



Full wwPDB EM Validation Report ⓘ

Apr 19, 2026 – 04:07 PM JST

PDB ID : 9LWI / pdb_00009lwi
EMDB ID : EMD-63446
Title : The head region of HBx-Smc5/6 ubiquitination complex
Authors : Tong, C.; Lili, D.; Hongshuai, L.; Jinhong, Z.; Qian, X.; Lanfeng, W.
Deposited on : 2025-02-15
Resolution : 3.12 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:

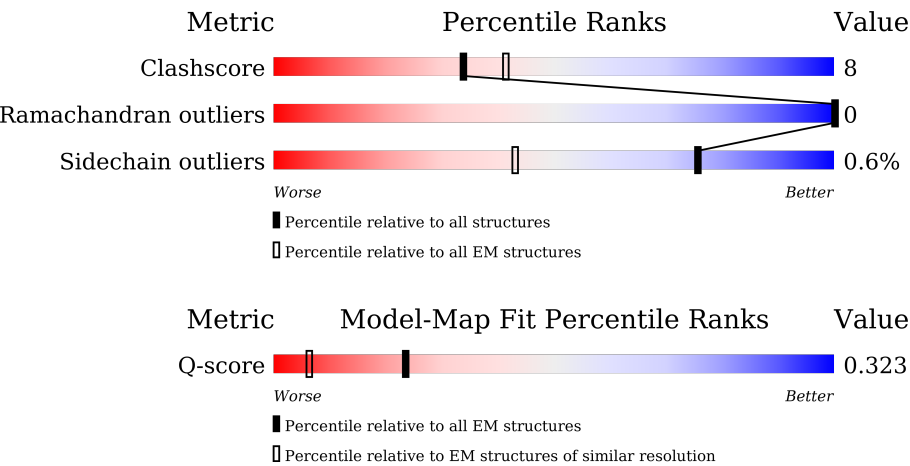
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.12 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	14478 (2.62 - 3.62)

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	1091	
2	B	1140	
3	C	154	
4	D	333	

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Mol	Chain	Length	Quality of chain
5	E	304	<div> <div>5%</div> <div>58%</div> <div>13%</div> <div>29%</div> </div>
6	F	266	<div> <div>14%</div> <div>75%</div> <div>14%</div> <div>11%</div> </div>
7	G	760	<div> <div>6%</div> <div>79%</div> <div>16%</div> <div>5%</div> </div>
8	H	108	<div> <div>17%</div> <div>73%</div> <div>10%</div> <div>17%</div> </div>
9	I	1101	<div> <div>23%</div> <div>29%</div> <div>6%</div> <div>65%</div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28124 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 Structural maintenance of chromosomes protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	392	Total	C	N	O	S	0	0
			3137	1971	557	586	23		

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1140	Total	C	N	O	S	0	0
			8918	5642	1503	1724	49		

- Molecule 3 is a protein called Protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	103	Total	C	N	O	S	0	0
			793	504	143	139	7		

- Molecule 4 is a protein called EP300-interacting inhibitor of differentiation 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	225	Total	C	N	O	S	0	0
			1840	1176	307	348	9		

- Molecule 5 is a protein called Non-structural maintenance of chromosomes element 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1787	1154	306	322	5		

- Molecule 6 is a protein called Non-structural maintenance of chromosomes element 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	237	Total	C	N	O	S	0	0
			1928	1220	333	361	14		

- Molecule 7 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	719	Total	C	N	O	S	0	0
			5898	3753	1023	1088	34		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	760	GLY	-	expression tag	UNP Q13619

- Molecule 8 is a protein called E3 ubiquitin-protein ligase RBX1.

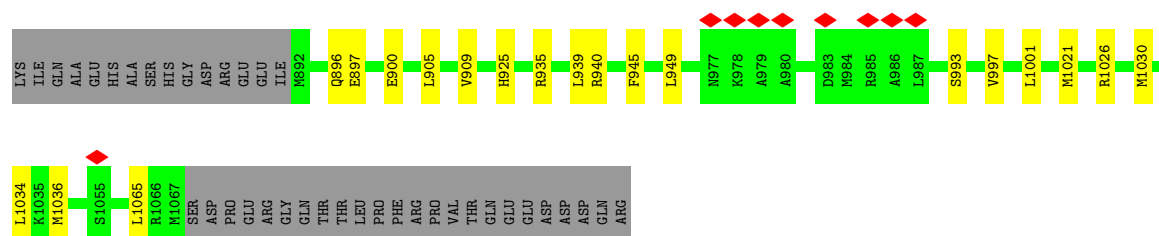
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	90	Total	C	N	O	S	0	0
			746	472	137	128	9		

- Molecule 9 is a protein called Structural maintenance of chromosomes protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	381	Total	C	N	O	S	0	0
			3071	1945	523	581	22		

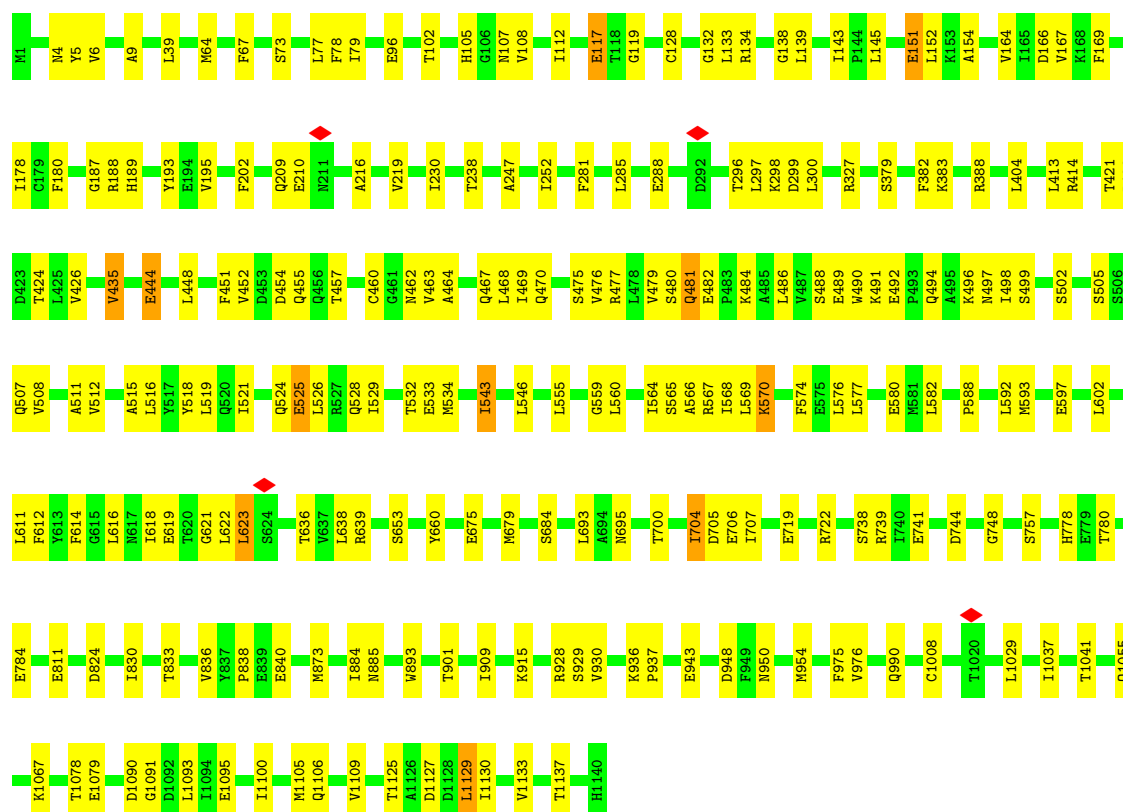
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Zn	0
			1	1	
10	F	2	Total	Zn	0
			2	2	
10	H	3	Total	Zn	0
			3	3	



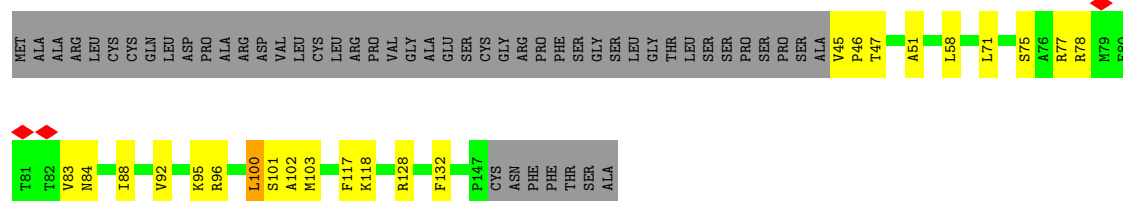
• Molecule 2: DNA damage-binding protein 1

Chain B: 80% 19%



• Molecule 3: Protein X

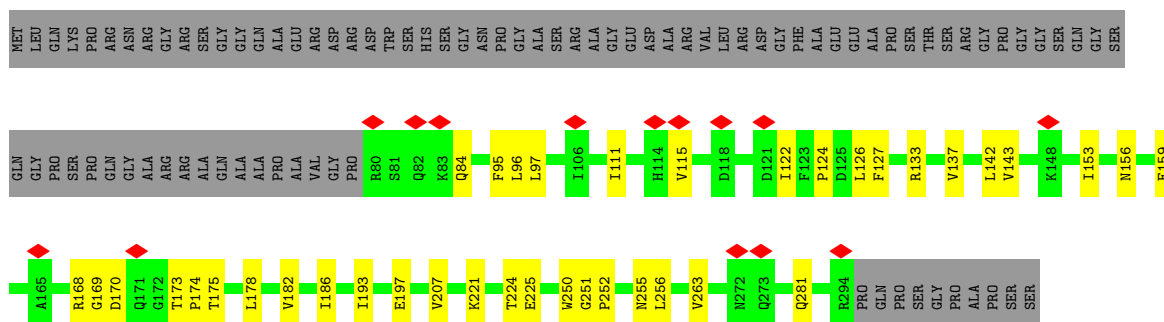
Chain C: 52% 14% 33%



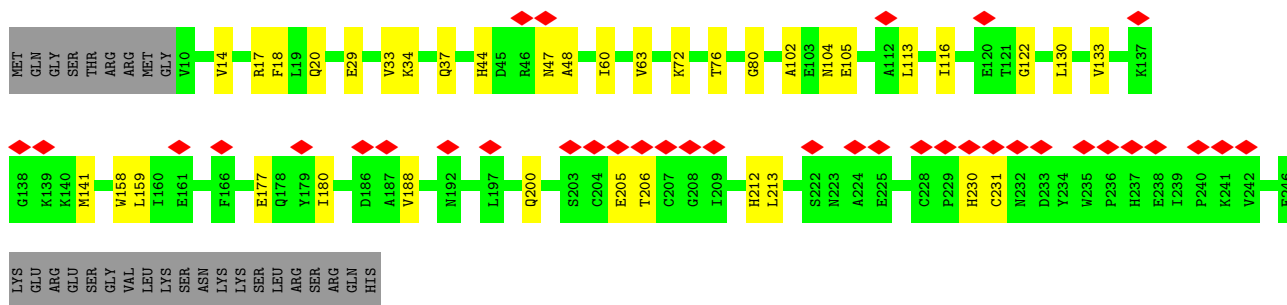
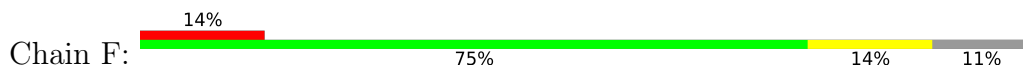
• Molecule 4: EP300-interacting inhibitor of differentiation 3

Chain D: 26% 59% 8% 32%

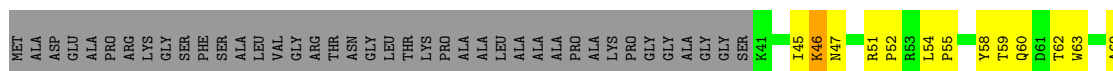
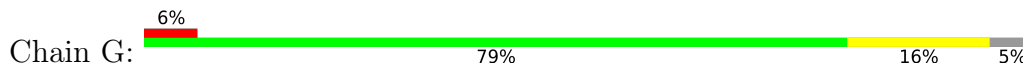
- Molecule 5: Non-structural maintenance of chromosomes element 3 homolog

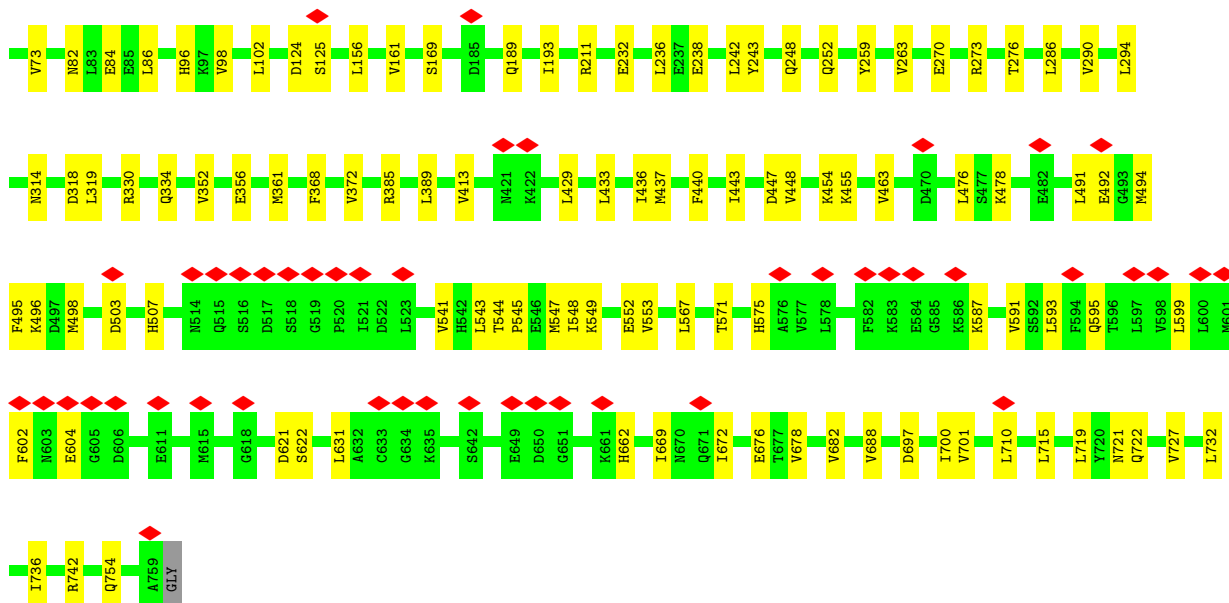


- Molecule 6: Non-structural maintenance of chromosomes element 1 homolog

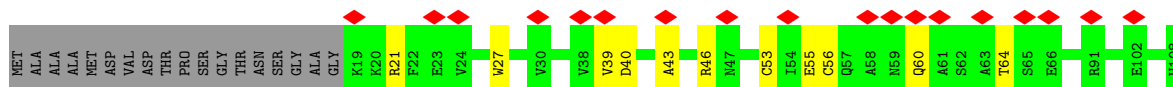
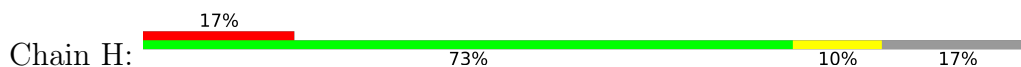


- Molecule 7: Cullin-4A

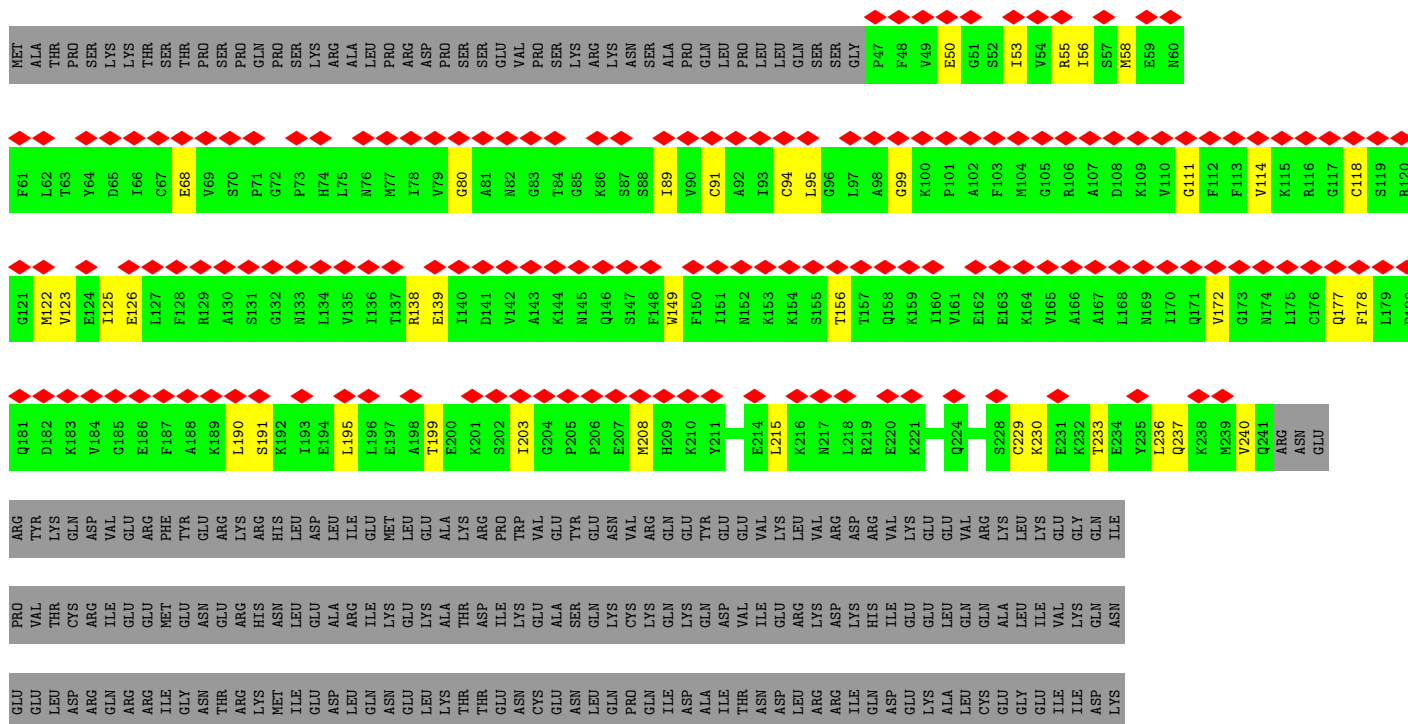




- Molecule 8: E3 ubiquitin-protein ligase RBX1



- Molecule 9: Structural maintenance of chromosomes protein 5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	401828	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	4.126	Depositor
Minimum map value	-2.523	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	477.184, 477.184, 477.184	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.932, 0.932, 0.932	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	1/3183 (0.0%)	0.61	2/4258 (0.0%)
2	B	0.55	0/9083	0.77	7/12306 (0.1%)
3	C	0.95	0/811	1.26	4/1097 (0.4%)
4	D	0.29	0/1874	0.41	0/2522
5	E	0.11	0/1827	0.27	0/2465
6	F	0.29	1/1966 (0.1%)	0.34	1/2656 (0.0%)
7	G	0.27	0/6006	0.43	4/8068 (0.0%)
8	H	0.50	0/768	0.64	1/1040 (0.1%)
9	I	0.19	0/3124	0.32	0/4197
All	All	0.43	2/28642 (0.0%)	0.60	19/38609 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	939	LEU	C-O	-5.86	1.16	1.24
6	F	213	LEU	N-CA	5.24	1.51	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	619	GLU	N-CA-C	-7.89	102.37	110.97
1	A	216	LEU	N-CA-C	-7.51	103.58	112.89
3	C	84	ASN	N-CA-C	-6.76	104.62	112.86
2	B	525	GLU	N-CA-C	6.53	119.12	108.55
3	C	102	ALA	N-CA-C	-6.38	105.07	112.92
7	G	55	PRO	N-CA-C	6.33	120.91	111.41
8	H	40	ASP	N-CA-C	-6.28	103.27	111.74
7	G	58	TYR	N-CA-C	-6.18	104.54	111.28
1	A	57	MET	CB-CA-C	-5.80	109.88	116.54
2	B	151	GLU	N-CA-C	-5.67	101.04	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	LEU	N-CA-CB	-5.46	102.70	110.46
2	B	73	SER	N-CA-C	-5.41	106.36	113.12
6	F	212	HIS	CA-C-O	-5.39	115.22	121.15
3	C	75	SER	CA-C-O	-5.37	115.00	120.80
3	C	100	LEU	N-CA-C	-5.32	103.62	111.81
2	B	937	PRO	N-CA-C	-5.26	106.34	113.40
7	G	46	LYS	CA-C-N	-5.10	113.59	122.37
7	G	46	LYS	C-N-CA	-5.10	113.59	122.37
2	B	704	ILE	N-CA-CB	5.02	116.01	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3137	0	3173	37	0
2	B	8918	0	8879	214	0
3	C	793	0	804	38	0
4	D	1840	0	1801	21	0
5	E	1787	0	1824	26	0
6	F	1928	0	1910	21	0
7	G	5898	0	5977	86	0
8	H	746	0	699	6	0
9	I	3071	0	3092	47	0
10	C	1	0	0	0	0
10	F	2	0	0	0	0
10	H	3	0	0	0	0
All	All	28124	0	28159	459	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 8.

All (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:SER:HB3	2:B:491:LYS:HG2	1.45	0.98
2:B:705:ASP:O	2:B:706:GLU:HG3	1.64	0.96
1:A:53:LEU:HD22	1:A:62:LEU:HD13	1.48	0.94
2:B:780:THR:HB	2:B:784:GLU:HB3	1.48	0.94
2:B:475:SER:CB	2:B:491:LYS:HG2	1.96	0.94
2:B:138:GLY:O	2:B:139:LEU:HD12	1.70	0.92
2:B:252:ILE:HD12	2:B:281:PHE:CE1	2.06	0.91
2:B:452:VAL:HG13	2:B:454:ASP:OD2	1.73	0.89
2:B:463:VAL:HG13	2:B:505:SER:O	1.74	0.88
7:G:719:LEU:HD13	7:G:732:LEU:HD22	1.55	0.88
2:B:836:VAL:HG13	3:C:88:ILE:HG21	1.53	0.87
2:B:476:VAL:HG11	2:B:526:LEU:HD21	1.57	0.87
3:C:100:LEU:HD12	3:C:100:LEU:O	1.75	0.86
2:B:382:PHE:HE2	3:C:100:LEU:CD2	1.88	0.86
2:B:138:GLY:C	2:B:139:LEU:HD12	2.02	0.84
2:B:566:ALA:HB2	2:B:582:LEU:HD11	1.60	0.83
2:B:467:GLN:C	2:B:468:LEU:HD12	2.03	0.83
2:B:102:THR:HG21	2:B:1067:LYS:CG	2.10	0.82
2:B:288:GLU:HB2	2:B:298:LYS:HB2	1.62	0.81
9:I:122:MET:HG2	9:I:139:GLU:OE1	1.80	0.81
2:B:102:THR:HG21	2:B:1067:LYS:HG2	1.63	0.80
7:G:700:ILE:HD11	7:G:719:LEU:HD11	1.65	0.79
2:B:780:THR:HB	2:B:784:GLU:CB	2.13	0.78
2:B:166:ASP:OD1	2:B:167:VAL:N	2.17	0.77
2:B:452:VAL:HG11	2:B:455:GLN:NE2	2.00	0.77
2:B:836:VAL:CG1	3:C:88:ILE:HG21	2.15	0.77
7:G:476:LEU:HD21	7:G:495:PHE:CZ	2.19	0.77
2:B:559:GLY:O	2:B:560:LEU:HD12	1.87	0.74
2:B:238:THR:HG23	2:B:247:ALA:HB2	1.70	0.74
1:A:52:HIS:C	1:A:53:LEU:HD12	2.13	0.74
2:B:252:ILE:HD12	2:B:281:PHE:HE1	1.51	0.73
7:G:727:VAL:HG11	7:G:732:LEU:HD21	1.71	0.73
3:C:92:VAL:HG12	3:C:103:MET:CE	2.19	0.72
3:C:92:VAL:HG12	3:C:103:MET:HE2	1.69	0.72
2:B:492:GLU:HG2	2:B:496:LYS:HB2	1.72	0.72
2:B:675:GLU:O	2:B:695:ASN:ND2	2.23	0.72
7:G:82:ASN:O	7:G:86:LEU:HD13	1.89	0.72
7:G:248:GLN:O	7:G:252:GLN:NE2	2.23	0.72
2:B:452:VAL:CG1	2:B:454:ASP:OD2	2.37	0.72
2:B:481:GLN:O	2:B:484:LYS:HG3	1.88	0.72
2:B:559:GLY:C	2:B:560:LEU:HD12	2.15	0.71
7:G:161:VAL:HG11	7:G:169:SER:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:660:TYR:CD1	2:B:707:ILE:CG2	2.73	0.71
7:G:51:ARG:HB3	7:G:52:PRO:HD2	1.73	0.71
9:I:199:THR:O	9:I:203:ILE:HG22	1.90	0.71
7:G:454:LYS:NZ	7:G:494:MET:SD	2.64	0.70
2:B:426:VAL:HG22	2:B:435:VAL:HG13	1.72	0.70
9:I:203:ILE:O	9:I:1012:ARG:NH1	2.24	0.70
2:B:188:ARG:NH1	2:B:216:ALA:O	2.25	0.70
7:G:286:LEU:O	7:G:290:VAL:HG23	1.92	0.70
2:B:660:TYR:CG	2:B:707:ILE:HG21	2.26	0.69
2:B:463:VAL:HG23	2:B:469:ILE:HG22	1.75	0.69
1:A:1021:MET:O	1:A:1026:ARG:NH1	2.24	0.69
2:B:382:PHE:CE2	3:C:100:LEU:HD21	2.28	0.69
2:B:576:LEU:N	2:B:576:LEU:HD12	2.08	0.69
2:B:616:LEU:HD13	2:B:623:LEU:CD1	2.22	0.69
2:B:169:PHE:CE1	2:B:178:ILE:CG2	2.76	0.69
7:G:59:THR:HG23	7:G:60:GLN:HE21	1.57	0.69
3:C:95:LYS:HG2	3:C:100:LEU:HD11	1.75	0.69
7:G:243:TYR:HE2	7:G:290:VAL:HG22	1.59	0.68
7:G:587:LYS:NZ	7:G:662:HIS:O	2.26	0.68
2:B:722:ARG:NH1	2:B:738:SER:OG	2.26	0.68
2:B:1055:GLN:NE2	2:B:1090:ASP:OD1	2.27	0.67
9:I:236:LEU:O	9:I:240:VAL:HG23	1.94	0.67
9:I:215:LEU:HD21	9:I:924:VAL:HB	1.77	0.67
9:I:229:CYS:O	9:I:233:THR:HG23	1.95	0.67
1:A:54:LYS:HG3	1:A:118:ASP:HB2	1.77	0.67
2:B:705:ASP:O	2:B:706:GLU:CG	2.42	0.67
2:B:616:LEU:CD1	2:B:623:LEU:HD12	2.26	0.66
2:B:580:GLU:OE1	2:B:623:LEU:CD2	2.44	0.66
2:B:448:LEU:HD23	2:B:451:PHE:CD1	2.31	0.65
5:E:95:PHE:HE2	5:E:111:ILE:HG22	1.62	0.65
2:B:382:PHE:HE2	3:C:100:LEU:HD21	1.59	0.65
2:B:180:PHE:HE2	2:B:193:TYR:HD2	1.45	0.65
2:B:519:LEU:HD23	2:B:528:GLN:HA	1.77	0.65
7:G:243:TYR:CE2	7:G:290:VAL:HG22	2.32	0.65
7:G:263:VAL:HG13	7:G:294:LEU:HD23	1.79	0.64
2:B:444:GLU:HB2	7:G:46:LYS:HE3	1.79	0.64
2:B:660:TYR:CE1	2:B:707:ILE:CG2	2.79	0.64
8:H:43:ALA:O	8:H:46:ARG:NH1	2.31	0.64
4:D:37:CYS:SG	4:D:82:ARG:NH1	2.70	0.64
2:B:593:MET:HB3	2:B:602:LEU:HD13	1.78	0.64
2:B:597:GLU:OE1	2:B:597:GLU:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:448:VAL:HG22	7:G:688:VAL:HG11	1.79	0.64
9:I:56:ILE:HG23	9:I:125:ILE:CD1	2.28	0.64
2:B:467:GLN:HA	2:B:480:SER:HA	1.78	0.64
6:F:47:ASN:OD1	6:F:48:ALA:N	2.31	0.63
2:B:555:LEU:HD22	2:B:618:ILE:HG22	1.80	0.63
2:B:623:LEU:HD12	2:B:623:LEU:N	2.13	0.62
2:B:824:ASP:OD2	2:B:893:TRP:NE1	2.32	0.62
2:B:499:SER:HB3	7:G:84:GLU:HB3	1.81	0.62
2:B:467:GLN:O	2:B:468:LEU:HD12	1.98	0.62
9:I:929:LEU:O	9:I:933:LYS:N	2.32	0.61
7:G:270:GLU:OE2	7:G:286:LEU:HD21	2.01	0.61
9:I:230:LYS:HE3	9:I:230:LYS:HA	1.82	0.61
1:A:53:LEU:HD22	1:A:62:LEU:CD1	2.26	0.61
7:G:270:GLU:OE1	7:G:273:ARG:NH2	2.33	0.61
2:B:884:ILE:HG22	2:B:885:ASN:H	1.64	0.61
9:I:920:ASN:O	9:I:924:VAL:HG23	2.01	0.61
4:D:55:ARG:NH2	4:D:121:ASP:OD2	2.32	0.61
2:B:636:THR:HG22	2:B:653:SER:HB3	1.83	0.61
5:E:95:PHE:CD2	5:E:115:VAL:HG21	2.36	0.60
2:B:102:THR:HG21	2:B:1067:LYS:HG3	1.83	0.60
7:G:495:PHE:HA	7:G:498:MET:SD	2.41	0.60
2:B:576:LEU:N	2:B:576:LEU:CD1	2.63	0.60
2:B:564:ILE:HG23	2:B:588:PRO:HD3	1.83	0.60
2:B:616:LEU:HD13	2:B:623:LEU:HD12	1.83	0.60
2:B:169:PHE:CE1	2:B:178:ILE:HG22	2.36	0.60
5:E:95:PHE:CE2	5:E:111:ILE:HG22	2.36	0.60
7:G:429:LEU:HD23	7:G:433:LEU:HD13	1.83	0.60
9:I:50:GLU:N	9:I:50:GLU:OE1	2.35	0.59
1:A:179:ASN:OD1	4:D:84:ARG:NH1	2.35	0.59
5:E:174:PRO:O	5:E:175:THR:OG1	2.17	0.59
1:A:53:LEU:CD2	1:A:62:LEU:HD13	2.28	0.59
2:B:943:GLU:HB2	3:C:51:ALA:HB3	1.85	0.59
2:B:569:LEU:HD12	2:B:569:LEU:O	2.03	0.59
2:B:660:TYR:CE1	2:B:707:ILE:HG23	2.36	0.59
5:E:84:GLN:OE1	5:E:84:GLN:N	2.36	0.59
9:I:149:TRP:CD1	9:I:156:THR:HG1	2.20	0.59
2:B:105:HIS:O	2:B:151:GLU:HG2	2.02	0.59
1:A:1030:MET:O	1:A:1034:LEU:HD23	2.03	0.58
2:B:623:LEU:CD1	2:B:623:LEU:N	2.66	0.58
7:G:548:ILE:O	7:G:552:GLU:OE1	2.21	0.58
7:G:697:ASP:O	7:G:701:VAL:HG23	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:VAL:CG1	2:B:526:LEU:HD21	2.29	0.58
6:F:130:LEU:O	6:F:133:VAL:HG22	2.04	0.58
9:I:191:SER:O	9:I:195:LEU:HD23	2.03	0.58
2:B:382:PHE:CE2	3:C:100:LEU:CD2	2.76	0.58
2:B:593:MET:HB3	2:B:602:LEU:CD1	2.33	0.58
9:I:123:VAL:CG2	9:I:138:ARG:HB3	2.33	0.58
2:B:534:MET:HE3	2:B:560:LEU:HD21	1.85	0.58
7:G:259:TYR:O	7:G:263:VAL:HG23	2.03	0.58
2:B:954:MET:HE1	2:B:975:PHE:CE1	2.39	0.58
5:E:197:GLU:OE1	5:E:197:GLU:N	2.36	0.58
6:F:200:GLN:OE1	6:F:200:GLN:N	2.36	0.58
5:E:142:LEU:HD13	5:E:153:ILE:O	2.04	0.57
7:G:544:THR:HB	7:G:547:MET:HE2	1.86	0.57
2:B:219:VAL:HG22	2:B:219:VAL:O	2.04	0.57
4:D:235:TYR:HH	4:D:242:TYR:N	2.01	0.57
1:A:54:LYS:HD3	1:A:61:MET:HE1	1.86	0.57
2:B:195:VAL:HG22	2:B:202:PHE:CE1	2.39	0.57
7:G:263:VAL:HG13	7:G:294:LEU:CD2	2.34	0.57
2:B:901:THR:HG23	3:C:46:PRO:CD	2.34	0.57
3:C:100:LEU:O	3:C:100:LEU:CD1	2.52	0.57
6:F:18:PHE:HZ	6:F:33:VAL:HG13	1.69	0.57
2:B:112:ILE:HG23	2:B:112:ILE:O	2.05	0.57
5:E:159:GLU:O	6:F:17:ARG:NH2	2.38	0.57
2:B:636:THR:HG22	2:B:653:SER:CB	2.35	0.56
2:B:705:ASP:C	2:B:706:GLU:HG3	2.30	0.56
5:E:168:ARG:NH2	5:E:170:ASP:OD2	2.38	0.56
2:B:494:GLN:CD	2:B:496:LYS:HE2	2.29	0.56
2:B:577:LEU:HD23	2:B:621:GLY:HA3	1.87	0.56
2:B:929:SER:O	2:B:930:VAL:HG13	2.05	0.56
5:E:96:LEU:HD12	5:E:97:LEU:N	2.20	0.56
2:B:518:TYR:CE2	2:B:529:ILE:HG21	2.41	0.56
2:B:143:ILE:HG12	2:B:154:ALA:HB2	1.88	0.56
2:B:476:VAL:HG11	2:B:526:LEU:CD2	2.31	0.56
2:B:901:THR:HG23	3:C:46:PRO:HD3	1.88	0.56
2:B:414:ARG:N	2:B:462:ASN:HD21	2.03	0.56
2:B:169:PHE:CE1	2:B:178:ILE:HG23	2.41	0.56
2:B:660:TYR:CD1	2:B:707:ILE:HG23	2.41	0.56
2:B:840:GLU:OE1	2:B:840:GLU:N	2.39	0.56
2:B:901:THR:HG21	3:C:45:VAL:HA	1.88	0.55
7:G:232:GLU:O	7:G:236:LEU:HD23	2.06	0.55
2:B:486:LEU:HD11	2:B:489:GLU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:189:GLN:NE2	7:G:193:ILE:HD11	2.21	0.55
2:B:39:LEU:HD13	2:B:64:MET:HE1	1.88	0.55
7:G:549:LYS:O	7:G:553:VAL:HG23	2.06	0.55
9:I:56:ILE:HA	9:I:125:ILE:HD13	1.89	0.55
1:A:896:GLN:O	1:A:900:GLU:HG2	2.06	0.55
7:G:669:ILE:O	7:G:669:ILE:HG22	2.07	0.55
2:B:639:ARG:NH1	2:B:679:MET:O	2.40	0.55
2:B:463:VAL:CG2	2:B:469:ILE:HG22	2.36	0.54
7:G:455:LYS:NZ	7:G:676:GLU:OE1	2.39	0.54
2:B:457:THR:HG21	2:B:460:CYS:HB2	1.89	0.54
2:B:660:TYR:CD1	2:B:707:ILE:HG21	2.40	0.54
2:B:494:GLN:O	2:B:494:GLN:HG2	2.07	0.54
2:B:780:THR:HG22	2:B:784:GLU:HG2	1.89	0.54
7:G:541:VAL:HG11	7:G:571:THR:OG1	2.07	0.54
2:B:929:SER:O	2:B:930:VAL:CG1	2.55	0.54
7:G:503:ASP:O	7:G:507:HIS:ND1	2.25	0.54
1:A:897:GLU:N	1:A:897:GLU:OE1	2.41	0.54
2:B:463:VAL:HG12	2:B:464:ALA:N	2.23	0.54
6:F:72:LYS:NZ	6:F:177:GLU:OE2	2.40	0.54
2:B:580:GLU:CD	2:B:623:LEU:CD2	2.81	0.54
2:B:77:LEU:HD13	2:B:79:ILE:HD11	1.88	0.54
2:B:744:ASP:O	2:B:748:GLY:N	2.41	0.54
5:E:124:PRO:HA	5:E:127:PHE:CE1	2.43	0.54
7:G:591:VAL:HG12	7:G:631:LEU:HD11	1.89	0.54
7:G:47:ASN:OD1	7:G:47:ASN:O	2.26	0.53
2:B:838:PRO:HA	3:C:88:ILE:HD11	1.91	0.53
5:E:251:GLY:O	5:E:255:ASN:ND2	2.42	0.53
2:B:490:TRP:CD2	2:B:519:LEU:HD11	2.43	0.53
2:B:580:GLU:CD	2:B:623:LEU:HD22	2.34	0.53
2:B:414:ARG:H	2:B:462:ASN:HD21	1.54	0.53
9:I:56:ILE:HG23	9:I:125:ILE:HD11	1.90	0.53
2:B:1008:CYS:O	2:B:1029:LEU:N	2.40	0.53
9:I:215:LEU:HD11	9:I:924:VAL:HG12	1.89	0.53
2:B:1078:THR:HG22	2:B:1079:GLU:N	2.23	0.52
7:G:721:ASN:OD1	7:G:722:GLN:N	2.41	0.52
2:B:382:PHE:HE2	3:C:100:LEU:HD22	1.71	0.52
1:A:54:LYS:HB2	1:A:118:ASP:O	2.10	0.52
5:E:207:VAL:O	5:E:207:VAL:HG13	2.08	0.52
7:G:102:LEU:HD22	7:G:156:LEU:HD13	1.91	0.52
7:G:368:PHE:O	7:G:372:VAL:HG23	2.10	0.52
7:G:541:VAL:HG21	7:G:571:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:215:LEU:HD11	9:I:924:VAL:CG1	2.39	0.52
2:B:424:THR:HG23	2:B:435:VAL:HG12	1.92	0.52
2:B:477:ARG:HG2	2:B:489:GLU:HG3	1.92	0.52
7:G:742:ARG:NH1	8:H:64:THR:OG1	2.43	0.52
1:A:1001:LEU:HD22	1:A:1036:MET:SD	2.50	0.52
2:B:424:THR:CG2	2:B:435:VAL:HG12	2.40	0.51
5:E:122:ILE:HG23	5:E:126:LEU:HD23	1.92	0.51
9:I:178:PHE:CD1	9:I:1021:ILE:HD11	2.44	0.51
2:B:96:GLU:OE1	2:B:96:GLU:N	2.43	0.51
7:G:602:PHE:O	8:H:21:ARG:NH2	2.43	0.51
2:B:707:ILE:HG22	2:B:707:ILE:O	2.09	0.51
2:B:492:GLU:HG3	2:B:494:GLN:H	1.75	0.51
2:B:519:LEU:CD2	2:B:528:GLN:HA	2.40	0.51
1:A:234:LYS:O	1:A:238:HIS:ND1	2.43	0.51
2:B:128:CYS:O	2:B:145:LEU:HD23	2.10	0.51
7:G:604:GLU:N	7:G:604:GLU:OE1	2.44	0.51
7:G:621:ASP:OD1	7:G:622:SER:N	2.44	0.51
2:B:518:TYR:HE2	2:B:529:ILE:HG21	1.77	0.50
2:B:660:TYR:CG	2:B:707:ILE:CG2	2.94	0.50
2:B:134:ARG:NH1	2:B:164:VAL:O	2.45	0.50
5:E:224:THR:OG1	5:E:225:GLU:OE1	2.25	0.50
2:B:836:VAL:HG13	3:C:88:ILE:CG2	2.35	0.50
7:G:710:LEU:N	7:G:754:GLN:OE1	2.45	0.50
9:I:111:GLY:O	9:I:114:VAL:HG22	2.10	0.50
9:I:902:GLN:O	9:I:905:GLU:HG3	2.12	0.50
3:C:83:VAL:O	3:C:83:VAL:HG13	2.12	0.50
4:D:271:ALA:O	4:D:302:ARG:NH1	2.45	0.50
1:A:993:SER:O	1:A:997:VAL:HG23	2.12	0.49
2:B:132:GLY:C	2:B:133:LEU:HD12	2.37	0.49
2:B:488:SER:CB	2:B:525:GLU:HA	2.42	0.49
5:E:133:ARG:O	5:E:137:VAL:HG22	2.12	0.49
2:B:660:TYR:CZ	2:B:707:ILE:HG22	2.47	0.49
4:D:90:ALA:O	4:D:94:VAL:HG23	2.13	0.49
2:B:612:PHE:HB3	2:B:614:PHE:CZ	2.48	0.49
7:G:356:GLU:OE1	7:G:356:GLU:N	2.45	0.49
2:B:1095:GLU:HG2	2:B:1137:THR:HG22	1.95	0.49
7:G:543:LEU:O	7:G:548:ILE:HD11	2.13	0.49
2:B:928:ARG:NH2	3:C:132:PHE:O	2.45	0.49
6:F:102:ALA:HB3	6:F:105:GLU:OE1	2.12	0.49
2:B:413:LEU:HD23	2:B:424:THR:HG21	1.94	0.49
2:B:811:GLU:HG2	2:B:833:THR:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:929:SER:C	2:B:930:VAL:HG13	2.37	0.49
1:A:45:VAL:HG11	1:A:129:ASP:O	2.12	0.49
2:B:616:LEU:HD13	2:B:623:LEU:HD11	1.94	0.49
7:G:238:GLU:O	7:G:242:LEU:HD13	2.13	0.49
1:A:940:ARG:HG3	3:C:71:LEU:HD12	1.94	0.48
7:G:318:ASP:OD1	7:G:319:LEU:N	2.45	0.48
2:B:230:ILE:HD11	2:B:285:LEU:HD11	1.94	0.48
2:B:499:SER:HB3	7:G:84:GLU:CB	2.42	0.48
1:A:52:HIS:O	1:A:53:LEU:HD12	2.12	0.48
2:B:580:GLU:OE1	2:B:623:LEU:HD23	2.12	0.48
4:D:314:TRP:O	4:D:318:VAL:HG23	2.13	0.48
9:I:89:ILE:CD1	9:I:1071:VAL:HG11	2.44	0.48
1:A:228:GLU:OE2	1:A:232:ARG:NH2	2.46	0.48
6:F:205:GLU:HG3	6:F:206:THR:HG23	1.94	0.48
2:B:901:THR:CG2	3:C:45:VAL:HA	2.43	0.48
6:F:230:HIS:O	6:F:231:CYS:SG	2.72	0.48
2:B:67:PHE:HE1	2:B:78:PHE:HB2	1.79	0.48
5:E:156:ASN:OD1	6:F:20:GLN:NE2	2.46	0.48
2:B:569:LEU:HD12	2:B:569:LEU:C	2.38	0.47
3:C:96:ARG:HA	3:C:101:SER:HB3	1.95	0.47
5:E:186:ILE:HG12	5:E:193:ILE:HG22	1.96	0.47
2:B:4:ASN:HD21	2:B:976:VAL:HG21	1.78	0.47
6:F:180:ILE:HG22	6:F:188:VAL:HG11	1.96	0.47
2:B:498:ILE:HG22	2:B:512:VAL:HG12	1.96	0.47
7:G:491:LEU:O	7:G:494:MET:HG2	2.15	0.47
7:G:463:VAL:HG12	7:G:575:HIS:ND1	2.29	0.47
1:A:77:ASN:OD1	1:A:78:ASN:N	2.46	0.47
2:B:780:THR:CG2	2:B:784:GLU:HG2	2.43	0.47
2:B:1105:MET:HE1	2:B:1130:ILE:HD11	1.96	0.47
4:D:306:VAL:HG22	4:D:306:VAL:O	2.15	0.47
9:I:1018:VAL:HG13	9:I:1021:ILE:HD12	1.97	0.47
1:A:248:LYS:O	1:A:252:VAL:HG23	2.14	0.47
1:A:157:LYS:NZ	1:A:161:GLY:O	2.31	0.47
4:D:111:MET:SD	4:D:111:MET:N	2.87	0.47
9:I:190:LEU:HB3	9:I:195:LEU:HD21	1.97	0.47
5:E:281:GLN:N	5:E:281:GLN:OE1	2.48	0.46
9:I:1020:GLU:OE1	9:I:1023:GLN:NE2	2.48	0.46
2:B:463:VAL:CG2	2:B:469:ILE:CG2	2.94	0.46
2:B:502:SER:OG	2:B:543:ILE:HG13	2.14	0.46
2:B:488:SER:HB2	2:B:525:GLU:HG3	1.97	0.46
2:B:515:ALA:HA	2:B:533:GLU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:242:TYR:N	4:D:244:GLU:OE1	2.49	0.46
9:I:172:VAL:HG22	9:I:177:GLN:NE2	2.30	0.46
9:I:1025:MET:SD	9:I:1025:MET:N	2.88	0.46
1:A:62:LEU:HD23	1:A:63:GLY:O	2.15	0.46
6:F:14:VAL:HG22	6:F:44:HIS:CB	2.45	0.46
2:B:592:LEU:O	2:B:602:LEU:HD12	2.15	0.46
2:B:830:ILE:HG22	2:B:873:MET:HE1	1.96	0.46
7:G:541:VAL:HG11	7:G:571:THR:CB	2.46	0.46
2:B:475:SER:HB2	2:B:490:TRP:O	2.16	0.46
2:B:532:THR:OG1	2:B:574:PHE:HD1	1.99	0.46
7:G:545:PRO:HA	7:G:548:ILE:HD12	1.97	0.46
2:B:884:ILE:HG22	2:B:885:ASN:N	2.30	0.46
2:B:1125:THR:HG23	2:B:1127:ASP:H	1.81	0.46
4:D:124:PHE:O	4:D:127:VAL:HG12	2.16	0.46
2:B:565:SER:HA	2:B:580:GLU:O	2.16	0.46
2:B:707:ILE:CG2	2:B:707:ILE:O	2.64	0.45
7:G:544:THR:CB	7:G:547:MET:HE2	2.46	0.45
7:G:447:ASP:OD1	7:G:448:VAL:N	2.47	0.45
7:G:211:ARG:HD2	7:G:276:THR:HG21	1.97	0.45
8:H:53:CYS:H	8:H:56:CYS:HB2	1.80	0.45
1:A:935:ARG:NH1	3:C:117:PHE:HB3	2.32	0.45
2:B:463:VAL:CG1	2:B:464:ALA:N	2.79	0.45
2:B:576:LEU:CD1	2:B:576:LEU:H	2.30	0.45
9:I:53:ILE:CG2	9:I:125:ILE:HG23	2.47	0.45
6:F:113:LEU:HD11	6:F:180:ILE:CG1	2.47	0.45
7:G:491:LEU:O	7:G:495:PHE:CD2	2.69	0.45
2:B:468:LEU:HD12	2:B:468:LEU:N	2.30	0.45
2:B:102:THR:HG23	2:B:102:THR:O	2.16	0.45
2:B:180:PHE:CE2	2:B:193:TYR:HD2	2.29	0.45
2:B:512:VAL:HG23	2:B:512:VAL:O	2.16	0.45
2:B:719:GLU:OE2	2:B:757:SER:OG	2.32	0.45
3:C:45:VAL:HG23	3:C:47:THR:HG23	1.98	0.45
7:G:96:HIS:O	7:G:98:VAL:HG23	2.16	0.45
7:G:385:ARG:O	7:G:389:LEU:HD23	2.17	0.45
9:I:91:CYS:O	9:I:95:LEU:HD23	2.17	0.45
3:C:92:VAL:CG1	3:C:103:MET:SD	3.05	0.45
2:B:739:ARG:NH2	2:B:741:GLU:OE2	2.48	0.45
3:C:95:LYS:HG2	3:C:100:LEU:CD1	2.44	0.45
4:D:246:VAL:HG11	9:I:80:GLY:C	2.42	0.45
2:B:521:ILE:HG22	2:B:526:LEU:HG	1.99	0.44
2:B:693:LEU:N	2:B:700:THR:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:VAL:O	4:D:163:VAL:HG12	2.17	0.44
6:F:116:ILE:HD11	6:F:122:GLY:O	2.17	0.44
7:G:69:ALA:HB1	7:G:86:LEU:HD21	1.98	0.44
2:B:421:THR:HB	2:B:684:SER:HA	2.00	0.44
4:D:233:ARG:NH2	9:I:68:GLU:OE1	2.50	0.44
2:B:404:LEU:HD21	7:G:45:ILE:HD13	1.99	0.44
5:E:173:THR:N	5:E:174:PRO:HD2	2.32	0.44
7:G:413:VAL:CG2	7:G:436:ILE:HG21	2.47	0.44
1:A:925:HIS:CE1	3:C:77:ARG:HG3	2.53	0.44
2:B:5:TYR:N	2:B:1041:THR:O	2.46	0.44
2:B:379:SER:HB2	2:B:388:ARG:HG3	2.00	0.44
2:B:451:PHE:CE2	2:B:470:GLN:HB2	2.52	0.44
2:B:1106:GLN:HA	2:B:1109:VAL:HG12	1.99	0.44
7:G:440:PHE:O	7:G:443:ILE:HG22	2.18	0.44
7:G:440:PHE:HA	7:G:443:ILE:HG22	2.00	0.44
1:A:72:ASN:HD21	1:A:1065:LEU:HD11	1.83	0.44
2:B:507:GLN:HB3	2:B:518:TYR:HE1	1.82	0.44
9:I:58:MET:HA	9:I:123:VAL:HG12	2.00	0.44
3:C:92:VAL:CG1	3:C:103:MET:CE	2.93	0.43
7:G:700:ILE:HD13	7:G:715:LEU:HD12	2.00	0.43
1:A:114:GLN:N	1:A:114:GLN:OE1	2.51	0.43
5:E:221:LYS:O	5:E:225:GLU:OE1	2.36	0.43
2:B:494:GLN:OE1	2:B:496:LYS:HE2	2.19	0.43
2:B:901:THR:HG23	3:C:46:PRO:HD2	1.98	0.43
2:B:1100:ILE:HG13	2:B:1105:MET:HG2	1.99	0.43
6:F:14:VAL:HG22	6:F:44:HIS:HB2	1.99	0.43
6:F:104:ASN:OD1	6:F:141:MET:HE3	2.17	0.43
2:B:469:ILE:CD1	2:B:508:VAL:HG21	2.48	0.43
9:I:215:LEU:HD21	9:I:924:VAL:CB	2.47	0.43
2:B:6:VAL:O	2:B:1091:GLY:N	2.43	0.43
2:B:178:ILE:HD11	2:B:202:PHE:CE2	2.54	0.43
4:D:146:ILE:HG22	4:D:146:ILE:O	2.19	0.43
7:G:330:ARG:O	7:G:334:GLN:NE2	2.51	0.43
2:B:296:THR:HG22	2:B:297:LEU:N	2.34	0.43
2:B:382:PHE:O	2:B:383:LYS:HG2	2.18	0.43
2:B:780:THR:HB	2:B:784:GLU:CG	2.49	0.43
5:E:143:VAL:HG21	5:E:256:LEU:HD12	2.01	0.43
9:I:114:VAL:HG21	9:I:118:CYS:O	2.19	0.43
2:B:611:LEU:HD11	2:B:638:LEU:HD21	2.01	0.43
3:C:58:LEU:HD23	3:C:58:LEU:HA	1.87	0.43
1:A:935:ARG:HH11	3:C:117:PHE:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:LEU:HD23	2:B:424:THR:CG2	2.49	0.43
2:B:468:LEU:HB2	2:B:479:VAL:O	2.18	0.43
7:G:492:GLU:O	7:G:496:LYS:HG2	2.19	0.43
7:G:700:ILE:HD12	7:G:736:ILE:HD11	2.00	0.43
2:B:67:PHE:CD2	2:B:145:LEU:HD21	2.54	0.42
2:B:479:VAL:HG22	2:B:486:LEU:HA	2.00	0.42
2:B:948:ASP:OD1	2:B:950:ASN:ND2	2.49	0.42
3:C:92:VAL:HG13	3:C:103:MET:HA	2.01	0.42
3:C:92:VAL:HG11	3:C:103:MET:SD	2.59	0.42
7:G:59:THR:O	7:G:63:TRP:HD1	2.02	0.42
1:A:905:LEU:O	1:A:909:VAL:HG23	2.19	0.42
2:B:187:GLY:O	2:B:189:HIS:ND1	2.52	0.42
2:B:593:MET:CB	2:B:602:LEU:HD13	2.49	0.42
2:B:954:MET:HE1	2:B:975:PHE:CZ	2.53	0.42
2:B:1055:GLN:HG3	2:B:1093:LEU:HD23	2.01	0.42
6:F:34:LYS:O	6:F:37:GLN:HG3	2.20	0.42
2:B:421:THR:O	2:B:422:ASP:C	2.61	0.42
7:G:124:ASP:OD1	7:G:125:SER:N	2.50	0.42
2:B:570:LYS:HB2	2:B:577:LEU:CD1	2.50	0.42
3:C:45:VAL:HG23	3:C:47:THR:CG2	2.50	0.42
7:G:678:VAL:O	7:G:682:VAL:HG23	2.20	0.42
2:B:209:GLN:NE2	2:B:210:GLU:O	2.53	0.42
2:B:511:ALA:HB2	2:B:516:LEU:HD12	2.02	0.42
7:G:413:VAL:HG22	7:G:436:ILE:HG21	2.00	0.42
8:H:55:GLU:OE2	8:H:60:GLN:HG3	2.19	0.42
2:B:568:ILE:HG13	2:B:623:LEU:HD11	2.01	0.42
2:B:1078:THR:CG2	2:B:1079:GLU:N	2.83	0.42
6:F:60:ILE:HA	6:F:63:VAL:HG12	2.02	0.42
7:G:491:LEU:O	7:G:495:PHE:HD2	2.03	0.42
2:B:1129:LEU:HD13	2:B:1129:LEU:HA	1.90	0.42
9:I:53:ILE:HG23	9:I:125:ILE:CG2	2.50	0.42
1:A:119:ILE:O	1:A:144:GLN:N	2.48	0.41
1:A:226:ILE:HG13	4:D:94:VAL:HG22	2.02	0.41
1:A:249:ARG:HD2	1:A:249:ARG:HA	1.87	0.41
2:B:915:LYS:HD3	2:B:915:LYS:HA	1.83	0.41
2:B:936:LYS:HA	2:B:936:LYS:HD2	1.81	0.41
7:G:352:VAL:HG12	7:G:361:MET:HE1	2.01	0.41
7:G:567:LEU:HD23	7:G:567:LEU:H	1.84	0.41
9:I:208:MET:CE	9:I:928:TRP:HB2	2.50	0.41
9:I:955:GLU:OE2	9:I:974:ARG:NH2	2.53	0.41
9:I:1005:MET:HE1	9:I:1040:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:ASP:OD1	2:B:300:LEU:N	2.51	0.41
4:D:221:VAL:HG23	4:D:228:LEU:HD13	2.03	0.41
1:A:54:LYS:CE	1:A:61:MET:HE1	2.50	0.41
4:D:254:ARG:NH1	9:I:1062:TYR:OH	2.53	0.41
7:G:69:ALA:O	7:G:73:VAL:HG23	2.20	0.41
7:G:593:LEU:HD11	8:H:27:TRP:HE1	1.85	0.41
9:I:55:ARG:H	9:I:126:GLU:HB3	1.84	0.41
9:I:1013:CYS:O	9:I:1047:SER:OG	2.24	0.41
5:E:252:PRO:O	5:E:256:LEU:HD23	2.20	0.41
7:G:669:ILE:HG23	7:G:672:ILE:HD12	2.02	0.41
1:A:72:ASN:OD1	1:A:73:PHE:N	2.54	0.41
1:A:945:PHE:CE2	1:A:949:LEU:HD11	2.56	0.41
7:G:69:ALA:CB	7:G:86:LEU:HD21	2.51	0.41
1:A:940:ARG:HG3	3:C:71:LEU:CD1	2.50	0.41
2:B:107:ASN:OD1	2:B:108:VAL:N	2.54	0.41
4:D:244:GLU:OE1	4:D:244:GLU:N	2.48	0.41
7:G:314:ASN:ND2	7:G:314:ASN:O	2.54	0.41
9:I:237:GLN:HA	9:I:237:GLN:OE1	2.20	0.41
4:D:262:VAL:HA	4:D:265:ILE:HG22	2.02	0.41
5:E:178:LEU:O	5:E:182:VAL:HG23	2.21	0.41
5:E:169:GLY:HA2	5:E:173:THR:HG21	2.02	0.41
7:G:595:GLN:HE22	7:G:599:LEU:HD22	1.85	0.41
2:B:909:ILE:HA	3:C:128:ARG:HH11	1.86	0.41
2:B:990:GLN:HE21	2:B:990:GLN:HB2	1.71	0.41
2:B:1133:VAL:O	2:B:1137:THR:HG23	2.20	0.41
7:G:448:VAL:HG22	7:G:688:VAL:CG1	2.46	0.41
9:I:94:CYS:O	9:I:99:GLY:N	2.51	0.41
9:I:1029:ASN:O	9:I:1033:VAL:HG23	2.20	0.41
2:B:169:PHE:HE1	2:B:178:ILE:HG23	1.86	0.41
7:G:429:LEU:O	7:G:433:LEU:HD13	2.20	0.41
7:G:437:MET:HE3	7:G:478:LYS:HB3	2.03	0.41
9:I:1066:MET:CG	9:I:1066:MET:O	2.69	0.41
2:B:467:GLN:HG2	2:B:480:SER:HB3	2.03	0.40
6:F:76:THR:O	6:F:80:GLY:N	2.52	0.40
6:F:158:TRP:C	6:F:159:LEU:HD12	2.46	0.40
1:A:935:ARG:HD3	3:C:117:PHE:CG	2.56	0.40
2:B:9:ALA:N	2:B:1037:ILE:O	2.54	0.40
4:D:163:VAL:O	4:D:164:LYS:C	2.64	0.40
6:F:29:GLU:O	6:F:33:VAL:HG23	2.21	0.40
2:B:117:GLU:C	2:B:119:GLY:H	2.30	0.40
2:B:570:LYS:HD3	2:B:577:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:250:TRP:CH2	5:E:263:VAL:HG21	2.57	0.40
9:I:1008:GLN:OE1	9:I:1008:GLN:N	2.48	0.40
2:B:560:LEU:HD22	2:B:567:ARG:HH11	1.87	0.40
2:B:580:GLU:CD	2:B:623:LEU:HD23	2.46	0.40
2:B:778:HIS:ND1	2:B:838:PRO:HD2	2.37	0.40
7:G:595:GLN:NE2	7:G:599:LEU:HD13	2.37	0.40
9:I:208:MET:HE2	9:I:928:TRP:HA	2.03	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	A	388/1091 (36%)	378 (97%)	10 (3%)	0	100	100
2	B	1138/1140 (100%)	1086 (95%)	52 (5%)	0	100	100
3	C	101/154 (66%)	96 (95%)	5 (5%)	0	100	100
4	D	217/333 (65%)	206 (95%)	11 (5%)	0	100	100
5	E	213/304 (70%)	205 (96%)	8 (4%)	0	100	100
6	F	235/266 (88%)	230 (98%)	5 (2%)	0	100	100
7	G	717/760 (94%)	700 (98%)	17 (2%)	0	100	100
8	H	88/108 (82%)	84 (96%)	4 (4%)	0	100	100
9	I	377/1101 (34%)	371 (98%)	6 (2%)	0	100	100
All	All	3474/5257 (66%)	3356 (97%)	118 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	348/979 (36%)	348 (100%)	0	100	100
2	B	999/999 (100%)	984 (98%)	15 (2%)	57	73
3	C	86/127 (68%)	84 (98%)	2 (2%)	44	68
4	D	200/296 (68%)	200 (100%)	0	100	100
5	E	195/257 (76%)	195 (100%)	0	100	100
6	F	216/242 (89%)	216 (100%)	0	100	100
7	G	656/679 (97%)	654 (100%)	2 (0%)	86	86
8	H	79/90 (88%)	78 (99%)	1 (1%)	61	75
9	I	346/1023 (34%)	346 (100%)	0	100	100
All	All	3125/4692 (67%)	3105 (99%)	20 (1%)	76	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	117	GLU
2	B	327	ARG
2	B	435	VAL
2	B	444	GLU
2	B	481	GLN
2	B	482	GLU
2	B	497	ASN
2	B	524	GLN
2	B	543	ILE
2	B	546	LEU
2	B	570	LYS
2	B	622	LEU
2	B	623	LEU
2	B	704	ILE
2	B	1129	LEU
3	C	78	ARG
3	C	118	LYS
7	G	54	LEU

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Mol	Chain	Res	Type
7	G	62	THR
8	H	39	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	964	ASN
2	B	4	ASN
2	B	30	ASN
2	B	105	HIS
2	B	156	ASN
2	B	240	HIS
2	B	261	HIS
2	B	455	GLN
2	B	462	ASN
2	B	465	HIS
2	B	467	GLN
2	B	578	HIS
2	B	617	ASN
2	B	796	GLN
2	B	852	GLN
2	B	952	ASN
2	B	990	GLN
3	C	87	GLN
6	F	25	HIS
7	G	60	GLN
7	G	673	GLN
7	G	712	HIS
8	H	41	ASN
8	H	47	ASN
9	I	1059	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

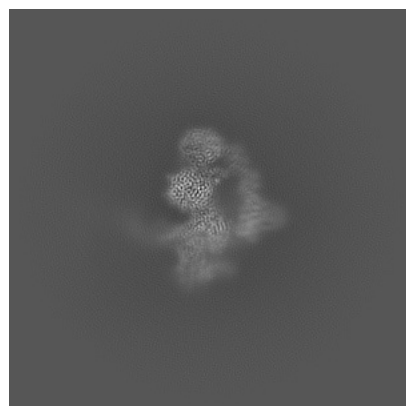
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63446. These allow visual inspection of the internal detail of the map and identification of artifacts.

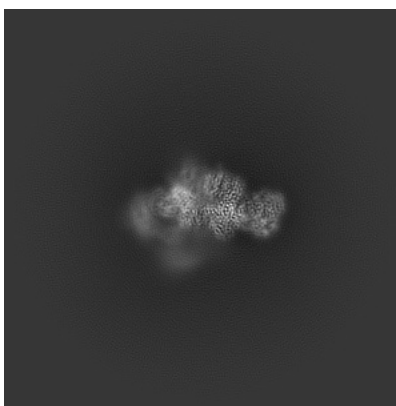
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

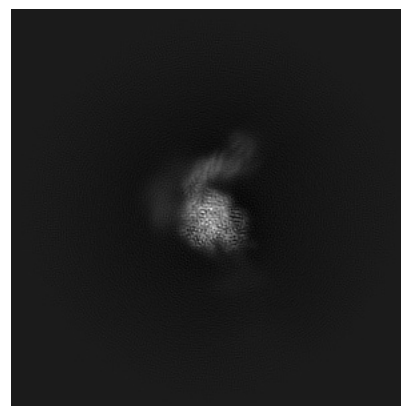
6.1.1 Primary map



X

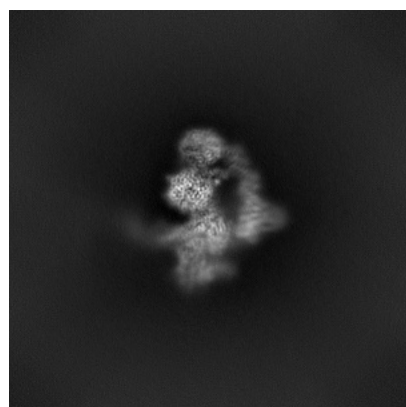


Y

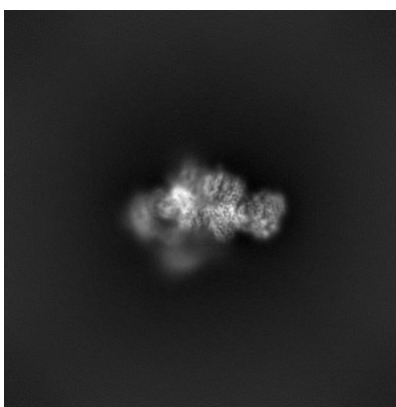


Z

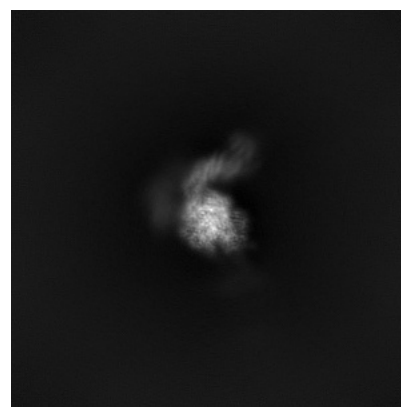
6.1.2 Raw map



X



Y

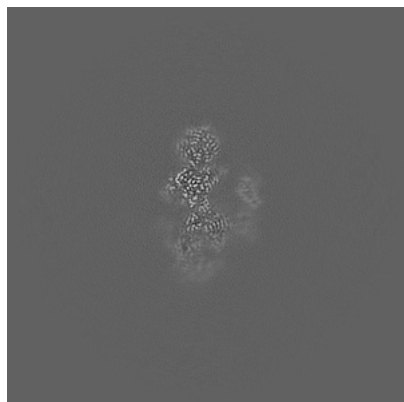


Z

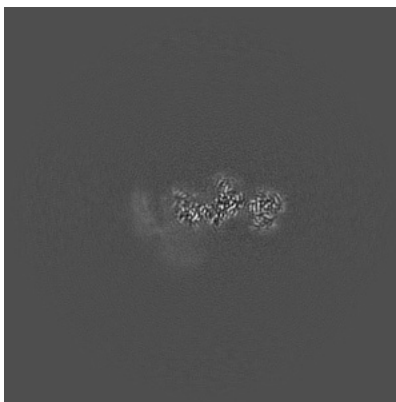
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

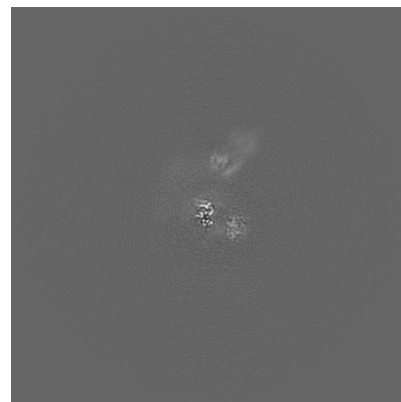
6.2.1 Primary map



X Index: 256

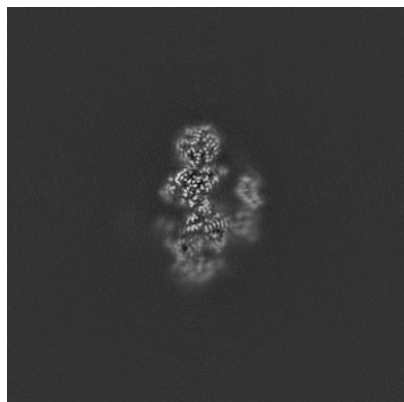


Y Index: 256

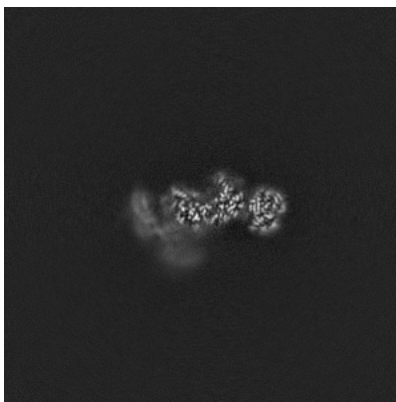


Z Index: 256

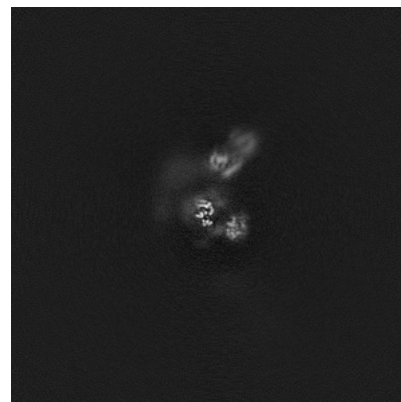
6.2.2 Raw map



X Index: 256



Y Index: 256

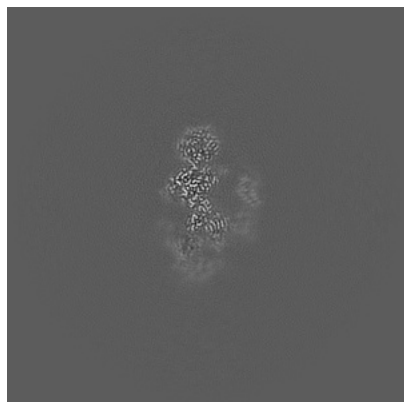


Z Index: 256

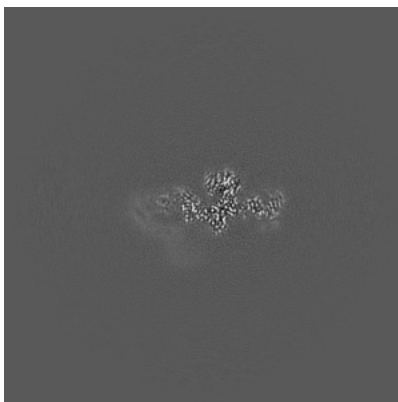
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

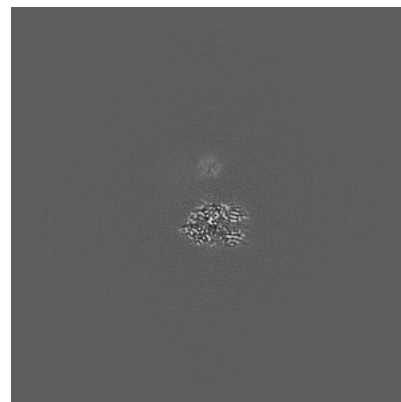
6.3.1 Primary map



X Index: 255

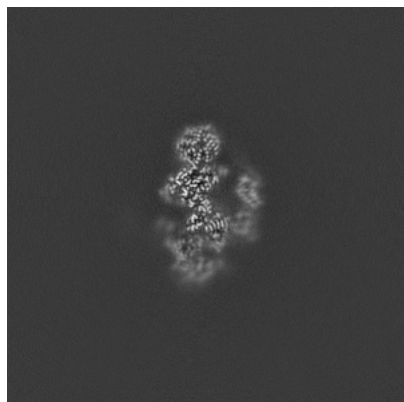


Y Index: 242

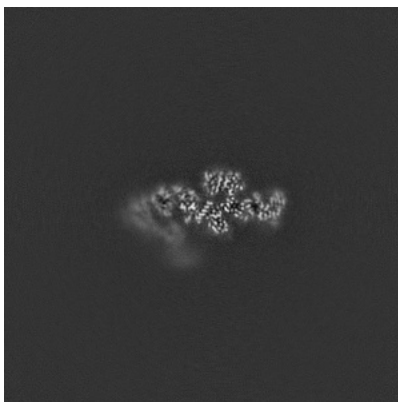


Z Index: 283

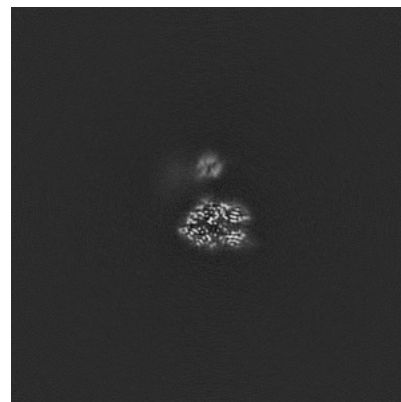
6.3.2 Raw map



X Index: 255



Y Index: 237

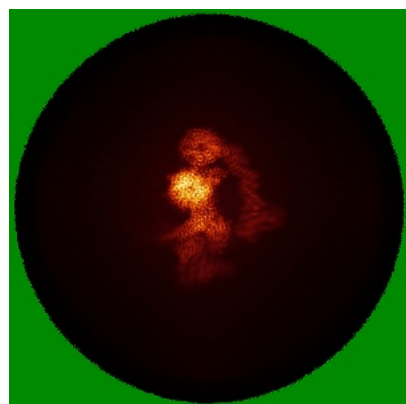


Z Index: 283

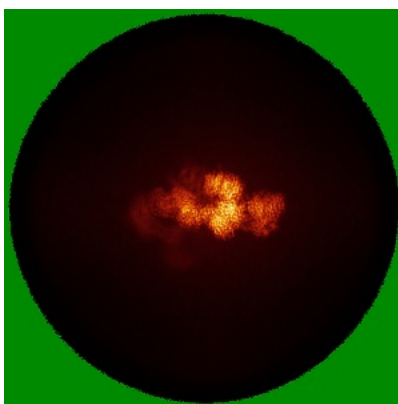
The images above show the largest variance slices of the map in three orthogonal directions.

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

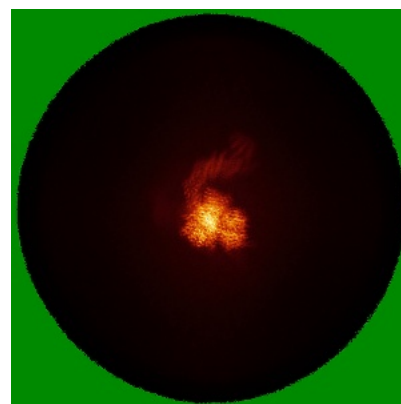
6.4.1 Primary map



X

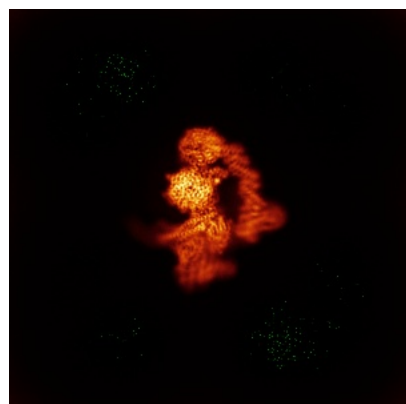


Y

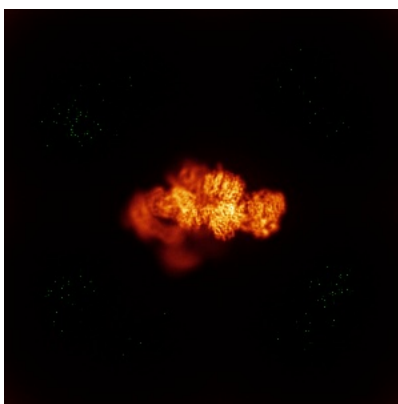


Z

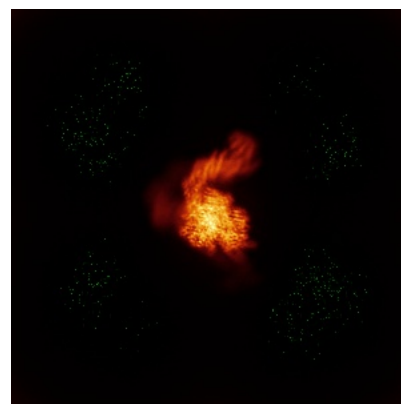
6.4.2 Raw map



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.

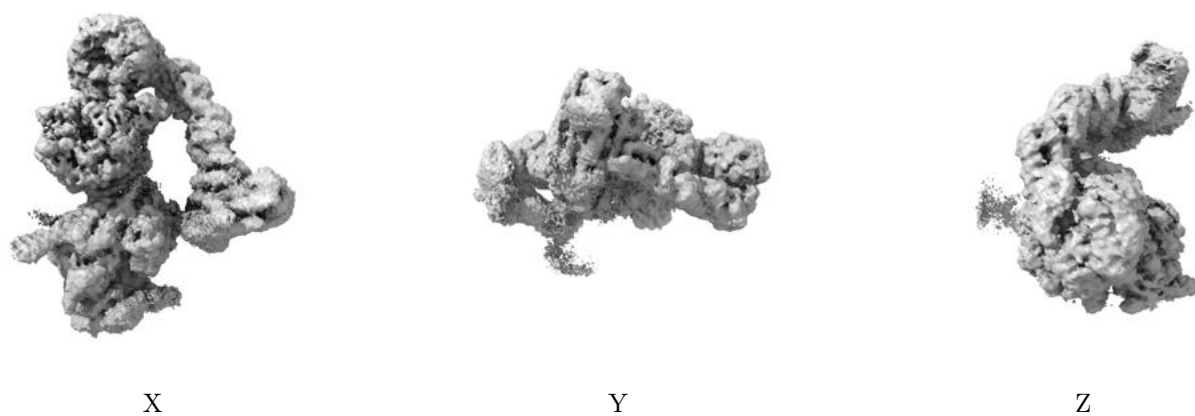
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

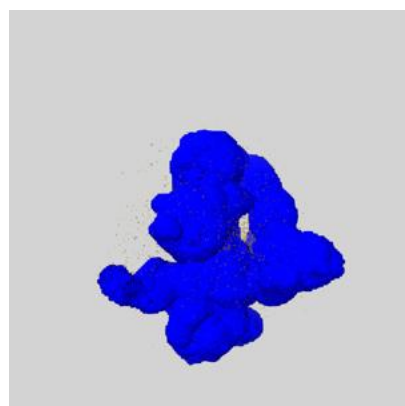
6.6 Mask visualisation [i](#)

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

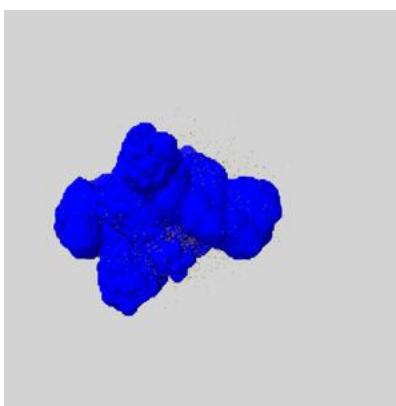
A mask typically either:

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

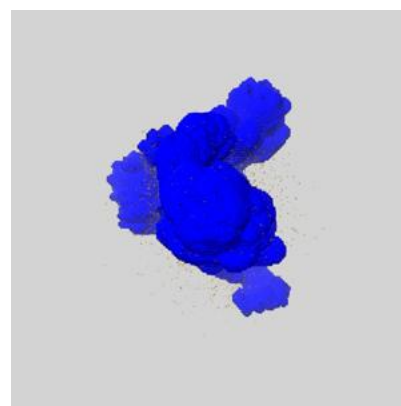
6.6.1 emd_63446_msk_1.map [i](#)



X



Y

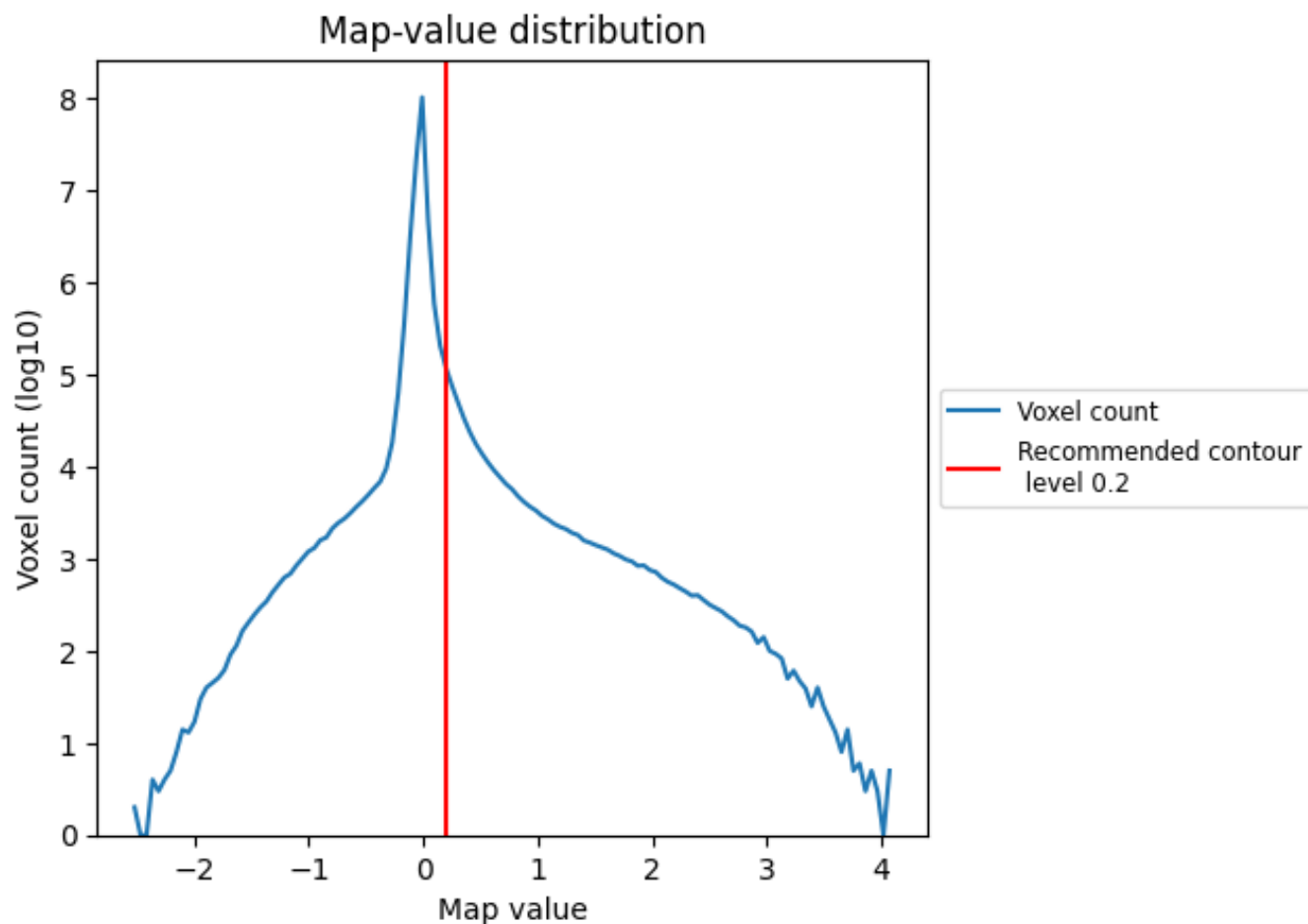


Z

7 Map analysis [i](#)

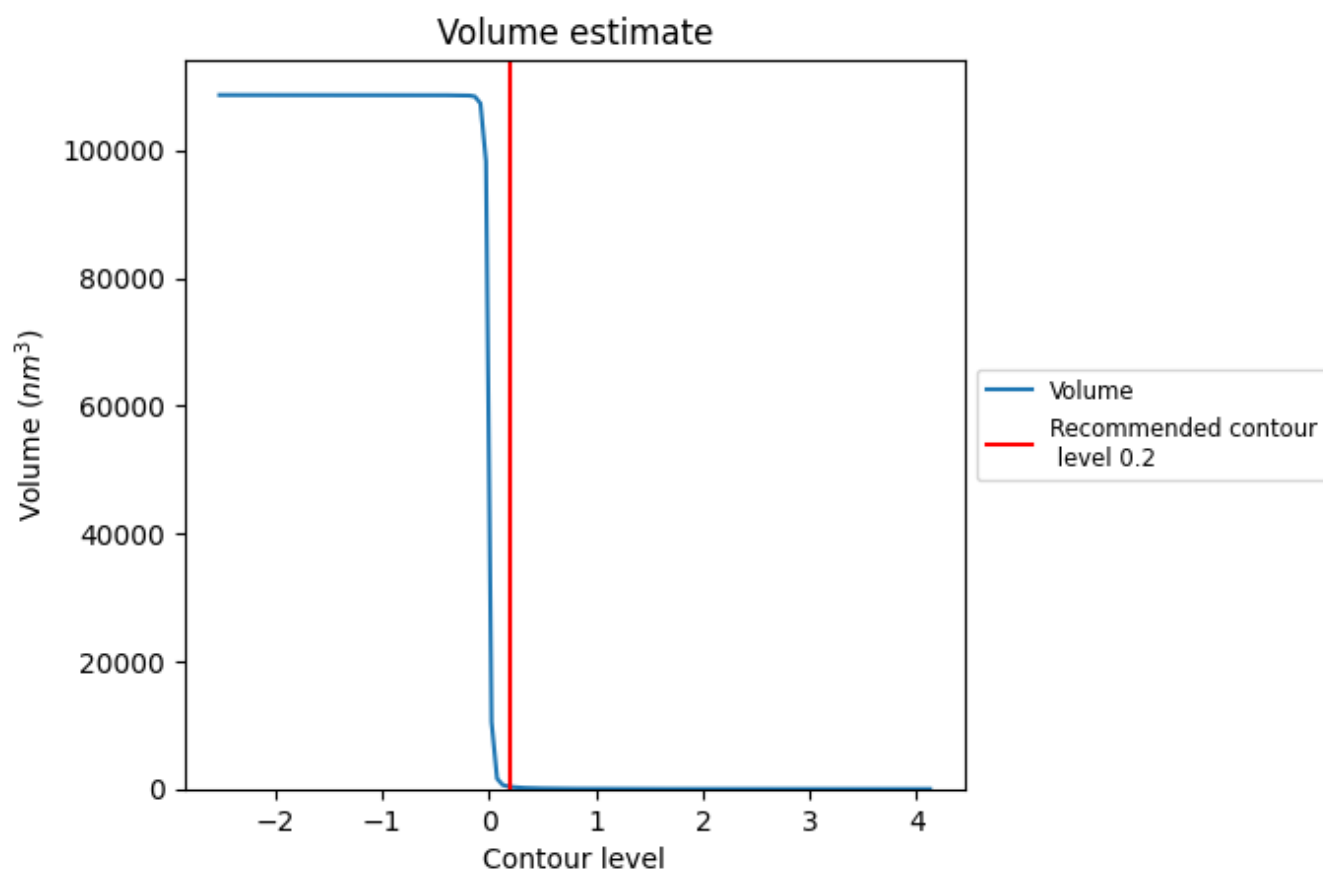
This section contains the results of statistical analysis of the map.

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.

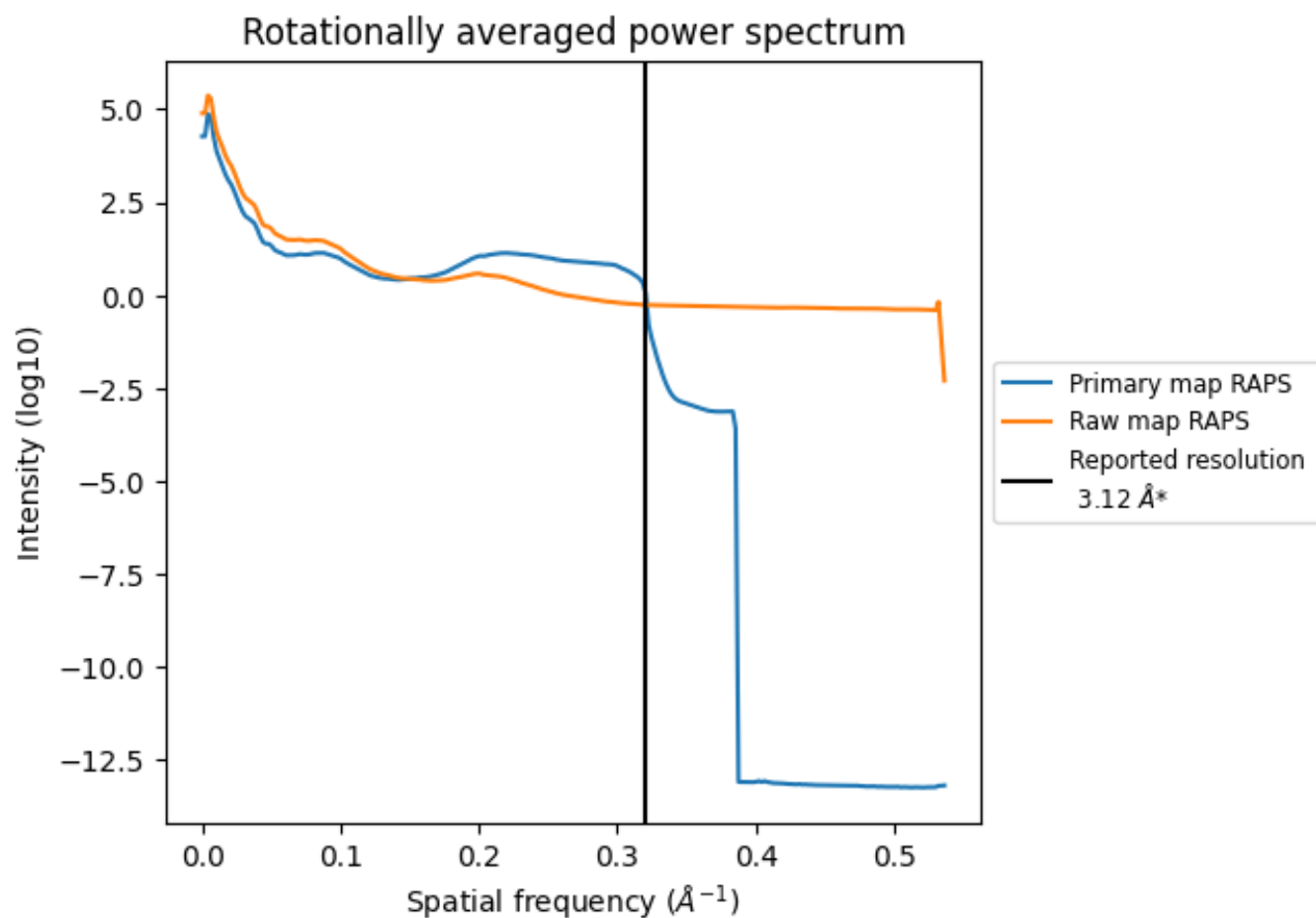
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm^3 ; this corresponds to an approximate mass of 316 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 ⓘ

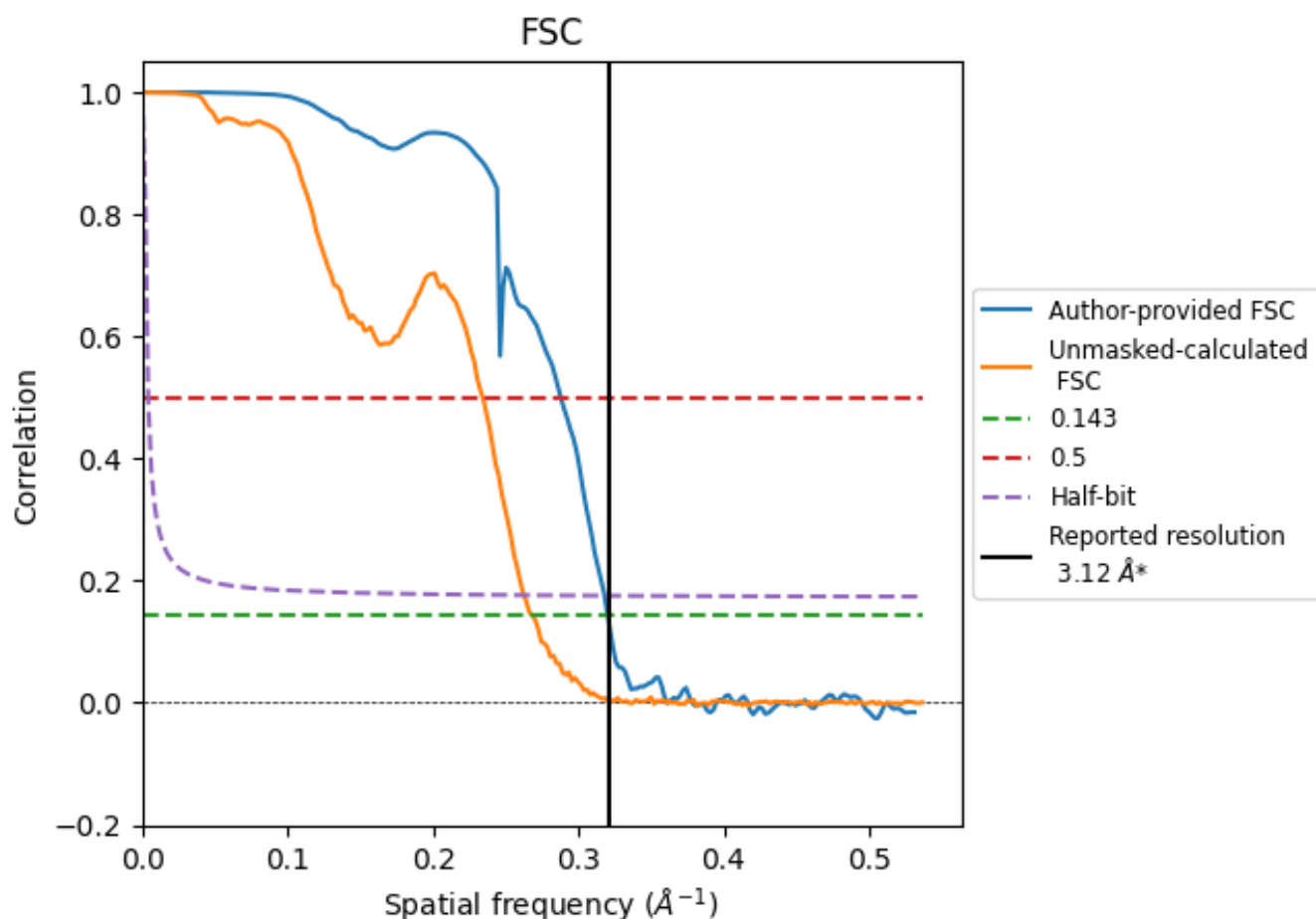


*Reported resolution corresponds to spatial frequency of 0.321 Å⁻¹

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 0.321 \AA^{-1}

8.2 Resolution estimates [i](#)

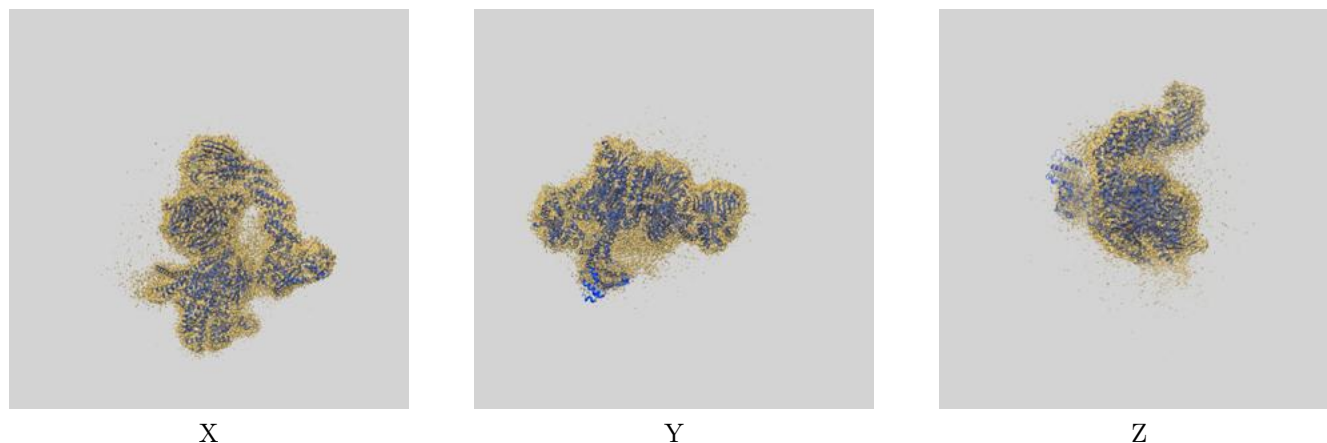
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	3.12	3.47	3.15
Unmasked-calculated*	3.73	4.27	3.81

*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 3.73 differs from the reported value 3.12 by more than 10 %

9 Map-model fit [i](#)

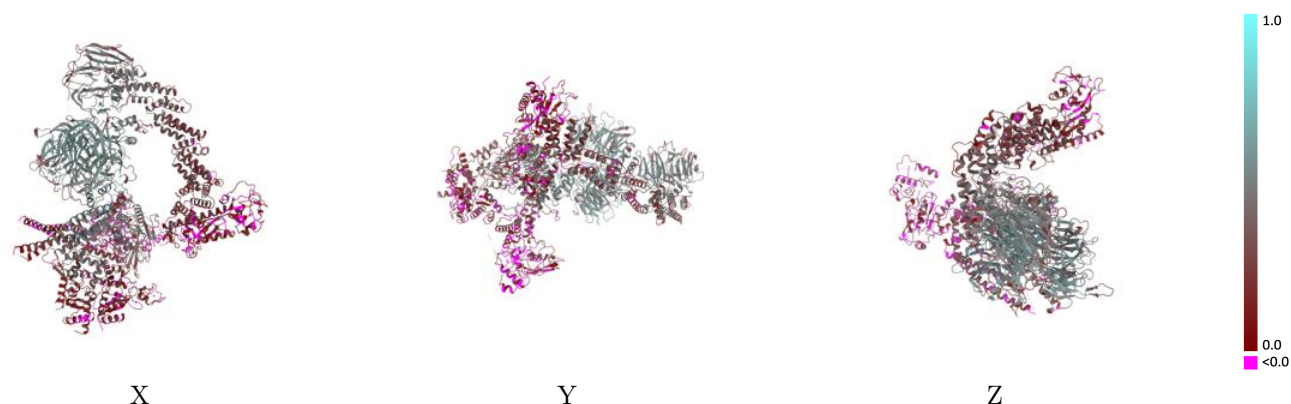
This section contains information regarding the fit between EMDB map EMD-63446 and PDB model 9LWI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



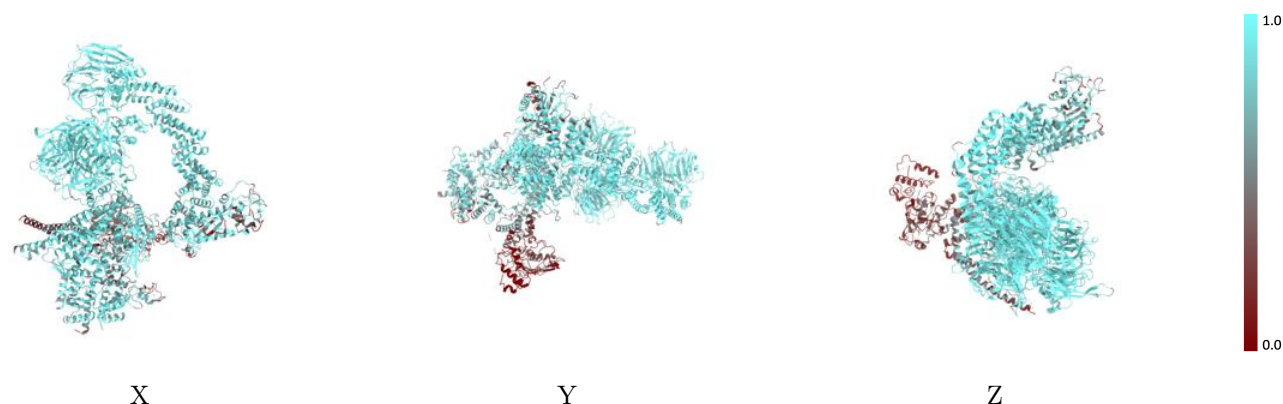
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



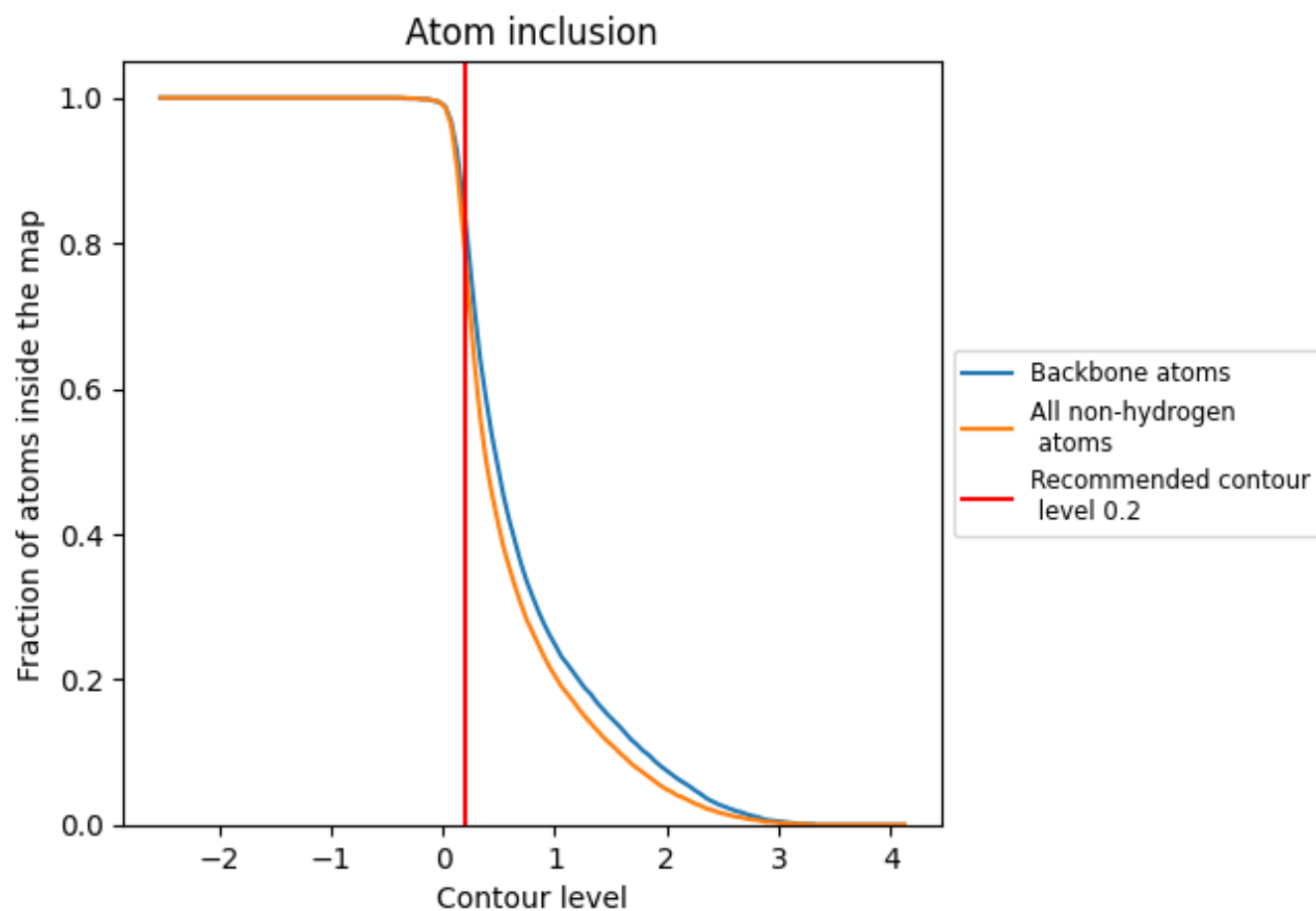
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7850	<div></div> 0.3230
A	<div></div> 0.8860	<div></div> 0.3990
B	<div></div> 0.9350	<div></div> 0.4930
C	<div></div> 0.8970	<div></div> 0.4960
D	<div></div> 0.5660	<div></div> 0.2530
E	<div></div> 0.7900	<div></div> 0.2300
F	<div></div> 0.6970	<div></div> 0.1350
G	<div></div> 0.8320	<div></div> 0.2590
H	<div></div> 0.6860	<div></div> 0.1030
I	<div></div> 0.3300	<div></div> 0.0930

1.0

0.0

<0.0