



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:51 AM UTC

PDB ID : 6VOA / pdb_00006voa
EMDB ID : EMD-21259
Title : Cryo-EM structure of the BBSome-ARL6 complex
Authors : Yang, S.; Walz, T.; Nachury, M.V.
Deposited on : 2020-01-30
Resolution : 4.00 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:

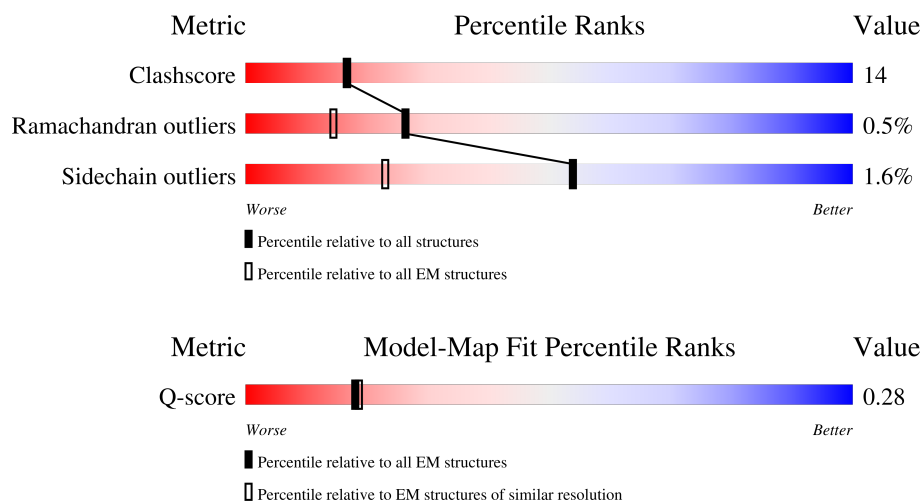
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	H	69	12% 45% 29% • 25%
2	B	721	16% 81% 5% 14%
3	E	519	10% 56% 18% • 25%
4	G	341	22% 57% 30% • 12%

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Mol	Chain	Length	Quality of chain
5	C	715	
6	F	501	
7	I	887	
8	A	186	
9	D	592	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26824 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 Bardet-Biedl syndrome 18 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	52	Total	C	N	O	S	0	0
			421	270	70	77	4		

- Molecule 2 is a protein called Bardet-Biedl syndrome 2 protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	619	Total	C	N	O	S	0	0
			3465	2088	691	678	8		

- Molecule 3 is a protein called Bardet-Biedl syndrome 4 protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	388	Total	C	N	O	S	0	0
			3114	2013	513	568	20		

- Molecule 4 is a protein called Bardet-Biedl syndrome 5 protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	300	Total	C	N	O	S	0	0
			2411	1533	422	450	6		

- Molecule 5 is a protein called Bardet-Biedl syndrome 7 protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	667	Total	C	N	O	S	0	0
			3676	2241	707	726	2		

- Molecule 6 is a protein called Tetratricopeptide repeat domain 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	475	Total	C	N	O	S	0	0
			3797	2417	655	705	20		

- Molecule 7 is a protein called Bardet-Biedl syndrome 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	764	Total	C	N	O	S	0	0
			6034	3857	1018	1128	31		

- Molecule 8 is a protein called ADP-ribosylation factor-like protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	A	165	Total	C	N	O	0	0
			816	486	165	165		

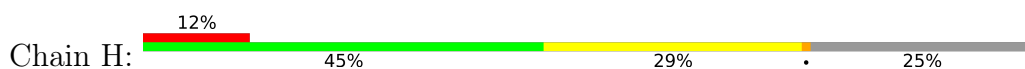
- Molecule 9 is a protein called BBS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	528	Total	C	N	O	S	0	0
			3090	1905	591	590	4		

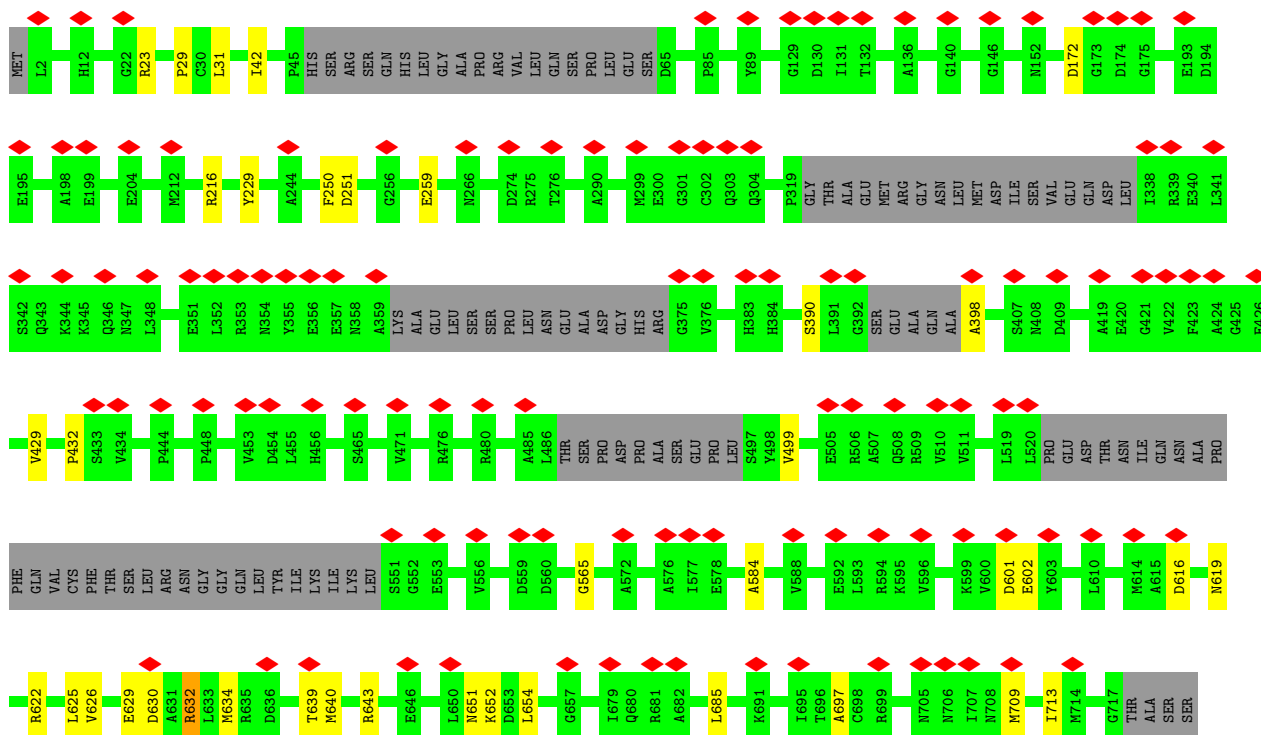
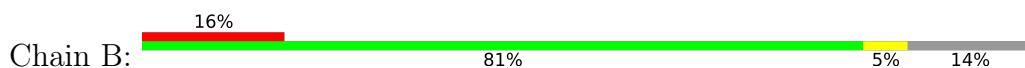
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Bardet-Biedl syndrome 18 protein



- Molecule 2: Bardet-Biedl syndrome 2 protein homolog

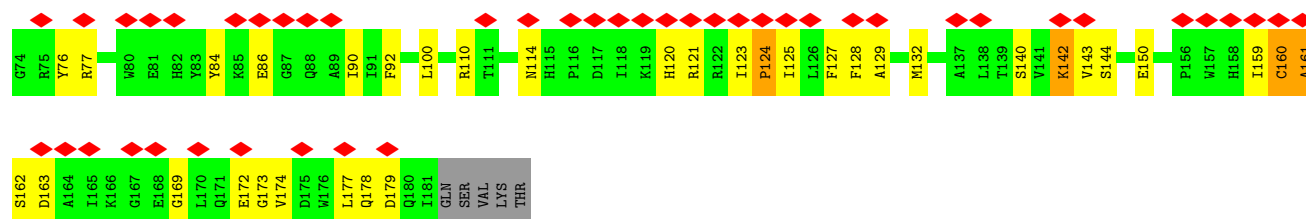


- Molecule 3: Bardet-Biedl syndrome 4 protein homolog

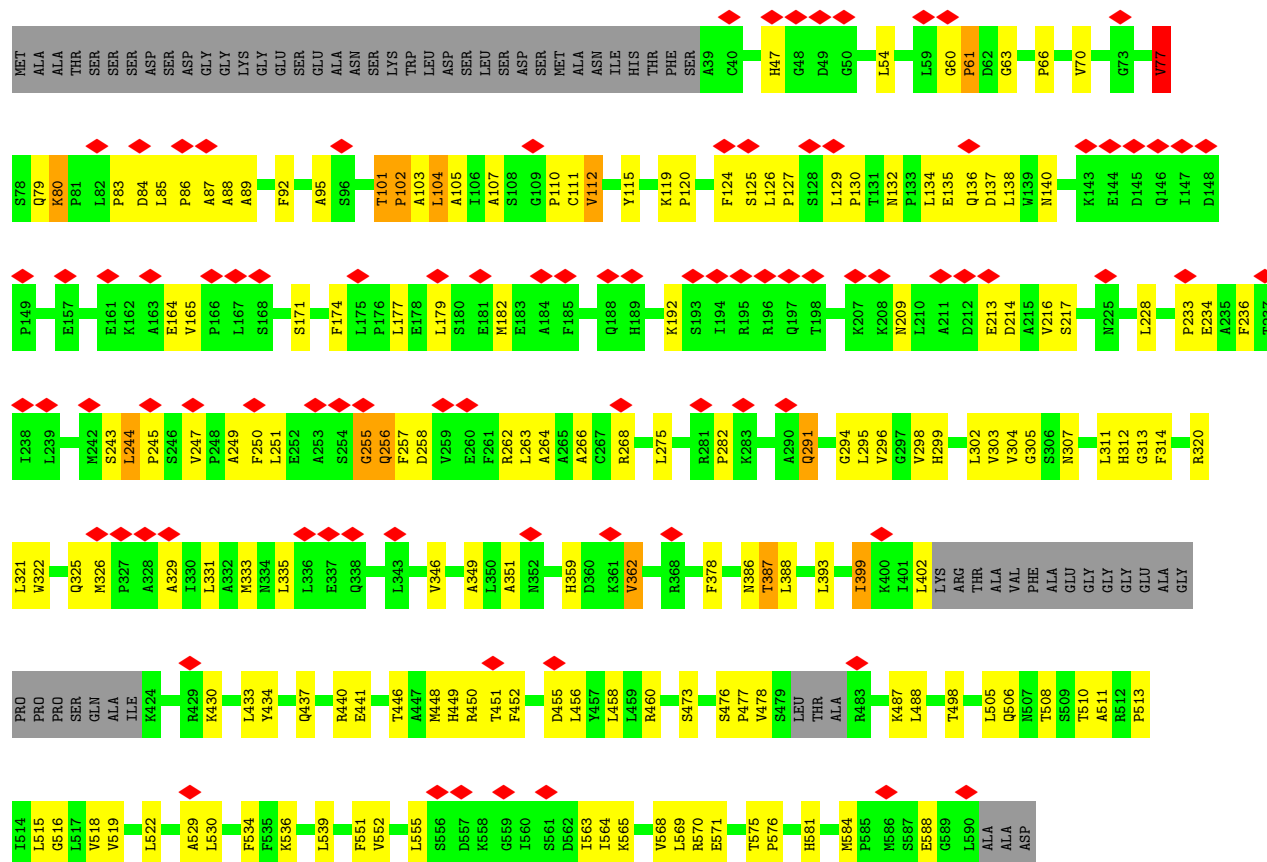


Chain I:





• Molecule 9: BBS1 domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	546186	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 ($e^-/\text{\AA}^2$)	75.2, 51.44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	378.0, 378.0, 378.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	H	0.50	0/426	0.59	0/572
2	B	0.34	0/3471	0.62	2/4763 (0.0%)
3	E	0.23	0/3177	0.43	1/4294 (0.0%)
4	G	0.20	0/2456	0.43	0/3324
5	C	0.20	0/3687	0.51	2/5073 (0.0%)
6	F	0.22	0/3883	0.43	3/5262 (0.1%)
7	I	0.21	0/6153	0.42	1/8325 (0.0%)
8	A	0.39	0/815	1.14	11/1134 (1.0%)
9	D	0.30	0/3114	0.89	23/4287 (0.5%)
All	All	0.25	0/27182	0.57	43/37034 (0.1%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	327	GLY	CA-C-N	11.07	133.68	119.84
5	C	327	GLY	C-N-CA	11.07	133.68	119.84
2	B	172	ASP	CB-CA-C	8.39	118.14	109.83
9	D	326	MET	CA-C-N	7.70	127.59	119.05
9	D	326	MET	C-N-CA	7.70	127.59	119.05
9	D	164	GLU	N-CA-C	7.35	119.29	111.28
8	A	160	CYS	N-CA-C	7.30	117.65	108.45
8	A	162	SER	N-CA-C	7.22	121.22	109.59
9	D	386	ASN	N-CA-C	7.14	120.56	110.50
8	A	161	ALA	N-CA-C	7.01	121.34	111.52
9	D	85	LEU	CA-C-N	6.99	126.81	119.05
9	D	85	LEU	C-N-CA	6.99	126.81	119.05
9	D	387	THR	N-CA-C	6.98	118.97	111.36
9	D	80	LYS	CA-C-N	6.83	126.80	119.76
9	D	80	LYS	C-N-CA	6.83	126.80	119.76
9	D	119	LYS	CA-C-N	6.61	128.10	119.84
9	D	119	LYS	C-N-CA	6.61	128.10	119.84
9	D	362	VAL	N-CA-C	6.55	117.06	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	84	TYR	N-CA-C	6.53	118.40	111.28
9	D	129	LEU	CA-C-N	6.51	126.28	119.05
9	D	129	LEU	C-N-CA	6.51	126.28	119.05
9	D	101	THR	CA-C-N	6.18	127.57	119.84
9	D	101	THR	C-N-CA	6.18	127.57	119.84
8	A	120	HIS	N-CA-C	6.10	117.93	111.28
9	D	256	GLN	N-CA-C	5.90	119.54	112.93
9	D	291	GLN	CA-C-N	5.89	127.21	119.84
9	D	291	GLN	C-N-CA	5.89	127.21	119.84
8	A	159	ILE	N-CA-C	5.88	117.21	108.46
9	D	249	ALA	N-CA-C	5.79	118.10	108.20
2	B	251	ASP	CB-CA-C	-5.77	103.16	111.70
9	D	393	LEU	N-CA-C	-5.58	104.58	111.33
7	I	362	ASP	CB-CA-C	-5.51	102.28	110.71
9	D	104	LEU	N-CA-C	5.50	118.44	109.59
6	F	17	GLN	N-CA-C	-5.49	105.69	112.72
6	F	24	THR	N-CA-C	-5.47	105.21	111.07
6	F	25	GLN	N-CA-C	-5.46	105.02	110.97
8	A	125	ILE	N-CA-C	5.35	114.50	106.42
8	A	86	GLU	N-CA-C	5.26	118.51	110.36
9	D	77	VAL	N-CA-C	5.23	120.21	109.34
8	A	76	TYR	N-CA-C	5.18	119.60	113.28
8	A	72	GLY	N-CA-C	5.15	125.38	113.18
8	A	121	ARG	N-CA-C	5.10	117.28	109.07
3	E	37	TRP	N-CA-C	5.00	116.81	111.36

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	H	421	0	450	41	0
2	B	3465	0	2204	22	0
3	E	3114	0	3124	130	0
4	G	2411	0	2412	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	3676	0	2182	34	0
6	F	3797	0	3740	125	0
7	I	6034	0	6068	197	0
8	A	816	0	354	47	0
9	D	3090	0	2188	178	0
All	All	26824	0	22722	694	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 14.

All (694) 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)
3:E:351:LEU:HD21	9:D:449:HIS:CG	1.33	1.62
3:E:40:HIS:CE1	3:E:44:ILE:HD11	1.07	1.59
8:A:161:ALA:HB2	8:A:172:GLU:CB	1.30	1.58
8:A:92:PHE:CB	8:A:127:PHE:HA	1.29	1.57
8:A:161:ALA:CB	8:A:172:GLU:CB	1.81	1.56
9:D:256:GLN:CB	9:D:263:LEU:HA	1.27	1.55
3:E:40:HIS:CE1	3:E:44:ILE:CD1	1.88	1.51
3:E:351:LEU:CD2	9:D:449:HIS:CD2	1.95	1.49
8:A:92:PHE:CB	8:A:127:PHE:CA	1.88	1.47
9:D:256:GLN:CB	9:D:263:LEU:CA	1.88	1.46
9:D:216:VAL:O	9:D:233:PRO:CB	1.66	1.41
9:D:256:GLN:CB	9:D:263:LEU:C	2.01	1.31
6:F:59:GLY:O	6:F:63:MET:CE	1.80	1.30
3:E:44:ILE:CG2	9:D:250:PHE:HA	1.62	1.29
3:E:351:LEU:CD2	9:D:449:HIS:CG	2.10	1.28
9:D:256:GLN:CB	9:D:264:ALA:N	1.97	1.27
3:E:99:GLN:NE2	9:D:192:LYS:CB	1.99	1.23
9:D:214:ASP:CB	9:D:234:GLU:CB	2.14	1.23
8:A:90:ILE:CB	8:A:124:PRO:O	1.87	1.21
3:E:40:HIS:ND1	3:E:44:ILE:CD1	2.06	1.18
9:D:88:ALA:O	9:D:107:ALA:HA	1.44	1.18
9:D:63:GLY:O	9:D:87:ALA:HA	1.45	1.14
8:A:161:ALA:HB3	8:A:172:GLU:CB	1.78	1.11
8:A:161:ALA:HB1	8:A:169:GLY:CA	1.78	1.11
3:E:351:LEU:HD21	9:D:449:HIS:CD2	1.72	1.10
9:D:136:GLN:O	9:D:140:ASN:N	1.85	1.09
9:D:214:ASP:HA	9:D:234:GLU:CB	1.84	1.08
8:A:161:ALA:O	8:A:169:GLY:HA3	1.52	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:CYS:N	6:F:422:ASN:HD21	1.51	1.07
9:D:86:PRO:CB	9:D:132:ASN:HA	1.84	1.07
3:E:44:ILE:HG23	9:D:250:PHE:CA	1.84	1.07
8:A:161:ALA:HB3	8:A:169:GLY:O	1.54	1.05
9:D:214:ASP:CA	9:D:234:GLU:CB	2.34	1.04
8:A:161:ALA:HB1	8:A:169:GLY:HA2	1.37	1.04
9:D:311:LEU:CB	9:D:325:GLN:H	1.69	1.03
3:E:351:LEU:HD23	9:D:449:HIS:CD2	1.93	1.03
3:E:40:HIS:NE2	3:E:44:ILE:HD11	1.73	1.02
9:D:217:SER:HA	9:D:233:PRO:CB	1.90	1.01
4:G:82:ARG:HE	6:F:375:LEU:HD13	1.26	1.01
1:H:29:CYS:H	6:F:422:ASN:ND2	1.59	1.00
3:E:351:LEU:HD21	9:D:449:HIS:CB	1.92	1.00
3:E:351:LEU:HD22	9:D:449:HIS:CD2	1.95	1.00
6:F:59:GLY:O	6:F:63:MET:HE3	0.84	1.00
3:E:99:GLN:HE21	9:D:192:LYS:CB	1.74	1.00
9:D:295:LEU:HA	9:D:304:VAL:HA	1.40	0.99
1:H:16:GLY:HA3	3:E:278:MET:HE2	1.43	0.99
9:D:296:VAL:O	9:D:303:VAL:N	1.97	0.97
1:H:29:CYS:H	6:F:422:ASN:HD21	0.98	0.97
3:E:44:ILE:HG23	9:D:250:PHE:HA	0.97	0.97
3:E:40:HIS:ND1	3:E:44:ILE:HD12	1.79	0.96
9:D:136:GLN:O	9:D:140:ASN:CB	2.13	0.96
9:D:95:ALA:HB2	9:D:102:PRO:CB	1.96	0.96
7:I:724:PHE:HZ	7:I:759:LEU:O	1.48	0.95
3:E:33:GLU:CG	3:E:36:ASN:HB2	1.94	0.95
3:E:34:LYS:CB	9:D:61:PRO:HA	1.97	0.94
7:I:724:PHE:CZ	7:I:759:LEU:O	2.21	0.94
9:D:296:VAL:O	9:D:303:VAL:CB	2.17	0.93
9:D:47:HIS:CB	9:D:54:LEU:O	2.17	0.92
3:E:320:TYR:O	3:E:351:LEU:CD1	2.19	0.91
9:D:311:LEU:CB	9:D:325:GLN:N	2.35	0.90
8:A:92:PHE:CA	8:A:127:PHE:HA	2.02	0.90
3:E:40:HIS:HE1	3:E:44:ILE:HD11	1.34	0.89
7:I:515:ASN:ND2	9:D:473:SER:OG	2.03	0.89
3:E:322:SER:HG	6:F:362:TYR:HE2	0.90	0.89
9:D:256:GLN:CB	9:D:264:ALA:H	1.79	0.89
8:A:161:ALA:CB	8:A:169:GLY:O	2.21	0.89
3:E:34:LYS:CB	9:D:60:GLY:O	2.20	0.89
3:E:351:LEU:HD22	9:D:449:HIS:NE2	1.88	0.88
9:D:216:VAL:C	9:D:233:PRO:CB	2.48	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:370:LYS:HB2	7:I:370:LYS:NZ	1.90	0.86
9:D:214:ASP:O	9:D:233:PRO:O	1.93	0.86
9:D:291:GLN:O	9:D:307:ASN:CB	2.23	0.86
3:E:46:LYS:HE3	9:D:291:GLN:CB	2.06	0.86
8:A:73:GLN:O	8:A:77:ARG:N	2.10	0.84
3:E:351:LEU:HD22	9:D:449:HIS:CE1	2.12	0.84
3:E:41:LEU:O	3:E:45:GLN:NE2	2.09	0.84
8:A:161:ALA:CA	8:A:172:GLU:CB	2.56	0.84
8:A:161:ALA:N	8:A:172:GLU:CB	2.41	0.84
6:F:19:CYS:SG	6:F:43:ALA:CB	2.67	0.83
8:A:52:GLY:HA2	8:A:69:ASP:CB	1.98	0.83
9:D:138:LEU:CB	9:D:174:PHE:HA	2.07	0.83
8:A:161:ALA:O	8:A:169:GLY:CA	2.26	0.83
6:F:340:GLN:O	7:I:325:GLN:NE2	2.13	0.81
3:E:40:HIS:ND1	3:E:44:ILE:HD11	1.77	0.81
9:D:256:GLN:CB	9:D:262:ARG:O	2.29	0.81
9:D:296:VAL:O	9:D:303:VAL:CA	2.28	0.80
3:E:291:SER:OG	9:D:430:LYS:NZ	2.12	0.80
3:E:352:GLU:HB2	9:D:450:ARG:HH21	1.45	0.79
9:D:111:CYS:CB	9:D:126:LEU:HA	2.12	0.79
9:D:177:LEU:CB	9:D:182:MET:CB	2.62	0.78
4:G:145:ALA:HB2	7:I:71:GLU:O	1.84	0.78
3:E:87:LEU:HD21	7:I:793:LEU:HD23	1.64	0.78
6:F:58:GLU:OE2	6:F:114:GLN:NE2	2.16	0.78
8:A:129:ALA:HB2	8:A:142:LYS:CB	2.13	0.78
1:H:26:MET:SD	6:F:428:MET:HG2	2.24	0.77
7:I:370:LYS:HB2	7:I:370:LYS:HZ3	1.50	0.77
4:G:82:ARG:NE	6:F:375:LEU:HD13	2.00	0.76
9:D:88:ALA:O	9:D:107:ALA:CA	2.32	0.75
9:D:86:PRO:HA	9:D:132:ASN:CB	2.16	0.74
6:F:19:CYS:SG	6:F:43:ALA:HB1	2.27	0.74
8:A:92:PHE:CB	8:A:127:PHE:C	2.61	0.74
4:G:194:ASN:OD1	7:I:124:LYS:NZ	2.19	0.74
3:E:46:LYS:NZ	9:D:291:GLN:CB	2.51	0.73
8:A:144:SER:O	8:A:150:GLU:HA	1.88	0.73
3:E:46:LYS:CE	9:D:291:GLN:CB	2.67	0.73
4:G:17:VAL:HB	4:G:68:ASN:HD21	1.52	0.73
6:F:19:CYS:SG	6:F:43:ALA:HB2	2.29	0.72
4:G:79:ILE:HG22	4:G:97:VAL:HG12	1.70	0.72
3:E:33:GLU:HG3	3:E:36:ASN:HB2	1.71	0.72
9:D:89:ALA:HB1	9:D:105:ALA:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:63:MET:HG2	6:F:117:ARG:HH21	1.53	0.71
3:E:40:HIS:CE1	3:E:44:ILE:HD13	2.20	0.71
4:G:300:VAL:HG11	7:I:370:LYS:O	1.90	0.71
7:I:376:LEU:HD11	9:D:458:LEU:HD21	1.71	0.71
9:D:255:GLY:C	9:D:264:ALA:HB3	2.16	0.71
7:I:245:ALA:HA	7:I:264:GLY:HA2	1.72	0.71
9:D:47:HIS:CB	9:D:54:LEU:C	2.63	0.71
1:H:26:MET:SD	6:F:428:MET:CG	2.78	0.71
9:D:136:GLN:O	9:D:140:ASN:CA	2.38	0.71
7:I:456:LYS:NZ	7:I:458:SER:OG	2.23	0.70
8:A:127:PHE:CB	8:A:143:VAL:CB	2.69	0.70
9:D:228:LEU:H	9:D:243:SER:CB	2.04	0.70
9:D:313:GLY:HA3	9:D:322:TRP:CB	2.21	0.70
6:F:18:LEU:H	6:F:18:LEU:CD2	2.04	0.70
6:F:411:VAL:HG23	9:D:476:SER:HA	1.71	0.70
7:I:41:ILE:HG21	7:I:95:LEU:HD11	1.73	0.70
6:F:18:LEU:CD2	6:F:18:LEU:N	2.55	0.69
7:I:513:GLU:H	7:I:513:GLU:CD	2.00	0.69
3:E:91:GLN:CD	7:I:793:LEU:HD22	2.17	0.69
6:F:1:MET:HB2	7:I:77:PRO:HG2	1.74	0.69
1:H:26:MET:SD	6:F:428:MET:HB3	2.32	0.69
2:B:651:ASN:HD21	7:I:677:GLN:HE22	1.40	0.69
4:G:169:ASN:O	4:G:176:ASN:ND2	2.26	0.69
7:I:371:VAL:HG22	7:I:374:ARG:H	1.58	0.69
9:D:519:VAL:HG22	9:D:568:VAL:HG22	1.75	0.69
9:D:84:ASP:O	9:D:130:PRO:O	2.11	0.68
3:E:414:ASP:HB2	3:E:415:PRO:HD3	1.75	0.68
3:E:44:ILE:CG2	9:D:250:PHE:CA	2.57	0.68
3:E:320:TYR:O	3:E:351:LEU:HD11	1.92	0.68
9:D:217:SER:CA	9:D:233:PRO:CB	2.70	0.68
8:A:161:ALA:CB	8:A:169:GLY:CA	2.65	0.68
7:I:498:PRO:O	7:I:610:TRP:NE1	2.26	0.68
3:E:247:GLN:NE2	3:E:279:CYS:SG	2.63	0.68
6:F:80:LEU:HG	6:F:260:PRO:HG3	1.74	0.68
9:D:95:ALA:CB	9:D:102:PRO:CB	2.72	0.68
6:F:359:ALA:O	9:D:437:GLN:NE2	2.26	0.67
1:H:41:LEU:HD11	6:F:134:ALA:HB1	1.74	0.67
9:D:111:CYS:O	9:D:127:PRO:CB	2.42	0.67
4:G:105:ARG:HH11	7:I:7:ARG:HH22	1.41	0.67
6:F:18:LEU:N	6:F:18:LEU:HD22	2.10	0.67
3:E:40:HIS:O	3:E:44:ILE:HD12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:314:ILE:HD12	7:I:322:TRP:HB3	1.76	0.67
7:I:102:LYS:NZ	7:I:104:CYS:SG	2.61	0.66
6:F:42:ARG:NH1	7:I:265:GLU:OE2	2.28	0.66
7:I:448:ASN:ND2	7:I:477:MET:SD	2.68	0.66
2:B:250:PHE:O	2:B:259:GLU:N	2.27	0.66
3:E:74:ALA:HB2	3:E:89:LEU:HB2	1.78	0.66
5:C:549:PHE:O	5:C:612:LYS:NZ	2.29	0.66
1:H:8:PHE:CZ	3:E:419:GLU:HB3	2.31	0.65
3:E:266:VAL:HG12	6:F:485:VAL:HG11	1.78	0.65
7:I:183:PRO:HB2	7:I:248:ILE:HG22	1.78	0.65
7:I:80:GLN:OE1	7:I:138:MET:N	2.29	0.65
3:E:33:GLU:OE1	3:E:68:TYR:HB3	1.96	0.65
3:E:302:LEU:HB3	6:F:429:ARG:NH2	2.11	0.65
3:E:83:ILE:HD12	6:F:468:GLN:HB2	1.79	0.65
7:I:2:SER:HB2	7:I:7:ARG:HH11	1.61	0.65
4:G:88:LEU:N	6:F:379:GLU:OE2	2.22	0.65
4:G:324:ILE:HD11	7:I:361:THR:HG21	1.79	0.65
8:A:161:ALA:HB1	8:A:169:GLY:HA3	1.75	0.65
3:E:352:GLU:HG3	9:D:446:THR:HG21	1.79	0.64
7:I:513:GLU:OE1	7:I:513:GLU:N	2.22	0.64
7:I:491:LEU:HD22	7:I:534:VAL:HG23	1.80	0.64
9:D:256:GLN:O	9:D:262:ARG:O	2.14	0.64
9:D:440:ARG:NH1	9:D:448:MET:SD	2.71	0.64
7:I:365:LEU:HD12	7:I:365:LEU:H	1.61	0.64
7:I:45:PHE:HA	7:I:78:ILE:H	1.63	0.64
8:A:50:THR:O	8:A:70:MET:C	2.40	0.64
1:H:29:CYS:N	6:F:422:ASN:ND2	2.28	0.64
4:G:297:ASP:O	4:G:300:VAL:HG12	1.97	0.64
1:H:34:LEU:HD21	6:F:384:ASP:CB	2.28	0.64
9:D:255:GLY:O	9:D:302:LEU:CB	2.45	0.64
7:I:68:LEU:HD21	7:I:71:GLU:HB2	1.79	0.64
4:G:131:TYR:O	4:G:138:ARG:NH1	2.31	0.64
7:I:103:LEU:HB3	7:I:129:HIS:HB2	1.80	0.64
9:D:245:PRO:C	9:D:247:VAL:H	2.04	0.64
3:E:33:GLU:HG2	3:E:36:ASN:HB2	1.80	0.63
7:I:80:GLN:NE2	7:I:138:MET:O	2.27	0.63
6:F:414:ASN:HD22	9:D:477:PRO:HG3	1.62	0.63
8:A:161:ALA:O	8:A:169:GLY:C	2.42	0.63
6:F:363:ASP:HB2	7:I:368:ALA:HB2	1.81	0.63
6:F:57:GLU:O	6:F:141:SER:HB2	1.99	0.63
1:H:26:MET:SD	6:F:428:MET:CB	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:87:VAL:O	7:I:166:GLN:NE2	2.32	0.62
9:D:515:LEU:HD23	9:D:539:LEU:HD13	1.80	0.62
9:D:530:LEU:HD21	9:D:552:VAL:HG22	1.81	0.62
7:I:760:GLN:O	7:I:760:GLN:HG2	1.99	0.62
7:I:524:GLN:NE2	9:D:571:GLU:HG3	2.13	0.62
3:E:412:GLU:C	3:E:415:PRO:HD2	2.25	0.62
7:I:460:TYR:CZ	9:D:534:PHE:HB3	2.35	0.62
3:E:99:GLN:HE22	9:D:192:LYS:CB	2.08	0.62
7:I:85:LYS:O	7:I:166:GLN:NE2	2.33	0.62
3:E:44:ILE:HG21	9:D:250:PHE:HA	1.74	0.61
1:H:27:VAL:HG22	6:F:456:ASN:HD21	1.65	0.61
8:A:161:ALA:CB	8:A:169:GLY:C	2.73	0.61
6:F:363:ASP:HB2	7:I:368:ALA:CB	2.30	0.61
7:I:14:LEU:HD11	7:I:52:PHE:HZ	1.65	0.61
7:I:521:ARG:CZ	9:D:575:THR:HG22	2.30	0.61
1:H:17:GLN:HE21	1:H:17:GLN:HA	1.66	0.61
3:E:213:LEU:HD12	3:E:221:ALA:HB1	1.83	0.61
5:C:623:VAL:HG11	5:C:660:TYR:HB2	1.83	0.61
6:F:231:GLU:HB2	6:F:253:VAL:HG11	1.82	0.61
7:I:162:MET:HB2	7:I:169:TYR:HE1	1.65	0.61
6:F:18:LEU:H	6:F:18:LEU:HD23	1.66	0.60
9:D:305:GLY:HA2	9:D:312:HIS:CB	2.31	0.60
7:I:515:ASN:HD22	9:D:473:SER:HG	1.47	0.60
7:I:589:THR:HB	7:I:602:GLN:HG2	1.83	0.60
6:F:182:PHE:HE2	6:F:216:GLN:HE21	1.48	0.60
2:B:390:SER:O	2:B:398:ALA:N	2.34	0.60
5:C:643:ILE:HB	7:I:672:GLN:HE22	1.67	0.60
7:I:724:PHE:HE1	7:I:768:TRP:HB2	1.67	0.60
3:E:33:GLU:CD	3:E:36:ASN:HB2	2.26	0.59
9:D:111:CYS:CB	9:D:125:SER:O	2.50	0.59
3:E:325:HIS:CD2	6:F:396:THR:HG23	2.37	0.59
4:G:322:LEU:HD12	7:I:359:LEU:HD11	1.84	0.59
8:A:160:CYS:C	8:A:172:GLU:CB	2.75	0.59
4:G:134:SER:O	4:G:138:ARG:NH2	2.36	0.59
6:F:63:MET:HG2	6:F:117:ARG:NH2	2.17	0.59
7:I:545:SER:HB3	7:I:604:GLU:HA	1.84	0.59
6:F:16:PHE:HB3	6:F:47:MET:HG2	1.83	0.58
6:F:305:LEU:HD21	6:F:315:ILE:HG13	1.85	0.58
8:A:161:ALA:HB1	8:A:169:GLY:C	2.27	0.58
4:G:83:THR:OG1	4:G:93:GLU:OE1	2.21	0.58
4:G:88:LEU:HB2	6:F:379:GLU:OE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:VAL:H	5:C:430:SER:CB	2.16	0.58
7:I:519:ILE:HG22	9:D:473:SER:HA	1.84	0.58
7:I:748:GLN:HE22	7:I:824:ARG:HD2	1.68	0.58
4:G:237:ILE:HG22	4:G:238:ASP:H	1.69	0.58
3:E:87:LEU:HD21	7:I:793:LEU:CD2	2.33	0.58
6:F:396:THR:HG21	9:D:456:LEU:HD11	1.85	0.58
6:F:414:ASN:ND2	9:D:477:PRO:HG3	2.19	0.57
3:E:411:LEU:O	3:E:415:PRO:HD3	2.04	0.57
8:A:92:PHE:C	8:A:128:PHE:H	2.12	0.57
9:D:563:ILE:HD11	9:D:581:HIS:HB3	1.84	0.57
4:G:190:HIS:HD2	4:G:192:ASN:H	1.50	0.57
5:C:632:LEU:HD21	7:I:676:ILE:HG12	1.85	0.57
1:H:28:LEU:HD11	3:E:302:LEU:HD12	1.87	0.57
6:F:444:SER:HB2	6:F:454:HIS:CE1	2.40	0.57
7:I:189:ARG:HD3	7:I:258:SER:HB2	1.85	0.57
7:I:371:VAL:HG22	7:I:371:VAL:O	2.02	0.57
1:H:19:TYR:CZ	3:E:305:LYS:HB2	2.40	0.57
1:H:34:LEU:HD21	6:F:384:ASP:HB3	1.86	0.57
6:F:332:LEU:HD21	6:F:336:ARG:HH21	1.69	0.57
7:I:196:VAL:HG22	7:I:202:VAL:HG22	1.85	0.57
1:H:28:LEU:HB3	6:F:422:ASN:ND2	2.18	0.57
7:I:607:GLU:HG2	7:I:726:ARG:HB3	1.86	0.57
5:C:620:ALA:HB2	5:C:663:GLN:HE22	1.69	0.56
3:E:322:SER:OG	6:F:362:TYR:HE2	1.71	0.56
7:I:461:VAL:HG23	7:I:462:GLN:H	1.70	0.56
3:E:46:LYS:HE2	9:D:268:ARG:O	2.05	0.56
3:E:65:LEU:HD11	9:D:179:LEU:CB	2.34	0.56
3:E:140:ASN:HA	3:E:143:VAL:HG12	1.86	0.56
7:I:77:PRO:O	7:I:99:HIS:ND1	2.31	0.56
1:H:7:MET:HG3	1:H:7:MET:O	2.04	0.56
7:I:490:TYR:HA	7:I:533:LEU:HD11	1.87	0.56
4:G:212:ARG:HD2	4:G:221:VAL:HG21	1.86	0.56
4:G:239:PRO:O	4:G:242:LYS:NZ	2.39	0.56
4:G:243:LEU:O	4:G:247:VAL:HG23	2.05	0.55
7:I:72:VAL:HG21	7:I:123:ILE:HD11	1.87	0.55
7:I:304:LEU:HA	7:I:313:HIS:O	2.07	0.55
9:D:137:ASP:CB	9:D:165:VAL:CB	2.84	0.55
5:C:681:LYS:NZ	5:C:712:PHE:O	2.32	0.55
7:I:333:VAL:HG12	7:I:347:THR:HG22	1.88	0.55
7:I:535:CYS:SG	7:I:536:LEU:N	2.79	0.55
5:C:603:LYS:HG3	5:C:709:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:70:VAL:CB	9:D:79:GLN:O	2.54	0.55
6:F:14:ARG:HD3	7:I:308:HIS:CE1	2.40	0.55
7:I:481:MET:SD	7:I:483:ARG:NH2	2.80	0.55
7:I:263:LEU:HD13	7:I:290:PHE:HB3	1.87	0.55
9:D:296:VAL:CB	9:D:333:MET:CB	2.84	0.54
3:E:168:ASP:N	3:E:168:ASP:OD1	2.41	0.54
8:A:174:VAL:O	8:A:179:ASP:N	2.39	0.54
1:H:28:LEU:HD11	3:E:302:LEU:CD1	2.37	0.54
3:E:351:LEU:CD2	9:D:449:HIS:ND1	2.65	0.54
4:G:238:ASP:HB3	4:G:239:PRO:HD2	1.88	0.54
7:I:519:ILE:CG2	9:D:473:SER:HA	2.37	0.54
3:E:319:GLN:OE1	9:D:441:GLU:CD	2.51	0.54
4:G:324:ILE:HD11	7:I:361:THR:CG2	2.37	0.54
7:I:304:LEU:HD12	7:I:312:LEU:HD13	1.88	0.54
9:D:335:LEU:HA	9:D:346:VAL:HA	1.88	0.54
7:I:20:PHE:HE2	7:I:352:GLY:HA2	1.70	0.54
3:E:267:ILE:HG23	3:E:268:GLU:HG3	1.90	0.54
1:H:20:VAL:HG12	1:H:20:VAL:O	2.08	0.54
1:H:49:GLN:NE2	1:H:53:ASP:OD1	2.41	0.54
4:G:207:ARG:HD3	4:G:225:SER:HA	1.89	0.54
7:I:724:PHE:CE2	7:I:759:LEU:O	2.60	0.54
3:E:152:ASP:OD1	3:E:153:LYS:N	2.39	0.54
4:G:17:VAL:N	4:G:68:ASN:OD1	2.40	0.54
7:I:550:ILE:HD11	7:I:613:THR:HG23	1.90	0.54
9:D:295:LEU:CA	9:D:304:VAL:HA	2.27	0.54
6:F:64:ILE:HD11	6:F:118:PRO:HG2	1.89	0.54
8:A:161:ALA:C	8:A:169:GLY:HA3	2.29	0.54
9:D:256:GLN:CB	9:D:262:ARG:C	2.81	0.53
3:E:222:PHE:HB2	3:E:245:MET:HE1	1.89	0.53
6:F:110:ARG:HG2	6:F:113:THR:HG23	1.90	0.53
3:E:46:LYS:HZ1	9:D:291:GLN:CB	2.20	0.53
3:E:320:TYR:O	3:E:351:LEU:HD12	2.06	0.53
3:E:352:GLU:HB2	9:D:450:ARG:NH2	2.21	0.53
6:F:166:LEU:HD23	6:F:166:LEU:H	1.74	0.53
6:F:212:TRP:O	6:F:216:GLN:HG2	2.09	0.53
6:F:336:ARG:HD3	7:I:366:PHE:CD2	2.44	0.53
4:G:30:LEU:HD11	4:G:51:LEU:HD22	1.91	0.53
7:I:18:GLU:OE2	7:I:50:ARG:NH1	2.38	0.53
8:A:20:VAL:O	8:A:68:PHE:N	2.42	0.53
7:I:112:LEU:HA	7:I:119:ASN:HB3	1.89	0.53
3:E:40:HIS:CG	3:E:44:ILE:HD12	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:815:PHE:HZ	7:I:825:LEU:HD11	1.74	0.52
9:D:313:GLY:O	9:D:320:ARG:HA	2.09	0.52
7:I:521:ARG:HH11	9:D:575:THR:HA	1.75	0.52
8:A:50:THR:O	8:A:70:MET:O	2.28	0.52
9:D:378:PHE:HA	9:D:387:THR:HA	1.90	0.52
3:E:33:GLU:HG3	3:E:33:GLU:O	2.10	0.52
3:E:42:TYR:HB3	3:E:51:CYS:HB2	1.91	0.52
3:E:274:ASN:OD1	3:E:309:ASN:ND2	2.40	0.52
3:E:372:PRO:HB2	3:E:398:MET:HG3	1.89	0.52
4:G:182:ILE:HA	4:G:187:ILE:HD12	1.91	0.52
7:I:455:ILE:HB	7:I:474:PHE:HB2	1.91	0.52
1:H:50:ALA:O	1:H:54:THR:HG23	2.10	0.52
5:C:704:ASP:HB3	5:C:707:ALA:HB3	1.92	0.52
6:F:366:LEU:HD12	9:D:455:ASP:HB3	1.92	0.52
7:I:250:ILE:HG12	7:I:260:VAL:HG22	1.92	0.52
9:D:86:PRO:CA	9:D:132:ASN:HA	2.39	0.52
4:G:19:SER:HA	4:G:22:MET:HE2	1.90	0.52
4:G:205:GLN:HE22	4:G:227:GLN:HB2	1.74	0.52
4:G:324:ILE:HG12	7:I:361:THR:OG1	2.10	0.52
8:A:174:VAL:HA	8:A:178:GLN:H	1.74	0.52
9:D:92:PHE:HA	9:D:104:LEU:O	2.08	0.52
7:I:724:PHE:HE2	7:I:760:GLN:HA	1.74	0.52
7:I:770:GLU:HG3	7:I:802:PRO:HD3	1.92	0.52
4:G:155:LEU:HG	4:G:186:ARG:HH11	1.75	0.51
4:G:181:PHE:HB2	4:G:188:VAL:HG22	1.92	0.51
6:F:169:ALA:O	6:F:173:GLN:NE2	2.39	0.51
7:I:575:VAL:HG12	7:I:576:ASN:H	1.75	0.51
9:D:70:VAL:CB	9:D:80:LYS:HA	2.40	0.51
6:F:2:GLU:OE1	7:I:134:THR:OG1	2.20	0.51
4:G:50:LEU:HD11	4:G:57:ILE:HD11	1.92	0.51
2:B:216:ARG:HA	2:B:229:TYR:O	2.11	0.51
3:E:351:LEU:HD21	9:D:449:HIS:HB3	1.86	0.51
4:G:8:TRP:HZ2	4:G:21:GLN:HB3	1.75	0.51
7:I:157:VAL:HA	7:I:181:PRO:HG3	1.93	0.51
8:A:161:ALA:O	8:A:169:GLY:O	2.29	0.51
2:B:619:ASN:OD1	2:B:622:ARG:NH1	2.44	0.51
9:D:101:THR:C	9:D:103:ALA:H	2.18	0.51
4:G:22:MET:SD	4:G:68:ASN:ND2	2.84	0.51
4:G:25:ARG:HG2	4:G:26:PRO:HD2	1.93	0.51
6:F:400:ASN:OD1	6:F:430:ARG:NH2	2.44	0.51
6:F:410:LEU:HD13	9:D:478:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:201:LEU:O	6:F:204:GLU:HG3	2.10	0.50
8:A:100:LEU:N	9:D:402:LEU:O	2.44	0.50
3:E:40:HIS:CG	3:E:44:ILE:CD1	2.91	0.50
5:C:597:ILE:HD11	5:C:684:PHE:HD2	1.77	0.50
4:G:162:ASN:HB3	4:G:164:ILE:HD11	1.93	0.50
4:G:336:LEU:HD21	7:I:363:PRO:HG3	1.93	0.50
7:I:558:SER:O	7:I:561:SER:OG	2.27	0.50
1:H:31:PRO:HD3	6:F:391:HIS:CE1	2.47	0.50
6:F:176:LYS:HG3	6:F:177:LEU:HD12	1.93	0.50
7:I:133:ARG:HH21	7:I:174:PHE:HZ	1.59	0.50
7:I:410:ASP:OD1	7:I:410:ASP:N	2.44	0.50
9:D:245:PRO:C	9:D:247:VAL:N	2.66	0.50
9:D:565:LYS:HG2	9:D:581:HIS:CD2	2.46	0.50
4:G:339:VAL:HG12	6:F:333:ARG:HD3	1.93	0.50
6:F:401:LEU:HD22	9:D:460:ARG:HG2	1.94	0.50
8:A:59:LYS:HA	8:A:64:SER:HA	1.93	0.50
9:D:132:ASN:CB	9:D:135:GLU:CB	2.90	0.50
9:D:256:GLN:CB	9:D:263:LEU:N	2.69	0.50
2:B:639:THR:O	2:B:643:ARG:HG2	2.11	0.50
5:C:428:SER:O	5:C:444:THR:N	2.45	0.50
7:I:642:LEU:HD11	7:I:812:ILE:HG22	1.93	0.50
9:D:209:ASN:O	9:D:213:GLU:N	2.42	0.50
9:D:536:LYS:NZ	9:D:571:GLU:OE1	2.45	0.50
3:E:87:LEU:HD11	3:E:111:LEU:HD23	1.93	0.50
3:E:119:ALA:HB2	7:I:788:SER:O	2.11	0.50
6:F:333:ARG:HD2	9:D:433:LEU:HD11	1.92	0.50
7:I:20:PHE:CE1	7:I:44:SER:HB2	2.47	0.50
7:I:554:LYS:NZ	7:I:632:PHE:HB2	2.27	0.50
8:A:50:THR:CB	8:A:70:MET:O	2.59	0.50
3:E:55:ILE:HG23	3:E:69:ALA:HB1	1.94	0.50
4:G:228:SER:O	4:G:228:SER:OG	2.30	0.50
3:E:83:ILE:HD13	3:E:113:LEU:HB3	1.93	0.50
3:E:183:ASP:OD1	3:E:184:LEU:N	2.45	0.49
5:C:190:PRO:HA	5:C:211:THR:HA	1.94	0.49
2:B:601:ASP:OD1	2:B:602:GLU:N	2.44	0.49
2:B:697:ALA:HB1	2:B:713:ILE:HD13	1.93	0.49
4:G:337:TRP:CZ3	7:I:4:PHE:CE2	2.99	0.49
6:F:366:LEU:HB2	9:D:455:ASP:HB3	1.94	0.49
8:A:52:GLY:CA	8:A:69:ASP:CB	2.83	0.49
9:D:513:PRO:HB2	9:D:539:LEU:HD11	1.93	0.49
4:G:49:ARG:HE	4:G:51:LEU:HD21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:19:CYS:SG	6:F:20:ALA:N	2.85	0.49
7:I:521:ARG:NH1	9:D:575:THR:HA	2.28	0.49
7:I:524:GLN:HE22	9:D:571:GLU:HG3	1.77	0.49
7:I:679:ARG:O	7:I:683:ARG:HG2	2.12	0.49
9:D:359:HIS:N	9:D:362:VAL:O	2.38	0.49
5:C:600:VAL:HA	5:C:603:LYS:HE2	1.93	0.49
6:F:54:ASP:OD1	6:F:54:ASP:N	2.36	0.49
1:H:14:LYS:CG	1:H:14:LYS:O	2.60	0.49
9:D:244:LEU:CB	9:D:275:LEU:CB	2.91	0.49
9:D:256:GLN:O	9:D:258:ASP:N	2.45	0.49
9:D:569:LEU:HB3	9:D:576:PRO:HA	1.93	0.49
7:I:510:ARG:O	7:I:518:GLY:HA2	2.13	0.49
7:I:510:ARG:NH2	7:I:519:ILE:CD1	2.75	0.49
1:H:14:LYS:O	1:H:14:LYS:HG3	2.13	0.49
3:E:342:MET:HG3	3:E:374:VAL:HA	1.93	0.49
5:C:644:PRO:HA	5:C:647:ARG:HB2	1.94	0.49
3:E:287:VAL:HG13	9:D:434:TYR:CE2	2.48	0.49
5:C:623:VAL:HG21	5:C:660:TYR:CG	2.48	0.49
6:F:59:GLY:HA2	6:F:137:ILE:HG23	1.94	0.49
7:I:204:SER:HG	7:I:237:TRP:CD1	2.31	0.49
1:H:17:GLN:HA	1:H:17:GLN:NE2	2.27	0.48
6:F:241:GLN:HG2	6:F:243:MET:HE2	1.94	0.48
7:I:826:CYS:SG	7:I:827:LEU:N	2.87	0.48
9:D:510:THR:OG1	9:D:511:ALA:N	2.46	0.48
4:G:154:LEU:HD21	4:G:160:VAL:HG13	1.95	0.48
9:D:77:VAL:C	9:D:79:GLN:H	2.20	0.48
1:H:14:LYS:O	1:H:14:LYS:HD2	2.14	0.48
1:H:27:VAL:O	6:F:425:VAL:HG21	2.13	0.48
5:C:323:HIS:O	8:A:140:SER:CB	2.62	0.48
6:F:5:LEU:HD21	7:I:79:LEU:HD11	1.95	0.48
7:I:44:SER:O	7:I:78:ILE:HB	2.13	0.48
7:I:108:VAL:HG22	7:I:123:ILE:HG22	1.95	0.48
7:I:417:VAL:HG13	7:I:442:VAL:HG22	1.95	0.48
7:I:548:LEU:HD23	7:I:609:LEU:HD23	1.95	0.48
6:F:99:THR:HG23	6:F:105:ILE:HG22	1.95	0.48
6:F:42:ARG:NH2	6:F:183:GLU:OE1	2.47	0.48
7:I:20:PHE:CE2	7:I:352:GLY:HA2	2.48	0.48
6:F:53:ILE:O	6:F:252:LYS:HD2	2.14	0.48
7:I:599:TYR:HE2	7:I:620:LEU:HD21	1.79	0.48
3:E:128:ALA:HB2	3:E:137:ILE:HG21	1.96	0.48
3:E:322:SER:OG	6:F:362:TYR:CE2	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:324:ILE:CD1	7:I:361:THR:HG21	2.44	0.48
4:G:337:TRP:HZ3	7:I:4:PHE:CE2	2.32	0.47
6:F:336:ARG:HD3	7:I:366:PHE:CG	2.49	0.47
6:F:362:TYR:HB3	9:D:452:PHE:CG	2.49	0.47
7:I:588:VAL:HA	7:I:603:SER:OG	2.14	0.47
8:A:173:GLY:O	8:A:177:LEU:N	2.44	0.47
4:G:305:ASP:OD1	7:I:7:ARG:NH1	2.37	0.47
7:I:497:PRO:HD2	7:I:534:VAL:HG21	1.96	0.47
9:D:111:CYS:O	9:D:112:VAL:O	2.32	0.47
7:I:98:LEU:HD13	7:I:154:ILE:HD13	1.96	0.47
7:I:371:VAL:CG2	7:I:374:ARG:HB2	2.44	0.47
7:I:453:GLN:HG3	7:I:509:SER:HB2	1.95	0.47
3:E:351:LEU:HD22	9:D:449:HIS:ND1	2.30	0.47
4:G:245:GLU:O	4:G:248:LYS:HG3	2.14	0.47
9:D:329:ALA:O	9:D:351:ALA:N	2.48	0.47
3:E:82:ASN:HD21	3:E:85:GLU:HG2	1.79	0.47
9:D:134:LEU:O	9:D:171:SER:CB	2.63	0.47
3:E:361:TYR:OH	3:E:377:ASN:HB3	2.14	0.47
4:G:57:ILE:HG23	4:G:71:ILE:HB	1.96	0.47
4:G:76:ILE:HG22	4:G:99:THR:HG22	1.95	0.47
9:D:522:LEU:HB2	9:D:565:LYS:HB2	1.96	0.47
3:E:40:HIS:HE1	3:E:44:ILE:CD1	1.99	0.47
3:E:113:LEU:HD22	6:F:467:LEU:HD12	1.97	0.47
4:G:333:LEU:HD21	7:I:361:THR:HG21	1.95	0.47
7:I:324:THR:HG21	7:I:359:LEU:HD22	1.97	0.47
7:I:367:GLN:HG3	9:D:440:ARG:HE	1.80	0.47
7:I:554:LYS:HZ2	7:I:632:PHE:HB2	1.79	0.47
9:D:111:CYS:CB	9:D:126:LEU:CA	2.89	0.47
4:G:105:ARG:NH1	7:I:7:ARG:HH22	2.10	0.47
6:F:43:ALA:O	6:F:47:MET:HG3	2.14	0.47
1:H:17:GLN:HG2	3:E:308:TYR:CE1	2.50	0.47
3:E:36:ASN:C	3:E:36:ASN:ND2	2.73	0.47
6:F:139:SER:OG	9:D:588:GLU:OE1	2.33	0.47
7:I:367:GLN:NE2	9:D:440:ARG:HG3	2.30	0.47
3:E:414:ASP:N	3:E:415:PRO:CD	2.78	0.47
4:G:189:TRP:O	4:G:198:ASN:HA	2.15	0.47
5:C:655:HIS:HA	5:C:658:GLU:HG3	1.97	0.47
6:F:60:ILE:HD13	6:F:124:ALA:CB	2.45	0.47
1:H:28:LEU:HD13	3:E:301:PRO:HD2	1.96	0.46
4:G:86:SER:OG	4:G:87:LYS:N	2.43	0.46
7:I:808:LEU:O	7:I:812:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:124:PHE:CB	9:D:236:PHE:CB	2.93	0.46
3:E:35:GLN:HB2	3:E:58:GLN:NE2	2.31	0.46
6:F:234:PHE:CE2	6:F:249:TYR:HB3	2.49	0.46
7:I:199:CYS:O	7:I:201:GLN:HG2	2.15	0.46
3:E:91:GLN:NE2	7:I:793:LEU:HD22	2.29	0.46
2:B:23:ARG:HA	2:B:29:PRO:HA	1.98	0.46
3:E:143:VAL:HG23	3:E:173:MET:HE2	1.98	0.46
1:H:40:THR:HG22	6:F:111:PRO:HG3	1.98	0.46
7:I:535:CYS:SG	7:I:580:PHE:HB3	2.56	0.46
4:G:194:ASN:OD1	7:I:122:GLN:HB3	2.16	0.46
6:F:424:ALA:HB2	6:F:439:LEU:HB2	1.98	0.46
2:B:654:LEU:HD23	2:B:654:LEU:HA	1.75	0.46
7:I:661:LYS:O	7:I:664:GLU:HG3	2.15	0.46
9:D:331:LEU:H	9:D:349:ALA:HB3	1.80	0.46
3:E:319:GLN:OE1	9:D:441:GLU:HG2	2.15	0.46
3:E:324:PHE:CD2	9:D:449:HIS:HE1	2.33	0.46
3:E:325:HIS:HD2	6:F:396:THR:HG23	1.79	0.46
7:I:307:ASN:HB3	7:I:309:ASN:H	1.81	0.46
7:I:537:PRO:HB3	7:I:566:PHE:HB3	1.98	0.46
2:B:625:LEU:HD13	7:I:674:ARG:HG3	1.97	0.46
3:E:324:PHE:CD2	9:D:449:HIS:CE1	3.03	0.46
9:D:251:LEU:H	9:D:266:ALA:HB3	1.80	0.46
3:E:342:MET:HG3	3:E:374:VAL:HG22	1.98	0.46
5:C:643:ILE:HG12	5:C:645:GLU:H	1.79	0.46
7:I:154:ILE:HD12	7:I:164:PHE:HE2	1.81	0.46
1:H:29:CYS:O	6:F:391:HIS:CE1	2.69	0.45
7:I:204:SER:O	7:I:236:ASP:HB3	2.16	0.45
9:D:84:ASP:O	9:D:130:PRO:C	2.59	0.45
1:H:35:PRO:HB2	6:F:109:LEU:HG	1.98	0.45
4:G:299:PHE:HD1	4:G:299:PHE:H	1.64	0.45
7:I:27:LEU:HD21	7:I:336:GLY:HA3	1.99	0.45
2:B:634:MET:HE1	9:D:498:THR:O	2.15	0.45
5:C:628:ALA:HB2	7:I:693:GLN:O	2.15	0.45
5:C:681:LYS:HE2	5:C:712:PHE:HD1	1.81	0.45
6:F:4:LEU:HB2	6:F:26:MET:HE1	1.99	0.45
6:F:59:GLY:C	6:F:137:ILE:CG2	2.90	0.45
6:F:411:VAL:CG2	9:D:476:SER:HA	2.43	0.45
7:I:187:SER:HA	7:I:250:ILE:HG21	1.98	0.45
7:I:205:TYR:CE1	7:I:235:VAL:HG22	2.51	0.45
1:H:17:GLN:HE21	1:H:17:GLN:CA	2.25	0.45
1:H:29:CYS:SG	6:F:418:GLU:HA	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:371:VAL:O	7:I:371:VAL:HG13	2.17	0.45
4:G:136:MET:HE3	4:G:146:LEU:HD21	1.98	0.45
6:F:294:ILE:O	6:F:298:THR:HG23	2.17	0.45
7:I:49:LEU:HD11	7:I:95:LEU:HD21	1.98	0.45
7:I:342:LYS:HB3	7:I:342:LYS:HE2	1.73	0.45
7:I:368:ALA:HA	7:I:369:PRO:HD3	1.87	0.45
3:E:319:GLN:OE1	9:D:441:GLU:CG	2.65	0.45
4:G:88:LEU:HD12	6:F:382:VAL:HG11	1.99	0.45
7:I:99:HIS:HB2	7:I:102:LYS:HB3	1.99	0.45
7:I:411:LEU:HD12	7:I:452:LEU:HD12	1.99	0.45
4:G:297:ASP:N	7:I:373:SER:OG	2.43	0.45
6:F:210:ASP:OD2	6:F:213:TRP:HD1	1.98	0.45
7:I:374:ARG:HA	7:I:374:ARG:HD3	1.81	0.44
7:I:701:GLY:O	7:I:705:GLN:HG2	2.16	0.44
7:I:460:TYR:CE2	9:D:534:PHE:HB3	2.51	0.44
7:I:588:VAL:HG22	7:I:608:ASP:HB3	1.97	0.44
3:E:352:GLU:CB	9:D:450:ARG:NH2	2.80	0.44
5:C:629:LEU:HB3	5:C:650:LEU:HD21	1.98	0.44
6:F:411:VAL:HG23	9:D:476:SER:CA	2.43	0.44
8:A:92:PHE:CB	8:A:128:PHE:N	2.79	0.44
2:B:632:ARG:HB2	2:B:640:MET:SD	2.58	0.44
4:G:149:ASN:OD1	4:G:150:LYS:N	2.49	0.44
4:G:171:SER:HB3	7:I:115:VAL:HG11	1.98	0.44
6:F:278:VAL:HG13	6:F:304:VAL:HG13	1.99	0.44
7:I:739:GLY:HA2	7:I:744:LEU:HB2	1.99	0.44
9:D:508:THR:O	9:D:508:THR:OG1	2.36	0.44
3:E:268:GLU:OE1	6:F:94:ALA:HB3	2.17	0.44
6:F:461:SER:O	6:F:465:GLY:N	2.43	0.44
7:I:389:GLN:HG2	7:I:393:LYS:HZ3	1.83	0.44
2:B:616:ASP:OD2	6:F:193:LYS:HD3	2.18	0.44
3:E:40:HIS:C	3:E:44:ILE:HD12	2.42	0.44
6:F:162:ASN:HB3	6:F:165:ARG:HG2	1.99	0.44
3:E:90:PHE:CD2	3:E:106:GLN:HB3	2.52	0.44
6:F:37:TRP:HZ2	6:F:161:ILE:HD12	1.83	0.44
6:F:196:LEU:HD12	6:F:220:CYS:HB3	1.99	0.44
6:F:196:LEU:HD11	6:F:221:TYR:CE1	2.53	0.44
7:I:376:LEU:HD23	7:I:378:TYR:HE1	1.83	0.44
9:D:314:PHE:HA	9:D:321:LEU:H	1.82	0.44
2:B:634:MET:O	9:D:551:PHE:HZ	2.00	0.44
3:E:314:HIS:CD2	3:E:322:SER:HB3	2.53	0.44
7:I:456:LYS:O	7:I:506:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:TYR:OH	3:E:303:ASP:HB3	2.18	0.44
4:G:308:LYS:NZ	7:I:362:ASP:OD1	2.49	0.44
7:I:278:GLN:HG2	7:I:279:PHE:CD2	2.52	0.44
9:D:505:LEU:HD23	9:D:506:GLN:N	2.33	0.44
3:E:415:PRO:O	3:E:418:VAL:HG22	2.18	0.43
2:B:565:GLY:HA2	2:B:685:LEU:HD12	1.99	0.43
3:E:311:GLY:HA3	3:E:327:LEU:HG	2.00	0.43
9:D:430:LYS:HA	9:D:430:LYS:HD3	1.81	0.43
3:E:46:LYS:HA	3:E:48:TYR:CZ	2.54	0.43
4:G:253:LEU:HA	4:G:256:VAL:HG12	2.00	0.43
7:I:9:TRP:HE3	7:I:356:CYS:HB2	1.83	0.43
7:I:464:PRO:HG2	7:I:497:PRO:HA	2.00	0.43
7:I:513:GLU:CD	7:I:513:GLU:N	2.73	0.43
7:I:610:TRP:HB2	7:I:733:LEU:HB2	2.01	0.43
9:D:101:THR:O	9:D:115:TYR:N	2.50	0.43
9:D:518:VAL:HG21	9:D:534:PHE:CZ	2.53	0.43
3:E:203:GLU:OE2	3:E:237:LYS:NZ	2.52	0.43
5:C:654:ASP:OD1	5:C:654:ASP:N	2.51	0.43
7:I:10:TRP:NE1	7:I:67:ASP:OD2	2.52	0.43
7:I:129:HIS:NE2	7:I:168:SER:HA	2.34	0.43
1:H:20:VAL:O	1:H:20:VAL:CG1	2.67	0.43
4:G:299:PHE:CD1	4:G:299:PHE:N	2.85	0.43
6:F:210:ASP:OD1	6:F:210:ASP:N	2.51	0.43
4:G:161:TYR:CE1	4:G:184:ASN:HB3	2.53	0.43
6:F:24:THR:O	6:F:28:GLU:HG2	2.19	0.43
6:F:363:ASP:HB2	7:I:368:ALA:HB3	2.01	0.43
4:G:190:HIS:HA	4:G:198:ASN:HB3	2.00	0.43
5:C:208:LEU:HA	5:C:217:GLY:O	2.18	0.43
3:E:314:HIS:NE2	6:F:360:GLN:OE1	2.52	0.43
5:C:613:LEU:HG	5:C:670:LEU:HD13	2.01	0.43
7:I:814:LEU:HD21	7:I:818:ARG:CZ	2.48	0.43
3:E:85:GLU:OE1	3:E:88:ARG:NH1	2.51	0.43
5:C:643:ILE:HG23	5:C:646:TYR:H	1.83	0.43
5:C:704:ASP:O	5:C:708:LEU:N	2.48	0.43
7:I:656:ARG:NH2	7:I:770:GLU:OE2	2.48	0.43
4:G:191:ALA:C	4:G:193:MET:H	2.26	0.43
4:G:323:ALA:O	7:I:358:TYR:HB2	2.19	0.43
6:F:332:LEU:HB2	6:F:355:CYS:HB3	2.00	0.43
7:I:272:LYS:HG3	7:I:278:GLN:HB2	2.01	0.43
7:I:821:LYS:H	7:I:821:LYS:HG2	1.65	0.43
9:D:564:ILE:HD12	9:D:584:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:GLY:HA3	3:E:278:MET:CE	2.31	0.42
7:I:326:LEU:HD23	7:I:326:LEU:HA	1.90	0.42
2:B:652:LYS:HA	2:B:652:LYS:HD3	1.66	0.42
3:E:191:TYR:O	3:E:195:VAL:HG23	2.19	0.42
4:G:99:THR:OG1	4:G:106:PHE:HB2	2.19	0.42
5:C:266:VAL:O	5:C:282:ASP:HA	2.20	0.42
9:D:63:GLY:O	9:D:87:ALA:CA	2.39	0.42
9:D:294:GLY:C	9:D:305:GLY:H	2.28	0.42
2:B:709:MET:O	2:B:713:ILE:HG13	2.20	0.42
6:F:333:ARG:HE	9:D:433:LEU:HD21	1.83	0.42
7:I:743:LYS:HA	7:I:743:LYS:HD3	1.80	0.42
9:D:516:GLY:O	9:D:570:ARG:HD3	2.19	0.42
5:C:13:VAL:O	5:C:312:GLY:HA3	2.20	0.42
5:C:326:SER:H	8:A:160:CYS:CB	2.32	0.42
5:C:669:ARG:HA	5:C:669:ARG:HD3	1.92	0.42
8:A:100:LEU:CB	9:D:402:LEU:C	2.93	0.42
3:E:210:LEU:O	3:E:214:GLN:HG2	2.20	0.42
3:E:247:GLN:NE2	3:E:275:ASN:O	2.50	0.42
5:C:689:VAL:HG13	5:C:692:LYS:HD3	2.01	0.42
6:F:59:GLY:HA2	6:F:137:ILE:CG2	2.50	0.42
6:F:75:ARG:O	6:F:78:THR:HG22	2.20	0.42
7:I:154:ILE:HD12	7:I:164:PHE:CE2	2.54	0.42
7:I:548:LEU:HD22	7:I:737:LEU:HD11	2.00	0.42
9:D:132:ASN:O	9:D:136:GLN:CB	2.67	0.42
2:B:31:LEU:O	2:B:42:ILE:HA	2.20	0.42
4:G:8:TRP:CZ2	4:G:21:GLN:HB3	2.55	0.42
4:G:137:TYR:CD1	4:G:264:GLY:HA3	2.55	0.42
7:I:48:TYR:CD1	7:I:73:HIS:HB2	2.54	0.42
4:G:179:THR:HB	4:G:190:HIS:CE1	2.54	0.42
9:D:245:PRO:O	9:D:247:VAL:N	2.53	0.42
9:D:487:LYS:HE3	9:D:506:GLN:HB3	2.02	0.42
3:E:108:ALA:HB2	3:E:123:VAL:HB	2.02	0.41
7:I:519:ILE:H	7:I:519:ILE:HG13	1.46	0.41
7:I:593:SER:HB3	7:I:598:ARG:O	2.19	0.41
4:G:105:ARG:HD3	7:I:7:ARG:HH22	1.85	0.41
6:F:234:PHE:HB3	6:F:250:LEU:HG	2.02	0.41
7:I:312:LEU:HG	7:I:326:LEU:HD11	2.03	0.41
9:D:111:CYS:C	9:D:112:VAL:O	2.63	0.41
4:G:183:THR:OG1	4:G:186:ARG:O	2.27	0.41
6:F:381:GLU:O	6:F:385:VAL:HG23	2.20	0.41
8:A:110:ARG:O	8:A:114:ASN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:174:VAL:O	8:A:178:GLN:N	2.53	0.41
4:G:9:GLU:HB3	4:G:56:ARG:HD3	2.00	0.41
4:G:22:MET:HA	4:G:56:ARG:NH1	2.36	0.41
4:G:48:GLY:HA2	4:G:61:SER:C	2.46	0.41
5:C:381:VAL:HA	5:C:399:GLU:O	2.19	0.41
6:F:22:LEU:O	6:F:25:GLN:HB2	2.20	0.41
4:G:15:PHE:HD1	4:G:69:LEU:HD23	1.84	0.41
4:G:113:LEU:HD23	4:G:113:LEU:HA	1.92	0.41
6:F:182:PHE:CE2	6:F:216:GLN:HB3	2.56	0.41
7:I:14:LEU:HA	7:I:14:LEU:HD12	1.73	0.41
3:E:218:TYR:CE1	3:E:245:MET:HG2	2.55	0.41
4:G:159:ASN:OD1	4:G:160:VAL:N	2.53	0.41
7:I:103:LEU:HD13	7:I:154:ILE:HD11	2.02	0.41
7:I:370:LYS:HB2	7:I:370:LYS:HZ2	1.76	0.41
7:I:709:LEU:HD23	7:I:709:LEU:HA	1.83	0.41
4:G:41:LYS:HG2	4:G:107:GLU:O	2.21	0.41
4:G:190:HIS:HD2	4:G:192:ASN:N	2.19	0.41
4:G:220:LEU:HD11	4:G:243:LEU:HG	2.02	0.41
4:G:308:LYS:HE3	4:G:310:GLN:O	2.20	0.41
5:C:506:MET:HA	5:C:567:SER:O	2.20	0.41
6:F:16:PHE:HA	6:F:19:CYS:SG	2.60	0.41
7:I:27:LEU:HD11	7:I:338:LEU:HD21	2.02	0.41
9:D:529:ALA:HB2	9:D:555:LEU:HD11	2.03	0.41
4:G:47:ARG:NH2	7:I:380:GLU:OE2	2.54	0.41
4:G:246:SER:O	4:G:249:GLU:HG3	2.21	0.41
7:I:79:LEU:O	7:I:98:LEU:HB3	2.20	0.41
7:I:686:ASP:OD1	7:I:687:LYS:N	2.54	0.41
3:E:247:GLN:NE2	3:E:259:TYR:HE2	2.19	0.41
6:F:458:ALA:HB2	6:F:473:ALA:HB3	2.02	0.41
8:A:132:MET:CB	8:A:163:ASP:HA	2.51	0.41
7:I:788:SER:HA	7:I:791:GLN:HB2	2.03	0.40
3:E:317:MET:HE3	3:E:317:MET:HB3	1.87	0.40
6:F:363:ASP:HA	9:D:451:THR:HG23	2.03	0.40
7:I:809:LYS:O	7:I:813:THR:HG23	2.22	0.40
1:H:44:LEU:HD23	1:H:44:LEU:HA	1.95	0.40
2:B:634:MET:O	9:D:551:PHE:CZ	2.75	0.40
7:I:577:VAL:HG13	7:I:591:LEU:HD23	2.02	0.40
9:D:388:LEU:C	9:D:399:ILE:HA	2.46	0.40
1:H:44:LEU:HD13	6:F:135:ARG:NH1	2.36	0.40
3:E:266:VAL:HG23	3:E:266:VAL:O	2.21	0.40
3:E:412:GLU:O	3:E:415:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:298:ALA:O	4:G:299:PHE:C	2.61	0.40
5:C:643:ILE:N	7:I:672:GLN:NE2	2.68	0.40
7:I:333:VAL:O	7:I:334:ARG:NH1	2.51	0.40
7:I:599:TYR:CD2	7:I:616:LEU:HD11	2.57	0.40
2:B:499:VAL:HA	2:B:584:ALA:HA	2.03	0.40
4:G:173:ASP:OD1	4:G:173:ASP:N	2.51	0.40
7:I:17:LYS:HE3	7:I:17:LYS:HB2	1.89	0.40
7:I:728:LYS:HD2	7:I:757:LEU:HD23	2.03	0.40
9:D:298:VAL:O	9:D:299:HIS:CB	2.68	0.40
9:D:456:LEU:HD23	9:D:456:LEU:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	50/69 (72%)	49 (98%)	1 (2%)	0	100	100
2	B	605/721 (84%)	561 (93%)	43 (7%)	1 (0%)	43	75
3	E	384/519 (74%)	368 (96%)	16 (4%)	0	100	100
4	G	294/341 (86%)	259 (88%)	34 (12%)	1 (0%)	36	70
5	C	649/715 (91%)	588 (91%)	60 (9%)	1 (0%)	43	75
6	F	469/501 (94%)	451 (96%)	18 (4%)	0	100	100
7	I	752/887 (85%)	704 (94%)	47 (6%)	1 (0%)	48	81
8	A	163/186 (88%)	131 (80%)	29 (18%)	3 (2%)	6	34
9	D	522/592 (88%)	416 (80%)	93 (18%)	13 (2%)	4	29
All	All	3888/4531 (86%)	3527 (91%)	341 (9%)	20 (0%)	26	60

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	328	PRO
8	A	123	ILE
9	D	110	PRO
9	D	112	VAL
9	D	282	PRO
8	A	142	LYS
9	D	61	PRO
9	D	257	PHE
4	G	87	LYS
8	A	124	PRO
2	B	432	PRO
9	D	77	VAL
9	D	83	PRO
9	D	102	PRO
9	D	399	ILE
9	D	66	PRO
9	D	255	GLY
9	D	244	LEU
7	I	516	PRO
9	D	120	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	49/65 (75%)	48 (98%)	1 (2%)	48	66
2	B	117/618 (19%)	113 (97%)	4 (3%)	32	55
3	E	330/438 (75%)	319 (97%)	11 (3%)	33	56
4	G	268/307 (87%)	267 (100%)	1 (0%)	84	84
5	C	108/638 (17%)	108 (100%)	0	100	100
6	F	402/423 (95%)	393 (98%)	9 (2%)	45	65
7	I	680/787 (86%)	674 (99%)	6 (1%)	70	76
9	D	144/499 (29%)	143 (99%)	1 (1%)	76	79
All	All	2098/3775 (56%)	2065 (98%)	33 (2%)	54	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	17	GLN
2	B	626	VAL
2	B	629	GLU
2	B	630	ASP
2	B	632	ARG
3	E	36	ASN
3	E	44	ILE
3	E	99	GLN
3	E	100	CYS
3	E	322	SER
3	E	351	LEU
3	E	352	GLU
3	E	409	SER
3	E	410	SER
3	E	411	LEU
3	E	413	PHE
4	G	299	PHE
6	F	18	LEU
6	F	22	LEU
6	F	57	GLU
6	F	60	ILE
6	F	62	GLU
6	F	137	ILE
6	F	139	SER
6	F	411	VAL
6	F	412	SER
7	I	361	THR
7	I	364	SER
7	I	365	LEU
7	I	370	LYS
7	I	519	ILE
7	I	759	LEU
9	D	488	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	17	GLN
2	B	608	GLN
2	B	642	ASN
2	B	651	ASN

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Mol	Chain	Res	Type
2	B	656	ASN
2	B	665	HIS
2	B	684	HIS
3	E	35	GLN
3	E	36	ASN
3	E	58	GLN
3	E	99	GLN
3	E	103	ASN
3	E	224	HIS
3	E	297	ASN
3	E	375	ASN
3	E	377	ASN
4	G	165	ASN
4	G	176	ASN
4	G	190	HIS
4	G	192	ASN
4	G	205	GLN
4	G	251	ASN
5	C	604	HIS
5	C	610	HIS
5	C	663	GLN
6	F	187	HIS
6	F	216	GLN
6	F	233	GLN
6	F	241	GLN
6	F	259	GLN
6	F	350	ASN
6	F	351	ASN
6	F	388	ASN
6	F	422	ASN
6	F	435	GLN
6	F	449	HIS
6	F	454	HIS
6	F	456	ASN
6	F	496	GLN
7	I	22	GLN
7	I	37	GLN
7	I	120	GLN
7	I	201	GLN
7	I	276	GLN
7	I	313	HIS
7	I	515	ASN

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Mol	Chain	Res	Type
7	I	652	HIS
7	I	672	GLN
7	I	693	GLN
7	I	705	GLN
7	I	742	GLN
7	I	748	GLN
7	I	778	HIS
7	I	796	ASN
9	D	449	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

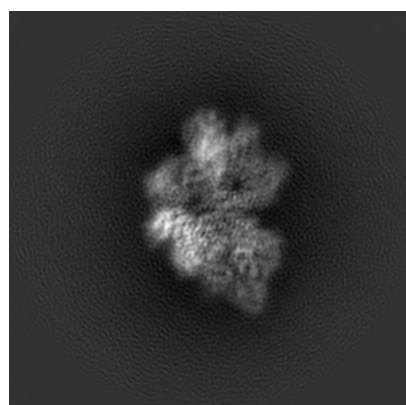
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21259. These allow visual inspection of the internal detail of the map and identification of artifacts.

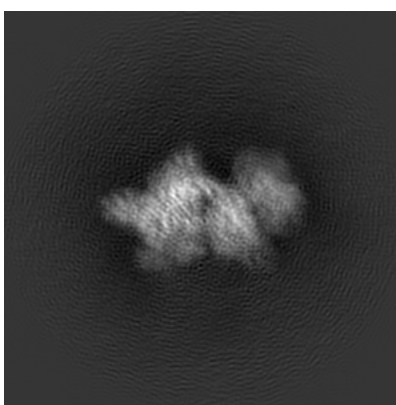
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

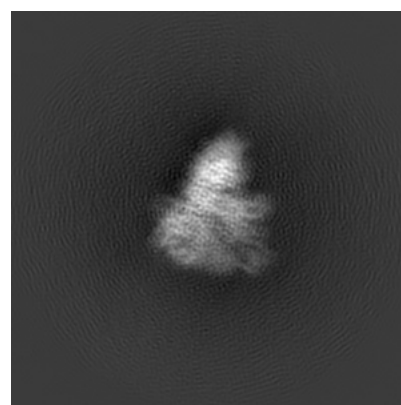
6.1.1 Primary map



X



Y

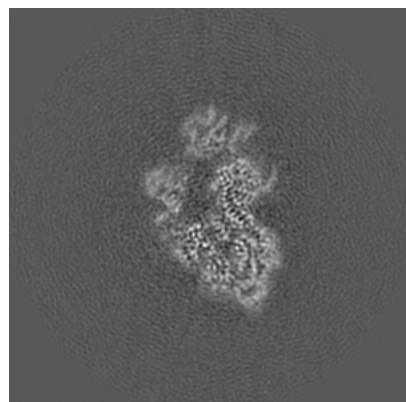


Z

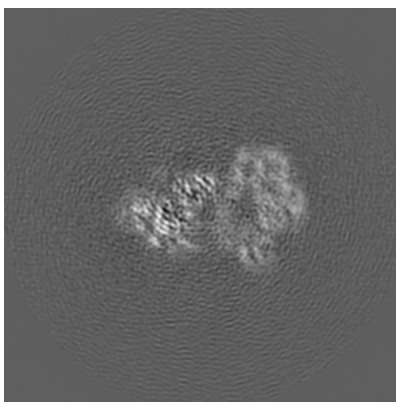
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

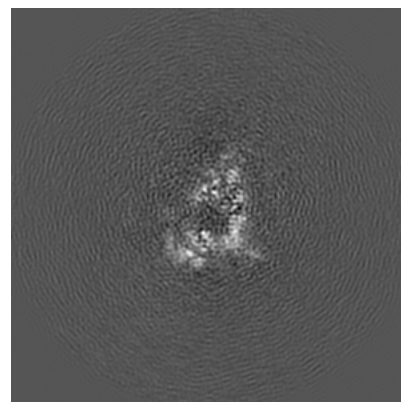
6.2.1 Primary map



X Index: 175



Y Index: 175

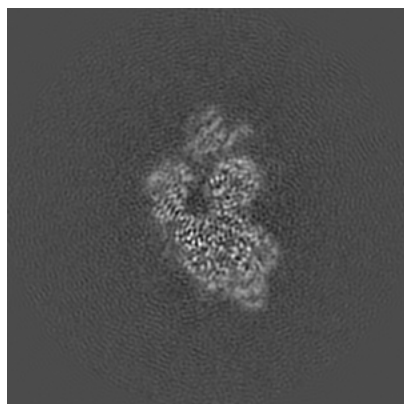


Z Index: 175

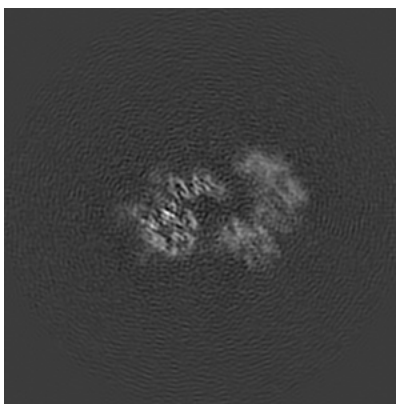
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

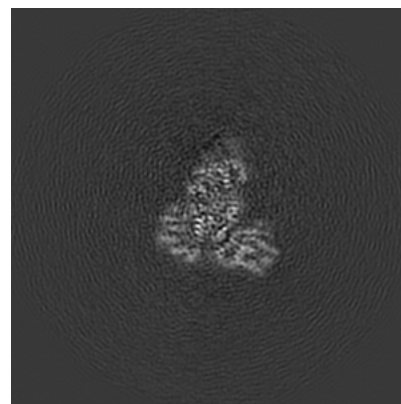
6.3.1 Primary map



X Index: 169



Y Index: 168

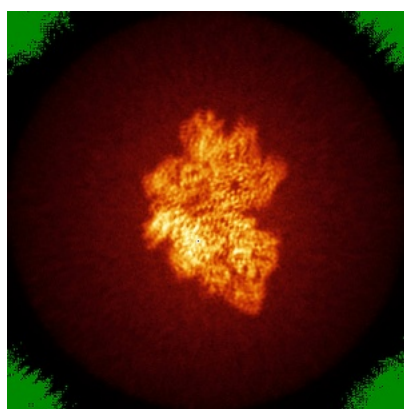


Z Index: 159

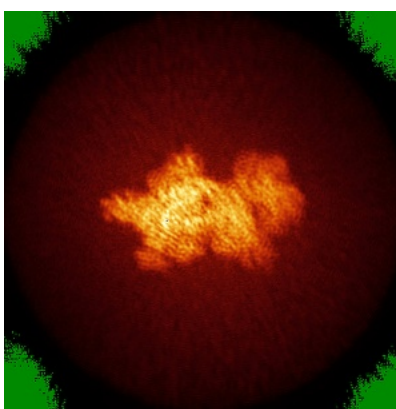
The images above show the largest variance slices of the map in three orthogonal directions.

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

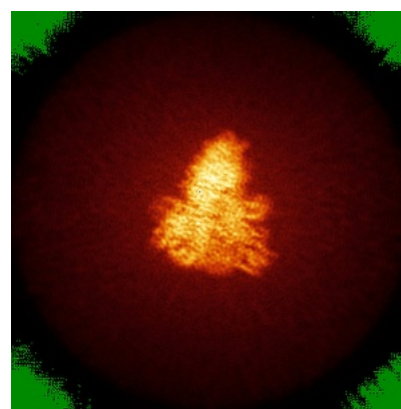
6.4.1 Primary map



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

This section was not generated.

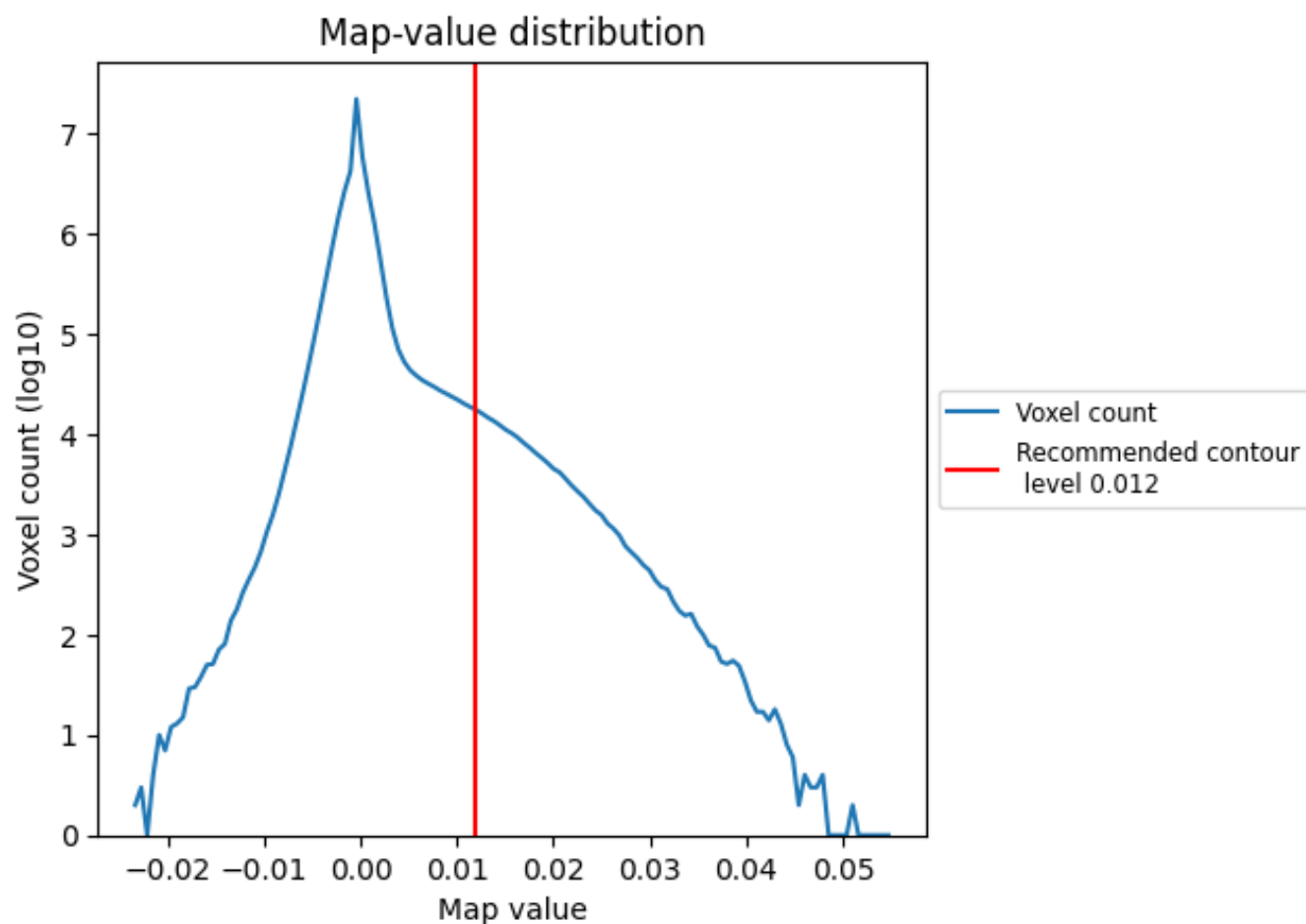
6.6 Mask visualisation

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

7 Map analysis [i](#)

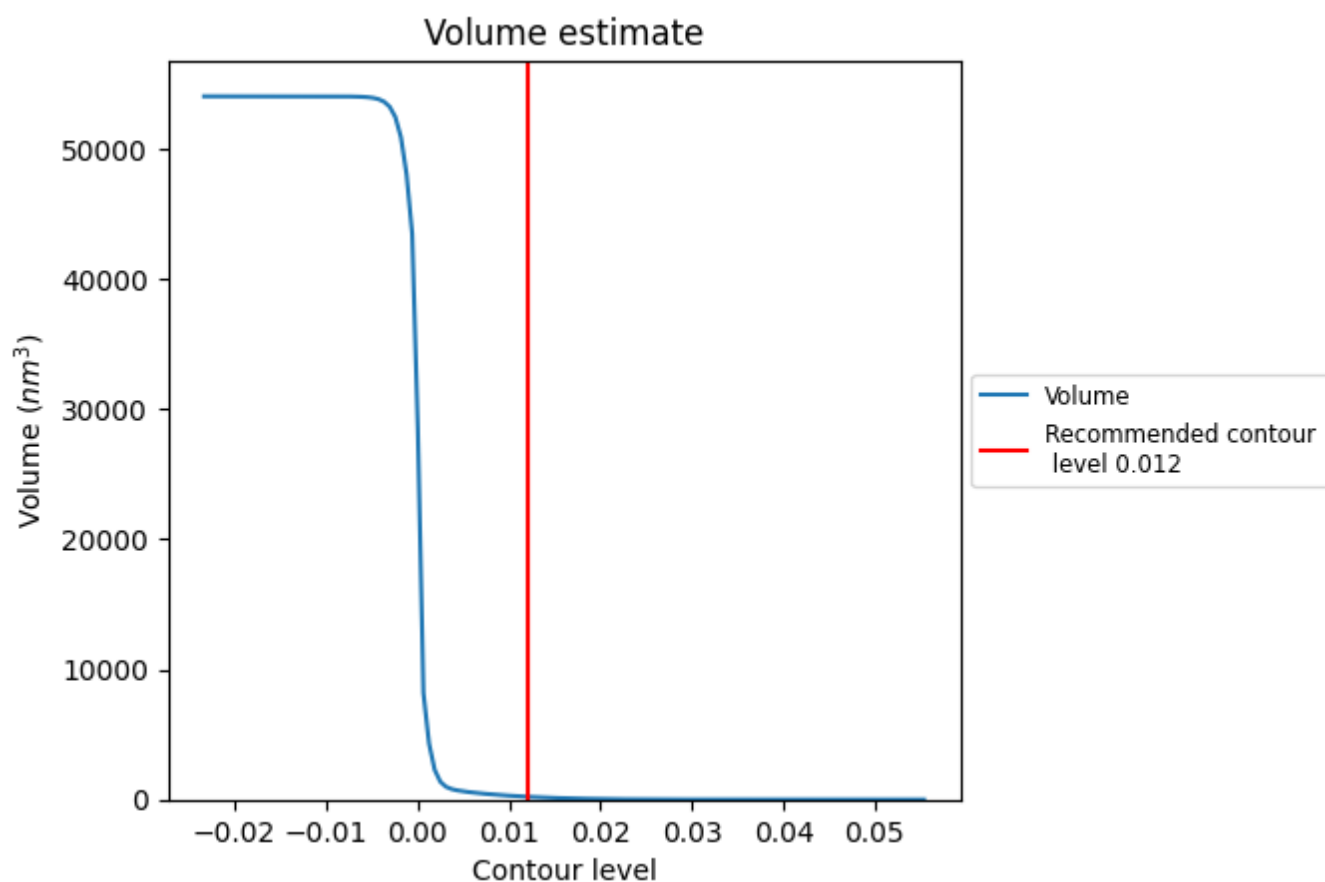
This section contains the results of statistical analysis of the map.

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.

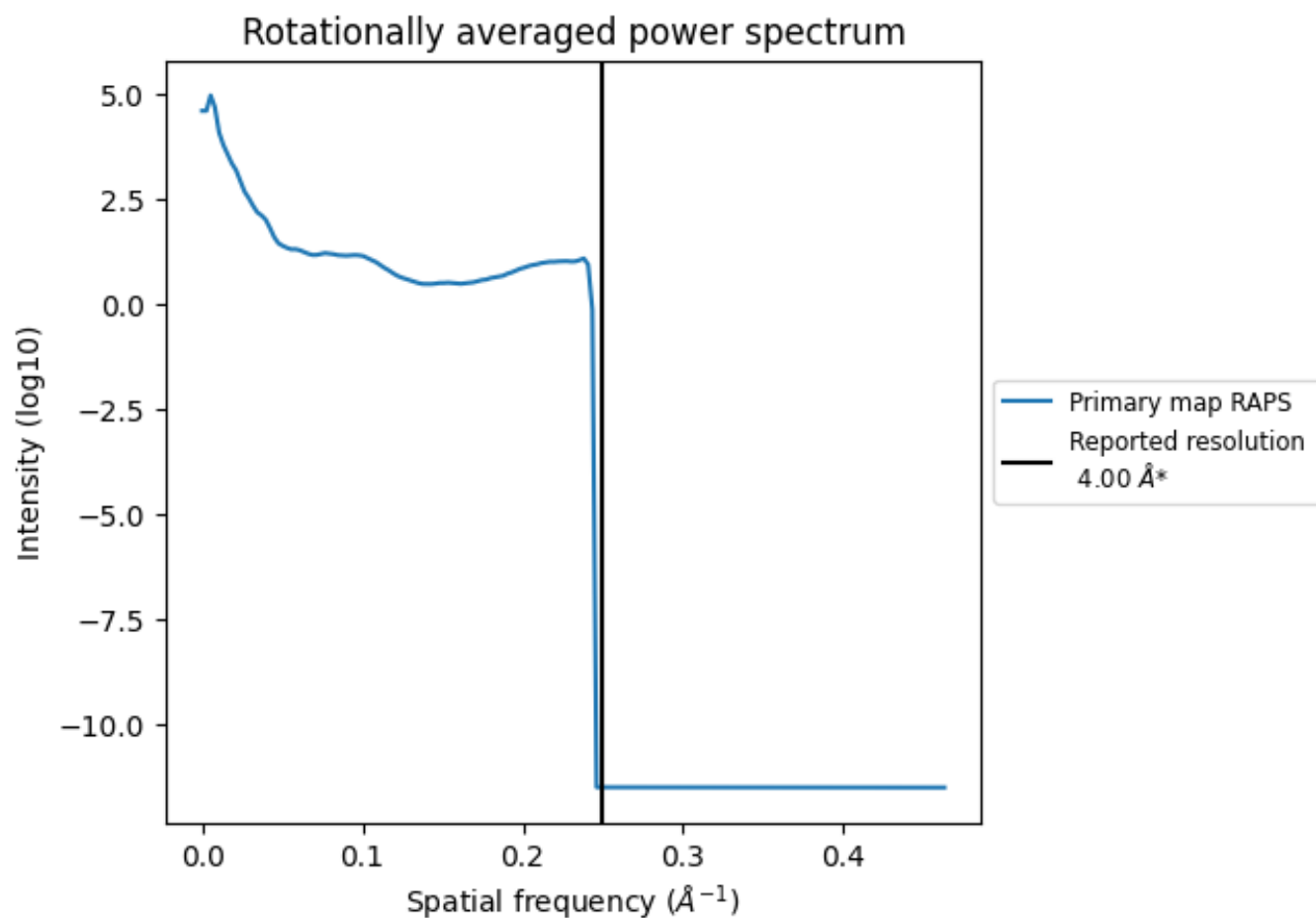
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 216 nm³; this corresponds to an approximate mass of 195 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 0.250 $\text{\AA}^{-1}$

8 Fourier-Shell correlation ⓘ

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

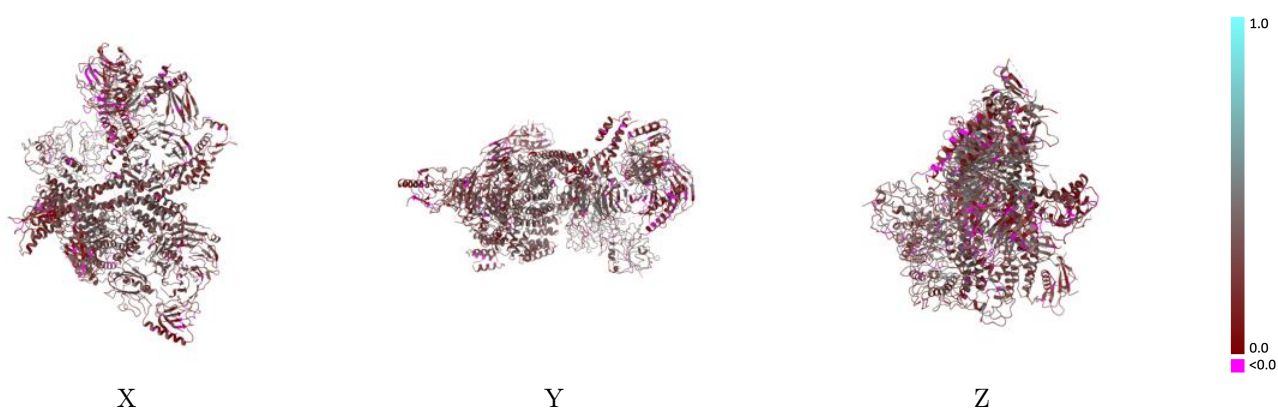
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21259 and PDB model 6VOA. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

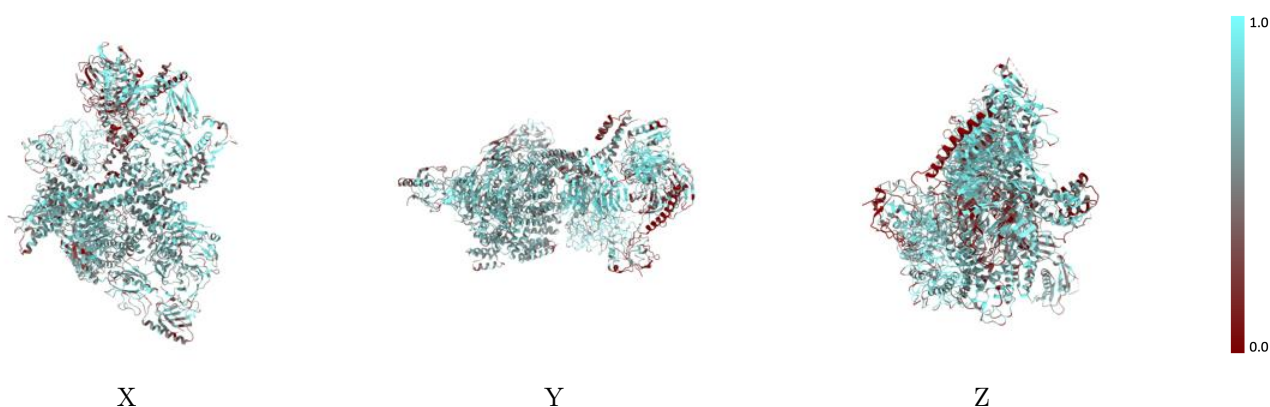
This section was not generated.

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



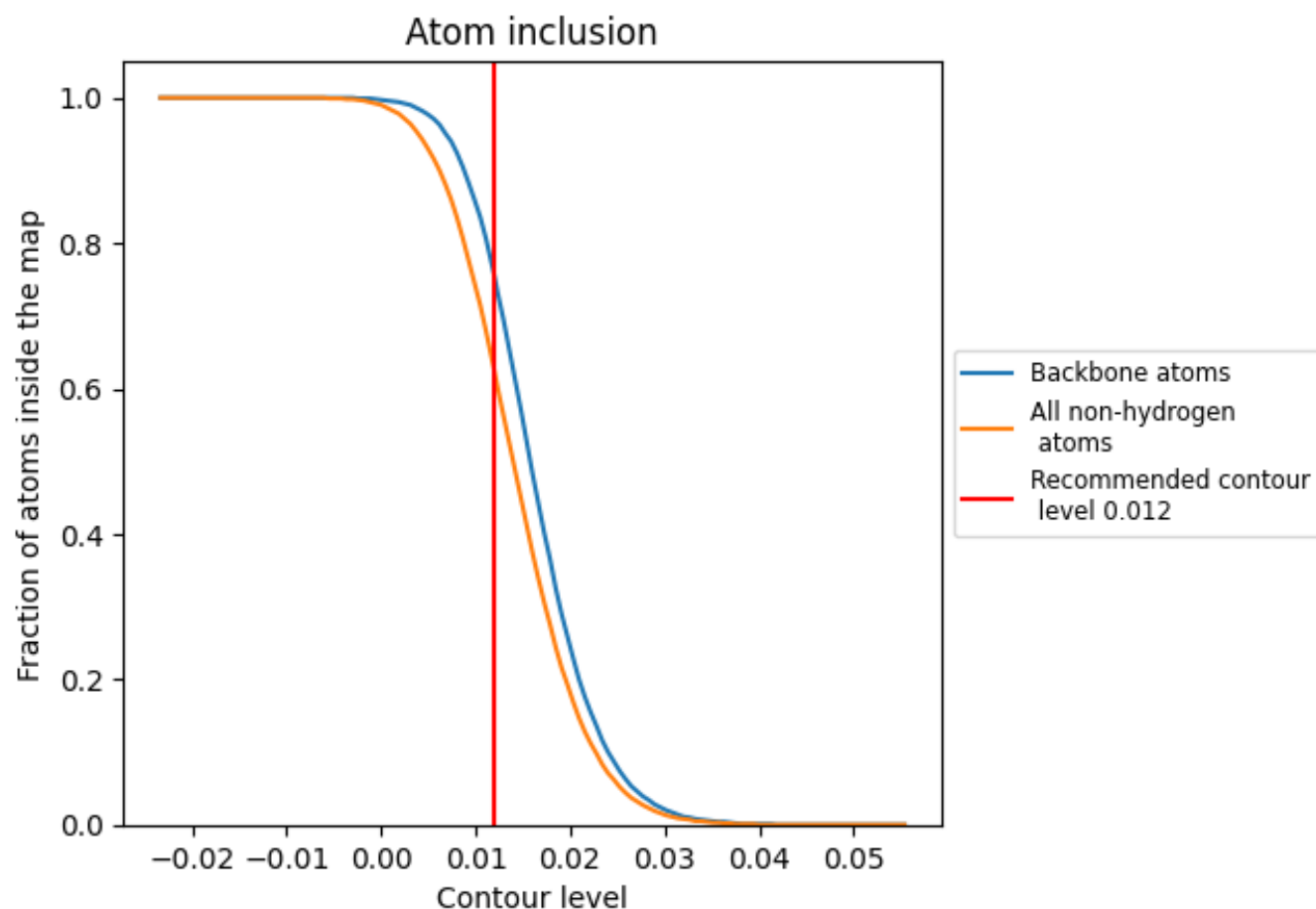
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 62% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6230	0.2800
A	0.4710	0.3370
B	0.7030	0.3060
C	0.4700	0.2270
D	0.7000	0.3240
E	0.6360	0.2710
F	0.6820	0.3170
G	0.5700	0.2340
H	0.5910	0.2950
I	0.6300	0.2670

1.0

0.0

<0.0