Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 07:15 pm BST

PDB ID	:	9F5W / pdb_00009f5w
EMDB ID	:	EMD-50201
Title	:	Human condensin II - M18BP1 complex
Authors	:	Borsellini, A.; Vannini, A.
Deposited on	:	2024-04-30
Resolution	:	7.50 Å(reported)
Based on initial model	:	.

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:

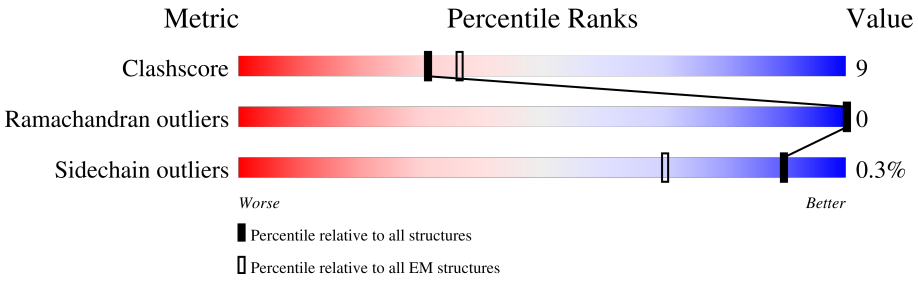
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 7.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	1197	34% 8% 57%
2	B	1305	29% 11% 59%
3	D	1498	57% 16% 26%
4	H	640	32% 8% 61%
5	M	652	99%
6	G	1143	30% 7% 62%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23030 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			4087	2587	709	773	18		

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	533	Total	C	N	O	S	0	0
			4344	2767	742	815	20		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q9NTJ3
B	-15	HIS	-	expression tag	UNP Q9NTJ3
B	-14	HIS	-	expression tag	UNP Q9NTJ3
B	-13	HIS	-	expression tag	UNP Q9NTJ3
B	-12	HIS	-	expression tag	UNP Q9NTJ3
B	-11	HIS	-	expression tag	UNP Q9NTJ3
B	-10	HIS	-	expression tag	UNP Q9NTJ3
B	-9	HIS	-	expression tag	UNP Q9NTJ3
B	-8	HIS	-	expression tag	UNP Q9NTJ3
B	-7	HIS	-	expression tag	UNP Q9NTJ3
B	-6	LEU	-	expression tag	UNP Q9NTJ3
B	-5	GLU	-	expression tag	UNP Q9NTJ3
B	-4	VAL	-	expression tag	UNP Q9NTJ3
B	-3	LEU	-	expression tag	UNP Q9NTJ3
B	-2	PHE	-	expression tag	UNP Q9NTJ3
B	-1	GLN	-	expression tag	UNP Q9NTJ3
B	0	GLY	-	expression tag	UNP Q9NTJ3
B	1	PRO	-	expression tag	UNP Q9NTJ3

- Molecule 3 is a protein called Condensin-2 complex subunit D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1113	Total	C	N	O	S	0	0
			8964	5760	1531	1618	55		

- Molecule 4 is a protein called Condensin-2 complex subunit H2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	252	Total	C	N	O	S	0	0
			2034	1303	334	381	16		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	606	GLU	-	expression tag	UNP Q6IBW4
H	607	ASN	-	expression tag	UNP Q6IBW4
H	608	LEU	-	expression tag	UNP Q6IBW4
H	609	TYR	-	expression tag	UNP Q6IBW4
H	610	PHE	-	expression tag	UNP Q6IBW4
H	611	GLN	-	expression tag	UNP Q6IBW4
H	612	SER	-	expression tag	UNP Q6IBW4
H	613	TRP	-	expression tag	UNP Q6IBW4
H	614	SER	-	expression tag	UNP Q6IBW4
H	615	HIS	-	expression tag	UNP Q6IBW4
H	616	PRO	-	expression tag	UNP Q6IBW4
H	617	GLN	-	expression tag	UNP Q6IBW4
H	618	PHE	-	expression tag	UNP Q6IBW4
H	619	GLU	-	expression tag	UNP Q6IBW4
H	620	LYS	-	expression tag	UNP Q6IBW4
H	621	GLY	-	expression tag	UNP Q6IBW4
H	622	GLY	-	expression tag	UNP Q6IBW4
H	623	GLY	-	expression tag	UNP Q6IBW4
H	624	SER	-	expression tag	UNP Q6IBW4
H	625	GLY	-	expression tag	UNP Q6IBW4
H	626	GLY	-	expression tag	UNP Q6IBW4
H	627	GLY	-	expression tag	UNP Q6IBW4
H	628	SER	-	expression tag	UNP Q6IBW4
H	629	GLY	-	expression tag	UNP Q6IBW4
H	630	GLY	-	expression tag	UNP Q6IBW4
H	631	GLY	-	expression tag	UNP Q6IBW4
H	632	SER	-	expression tag	UNP Q6IBW4
H	633	TRP	-	expression tag	UNP Q6IBW4
H	634	SER	-	expression tag	UNP Q6IBW4
H	635	HIS	-	expression tag	UNP Q6IBW4
H	636	PRO	-	expression tag	UNP Q6IBW4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	637	GLN	-	expression tag	UNP Q6IBW4
H	638	PHE	-	expression tag	UNP Q6IBW4
H	639	GLU	-	expression tag	UNP Q6IBW4
H	640	LYS	-	expression tag	UNP Q6IBW4

- Molecule 5 is a protein called Maltose/maltodextrin-binding periplasmic protein,Mis18-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	5	Total	C	N	O	0	0
			48	32	7	9		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	491	MET	-	initiating methionine	UNP P0AEX9
M	863	GLY	-	linker	UNP P0AEX9
M	864	SER	-	linker	UNP P0AEX9
M	865	GLU	-	linker	UNP P0AEX9
M	866	ASN	-	linker	UNP P0AEX9
M	867	LEU	-	linker	UNP P0AEX9
M	868	TYR	-	linker	UNP P0AEX9
M	869	PHE	-	linker	UNP P0AEX9
M	870	GLN	-	linker	UNP P0AEX9
M	871	GLY	-	linker	UNP P0AEX9
M	872	SER	-	linker	UNP P0AEX9
M	1133	LEU	-	expression tag	UNP Q6P0N0
M	1134	GLU	-	expression tag	UNP Q6P0N0
M	1135	HIS	-	expression tag	UNP Q6P0N0
M	1136	HIS	-	expression tag	UNP Q6P0N0
M	1137	HIS	-	expression tag	UNP Q6P0N0
M	1138	HIS	-	expression tag	UNP Q6P0N0
M	1139	HIS	-	expression tag	UNP Q6P0N0
M	1140	HIS	-	expression tag	UNP Q6P0N0
M	1141	HIS	-	expression tag	UNP Q6P0N0
M	1142	HIS	-	expression tag	UNP Q6P0N0

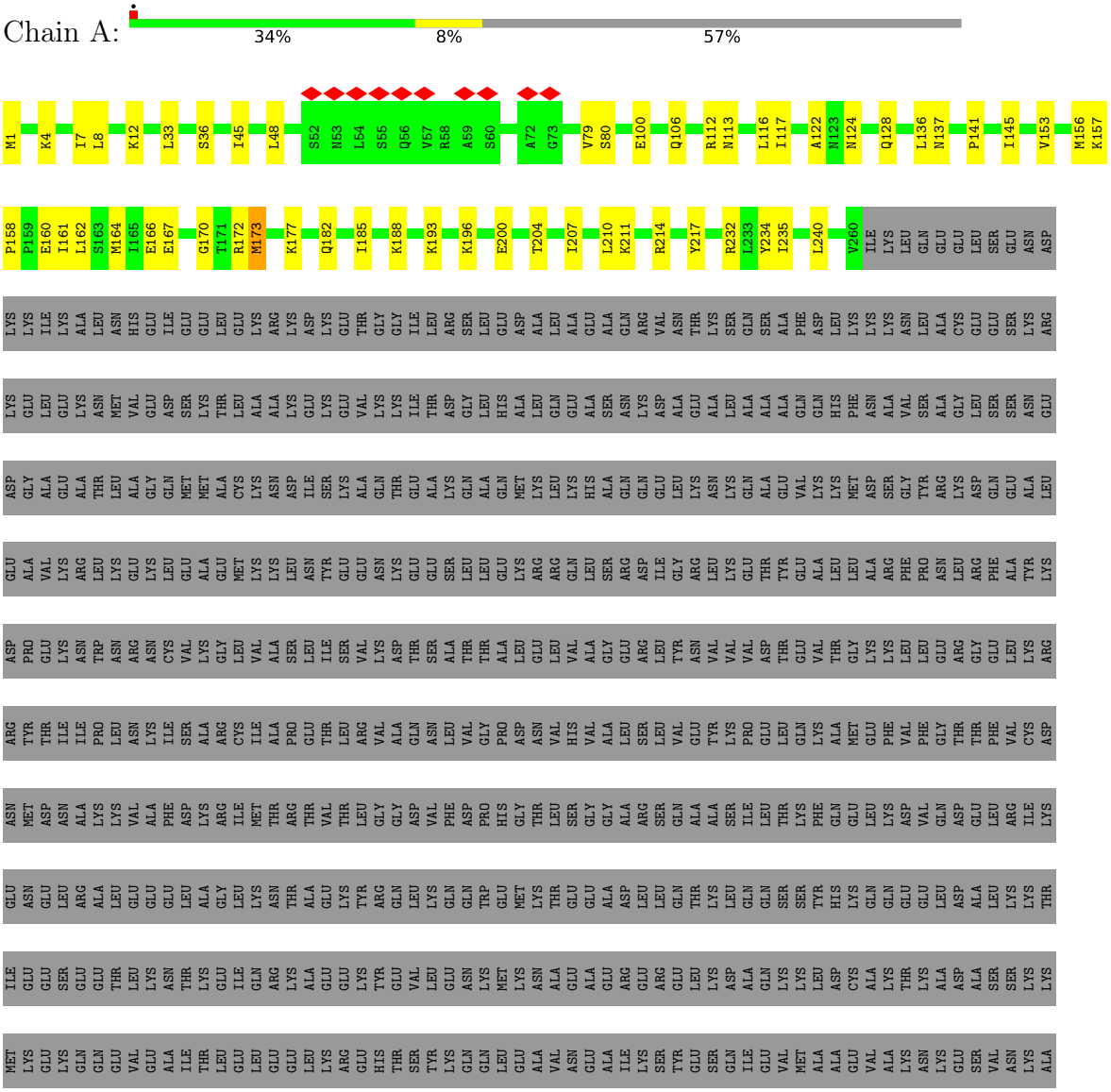
- Molecule 6 is a protein called Condensin-2 complex subunit G2.

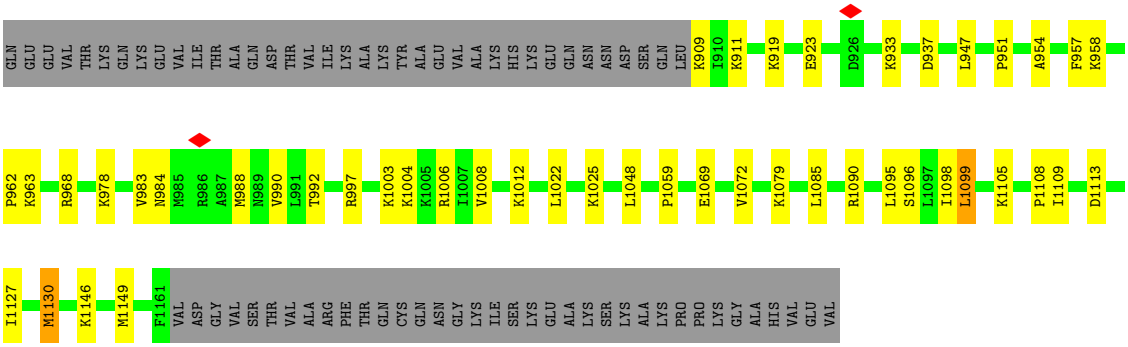
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	433	Total	C	N	O	S	0	0
			3553	2289	622	614	28		

3 Residue-property plots (i)

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

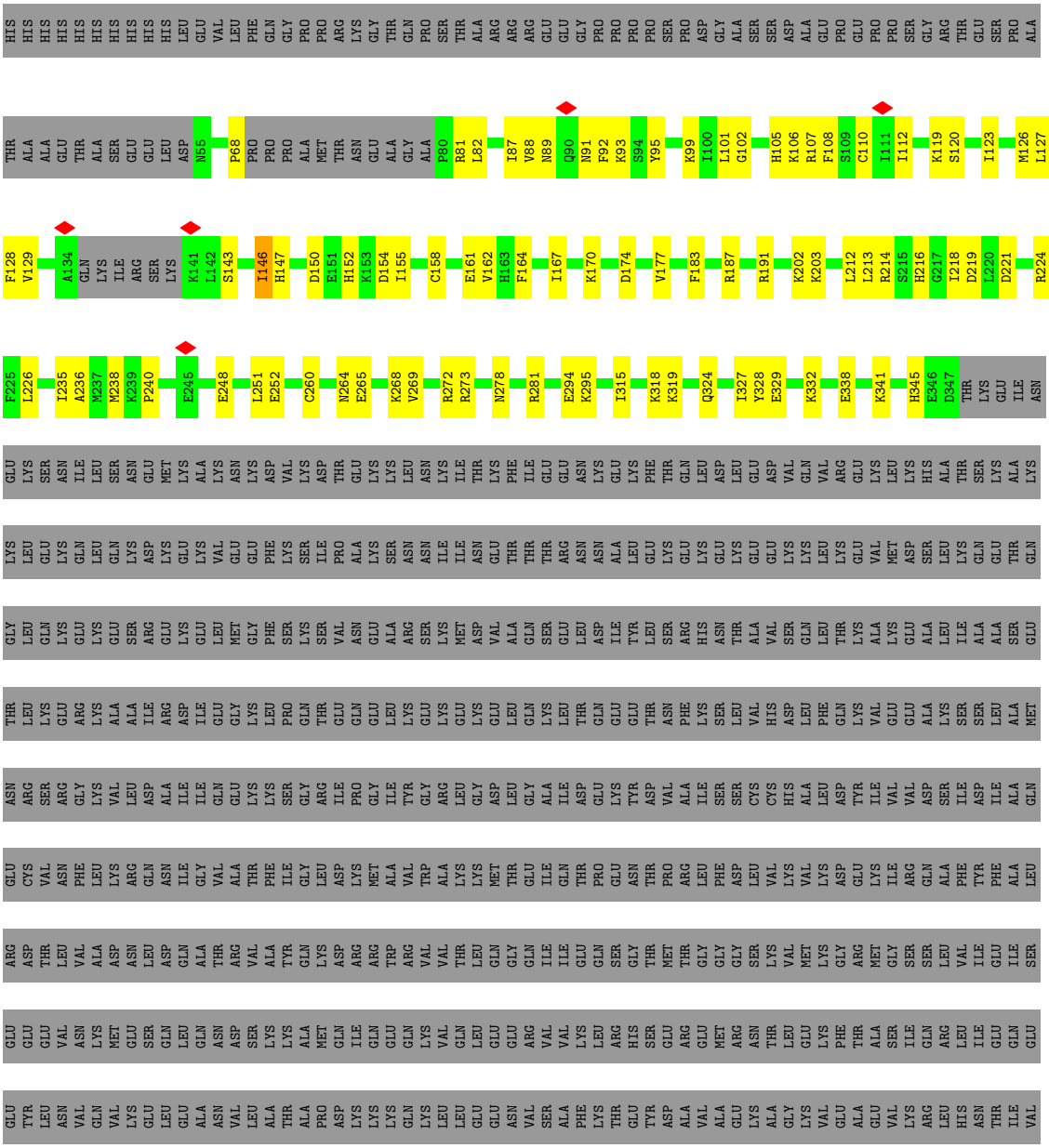
- Molecule 1: Structural maintenance of chromosomes protein 2

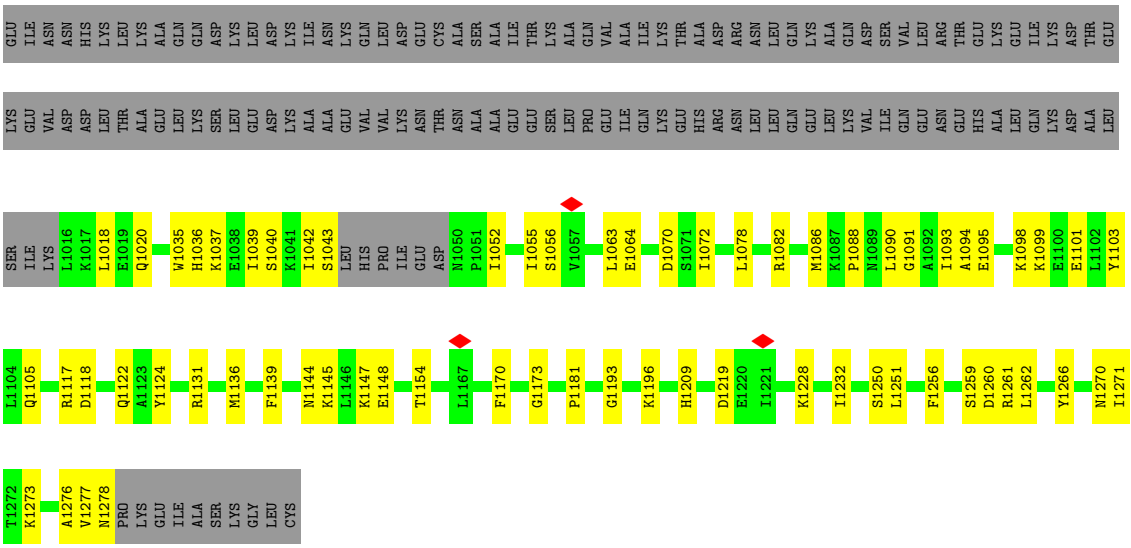




• Molecule 2: Structural maintenance of chromosomes protein 4

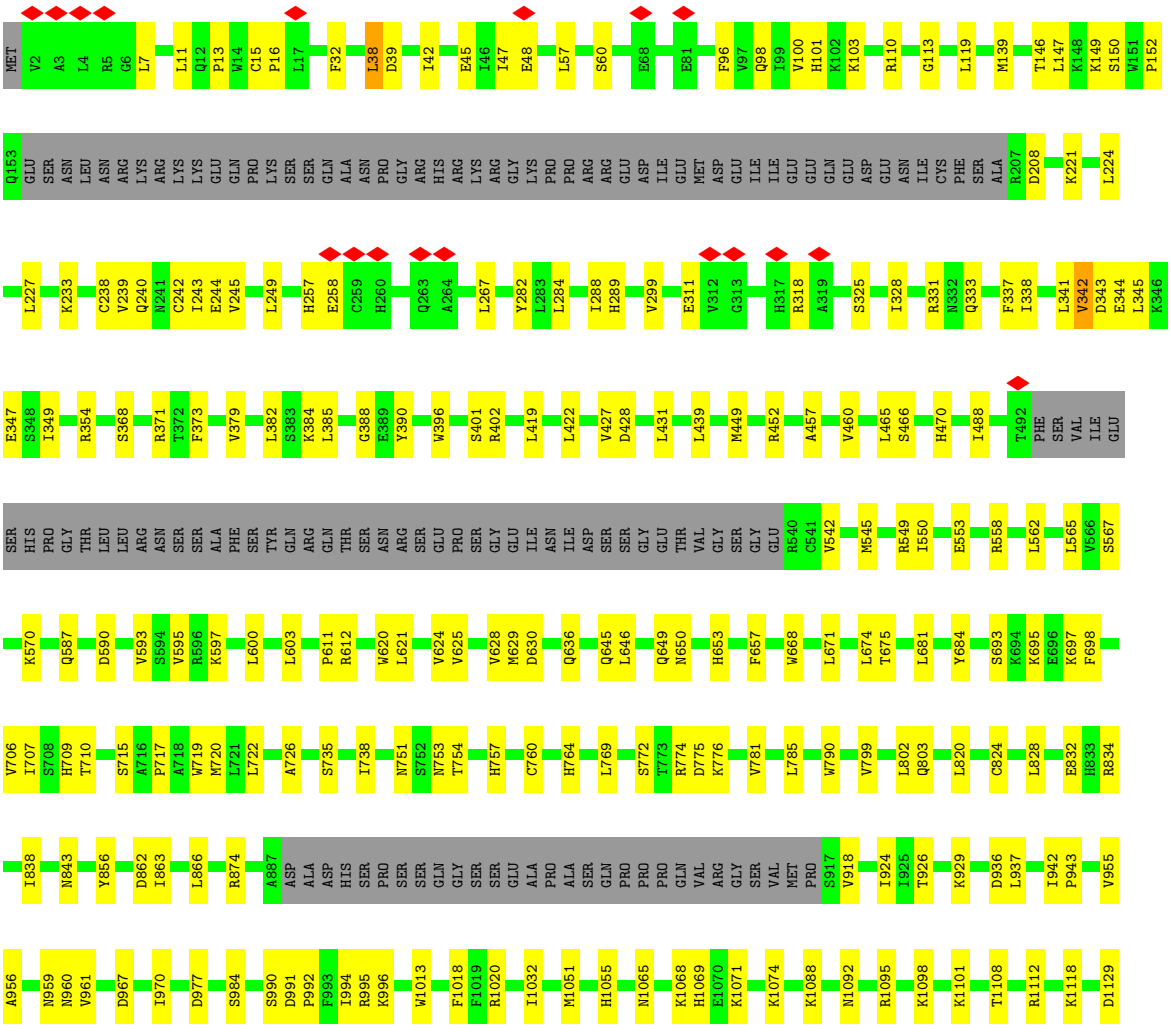
Chain B:

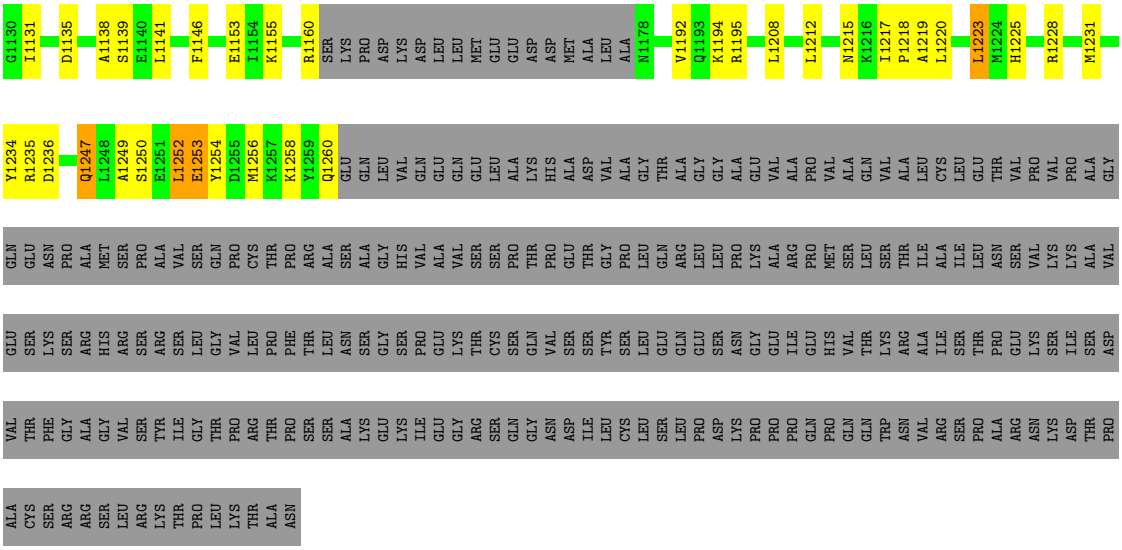




• Molecule 3: Condensin-2 complex subunit D3

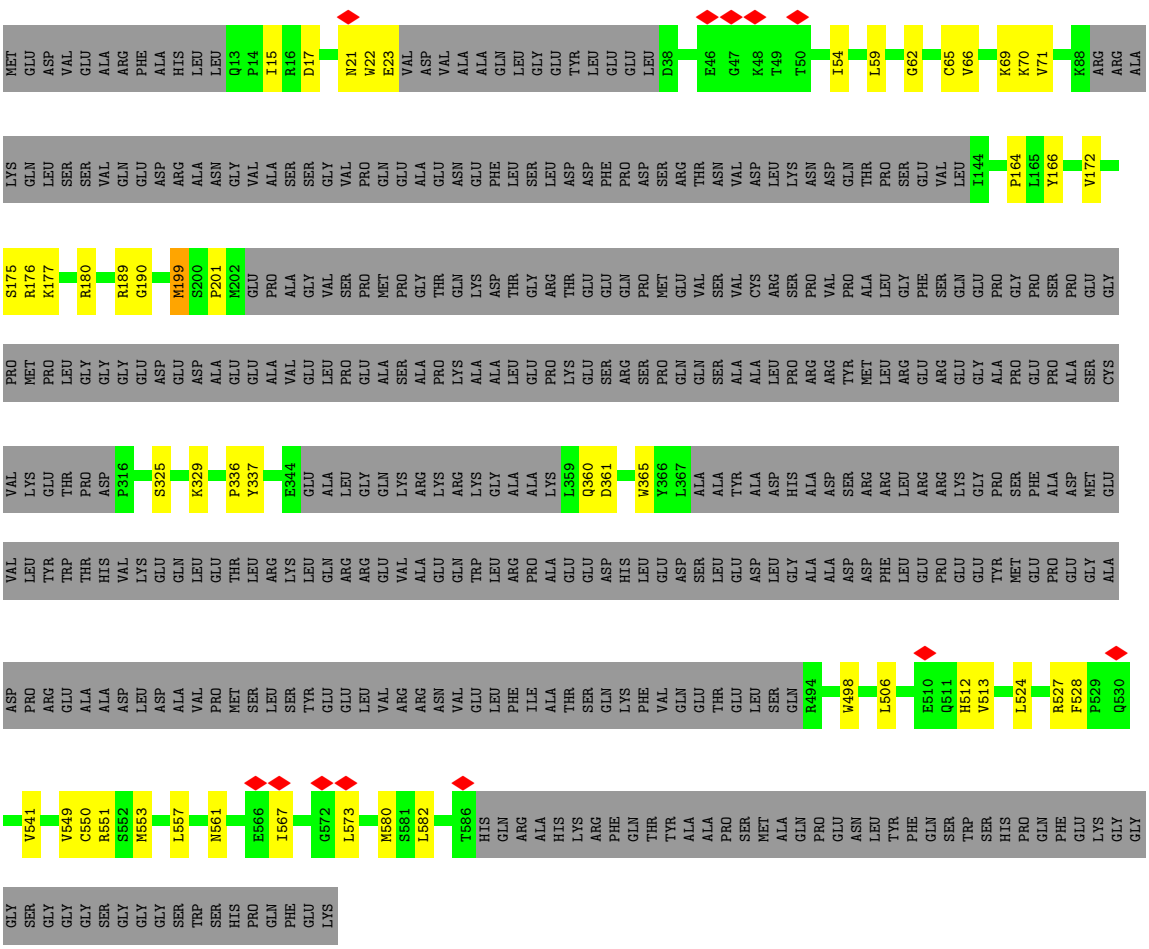
Chain D:





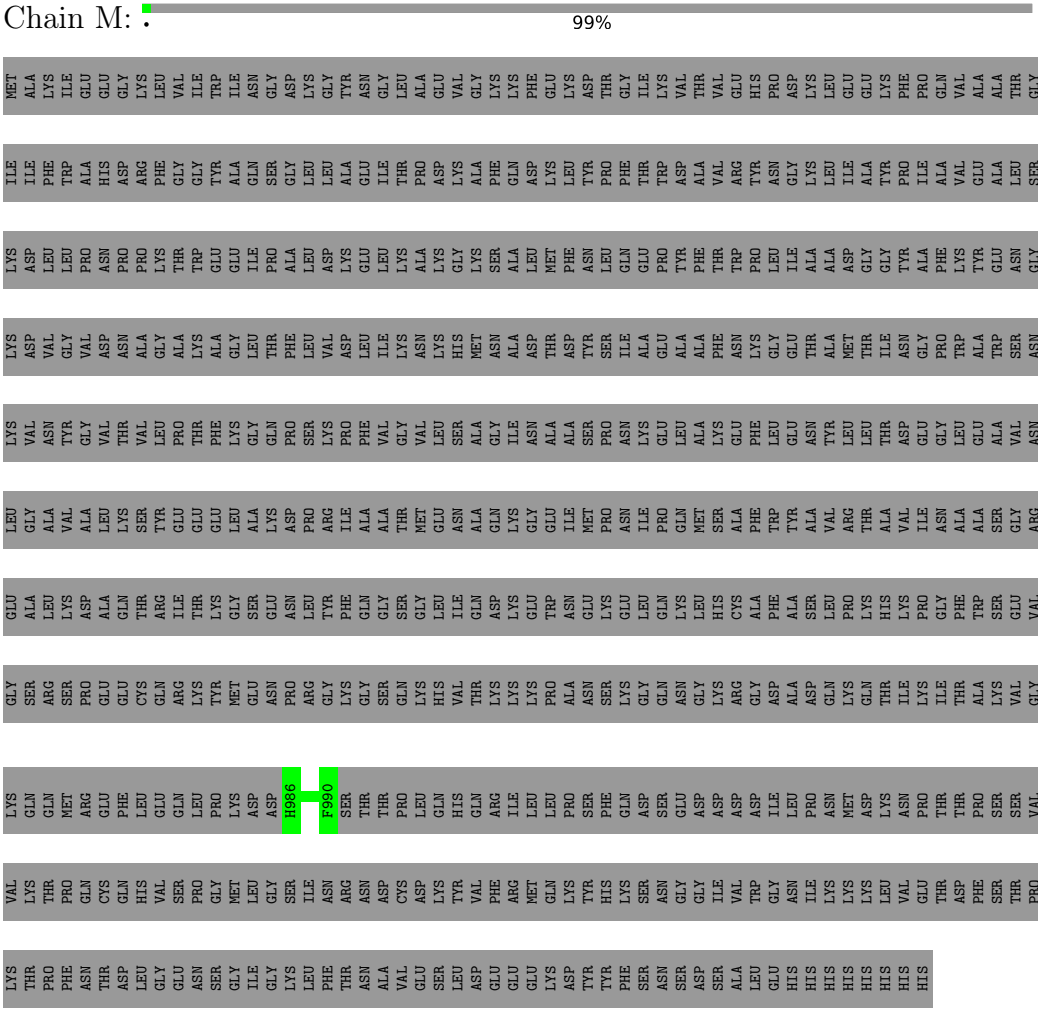
• Molecule 4: Condensin-2 complex subunit H2

Chain H:



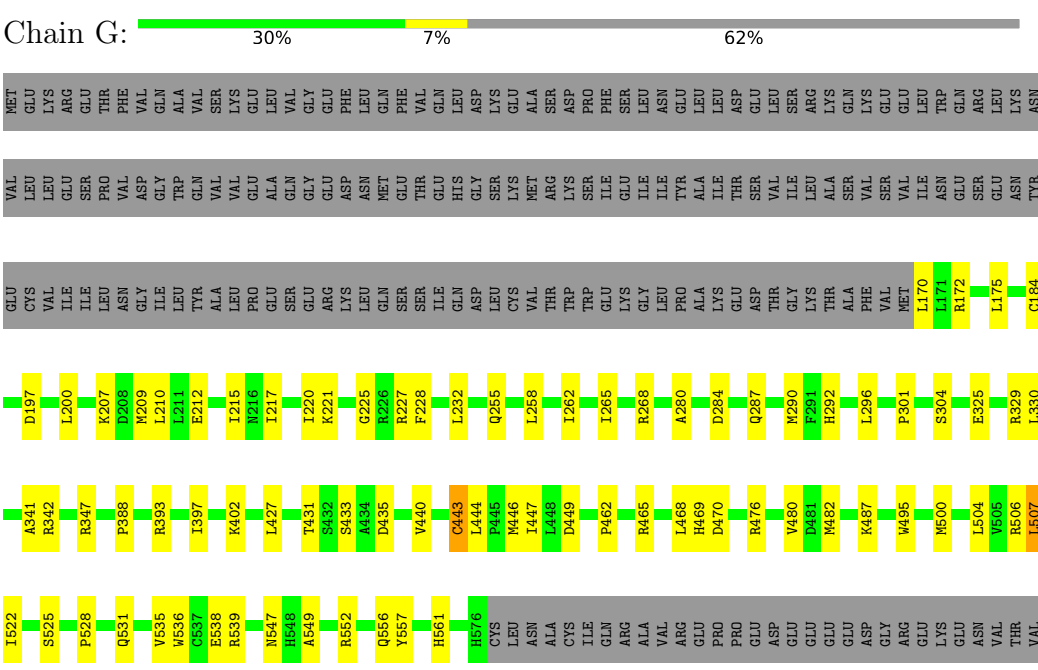
• Molecule 5: Maltose/maltodextrin-binding periplasmic protein,Mis18-binding protein 1

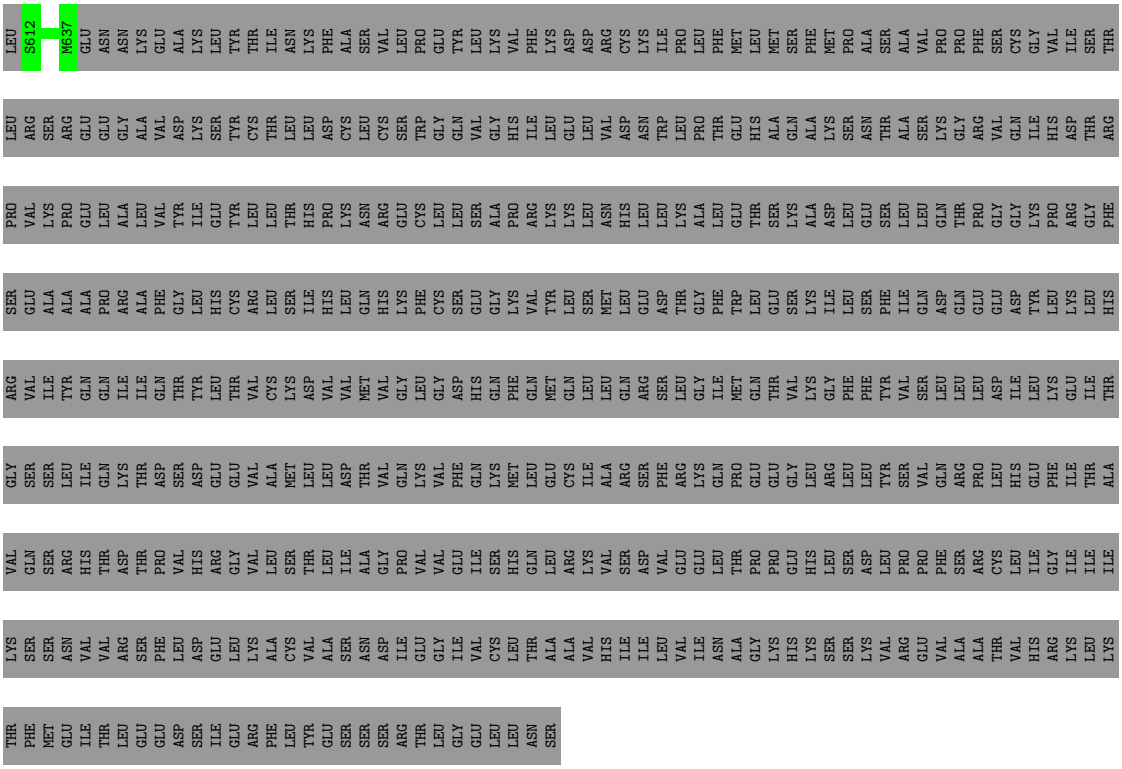
Chain M:



• Molecule 6: Condensin-2 complex subunit G2

Chain G:




LEU S612 M637 GLU ASN ASN LYS GLU ALA LYS LEU TYR THR ILE ASN LYS PHE ALA SER VAL LEU PRO GLU TYR LEU LYS VAL PHE LYS ASP ASP ARG CYS LYS ILE PRO LEU PHE MET LEU MET SER PHE MET PRO ALA SER ALA VAL PRO PRO PHE SER CYS GLY VAL ILE SER THR
LEU ARG SER ARG GLU GLU GLY ALA VAL ASP LYS SER TYR CYS THR LEU LEU ASP CYS LEU CYS SER TRP GLY GLN VAL GLY HIS ILE LEU GLU LEU VAL ASP ASN TRP LEU PRO THR GLU HIS ALA GLN ALA LYS SER ASN THR ALA SER LYS GLY ARG VAL GLN ILE HIS ASP THR ARG
PRO VAL LYS PRO GLU LEU ALA LEU VAL TYR ILE GLU TYR LEU LEU THR HIS PRO LYS ASN ARG GLU CYS LEU LEU SER ALA PRO ARG LYS LYS LEU ASN HIS LEU LEU LYS ALA LEU GLU THR SER LYS ALA ASP LEU GLU SER LEU LEU GLN THR PRO GLY GLY LYS PRO ARG GLY PHE
SER GLU ALA ALA ALA PRO ARG ALA PHE GLY LEU HIS CYS ARG LEU SER ILE HIS LEU GLN HIS LYS PHE CYS SER GLU GLY LYS VAL TYR LEU SER MET LEU GLU ASP THR GLY PHE TRP LEU GLU SER LYS ILE LEU SER PHE ILE GLN ASP GLN GLU GLU ASP TYR LEU LYS GLU HIS
ARG VAL ILE TYR GLN GLN ILE ILE GLN THR TYR LEU THR VAL CYS LYS ASP VAL VAL MET VAL GLY LEU GLY ASP HIS GLN PHE GLN MET GLN LEU LEU GLN ARG SER LEU GLY ILE MET GLN THR VAL LYS GLY PHE PHE TYR VAL SER LEU LEU LEU ASP ILE LEU LYS GLU ILE THR
GLY SER SER LEU ILE GLN LYS THR ASP SER ASP GLU GLU VAL ALA MET LEU LEU ASP THR VAL GLN LYS VAL PHE GLN LYS MET LEU GLU CYS ILE ALA ARG SER PHE ARG LYS GLN PRO GLU GLU GLY LEU ARG LEU LEU TYR SER VAL GLN ARG PRO LEU HIS GLU ILE ALA THR
VAL GLN SER ARG HIS THR ASP THR PRO VAL HIS ARG GLY VAL LEU SER THR LEU ILE ALA GLY PRO VAL VAL GLU ILE SER HIS GLN LEU ARG LYS VAL SER ASP VAL GLU GLU LEU THR PRO PRO GLU HIS LEU SER ASP LEU PRO PRO PHE SER ARG CYS LEU ILE GLY ILE ILE ILE
LYS SER SER ASN VAL VAL ARG SER PHE LEU ASP GLU LEU LYS ALA CYS VAL ALA SER ASN ASP ILE GLU GLY ILE VAL CYS LEU THR ALA ALA VAL HIS ILE ILE LEU VAL ILE ASN ALA GLY LYS HIS LYS SER SER LYS VAL ARG GLU VAL ALA ALA THR VAL HIS ARG LYS LEU LYS
THR PHE MET GLU ILE THR LEU GLU GLU ASP SER ILE GLU ARG PHE LEU TYR GLU SER SER SER ARG THR LEU GLY GLU LEU LEU ASN SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24490	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0248	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.4, 2.4, 2.4	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/4147	0.60	0/5574
2	B	0.30	0/4424	0.60	0/5945
3	D	0.31	0/9144	0.64	8/12363 (0.1%)
4	H	0.24	0/2084	0.52	0/2826
5	M	0.12	0/50	0.32	0/66
6	G	0.26	0/3632	0.58	0/4902
All	All	0.29	0/23481	0.61	8/31676 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	344	GLU	CA-C-O	-7.12	113.37	120.70
3	D	1247	GLN	CA-C-O	-6.68	112.44	120.32
3	D	1252	LEU	CA-C-O	-5.76	114.77	120.82
3	D	1253	GLU	N-CA-CB	5.73	118.64	110.16
3	D	342	VAL	CA-C-N	-5.68	113.05	120.44
3	D	342	VAL	C-N-CA	-5.68	113.05	120.44
3	D	1252	LEU	CA-C-N	-5.37	112.67	120.29
3	D	1252	LEU	C-N-CA	-5.37	112.67	120.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4087	0	4187	69	0
2	B	4344	0	4363	106	0
3	D	8964	0	9157	154	0
4	H	2034	0	1982	35	0
5	M	48	0	32	0	0
6	G	3553	0	3634	56	0
All	All	23030	0	23355	397	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (397) 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:143:SER:HA	2:B:146:ILE:HD12	1.60	0.83
2:B:1094:ALA:O	2:B:1098:LYS:HB3	1.78	0.82
1:A:1096:SER:HA	1:A:1099:LEU:HD23	1.69	0.74
2:B:1232:ILE:HG23	4:H:498:TRP:HE1	1.53	0.73
1:A:963:LYS:HD3	2:B:1035:TRP:HZ3	1.55	0.72
3:D:345:LEU:HD12	3:D:349:ILE:HB	1.72	0.71
3:D:1247:GLN:HG3	6:G:336:TRP:CZ3	2.26	0.70
2:B:327:ILE:HG22	2:B:1036:HIS:ND1	2.07	0.69
2:B:219:ASP:H	2:B:224:ARG:HH12	1.39	0.69
3:D:7:LEU:HA	3:D:60:SER:HB2	1.76	0.68
3:D:488:ILE:HG13	3:D:542:VAL:HB	1.74	0.68
2:B:327:ILE:HG21	2:B:1037:LYS:HA	1.76	0.68
3:D:96:PHE:HB3	3:D:113:GLY:HA2	1.76	0.67
2:B:345:HIS:HB2	2:B:1020:GLN:HG3	1.76	0.66
1:A:167:GLU:HA	1:A:172:ARG:HD2	1.78	0.65
1:A:173:MET:HE1	4:H:59:LEU:HG	1.79	0.65
1:A:214:ARG:HB3	1:A:983:VAL:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:VAL:O	1:A:1012:LYS:HB2	1.97	0.64
3:D:593:VAL:O	3:D:597:LYS:HB2	1.97	0.64
2:B:164:PHE:HB2	2:B:183:PHE:HB2	1.82	0.62
2:B:1193:GLY:HA2	2:B:1196:LYS:HD2	1.80	0.62
2:B:278:ASN:HA	2:B:281:ARG:HD2	1.82	0.62
3:D:645:GLN:HA	3:D:649:GLN:HB2	1.82	0.62
3:D:967:ASP:HA	3:D:970:ILE:HD12	1.82	0.61
2:B:82:LEU:HD11	2:B:164:PHE:HB3	1.83	0.61
1:A:196:LYS:HB3	1:A:1004:LYS:HE2	1.82	0.61
2:B:87:ILE:HG12	2:B:162:VAL:HG23	1.83	0.61
2:B:1099:LYS:HA	2:B:1103:TYR:HB2	1.82	0.61
4:H:22:TRP:HD1	4:H:23:GLU:HG2	1.66	0.60
2:B:150:ASP:OD1	2:B:1270:ASN:ND2	2.35	0.60
2:B:251:LEU:HD21	2:B:1170:PHE:HA	1.84	0.60
3:D:828:LEU:HB2	3:D:863:ILE:HG21	1.82	0.60
6:G:443:CYS:O	6:G:447:ILE:HD12	2.02	0.59
1:A:1048:LEU:HD22	1:A:1127:ILE:HG22	1.83	0.59
2:B:248:GLU:HG3	2:B:252:GLU:HB2	1.84	0.59
2:B:1261:ARG:NH1	2:B:1276:ALA:O	2.36	0.59
1:A:968:ARG:NH2	2:B:1040:SER:O	2.35	0.59
6:G:292:HIS:O	6:G:296:LEU:N	2.36	0.58
2:B:127:LEU:HD21	2:B:226:LEU:HD22	1.85	0.58
2:B:295:LYS:HG2	2:B:1099:LYS:HD2	1.85	0.58
2:B:332:LYS:NZ	2:B:1064:GLU:OE1	2.38	0.57
1:A:978:LYS:HA	2:B:1088:PRO:HD2	1.86	0.57
1:A:177:LYS:HE3	4:H:54:ILE:HG13	1.87	0.57
3:D:769:LEU:O	3:D:774:ARG:NH2	2.38	0.57
4:H:164:PRO:O	4:H:176:ARG:NH1	2.38	0.57
1:A:1149:MET:SD	1:A:1149:MET:N	2.79	0.56
2:B:154:ASP:O	2:B:191:ARG:NH2	2.39	0.56
2:B:240:PRO:HB2	2:B:1173:GLY:HA3	1.87	0.56
2:B:1039:ILE:HB	2:B:1052:ILE:HD12	1.87	0.56
2:B:1118:ASP:O	2:B:1122:GLN:NE2	2.38	0.56
6:G:444:LEU:HD12	6:G:482:MET:HE3	1.88	0.56
2:B:146:ILE:HG22	2:B:147:HIS:H	1.69	0.56
3:D:717:PRO:HA	3:D:720:MET:HG2	1.86	0.56
1:A:1059:PRO:HG3	1:A:1069:GLU:HB2	1.87	0.56
6:G:341:ALA:O	6:G:347:ARG:NH1	2.39	0.56
3:D:706:VAL:HG11	3:D:722:LEU:HD21	1.88	0.56
6:G:287:GLN:HB3	6:G:330:LEU:HD11	1.87	0.56
1:A:137:ASN:ND2	4:H:62:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:175:LEU:HG	6:G:209:MET:HB3	1.88	0.56
3:D:221:LYS:HG2	3:D:267:LEU:HB3	1.86	0.56
3:D:924:ILE:HG21	3:D:961:VAL:HG22	1.88	0.56
1:A:7:ILE:HB	1:A:80:SER:H	1.70	0.56
1:A:1003:LYS:HG2	1:A:1006:ARG:HH21	1.69	0.56
3:D:257:HIS:O	3:D:333:GLN:NE2	2.38	0.56
1:A:963:LYS:HD3	2:B:1035:TRP:CZ3	2.39	0.56
2:B:93:LYS:HA	2:B:147:HIS:HA	1.88	0.56
6:G:487:LYS:NZ	6:G:521:LEU:O	2.39	0.56
4:H:557:LEU:O	4:H:561:ASN:ND2	2.39	0.55
3:D:550:ILE:HG21	3:D:587:GLN:HE21	1.72	0.55
3:D:311:GLU:O	3:D:318:ARG:NH1	2.38	0.55
3:D:1135:ASP:H	3:D:1138:ALA:HB3	1.72	0.55
1:A:8:LEU:HA	1:A:79:VAL:HG12	1.87	0.55
3:D:1256:MET:SD	3:D:1260:GLN:NE2	2.78	0.55
1:A:4:LYS:NZ	1:A:100:GLU:OE1	2.39	0.55
2:B:1042:ILE:HG22	2:B:1052:ILE:HD11	1.88	0.55
3:D:542:VAL:HA	3:D:545:MET:HG3	1.88	0.55
3:D:550:ILE:HA	3:D:558:ARG:HG2	1.88	0.55
3:D:926:THR:HA	3:D:929:LYS:HD3	1.89	0.54
3:D:379:VAL:HG13	3:D:422:LEU:HD11	1.90	0.54
6:G:433:SER:OG	6:G:435:ASP:OD1	2.25	0.54
3:D:824:CYS:HB3	3:D:863:ILE:HG23	1.88	0.54
3:D:722:LEU:HD22	3:D:726:ALA:HB2	1.90	0.54
3:D:668:TRP:HE3	3:D:671:LEU:HD11	1.73	0.54
2:B:92:PHE:HB3	2:B:95:TYR:HB2	1.89	0.54
3:D:146:THR:HA	3:D:149:LYS:HB2	1.89	0.54
3:D:956:ALA:O	3:D:960:ASN:ND2	2.41	0.54
1:A:145:ILE:HB	1:A:1113:ASP:HB3	1.90	0.53
1:A:182:GLN:HA	1:A:185:ILE:HG12	1.90	0.53
3:D:955:VAL:HB	3:D:994:ILE:HD11	1.90	0.53
3:D:1112:ARG:NH1	3:D:1155:LYS:O	2.42	0.53
1:A:157:LYS:HB2	1:A:160:GLU:HB2	1.90	0.53
3:D:110:ARG:HH22	3:D:152:PRO:HA	1.73	0.53
3:D:772:SER:O	3:D:776:LYS:NZ	2.40	0.53
3:D:1231:MET:HE1	3:D:1256:MET:HB2	1.91	0.53
6:G:462:PRO:O	6:G:465:ARG:NH1	2.41	0.53
3:D:646:LEU:O	3:D:650:ASN:ND2	2.42	0.53
3:D:1112:ARG:HH12	3:D:1160:ARG:HH22	1.56	0.53
3:D:16:PRO:HG3	3:D:42:ILE:HG12	1.91	0.53
2:B:1145:LYS:HD3	2:B:1209:HIS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:HIS:O	3:D:715:SER:OG	2.24	0.53
3:D:781:VAL:HG11	3:D:802:LEU:HD21	1.90	0.53
3:D:110:ARG:NH1	3:D:150:SER:O	2.42	0.53
2:B:278:ASN:HB3	2:B:1117:ARG:HD3	1.91	0.53
6:G:402:LYS:HA	6:G:446:MET:HE1	1.90	0.53
2:B:1086:MET:HB3	2:B:1088:PRO:HD3	1.91	0.52
1:A:185:ILE:HA	1:A:188:LYS:HG2	1.92	0.52
2:B:213:LEU:HD22	2:B:218:ILE:HD12	1.91	0.52
2:B:338:GLU:HA	2:B:341:LYS:HE2	1.90	0.52
3:D:1013:TRP:HB3	3:D:1018:PHE:HE1	1.74	0.52
3:D:693:SER:HA	3:D:698:PHE:HE2	1.74	0.52
4:H:512:HIS:HB3	4:H:551:ARG:HH12	1.73	0.52
6:G:184:CYS:SG	6:G:188:ARG:NH1	2.81	0.52
2:B:278:ASN:HB3	2:B:1117:ARG:CD	2.39	0.52
3:D:284:LEU:HD23	3:D:289:HIS:HB3	1.91	0.52
3:D:628:VAL:HA	3:D:636:GLN:HG2	1.91	0.52
6:G:225:GLY:HA2	6:G:228:PHE:CE1	2.45	0.52
2:B:81:ARG:NH1	2:B:82:LEU:O	2.42	0.52
2:B:269:VAL:HG12	2:B:273:ARG:HE	1.75	0.52
6:G:504:LEU:HD22	6:G:547:ASN:HD22	1.75	0.52
2:B:1055:ILE:HB	2:B:1063:LEU:HD21	1.91	0.52
4:H:65:CYS:HB2	4:H:70:LYS:HG3	1.91	0.52
2:B:214:ARG:NH2	2:B:221:ASP:OD1	2.43	0.51
2:B:1082:ARG:O	2:B:1086:MET:HG2	2.10	0.51
3:D:57:LEU:HD23	3:D:119:LEU:HD13	1.91	0.51
3:D:233:LYS:HE3	3:D:288:ILE:HG13	1.91	0.51
1:A:158:PRO:HA	1:A:161:ILE:HG22	1.91	0.51
6:G:522:ILE:HG22	6:G:525:SER:HB2	1.91	0.51
1:A:170:GLY:HA2	1:A:172:ARG:HH11	1.76	0.51
6:G:220:ILE:HG23	6:G:265:ILE:HD11	1.92	0.51
6:G:262:ILE:HD13	6:G:265:ILE:HD12	1.92	0.51
2:B:108:PHE:HB2	2:B:1260:ASP:H	1.76	0.50
3:D:977:ASP:N	3:D:977:ASP:OD1	2.43	0.50
1:A:954:ALA:O	1:A:958:LYS:NZ	2.44	0.50
4:H:360:GLN:HG2	6:G:549:ALA:HB2	1.93	0.50
1:A:1095:LEU:HD12	1:A:1096:SER:N	2.26	0.50
2:B:68:PRO:HB3	2:B:1131:ARG:HH22	1.77	0.50
2:B:87:ILE:HD12	2:B:101:LEU:HD22	1.94	0.50
2:B:1256:PHE:HB2	2:B:1262:LEU:HD22	1.93	0.50
2:B:89:ASN:HB3	2:B:92:PHE:HB2	1.94	0.50
6:G:227:ARG:HH21	6:G:268:ARG:HG2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HA	1:A:48:LEU:HG	1.94	0.49
2:B:1101:GLU:O	2:B:1105:GLN:N	2.44	0.49
2:B:1250:SER:OG	2:B:1251:LEU:N	2.45	0.49
3:D:224:LEU:HD23	3:D:227:LEU:HD12	1.94	0.49
2:B:106:LYS:HE3	2:B:107:ARG:HH11	1.76	0.49
3:D:1155:LYS:O	3:D:1160:ARG:NH1	2.46	0.49
1:A:7:ILE:HG13	1:A:80:SER:HB3	1.93	0.49
2:B:1091:GLY:HA2	2:B:1094:ALA:HB3	1.95	0.49
2:B:1094:ALA:O	2:B:1098:LYS:CB	2.58	0.49
3:D:695:LYS:HB3	3:D:697:LYS:HG2	1.93	0.49
3:D:1138:ALA:HA	3:D:1141:LEU:HD12	1.95	0.49
6:G:557:TYR:O	6:G:561:HIS:ND1	2.46	0.49
1:A:240:LEU:HD22	1:A:947:LEU:HB3	1.94	0.49
3:D:243:ILE:HG21	3:D:299:VAL:HG23	1.95	0.49
3:D:1250:SER:HA	3:D:1253:GLU:OE1	2.13	0.49
4:H:177:LYS:O	4:H:180:ARG:NH2	2.41	0.49
2:B:329:GLU:HB2	2:B:1064:GLU:HA	1.95	0.49
1:A:200:GLU:O	1:A:204:THR:OG1	2.31	0.49
1:A:1108:PRO:HG2	1:A:1109:ILE:HD12	1.95	0.49
2:B:265:GLU:HA	2:B:268:LYS:HD2	1.94	0.49
4:H:164:PRO:HA	4:H:175:SER:HA	1.95	0.49
3:D:832:GLU:OE2	3:D:874:ARG:NH1	2.46	0.49
6:G:280:ALA:O	6:G:284:ASP:HB2	2.13	0.48
3:D:32:PHE:HB3	3:D:139:MET:HB3	1.94	0.48
1:A:211:LYS:HA	1:A:214:ARG:HG2	1.95	0.48
2:B:236:ALA:HB1	2:B:1196:LYS:HD3	1.95	0.48
2:B:278:ASN:OD1	2:B:281:ARG:NH1	2.46	0.48
3:D:342:VAL:O	3:D:343:ASP:C	2.55	0.48
3:D:838:ILE:O	3:D:843:ASN:ND2	2.41	0.48
3:D:1235:ARG:CZ	3:D:1256:MET:HE2	2.44	0.48
3:D:567:SER:O	3:D:570:LYS:NZ	2.36	0.48
3:D:603:LEU:HD13	3:D:620:TRP:CD1	2.49	0.48
2:B:1090:LEU:HD22	2:B:1093:ILE:HD12	1.96	0.48
3:D:1235:ARG:NH1	3:D:1256:MET:HG3	2.29	0.48
1:A:1022:LEU:HA	1:A:1025:LYS:HB2	1.95	0.48
3:D:449:MET:HA	3:D:452:ARG:HB2	1.95	0.48
1:A:124:ASN:OD1	1:A:128:GLN:NE2	2.45	0.48
3:D:1217:ILE:HG22	3:D:1219:ALA:H	1.79	0.47
3:D:100:VAL:HG22	3:D:110:ARG:HA	1.96	0.47
6:G:528:PRO:HD3	6:G:539:ARG:HD2	1.95	0.47
1:A:217:TYR:HD2	1:A:984:ASN:HD22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:440:VAL:O	6:G:443:CYS:HB2	2.14	0.47
1:A:162:LEU:O	1:A:166:GLU:HB2	2.14	0.47
3:D:427:VAL:HA	3:D:439:LEU:HD13	1.95	0.47
6:G:468:LEU:HD21	6:G:506:ARG:HB2	1.96	0.47
2:B:167:ILE:HD12	2:B:177:VAL:HG12	1.97	0.47
3:D:590:ASP:HB2	3:D:595:VAL:HG11	1.96	0.47
3:D:1098:LYS:HG2	3:D:1101:LYS:HZ3	1.79	0.47
1:A:909:LYS:HD3	2:B:1018:LEU:HD22	1.97	0.47
2:B:315:ILE:HA	2:B:318:LYS:HD2	1.97	0.47
3:D:625:VAL:HG11	3:D:681:LEU:HD22	1.96	0.47
3:D:834:ARG:NH1	3:D:856:TYR:OH	2.48	0.47
3:D:1051:MET:O	3:D:1055:HIS:ND1	2.44	0.47
3:D:1236:ASP:OD1	3:D:1236:ASP:N	2.46	0.47
2:B:319:LYS:NZ	2:B:1072:ILE:O	2.48	0.47
2:B:1136:MET:HA	2:B:1139:PHE:HB3	1.96	0.47
3:D:466:SER:O	3:D:470:HIS:ND1	2.48	0.47
3:D:1069:HIS:O	3:D:1074:LYS:NZ	2.48	0.47
3:D:242:CYS:HA	3:D:245:VAL:HG22	1.97	0.47
3:D:1112:ARG:NH1	3:D:1153:GLU:O	2.42	0.47
4:H:329:LYS:O	6:G:393:ARG:NH2	2.48	0.47
3:D:629:MET:HB3	3:D:684:TYR:HE1	1.80	0.46
4:H:17:ASP:O	4:H:21:ASN:N	2.47	0.46
6:G:528:PRO:HB2	6:G:531:GLN:HB2	1.96	0.46
3:D:674:LEU:HD22	3:D:681:LEU:HD11	1.96	0.46
3:D:1135:ASP:N	3:D:1135:ASP:OD1	2.48	0.46
3:D:1254:TYR:CZ	3:D:1258:LYS:HD2	2.51	0.46
6:G:397:ILE:HD11	6:G:427:LEU:HD11	1.97	0.46
3:D:918:VAL:HG13	4:H:190:GLY:HA3	1.96	0.46
6:G:528:PRO:HG2	6:G:536:TRP:HD1	1.80	0.46
3:D:653:HIS:O	3:D:657:PHE:N	2.48	0.46
6:G:217:ILE:HG22	6:G:221:LYS:HE3	1.98	0.46
2:B:324:GLN:HA	2:B:327:ILE:HG12	1.96	0.46
2:B:1154:THR:HB	2:B:1181:PRO:HG3	1.97	0.46
3:D:1146:PHE:CZ	3:D:1223:LEU:HG	2.51	0.46
3:D:1208:LEU:O	3:D:1212:LEU:HB2	2.16	0.46
1:A:161:ILE:HA	1:A:164:MET:HG3	1.98	0.46
2:B:105:HIS:ND1	2:B:1261:ARG:HG2	2.31	0.46
2:B:128:PHE:HB3	2:B:187:ARG:HH12	1.80	0.46
2:B:327:ILE:HG22	2:B:1036:HIS:CE1	2.51	0.46
3:D:11:LEU:O	3:D:15:CYS:N	2.47	0.46
3:D:785:LEU:HD23	3:D:790:TRP:HZ3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:NH1	1:A:113:ASN:O	2.49	0.46
1:A:117:ILE:HG12	1:A:122:ALA:HB2	1.96	0.46
2:B:1043:SER:HB3	2:B:1052:ILE:HG13	1.98	0.46
3:D:98:GLN:HA	3:D:101:HIS:HD2	1.79	0.46
3:D:390:TYR:HE1	3:D:419:LEU:HD11	1.81	0.45
4:H:166:TYR:HA	4:H:172:VAL:HA	1.98	0.45
4:H:189:ARG:NH2	4:H:201:PRO:O	2.47	0.45
3:D:147:LEU:HB3	3:D:249:LEU:HD11	1.99	0.45
2:B:202:LYS:NZ	2:B:203:LYS:O	2.49	0.45
2:B:1266:TYR:HB3	4:H:557:LEU:HD23	1.98	0.45
3:D:760:CYS:O	3:D:764:HIS:ND1	2.50	0.45
1:A:911:LYS:HD2	1:A:911:LYS:HA	1.75	0.45
2:B:88:VAL:HG23	2:B:161:GLU:HB2	1.98	0.45
2:B:91:ASN:HB2	2:B:158:CYS:HA	1.97	0.45
3:D:368:SER:HA	3:D:371:ARG:HE	1.82	0.45
6:G:255:GLN:H	6:G:258:LEU:HD12	1.82	0.45
6:G:388:PRO:O	6:G:393:ARG:NH2	2.49	0.45
2:B:235:ILE:HA	2:B:238:MET:HG3	1.99	0.45
3:D:707:ILE:O	3:D:710:THR:OG1	2.29	0.45
2:B:120:SER:HA	2:B:123:ILE:HG22	1.98	0.45
3:D:258:GLU:HA	3:D:333:GLN:HG2	1.98	0.45
3:D:1249:ALA:O	3:D:1252:LEU:HB2	2.16	0.45
2:B:1219:ASP:OD1	2:B:1219:ASP:N	2.48	0.45
3:D:208:ASP:OD1	3:D:208:ASP:N	2.49	0.45
3:D:282:TYR:HB2	3:D:337:PHE:HE1	1.82	0.45
2:B:102:GLY:HA2	4:H:573:LEU:HD11	1.98	0.45
2:B:212:LEU:O	2:B:216:HIS:ND1	2.45	0.45
3:D:331:ARG:NH1	3:D:373:PHE:O	2.49	0.45
4:H:361:ASP:O	6:G:552:ARG:NH1	2.49	0.45
6:G:301:PRO:O	6:G:304:SER:OG	2.32	0.45
1:A:106:GLN:HE22	1:A:116:LEU:HB2	1.82	0.45
3:D:611:PRO:HG2	3:D:612:ARG:HG3	1.99	0.45
4:H:550:CYS:HA	4:H:553:MET:HG2	1.99	0.45
2:B:260:CYS:HA	2:B:1131:ARG:HE	1.82	0.45
3:D:715:SER:O	3:D:719:TRP:N	2.48	0.45
3:D:751:ASN:O	3:D:754:THR:OG1	2.33	0.45
3:D:984:SER:HB2	3:D:1020:ARG:HD2	1.99	0.45
1:A:153:VAL:HA	1:A:156:MET:HG2	2.00	0.44
3:D:671:LEU:HD13	3:D:717:PRO:HB2	1.98	0.44
3:D:942:ILE:HG13	3:D:943:PRO:HD3	1.99	0.44
2:B:328:TYR:CG	2:B:1063:LEU:HD23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:15:ILE:HD12	4:H:71:VAL:HG23	1.99	0.44
3:D:562:LEU:HA	3:D:565:LEU:HG	1.99	0.44
3:D:990:SER:O	3:D:995:ARG:NH2	2.50	0.44
4:H:337:TYR:HB3	6:G:469:HIS:HB2	1.98	0.44
6:G:212:GLU:HA	6:G:215:ILE:HD12	2.00	0.44
1:A:962:PRO:HD2	2:B:1035:TRP:CZ2	2.52	0.44
2:B:1070:ASP:OD1	2:B:1070:ASP:N	2.47	0.44
2:B:1261:ARG:NH1	2:B:1278:ASN:OD1	2.51	0.44
1:A:136:LEU:HG	1:A:141:PRO:HD3	1.99	0.44
3:D:866:LEU:O	4:H:166:TYR:OH	2.34	0.44
3:D:238:CYS:O	3:D:242:CYS:SG	2.75	0.44
3:D:457:ALA:HB3	3:D:460:VAL:HB	1.99	0.44
3:D:1108:THR:O	3:D:1112:ARG:N	2.48	0.44
6:G:172:ARG:HA	6:G:209:MET:HE1	1.98	0.44
3:D:799:VAL:HG21	3:D:862:ASP:HB3	1.99	0.44
3:D:955:VAL:O	3:D:959:ASN:ND2	2.51	0.44
1:A:1130:MET:HE3	1:A:1130:MET:HB3	1.85	0.44
3:D:103:LYS:O	3:D:110:ARG:NH2	2.51	0.44
3:D:996:LYS:HB3	3:D:1032:ILE:HG12	1.99	0.44
3:D:1071:LYS:HE2	3:D:1071:LYS:HB3	1.84	0.44
3:D:1194:LYS:HB3	3:D:1194:LYS:HE3	1.88	0.44
1:A:210:LEU:HD22	1:A:990:VAL:HG11	2.00	0.43
2:B:147:HIS:CD2	2:B:152:HIS:HB3	2.53	0.43
3:D:1129:ASP:HB3	3:D:1131:ILE:HG13	2.00	0.43
4:H:199:MET:HE3	4:H:199:MET:HB3	1.76	0.43
4:H:541:VAL:HB	4:H:549:VAL:HG22	2.00	0.43
1:A:1085:LEU:O	1:A:1090:ARG:NH2	2.47	0.43
3:D:1068:LYS:HE2	3:D:1068:LYS:HB2	1.86	0.43
6:G:528:PRO:O	6:G:536:TRP:NE1	2.51	0.43
3:D:428:ASP:HB3	3:D:431:LEU:HD12	2.01	0.43
6:G:435:ASP:OD1	6:G:435:ASP:N	2.50	0.43
6:G:535:VAL:HA	6:G:538:GLU:HG3	2.01	0.43
1:A:232:ARG:HA	1:A:235:ILE:HB	1.98	0.43
2:B:1145:LYS:HA	2:B:1148:GLU:HG2	2.01	0.43
3:D:345:LEU:O	3:D:347:GLU:N	2.51	0.43
6:G:449:ASP:OD1	6:G:449:ASP:N	2.52	0.43
1:A:933:LYS:NZ	1:A:937:ASP:OD1	2.51	0.43
1:A:947:LEU:HD22	1:A:951:PRO:HG3	1.99	0.43
3:D:13:PRO:HA	3:D:45:GLU:HG2	2.01	0.43
3:D:1139:SER:HB2	3:D:1218:PRO:HD2	1.99	0.43
4:H:325:SER:HB2	6:G:342:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:470:ASP:O	6:G:476:ARG:NH1	2.52	0.43
1:A:207:ILE:HD11	1:A:997:ARG:HH21	1.83	0.43
1:A:33:LEU:HB2	1:A:36:SER:HB2	2.00	0.43
1:A:988:MET:O	1:A:992:THR:OG1	2.20	0.43
2:B:1259:SER:OG	2:B:1261:ARG:O	2.34	0.43
1:A:1146:LYS:HB2	1:A:1149:MET:HE1	2.00	0.42
2:B:1262:LEU:HB2	2:B:1277:VAL:HG23	2.02	0.42
6:G:482:MET:HE2	6:G:482:MET:HB2	1.86	0.42
2:B:294:GLU:HG3	2:B:295:LYS:HD3	2.00	0.42
2:B:269:VAL:O	2:B:273:ARG:HG3	2.18	0.42
3:D:775:ASP:OD1	3:D:776:LYS:N	2.52	0.42
3:D:1215:ASN:HB3	3:D:1217:ILE:HG13	2.01	0.42
1:A:1095:LEU:HA	1:A:1098:ILE:HG12	2.00	0.42
2:B:1039:ILE:HB	2:B:1052:ILE:HG23	2.00	0.42
1:A:1072:VAL:O	1:A:1079:LYS:N	2.53	0.42
3:D:710:THR:HG22	3:D:719:TRP:HE1	1.85	0.42
4:H:365:TRP:HZ2	6:G:556:GLN:HB2	1.84	0.42
2:B:146:ILE:HG22	2:B:147:HIS:N	2.34	0.42
6:G:207:LYS:HA	6:G:210:LEU:HD12	2.00	0.42
6:G:325:GLU:HG3	6:G:329:ARG:HH21	1.84	0.42
1:A:4:LYS:HB2	1:A:4:LYS:HE2	1.83	0.42
6:G:507:LEU:HD13	6:G:507:LEU:HA	1.80	0.42
2:B:268:LYS:HA	2:B:1124:TYR:CE1	2.54	0.42
3:D:936:ASP:OD1	3:D:937:LEU:N	2.53	0.42
4:H:336:PRO:HG3	6:G:431:THR:HG22	2.02	0.42
6:G:290:MET:SD	6:G:334:ILE:HD12	2.60	0.42
6:G:334:ILE:H	6:G:334:ILE:HG12	1.69	0.42
6:G:480:VAL:HG11	6:G:518:LEU:HD22	2.02	0.42
2:B:126:MET:HA	2:B:129:VAL:HG22	2.01	0.42
2:B:99:LYS:HA	2:B:99:LYS:HD3	1.86	0.42
3:D:382:LEU:HD11	3:D:390:TYR:HD1	1.84	0.41
3:D:675:THR:HG22	3:D:717:PRO:HG3	2.02	0.41
4:H:524:LEU:HD23	4:H:527:ARG:HE	1.85	0.41
6:G:210:LEU:HD22	6:G:232:LEU:HD11	2.02	0.41
2:B:110:CYS:HB3	2:B:112:ILE:HG23	2.02	0.41
3:D:38:LEU:CD2	3:D:39:ASP:H	2.33	0.41
4:H:513:VAL:O	4:H:551:ARG:NH1	2.53	0.41
1:A:234:TYR:CG	1:A:957:PHE:HB3	2.55	0.41
3:D:384:LYS:HA	3:D:384:LYS:HD3	1.85	0.41
3:D:621:LEU:HA	3:D:624:VAL:HG22	2.01	0.41
1:A:12:LYS:HB2	1:A:12:LYS:HE3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:LYS:NZ	2:B:174:ASP:OD2	2.51	0.41
3:D:550:ILE:HD13	3:D:587:GLN:HE21	1.84	0.41
3:D:553:GLU:O	3:D:558:ARG:NH2	2.53	0.41
3:D:803:GLN:HB2	3:D:866:LEU:HD11	2.02	0.41
3:D:1225:HIS:O	3:D:1228:ARG:HG3	2.20	0.41
1:A:1:MET:HE2	1:A:1108:PRO:HB2	2.01	0.41
2:B:1056:SER:HB2	2:B:1063:LEU:HD11	2.02	0.41
3:D:1220:LEU:HA	3:D:1223:LEU:HB2	2.01	0.41
4:H:567:ILE:HG23	4:H:580:MET:HB2	2.03	0.41
1:A:234:TYR:HE1	1:A:954:ALA:HA	1.85	0.41
2:B:1091:GLY:O	2:B:1095:GLU:HB2	2.20	0.41
3:D:600:LEU:HD12	3:D:603:LEU:HD11	2.03	0.41
4:H:528:PHE:CE2	4:H:582:LEU:HB2	2.55	0.41
6:G:197:ASP:HB3	6:G:200:LEU:HG	2.02	0.41
2:B:146:ILE:HD13	2:B:155:ILE:O	2.20	0.41
3:D:1065:ASN:HB2	3:D:1088:LYS:HE2	2.02	0.41
6:G:170:LEU:HG	6:G:186:LEU:HD21	2.01	0.41
1:A:172:ARG:HG2	1:A:173:MET:N	2.36	0.41
2:B:1271:ILE:O	2:B:1273:LYS:NZ	2.53	0.41
3:D:325:SER:HA	3:D:328:ILE:HD12	2.03	0.41
3:D:338:ILE:HA	3:D:341:LEU:HD12	2.02	0.41
3:D:388:GLY:HA2	3:D:431:LEU:HD21	2.03	0.41
3:D:630:ASP:O	3:D:636:GLN:NE2	2.53	0.41
3:D:1092:ASN:OD1	3:D:1095:ARG:NH1	2.52	0.41
6:G:495:TRP:HA	6:G:500:MET:HE3	2.02	0.41
1:A:1105:LYS:HA	1:A:1105:LYS:HD2	1.95	0.41
2:B:129:VAL:HG12	2:B:187:ARG:HD3	2.02	0.41
2:B:260:CYS:O	2:B:264:ASN:N	2.53	0.41
3:D:735:SER:HA	3:D:738:ILE:HD12	2.03	0.41
3:D:47:ILE:O	3:D:48:GLU:C	2.63	0.41
2:B:119:LYS:HE2	2:B:119:LYS:HB2	1.91	0.40
3:D:239:VAL:O	3:D:243:ILE:HB	2.20	0.40
3:D:1192:VAL:HA	3:D:1195:ARG:HG2	2.03	0.40
1:A:193:LYS:HA	1:A:1004:LYS:HD3	2.03	0.40
2:B:315:ILE:HD13	2:B:1078:LEU:HB3	2.02	0.40
2:B:1144:ASN:HA	2:B:1147:LYS:HG2	2.02	0.40
2:B:1228:LYS:HG2	4:H:506:LEU:HD13	2.03	0.40
3:D:401:SER:OG	3:D:402:ARG:NH1	2.54	0.40
3:D:820:LEU:HD21	3:D:866:LEU:HD12	2.04	0.40
3:D:1194:LYS:HD2	3:D:1234:TYR:CZ	2.57	0.40
6:G:487:LYS:HE3	6:G:487:LYS:HB2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HH21	1:A:124:ASN:HB2	1.87	0.40
1:A:988:MET:O	1:A:992:THR:N	2.51	0.40
3:D:354:ARG:HH21	3:D:396:TRP:HB2	1.87	0.40
3:D:753:ASN:O	3:D:757:HIS:ND1	2.55	0.40
3:D:1118:LYS:HD2	3:D:1118:LYS:HA	1.91	0.40
4:H:66:VAL:HG23	4:H:69:LYS:H	1.87	0.40
1:A:919:LYS:O	1:A:923:GLU:HB2	2.22	0.40
3:D:240:GLN:O	3:D:244:GLU:HB2	2.21	0.40
3:D:382:LEU:HD12	3:D:385:LEU:HD12	2.04	0.40
3:D:465:LEU:HD11	3:D:549:ARG:HG3	2.03	0.40
3:D:991:ASP:HA	3:D:992:PRO:HD3	1.97	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	509/1197 (42%)	497 (98%)	12 (2%)	0	100	100
2	B	523/1305 (40%)	507 (97%)	16 (3%)	0	100	100
3	D	1103/1498 (74%)	1078 (98%)	25 (2%)	0	100	100
4	H	240/640 (38%)	231 (96%)	9 (4%)	0	100	100
5	M	3/652 (0%)	3 (100%)	0	0	100	100
6	G	429/1143 (38%)	424 (99%)	5 (1%)	0	100	100
All	All	2807/6435 (44%)	2740 (98%)	67 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	452/1040 (44%)	449 (99%)	3 (1%)	81 87
2	B	483/1165 (42%)	482 (100%)	1 (0%)	92 94
3	D	1014/1345 (75%)	1012 (100%)	2 (0%)	92 94
4	H	228/548 (42%)	227 (100%)	1 (0%)	89 91
5	M	5/549 (1%)	5 (100%)	0	100 100
6	G	394/1035 (38%)	392 (100%)	2 (0%)	86 89
All	All	2576/5682 (45%)	2567 (100%)	9 (0%)	90 92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	MET
1	A	1099	LEU
1	A	1130	MET
2	B	146	ILE
3	D	38	LEU
3	D	1223	LEU
4	H	199	MET
6	G	443	CYS
6	G	507	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	56	GLN
1	A	69	ASN
1	A	106	GLN
1	A	229	HIS
1	A	257	GLN
1	A	916	ASN
1	A	920	HIS

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Mol	Chain	Res	Type
1	A	961	ASN
2	B	223	ASN
2	B	229	GLN
2	B	234	GLN
2	B	320	ASN
2	B	1075	GLN
2	B	1245	GLN
3	D	240	GLN
3	D	435	HIS
3	D	704	ASN
3	D	786	ASN
3	D	880	GLN
3	D	982	ASN
3	D	1182	GLN
3	D	1185	GLN
3	D	1225	HIS
3	D	1247	GLN
4	H	558	GLN
6	G	283	ASN
6	G	349	ASN
6	G	377	GLN
6	G	454	HIS

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

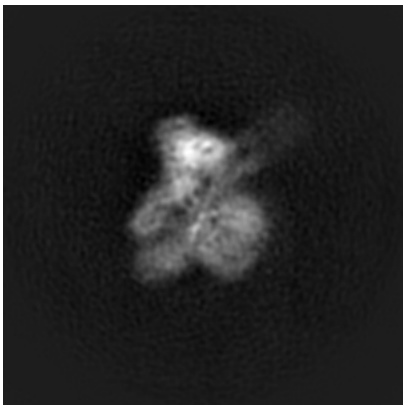
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50201. These allow visual inspection of the internal detail of the map and identification of artifacts.

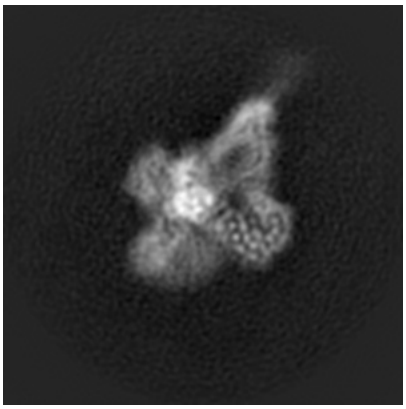
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

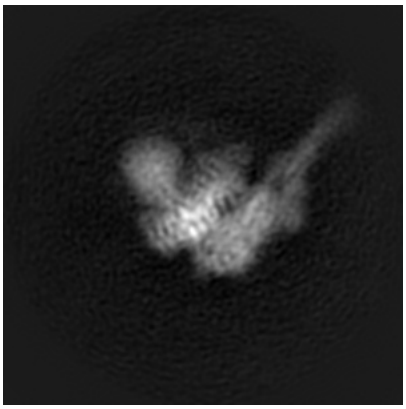
6.1.1 Primary map



X

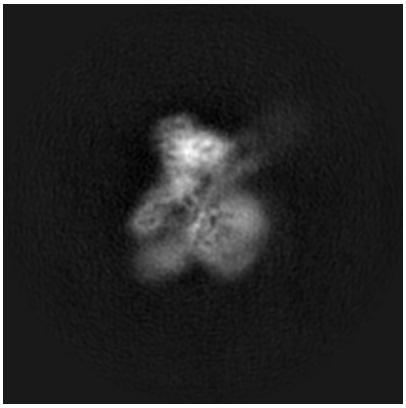


Y

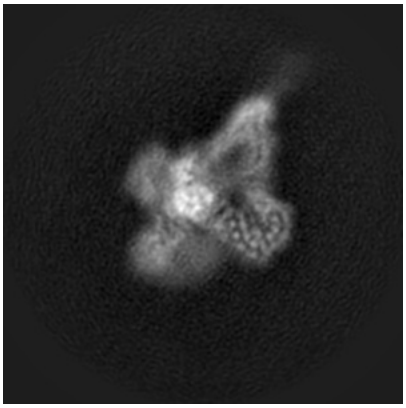


Z

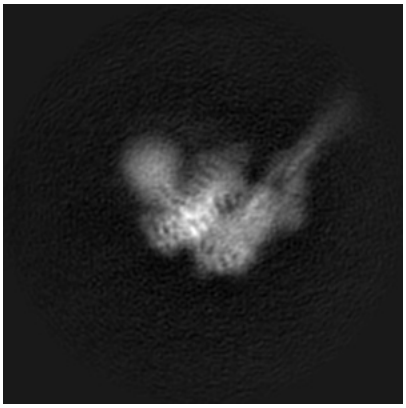
6.1.2 Raw map



X



Y

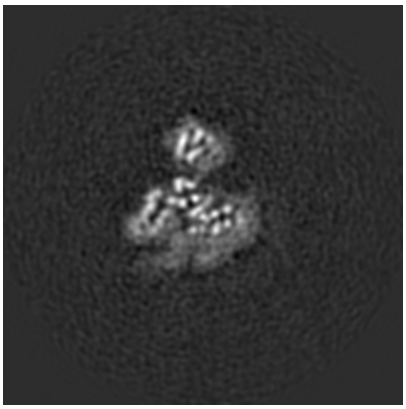


Z

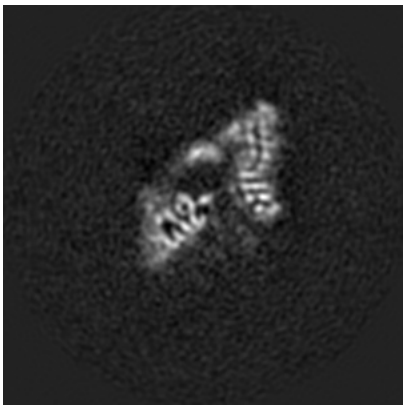
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

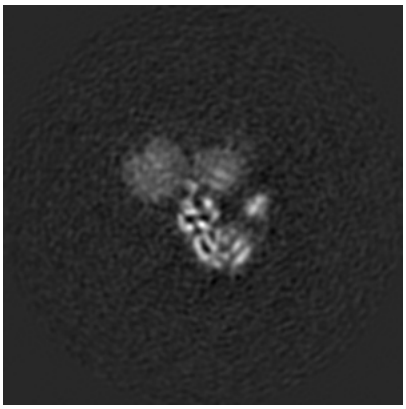
6.2.1 Primary map



X Index: 80

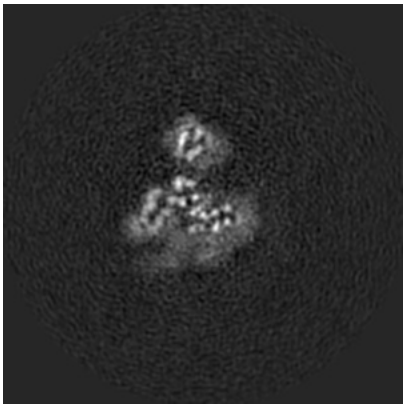


Y Index: 80

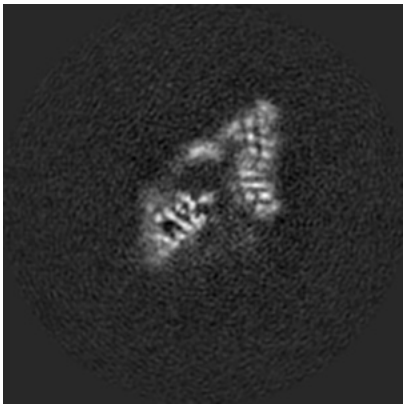


Z Index: 80

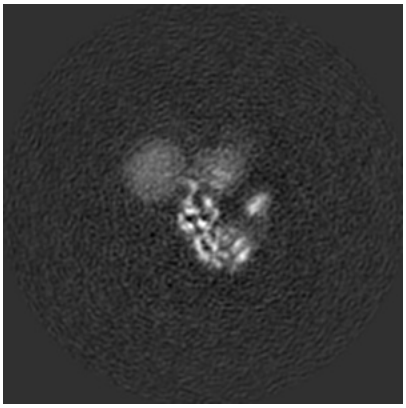
6.2.2 Raw map



X Index: 80



Y Index: 80

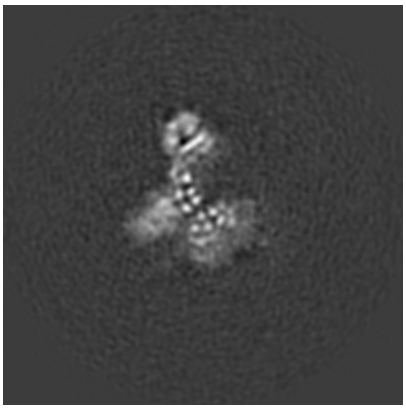


Z Index: 80

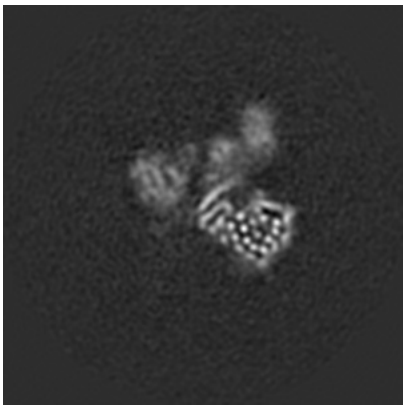
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

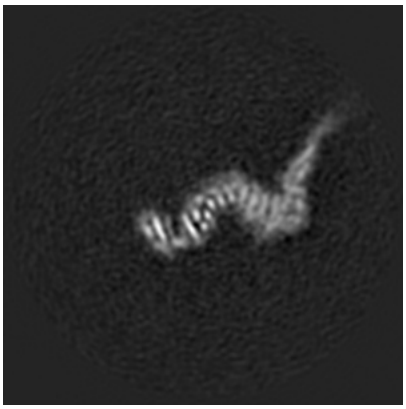
6.3.1 Primary map



X Index: 77

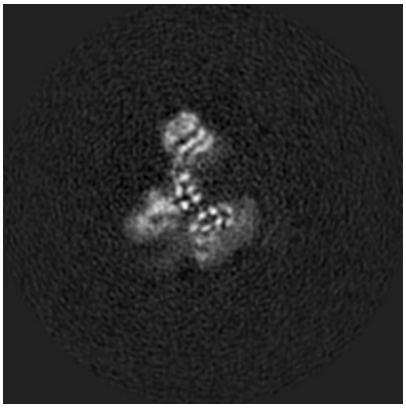


Y Index: 71

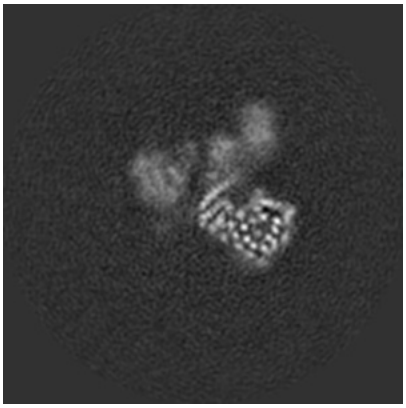


Z Index: 104

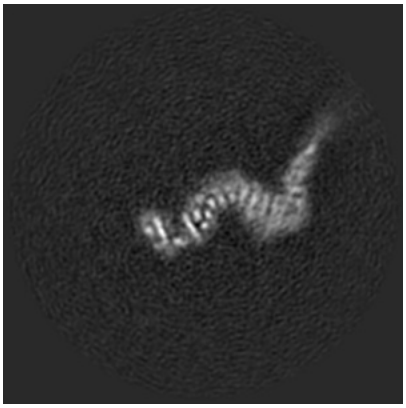
6.3.2 Raw map



X Index: 78



Y Index: 71

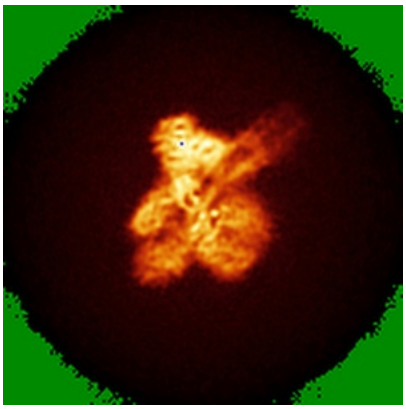


Z Index: 104

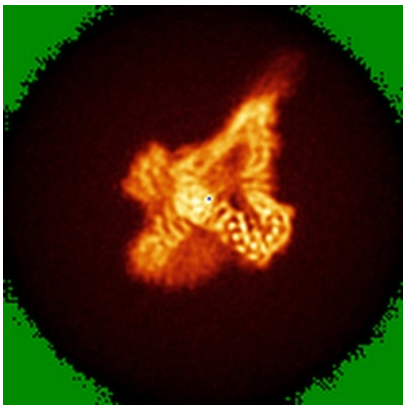
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

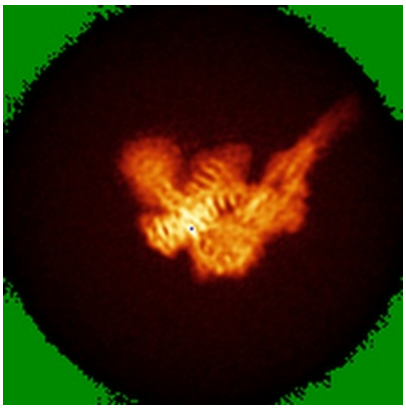
6.4.1 Primary map



X

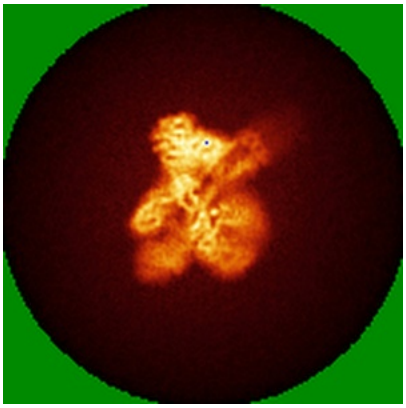


Y

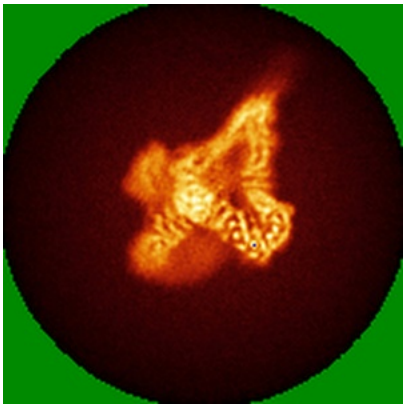


Z

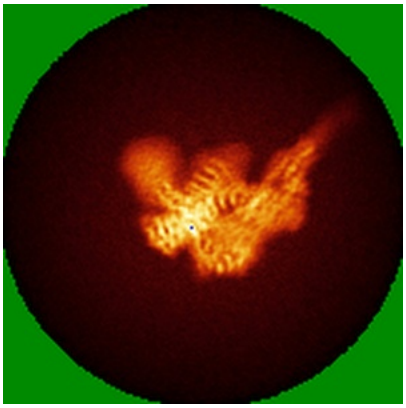
6.4.2 Raw map



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.

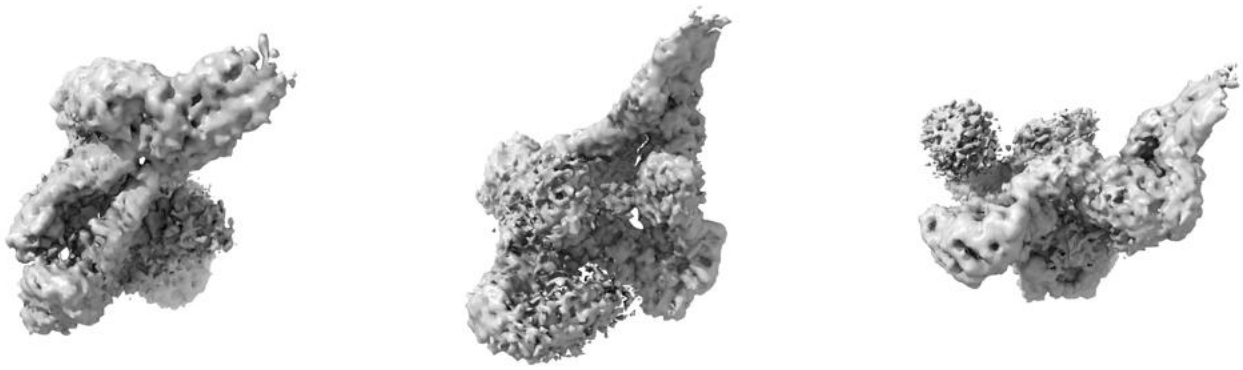
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0248. 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



X Y Z

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.

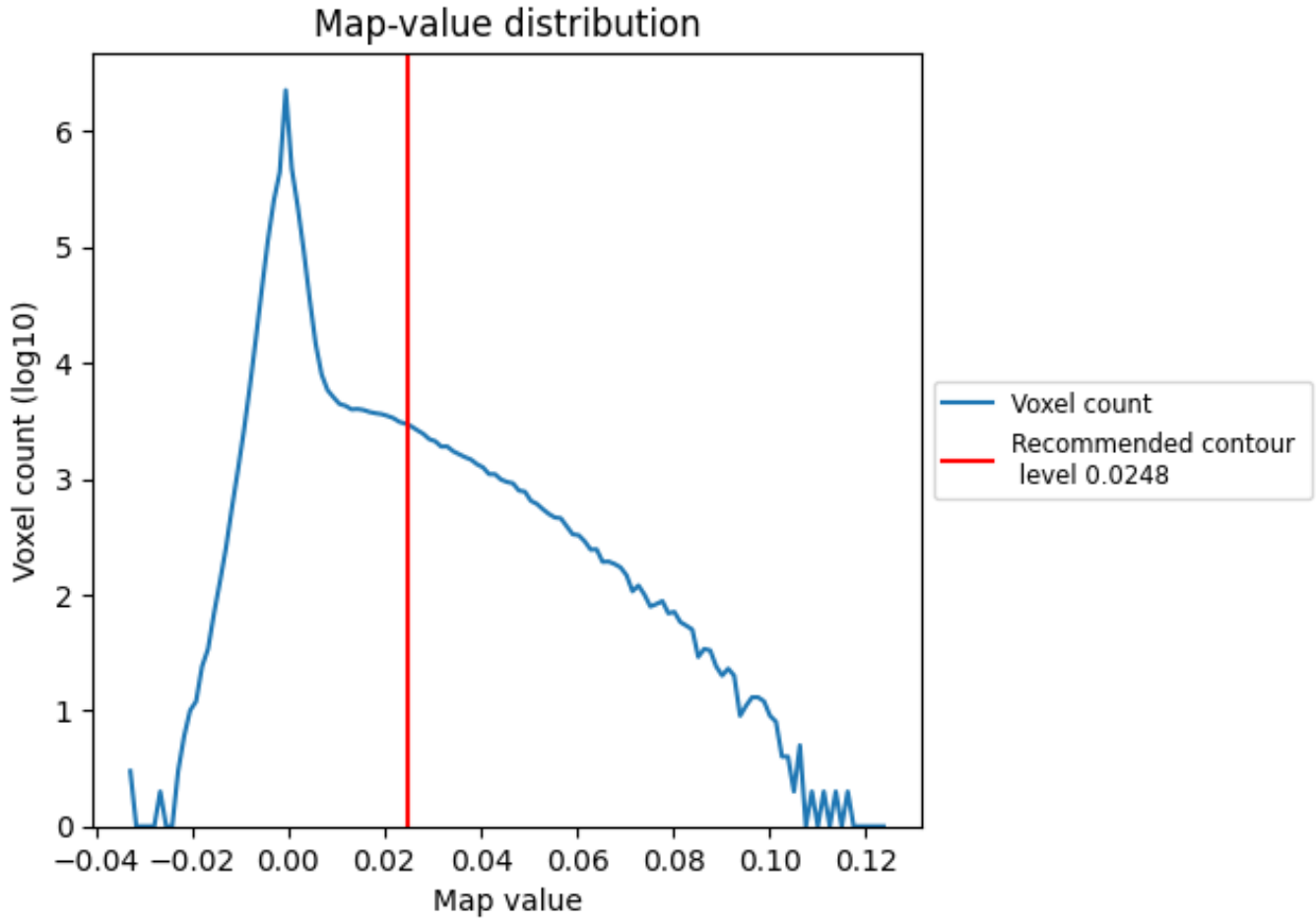
6.6 Mask visualisation (i)

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

7 Map analysis

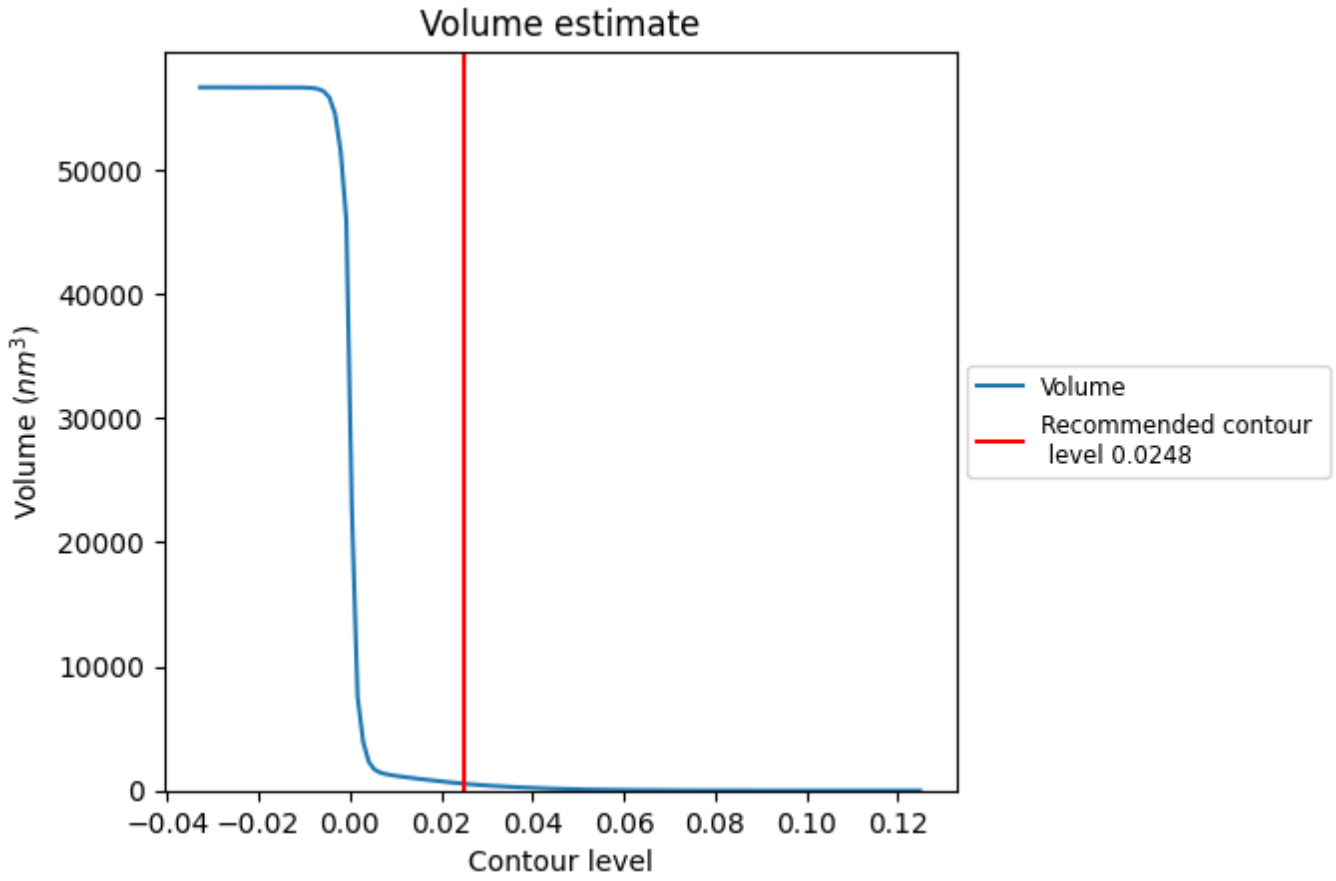
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

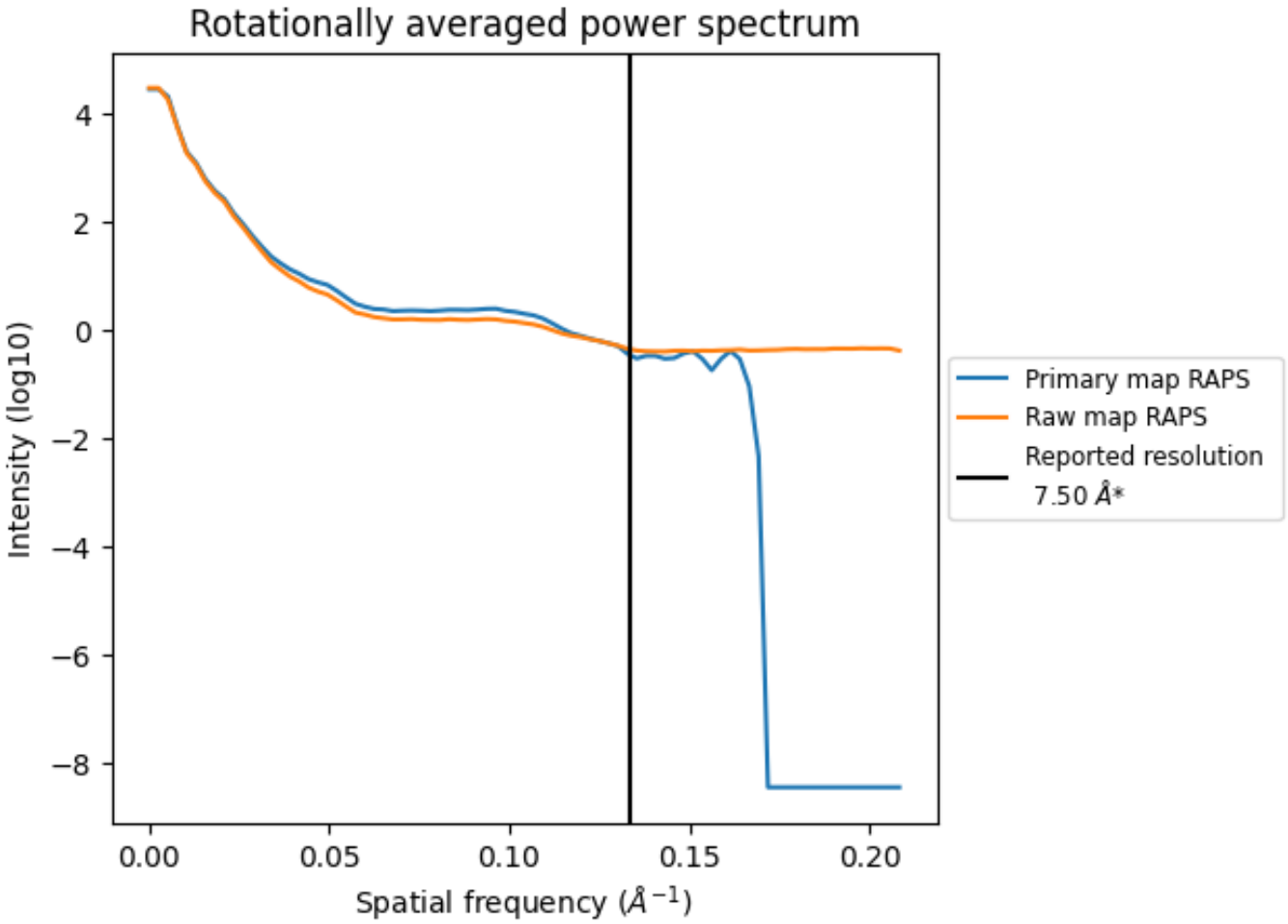
7.2 Volume estimate (i)



The volume at the recommended contour level is 560 nm^3; this corresponds to an approximate mass of 506 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 (i)

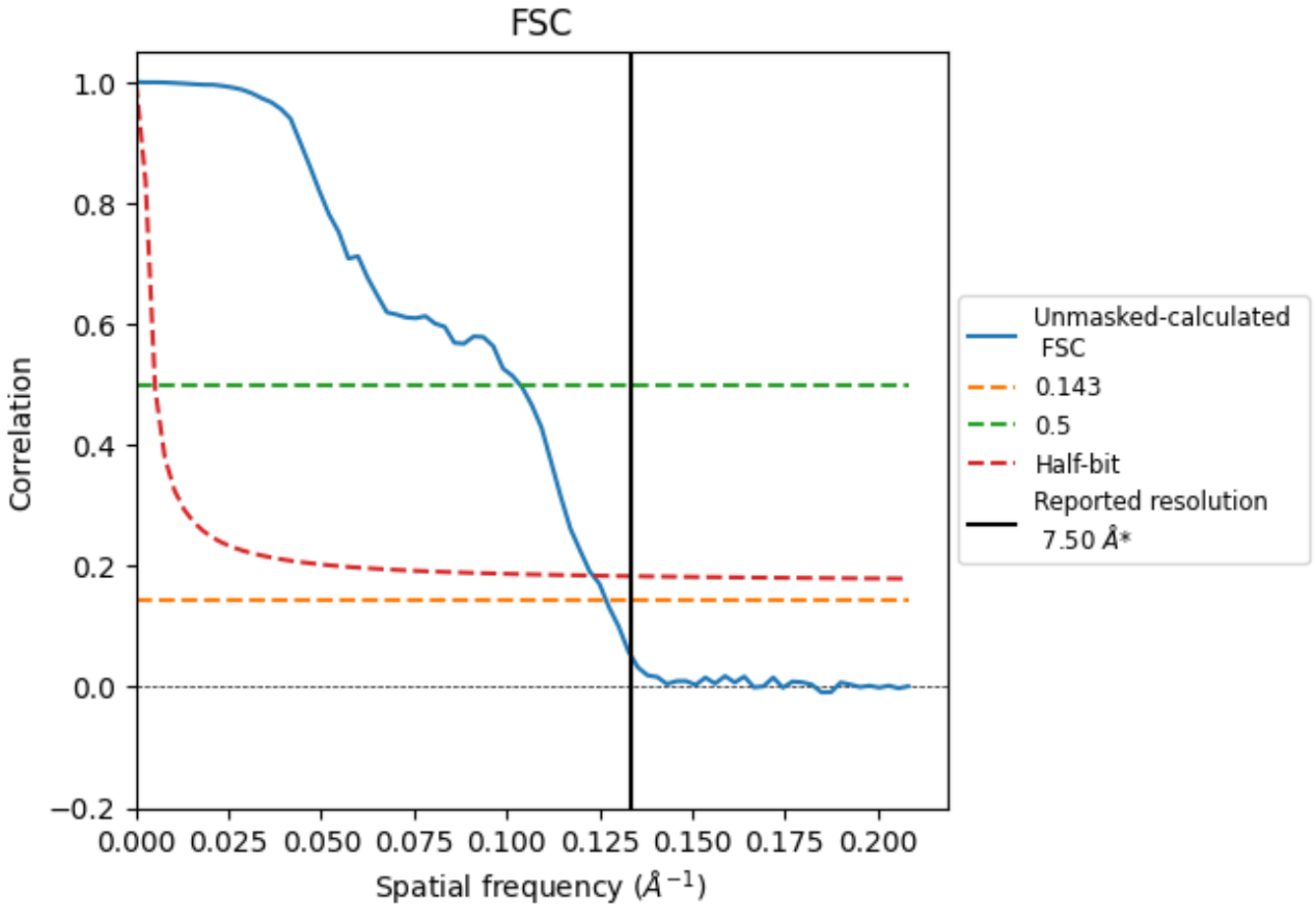


*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

8.2 Resolution estimates (i)

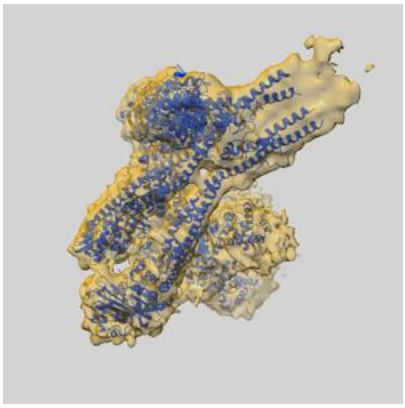
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.89	9.66	8.11

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

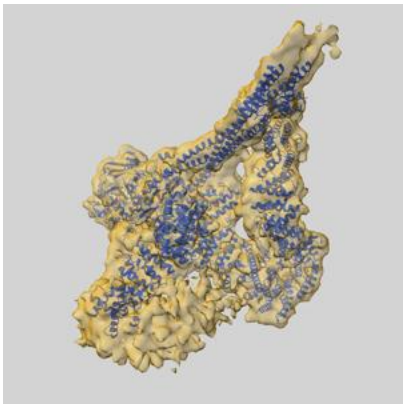
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50201 and PDB model 9F5W. Per-residue inclusion information can be found in section 3 on page 6.

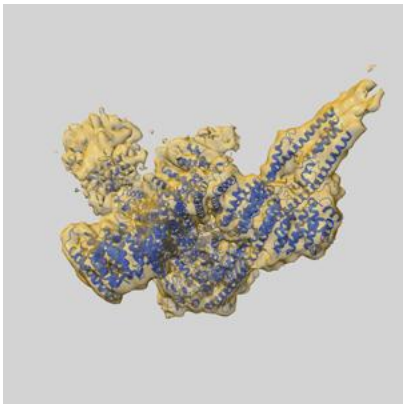
9.1 Map-model overlay



X



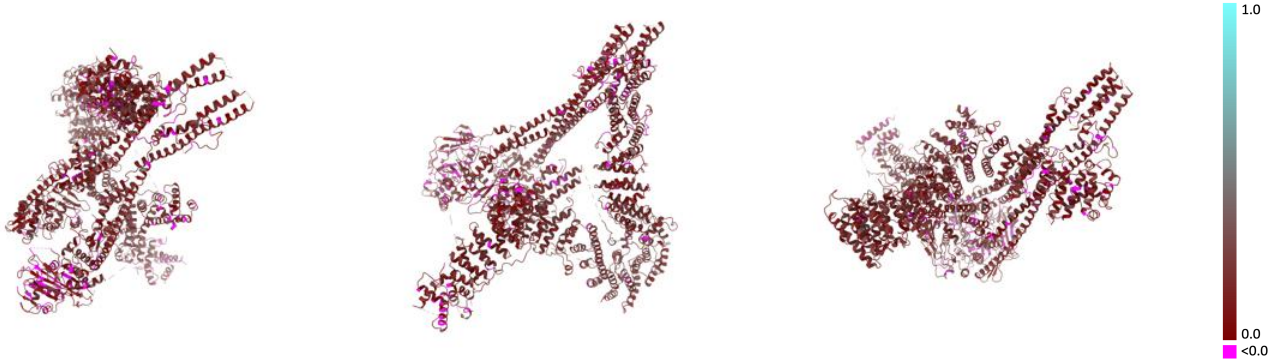
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0248 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.

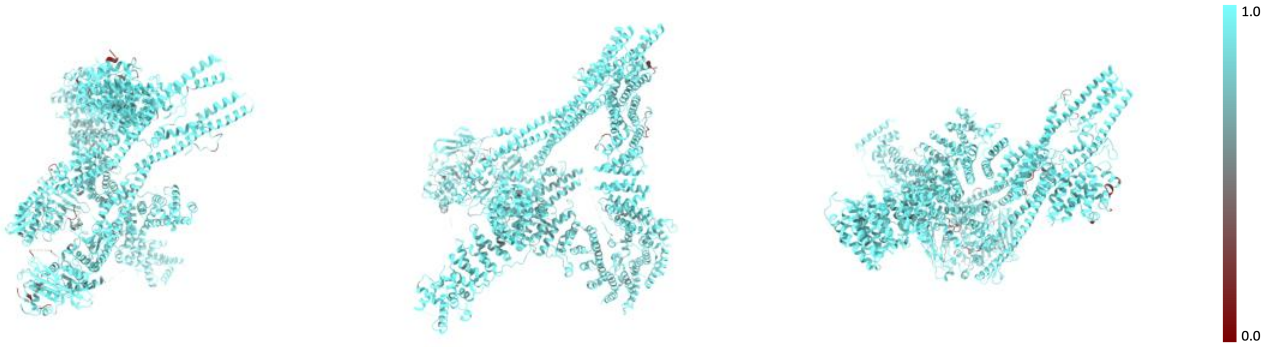
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

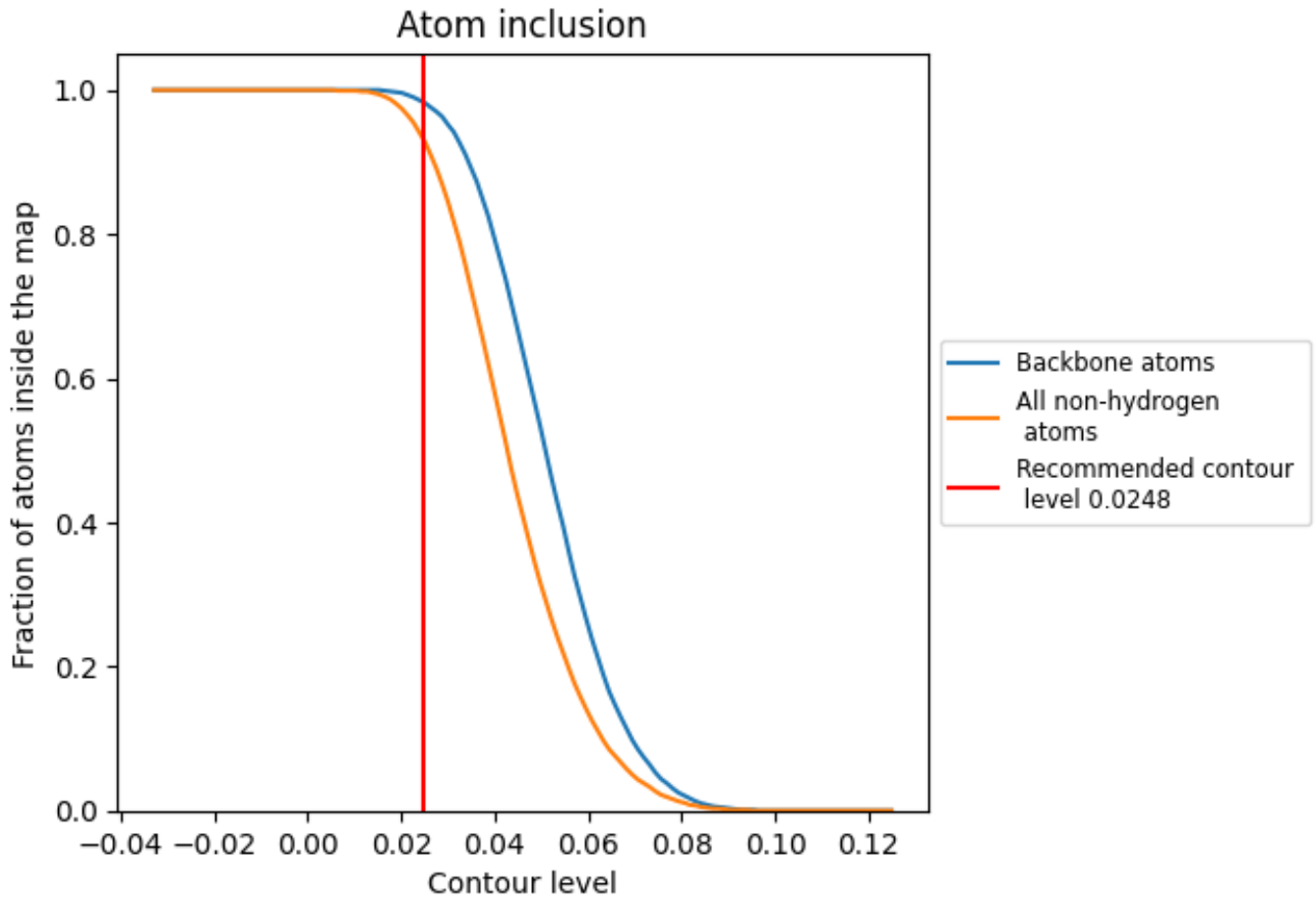
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0248).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.0248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9320	0.1550
A	0.9390	0.1600
B	0.9320	0.1340
D	0.9340	0.1630
G	0.9380	0.1560
H	0.8970	0.1580
M	0.9790	0.0820