



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 02:58 PM UTC

PDB ID : 8XXT / pdb_00008xxt
EMDB ID : EMD-38760
Title : ASFV RNAP M1249L C-tail occupied complex2 (MCOC2)
Authors : Zhu, G.L.; Zhu, Y.; Zhu, Z.X.; Sun, F.; Zheng, H.X.
Deposited on : 2024-01-19
Resolution : 2.85 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

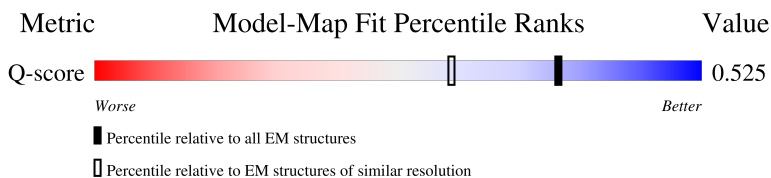
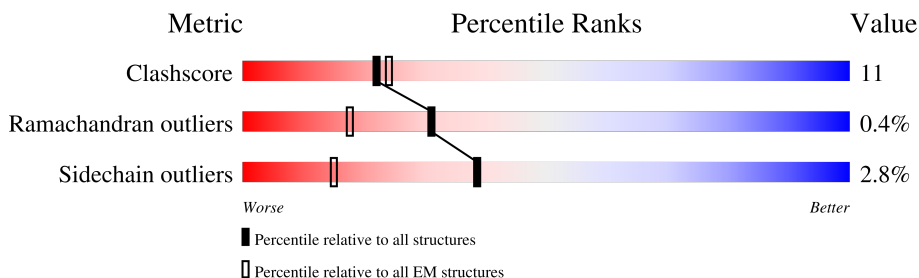
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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	11965 (2.35 - 3.35)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1441	
2	B	1235	
3	C	358	
4	D	205	

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Mol	Chain	Length	Quality of chain
5	E	139	15% 68% 23% 7%
6	F	334	32% 63% 35%
7	G	105	10% 68% 31%
8	H	80	64% 22% 14%
9	I	1170	23% 39% 15% 45%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 35783 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1415	Total	C	N	O	S	0	0
			11244	7135	1955	2092	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1226	Total	C	N	O	S	0	0
			9701	6124	1706	1819	52		

- Molecule 3 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	358	Total	C	N	O	S	0	0
			2907	1885	481	529	12		

- Molecule 4 is a protein called DNA-directed RNA polymerase RPB5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	205	Total	C	N	O	S	0	0
			1669	1088	278	295	8		

- Molecule 5 is a protein called C147L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	129	Total	C	N	O	S	0	0
			1021	648	167	200	6		

- Molecule 6 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	334	Total	C	N	O	S	0	0
			2687	1726	444	503	14		

- Molecule 7 is a protein called C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	105	Total	C	N	O	S	0	0
			816	507	141	153	15		

- Molecule 8 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	69	Total	C	N	O	S	0	0
			553	362	89	95	7		

- Molecule 9 is a protein called M1249L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	638	Total	C	N	O	S	0	0
			5177	3329	858	968	22		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	3	Total	Zn	0
			3	3	
10	B	1	Total	Zn	0
			1	1	
10	G	2	Total	Zn	0
			2	2	
10	H	1	Total	Zn	0
			1	1	

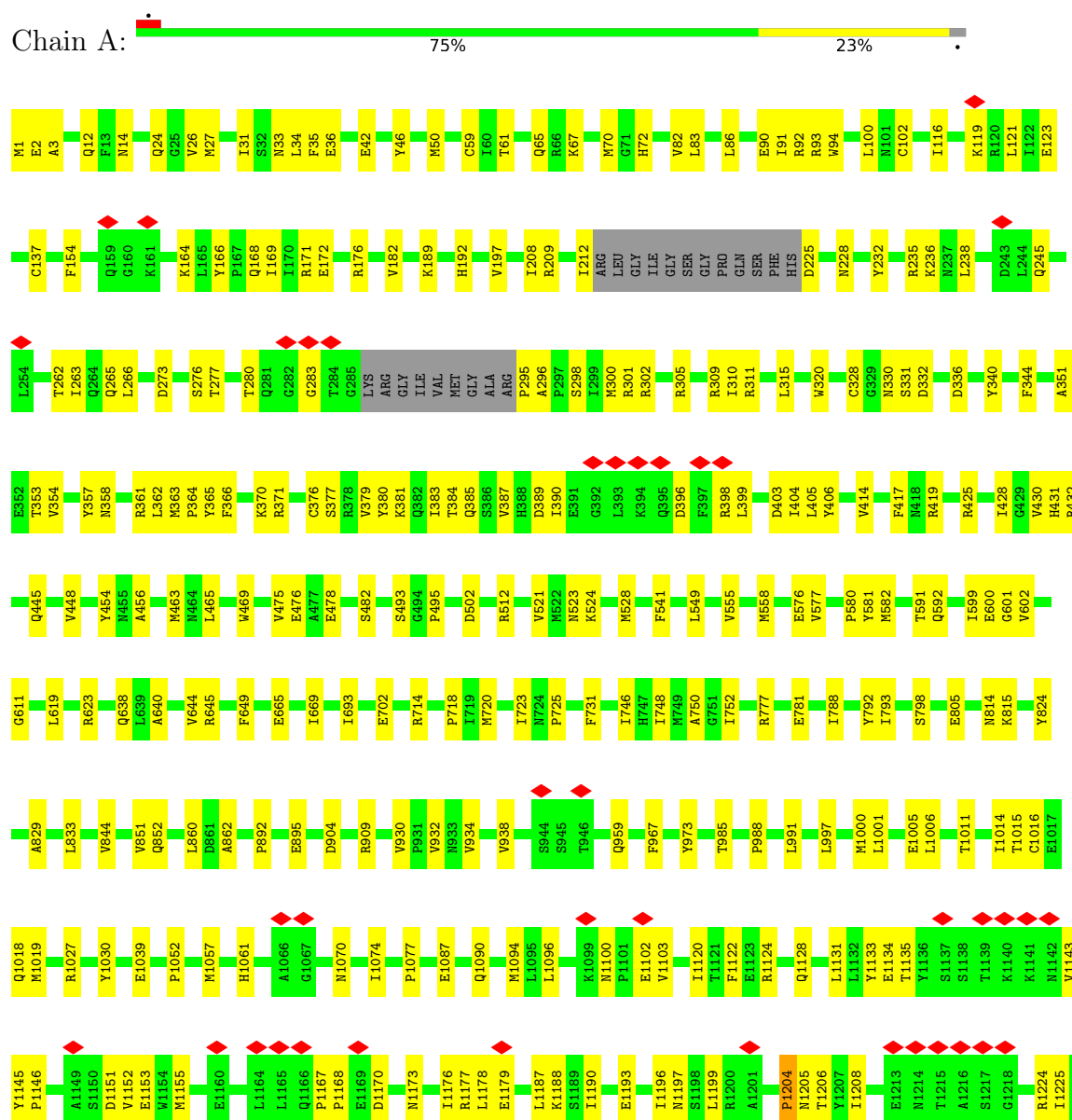
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

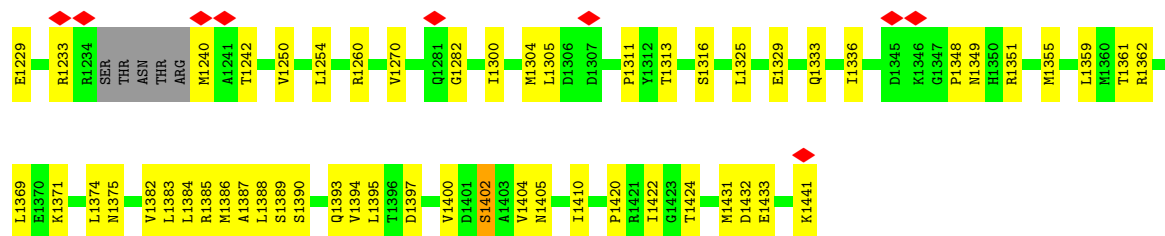
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

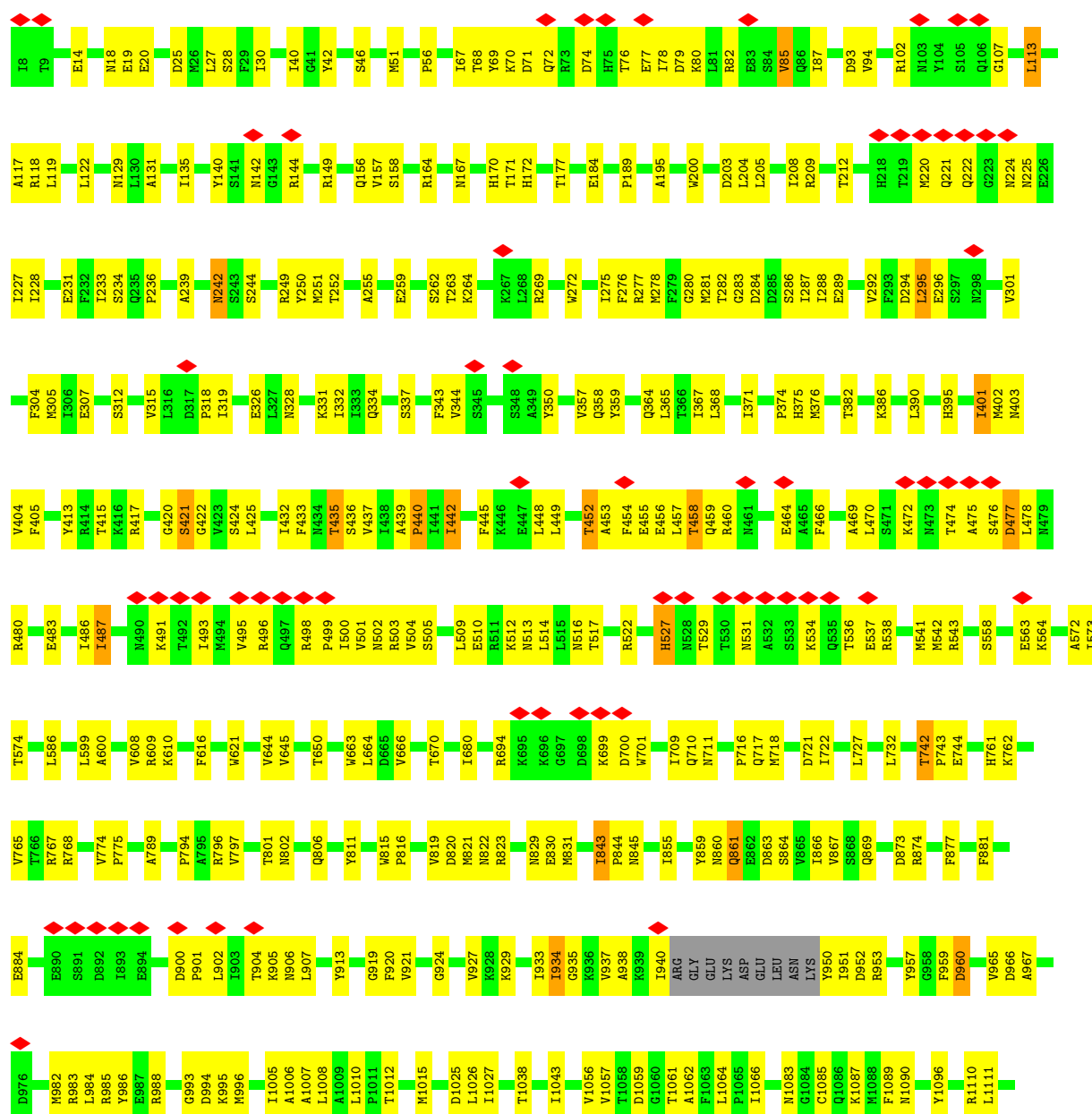
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



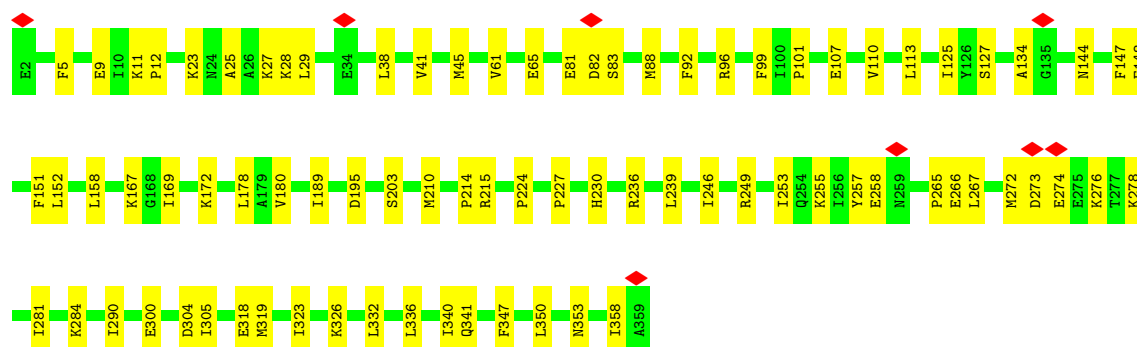
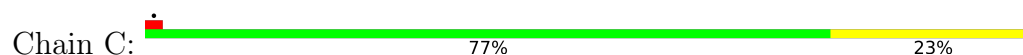


• Molecule 2: DNA-directed RNA polymerase subunit beta

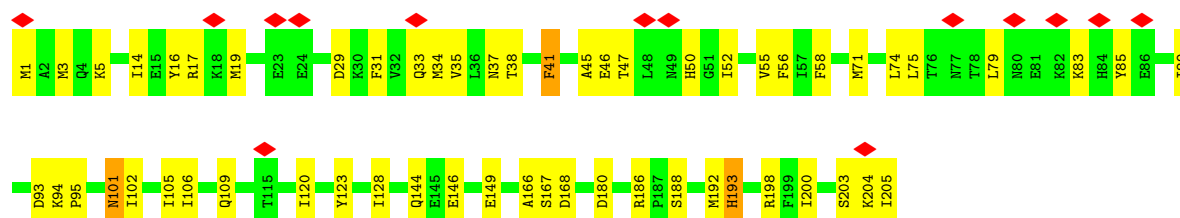




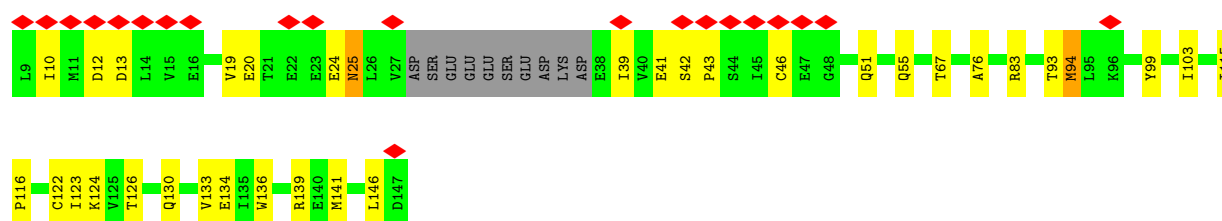
- Molecule 3: DNA-directed RNA polymerase RPB3-11 homolog



- Molecule 4: DNA-directed RNA polymerase RPB5 homolog



- Molecule 5: C147L



- Molecule 6: D339L



V1161	V1162	V1165	R1166	E1172	I1177	K1181	L1182	P1186	M1192	I1193	F1194	G1195	E1196	D1197	F1198	V1199	C1200	S1206	M1207	D1208	D1209	I1210	P1216	G1217	F1219	G1220	E1221	D1222	I1223	I1224	D1225	R1226	L1227	D1228	S1232	I1233	E1234	D1235	V1236	S1239	L1240	D1241	V1242	P1248	Q1249																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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LVS	ASN	THR	ILE	THR	GLN	ASN	THR	GLN	ASP	LEU	LEU	GLN	ALA	ALA	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83920	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.226	Depositor
Minimum map value	-1.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.19	0/11462	0.32	1/15525 (0.0%)
2	B	0.20	0/9896	0.36	1/13394 (0.0%)
3	C	0.20	0/2969	0.33	0/4012
4	D	0.17	0/1708	0.37	0/2311
5	E	0.20	0/1033	0.36	0/1398
6	F	0.17	0/2740	0.42	0/3709
7	G	0.19	0/828	0.42	0/1109
8	H	0.24	0/563	0.41	0/758
9	I	0.17	0/5298	0.39	1/7172 (0.0%)
All	All	0.19	0/36497	0.36	3/49388 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	124	PRO	CA-N-CD	-9.28	99.01	112.00
1	A	1204	PRO	CA-N-CD	-8.63	99.92	112.00
2	B	440	PRO	CA-N-CD	-5.94	103.68	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11244	0	11362	231	0
2	B	9701	0	9657	304	0
3	C	2907	0	2982	56	0
4	D	1669	0	1713	44	0
5	E	1021	0	1054	25	0
6	F	2687	0	2721	88	0
7	G	816	0	814	23	0
8	H	553	0	580	28	0
9	I	5177	0	5136	140	0
10	A	3	0	0	0	0
10	B	1	0	0	0	0
10	G	2	0	0	0	0
10	H	1	0	0	0	0
11	A	1	0	0	0	0
All	All	35783	0	36019	824	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 11.

All (824) 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)
8:H:48:GLN:HB2	9:I:821:PHE:H	1.24	1.03
3:C:29:LEU:HD22	8:H:23:LYS:HD3	1.54	0.88
4:D:192:MET:O	4:D:193:HIS:ND1	2.08	0.86
2:B:491:LYS:HE2	2:B:527:HIS:HB3	1.60	0.84
2:B:1161:MET:O	2:B:1163:THR:N	2.13	0.81
9:I:912:ASN:HD22	9:I:915:LYS:HE2	1.46	0.80
9:I:952:LYS:HG3	9:I:954:GLY:H	1.47	0.80
1:A:1227:LEU:HD11	1:A:1250:VAL:HG11	1.65	0.77
1:A:419:ARG:HG3	1:A:463:MET:HG2	1.66	0.77
9:I:840:GLU:HG3	9:I:842:LYS:HG3	1.65	0.77
9:I:222:LEU:O	9:I:226:MET:HG3	1.85	0.76
6:F:157:PRO:HB2	6:F:209:THR:HG22	1.68	0.75
8:H:48:GLN:H	9:I:820:GLY:HA3	1.53	0.73
7:G:33:ASP:O	7:G:35:GLN:NE2	2.20	0.73
2:B:276:PHE:HB3	2:B:287:ILE:HD12	1.68	0.73
2:B:249:ARG:NH1	2:B:259:GLU:OE1	2.22	0.73
9:I:1070:ASP:OD2	9:I:1074:ARG:NH2	2.22	0.72
8:H:23:LYS:HB3	8:H:23:LYS:HZ3	1.53	0.72
9:I:817:ALA:O	9:I:819:GLN:NE2	2.22	0.72
1:A:1070:ASN:ND2	1:A:1090:GLN:OE1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:ASN:HA	9:I:1075:ILE:HD11	1.72	0.71
2:B:14:GLU:HG3	2:B:709:ILE:HG21	1.73	0.71
2:B:20:GLU:HG2	2:B:716:PRO:HG2	1.72	0.71
1:A:693:ILE:HD12	1:A:693:ILE:H	1.55	0.71
1:A:59:CYS:SG	1:A:72:HIS:CD2	2.84	0.71
6:F:1:MET:SD	6:F:298:LYS:NZ	2.64	0.71
1:A:1128:GLN:HB3	7:G:43:VAL:HG13	1.74	0.70
3:C:83:SER:HB2	9:I:703:HIS:HA	1.72	0.70
1:A:1441:LYS:HD2	6:F:21:THR:HB	1.73	0.70
2:B:20:GLU:N	2:B:20:GLU:OE1	2.22	0.70
6:F:221:LYS:HG3	6:F:227:LYS:HD2	1.75	0.69
2:B:164:ARG:NH1	2:B:171:THR:OG1	2.26	0.69
2:B:938:ALA:HB3	2:B:951:ILE:HG22	1.76	0.68
2:B:543:ARG:NH2	2:B:563:GLU:OE1	2.26	0.68
2:B:586:LEU:HD23	2:B:664:LEU:HD11	1.74	0.68
1:A:189:LYS:NZ	5:E:41:GLU:O	2.25	0.68
1:A:331:SER:O	1:A:638:GLN:NE2	2.28	0.67
6:F:157:PRO:HD2	6:F:330:ILE:HD11	1.74	0.67
2:B:135:ILE:HG13	2:B:149:ARG:HG2	1.74	0.67
1:A:824:TYR:OH	9:I:1232:SER:OG	2.11	0.67
1:A:1329:GLU:OE2	4:D:186:ARG:NH2	2.28	0.67
2:B:558:SER:O	2:B:802:ASN:ND2	2.28	0.67
9:I:1155:ILE:HD12	9:I:1165:VAL:HG11	1.76	0.67
1:A:328:CYS:HB2	2:B:1007:ALA:HB2	1.75	0.66
2:B:404:VAL:O	7:G:52:LYS:NZ	2.24	0.66
2:B:1238:VAL:HG12	5:E:55:GLN:HB2	1.77	0.66
3:C:127:SER:HB2	3:C:147:PHE:HB2	1.77	0.66
2:B:929:LYS:NZ	2:B:960:ASP:OD1	2.28	0.66
1:A:12:GLN:HG3	1:A:1404:VAL:HG22	1.76	0.66
3:C:61:VAL:HA	3:C:65:GLU:HB2	1.77	0.66
6:F:46:LEU:HD11	6:F:79:SER:HB3	1.78	0.66
7:G:21:ILE:HA	7:G:31:GLN:HA	1.78	0.66
9:I:1029:ILE:HD13	9:I:1033:VAL:HB	1.78	0.66
6:F:243:LEU:HD11	6:F:297:LEU:HD11	1.77	0.66
2:B:239:ALA:HB2	2:B:666:VAL:HG11	1.79	0.65
2:B:118:ARG:NH2	2:B:184:GLU:OE2	2.29	0.65
2:B:476:SER:OG	2:B:480:ARG:NH1	2.30	0.65
1:A:232:TYR:HB3	1:A:266:LEU:HD21	1.77	0.65
7:G:35:GLN:CD	7:G:35:GLN:H	2.04	0.65
1:A:50:MET:SD	1:A:209:ARG:NH2	2.70	0.65
2:B:417:ARG:NH1	2:B:744:GLU:OE2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:PHE:HB3	2:B:1110:ARG:HD2	1.79	0.64
4:D:1:MET:HE2	4:D:3:MET:H	1.62	0.64
4:D:52:ILE:HG21	4:D:83:LYS:HD3	1.79	0.64
7:G:11:MET:HE3	7:G:24:CYS:HB2	1.79	0.64
1:A:176:ARG:HE	9:I:120:PRO:HD3	1.63	0.64
1:A:166:TYR:H	1:A:169:ILE:HD12	1.61	0.64
8:H:17:TYR:HB3	8:H:58:LEU:HD22	1.80	0.64
2:B:82:ARG:HH22	2:B:455:GLU:CD	2.06	0.64
2:B:19:GLU:OE2	2:B:762:LYS:NZ	2.26	0.64
2:B:877:PHE:O	2:B:1110:ARG:NH1	2.29	0.64
2:B:227:ILE:HG22	2:B:228:ILE:H	1.63	0.63
3:C:266:GLU:N	3:C:266:GLU:OE2	2.31	0.63
8:H:75:ASP:HB3	8:H:78:LYS:HD3	1.79	0.63
4:D:93:ASP:OD1	4:D:94:LYS:N	2.31	0.63
2:B:844:PRO:HD2	8:H:74:LEU:HD11	1.80	0.63
1:A:938:VAL:HG13	1:A:1014:ILE:HD11	1.81	0.62
1:A:576:GLU:HG3	9:I:880:ARG:HG2	1.81	0.62
2:B:510:GLU:O	2:B:516:ASN:ND2	2.31	0.62
1:A:475:VAL:HG22	5:E:103:ILE:HG23	1.81	0.62
6:F:200:ILE:HD12	6:F:200:ILE:H	1.65	0.62
1:A:27:MET:HE2	1:A:50:MET:HE3	1.82	0.62
3:C:249:ARG:O	3:C:253:ILE:HD12	1.99	0.62
2:B:453:ALA:HB3	2:B:456:GLU:HB3	1.82	0.61
2:B:491:LYS:HD2	2:B:529:THR:HG22	1.82	0.61
6:F:208:TYR:OH	6:F:262:ASN:O	2.18	0.61
7:G:73:CYS:HB2	7:G:81:LEU:HD21	1.80	0.61
2:B:474:THR:HG23	2:B:477:ASP:HB2	1.82	0.61
6:F:322:ARG:O	6:F:322:ARG:NH1	2.33	0.61
2:B:220:MET:SD	2:B:220:MET:N	2.73	0.61
6:F:179:THR:HA	6:F:182:VAL:HG12	1.82	0.61
1:A:523:ASN:ND2	3:C:210:MET:O	2.34	0.61
2:B:289:GLU:HB2	2:B:295:LEU:HD11	1.83	0.60
2:B:67:ILE:HD11	9:I:1198:PHE:HB2	1.82	0.60
2:B:113:LEU:HD23	9:I:686:MET:HE3	1.81	0.60
7:G:61:PRO:O	7:G:97:ARG:NH1	2.34	0.60
2:B:722:ILE:HD11	2:B:732:LEU:HD11	1.83	0.60
1:A:33:ASN:ND2	1:A:36:GLU:OE2	2.35	0.60
1:A:1196:ILE:HG23	1:A:1208:ILE:HG21	1.84	0.60
1:A:1305:LEU:HA	4:D:5:LYS:HD2	1.84	0.60
6:F:176:LEU:O	6:F:179:THR:HG22	2.02	0.60
2:B:522:ARG:NH2	2:B:572:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1057:VAL:HB	8:H:47:LEU:HG	1.83	0.60
6:F:182:VAL:HA	6:F:185:ILE:HG22	1.84	0.59
2:B:866:ILE:HB	2:B:1027:ILE:HB	1.84	0.59
3:C:236:ARG:HG3	3:C:358:ILE:HB	1.84	0.59
9:I:932:PHE:O	9:I:936:ARG:NH1	2.30	0.59
1:A:904:ASP:HB3	1:A:1000:MET:HG3	1.83	0.59
2:B:203:ASP:N	2:B:505:SER:O	2.28	0.59
2:B:821:MET:HB2	2:B:884:GLU:HG3	1.83	0.59
1:A:353:THR:O	1:A:358:ASN:ND2	2.29	0.59
2:B:432:ILE:HG22	2:B:478:LEU:HD12	1.85	0.59
1:A:844:VAL:HB	1:A:852:GLN:HB2	1.85	0.59
2:B:420:GLY:O	2:B:422:GLY:N	2.35	0.59
2:B:452:THR:HG23	2:B:456:GLU:HG2	1.84	0.59
9:I:792:ALA:HB3	9:I:795:PHE:HB2	1.84	0.59
2:B:493:ILE:HD13	2:B:502:ASN:HB2	1.84	0.59
6:F:180:LYS:HA	6:F:180:LYS:HE2	1.84	0.59
2:B:221:GLN:HA	2:B:224:ASN:HD21	1.67	0.59
1:A:208:ILE:O	1:A:302:ARG:NH2	2.36	0.59
1:A:493:SER:OG	1:A:1349:ASN:ND2	2.36	0.59
6:F:217:ILE:HD12	6:F:218:LEU:HD23	1.85	0.59
1:A:1187:LEU:HG	1:A:1188:LYS:HG2	1.84	0.58
2:B:404:VAL:HG12	2:B:405:PHE:HD1	1.67	0.58
2:B:994:ASP:OD2	2:B:1110:ARG:NH2	2.36	0.58
4:D:204:LYS:HG2	4:D:205:ILE:HG13	1.86	0.58
1:A:332:ASP:OD2	2:B:859:TYR:OH	2.21	0.58
2:B:205:LEU:HD23	2:B:505:SER:HB2	1.86	0.58
3:C:284:LYS:HD2	3:C:318:GLU:HB3	1.84	0.58
2:B:40:ILE:HG13	2:B:189:PRO:HG3	1.85	0.58
2:B:326:GLU:HG3	2:B:328:ASN:H	1.67	0.58
9:I:918:THR:OG1	9:I:921:LYS:NZ	2.37	0.58
2:B:491:LYS:HB3	2:B:529:THR:HA	1.86	0.58
8:H:48:GLN:HB2	9:I:821:PHE:N	2.08	0.58
1:A:448:VAL:HG11	2:B:861:GLN:HB3	1.86	0.57
2:B:242:ASN:OD1	2:B:242:ASN:N	2.31	0.57
9:I:106:ARG:NH2	9:I:119:VAL:O	2.37	0.57
1:A:1204:PRO:HD2	1:A:1205:ASN:N	2.19	0.57
9:I:92:VAL:HG22	9:I:125:ILE:HG21	1.85	0.57
3:C:9:GLU:HG3	3:C:11:LYS:HE2	1.87	0.57
4:D:34:MET:O	4:D:38:THR:OG1	2.22	0.57
6:F:195:LYS:HB2	6:F:200:ILE:HD11	1.87	0.57
6:F:209:THR:OG1	6:F:261:PRO:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:263:LEU:HD11	6:F:271:TYR:CE2	2.39	0.57
7:G:1:MET:HE3	7:G:3:ILE:HD13	1.85	0.57
2:B:404:VAL:HA	7:G:52:LYS:HD2	1.85	0.57
6:F:263:LEU:HD11	6:F:271:TYR:HE2	1.70	0.57
1:A:798:SER:HB2	2:B:775:PRO:HB3	1.85	0.57
1:A:1015:THR:HG23	1:A:1018:GLN:H	1.69	0.57
2:B:301:VAL:HG22	2:B:305:MET:HE3	1.85	0.57
3:C:305:ILE:HD11	3:C:323:ILE:HG23	1.86	0.57
4:D:101:ASN:O	4:D:105:ILE:HG12	2.03	0.57
1:A:1240:MET:SD	1:A:1240:MET:N	2.78	0.57
2:B:251:MET:HE1	2:B:269:ARG:HH21	1.70	0.57
2:B:343:PHE:HA	9:I:1196:GLU:HG3	1.87	0.57
2:B:650:THR:HB	2:B:663:TRP:HB2	1.87	0.57
1:A:1011:THR:HG22	1:A:1014:ILE:HD12	1.85	0.57
2:B:82:ARG:HB2	2:B:140:TYR:CD2	2.40	0.57
2:B:255:ALA:HB2	2:B:315:VAL:HG11	1.87	0.57
2:B:296:GLU:OE1	2:B:609:ARG:NH2	2.38	0.57
2:B:934:ILE:HG23	2:B:982:MET:HE3	1.86	0.57
6:F:171:THR:HG22	6:F:174:GLN:HG3	1.87	0.57
1:A:431:HIS:NE2	1:A:454:TYR:OH	2.29	0.57
4:D:58:PHE:O	4:D:123:TYR:OH	2.21	0.56
4:D:180:ASP:HB3	4:D:200:ILE:HD12	1.87	0.56
1:A:300:MET:HE1	1:A:1395:LEU:HD23	1.86	0.56
2:B:509:LEU:HD11	2:B:517:THR:HG23	1.86	0.56
1:A:168:GLN:HE22	1:A:245:GLN:HA	1.70	0.56
2:B:404:VAL:HG12	2:B:405:PHE:CD1	2.40	0.56
6:F:204:GLU:HG3	6:F:264:LEU:HD21	1.87	0.56
2:B:573:ILE:HG23	2:B:574:THR:HG23	1.86	0.56
2:B:830:GLU:HG2	8:H:73:THR:HA	1.87	0.56
9:I:106:ARG:NH2	9:I:120:PRO:O	2.39	0.56
1:A:377:SER:HA	1:A:390:ILE:HB	1.88	0.56
1:A:383:ILE:HG13	1:A:384:THR:HG23	1.88	0.56
1:A:1177:ARG:HG3	1:A:1224:ARG:HG2	1.87	0.56
2:B:700:ASP:OD1	2:B:700:ASP:N	2.36	0.56
2:B:904:THR:HG23	2:B:907:LEU:HD13	1.88	0.56
3:C:113:LEU:HD21	3:C:125:ILE:HG21	1.87	0.56
4:D:75:LEU:O	4:D:79:LEU:HG	2.05	0.56
9:I:221:ARG:HG2	9:I:221:ARG:HH11	1.71	0.56
1:A:959:GLN:NE2	1:A:1016:CYS:SG	2.78	0.56
1:A:1300:ILE:HB	1:A:1325:LEU:HG	1.87	0.56
2:B:600:ALA:HB1	9:I:1060:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:ARG:HH21	5:E:24:GLU:HG2	1.71	0.56
2:B:77:GLU:HA	2:B:80:LYS:HD2	1.88	0.56
9:I:695:ARG:NH2	9:I:703:HIS:O	2.39	0.56
1:A:336:ASP:OD1	1:A:432:ARG:NH2	2.37	0.55
2:B:913:TYR:OH	2:B:952:ASP:OD2	2.19	0.55
6:F:320:ILE:O	6:F:327:TRP:NE1	2.27	0.55
2:B:69:TYR:OH	2:B:442:ILE:HG23	2.07	0.55
2:B:498:ARG:NH2	9:I:1209:ASP:OD1	2.39	0.55
9:I:1239:SER:HB3	9:I:1242:VAL:HG22	1.88	0.55
1:A:599:ILE:HD12	1:A:600:GLU:HG2	1.87	0.55
1:A:1120:ILE:HG23	1:A:1124:ARG:HD3	1.89	0.55
1:A:1120:ILE:HG23	1:A:1124:ARG:HH11	1.70	0.55
2:B:988:ARG:NH2	2:B:1117:ASP:OD1	2.36	0.55
2:B:40:ILE:HG21	2:B:189:PRO:HB2	1.87	0.55
1:A:425:ARG:NH2	1:A:1039:GLU:OE2	2.36	0.55
2:B:301:VAL:HG23	2:B:402:MET:SD	2.47	0.55
2:B:531:ASN:ND2	9:I:1221:GLU:O	2.39	0.55
9:I:179:GLU:O	9:I:182:LYS:NZ	2.31	0.55
3:C:81:GLU:HG2	3:C:82:ASP:H	1.72	0.55
5:E:126:THR:HB	5:E:130:GLN:HB3	1.87	0.55
1:A:1371:LYS:HD3	1:A:1388:LEU:HD23	1.88	0.55
2:B:512:LYS:HD2	2:B:806:GLN:HA	1.90	0.54
5:E:83:ARG:HD3	5:E:116:PRO:HD2	1.89	0.54
1:A:1170:ASP:HB2	1:A:1229:GLU:HG2	1.88	0.54
2:B:200:TRP:CE2	2:B:487:ILE:HG13	2.42	0.54
1:A:100:LEU:O	1:A:176:ARG:NH1	2.38	0.54
1:A:1311:PRO:HB2	4:D:128:ILE:HD12	1.88	0.54
2:B:277:ARG:HB2	2:B:282:THR:HG22	1.89	0.54
2:B:768:ARG:NH2	7:G:68:GLN:HE22	2.05	0.54
9:I:124:PRO:HD2	9:I:124:PRO:O	2.08	0.54
2:B:231:GLU:HG3	9:I:1219:PHE:CE1	2.43	0.54
2:B:796:ARG:HG3	2:B:1038:THR:HG22	1.90	0.54
9:I:1233:ILE:HG23	9:I:1236:VAL:HB	1.88	0.54
1:A:70:MET:HG2	2:B:1217:ILE:HG21	1.90	0.54
2:B:278:MET:HE2	2:B:332:ILE:HG22	1.89	0.54
2:B:281:MET:HG2	2:B:281:MET:O	2.08	0.54
2:B:866:ILE:HG23	2:B:1008:LEU:HB3	1.91	0.54
9:I:132:LEU:HD22	9:I:173:MET:HG3	1.90	0.54
3:C:265:PRO:HD2	3:C:266:GLU:OE2	2.08	0.53
6:F:241:SER:HA	6:F:244:TYR:HD1	1.71	0.53
9:I:695:ARG:NE	9:I:702:MET:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:ASN:HB3	2:B:952:ASP:H	1.72	0.53
6:F:204:GLU:CG	6:F:264:LEU:HD21	2.37	0.53
9:I:1019:LYS:HD2	9:I:1150:LEU:HD21	1.89	0.53
1:A:65:GLN:O	1:A:67:LYS:N	2.41	0.53
2:B:236:PRO:HG3	2:B:374:PRO:HB2	1.90	0.53
9:I:966:GLN:HB2	9:I:967:PRO:HD3	1.90	0.53
1:A:997:LEU:HD13	4:D:192:MET:HB2	1.90	0.53
2:B:93:ASP:HB3	2:B:131:ALA:HB3	1.90	0.53
2:B:797:VAL:O	2:B:801:THR:HG23	2.08	0.53
5:E:123:ILE:O	5:E:124:LYS:HB2	2.09	0.53
1:A:330:ASN:ND2	1:A:445:GLN:OE1	2.41	0.53
8:H:29:ILE:CD1	8:H:49:ILE:HD13	2.39	0.53
9:I:884:ILE:HG23	9:I:885:LYS:HD2	1.90	0.53
1:A:1386:MET:HG2	1:A:1394:VAL:HG23	1.89	0.53
1:A:276:SER:O	1:A:280:THR:OG1	2.19	0.53
1:A:714:ARG:NH1	9:I:905:GLN:HE22	2.07	0.53
1:A:973:TYR:OH	1:A:985:THR:O	2.26	0.53
1:A:1383:LEU:H	1:A:1405:ASN:ND2	2.06	0.53
5:E:67:THR:OG1	5:E:134:GLU:OE1	2.24	0.53
1:A:892:PRO:HA	1:A:895:GLU:HG2	1.90	0.53
1:A:1057:MET:SD	1:A:1057:MET:N	2.81	0.53
8:H:68:THR:O	8:H:72:THR:OG1	2.18	0.53
1:A:862:ALA:HB2	1:A:1351:ARG:HD2	1.90	0.53
2:B:382:THR:O	2:B:386:LYS:HG3	2.09	0.53
4:D:75:LEU:HD13	4:D:109:GLN:HG3	1.91	0.53
1:A:430:VAL:HB	1:A:482:SER:HA	1.91	0.52
2:B:344:VAL:HA	9:I:1194:PHE:HB3	1.91	0.52
9:I:83:LEU:HD12	9:I:107:LYS:HE3	1.91	0.52
2:B:829:ASN:ND2	2:B:845:ASN:HA	2.24	0.52
2:B:937:VAL:HG23	2:B:940:ILE:HD11	1.91	0.52
6:F:324:GLU:HA	6:F:327:TRP:CD1	2.43	0.52
7:G:52:LYS:HE3	7:G:53:TYR:CZ	2.44	0.52
1:A:86:LEU:HD21	1:A:300:MET:HE2	1.90	0.52
1:A:320:TRP:CE2	2:B:1135:PRO:HG3	2.44	0.52
1:A:1019:MET:HE3	1:A:1019:MET:HA	1.90	0.52
2:B:829:ASN:ND2	2:B:844:PRO:O	2.39	0.52
2:B:1059:ASP:OD1	2:B:1061:THR:OG1	2.25	0.52
3:C:110:VAL:H	3:C:134:ALA:HB3	1.74	0.52
6:F:191:SER:OG	6:F:308:ASN:ND2	2.43	0.52
1:A:171:ARG:HB2	1:A:197:VAL:HG11	1.92	0.52
1:A:414:VAL:HG11	1:A:478:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:SER:OG	2:B:375:HIS:ND1	2.41	0.52
4:D:17:ARG:HB2	4:D:19:MET:HE2	1.92	0.52
4:D:146:GLU:HA	4:D:149:GLU:HG2	1.91	0.52
9:I:132:LEU:HB2	9:I:199:PHE:HZ	1.75	0.52
2:B:644:VAL:HG23	2:B:645:VAL:HG23	1.91	0.52
9:I:955:LEU:HD13	9:I:963:HIS:CE1	2.44	0.52
6:F:220:LEU:HD11	6:F:229:LYS:HG2	1.92	0.52
9:I:1090:ASN:OD1	9:I:1091:LYS:N	2.43	0.52
1:A:502:ASP:OD2	2:B:861:GLN:HG3	2.10	0.51
2:B:460:ARG:NH2	2:B:464:GLU:HG2	2.24	0.51
6:F:105:LEU:HD23	6:F:105:LEU:H	1.75	0.51
6:F:185:ILE:HD13	6:F:301:ILE:HD13	1.92	0.51
9:I:172:PHE:O	9:I:202:GLN:NE2	2.41	0.51
9:I:223:ALA:O	9:I:227:VAL:HG13	2.11	0.51
9:I:866:ALA:HB2	9:I:874:ALA:HA	1.92	0.51
9:I:885:LYS:HD2	9:I:885:LYS:N	2.26	0.51
1:A:1193:GLU:O	1:A:1197:ASN:ND2	2.34	0.51
1:A:311:ARG:HH22	9:I:1235:ASP:HA	1.75	0.51
1:A:1134:GLU:OE2	1:A:1224:ARG:NH2	2.40	0.51
2:B:921:VAL:HG21	2:B:933:ILE:HG22	1.92	0.51
2:B:1057:VAL:H	8:H:47:LEU:HD12	1.74	0.51
6:F:298:LYS:HA	6:F:301:ILE:HG12	1.92	0.51
9:I:1162:VAL:HG12	9:I:1166:ARG:HD2	1.90	0.51
1:A:363:MET:HE3	1:A:363:MET:HA	1.92	0.51
2:B:69:TYR:O	2:B:85:VAL:N	2.43	0.51
2:B:359:TYR:OH	9:I:1200:CYS:O	2.24	0.51
1:A:315:LEU:HD11	1:A:1387:ALA:HB1	1.93	0.51
2:B:819:VAL:HG13	2:B:983:ARG:HB2	1.91	0.51
3:C:276:LYS:HG3	3:C:326:LYS:HD3	1.93	0.51
9:I:832:ALA:O	9:I:834:GLN:NE2	2.44	0.51
2:B:965:VAL:HG22	2:B:984:LEU:HD23	1.91	0.51
9:I:895:ASP:OD2	9:I:904:LEU:HB3	2.11	0.51
9:I:903:VAL:HG11	9:I:911:LEU:HD21	1.93	0.51
1:A:752:ILE:HB	1:A:788:ILE:HB	1.92	0.51
9:I:686:MET:N	9:I:686:MET:SD	2.83	0.51
9:I:1023:THR:HG23	9:I:1149:PHE:CD2	2.45	0.51
1:A:419:ARG:HD3	1:A:456:ALA:HB2	1.92	0.51
3:C:107:GLU:OE2	3:C:167:LYS:NZ	2.39	0.51
4:D:193:HIS:ND1	4:D:193:HIS:O	2.44	0.51
7:G:49:MET:HE1	7:G:57:ILE:HD11	1.92	0.51
1:A:1094:MET:HE2	1:A:1096:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:THR:HA	1:A:601:GLY:HA3	1.94	0.50
1:A:591:THR:OG1	1:A:602:VAL:O	2.25	0.50
1:A:829:ALA:HA	1:A:1369:LEU:HD13	1.94	0.50
1:A:1225:ILE:HD12	1:A:1225:ILE:O	2.11	0.50
2:B:170:HIS:ND1	9:I:788:TYR:OH	2.37	0.50
2:B:995:LYS:HG2	2:B:1111:LEU:HD12	1.92	0.50
5:E:115:ILE:O	5:E:139:ARG:NH1	2.44	0.50
1:A:320:TRP:O	2:B:1167:LYS:NZ	2.44	0.50
1:A:1371:LYS:NZ	1:A:1389:SER:O	2.45	0.50
1:A:1433:GLU:HG2	6:F:23:VAL:HG21	1.93	0.50
9:I:1098:ARG:O	9:I:1101:LYS:HD2	2.11	0.50
1:A:502:ASP:HB2	2:B:861:GLN:CD	2.36	0.50
1:A:645:ARG:HG2	2:B:1090:ASN:ND2	2.26	0.50
2:B:503:ARG:NH2	9:I:1216:PRO:HA	2.26	0.50
1:A:1204:PRO:HD2	1:A:1205:ASN:H	1.77	0.50
6:F:287:CYS:SG	6:F:292:MET:HE1	2.51	0.50
3:C:332:LEU:O	3:C:336:LEU:HG	2.10	0.50
6:F:118:GLU:HG3	6:F:121:ASN:HD21	1.75	0.50
6:F:233:ARG:NH1	6:F:234:LEU:H	2.09	0.50
8:H:25:ARG:O	8:H:29:ILE:HG12	2.11	0.50
9:I:92:VAL:HG12	9:I:94:GLU:H	1.77	0.50
1:A:417:PHE:CZ	1:A:463:MET:HE2	2.47	0.50
1:A:815:LYS:NZ	9:I:1248:PRO:HD3	2.27	0.50
1:A:1390:SER:O	1:A:1394:VAL:HG22	2.11	0.50
2:B:46:SER:OG	2:B:421:SER:OG	2.29	0.50
2:B:334:GLN:NE2	2:B:357:VAL:HG13	2.26	0.50
2:B:514:LEU:HD23	2:B:843:ILE:HD11	1.94	0.50
2:B:402:MET:HB3	2:B:404:VAL:HG23	1.94	0.50
9:I:85:ASP:O	9:I:107:LYS:NZ	2.43	0.50
2:B:874:ARG:NE	8:H:8:PHE:O	2.38	0.49
6:F:27:LEU:HD13	6:F:70:MET:HE3	1.93	0.49
6:F:164:TYR:N	6:F:257:TRP:O	2.42	0.49
8:H:47:LEU:C	9:I:822:TYR:HB2	2.37	0.49
1:A:1313:THR:O	1:A:1313:THR:HG22	2.12	0.49
2:B:85:VAL:HB	2:B:454:PHE:CE2	2.47	0.49
2:B:670:THR:HG22	2:B:742:THR:HG23	1.93	0.49
2:B:1190:ASN:HB3	2:B:1195:ILE:HG22	1.94	0.49
3:C:82:ASP:HB3	9:I:704:LYS:HD3	1.95	0.49
6:F:197:PHE:HA	6:F:200:ILE:HD13	1.94	0.49
4:D:29:ASP:N	4:D:29:ASP:OD1	2.45	0.49
6:F:25:ALA:O	6:F:29:LYS:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:ALA:HA	2:B:472:LYS:HE2	1.94	0.49
3:C:110:VAL:HB	3:C:134:ALA:HB2	1.95	0.49
2:B:796:ARG:NH1	9:I:1249:GLN:OXT	2.38	0.49
4:D:166:ALA:HB3	4:D:203:SER:HB2	1.94	0.49
6:F:46:LEU:N	6:F:77:VAL:O	2.35	0.49
2:B:67:ILE:HG21	2:B:442:ILE:HD12	1.95	0.49
2:B:292:VAL:HG23	2:B:294:ASP:H	1.76	0.49
2:B:368:LEU:HA	2:B:371:ILE:HG22	1.93	0.49
2:B:491:LYS:O	2:B:501:VAL:HG23	2.13	0.49
2:B:1144:GLY:O	2:B:1145:LEU:HB2	2.13	0.49
1:A:92:ARG:HB2	1:A:154:PHE:HZ	1.77	0.49
1:A:860:LEU:HD21	1:A:1030:TYR:HE1	1.77	0.49
2:B:742:THR:HG22	2:B:743:PRO:HD2	1.94	0.49
6:F:9:THR:OG1	6:F:35:TYR:OH	2.25	0.49
1:A:380:TYR:HB3	1:A:404:ILE:HB	1.94	0.49
2:B:445:PHE:HE2	2:B:466:PHE:HD2	1.59	0.49
1:A:580:PRO:O	9:I:864:TYR:OH	2.21	0.49
1:A:1382:VAL:O	1:A:1386:MET:HG3	2.13	0.49
2:B:616:PHE:CE2	2:B:621:TRP:HB2	2.47	0.49
3:C:61:VAL:HG21	3:C:246:ILE:HG12	1.95	0.49
3:C:12:PRO:HA	3:C:41:VAL:HA	1.95	0.49
9:I:94:GLU:OE2	9:I:94:GLU:N	2.46	0.49
1:A:1131:LEU:HD13	1:A:1176:ILE:HG12	1.96	0.48
1:A:1225:ILE:HD12	1:A:1225:ILE:C	2.38	0.48
9:I:684:ASP:HB3	9:I:686:MET:SD	2.53	0.48
3:C:5:PHE:CE1	3:C:45:MET:HB3	2.49	0.48
1:A:1410:ILE:HG12	2:B:1156:THR:HG21	1.95	0.48
3:C:319:MET:HE3	3:C:319:MET:HB3	1.74	0.48
8:H:45:ALA:HA	9:I:821:PHE:HA	1.95	0.48
9:I:1037:ILE:HB	9:I:1142:ILE:HD11	1.94	0.48
2:B:599:LEU:HD11	2:B:621:TRP:O	2.14	0.48
2:B:904:THR:HG23	2:B:907:LEU:HB2	1.94	0.48
2:B:1056:VAL:HA	8:H:47:LEU:HD11	1.96	0.48
3:C:101:PRO:HD2	3:C:147:PHE:CZ	2.49	0.48
1:A:1006:LEU:HD22	1:A:1019:MET:HE1	1.95	0.48
3:C:38:LEU:HB2	3:C:144:ASN:ND2	2.29	0.48
3:C:45:MET:HE1	3:C:239:LEU:HD21	1.96	0.48
6:F:166:VAL:HG11	6:F:289:ALA:HB2	1.96	0.48
9:I:1016:ASP:OD2	9:I:1019:LYS:NZ	2.37	0.48
2:B:337:SER:HB3	2:B:364:GLN:HB2	1.96	0.48
2:B:401:ILE:HD13	2:B:401:ILE:HA	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:ARG:HD3	2:B:701:TRP:CD1	2.49	0.48
3:C:178:LEU:O	3:C:224:PRO:HD3	2.14	0.48
1:A:580:PRO:HA	9:I:883:VAL:HG11	1.96	0.48
1:A:988:PRO:HD2	1:A:991:LEU:HD12	1.96	0.48
2:B:222:GLN:HB3	9:I:1226:ARG:NH1	2.29	0.48
3:C:257:TYR:HD2	3:C:340:ILE:HD12	1.78	0.48
1:A:833:LEU:HG	1:A:1359:LEU:HD22	1.96	0.47
2:B:1089:PHE:HA	2:B:1096:TYR:HA	1.96	0.47
3:C:189:ILE:HD11	3:C:214:PRO:HB3	1.95	0.47
4:D:56:PHE:CE2	4:D:74:LEU:HD21	2.48	0.47
9:I:229:ARG:HH12	9:I:230:LYS:HB2	1.79	0.47
2:B:263:THR:HG23	9:I:1209:ASP:H	1.79	0.47
2:B:359:TYR:HA	9:I:1186:PRO:HG3	1.96	0.47
6:F:182:VAL:O	6:F:186:GLU:HG3	2.14	0.47
9:I:871:GLN:HG3	9:I:873:PRO:HD2	1.95	0.47
1:A:31:ILE:HG13	1:A:33:ASN:H	1.79	0.47
1:A:1128:GLN:NE2	1:A:1179:GLU:OE1	2.47	0.47
6:F:164:TYR:HB3	6:F:292:MET:HG3	1.97	0.47
7:G:14:THR:HG22	7:G:14:THR:O	2.14	0.47
8:H:47:LEU:O	9:I:822:TYR:HB2	2.14	0.47
1:A:235:ARG:HA	1:A:238:LEU:HD12	1.96	0.47
1:A:1133:TYR:OH	7:G:17:ASP:O	2.32	0.47
2:B:376:MET:HB3	2:B:386:LYS:HG2	1.96	0.47
4:D:14:ILE:HD13	4:D:45:ALA:HB2	1.96	0.47
1:A:305:ARG:HG3	1:A:305:ARG:HH11	1.78	0.47
2:B:227:ILE:HD11	2:B:252:THR:HA	1.96	0.47
4:D:37:ASN:ND2	4:D:38:THR:HG23	2.30	0.47
1:A:189:LYS:NZ	5:E:43:PRO:HD2	2.29	0.47
2:B:367:ILE:O	2:B:371:ILE:HG22	2.14	0.47
2:B:860:ASN:OD1	2:B:860:ASN:N	2.47	0.47
4:D:188:SER:HB3	4:D:193:HIS:H	1.78	0.47
9:I:143:MET:HE1	9:I:226:MET:HB2	1.96	0.47
9:I:879:THR:HG22	9:I:880:ARG:H	1.80	0.47
1:A:14:ASN:O	2:B:1229:ASN:N	2.38	0.47
1:A:644:VAL:HG11	2:B:855:ILE:HD12	1.97	0.47
1:A:665:GLU:HG2	1:A:718:PRO:HG3	1.97	0.47
1:A:720:MET:HA	1:A:720:MET:HE2	1.97	0.47
1:A:777:ARG:NH2	7:G:65:THR:OG1	2.47	0.47
2:B:1087:LYS:HG3	3:C:203:SER:HB2	1.96	0.47
6:F:14:ASP:HA	6:F:67:ARG:HD2	1.97	0.47
6:F:178:LEU:O	6:F:182:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1397:ASP:HA	1:A:1400:VAL:HG22	1.97	0.47
2:B:365:LEU:HD23	2:B:365:LEU:HA	1.79	0.47
4:D:19:MET:HG2	4:D:47:THR:HG22	1.97	0.47
1:A:725:PRO:HB3	1:A:731:PHE:CE2	2.50	0.47
6:F:158:LYS:O	6:F:160:THR:N	2.39	0.47
9:I:806:GLU:O	9:I:810:GLY:N	2.45	0.47
1:A:276:SER:HB2	5:E:19:VAL:HA	1.97	0.47
1:A:428:ILE:O	2:B:1158:GLN:NE2	2.39	0.47
1:A:669:ILE:HG12	1:A:714:ARG:NH2	2.30	0.47
2:B:208:ILE:HD11	2:B:233:ILE:HD12	1.97	0.47
2:B:874:ARG:HG2	3:C:99:PHE:CE2	2.50	0.47
3:C:151:PHE:CZ	8:H:76:TYR:HB3	2.50	0.47
1:A:379:VAL:HG22	1:A:405:LEU:HD12	1.96	0.46
6:F:41:LYS:NZ	9:I:148:ILE:O	2.39	0.46
7:G:13:ARG:HD3	7:G:15:TYR:OH	2.16	0.46
8:H:47:LEU:HD22	8:H:49:ILE:HD11	1.97	0.46
1:A:851:VAL:HG22	1:A:1362:ARG:HD2	1.98	0.46
2:B:358:GLN:HB3	9:I:1186:PRO:HB3	1.97	0.46
4:D:1:MET:CE	4:D:3:MET:H	2.28	0.46
6:F:41:LYS:HD2	9:I:150:SER:HB2	1.98	0.46
9:I:826:ASP:HB2	9:I:833:ASP:HA	1.97	0.46
1:A:645:ARG:HG2	2:B:1090:ASN:HD21	1.79	0.46
6:F:90:VAL:HG11	6:F:112:ILE:HG21	1.97	0.46
6:F:179:THR:HA	6:F:182:VAL:CG1	2.45	0.46
1:A:164:LYS:HE3	1:A:164:LYS:HB2	1.83	0.46
1:A:555:VAL:HA	1:A:558:MET:HG3	1.98	0.46
2:B:1223:MET:HB3	2:B:1230:ILE:HD11	1.96	0.46
5:E:12:ASP:OD1	5:E:13:ASP:N	2.45	0.46
7:G:70:LYS:NZ	7:G:79:ASP:HB3	2.30	0.46
2:B:437:VAL:HA	2:B:470:LEU:HD21	1.96	0.46
2:B:513:ASN:HA	2:B:811:TYR:HA	1.98	0.46
2:B:718:MET:HB3	2:B:727:LEU:HD22	1.97	0.46
6:F:60:MET:HE3	6:F:67:ARG:HB2	1.98	0.46
1:A:302:ARG:O	1:A:309:ARG:N	2.45	0.46
2:B:42:TYR:HE1	2:B:204:LEU:HD21	1.81	0.46
6:F:112:ILE:HG12	6:F:132:VAL:HG11	1.97	0.46
6:F:265:LYS:HD3	6:F:265:LYS:HA	1.62	0.46
8:H:23:LYS:HB3	8:H:23:LYS:NZ	2.28	0.46
9:I:93:SER:O	9:I:95:LYS:N	2.49	0.46
1:A:909:ARG:NH1	1:A:1282:GLY:O	2.42	0.46
1:A:1135:THR:HB	1:A:1173:ASN:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ASP:OD1	2:B:72:GLN:N	2.45	0.46
2:B:900:ASP:OD2	2:B:902:LEU:HB2	2.16	0.46
9:I:1079:ASN:HB2	9:I:1172:GLU:OE2	2.16	0.46
1:A:24:GLN:NE2	2:B:1185:GLU:OE2	2.48	0.46
1:A:748:ILE:HA	1:A:792:TYR:HB2	1.96	0.46
2:B:70:LYS:HB2	2:B:70:LYS:HE2	1.76	0.46
4:D:71:MET:HE3	4:D:71:MET:O	2.16	0.46
1:A:305:ARG:HG3	1:A:305:ARG:NH1	2.31	0.46
2:B:262:SER:OG	2:B:263:THR:N	2.48	0.46
2:B:1223:MET:HE3	2:B:1230:ILE:HG12	1.98	0.46
3:C:274:GLU:C	3:C:276:LYS:H	2.23	0.46
1:A:12:GLN:OE1	1:A:14:ASN:ND2	2.38	0.45
1:A:1375:ASN:HD21	5:E:24:GLU:HG3	1.81	0.45
2:B:920:PHE:CD2	2:B:934:ILE:HG22	2.51	0.45
6:F:259:ARG:NH2	6:F:265:LYS:O	2.47	0.45
9:I:209:PHE:CZ	9:I:215:HIS:HB2	2.51	0.45
9:I:1233:ILE:O	9:I:1233:ILE:HG22	2.17	0.45
1:A:83:LEU:HD22	1:A:91:ILE:HD13	1.98	0.45
1:A:389:ASP:OD1	1:A:390:ILE:N	2.49	0.45
2:B:225:ASN:N	2:B:225:ASN:OD1	2.50	0.45
2:B:1180:CYS:C	2:B:1182:ASN:H	2.23	0.45
4:D:3:MET:HG3	4:D:31:PHE:CE2	2.51	0.45
1:A:310:ILE:HG21	1:A:1387:ALA:HA	1.98	0.45
2:B:1161:MET:SD	2:B:1161:MET:N	2.88	0.45
4:D:55:VAL:HG22	4:D:89:ILE:HD12	1.98	0.45
1:A:301:ARG:HD2	1:A:301:ARG:HA	1.77	0.45
2:B:860:ASN:HA	2:B:864:SER:HB2	1.98	0.45
1:A:1120:ILE:HD13	1:A:1260:ARG:HE	1.80	0.45
2:B:940:ILE:HA	2:B:950:TYR:CE1	2.52	0.45
4:D:46:GLU:OE2	4:D:50:HIS:ND1	2.44	0.45
9:I:145:MET:HA	9:I:148:ILE:HD12	1.99	0.45
3:C:215:ARG:NH1	3:C:300:GLU:OE2	2.47	0.45
1:A:340:TYR:CE1	1:A:465:LEU:HD22	2.52	0.45
2:B:195:ALA:HB1	2:B:483:GLU:HG2	1.99	0.45
2:B:822:ASN:HA	2:B:881:PHE:CZ	2.52	0.45
3:C:92:PHE:O	3:C:96:ARG:HG2	2.17	0.45
1:A:361:ARG:O	1:A:364:PRO:HD2	2.17	0.45
2:B:142:ASN:OD1	2:B:144:ARG:HG3	2.17	0.45
2:B:867:VAL:HG22	2:B:1026:LEU:HD22	1.99	0.45
2:B:1008:LEU:HD12	2:B:1008:LEU:HA	1.81	0.45
5:E:76:ALA:HB1	5:E:146:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:171:THR:HG23	6:F:173:GLU:H	1.82	0.45
6:F:310:LEU:HD23	6:F:310:LEU:HA	1.82	0.45
9:I:221:ARG:HG2	9:I:221:ARG:NH1	2.32	0.45
2:B:85:VAL:HB	2:B:454:PHE:HE2	1.81	0.45
6:F:328:MET:SD	6:F:329:LEU:N	2.89	0.45
1:A:370:LYS:HG3	1:A:377:SER:HB3	1.98	0.45
1:A:1190:ILE:N	1:A:1190:ILE:HD12	2.32	0.45
2:B:69:TYR:HB2	2:B:85:VAL:HG13	1.98	0.45
2:B:234:SER:HB3	2:B:374:PRO:HD2	1.99	0.45
2:B:368:LEU:HA	2:B:368:LEU:HD23	1.80	0.45
2:B:209:ARG:NE	2:B:212:THR:OG1	2.45	0.44
2:B:263:THR:HB	2:B:264:LYS:HD2	1.99	0.44
2:B:680:ILE:HD12	2:B:680:ILE:HA	1.84	0.44
3:C:267:LEU:HD13	3:C:281:ILE:HG13	1.98	0.44
9:I:895:ASP:HB3	9:I:906:HIS:CD2	2.52	0.44
1:A:93:ARG:HH11	1:A:121:LEU:HD12	1.82	0.44
1:A:119:LYS:HG2	1:A:123:GLU:HG3	2.00	0.44
2:B:343:PHE:HB3	9:I:1198:PHE:CE1	2.52	0.44
2:B:1083:ASN:ND2	2:B:1085:CYS:SG	2.90	0.44
6:F:28:LEU:HD21	6:F:50:GLY:HA2	1.99	0.44
6:F:242:PHE:HA	6:F:245:ASP:OD2	2.16	0.44
9:I:777:ILE:HG21	9:I:809:TYR:CE2	2.52	0.44
9:I:1027:LEU:O	9:I:1029:ILE:HG23	2.18	0.44
1:A:381:LYS:O	1:A:385:GLN:N	2.49	0.44
1:A:1433:GLU:CD	6:F:54:ARG:HH22	2.25	0.44
2:B:85:VAL:HG11	2:B:449:LEU:HD13	1.99	0.44
2:B:448:LEU:HD21	2:B:457:LEU:HD21	1.98	0.44
3:C:5:PHE:HE1	3:C:45:MET:HB3	1.82	0.44
6:F:304:LEU:O	6:F:307:ILE:HG13	2.17	0.44
9:I:1076:PHE:HZ	9:I:1152:LEU:HD22	1.82	0.44
9:I:1206:SER:OG	9:I:1207:MET:HE3	2.17	0.44
2:B:710:GLN:NE2	2:B:767:ARG:O	2.51	0.44
3:C:195:ASP:OD1	3:C:195:ASP:N	2.42	0.44
1:A:640:ALA:O	1:A:644:VAL:HG23	2.17	0.44
1:A:1361:THR:O	4:D:198:ARG:NH2	2.44	0.44
2:B:42:TYR:OH	2:B:522:ARG:HA	2.18	0.44
2:B:501:VAL:HG11	2:B:503:ARG:CZ	2.48	0.44
2:B:966:ASP:OD2	2:B:985:ARG:NE	2.42	0.44
6:F:88:ALA:HA	6:F:131:PRO:HB3	1.99	0.44
6:F:88:ALA:HB1	6:F:310:LEU:HG	2.00	0.44
1:A:330:ASN:HB2	1:A:445:GLN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:GLU:HG2	2:B:794:PRO:HB3	1.98	0.44
2:B:70:LYS:HE3	9:I:1192:MET:HA	1.99	0.44
2:B:283:GLY:O	2:B:287:ILE:HG12	2.18	0.44
2:B:1043:ILE:HG21	2:B:1066:ILE:HD11	1.98	0.44
3:C:23:LYS:O	3:C:27:LYS:HG2	2.17	0.44
5:E:25:ASN:OD1	5:E:25:ASN:N	2.51	0.44
1:A:168:GLN:O	1:A:172:GLU:HG2	2.18	0.44
1:A:1422:ILE:CD1	2:B:1156:THR:HG23	2.48	0.44
2:B:76:THR:H	2:B:79:ASP:HB2	1.82	0.44
2:B:272:TRP:NE1	2:B:312:SER:OG	2.49	0.44
2:B:304:PHE:O	2:B:307:GLU:HG2	2.17	0.44
2:B:564:LYS:HB3	2:B:564:LYS:HE2	1.69	0.44
2:B:967:ALA:HB3	2:B:983:ARG:H	1.82	0.44
2:B:993:GLY:HA2	2:B:1005:ILE:HG23	1.99	0.44
4:D:144:GLN:NE2	4:D:180:ASP:OD1	2.51	0.44
1:A:176:ARG:HE	9:I:120:PRO:CD	2.27	0.44
1:A:967:PHE:HE1	1:A:1027:ARG:HE	1.65	0.44
1:A:1176:ILE:HG13	1:A:1225:ILE:HD11	1.99	0.44
3:C:257:TYR:CD2	3:C:340:ILE:HD12	2.52	0.44
2:B:500:ILE:HG21	9:I:1210:ILE:HD13	2.00	0.44
2:B:1007:ALA:O	2:B:1008:LEU:HB2	2.18	0.44
3:C:169:ILE:HG12	3:C:172:LYS:HG2	2.00	0.44
6:F:235:LYS:H	6:F:235:LYS:HG2	1.64	0.44
6:F:292:MET:O	6:F:296:LEU:HG	2.17	0.44
6:F:297:LEU:O	6:F:301:ILE:HG12	2.18	0.44
1:A:26:VAL:HG12	2:B:1199:MET:HE2	1.99	0.43
1:A:396:ASP:C	1:A:398:ARG:H	2.26	0.43
1:A:814:ASN:HD21	1:A:1061:HIS:HB3	1.82	0.43
1:A:1402:SER:O	1:A:1402:SER:OG	2.26	0.43
2:B:227:ILE:HB	2:B:250:TYR:HD1	1.83	0.43
2:B:820:ASP:HB3	2:B:823:ARG:HG2	2.00	0.43
7:G:49:MET:HE2	7:G:105:GLY:HA2	2.00	0.43
7:G:84:ILE:CG2	7:G:86:ILE:HD13	2.48	0.43
9:I:897:ARG:HB2	9:I:904:LEU:HD13	2.00	0.43
9:I:951:VAL:O	9:I:958:TYR:HB3	2.17	0.43
1:A:781:GLU:OE1	2:B:767:ARG:NH2	2.43	0.43
1:A:1152:VAL:HA	1:A:1155:MET:HB2	2.01	0.43
9:I:102:ARG:HA	9:I:103:PRO:HD3	1.87	0.43
1:A:814:ASN:ND2	1:A:1061:HIS:HB3	2.34	0.43
2:B:244:SER:HB2	2:B:262:SER:HB2	2.00	0.43
2:B:294:ASP:HB2	2:B:608:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:182:VAL:HG23	6:F:240:LEU:HG	2.00	0.43
6:F:219:ASP:OD1	6:F:220:LEU:N	2.52	0.43
1:A:90:GLU:HG3	1:A:94:TRP:HD1	1.84	0.43
2:B:82:ARG:NH2	2:B:455:GLU:OE1	2.37	0.43
2:B:477:ASP:OD1	2:B:480:ARG:NH2	2.51	0.43
2:B:717:GLN:NE2	2:B:721:ASP:OD1	2.52	0.43
4:D:52:ILE:HB	4:D:85:TYR:H	1.84	0.43
4:D:83:LYS:HB2	4:D:85:TYR:CE2	2.53	0.43
1:A:777:ARG:NH2	7:G:63:ASP:OD2	2.50	0.43
2:B:25:ASP:O	2:B:28:SER:OG	2.30	0.43
2:B:278:MET:HB2	2:B:278:MET:HE3	1.84	0.43
2:B:474:THR:O	2:B:476:SER:N	2.45	0.43
2:B:881:PHE:HB3	2:B:986:TYR:HB2	2.01	0.43
3:C:304:ASP:OD1	3:C:304:ASP:N	2.46	0.43
6:F:205:LYS:HE3	6:F:205:LYS:HB3	1.90	0.43
9:I:1070:ASP:OD1	9:I:1122:TYR:OH	2.27	0.43
1:A:182:VAL:HG21	1:A:192:HIS:CD2	2.53	0.43
1:A:363:MET:HE1	1:A:366:PHE:HD2	1.83	0.43
1:A:649:PHE:HB3	2:B:855:ILE:HG13	2.00	0.43
1:A:793:ILE:HD12	1:A:793:ILE:HA	1.91	0.43
2:B:458:THR:OG1	2:B:459:GLN:N	2.51	0.43
9:I:102:ARG:HH22	9:I:104:SER:HB3	1.84	0.43
1:A:376:CYS:SG	1:A:405:LEU:HD11	2.59	0.43
2:B:455:GLU:OE1	2:B:455:GLU:N	2.23	0.43
2:B:1224:ARG:HG3	2:B:1230:ILE:HD12	2.00	0.43
4:D:5:LYS:HE3	4:D:5:LYS:HB3	1.90	0.43
4:D:19:MET:HB3	4:D:45:ALA:HB1	2.00	0.43
1:A:92:ARG:HB2	1:A:154:PHE:CZ	2.54	0.43
1:A:1102:GLU:HG2	1:A:1103:VAL:N	2.32	0.43
1:A:1422:ILE:HD13	2:B:1156:THR:HG23	1.99	0.43
2:B:455:GLU:CD	2:B:455:GLU:H	2.18	0.43
2:B:610:LYS:HD3	2:B:610:LYS:N	2.33	0.43
2:B:957:TYR:CZ	2:B:959:PHE:HB2	2.54	0.43
2:B:1010:LEU:HB2	2:B:1015:MET:HE3	2.01	0.43
3:C:255:LYS:O	3:C:258:GLU:HG3	2.18	0.43
7:G:2:LYS:HZ2	7:G:30:VAL:HG11	1.83	0.43
9:I:229:ARG:NH1	9:I:230:LYS:HB2	2.33	0.43
1:A:102:CYS:HB3	1:A:137:CYS:SG	2.58	0.43
1:A:1145:TYR:CG	1:A:1146:PRO:HD2	2.53	0.43
2:B:30:ILE:HD11	2:B:774:VAL:HB	2.01	0.43
2:B:56:PRO:HA	2:B:94:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:ALA:O	2:B:457:LEU:HD12	2.19	0.43
2:B:503:ARG:HH22	9:I:1221:GLU:CD	2.27	0.43
2:B:953:ARG:HD3	2:B:953:ARG:HA	1.79	0.43
2:B:1203:VAL:HA	6:F:143:PRO:HD3	1.99	0.43
6:F:166:VAL:HG22	6:F:292:MET:HG2	2.00	0.43
6:F:182:VAL:O	6:F:185:ILE:HG22	2.18	0.43
9:I:1160:TRP:H	9:I:1160:TRP:CD1	2.37	0.43
1:A:34:LEU:HD13	1:A:46:TYR:HE2	1.84	0.43
1:A:46:TYR:CZ	1:A:212:ILE:HG12	2.54	0.43
1:A:236:LYS:HB3	1:A:263:ILE:CD1	2.49	0.43
2:B:538:ARG:O	2:B:542:MET:HG2	2.19	0.43
2:B:901:PRO:O	2:B:904:THR:OG1	2.35	0.43
6:F:164:TYR:HB3	6:F:292:MET:HE3	2.01	0.43
6:F:299:GLU:HA	6:F:302:ASN:OD1	2.19	0.43
8:H:47:LEU:C	8:H:49:ILE:H	2.27	0.43
9:I:112:ILE:O	9:I:183:LYS:NZ	2.52	0.43
9:I:145:MET:H	9:I:145:MET:HG2	1.69	0.43
9:I:158:TYR:CD1	9:I:158:TYR:C	2.97	0.43
1:A:512:ARG:HA	1:A:602:VAL:HG12	2.00	0.42
2:B:51:MET:HE2	2:B:51:MET:HA	2.01	0.42
2:B:78:ILE:HD12	2:B:78:ILE:HA	1.82	0.42
2:B:460:ARG:CZ	2:B:464:GLU:HG2	2.49	0.42
5:E:136:TRP:HB3	5:E:141:MET:SD	2.59	0.42
9:I:864:TYR:O	9:I:875:GLU:HA	2.19	0.42
1:A:1122:PHE:CE2	1:A:1199:LEU:HD11	2.53	0.42
2:B:1176:ILE:HD11	2:B:1209:MET:CG	2.49	0.42
9:I:178:GLN:HE21	9:I:192:THR:HG23	1.84	0.42
9:I:179:GLU:OE1	9:I:179:GLU:N	2.52	0.42
9:I:196:ILE:O	9:I:200:THR:HG22	2.18	0.42
9:I:693:VAL:HG11	9:I:782:TYR:CE2	2.54	0.42
1:A:1333:GLN:HA	1:A:1336:ILE:HD12	2.02	0.42
2:B:863:ASP:OD2	9:I:1249:GLN:HG2	2.19	0.42
2:B:1202:ASP:OD1	2:B:1203:VAL:N	2.43	0.42
5:E:93:THR:OG1	5:E:94:MET:N	2.52	0.42
6:F:156:ILE:HG22	6:F:158:LYS:H	1.84	0.42
6:F:241:SER:HA	6:F:244:TYR:CD1	2.53	0.42
1:A:351:ALA:H	1:A:469:TRP:HB2	1.84	0.42
1:A:1167:PRO:HA	1:A:1168:PRO:HD3	1.91	0.42
3:C:152:LEU:HD21	3:C:158:LEU:HB2	2.00	0.42
6:F:101:LEU:HD12	6:F:101:LEU:HA	1.82	0.42
2:B:27:LEU:HD11	2:B:1064:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:ARG:HD2	2:B:499:PRO:HD2	2.01	0.42
2:B:537:GLU:O	2:B:541:MET:HG2	2.20	0.42
2:B:996:MET:HE1	2:B:1006:ALA:HB2	2.01	0.42
3:C:25:ALA:O	3:C:29:LEU:HD23	2.20	0.42
3:C:88:MET:HE3	3:C:151:PHE:H	1.83	0.42
5:E:124:LYS:HD2	5:E:124:LYS:HA	1.60	0.42
1:A:1:MET:HB3	1:A:2:GLU:H	1.68	0.42
1:A:35:PHE:HE2	1:A:212:ILE:HG21	1.83	0.42
1:A:119:LYS:HE3	1:A:119:LYS:HB2	1.77	0.42
1:A:371:ARG:HA	1:A:371:ARG:HD3	1.71	0.42
1:A:1304:MET:HE2	1:A:1325:LEU:HD12	2.00	0.42
2:B:276:PHE:CE1	2:B:390:LEU:HD23	2.54	0.42
2:B:710:GLN:NE2	2:B:761:HIS:O	2.42	0.42
9:I:1076:PHE:HD1	9:I:1172:GLU:HG2	1.84	0.42
1:A:59:CYS:O	1:A:61:THR:N	2.46	0.42
2:B:167:ASN:HA	2:B:172:HIS:CG	2.54	0.42
2:B:433:PHE:O	2:B:437:VAL:HB	2.18	0.42
2:B:460:ARG:HH21	2:B:464:GLU:N	2.17	0.42
9:I:93:SER:HB2	9:I:96:LYS:HB3	2.00	0.42
9:I:1029:ILE:C	9:I:1029:ILE:HD12	2.45	0.42
1:A:619:LEU:O	1:A:623:ARG:HG2	2.20	0.42
1:A:1420:PRO:HD2	2:B:1161:MET:HE2	2.02	0.42
1:A:1432:ASP:OD2	5:E:139:ARG:NH2	2.36	0.42
2:B:432:ILE:HD11	5:E:10:ILE:HD11	2.01	0.42
9:I:1076:PHE:CZ	9:I:1152:LEU:HD22	2.55	0.42
9:I:1100:VAL:HG13	9:I:1103:LEU:HD12	2.01	0.42
1:A:3:ALA:O	2:B:1209:MET:HE3	2.20	0.42
1:A:1074:ILE:C	1:A:1077:PRO:HD2	2.45	0.42
2:B:94:VAL:HA	2:B:129:ASN:O	2.20	0.42
3:C:272:MET:HE3	3:C:278:LYS:HB2	2.02	0.42
4:D:94:LYS:HB3	4:D:95:PRO:HD3	2.01	0.42
6:F:39:CYS:HA	6:F:44:PHE:HA	2.00	0.42
1:A:265:GLN:O	1:A:265:GLN:NE2	2.51	0.42
1:A:1052:PRO:HG2	1:A:1348:PRO:HD3	2.02	0.42
2:B:331:LYS:N	2:B:331:LYS:HD2	2.33	0.42
2:B:404:VAL:HG13	7:G:52:LYS:HG3	2.02	0.42
2:B:424:SER:HB3	2:B:504:VAL:HA	2.01	0.42
2:B:924:GLY:N	2:B:965:VAL:O	2.29	0.42
3:C:273:ASP:OD1	3:C:273:ASP:C	2.63	0.42
3:C:290:ILE:HD13	3:C:290:ILE:HA	1.87	0.42
4:D:34:MET:HE2	4:D:34:MET:HB2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:183:ASN:HA	6:F:186:GLU:OE1	2.20	0.42
1:A:340:TYR:CZ	1:A:344:PHE:HB3	2.55	0.41
1:A:528:MET:HG2	1:A:541:PHE:CD2	2.55	0.41
2:B:69:TYR:CD1	2:B:87:ILE:HD12	2.55	0.41
2:B:263:THR:HG21	9:I:1208:ASP:CG	2.45	0.41
4:D:83:LYS:HB2	4:D:85:TYR:CZ	2.55	0.41
9:I:1029:ILE:HD11	9:I:1034:ILE:HG12	2.02	0.41
1:A:93:ARG:NH1	1:A:121:LEU:HD12	2.35	0.41
1:A:521:VAL:HG21	1:A:549:LEU:HD13	2.03	0.41
2:B:164:ARG:NH2	2:B:184:GLU:HB3	2.34	0.41
2:B:277:ARG:HA	2:B:280:GLY:O	2.20	0.41
2:B:328:ASN:O	2:B:332:ILE:HG13	2.20	0.41
2:B:436:SER:OG	2:B:477:ASP:HB3	2.19	0.41
4:D:102:ILE:HD12	4:D:102:ILE:H	1.83	0.41
1:A:1151:ASP:OD2	1:A:1177:ARG:HD2	2.20	0.41
2:B:74:ASP:N	2:B:74:ASP:OD1	2.52	0.41
2:B:281:MET:O	2:B:287:ILE:HD11	2.19	0.41
2:B:318:PRO:HB2	2:B:319:ILE:HD13	2.02	0.41
2:B:534:LYS:HB2	9:I:1227:LEU:HB2	2.02	0.41
2:B:920:PHE:CE2	2:B:934:ILE:HG22	2.55	0.41
4:D:41:PHE:CD1	4:D:41:PHE:C	2.98	0.41
5:E:122:CYS:HA	5:E:133:VAL:HG12	2.02	0.41
6:F:325:ASN:O	6:F:325:ASN:ND2	2.52	0.41
6:F:326:ILE:O	6:F:330:ILE:HG22	2.20	0.41
9:I:80:ARG:HD2	9:I:80:ARG:HA	1.68	0.41
9:I:691:ALA:O	9:I:695:ARG:HG3	2.20	0.41
9:I:788:TYR:HB2	9:I:795:PHE:CZ	2.55	0.41
1:A:42:GLU:CD	1:A:42:GLU:H	2.29	0.41
2:B:18:ASN:ND2	2:B:711:ASN:OD1	2.53	0.41
2:B:67:ILE:HD12	2:B:68:THR:H	1.84	0.41
2:B:815:TRP:CG	2:B:816:PRO:HD3	2.54	0.41
4:D:16:TYR:CD1	4:D:16:TYR:C	2.98	0.41
4:D:33:GLN:OE1	4:D:33:GLN:HA	2.19	0.41
6:F:161:PHE:CG	6:F:260:PRO:HA	2.56	0.41
1:A:70:MET:SD	2:B:1214:ARG:NH1	2.94	0.41
1:A:1374:LEU:HD11	1:A:1384:LEU:HD21	2.02	0.41
2:B:305:MET:HE1	2:B:395:HIS:CE1	2.54	0.41
4:D:106:ILE:HD12	4:D:106:ILE:HA	1.84	0.41
6:F:221:LYS:O	6:F:223:TRP:N	2.46	0.41
9:I:90:PRO:HD2	9:I:109:ILE:HG22	2.02	0.41
1:A:524:LYS:HE3	1:A:541:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1233:ARG:O	1:A:1233:ARG:NE	2.53	0.41
2:B:401:ILE:C	2:B:403:ASN:H	2.28	0.41
2:B:495:VAL:HG12	2:B:500:ILE:HG12	2.03	0.41
3:C:227:PRO:HG2	3:C:230:HIS:HB2	2.01	0.41
6:F:174:GLN:O	6:F:178:LEU:HD22	2.20	0.41
1:A:376:CYS:HB2	1:A:406:TYR:O	2.21	0.41
1:A:1431:MET:SD	6:F:59:ILE:HD11	2.61	0.41
2:B:357:VAL:CG1	9:I:1182:LEU:HD22	2.51	0.41
2:B:435:THR:HG23	2:B:496:ARG:HD3	2.03	0.41
2:B:445:PHE:HE2	2:B:466:PHE:CD2	2.39	0.41
2:B:881:PHE:HB2	2:B:988:ARG:HG3	2.01	0.41
9:I:207:TYR:O	9:I:211:ARG:HD3	2.21	0.41
1:A:354:VAL:N	1:A:403:ASP:O	2.41	0.41
1:A:592:GLN:CD	1:A:599:ILE:HD11	2.46	0.41
1:A:934:VAL:HB	1:A:1005:GLU:HG3	2.03	0.41
1:A:1355:MET:HA	1:A:1355:MET:HE3	2.03	0.41
1:A:1386:MET:HE3	1:A:1386:MET:HB3	1.94	0.41
3:C:28:LYS:HD2	8:H:23:LYS:HZ1	1.85	0.41
5:E:83:ARG:HD3	5:E:115:ILE:HG13	2.03	0.41
6:F:141:TYR:CE1	6:F:148:ALA:HB2	2.55	0.41
1:A:295:PRO:HB2	1:A:296:ALA:H	1.65	0.41
1:A:930:VAL:HG21	1:A:1001:LEU:HD22	2.03	0.41
1:A:1441:LYS:HB3	1:A:1441:LYS:HE3	1.71	0.41
2:B:157:VAL:O	2:B:158:SER:OG	2.35	0.41
2:B:350:TYR:HA	9:I:1193:ILE:HG12	2.03	0.41
3:C:5:PHE:HB3	3:C:353:ASN:CB	2.51	0.41
8:H:45:ALA:HA	9:I:821:PHE:HD1	1.85	0.41
8:H:47:LEU:O	8:H:47:LEU:HD13	2.21	0.41
2:B:789:ALA:HB3	2:B:1062:ALA:HB2	2.02	0.41
2:B:829:ASN:HD21	2:B:845:ASN:HA	1.85	0.41
3:C:350:LEU:HD23	3:C:350:LEU:HA	1.94	0.41
8:H:48:GLN:NE2	9:I:821:PHE:HB3	2.35	0.41
1:A:189:LYS:NZ	5:E:42:SER:HA	2.35	0.40
1:A:1393:GLN:HB2	5:E:20:GLU:OE1	2.21	0.40
2:B:831:MET:O	8:H:72:THR:HB	2.22	0.40
2:B:1089:PHE:CE2	2:B:1096:TYR:HB3	2.55	0.40
3:C:246:ILE:HD12	3:C:347:PHE:CE1	2.56	0.40
1:A:362:LEU:HA	1:A:365:TYR:HD2	1.87	0.40
1:A:398:ARG:HA	1:A:398:ARG:HD2	1.89	0.40
1:A:495:PRO:O	1:A:611:GLY:HA2	2.21	0.40
1:A:1145:TYR:CD1	1:A:1146:PRO:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:919:GLY:O	2:B:935:GLY:N	2.54	0.40
1:A:357:TYR:HB2	5:E:99:TYR:O	2.21	0.40
2:B:117:ALA:HA	2:B:122:LEU:HB2	2.04	0.40
2:B:281:MET:HG3	2:B:286:SER:HB3	2.03	0.40
2:B:284:ASP:O	2:B:288:ILE:HG12	2.21	0.40
1:A:273:ASP:HB3	1:A:298:SER:HB3	2.03	0.40
2:B:262:SER:HB3	2:B:371:ILE:HD11	2.02	0.40
2:B:304:PHE:HA	2:B:307:GLU:CD	2.46	0.40
2:B:425:LEU:HD21	2:B:486:ILE:HD11	2.04	0.40
2:B:439:ALA:HB3	2:B:440:PRO:HD2	2.02	0.40
2:B:699:LYS:HA	2:B:699:LYS:HD3	1.90	0.40
2:B:869:GLN:HE21	2:B:873:ASP:CG	2.30	0.40
3:C:96:ARG:NH2	3:C:148:GLU:O	2.28	0.40
9:I:90:PRO:HB3	9:I:127:ILE:HG21	2.02	0.40
9:I:128:TYR:CG	9:I:128:TYR:O	2.74	0.40
9:I:951:VAL:HG13	9:I:952:LYS:N	2.37	0.40
1:A:67:LYS:HE2	1:A:67:LYS:HB2	1.91	0.40
1:A:225:ASP:OD1	1:A:228:ASN:ND2	2.54	0.40
1:A:746:ILE:HG23	1:A:750:ALA:HB3	2.04	0.40
2:B:102:ARG:NH2	2:B:107:GLY:O	2.55	0.40
2:B:304:PHE:CE2	2:B:402:MET:HG3	2.57	0.40
2:B:904:THR:HG22	2:B:905:LYS:N	2.36	0.40
6:F:145:ARG:HA	6:F:145:ARG:HD2	1.71	0.40
6:F:273:GLN:OE1	6:F:276:ASN:N	2.54	0.40
9:I:1177:ILE:O	9:I:1181:LYS:N	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1407/1441 (98%)	1351 (96%)	51 (4%)	5 (0%)	30 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1222/1235 (99%)	1130 (92%)	86 (7%)	6 (0%)	24	42
3	C	356/358 (99%)	338 (95%)	18 (5%)	0	100	100
4	D	203/205 (99%)	196 (97%)	7 (3%)	0	100	100
5	E	125/139 (90%)	108 (86%)	17 (14%)	0	100	100
6	F	332/334 (99%)	298 (90%)	30 (9%)	4 (1%)	10	22
7	G	103/105 (98%)	95 (92%)	7 (7%)	1 (1%)	12	25
8	H	65/80 (81%)	59 (91%)	6 (9%)	0	100	100
9	I	630/1170 (54%)	588 (93%)	40 (6%)	2 (0%)	36	54
All	All	4443/5067 (88%)	4163 (94%)	262 (6%)	18 (0%)	31	48

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	582	MET
2	B	421	SER
2	B	1162	GLN
2	B	1202	ASP
9	I	94	GLU
6	F	70	MET
7	G	34	SER
1	A	277	THR
2	B	475	ALA
6	F	100	ILE
6	F	138	SER
6	F	45	ILE
9	I	183	LYS
1	A	283	GLY
1	A	1143	VAL
2	B	1145	LEU
1	A	1100	ASN
2	B	934	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1250/1270 (98%)	1229 (98%)	21 (2%)	53	75
2	B	1066/1074 (99%)	1034 (97%)	32 (3%)	36	61
3	C	327/327 (100%)	325 (99%)	2 (1%)	78	89
4	D	185/185 (100%)	178 (96%)	7 (4%)	29	54
5	E	119/129 (92%)	114 (96%)	5 (4%)	26	51
6	F	308/308 (100%)	292 (95%)	16 (5%)	21	43
7	G	96/96 (100%)	93 (97%)	3 (3%)	35	60
8	H	61/70 (87%)	60 (98%)	1 (2%)	55	76
9	I	572/1057 (54%)	549 (96%)	23 (4%)	28	53
All	All	3984/4516 (88%)	3874 (97%)	110 (3%)	38	62

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	116	ILE
1	A	262	THR
1	A	387	VAL
1	A	399	LEU
1	A	476	GLU
1	A	577	VAL
1	A	581	TYR
1	A	702	GLU
1	A	723	ILE
1	A	932	VAL
1	A	1087	GLU
1	A	1153	GLU
1	A	1178	LEU
1	A	1206	THR
1	A	1242	THR
1	A	1254	LEU
1	A	1270	VAL
1	A	1316	SER
1	A	1402	SER
1	A	1424	THR
2	B	85	VAL
2	B	113	LEU
2	B	119	LEU

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Mol	Chain	Res	Type
2	B	156	GLN
2	B	177	THR
2	B	242	ASN
2	B	275	ILE
2	B	295	LEU
2	B	401	ILE
2	B	413	TYR
2	B	415	THR
2	B	435	THR
2	B	442	ILE
2	B	452	THR
2	B	458	THR
2	B	477	ASP
2	B	487	ILE
2	B	527	HIS
2	B	536	THR
2	B	742	THR
2	B	765	VAL
2	B	843	ILE
2	B	861	GLN
2	B	927	VAL
2	B	960	ASP
2	B	1012	THR
2	B	1025	ASP
2	B	1124	SER
2	B	1137	ASP
2	B	1161	MET
2	B	1200	ASN
2	B	1231	THR
3	C	180	VAL
3	C	341	GLN
4	D	35	VAL
4	D	41	PHE
4	D	101	ASN
4	D	120	ILE
4	D	167	SER
4	D	168	ASP
4	D	193	HIS
5	E	25	ASN
5	E	39	ILE
5	E	46	CYS
5	E	51	GLN

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Mol	Chain	Res	Type
5	E	94	MET
6	F	17	THR
6	F	70	MET
6	F	72	VAL
6	F	85	ASP
6	F	93	ILE
6	F	101	LEU
6	F	108	GLU
6	F	121	ASN
6	F	147	GLN
6	F	162	SER
6	F	215	ASP
6	F	218	LEU
6	F	221	LYS
6	F	224	LYS
6	F	245	ASP
6	F	286	ILE
7	G	21	ILE
7	G	40	SER
7	G	72	ASP
8	H	7	CYS
9	I	83	LEU
9	I	102	ARG
9	I	104	SER
9	I	105	THR
9	I	152	SER
9	I	154	GLU
9	I	155	THR
9	I	171	VAL
9	I	176	VAL
9	I	189	VAL
9	I	191	THR
9	I	211	ARG
9	I	775	THR
9	I	794	ASN
9	I	801	GLU
9	I	836	THR
9	I	847	SER
9	I	876	ILE
9	I	1034	ILE
9	I	1094	ILE
9	I	1161	VAL

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Mol	Chain	Res	Type
9	I	1199	VAL
9	I	1218	LEU

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

Mol	Chain	Res	Type
1	A	190	ASN
1	A	265	GLN
1	A	385	GLN
1	A	418	ASN
1	A	664	GLN
1	A	667	GLN
1	A	721	ASN
1	A	814	ASN
1	A	852	GLN
1	A	959	GLN
1	A	980	GLN
1	A	1018	GLN
1	A	1055	GLN
1	A	1062	HIS
1	A	1078	GLN
1	A	1128	GLN
1	A	1173	ASN
1	A	1269	ASN
1	A	1349	ASN
2	B	95	ASN
2	B	172	HIS
2	B	235	GLN
2	B	290	GLN
2	B	298	ASN
2	B	328	ASN
2	B	395	HIS
2	B	451	GLN
2	B	525	ASN
2	B	598	GLN
2	B	627	ASN
2	B	829	ASN
2	B	845	ASN
2	B	912	ASN
2	B	1112	GLN
2	B	1220	GLN
2	B	1227	ASN

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Mol	Chain	Res	Type
3	C	144	ASN
3	C	230	HIS
4	D	37	ASN
6	F	4	GLN
6	F	47	ASN
6	F	121	ASN
6	F	305	GLN
6	F	323	HIS
7	G	35	GLN
8	H	48	GLN
8	H	69	HIS
9	I	113	ASN
9	I	195	ASN
9	I	812	GLN
9	I	819	GLN
9	I	905	GLN
9	I	906	HIS
9	I	912	ASN
9	I	1085	HIS
9	I	1123	HIS
9	I	1163	ASN
9	I	1174	ASN
9	I	1190	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

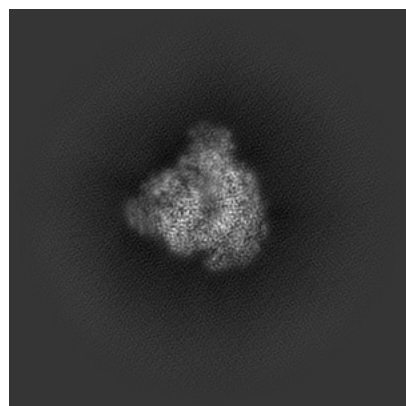
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38760. These allow visual inspection of the internal detail of the map and identification of artifacts.

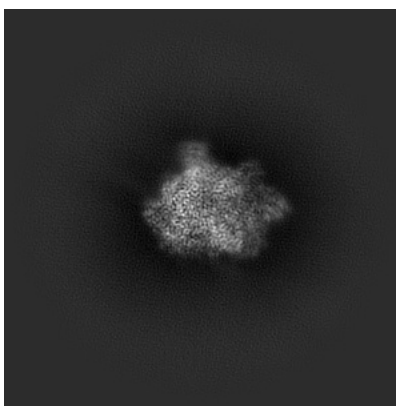
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

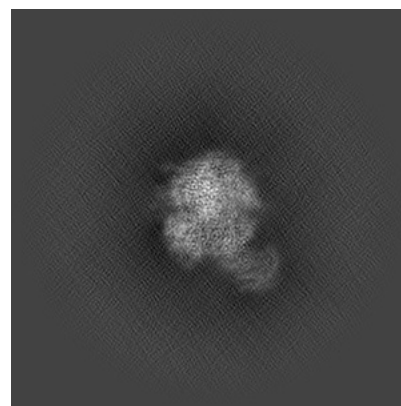
6.1.1 Primary map



X

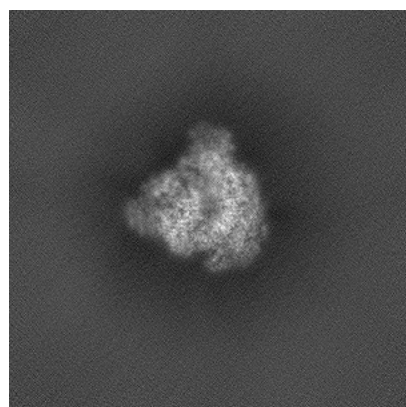


Y

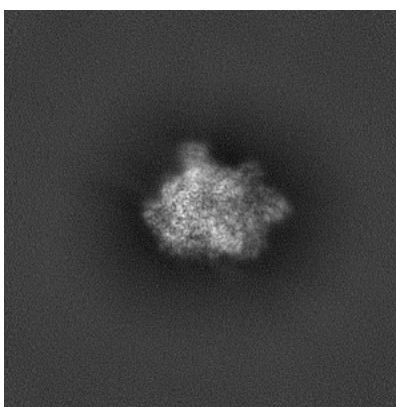


Z

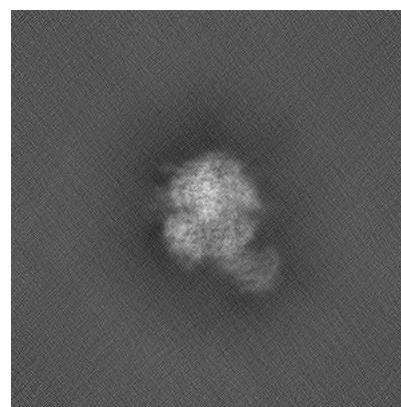
6.1.2 Raw map



X



Y

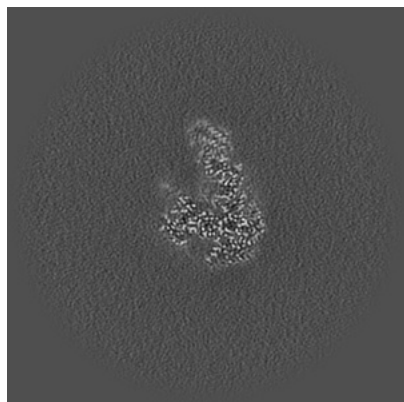


Z

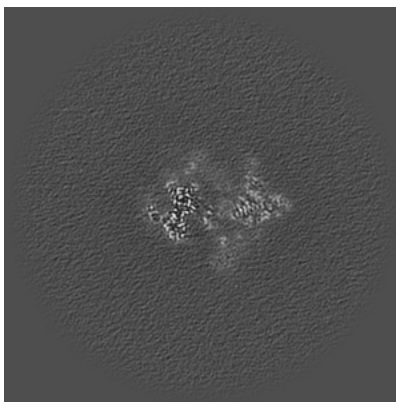
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

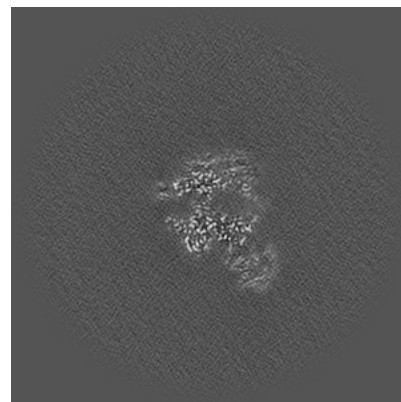
6.2.1 Primary map



X Index: 256

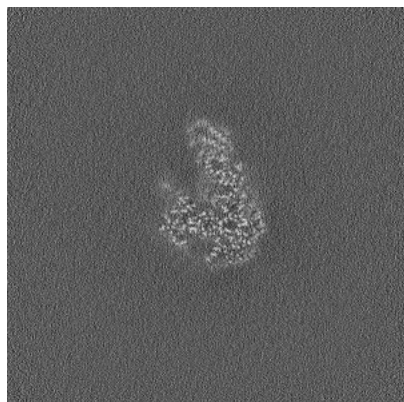


Y Index: 256

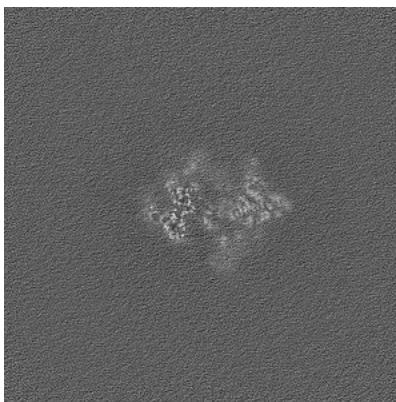


Z Index: 256

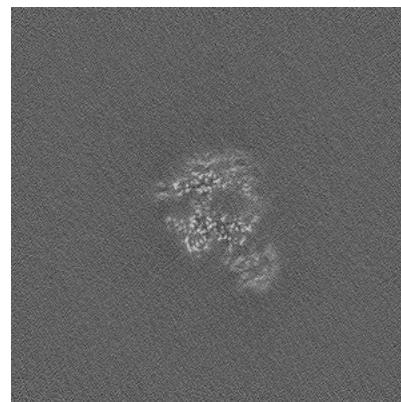
6.2.2 Raw map



X Index: 256



Y Index: 256

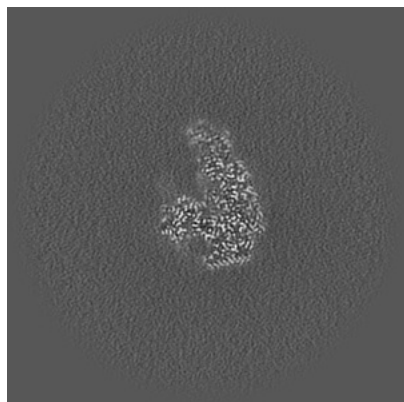


Z Index: 256

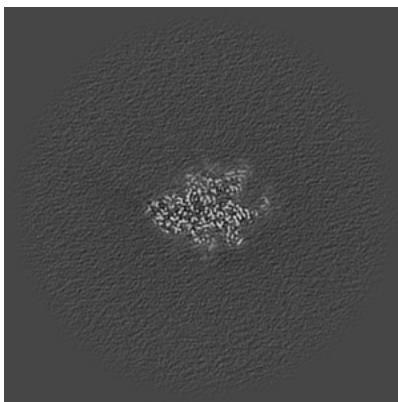
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

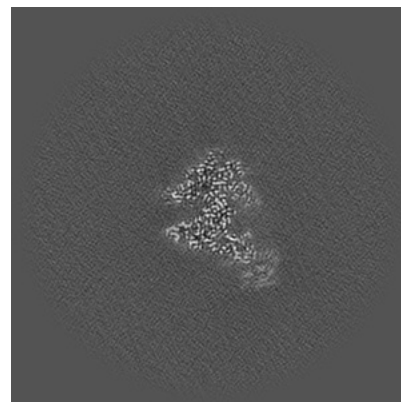
6.3.1 Primary map



X Index: 252

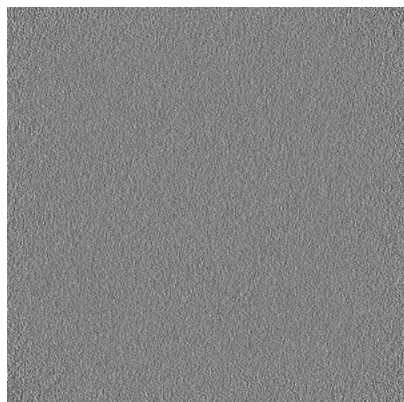


Y Index: 287

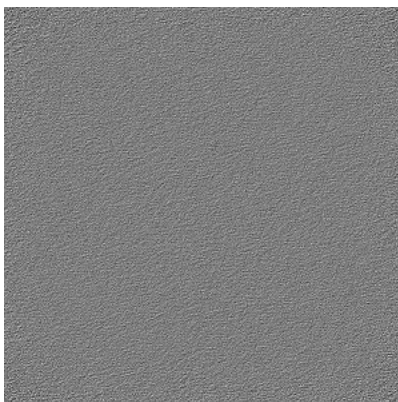


Z Index: 236

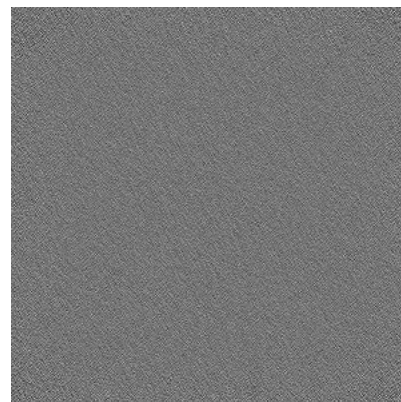
6.3.2 Raw map



X Index: 0



Y Index: 0

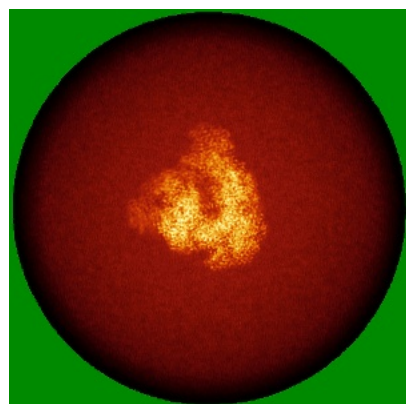


Z Index: 0

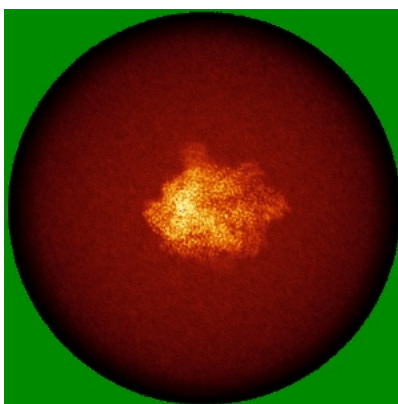
The images above show the largest variance slices of the map in three orthogonal directions.

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

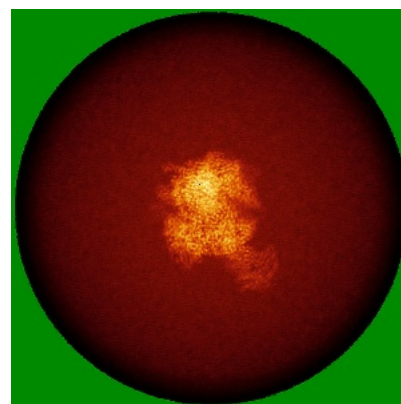
6.4.1 Primary map



X

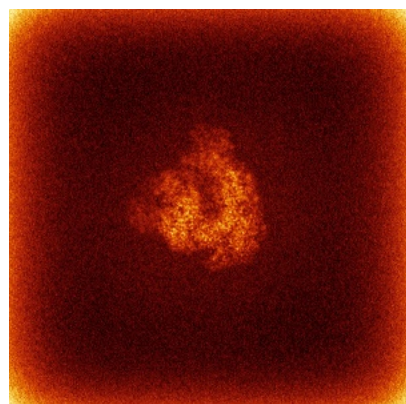


Y

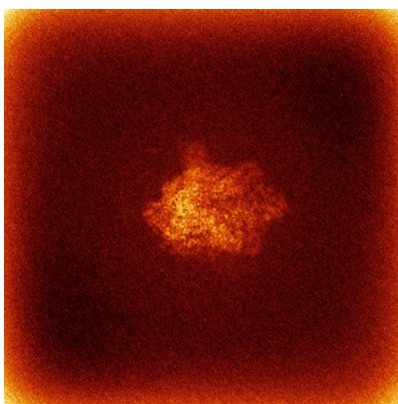


Z

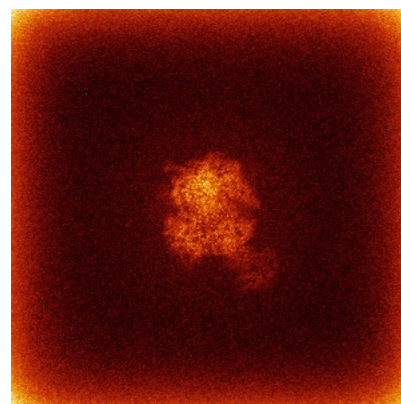
6.4.2 Raw map



X



Y

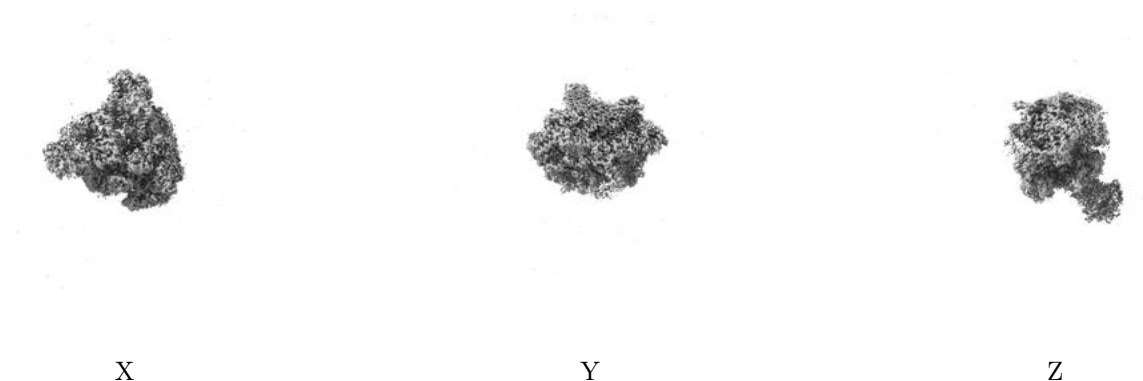


Z

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.

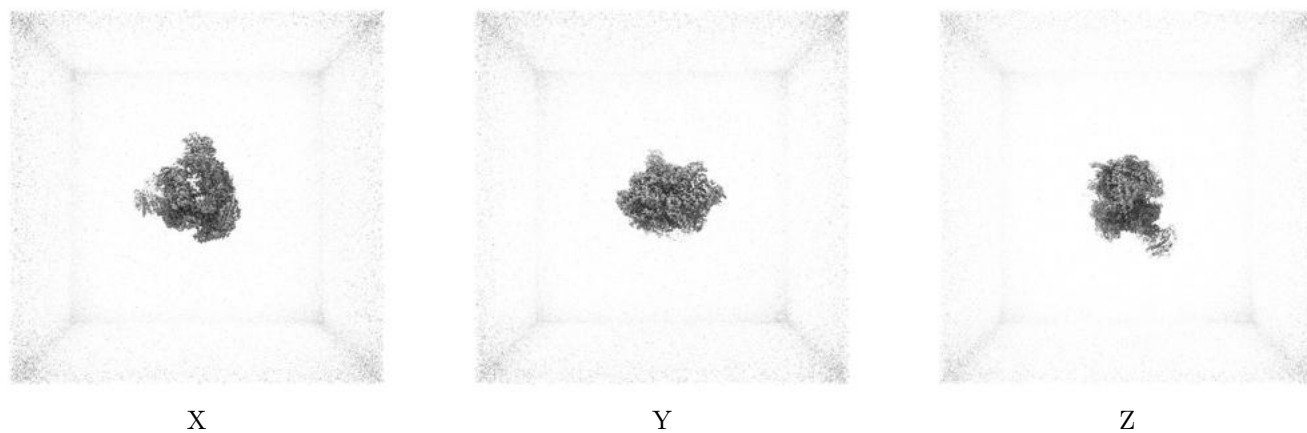
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

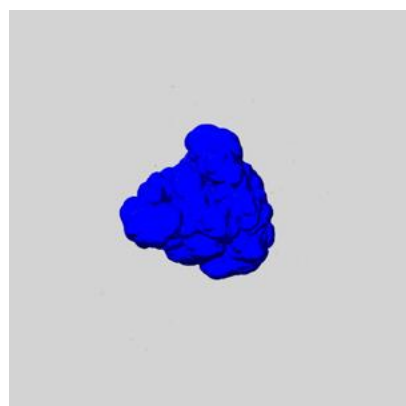
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

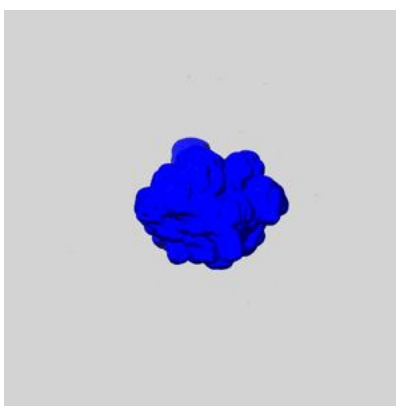
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

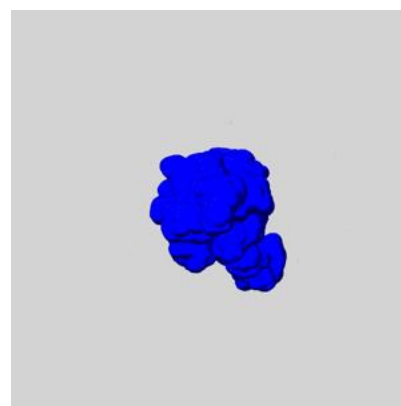
6.6.1 emd_38760_msk_1.map [i](#)



X



Y

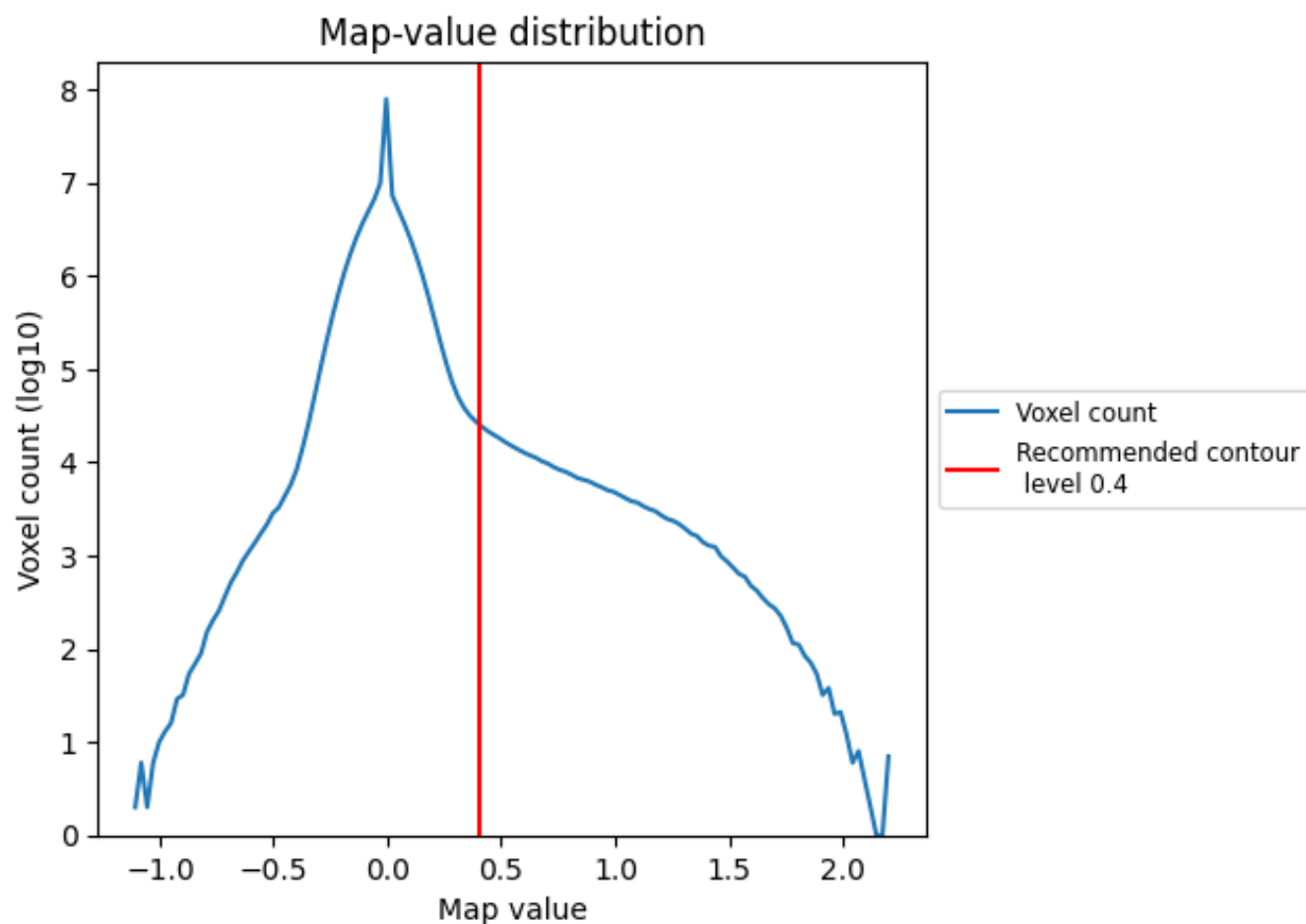


Z

7 Map analysis [i](#)

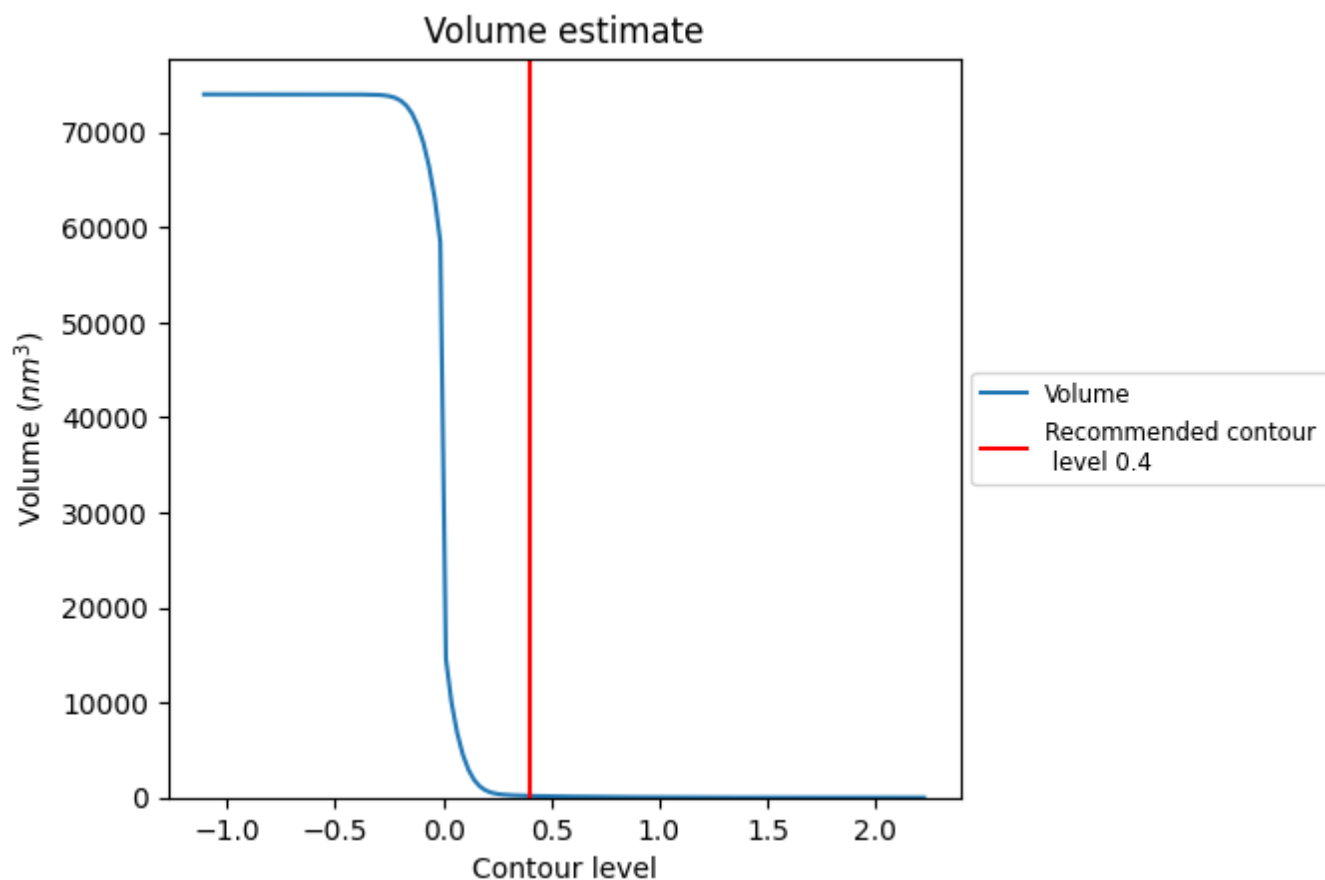
This section contains the results of statistical analysis of the map.

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.

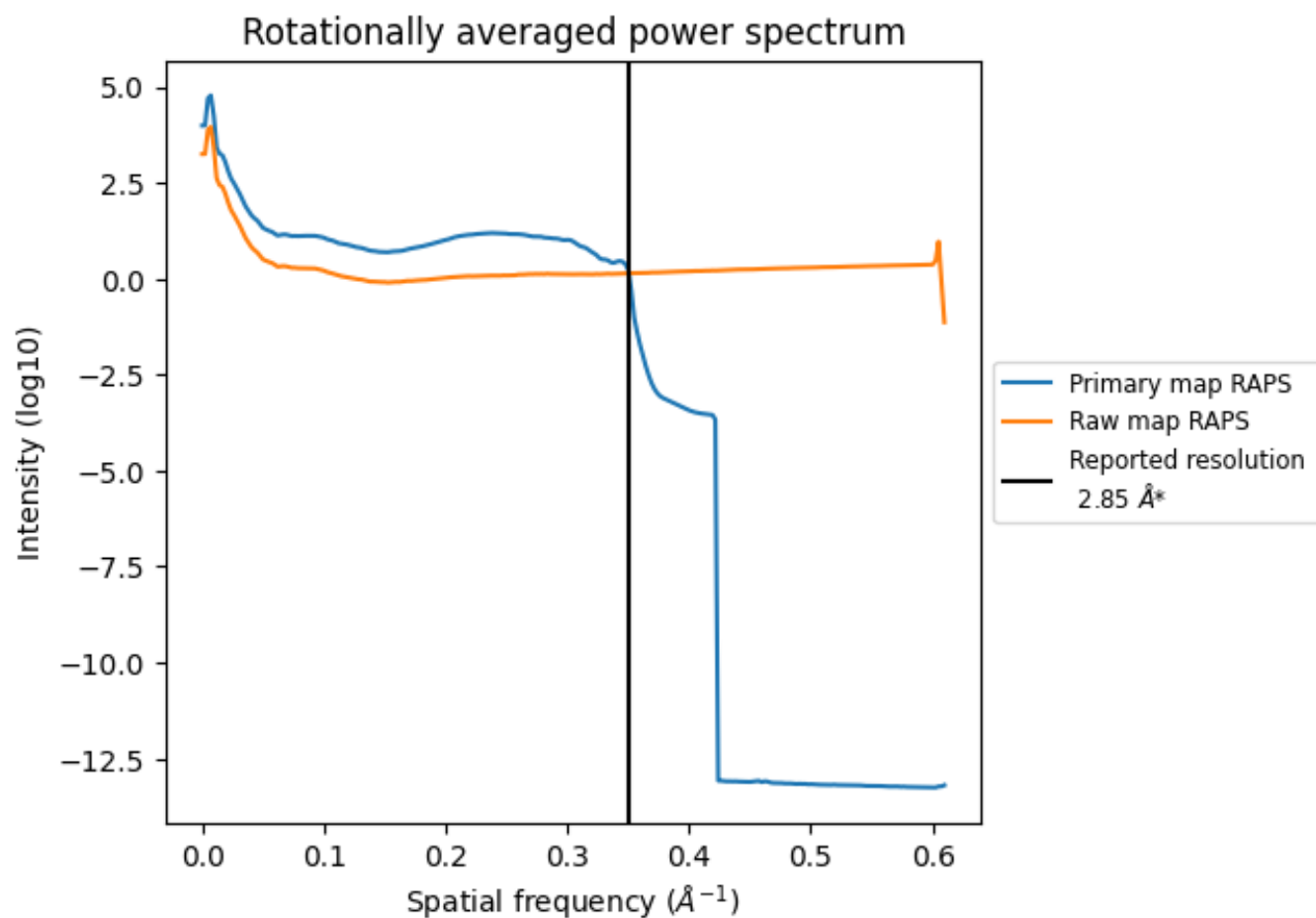
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179 nm³; this corresponds to an approximate mass of 162 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 ⓘ

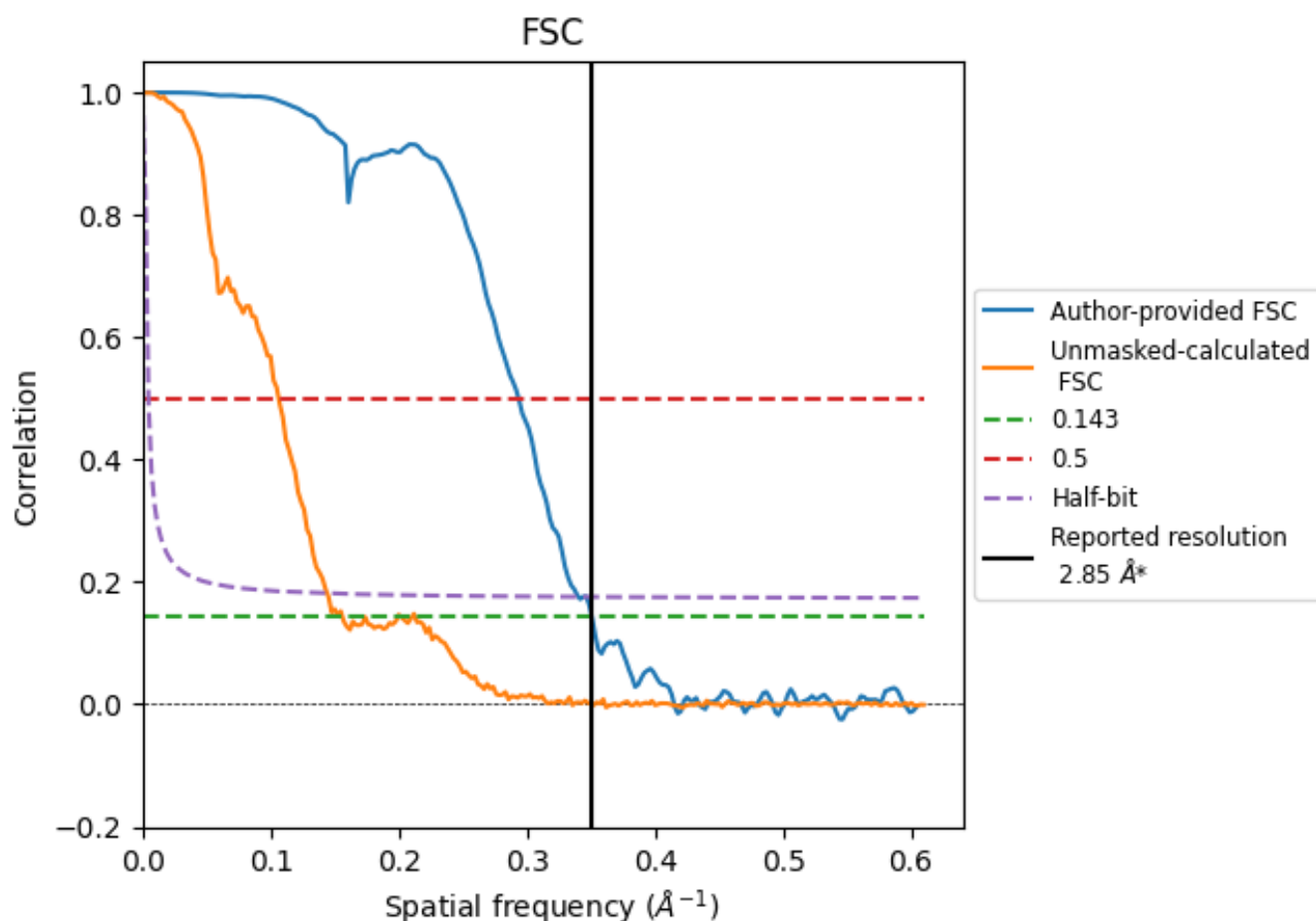


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.351 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

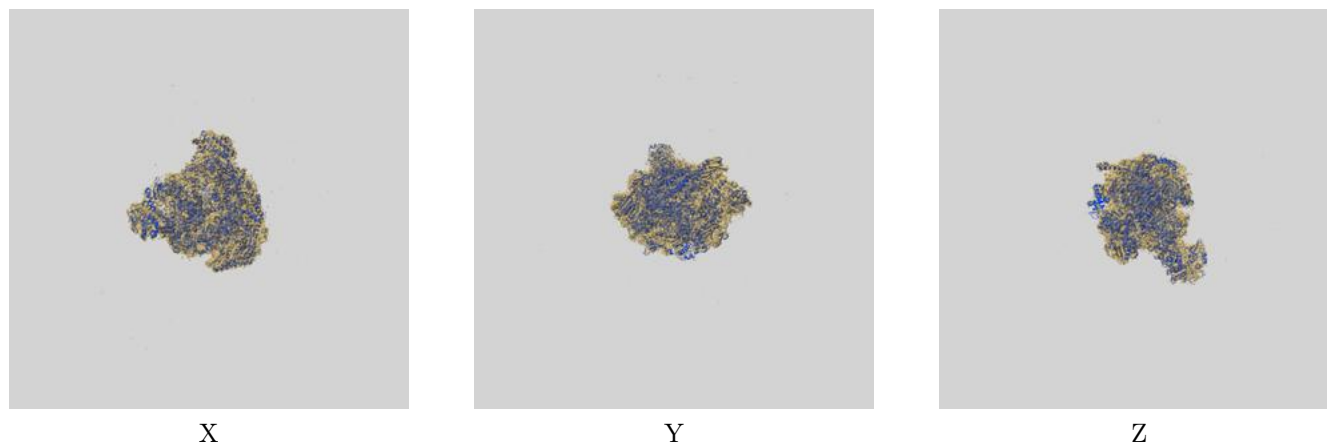
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.41	2.94
Unmasked-calculated*	6.41	9.40	6.93

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

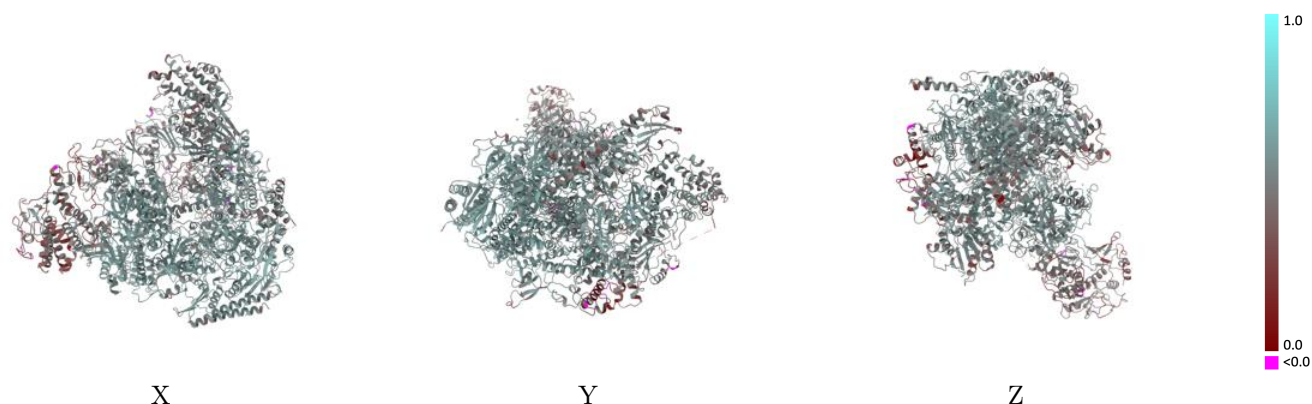
This section contains information regarding the fit between EMDB map EMD-38760 and PDB model 8XXT. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



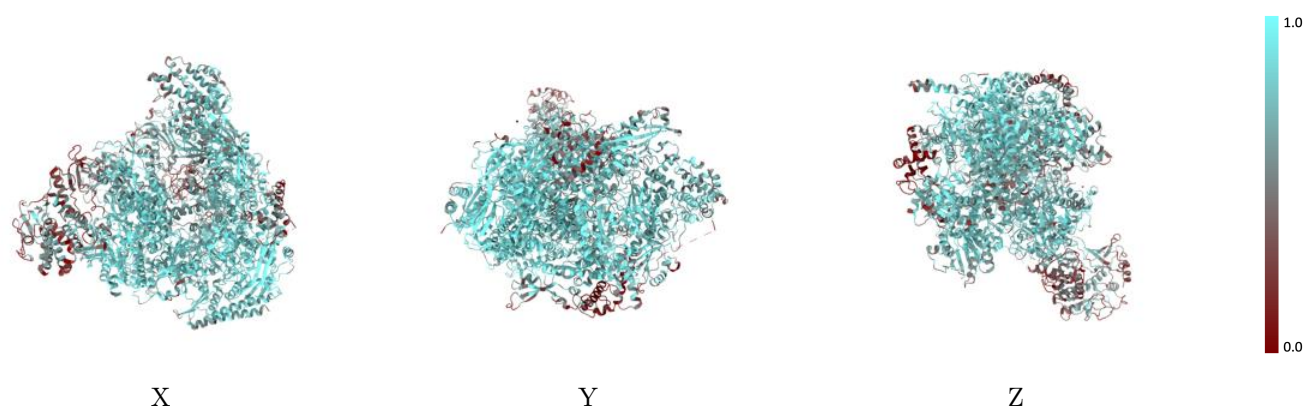
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



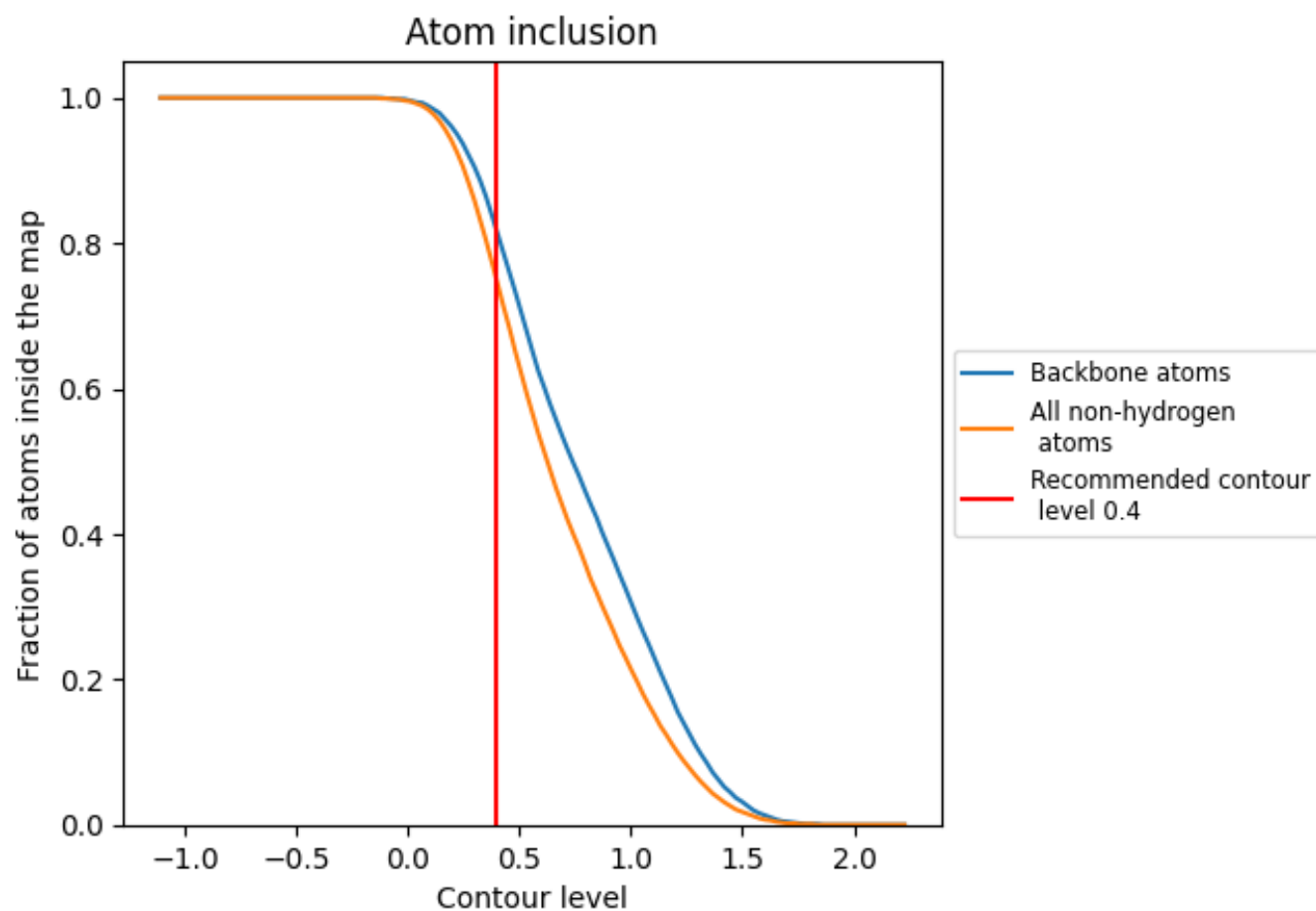
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7480	0.5250
A	0.8320	0.5600
B	0.8140	0.5490
C	0.8440	0.5700
D	0.7550	0.5130
E	0.7370	0.5400
F	0.5570	0.4370
G	0.7750	0.5230
H	0.8730	0.5620
I	0.4670	0.4200

1.0

0.0

<0.0