	0.59
1:D:618:CYS:HB2	1:D:629:GLN:HG2	1.84	0.59
1:G:1792:ILE:HG23	1:G:1842:ILE:HD13	1.84	0.59
1:G:3854:ASP:OD1	1:G:3854:ASP:N	2.33	0.59
1:J:1006:VAL:HA	1:J:1009:ARG:HD3	1.85	0.59
1:J:2838:LEU:HD12	1:J:2904:VAL:HG11	1.84	0.59
1:A:2425:ARG:NH2	1:A:2476:VAL:O	2.35	0.59
1:A:2782:THR:OG1	1:A:2848:ASN:ND2	2.36	0.59
1:D:3761:LYS:NZ	1:D:3839:ASP:OD2	2.36	0.59
1:D:4858:ILE:HD12	1:G:4867:ILE:HG21	1.84	0.59
1:J:697:TRP:NE1	1:J:757:CYS:SG	2.75	0.59
1:J:1272:ARG:HH11	1:J:1586:LEU:HD21	1.67	0.59
1:G:4113:ASP:O	1:G:4117:GLN:NE2	2.36	0.59
1:G:4957:ASP:OD1	1:G:4957:ASP:N	2.34	0.59
1:A:1272:ARG:HH11	1:A:1586:LEU:HD21	1.67	0.59
1:A:2327:ARG:HG2	1:J:207:PHE:O	2.02	0.59
1:D:1205:CYS:SG	1:D:1206:SER:N	2.75	0.59
1:G:335:LYS:NZ	1:G:398:HIS:O	2.33	0.59
1:D:2782:THR:OG1	1:D:2848:ASN:ND2	2.36	0.59
1:G:207:PHE:O	1:J:2327:ARG:HG2	2.02	0.59
1:G:231:GLY:O	1:G:276:ARG:NH1	2.35	0.59
1:G:3761:LYS:NZ	1:G:3839:ASP:OD2	2.36	0.59
1:J:4024:LEU:HG	1:J:4085:VAL:HG12	1.85	0.59
1:A:618:CYS:HB2	1:A:629:GLN:HG2	1.84	0.59
1:A:2838:LEU:HD12	1:A:2904:VAL:HG11	1.84	0.59
1:A:4791:ARG:NH2	1:D:4523:VAL:HG21	2.17	0.59
1:A:4858:ILE:HD12	1:D:4867:ILE:HG21	1.84	0.59
1:A:4867:ILE:HG21	1:J:4858:ILE:HD12	1.83	0.59
2:B:7:ILE:HB	2:B:71:ARG:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:697:TRP:NE1	1:D:757:CYS:SG	2.75	0.59
2:E:7:ILE:HB	2:E:71:ARG:HG3	1.85	0.59
1:J:231:GLY:O	1:J:276:ARG:NH1	2.35	0.59
1:D:881:ILE:HA	1:D:884:LYS:HD2	1.84	0.58
1:D:1272:ARG:HH11	1:D:1586:LEU:HD21	1.67	0.58
1:G:1205:CYS:SG	1:G:1206:SER:N	2.75	0.58
1:G:4788:ASN:OD1	1:J:4738:PHE:CE2	2.56	0.58
1:G:4879:GLU:OE1	1:G:4879:GLU:HA	1.97	0.58
1:J:2427:LEU:HD11	1:J:2428:ILE:HG22	1.84	0.58
1:J:4113:ASP:O	1:J:4117:GLN:NE2	2.36	0.58
1:A:1100:ARG:HH12	1:A:1170:GLU:H	1.51	0.58
1:A:2326:ILE:HG21	1:J:207:PHE:CE1	2.38	0.58
1:G:207:PHE:CE1	1:J:2326:ILE:HG21	2.38	0.58
1:J:1792:ILE:HG23	1:J:1842:ILE:HD13	1.84	0.58
1:D:207:PHE:CE1	1:G:2326:ILE:HG21	2.38	0.58
1:D:867:VAL:O	1:D:1002:ASN:ND2	2.36	0.58
1:G:694:ARG:NH1	1:G:716:ASN:O	2.35	0.58
1:J:694:ARG:NH1	1:J:716:ASN:O	2.35	0.58
2:K:7:ILE:HB	2:K:71:ARG:HG3	1.85	0.58
1:A:207:PHE:CE1	1:D:2326:ILE:HG21	2.39	0.58
1:A:1916:ASP:OD1	1:A:2091:ARG:NH1	2.37	0.58
1:D:503:ASP:OD1	1:D:561:ARG:NH2	2.37	0.58
1:G:867:VAL:O	1:G:1002:ASN:ND2	2.37	0.58
1:J:867:VAL:O	1:J:1002:ASN:ND2	2.37	0.58
1:A:180:ASP:HB3	1:A:211:LEU:HD12	1.86	0.58
1:A:231:GLY:O	1:A:276:ARG:NH1	2.35	0.58
1:A:1106:GLU:HB3	1:A:1214:ARG:HB2	1.86	0.58
1:D:231:GLY:O	1:D:276:ARG:NH1	2.35	0.58
1:D:4577:ALA:O	1:D:4734:HIS:NE2	2.35	0.58
1:A:4113:ASP:O	1:A:4117:GLN:NE2	2.36	0.58
2:H:7:ILE:HB	2:H:71:ARG:HG3	1.85	0.58
1:A:3761:LYS:NZ	1:A:3839:ASP:OD2	2.36	0.58
1:D:180:ASP:HB3	1:D:211:LEU:HD12	1.86	0.58
1:D:207:PHE:O	1:G:2327:ARG:HG2	2.03	0.58
1:D:1250:TRP:HE1	1:D:1602:GLN:HG3	1.68	0.58
1:J:734:SER:OG	1:J:739:ARG:NH1	2.37	0.58
1:D:734:SER:OG	1:D:739:ARG:NH1	2.37	0.58
1:D:4808:ASP:HB2	1:G:4523:VAL:CG1	2.34	0.58
1:G:1250:TRP:HE1	1:G:1602:GLN:HG3	1.68	0.58
1:J:1100:ARG:HH12	1:J:1170:GLU:H	1.51	0.58
1:A:867:VAL:O	1:A:1002:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1482:ARG:NH1	1:A:1530:TYR:O	2.37	0.58
1:A:4523:VAL:CG1	1:J:4808:ASP:HB2	2.34	0.58
1:G:207:PHE:HB3	1:J:2326:ILE:HD12	1.86	0.58
1:G:734:SER:OG	1:G:739:ARG:NH1	2.37	0.58
1:G:1006:VAL:HA	1:G:1009:ARG:HD3	1.85	0.58
1:G:4808:ASP:HB2	1:J:4523:VAL:CG1	2.34	0.58
1:J:180:ASP:HB3	1:J:211:LEU:HD12	1.86	0.58
1:J:834:VAL:H	1:J:1614:ARG:HH22	1.51	0.58
1:A:1006:VAL:HA	1:A:1009:ARG:HD3	1.85	0.57
1:A:3599:ALA:HB1	3:C:76:LYS:HE2	1.86	0.57
1:D:3599:ALA:HB1	3:F:76:LYS:HE2	1.86	0.57
1:D:4094:ASP:OD1	1:D:4094:ASP:N	2.33	0.57
1:D:4113:ASP:O	1:D:4117:GLN:NE2	2.36	0.57
1:G:503:ASP:OD1	1:G:561:ARG:NH2	2.37	0.57
1:G:510:SER:O	1:G:520:ARG:NH2	2.37	0.57
1:D:1006:VAL:HA	1:D:1009:ARG:HD3	1.85	0.57
1:D:1482:ARG:NH1	1:D:1530:TYR:O	2.37	0.57
1:G:1916:ASP:OD1	1:G:2091:ARG:NH1	2.37	0.57
1:G:4024:LEU:HG	1:G:4085:VAL:HG12	1.85	0.57
1:J:1304:LEU:HB2	1:J:1541:PRO:HG2	1.87	0.57
1:J:1482:ARG:NH1	1:J:1530:TYR:O	2.37	0.57
1:A:143:LEU:HD22	1:D:2427:LEU:CA	2.31	0.57
1:D:834:VAL:H	1:D:1614:ARG:HH22	1.51	0.57
1:G:180:ASP:HB3	1:G:211:LEU:HD12	1.86	0.57
1:A:694:ARG:NH1	1:A:716:ASN:O	2.35	0.57
1:G:1482:ARG:NH1	1:G:1530:TYR:O	2.37	0.57
1:G:4195:GLU:OE1	1:G:4948:ARG:NH2	2.37	0.57
1:A:4788:ASN:OD1	1:D:4738:PHE:CD2	2.57	0.57
1:D:510:SER:O	1:D:520:ARG:NH2	2.37	0.57
1:D:4024:LEU:HG	1:D:4085:VAL:HG12	1.85	0.57
2:E:38:SER:OG	2:E:39:SER:N	2.37	0.57
1:J:3761:LYS:NZ	1:J:3839:ASP:OD2	2.36	0.57
1:A:1250:TRP:HE1	1:A:1602:GLN:HG3	1.68	0.57
1:A:4195:GLU:OE1	1:A:4948:ARG:NH2	2.37	0.57
1:D:1916:ASP:OD1	1:D:2091:ARG:NH1	2.37	0.57
1:D:3939:SER:OG	1:D:3940:ARG:N	2.33	0.57
1:G:1172:THR:HG22	1:G:1193:LYS:HG2	1.87	0.57
1:J:1916:ASP:OD1	1:J:2091:ARG:NH1	2.37	0.57
1:A:4024:LEU:HG	1:A:4085:VAL:HG12	1.85	0.57
1:G:1106:GLU:HB3	1:G:1214:ARG:HB2	1.86	0.57
2:H:38:SER:OG	2:H:39:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:510:SER:O	1:J:520:ARG:NH2	2.37	0.57
1:J:1106:GLU:HB3	1:J:1214:ARG:HB2	1.86	0.57
1:J:1250:TRP:HE1	1:J:1602:GLN:HG3	1.68	0.57
2:K:38:SER:OG	2:K:39:SER:N	2.37	0.57
1:A:1304:LEU:HB2	1:A:1541:PRO:HG2	1.87	0.57
1:D:4845:ILE:HD12	1:G:4819:TYR:CD1	2.40	0.57
1:G:556:ASP:OD1	1:G:593:HIS:NE2	2.38	0.57
1:A:510:SER:O	1:A:520:ARG:NH2	2.37	0.56
1:A:556:ASP:OD1	1:A:593:HIS:NE2	2.38	0.56
1:A:3862:GLN:HE21	1:A:3865:ASN:HD22	1.53	0.56
1:D:3862:GLN:HE21	1:D:3865:ASN:HD22	1.53	0.56
1:A:834:VAL:H	1:A:1614:ARG:HH22	1.51	0.56
1:D:1100:ARG:HH12	1:D:1170:GLU:H	1.51	0.56
1:J:1172:THR:HG22	1:J:1193:LYS:HG2	1.87	0.56
1:A:467:ASP:N	1:A:467:ASP:OD1	2.38	0.56
1:A:734:SER:OG	1:A:739:ARG:NH1	2.37	0.56
1:A:756:SER:HB2	1:A:769:ARG:HB2	1.87	0.56
1:A:2326:ILE:HD12	1:J:207:PHE:HB3	1.87	0.56
1:D:1304:LEU:HB2	1:D:1541:PRO:HG2	1.87	0.56
1:D:4195:GLU:OE1	1:D:4948:ARG:NH2	2.37	0.56
1:G:834:VAL:H	1:G:1614:ARG:HH22	1.51	0.56
1:G:1100:ARG:HH12	1:G:1170:GLU:H	1.51	0.56
1:A:1172:THR:HG22	1:A:1193:LYS:HG2	1.87	0.56
2:B:38:SER:OG	2:B:39:SER:N	2.37	0.56
1:J:2883:LYS:O	1:J:2887:ARG:N	2.37	0.56
1:J:4195:GLU:OE1	1:J:4948:ARG:NH2	2.37	0.56
1:A:2427:LEU:HD11	1:A:2428:ILE:HG22	1.84	0.56
1:A:2712:ILE:O	1:A:2781:LYS:NZ	2.35	0.56
1:D:694:ARG:NH1	1:D:716:ASN:O	2.35	0.56
1:D:3856:GLN:O	1:D:3932:ASN:ND2	2.39	0.56
1:G:3862:GLN:HE21	1:G:3865:ASN:HD22	1.53	0.56
1:D:207:PHE:HB3	1:G:2326:ILE:HD12	1.87	0.56
1:D:748:LEU:HB2	1:D:750:ARG:HG3	1.88	0.56
1:J:503:ASP:OD1	1:J:561:ARG:NH2	2.37	0.56
1:J:3862:GLN:HE21	1:J:3865:ASN:HD22	1.53	0.56
1:A:207:PHE:HB3	1:D:2326:ILE:HD12	1.86	0.56
1:A:3856:GLN:O	1:A:3932:ASN:ND2	2.39	0.56
1:D:1106:GLU:HB3	1:D:1214:ARG:HB2	1.86	0.56
1:G:3599:ALA:HB1	3:I:76:LYS:HE2	1.86	0.56
1:G:4094:ASP:OD1	1:G:4094:ASP:N	2.33	0.56
1:J:1465:VAL:N	1:J:1483:SER:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2793:THR:HG23	1:J:2903:ALA:HB2	1.88	0.56
1:G:2793:THR:HG23	1:G:2903:ALA:HB2	1.88	0.56
1:J:3599:ALA:HB1	3:L:76:LYS:HE2	1.86	0.56
1:A:1465:VAL:N	1:A:1483:SER:O	2.39	0.56
1:A:4808:ASP:HB2	1:D:4523:VAL:CG1	2.36	0.56
1:A:4819:TYR:CD1	1:J:4845:ILE:HD12	2.41	0.56
1:D:756:SER:HB2	1:D:769:ARG:HB2	1.87	0.56
1:D:2427:LEU:HD11	1:D:2428:ILE:HG22	1.84	0.56
1:G:143:LEU:HD22	1:J:2427:LEU:CA	2.30	0.56
1:G:4020:MET:HB3	1:G:4067:LEU:HD21	1.88	0.56
1:A:4845:ILE:HD12	1:D:4819:TYR:CD1	2.41	0.55
1:D:2326:ILE:HD11	1:D:2327:ARG:HG3	1.88	0.55
1:D:2883:LYS:O	1:D:2887:ARG:N	2.37	0.55
1:A:503:ASP:OD1	1:A:561:ARG:NH2	2.37	0.55
1:A:2892:ASP:HA	1:A:2895:LYS:HB2	1.88	0.55
1:D:4031:ASP:HA	1:D:4034:LYS:HB2	1.89	0.55
3:F:51:ASP:O	3:F:55:GLU:N	2.39	0.55
1:G:4858:ILE:HD12	1:J:4867:ILE:CG2	2.37	0.55
1:J:2712:ILE:O	1:J:2781:LYS:NZ	2.35	0.55
1:J:2892:ASP:HA	1:J:2895:LYS:HB2	1.88	0.55
1:A:748:LEU:HB2	1:A:750:ARG:HG3	1.88	0.55
1:D:2025:THR:O	1:D:2029:ARG:NH1	2.40	0.55
1:G:1304:LEU:HB2	1:G:1541:PRO:HG2	1.87	0.55
1:J:2326:ILE:HD11	1:J:2327:ARG:HG3	1.89	0.55
1:J:3854:ASP:OD1	1:J:3854:ASP:N	2.33	0.55
1:A:1432:ILE:HG22	1:A:1434:PRO:HD2	1.89	0.55
1:D:1172:THR:HG22	1:D:1193:LYS:HG2	1.87	0.55
1:G:2427:LEU:HD12	1:G:2428:ILE:N	2.22	0.55
1:G:3623:GLN:NE2	1:G:3626:GLU:OE2	2.40	0.55
1:J:1112:ASP:H	1:J:1211:GLN:HE21	1.55	0.55
1:A:188:SER:OG	1:A:190:ARG:NH2	2.36	0.55
1:A:2793:THR:HG23	1:A:2903:ALA:HB2	1.88	0.55
1:A:4020:MET:HB3	1:A:4067:LEU:HD21	1.88	0.55
1:D:3623:GLN:NE2	1:D:3626:GLU:OE2	2.40	0.55
1:G:474:ASP:OD1	1:G:478:ARG:NH1	2.40	0.55
1:G:4146:ILE:H	1:G:4962:GLN:HE22	1.54	0.55
1:J:3856:GLN:O	1:J:3932:ASN:ND2	2.39	0.55
1:A:2025:THR:O	1:A:2029:ARG:NH1	2.40	0.55
1:J:1643:GLU:O	1:J:1647:GLN:NE2	2.40	0.55
1:J:4146:ILE:H	1:J:4962:GLN:HE22	1.54	0.55
1:A:1643:GLU:O	1:A:1647:GLN:NE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2892:ASP:HA	1:D:2895:LYS:HB2	1.88	0.55
1:G:2025:THR:O	1:G:2029:ARG:NH1	2.40	0.55
1:G:4031:ASP:HA	1:G:4034:LYS:HB2	1.89	0.55
1:A:3623:GLN:NE2	1:A:3626:GLU:OE2	2.40	0.55
1:D:394:HIS:CD2	1:D:397:GLY:H	2.25	0.55
1:D:2257:ALA:O	1:D:2259:ARG:NH1	2.40	0.55
1:D:2793:THR:HG23	1:D:2903:ALA:HB2	1.88	0.55
1:G:2892:ASP:HA	1:G:2895:LYS:HB2	1.88	0.55
1:G:3856:GLN:O	1:G:3932:ASN:ND2	2.39	0.55
1:J:748:LEU:HB2	1:J:750:ARG:HG3	1.88	0.55
1:J:2427:LEU:HD12	1:J:2428:ILE:N	2.22	0.55
1:J:4518:LEU:HD21	1:J:4738:PHE:CD1	2.42	0.55
1:A:2257:ALA:O	1:A:2259:ARG:NH1	2.40	0.55
1:A:4577:ALA:O	1:A:4734:HIS:NE2	2.35	0.55
1:G:4577:ALA:O	1:G:4734:HIS:NE2	2.35	0.55
1:G:4926:LEU:HD13	1:G:4942:TRP:HB2	1.89	0.55
1:J:756:SER:HB2	1:J:769:ARG:HB2	1.87	0.55
1:J:4926:LEU:HD13	1:J:4942:TRP:HB2	1.89	0.55
3:L:51:ASP:O	3:L:55:GLU:N	2.39	0.55
1:D:699:SER:OG	1:D:700:THR:N	2.40	0.55
1:D:1432:ILE:HG22	1:D:1434:PRO:HD2	1.89	0.55
1:G:2257:ALA:O	1:G:2259:ARG:NH1	2.40	0.55
1:G:4845:ILE:HD12	1:J:4819:TYR:CD1	2.42	0.55
1:J:556:ASP:OD1	1:J:593:HIS:NE2	2.38	0.55
1:J:2025:THR:O	1:J:2029:ARG:NH1	2.40	0.55
1:J:3623:GLN:NE2	1:J:3626:GLU:OE2	2.40	0.55
1:A:474:ASP:OD1	1:A:478:ARG:NH1	2.40	0.54
1:A:1112:ASP:H	1:A:1211:GLN:HE21	1.55	0.54
1:A:4867:ILE:CG2	1:J:4858:ILE:HD12	2.37	0.54
1:D:1465:VAL:N	1:D:1483:SER:O	2.39	0.54
1:G:748:LEU:HB2	1:G:750:ARG:HG3	1.88	0.54
1:J:394:HIS:CD2	1:J:397:GLY:H	2.25	0.54
1:A:1589:GLN:NE2	1:A:1634:GLU:OE2	2.40	0.54
1:A:1756:SER:OG	1:A:1757:LEU:N	2.40	0.54
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.89	0.54
1:G:290:ARG:H	1:G:293:GLN:HE22	1.55	0.54
1:J:290:ARG:H	1:J:293:GLN:HE22	1.56	0.54
1:J:1432:ILE:HG22	1:J:1434:PRO:HD2	1.89	0.54
1:A:699:SER:OG	1:A:700:THR:N	2.40	0.54
1:A:2645:LEU:O	1:A:2649:ILE:N	2.40	0.54
1:A:4146:ILE:H	1:A:4962:GLN:HE22	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1589:GLN:NE2	1:D:1634:GLU:OE2	2.40	0.54
1:D:4518:LEU:HD21	1:D:4738:PHE:CD1	2.42	0.54
1:G:756:SER:HB2	1:G:769:ARG:HB2	1.87	0.54
1:G:1465:VAL:N	1:G:1483:SER:O	2.39	0.54
1:J:1589:GLN:NE2	1:J:1634:GLU:OE2	2.40	0.54
1:J:4154:SER:OG	1:J:4155:GLU:N	2.41	0.54
1:A:290:ARG:H	1:A:293:GLN:HE22	1.56	0.54
1:D:2427:LEU:HD12	1:D:2428:ILE:N	2.22	0.54
1:D:4020:MET:HB3	1:D:4067:LEU:HD21	1.88	0.54
1:G:228:LEU:HB3	1:G:289:ILE:HD12	1.89	0.54
1:G:676:GLU:HB2	1:G:803:LEU:HB2	1.89	0.54
1:J:2317:ASN:HA	1:J:2320:VAL:HG12	1.90	0.54
1:J:2423:ILE:HG23	1:J:2427:LEU:HD23	1.89	0.54
1:J:4020:MET:HB3	1:J:4067:LEU:HD21	1.88	0.54
1:J:4577:ALA:O	1:J:4734:HIS:NE2	2.35	0.54
1:A:2423:ILE:HG23	1:A:2427:LEU:HD23	1.89	0.54
1:D:300:VAL:O	1:D:420:ARG:NE	2.34	0.54
1:D:556:ASP:OD1	1:D:593:HIS:NE2	2.38	0.54
1:A:2317:ASN:HA	1:A:2320:VAL:HG12	1.90	0.54
1:A:2893:ILE:HG13	1:A:2894:LEU:HG	1.90	0.54
1:D:290:ARG:H	1:D:293:GLN:HE22	1.55	0.54
1:D:4858:ILE:HD12	1:G:4867:ILE:CG2	2.37	0.54
1:G:4154:SER:OG	1:G:4155:GLU:N	2.41	0.54
1:J:115:TYR:HE2	1:J:175:VAL:HA	1.73	0.54
1:J:699:SER:OG	1:J:700:THR:N	2.40	0.54
1:J:2138:GLU:O	1:J:2141:LYS:NZ	2.37	0.54
1:A:394:HIS:CD2	1:A:397:GLY:H	2.25	0.54
1:A:4031:ASP:HA	1:A:4034:LYS:HB2	1.89	0.54
3:C:51:ASP:O	3:C:55:GLU:N	2.39	0.54
1:G:115:TYR:HE2	1:G:175:VAL:HA	1.73	0.54
1:G:2326:ILE:HD11	1:G:2327:ARG:HG3	1.89	0.54
3:I:51:ASP:O	3:I:55:GLU:N	2.39	0.54
1:J:467:ASP:N	1:J:467:ASP:OD1	2.38	0.54
1:J:676:GLU:HB2	1:J:803:LEU:HB2	1.89	0.54
1:J:2257:ALA:O	1:J:2259:ARG:NH1	2.40	0.54
1:A:411:GLU:OE2	1:A:484:ASN:ND2	2.41	0.54
1:A:1445:TRP:O	1:A:1486:TYR:N	2.41	0.54
1:D:680:ASP:O	1:D:799:LYS:NZ	2.41	0.54
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.40	0.54
1:D:2893:ILE:HG13	1:D:2894:LEU:HG	1.90	0.54
1:G:394:HIS:CD2	1:G:397:GLY:H	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:699:SER:OG	1:G:700:THR:N	2.40	0.54
1:G:1432:ILE:HG22	1:G:1434:PRO:HD2	1.89	0.54
1:J:2321:VAL:HG12	1:J:2324:LEU:HD12	1.90	0.54
1:J:2423:ILE:O	1:J:2427:LEU:CG	2.54	0.54
1:A:2326:ILE:HD11	1:A:2327:ARG:HG3	1.89	0.54
1:A:2427:LEU:HD12	1:A:2428:ILE:N	2.22	0.54
1:A:4094:ASP:OD1	1:A:4094:ASP:N	2.33	0.54
1:A:4518:LEU:HD21	1:A:4738:PHE:CD1	2.42	0.54
1:D:474:ASP:OD1	1:D:478:ARG:NH1	2.40	0.54
1:D:2317:ASN:HA	1:D:2320:VAL:HG12	1.89	0.54
1:D:4146:ILE:H	1:D:4962:GLN:HE22	1.54	0.54
1:G:62:LEU:HB3	1:G:276:ARG:HH21	1.73	0.54
1:G:143:LEU:HD22	1:J:2427:LEU:HB3	0.70	0.54
1:G:1112:ASP:H	1:G:1211:GLN:HE21	1.55	0.54
1:G:2317:ASN:HA	1:G:2320:VAL:HG12	1.90	0.54
1:J:3733:HIS:O	1:J:3777:LYS:NZ	2.40	0.54
1:J:4031:ASP:HA	1:J:4034:LYS:HB2	1.89	0.54
1:A:62:LEU:HB3	1:A:276:ARG:HH21	1.73	0.54
1:D:1112:ASP:H	1:D:1211:GLN:HE21	1.55	0.54
1:D:3733:HIS:O	1:D:3777:LYS:NZ	2.40	0.54
1:G:1756:SER:OG	1:G:1757:LEU:N	2.40	0.54
1:G:2844:MET:O	1:G:2848:ASN:N	2.40	0.54
1:J:411:GLU:OE2	1:J:484:ASN:ND2	2.41	0.54
1:J:474:ASP:OD1	1:J:478:ARG:NH1	2.40	0.54
1:J:2893:ILE:HG13	1:J:2894:LEU:HG	1.90	0.54
1:D:1643:GLU:O	1:D:1647:GLN:NE2	2.40	0.53
1:G:2893:ILE:HG13	1:G:2894:LEU:HG	1.90	0.53
1:A:2321:VAL:HG12	1:A:2324:LEU:HD12	1.90	0.53
1:D:4926:LEU:HD13	1:D:4942:TRP:HB2	1.89	0.53
1:G:1589:GLN:NE2	1:G:1634:GLU:OE2	2.40	0.53
1:D:115:TYR:HE2	1:D:175:VAL:HA	1.73	0.53
1:D:411:GLU:OE2	1:D:484:ASN:ND2	2.41	0.53
1:D:499:LEU:HD22	1:D:557:TRP:HZ3	1.74	0.53
1:D:3845:GLN:HG3	1:D:3923:GLU:HG3	1.90	0.53
1:G:4060:THR:OG1	1:G:4063:GLU:OE2	2.27	0.53
1:A:115:TYR:HE2	1:A:175:VAL:HA	1.73	0.53
1:A:4926:LEU:HD13	1:A:4942:TRP:HB2	1.89	0.53
1:D:62:LEU:HB3	1:D:276:ARG:HH21	1.73	0.53
1:D:228:LEU:HB3	1:D:289:ILE:HD12	1.89	0.53
1:D:1445:TRP:O	1:D:1486:TYR:N	2.41	0.53
1:D:2138:GLU:O	1:D:2141:LYS:NZ	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4518:LEU:HD21	1:G:4738:PHE:CD1	2.43	0.53
1:A:2593:LEU:O	1:A:2597:VAL:N	2.42	0.53
1:D:188:SER:OG	1:D:190:ARG:NH2	2.36	0.53
1:G:1643:GLU:O	1:G:1647:GLN:NE2	2.40	0.53
1:G:2645:LEU:O	1:G:2649:ILE:N	2.40	0.53
1:J:654:SER:HB3	1:J:791:VAL:HG12	1.91	0.53
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.89	0.53
1:A:4154:SER:OG	1:A:4155:GLU:N	2.41	0.53
1:J:671:LYS:N	1:J:819:TYR:O	2.42	0.53
1:J:1445:TRP:O	1:J:1486:TYR:N	2.41	0.53
1:J:3787:ASP:O	1:J:3865:ASN:ND2	2.42	0.53
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.42	0.53
1:A:4060:THR:OG1	1:A:4063:GLU:OE2	2.27	0.53
1:D:671:LYS:N	1:D:819:TYR:O	2.42	0.53
1:D:847:THR:OG1	1:D:1216:ASN:OD1	2.27	0.53
1:D:3956:GLN:NE2	1:D:3973:MET:SD	2.82	0.53
1:G:300:VAL:O	1:G:420:ARG:NE	2.34	0.53
1:A:2883:LYS:O	1:A:2887:ARG:N	2.37	0.53
1:A:4858:ILE:HD12	1:D:4867:ILE:CG2	2.38	0.53
1:D:2844:MET:O	1:D:2848:ASN:N	2.40	0.53
1:G:654:SER:HB3	1:G:791:VAL:HG12	1.91	0.53
1:G:411:GLU:OE2	1:G:484:ASN:ND2	2.41	0.53
1:G:1445:TRP:O	1:G:1486:TYR:N	2.41	0.53
1:J:62:LEU:HB3	1:J:276:ARG:HH21	1.73	0.53
1:D:420:ARG:HA	1:D:423:VAL:HB	1.91	0.53
1:D:4154:SER:OG	1:D:4155:GLU:N	2.41	0.53
1:G:207:PHE:HD1	1:J:2326:ILE:CD1	1.99	0.53
1:G:2423:ILE:HG23	1:G:2427:LEU:HD23	1.89	0.53
1:J:629:GLN:OE1	1:J:1669:ASN:ND2	2.42	0.53
1:A:228:LEU:HB3	1:A:289:ILE:HD12	1.89	0.52
1:A:4957:ASP:OD1	1:A:4957:ASP:N	2.34	0.52
1:G:188:SER:OG	1:G:190:ARG:NH2	2.36	0.52
1:G:680:ASP:O	1:G:799:LYS:NZ	2.41	0.52
1:G:847:THR:OG1	1:G:1216:ASN:OD1	2.27	0.52
1:G:3733:HIS:O	1:G:3777:LYS:NZ	2.40	0.52
1:G:3787:ASP:O	1:G:3865:ASN:ND2	2.42	0.52
1:J:499:LEU:HD22	1:J:557:TRP:HZ3	1.74	0.52
1:J:2844:MET:O	1:J:2848:ASN:N	2.40	0.52
1:A:671:LYS:N	1:A:819:TYR:O	2.42	0.52
1:A:1293:GLN:NE2	1:A:1548:THR:O	2.43	0.52
1:A:3787:ASP:O	1:A:3865:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2321:VAL:HG12	1:D:2324:LEU:HD12	1.90	0.52
1:G:629:GLN:OE1	1:G:1669:ASN:ND2	2.42	0.52
1:G:2593:LEU:O	1:G:2597:VAL:N	2.42	0.52
1:J:228:LEU:HB3	1:J:289:ILE:HD12	1.89	0.52
1:A:847:THR:OG1	1:A:1216:ASN:OD1	2.27	0.52
1:D:1811:GLY:HA3	1:D:1816:PHE:HB2	1.92	0.52
1:D:4060:THR:OG1	1:D:4063:GLU:OE2	2.27	0.52
1:G:2423:ILE:O	1:G:2427:LEU:CG	2.54	0.52
1:G:3845:GLN:HG3	1:G:3923:GLU:HG3	1.90	0.52
1:J:1938:GLN:HG3	1:J:3611:ASN:HA	1.91	0.52
1:J:3845:GLN:HG3	1:J:3923:GLU:HG3	1.90	0.52
1:A:499:LEU:HD22	1:A:557:TRP:HZ3	1.74	0.52
1:A:1811:GLY:HA3	1:A:1816:PHE:HB2	1.92	0.52
3:C:61:ASN:ND2	3:C:63:THR:O	2.43	0.52
1:G:2321:VAL:HG12	1:G:2324:LEU:HD12	1.90	0.52
1:G:3956:GLN:NE2	1:G:3973:MET:SD	2.82	0.52
1:J:2593:LEU:O	1:J:2597:VAL:N	2.42	0.52
1:J:2645:LEU:O	1:J:2649:ILE:N	2.40	0.52
1:A:1938:GLN:HG3	1:A:3611:ASN:HA	1.91	0.52
1:A:2427:LEU:HB3	1:J:143:LEU:HD22	0.69	0.52
1:D:467:ASP:N	1:D:467:ASP:OD1	2.38	0.52
1:D:654:SER:HB3	1:D:791:VAL:HG12	1.91	0.52
1:D:2645:LEU:O	1:D:2649:ILE:N	2.40	0.52
1:D:2712:ILE:O	1:D:2781:LYS:NZ	2.35	0.52
1:G:420:ARG:HA	1:G:423:VAL:HB	1.91	0.52
1:G:499:LEU:HD22	1:G:557:TRP:HZ3	1.74	0.52
1:G:620:CYS:SG	1:G:621:HIS:N	2.82	0.52
1:G:1293:GLN:NE2	1:G:1548:THR:O	2.43	0.52
1:G:3875:THR:HG21	1:G:3924:TYR:HE2	1.75	0.52
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.75	0.52
1:D:629:GLN:OE1	1:D:1669:ASN:ND2	2.42	0.52
1:G:671:LYS:N	1:G:819:TYR:O	2.42	0.52
1:J:420:ARG:HA	1:J:423:VAL:HB	1.91	0.52
1:J:680:ASP:O	1:J:799:LYS:NZ	2.41	0.52
1:D:207:PHE:HD1	1:G:2326:ILE:CD1	2.00	0.52
1:D:1938:GLN:HG3	1:D:3611:ASN:HA	1.91	0.52
1:D:3787:ASP:O	1:D:3865:ASN:ND2	2.42	0.52
1:G:467:ASP:N	1:G:467:ASP:OD1	2.38	0.52
1:G:4630:GLN:OE1	1:G:4633:ARG:NH2	2.43	0.52
1:J:1293:GLN:NE2	1:J:1548:THR:O	2.43	0.52
1:A:300:VAL:O	1:A:420:ARG:NE	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2423:ILE:HG23	1:D:2427:LEU:HD23	1.89	0.52
1:D:2832:VAL:O	1:D:2895:LYS:NZ	2.38	0.52
1:A:3956:GLN:NE2	1:A:3973:MET:SD	2.82	0.52
1:D:1293:GLN:NE2	1:D:1548:THR:O	2.43	0.52
1:D:2423:ILE:O	1:D:2427:LEU:CG	2.54	0.52
3:F:61:ASN:ND2	3:F:63:THR:O	2.43	0.52
1:A:4634:LEU:O	1:A:4705:LYS:NZ	2.43	0.52
1:D:4630:GLN:OE1	1:D:4633:ARG:NH2	2.43	0.52
1:G:1811:GLY:HA3	1:G:1816:PHE:HB2	1.92	0.52
1:G:4634:LEU:O	1:G:4705:LYS:NZ	2.43	0.52
3:I:61:ASN:ND2	3:I:63:THR:O	2.43	0.52
1:J:3956:GLN:NE2	1:J:3973:MET:SD	2.82	0.52
1:A:654:SER:HB3	1:A:791:VAL:HG12	1.91	0.51
1:A:4630:GLN:OE1	1:A:4633:ARG:NH2	2.43	0.51
1:D:1440:ASN:N	1:D:1440:ASN:OD1	2.43	0.51
1:D:2593:LEU:O	1:D:2597:VAL:N	2.42	0.51
1:D:3875:THR:HG21	1:D:3924:TYR:HE2	1.75	0.51
1:G:681:HIS:ND1	1:G:797:GLY:O	2.44	0.51
1:G:956:HIS:HA	1:G:1060:TYR:HB3	1.92	0.51
1:J:620:CYS:SG	1:J:621:HIS:N	2.82	0.51
1:J:1209:VAL:N	1:J:1211:GLN:OE1	2.43	0.51
1:J:1811:GLY:HA3	1:J:1816:PHE:HB2	1.92	0.51
1:J:4634:LEU:O	1:J:4705:LYS:NZ	2.43	0.51
3:L:61:ASN:ND2	3:L:63:THR:O	2.43	0.51
1:A:1209:VAL:N	1:A:1211:GLN:OE1	2.43	0.51
1:A:3845:GLN:HG3	1:A:3923:GLU:HG3	1.90	0.51
1:J:300:VAL:O	1:J:420:ARG:NE	2.34	0.51
1:J:847:THR:OG1	1:J:1216:ASN:OD1	2.27	0.51
1:A:420:ARG:HA	1:A:423:VAL:HB	1.91	0.51
1:A:1440:ASN:N	1:A:1440:ASN:OD1	2.43	0.51
1:D:681:HIS:ND1	1:D:797:GLY:O	2.44	0.51
1:G:245:LEU:HD12	1:G:262:TYR:HE1	1.75	0.51
1:G:4497:ALA:HB2	1:G:4593:CYS:HB2	1.93	0.51
1:A:2138:GLU:O	1:A:2141:LYS:NZ	2.37	0.51
1:A:4497:ALA:HB2	1:A:4593:CYS:HB2	1.93	0.51
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.93	0.51
1:G:1440:ASN:N	1:G:1440:ASN:OD1	2.43	0.51
1:J:1756:SER:OG	1:J:1757:LEU:N	2.40	0.51
1:J:4094:ASP:OD1	1:J:4094:ASP:N	2.33	0.51
1:A:288:HIS:ND1	1:A:349:MET:O	2.37	0.51
1:A:618:CYS:O	1:A:629:GLN:NE2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1938:GLN:HG3	1:G:3611:ASN:HA	1.91	0.51
1:J:3875:THR:HG21	1:J:3924:TYR:HE2	1.75	0.51
1:J:4046:LYS:NZ	1:J:4072:GLU:OE2	2.43	0.51
1:J:4497:ALA:HB2	1:J:4593:CYS:HB2	1.93	0.51
1:J:4630:GLN:OE1	1:J:4633:ARG:NH2	2.43	0.51
1:A:4958:CYS:SG	1:A:4959:PHE:N	2.84	0.51
1:D:1429:SER:HA	1:D:1507:ILE:HG12	1.93	0.51
2:E:25:HIS:ND1	2:E:39:SER:OG	2.40	0.51
1:A:611:LEU:HD22	1:A:1660:LEU:HD22	1.92	0.51
1:D:731:HIS:HB2	1:D:740:THR:HA	1.93	0.51
1:D:1053:ALA:O	1:D:1056:THR:OG1	2.29	0.51
1:D:4497:ALA:HB2	1:D:4593:CYS:HB2	1.93	0.51
1:D:3788:VAL:HG22	1:D:3865:ASN:HB3	1.93	0.51
1:G:700:THR:HG22	1:G:787:LEU:H	1.76	0.51
1:G:1053:ALA:O	1:G:1056:THR:OG1	2.29	0.51
1:G:2213:LYS:HA	1:G:2254:LEU:HD21	1.93	0.51
1:J:1119:ARG:NH2	1:J:1196:ASP:O	2.40	0.51
1:A:245:LEU:HD12	1:A:262:TYR:HE1	1.75	0.51
1:A:3798:MET:HG2	1:A:3840:LEU:HD21	1.92	0.51
1:G:674:TYR:HE2	1:G:814:LEU:HB2	1.76	0.51
1:G:2883:LYS:O	1:G:2887:ARG:N	2.37	0.51
1:J:674:TYR:HE2	1:J:814:LEU:HB2	1.76	0.51
1:J:1440:ASN:N	1:J:1440:ASN:OD1	2.43	0.51
1:J:2213:LYS:HA	1:J:2254:LEU:HD21	1.93	0.51
1:A:620:CYS:SG	1:A:621:HIS:N	2.82	0.51
1:A:2423:ILE:O	1:A:2427:LEU:CG	2.54	0.51
1:D:956:HIS:HA	1:D:1060:TYR:HB3	1.92	0.51
1:G:611:LEU:HD22	1:G:1660:LEU:HD22	1.92	0.51
1:G:2712:ILE:O	1:G:2781:LYS:NZ	2.35	0.51
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.93	0.51
1:J:2832:VAL:O	1:J:2895:LYS:NZ	2.38	0.51
1:A:681:HIS:ND1	1:A:797:GLY:O	2.44	0.50
1:A:920:GLU:OE2	1:A:976:TYR:OH	2.29	0.50
1:D:4634:LEU:O	1:D:4705:LYS:NZ	2.43	0.50
1:G:4897:ASP:OD1	1:G:4897:ASP:N	2.43	0.50
1:J:188:SER:OG	1:J:190:ARG:NH2	2.36	0.50
1:J:190:ARG:NE	1:J:207:PHE:CZ	2.79	0.50
1:J:681:HIS:ND1	1:J:797:GLY:O	2.44	0.50
1:J:1429:SER:HA	1:J:1507:ILE:HG12	1.93	0.50
1:A:680:ASP:O	1:A:799:LYS:NZ	2.41	0.50
1:A:956:HIS:HA	1:A:1060:TYR:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1429:SER:HA	1:A:1507:ILE:HG12	1.93	0.50
1:A:3797:LEU:HD22	1:A:3836:PHE:HZ	1.77	0.50
2:B:7:ILE:HD11	2:B:73:LYS:HB2	1.93	0.50
1:D:355:LYS:O	1:D:359:SER:OG	2.27	0.50
1:D:674:TYR:HE2	1:D:814:LEU:HB2	1.76	0.50
1:D:1298:ASP:OD1	1:D:1298:ASP:N	2.44	0.50
1:G:3788:VAL:HG22	1:G:3865:ASN:HB3	1.93	0.50
1:J:700:THR:HG22	1:J:787:LEU:H	1.76	0.50
1:A:1053:ALA:O	1:A:1056:THR:OG1	2.29	0.50
1:G:4797:SER:OG	1:G:4805:MET:N	2.45	0.50
1:J:956:HIS:HA	1:J:1060:TYR:HB3	1.92	0.50
1:J:1434:PRO:HB2	1:J:1440:ASN:HD21	1.76	0.50
1:A:1434:PRO:HB2	1:A:1440:ASN:HD21	1.76	0.50
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.45	0.50
1:D:394:HIS:HD2	1:D:396:GLU:H	1.59	0.50
1:D:920:GLU:OE2	1:D:976:TYR:OH	2.29	0.50
1:D:3927:GLY:O	1:D:3929:CYS:N	2.44	0.50
1:G:920:GLU:OE2	1:G:976:TYR:OH	2.29	0.50
1:G:1091:GLU:OE1	1:G:1248:THR:OG1	2.30	0.50
1:G:3690:MET:HE1	1:G:3754:PRO:HG2	1.93	0.50
1:J:245:LEU:HD12	1:J:262:TYR:HE1	1.75	0.50
1:J:611:LEU:HD22	1:J:1660:LEU:HD22	1.92	0.50
1:J:3690:MET:HE1	1:J:3754:PRO:HG2	1.93	0.50
1:A:190:ARG:NE	1:A:207:PHE:CZ	2.80	0.50
1:A:271:ALA:O	1:A:301:THR:OG1	2.25	0.50
1:A:2213:LYS:HA	1:A:2254:LEU:HD21	1.93	0.50
1:D:3798:MET:HG2	1:D:3840:LEU:HD21	1.92	0.50
2:E:27:THR:HG23	2:E:100:ASP:HB3	1.93	0.50
1:G:1119:ARG:NH2	1:G:1196:ASP:O	2.40	0.50
1:G:1209:VAL:N	1:G:1211:GLN:OE1	2.43	0.50
1:J:1053:ALA:O	1:J:1056:THR:OG1	2.29	0.50
1:J:4958:CYS:SG	1:J:4959:PHE:N	2.84	0.50
1:A:673:TRP:HA	1:A:820:ALA:HB3	1.94	0.50
1:A:674:TYR:HE2	1:A:814:LEU:HB2	1.76	0.50
1:A:700:THR:HG22	1:A:787:LEU:H	1.76	0.50
1:A:1091:GLU:OE1	1:A:1248:THR:OG1	2.30	0.50
2:B:27:THR:HG23	2:B:100:ASP:HB3	1.93	0.50
1:D:1209:VAL:N	1:D:1211:GLN:OE1	2.43	0.50
1:J:3686:ASP:HB3	1:J:3755:MET:HE1	1.94	0.50
1:A:355:LYS:O	1:A:359:SER:OG	2.27	0.50
1:D:190:ARG:NE	1:D:207:PHE:CZ	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3798:MET:HG2	1:G:3840:LEU:HD21	1.92	0.50
1:J:731:HIS:HB2	1:J:740:THR:HA	1.93	0.50
1:J:1298:ASP:OD1	1:J:1298:ASP:N	2.44	0.50
1:J:2793:THR:OG1	1:J:2901:GLY:O	2.29	0.50
1:J:3798:MET:HG2	1:J:3840:LEU:HD21	1.92	0.50
2:K:7:ILE:HD11	2:K:73:LYS:HB2	1.93	0.50
1:A:2067:MET:HE2	1:A:2088:LEU:HB3	1.94	0.50
1:D:2213:LYS:HA	1:D:2254:LEU:HD21	1.93	0.50
1:G:394:HIS:HD2	1:G:396:GLU:H	1.59	0.50
1:G:1298:ASP:OD1	1:G:1298:ASP:N	2.44	0.50
1:G:1434:PRO:HB2	1:G:1440:ASN:HD21	1.76	0.50
1:G:2832:VAL:O	1:G:2895:LYS:NZ	2.38	0.50
1:G:3945:VAL:HG13	1:G:4003:MET:HE3	1.94	0.50
2:H:25:HIS:ND1	2:H:39:SER:OG	2.40	0.50
1:J:920:GLU:OE2	1:J:976:TYR:OH	2.29	0.50
1:J:3797:LEU:HD22	1:J:3836:PHE:HZ	1.77	0.50
1:A:3733:HIS:O	1:A:3777:LYS:NZ	2.40	0.50
1:D:245:LEU:HD12	1:D:262:TYR:HE1	1.75	0.50
1:D:611:LEU:HD22	1:D:1660:LEU:HD22	1.92	0.50
1:D:700:THR:HG22	1:D:787:LEU:H	1.76	0.50
1:D:2067:MET:HE2	1:D:2088:LEU:HB3	1.94	0.50
1:D:2132:SER:O	1:D:2132:SER:OG	2.30	0.50
1:G:731:HIS:HB2	1:G:740:THR:HA	1.93	0.50
1:G:3686:ASP:HB3	1:G:3755:MET:HE1	1.94	0.50
1:G:3927:GLY:O	1:G:3929:CYS:N	2.45	0.50
1:J:1449:ASP:OD1	1:J:1449:ASP:N	2.45	0.50
1:A:1044:LYS:HA	1:A:1047:LYS:HB2	1.94	0.49
1:D:431:ARG:HA	1:D:434:ASP:HB2	1.94	0.49
1:D:3945:VAL:HG13	1:D:4003:MET:HE3	1.94	0.49
1:G:249:SER:OG	1:G:250:GLY:N	2.45	0.49
1:G:1429:SER:HA	1:G:1507:ILE:HG12	1.93	0.49
1:A:3686:ASP:HB3	1:A:3755:MET:HE1	1.94	0.49
1:A:3927:GLY:O	1:A:3929:CYS:N	2.45	0.49
1:D:673:TRP:HA	1:D:820:ALA:HB3	1.94	0.49
1:D:3800:SER:OG	1:D:3801:CYS:N	2.44	0.49
2:H:27:THR:HG23	2:H:100:ASP:HB3	1.93	0.49
1:J:1044:LYS:HA	1:J:1047:LYS:HB2	1.94	0.49
1:A:394:HIS:HD2	1:A:396:GLU:H	1.59	0.49
1:J:1091:GLU:OE1	1:J:1248:THR:OG1	2.30	0.49
1:A:2838:LEU:HD21	1:A:2894:LEU:HB2	1.94	0.49
1:A:3788:VAL:HG22	1:A:3865:ASN:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3945:VAL:HG13	1:A:4003:MET:HE3	1.94	0.49
1:D:2793:THR:OG1	1:D:2901:GLY:O	2.29	0.49
1:D:2838:LEU:HD21	1:D:2894:LEU:HB2	1.94	0.49
1:D:3797:LEU:HD22	1:D:3836:PHE:HZ	1.77	0.49
1:G:190:ARG:NE	1:G:207:PHE:CZ	2.80	0.49
1:J:394:HIS:HD2	1:J:396:GLU:H	1.59	0.49
1:J:431:ARG:HA	1:J:434:ASP:HB2	1.94	0.49
1:J:3604:PHE:HB2	3:L:52:MET:HG2	1.95	0.49
1:J:3945:VAL:HG13	1:J:4003:MET:HE3	1.94	0.49
1:A:1265:HIS:CD2	1:A:1267:HIS:H	2.31	0.49
1:D:1058:LEU:HA	1:D:1062:TYR:H	1.78	0.49
1:G:431:ARG:HA	1:G:434:ASP:HB2	1.94	0.49
1:G:673:TRP:HA	1:G:820:ALA:HB3	1.94	0.49
1:G:4078:THR:OG1	1:G:4079:LEU:N	2.46	0.49
1:J:3788:VAL:HG22	1:J:3865:ASN:HB3	1.93	0.49
1:J:4922:PHE:HE2	1:J:4941:VAL:HG11	1.77	0.49
1:A:731:HIS:HB2	1:A:740:THR:HA	1.93	0.49
1:D:288:HIS:ND1	1:D:349:MET:O	2.37	0.49
1:D:1044:LYS:HA	1:D:1047:LYS:HB2	1.94	0.49
1:D:3646:ALA:HB1	1:D:3735:ARG:HH22	1.78	0.49
1:D:3690:MET:HE1	1:D:3754:PRO:HG2	1.93	0.49
1:D:3759:THR:O	1:D:3759:THR:OG1	2.28	0.49
1:G:618:CYS:O	1:G:629:GLN:NE2	2.38	0.49
1:G:2838:LEU:HD21	1:G:2894:LEU:HB2	1.94	0.49
1:J:279:THR:HG22	1:J:281:ARG:H	1.78	0.49
1:J:2731:ASP:O	1:J:2735:MET:N	2.44	0.49
1:J:2838:LEU:HD21	1:J:2894:LEU:HB2	1.94	0.49
1:J:4060:THR:OG1	1:J:4063:GLU:OE2	2.27	0.49
1:A:2710:SER:HA	1:A:2781:LYS:HD3	1.93	0.49
1:A:4605:LYS:HG3	1:A:4609:ARG:HH21	1.77	0.49
1:D:1434:PRO:HB2	1:D:1440:ASN:HD21	1.76	0.49
1:D:2710:SER:HA	1:D:2781:LYS:HD3	1.93	0.49
1:D:4958:CYS:SG	1:D:4959:PHE:N	2.84	0.49
1:G:279:THR:HG22	1:G:281:ARG:H	1.78	0.49
1:G:1044:LYS:HA	1:G:1047:LYS:HB2	1.94	0.49
1:J:3646:ALA:HB1	1:J:3735:ARG:HH22	1.78	0.49
2:K:27:THR:HG23	2:K:100:ASP:HB3	1.93	0.49
1:A:1911:LEU:HB2	1:A:2088:LEU:HD21	1.95	0.49
1:A:3604:PHE:HB2	3:C:52:MET:HG2	1.95	0.49
1:A:3690:MET:HE1	1:A:3754:PRO:HG2	1.93	0.49
1:A:4922:PHE:HE2	1:A:4941:VAL:HG11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1091:GLU:OE1	1:D:1248:THR:OG1	2.30	0.49
1:D:2731:ASP:O	1:D:2735:MET:N	2.44	0.49
1:D:3604:PHE:HB2	3:F:52:MET:HG2	1.95	0.49
1:D:4797:SER:OG	1:D:4805:MET:N	2.45	0.49
1:D:4862:ILE:HD11	1:G:4757:ILE:HD13	1.93	0.49
1:G:844:ARG:NH1	1:G:849:ASP:OD1	2.46	0.49
1:G:2793:THR:OG1	1:G:2901:GLY:O	2.29	0.49
1:A:125:TYR:O	1:A:414:ARG:NH1	2.46	0.49
1:D:279:THR:HG22	1:D:281:ARG:H	1.78	0.49
1:G:248:PRO:HD3	1:G:261:HIS:CD2	2.48	0.49
1:G:3604:PHE:HB2	3:I:52:MET:HG2	1.95	0.49
1:G:3646:ALA:HB1	1:G:3735:ARG:HH22	1.78	0.49
1:J:125:TYR:O	1:J:414:ARG:NH1	2.46	0.49
1:J:248:PRO:HD3	1:J:261:HIS:CD2	2.48	0.49
1:J:1930:SER:O	1:J:1930:SER:OG	2.24	0.49
1:J:2774:TRP:HA	1:J:2777:LYS:HG2	1.95	0.49
1:J:4078:THR:OG1	1:J:4079:LEU:N	2.46	0.49
1:J:4957:ASP:OD1	1:J:4957:ASP:N	2.34	0.49
1:A:844:ARG:NH1	1:A:849:ASP:OD1	2.46	0.49
1:A:1298:ASP:OD1	1:A:1298:ASP:N	2.44	0.49
1:A:4757:ILE:HD13	1:J:4862:ILE:HD11	1.94	0.49
1:D:606:ARG:HH21	1:D:1632:ILE:HG23	1.78	0.49
1:D:4788:ASN:CG	1:G:4738:PHE:CD2	2.88	0.49
1:G:1556:GLU:O	1:G:1572:LYS:NZ	2.45	0.49
1:G:1911:LEU:HB2	1:G:2088:LEU:HD21	1.95	0.49
1:G:2132:SER:O	1:G:2132:SER:OG	2.30	0.49
1:G:2138:GLU:O	1:G:2141:LYS:NZ	2.37	0.49
1:G:3797:LEU:HD22	1:G:3836:PHE:HZ	1.77	0.49
1:J:2067:MET:HE2	1:J:2088:LEU:HB3	1.94	0.49
1:J:3927:GLY:O	1:J:3929:CYS:N	2.45	0.49
1:A:1210:ALA:N	1:A:1211:GLN:OE1	2.46	0.48
1:A:2774:TRP:HA	1:A:2777:LYS:HG2	1.95	0.48
1:A:2844:MET:O	1:A:2848:ASN:N	2.40	0.48
1:A:4797:SER:OG	1:A:4805:MET:N	2.45	0.48
1:D:125:TYR:O	1:D:414:ARG:NH1	2.46	0.48
1:D:1210:ALA:N	1:D:1211:GLN:OE1	2.46	0.48
1:D:4922:PHE:HE2	1:D:4941:VAL:HG11	1.77	0.48
1:G:1058:LEU:HA	1:G:1062:TYR:H	1.78	0.48
1:G:2852:ILE:O	1:G:2856:LYS:N	2.44	0.48
1:J:1058:LEU:HA	1:J:1062:TYR:H	1.78	0.48
1:A:4738:PHE:CD2	1:J:4788:ASN:CG	2.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1556:GLU:O	1:D:1572:LYS:NZ	2.45	0.48
1:D:2834:LEU:HD21	1:D:2838:LEU:HD22	1.95	0.48
1:G:1629:SER:HA	1:G:1640:ASP:HA	1.95	0.48
1:G:4605:LYS:HG3	1:G:4609:ARG:HH21	1.77	0.48
1:J:673:TRP:HA	1:J:820:ALA:HB3	1.94	0.48
1:J:1210:ALA:N	1:J:1211:GLN:OE1	2.46	0.48
1:A:143:LEU:HD23	1:A:207:PHE:CE2	2.49	0.48
1:A:2314:VAL:HG23	1:A:2317:ASN:HB2	1.95	0.48
1:D:618:CYS:O	1:D:629:GLN:NE2	2.38	0.48
1:G:125:TYR:O	1:G:414:ARG:NH1	2.46	0.48
1:G:143:LEU:HD23	1:G:207:PHE:CE2	2.49	0.48
1:G:1210:ALA:N	1:G:1211:GLN:OE1	2.46	0.48
1:G:4922:PHE:HE2	1:G:4941:VAL:HG11	1.77	0.48
1:J:143:LEU:HD23	1:J:207:PHE:CE2	2.49	0.48
1:J:1011:ARG:HA	1:J:1014:GLN:HB3	1.95	0.48
1:J:1691:ASN:HB3	1:J:1694:MET:HG3	1.96	0.48
1:A:431:ARG:HA	1:A:434:ASP:HB2	1.94	0.48
1:D:248:PRO:HD3	1:D:261:HIS:CD2	2.48	0.48
1:D:1691:ASN:HB3	1:D:1694:MET:HG3	1.95	0.48
1:D:1911:LEU:HB2	1:D:2088:LEU:HD21	1.95	0.48
1:D:3686:ASP:HB3	1:D:3755:MET:HE1	1.94	0.48
1:G:1265:HIS:CD2	1:G:1267:HIS:H	2.31	0.48
1:G:2067:MET:HE2	1:G:2088:LEU:HB3	1.94	0.48
1:J:727:PHE:H	1:J:730:LEU:HD13	1.78	0.48
1:J:894:VAL:O	1:J:898:ILE:N	2.47	0.48
1:J:1911:LEU:HB2	1:J:2088:LEU:HD21	1.95	0.48
1:J:2314:VAL:HG23	1:J:2317:ASN:HB2	1.95	0.48
1:J:2710:SER:HA	1:J:2781:LYS:HD3	1.93	0.48
1:A:894:VAL:O	1:A:898:ILE:N	2.47	0.48
1:D:844:ARG:NH1	1:D:849:ASP:OD1	2.46	0.48
1:D:4074:ASP:O	1:D:4076:ASN:N	2.47	0.48
1:G:727:PHE:H	1:G:730:LEU:HD13	1.78	0.48
1:G:2731:ASP:O	1:G:2735:MET:N	2.44	0.48
1:G:2834:LEU:HD21	1:G:2838:LEU:HD22	1.95	0.48
1:J:1265:HIS:CD2	1:J:1267:HIS:H	2.31	0.48
1:J:1292:SER:O	1:J:1292:SER:OG	2.32	0.48
1:J:4605:LYS:HG3	1:J:4609:ARG:HH21	1.77	0.48
1:A:248:PRO:HD3	1:A:261:HIS:CD2	2.48	0.48
1:A:606:ARG:HH21	1:A:1632:ILE:HG23	1.78	0.48
1:D:4897:ASP:OD1	1:D:4897:ASP:N	2.43	0.48
1:J:844:ARG:NH1	1:J:849:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:PHE:H	1:A:730:LEU:HD13	1.78	0.48
1:A:1086:ARG:HH11	1:A:1251:LEU:HD12	1.79	0.48
1:D:620:CYS:SG	1:D:621:HIS:N	2.82	0.48
1:D:1629:SER:HA	1:D:1640:ASP:HA	1.95	0.48
1:G:2710:SER:HA	1:G:2781:LYS:HD3	1.94	0.48
1:J:355:LYS:O	1:J:359:SER:OG	2.27	0.48
1:J:422:THR:HG21	1:J:459:LEU:HD11	1.96	0.48
2:K:25:HIS:ND1	2:K:39:SER:OG	2.40	0.48
1:D:1265:HIS:CD2	1:D:1267:HIS:H	2.31	0.48
1:G:207:PHE:CE1	1:J:2326:ILE:CG2	2.97	0.48
1:G:332:ARG:NE	1:G:364:GLN:OE1	2.47	0.48
1:G:606:ARG:HH21	1:G:1632:ILE:HG23	1.78	0.48
1:G:4862:ILE:HD11	1:J:4757:ILE:HD13	1.95	0.48
1:J:249:SER:OG	1:J:250:GLY:N	2.45	0.48
1:J:2132:SER:O	1:J:2132:SER:OG	2.30	0.48
1:A:1011:ARG:HA	1:A:1014:GLN:HB3	1.95	0.48
1:A:1058:LEU:HA	1:A:1062:TYR:H	1.78	0.48
1:A:2731:ASP:O	1:A:2735:MET:N	2.44	0.48
1:D:143:LEU:HD23	1:D:207:PHE:CE2	2.49	0.48
1:D:2774:TRP:HA	1:D:2777:LYS:HG2	1.95	0.48
1:D:4900:ASP:O	1:D:4902:VAL:N	2.47	0.48
1:G:55:SER:O	1:G:296:ARG:NH2	2.41	0.48
1:G:725:TYR:HD1	1:G:732:LEU:HB3	1.79	0.48
1:J:4900:ASP:O	1:J:4902:VAL:N	2.47	0.48
1:A:717:GLY:O	1:A:735:GLY:N	2.47	0.48
1:A:3724:LYS:HB3	1:A:3724:LYS:HE2	1.69	0.48
1:G:2774:TRP:HA	1:G:2777:LYS:HG2	1.95	0.48
1:G:4788:ASN:CG	1:J:4738:PHE:CD2	2.90	0.48
1:J:1556:GLU:O	1:J:1572:LYS:NZ	2.45	0.48
1:J:1629:SER:HA	1:J:1640:ASP:HA	1.95	0.48
2:K:78:PRO:HA	2:K:81:ALA:HB3	1.96	0.48
1:A:302:THR:OG1	1:A:304:LYS:NZ	2.47	0.47
1:A:1116:GLY:HA3	1:A:1136:ALA:HA	1.96	0.47
1:A:2326:ILE:CG2	1:J:207:PHE:CE1	2.97	0.47
1:A:4074:ASP:O	1:A:4076:ASN:N	2.47	0.47
1:D:725:TYR:HD1	1:D:732:LEU:HB3	1.79	0.47
1:D:3854:ASP:OD1	1:D:3854:ASP:N	2.33	0.47
1:G:1177:LEU:N	1:G:1180:GLU:O	2.44	0.47
1:G:4818:MET:HE3	1:G:4818:MET:HB2	1.72	0.47
1:J:302:THR:OG1	1:J:304:LYS:NZ	2.47	0.47
1:A:207:PHE:CE1	1:D:2326:ILE:CG2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:TYR:HD1	1:A:732:LEU:HB3	1.79	0.47
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.95	0.47
1:A:2834:LEU:HD21	1:A:2838:LEU:HD22	1.95	0.47
1:A:3646:ALA:HB1	1:A:3735:ARG:HH22	1.78	0.47
1:A:4900:ASP:O	1:A:4902:VAL:N	2.47	0.47
1:D:2314:VAL:HG23	1:D:2317:ASN:HB2	1.95	0.47
1:D:4605:LYS:HG3	1:D:4609:ARG:HH21	1.77	0.47
1:G:1691:ASN:HB3	1:G:1694:MET:HG3	1.95	0.47
1:G:4900:ASP:O	1:G:4902:VAL:N	2.47	0.47
1:J:1116:GLY:HA3	1:J:1136:ALA:HA	1.96	0.47
1:A:279:THR:HG22	1:A:281:ARG:H	1.78	0.47
1:A:1107:ALA:HA	1:A:1113:MET:HE3	1.97	0.47
1:D:727:PHE:H	1:D:730:LEU:HD13	1.78	0.47
1:D:4804:ASP:OD1	1:D:4804:ASP:N	2.47	0.47
1:G:1011:ARG:HA	1:G:1014:GLN:HB3	1.95	0.47
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.96	0.47
1:J:394:HIS:HD2	1:J:397:GLY:H	1.62	0.47
1:J:725:TYR:HD1	1:J:732:LEU:HB3	1.79	0.47
1:J:4804:ASP:N	1:J:4804:ASP:OD1	2.47	0.47
1:D:249:SER:OG	1:D:250:GLY:N	2.45	0.47
1:D:332:ARG:NE	1:D:364:GLN:OE1	2.47	0.47
1:D:2156:PHE:HA	1:D:2163:MET:HE3	1.97	0.47
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.96	0.47
1:G:2427:LEU:HD12	1:G:2428:ILE:CG2	2.35	0.47
1:G:4074:ASP:O	1:G:4076:ASN:N	2.47	0.47
1:J:1219:LYS:HD3	1:J:1243:THR:HG23	1.96	0.47
1:J:2834:LEU:HD21	1:J:2838:LEU:HD22	1.95	0.47
1:J:2852:ILE:O	1:J:2856:LYS:N	2.44	0.47
1:A:332:ARG:NE	1:A:364:GLN:OE1	2.47	0.47
1:A:422:THR:HG21	1:A:459:LEU:HD11	1.96	0.47
1:A:1089:ARG:HH22	1:A:1600:PRO:HG3	1.80	0.47
1:A:1173:MET:HB3	1:A:1192:PHE:HB2	1.96	0.47
1:A:1691:ASN:HB3	1:A:1694:MET:HG3	1.95	0.47
2:B:25:HIS:ND1	2:B:39:SER:OG	2.40	0.47
1:D:422:THR:HG21	1:D:459:LEU:HD11	1.96	0.47
1:G:394:HIS:HD2	1:G:397:GLY:H	1.62	0.47
1:J:1086:ARG:HH11	1:J:1251:LEU:HD12	1.79	0.47
1:J:2156:PHE:HA	1:J:2163:MET:HE3	1.97	0.47
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.40	0.47
1:A:2156:PHE:HA	1:A:2163:MET:HE3	1.97	0.47
1:D:298:ARG:HE	1:D:303:GLY:HA2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:717:GLY:O	1:D:735:GLY:N	2.47	0.47
1:D:1011:ARG:HA	1:D:1014:GLN:HB3	1.95	0.47
1:D:1107:ALA:HA	1:D:1113:MET:HE3	1.97	0.47
1:D:1173:MET:HB3	1:D:1192:PHE:HB2	1.96	0.47
1:D:2400:LEU:HD12	1:D:2424:LEU:HD22	1.97	0.47
1:D:3966:ILE:HD12	1:D:3966:ILE:HA	1.80	0.47
1:G:2314:VAL:HG23	1:G:2317:ASN:HB2	1.95	0.47
3:I:54:ASN:ND2	3:I:62:GLY:O	2.47	0.47
1:J:4074:ASP:O	1:J:4076:ASN:N	2.47	0.47
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.97	0.47
2:B:78:PRO:HA	2:B:81:ALA:HB3	1.96	0.47
1:D:1140:PHE:HB2	1:D:1156:TRP:HE1	1.79	0.47
1:G:302:THR:OG1	1:G:304:LYS:NZ	2.47	0.47
1:G:355:LYS:O	1:G:359:SER:OG	2.27	0.47
1:G:1089:ARG:HH22	1:G:1600:PRO:HG3	1.80	0.47
1:G:1116:GLY:HA3	1:G:1136:ALA:HA	1.96	0.47
1:G:1714:TYR:CZ	1:G:1761:MET:HB3	2.50	0.47
1:G:2143:MET:HB3	1:G:2143:MET:HE3	1.73	0.47
1:G:2156:PHE:HA	1:G:2163:MET:HE3	1.97	0.47
1:J:993:GLU:O	1:J:1051:ARG:NE	2.46	0.47
1:J:1089:ARG:HH22	1:J:1600:PRO:HG3	1.80	0.47
1:J:1104:GLU:HA	1:J:1163:GLY:HA2	1.97	0.47
1:J:1140:PHE:HB2	1:J:1156:TRP:HE1	1.79	0.47
1:J:2627:GLY:HA3	1:J:2677:LEU:HA	1.97	0.47
1:J:4797:SER:OG	1:J:4805:MET:N	2.45	0.47
1:A:1140:PHE:HB2	1:A:1156:TRP:HE1	1.79	0.47
1:A:1219:LYS:HD3	1:A:1243:THR:HG23	1.96	0.47
1:D:1086:ARG:HH11	1:D:1251:LEU:HD12	1.79	0.47
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.97	0.47
1:D:1253:LYS:HD3	1:D:1601:ASN:HD21	1.80	0.47
1:D:4046:LYS:NZ	1:D:4072:GLU:OE2	2.43	0.47
3:F:54:ASN:ND2	3:F:62:GLY:O	2.47	0.47
1:G:422:THR:HG21	1:G:459:LEU:HD11	1.96	0.47
1:G:3919:ASN:O	1:G:3922:THR:OG1	2.32	0.47
1:G:4507:ALA:O	1:G:4726:TYR:OH	2.33	0.47
1:G:4804:ASP:N	1:G:4804:ASP:OD1	2.47	0.47
2:H:29:MET:HE2	2:H:29:MET:HB3	1.81	0.47
1:J:332:ARG:NE	1:J:364:GLN:OE1	2.47	0.47
1:J:606:ARG:HH21	1:J:1632:ILE:HG23	1.78	0.47
1:J:717:GLY:O	1:J:735:GLY:N	2.47	0.47
1:J:1510:VAL:HG12	1:J:1511:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1714:TYR:CZ	1:J:1761:MET:HB3	2.50	0.47
2:K:29:MET:HE2	2:K:29:MET:HB3	1.81	0.47
1:A:55:SER:O	1:A:296:ARG:NH2	2.41	0.47
1:D:207:PHE:CE1	1:G:2326:ILE:CG2	2.97	0.47
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.97	0.47
1:D:1219:LYS:HD3	1:D:1243:THR:HG23	1.96	0.47
1:G:681:HIS:HB3	1:G:798:ILE:HA	1.97	0.47
1:G:1292:SER:O	1:G:1292:SER:OG	2.32	0.47
1:G:4627:ILE:O	1:G:4631:TRP:N	2.46	0.47
1:A:123:HIS:HD2	1:A:125:TYR:H	1.63	0.47
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.97	0.47
1:A:2627:GLY:HA3	1:A:2677:LEU:HA	1.97	0.47
1:A:4507:ALA:O	1:A:4726:TYR:OH	2.33	0.47
1:D:123:HIS:HD2	1:D:125:TYR:H	1.63	0.47
1:D:1116:GLY:HA3	1:D:1136:ALA:HA	1.96	0.47
1:D:4078:THR:OG1	1:D:4079:LEU:N	2.46	0.47
1:G:717:GLY:O	1:G:735:GLY:N	2.47	0.47
1:G:802:PHE:HB2	1:G:1617:TRP:HB2	1.97	0.47
1:G:1253:LYS:HD3	1:G:1601:ASN:HD21	1.80	0.47
1:J:370:LEU:HB2	1:J:393:MET:HB3	1.97	0.47
1:J:1131:ASP:OD1	1:J:1131:ASP:N	2.48	0.47
1:A:1253:LYS:HD3	1:A:1601:ASN:HD21	1.80	0.46
1:D:681:HIS:HB3	1:D:798:ILE:HA	1.97	0.46
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.48	0.46
1:G:299:HIS:CD2	1:G:302:THR:HG22	2.50	0.46
1:G:2627:GLY:HA3	1:G:2677:LEU:HA	1.97	0.46
1:J:1107:ALA:HA	1:J:1113:MET:HE3	1.97	0.46
1:J:4584:SER:O	1:J:4584:SER:OG	2.33	0.46
1:A:249:SER:OG	1:A:250:GLY:N	2.45	0.46
1:A:2400:LEU:HD12	1:A:2424:LEU:HD22	1.97	0.46
1:G:143:LEU:HD23	1:G:207:PHE:HE2	1.80	0.46
1:G:298:ARG:HE	1:G:303:GLY:HA2	1.80	0.46
1:G:894:VAL:O	1:G:898:ILE:N	2.47	0.46
1:J:1173:MET:HB3	1:J:1192:PHE:HB2	1.96	0.46
1:A:1556:GLU:O	1:A:1572:LYS:NZ	2.45	0.46
1:A:1714:TYR:CZ	1:A:1761:MET:HB3	2.50	0.46
1:A:4638:THR:O	1:A:4651:LYS:NZ	2.39	0.46
1:D:370:LEU:HB2	1:D:393:MET:HB3	1.97	0.46
1:D:1272:ARG:HD2	1:D:1586:LEU:HD21	1.98	0.46
1:G:1086:ARG:HH11	1:G:1251:LEU:HD12	1.79	0.46
1:G:1104:GLU:HA	1:G:1163:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1173:MET:HB3	1:G:1192:PHE:HB2	1.96	0.46
1:J:143:LEU:HD23	1:J:207:PHE:HE2	1.80	0.46
3:L:54:ASN:ND2	3:L:62:GLY:O	2.47	0.46
1:A:693:LEU:HD22	1:A:798:ILE:HG21	1.98	0.46
1:A:1272:ARG:HD2	1:A:1586:LEU:HD21	1.98	0.46
1:A:4584:SER:O	1:A:4584:SER:OG	2.33	0.46
1:D:894:VAL:O	1:D:898:ILE:N	2.47	0.46
1:D:3919:ASN:O	1:D:3922:THR:OG1	2.32	0.46
1:G:1107:ALA:HA	1:G:1113:MET:HE3	1.97	0.46
1:G:1140:PHE:HB2	1:G:1156:TRP:HE1	1.79	0.46
1:G:1219:LYS:HD3	1:G:1243:THR:HG23	1.96	0.46
1:J:298:ARG:HE	1:J:303:GLY:HA2	1.80	0.46
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.97	0.46
1:D:1714:TYR:CZ	1:D:1761:MET:HB3	2.50	0.46
1:G:123:HIS:HD2	1:G:125:TYR:H	1.63	0.46
1:G:1510:VAL:HG12	1:G:1511:VAL:HG23	1.97	0.46
1:A:2832:VAL:O	1:A:2895:LYS:NZ	2.38	0.46
1:A:4861:ALA:HB2	1:D:4864:GLN:HE21	1.80	0.46
2:B:38:SER:O	2:B:42:ARG:NH1	2.49	0.46
3:C:54:ASN:ND2	3:C:62:GLY:O	2.47	0.46
1:D:302:THR:OG1	1:D:304:LYS:NZ	2.47	0.46
1:D:1089:ARG:HH22	1:D:1600:PRO:HG3	1.80	0.46
1:D:2427:LEU:HD12	1:D:2428:ILE:CG2	2.35	0.46
1:D:2627:GLY:HA3	1:D:2677:LEU:HA	1.97	0.46
1:D:3072:THR:O	1:D:3076:LEU:N	2.49	0.46
1:D:4515:ASN:ND2	1:D:4740:PHE:O	2.33	0.46
1:G:4861:ALA:HB2	1:J:4864:GLN:HE21	1.81	0.46
1:J:693:LEU:HD22	1:J:798:ILE:HG21	1.98	0.46
1:J:1272:ARG:HD2	1:J:1586:LEU:HD21	1.98	0.46
1:A:298:ARG:HE	1:A:303:GLY:HA2	1.80	0.46
1:G:1272:ARG:HD2	1:G:1586:LEU:HD21	1.98	0.46
1:G:4110:MET:HE2	1:G:4110:MET:HB2	1.78	0.46
1:J:190:ARG:CZ	1:J:207:PHE:CZ	2.99	0.46
1:J:2400:LEU:HD12	1:J:2424:LEU:HD22	1.97	0.46
1:J:3072:THR:O	1:J:3076:LEU:N	2.49	0.46
1:A:190:ARG:CZ	1:A:207:PHE:CZ	2.99	0.46
1:A:2777:LYS:NZ	1:A:2778:GLU:OE2	2.49	0.46
2:B:78:PRO:HD3	2:B:96:THR:HG22	1.98	0.46
1:G:2400:LEU:HD12	1:G:2424:LEU:HD22	1.97	0.46
1:G:2777:LYS:NZ	1:G:2778:GLU:OE2	2.49	0.46
1:J:66:THR:OG1	1:J:124:SER:OG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:HIS:HD2	1:J:125:TYR:H	1.63	0.46
1:J:2777:LYS:NZ	1:J:2778:GLU:OE2	2.49	0.46
1:J:4507:ALA:O	1:J:4726:TYR:OH	2.33	0.46
1:A:299:HIS:CD2	1:A:302:THR:HG22	2.50	0.46
1:A:1907:MET:HE3	1:A:1907:MET:HB2	1.89	0.46
1:A:3072:THR:O	1:A:3076:LEU:N	2.49	0.46
1:D:992:GLN:HB2	1:D:1054:VAL:HG11	1.98	0.46
1:D:1299:ILE:HG13	1:D:1455:THR:HG23	1.98	0.46
2:E:78:PRO:HD3	2:E:96:THR:HG22	1.98	0.46
1:G:993:GLU:O	1:G:1051:ARG:NE	2.46	0.46
1:J:802:PHE:HB2	1:J:1617:TRP:HB2	1.97	0.46
1:J:4050:HIS:ND1	1:J:4054:GLU:OE2	2.48	0.46
1:A:370:LEU:HB2	1:A:393:MET:HB3	1.97	0.46
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.32	0.46
1:A:4862:ILE:HD11	1:D:4757:ILE:HD13	1.96	0.46
1:D:1310:CYS:HB2	1:D:1536:SER:HA	1.98	0.46
1:D:4808:ASP:HB2	1:G:4523:VAL:HG12	1.97	0.46
2:E:38:SER:O	2:E:42:ARG:NH1	2.49	0.46
1:G:1670:HIS:ND1	1:G:1778:TYR:O	2.49	0.46
1:G:2313:SER:OG	1:G:2402:ARG:O	2.31	0.46
1:A:394:HIS:HD2	1:A:397:GLY:H	1.62	0.45
1:A:681:HIS:HB3	1:A:798:ILE:HA	1.97	0.45
1:D:4507:ALA:O	1:D:4726:TYR:OH	2.33	0.45
1:D:4725:TRP:HA	1:D:4728:THR:HG22	1.98	0.45
1:G:4589:ILE:HD13	1:G:4589:ILE:HA	1.83	0.45
1:J:1310:CYS:HB2	1:J:1536:SER:HA	1.98	0.45
1:J:3724:LYS:HB3	1:J:3724:LYS:HE2	1.69	0.45
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.97	0.45
1:A:878:LEU:HA	1:A:881:ILE:HB	1.98	0.45
1:A:1299:ILE:HG13	1:A:1455:THR:HG23	1.98	0.45
1:D:236:LEU:HD22	1:D:245:LEU:HD13	1.98	0.45
1:D:2777:LYS:NZ	1:D:2778:GLU:OE2	2.49	0.45
1:D:3911:ILE:HG23	1:D:3975:LEU:HD22	1.98	0.45
1:G:370:LEU:HB2	1:G:393:MET:HB3	1.97	0.45
1:G:878:LEU:HA	1:G:881:ILE:HB	1.98	0.45
1:G:4725:TRP:HA	1:G:4728:THR:HG22	1.99	0.45
1:J:681:HIS:HB3	1:J:798:ILE:HA	1.97	0.45
1:J:1253:LYS:HD3	1:J:1601:ASN:HD21	1.80	0.45
2:K:38:SER:O	2:K:42:ARG:NH1	2.49	0.45
1:A:27:THR:OG1	1:A:32:GLN:OE1	2.26	0.45
1:A:259:THR:HG1	1:A:261:HIS:CE1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:HIS:HD2	1:D:397:GLY:H	1.62	0.45
1:D:993:GLU:O	1:D:1051:ARG:NE	2.46	0.45
1:D:2106:THR:OG1	1:D:2107:TYR:N	2.50	0.45
1:D:2852:ILE:O	1:D:2856:LYS:N	2.44	0.45
1:D:3666:HIS:HD2	1:D:3735:ARG:HG3	1.82	0.45
1:D:4775:LEU:HD12	1:D:4775:LEU:HA	1.82	0.45
1:G:236:LEU:HD22	1:G:245:LEU:HD13	1.98	0.45
1:G:630:HIS:CE1	1:G:1671:ARG:HD3	2.52	0.45
1:J:236:LEU:HD22	1:J:245:LEU:HD13	1.98	0.45
1:J:1299:ILE:HG13	1:J:1455:THR:HG23	1.98	0.45
2:K:78:PRO:HD3	2:K:96:THR:HG22	1.98	0.45
1:A:993:GLU:O	1:A:1051:ARG:NE	2.46	0.45
1:A:4788:ASN:CG	1:D:4738:PHE:CD2	2.94	0.45
1:D:630:HIS:CE1	1:D:1671:ARG:HD3	2.52	0.45
1:D:878:LEU:HA	1:D:881:ILE:HB	1.98	0.45
1:G:3072:THR:O	1:G:3076:LEU:N	2.49	0.45
1:J:2110:ASN:HB3	1:J:3615:HIS:CE1	2.52	0.45
1:A:2106:THR:OG1	1:A:2107:TYR:N	2.50	0.45
1:A:2852:ILE:O	1:A:2856:LYS:N	2.44	0.45
1:A:3911:ILE:HG23	1:A:3975:LEU:HD22	1.98	0.45
1:A:4725:TRP:HA	1:A:4728:THR:HG22	1.99	0.45
1:D:27:THR:OG1	1:D:32:GLN:OE1	2.26	0.45
1:D:271:ALA:O	1:D:301:THR:OG1	2.25	0.45
1:D:374:TYR:HA	1:D:391:ALA:HA	1.99	0.45
1:G:1299:ILE:HG13	1:G:1455:THR:HG23	1.98	0.45
1:G:4050:HIS:ND1	1:G:4054:GLU:OE2	2.48	0.45
1:J:374:TYR:HA	1:J:391:ALA:HA	1.99	0.45
1:J:2106:THR:OG1	1:J:2107:TYR:N	2.50	0.45
1:J:2846:ALA:O	1:J:2850:HIS:N	2.50	0.45
1:A:1310:CYS:HB2	1:A:1536:SER:HA	1.98	0.45
1:A:1670:HIS:ND1	1:A:1778:TYR:O	2.49	0.45
1:A:2110:ASN:HB3	1:A:3615:HIS:CE1	2.52	0.45
1:A:3631:GLU:OE1	1:A:3631:GLU:N	2.48	0.45
1:A:4753:THR:O	1:A:4753:THR:OG1	2.34	0.45
1:D:55:SER:O	1:D:296:ARG:NH2	2.41	0.45
1:D:299:HIS:CD2	1:D:302:THR:HG22	2.50	0.45
1:D:1670:HIS:ND1	1:D:1778:TYR:O	2.49	0.45
1:D:4818:MET:HE3	1:D:4818:MET:HB2	1.72	0.45
1:D:4880:GLN:OE1	1:D:4880:GLN:HA	2.17	0.45
1:G:1131:ASP:OD1	1:G:1131:ASP:N	2.48	0.45
2:H:38:SER:O	2:H:42:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3986:MET:HE3	1:J:3986:MET:HB3	1.79	0.45
1:A:2793:THR:OG1	1:A:2901:GLY:O	2.29	0.45
1:A:3666:HIS:HD2	1:A:3735:ARG:HG3	1.82	0.45
1:A:4627:ILE:O	1:A:4631:TRP:N	2.46	0.45
1:A:4880:GLN:OE1	1:A:4880:GLN:HA	2.17	0.45
1:D:190:ARG:CZ	1:D:207:PHE:CZ	2.99	0.45
1:D:3631:GLU:OE1	1:D:3631:GLU:N	2.48	0.45
1:G:1310:CYS:HB2	1:G:1536:SER:HA	1.98	0.45
1:G:2767:LYS:HD2	1:G:2767:LYS:HA	1.73	0.45
1:G:3911:ILE:HG23	1:G:3975:LEU:HD22	1.98	0.45
1:G:4880:GLN:OE1	1:G:4880:GLN:HA	2.17	0.45
1:A:143:LEU:HD23	1:A:207:PHE:HE2	1.80	0.45
1:D:874:LEU:HD21	1:D:941:LYS:HA	1.99	0.45
1:D:1057:LEU:O	1:D:1061:GLY:N	2.50	0.45
1:D:1907:MET:HE3	1:D:1907:MET:HB2	1.89	0.45
1:D:4627:ILE:O	1:D:4631:TRP:N	2.46	0.45
1:G:271:ALA:O	1:G:301:THR:OG1	2.25	0.45
1:G:1057:LEU:O	1:G:1061:GLY:N	2.50	0.45
1:J:4725:TRP:HA	1:J:4728:THR:HG22	1.99	0.45
1:J:4880:GLN:OE1	1:J:4880:GLN:HA	2.17	0.45
1:A:236:LEU:HD22	1:A:245:LEU:HD13	1.98	0.45
1:A:374:TYR:HA	1:A:391:ALA:HA	1.99	0.45
1:A:992:GLN:HB2	1:A:1054:VAL:HG21	1.98	0.45
1:A:2270:LEU:HD23	1:A:2270:LEU:HA	1.84	0.45
1:D:3724:LYS:HB3	1:D:3724:LYS:HE2	1.69	0.45
1:G:992:GLN:HB2	1:G:1054:VAL:HG21	1.98	0.45
1:G:3666:HIS:HD2	1:G:3735:ARG:HG3	1.82	0.45
1:G:4775:LEU:HD12	1:G:4775:LEU:HA	1.82	0.45
1:J:299:HIS:CD2	1:J:302:THR:HG22	2.50	0.45
1:J:1111:GLY:HA3	1:J:1211:GLN:HE21	1.82	0.45
1:J:1670:HIS:ND1	1:J:1778:TYR:O	2.49	0.45
1:A:1111:GLY:HA3	1:A:1211:GLN:HE21	1.82	0.45
1:A:1131:ASP:N	1:A:1131:ASP:OD1	2.48	0.45
1:A:4804:ASP:OD1	1:A:4804:ASP:N	2.47	0.45
1:D:365:HIS:HD2	1:D:368:THR:HG23	1.82	0.45
1:D:1177:LEU:N	1:D:1180:GLU:O	2.44	0.45
1:D:2110:ASN:HB3	1:D:3615:HIS:CE1	2.52	0.45
1:D:2857:LYS:HE3	1:D:2858:LYS:HD2	1.99	0.45
1:G:190:ARG:CZ	1:G:207:PHE:CZ	2.99	0.45
1:G:2853:TRP:HA	1:G:2856:LYS:HB2	1.99	0.45
1:G:3986:MET:HE3	1:G:3986:MET:HB3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4808:ASP:HB2	1:J:4523:VAL:HG12	1.99	0.45
1:J:992:GLN:HB2	1:J:1054:VAL:HG11	1.98	0.45
1:J:2853:TRP:HA	1:J:2856:LYS:HB2	1.99	0.45
1:A:270:HIS:ND1	1:A:491:GLU:OE1	2.51	0.44
1:A:594:ILE:HD12	1:A:631:LEU:HD23	2.00	0.44
1:A:2846:ALA:O	1:A:2850:HIS:N	2.50	0.44
1:D:270:HIS:ND1	1:D:491:GLU:OE1	2.51	0.44
1:D:1756:SER:OG	1:D:1757:LEU:N	2.40	0.44
1:D:4810:MET:HB3	1:G:4519:LEU:O	2.16	0.44
1:G:374:TYR:HA	1:G:391:ALA:HA	1.99	0.44
1:J:618:CYS:O	1:J:629:GLN:NE2	2.38	0.44
1:J:1177:LEU:N	1:J:1180:GLU:O	2.44	0.44
1:J:4945:TYR:OH	7:J:6003:CFF:H81	2.17	0.44
1:A:630:HIS:CE1	1:A:1671:ARG:HD3	2.52	0.44
1:A:874:LEU:HD21	1:A:941:LYS:HA	1.99	0.44
1:A:1614:ARG:HA	1:A:1614:ARG:HD3	1.83	0.44
1:A:2853:TRP:HA	1:A:2856:LYS:HB2	1.99	0.44
1:A:4078:THR:OG1	1:A:4079:LEU:N	2.46	0.44
1:A:4110:MET:HE2	1:A:4110:MET:HB2	1.78	0.44
1:A:4864:GLN:HE21	1:J:4861:ALA:HB2	1.82	0.44
1:A:4943:LYS:HB3	1:A:4943:LYS:HE2	1.81	0.44
1:D:693:LEU:HD22	1:D:798:ILE:HG21	1.98	0.44
1:D:4050:HIS:ND1	1:D:4054:GLU:OE2	2.48	0.44
1:G:693:LEU:HD22	1:G:798:ILE:HG21	1.98	0.44
1:G:2110:ASN:HB3	1:G:3615:HIS:CE1	2.52	0.44
1:G:2857:LYS:HE3	1:G:2858:LYS:HD2	2.00	0.44
1:G:3724:LYS:HB3	1:G:3724:LYS:HE2	1.69	0.44
1:G:4515:ASN:ND2	1:G:4740:PHE:O	2.33	0.44
1:G:4638:THR:O	1:G:4651:LYS:NZ	2.39	0.44
2:H:78:PRO:HD3	2:H:96:THR:HG22	1.98	0.44
1:J:594:ILE:HD12	1:J:631:LEU:HD23	2.00	0.44
1:J:2143:MET:HE3	1:J:2143:MET:HB3	1.73	0.44
1:J:2156:PHE:HD1	1:J:2163:MET:HG2	1.82	0.44
1:J:2871:LEU:HG	1:J:2878:LEU:HD21	2.00	0.44
1:J:2891:GLN:O	1:J:2895:LYS:N	2.48	0.44
1:A:616:SER:O	1:A:616:SER:OG	2.35	0.44
1:A:2714:ILE:HD13	1:A:2780:LEU:HD11	2.00	0.44
1:A:2767:LYS:HD2	1:A:2767:LYS:HA	1.73	0.44
1:A:3762:LEU:HD12	1:A:3762:LEU:HA	1.83	0.44
1:A:4945:TYR:OH	7:A:6003:CFF:H81	2.17	0.44
1:D:143:LEU:HD23	1:D:207:PHE:HE2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1169:THR:OG1	1:D:1170:GLU:N	2.51	0.44
1:D:2391:THR:HA	1:D:2394:ALA:HB3	1.99	0.44
1:D:2714:ILE:HD13	1:D:2780:LEU:HD11	2.00	0.44
1:G:470:LEU:HD12	1:G:470:LEU:HA	1.87	0.44
1:G:2024:LEU:HB3	1:G:2025:THR:H	1.47	0.44
1:G:4945:TYR:OH	7:G:6003:CFF:H81	2.17	0.44
1:J:270:HIS:ND1	1:J:491:GLU:OE1	2.51	0.44
1:J:878:LEU:HA	1:J:881:ILE:HB	1.98	0.44
1:J:3666:HIS:HD2	1:J:3735:ARG:HG3	1.82	0.44
1:J:3911:ILE:HG23	1:J:3975:LEU:HD22	1.98	0.44
1:J:4627:ILE:O	1:J:4631:TRP:N	2.46	0.44
1:J:4897:ASP:N	1:J:4897:ASP:OD1	2.43	0.44
1:A:4934:HIS:HB3	1:A:4939:SER:HB2	2.00	0.44
1:D:757:CYS:SG	1:D:758:CYS:N	2.90	0.44
1:D:1111:GLY:HA3	1:D:1211:GLN:HE21	1.82	0.44
1:D:2767:LYS:HA	1:D:2767:LYS:HD2	1.73	0.44
1:D:2846:ALA:O	1:D:2850:HIS:N	2.50	0.44
1:D:2853:TRP:HA	1:D:2856:LYS:HB2	1.99	0.44
1:D:4589:ILE:HD13	1:D:4589:ILE:HA	1.83	0.44
1:G:188:SER:O	1:G:190:ARG:NH2	2.51	0.44
1:G:2846:ALA:O	1:G:2850:HIS:N	2.50	0.44
1:G:3966:ILE:HD12	1:G:3966:ILE:HA	1.80	0.44
1:J:365:HIS:HD2	1:J:368:THR:HG23	1.82	0.44
1:J:630:HIS:CE1	1:J:1671:ARG:HD3	2.52	0.44
1:J:1169:THR:OG1	1:J:1170:GLU:N	2.51	0.44
1:A:2173:MET:HE1	1:A:2215:MET:HE1	1.99	0.44
1:A:2857:LYS:HE3	1:A:2858:LYS:HD2	2.00	0.44
1:D:842:GLN:H	1:D:848:ARG:HD3	1.83	0.44
1:J:2270:LEU:HD23	1:J:2270:LEU:HA	1.84	0.44
1:J:4638:THR:O	1:J:4651:LYS:NZ	2.39	0.44
1:A:900:LEU:HB3	1:A:902:TRP:CD1	2.53	0.44
1:D:2227:SER:OG	1:D:2228:VAL:N	2.51	0.44
1:G:270:HIS:ND1	1:G:491:GLU:OE1	2.51	0.44
1:G:1111:GLY:HA3	1:G:1211:GLN:HE21	1.82	0.44
1:G:2156:PHE:HD1	1:G:2163:MET:HG2	1.82	0.44
1:J:762:SER:O	1:J:762:SER:OG	2.33	0.44
1:D:2156:PHE:HD1	1:D:2163:MET:HG2	1.82	0.44
1:G:4958:CYS:SG	1:G:4959:PHE:N	2.84	0.44
1:J:27:THR:OG1	1:J:32:GLN:OE1	2.26	0.44
1:J:3640:LYS:HA	1:J:3640:LYS:HD2	1.81	0.44
1:A:66:THR:OG1	1:A:124:SER:OG	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:LEU:O	1:A:1061:GLY:N	2.50	0.44
1:A:4519:LEU:O	1:J:4810:MET:HB3	2.18	0.44
1:A:4523:VAL:HG12	1:J:4808:ASP:HB2	1.98	0.44
1:G:624:ALA:HB2	1:G:1667:LEU:HD12	2.00	0.44
1:J:900:LEU:HB3	1:J:902:TRP:CD1	2.53	0.44
1:J:1057:LEU:O	1:J:1061:GLY:N	2.50	0.44
1:J:2714:ILE:HD13	1:J:2780:LEU:HD11	2.00	0.44
1:J:2857:LYS:HE3	1:J:2858:LYS:HD2	1.99	0.44
1:J:4934:HIS:HB3	1:J:4939:SER:HB2	2.00	0.44
1:A:1169:THR:OG1	1:A:1170:GLU:N	2.51	0.44
1:A:1757:LEU:HD12	1:A:1757:LEU:HA	1.88	0.44
1:A:2227:SER:OG	1:A:2228:VAL:N	2.51	0.44
1:A:4775:LEU:HD12	1:A:4775:LEU:HA	1.82	0.44
1:A:4897:ASP:OD1	1:A:4897:ASP:N	2.43	0.44
1:D:734:SER:OG	1:D:734:SER:O	2.36	0.44
1:G:594:ILE:HD12	1:G:631:LEU:HD23	2.00	0.44
1:G:757:CYS:SG	1:G:758:CYS:N	2.90	0.44
1:G:831:LYS:HE3	1:G:831:LYS:HB2	1.80	0.44
1:G:2173:MET:HE1	1:G:2215:MET:HE1	1.99	0.44
1:G:2714:ILE:HD13	1:G:2780:LEU:HD11	2.00	0.44
1:J:558:LEU:HD23	1:J:558:LEU:HA	1.88	0.44
1:J:1224:LEU:HD23	1:J:1224:LEU:HA	1.85	0.44
1:J:4752:LYS:HD2	1:J:4752:LYS:HA	1.75	0.44
1:A:365:HIS:HD2	1:A:368:THR:HG23	1.82	0.43
1:A:757:CYS:SG	1:A:758:CYS:N	2.90	0.43
1:A:1610:ARG:HE	1:A:1610:ARG:HB3	1.64	0.43
1:A:3786:LYS:HE2	1:A:3786:LYS:HB3	1.79	0.43
2:B:17:LYS:N	2:B:20:GLN:OE1	2.50	0.43
1:D:169:ARG:HH21	1:D:176:ARG:HH11	1.66	0.43
1:D:2173:MET:HE1	1:D:2215:MET:HE1	1.99	0.43
1:D:4792:LYS:H	1:D:4792:LYS:HG2	1.57	0.43
1:G:1169:THR:OG1	1:G:1170:GLU:N	2.51	0.43
1:G:4046:LYS:HB2	1:G:4046:LYS:HE3	1.81	0.43
1:J:757:CYS:SG	1:J:758:CYS:N	2.90	0.43
1:A:2871:LEU:HG	1:A:2878:LEU:HD21	2.00	0.43
1:A:4613:PHE:HE2	1:A:4948:ARG:HD2	1.83	0.43
1:D:900:LEU:HB3	1:D:902:TRP:CD1	2.53	0.43
1:D:3665:LEU:HD11	1:D:3696:MET:HE2	2.00	0.43
1:D:4584:SER:O	1:D:4584:SER:OG	2.33	0.43
1:D:4934:HIS:HB3	1:D:4939:SER:HB2	2.00	0.43
1:G:3762:LEU:HD12	1:G:3762:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4613:PHE:HE2	1:G:4948:ARG:HD2	1.83	0.43
1:J:188:SER:O	1:J:190:ARG:NH2	2.51	0.43
1:A:188:SER:O	1:A:190:ARG:NH2	2.51	0.43
1:A:938:GLU:HA	1:A:941:LYS:HG3	2.00	0.43
1:A:1224:LEU:HD23	1:A:1224:LEU:HA	1.85	0.43
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	2.00	0.43
1:A:3920:THR:O	1:A:3920:THR:OG1	2.32	0.43
1:D:594:ILE:HD12	1:D:631:LEU:HD23	2.00	0.43
1:J:3631:GLU:OE1	1:J:3631:GLU:N	2.48	0.43
1:A:677:LEU:HD23	1:A:677:LEU:HA	1.87	0.43
1:A:1764:SER:OG	1:A:1779:SER:O	2.36	0.43
1:D:4801:ASP:OD1	1:D:4801:ASP:N	2.51	0.43
1:G:335:LYS:HZ3	1:G:401:ASP:HB2	1.83	0.43
1:G:365:HIS:HD2	1:G:368:THR:HG23	1.82	0.43
1:G:874:LEU:HD21	1:G:941:LYS:HA	1.99	0.43
1:G:2871:LEU:HG	1:G:2878:LEU:HD21	2.00	0.43
1:J:616:SER:O	1:J:616:SER:OG	2.35	0.43
1:J:1764:SER:OG	1:J:1779:SER:O	2.36	0.43
1:J:2173:MET:HE1	1:J:2215:MET:HE1	1.99	0.43
1:A:836:HIS:HB2	1:A:839:GLU:CD	2.44	0.43
1:A:2103:LEU:HA	1:A:2106:THR:HG22	2.00	0.43
1:A:2156:PHE:HD1	1:A:2163:MET:HG2	1.82	0.43
1:A:2391:THR:HA	1:A:2394:ALA:HB3	1.99	0.43
1:D:3760:LEU:HD23	1:D:3760:LEU:HA	1.78	0.43
1:G:123:HIS:CD2	1:G:125:TYR:H	2.37	0.43
1:G:2227:SER:OG	1:G:2228:VAL:N	2.51	0.43
1:G:2308:PHE:HE1	1:G:2475:ARG:HH22	1.67	0.43
1:G:4943:LYS:HB3	1:G:4943:LYS:HE2	1.81	0.43
1:J:734:SER:OG	1:J:734:SER:O	2.36	0.43
1:J:874:LEU:HD21	1:J:941:LYS:HA	1.99	0.43
1:J:2391:THR:HA	1:J:2394:ALA:HB3	1.99	0.43
1:J:2427:LEU:HD12	1:J:2428:ILE:CG2	2.35	0.43
1:J:3804:LEU:HD13	1:J:3910:ALA:HB2	2.00	0.43
1:J:4613:PHE:HE2	1:J:4948:ARG:HD2	1.83	0.43
1:A:2308:PHE:HE1	1:A:2475:ARG:HH22	1.67	0.43
1:A:3665:LEU:HD11	1:A:3696:MET:HE2	2.00	0.43
1:A:4845:ILE:CD1	1:D:4819:TYR:CD1	3.02	0.43
1:D:188:SER:O	1:D:190:ARG:NH2	2.51	0.43
1:D:4835:PRO:HG3	1:D:4844:ARG:HG2	2.01	0.43
1:D:4845:ILE:CD1	1:G:4819:TYR:CD1	3.01	0.43
1:D:4945:TYR:OH	7:D:6003:CFF:H81	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2391:THR:HA	1:G:2394:ALA:HB3	1.99	0.43
1:G:3804:LEU:HD13	1:G:3910:ALA:HB2	2.00	0.43
1:G:3890:TYR:O	1:G:3894:SER:N	2.52	0.43
1:J:169:ARG:HH21	1:J:176:ARG:HH11	1.66	0.43
1:J:2173:MET:HE2	1:J:2173:MET:HB2	1.83	0.43
1:J:2227:SER:OG	1:J:2228:VAL:N	2.51	0.43
1:J:4801:ASP:OD1	1:J:4801:ASP:N	2.51	0.43
3:L:45:THR:HG23	3:L:48:GLU:H	1.84	0.43
1:A:25:THR:HG22	1:A:34:LYS:HA	2.01	0.43
1:A:4894:ILE:HD13	1:A:4894:ILE:HA	1.89	0.43
1:D:679:VAL:HA	1:D:800:VAL:HG23	2.01	0.43
1:D:836:HIS:HB2	1:D:839:GLU:CD	2.44	0.43
1:G:1690:GLU:HG2	1:G:1790:LYS:HE3	2.01	0.43
1:J:1842:ILE:HD12	1:J:1845:LEU:HD23	2.01	0.43
1:J:2103:LEU:HA	1:J:2106:THR:HG22	2.00	0.43
1:J:4504:ARG:NH1	1:J:4746:ASP:OD1	2.52	0.43
1:J:4775:LEU:HD12	1:J:4775:LEU:HA	1.82	0.43
1:A:123:HIS:CD2	1:A:125:TYR:H	2.37	0.43
1:A:207:PHE:HB3	1:D:2326:ILE:CD1	2.49	0.43
1:A:1112:ASP:H	1:A:1211:GLN:NE2	2.17	0.43
1:A:4801:ASP:OD1	1:A:4801:ASP:N	2.51	0.43
3:C:45:THR:HG23	3:C:48:GLU:H	1.84	0.43
1:D:4504:ARG:NH1	1:D:4746:ASP:OD1	2.52	0.43
1:D:4791:ARG:HH22	1:G:4523:VAL:HG21	1.83	0.43
1:D:4861:ALA:HB2	1:G:4864:GLN:HE21	1.84	0.43
1:G:842:GLN:H	1:G:848:ARG:HD3	1.83	0.43
1:G:1764:SER:OG	1:G:1779:SER:O	2.36	0.43
1:G:4835:PRO:HG3	1:G:4844:ARG:HG2	2.01	0.43
1:J:799:LYS:HB2	1:J:1618:LEU:HD11	2.00	0.43
1:A:842:GLN:H	1:A:848:ARG:HD3	1.83	0.43
1:A:1177:LEU:N	1:A:1180:GLU:O	2.44	0.43
1:A:1690:GLU:HG2	1:A:1790:LYS:HE3	2.01	0.43
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	2.00	0.43
1:D:4613:PHE:HE2	1:D:4948:ARG:HD2	1.83	0.43
1:G:679:VAL:HA	1:G:800:VAL:HG23	2.01	0.43
1:G:900:LEU:HB3	1:G:902:TRP:CD1	2.53	0.43
1:G:938:GLU:HA	1:G:941:LYS:HG3	2.00	0.43
1:G:1255:LEU:HD22	1:G:1451:HIS:HB2	2.01	0.43
1:J:679:VAL:HA	1:J:800:VAL:HG23	2.01	0.43
1:J:706:TYR:HA	1:J:707:PRO:HD3	1.85	0.43
1:J:2770:GLU:HA	1:J:2773:ARG:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2988:SER:O	1:J:2992:CYS:N	2.52	0.43
1:J:4835:PRO:HG3	1:J:4844:ARG:HG2	2.01	0.43
1:A:1255:LEU:HD22	1:A:1451:HIS:HB2	2.01	0.43
1:A:2427:LEU:HD12	1:A:2427:LEU:C	2.44	0.43
1:A:2718:LEU:HA	1:A:2721:PHE:HB3	2.01	0.43
1:A:3760:LEU:HD23	1:A:3760:LEU:HA	1.78	0.43
1:A:4835:PRO:HG3	1:A:4844:ARG:HG2	2.01	0.43
1:G:1040:ASP:HA	1:G:1043:LYS:HB2	2.01	0.43
1:G:1097:LYS:HA	1:G:1168:MET:HE2	2.01	0.43
1:G:4934:HIS:HB3	1:G:4939:SER:HB2	2.00	0.43
1:J:25:THR:HG22	1:J:34:LYS:HA	2.01	0.43
1:J:135:THR:OG1	1:J:146:ASP:OD2	2.36	0.43
1:J:842:GLN:H	1:J:848:ARG:HD3	1.83	0.43
1:J:1107:ALA:HB3	1:J:1160:ASP:HB2	2.01	0.43
1:J:1255:LEU:HD22	1:J:1451:HIS:HB2	2.01	0.43
1:J:1614:ARG:HA	1:J:1614:ARG:HD3	1.83	0.43
1:J:2718:LEU:HA	1:J:2721:PHE:HB3	2.01	0.43
1:A:135:THR:OG1	1:A:146:ASP:OD2	2.36	0.42
1:A:760:ASP:HB3	1:A:763:ALA:HB3	2.01	0.42
1:A:1842:ILE:HD12	1:A:1845:LEU:HD23	2.01	0.42
1:A:2777:LYS:HE2	1:A:2781:LYS:HE3	2.01	0.42
1:A:3617:ALA:O	1:A:3621:PHE:N	2.51	0.42
1:D:1097:LYS:HA	1:D:1168:MET:HE2	2.01	0.42
1:D:1255:LEU:HD22	1:D:1451:HIS:HB2	2.01	0.42
1:D:2718:LEU:HA	1:D:2721:PHE:HB3	2.01	0.42
1:D:2770:GLU:HA	1:D:2773:ARG:HB3	2.01	0.42
1:D:3592:LEU:HD23	1:D:3592:LEU:HA	1.91	0.42
1:D:4610:LYS:HD3	1:D:4616:LEU:HD22	2.01	0.42
1:G:498:VAL:HG23	1:G:533:LEU:HD22	2.01	0.42
1:G:2106:THR:OG1	1:G:2107:TYR:N	2.50	0.42
1:G:4885:MET:O	6:G:6002:ATP:H1'	2.18	0.42
1:J:836:HIS:HB2	1:J:839:GLU:CD	2.44	0.42
1:J:938:GLU:HA	1:J:941:LYS:HG3	2.00	0.42
1:J:2308:PHE:HE1	1:J:2475:ARG:HH22	1.67	0.42
1:J:2427:LEU:HD12	1:J:2427:LEU:C	2.44	0.42
1:A:1086:ARG:NH1	1:A:1252:SER:O	2.53	0.42
1:A:2326:ILE:CD1	1:J:207:PHE:HB3	2.50	0.42
1:A:2770:GLU:HA	1:A:2773:ARG:HB3	2.01	0.42
1:A:4000:MET:HE3	1:A:4000:MET:HB2	1.95	0.42
1:A:4020:MET:HE1	1:A:4063:GLU:HG2	2.01	0.42
1:A:4610:LYS:HD3	1:A:4616:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:THR:HG22	1:D:34:LYS:HA	2.01	0.42
1:D:555:LEU:HD23	1:D:555:LEU:HA	1.87	0.42
1:D:799:LYS:HB2	1:D:1618:LEU:HD11	2.00	0.42
1:D:915:HIS:CE1	1:D:917:CYS:HB2	2.54	0.42
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	2.00	0.42
1:G:915:HIS:CE1	1:G:917:CYS:HB2	2.54	0.42
1:G:2718:LEU:HA	1:G:2721:PHE:HB3	2.01	0.42
1:G:2770:GLU:HA	1:G:2773:ARG:HB3	2.01	0.42
1:G:4584:SER:O	1:G:4584:SER:OG	2.33	0.42
1:G:4723:LEU:HD13	1:G:4723:LEU:HA	1.88	0.42
1:G:4810:MET:HB3	1:J:4519:LEU:O	2.19	0.42
1:J:1040:ASP:HA	1:J:1043:LYS:HB2	2.01	0.42
1:J:1112:ASP:H	1:J:1211:GLN:NE2	2.17	0.42
1:J:1685:LEU:HD23	1:J:1685:LEU:HA	1.88	0.42
1:J:2317:ASN:HA	1:J:2317:ASN:HD22	1.66	0.42
1:J:3759:THR:O	1:J:3759:THR:OG1	2.28	0.42
1:J:4045:SER:C	1:J:4078:THR:HA	2.45	0.42
1:A:915:HIS:CE1	1:A:917:CYS:HB2	2.54	0.42
1:A:1605:LYS:HA	1:A:1605:LYS:HD3	1.83	0.42
1:A:4504:ARG:NH1	1:A:4746:ASP:OD1	2.52	0.42
1:A:4589:ILE:HD13	1:A:4589:ILE:HA	1.83	0.42
1:A:4836:ALA:HB1	1:D:4805:MET:HE1	2.01	0.42
1:D:1730:THR:O	1:D:1733:THR:OG1	2.35	0.42
1:D:1764:SER:OG	1:D:1779:SER:O	2.36	0.42
1:D:2169:HIS:HB3	1:D:2204:PHE:CE2	2.55	0.42
1:D:2871:LEU:HG	1:D:2878:LEU:HD21	1.99	0.42
3:F:45:THR:HG23	3:F:48:GLU:H	1.84	0.42
1:G:4610:LYS:HD3	1:G:4616:LEU:HD22	2.01	0.42
1:G:4753:THR:O	1:G:4753:THR:OG1	2.34	0.42
1:J:306:LEU:O	1:J:327:THR:OG1	2.32	0.42
1:J:624:ALA:HB2	1:J:1667:LEU:HD12	2.00	0.42
1:J:1097:LYS:HA	1:J:1168:MET:HE2	2.01	0.42
1:J:1709:ILE:HD13	1:J:1709:ILE:HA	1.92	0.42
1:J:4610:LYS:HD3	1:J:4616:LEU:HD22	2.01	0.42
1:A:309:MET:O	1:A:313:SER:N	2.53	0.42
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	2.00	0.42
1:A:4050:HIS:ND1	1:A:4054:GLU:OE2	2.48	0.42
1:D:1112:ASP:H	1:D:1211:GLN:NE2	2.17	0.42
1:D:1732:GLU:O	1:D:1735:SER:OG	2.31	0.42
1:D:2397:ILE:HD13	1:D:2397:ILE:HA	1.88	0.42
1:D:2788:TRP:NE1	1:D:2906:ARG:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4770:LEU:HD13	1:G:4751:PHE:CD1	2.55	0.42
1:G:169:ARG:HH21	1:G:176:ARG:HH11	1.66	0.42
1:G:675:TYR:HB2	1:G:804:LEU:HD21	2.01	0.42
1:G:836:HIS:HB2	1:G:839:GLU:CD	2.44	0.42
1:G:2169:HIS:HB3	1:G:2204:PHE:CE2	2.55	0.42
1:G:2427:LEU:HD12	1:G:2427:LEU:C	2.44	0.42
1:G:4020:MET:HE1	1:G:4063:GLU:HG2	2.01	0.42
1:G:4160:GLN:HE22	1:G:4205:ALA:HA	1.85	0.42
1:G:4504:ARG:NH1	1:G:4746:ASP:OD1	2.52	0.42
1:G:4651:LYS:HG2	1:G:4671:LEU:HD23	2.01	0.42
2:H:17:LYS:N	2:H:20:GLN:OE1	2.50	0.42
1:J:498:VAL:HG23	1:J:533:LEU:HD22	2.01	0.42
1:J:1690:GLU:HG2	1:J:1790:LYS:HE3	2.01	0.42
1:A:169:ARG:HH21	1:A:176:ARG:HH11	1.66	0.42
1:A:1097:LYS:HA	1:A:1168:MET:HE2	2.01	0.42
1:A:1107:ALA:HB3	1:A:1160:ASP:HB2	2.01	0.42
1:A:1256:PRO:HB3	1:A:1597:SER:HA	2.02	0.42
1:A:2788:TRP:NE1	1:A:2906:ARG:O	2.53	0.42
1:A:4045:SER:C	1:A:4078:THR:HA	2.45	0.42
1:D:470:LEU:HD12	1:D:470:LEU:HA	1.87	0.42
1:D:616:SER:O	1:D:616:SER:OG	2.34	0.42
1:D:760:ASP:HB3	1:D:763:ALA:HB3	2.01	0.42
1:D:1086:ARG:NH1	1:D:1252:SER:O	2.53	0.42
1:D:2308:PHE:HE1	1:D:2475:ARG:HH22	1.67	0.42
1:D:2427:LEU:HD12	1:D:2427:LEU:C	2.44	0.42
1:D:4020:MET:HE1	1:D:4063:GLU:HG2	2.01	0.42
1:D:4518:LEU:HD21	1:D:4738:PHE:CE1	2.54	0.42
1:G:343:ARG:HB3	1:G:344:LYS:H	1.60	0.42
1:G:883:GLU:HA	1:G:886:ALA:HB3	2.02	0.42
1:G:1224:LEU:HD23	1:G:1224:LEU:HA	1.85	0.42
1:G:1610:ARG:HE	1:G:1610:ARG:HB3	1.64	0.42
1:G:3665:LEU:HD11	1:G:3696:MET:HE2	2.00	0.42
1:G:4052:ALA:O	1:G:4056:HIS:ND1	2.52	0.42
1:G:4617:TYR:OH	1:G:4629:GLY:O	2.36	0.42
3:I:45:THR:HG23	3:I:48:GLU:H	1.84	0.42
1:J:246:THR:HG22	1:J:247:VAL:H	1.84	0.42
1:J:3890:TYR:O	1:J:3894:SER:N	2.52	0.42
1:A:59:PRO:HD3	1:A:322:ALA:HB3	2.01	0.42
1:A:246:THR:HG22	1:A:247:VAL:H	1.84	0.42
1:A:470:LEU:HD12	1:A:470:LEU:HA	1.87	0.42
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:VAL:HA	1:A:800:VAL:HG23	2.01	0.42
1:A:3829:LYS:HE3	1:A:3829:LYS:HB3	1.83	0.42
1:A:3890:TYR:O	1:A:3894:SER:N	2.52	0.42
1:A:4518:LEU:HD21	1:A:4738:PHE:CE1	2.55	0.42
1:D:259:THR:HG1	1:D:261:HIS:CE1	2.31	0.42
1:D:1690:GLU:HG2	1:D:1790:LYS:HE3	2.01	0.42
1:G:59:PRO:HD3	1:G:322:ALA:HB3	2.01	0.42
1:J:883:GLU:HA	1:J:886:ALA:HB3	2.02	0.42
1:J:2788:TRP:NE1	1:J:2906:ARG:O	2.53	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.91	0.42
1:A:1157:GLN:N	1:A:1160:ASP:OD2	2.42	0.42
1:A:4867:ILE:HG21	1:J:4858:ILE:CD1	2.49	0.42
1:D:3640:LYS:HA	1:D:3640:LYS:HD2	1.81	0.42
1:D:3890:TYR:O	1:D:3894:SER:N	2.52	0.42
1:D:4858:ILE:CD1	1:G:4867:ILE:HG21	2.50	0.42
1:G:1086:ARG:NH1	1:G:1252:SER:O	2.53	0.42
1:G:1112:ASP:H	1:G:1211:GLN:NE2	2.17	0.42
1:G:1730:THR:O	1:G:1733:THR:OG1	2.35	0.42
1:G:3592:LEU:HD23	1:G:3592:LEU:HA	1.91	0.42
1:G:3631:GLU:OE1	1:G:3631:GLU:N	2.48	0.42
1:J:675:TYR:HB2	1:J:804:LEU:HD21	2.01	0.42
1:A:290:ARG:HA	1:A:353:GLU:HG2	2.02	0.42
1:A:831:LYS:HE3	1:A:831:LYS:HB2	1.80	0.42
1:A:2154:LYS:HB2	1:A:2154:LYS:HE2	1.79	0.42
1:A:4819:TYR:CD1	1:J:4845:ILE:CD1	3.02	0.42
1:D:883:GLU:HA	1:D:886:ALA:HB3	2.02	0.42
1:D:938:GLU:HA	1:D:941:LYS:HG3	2.00	0.42
1:D:1610:ARG:HE	1:D:1610:ARG:HB3	1.64	0.42
1:D:1843:LEU:HD23	1:D:1843:LEU:HA	1.93	0.42
1:D:2103:LEU:HA	1:D:2106:THR:HG22	2.00	0.42
1:D:2988:SER:O	1:D:2992:CYS:N	2.52	0.42
1:D:3986:MET:HE3	1:D:3986:MET:HB3	1.79	0.42
1:D:4943:LYS:HE2	1:D:4943:LYS:HB3	1.81	0.42
1:G:25:THR:HG22	1:G:34:LYS:HA	2.01	0.42
1:G:162:ILE:O	1:G:163:HIS:ND1	2.53	0.42
1:G:799:LYS:HB2	1:G:1618:LEU:HD11	2.00	0.42
1:G:1107:ALA:HB3	1:G:1160:ASP:HB2	2.01	0.42
1:G:1165:MET:HB3	1:G:1236:TYR:CE1	2.55	0.42
1:G:1842:ILE:HD12	1:G:1845:LEU:HD23	2.01	0.42
1:G:2788:TRP:NE1	1:G:2906:ARG:O	2.53	0.42
1:G:4045:SER:C	1:G:4078:THR:HA	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:37:MET:HG2	3:I:44:PRO:HG3	2.02	0.42
1:J:309:MET:O	1:J:313:SER:N	2.53	0.42
1:J:677:LEU:HD23	1:J:677:LEU:HA	1.87	0.42
1:J:915:HIS:CE1	1:J:917:CYS:HB2	2.54	0.42
1:J:1086:ARG:NH1	1:J:1252:SER:O	2.53	0.42
1:J:1256:PRO:HB3	1:J:1597:SER:HA	2.02	0.42
1:J:4160:GLN:HE22	1:J:4205:ALA:HA	1.85	0.42
1:A:1292:SER:O	1:A:1292:SER:OG	2.32	0.42
1:A:2143:MET:HE2	1:A:2175:VAL:HG11	2.02	0.42
1:A:4515:ASN:ND2	1:A:4740:PHE:O	2.33	0.42
1:D:309:MET:O	1:D:313:SER:N	2.53	0.42
1:D:2313:SER:OG	1:D:2402:ARG:O	2.31	0.42
1:D:4046:LYS:HE3	1:D:4046:LYS:HB2	1.81	0.42
1:G:2103:LEU:HA	1:G:2106:THR:HG22	2.00	0.42
1:G:4836:ALA:HB1	1:J:4805:MET:HE1	2.02	0.42
1:G:4845:ILE:CD1	1:J:4819:TYR:CD1	3.03	0.42
1:J:271:ALA:O	1:J:301:THR:OG1	2.25	0.42
1:J:559:ILE:H	1:J:559:ILE:HG13	1.72	0.42
1:J:1165:MET:HB3	1:J:1236:TYR:CE1	2.55	0.42
1:J:2313:SER:OG	1:J:2402:ARG:O	2.31	0.42
1:J:3617:ALA:O	1:J:3621:PHE:N	2.51	0.42
1:J:3762:LEU:HD12	1:J:3762:LEU:HA	1.83	0.42
1:J:4046:LYS:HE3	1:J:4046:LYS:HB2	1.81	0.42
1:J:4885:MET:O	6:J:6002:ATP:H1'	2.20	0.42
1:A:853:PRO:HD2	1:A:1209:VAL:HA	2.02	0.42
1:A:883:GLU:HA	1:A:886:ALA:HB3	2.02	0.42
1:A:1768:PHE:HE1	2:B:90:VAL:HG21	1.85	0.42
1:A:2427:LEU:HD12	1:A:2428:ILE:CG2	2.35	0.42
1:D:1107:ALA:HB3	1:D:1160:ASP:HB2	2.01	0.42
1:D:2764:LEU:HD23	1:D:2764:LEU:HA	1.91	0.42
1:D:3794:LEU:HD23	1:D:3794:LEU:HA	1.81	0.42
1:G:448:PRO:HB2	1:G:451:SER:HB3	2.02	0.42
1:G:4600:ILE:HD13	1:G:4600:ILE:HA	1.88	0.42
1:J:59:PRO:HD3	1:J:322:ALA:HB3	2.01	0.42
1:J:290:ARG:HA	1:J:353:GLU:HG2	2.02	0.42
1:J:760:ASP:HB3	1:J:763:ALA:HB3	2.01	0.42
1:J:2777:LYS:HE2	1:J:2781:LYS:HE3	2.02	0.42
1:J:3665:LEU:HD11	1:J:3696:MET:HE2	2.00	0.42
1:J:4943:LYS:HE2	1:J:4943:LYS:HB3	1.81	0.42
1:A:2313:SER:OG	1:A:2402:ARG:O	2.31	0.41
1:D:59:PRO:HD3	1:D:322:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:HIS:CD2	1:D:125:TYR:H	2.37	0.41
1:D:162:ILE:O	1:D:163:HIS:ND1	2.53	0.41
1:D:498:VAL:HG23	1:D:533:LEU:HD22	2.01	0.41
1:D:706:TYR:HA	1:D:707:PRO:HD3	1.85	0.41
1:D:995:MET:HE3	1:D:995:MET:HB3	1.98	0.41
1:D:1040:ASP:HA	1:D:1043:LYS:HB2	2.01	0.41
1:D:1256:PRO:HB3	1:D:1597:SER:HA	2.02	0.41
1:D:1809:PRO:HB2	1:D:1817:LEU:HD22	2.02	0.41
1:D:1842:ILE:HD12	1:D:1845:LEU:HD23	2.01	0.41
1:D:2259:ARG:HA	1:D:2259:ARG:HD3	1.87	0.41
1:D:4638:THR:O	1:D:4651:LYS:NZ	2.39	0.41
1:G:66:THR:OG1	1:G:124:SER:OG	2.29	0.41
1:G:246:THR:HG22	1:G:247:VAL:H	1.84	0.41
1:G:995:MET:HE3	1:G:995:MET:HB3	1.98	0.41
1:G:1843:LEU:HD23	1:G:1843:LEU:HA	1.93	0.41
1:G:4858:ILE:CD1	1:J:4867:ILE:HG21	2.49	0.41
1:J:1809:PRO:HB2	1:J:1817:LEU:HD22	2.02	0.41
1:J:4020:MET:HE1	1:J:4063:GLU:HG2	2.01	0.41
2:K:17:LYS:N	2:K:20:GLN:OE1	2.50	0.41
1:A:162:ILE:O	1:A:163:HIS:ND1	2.53	0.41
1:A:1040:ASP:HA	1:A:1043:LYS:HB2	2.01	0.41
1:A:1165:MET:HB3	1:A:1236:TYR:CE1	2.55	0.41
1:A:4885:MET:O	6:A:6002:ATP:H1'	2.21	0.41
2:B:40:ARG:H	2:B:40:ARG:HG2	1.64	0.41
1:D:448:PRO:HB2	1:D:451:SER:HB3	2.02	0.41
1:D:1157:GLN:N	1:D:1160:ASP:OD2	2.42	0.41
1:D:1165:MET:HB3	1:D:1236:TYR:CE1	2.55	0.41
1:D:3786:LYS:HB3	1:D:3786:LYS:HE2	1.79	0.41
1:D:3829:LYS:HE3	1:D:3829:LYS:HB3	1.83	0.41
1:D:4752:LYS:HA	1:D:4752:LYS:HD2	1.75	0.41
1:G:309:MET:O	1:G:313:SER:N	2.53	0.41
1:G:2143:MET:HE2	1:G:2175:VAL:HG11	2.02	0.41
1:G:4801:ASP:OD1	1:G:4801:ASP:N	2.51	0.41
1:J:1610:ARG:HE	1:J:1610:ARG:HB3	1.64	0.41
1:J:4651:LYS:HG2	1:J:4671:LEU:HD23	2.01	0.41
1:A:498:VAL:HG23	1:A:533:LEU:HD22	2.01	0.41
1:A:1685:LEU:HA	1:A:1685:LEU:HD23	1.88	0.41
1:A:3669:ILE:HD12	1:A:3735:ARG:HB3	2.02	0.41
1:A:4911:LEU:O	1:A:4915:ASN:ND2	2.42	0.41
1:D:156:GLU:HG3	1:D:187:SER:HB3	2.02	0.41
1:D:1757:LEU:HD12	1:D:1757:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1822:ILE:O	1:D:1826:TYR:N	2.47	0.41
1:G:1118:SER:OG	1:G:1122:CYS:SG	2.78	0.41
1:G:1256:PRO:HB3	1:G:1597:SER:HA	2.02	0.41
1:G:1809:PRO:HB2	1:G:1817:LEU:HD22	2.02	0.41
1:G:2891:GLN:O	1:G:2895:LYS:N	2.48	0.41
1:G:4896:ASN:O	1:G:4900:ASP:HB2	2.20	0.41
1:J:143:LEU:O	1:J:143:LEU:CG	2.68	0.41
1:J:1182:LEU:HD23	1:J:1182:LEU:HA	1.90	0.41
1:J:2143:MET:HE2	1:J:2175:VAL:HG11	2.02	0.41
1:A:799:LYS:HB2	1:A:1618:LEU:HD11	2.00	0.41
1:A:1809:PRO:HB2	1:A:1817:LEU:HD22	2.02	0.41
1:A:1942:ARG:HG3	1:A:3611:ASN:HB2	2.02	0.41
1:A:3640:LYS:HA	1:A:3640:LYS:HD2	1.81	0.41
1:A:4896:ASN:O	1:A:4900:ASP:HB2	2.20	0.41
1:D:135:THR:OG1	1:D:146:ASP:OD2	2.36	0.41
1:D:246:THR:HG22	1:D:247:VAL:H	1.84	0.41
1:D:290:ARG:HA	1:D:353:GLU:HG2	2.02	0.41
1:D:1091:GLU:HG3	1:D:1250:TRP:CH2	2.55	0.41
1:D:2777:LYS:HE2	1:D:2781:LYS:HE3	2.02	0.41
1:D:3689:TYR:HE2	1:D:3759:THR:HB	1.86	0.41
1:G:558:LEU:HD22	1:G:571:ILE:HG12	2.03	0.41
1:G:2512:ASP:N	1:G:2512:ASP:OD1	2.54	0.41
1:J:123:HIS:CD2	1:J:125:TYR:H	2.37	0.41
1:J:4518:LEU:HD21	1:J:4738:PHE:CE1	2.55	0.41
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.88	0.41
1:A:565:LEU:HD22	1:A:604:HIS:HE1	1.86	0.41
1:A:2058:THR:N	1:A:2061:GLN:OE1	2.54	0.41
1:A:2169:HIS:HB3	1:A:2204:PHE:CE2	2.55	0.41
1:A:4651:LYS:HG2	1:A:4671:LEU:HD23	2.01	0.41
1:D:831:LYS:HB2	1:D:831:LYS:HE3	1.80	0.41
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.52	0.41
1:G:760:ASP:HB3	1:G:763:ALA:HB3	2.01	0.41
1:G:1273:ILE:HD11	1:G:1287:GLN:HB2	2.03	0.41
1:G:2076:ILE:HD12	1:G:2085:MET:HE1	2.03	0.41
1:G:2764:LEU:HD23	1:G:2764:LEU:HA	1.91	0.41
1:G:2777:LYS:HE2	1:G:2781:LYS:HE3	2.01	0.41
1:G:2988:SER:O	1:G:2992:CYS:N	2.52	0.41
1:J:555:LEU:HD23	1:J:555:LEU:HA	1.87	0.41
1:J:1732:GLU:O	1:J:1735:SER:OG	2.31	0.41
1:J:2169:HIS:HB3	1:J:2204:PHE:CE2	2.55	0.41
1:J:2823:SER:O	1:J:2823:SER:OG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:37:MET:HG2	3:L:44:PRO:HG3	2.02	0.41
1:A:448:PRO:HB2	1:A:451:SER:HB3	2.02	0.41
1:A:1182:LEU:HD23	1:A:1182:LEU:HA	1.91	0.41
1:A:2150:ILE:HG21	1:A:2168:MET:HE1	2.03	0.41
1:A:4041:LYS:HB3	1:A:4043:VAL:HG12	2.02	0.41
1:A:4160:GLN:HE22	1:A:4205:ALA:HA	1.85	0.41
1:A:4618:ILE:HD13	1:A:4618:ILE:HA	1.87	0.41
1:A:4818:MET:HE3	1:A:4818:MET:HB2	1.72	0.41
1:D:675:TYR:HB2	1:D:804:LEU:HD21	2.01	0.41
1:D:1548:THR:OG1	1:D:1549:SER:N	2.54	0.41
1:D:1625:LEU:HD23	1:D:1625:LEU:HA	1.90	0.41
1:D:1768:PHE:HE1	2:E:90:VAL:HG21	1.85	0.41
1:D:1796:THR:HG22	1:D:1845:LEU:HD11	2.03	0.41
1:D:1942:ARG:HG3	1:D:3611:ASN:HB2	2.02	0.41
1:D:4045:SER:C	1:D:4078:THR:HA	2.45	0.41
1:D:4160:GLN:HE22	1:D:4205:ALA:HA	1.85	0.41
3:F:49:LEU:HD12	3:F:49:LEU:HA	1.92	0.41
1:G:288:HIS:ND1	1:G:349:MET:O	2.37	0.41
1:G:1768:PHE:HE1	2:H:90:VAL:HG21	1.85	0.41
1:G:1796:THR:HG22	1:G:1845:LEU:HD11	2.03	0.41
1:G:2058:THR:N	1:G:2061:GLN:OE1	2.54	0.41
1:G:4137:ILE:HG23	1:G:4151:PHE:HE1	1.86	0.41
1:G:4770:LEU:HD13	1:J:4751:PHE:CD1	2.56	0.41
1:J:558:LEU:HD22	1:J:571:ILE:HG12	2.03	0.41
1:J:2058:THR:N	1:J:2061:GLN:OE1	2.54	0.41
1:J:3669:ILE:HD12	1:J:3735:ARG:HB3	2.02	0.41
1:J:3919:ASN:O	1:J:3922:THR:OG1	2.32	0.41
1:A:1548:THR:OG1	1:A:1549:SER:N	2.54	0.41
1:A:4751:PHE:CD1	1:J:4770:LEU:HD13	2.55	0.41
1:A:4808:ASP:HB2	1:D:4523:VAL:HG12	2.01	0.41
1:D:228:LEU:HD23	1:D:228:LEU:HA	1.91	0.41
1:D:853:PRO:HD2	1:D:1209:VAL:HA	2.03	0.41
1:D:1273:ILE:HD11	1:D:1287:GLN:HB2	2.03	0.41
1:D:2143:MET:HE3	1:D:2143:MET:HB3	1.73	0.41
1:D:4041:LYS:HB3	1:D:4043:VAL:HG12	2.02	0.41
1:D:4753:THR:O	1:D:4753:THR:OG1	2.34	0.41
3:F:37:MET:HG2	3:F:44:PRO:HG3	2.02	0.41
1:G:734:SER:OG	1:G:734:SER:O	2.36	0.41
1:G:3689:TYR:HE2	1:G:3759:THR:HB	1.86	0.41
1:J:162:ILE:O	1:J:163:HIS:ND1	2.53	0.41
1:J:288:HIS:ND1	1:J:349:MET:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:853:PRO:HD2	1:J:1209:VAL:HA	2.02	0.41
1:J:2767:LYS:HD2	1:J:2767:LYS:HA	1.73	0.41
1:J:3636:TYR:HD1	1:J:3636:TYR:HA	1.78	0.41
1:J:4896:ASN:O	1:J:4900:ASP:HB2	2.20	0.41
1:A:675:TYR:HB2	1:A:804:LEU:HD21	2.01	0.41
1:A:4029:SER:HA	1:A:4034:LYS:HE2	2.02	0.41
1:A:4723:LEU:HD13	1:A:4723:LEU:HA	1.88	0.41
1:A:4810:MET:HB3	1:D:4519:LEU:O	2.20	0.41
1:A:4845:ILE:HD12	1:D:4819:TYR:CG	2.55	0.41
1:D:2512:ASP:N	1:D:2512:ASP:OD1	2.54	0.41
1:D:3742:LEU:HD12	1:D:3742:LEU:HA	1.89	0.41
1:D:3762:LEU:HA	1:D:3762:LEU:HD12	1.83	0.41
1:G:259:THR:HG1	1:G:261:HIS:CE1	2.33	0.41
1:G:3759:THR:O	1:G:3759:THR:OG1	2.28	0.41
1:G:3829:LYS:HB3	1:G:3829:LYS:HE3	1.83	0.41
1:J:1091:GLU:HG3	1:J:1250:TRP:CH2	2.56	0.41
1:J:1548:THR:OG1	1:J:1549:SER:N	2.54	0.41
1:J:2742:TRP:HB2	1:J:2758:MET:HE3	2.03	0.41
1:J:3966:ILE:HA	1:J:3966:ILE:HD12	1.80	0.41
1:A:1796:THR:HG22	1:A:1845:LEU:HD11	2.03	0.41
1:A:3689:TYR:HE2	1:A:3759:THR:HB	1.86	0.41
1:D:70:GLU:HG3	1:D:71:GLN:HG3	2.03	0.41
1:D:1181:ILE:H	1:D:1181:ILE:HG13	1.74	0.41
1:D:1710:HIS:CD2	1:D:1782:PHE:HB3	2.56	0.41
1:D:2143:MET:HE2	1:D:2175:VAL:HG11	2.02	0.41
1:D:3998:LYS:HB2	1:D:3998:LYS:HE3	1.85	0.41
1:D:4110:MET:HE2	1:D:4110:MET:HB2	1.79	0.41
1:D:4651:LYS:HG2	1:D:4671:LEU:HD23	2.01	0.41
1:D:4896:ASN:O	1:D:4900:ASP:HB2	2.20	0.41
1:G:156:GLU:HG3	1:G:187:SER:HB3	2.02	0.41
1:G:693:LEU:HD22	1:G:798:ILE:HD13	2.03	0.41
1:G:1262:PRO:HG2	1:G:1264:SER:H	1.86	0.41
1:G:3617:ALA:O	1:G:3621:PHE:N	2.51	0.41
3:I:49:LEU:HD12	3:I:49:LEU:HA	1.92	0.41
1:J:35:LEU:H	1:J:35:LEU:HG	1.75	0.41
1:J:448:PRO:HB2	1:J:451:SER:HB3	2.02	0.41
1:J:693:LEU:HD22	1:J:798:ILE:HD13	2.03	0.41
1:J:3760:LEU:HD23	1:J:3760:LEU:HA	1.78	0.41
1:A:1709:ILE:HD13	1:A:1709:ILE:HA	1.92	0.41
1:A:2988:SER:O	1:A:2992:CYS:N	2.52	0.41
1:D:1167:ASP:OD1	1:D:1236:TYR:OH	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:GLU:HG3	1:G:71:GLN:HG3	2.03	0.41
1:G:290:ARG:HA	1:G:353:GLU:HG2	2.02	0.41
1:G:2323:ARG:HE	1:G:2323:ARG:HB3	1.71	0.41
1:J:55:SER:O	1:J:296:ARG:NH2	2.41	0.41
1:J:156:GLU:HG3	1:J:187:SER:HB3	2.02	0.41
1:J:565:LEU:HD22	1:J:604:HIS:HE1	1.86	0.41
1:J:833:LYS:HE2	1:J:833:LYS:HB2	1.90	0.41
1:J:1796:THR:HG22	1:J:1845:LEU:HD11	2.03	0.41
1:J:2150:ILE:HG21	1:J:2168:MET:HE1	2.03	0.41
1:J:4010:ASN:OD1	1:J:4010:ASN:N	2.41	0.41
1:A:558:LEU:HD22	1:A:571:ILE:HG12	2.03	0.40
1:D:1709:ILE:HD13	1:D:1709:ILE:HA	1.92	0.40
1:D:3669:ILE:HD12	1:D:3735:ARG:HB3	2.02	0.40
2:E:40:ARG:H	2:E:40:ARG:HG2	1.64	0.40
1:G:1091:GLU:HG3	1:G:1250:TRP:CH2	2.56	0.40
1:G:1548:THR:OG1	1:G:1549:SER:N	2.54	0.40
1:G:4029:SER:HA	1:G:4034:LYS:HE2	2.02	0.40
1:J:35:LEU:HD13	1:J:49:LEU:HD22	2.03	0.40
1:J:673:TRP:N	1:J:759:LEU:O	2.51	0.40
1:J:1768:PHE:HE1	2:K:90:VAL:HG21	1.85	0.40
1:J:3689:TYR:HE2	1:J:3759:THR:HB	1.86	0.40
1:A:1091:GLU:HG3	1:A:1250:TRP:CH2	2.56	0.40
1:A:2742:TRP:HB2	1:A:2758:MET:HE3	2.03	0.40
1:D:558:LEU:HD22	1:D:571:ILE:HG12	2.03	0.40
1:D:752:ASP:N	1:D:752:ASP:OD1	2.55	0.40
1:D:1118:SER:OG	1:D:1122:CYS:SG	2.78	0.40
1:D:2150:ILE:HD13	1:D:2168:MET:HE1	2.04	0.40
1:D:3943:ASP:OD1	1:D:3943:ASP:N	2.54	0.40
1:D:4845:ILE:HD12	1:G:4819:TYR:CG	2.56	0.40
1:G:673:TRP:N	1:G:759:LEU:O	2.51	0.40
1:G:4808:ASP:HB2	1:J:4523:VAL:HG11	2.04	0.40
1:J:1454:ASP:OD1	1:J:1454:ASP:N	2.54	0.40
1:J:1605:LYS:HA	1:J:1605:LYS:HD3	1.83	0.40
1:J:2076:ILE:HD12	1:J:2085:MET:HE1	2.03	0.40
1:J:4002:ASP:HA	1:J:4005:VAL:HG22	2.02	0.40
1:A:156:GLU:HG3	1:A:187:SER:HB3	2.02	0.40
1:A:646:THR:OG1	1:A:647:ARG:N	2.55	0.40
1:A:1710:HIS:CD2	1:A:1782:PHE:HB3	2.56	0.40
1:A:2259:ARG:HD3	1:A:2259:ARG:HA	1.87	0.40
1:A:3620:LEU:HD23	1:A:3620:LEU:HA	1.93	0.40
1:A:4752:LYS:HD2	1:A:4752:LYS:HA	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:PHE:O	1:D:205:ALA:N	2.51	0.40
1:D:646:THR:OG1	1:D:647:ARG:N	2.55	0.40
1:D:1262:PRO:HG2	1:D:1264:SER:H	1.86	0.40
1:D:1614:ARG:HA	1:D:1614:ARG:HD3	1.83	0.40
1:G:135:THR:OG1	1:G:146:ASP:OD2	2.36	0.40
1:G:2742:TRP:HB2	1:G:2758:MET:HE3	2.03	0.40
1:G:3669:ILE:HD12	1:G:3735:ARG:HB3	2.02	0.40
1:J:70:GLU:HG3	1:J:71:GLN:HG3	2.03	0.40
1:J:1262:PRO:HG2	1:J:1264:SER:H	1.86	0.40
1:J:1710:HIS:CD2	1:J:1782:PHE:HB3	2.56	0.40
1:J:2154:LYS:HB2	1:J:2154:LYS:HE2	1.79	0.40
1:J:4110:MET:HE2	1:J:4110:MET:HB2	1.78	0.40
1:A:559:ILE:H	1:A:559:ILE:HG13	1.72	0.40
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.54	0.40
1:A:3966:ILE:HD12	1:A:3966:ILE:HA	1.80	0.40
1:A:4002:ASP:HA	1:A:4005:VAL:HG22	2.02	0.40
1:A:4849:ILE:HD13	1:D:4823:ARG:HD3	2.04	0.40
3:C:37:MET:HG2	3:C:44:PRO:HG3	2.02	0.40
1:D:66:THR:OG1	1:D:124:SER:OG	2.29	0.40
1:D:1255:LEU:HD23	1:D:1255:LEU:HA	1.91	0.40
1:D:4029:SER:HA	1:D:4034:LYS:HE2	2.02	0.40
1:G:355:LYS:HE3	1:G:355:LYS:HB3	1.91	0.40
1:G:565:LEU:HD22	1:G:604:HIS:HE1	1.86	0.40
1:G:740:THR:O	1:G:740:THR:OG1	2.35	0.40
1:G:853:PRO:HD2	1:G:1209:VAL:HA	2.02	0.40
1:G:3760:LEU:HD23	1:G:3760:LEU:HA	1.78	0.40
1:J:35:LEU:HD13	1:J:49:LEU:HD13	2.04	0.40
1:J:355:LYS:HE3	1:J:355:LYS:HB3	1.91	0.40
1:J:3598:ARG:HG2	3:L:40:LEU:HD11	2.04	0.40
1:J:3860:ARG:HH11	1:J:3860:ARG:HD3	1.76	0.40
1:J:3957:MET:O	1:J:3960:SER:OG	2.36	0.40
1:A:1273:ILE:HD11	1:A:1287:GLN:HB2	2.03	0.40
1:A:2173:MET:HE2	1:A:2173:MET:HB2	1.83	0.40
1:A:4819:TYR:CG	1:J:4845:ILE:HD12	2.56	0.40
3:C:49:LEU:HD12	3:C:49:LEU:HA	1.92	0.40
1:D:565:LEU:HD22	1:D:604:HIS:HE1	1.86	0.40
1:D:2076:ILE:HD12	1:D:2085:MET:HE1	2.03	0.40
1:D:2127:ILE:HD11	1:D:2146:GLY:HA3	2.04	0.40
1:D:4137:ILE:HG23	1:D:4151:PHE:HE1	1.86	0.40
1:D:4860:LEU:HD12	1:D:4860:LEU:HA	1.84	0.40
1:G:687:THR:OG1	1:G:689:GLU:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1830:ILE:H	1:G:1830:ILE:HG13	1.72	0.40
1:G:1942:ARG:HG3	1:G:3611:ASN:HB2	2.02	0.40
1:G:2157:TYR:HE1	1:G:2203:TYR:HE2	1.70	0.40
1:G:4002:ASP:HA	1:G:4005:VAL:HG22	2.02	0.40
1:G:4845:ILE:HD12	1:J:4819:TYR:CG	2.57	0.40
1:G:4860:LEU:HD12	1:G:4860:LEU:HA	1.84	0.40
1:J:1166:VAL:HG22	1:J:1173:MET:HG3	2.04	0.40
1:J:1273:ILE:HD11	1:J:1287:GLN:HB2	2.03	0.40
1:J:3984:LEU:HA	1:J:3984:LEU:HD23	1.93	0.40
1:J:4137:ILE:HG23	1:J:4151:PHE:HE1	1.86	0.40
1:J:4627:ILE:H	1:J:4627:ILE:HG12	1.66	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 PDB entries followed by that with respect to all EM entries.

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	3366/4968 (68%)	2925 (87%)	429 (13%)	12 (0%)	30	60
1	D	3366/4968 (68%)	2927 (87%)	428 (13%)	11 (0%)	36	65
1	G	3366/4968 (68%)	2925 (87%)	429 (13%)	12 (0%)	30	60
1	J	3366/4968 (68%)	2927 (87%)	427 (13%)	12 (0%)	30	60
2	B	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	E	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	K	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
3	C	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	F	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	I	66/149 (44%)	63 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
All	All	14148/20900 (68%)	12344 (87%)	1757 (12%)	47 (0%)	37	65

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2321	VAL
1	A	4901	THR
1	D	2321	VAL
1	D	4901	THR
1	G	2321	VAL
1	G	4901	THR
1	J	2321	VAL
1	J	4901	THR
1	A	4075	GLU
1	D	4075	GLU
1	G	4075	GLU
1	J	4075	GLU
1	A	730	LEU
1	A	853	PRO
1	A	1580	PRO
1	A	2309	CYS
1	D	730	LEU
1	D	853	PRO
1	D	1580	PRO
1	D	2309	CYS
1	G	730	LEU
1	G	853	PRO
1	G	1580	PRO
1	G	2309	CYS
1	J	730	LEU
1	J	853	PRO
1	J	1580	PRO
1	J	2309	CYS
1	A	1848	PRO
1	A	1990	PRO
1	A	4916	LEU
1	D	1848	PRO
1	D	1990	PRO
1	G	1848	PRO
1	G	1990	PRO
1	G	4916	LEU

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Mol	Chain	Res	Type
1	J	1848	PRO
1	J	1990	PRO
1	J	4916	LEU
1	A	1535	PRO
1	A	2320	VAL
1	D	1535	PRO
1	D	2320	VAL
1	G	1535	PRO
1	G	2320	VAL
1	J	1535	PRO
1	J	2320	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 PDB entries followed by that with respect to all EM entries.

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	2677/4355 (62%)	2650 (99%)	27 (1%)	68	74
1	D	2678/4355 (62%)	2651 (99%)	27 (1%)	68	74
1	G	2677/4355 (62%)	2650 (99%)	27 (1%)	68	74
1	J	2678/4355 (62%)	2650 (99%)	28 (1%)	68	74
2	B	88/89 (99%)	88 (100%)	0	100	100
2	E	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
2	K	88/89 (99%)	88 (100%)	0	100	100
3	C	57/127 (45%)	57 (100%)	0	100	100
3	F	57/127 (45%)	57 (100%)	0	100	100
3	I	57/127 (45%)	57 (100%)	0	100	100
3	L	57/127 (45%)	57 (100%)	0	100	100
All	All	11290/18284 (62%)	11181 (99%)	109 (1%)	65	74

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	360	VAL
1	A	718	VAL
1	A	855	VAL
1	A	925	PRO
1	A	950	VAL
1	A	990	PRO
1	A	1167	ASP
1	A	1246	ASP
1	A	1521	THR
1	A	1782	PHE
1	A	3803	VAL
1	A	3899	ILE
1	A	3936	LEU
1	A	3992	VAL
1	A	4588	ILE
1	A	4596	VAL
1	A	4638	THR
1	A	4832	ILE
1	A	4877	GLN
1	A	4878	GLN
1	A	4879	GLU
1	A	4881	VAL
1	A	4882	LYS
1	A	4884	ASP
1	A	4885	MET
1	A	4886	GLU
1	D	35	LEU
1	D	360	VAL
1	D	718	VAL
1	D	855	VAL
1	D	925	PRO
1	D	950	VAL
1	D	990	PRO
1	D	1054	VAL
1	D	1167	ASP
1	D	1246	ASP
1	D	1521	THR
1	D	1782	PHE
1	D	3803	VAL
1	D	3899	ILE
1	D	3936	LEU
1	D	3992	VAL

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Mol	Chain	Res	Type
1	D	4588	ILE
1	D	4596	VAL
1	D	4638	THR
1	D	4832	ILE
1	D	4877	GLN
1	D	4878	GLN
1	D	4879	GLU
1	D	4882	LYS
1	D	4884	ASP
1	D	4885	MET
1	D	4886	GLU
1	G	35	LEU
1	G	360	VAL
1	G	718	VAL
1	G	855	VAL
1	G	925	PRO
1	G	950	VAL
1	G	990	PRO
1	G	1167	ASP
1	G	1246	ASP
1	G	1521	THR
1	G	1782	PHE
1	G	3803	VAL
1	G	3899	ILE
1	G	3936	LEU
1	G	3992	VAL
1	G	4588	ILE
1	G	4596	VAL
1	G	4638	THR
1	G	4832	ILE
1	G	4877	GLN
1	G	4878	GLN
1	G	4879	GLU
1	G	4881	VAL
1	G	4882	LYS
1	G	4884	ASP
1	G	4885	MET
1	G	4886	GLU
1	J	35	LEU
1	J	360	VAL
1	J	718	VAL
1	J	855	VAL

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Mol	Chain	Res	Type
1	J	925	PRO
1	J	950	VAL
1	J	990	PRO
1	J	1054	VAL
1	J	1167	ASP
1	J	1246	ASP
1	J	1521	THR
1	J	1782	PHE
1	J	3803	VAL
1	J	3899	ILE
1	J	3936	LEU
1	J	3992	VAL
1	J	4588	ILE
1	J	4596	VAL
1	J	4638	THR
1	J	4832	ILE
1	J	4877	GLN
1	J	4878	GLN
1	J	4879	GLU
1	J	4881	VAL
1	J	4882	LYS
1	J	4884	ASP
1	J	4885	MET
1	J	4886	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (234) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	123	HIS
1	A	293	GLN
1	A	365	HIS
1	A	394	HIS
1	A	477	ASN
1	A	484	ASN
1	A	604	HIS
1	A	630	HIS
1	A	651	HIS
1	A	746	GLN
1	A	771	ASN
1	A	890	HIS
1	A	915	HIS

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Mol	Chain	Res	Type
1	A	1265	HIS
1	A	1267	HIS
1	A	1294	ASN
1	A	1440	ASN
1	A	1503	ASN
1	A	1551	ASN
1	A	1554	GLN
1	A	1762	GLN
1	A	1906	GLN
1	A	1918	GLN
1	A	1946	ASN
1	A	1950	GLN
1	A	2061	GLN
1	A	2072	GLN
1	A	2119	ASN
1	A	2218	HIS
1	A	2225	ASN
1	A	2317	ASN
1	A	2465	HIS
1	A	2518	ASN
1	A	2839	HIS
1	A	2848	ASN
1	A	2891	GLN
1	A	3595	GLN
1	A	3635	HIS
1	A	3666	HIS
1	A	3865	ASN
1	A	3906	ASN
1	A	3916	GLN
1	A	3961	GLN
1	A	3993	ASN
1	A	4109	HIS
1	A	4172	GLN
1	A	4490	GLN
1	A	4494	ASN
1	A	4643	ASN
1	A	4763	HIS
1	A	4764	ASN
1	A	4788	ASN
1	A	4864	GLN
1	A	4934	HIS
1	A	4962	GLN

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Mol	Chain	Res	Type
2	B	31	GLN
3	C	42	GLN
3	C	50	GLN
1	D	79	GLN
1	D	123	HIS
1	D	293	GLN
1	D	365	HIS
1	D	394	HIS
1	D	477	ASN
1	D	484	ASN
1	D	604	HIS
1	D	630	HIS
1	D	651	HIS
1	D	692	HIS
1	D	746	GLN
1	D	771	ASN
1	D	890	HIS
1	D	915	HIS
1	D	1265	HIS
1	D	1267	HIS
1	D	1294	ASN
1	D	1440	ASN
1	D	1551	ASN
1	D	1554	GLN
1	D	1762	GLN
1	D	1906	GLN
1	D	1918	GLN
1	D	1946	ASN
1	D	1950	GLN
1	D	2061	GLN
1	D	2072	GLN
1	D	2119	ASN
1	D	2218	HIS
1	D	2225	ASN
1	D	2317	ASN
1	D	2465	HIS
1	D	2518	ASN
1	D	2839	HIS
1	D	2848	ASN
1	D	2891	GLN
1	D	3595	GLN
1	D	3623	GLN

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Mol	Chain	Res	Type
1	D	3635	HIS
1	D	3666	HIS
1	D	3865	ASN
1	D	3906	ASN
1	D	3916	GLN
1	D	3961	GLN
1	D	3993	ASN
1	D	4109	HIS
1	D	4172	GLN
1	D	4490	GLN
1	D	4494	ASN
1	D	4643	ASN
1	D	4763	HIS
1	D	4764	ASN
1	D	4864	GLN
1	D	4934	HIS
1	D	4962	GLN
2	E	31	GLN
3	F	42	GLN
3	F	50	GLN
1	G	79	GLN
1	G	123	HIS
1	G	293	GLN
1	G	365	HIS
1	G	394	HIS
1	G	477	ASN
1	G	484	ASN
1	G	604	HIS
1	G	628	ASN
1	G	630	HIS
1	G	651	HIS
1	G	692	HIS
1	G	746	GLN
1	G	771	ASN
1	G	890	HIS
1	G	914	GLN
1	G	915	HIS
1	G	1265	HIS
1	G	1267	HIS
1	G	1294	ASN
1	G	1440	ASN
1	G	1551	ASN

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Mol	Chain	Res	Type
1	G	1554	GLN
1	G	1762	GLN
1	G	1906	GLN
1	G	1918	GLN
1	G	1946	ASN
1	G	1950	GLN
1	G	2061	GLN
1	G	2072	GLN
1	G	2119	ASN
1	G	2317	ASN
1	G	2465	HIS
1	G	2518	ASN
1	G	2839	HIS
1	G	2848	ASN
1	G	2891	GLN
1	G	3635	HIS
1	G	3666	HIS
1	G	3865	ASN
1	G	3906	ASN
1	G	3916	GLN
1	G	3961	GLN
1	G	3993	ASN
1	G	4061	GLN
1	G	4109	HIS
1	G	4172	GLN
1	G	4490	GLN
1	G	4494	ASN
1	G	4643	ASN
1	G	4764	ASN
1	G	4864	GLN
1	G	4904	HIS
1	G	4934	HIS
1	G	4962	GLN
2	H	31	GLN
3	I	42	GLN
3	I	50	GLN
1	J	79	GLN
1	J	123	HIS
1	J	293	GLN
1	J	365	HIS
1	J	394	HIS
1	J	477	ASN

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Mol	Chain	Res	Type
1	J	484	ASN
1	J	604	HIS
1	J	628	ASN
1	J	630	HIS
1	J	651	HIS
1	J	746	GLN
1	J	771	ASN
1	J	890	HIS
1	J	914	GLN
1	J	915	HIS
1	J	1265	HIS
1	J	1267	HIS
1	J	1294	ASN
1	J	1440	ASN
1	J	1551	ASN
1	J	1554	GLN
1	J	1762	GLN
1	J	1906	GLN
1	J	1918	GLN
1	J	1946	ASN
1	J	1950	GLN
1	J	2061	GLN
1	J	2072	GLN
1	J	2119	ASN
1	J	2218	HIS
1	J	2317	ASN
1	J	2465	HIS
1	J	2518	ASN
1	J	2839	HIS
1	J	2848	ASN
1	J	2891	GLN
1	J	3595	GLN
1	J	3623	GLN
1	J	3635	HIS
1	J	3666	HIS
1	J	3865	ASN
1	J	3906	ASN
1	J	3916	GLN
1	J	3961	GLN
1	J	3993	ASN
1	J	4109	HIS
1	J	4172	GLN

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Mol	Chain	Res	Type
1	J	4490	GLN
1	J	4494	ASN
1	J	4643	ASN
1	J	4764	ASN
1	J	4864	GLN
1	J	4934	HIS
1	J	4962	GLN
2	K	31	GLN
3	L	42	GLN
3	L	50	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CFF	D	6003	-	15,15,15	2.24	8 (53%)	23,23,23	2.73	9 (39%)
7	CFF	J	6003	-	15,15,15	2.24	8 (53%)	23,23,23	2.73	9 (39%)
6	ATP	J	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.66	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CFF	G	6003	-	15,15,15	2.24	8 (53%)	23,23,23	2.73	9 (39%)
6	ATP	D	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.66	6 (12%)
7	CFF	A	6003	-	15,15,15	2.24	8 (53%)	23,23,23	2.73	9 (39%)
6	ATP	G	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.66	6 (12%)
6	ATP	A	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.66	6 (12%)

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
7	CFF	D	6003	-	-	-	0/2/2/2
7	CFF	J	6003	-	-	-	0/2/2/2
6	ATP	J	6002	-	-	7/22/38/38	0/3/3/3
7	CFF	G	6003	-	-	-	0/2/2/2
6	ATP	D	6002	-	-	7/22/38/38	0/3/3/3
7	CFF	A	6003	-	-	-	0/2/2/2
6	ATP	G	6002	-	-	7/22/38/38	0/3/3/3
6	ATP	A	6002	-	-	7/22/38/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	6003	CFF	C6-N1	-4.46	1.31	1.40
7	D	6003	CFF	C6-N1	-4.46	1.31	1.40
7	G	6003	CFF	C6-N1	-4.46	1.31	1.40
7	J	6003	CFF	C6-N1	-4.46	1.31	1.40
6	A	6002	ATP	C5-C4	3.68	1.45	1.39
6	D	6002	ATP	C5-C4	3.68	1.45	1.39
6	G	6002	ATP	C5-C4	3.68	1.45	1.39
6	J	6002	ATP	C5-C4	3.68	1.45	1.39
6	A	6002	ATP	C5-N7	-3.61	1.32	1.39
6	D	6002	ATP	C5-N7	-3.61	1.32	1.39
6	G	6002	ATP	C5-N7	-3.61	1.32	1.39
6	J	6002	ATP	C5-N7	-3.61	1.32	1.39
7	A	6003	CFF	C5-N7	-3.06	1.33	1.38
7	D	6003	CFF	C5-N7	-3.06	1.33	1.38
7	G	6003	CFF	C5-N7	-3.06	1.33	1.38
7	J	6003	CFF	C5-N7	-3.06	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6002	ATP	C4-N9	-2.93	1.31	1.37
6	D	6002	ATP	C4-N9	-2.93	1.31	1.37
6	G	6002	ATP	C4-N9	-2.93	1.31	1.37
6	J	6002	ATP	C4-N9	-2.93	1.31	1.37
7	A	6003	CFF	C2-N1	-2.64	1.33	1.39
7	D	6003	CFF	C2-N1	-2.64	1.33	1.39
7	G	6003	CFF	C2-N1	-2.64	1.33	1.39
7	J	6003	CFF	C2-N1	-2.64	1.33	1.39
7	D	6003	CFF	C4-N3	-2.57	1.33	1.38
7	A	6003	CFF	C4-N3	-2.54	1.34	1.38
7	G	6003	CFF	C4-N3	-2.54	1.34	1.38
7	J	6003	CFF	C4-N3	-2.54	1.34	1.38
7	D	6003	CFF	O13-C6	-2.48	1.18	1.23
7	A	6003	CFF	O13-C6	-2.46	1.18	1.23
7	G	6003	CFF	O13-C6	-2.46	1.18	1.23
7	J	6003	CFF	O13-C6	-2.46	1.18	1.23
7	A	6003	CFF	C5-C6	-2.45	1.36	1.43
7	G	6003	CFF	C5-C6	-2.45	1.36	1.43
7	J	6003	CFF	C5-C6	-2.45	1.36	1.43
7	D	6003	CFF	C5-C6	-2.43	1.36	1.43
7	A	6003	CFF	O11-C2	-2.34	1.18	1.22
7	D	6003	CFF	O11-C2	-2.34	1.18	1.22
7	G	6003	CFF	O11-C2	-2.34	1.18	1.22
7	J	6003	CFF	O11-C2	-2.34	1.18	1.22
7	A	6003	CFF	C2-N3	-2.20	1.34	1.39
7	D	6003	CFF	C2-N3	-2.20	1.34	1.39
7	G	6003	CFF	C2-N3	-2.20	1.34	1.39
7	J	6003	CFF	C2-N3	-2.20	1.34	1.39
6	A	6002	ATP	C8-N9	-2.03	1.34	1.37
6	D	6002	ATP	C8-N9	-2.03	1.34	1.37
6	G	6002	ATP	C8-N9	-2.03	1.34	1.37
6	J	6002	ATP	C8-N9	-2.03	1.34	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	6003	CFF	C14-N7-C8	-7.57	112.12	126.28
7	A	6003	CFF	C14-N7-C8	-7.55	112.15	126.28
7	G	6003	CFF	C14-N7-C8	-7.55	112.15	126.28
7	J	6003	CFF	C14-N7-C8	-7.55	112.15	126.28
6	A	6002	ATP	C5-C4-N3	-5.17	119.59	126.72
6	D	6002	ATP	C5-C4-N3	-5.17	119.59	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	6002	ATP	C5-C4-N3	-5.17	119.59	126.72
6	J	6002	ATP	C5-C4-N3	-5.17	119.59	126.72
7	D	6003	CFF	C14-N7-C5	4.99	139.66	127.77
7	A	6003	CFF	C14-N7-C5	4.98	139.62	127.77
7	G	6003	CFF	C14-N7-C5	4.98	139.62	127.77
7	J	6003	CFF	C14-N7-C5	4.98	139.62	127.77
7	A	6003	CFF	C5-C6-N1	4.36	120.05	112.06
7	G	6003	CFF	C5-C6-N1	4.36	120.05	112.06
7	J	6003	CFF	C5-C6-N1	4.36	120.05	112.06
7	D	6003	CFF	C5-C6-N1	4.34	120.01	112.06
6	A	6002	ATP	N3-C4-N9	4.27	134.42	127.17
6	D	6002	ATP	N3-C4-N9	4.27	134.42	127.17
6	G	6002	ATP	N3-C4-N9	4.27	134.42	127.17
6	J	6002	ATP	N3-C4-N9	4.27	134.42	127.17
6	A	6002	ATP	N3-C2-N1	-4.19	122.24	128.58
6	D	6002	ATP	N3-C2-N1	-4.19	122.24	128.58
6	G	6002	ATP	N3-C2-N1	-4.19	122.24	128.58
6	J	6002	ATP	N3-C2-N1	-4.19	122.24	128.58
6	A	6002	ATP	C2-N3-C4	3.71	120.89	111.83
6	D	6002	ATP	C2-N3-C4	3.71	120.89	111.83
6	G	6002	ATP	C2-N3-C4	3.71	120.89	111.83
6	J	6002	ATP	C2-N3-C4	3.71	120.89	111.83
7	D	6003	CFF	N3-C4-N9	3.40	131.62	126.27
7	A	6003	CFF	N3-C4-N9	3.38	131.59	126.27
7	G	6003	CFF	N3-C4-N9	3.38	131.59	126.27
7	J	6003	CFF	N3-C4-N9	3.38	131.59	126.27
7	A	6003	CFF	C6-N1-C2	-3.16	120.53	125.66
7	D	6003	CFF	C6-N1-C2	-3.16	120.53	125.66
7	G	6003	CFF	C6-N1-C2	-3.16	120.53	125.66
7	J	6003	CFF	C6-N1-C2	-3.16	120.53	125.66
7	A	6003	CFF	N7-C8-N9	-2.97	108.09	113.48
7	D	6003	CFF	N7-C8-N9	-2.97	108.09	113.48
7	G	6003	CFF	N7-C8-N9	-2.97	108.09	113.48
7	J	6003	CFF	N7-C8-N9	-2.97	108.09	113.48
7	A	6003	CFF	O13-C6-C5	-2.80	120.65	126.38
7	D	6003	CFF	O13-C6-C5	-2.80	120.65	126.38
7	G	6003	CFF	O13-C6-C5	-2.80	120.65	126.38
7	J	6003	CFF	O13-C6-C5	-2.80	120.65	126.38
7	A	6003	CFF	C6-C5-C4	-2.62	119.62	122.92
7	G	6003	CFF	C6-C5-C4	-2.62	119.62	122.92
7	J	6003	CFF	C6-C5-C4	-2.62	119.62	122.92
7	D	6003	CFF	C6-C5-C4	-2.59	119.65	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6002	ATP	C3'-C2'-C1'	2.53	106.25	101.46
6	D	6002	ATP	C3'-C2'-C1'	2.53	106.25	101.46
6	G	6002	ATP	C3'-C2'-C1'	2.53	106.25	101.46
6	J	6002	ATP	C3'-C2'-C1'	2.53	106.25	101.46
6	A	6002	ATP	C2-N1-C6	2.30	122.51	118.73
6	D	6002	ATP	C2-N1-C6	2.30	122.51	118.73
6	G	6002	ATP	C2-N1-C6	2.30	122.51	118.73
6	J	6002	ATP	C2-N1-C6	2.30	122.51	118.73
7	A	6003	CFF	N3-C2-N1	2.15	119.82	117.14
7	D	6003	CFF	N3-C2-N1	2.15	119.82	117.14
7	G	6003	CFF	N3-C2-N1	2.15	119.82	117.14
7	J	6003	CFF	N3-C2-N1	2.15	119.82	117.14

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C5'-O5'-PA-O3A
6	D	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C5'-O5'-PA-O3A
6	G	6002	ATP	C5'-O5'-PA-O2A
6	G	6002	ATP	C5'-O5'-PA-O3A
6	J	6002	ATP	C5'-O5'-PA-O2A
6	J	6002	ATP	C5'-O5'-PA-O3A
6	A	6002	ATP	C3'-C4'-C5'-O5'
6	D	6002	ATP	C3'-C4'-C5'-O5'
6	G	6002	ATP	C3'-C4'-C5'-O5'
6	J	6002	ATP	C3'-C4'-C5'-O5'
6	A	6002	ATP	O4'-C4'-C5'-O5'
6	D	6002	ATP	O4'-C4'-C5'-O5'
6	G	6002	ATP	O4'-C4'-C5'-O5'
6	J	6002	ATP	O4'-C4'-C5'-O5'
6	A	6002	ATP	PB-O3A-PA-O5'
6	D	6002	ATP	PB-O3A-PA-O5'
6	G	6002	ATP	PB-O3A-PA-O5'
6	J	6002	ATP	PB-O3A-PA-O5'
6	A	6002	ATP	C5'-O5'-PA-O1A
6	D	6002	ATP	C5'-O5'-PA-O1A
6	G	6002	ATP	C5'-O5'-PA-O1A
6	J	6002	ATP	C5'-O5'-PA-O1A
6	A	6002	ATP	O4'-C1'-N9-C8

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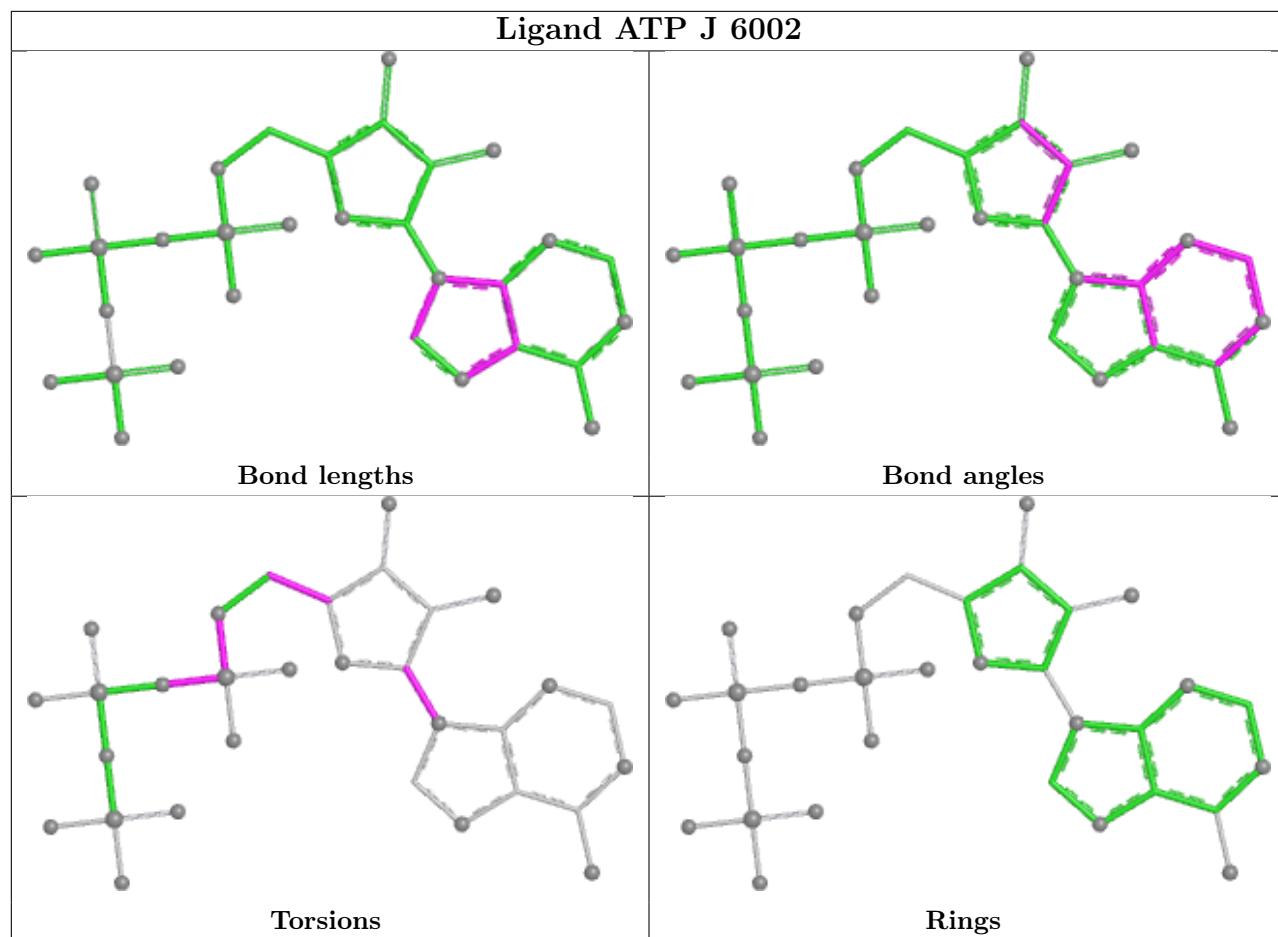
Mol	Chain	Res	Type	Atoms
6	D	6002	ATP	O4'-C1'-N9-C8
6	G	6002	ATP	O4'-C1'-N9-C8
6	J	6002	ATP	O4'-C1'-N9-C8

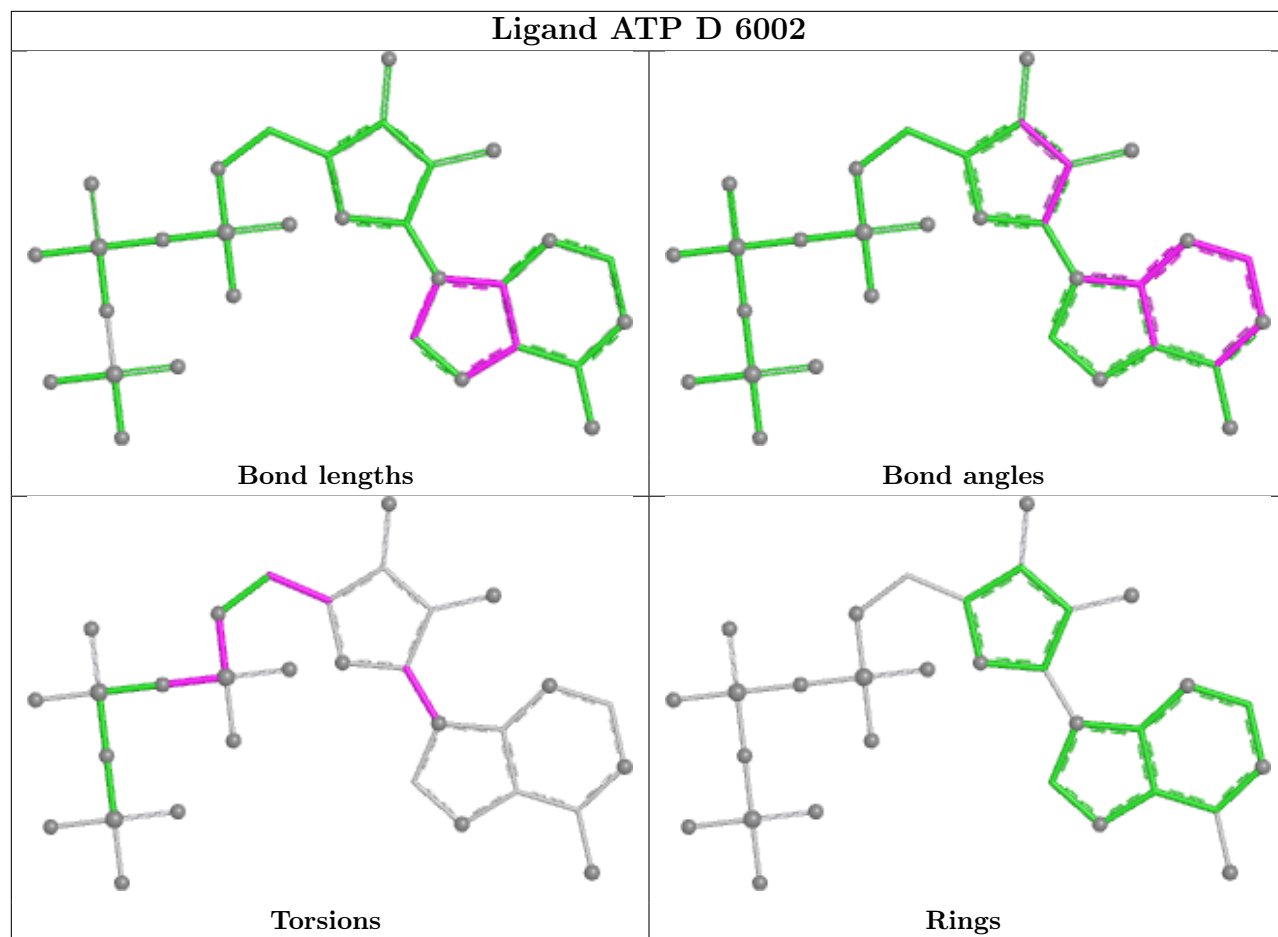
There are no ring outliers.

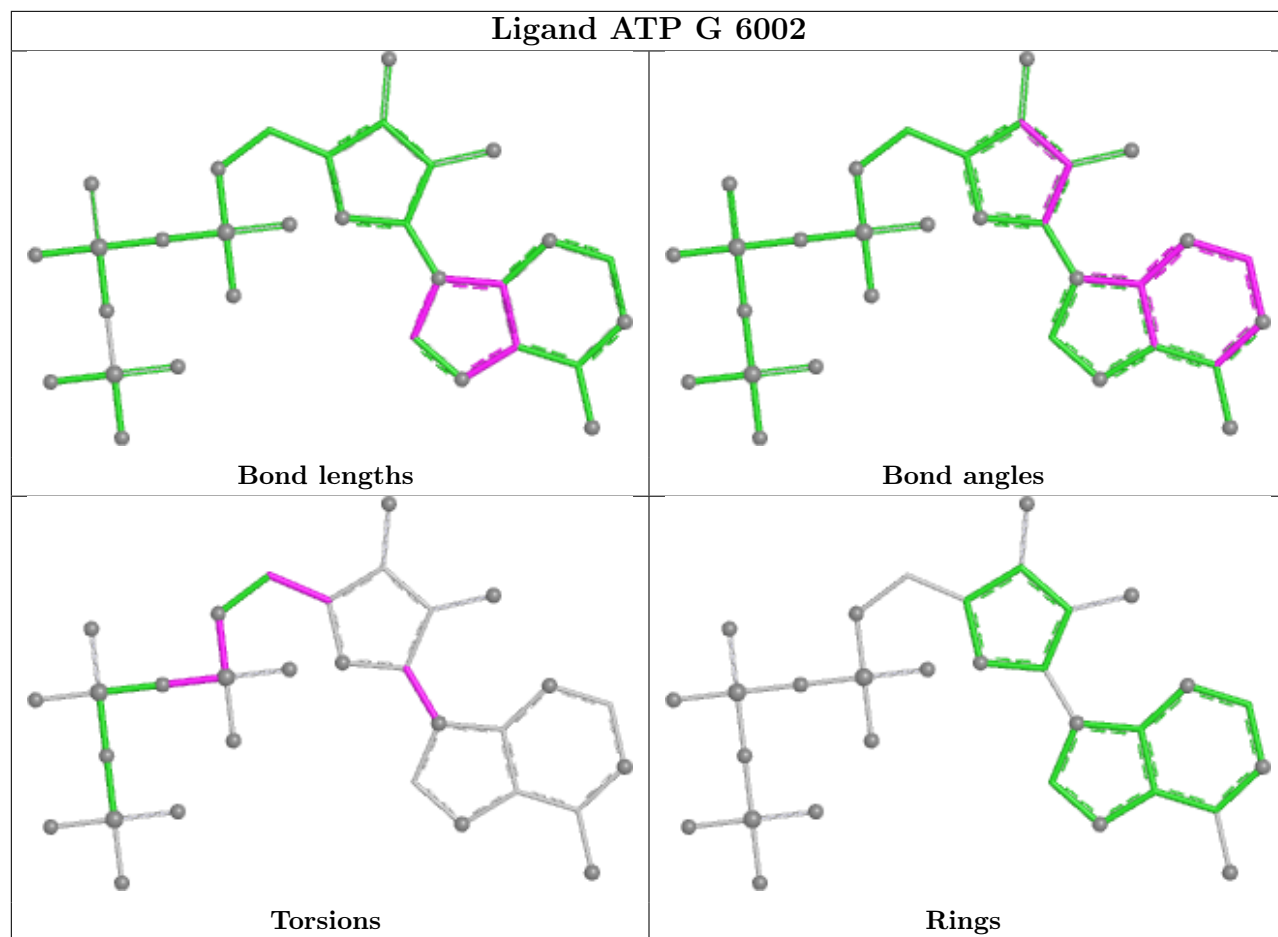
7 monomers are involved in 7 short contacts:

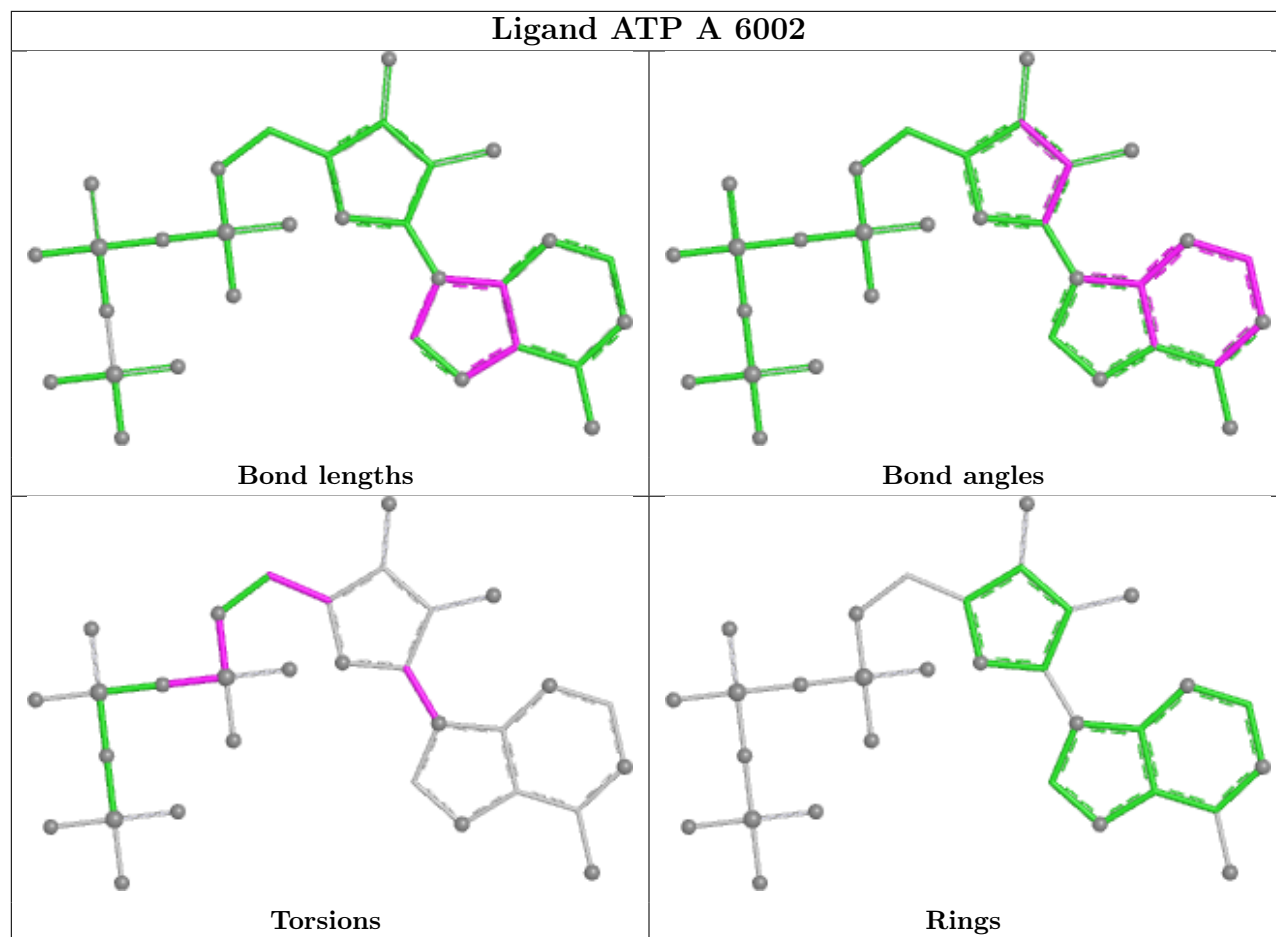
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	6003	CFF	1	0
7	J	6003	CFF	1	0
6	J	6002	ATP	1	0
7	G	6003	CFF	1	0
7	A	6003	CFF	1	0
6	G	6002	ATP	1	0
6	A	6002	ATP	1	0

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 than 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.









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.

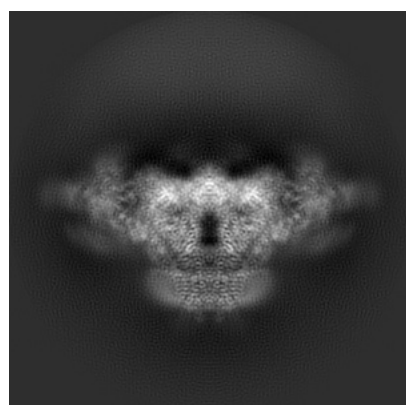
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9880. These allow visual inspection of the internal detail of the map and identification of artifacts.

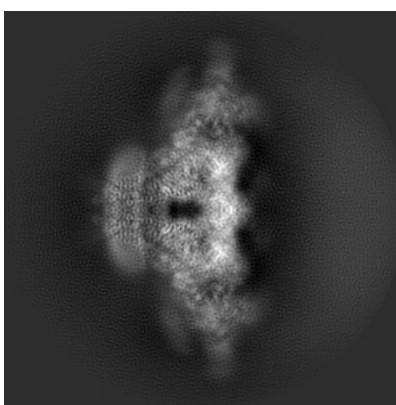
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

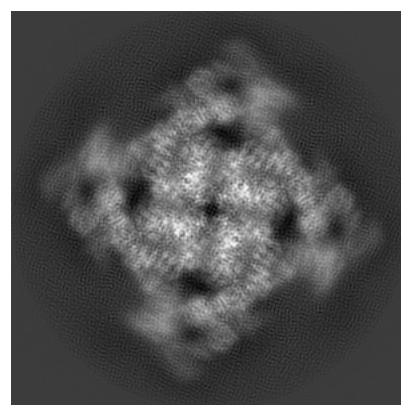
6.1.1 Primary map



X



Y

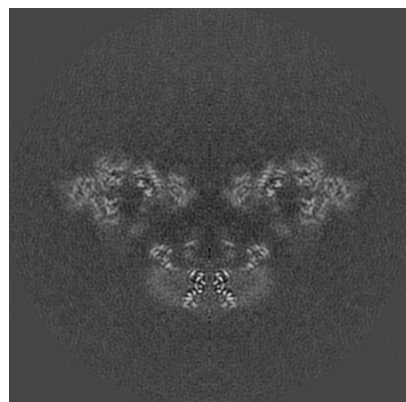


Z

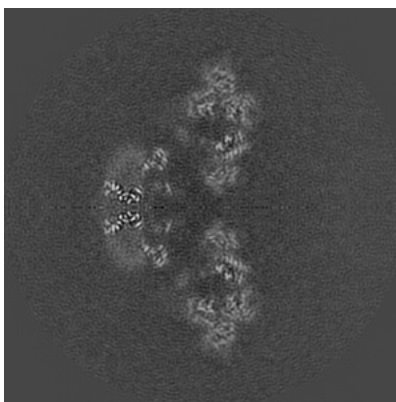
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

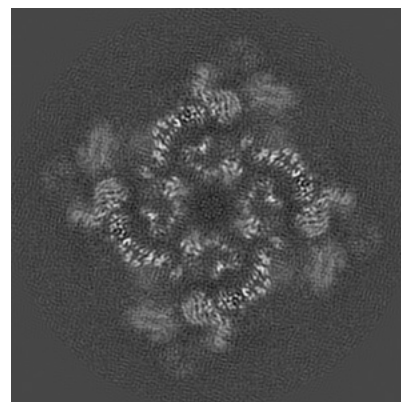
6.2.1 Primary map



X Index: 200



Y Index: 200

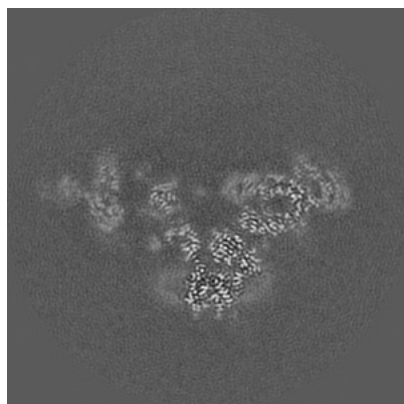


Z Index: 200

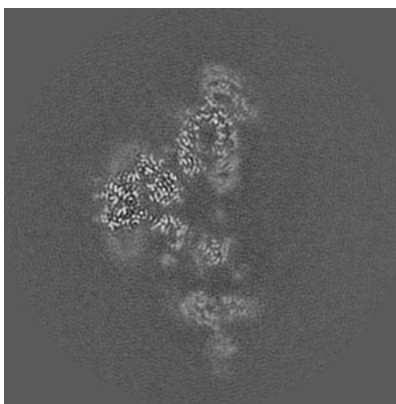
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

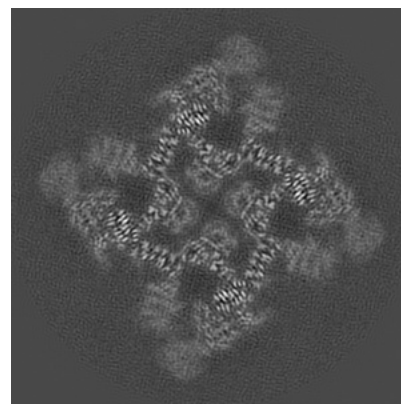
6.3.1 Primary map



X Index: 187



Y Index: 213

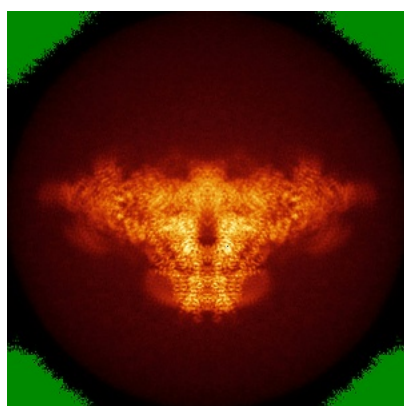


Z Index: 212

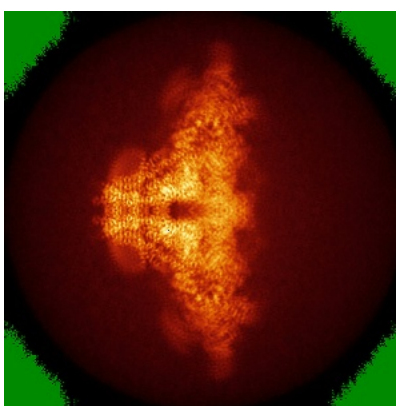
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

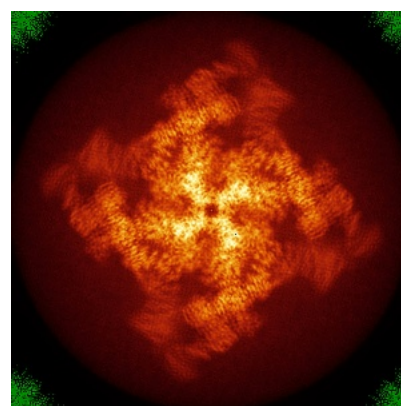
6.4.1 Primary map



X



Y

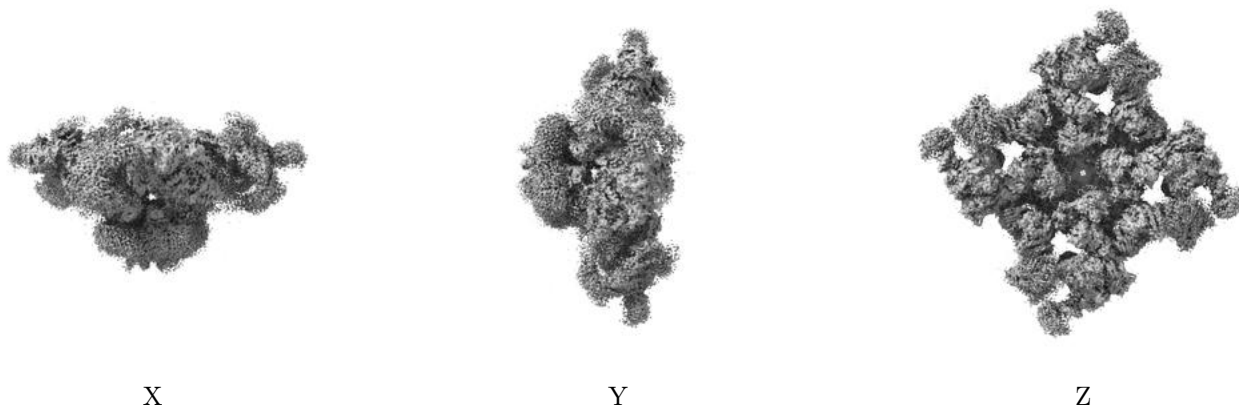


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

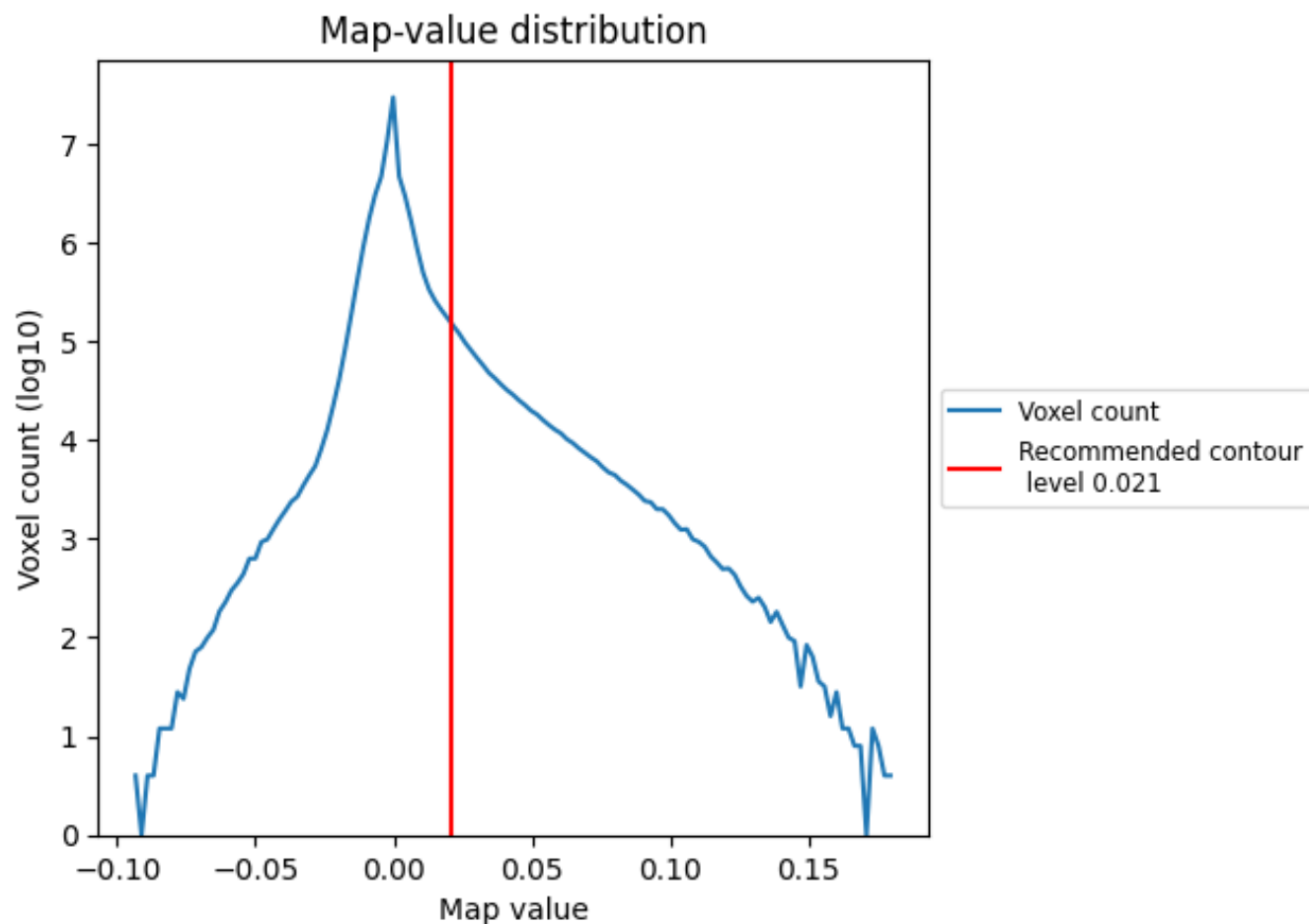
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

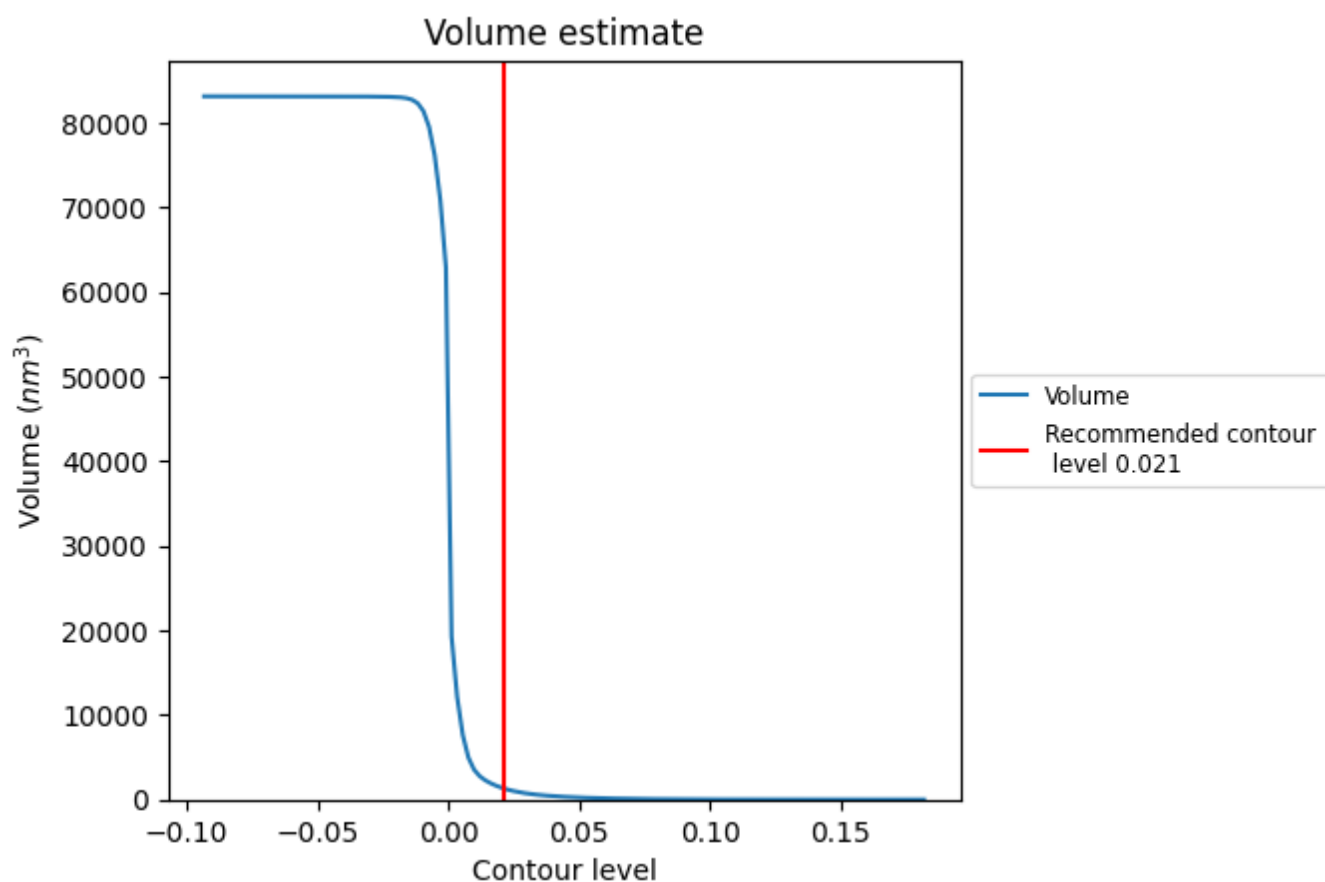
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

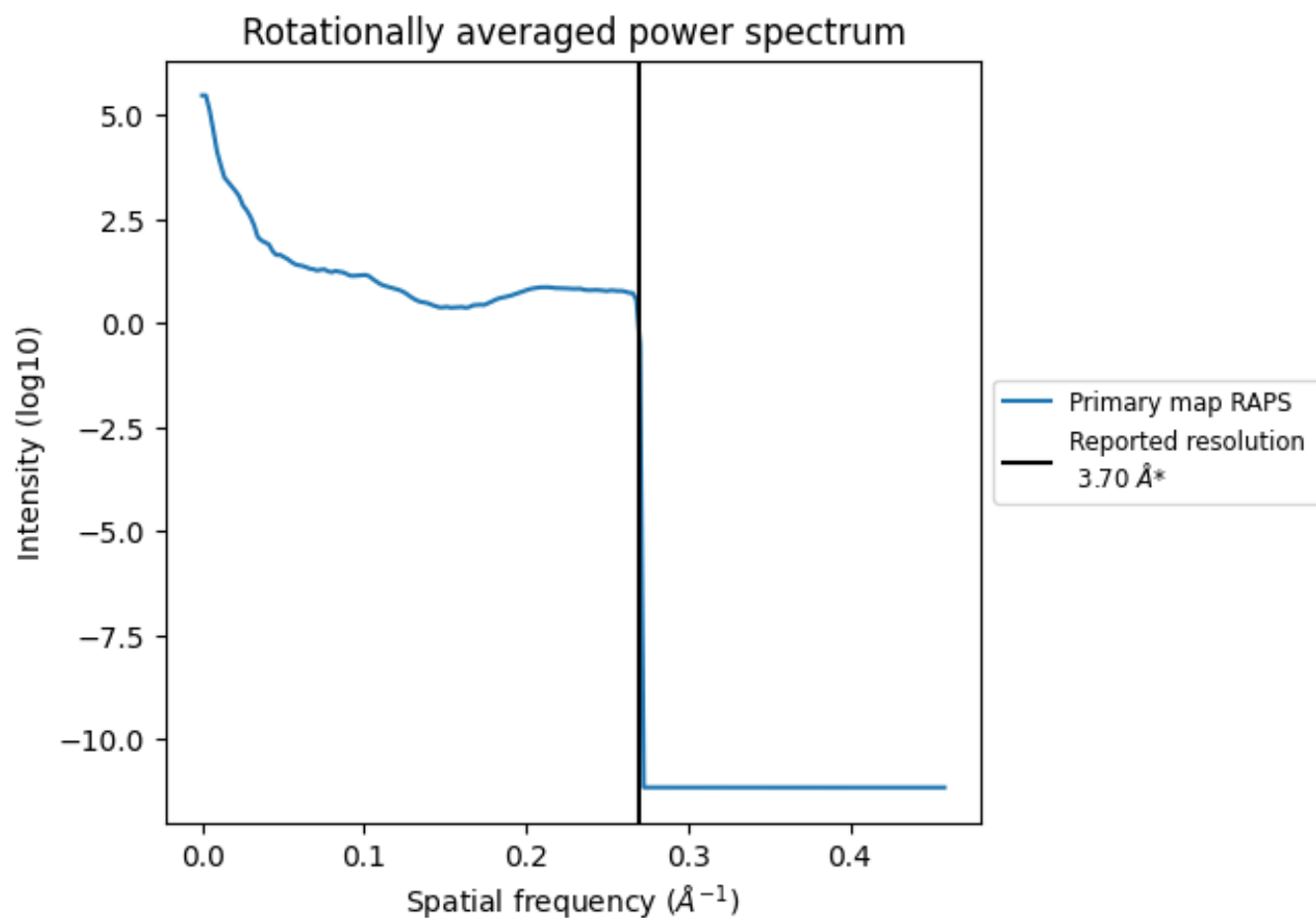
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1340 nm³; this corresponds to an approximate mass of 1210 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

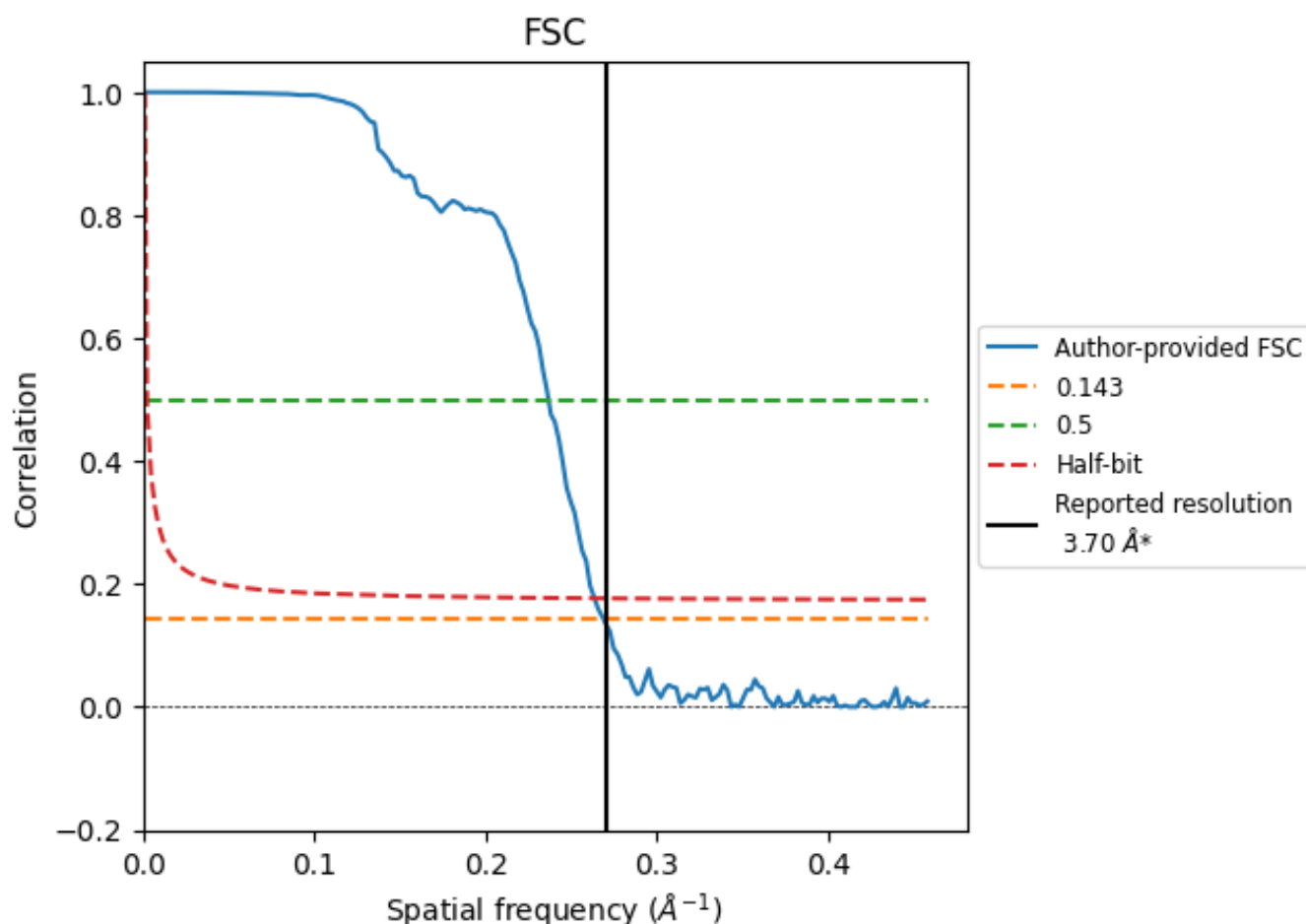


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

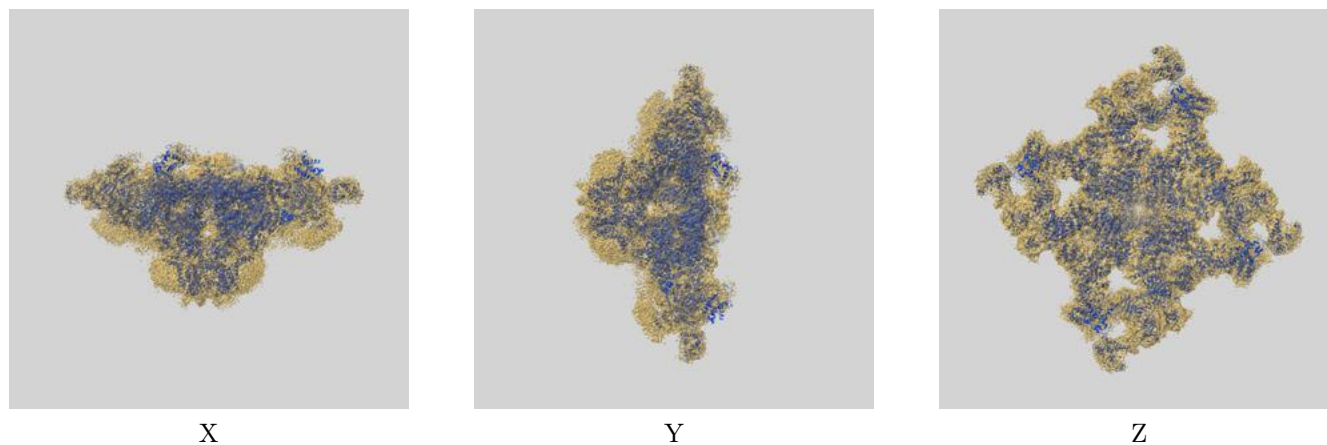
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.22	3.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

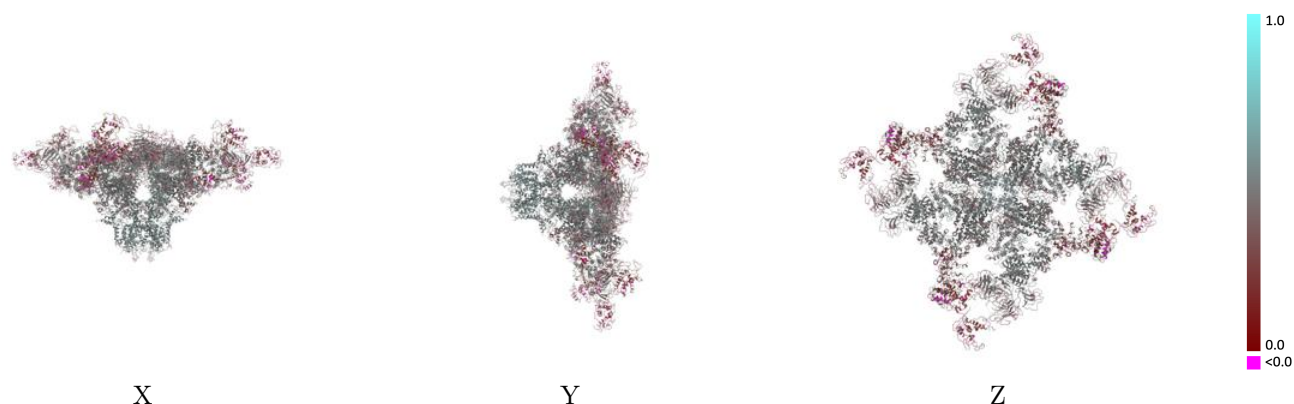
This section contains information regarding the fit between EMDB map EMD-9880 and PDB model 6JRS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

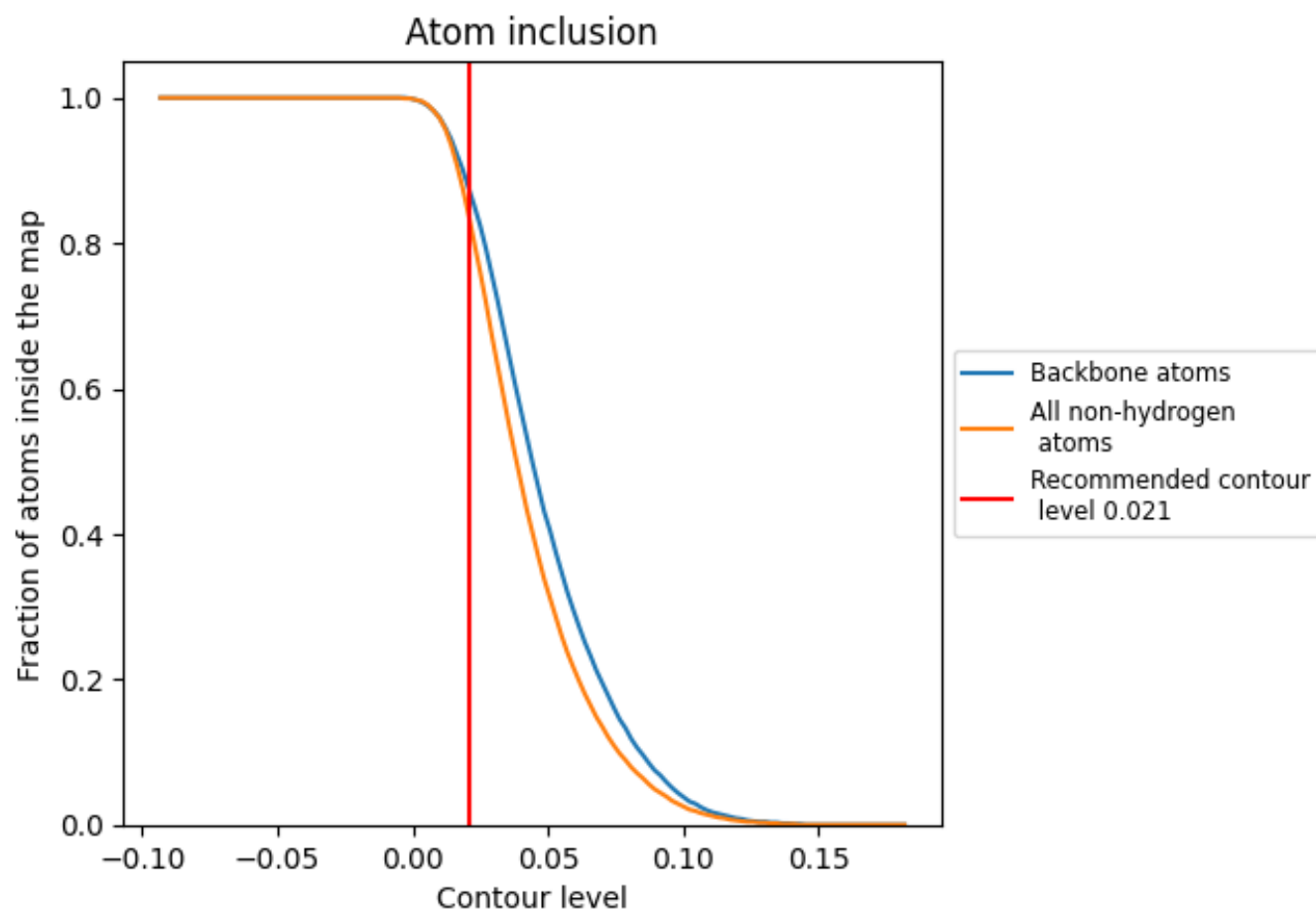


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8320	0.4210
A	0.8420	0.4240
B	0.9010	0.4500
C	0.2030	0.2530
D	0.8430	0.4240
E	0.9010	0.4470
F	0.2050	0.2570
G	0.8420	0.4240
H	0.9060	0.4470
I	0.2050	0.2560
J	0.8430	0.4230
K	0.9000	0.4460
L	0.2010	0.2520

