



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:19 AM UTC

PDB ID : 7YZY / pdb_00007zyz
EMDB ID : EMD-14399
Title : pMMO structure from native membranes by cryoET and STA
Authors : Zhu, Y.; Ni, T.; Zhang, P.
Deposited on : 2022-02-21
Resolution : 4.80 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
MolProbity : 4-5-2 with Phenix2.0
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

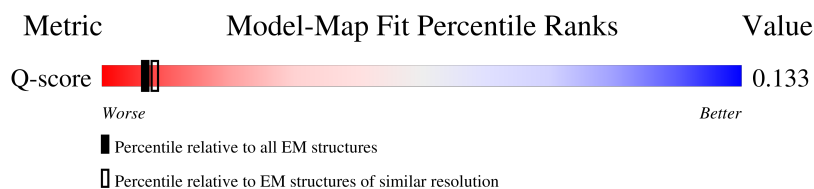
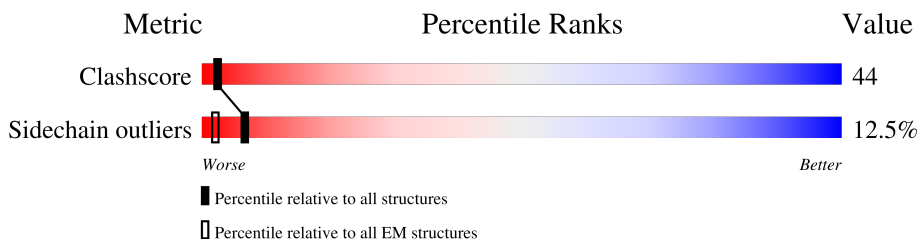
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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	B	247	
1	F	247	
1	J	247	
2	C	289	
2	G	289	

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Mol	Chain	Length	Quality of chain
2	K	289	32% 43% 32% 7% 18%
3	A	414	33% 55% 32% 6% 8%
3	E	414	33% 54% 32% 6% 8%
3	I	414	33% 55% 32% 6% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20364 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 Particulate methane monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	218	Total	C	N	O	S	0	0
			1796	1216	284	286	10		
1	F	218	Total	C	N	O	S	0	0
			1796	1216	284	286	10		
1	J	218	Total	C	N	O	S	0	0
			1796	1216	284	286	10		

- Molecule 2 is a protein called Methane monooxygenase subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	238	Total	C	N	O	S	0	0
			1975	1339	300	331	5		
2	G	238	Total	C	N	O	S	0	0
			1975	1339	300	331	5		
2	K	238	Total	C	N	O	S	0	0
			1975	1339	300	331	5		

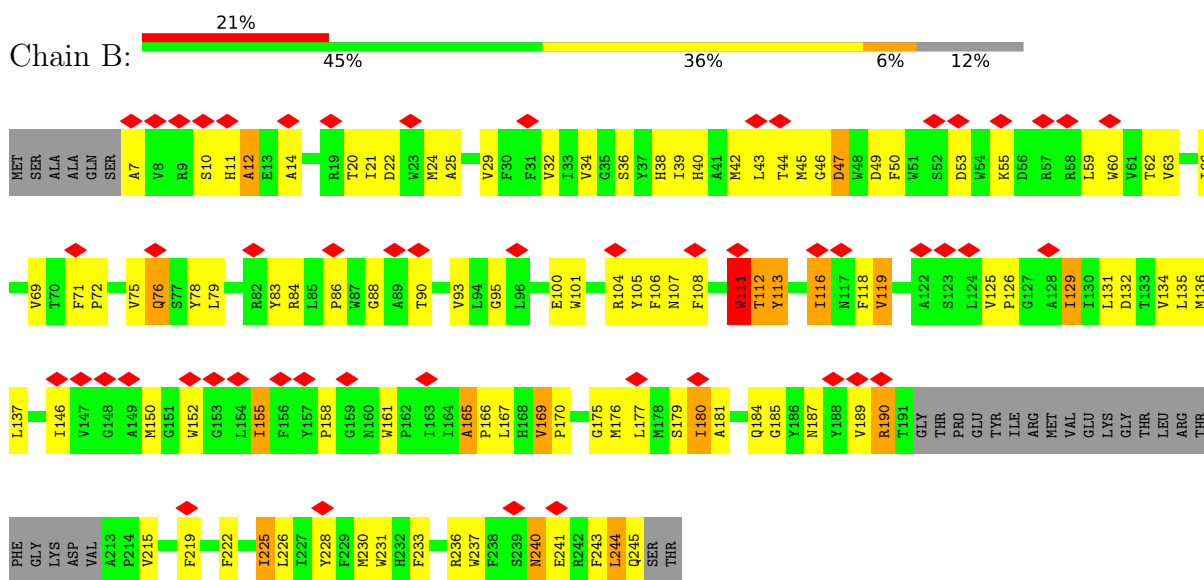
- Molecule 3 is a protein called Particulate methane monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
3	E	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
3	I	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		

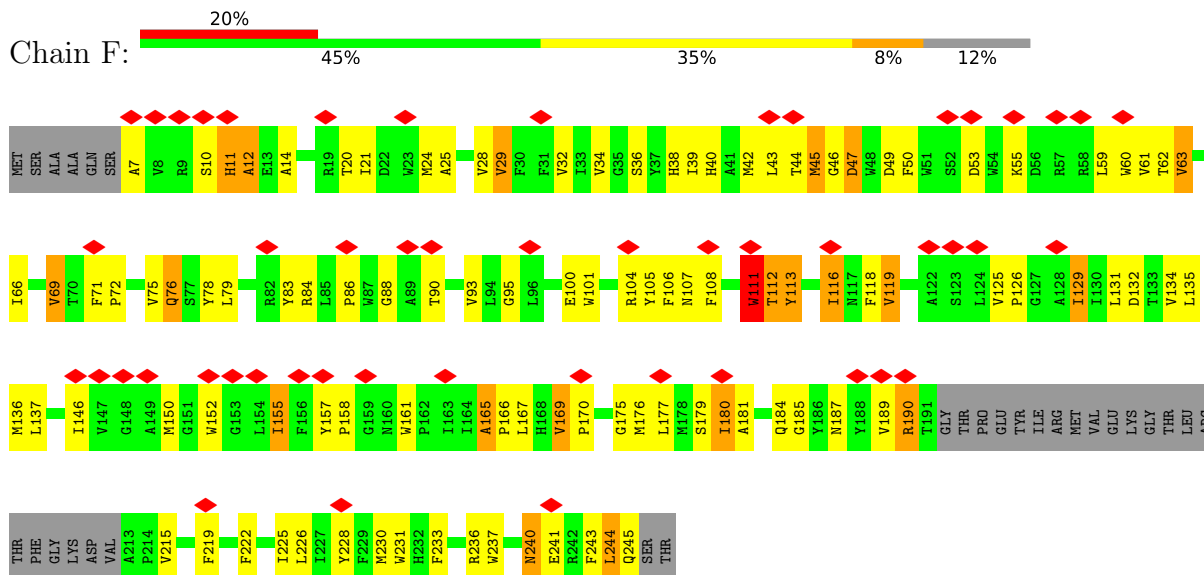
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

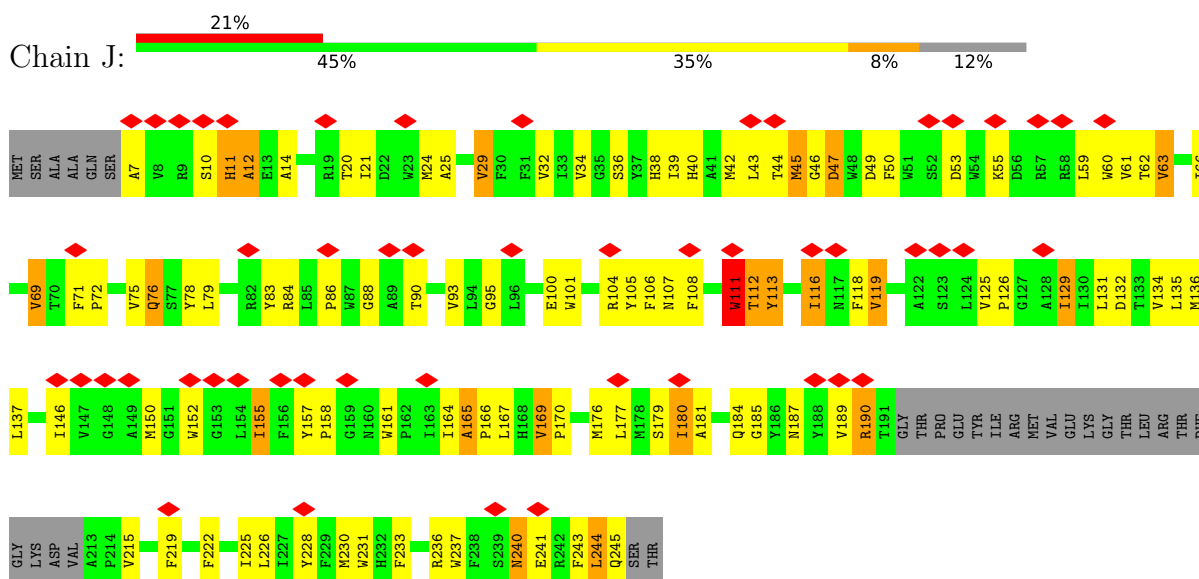
- Molecule 1: Particulate methane monooxygenase beta subunit



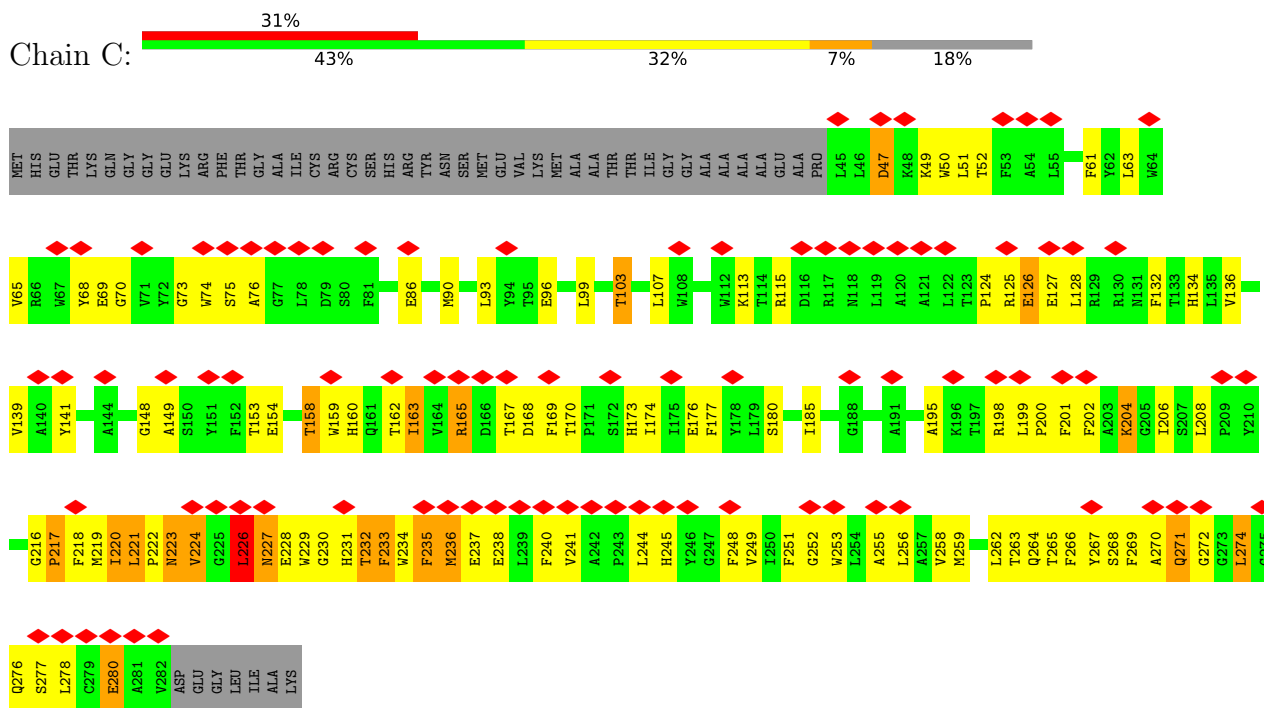
- Molecule 1: Particulate methane monooxygenase beta subunit



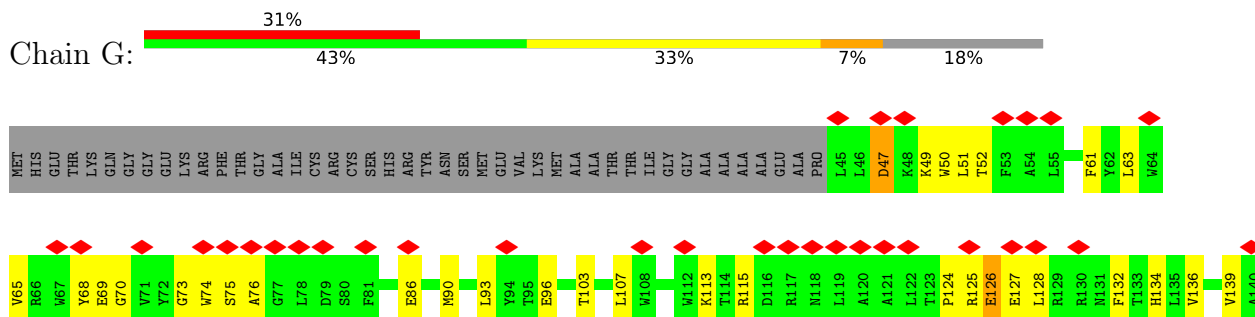
- Molecule 1: Particulate methane monooxygenase beta subunit

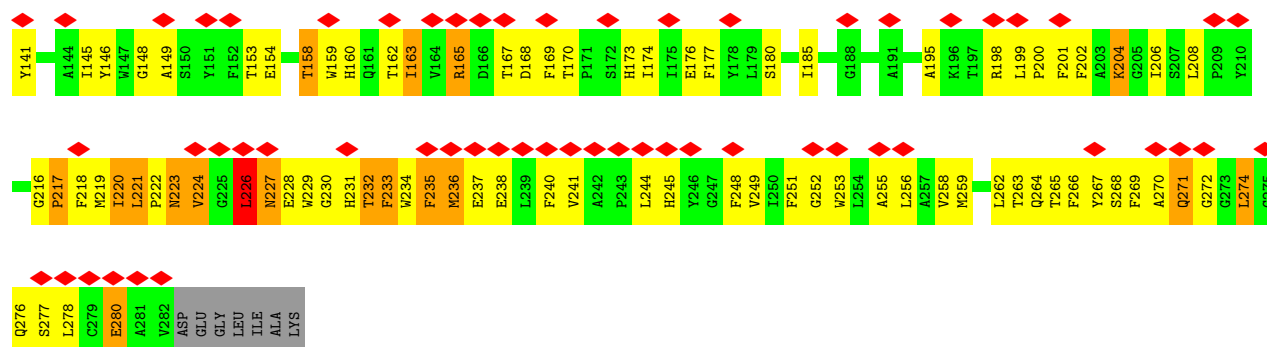


• Molecule 2: Methane monooxygenase subunit C2

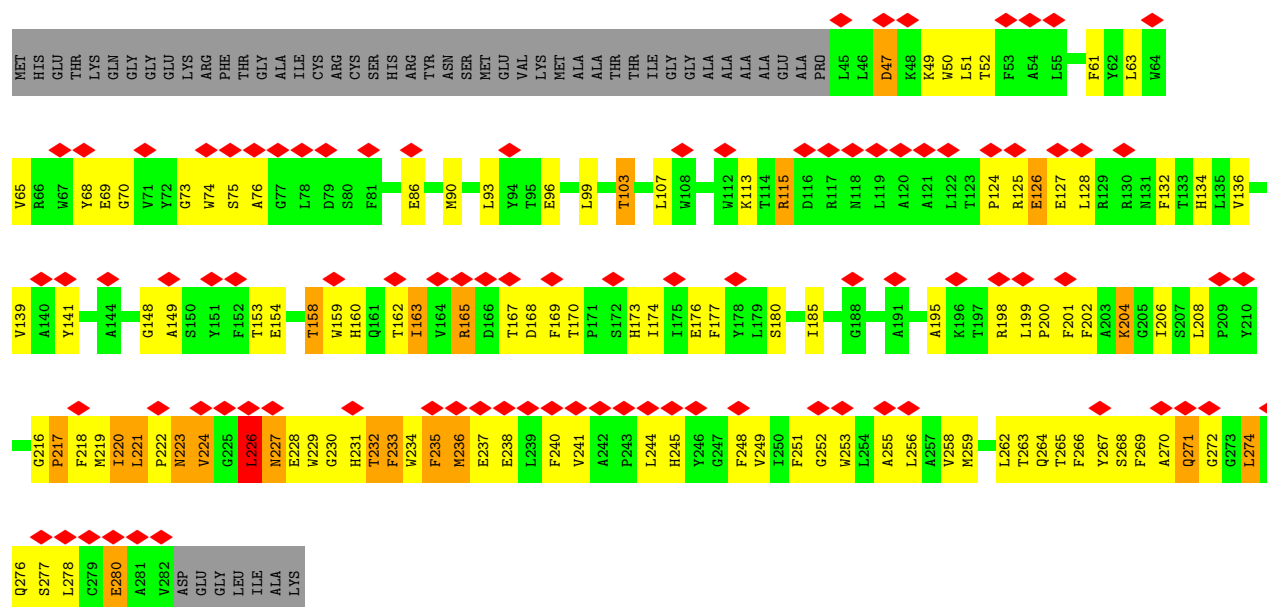
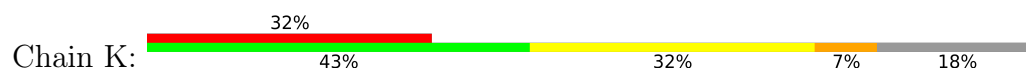


• Molecule 2: Methane monooxygenase subunit C2

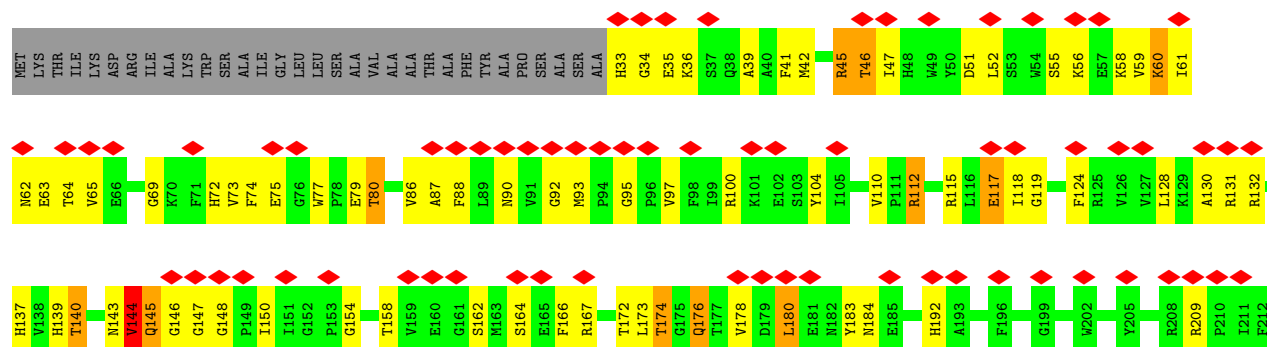


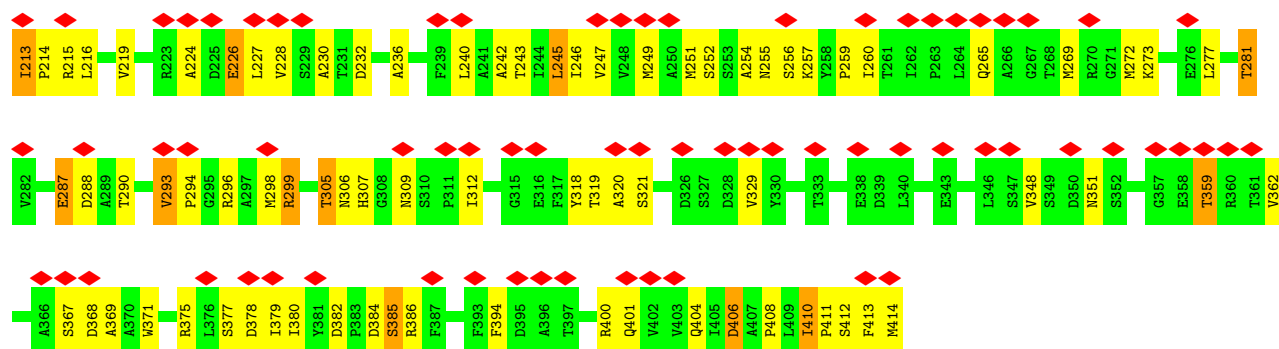


• Molecule 2: Methane monooxygenase subunit C2

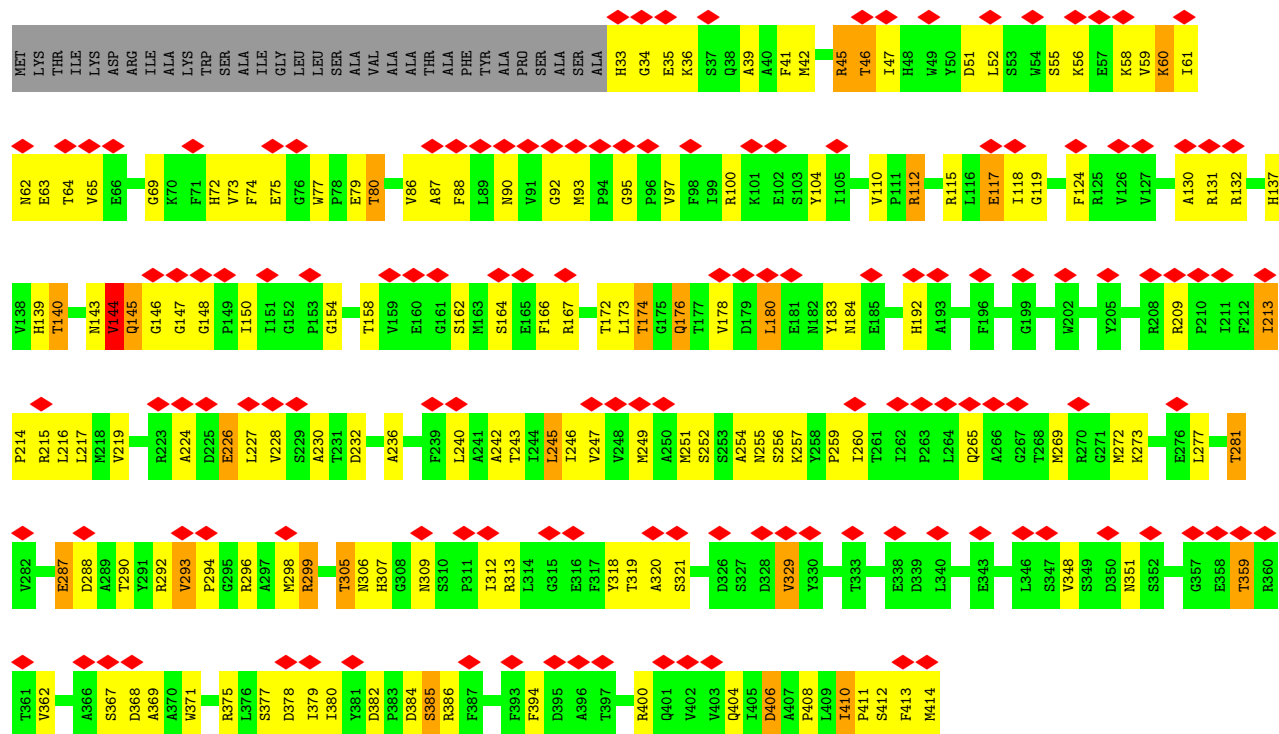


• Molecule 3: Particulate methane monooxygenase alpha subunit

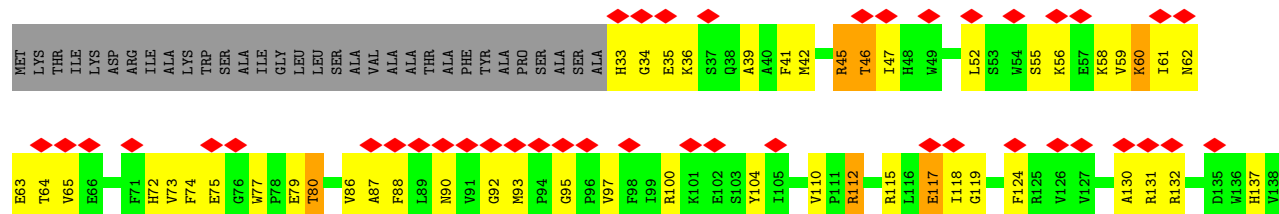


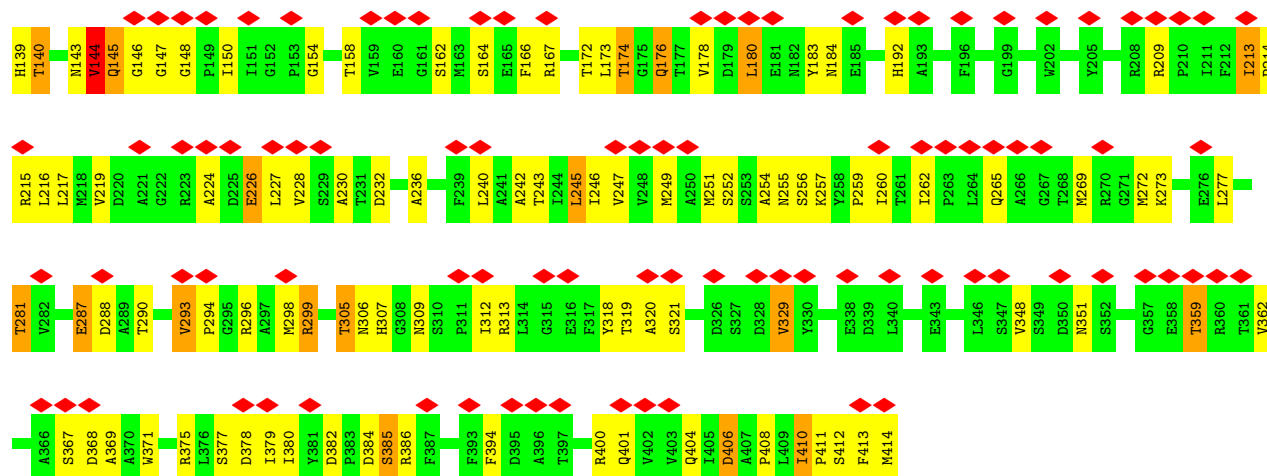


• Molecule 3: Particulate methane monooxygenase alpha subunit



• Molecule 3: Particulate methane monooxygenase alpha subunit





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	127417	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 ($e^-/\text{\AA}^2$)	129	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0109	Depositor
Map size (Å)	241.20001, 241.20001, 241.20001	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.87	0/1868	1.09	12/2560 (0.5%)
1	F	0.87	0/1868	1.10	11/2560 (0.4%)
1	J	0.87	0/1868	1.10	11/2560 (0.4%)
2	C	0.71	0/2052	1.04	5/2811 (0.2%)
2	G	0.71	0/2052	1.04	5/2811 (0.2%)
2	K	0.71	0/2052	1.04	5/2811 (0.2%)
3	A	0.97	1/3099 (0.0%)	1.14	9/4215 (0.2%)
3	E	0.97	1/3099 (0.0%)	1.14	9/4215 (0.2%)
3	I	0.97	1/3099 (0.0%)	1.14	9/4215 (0.2%)
All	All	0.87	3/21057 (0.0%)	1.10	76/28758 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	130	ALA	CA-CB	-5.06	1.45	1.53
3	E	130	ALA	CA-CB	-5.04	1.45	1.53
3	I	130	ALA	CA-CB	-5.04	1.45	1.53

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	50	TRP	N-CA-C	-9.23	101.79	113.23
2	G	50	TRP	N-CA-C	-9.22	101.80	113.23
2	K	50	TRP	N-CA-C	-9.22	101.80	113.23
1	B	113	TYR	N-CA-C	7.89	120.59	110.65
1	J	113	TYR	N-CA-C	7.87	120.57	110.65
1	F	113	TYR	N-CA-C	7.86	120.55	110.65
3	A	80	THR	CA-C-N	-6.72	114.16	123.10
3	A	80	THR	C-N-CA	-6.72	114.16	123.10
3	I	80	THR	CA-C-N	-6.71	114.17	123.10
3	I	80	THR	C-N-CA	-6.71	114.17	123.10
3	E	80	THR	CA-C-N	-6.71	114.18	123.10
3	E	80	THR	C-N-CA	-6.71	114.18	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	144	VAL	N-CA-C	6.55	122.97	109.34
3	I	144	VAL	N-CA-C	6.53	122.93	109.34
3	A	144	VAL	N-CA-C	6.53	122.92	109.34
3	A	329	VAL	N-CA-C	6.40	117.50	112.12
3	I	329	VAL	N-CA-C	6.37	117.47	112.12
3	E	329	VAL	N-CA-C	6.32	117.43	112.12
3	A	309	ASN	N-CA-C	6.31	118.91	108.49
3	I	309	ASN	N-CA-C	6.31	118.89	108.49
2	C	168	ASP	N-CA-C	-6.30	105.65	113.15
3	E	309	ASN	N-CA-C	6.30	118.88	108.49
2	K	168	ASP	N-CA-C	-6.29	105.66	113.15
2	G	168	ASP	N-CA-C	-6.28	105.67	113.15
2	K	226	LEU	CA-C-N	6.26	128.99	120.54
2	K	226	LEU	C-N-CA	6.26	128.99	120.54
2	C	226	LEU	CA-C-N	6.25	128.98	120.54
2	C	226	LEU	C-N-CA	6.25	128.98	120.54
2	G	226	LEU	CA-C-N	6.24	128.96	120.54
2	G	226	LEU	C-N-CA	6.24	128.96	120.54
1	B	47	ASP	N-CA-C	5.97	119.88	112.24
1	F	12	ALA	N-CA-C	-5.96	106.65	114.04
1	B	12	ALA	N-CA-C	-5.95	106.66	114.04
1	F	47	ASP	N-CA-C	5.95	119.86	112.24
1	J	12	ALA	N-CA-C	-5.95	106.67	114.04
1	J	47	ASP	N-CA-C	5.95	119.85	112.24
3	E	329	VAL	CB-CA-C	-5.67	105.35	110.91
3	A	329	VAL	CB-CA-C	-5.64	105.38	110.91
2	G	271	GLN	OE1-CD-NE2	-5.63	116.97	122.60
3	I	329	VAL	CB-CA-C	-5.62	105.40	110.91
2	K	271	GLN	OE1-CD-NE2	-5.59	117.01	122.60
2	C	271	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	F	165	ALA	CA-C-N	-5.38	113.11	119.84
1	F	165	ALA	C-N-CA	-5.38	113.11	119.84
3	E	226	GLU	N-CA-C	-5.38	106.56	113.23
1	J	165	ALA	CA-C-N	-5.38	113.12	119.84
1	J	165	ALA	C-N-CA	-5.38	113.12	119.84
3	I	226	GLU	N-CA-C	-5.36	106.58	113.23
3	A	226	GLU	N-CA-C	-5.35	106.59	113.23
1	F	112	THR	CA-C-N	-5.35	114.43	122.24
1	F	112	THR	C-N-CA	-5.35	114.43	122.24
1	B	165	ALA	CA-C-N	-5.34	113.17	119.84
1	B	165	ALA	C-N-CA	-5.34	113.17	119.84
1	B	112	THR	CA-C-N	-5.33	114.45	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	THR	C-N-CA	-5.33	114.45	122.24
1	J	112	THR	CA-C-N	-5.33	114.46	122.24
1	J	112	THR	C-N-CA	-5.33	114.46	122.24
1	J	119	VAL	N-CA-C	5.27	116.60	111.91
1	F	119	VAL	N-CA-C	5.27	116.60	111.91
1	B	119	VAL	N-CA-C	5.23	116.57	111.91
1	J	189	VAL	N-CA-C	5.18	115.06	108.12
1	F	189	VAL	N-CA-C	5.17	115.05	108.12
1	B	189	VAL	N-CA-C	5.17	115.04	108.12
1	J	111	TRP	CA-CB-CG	5.15	123.39	113.60
1	F	111	TRP	CA-CB-CG	5.14	123.38	113.60
1	B	111	TRP	CA-CB-CG	5.13	123.36	113.60
3	E	410	ILE	N-CA-C	5.08	113.43	107.89
3	I	410	ILE	N-CA-C	5.07	113.41	107.89
3	A	410	ILE	N-CA-C	5.07	113.41	107.89
3	I	176	GLN	N-CA-C	5.06	117.23	110.35
3	A	176	GLN	N-CA-C	5.06	117.23	110.35
3	E	176	GLN	N-CA-C	5.04	117.21	110.35
1	F	244	LEU	N-CA-C	5.03	121.52	110.80
1	J	244	LEU	N-CA-C	5.03	121.52	110.80
1	B	244	LEU	N-CA-C	5.03	121.51	110.80
1	B	225	ILE	N-CA-C	-5.02	105.81	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1796	0	1751	272	0
1	F	1796	0	1751	275	0
1	J	1796	0	1751	270	0
2	C	1975	0	1908	383	0
2	G	1975	0	1908	390	0
2	K	1975	0	1908	382	0
3	A	3017	0	2980	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3017	0	2980	162	0
3	I	3017	0	2980	164	0
All	All	20364	0	19917	1766	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 44.

All (1766) 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)
2:C:235:PHE:CE1	3:A:146:GLY:HA2	1.22	1.74
2:K:235:PHE:CE1	3:I:146:GLY:HA2	1.22	1.71
1:B:40:HIS:CE1	2:C:253:TRP:CZ2	1.78	1.68
2:G:222:PRO:HB3	1:J:222:PHE:CG	1.29	1.67
1:F:40:HIS:CE1	2:G:253:TRP:CZ2	1.78	1.66
2:G:222:PRO:HB3	1:J:222:PHE:CB	1.22	1.65
2:K:230:GLY:HA3	2:K:244:LEU:CD1	1.18	1.65
2:K:223:ASN:HD21	2:K:248:PHE:CA	1.01	1.64
2:K:231:HIS:H	2:K:244:LEU:CD2	1.04	1.63
1:B:222:PHE:CB	2:K:222:PRO:HB3	1.21	1.62
1:J:40:HIS:CE1	2:K:253:TRP:CZ2	1.78	1.62
2:G:235:PHE:CE1	3:E:146:GLY:HA2	1.22	1.61
1:B:45:MET:SD	1:B:47:ASP:HA	1.40	1.60
2:G:222:PRO:CG	1:J:222:PHE:CD1	1.75	1.60
1:B:222:PHE:CG	2:K:222:PRO:HB3	1.32	1.60
2:C:230:GLY:HA3	2:C:244:LEU:CD1	1.18	1.60
1:F:39:ILE:HG23	2:G:248:PHE:CE2	1.07	1.60
2:C:222:PRO:HB3	1:F:222:PHE:CB	1.22	1.59
2:C:231:HIS:H	2:C:244:LEU:CD2	1.04	1.59
2:G:230:GLY:HA3	2:G:244:LEU:CD1	1.18	1.58
1:B:222:PHE:CD1	2:K:222:PRO:CG	1.79	1.58
2:C:222:PRO:HB3	1:F:222:PHE:CG	1.34	1.58
1:J:43:LEU:HB3	2:K:249:VAL:CG2	1.34	1.57
2:G:231:HIS:H	2:G:244:LEU:CD2	1.04	1.57
1:F:45:MET:SD	1:F:47:ASP:HA	1.41	1.57
1:J:39:ILE:HG23	2:K:248:PHE:CE2	1.07	1.57
1:J:45:MET:SD	1:J:47:ASP:HA	1.41	1.57
1:B:39:ILE:HG23	2:C:248:PHE:CE2	1.07	1.56
2:C:222:PRO:CG	1:F:222:PHE:CD1	1.80	1.56
2:C:223:ASN:HD21	2:C:248:PHE:CA	1.01	1.56
2:G:223:ASN:HD21	2:G:248:PHE:CA	1.01	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:GLY:CA	2:C:244:LEU:HD13	1.37	1.54
1:F:43:LEU:HB3	2:G:249:VAL:CG2	1.34	1.54
1:B:43:LEU:HB3	2:C:249:VAL:CG2	1.34	1.53
2:K:230:GLY:CA	2:K:244:LEU:HD13	1.37	1.53
2:G:230:GLY:CA	2:G:244:LEU:HD13	1.37	1.50
1:B:222:PHE:CD1	2:K:222:PRO:HG3	0.98	1.48
2:C:222:PRO:HG3	1:F:222:PHE:CD1	0.97	1.48
1:J:39:ILE:CG2	2:K:248:PHE:CE2	1.98	1.47
3:E:144:VAL:HG21	3:E:150:ILE:CD1	1.41	1.46
3:I:144:VAL:HG21	3:I:150:ILE:CD1	1.41	1.46
2:G:222:PRO:HG3	1:J:222:PHE:CD1	0.93	1.46
3:A:144:VAL:HG21	3:A:150:ILE:CD1	1.41	1.46
2:K:235:PHE:CE1	3:I:146:GLY:CA	1.99	1.44
2:G:235:PHE:CE1	3:E:146:GLY:CA	1.99	1.44
1:B:39:ILE:CG2	2:C:248:PHE:CE2	1.98	1.44
2:G:235:PHE:HE1	3:E:146:GLY:CA	1.32	1.43
2:C:235:PHE:CE1	3:A:146:GLY:CA	1.99	1.43
1:F:39:ILE:CG2	2:G:248:PHE:CE2	1.98	1.43
2:G:222:PRO:CB	1:J:222:PHE:HB3	1.50	1.42
2:C:173:HIS:CE1	2:C:228:GLU:OE2	1.72	1.42
2:G:222:PRO:CB	1:J:222:PHE:CG	2.02	1.42
1:B:222:PHE:HB3	2:K:222:PRO:CB	1.49	1.42
2:G:173:HIS:CE1	2:G:228:GLU:OE2	1.72	1.41
2:K:235:PHE:HE1	3:I:146:GLY:CA	1.32	1.41
2:K:173:HIS:CE1	2:K:228:GLU:OE2	1.72	1.41
2:G:223:ASN:ND2	2:G:248:PHE:CA	1.84	1.40
2:C:223:ASN:ND2	2:C:248:PHE:HA	1.38	1.39
2:C:222:PRO:CB	1:F:222:PHE:HB3	1.48	1.39
2:C:235:PHE:HE1	3:A:146:GLY:CA	1.32	1.39
2:C:230:GLY:CA	2:C:244:LEU:CD1	1.94	1.38
2:K:230:GLY:CA	2:K:244:LEU:CD1	1.94	1.38
1:B:222:PHE:CG	2:K:222:PRO:CB	2.05	1.37
2:G:223:ASN:ND2	2:G:248:PHE:HA	1.38	1.37
1:B:146:ILE:HG21	2:K:218:PHE:CE2	1.60	1.37
2:C:222:PRO:CB	1:F:222:PHE:CG	2.06	1.35
2:C:223:ASN:ND2	2:C:248:PHE:CA	1.84	1.35
2:K:223:ASN:ND2	2:K:248:PHE:CA	1.84	1.35
2:C:218:PHE:CE2	1:F:146:ILE:HG21	1.61	1.35
2:G:230:GLY:C	2:G:244:LEU:HD22	1.51	1.35
2:K:230:GLY:C	2:K:244:LEU:HD22	1.51	1.35
2:G:218:PHE:CE2	1:J:146:ILE:HG21	1.60	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:223:ASN:ND2	2:K:248:PHE:HA	1.38	1.34
1:J:45:MET:SD	1:J:47:ASP:CA	2.16	1.33
2:G:230:GLY:CA	2:G:244:LEU:CD1	1.94	1.32
2:C:230:GLY:C	2:C:244:LEU:HD22	1.51	1.32
1:B:45:MET:SD	1:B:47:ASP:CA	2.16	1.31
1:F:40:HIS:CE1	2:G:253:TRP:HZ2	1.25	1.30
1:B:39:ILE:HG23	2:C:248:PHE:CD2	1.65	1.30
1:F:45:MET:SD	1:F:47:ASP:CA	2.17	1.30
1:F:39:ILE:HG23	2:G:248:PHE:CD2	1.65	1.29
1:F:78:TYR:CD2	2:G:259:MET:HE3	1.68	1.29
1:J:39:ILE:HG23	2:K:248:PHE:CD2	1.65	1.29
2:K:231:HIS:N	2:K:244:LEU:HD22	0.96	1.29
1:B:78:TYR:CD2	2:C:259:MET:HE3	1.68	1.28
3:A:293:VAL:HB	3:A:294:PRO:CD	1.63	1.28
2:G:231:HIS:N	2:G:244:LEU:HD22	0.96	1.28
1:J:78:TYR:CD2	2:K:259:MET:HE3	1.68	1.28
2:K:201:PHE:CE1	2:K:267:TYR:HD2	1.52	1.28
2:C:235:PHE:CZ	3:A:146:GLY:HA2	1.69	1.28
2:C:231:HIS:N	2:C:244:LEU:HD22	0.96	1.27
2:K:235:PHE:CE1	3:I:147:GLY:N	2.02	1.27
2:G:235:PHE:CZ	3:E:146:GLY:HA2	1.69	1.27
2:C:226:LEU:O	2:C:244:LEU:HG	1.35	1.26
2:G:177:PHE:CE1	2:G:224:VAL:CG1	2.18	1.26
2:C:201:PHE:CE1	2:C:267:TYR:HD2	1.52	1.26
3:E:293:VAL:HB	3:E:294:PRO:CD	1.63	1.26
2:K:269:PHE:CA	2:K:274:LEU:HD21	1.65	1.26
1:B:40:HIS:CE1	2:C:253:TRP:HZ2	1.25	1.26
1:B:78:TYR:CE2	2:C:259:MET:HE3	1.71	1.25
2:C:177:PHE:CE1	2:C:224:VAL:CG1	2.18	1.25
2:C:235:PHE:CE1	3:A:147:GLY:N	2.02	1.25
2:C:269:PHE:CA	2:C:274:LEU:HD21	1.65	1.25
2:G:201:PHE:CE1	2:G:267:TYR:HD2	1.52	1.25
2:G:235:PHE:CE1	3:E:147:GLY:N	2.02	1.25
2:K:226:LEU:O	2:K:244:LEU:HG	1.35	1.25
2:G:269:PHE:CA	2:G:274:LEU:HD21	1.65	1.25
2:K:177:PHE:CE1	2:K:224:VAL:CG1	2.18	1.25
1:F:78:TYR:CE2	2:G:259:MET:HE3	1.71	1.24
1:J:39:ILE:HG23	2:K:248:PHE:CZ	1.73	1.24
2:K:226:LEU:O	2:K:244:LEU:CG	1.85	1.24
2:C:226:LEU:O	2:C:244:LEU:CG	1.85	1.24
2:K:235:PHE:CZ	3:I:146:GLY:HA2	1.69	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:235:PHE:HE1	3:I:146:GLY:C	1.46	1.24
1:J:40:HIS:CE1	2:K:253:TRP:HZ2	1.25	1.24
1:F:39:ILE:HG23	2:G:248:PHE:CZ	1.73	1.23
2:G:226:LEU:O	2:G:244:LEU:CG	1.85	1.23
2:G:235:PHE:HE1	3:E:146:GLY:C	1.46	1.23
1:J:78:TYR:CE2	2:K:259:MET:HE3	1.71	1.23
1:B:39:ILE:HG23	2:C:248:PHE:CZ	1.73	1.22
2:C:201:PHE:CE1	2:C:267:TYR:CD2	2.27	1.22
2:C:235:PHE:HE1	3:A:146:GLY:C	1.46	1.22
1:J:43:LEU:CD1	2:K:248:PHE:HB3	1.69	1.22
2:G:201:PHE:CE1	2:G:267:TYR:CD2	2.27	1.22
3:I:293:VAL:HB	3:I:294:PRO:CD	1.63	1.22
2:G:226:LEU:O	2:G:244:LEU:HG	1.35	1.22
2:K:224:VAL:CG2	2:K:248:PHE:HD1	1.54	1.21
1:B:43:LEU:CD1	2:C:248:PHE:HB3	1.69	1.21
1:F:43:LEU:CD1	2:G:248:PHE:HB3	1.69	1.21
2:K:201:PHE:CE1	2:K:267:TYR:CD2	2.27	1.21
2:G:269:PHE:CB	2:G:274:LEU:HD21	1.71	1.21
1:B:40:HIS:CE1	2:C:253:TRP:CE2	2.30	1.20
2:C:224:VAL:CG2	2:C:248:PHE:HD1	1.54	1.20
1:F:40:HIS:CE1	2:G:253:TRP:CE2	2.30	1.19
2:C:269:PHE:CB	2:C:274:LEU:HD21	1.71	1.19
2:G:224:VAL:CG2	2:G:248:PHE:HD1	1.54	1.19
2:G:224:VAL:CG2	2:G:248:PHE:CD1	2.25	1.19
2:K:224:VAL:CG2	2:K:248:PHE:CD1	2.25	1.19
2:K:231:HIS:N	2:K:244:LEU:CD2	1.76	1.18
2:K:269:PHE:CB	2:K:274:LEU:HD21	1.71	1.18
2:C:224:VAL:CG2	2:C:248:PHE:CD1	2.25	1.18
1:F:46:GLY:N	2:G:241:VAL:HG13	1.59	1.18
1:J:40:HIS:CE1	2:K:253:TRP:CE2	2.30	1.18
1:B:46:GLY:N	2:C:241:VAL:HG13	1.59	1.18
2:G:219:MET:HE1	1:J:225:ILE:HG21	1.18	1.17
1:J:231:TRP:HZ2	2:K:253:TRP:CH2	1.63	1.17
1:F:43:LEU:CB	2:G:249:VAL:CG2	2.22	1.17
1:B:231:TRP:HZ2	2:C:253:TRP:CH2	1.63	1.17
1:F:43:LEU:CD2	2:G:249:VAL:HG23	1.75	1.17
2:C:219:MET:HE1	1:F:225:ILE:HG21	1.21	1.16
1:J:43:LEU:CB	2:K:249:VAL:CG2	2.22	1.16
1:B:43:LEU:CB	2:C:249:VAL:CG2	2.23	1.16
2:C:231:HIS:N	2:C:244:LEU:CD2	1.76	1.16
1:J:43:LEU:CD2	2:K:249:VAL:HG23	1.75	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HG12	2:C:248:PHE:HZ	1.09	1.16
1:F:46:GLY:N	2:G:241:VAL:CG1	2.09	1.16
1:B:40:HIS:HE1	2:C:253:TRP:CZ2	1.33	1.15
1:B:43:LEU:CD2	2:C:249:VAL:HG23	1.75	1.15
3:E:144:VAL:HG21	3:E:150:ILE:CG1	1.76	1.15
1:F:231:TRP:HZ2	2:G:253:TRP:CH2	1.63	1.15
1:B:222:PHE:HD1	2:K:222:PRO:CG	1.30	1.15
1:J:46:GLY:N	2:K:241:VAL:CG1	2.09	1.15
1:J:46:GLY:N	2:K:241:VAL:HG13	1.59	1.15
1:B:39:ILE:HG12	2:C:248:PHE:CZ	1.82	1.15
2:G:223:ASN:HD21	2:G:248:PHE:N	1.24	1.15
2:K:224:VAL:HG23	2:K:248:PHE:HD1	1.11	1.15
2:G:221:LEU:HB2	2:G:222:PRO:HD3	1.20	1.14
1:B:46:GLY:N	2:C:241:VAL:CG1	2.09	1.14
2:G:269:PHE:HB3	2:G:274:LEU:CD2	1.77	1.14
2:K:173:HIS:HE1	2:K:228:GLU:OE2	0.79	1.14
2:K:269:PHE:HB3	2:K:274:LEU:CD2	1.77	1.14
2:G:173:HIS:HE1	2:G:228:GLU:OE2	0.79	1.14
1:J:39:ILE:HG12	2:K:248:PHE:HZ	1.09	1.14
1:J:43:LEU:HD23	2:K:249:VAL:HG23	1.26	1.14
3:A:144:VAL:HG21	3:A:150:ILE:CG1	1.76	1.14
1:B:43:LEU:HB3	2:C:249:VAL:HG23	1.28	1.14
2:C:269:PHE:HB3	2:C:274:LEU:CD2	1.77	1.14
1:F:43:LEU:CD2	2:G:245:HIS:O	1.96	1.14
2:C:173:HIS:HE1	2:C:228:GLU:OE2	0.79	1.13
2:C:227:ASN:OD1	2:C:238:GLU:OE1	1.67	1.13
1:J:39:ILE:HG12	2:K:248:PHE:CZ	1.82	1.13
1:J:43:LEU:CD2	2:K:245:HIS:O	1.96	1.13
1:F:39:ILE:HG12	2:G:248:PHE:CZ	1.82	1.13
1:F:44:THR:HG23	2:G:249:VAL:HG21	1.28	1.13
1:F:45:MET:SD	1:F:47:ASP:N	2.22	1.13
2:G:201:PHE:CZ	2:G:267:TYR:HD2	1.66	1.12
2:G:219:MET:HE1	1:J:225:ILE:CG2	1.79	1.12
1:J:45:MET:SD	1:J:47:ASP:N	2.22	1.12
1:B:225:ILE:CG2	2:K:219:MET:HE1	1.78	1.12
2:C:127:GLU:OE2	2:C:272:GLY:CA	1.97	1.12
1:J:231:TRP:CZ2	2:K:253:TRP:CH2	2.38	1.12
3:I:144:VAL:HG21	3:I:150:ILE:HD12	1.13	1.12
1:B:43:LEU:CD2	2:C:245:HIS:O	1.96	1.12
1:B:44:THR:HG23	2:C:249:VAL:HG21	1.28	1.12
3:I:144:VAL:HG21	3:I:150:ILE:CG1	1.77	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:HIS:CE1	2:C:238:GLU:OE2	2.02	1.12
2:K:127:GLU:OE2	2:K:272:GLY:CA	1.98	1.12
2:K:160:HIS:CE1	2:K:238:GLU:OE2	2.02	1.12
1:B:231:TRP:CZ2	2:C:253:TRP:CH2	2.38	1.12
2:G:160:HIS:CE1	2:G:238:GLU:OE2	2.02	1.12
1:J:43:LEU:HD21	2:K:245:HIS:O	1.50	1.12
2:K:201:PHE:CZ	2:K:267:TYR:HD2	1.66	1.12
3:I:293:VAL:CG2	3:I:413:PHE:HA	1.80	1.12
2:C:201:PHE:CZ	2:C:267:TYR:HD2	1.66	1.11
2:G:127:GLU:OE2	2:G:272:GLY:CA	1.98	1.11
1:B:45:MET:SD	1:B:47:ASP:N	2.22	1.11
2:C:177:PHE:CE1	2:C:224:VAL:HG11	1.84	1.11
1:F:231:TRP:CZ2	2:G:253:TRP:CH2	2.38	1.11
2:K:165:ARG:NH2	2:K:228:GLU:OE1	1.84	1.11
2:K:227:ASN:OD1	2:K:238:GLU:OE1	1.67	1.11
3:A:293:VAL:CG2	3:A:413:PHE:HA	1.80	1.11
2:G:231:HIS:N	2:G:244:LEU:CD2	1.76	1.11
2:C:219:MET:HE1	1:F:225:ILE:CG2	1.79	1.10
2:C:224:VAL:HG23	2:C:248:PHE:HD1	1.10	1.10
3:A:144:VAL:HG21	3:A:150:ILE:HD12	1.12	1.10
1:F:40:HIS:HE1	2:G:253:TRP:CZ2	1.33	1.10
3:E:144:VAL:HG21	3:E:150:ILE:HD12	1.13	1.10
1:B:222:PHE:CD1	2:K:222:PRO:CB	2.29	1.10
2:C:165:ARG:NH2	2:C:228:GLU:OE1	1.84	1.10
1:F:43:LEU:CG	2:G:245:HIS:O	1.99	1.10
1:B:43:LEU:CG	2:C:245:HIS:O	1.99	1.10
2:G:227:ASN:OD1	2:G:238:GLU:OE1	1.67	1.10
1:J:43:LEU:HB3	2:K:249:VAL:HG23	1.28	1.10
1:J:43:LEU:CB	2:K:249:VAL:HG23	1.81	1.10
1:J:44:THR:HG23	2:K:249:VAL:HG21	1.28	1.10
2:K:177:PHE:CE1	2:K:224:VAL:HG11	1.84	1.10
2:G:165:ARG:NH2	2:G:228:GLU:OE1	1.84	1.09
3:E:293:VAL:CG2	3:E:413:PHE:HA	1.80	1.09
1:J:43:LEU:CG	2:K:245:HIS:O	1.99	1.09
1:F:43:LEU:HD21	2:G:245:HIS:O	1.50	1.09
1:F:43:LEU:HD23	2:G:249:VAL:HG23	1.26	1.09
1:B:43:LEU:CG	2:C:249:VAL:HG23	1.82	1.09
2:C:221:LEU:HB2	2:C:222:PRO:HD3	1.20	1.09
2:K:223:ASN:HD21	2:K:248:PHE:N	1.24	1.09
1:F:43:LEU:CG	2:G:249:VAL:HG23	1.82	1.08
2:C:222:PRO:CG	1:F:222:PHE:HD1	1.32	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:LEU:CB	2:G:249:VAL:HG23	1.81	1.08
2:G:222:PRO:CB	1:J:222:PHE:CD1	2.28	1.08
1:J:43:LEU:CG	2:K:249:VAL:HG23	1.82	1.08
1:B:43:LEU:HD23	2:C:249:VAL:HG23	1.26	1.08
2:G:222:PRO:CG	1:J:222:PHE:HD1	1.29	1.08
2:K:221:LEU:HB2	2:K:222:PRO:HD3	1.20	1.08
1:B:45:MET:C	2:C:241:VAL:CG1	2.27	1.08
1:B:225:ILE:HG21	2:K:219:MET:HE1	1.20	1.07
1:B:222:PHE:CB	2:K:222:PRO:CB	2.06	1.07
2:C:223:ASN:HD21	2:C:248:PHE:N	1.24	1.07
1:J:45:MET:C	2:K:241:VAL:HG13	1.80	1.07
1:J:45:MET:C	2:K:241:VAL:CG1	2.27	1.07
1:F:45:MET:C	2:G:241:VAL:CG1	2.27	1.07
1:B:45:MET:C	2:C:241:VAL:HG13	1.80	1.07
2:C:230:GLY:N	2:C:244:LEU:HD11	1.70	1.07
1:F:231:TRP:HH2	2:G:253:TRP:CD2	1.72	1.06
2:G:177:PHE:CE1	2:G:224:VAL:HG11	1.85	1.06
2:C:218:PHE:HE2	1:F:146:ILE:CG2	1.69	1.06
2:G:218:PHE:HE2	1:J:146:ILE:CG2	1.67	1.06
1:B:40:HIS:ND1	2:C:253:TRP:NE1	2.03	1.06
2:C:222:PRO:CB	1:F:222:PHE:CD1	2.32	1.06
1:J:40:HIS:ND1	2:K:253:TRP:NE1	2.03	1.06
1:B:43:LEU:CB	2:C:249:VAL:HG23	1.81	1.05
1:F:45:MET:C	2:G:241:VAL:HG13	1.79	1.05
3:A:144:VAL:CG2	3:A:150:ILE:HD12	1.86	1.05
2:K:230:GLY:N	2:K:244:LEU:HD11	1.70	1.05
3:A:293:VAL:CB	3:A:294:PRO:HD3	1.86	1.05
1:F:40:HIS:ND1	2:G:253:TRP:NE1	2.03	1.05
2:G:224:VAL:HG23	2:G:248:PHE:HD1	1.11	1.05
3:E:144:VAL:CG2	3:E:150:ILE:HD12	1.86	1.05
3:E:293:VAL:CB	3:E:294:PRO:HD3	1.86	1.05
1:B:231:TRP:HH2	2:C:253:TRP:CD2	1.72	1.05
1:J:231:TRP:HH2	2:K:253:TRP:CD2	1.72	1.05
1:F:43:LEU:HB3	2:G:249:VAL:HG23	1.28	1.05
2:C:127:GLU:OE2	2:C:272:GLY:HA3	1.57	1.04
2:C:230:GLY:CA	2:C:244:LEU:CD2	2.35	1.04
2:G:230:GLY:N	2:G:244:LEU:HD11	1.70	1.04
2:K:127:GLU:OE2	2:K:272:GLY:HA3	1.57	1.04
2:C:231:HIS:H	2:C:244:LEU:HD23	1.21	1.04
1:F:36:SER:HB3	2:G:255:ALA:HB3	1.39	1.04
1:J:40:HIS:HE1	2:K:253:TRP:CZ2	1.33	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:144:VAL:CG2	3:I:150:ILE:HD12	1.86	1.04
1:B:146:ILE:CG2	2:K:218:PHE:HE2	1.69	1.04
2:C:220:ILE:H	2:C:220:ILE:HD12	1.22	1.04
1:B:46:GLY:CA	2:C:241:VAL:HG13	1.88	1.04
1:F:39:ILE:HG12	2:G:248:PHE:HZ	1.09	1.04
1:B:43:LEU:HD21	2:C:245:HIS:O	1.50	1.03
2:G:127:GLU:OE2	2:G:272:GLY:HA3	1.57	1.03
2:G:230:GLY:CA	2:G:244:LEU:CD2	2.35	1.03
2:G:230:GLY:N	2:G:244:LEU:HD21	1.72	1.03
1:J:43:LEU:HB3	2:K:249:VAL:HG22	1.06	1.03
3:I:293:VAL:CB	3:I:294:PRO:HD3	1.86	1.03
1:B:36:SER:HB3	2:C:255:ALA:HB3	1.39	1.03
2:G:231:HIS:H	2:G:244:LEU:HD23	1.21	1.03
1:J:46:GLY:CA	2:K:241:VAL:HG13	1.88	1.03
2:C:230:GLY:N	2:C:244:LEU:HD21	1.72	1.03
2:G:220:ILE:H	2:G:220:ILE:HD12	1.22	1.03
3:E:144:VAL:CG2	3:E:150:ILE:CD1	2.37	1.03
2:K:230:GLY:CA	2:K:244:LEU:CD2	2.35	1.03
1:B:36:SER:CB	2:C:255:ALA:HB3	1.89	1.03
1:F:46:GLY:CA	2:G:241:VAL:HG13	1.88	1.03
1:J:231:TRP:HH2	2:K:253:TRP:CE3	1.77	1.03
2:C:230:GLY:H	2:C:244:LEU:HD11	1.20	1.03
2:G:201:PHE:HE1	2:G:267:TYR:CD2	1.70	1.03
1:J:244:LEU:HB2	2:K:206:ILE:HB	1.41	1.03
2:K:230:GLY:H	2:K:244:LEU:HD11	1.20	1.03
2:K:230:GLY:N	2:K:244:LEU:HD21	1.72	1.02
3:I:144:VAL:CG2	3:I:150:ILE:CD1	2.37	1.02
1:B:231:TRP:HH2	2:C:253:TRP:CE3	1.77	1.02
3:A:144:VAL:CG2	3:A:150:ILE:CD1	2.37	1.02
1:B:222:PHE:HB3	2:K:222:PRO:HB2	1.42	1.02
1:F:231:TRP:HH2	2:G:253:TRP:CE3	1.77	1.02
1:J:7:ALA:HA	2:K:125:ARG:HG2	1.41	1.02
2:K:235:PHE:HE1	3:I:147:GLY:N	1.46	1.02
1:B:244:LEU:HB2	2:C:206:ILE:HB	1.41	1.02
1:J:36:SER:HB3	2:K:255:ALA:HB3	1.39	1.02
1:J:36:SER:CB	2:K:255:ALA:HB3	1.89	1.02
2:K:201:PHE:HE1	2:K:267:TYR:CD2	1.70	1.01
2:K:231:HIS:H	2:K:244:LEU:HD23	1.21	1.01
1:B:43:LEU:HB3	2:C:249:VAL:HG22	1.06	1.01
1:F:36:SER:CB	2:G:255:ALA:HB3	1.89	1.01
2:G:222:PRO:CB	1:J:222:PHE:CB	2.05	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:HIS:CG	2:C:253:TRP:HE1	1.78	1.01
1:F:7:ALA:HA	2:G:125:ARG:HG2	1.41	1.00
2:K:220:ILE:H	2:K:220:ILE:HD12	1.22	1.00
1:F:40:HIS:CG	2:G:253:TRP:HE1	1.78	1.00
1:F:244:LEU:HB2	2:G:206:ILE:HB	1.41	1.00
2:G:177:PHE:HE1	2:G:224:VAL:CG1	1.63	1.00
1:J:40:HIS:CG	2:K:253:TRP:HE1	1.78	1.00
2:C:177:PHE:HE1	2:C:224:VAL:CG1	1.63	1.00
1:B:7:ALA:HA	2:C:125:ARG:HG2	1.41	1.00
2:C:218:PHE:CE2	1:F:146:ILE:CG2	2.43	1.00
1:F:43:LEU:HB3	2:G:249:VAL:HG22	1.06	1.00
2:C:235:PHE:HE1	3:A:147:GLY:N	1.46	1.00
2:G:222:PRO:HB2	1:J:222:PHE:HB3	1.40	1.00
2:C:223:ASN:HD21	2:C:248:PHE:HA	0.94	0.99
2:G:218:PHE:CE2	1:J:146:ILE:CG2	2.43	0.99
2:G:223:ASN:HD21	2:G:248:PHE:HA	0.94	0.99
2:K:223:ASN:ND2	2:K:248:PHE:N	1.84	0.99
1:B:231:TRP:CZ2	2:C:253:TRP:CZ3	2.51	0.99
1:B:78:TYR:CD2	2:C:259:MET:CE	2.46	0.99
1:F:231:TRP:CZ2	2:G:253:TRP:CZ3	2.51	0.99
1:F:71:PHE:HE1	2:G:253:TRP:CD1	1.80	0.98
2:G:237:GLU:OE2	3:E:148:GLY:N	1.96	0.98
3:I:293:VAL:HG21	3:I:413:PHE:HA	1.44	0.98
1:F:78:TYR:CD2	2:G:259:MET:CE	2.46	0.98
1:J:36:SER:HB3	2:K:255:ALA:CB	1.94	0.98
2:K:177:PHE:HE1	2:K:224:VAL:CG1	1.63	0.98
1:B:146:ILE:CG2	2:K:218:PHE:CE2	2.43	0.98
3:A:293:VAL:HG21	3:A:413:PHE:HA	1.44	0.98
1:J:78:TYR:CD2	2:K:259:MET:CE	2.46	0.98
2:C:237:GLU:OE2	3:A:148:GLY:N	1.96	0.98
1:J:71:PHE:HE1	2:K:253:TRP:CD1	1.80	0.98
1:F:71:PHE:CE1	2:G:253:TRP:CD1	2.52	0.98
2:G:230:GLY:H	2:G:244:LEU:HD11	1.20	0.98
1:B:71:PHE:HE1	2:C:253:TRP:CD1	1.80	0.97
1:B:36:SER:HB3	2:C:255:ALA:CB	1.94	0.97
3:A:112:ARG:HB2	3:A:269:MET:CE	1.94	0.97
2:G:222:PRO:HG3	1:J:222:PHE:CE1	1.98	0.97
3:E:293:VAL:HB	3:E:294:PRO:HD3	0.98	0.97
2:C:165:ARG:CZ	2:C:228:GLU:OE1	2.13	0.97
1:J:71:PHE:CE1	2:K:253:TRP:CD1	2.52	0.97
1:F:7:ALA:HB2	2:G:125:ARG:N	1.80	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:SER:HB3	2:G:255:ALA:CB	1.94	0.97
2:G:165:ARG:CZ	2:G:228:GLU:OE1	2.13	0.97
1:J:231:TRP:CZ2	2:K:253:TRP:CZ3	2.51	0.97
2:K:165:ARG:CZ	2:K:228:GLU:OE1	2.13	0.97
3:E:112:ARG:HB2	3:E:269:MET:CE	1.94	0.97
3:I:112:ARG:HB2	3:I:269:MET:CE	1.94	0.97
1:B:71:PHE:CE1	2:C:253:TRP:CD1	2.52	0.96
2:C:222:PRO:HB3	1:F:222:PHE:HB3	1.00	0.96
2:C:230:GLY:HA3	2:C:244:LEU:CG	1.95	0.96
2:K:237:GLU:OE2	3:I:148:GLY:N	1.96	0.96
2:G:230:GLY:CA	2:G:244:LEU:HD22	1.95	0.96
2:C:230:GLY:CA	2:C:244:LEU:HD22	1.95	0.96
3:E:293:VAL:HG21	3:E:413:PHE:HA	1.44	0.96
2:K:230:GLY:N	2:K:244:LEU:CD1	2.27	0.96
2:G:235:PHE:HE1	3:E:147:GLY:N	1.46	0.96
1:J:7:ALA:HB2	2:K:125:ARG:N	1.80	0.96
1:B:7:ALA:HB2	2:C:125:ARG:N	1.80	0.96
2:K:230:GLY:HA3	2:K:244:LEU:CG	1.95	0.96
2:C:222:PRO:HB2	1:F:222:PHE:HB3	1.42	0.96
1:F:78:TYR:OH	2:G:263:THR:OG1	1.83	0.96
1:J:43:LEU:HG	2:K:245:HIS:O	1.64	0.96
2:K:230:GLY:CA	2:K:244:LEU:HD22	1.95	0.96
1:B:40:HIS:ND1	2:C:253:TRP:CE2	2.33	0.96
2:K:223:ASN:HD21	2:K:248:PHE:HA	0.94	0.96
1:B:43:LEU:HD23	2:C:249:VAL:CG2	1.88	0.95
1:B:222:PHE:HB3	2:K:222:PRO:HB3	1.00	0.95
3:A:293:VAL:HB	3:A:294:PRO:HD3	0.98	0.95
1:F:40:HIS:ND1	2:G:253:TRP:CE2	2.33	0.95
2:G:269:PHE:HB3	2:G:274:LEU:HD21	1.40	0.95
1:J:43:LEU:HD23	2:K:249:VAL:CG2	1.88	0.95
2:C:201:PHE:HE1	2:C:267:TYR:CD2	1.70	0.95
2:G:201:PHE:HE1	2:G:267:TYR:CE2	1.84	0.95
2:G:230:GLY:HA3	2:G:244:LEU:CG	1.95	0.95
2:G:270:ALA:HA	2:G:274:LEU:CD1	1.96	0.95
1:J:40:HIS:ND1	2:K:253:TRP:CE2	2.33	0.95
3:I:293:VAL:HB	3:I:294:PRO:HD3	0.98	0.95
2:C:230:GLY:N	2:C:244:LEU:CD1	2.27	0.95
2:G:223:ASN:ND2	2:G:248:PHE:N	1.84	0.95
1:B:146:ILE:HG21	2:K:218:PHE:HE2	1.01	0.94
2:C:269:PHE:C	2:C:274:LEU:HD21	1.87	0.94
1:F:43:LEU:CB	2:G:249:VAL:HG22	1.93	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:224:VAL:HG22	2:K:248:PHE:CD1	2.00	0.94
1:B:231:TRP:CH2	2:C:253:TRP:CE3	2.55	0.94
2:C:201:PHE:HE1	2:C:267:TYR:CE2	1.84	0.94
1:J:231:TRP:CH2	2:K:253:TRP:CE3	2.55	0.94
1:B:43:LEU:HG	2:C:245:HIS:O	1.65	0.94
2:C:270:ALA:HA	2:C:274:LEU:CD1	1.96	0.94
2:K:201:PHE:HE1	2:K:267:TYR:CE2	1.84	0.94
2:G:177:PHE:HE1	2:G:224:VAL:HG11	1.21	0.94
2:K:127:GLU:OE2	2:K:272:GLY:HA2	1.67	0.94
1:B:43:LEU:CB	2:C:249:VAL:HG22	1.94	0.94
1:B:222:PHE:CE1	2:K:222:PRO:HG3	2.02	0.94
2:C:224:VAL:HG22	2:C:248:PHE:CD1	2.00	0.94
1:F:231:TRP:CH2	2:G:253:TRP:CE3	2.55	0.94
2:C:177:PHE:HE1	2:C:224:VAL:HG11	1.21	0.93
3:A:112:ARG:NH2	3:I:384:ASP:OD1	2.01	0.93
2:K:269:PHE:HB3	2:K:274:LEU:HD21	1.40	0.93
1:F:43:LEU:HG	2:G:245:HIS:O	1.64	0.93
2:G:127:GLU:OE2	2:G:272:GLY:HA2	1.67	0.93
2:G:224:VAL:HG22	2:G:248:PHE:CD1	2.00	0.93
1:F:43:LEU:HD11	2:G:248:PHE:HB3	1.51	0.93
2:K:270:ALA:HA	2:K:274:LEU:CD1	1.96	0.92
1:J:43:LEU:CB	2:K:249:VAL:HG22	1.94	0.92
2:K:269:PHE:C	2:K:274:LEU:HD21	1.87	0.92
2:G:230:GLY:N	2:G:244:LEU:CD1	2.27	0.92
2:G:230:GLY:N	2:G:244:LEU:CD2	2.32	0.92
1:J:43:LEU:HD11	2:K:248:PHE:HB3	1.51	0.92
1:B:78:TYR:OH	2:C:263:THR:OG1	1.83	0.92
3:A:384:ASP:OD1	3:E:112:ARG:NH2	2.03	0.92
2:K:160:HIS:HE1	2:K:238:GLU:OE2	1.53	0.92
2:C:127:GLU:OE2	2:C:272:GLY:HA2	1.67	0.92
1:J:11:HIS:HB3	2:K:277:SER:C	1.95	0.92
1:J:43:LEU:O	2:K:240:PHE:O	1.88	0.92
2:K:270:ALA:HA	2:K:274:LEU:HD13	1.52	0.92
1:B:11:HIS:HB3	2:C:277:SER:C	1.95	0.91
2:C:230:GLY:N	2:C:244:LEU:CD2	2.32	0.91
1:J:43:LEU:HD13	2:K:248:PHE:HB3	1.50	0.91
1:B:43:LEU:HD13	2:C:248:PHE:HB3	1.50	0.91
3:E:305:THR:HB	3:E:359:THR:HB	1.52	0.91
2:K:230:GLY:N	2:K:244:LEU:CD2	2.32	0.91
2:C:270:ALA:HA	2:C:274:LEU:HD13	1.52	0.91
1:B:43:LEU:HD11	2:C:248:PHE:HB3	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:230:GLY:CA	2:G:244:LEU:HD11	1.97	0.91
3:I:305:THR:HB	3:I:359:THR:HB	1.53	0.91
1:F:39:ILE:CG2	2:G:248:PHE:CZ	2.44	0.91
3:A:305:THR:HB	3:A:359:THR:HB	1.52	0.91
1:B:146:ILE:HG21	2:K:218:PHE:CZ	2.05	0.91
2:C:218:PHE:CZ	1:F:146:ILE:HG21	2.05	0.91
1:F:11:HIS:HB3	2:G:277:SER:C	1.95	0.91
2:G:269:PHE:C	2:G:274:LEU:HD21	1.87	0.90
1:B:43:LEU:O	2:C:240:PHE:O	1.88	0.90
1:F:43:LEU:HD13	2:G:248:PHE:HB3	1.50	0.90
2:G:231:HIS:CD2	2:G:245:HIS:CE1	2.60	0.90
2:C:235:PHE:CD1	3:A:147:GLY:N	2.34	0.90
2:G:160:HIS:HE1	2:G:238:GLU:OE2	1.53	0.90
2:C:160:HIS:HE1	2:C:238:GLU:OE2	1.53	0.90
2:C:222:PRO:CB	1:F:222:PHE:CB	2.06	0.90
2:K:231:HIS:CD2	2:K:245:HIS:CE1	2.60	0.90
2:G:270:ALA:HA	2:G:274:LEU:HD13	1.52	0.90
3:E:384:ASP:OD1	3:I:112:ARG:NH2	2.05	0.90
1:J:90:THR:HG23	1:J:132:ASP:OD2	1.72	0.89
1:B:90:THR:HG23	1:B:132:ASP:OD2	1.72	0.89
1:F:90:THR:HG23	1:F:132:ASP:OD2	1.72	0.89
2:G:223:ASN:HB2	2:G:251:PHE:CD2	2.07	0.89
2:C:222:PRO:HG3	1:F:222:PHE:CE1	2.03	0.89
2:C:223:ASN:HB2	2:C:251:PHE:CD2	2.07	0.89
1:B:78:TYR:HH	2:C:263:THR:HG1	1.08	0.89
2:C:231:HIS:CD2	2:C:245:HIS:CE1	2.60	0.89
2:G:222:PRO:HB3	1:J:222:PHE:HB3	1.04	0.89
1:F:43:LEU:O	2:G:240:PHE:O	1.88	0.89
2:K:223:ASN:HB2	2:K:251:PHE:CD2	2.07	0.89
2:K:177:PHE:HE1	2:K:224:VAL:HG11	1.21	0.89
2:K:235:PHE:CD1	3:I:147:GLY:N	2.34	0.89
1:F:45:MET:C	2:G:241:VAL:HG12	1.98	0.89
2:C:223:ASN:ND2	2:C:248:PHE:N	1.84	0.88
1:J:78:TYR:OH	2:K:263:THR:OG1	1.83	0.88
2:C:270:ALA:CA	2:C:274:LEU:CD1	2.51	0.88
2:G:218:PHE:O	2:G:221:LEU:HD23	1.74	0.88
2:G:218:PHE:CZ	1:J:146:ILE:HG21	2.08	0.88
1:J:39:ILE:CG2	2:K:248:PHE:CZ	2.44	0.88
2:C:218:PHE:O	2:C:221:LEU:HD23	1.74	0.88
3:I:144:VAL:HG21	3:I:150:ILE:HG13	1.56	0.88
2:C:269:PHE:HB3	2:C:274:LEU:HD22	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:ILE:CG1	2:K:248:PHE:CZ	2.56	0.88
1:F:39:ILE:CG1	2:G:248:PHE:CZ	2.56	0.88
2:K:270:ALA:CA	2:K:274:LEU:CD1	2.51	0.87
1:F:40:HIS:ND1	2:G:249:VAL:HG13	1.90	0.87
1:B:39:ILE:CG1	2:C:248:PHE:CZ	2.56	0.87
2:G:201:PHE:CZ	2:G:267:TYR:CD2	2.58	0.87
3:E:144:VAL:CG2	3:E:150:ILE:HG13	2.04	0.87
3:A:144:VAL:CG2	3:A:150:ILE:HG13	2.04	0.87
1:B:40:HIS:ND1	2:C:249:VAL:HG13	1.90	0.87
1:F:43:LEU:HD23	2:G:249:VAL:CG2	1.88	0.87
2:G:269:PHE:HB3	2:G:274:LEU:HD22	1.55	0.87
3:A:144:VAL:HG21	3:A:150:ILE:HG13	1.56	0.87
2:C:201:PHE:CZ	2:C:267:TYR:CD2	2.58	0.87
2:C:269:PHE:CB	2:C:274:LEU:CD2	2.43	0.87
2:K:269:PHE:HB3	2:K:274:LEU:HD22	1.55	0.87
1:F:39:ILE:HD11	2:G:149:ALA:CB	2.05	0.86
2:C:221:LEU:CB	2:C:222:PRO:HD3	2.05	0.86
1:J:40:HIS:ND1	2:K:249:VAL:HG13	1.90	0.86
1:J:79:LEU:HD21	2:K:259:MET:HE1	1.57	0.86
2:K:218:PHE:O	2:K:221:LEU:HD23	1.74	0.86
2:G:224:VAL:HG23	2:G:248:PHE:CD1	2.03	0.86
2:G:269:PHE:CB	2:G:274:LEU:CD2	2.43	0.86
1:J:39:ILE:HD11	2:K:149:ALA:CB	2.05	0.86
1:B:40:HIS:ND1	2:C:249:VAL:CG1	2.38	0.86
1:B:45:MET:C	2:C:241:VAL:HG12	1.98	0.86
3:I:144:VAL:CG2	3:I:150:ILE:HG13	2.04	0.86
2:C:226:LEU:O	2:C:244:LEU:CD2	2.24	0.86
2:C:269:PHE:HB3	2:C:274:LEU:HD21	1.40	0.86
1:J:45:MET:C	2:K:241:VAL:HG12	1.98	0.86
1:B:39:ILE:HD11	2:C:149:ALA:CB	2.05	0.86
1:B:79:LEU:HD21	2:C:259:MET:HE1	1.57	0.86
2:G:226:LEU:O	2:G:244:LEU:CD2	2.24	0.86
3:E:144:VAL:HG21	3:E:150:ILE:HG13	1.55	0.86
1:J:40:HIS:ND1	2:K:249:VAL:CG1	2.38	0.86
2:K:226:LEU:O	2:K:244:LEU:CD2	2.24	0.86
1:F:40:HIS:ND1	2:G:249:VAL:CG1	2.38	0.86
2:G:223:ASN:CG	2:G:251:PHE:HD2	1.84	0.85
2:K:223:ASN:CB	2:K:251:PHE:HD2	1.89	0.85
2:G:270:ALA:CA	2:G:274:LEU:CD1	2.51	0.85
1:B:146:ILE:HD13	2:K:218:PHE:CE2	2.11	0.85
2:C:223:ASN:CG	2:C:251:PHE:HD2	1.84	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:144:VAL:CG2	3:A:150:ILE:CG1	2.54	0.85
1:J:43:LEU:HD13	2:K:248:PHE:CD2	2.11	0.85
3:I:144:VAL:CG2	3:I:150:ILE:CG1	2.54	0.85
2:C:218:PHE:CE2	1:F:146:ILE:HD13	2.12	0.85
1:F:43:LEU:HD13	2:G:248:PHE:CD2	2.11	0.85
3:E:144:VAL:CG2	3:E:150:ILE:CG1	2.54	0.85
2:C:223:ASN:CB	2:C:251:PHE:HD2	1.89	0.85
1:F:231:TRP:CH2	2:G:253:TRP:CD2	2.64	0.85
1:B:43:LEU:HD13	2:C:248:PHE:CD2	2.11	0.84
2:G:221:LEU:CB	2:G:222:PRO:HD3	2.05	0.84
1:F:79:LEU:HD21	2:G:259:MET:HE1	1.57	0.84
2:G:220:ILE:HA	2:G:223:ASN:HB3	1.59	0.84
3:A:224:ALA:O	3:A:226:GLU:N	2.11	0.84
3:E:224:ALA:O	3:E:226:GLU:N	2.11	0.84
1:J:231:TRP:CH2	2:K:253:TRP:CD2	2.64	0.84
2:K:269:PHE:CB	2:K:274:LEU:CD2	2.43	0.84
1:F:231:TRP:CH2	2:G:253:TRP:CZ3	2.66	0.84
2:G:223:ASN:CB	2:G:251:PHE:HD2	1.89	0.84
3:E:242:ALA:O	3:E:246:ILE:HG13	1.78	0.84
2:G:235:PHE:CD1	3:E:147:GLY:N	2.34	0.84
1:J:231:TRP:CH2	2:K:253:TRP:CZ3	2.66	0.84
2:K:221:LEU:CB	2:K:222:PRO:HD3	2.05	0.84
2:K:223:ASN:CG	2:K:251:PHE:HD2	1.84	0.84
3:I:242:ALA:O	3:I:246:ILE:HG13	1.78	0.84
1:B:39:ILE:CG2	2:C:248:PHE:CZ	2.43	0.84
2:C:274:LEU:H	2:C:274:LEU:HD12	1.43	0.84
1:F:62:THR:HG23	1:F:219:PHE:HD2	1.41	0.84
2:K:201:PHE:CZ	2:K:267:TYR:CD2	2.58	0.84
3:A:242:ALA:O	3:A:246:ILE:HG13	1.78	0.83
1:J:62:THR:HG23	1:J:219:PHE:HD2	1.41	0.83
3:I:224:ALA:O	3:I:226:GLU:N	2.11	0.83
1:B:43:LEU:CD2	2:C:248:PHE:HB3	2.08	0.83
1:B:231:TRP:CH2	2:C:253:TRP:CZ3	2.66	0.83
1:B:231:TRP:CH2	2:C:253:TRP:CD2	2.64	0.83
2:G:231:HIS:HD2	2:G:245:HIS:HE1	1.27	0.83
1:J:43:LEU:CD2	2:K:248:PHE:HB3	2.08	0.83
1:F:43:LEU:CD2	2:G:248:PHE:HB3	2.08	0.83
2:K:231:HIS:HD2	2:K:245:HIS:HE1	1.27	0.83
2:K:274:LEU:H	2:K:274:LEU:HD12	1.43	0.83
1:B:62:THR:HG23	1:B:219:PHE:HD2	1.41	0.83
2:G:274:LEU:H	2:G:274:LEU:HD12	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:LEU:CD1	2:G:248:PHE:CB	2.56	0.82
2:C:220:ILE:HA	2:C:223:ASN:HB3	1.59	0.82
1:B:43:LEU:CD1	2:C:248:PHE:CB	2.56	0.82
2:C:224:VAL:HG23	2:C:248:PHE:CD1	2.02	0.82
2:K:220:ILE:HA	2:K:223:ASN:HB3	1.59	0.82
2:K:224:VAL:HG23	2:K:248:PHE:CD1	2.03	0.82
2:K:230:GLY:CA	2:K:244:LEU:HD11	1.97	0.82
2:C:231:HIS:HD2	2:C:245:HIS:HE1	1.27	0.81
2:C:269:PHE:C	2:C:274:LEU:CD2	2.49	0.81
1:B:7:ALA:HB2	2:C:124:PRO:C	2.05	0.81
2:C:177:PHE:CE1	2:C:224:VAL:HG12	2.14	0.81
1:J:7:ALA:HB2	2:K:124:PRO:C	2.05	0.81
1:J:43:LEU:CD1	2:K:248:PHE:CB	2.56	0.81
2:K:232:THR:HA	2:K:236:MET:HG3	1.62	0.81
3:I:73:VAL:HG23	3:I:118:ILE:HA	1.63	0.81
2:C:223:ASN:HB2	2:C:251:PHE:CE2	2.16	0.81
3:E:73:VAL:HG23	3:E:118:ILE:HA	1.62	0.81
2:K:223:ASN:HB2	2:K:251:PHE:CE2	2.16	0.81
2:C:251:PHE:HZ	1:F:226:LEU:HD21	1.45	0.81
2:G:177:PHE:CE1	2:G:224:VAL:HG12	2.14	0.81
2:G:223:ASN:OD1	2:G:251:PHE:CD2	2.34	0.81
2:K:223:ASN:OD1	2:K:251:PHE:CD2	2.34	0.81
3:E:110:VAL:O	3:E:110:VAL:HG12	1.81	0.81
1:B:39:ILE:CG2	2:C:248:PHE:CD2	2.47	0.81
2:C:223:ASN:OD1	2:C:251:PHE:CD2	2.34	0.80
1:F:7:ALA:HB2	2:G:124:PRO:C	2.05	0.80
2:C:232:THR:HA	2:C:236:MET:HG3	1.62	0.80
3:A:110:VAL:O	3:A:110:VAL:HG12	1.81	0.80
2:G:218:PHE:CE2	1:J:146:ILE:HD13	2.16	0.80
1:J:43:LEU:HD13	2:K:248:PHE:CB	2.12	0.80
2:K:223:ASN:CB	2:K:251:PHE:CD2	2.65	0.80
2:G:223:ASN:CB	2:G:251:PHE:CD2	2.65	0.80
2:G:223:ASN:HB2	2:G:251:PHE:CE2	2.16	0.80
2:K:177:PHE:CE1	2:K:224:VAL:HG12	2.14	0.80
1:B:226:LEU:HD21	2:K:251:PHE:HZ	1.45	0.80
1:B:231:TRP:HZ2	2:C:253:TRP:CZ3	1.95	0.80
3:A:42:MET:HE1	3:A:80:THR:OG1	1.82	0.79
2:C:231:HIS:HD2	2:C:245:HIS:CE1	2.00	0.79
3:A:73:VAL:HG23	3:A:118:ILE:HA	1.62	0.79
1:F:43:LEU:HD13	2:G:248:PHE:CB	2.12	0.79
3:I:110:VAL:O	3:I:110:VAL:HG12	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:251:PHE:HZ	1:J:226:LEU:HD21	1.46	0.79
1:J:40:HIS:NE2	2:K:253:TRP:HZ2	1.80	0.79
1:F:39:ILE:CB	2:G:248:PHE:CE2	2.66	0.79
2:G:232:THR:HA	2:G:236:MET:HG3	1.62	0.79
2:K:231:HIS:HD2	2:K:245:HIS:CE1	2.00	0.79
3:E:42:MET:HE1	3:E:80:THR:OG1	1.82	0.78
1:B:40:HIS:NE2	2:C:253:TRP:HZ2	1.80	0.78
1:B:43:LEU:HD13	2:C:248:PHE:CB	2.12	0.78
1:B:111:TRP:O	2:C:74:TRP:HH2	1.67	0.78
1:B:222:PHE:CG	2:K:222:PRO:CG	2.48	0.78
1:F:40:HIS:NE2	2:G:253:TRP:HZ2	1.80	0.78
1:F:111:TRP:O	2:G:74:TRP:HH2	1.66	0.78
1:J:39:ILE:CB	2:K:248:PHE:CE2	2.66	0.78
2:C:221:LEU:HB2	2:C:222:PRO:CD	2.09	0.78
3:I:42:MET:HE1	3:I:80:THR:OG1	1.82	0.78
2:C:218:PHE:HE2	1:F:146:ILE:HG21	1.02	0.78
2:C:223:ASN:CB	2:C:251:PHE:CD2	2.65	0.77
1:B:36:SER:HB2	2:C:252:GLY:O	1.85	0.77
1:B:39:ILE:CB	2:C:248:PHE:CE2	2.66	0.77
3:E:144:VAL:HG21	3:E:150:ILE:HD11	1.65	0.77
2:K:221:LEU:HB2	2:K:222:PRO:CD	2.09	0.77
3:E:73:VAL:CG2	3:E:118:ILE:HA	2.15	0.77
1:B:39:ILE:HD11	2:C:149:ALA:HB1	1.68	0.77
1:J:111:TRP:O	2:K:74:TRP:HH2	1.67	0.77
3:I:88:PHE:HD2	3:I:143:ASN:HD22	1.34	0.76
2:C:200:PRO:O	2:C:201:PHE:HB3	1.84	0.76
1:F:39:ILE:CG2	2:G:248:PHE:CD2	2.47	0.76
1:J:78:TYR:HH	2:K:263:THR:HG1	1.11	0.76
3:I:73:VAL:CG2	3:I:118:ILE:HA	2.15	0.76
1:F:36:SER:HB2	2:G:252:GLY:O	1.85	0.76
1:F:78:TYR:HD2	2:G:259:MET:CE	1.99	0.76
2:K:269:PHE:C	2:K:274:LEU:CD2	2.49	0.76
2:G:200:PRO:O	2:G:201:PHE:HB3	1.84	0.76
1:B:43:LEU:HD13	2:C:248:PHE:CG	2.21	0.76
2:K:200:PRO:O	2:K:201:PHE:HB3	1.84	0.76
2:K:230:GLY:CA	2:K:244:LEU:CG	2.61	0.76
3:A:272:MET:HE3	3:A:272:MET:HA	1.68	0.76
2:K:230:GLY:H	2:K:244:LEU:CD1	1.93	0.76
1:J:39:ILE:CG2	2:K:248:PHE:CD2	2.47	0.75
1:J:39:ILE:CD1	2:K:149:ALA:HB1	2.16	0.75
3:A:88:PHE:HD2	3:A:143:ASN:HD22	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:LEU:CD2	2:G:249:VAL:CG2	2.54	0.75
2:C:274:LEU:HD12	2:C:274:LEU:N	2.02	0.75
2:G:231:HIS:HD2	2:G:245:HIS:CE1	2.00	0.75
1:J:43:LEU:HD13	2:K:248:PHE:CG	2.21	0.75
1:B:78:TYR:HD2	2:C:259:MET:CE	1.98	0.75
3:A:112:ARG:HB2	3:A:269:MET:HE2	1.69	0.75
1:B:39:ILE:CD1	2:C:149:ALA:HB1	2.16	0.75
1:F:39:ILE:CD1	2:G:149:ALA:HB1	2.16	0.75
2:K:274:LEU:HD12	2:K:274:LEU:N	2.02	0.75
1:F:43:LEU:HD13	2:G:248:PHE:CG	2.21	0.75
1:J:36:SER:HB2	2:K:252:GLY:O	1.85	0.75
2:K:226:LEU:C	2:K:244:LEU:HG	2.12	0.75
3:E:112:ARG:HB2	3:E:269:MET:HE2	1.68	0.75
1:F:39:ILE:HD11	2:G:149:ALA:HB1	1.67	0.74
3:E:88:PHE:HD2	3:E:143:ASN:HD22	1.33	0.74
3:E:272:MET:HA	3:E:272:MET:HE3	1.68	0.74
2:K:269:PHE:HA	2:K:274:LEU:HD21	1.67	0.74
2:C:226:LEU:C	2:C:244:LEU:HG	2.12	0.74
2:G:230:GLY:CA	2:G:244:LEU:CG	2.61	0.74
1:J:40:HIS:CG	2:K:253:TRP:NE1	2.51	0.74
1:J:47:ASP:CG	1:J:50:PHE:CD2	2.65	0.74
2:G:201:PHE:CD2	2:G:268:SER:HB2	2.22	0.74
3:I:272:MET:HE3	3:I:272:MET:HA	1.68	0.74
3:A:73:VAL:CG2	3:A:118:ILE:HA	2.15	0.74
1:J:78:TYR:HD2	2:K:259:MET:CE	1.98	0.74
1:B:47:ASP:CG	1:B:50:PHE:CD2	2.65	0.74
2:G:221:LEU:HB2	2:G:222:PRO:CD	2.09	0.74
1:F:237:TRP:O	1:F:240:ASN:HB3	1.88	0.74
1:J:39:ILE:HD11	2:K:149:ALA:HB1	1.68	0.74
1:J:46:GLY:CA	2:K:241:VAL:CG1	2.63	0.74
2:K:216:GLY:O	2:K:220:ILE:CD1	2.36	0.74
2:K:226:LEU:O	2:K:244:LEU:CD1	2.35	0.74
2:C:201:PHE:CD2	2:C:268:SER:HB2	2.23	0.74
1:F:47:ASP:CG	1:F:50:PHE:CD2	2.65	0.74
1:J:231:TRP:HZ2	2:K:253:TRP:CZ3	1.95	0.74
2:G:216:GLY:O	2:G:220:ILE:CD1	2.36	0.73
1:J:237:TRP:O	1:J:240:ASN:HB3	1.88	0.73
1:F:71:PHE:HE1	2:G:253:TRP:NE1	1.87	0.73
2:G:226:LEU:O	2:G:244:LEU:CD1	2.35	0.73
2:C:216:GLY:O	2:C:220:ILE:CD1	2.36	0.73
2:C:226:LEU:O	2:C:244:LEU:CD1	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:PHE:HE1	2:K:253:TRP:NE1	1.86	0.73
3:I:112:ARG:HB2	3:I:269:MET:HE2	1.68	0.73
1:J:243:PHE:HA	2:K:206:ILE:O	1.88	0.73
3:I:144:VAL:HG21	3:I:150:ILE:HD11	1.65	0.73
1:B:243:PHE:HA	2:C:206:ILE:O	1.88	0.73
2:C:224:VAL:O	2:C:227:ASN:HB3	1.89	0.73
3:E:88:PHE:HB3	3:E:143:ASN:HB2	1.71	0.73
2:C:230:GLY:CA	2:C:244:LEU:HD11	1.97	0.73
2:C:230:GLY:CA	2:C:244:LEU:CG	2.61	0.73
3:A:88:PHE:HB3	3:A:143:ASN:HB2	1.71	0.73
1:F:62:THR:CG2	1:F:219:PHE:CD2	2.72	0.73
2:G:224:VAL:O	2:G:227:ASN:HB3	1.89	0.73
2:G:269:PHE:HA	2:G:274:LEU:HD21	1.67	0.73
2:K:201:PHE:CD2	2:K:268:SER:HB2	2.23	0.73
1:B:47:ASP:CG	1:B:50:PHE:CE2	2.67	0.72
1:B:237:TRP:O	1:B:240:ASN:HB3	1.88	0.72
2:G:218:PHE:HE2	1:J:146:ILE:HG21	1.00	0.72
1:F:47:ASP:CG	1:F:50:PHE:CE2	2.67	0.72
1:J:47:ASP:CG	1:J:50:PHE:CE2	2.67	0.72
1:B:62:THR:CG2	1:B:219:PHE:CD2	2.72	0.72
1:B:244:LEU:O	1:B:245:GLN:HB2	1.90	0.72
2:C:230:GLY:H	2:C:244:LEU:CD1	1.93	0.72
2:G:222:PRO:CG	1:J:222:PHE:CG	2.43	0.72
1:J:62:THR:CG2	1:J:219:PHE:CD2	2.72	0.72
1:F:244:LEU:O	1:F:245:GLN:HB2	1.90	0.72
1:F:243:PHE:HA	2:G:206:ILE:O	1.88	0.72
3:I:293:VAL:HG21	3:I:413:PHE:CA	2.19	0.72
2:G:226:LEU:C	2:G:244:LEU:HG	2.12	0.72
2:G:274:LEU:HD12	2:G:274:LEU:N	2.02	0.72
1:J:244:LEU:O	1:J:245:GLN:HB2	1.89	0.72
1:J:169:VAL:HG23	1:J:180:ILE:HG13	1.72	0.72
1:B:29:VAL:HG23	2:C:262:LEU:CD1	2.20	0.72
2:C:218:PHE:O	2:C:221:LEU:CD2	2.38	0.72
2:G:269:PHE:C	2:G:274:LEU:CD2	2.49	0.72
3:I:62:ASN:HD21	3:I:167:ARG:H	1.37	0.72
1:B:71:PHE:HE1	2:C:253:TRP:NE1	1.86	0.72
3:E:305:THR:HB	3:E:359:THR:CB	2.20	0.72
2:K:177:PHE:CE1	2:K:224:VAL:HG13	2.22	0.71
3:A:305:THR:HB	3:A:359:THR:CB	2.20	0.71
2:K:224:VAL:O	2:K:227:ASN:HB3	1.89	0.71
1:J:29:VAL:HG23	2:K:262:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:222:PRO:CG	1:F:222:PHE:CG	2.46	0.71
1:F:29:VAL:HG23	2:G:262:LEU:CD1	2.20	0.71
2:G:230:GLY:H	2:G:244:LEU:CD1	1.93	0.71
1:B:62:THR:HG23	1:B:219:PHE:CD2	2.26	0.71
1:B:225:ILE:HG22	2:K:219:MET:HE1	1.72	0.71
2:C:269:PHE:HD1	2:C:274:LEU:HD23	1.55	0.71
2:G:177:PHE:CE1	2:G:224:VAL:HG13	2.22	0.71
2:G:216:GLY:C	2:G:220:ILE:HD11	2.15	0.71
3:I:88:PHE:HB3	3:I:143:ASN:HB2	1.71	0.71
1:B:46:GLY:CA	2:C:241:VAL:CG1	2.63	0.71
2:K:218:PHE:O	2:K:221:LEU:CD2	2.38	0.71
3:A:144:VAL:HG21	3:A:150:ILE:HD11	1.65	0.71
1:J:112:THR:HG21	2:K:162:THR:HG21	1.73	0.71
1:F:40:HIS:CG	2:G:253:TRP:NE1	2.51	0.70
3:I:305:THR:HB	3:I:359:THR:CB	2.20	0.70
2:G:269:PHE:HD1	2:G:274:LEU:HD23	1.55	0.70
2:C:216:GLY:O	2:C:220:ILE:HD11	1.92	0.70
2:C:219:MET:HE1	1:F:225:ILE:HG22	1.73	0.70
2:K:216:GLY:O	2:K:220:ILE:HD11	1.92	0.70
2:K:216:GLY:C	2:K:220:ILE:HD11	2.16	0.70
2:C:202:PHE:HZ	2:C:265:THR:HA	1.56	0.70
1:J:78:TYR:CE2	2:K:259:MET:CE	2.64	0.70
1:B:112:THR:HG21	2:C:162:THR:HG21	1.73	0.70
1:B:169:VAL:HG23	1:B:180:ILE:HG13	1.72	0.70
1:F:169:VAL:HG23	1:F:180:ILE:HG13	1.72	0.70
3:A:62:ASN:HD21	3:A:167:ARG:H	1.37	0.70
1:F:78:TYR:CE2	2:G:259:MET:CE	2.64	0.70
2:G:216:GLY:O	2:G:220:ILE:HD11	1.91	0.70
2:G:218:PHE:O	2:G:221:LEU:CD2	2.38	0.70
3:E:35:GLU:O	3:E:36:LYS:HB2	1.90	0.70
1:F:112:THR:HG21	2:G:162:THR:HG21	1.73	0.69
2:K:202:PHE:HZ	2:K:265:THR:HA	1.56	0.69
1:F:62:THR:HG23	1:F:219:PHE:CD2	2.26	0.69
2:K:269:PHE:HD1	2:K:274:LEU:HD23	1.55	0.69
3:A:35:GLU:O	3:A:36:LYS:HB2	1.90	0.69
2:C:177:PHE:CE1	2:C:224:VAL:HG13	2.22	0.69
3:E:293:VAL:HG21	3:E:413:PHE:CA	2.20	0.69
1:B:231:TRP:CH2	2:C:253:TRP:CE2	2.81	0.69
1:J:231:TRP:CH2	2:K:253:TRP:CE2	2.81	0.69
1:F:231:TRP:HZ2	2:G:253:TRP:CZ3	1.95	0.69
2:K:223:ASN:CG	2:K:251:PHE:CD2	2.69	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:216:GLY:C	2:C:220:ILE:HD11	2.16	0.69
2:C:269:PHE:HA	2:C:274:LEU:HD21	1.67	0.69
3:E:62:ASN:HD21	3:E:167:ARG:H	1.37	0.69
1:F:231:TRP:CH2	2:G:253:TRP:CE2	2.81	0.69
3:I:35:GLU:O	3:I:36:LYS:HB2	1.90	0.69
3:A:293:VAL:HG21	3:A:413:PHE:CA	2.19	0.68
2:G:202:PHE:HZ	2:G:265:THR:HA	1.56	0.68
3:I:112:ARG:HB2	3:I:269:MET:HE3	1.75	0.68
3:A:112:ARG:HB2	3:A:269:MET:HE3	1.75	0.68
2:G:270:ALA:CA	2:G:274:LEU:HD11	2.08	0.68
1:B:71:PHE:CZ	2:C:253:TRP:CD1	2.82	0.68
1:J:62:THR:HG23	1:J:219:PHE:CD2	2.26	0.68
3:I:293:VAL:HG23	3:I:413:PHE:HA	1.73	0.68
2:G:223:ASN:CG	2:G:251:PHE:CD2	2.69	0.67
1:F:71:PHE:CZ	2:G:253:TRP:CD1	2.82	0.67
2:G:223:ASN:HD21	2:G:248:PHE:CB	2.02	0.67
3:E:112:ARG:HB2	3:E:269:MET:HE3	1.75	0.67
1:J:43:LEU:HD21	2:K:248:PHE:N	2.09	0.67
1:J:71:PHE:CZ	2:K:253:TRP:CD1	2.82	0.67
2:K:226:LEU:O	2:K:244:LEU:HD21	1.94	0.67
2:K:170:THR:O	2:K:174:ILE:HG12	1.95	0.67
3:A:293:VAL:HG23	3:A:413:PHE:HA	1.74	0.67
2:G:222:PRO:CA	1:J:222:PHE:CG	2.78	0.67
1:B:45:MET:CA	2:C:241:VAL:HG12	2.24	0.67
1:B:111:TRP:CZ3	2:C:70:GLY:HA2	2.30	0.67
2:C:170:THR:O	2:C:174:ILE:HG12	1.95	0.67
1:F:43:LEU:HD21	2:G:248:PHE:N	2.09	0.67
1:J:111:TRP:CZ3	2:K:70:GLY:HA2	2.30	0.67
1:B:104:ARG:NH1	2:C:154:GLU:OE1	2.28	0.67
1:F:104:ARG:NH1	2:G:154:GLU:OE1	2.28	0.67
2:G:226:LEU:O	2:G:244:LEU:HD21	1.94	0.67
2:G:219:MET:HE1	1:J:225:ILE:HG22	1.75	0.67
1:J:104:ARG:NH1	2:K:154:GLU:OE1	2.28	0.67
1:J:62:THR:CG2	1:J:219:PHE:HD2	2.07	0.67
1:F:62:THR:CG2	1:F:219:PHE:HD2	2.07	0.66
2:G:165:ARG:NH2	2:G:228:GLU:CD	2.53	0.66
1:J:43:LEU:CD1	2:K:245:HIS:HB3	2.26	0.66
2:C:235:PHE:CE1	3:A:146:GLY:C	2.37	0.66
3:A:293:VAL:CG2	3:A:413:PHE:CA	2.69	0.66
3:E:293:VAL:HG23	3:E:413:PHE:HA	1.74	0.66
1:F:45:MET:CA	2:G:241:VAL:HG12	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:LEU:CD1	2:G:245:HIS:HB3	2.26	0.66
2:G:170:THR:O	2:G:174:ILE:HG12	1.95	0.66
1:B:222:PHE:CG	2:K:222:PRO:CA	2.78	0.66
1:J:45:MET:CA	2:K:241:VAL:HG12	2.24	0.66
2:K:235:PHE:CE1	3:I:146:GLY:C	2.37	0.66
1:B:43:LEU:CG	2:C:248:PHE:HB3	2.26	0.66
1:F:111:TRP:HZ3	2:G:70:GLY:HA2	1.61	0.66
1:F:111:TRP:CZ3	2:G:70:GLY:HA2	2.30	0.66
1:J:43:LEU:CG	2:K:248:PHE:HB3	2.26	0.66
1:J:90:THR:HG21	1:J:129:ILE:HD12	1.78	0.66
2:K:235:PHE:CZ	3:I:146:GLY:CA	2.54	0.66
1:F:244:LEU:H	2:G:206:ILE:H	1.44	0.66
1:B:43:LEU:HD12	2:C:245:HIS:HB3	1.78	0.66
2:C:226:LEU:O	2:C:244:LEU:HD21	1.94	0.66
1:J:43:LEU:HD12	2:K:245:HIS:HB3	1.78	0.66
2:G:222:PRO:CD	1:J:222:PHE:CD1	2.76	0.65
1:B:43:LEU:CD2	2:C:249:VAL:CG2	2.54	0.65
1:B:111:TRP:HZ3	2:C:70:GLY:HA2	1.61	0.65
2:C:165:ARG:NH2	2:C:228:GLU:CD	2.53	0.65
1:F:231:TRP:CH2	2:G:253:TRP:CH2	2.84	0.65
2:K:165:ARG:NH2	2:K:228:GLU:CD	2.53	0.65
1:B:43:LEU:HD21	2:C:248:PHE:N	2.09	0.65
1:F:11:HIS:CB	2:G:277:SER:C	2.70	0.65
1:F:231:TRP:HH2	2:G:253:TRP:CE2	2.14	0.65
2:G:235:PHE:CE1	3:E:146:GLY:C	2.37	0.65
1:B:226:LEU:HD21	2:K:251:PHE:CZ	2.31	0.65
1:B:244:LEU:H	2:C:206:ILE:H	1.44	0.65
1:F:7:ALA:HA	2:G:125:ARG:CG	2.23	0.65
1:F:43:LEU:HD12	2:G:245:HIS:HB3	1.78	0.65
1:B:43:LEU:CD1	2:C:245:HIS:HB3	2.26	0.65
1:J:111:TRP:HZ3	2:K:70:GLY:HA2	1.61	0.65
1:B:71:PHE:CD2	2:C:256:LEU:HD21	2.32	0.65
2:C:222:PRO:CA	1:F:222:PHE:CG	2.80	0.65
2:C:235:PHE:CZ	3:A:146:GLY:CA	2.54	0.65
2:G:148:GLY:HA2	2:G:180:SER:OG	1.97	0.65
1:F:46:GLY:CA	2:G:241:VAL:CG1	2.63	0.65
1:F:43:LEU:CG	2:G:248:PHE:HB3	2.26	0.64
1:J:71:PHE:CD2	2:K:256:LEU:HD21	2.32	0.64
1:J:244:LEU:H	2:K:206:ILE:H	1.44	0.64
1:F:71:PHE:CD2	2:G:256:LEU:HD21	2.32	0.64
1:J:42:MET:SD	2:K:154:GLU:HG3	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:MET:SD	2:C:154:GLU:HG3	2.37	0.64
1:F:233:PHE:HA	1:F:236:ARG:HG2	1.79	0.64
1:J:231:TRP:CH2	2:K:253:TRP:CH2	2.84	0.64
3:I:215:ARG:NH2	3:I:227:LEU:HB3	2.13	0.64
1:F:90:THR:HG21	1:F:129:ILE:HD12	1.78	0.64
1:B:90:THR:HG21	1:B:129:ILE:HD12	1.78	0.64
1:F:42:MET:SD	2:G:154:GLU:HG3	2.37	0.64
2:G:201:PHE:HD1	2:G:271:GLN:OE1	1.81	0.64
1:J:7:ALA:CB	2:K:125:ARG:HA	2.28	0.64
1:B:39:ILE:HD11	2:C:149:ALA:HB2	1.80	0.64
3:E:215:ARG:NH2	3:E:227:LEU:HB3	2.13	0.64
1:J:43:LEU:CD2	2:K:248:PHE:CB	2.75	0.64
1:J:233:PHE:HA	1:J:236:ARG:HG2	1.79	0.64
2:K:148:GLY:HA2	2:K:180:SER:OG	1.97	0.64
1:B:11:HIS:CB	2:C:277:SER:C	2.70	0.63
1:B:78:TYR:CE2	2:C:259:MET:CE	2.64	0.63
2:C:200:PRO:O	2:C:201:PHE:CB	2.46	0.63
2:G:47:ASP:C	2:G:47:ASP:OD1	2.42	0.63
2:G:200:PRO:O	2:G:201:PHE:CB	2.46	0.63
1:B:233:PHE:HA	1:B:236:ARG:HG2	1.79	0.63
3:A:215:ARG:NH2	3:A:227:LEU:HB3	2.13	0.63
1:F:39:ILE:HD11	2:G:149:ALA:HB2	1.80	0.63
1:J:39:ILE:HD11	2:K:149:ALA:HB2	1.80	0.63
1:B:44:THR:HG23	2:C:249:VAL:CG2	2.19	0.63
2:K:201:PHE:HD1	2:K:271:GLN:OE1	1.81	0.63
1:B:7:ALA:CB	2:C:125:ARG:HA	2.28	0.63
2:C:148:GLY:HA2	2:C:180:SER:OG	1.97	0.63
3:A:144:VAL:HG23	3:A:150:ILE:HG13	1.81	0.63
1:F:231:TRP:CZ2	2:G:253:TRP:CZ2	2.87	0.63
1:B:29:VAL:HG23	2:C:262:LEU:HD12	1.81	0.63
1:F:111:TRP:O	2:G:74:TRP:CH2	2.50	0.63
2:G:251:PHE:CZ	1:J:226:LEU:HD21	2.33	0.63
1:J:111:TRP:O	2:K:74:TRP:CH2	2.50	0.63
3:I:293:VAL:CG2	3:I:413:PHE:CA	2.69	0.63
1:F:7:ALA:CB	2:G:125:ARG:HA	2.28	0.63
3:I:46:THR:HG23	3:I:47:ILE:N	2.14	0.63
3:I:319:THR:HG23	3:I:320:ALA:N	2.13	0.63
2:C:134:HIS:CE1	2:C:195:ALA:HB2	2.34	0.62
3:E:319:THR:HG23	3:E:320:ALA:N	2.14	0.62
1:J:7:ALA:HA	2:K:125:ARG:CG	2.23	0.62
2:K:200:PRO:O	2:K:201:PHE:CB	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:PHE:CE2	2:C:268:SER:CB	2.82	0.62
2:C:251:PHE:CZ	1:F:226:LEU:HD21	2.32	0.62
3:A:46:THR:CG2	3:A:47:ILE:H	2.12	0.62
3:A:305:THR:CB	3:A:359:THR:HB	2.29	0.62
1:F:71:PHE:CZ	2:G:253:TRP:HD1	2.18	0.62
2:G:202:PHE:CE2	2:G:268:SER:CB	2.82	0.62
1:J:43:LEU:CD2	2:K:249:VAL:CG2	2.54	0.62
2:C:47:ASP:C	2:C:47:ASP:OD1	2.41	0.62
1:F:39:ILE:CA	2:G:248:PHE:HE2	2.13	0.62
3:E:41:PHE:O	3:E:45:ARG:HG3	2.00	0.62
3:E:305:THR:CB	3:E:359:THR:HB	2.29	0.62
3:I:46:THR:CG2	3:I:47:ILE:H	2.12	0.62
2:C:201:PHE:HD1	2:C:271:GLN:OE1	1.81	0.62
1:F:38:HIS:NE2	2:G:154:GLU:HB2	2.14	0.62
2:G:201:PHE:CE1	2:G:267:TYR:CE2	2.73	0.62
3:E:296:ARG:HD2	3:E:369:ALA:HA	1.81	0.62
3:I:46:THR:HG23	3:I:47:ILE:H	1.64	0.62
1:B:39:ILE:HA	2:C:248:PHE:HE2	1.64	0.62
1:B:40:HIS:CG	2:C:253:TRP:NE1	2.51	0.62
3:I:41:PHE:O	3:I:45:ARG:HG3	2.00	0.62
1:J:39:ILE:CA	2:K:248:PHE:HE2	2.13	0.62
2:K:47:ASP:C	2:K:47:ASP:OD1	2.41	0.62
3:I:296:ARG:HD2	3:I:369:ALA:HA	1.81	0.62
1:B:14:ALA:HB3	2:C:278:LEU:HD13	1.82	0.62
1:B:39:ILE:CA	2:C:248:PHE:HE2	2.13	0.62
1:B:111:TRP:O	2:C:74:TRP:CH2	2.50	0.62
1:B:146:ILE:HD13	2:K:218:PHE:CD2	2.34	0.62
3:A:46:THR:HG23	3:A:47:ILE:N	2.14	0.62
1:B:20:THR:O	1:B:24:MET:HG3	2.00	0.62
1:B:38:HIS:NE2	2:C:154:GLU:HB2	2.14	0.62
3:A:46:THR:HG23	3:A:47:ILE:H	1.65	0.62
3:A:296:ARG:HD2	3:A:369:ALA:HA	1.81	0.62
1:B:231:TRP:CZ2	2:C:253:TRP:CZ2	2.87	0.62
1:F:43:LEU:CD2	2:G:248:PHE:CB	2.74	0.62
2:G:159:TRP:CZ2	2:G:163:ILE:HD11	2.35	0.62
1:J:20:THR:O	1:J:24:MET:HG3	2.00	0.62
1:J:29:VAL:HG23	2:K:262:LEU:HD12	1.81	0.62
3:A:319:THR:HG23	3:A:320:ALA:N	2.13	0.62
2:G:134:HIS:CE1	2:G:195:ALA:HB2	2.34	0.62
3:E:46:THR:HG23	3:E:47:ILE:N	2.14	0.62
3:E:46:THR:CG2	3:E:47:ILE:H	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:ILE:HA	2:K:248:PHE:HE2	1.64	0.61
2:K:134:HIS:CE1	2:K:195:ALA:HB2	2.34	0.61
3:I:386:ARG:HG2	3:I:408:PRO:HA	1.82	0.61
3:A:42:MET:O	3:A:46:THR:HB	2.00	0.61
3:E:42:MET:O	3:E:46:THR:HB	2.00	0.61
1:J:11:HIS:CB	2:K:277:SER:C	2.70	0.61
1:J:231:TRP:CZ2	2:K:253:TRP:CZ2	2.87	0.61
2:C:159:TRP:CZ2	2:C:163:ILE:HD11	2.35	0.61
1:F:29:VAL:HG23	2:G:262:LEU:HD12	1.81	0.61
1:F:39:ILE:HA	2:G:248:PHE:HE2	1.64	0.61
3:E:144:VAL:HG23	3:E:150:ILE:HG13	1.81	0.61
2:K:223:ASN:HD21	2:K:248:PHE:CB	2.02	0.61
3:A:41:PHE:O	3:A:45:ARG:HG3	2.00	0.61
1:J:38:HIS:NE2	2:K:154:GLU:HB2	2.14	0.61
2:K:159:TRP:CZ2	2:K:163:ILE:HD11	2.35	0.61
3:I:42:MET:O	3:I:46:THR:HB	2.00	0.61
2:C:218:PHE:CD2	1:F:146:ILE:HD13	2.35	0.61
1:F:14:ALA:HB3	2:G:278:LEU:HD13	1.82	0.61
1:J:44:THR:HG23	2:K:249:VAL:CG2	2.18	0.61
2:K:202:PHE:CE2	2:K:268:SER:CB	2.82	0.61
1:B:71:PHE:CZ	2:C:253:TRP:HD1	2.18	0.61
1:B:231:TRP:CH2	2:C:253:TRP:CH2	2.84	0.61
3:A:386:ARG:HG2	3:A:408:PRO:HA	1.82	0.61
2:G:223:ASN:ND2	2:G:248:PHE:CB	2.62	0.61
2:G:49:LYS:HB2	2:G:52:THR:OG1	2.01	0.61
2:G:231:HIS:NE2	2:G:245:HIS:ND1	2.49	0.61
3:E:46:THR:HG23	3:E:47:ILE:H	1.65	0.61
1:J:86:PRO:HB3	1:J:136:MET:HG3	1.83	0.61
2:K:223:ASN:ND2	2:K:248:PHE:CB	2.62	0.61
2:C:222:PRO:CD	1:F:222:PHE:CD1	2.79	0.60
1:J:39:ILE:CB	2:K:248:PHE:CZ	2.84	0.60
1:B:86:PRO:HB3	1:B:136:MET:HG3	1.83	0.60
2:C:231:HIS:NE2	2:C:245:HIS:ND1	2.49	0.60
2:K:231:HIS:NE2	2:K:245:HIS:ND1	2.49	0.60
3:I:72:HIS:HE1	3:I:404:GLN:HE22	1.49	0.60
1:F:20:THR:O	1:F:24:MET:HG3	2.00	0.60
3:E:293:VAL:CG2	3:E:413:PHE:CA	2.69	0.60
1:J:14:ALA:HB3	2:K:278:LEU:HD13	1.82	0.60
3:I:144:VAL:HG23	3:I:150:ILE:HG13	1.81	0.60
1:B:39:ILE:CB	2:C:248:PHE:CZ	2.84	0.60
1:J:71:PHE:CZ	2:K:253:TRP:HD1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:305:THR:CB	3:I:359:THR:HB	2.29	0.60
2:K:49:LYS:HB2	2:K:52:THR:OG1	2.01	0.60
1:B:7:ALA:HA	2:C:125:ARG:CG	2.23	0.60
2:K:69:GLU:O	2:K:73:GLY:N	2.35	0.60
3:A:254:ALA:O	3:A:257:LYS:O	2.20	0.60
1:F:45:MET:O	2:G:240:PHE:HB2	2.02	0.60
1:F:86:PRO:HB3	1:F:136:MET:HG3	1.83	0.60
3:I:319:THR:CG2	3:I:320:ALA:N	2.65	0.60
1:F:39:ILE:CB	2:G:248:PHE:CZ	2.84	0.60
2:G:231:HIS:CD2	2:G:245:HIS:HE1	2.07	0.60
2:K:231:HIS:CD2	2:K:245:HIS:HE1	2.07	0.60
1:J:155:ILE:O	1:J:158:PRO:HG2	2.02	0.59
1:B:155:ILE:O	1:B:158:PRO:HG2	2.02	0.59
2:C:49:LYS:HB2	2:C:52:THR:OG1	2.01	0.59
3:E:386:ARG:HG2	3:E:408:PRO:HA	1.82	0.59
2:C:222:PRO:CG	1:F:222:PHE:CB	2.79	0.59
1:F:40:HIS:CE1	2:G:253:TRP:NE1	2.60	0.59
3:E:72:HIS:HE1	3:E:404:GLN:HE22	1.49	0.59
2:C:218:PHE:CZ	1:F:146:ILE:CG2	2.82	0.59
2:G:218:PHE:CD2	1:J:146:ILE:HD13	2.37	0.59
2:G:220:ILE:HG22	2:G:224:VAL:HG23	1.83	0.59
3:E:86:VAL:HB	3:E:145:GLN:HG3	1.85	0.59
2:K:220:ILE:HG22	2:K:224:VAL:HG23	1.83	0.59
2:K:237:GLU:OE2	3:I:147:GLY:HA2	2.02	0.59
3:A:319:THR:CG2	3:A:320:ALA:N	2.65	0.59
1:F:155:ILE:O	1:F:158:PRO:HG2	2.02	0.59
3:E:254:ALA:O	3:E:257:LYS:O	2.20	0.59
2:C:220:ILE:HG22	2:C:224:VAL:HG23	1.83	0.59
3:A:86:VAL:HB	3:A:145:GLN:HG3	1.85	0.59
3:E:319:THR:CG2	3:E:320:ALA:N	2.65	0.59
2:C:237:GLU:OE2	3:A:147:GLY:HA2	2.02	0.59
2:G:237:GLU:OE2	3:E:147:GLY:HA2	2.02	0.59
3:E:243:THR:O	3:E:247:VAL:HG23	2.03	0.59
2:G:69:GLU:O	2:G:73:GLY:N	2.35	0.58
3:I:254:ALA:O	3:I:257:LYS:O	2.20	0.58
3:A:72:HIS:HE1	3:A:404:GLN:HE22	1.49	0.58
2:G:227:ASN:O	2:G:244:LEU:HD23	2.03	0.58
1:J:79:LEU:CD2	2:K:259:MET:HE1	2.31	0.58
2:C:227:ASN:CG	2:C:238:GLU:OE1	2.45	0.58
1:F:79:LEU:CD2	2:G:259:MET:HE1	2.31	0.58
2:K:227:ASN:O	2:K:244:LEU:HD23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:259:PRO:HG2	3:I:260:ILE:HD12	1.86	0.58
3:E:115:ARG:NH2	3:E:117:GLU:OE2	2.33	0.58
1:B:45:MET:O	2:C:240:PHE:HB2	2.02	0.58
3:A:259:PRO:HG2	3:A:260:ILE:HD12	1.86	0.58
1:F:231:TRP:CH2	2:G:253:TRP:CZ2	2.92	0.58
2:G:177:PHE:HE1	2:G:224:VAL:HG13	1.60	0.58
1:J:45:MET:O	2:K:240:PHE:HB2	2.02	0.58
2:C:177:PHE:CD1	2:C:224:VAL:HG11	2.39	0.57
2:G:235:PHE:CZ	3:E:146:GLY:CA	2.54	0.57
3:I:243:THR:O	3:I:247:VAL:HG23	2.04	0.57
1:B:79:LEU:CD2	2:C:259:MET:HE1	2.31	0.57
1:J:43:LEU:HG	2:K:245:HIS:C	2.29	0.57
2:K:227:ASN:CG	2:K:238:GLU:OE1	2.45	0.57
3:I:86:VAL:HB	3:I:145:GLN:HG3	1.85	0.57
2:K:233:PHE:N	2:K:233:PHE:CD1	2.73	0.57
2:C:69:GLU:O	2:C:73:GLY:N	2.35	0.57
3:A:243:THR:O	3:A:247:VAL:HG23	2.04	0.57
1:J:7:ALA:CB	2:K:124:PRO:C	2.78	0.57
1:J:231:TRP:CH2	2:K:253:TRP:CZ2	2.92	0.57
1:B:146:ILE:CG2	2:K:218:PHE:CZ	2.82	0.57
1:F:7:ALA:CB	2:G:124:PRO:C	2.78	0.57
2:C:223:ASN:ND2	2:C:248:PHE:CB	2.62	0.57
3:E:293:VAL:CB	3:E:294:PRO:CD	2.50	0.57
1:B:43:LEU:HG	2:C:245:HIS:C	2.29	0.57
3:A:371:TRP:CZ3	3:A:377:SER:HB3	2.40	0.57
1:F:39:ILE:CA	2:G:248:PHE:CE2	2.88	0.57
1:J:43:LEU:CD1	2:K:245:HIS:O	2.52	0.57
2:C:227:ASN:O	2:C:244:LEU:HD23	2.04	0.56
3:E:77:TRP:CZ2	3:E:144:VAL:HG11	2.40	0.56
2:K:177:PHE:CD1	2:K:224:VAL:HG11	2.39	0.56
2:K:230:GLY:H	2:K:244:LEU:HD21	1.69	0.56
1:B:39:ILE:CA	2:C:248:PHE:CE2	2.88	0.56
2:C:202:PHE:CE2	2:C:268:SER:HB2	2.40	0.56
1:F:14:ALA:HB3	2:G:278:LEU:HB2	1.88	0.56
3:E:259:PRO:HG2	3:E:260:ILE:HD12	1.86	0.56
1:B:43:LEU:CD1	2:C:245:HIS:O	2.52	0.56
1:B:231:TRP:CH2	2:C:253:TRP:CZ2	2.92	0.56
2:C:201:PHE:CE1	2:C:267:TYR:CE2	2.73	0.56
3:A:77:TRP:CZ2	3:A:144:VAL:HG11	2.40	0.56
3:A:87:ALA:HA	3:A:143:ASN:O	2.06	0.56
2:G:233:PHE:N	2:G:233:PHE:CD1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:371:TRP:CZ3	3:E:377:SER:HB3	2.40	0.56
1:J:107:ASN:HA	1:J:111:TRP:HB2	1.87	0.56
2:K:232:THR:HA	2:K:236:MET:HA	1.87	0.56
1:B:107:ASN:HA	1:B:111:TRP:HB2	1.87	0.56
1:F:161:TRP:HD1	3:E:251:MET:HG3	1.70	0.56
1:B:14:ALA:HB3	2:C:278:LEU:HB2	1.88	0.56
1:F:107:ASN:HA	1:F:111:TRP:HB2	1.87	0.56
3:E:87:ALA:HA	3:E:143:ASN:O	2.06	0.56
3:I:87:ALA:HA	3:I:143:ASN:O	2.06	0.56
3:I:115:ARG:NH2	3:I:117:GLU:OE2	2.33	0.56
2:C:231:HIS:CD2	2:C:245:HIS:HE1	2.07	0.56
1:F:43:LEU:CD1	2:G:245:HIS:O	2.52	0.56
2:G:227:ASN:CG	2:G:238:GLU:OE1	2.45	0.56
1:B:161:TRP:CD1	3:A:251:MET:HG3	2.41	0.56
1:B:222:PHE:CD1	2:K:222:PRO:CD	2.78	0.56
1:F:44:THR:HG23	2:G:249:VAL:CG2	2.19	0.56
1:J:161:TRP:CD1	3:I:251:MET:HG3	2.41	0.56
1:J:161:TRP:HD1	3:I:251:MET:HG3	1.70	0.56
1:B:83:TYR:CE1	3:A:216:LEU:HB2	2.41	0.56
1:F:161:TRP:CD1	3:E:251:MET:HG3	2.41	0.56
2:C:232:THR:HA	2:C:236:MET:HA	1.87	0.56
2:G:202:PHE:CE2	2:G:268:SER:HB2	2.40	0.56
2:G:218:PHE:CZ	1:J:146:ILE:CG2	2.84	0.56
1:J:46:GLY:HA2	2:K:241:VAL:HG13	1.84	0.56
3:I:77:TRP:CZ2	3:I:144:VAL:HG11	2.40	0.56
1:B:45:MET:O	2:C:241:VAL:N	2.39	0.55
3:I:245:LEU:HD13	3:I:249:MET:HG3	1.88	0.55
1:B:161:TRP:HD1	3:A:251:MET:HG3	1.70	0.55
2:G:226:LEU:O	2:G:244:LEU:HD11	2.06	0.55
1:B:43:LEU:HD22	2:C:248:PHE:CB	2.36	0.55
2:C:269:PHE:CD1	2:C:274:LEU:HD23	2.40	0.55
3:A:265:GLN:HE22	3:I:385:SER:H	1.54	0.55
2:K:202:PHE:CE2	2:K:268:SER:HB2	2.40	0.55
2:C:220:ILE:H	2:C:220:ILE:CD1	1.96	0.55
2:C:233:PHE:N	2:C:233:PHE:CD1	2.73	0.55
1:J:14:ALA:HB3	2:K:278:LEU:HB2	1.88	0.55
1:J:45:MET:O	2:K:241:VAL:N	2.39	0.55
1:J:83:TYR:CE1	3:I:216:LEU:HB2	2.41	0.55
1:B:7:ALA:HB1	2:C:125:ARG:HA	1.89	0.55
1:B:170:PRO:HG3	3:I:413:PHE:CE2	2.42	0.55
3:A:39:ALA:HB3	3:A:42:MET:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:141:TYR:OH	2:G:217:PRO:HG2	2.07	0.55
1:J:7:ALA:HB1	2:K:125:ARG:HA	1.89	0.55
3:I:371:TRP:CZ3	3:I:377:SER:HB3	2.40	0.55
3:A:265:GLN:HE22	3:I:385:SER:HB2	1.72	0.55
1:F:83:TYR:CE1	3:E:216:LEU:HB2	2.41	0.55
2:C:141:TYR:OH	2:C:217:PRO:HG2	2.07	0.55
2:C:226:LEU:O	2:C:244:LEU:HD11	2.06	0.55
1:F:45:MET:O	2:G:241:VAL:N	2.39	0.55
2:G:222:PRO:CG	1:J:222:PHE:CB	2.79	0.55
3:I:249:MET:HE2	3:I:249:MET:HA	1.89	0.55
1:F:7:ALA:CB	2:G:125:ARG:N	2.65	0.55
1:J:39:ILE:CA	2:K:248:PHE:CE2	2.88	0.55
1:F:43:LEU:HB2	2:G:248:PHE:HD2	1.71	0.55
1:J:86:PRO:CB	1:J:136:MET:HG3	2.37	0.55
1:B:108:PHE:HB3	1:B:119:VAL:HG21	1.90	0.54
1:F:86:PRO:CB	1:F:136:MET:HG3	2.37	0.54
1:F:7:ALA:HB1	2:G:125:ARG:HA	1.89	0.54
2:G:232:THR:HA	2:G:236:MET:HA	1.88	0.54
2:G:269:PHE:CD1	2:G:274:LEU:HD23	2.40	0.54
1:J:43:LEU:HB2	2:K:248:PHE:HD2	1.71	0.54
1:J:166:PRO:HG2	3:I:184:ASN:OD1	2.08	0.54
2:K:269:PHE:CD1	2:K:274:LEU:HD23	2.40	0.54
1:B:86:PRO:CB	1:B:136:MET:HG3	2.37	0.54
2:K:141:TYR:OH	2:K:217:PRO:HG2	2.07	0.54
3:I:110:VAL:O	3:I:110:VAL:CG1	2.54	0.54
3:A:245:LEU:HD13	3:A:249:MET:HG3	1.88	0.54
3:A:367:SER:O	3:A:368:ASP:HB2	2.07	0.54
3:I:46:THR:CG2	3:I:47:ILE:N	2.70	0.54
1:B:7:ALA:CB	2:C:124:PRO:C	2.78	0.54
1:B:166:PRO:HG2	3:A:184:ASN:OD1	2.08	0.54
1:F:108:PHE:HB3	1:F:119:VAL:HG21	1.90	0.54
3:A:110:VAL:O	3:A:110:VAL:CG1	2.54	0.54
2:K:202:PHE:CZ	2:K:265:THR:HA	2.41	0.54
2:C:269:PHE:CD1	2:C:274:LEU:CD2	2.91	0.54
3:A:385:SER:HB2	3:E:265:GLN:HE22	1.72	0.54
3:A:413:PHE:CE2	1:F:170:PRO:HG3	2.43	0.54
1:F:43:LEU:HG	2:G:245:HIS:C	2.29	0.54
3:I:39:ALA:HB3	3:I:42:MET:HG3	1.89	0.54
3:A:115:ARG:NH2	3:A:117:GLU:OE2	2.33	0.54
1:F:166:PRO:HG2	3:E:184:ASN:OD1	2.08	0.54
1:J:108:PHE:HB3	1:J:119:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:226:LEU:O	2:K:244:LEU:HD11	2.06	0.54
1:B:222:PHE:CB	2:K:222:PRO:CG	2.81	0.54
2:C:202:PHE:CZ	2:C:265:THR:HA	2.41	0.54
1:F:46:GLY:HA2	2:G:241:VAL:HG13	1.84	0.54
3:E:46:THR:CG2	3:E:47:ILE:N	2.70	0.54
1:J:43:LEU:HD11	2:K:248:PHE:CB	2.33	0.54
1:J:43:LEU:HD22	2:K:248:PHE:CB	2.37	0.54
2:K:230:GLY:HA2	2:K:244:LEU:HD13	1.71	0.54
1:B:146:ILE:HD13	2:K:218:PHE:HE2	1.69	0.54
2:G:202:PHE:CZ	2:G:265:THR:HA	2.41	0.54
2:K:269:PHE:CD1	2:K:274:LEU:CD2	2.91	0.54
3:A:249:MET:HE2	3:A:249:MET:HA	1.89	0.53
3:E:39:ALA:HB3	3:E:42:MET:HG3	1.89	0.53
1:B:7:ALA:CB	2:C:125:ARG:N	2.65	0.53
1:B:43:LEU:HB2	2:C:248:PHE:HD2	1.71	0.53
3:A:46:THR:CG2	3:A:47:ILE:N	2.70	0.53
2:C:218:PHE:HE2	1:F:146:ILE:HD13	1.71	0.53
2:G:86:GLU:HA	2:G:90:MET:HB2	1.89	0.53
3:E:245:LEU:HD13	3:E:249:MET:HG3	1.88	0.53
3:E:249:MET:HE2	3:E:249:MET:HA	1.89	0.53
1:J:47:ASP:OD1	1:J:50:PHE:CE2	2.62	0.53
1:J:53:ASP:OD1	1:J:190:ARG:NH2	2.41	0.53
2:C:167:THR:HB	2:C:169:PHE:H	1.73	0.53
1:F:47:ASP:OD1	1:F:50:PHE:CE2	2.62	0.53
1:F:108:PHE:CE2	2:G:158:THR:HG22	2.44	0.53
2:K:167:THR:HB	2:K:169:PHE:H	1.73	0.53
3:I:348:VAL:HG21	3:I:351:ASN:ND2	2.24	0.53
3:A:411:PRO:CD	1:F:177:LEU:HD22	2.38	0.53
2:G:269:PHE:CD1	2:G:274:LEU:CD2	2.91	0.53
3:E:367:SER:O	3:E:368:ASP:HB2	2.07	0.53
3:E:375:ARG:O	3:E:378:ASP:HB2	2.09	0.53
1:B:53:ASP:OD1	1:B:190:ARG:NH2	2.41	0.53
1:B:108:PHE:CE2	2:C:158:THR:HG22	2.44	0.53
1:B:146:ILE:O	1:B:150:MET:HB2	2.09	0.53
3:E:110:VAL:O	3:E:110:VAL:CG1	2.54	0.53
1:J:108:PHE:CE2	2:K:158:THR:HG22	2.44	0.53
2:C:223:ASN:CG	2:C:251:PHE:CD2	2.69	0.53
1:F:146:ILE:O	1:F:150:MET:HB2	2.09	0.53
3:E:299:ARG:HB3	3:E:299:ARG:HH11	1.74	0.53
3:E:348:VAL:HG21	3:E:351:ASN:ND2	2.24	0.53
1:J:45:MET:CG	1:J:47:ASP:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:367:SER:O	3:I:368:ASP:HB2	2.07	0.53
1:B:11:HIS:HB3	2:C:277:SER:O	2.09	0.53
1:B:45:MET:O	2:C:240:PHE:CB	2.57	0.53
3:A:348:VAL:HG21	3:A:351:ASN:ND2	2.24	0.53
3:A:375:ARG:O	3:A:378:ASP:HB2	2.09	0.53
2:K:86:GLU:HA	2:K:90:MET:HB2	1.89	0.53
2:K:201:PHE:CE1	2:K:267:TYR:CE2	2.73	0.53
1:F:11:HIS:HB3	2:G:277:SER:O	2.09	0.53
1:F:71:PHE:CE1	2:G:253:TRP:NE1	2.74	0.53
1:J:146:ILE:O	1:J:150:MET:HB2	2.09	0.53
1:F:45:MET:O	2:G:240:PHE:CB	2.57	0.52
2:K:74:TRP:O	2:K:75:SER:HB2	2.09	0.52
3:I:375:ARG:O	3:I:378:ASP:HB2	2.08	0.52
2:C:74:TRP:O	2:C:75:SER:HB2	2.09	0.52
2:G:222:PRO:CA	1:J:222:PHE:CD1	2.93	0.52
3:E:88:PHE:HD2	3:E:143:ASN:ND2	2.05	0.52
1:F:53:ASP:OD1	1:F:190:ARG:NH2	2.41	0.52
3:I:299:ARG:HB3	3:I:299:ARG:HH11	1.74	0.52
1:B:165:ALA:O	1:B:166:PRO:C	2.52	0.52
1:F:43:LEU:HD11	2:G:248:PHE:CB	2.33	0.52
3:I:348:VAL:HB	3:I:351:ASN:HB2	1.91	0.52
2:C:86:GLU:HA	2:C:90:MET:HB2	1.89	0.52
3:A:88:PHE:HD2	3:A:143:ASN:ND2	2.05	0.52
3:A:299:ARG:HB3	3:A:299:ARG:HH11	1.74	0.52
3:A:348:VAL:HB	3:A:351:ASN:HB2	1.91	0.52
1:F:45:MET:CG	1:F:47:ASP:H	2.22	0.52
1:J:40:HIS:CE1	2:K:253:TRP:NE1	2.60	0.52
1:B:47:ASP:OD1	1:B:50:PHE:CE2	2.62	0.52
2:C:221:LEU:HD23	2:C:221:LEU:N	2.25	0.52
3:A:260:ILE:HG21	3:I:413:PHE:CD2	2.45	0.52
2:G:221:LEU:CD2	2:G:221:LEU:N	2.73	0.52
1:B:78:TYR:HE2	2:C:259:MET:HE3	1.60	0.52
1:F:36:SER:CB	2:G:252:GLY:O	2.58	0.52
2:G:167:THR:HB	2:G:169:PHE:H	1.73	0.52
2:G:221:LEU:HD23	2:G:221:LEU:N	2.25	0.52
2:G:269:PHE:HD1	2:G:274:LEU:CD2	2.23	0.52
3:E:385:SER:H	3:I:265:GLN:HE22	1.57	0.52
1:J:40:HIS:CE1	2:K:249:VAL:CG1	2.93	0.52
1:B:43:LEU:CD2	2:C:248:PHE:CB	2.75	0.52
3:A:219:VAL:HG22	3:A:224:ALA:HB2	1.92	0.52
3:E:219:VAL:HG22	3:E:224:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:11:HIS:HB3	2:K:277:SER:O	2.09	0.52
1:J:165:ALA:O	1:J:166:PRO:C	2.52	0.52
1:B:100:GLU:O	1:B:104:ARG:HG2	2.11	0.52
1:B:177:LEU:HD22	3:I:411:PRO:CD	2.40	0.52
2:G:74:TRP:O	2:G:75:SER:HB2	2.09	0.52
2:K:269:PHE:HD1	2:K:274:LEU:CD2	2.23	0.52
1:B:45:MET:CG	1:B:47:ASP:H	2.22	0.51
2:G:177:PHE:CD1	2:G:224:VAL:HG11	2.39	0.51
1:J:45:MET:O	2:K:240:PHE:CB	2.57	0.51
2:K:221:LEU:CD2	2:K:221:LEU:N	2.73	0.51
3:A:45:ARG:NH1	3:A:406:ASP:OD2	2.43	0.51
1:F:165:ALA:O	1:F:166:PRO:C	2.52	0.51
3:E:348:VAL:HB	3:E:351:ASN:HB2	1.91	0.51
3:A:75:GLU:OE1	3:A:404:GLN:NE2	2.44	0.51
2:C:269:PHE:HD1	2:C:274:LEU:CD2	2.23	0.51
1:F:100:GLU:O	1:F:104:ARG:HG2	2.11	0.51
1:B:62:THR:CG2	1:B:219:PHE:HD2	2.07	0.51
2:C:230:GLY:HA3	2:C:244:LEU:HD13	0.52	0.51
1:F:45:MET:O	2:G:241:VAL:HG13	2.10	0.51
1:F:118:PHE:CZ	1:F:185:GLY:HA2	2.46	0.51
3:I:45:ARG:NH1	3:I:406:ASP:OD2	2.43	0.51
1:B:7:ALA:HB2	2:C:125:ARG:CA	2.41	0.51
1:B:222:PHE:CD1	2:K:222:PRO:CA	2.92	0.51
2:C:221:LEU:CD2	2:C:221:LEU:N	2.73	0.51
3:A:60:LYS:O	3:A:63:GLU:HB2	2.11	0.51
1:F:40:HIS:CE1	2:G:249:VAL:CG1	2.93	0.51
3:E:45:ARG:NH1	3:E:406:ASP:OD2	2.43	0.51
3:E:104:TYR:O	3:E:124:PHE:HA	2.11	0.51
1:J:45:MET:O	2:K:240:PHE:C	2.54	0.51
3:I:75:GLU:OE1	3:I:404:GLN:NE2	2.44	0.51
1:B:40:HIS:CE1	2:C:249:VAL:CG1	2.93	0.51
1:B:45:MET:O	2:C:240:PHE:C	2.54	0.51
1:J:7:ALA:CB	2:K:125:ARG:CA	2.89	0.51
1:B:43:LEU:HD21	2:C:248:PHE:HB3	1.92	0.51
1:B:118:PHE:CZ	1:B:185:GLY:HA2	2.46	0.51
2:C:270:ALA:CA	2:C:274:LEU:HD11	2.08	0.51
3:A:104:TYR:O	3:A:124:PHE:HA	2.11	0.51
1:F:43:LEU:HD22	2:G:248:PHE:CB	2.36	0.51
3:E:75:GLU:OE1	3:E:404:GLN:NE2	2.44	0.51
3:I:219:VAL:HG22	3:I:224:ALA:HB2	1.92	0.51
2:C:220:ILE:HD12	2:C:220:ILE:N	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:GLU:O	1:J:104:ARG:HG2	2.11	0.51
2:K:221:LEU:HD23	2:K:221:LEU:N	2.25	0.51
1:B:36:SER:CB	2:C:252:GLY:O	2.57	0.51
1:B:45:MET:O	2:C:241:VAL:HG13	2.10	0.51
2:C:201:PHE:CE2	2:C:264:GLN:O	2.64	0.51
2:G:230:GLY:C	2:G:244:LEU:CD2	2.38	0.51
1:B:7:ALA:CB	2:C:125:ARG:CA	2.89	0.50
3:E:60:LYS:O	3:E:63:GLU:HB2	2.11	0.50
1:J:7:ALA:CB	2:K:125:ARG:N	2.65	0.50
2:C:177:PHE:HE1	2:C:224:VAL:HG13	1.60	0.50
3:E:58:LYS:HG3	3:E:158:THR:HB	1.93	0.50
3:I:55:SER:O	3:I:56:LYS:HG3	2.12	0.50
1:B:40:HIS:CE1	2:C:253:TRP:NE1	2.60	0.50
3:A:58:LYS:HG3	3:A:158:THR:HB	1.93	0.50
3:A:306:ASN:ND2	3:A:307:HIS:O	2.44	0.50
1:F:45:MET:O	2:G:240:PHE:C	2.54	0.50
3:I:60:LYS:O	3:I:63:GLU:HB2	2.11	0.50
1:F:7:ALA:HB2	2:G:125:ARG:CA	2.41	0.50
2:K:201:PHE:CE2	2:K:264:GLN:O	2.64	0.50
3:I:306:ASN:ND2	3:I:307:HIS:O	2.44	0.50
3:A:55:SER:O	3:A:56:LYS:HG3	2.12	0.50
1:B:90:THR:CG2	1:B:129:ILE:HD12	2.42	0.50
2:G:201:PHE:CE2	2:G:264:GLN:O	2.64	0.50
1:J:38:HIS:CE1	2:K:154:GLU:CD	2.90	0.50
1:J:118:PHE:CZ	1:J:185:GLY:HA2	2.46	0.50
3:I:58:LYS:HG3	3:I:158:THR:HB	1.93	0.50
3:I:88:PHE:HD2	3:I:143:ASN:ND2	2.05	0.50
1:F:7:ALA:CB	2:G:125:ARG:CA	2.89	0.50
1:J:7:ALA:HB2	2:K:125:ARG:CA	2.41	0.50
3:I:104:TYR:O	3:I:124:PHE:HA	2.11	0.50
2:G:159:TRP:CE2	2:G:163:ILE:HD11	2.47	0.49
1:B:46:GLY:HA2	2:C:241:VAL:HG13	1.84	0.49
2:C:159:TRP:CE2	2:C:163:ILE:HD11	2.47	0.49
2:C:220:ILE:CD1	2:C:220:ILE:N	2.73	0.49
1:J:36:SER:OG	2:K:255:ALA:HB3	2.13	0.49
1:J:45:MET:O	2:K:241:VAL:HG13	2.10	0.49
1:F:38:HIS:CE1	2:G:154:GLU:CD	2.90	0.49
1:B:38:HIS:CE1	2:C:154:GLU:CD	2.90	0.49
3:E:306:ASN:ND2	3:E:307:HIS:O	2.44	0.49
3:I:230:ALA:C	3:I:232:ASP:N	2.70	0.49
3:A:230:ALA:C	3:A:232:ASP:N	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:THR:CG2	1:F:129:ILE:HD12	2.42	0.49
2:K:159:TRP:CE2	2:K:163:ILE:HD11	2.47	0.49
3:A:124:PHE:CE2	3:A:140:THR:HG21	2.47	0.49
3:E:93:MET:HG3	3:E:95:GLY:O	2.13	0.49
3:I:124:PHE:CE2	3:I:140:THR:HG21	2.47	0.49
2:G:230:GLY:HA3	2:G:244:LEU:HD13	0.52	0.49
3:E:55:SER:O	3:E:56:LYS:HG3	2.12	0.49
3:E:73:VAL:HG21	3:E:118:ILE:HA	1.94	0.49
3:E:124:PHE:CE2	3:E:140:THR:HG21	2.47	0.49
3:I:39:ALA:HB3	3:I:42:MET:CG	2.43	0.49
2:K:221:LEU:HD23	2:K:221:LEU:H	1.77	0.49
3:A:93:MET:HG3	3:A:95:GLY:O	2.13	0.49
3:E:72:HIS:CE1	3:E:404:GLN:HE22	2.29	0.49
3:E:413:PHE:CE2	1:J:170:PRO:HG3	2.47	0.49
1:J:36:SER:CB	2:K:252:GLY:O	2.57	0.49
3:A:72:HIS:CE1	3:A:404:GLN:HE22	2.29	0.49
3:E:230:ALA:C	3:E:232:ASP:N	2.70	0.49
2:G:132:PHE:O	2:G:136:VAL:HG23	2.13	0.48
3:E:60:LYS:O	3:E:61:ILE:C	2.56	0.48
1:J:29:VAL:HG22	2:K:259:MET:SD	2.53	0.48
3:A:60:LYS:O	3:A:61:ILE:C	2.56	0.48
2:G:221:LEU:HD23	2:G:221:LEU:H	1.77	0.48
2:G:230:GLY:N	2:G:244:LEU:CG	2.76	0.48
1:B:36:SER:OG	2:C:255:ALA:HB3	2.13	0.48
2:C:221:LEU:HD23	2:C:221:LEU:H	1.77	0.48
1:F:71:PHE:CE2	2:G:256:LEU:HD21	2.49	0.48
1:J:71:PHE:CE1	2:K:253:TRP:NE1	2.74	0.48
1:J:71:PHE:CE2	2:K:256:LEU:HD21	2.49	0.48
2:K:220:ILE:HD12	2:K:220:ILE:N	2.07	0.48
1:B:101:TRP:HE1	3:A:192:HIS:CD2	2.31	0.48
1:F:36:SER:OG	2:G:255:ALA:HB3	2.13	0.48
1:F:43:LEU:HD21	2:G:248:PHE:HB3	1.92	0.48
2:K:230:GLY:HA3	2:K:244:LEU:HD13	0.52	0.48
1:B:29:VAL:HG22	2:C:259:MET:SD	2.53	0.48
2:C:230:GLY:N	2:C:244:LEU:CG	2.77	0.48
2:G:224:VAL:HG21	2:G:248:PHE:CD1	2.39	0.48
3:E:45:ARG:HB3	3:E:74:PHE:CE2	2.48	0.48
1:B:11:HIS:HB3	2:C:277:SER:CA	2.44	0.48
2:C:222:PRO:CA	1:F:222:PHE:CD1	2.95	0.48
1:F:29:VAL:HG22	2:G:259:MET:SD	2.53	0.48
3:E:39:ALA:HB3	3:E:42:MET:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:78:TYR:HE2	2:K:259:MET:HE3	1.60	0.48
3:I:45:ARG:HB3	3:I:74:PHE:CE2	2.48	0.48
1:B:59:LEU:O	1:B:63:VAL:HG13	2.14	0.48
3:A:39:ALA:HB3	3:A:42:MET:CG	2.43	0.48
3:A:45:ARG:HB3	3:A:74:PHE:CE2	2.48	0.48
1:F:101:TRP:HE1	3:E:192:HIS:CD2	2.31	0.48
1:J:39:ILE:HA	2:K:248:PHE:CE2	2.47	0.48
1:J:71:PHE:HZ	2:K:253:TRP:HD1	1.62	0.48
2:K:132:PHE:O	2:K:136:VAL:HG23	2.13	0.48
2:K:201:PHE:CD1	2:K:271:GLN:OE1	2.66	0.48
2:C:132:PHE:O	2:C:136:VAL:HG23	2.13	0.48
3:E:385:SER:HB2	3:I:265:GLN:HE22	1.78	0.48
3:I:93:MET:HG3	3:I:95:GLY:O	2.13	0.48
3:I:380:ILE:HG13	3:I:380:ILE:O	2.13	0.48
3:A:385:SER:H	3:E:265:GLN:HE22	1.61	0.48
1:F:59:LEU:O	1:F:63:VAL:HG13	2.14	0.48
1:J:11:HIS:HB3	2:K:277:SER:CA	2.44	0.48
2:K:204:LYS:HD3	2:K:204:LYS:HA	1.40	0.48
1:B:71:PHE:HZ	2:C:253:TRP:HD1	1.62	0.47
1:F:71:PHE:HZ	2:G:253:TRP:HD1	1.62	0.47
1:F:190:ARG:HD2	1:F:190:ARG:H	1.79	0.47
2:G:201:PHE:CD1	2:G:271:GLN:OE1	2.66	0.47
3:E:137:HIS:NE2	3:E:154:GLY:O	2.44	0.47
1:J:47:ASP:OD2	1:J:50:PHE:CE2	2.67	0.47
1:B:190:ARG:H	1:B:190:ARG:HD2	1.79	0.47
3:A:33:HIS:N	3:A:33:HIS:HD1	2.12	0.47
3:A:230:ALA:C	3:A:232:ASP:H	2.22	0.47
3:E:33:HIS:N	3:E:33:HIS:HD1	2.12	0.47
3:I:72:HIS:CE1	3:I:404:GLN:HE22	2.29	0.47
3:I:318:TYR:CD1	3:I:318:TYR:C	2.92	0.47
3:E:213:ILE:N	3:E:214:PRO:HD2	2.30	0.47
3:E:287:GLU:O	3:E:288:ASP:O	2.33	0.47
1:J:59:LEU:O	1:J:63:VAL:HG13	2.14	0.47
1:J:90:THR:CG2	1:J:129:ILE:HD12	2.42	0.47
1:J:101:TRP:HE1	3:I:192:HIS:CD2	2.31	0.47
1:J:190:ARG:H	1:J:190:ARG:HD2	1.79	0.47
3:I:287:GLU:O	3:I:288:ASP:O	2.33	0.47
1:B:55:LYS:HD2	1:B:60:TRP:CZ2	2.50	0.47
2:C:229:TRP:C	2:C:244:LEU:HD21	2.38	0.47
3:A:380:ILE:HG13	3:A:380:ILE:O	2.13	0.47
3:E:380:ILE:O	3:E:380:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:45:MET:HA	2:K:241:VAL:HG12	1.96	0.47
1:J:55:LYS:HD2	1:J:60:TRP:CZ2	2.50	0.47
3:I:209:ARG:NH1	3:I:232:ASP:OD1	2.48	0.47
1:B:71:PHE:CE2	2:C:256:LEU:HD21	2.49	0.47
3:A:77:TRP:CH2	3:A:144:VAL:HG11	2.50	0.47
3:I:60:LYS:O	3:I:61:ILE:C	2.56	0.47
3:I:77:TRP:CH2	3:I:144:VAL:HG11	2.50	0.47
3:A:293:VAL:HG22	3:A:413:PHE:CD1	2.50	0.47
1:F:47:ASP:OD2	1:F:50:PHE:CE2	2.67	0.47
3:E:293:VAL:HG22	3:E:413:PHE:CD1	2.50	0.47
3:I:137:HIS:NE2	3:I:154:GLY:O	2.44	0.47
1:B:47:ASP:OD2	1:B:50:PHE:CE2	2.67	0.47
3:A:213:ILE:N	3:A:214:PRO:HD2	2.30	0.47
1:F:7:ALA:CA	2:G:125:ARG:HG2	2.29	0.47
1:F:55:LYS:HD2	1:F:60:TRP:CZ2	2.50	0.47
2:G:219:MET:CE	1:J:225:ILE:HG21	2.13	0.47
2:G:229:TRP:C	2:G:244:LEU:HD21	2.38	0.47
3:E:77:TRP:CH2	3:E:144:VAL:HG11	2.50	0.47
3:I:293:VAL:HG22	3:I:413:PHE:CD1	2.50	0.47
2:C:230:GLY:C	2:C:244:LEU:CD2	2.38	0.47
3:A:209:ARG:NH1	3:A:232:ASP:OD1	2.48	0.47
3:E:413:PHE:CD2	3:I:260:ILE:HG21	2.50	0.47
2:K:223:ASN:ND2	2:K:223:ASN:C	2.73	0.47
3:I:33:HIS:N	3:I:33:HIS:HD1	2.12	0.47
3:I:293:VAL:HG23	3:I:412:SER:O	2.15	0.47
3:E:318:TYR:CD1	3:E:318:TYR:C	2.92	0.47
3:I:230:ALA:C	3:I:232:ASP:H	2.22	0.47
2:C:223:ASN:ND2	2:C:223:ASN:C	2.73	0.47
3:A:287:GLU:O	3:A:288:ASP:O	2.33	0.47
3:E:293:VAL:HG23	3:E:412:SER:O	2.15	0.47
1:B:7:ALA:CA	2:C:125:ARG:HG2	2.29	0.46
1:B:43:LEU:HD11	2:C:248:PHE:CB	2.33	0.46
2:C:230:GLY:H	2:C:244:LEU:HD21	1.69	0.46
3:E:411:PRO:CD	1:J:177:LEU:HD22	2.45	0.46
2:K:220:ILE:H	2:K:220:ILE:CD1	1.96	0.46
2:C:224:VAL:HG21	2:C:248:PHE:CD1	2.39	0.46
3:A:265:GLN:NE2	3:I:385:SER:HB2	2.29	0.46
1:F:62:THR:HG21	1:F:219:PHE:CD2	2.49	0.46
2:G:231:HIS:CD2	2:G:245:HIS:ND1	2.83	0.46
2:G:231:HIS:CE1	2:G:244:LEU:HB3	2.50	0.46
2:K:230:GLY:N	2:K:244:LEU:CG	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:92:GLY:HA3	3:I:139:HIS:HB2	1.98	0.46
2:C:231:HIS:CE1	2:C:244:LEU:HB3	2.50	0.46
3:A:73:VAL:HG21	3:A:118:ILE:HA	1.94	0.46
2:G:220:ILE:HD12	2:G:220:ILE:N	2.07	0.46
3:A:293:VAL:CB	3:A:294:PRO:CD	2.50	0.46
3:A:293:VAL:HG23	3:A:412:SER:O	2.15	0.46
1:F:11:HIS:HB3	2:G:277:SER:CA	2.44	0.46
1:F:71:PHE:O	1:F:72:PRO:C	2.59	0.46
2:G:223:ASN:ND2	2:G:223:ASN:C	2.73	0.46
3:E:209:ARG:NH1	3:E:232:ASP:OD1	2.48	0.46
3:I:213:ILE:N	3:I:214:PRO:HD2	2.30	0.46
1:F:105:TYR:HD2	1:F:106:PHE:CD1	2.34	0.46
2:G:218:PHE:HE2	1:J:146:ILE:HD13	1.74	0.46
2:K:224:VAL:HG21	2:K:248:PHE:CD1	2.39	0.46
2:K:231:HIS:CE1	2:K:244:LEU:HB3	2.50	0.46
3:A:413:PHE:CD2	3:E:260:ILE:HG21	2.50	0.46
2:G:160:HIS:CE1	2:G:165:ARG:HD2	2.50	0.46
2:C:235:PHE:HD1	2:C:235:PHE:HA	1.65	0.46
2:G:274:LEU:CD1	2:G:274:LEU:N	2.73	0.46
3:E:35:GLU:O	3:E:36:LYS:CB	2.59	0.46
3:E:88:PHE:HB3	3:E:143:ASN:CB	2.44	0.46
1:B:62:THR:HG21	1:B:219:PHE:CD2	2.50	0.46
3:E:230:ALA:C	3:E:232:ASP:H	2.23	0.46
2:K:160:HIS:CE1	2:K:165:ARG:HD2	2.50	0.46
2:K:280:GLU:OE1	2:K:280:GLU:HA	2.15	0.46
1:B:69:VAL:HG22	1:B:152:TRP:NE1	2.31	0.46
1:B:71:PHE:CE1	2:C:253:TRP:NE1	2.74	0.46
2:G:75:SER:O	2:G:76:ALA:HB3	2.16	0.46
2:C:75:SER:O	2:C:76:ALA:HB3	2.16	0.46
2:C:280:GLU:OE1	2:C:280:GLU:HA	2.15	0.46
3:A:172:THR:C	3:A:174:THR:H	2.24	0.46
3:A:318:TYR:CD1	3:A:318:TYR:C	2.92	0.46
3:A:385:SER:HB2	3:E:265:GLN:NE2	2.30	0.46
1:F:39:ILE:HA	2:G:248:PHE:CE2	2.47	0.46
1:J:104:ARG:HA	1:J:108:PHE:HB2	1.98	0.46
3:I:293:VAL:HG21	3:I:413:PHE:CB	2.47	0.46
1:B:34:VAL:HG22	1:B:95:GLY:CA	2.46	0.45
2:C:160:HIS:CE1	2:C:165:ARG:HD2	2.50	0.45
2:C:201:PHE:CD1	2:C:271:GLN:OE1	2.66	0.45
3:A:92:GLY:HA3	3:A:139:HIS:HB2	1.98	0.45
3:A:411:PRO:HD2	1:F:177:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:10:SER:C	1:J:12:ALA:H	2.24	0.45
1:J:105:TYR:HD2	1:J:106:PHE:CD1	2.34	0.45
2:K:158:THR:O	2:K:162:THR:HG23	2.16	0.45
1:B:105:TYR:HD2	1:B:106:PHE:CD1	2.34	0.45
1:B:32:VAL:HG11	2:C:258:VAL:HB	1.99	0.45
1:F:34:VAL:HG22	1:F:95:GLY:CA	2.46	0.45
1:F:116:ILE:C	1:F:118:PHE:H	2.24	0.45
1:J:71:PHE:O	1:J:72:PRO:C	2.59	0.45
2:K:75:SER:O	2:K:76:ALA:HB3	2.16	0.45
2:C:231:HIS:CD2	2:C:245:HIS:ND1	2.83	0.45
2:G:280:GLU:OE1	2:G:280:GLU:HA	2.15	0.45
3:E:92:GLY:HA3	3:E:139:HIS:HB2	1.98	0.45
2:K:229:TRP:C	2:K:244:LEU:HD21	2.38	0.45
1:B:137:LEU:HD21	3:A:236:ALA:HB3	1.98	0.45
3:A:35:GLU:O	3:A:36:LYS:CB	2.59	0.45
3:A:124:PHE:HE2	3:A:140:THR:HG21	1.82	0.45
1:F:107:ASN:O	1:F:111:TRP:HB3	2.16	0.45
3:E:180:LEU:HA	3:E:180:LEU:HD12	1.68	0.45
1:J:137:LEU:HD21	3:I:236:ALA:HB3	1.98	0.45
3:E:293:VAL:HG21	3:E:413:PHE:CB	2.46	0.45
3:A:88:PHE:HB3	3:A:143:ASN:CB	2.44	0.45
1:F:69:VAL:HG22	1:F:152:TRP:NE1	2.31	0.45
3:E:281:THR:HG23	3:E:307:HIS:O	2.17	0.45
1:J:78:TYR:CZ	2:K:263:THR:OG1	2.69	0.45
1:B:10:SER:C	1:B:12:ALA:H	2.24	0.45
1:B:43:LEU:HD11	2:C:245:HIS:O	2.17	0.45
2:G:127:GLU:CD	2:G:272:GLY:HA2	2.41	0.45
2:G:222:PRO:HA	1:J:222:PHE:CD2	2.52	0.45
2:G:235:PHE:HD1	2:G:235:PHE:HA	1.65	0.45
1:J:34:VAL:HG22	1:J:95:GLY:CA	2.46	0.45
1:J:39:ILE:CD1	2:K:149:ALA:CB	2.81	0.45
1:J:32:VAL:HG11	2:K:258:VAL:HB	1.99	0.45
1:J:116:ILE:C	1:J:118:PHE:H	2.24	0.45
2:K:115:ARG:HE	2:K:115:ARG:HB3	1.69	0.45
3:I:33:HIS:N	3:I:139:HIS:HE2	2.15	0.45
3:I:281:THR:HG23	3:I:307:HIS:O	2.17	0.45
1:B:79:LEU:HD12	1:B:88:GLY:HA2	1.99	0.45
1:F:10:SER:C	1:F:12:ALA:H	2.24	0.45
1:F:79:LEU:HD12	1:F:88:GLY:HA2	1.99	0.45
2:G:158:THR:O	2:G:162:THR:HG23	2.16	0.45
2:G:223:ASN:C	2:G:223:ASN:HD22	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:THR:O	2:C:162:THR:HG23	2.16	0.44
3:A:34:GLY:C	3:A:35:GLU:O	2.58	0.44
3:A:293:VAL:HG21	3:A:413:PHE:CB	2.47	0.44
2:G:93:LEU:O	2:G:96:GLU:HG2	2.17	0.44
1:J:43:LEU:HD21	2:K:248:PHE:HB3	1.92	0.44
3:I:124:PHE:HE2	3:I:140:THR:HG21	1.82	0.44
1:B:107:ASN:O	1:B:111:TRP:HB3	2.16	0.44
1:B:177:LEU:HD22	3:I:411:PRO:HD2	1.98	0.44
1:F:104:ARG:HA	1:F:108:PHE:HB2	1.98	0.44
3:E:292:ARG:HD2	3:E:292:ARG:HA	1.85	0.44
1:J:69:VAL:HG22	1:J:152:TRP:NE1	2.31	0.44
1:J:107:ASN:O	1:J:111:TRP:HB3	2.16	0.44
2:K:93:LEU:O	2:K:96:GLU:HG2	2.17	0.44
2:K:177:PHE:HE1	2:K:224:VAL:HG13	1.60	0.44
1:B:104:ARG:HA	1:B:108:PHE:HB2	1.98	0.44
3:A:33:HIS:N	3:A:139:HIS:HE2	2.15	0.44
1:F:78:TYR:CZ	2:G:263:THR:OG1	2.70	0.44
3:E:33:HIS:N	3:E:139:HIS:HE2	2.15	0.44
3:E:124:PHE:HE2	3:E:140:THR:HG21	1.82	0.44
2:K:61:PHE:O	2:K:65:VAL:HG23	2.18	0.44
1:B:45:MET:HE2	1:B:45:MET:HB2	1.63	0.44
2:C:223:ASN:C	2:C:223:ASN:HD22	2.25	0.44
3:A:137:HIS:NE2	3:A:154:GLY:O	2.44	0.44
3:A:281:THR:HG23	3:A:307:HIS:O	2.17	0.44
1:F:32:VAL:HG11	2:G:258:VAL:HB	1.99	0.44
1:F:176:MET:HB3	1:F:176:MET:HE2	1.66	0.44
1:J:79:LEU:HD12	1:J:88:GLY:HA2	1.99	0.44
1:B:45:MET:HE1	1:B:49:ASP:H	1.83	0.44
1:B:45:MET:HA	2:C:241:VAL:HG12	1.97	0.44
1:B:71:PHE:O	1:B:72:PRO:C	2.58	0.44
2:C:93:LEU:O	2:C:96:GLU:HG2	2.17	0.44
1:F:45:MET:HA	2:G:241:VAL:HG12	1.96	0.44
1:F:137:LEU:HD21	3:E:236:ALA:HB3	1.98	0.44
2:G:61:PHE:O	2:G:65:VAL:HG23	2.17	0.44
2:K:223:ASN:C	2:K:223:ASN:HD22	2.25	0.44
3:I:172:THR:C	3:I:174:THR:H	2.24	0.44
2:C:167:THR:C	2:C:169:PHE:H	2.26	0.44
1:F:36:SER:HB3	2:G:255:ALA:HB2	1.93	0.44
3:E:137:HIS:CD2	3:E:154:GLY:C	2.96	0.44
1:J:113:TYR:CD1	3:I:132:ARG:HD2	2.53	0.44
2:K:167:THR:C	2:K:169:PHE:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:230:GLY:C	2:K:244:LEU:CD2	2.38	0.44
1:B:116:ILE:C	1:B:118:PHE:H	2.24	0.44
1:F:170:PRO:HB2	3:E:173:LEU:HD12	2.00	0.44
3:E:293:VAL:CG1	3:E:294:PRO:HD3	2.46	0.44
1:B:113:TYR:CD1	3:A:132:ARG:HD2	2.53	0.44
3:A:413:PHE:CE2	1:F:170:PRO:CG	3.01	0.44
1:F:43:LEU:HD11	2:G:245:HIS:O	2.17	0.44
3:E:172:THR:C	3:E:174:THR:H	2.24	0.44
3:I:290:THR:HA	3:I:410:ILE:O	2.18	0.44
2:C:127:GLU:CD	2:C:272:GLY:HA2	2.41	0.44
3:A:137:HIS:CD2	3:A:154:GLY:C	2.96	0.44
3:A:290:THR:HA	3:A:410:ILE:O	2.18	0.44
3:A:410:ILE:HD11	1:F:175:GLY:O	2.18	0.44
2:G:185:ILE:HD11	2:G:217:PRO:O	2.18	0.44
2:G:230:GLY:H	2:G:244:LEU:HD21	1.68	0.44
3:E:245:LEU:HD22	3:E:245:LEU:HA	1.90	0.44
3:I:73:VAL:HG21	3:I:118:ILE:HA	1.94	0.44
1:B:36:SER:HB3	2:C:255:ALA:HB2	1.93	0.43
1:B:222:PHE:CD2	2:K:222:PRO:HA	2.53	0.43
2:C:61:PHE:O	2:C:65:VAL:HG23	2.18	0.43
1:J:45:MET:HE1	1:J:49:ASP:H	1.83	0.43
3:I:371:TRP:CH2	3:I:377:SER:HA	2.53	0.43
1:F:25:ALA:HB2	2:G:266:PHE:HZ	1.84	0.43
1:F:45:MET:HE1	1:F:49:ASP:H	1.83	0.43
1:J:62:THR:HG21	1:J:219:PHE:CD2	2.50	0.43
1:J:170:PRO:HB2	3:I:173:LEU:HD12	2.00	0.43
3:I:293:VAL:CG2	3:I:412:SER:O	2.66	0.43
1:B:170:PRO:HB2	3:A:173:LEU:HD12	2.00	0.43
2:C:68:TYR:CD1	2:C:68:TYR:C	2.97	0.43
2:C:153:THR:HA	2:C:176:GLU:OE2	2.19	0.43
3:A:90:ASN:HA	3:A:100:ARG:HH22	1.83	0.43
1:F:78:TYR:HE2	2:G:259:MET:HE3	1.60	0.43
3:E:34:GLY:C	3:E:35:GLU:O	2.58	0.43
1:J:25:ALA:CB	2:K:266:PHE:HZ	2.32	0.43
1:B:170:PRO:CG	3:I:413:PHE:CE2	3.01	0.43
1:F:179:SER:O	1:F:180:ILE:C	2.61	0.43
1:F:187:ASN:ND2	3:E:100:ARG:O	2.52	0.43
3:E:371:TRP:CH2	3:E:377:SER:HA	2.53	0.43
1:J:43:LEU:HD11	2:K:245:HIS:O	2.17	0.43
1:J:176:MET:HE2	1:J:176:MET:HB3	1.66	0.43
2:K:185:ILE:HD11	2:K:217:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:224:VAL:CG2	2:C:248:PHE:CE1	2.96	0.43
3:I:90:ASN:HA	3:I:100:ARG:HH22	1.83	0.43
1:B:170:PRO:HG3	3:I:413:PHE:CZ	2.54	0.43
3:A:33:HIS:N	3:A:33:HIS:ND1	2.67	0.43
2:G:204:LYS:HA	2:G:204:LYS:HD3	1.40	0.43
2:G:220:ILE:HG13	2:G:251:PHE:HB3	2.01	0.43
3:E:90:ASN:HA	3:E:100:ARG:HH22	1.83	0.43
3:E:293:VAL:CG2	3:E:413:PHE:CD1	3.02	0.43
1:J:116:ILE:C	1:J:118:PHE:N	2.77	0.43
1:J:187:ASN:ND2	3:I:100:ARG:O	2.52	0.43
3:I:34:GLY:C	3:I:35:GLU:O	2.58	0.43
1:B:187:ASN:ND2	3:A:100:ARG:O	2.52	0.43
3:A:293:VAL:CG2	3:A:412:SER:O	2.66	0.43
3:A:371:TRP:CH2	3:A:377:SER:HA	2.53	0.43
1:F:125:VAL:O	1:F:126:PRO:C	2.62	0.43
2:G:153:THR:HA	2:G:176:GLU:OE2	2.19	0.43
1:J:25:ALA:HB2	2:K:266:PHE:HZ	1.84	0.43
1:J:179:SER:O	1:J:180:ILE:C	2.61	0.43
3:I:137:HIS:CD2	3:I:154:GLY:C	2.96	0.43
1:B:25:ALA:CB	2:C:266:PHE:HZ	2.32	0.43
1:B:25:ALA:HB2	2:C:266:PHE:HZ	1.84	0.43
1:B:179:SER:O	1:B:180:ILE:C	2.61	0.43
2:C:220:ILE:HG13	2:C:251:PHE:HB3	2.01	0.43
3:E:245:LEU:HD13	3:E:249:MET:CG	2.49	0.43
3:I:74:PHE:HD1	3:I:404:GLN:OE1	2.02	0.43
3:I:293:VAL:CG2	3:I:413:PHE:CD1	3.02	0.43
3:A:245:LEU:HD13	3:A:249:MET:CG	2.49	0.43
1:F:113:TYR:CD1	3:E:132:ARG:HD2	2.53	0.43
3:I:35:GLU:O	3:I:36:LYS:CB	2.59	0.43
1:B:176:MET:HE2	1:B:176:MET:HB3	1.66	0.43
1:F:116:ILE:C	1:F:118:PHE:N	2.77	0.43
3:E:290:THR:HA	3:E:410:ILE:O	2.18	0.43
3:E:293:VAL:CG2	3:E:412:SER:O	2.66	0.43
2:K:68:TYR:CD1	2:K:68:TYR:C	2.97	0.43
3:I:180:LEU:HD12	3:I:180:LEU:HA	1.69	0.43
1:B:66:ILE:O	1:B:69:VAL:HG23	2.19	0.42
3:E:131:ARG:HG3	3:E:166:PHE:CG	2.54	0.42
1:F:44:THR:CG2	2:G:249:VAL:HG21	2.21	0.42
1:F:62:THR:CG2	1:F:219:PHE:CE2	3.02	0.42
1:J:34:VAL:HG22	1:J:95:GLY:HA2	2.01	0.42
1:J:62:THR:CG2	1:J:219:PHE:CE2	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:220:ILE:HG13	2:K:251:PHE:HB3	2.01	0.42
1:B:241:GLU:C	2:C:264:GLN:HE21	2.27	0.42
3:E:97:VAL:HA	3:E:132:ARG:HB2	2.02	0.42
1:J:66:ILE:O	1:J:69:VAL:HG23	2.19	0.42
1:J:125:VAL:O	1:J:126:PRO:C	2.62	0.42
1:B:116:ILE:C	1:B:118:PHE:N	2.77	0.42
3:A:74:PHE:HD1	3:A:404:GLN:OE1	2.02	0.42
3:A:131:ARG:HG3	3:A:166:PHE:CG	2.54	0.42
1:F:45:MET:HE2	1:F:45:MET:HB2	1.63	0.42
3:I:131:ARG:HG3	3:I:166:PHE:CG	2.54	0.42
1:B:62:THR:CG2	1:B:219:PHE:CE2	3.02	0.42
1:B:165:ALA:O	1:B:167:LEU:N	2.53	0.42
1:B:228:TYR:CD1	1:B:228:TYR:C	2.97	0.42
2:C:280:GLU:N	2:C:280:GLU:CD	2.77	0.42
1:F:25:ALA:CB	2:G:266:PHE:HZ	2.32	0.42
1:F:241:GLU:C	2:G:264:GLN:HE21	2.27	0.42
2:G:68:TYR:CD1	2:G:68:TYR:C	2.97	0.42
2:G:222:PRO:CG	1:J:222:PHE:CE1	2.77	0.42
3:I:75:GLU:HG3	3:I:119:GLY:HA2	2.01	0.42
3:I:88:PHE:HB3	3:I:143:ASN:CB	2.44	0.42
2:C:99:LEU:O	2:C:103:THR:OG1	2.35	0.42
3:A:178:VAL:HG11	3:A:183:TYR:CE1	2.55	0.42
3:A:293:VAL:CG2	3:A:413:PHE:CD1	3.02	0.42
1:F:112:THR:CG2	2:G:162:THR:HG21	2.46	0.42
1:F:228:TYR:CD1	1:F:228:TYR:C	2.97	0.42
2:K:280:GLU:N	2:K:280:GLU:CD	2.77	0.42
2:C:185:ILE:HD11	2:C:217:PRO:O	2.18	0.42
1:F:21:ILE:CG2	2:G:266:PHE:HE1	2.33	0.42
3:E:77:TRP:HZ2	3:E:144:VAL:HG11	1.85	0.42
1:J:165:ALA:O	1:J:167:LEU:N	2.53	0.42
2:K:202:PHE:HE2	2:K:268:SER:CB	2.30	0.42
3:I:33:HIS:N	3:I:33:HIS:ND1	2.67	0.42
2:G:167:THR:C	2:G:169:PHE:H	2.26	0.42
2:G:280:GLU:N	2:G:280:GLU:CD	2.77	0.42
2:K:127:GLU:CD	2:K:272:GLY:HA2	2.41	0.42
3:I:245:LEU:HD13	3:I:249:MET:CG	2.49	0.42
1:B:39:ILE:HA	2:C:248:PHE:CE2	2.47	0.42
1:B:125:VAL:O	1:B:126:PRO:C	2.62	0.42
2:C:204:LYS:HA	2:C:204:LYS:HD3	1.40	0.42
2:C:226:LEU:HD12	2:C:226:LEU:HA	1.81	0.42
3:A:320:ALA:O	3:A:321:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ILE:CD1	2:G:149:ALA:CB	2.81	0.42
1:F:66:ILE:O	1:F:69:VAL:HG23	2.19	0.42
2:G:226:LEU:HD12	2:G:226:LEU:HA	1.81	0.42
3:E:74:PHE:HD1	3:E:404:GLN:OE1	2.02	0.42
3:E:385:SER:HB2	3:I:265:GLN:NE2	2.35	0.42
1:J:7:ALA:CA	2:K:125:ARG:HG2	2.29	0.42
1:J:228:TYR:CD1	1:J:228:TYR:C	2.97	0.42
1:J:241:GLU:C	2:K:264:GLN:HE21	2.27	0.42
1:B:34:VAL:HG22	1:B:95:GLY:HA2	2.01	0.42
1:B:78:TYR:CZ	2:C:263:THR:OG1	2.70	0.42
2:C:222:PRO:HA	1:F:222:PHE:CD2	2.54	0.42
2:G:165:ARG:H	2:G:165:ARG:HG3	1.50	0.42
3:E:394:PHE:CE2	3:E:400:ARG:HB3	2.55	0.42
1:J:181:ALA:O	1:J:184:GLN:HB2	2.20	0.42
2:K:153:THR:HA	2:K:176:GLU:OE2	2.19	0.42
2:C:226:LEU:HG	1:F:219:PHE:CE1	2.55	0.41
3:A:97:VAL:HA	3:A:132:ARG:HB2	2.02	0.41
1:F:34:VAL:HG22	1:F:95:GLY:HA2	2.01	0.41
3:E:75:GLU:HG3	3:E:119:GLY:HA2	2.01	0.41
3:I:394:PHE:CE2	3:I:400:ARG:HB3	2.55	0.41
1:F:165:ALA:O	1:F:167:LEU:N	2.53	0.41
3:I:77:TRP:HZ2	3:I:144:VAL:HG11	1.85	0.41
1:B:72:PRO:O	1:B:76:GLN:HB2	2.20	0.41
3:A:75:GLU:HG3	3:A:119:GLY:HA2	2.01	0.41
2:G:220:ILE:H	2:G:220:ILE:CD1	1.96	0.41
1:B:181:ALA:O	1:B:184:GLN:HB2	2.20	0.41
2:C:274:LEU:CD1	2:C:274:LEU:N	2.73	0.41
1:F:76:GLN:HE22	1:F:131:LEU:HD13	1.86	0.41
1:J:164:ILE:HD13	1:J:164:ILE:HA	1.88	0.41
3:I:178:VAL:HG11	3:I:183:TYR:CE1	2.55	0.41
1:B:21:ILE:CG2	2:C:266:PHE:HE1	2.33	0.41
1:F:240:ASN:ND2	2:G:208:LEU:HD23	2.36	0.41
3:E:213:ILE:O	3:E:217:LEU:HD12	2.21	0.41
2:K:221:LEU:CB	2:K:222:PRO:CD	2.80	0.41
3:I:33:HIS:N	3:I:139:HIS:NE2	2.69	0.41
3:A:252:SER:HA	3:A:255:ASN:HB2	2.02	0.41
3:E:178:VAL:HG11	3:E:183:TYR:CE1	2.55	0.41
3:E:379:ILE:HA	3:E:382:ASP:OD2	2.21	0.41
1:J:72:PRO:O	1:J:76:GLN:HB2	2.20	0.41
2:K:99:LEU:O	2:K:103:THR:OG1	2.35	0.41
1:B:240:ASN:ND2	2:C:208:LEU:HD23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:379:ILE:HA	3:A:382:ASP:OD2	2.21	0.41
3:E:252:SER:HA	3:E:255:ASN:HB2	2.02	0.41
1:J:21:ILE:CG2	2:K:266:PHE:HE1	2.33	0.41
2:K:231:HIS:CD2	2:K:245:HIS:ND1	2.83	0.41
3:I:379:ILE:HA	3:I:382:ASP:OD2	2.21	0.41
3:A:394:PHE:CE2	3:A:400:ARG:HB3	2.55	0.41
1:F:72:PRO:O	1:F:76:GLN:HB2	2.20	0.41
3:E:33:HIS:N	3:E:33:HIS:ND1	2.67	0.41
3:I:313:ARG:CZ	3:I:329:VAL:HG22	2.51	0.41
1:B:175:GLY:O	3:I:410:ILE:HD11	2.21	0.41
2:C:201:PHE:HE1	2:C:267:TYR:HE2	1.57	0.41
2:C:237:GLU:OE2	3:A:147:GLY:CA	2.68	0.41
3:A:413:PHE:CZ	1:F:170:PRO:HG3	2.55	0.41
1:F:61:VAL:HG22	1:F:157:TYR:CD1	2.56	0.41
2:G:126:GLU:C	2:G:128:LEU:N	2.78	0.41
2:G:226:LEU:HG	1:J:219:PHE:CE1	2.56	0.41
3:E:320:ALA:O	3:E:321:SER:HB2	2.20	0.41
1:J:76:GLN:HE22	1:J:131:LEU:HD13	1.86	0.41
1:J:240:ASN:ND2	2:K:208:LEU:HD23	2.36	0.41
3:I:97:VAL:HA	3:I:132:ARG:HB2	2.02	0.41
3:I:213:ILE:O	3:I:217:LEU:HD12	2.21	0.41
3:I:252:SER:HA	3:I:255:ASN:HB2	2.02	0.41
1:B:76:GLN:HE22	1:B:131:LEU:HD13	1.86	0.41
1:B:219:PHE:CE1	2:K:226:LEU:HG	2.56	0.41
2:C:126:GLU:C	2:C:128:LEU:N	2.77	0.41
2:K:126:GLU:C	2:K:128:LEU:N	2.78	0.41
3:A:51:ASP:O	3:A:69:GLY:HA2	2.21	0.40
3:A:281:THR:H	3:A:401:GLN:NE2	2.19	0.40
2:G:202:PHE:HE2	2:G:268:SER:CB	2.30	0.40
3:E:33:HIS:N	3:E:139:HIS:NE2	2.69	0.40
3:E:313:ARG:CZ	3:E:329:VAL:HG22	2.51	0.40
2:K:201:PHE:HE2	2:K:264:GLN:O	2.04	0.40
2:K:270:ALA:CA	2:K:274:LEU:HD11	2.08	0.40
1:B:21:ILE:O	1:B:22:ASP:C	2.65	0.40
2:C:230:GLY:HA2	2:C:244:LEU:HD13	1.71	0.40
3:A:180:LEU:HD12	3:A:180:LEU:HA	1.69	0.40
1:F:181:ALA:O	1:F:184:GLN:HB2	2.20	0.40
2:G:145:ILE:O	2:G:146:TYR:C	2.63	0.40
2:G:223:ASN:HB2	2:G:251:PHE:HE2	1.79	0.40
2:G:230:GLY:HA2	2:G:244:LEU:HD13	1.70	0.40
3:E:51:ASP:O	3:E:69:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:411:PRO:HD2	1:J:177:LEU:HD22	2.03	0.40
2:K:235:PHE:CZ	3:I:146:GLY:N	2.89	0.40
3:A:33:HIS:N	3:A:139:HIS:NE2	2.69	0.40
3:I:320:ALA:O	3:I:321:SER:HB2	2.20	0.40
3:A:128:LEU:HA	3:A:128:LEU:HD23	1.87	0.40
2:G:201:PHE:HE2	2:G:264:GLN:O	2.05	0.40
1:J:61:VAL:HG22	1:J:157:TYR:CD1	2.56	0.40
1:J:177:LEU:HD21	3:I:262:ILE:HG21	2.03	0.40
3:I:281:THR:H	3:I:401:GLN:NE2	2.19	0.40
1:B:177:LEU:HD13	3:I:411:PRO:HD2	2.04	0.40
1:B:180:ILE:HG23	3:A:180:LEU:HD11	2.03	0.40
1:F:12:ALA:HA	2:G:278:LEU:HD11	1.30	0.40
1:F:28:VAL:O	1:F:29:VAL:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	B	128/210 (61%)	112 (88%)	16 (12%)	4	17
1	F	186/210 (89%)	165 (89%)	21 (11%)	5	20
1	J	186/210 (89%)	165 (89%)	21 (11%)	5	20
2	C	200/237 (84%)	170 (85%)	30 (15%)	3	13
2	G	200/237 (84%)	170 (85%)	30 (15%)	3	13
2	K	200/237 (84%)	170 (85%)	30 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	323/345 (94%)	286 (88%)	37 (12%)	5	19
3	E	323/345 (94%)	286 (88%)	37 (12%)	5	19
3	I	323/345 (94%)	286 (88%)	37 (12%)	5	19
All	All	2069/2376 (87%)	1810 (88%)	259 (12%)	7	17

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	75	VAL
1	B	76	GLN
1	B	84	ARG
1	B	93	VAL
1	B	111	TRP
1	B	116	ILE
1	B	129	ILE
1	B	134	VAL
1	B	135	LEU
1	B	155	ILE
1	B	169	VAL
1	B	180	ILE
1	B	190	ARG
1	B	215	VAL
1	B	230	MET
1	B	240	ASN
2	C	47	ASP
2	C	51	LEU
2	C	63	LEU
2	C	103	THR
2	C	107	LEU
2	C	113	LYS
2	C	115	ARG
2	C	126	GLU
2	C	139	VAL
2	C	158	THR
2	C	163	ILE
2	C	165	ARG
2	C	198	ARG
2	C	199	LEU
2	C	204	LYS
2	C	217	PRO
2	C	220	ILE

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Mol	Chain	Res	Type
2	C	221	LEU
2	C	223	ASN
2	C	224	VAL
2	C	226	LEU
2	C	227	ASN
2	C	232	THR
2	C	233	PHE
2	C	234	TRP
2	C	235	PHE
2	C	236	MET
2	C	274	LEU
2	C	276	GLN
2	C	280	GLU
3	A	45	ARG
3	A	46	THR
3	A	52	LEU
3	A	59	VAL
3	A	60	LYS
3	A	64	THR
3	A	65	VAL
3	A	79	GLU
3	A	112	ARG
3	A	117	GLU
3	A	140	THR
3	A	144	VAL
3	A	145	GLN
3	A	162	SER
3	A	164	SER
3	A	174	THR
3	A	176	GLN
3	A	180	LEU
3	A	213	ILE
3	A	228	VAL
3	A	240	LEU
3	A	245	LEU
3	A	256	SER
3	A	273	LYS
3	A	277	LEU
3	A	281	THR
3	A	287	GLU
3	A	293	VAL
3	A	298	MET

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Mol	Chain	Res	Type
3	A	299	ARG
3	A	305	THR
3	A	312	ILE
3	A	359	THR
3	A	362	VAL
3	A	385	SER
3	A	406	ASP
3	A	414	MET
1	F	11	HIS
1	F	29	VAL
1	F	45	MET
1	F	63	VAL
1	F	69	VAL
1	F	75	VAL
1	F	76	GLN
1	F	84	ARG
1	F	93	VAL
1	F	111	TRP
1	F	116	ILE
1	F	129	ILE
1	F	134	VAL
1	F	135	LEU
1	F	155	ILE
1	F	169	VAL
1	F	180	ILE
1	F	190	ARG
1	F	215	VAL
1	F	230	MET
1	F	240	ASN
2	G	47	ASP
2	G	51	LEU
2	G	63	LEU
2	G	103	THR
2	G	107	LEU
2	G	113	LYS
2	G	115	ARG
2	G	126	GLU
2	G	139	VAL
2	G	158	THR
2	G	163	ILE
2	G	165	ARG
2	G	198	ARG

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Mol	Chain	Res	Type
2	G	199	LEU
2	G	204	LYS
2	G	217	PRO
2	G	220	ILE
2	G	221	LEU
2	G	223	ASN
2	G	224	VAL
2	G	226	LEU
2	G	227	ASN
2	G	232	THR
2	G	233	PHE
2	G	234	TRP
2	G	235	PHE
2	G	236	MET
2	G	274	LEU
2	G	276	GLN
2	G	280	GLU
3	E	45	ARG
3	E	46	THR
3	E	52	LEU
3	E	59	VAL
3	E	60	LYS
3	E	64	THR
3	E	65	VAL
3	E	79	GLU
3	E	112	ARG
3	E	117	GLU
3	E	140	THR
3	E	144	VAL
3	E	145	GLN
3	E	162	SER
3	E	164	SER
3	E	174	THR
3	E	176	GLN
3	E	180	LEU
3	E	213	ILE
3	E	228	VAL
3	E	240	LEU
3	E	245	LEU
3	E	256	SER
3	E	273	LYS
3	E	277	LEU

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Mol	Chain	Res	Type
3	E	281	THR
3	E	287	GLU
3	E	293	VAL
3	E	298	MET
3	E	299	ARG
3	E	305	THR
3	E	312	ILE
3	E	359	THR
3	E	362	VAL
3	E	385	SER
3	E	406	ASP
3	E	414	MET
1	J	11	HIS
1	J	29	VAL
1	J	45	MET
1	J	63	VAL
1	J	69	VAL
1	J	75	VAL
1	J	76	GLN
1	J	84	ARG
1	J	93	VAL
1	J	111	TRP
1	J	116	ILE
1	J	129	ILE
1	J	134	VAL
1	J	135	LEU
1	J	155	ILE
1	J	169	VAL
1	J	180	ILE
1	J	190	ARG
1	J	215	VAL
1	J	230	MET
1	J	240	ASN
2	K	47	ASP
2	K	51	LEU
2	K	63	LEU
2	K	103	THR
2	K	107	LEU
2	K	113	LYS
2	K	115	ARG
2	K	126	GLU
2	K	139	VAL

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Mol	Chain	Res	Type
2	K	158	THR
2	K	163	ILE
2	K	165	ARG
2	K	198	ARG
2	K	199	LEU
2	K	204	LYS
2	K	217	PRO
2	K	220	ILE
2	K	221	LEU
2	K	223	ASN
2	K	224	VAL
2	K	226	LEU
2	K	227	ASN
2	K	232	THR
2	K	233	PHE
2	K	234	TRP
2	K	235	PHE
2	K	236	MET
2	K	274	LEU
2	K	276	GLN
2	K	280	GLU
3	I	45	ARG
3	I	46	THR
3	I	52	LEU
3	I	59	VAL
3	I	60	LYS
3	I	64	THR
3	I	65	VAL
3	I	79	GLU
3	I	112	ARG
3	I	117	GLU
3	I	140	THR
3	I	144	VAL
3	I	145	GLN
3	I	162	SER
3	I	164	SER
3	I	174	THR
3	I	176	GLN
3	I	180	LEU
3	I	213	ILE
3	I	228	VAL
3	I	240	LEU

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Mol	Chain	Res	Type
3	I	245	LEU
3	I	256	SER
3	I	273	LYS
3	I	277	LEU
3	I	281	THR
3	I	287	GLU
3	I	293	VAL
3	I	298	MET
3	I	299	ARG
3	I	305	THR
3	I	312	ILE
3	I	359	THR
3	I	362	VAL
3	I	385	SER
3	I	406	ASP
3	I	414	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	GLN
1	B	103	ASN
1	B	174	ASN
1	B	187	ASN
1	B	240	ASN
2	C	91	ASN
2	C	134	HIS
2	C	155	GLN
2	C	160	HIS
2	C	173	HIS
2	C	223	ASN
3	A	33	HIS
3	A	62	ASN
3	A	72	HIS
3	A	143	ASN
3	A	168	ASN
3	A	192	HIS
3	A	265	GLN
3	A	306	ASN
3	A	401	GLN
1	F	40	HIS
1	F	76	GLN

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Mol	Chain	Res	Type
1	F	103	ASN
1	F	174	ASN
1	F	187	ASN
2	G	91	ASN
2	G	134	HIS
2	G	155	GLN
2	G	160	HIS
2	G	173	HIS
2	G	223	ASN
3	E	33	HIS
3	E	62	ASN
3	E	72	HIS
3	E	143	ASN
3	E	168	ASN
3	E	192	HIS
3	E	265	GLN
3	E	306	ASN
3	E	401	GLN
1	J	40	HIS
1	J	76	GLN
1	J	103	ASN
1	J	174	ASN
1	J	240	ASN
2	K	91	ASN
2	K	134	HIS
2	K	155	GLN
2	K	160	HIS
2	K	173	HIS
2	K	223	ASN
3	I	33	HIS
3	I	62	ASN
3	I	72	HIS
3	I	143	ASN
3	I	192	HIS
3	I	265	GLN
3	I	306	ASN
3	I	401	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

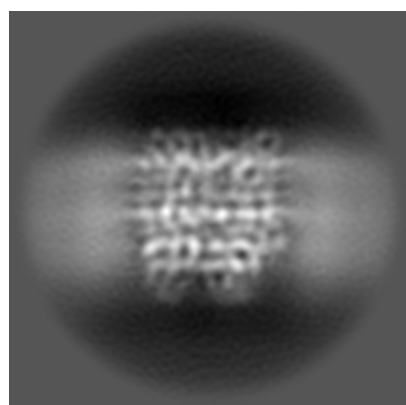
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14399. These allow visual inspection of the internal detail of the map and identification of artifacts.

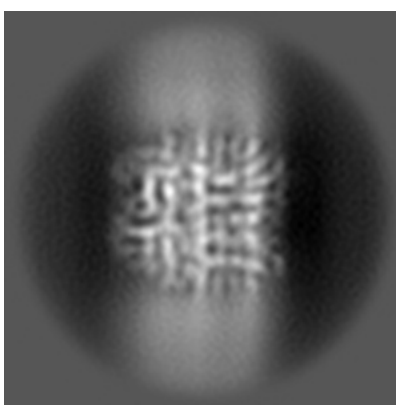
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

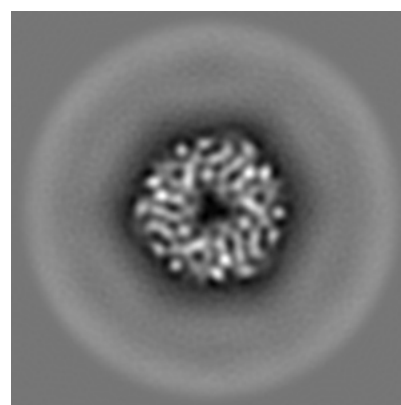
6.1.1 Primary map



X



Y

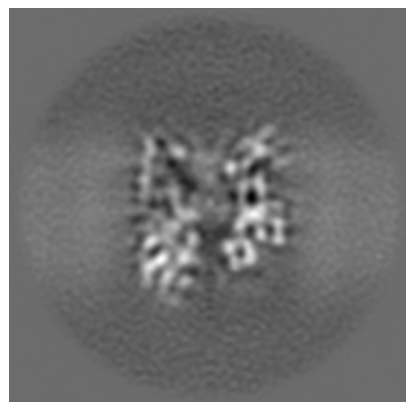


Z

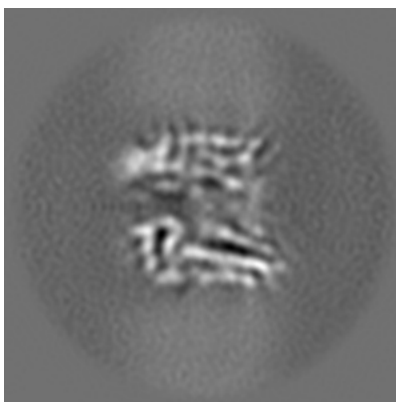
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

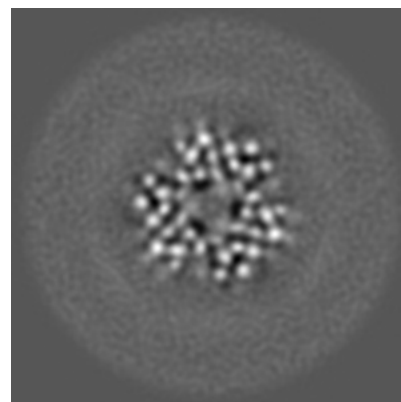
6.2.1 Primary map



X Index: 90



Y Index: 90

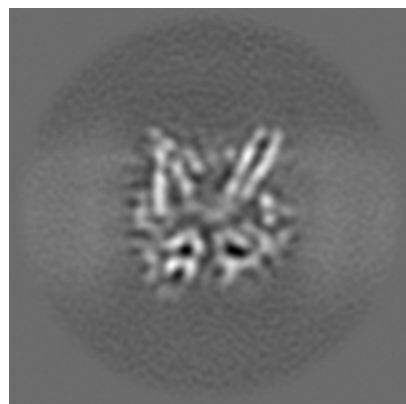


Z Index: 90

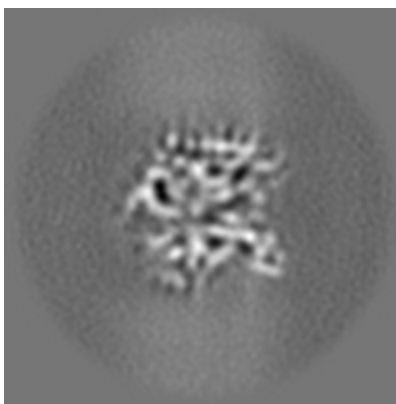
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

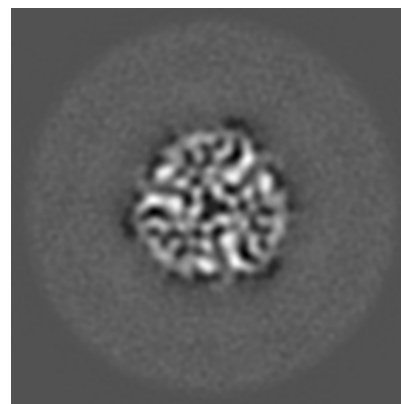
6.3.1 Primary map



X Index: 96



Y Index: 80

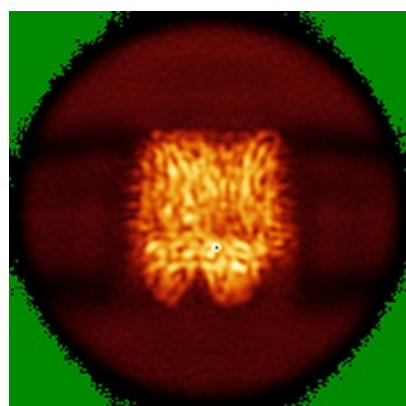


Z Index: 74

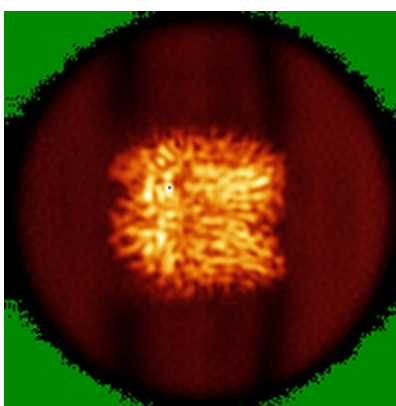
The images above show the largest variance slices of the map in three orthogonal directions.

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

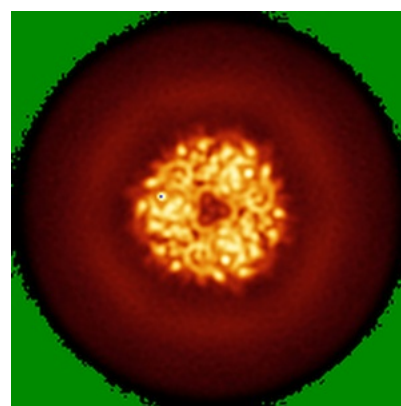
6.4.1 Primary map



X



Y

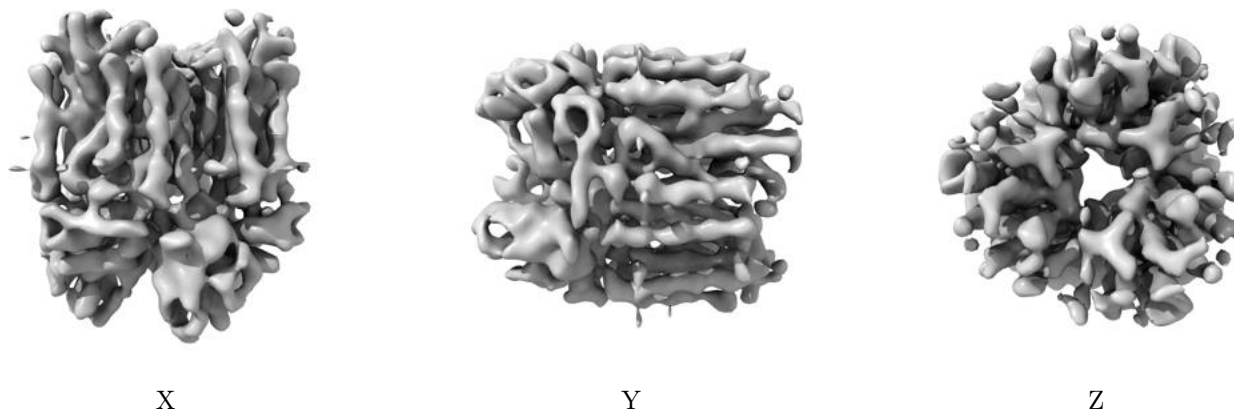


Z

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 0.0109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

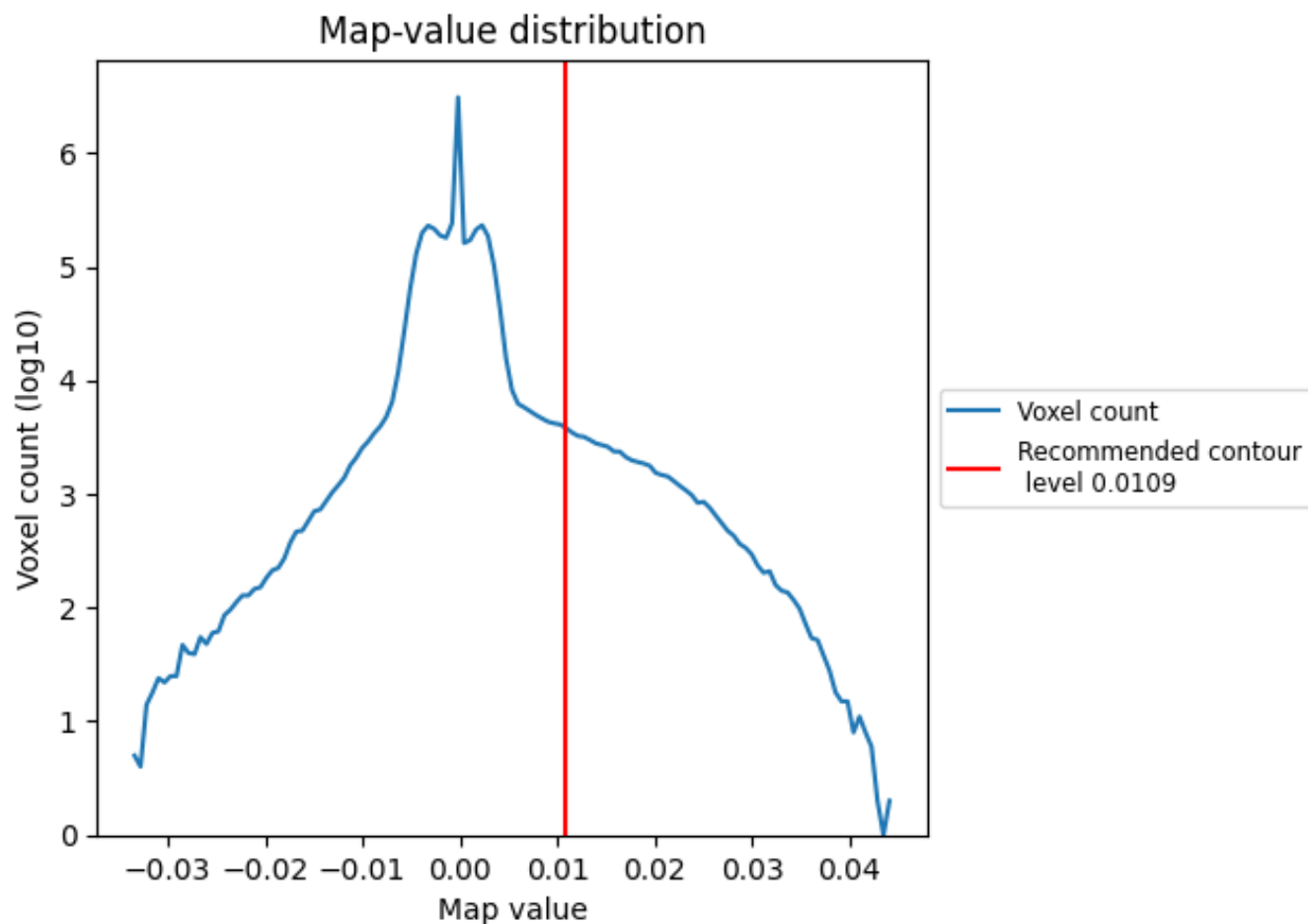
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

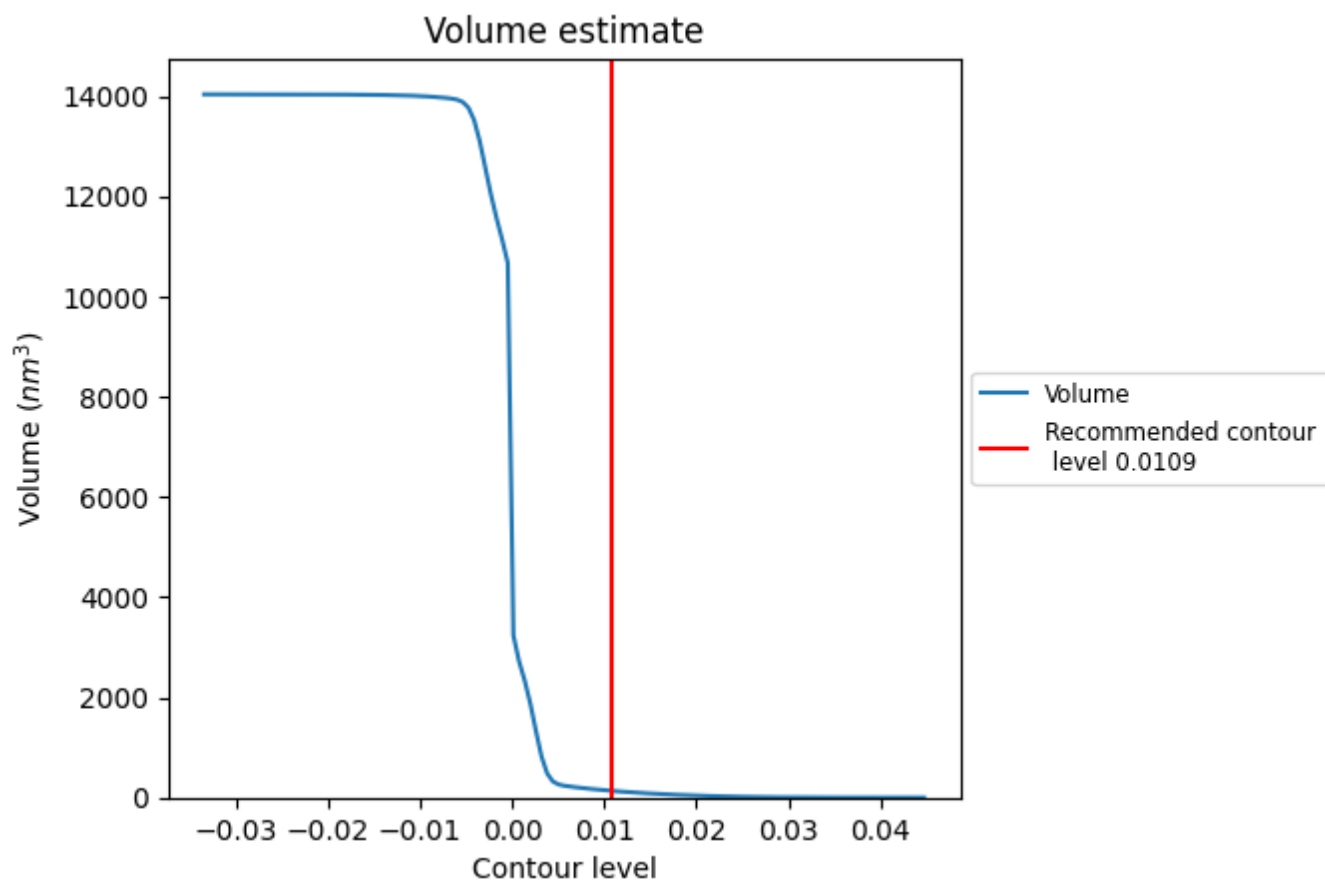
This section contains the results of statistical analysis of the map.

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.

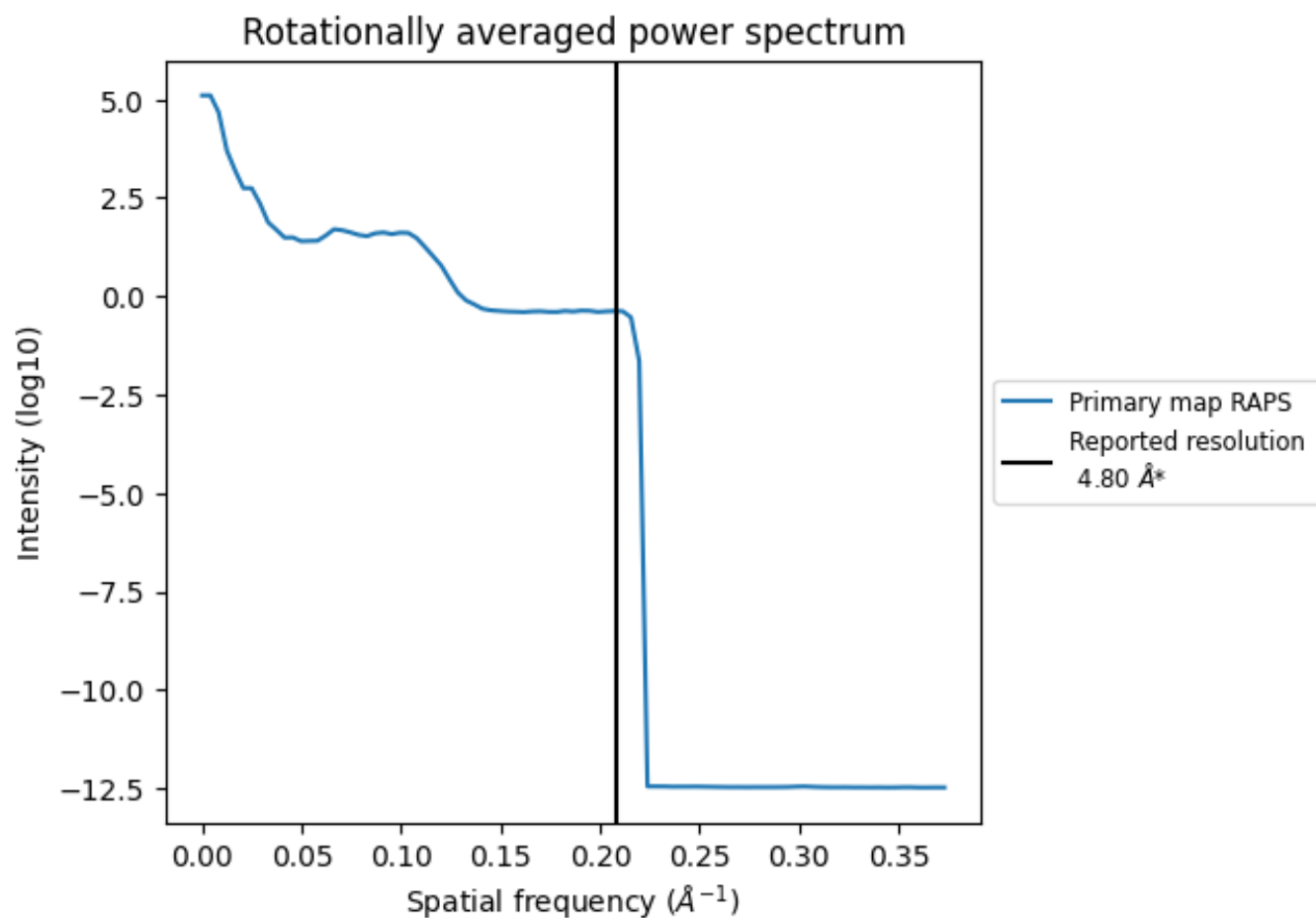
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm³; this corresponds to an approximate mass of 120 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 0.208 Å⁻¹

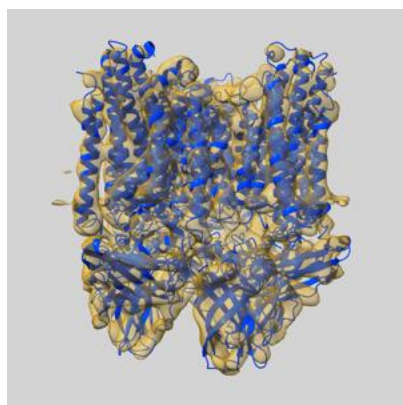
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

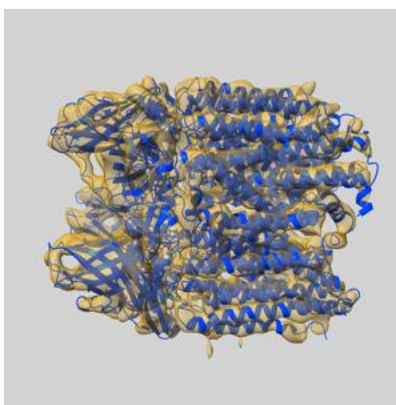
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14399 and PDB model 7YZY. Per-residue inclusion information can be found in section 3 on page 5.

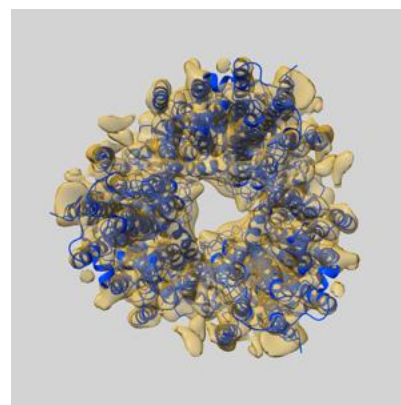
9.1 Map-model overlay [i](#)



X



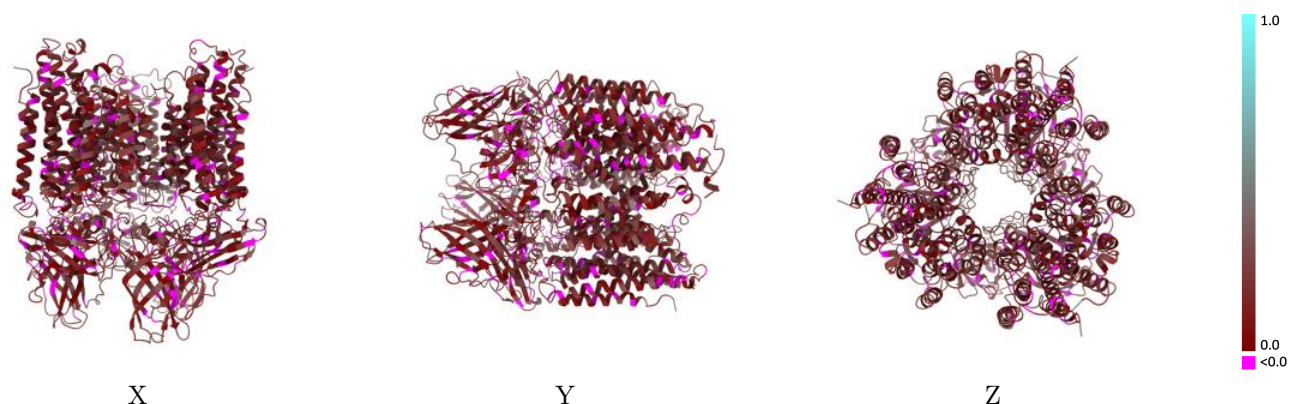
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0109 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](#)

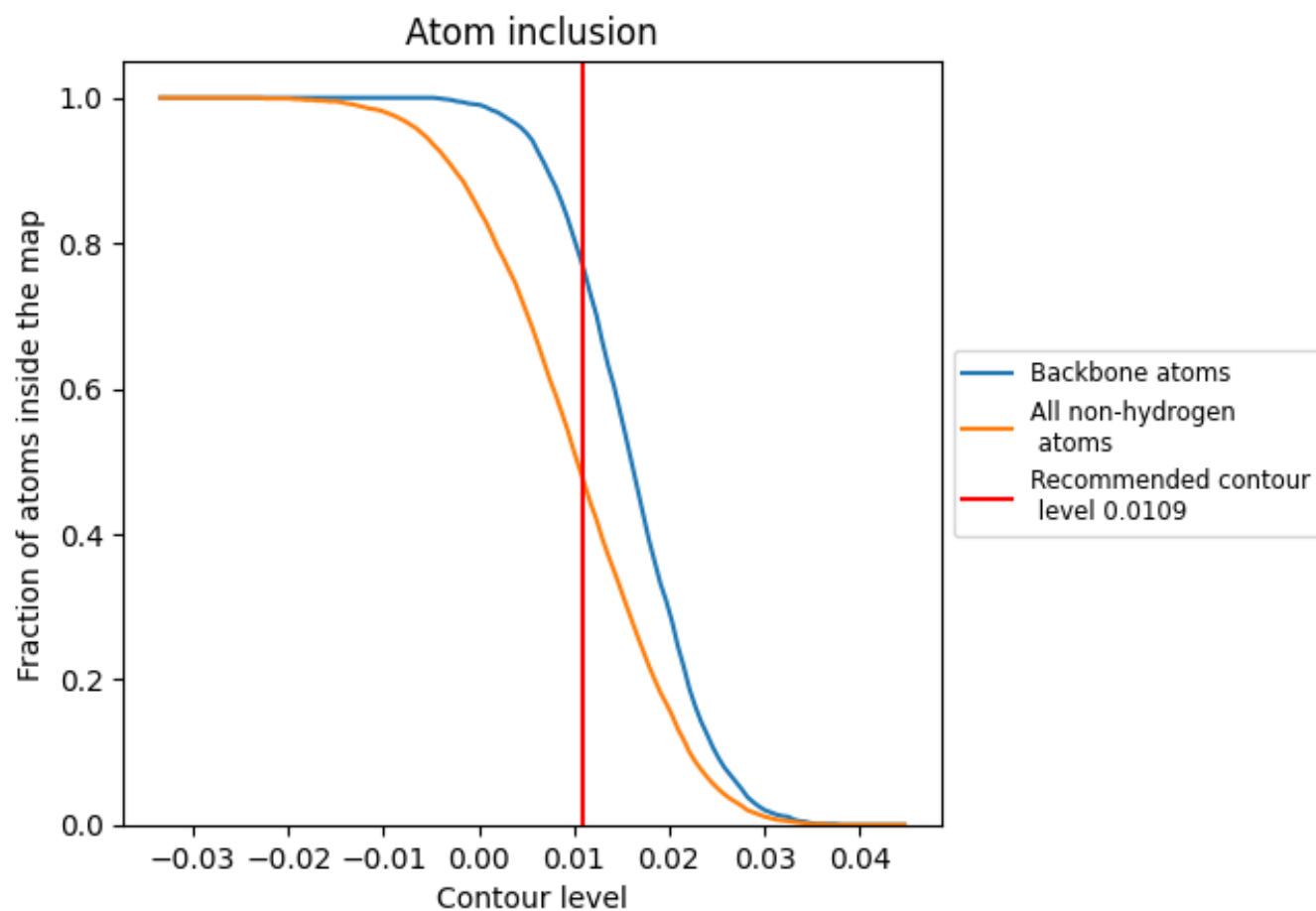


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 77% of all backbone atoms, 48% 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 (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4770	0.1330
A	0.4830	0.1370
B	0.5050	0.1340
C	0.4400	0.1280
E	0.4830	0.1370
F	0.5070	0.1330
G	0.4400	0.1270
I	0.4850	0.1360
J	0.5070	0.1300
K	0.4400	0.1270

1.0

0.0

<0.0