Full wwPDB EM Validation Report ⓘ

Jun 8, 2024 – 07:32 AM EDT

PDB ID	:	8EBT
EMDB ID	:	EMD-27997
Title	:	XPA repositioning Core7 of TFIIH relative to XPC-DNA lesion (Cy5)
Authors	:	Kim, J.; Yang, W.
Deposited on	:	2022-08-31
Resolution	:	3.90 Å(reported)
Based on initial model	:	6RO4

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:

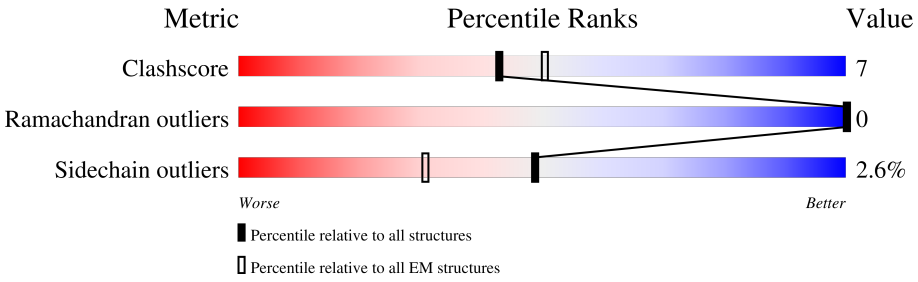
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	603	78% 21%
2	B	730	74% 18% 7%
3	C	438	36% 8% 56%
4	D	446	81% 16%
5	E	380	84% 16%
6	F	284	79% 12% 9%
7	G	66	77% 23%
8	H	274	14% 70% 29%

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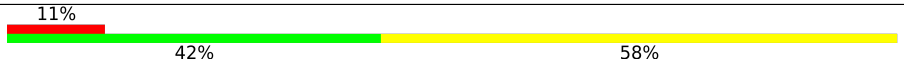
Mol	Chain	Length	Quality of chain
9	J	70	
10	K	172	
11	L	44	
12	M	45	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 27026 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 General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	603	4874	3113	844	888	29	0	0

- Molecule 2 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	677	5457	3502	948	978	29	0	0

- Molecule 3 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	191	1547	981	267	290	9	0	0

- Molecule 4 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	436	3499	2255	608	623	13	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	380	2989	1886	518	558	27	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	52	GLY	GLN	conflict	UNP Q13888

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	258	Total	C	N	O	S	0	0
			2034	1301	337	377	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	66	Total	C	N	O	S	0	0
			522	337	82	100	3		

- Molecule 8 is a protein called DNA repair protein complementing XP-C cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	274	Total	C	N	O	S	0	0
			2224	1420	401	395	8		

- Molecule 9 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	70	Total	C	N	O	S	1	0
			573	356	94	121	2		

- Molecule 10 is a protein called DNA repair protein complementing XP-A cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	172	Total	C	N	O	S	0	0
			1450	908	255	273	14		

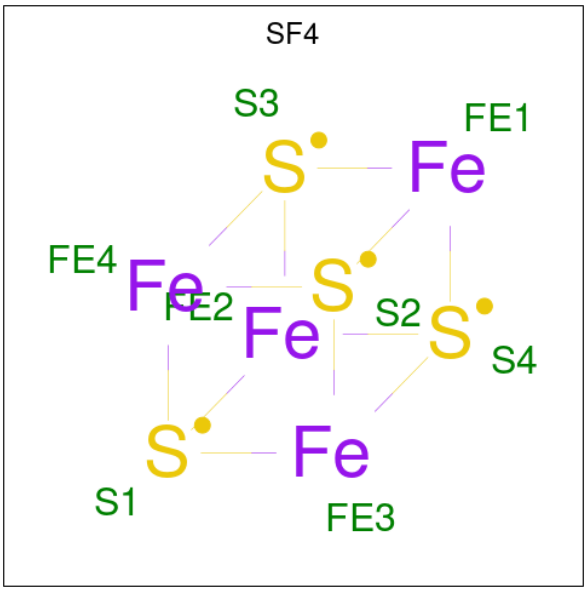
- Molecule 11 is a DNA chain called DNA (Cy5).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	44	Total	C	N	O	P	0	0
			930	454	170	262	44		

- Molecule 12 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	45	Total	C	N	O	P	0	0
			911	436	158	272	45		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	E	3	Total	Zn	0
			3	3	
14	F	2	Total	Zn	0
			2	2	
14	K	1	Total	Zn	0
			1	1	

- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

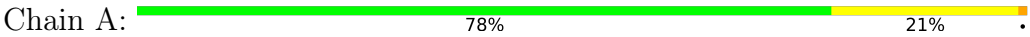
Mol	Chain	Residues	Atoms		AltConf
15	J	2	Total	Ca	0
			2	2	

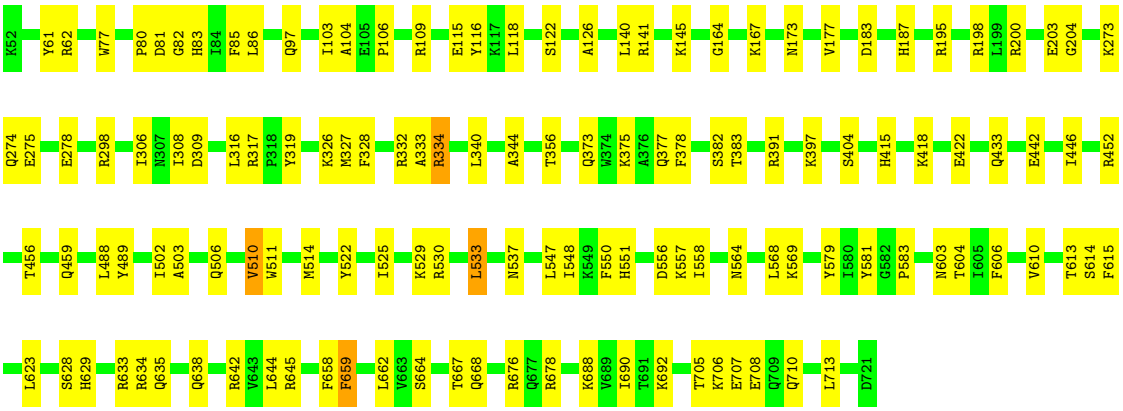
3 Residue-property plots (i)

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: General transcription and DNA repair factor IIH helicase subunit XPB

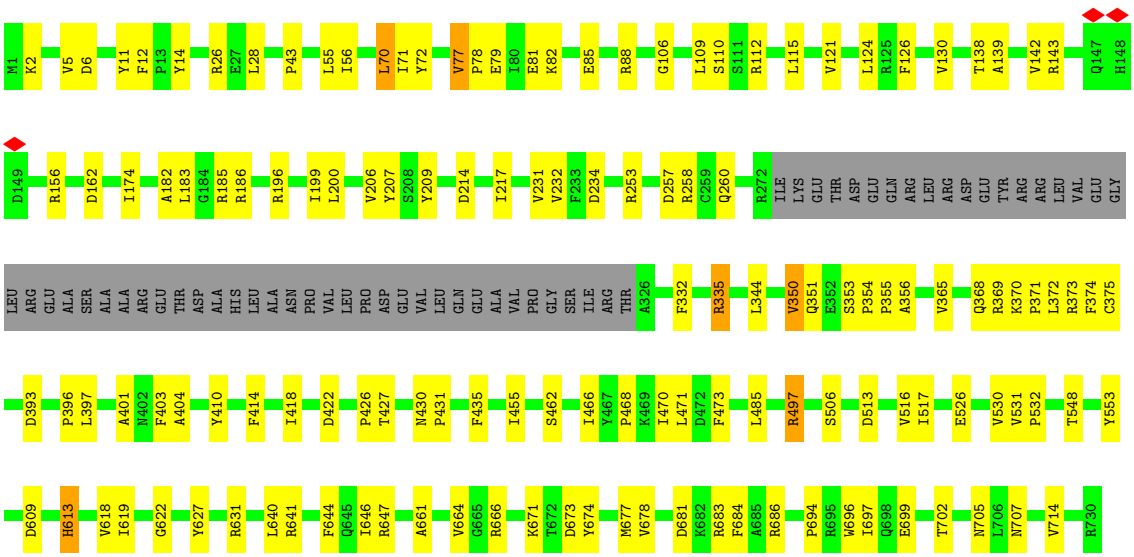
Chain A:





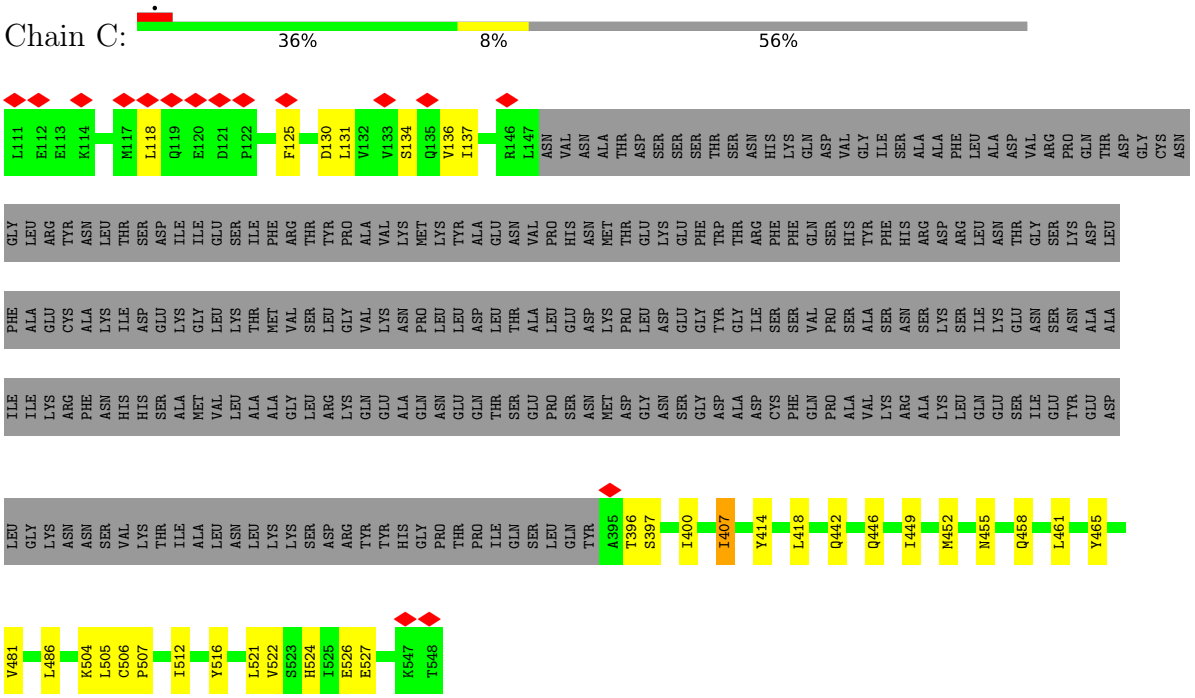
• Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD

Chain B:



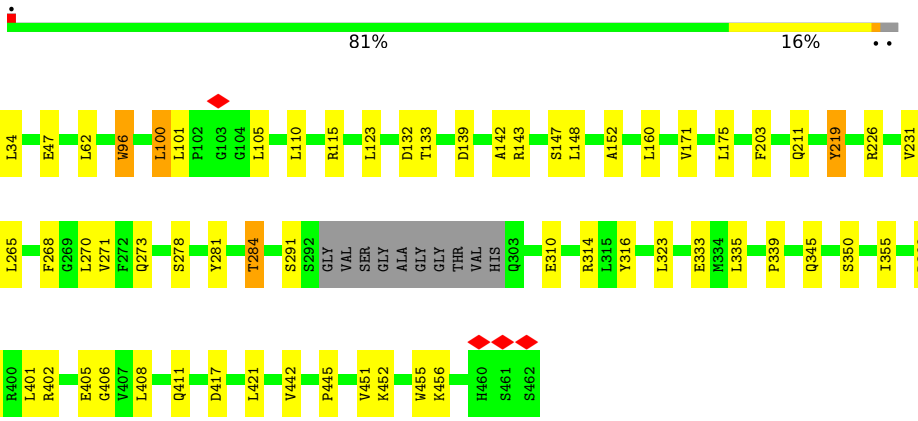
• Molecule 3: General transcription factor IIH subunit 1

Chain C:



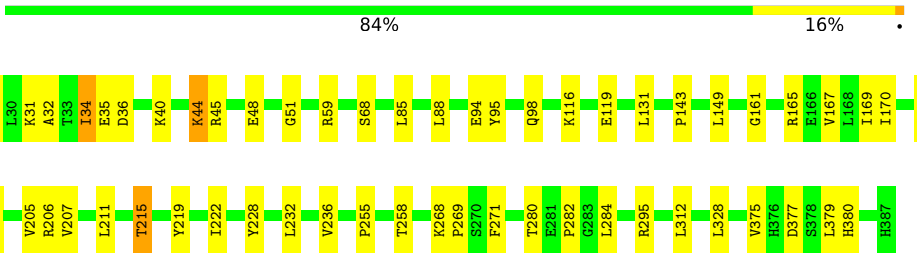
• Molecule 4: General transcription factor IIH subunit 4

Chain D:



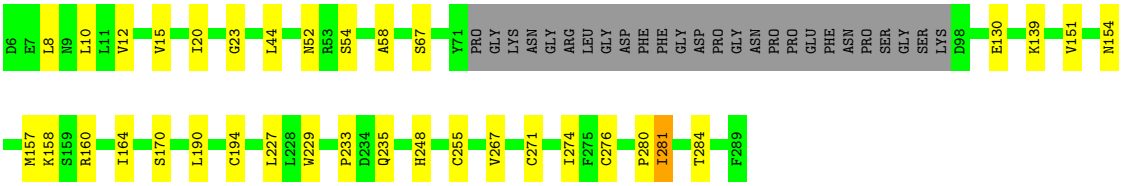
• Molecule 5: General transcription factor IIH subunit 2

Chain E:

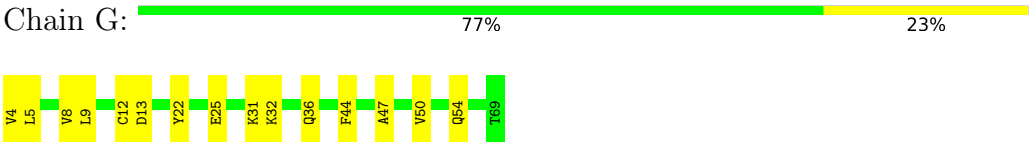


• Molecule 6: General transcription factor IIH subunit 3

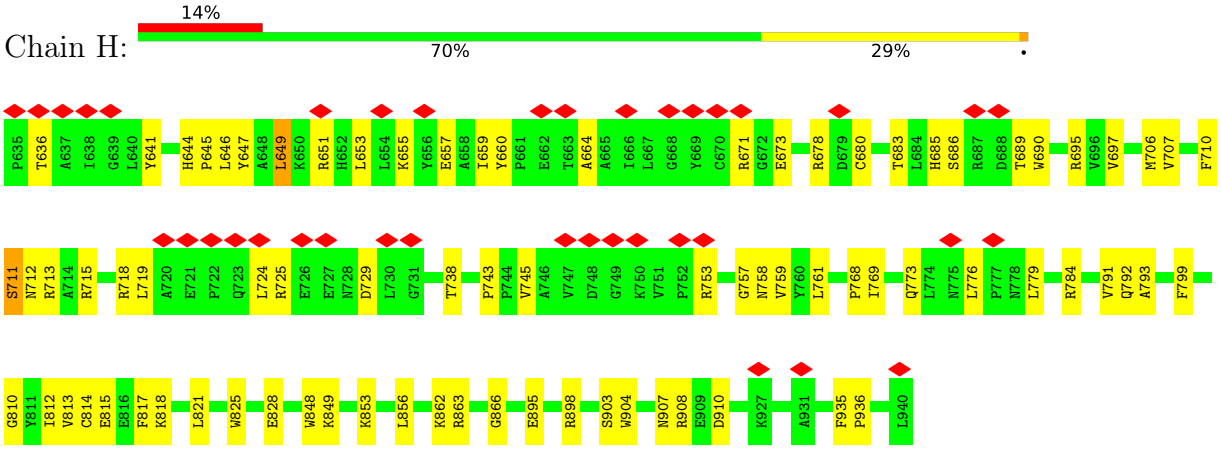
Chain F:



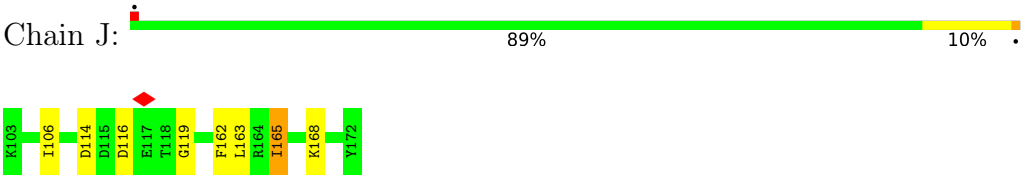
• Molecule 7: General transcription factor IIH subunit 5



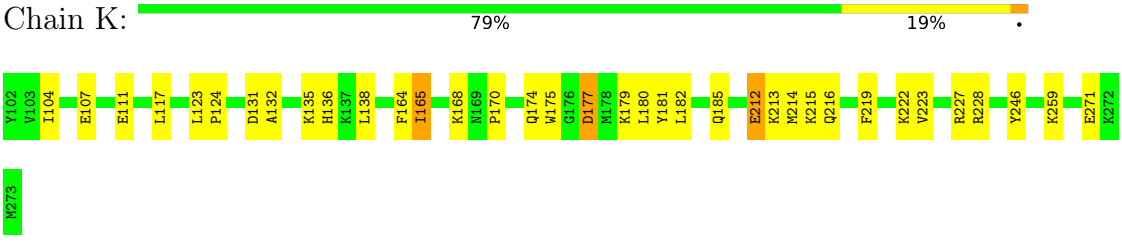
• Molecule 8: DNA repair protein complementing XP-C cells



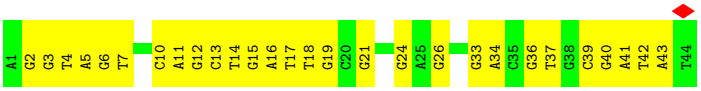
• Molecule 9: Centrin-2



• Molecule 10: DNA repair protein complementing XP-A cells



• Molecule 11: DNA (Cy5)



• Molecule 12: DNA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	173440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54.1	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	319.872, 319.872, 319.872	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, CA, VM6

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	0.24	0/4977	0.40	0/6723
2	B	0.24	0/5578	0.41	0/7551
3	C	0.23	0/1575	0.35	0/2125
4	D	0.24	0/3581	0.37	0/4851
5	E	0.24	0/3057	0.39	0/4136
6	F	0.24	0/2070	0.36	0/2803
7	G	0.24	0/528	0.41	0/713
8	H	0.23	0/2275	0.39	0/3064
9	J	0.24	0/577	0.37	0/762
10	K	0.23	0/1478	0.39	0/1974
11	L	0.53	0/1001	0.91	0/1543
12	M	0.54	0/1018	0.94	0/1566
All	All	0.27	0/27715	0.46	0/37811

There are no bond length outliers.

There are no bond angle outliers.

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	4874	0	4912	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5457	0	5499	86	0
3	C	1547	0	1561	20	0
4	D	3499	0	3541	44	0
5	E	2989	0	2950	36	0
6	F	2034	0	2050	21	0
7	G	522	0	531	13	0
8	H	2224	0	2239	52	0
9	J	573	0	555	6	0
10	K	1450	0	1434	24	0
11	L	930	0	485	24	0
12	M	911	0	509	22	0
13	B	8	0	0	0	0
14	E	3	0	0	0	0
14	F	2	0	0	0	0
14	K	1	0	0	0	0
15	J	2	0	0	0	0
All	All	27026	0	26266	380	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 7.

All (380) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:649:LEU:HD11	8:H:673:GLU:HB3	1.66	0.78
8:H:758:ASN:HD21	8:H:792:GLN:HB2	1.50	0.77
11:L:14:DT:H2'	11:L:15:DG:C8	2.25	0.71
2:B:353:SER:HB2	2:B:356:ALA:HB3	1.73	0.71
2:B:258:ARG:HE	2:B:393:ASP:HA	1.56	0.70
10:K:174:GLN:OE1	11:L:24:DG:N2	2.26	0.69
8:H:711:SER:O	8:H:715:ARG:N	2.17	0.69
2:B:258:ARG:HH21	2:B:393:ASP:H	1.41	0.69
2:B:109:LEU:HB2	2:B:207:TYR:HB3	1.74	0.68
11:L:6:DG:H2'	11:L:7:DT:H71	1.76	0.68
3:C:446:GLN:HB3	3:C:449:ILE:HB	1.76	0.68
1:A:115:GLU:OE1	4:D:314:ARG:NH1	2.26	0.67
2:B:232:VAL:HG12	2:B:455:ILE:HB	1.75	0.67
4:D:139:ASP:HB3	4:D:142:ALA:HB2	1.76	0.66
2:B:372:LEU:HD12	2:B:404:ALA:HB1	1.77	0.65
4:D:377:LEU:HB3	6:F:154:ASN:HB3	1.78	0.65
5:E:116:LYS:HE2	5:E:119:GLU:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4:VAL:N	10:K:271:GLU:O	2.29	0.65
1:A:633:ARG:HD3	1:A:678:ARG:HE	1.60	0.65
8:H:903:SER:O	8:H:907:ASN:ND2	2.30	0.65
1:A:308:ILE:HD11	1:A:382:SER:HB2	1.79	0.65
1:A:615:PHE:HB2	1:A:642:ARG:HH22	1.63	0.65
1:A:623:LEU:HB3	1:A:659:PHE:HB2	1.80	0.64
2:B:72:TYR:HB3	2:B:206:VAL:HG12	1.81	0.63
2:B:641:ARG:NH1	10:K:177:ASP:OD1	2.31	0.63
10:K:104:ILE:HG12	10:K:111:GLU:HG2	1.81	0.63
2:B:647:ARG:HH21	10:K:179:LYS:HE3	1.64	0.63
2:B:532:PRO:HB3	5:E:174:LEU:HB3	1.81	0.63
2:B:335:ARG:HG3	2:B:365:VAL:HG21	1.80	0.63
8:H:653:LEU:HD11	8:H:659:ILE:HG23	1.81	0.62
2:B:332:PHE:O	2:B:335:ARG:NH1	2.33	0.62
4:D:62:LEU:O	4:D:115:ARG:NH1	2.33	0.61
4:D:219:TYR:OH	4:D:264:HIS:ND1	2.30	0.61
4:D:19:LEU:HD23	4:D:47:GLU:HG3	1.83	0.61
1:A:278:GLU:OE2	1:A:452:ARG:NH2	2.34	0.61
3:C:136:VAL:HG12	3:C:137:ILE:HG23	1.82	0.60
1:A:378:PHE:O	1:A:382:SER:OG	2.17	0.60
8:H:649:LEU:HD12	8:H:651:ARG:HG2	1.82	0.60
10:K:174:GLN:HA	11:L:24:DG:H1'	1.84	0.60
1:A:82:GLY:O	1:A:83:HIS:ND1	2.34	0.60
1:A:183:ASP:O	1:A:187:HIS:ND1	2.35	0.60
8:H:706:MET:HB3	8:H:729:ASP:HB3	1.84	0.60
1:A:633:ARG:HG2	1:A:676:ARG:HA	1.83	0.59
2:B:28:LEU:HD23	2:B:55:LEU:HD23	1.82	0.59
4:D:30:VAL:HG22	4:D:33:ARG:HH21	1.66	0.59
1:A:547:LEU:O	1:A:551:HIS:ND1	2.33	0.59
2:B:350:VAL:HG11	2:B:631:ARG:HD3	1.83	0.59
8:H:712:ASN:N	12:M:28:DA:OP1	2.36	0.59
4:D:442:VAL:HG21	7:G:9:LEU:HD12	1.85	0.59
1:A:551:HIS:HB2	1:A:558:ILE:HD11	1.85	0.59
4:D:96:TRP:HB3	4:D:110:LEU:HD23	1.84	0.58
2:B:196:ARG:HH21	2:B:199:ILE:HD13	1.67	0.58
2:B:258:ARG:HD3	2:B:396:PRO:HG2	1.84	0.58
2:B:686:ARG:NH2	11:L:21:DG:O3'	2.36	0.58
11:L:13:DC:H2'	11:L:14:DT:C6	2.38	0.58
6:F:271:CYS:SG	6:F:284:THR:OG1	2.59	0.58
12:M:22:DT:H2"	12:M:23:DC:C5	2.38	0.58
4:D:241:SER:HB3	4:D:291:SER:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:267:VAL:HG22	6:F:274:ILE:HG12	1.86	0.58
7:G:36:GLN:HB3	7:G:44:PHE:HB3	1.86	0.57
2:B:622:GLY:HA2	2:B:681:ASP:HB2	1.86	0.57
1:A:103:ILE:HA	1:A:126:ALA:HB2	1.84	0.57
8:H:710:PHE:N	12:M:27:DT:OP2	2.37	0.57
10:K:165:ILE:HG23	10:K:180:LEU:HB2	1.87	0.57
2:B:5:VAL:HA	2:B:26:ARG:HH12	1.70	0.57
11:L:11:DA:H2'	11:L:12:DG:C8	2.40	0.57
1:A:710:GLN:HA	1:A:713:LEU:HD23	1.87	0.57
2:B:344:LEU:HA	2:B:431:PRO:HG2	1.87	0.57
3:C:481:VAL:HG13	3:C:486:LEU:HB2	1.86	0.56
3:C:505:LEU:HD11	3:C:522:VAL:HG13	1.87	0.56
11:L:40:DG:H2"	11:L:41:DA:C8	2.41	0.56
2:B:422:ASP:H	2:B:426:PRO:HA	1.70	0.56
5:E:174:LEU:HD21	5:E:202:SER:HB2	1.88	0.56
1:A:77:TRP:HB2	1:A:85:PHE:HB2	1.88	0.56
8:H:784:ARG:NH1	11:L:26:DG:OP1	2.39	0.56
12:M:21:DG:H2'	12:M:22:DT:C6	2.41	0.55
5:E:258:THR:HA	6:F:248:HIS:HB3	1.88	0.55
5:E:94:GLU:OE2	5:E:98:GLN:NE2	2.40	0.55
4:D:411:GLN:OE1	7:G:4:VAL:N	2.40	0.55
10:K:138:LEU:HB3	10:K:180:LEU:HB3	1.89	0.55
1:A:692:LYS:NZ	8:H:910:ASP:OD1	2.39	0.55
2:B:497:ARG:NH2	2:B:707:ASN:O	2.39	0.55
1:A:514:MET:HA	1:A:537:ASN:HD21	1.72	0.54
3:C:455:ASN:HA	3:C:458:GLN:HB2	1.89	0.54
11:L:12:DG:H2'	11:L:13:DC:C6	2.42	0.54
8:H:793:ALA:HB2	8:H:812:ILE:HG13	1.88	0.54
2:B:468:PRO:HA	2:B:473:PHE:HB3	1.89	0.54
4:D:232:GLU:HB3	4:D:258:LEU:HD11	1.88	0.54
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.90	0.54
2:B:370:LYS:HA	2:B:373:ARG:HH21	1.73	0.54
6:F:44:LEU:HD22	6:F:227:LEU:HB3	1.90	0.54
6:F:158:LYS:HD3	6:F:235:GLN:HE21	1.73	0.54
1:A:326:LYS:O	1:A:334:ARG:NH2	2.41	0.53
4:D:408:LEU:HD23	7:G:5:LEU:HD12	1.91	0.53
6:F:164:ILE:HG22	6:F:194:CYS:HB3	1.88	0.53
1:A:418:LYS:NZ	11:L:16:DA:OP1	2.41	0.53
1:A:510:VAL:HB	1:A:690:ILE:HB	1.90	0.53
1:A:581:TYR:HD1	1:A:583:PRO:HD2	1.73	0.53
6:F:280:PRO:HG2	6:F:281:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:ILE:HD11	2:B:548:THR:HG23	1.91	0.53
11:L:18:DT:H4'	11:L:19:DG:OP1	2.09	0.53
2:B:513:ASP:HB3	2:B:516:VAL:HG22	1.89	0.53
3:C:118:LEU:HB3	3:C:125:PHE:HD1	1.74	0.53
5:E:211:LEU:O	5:E:215:THR:OG1	2.16	0.53
5:E:284:LEU:HD23	5:E:284:LEU:H	1.74	0.53
5:E:375:VAL:HA	5:E:379:LEU:HB3	1.91	0.53
10:K:182:LEU:HD23	10:K:185:GLN:HG3	1.89	0.53
4:D:152:ALA:HB2	4:D:284:THR:HG21	1.90	0.52
5:E:26:GLU:HG2	5:E:29:SER:HB3	1.90	0.52
1:A:173:ASN:OD1	1:A:459:GLN:NE2	2.42	0.52
3:C:130:ASP:O	3:C:134:SER:OG	2.26	0.52
6:F:8:LEU:HB2	6:F:157:MET:HA	1.90	0.52
6:F:160:ARG:NH1	6:F:233:PRO:O	2.37	0.52
3:C:407:ILE:HB	6:F:23:GLY:HA2	1.91	0.52
10:K:174:GLN:HB2	12:M:34:DA:C2	2.44	0.52
1:A:628:SER:OG	1:A:635:GLN:OE1	2.27	0.52
5:E:271:PHE:HD2	5:E:282:PRO:HB2	1.73	0.52
11:L:36:DG:H2'	11:L:37:DT:C6	2.44	0.52
8:H:853:LYS:HE2	10:K:223:VAL:HG21	1.92	0.52
2:B:640:LEU:HB3	2:B:646:ILE:HB	1.92	0.52
1:A:550:PHE:HZ	8:H:936:PRO:HB2	1.75	0.51
9:J:116:ASP:OD1	9:J:116:ASP:N	2.36	0.51
1:A:195:ARG:HG2	1:A:198:ARG:HH21	1.75	0.51
4:D:369:ARG:HG3	4:D:382:VAL:HG11	1.92	0.51
6:F:151:VAL:HG21	6:F:157:MET:HB2	1.92	0.51
2:B:485:LEU:HD11	2:B:671:LYS:HD2	1.91	0.51
2:B:139:ALA:H	2:B:142:VAL:HB	1.75	0.51
8:H:815:GLU:O	8:H:818:LYS:NZ	2.40	0.51
12:M:37:DG:H2"	12:M:38:DC:C5	2.46	0.51
1:A:104:ALA:HA	1:A:122:SER:HB2	1.93	0.51
1:A:309:ASP:OD1	1:A:309:ASP:N	2.44	0.51
10:K:132:ALA:HA	10:K:136:HIS:HB2	1.93	0.51
1:A:274:GLN:NE2	1:A:456:THR:O	2.43	0.51
12:M:24:DT:H2"	12:M:25:DA:C8	2.46	0.51
1:A:525:ILE:HG12	1:A:529:LYS:HB2	1.93	0.50
2:B:5:VAL:HB	2:B:26:ARG:HH22	1.76	0.50
2:B:88:ARG:HA	2:B:174:ILE:HD11	1.92	0.50
2:B:530:VAL:HG11	2:B:714:VAL:HG13	1.92	0.50
11:L:10:DC:H2'	11:L:11:DA:C8	2.46	0.50
2:B:78:PRO:HA	2:B:81:GLU:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:PRO:HG2	2:B:355:PRO:HD3	1.93	0.50
8:H:907:ASN:OD1	8:H:908:ARG:NE	2.44	0.50
11:L:33:DG:H2"	11:L:34:DA:C8	2.47	0.50
3:C:461:LEU:HD22	3:C:521:LEU:HD13	1.94	0.50
11:L:5:DA:H2"	11:L:6:DG:C8	2.46	0.50
2:B:6:ASP:H	2:B:26:ARG:HH22	1.60	0.50
6:F:12:VAL:HG22	6:F:58:ALA:HB3	1.94	0.50
11:L:5:DA:H2"	11:L:6:DG:H8	1.77	0.50
2:B:77:VAL:HG13	2:B:78:PRO:HD3	1.93	0.50
4:D:160:LEU:HD12	4:D:323:LEU:HD21	1.93	0.49
8:H:719:LEU:HD12	8:H:725:ARG:HH11	1.76	0.49
2:B:12:PHE:HD1	2:B:14:TYR:H	1.58	0.49
1:A:569:LYS:NZ	1:A:579:TYR:OH	2.41	0.49
4:D:421:LEU:HD11	4:D:451:VAL:HG13	1.94	0.49
2:B:351:GLN:HB2	2:B:418:ILE:HD11	1.94	0.49
8:H:686:SER:O	8:H:690:TRP:N	2.43	0.49
4:D:401:LEU:HD13	7:G:12:CYS:HB3	1.95	0.49
11:L:42:DT:H2"	11:L:43:DA:N7	2.28	0.49
12:M:33:DC:H2"	12:M:34:DA:C8	2.47	0.49
1:A:164:GLY:O	1:A:167:LYS:NZ	2.42	0.49
8:H:895:GLU:OE2	8:H:898:ARG:NH2	2.38	0.49
4:D:132:ASP:OD1	4:D:133:THR:N	2.44	0.49
4:D:262:LEU:HD11	4:D:271:VAL:HG11	1.95	0.49
1:A:356:THR:HG21	5:E:11:TRP:HE1	1.78	0.48
2:B:699:GLU:OE1	2:B:699:GLU:N	2.45	0.48
4:D:355:ILE:HD13	4:D:395:GLU:HA	1.95	0.48
1:A:77:TRP:CE2	1:A:145:LYS:HD3	2.48	0.48
3:C:131:LEU:HB3	3:C:137:ILE:HG12	1.96	0.48
10:K:246:TYR:HB3	10:K:259:LYS:HB3	1.94	0.48
12:M:13:DT:H2"	12:M:14:DA:C8	2.48	0.48
7:G:47:ALA:HA	7:G:50:VAL:HG13	1.95	0.48
10:K:123:LEU:HD12	10:K:124:PRO:HD2	1.96	0.48
8:H:706:MET:SD	8:H:706:MET:N	2.86	0.48
11:L:18:DT:H2"	11:L:19:DG:C8	2.48	0.48
2:B:2:LYS:HZ3	2:B:11:TYR:HB3	1.79	0.48
10:K:107:GLU:OE2	10:K:135:LYS:NZ	2.41	0.48
1:A:568:LEU:HD11	1:A:606:PHE:HB3	1.95	0.48
8:H:848:TRP:CD2	9:J:165:ILE:HD11	2.49	0.48
11:L:18:DT:H2"	11:L:19:DG:H8	1.79	0.48
4:D:34:LEU:HD23	4:D:231:VAL:HG13	1.96	0.47
5:E:149:LEU:HD21	5:E:169:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:67:SER:HB2	6:F:139:LYS:HD2	1.96	0.47
1:A:397:LYS:HD2	1:A:422:GLU:HG2	1.97	0.47
1:A:514:MET:SD	1:A:537:ASN:ND2	2.87	0.47
5:E:31:LYS:O	5:E:34:ILE:HG12	2.14	0.47
2:B:109:LEU:HD13	2:B:196:ARG:HH22	1.80	0.47
5:E:143:PRO:HG3	5:E:173:SER:HB3	1.96	0.47
8:H:655:LYS:HE2	8:H:707:VAL:HB	1.96	0.47
12:M:42:DC:H2"	12:M:43:DA:C8	2.50	0.47
1:A:506:GLN:HB3	1:A:658:PHE:HB3	1.97	0.47
2:B:209:TYR:OH	2:B:234:ASP:O	2.32	0.47
2:B:71:ILE:HB	2:B:231:VAL:HG12	1.97	0.47
2:B:618:VAL:HG11	2:B:664:VAL:HA	1.97	0.47
3:C:418:LEU:HD22	4:D:123:LEU:HB3	1.97	0.47
10:K:131:ASP:HB3	10:K:135:LYS:HB3	1.96	0.47
10:K:213:LYS:O	10:K:216:GLN:HG3	2.15	0.47
12:M:54:DC:H2"	12:M:55:DC:C6	2.50	0.47
2:B:214:ASP:HB3	2:B:217:ILE:HG22	1.96	0.47
1:A:344:ALA:HB2	1:A:502:ILE:HD11	1.97	0.47
10:K:212:GLU:HA	10:K:215:LYS:HG2	1.96	0.47
10:K:219:PHE:HD1	10:K:222:LYS:HZ3	1.63	0.47
4:D:171:VAL:HB	4:D:175:LEU:HD23	1.97	0.47
11:L:2:DG:H2"	11:L:3:DG:C8	2.50	0.47
1:A:104:ALA:HB2	1:A:118:LEU:HD23	1.96	0.46
2:B:106:GLY:N	2:B:174:ILE:HG22	2.29	0.46
4:D:333:GLU:HG3	4:D:350:SER:HB3	1.97	0.46
12:M:53:DA:H2"	12:M:54:DC:C6	2.50	0.46
6:F:190:LEU:HD11	6:F:235:GLN:HB3	1.97	0.46
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.76	0.46
2:B:369:ARG:HA	2:B:372:LEU:HD23	1.96	0.46
8:H:712:ASN:HB2	12:M:28:DA:H5'	1.98	0.46
8:H:813:VAL:HG11	8:H:821:LEU:HD11	1.97	0.46
1:A:433:GLN:OE1	1:A:433:GLN:N	2.48	0.46
1:A:510:VAL:HG13	1:A:662:LEU:HD23	1.98	0.46
2:B:694:PRO:HB2	2:B:696:TRP:CD1	2.50	0.46
4:D:310:GLU:HG3	4:D:316:TYR:HE2	1.79	0.46
5:E:377:ASP:O	5:E:380:HIS:NE2	2.48	0.46
8:H:753:ARG:HB3	8:H:757:GLY:HA2	1.98	0.46
12:M:32:DT:H2"	12:M:33:DC:H5	1.80	0.46
2:B:43:PRO:HB3	2:B:696:TRP:CG	2.51	0.45
5:E:94:GLU:HG3	5:E:236:VAL:HG11	1.98	0.45
8:H:690:TRP:CZ3	8:H:695:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ARG:NH2	1:A:638:GLN:OE1	2.50	0.45
2:B:705:ASN:OD1	2:B:705:ASN:N	2.49	0.45
4:D:405:GLU:HG2	7:G:8:VAL:HG22	1.96	0.45
1:A:551:HIS:HB3	1:A:556:ASP:HB2	1.99	0.45
4:D:265:LEU:HD22	4:D:270:LEU:HD12	1.96	0.45
8:H:791:VAL:O	8:H:812:ILE:N	2.42	0.45
1:A:327:MET:HG2	1:A:488:LEU:HD23	1.99	0.45
6:F:15:VAL:HG22	6:F:164:ILE:HD11	1.98	0.45
8:H:645:PRO:O	8:H:678:ARG:HB2	2.16	0.45
2:B:613:HIS:ND1	2:B:613:HIS:O	2.50	0.45
1:A:62:ARG:HA	4:D:339:PRO:HG3	1.98	0.45
6:F:10:LEU:HD22	6:F:157:MET:HE1	1.99	0.45
2:B:677:MET:HE3	2:B:697:ILE:HD13	1.98	0.45
8:H:724:LEU:H	8:H:724:LEU:HD23	1.82	0.45
6:F:52:ASN:ND2	6:F:54:SER:OG	2.49	0.45
8:H:853:LYS:HD2	8:H:856:LEU:HD12	1.99	0.44
1:A:613:THR:OG1	1:A:614:SER:N	2.50	0.44
4:D:406:GLY:HA2	4:D:445:PRO:HD3	1.98	0.44
4:D:452:LYS:HE2	4:D:456:LYS:HE3	1.98	0.44
5:E:198:VAL:HB	5:E:219:TYR:HD1	1.81	0.44
12:M:36:DC:H2"	12:M:37:DG:C8	2.52	0.44
2:B:344:LEU:HD12	2:B:431:PRO:HG2	1.99	0.44
3:C:527:GLU:OE2	5:E:268:LYS:NZ	2.33	0.44
5:E:186:ILE:HG12	5:E:211:LEU:HD13	1.98	0.44
8:H:848:TRP:CE2	9:J:165:ILE:HD11	2.52	0.44
11:L:4:DT:H2"	11:L:5:DA:C8	2.52	0.44
2:B:613:HIS:CE1	5:E:206:ARG:HG2	2.52	0.44
7:G:31:LYS:HD3	7:G:32:LYS:H	1.82	0.44
8:H:664:ALA:HB2	8:H:680:CYS:SG	2.58	0.44
10:K:174:GLN:HB2	12:M:34:DA:H2	1.82	0.44
8:H:697:VAL:HA	8:H:738:THR:HG22	2.00	0.44
1:A:442:GLU:OE2	1:A:613:THR:OG1	2.34	0.44
1:A:664:SER:O	1:A:667:THR:OG1	2.30	0.44
8:H:743:PRO:HB2	8:H:768:PRO:HA	1.99	0.44
1:A:706:LYS:HE3	1:A:706:LYS:HB3	1.90	0.44
2:B:110:SER:HB2	2:B:115:LEU:HD13	1.99	0.44
2:B:702:THR:OG1	2:B:705:ASN:OD1	2.33	0.44
3:C:400:ILE:HG13	6:F:20:ILE:HG23	1.98	0.44
3:C:522:VAL:HG12	3:C:526:GLU:HG3	2.00	0.44
8:H:718:ARG:HG3	8:H:724:LEU:HG	1.99	0.44
8:H:784:ARG:NE	10:K:170:PRO:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:TYR:HA	1:A:533:LEU:HD23	2.00	0.44
5:E:44:LYS:HD2	5:E:45:ARG:HG2	1.99	0.44
8:H:657:GLU:HG2	8:H:683:THR:HG22	1.99	0.44
1:A:610:VAL:HG12	1:A:615:PHE:HE2	1.83	0.43
2:B:143:ARG:NH1	2:B:162:ASP:OD2	2.51	0.43
8:H:759:VAL:HG23	8:H:791:VAL:HG11	1.99	0.43
10:K:168:LYS:HA	10:K:177:ASP:H	1.81	0.43
1:A:306:ILE:HG21	1:A:404:SER:HB2	2.01	0.43
2:B:257:ASP:O	2:B:260:GLN:HG3	2.18	0.43
5:E:201:LEU:HG	5:E:222:ILE:HD12	1.99	0.43
1:A:203:GLU:HG2	1:A:204:GLY:H	1.83	0.43
1:A:446:ILE:HD13	1:A:446:ILE:HA	1.90	0.43
7:G:13:ASP:OD1	7:G:13:ASP:N	2.52	0.43
8:H:862:LYS:HA	8:H:866:GLY:HA2	1.99	0.43
2:B:644:PHE:HB2	2:B:646:ILE:HG12	2.00	0.43
2:B:673:ASP:OD1	2:B:674:TYR:N	2.51	0.43
10:K:164:PHE:HB3	10:K:181:TYR:CE2	2.53	0.43
2:B:403:PHE:HE1	2:B:435:PHE:HB2	1.83	0.43
1:A:97:GLN:NE2	1:A:116:TYR:OH	2.49	0.43
2:B:182:ALA:HA	2:B:185:ARG:HG2	2.00	0.43
2:B:371:PRO:HA	2:B:374:PHE:HD2	1.84	0.43
2:B:506:SER:OG	2:B:683:ARG:NH2	2.51	0.43
5:E:85:LEU:HD22	5:E:131:LEU:HD22	2.01	0.43
1:A:530:ARG:NH2	1:A:668:GLN:OE1	2.46	0.43
3:C:397:SER:O	3:C:400:ILE:HG22	2.19	0.43
6:F:255:CYS:SG	6:F:276:CYS:N	2.92	0.43
1:A:309:ASP:O	1:A:383:THR:OG1	2.36	0.43
1:A:375:LYS:HD3	1:A:391:ARG:HD3	2.00	0.43
1:A:81:ASP:N	1:A:81:ASP:OD1	2.52	0.43
1:A:317:ARG:HD3	1:A:319:TYR:HE1	1.83	0.43
2:B:199:ILE:HG13	2:B:200:LEU:HD22	1.99	0.43
4:D:175:LEU:HD13	4:D:268:PHE:HE1	1.83	0.43
8:H:776:LEU:HB2	8:H:779:LEU:HD22	2.00	0.43
12:M:49:DG:H2'	12:M:50:DA:C8	2.53	0.43
3:C:130:ASP:HB3	3:C:504:LYS:HE3	2.01	0.42
1:A:106:PRO:HG3	1:A:109:ARG:HE	1.83	0.42
5:E:88:LEU:HD21	5:E:170:ILE:HD11	2.01	0.42
1:A:548:ILE:HD12	1:A:604:THR:HG21	2.01	0.42
1:A:705:THR:OG1	1:A:708:GLU:OE1	2.37	0.42
3:C:521:LEU:HD23	5:E:269:PRO:HG2	2.01	0.42
4:D:399:ASP:O	8:H:908:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:GLN:OE1	2:B:369:ARG:N	2.52	0.42
1:A:62:ARG:HG3	4:D:339:PRO:HA	2.02	0.42
1:A:298:ARG:HA	1:A:298:ARG:HH11	1.83	0.42
3:C:506:CYS:HB3	3:C:507:PRO:HD3	2.01	0.42
5:E:48:GLU:OE1	5:E:51:GLY:N	2.49	0.42
5:E:59:ARG:HB2	5:E:95:TYR:OH	2.19	0.42
8:H:761:LEU:HD22	8:H:812:ILE:HD11	2.01	0.42
2:B:124:LEU:HD12	2:B:126:PHE:H	1.83	0.42
2:B:375:CYS:HB3	2:B:401:ALA:HB1	2.00	0.42
5:E:167:VAL:N	5:E:195:ARG:O	2.49	0.42
9:J:162:PHE:HA	9:J:165:ILE:HG22	2.00	0.42
1:A:319:TYR:HE2	1:A:340:LEU:HD22	1.84	0.42
5:E:32:ALA:O	5:E:35:GLU:HB3	2.19	0.42
8:H:644:HIS:CD2	8:H:646:LEU:HB2	2.54	0.42
11:L:39:DC:H2"	11:L:40:DG:C8	2.54	0.42
4:D:143:ARG:HB3	4:D:147:SER:OG	2.20	0.42
9:J:114:ASP:OD2	9:J:119:GLY:N	2.43	0.42
1:A:328:PHE:CE2	1:A:333:ALA:HB2	2.55	0.42
2:B:681:ASP:HB3	2:B:684:PHE:CD2	2.55	0.42
7:G:8:VAL:HG23	7:G:47:ALA:HB2	2.01	0.42
1:A:688:LYS:HD3	8:H:935:PHE:HE1	1.85	0.42
4:D:335:LEU:HD11	4:D:345:GLN:HB2	2.02	0.42
5:E:161:GLY:HA2	5:E:165:ARG:HH12	1.85	0.42
10:K:117:LEU:HD13	10:K:123:LEU:HD23	2.02	0.41
12:M:46:DT:H2"	12:M:47:DG:H8	1.85	0.41
2:B:82:LYS:O	2:B:85:GLU:HG3	2.20	0.41
11:L:16:DA:H2'	11:L:17:DT:C6	2.55	0.41
1:A:326:LYS:HZ3	1:A:489:TYR:HB2	1.84	0.41
4:D:101:LEU:HB3	4:D:105:LEU:HB2	2.00	0.41
7:G:22:TYR:HA	7:G:25:GLU:HG2	2.01	0.41
7:G:50:VAL:O	7:G:54:GLN:HG2	2.21	0.41
8:H:814:CYS:HB2	8:H:817:PHE:CD2	2.55	0.41
1:A:503:ALA:HB3	1:A:644:LEU:HA	2.01	0.41
2:B:370:LYS:HG3	2:B:374:PHE:HE2	1.85	0.41
12:M:55:DC:H2"	12:M:56:DT:C6	2.55	0.41
1:A:273:LYS:HG2	1:A:275:GLU:HG3	2.02	0.41
1:A:373:GLN:O	1:A:377:GLN:HG2	2.21	0.41
4:D:417:ASP:HB3	4:D:455:TRP:HH2	1.86	0.41
5:E:205:VAL:HG12	5:E:207:VAL:HG12	2.03	0.41
1:A:61:TYR:CD1	1:A:80:PRO:HG3	2.55	0.41
5:E:232:LEU:O	5:E:236:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:524:HIS:NE2	5:E:295:ARG:O	2.45	0.41
5:E:36:ASP:O	5:E:40:LYS:N	2.48	0.41
5:E:255:PRO:HG3	5:E:312:LEU:HB3	2.02	0.41
6:F:130:GLU:OE1	6:F:170:SER:OG	2.30	0.41
2:B:56:ILE:HG21	2:B:70:LEU:HG	2.03	0.41
2:B:79:GLU:HA	2:B:82:LYS:HG2	2.02	0.41
2:B:253:ARG:NH1	2:B:431:PRO:O	2.51	0.41
1:A:557:LYS:HD3	1:A:603:ASN:HB2	2.02	0.41
2:B:183:LEU:HA	2:B:186:ARG:HG2	2.02	0.41
2:B:354:PRO:CG	2:B:355:PRO:HD3	2.51	0.41
2:B:619:ILE:HA	2:B:678:VAL:HG22	2.02	0.41
4:D:249:TYR:HB2	4:D:281:TYR:CZ	2.56	0.41
8:H:711:SER:HA	12:M:27:DT:H5'	2.03	0.41
9:J:106:ILE:HG21	9:J:163:LEU:HD23	2.03	0.41
2:B:121:VAL:HG22	2:B:130:VAL:HG12	2.03	0.41
2:B:410:TYR:HB3	2:B:414:PHE:CE1	2.56	0.41
8:H:745:VAL:HG22	8:H:769:ILE:HB	2.03	0.41
12:M:46:DT:C2	12:M:47:DG:N7	2.89	0.41
2:B:427:THR:OG1	8:H:713:ARG:HD2	2.21	0.40
2:B:661:ALA:HA	2:B:664:VAL:HG12	2.03	0.40
4:D:203:PHE:O	4:D:211:GLN:NE2	2.53	0.40
2:B:6:ASP:H	2:B:26:ARG:NH2	2.19	0.40
2:B:43:PRO:HB3	2:B:696:TRP:CD2	2.57	0.40
4:D:380:THR:OG1	4:D:381:PRO:HD3	2.21	0.40
8:H:641:TYR:HA	8:H:647:TYR:CD2	2.56	0.40
4:D:100:LEU:HD13	4:D:100:LEU:H	1.86	0.40
4:D:148:LEU:HB3	4:D:284:THR:HG23	2.04	0.40
2:B:430:ASN:OD1	2:B:430:ASN:N	2.53	0.40
2:B:609:ASP:OD1	2:B:666:ARG:NH2	2.36	0.40
2:B:466:ILE:HG12	2:B:470:ILE:HG13	2.03	0.40
3:C:512:ILE:O	3:C:516:TYR:N	2.54	0.40
4:D:273:GLN:NE2	4:D:278:SER:O	2.55	0.40
8:H:689:THR:HG21	12:M:26:DT:H72	2.03	0.40
8:H:773:GLN:HE21	8:H:810:GLY:HA3	1.86	0.40
8:H:825:TRP:O	8:H:828:GLU:HG3	2.22	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	597/603 (99%)	544 (91%)	53 (9%)	0	100	100
2	B	673/730 (92%)	647 (96%)	26 (4%)	0	100	100
3	C	187/438 (43%)	179 (96%)	8 (4%)	0	100	100
4	D	432/446 (97%)	428 (99%)	4 (1%)	0	100	100
5	E	378/380 (100%)	369 (98%)	9 (2%)	0	100	100
6	F	254/284 (89%)	249 (98%)	5 (2%)	0	100	100
7	G	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
8	H	268/274 (98%)	262 (98%)	6 (2%)	0	100	100
9	J	69/70 (99%)	69 (100%)	0	0	100	100
10	K	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
All	All	3092/3463 (89%)	2969 (96%)	123 (4%)	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	535/535 (100%)	518 (97%)	17 (3%)	39	63
2	B	591/636 (93%)	575 (97%)	16 (3%)	44	67
3	C	175/389 (45%)	169 (97%)	6 (3%)	37	62
4	D	379/384 (99%)	372 (98%)	7 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	338/338 (100%)	332 (98%)	6 (2%)	59 77
6	F	230/250 (92%)	228 (99%)	2 (1%)	78 87
7	G	59/59 (100%)	59 (100%)	0	100 100
8	H	231/231 (100%)	221 (96%)	10 (4%)	29 57
9	J	61/63 (97%)	59 (97%)	2 (3%)	38 63
10	K	162/162 (100%)	155 (96%)	7 (4%)	29 57
All	All	2761/3047 (91%)	2688 (97%)	73 (3%)	49 68

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	140	LEU
1	A	141	ARG
1	A	177	VAL
1	A	200	ARG
1	A	316	LEU
1	A	332	ARG
1	A	334	ARG
1	A	415	HIS
1	A	510	VAL
1	A	511	TRP
1	A	533	LEU
1	A	564	ASN
1	A	629	HIS
1	A	645	ARG
1	A	659	PHE
1	A	707	GLU
2	B	70	LEU
2	B	77	VAL
2	B	112	ARG
2	B	138	THR
2	B	156	ARG
2	B	335	ARG
2	B	350	VAL
2	B	397	LEU
2	B	462	SER
2	B	471	LEU
2	B	497	ARG
2	B	526	GLU

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Mol	Chain	Res	Type
2	B	531	VAL
2	B	553	TYR
2	B	613	HIS
2	B	627	TYR
3	C	396	THR
3	C	407	ILE
3	C	414	TYR
3	C	442	GLN
3	C	452	MET
3	C	465	TYR
4	D	96	TRP
4	D	100	LEU
4	D	219	TYR
4	D	226	ARG
4	D	284	THR
4	D	380	THR
4	D	402	ARG
5	E	34	ILE
5	E	44	LYS
5	E	215	THR
5	E	228	TYR
5	E	280	THR
5	E	328	LEU
6	F	229	TRP
6	F	281	ILE
8	H	636	THR
8	H	649	LEU
8	H	660	TYR
8	H	671	ARG
8	H	685	HIS
8	H	711	SER
8	H	799	PHE
8	H	849	LYS
8	H	863	ARG
8	H	904	TRP
9	J	165	ILE
9	J	168	LYS
10	K	165	ILE
10	K	175	TRP
10	K	177	ASP
10	K	212	GLU
10	K	214	MET

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Mol	Chain	Res	Type
10	K	227	ARG
10	K	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	501	GLN
6	F	52	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	SF4	B	1000	2	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	B	1000	2	-	-	0/6/5/5

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	866:GLY	C	889:GLY	N	33.59
1	H	915:LYS	C	926:GLU	N	19.41
1	A	645:ARG	C	655:TYR	N	13.35
1	A	208:GLU	C	267:THR	N	6.37

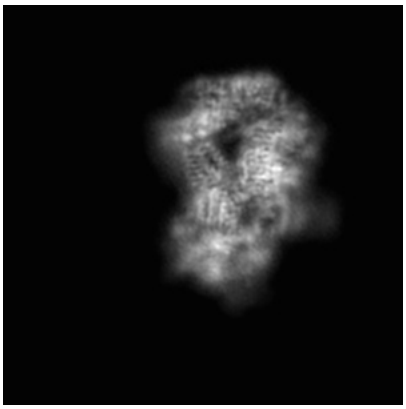
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27997. These allow visual inspection of the internal detail of the map and identification of artifacts.

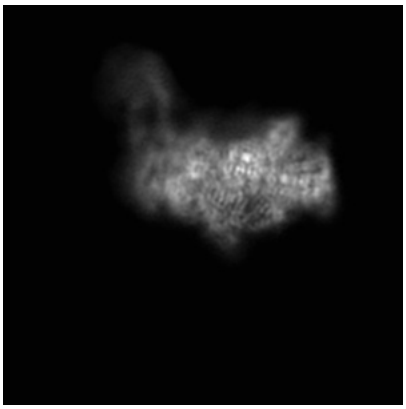
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

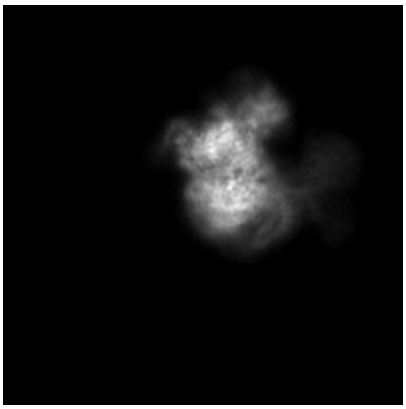
6.1.1 Primary map



X

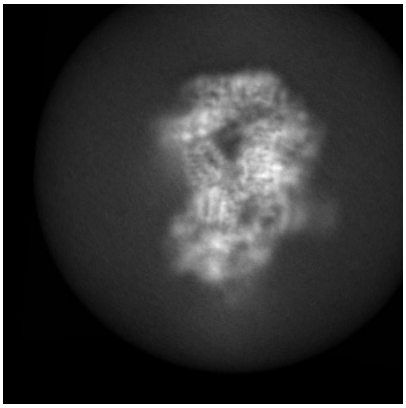


Y

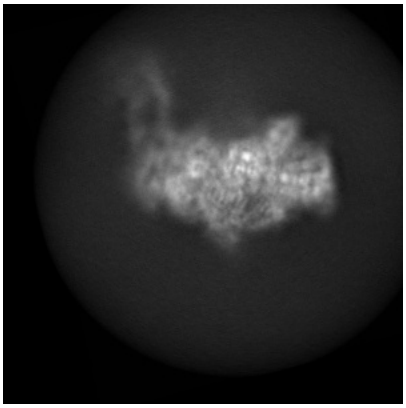


Z

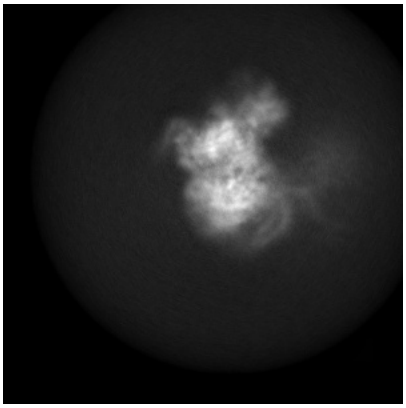
6.1.2 Raw map



X



Y

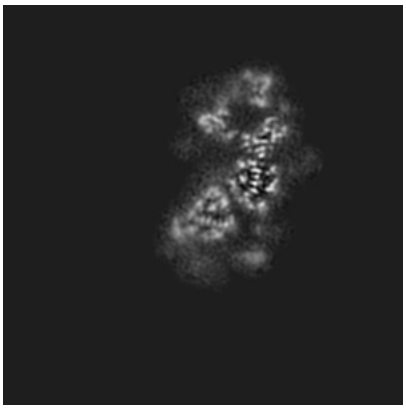


Z

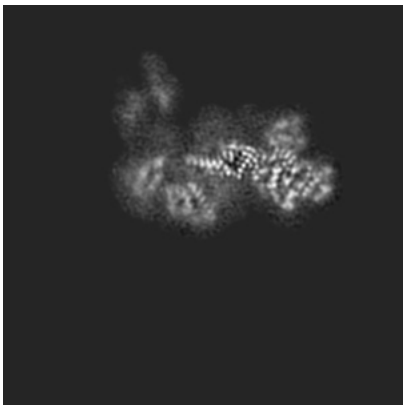
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

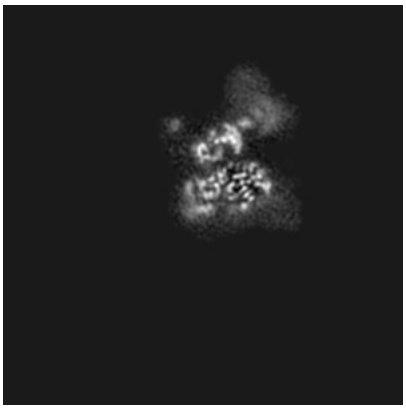
6.2.1 Primary map



X Index: 192

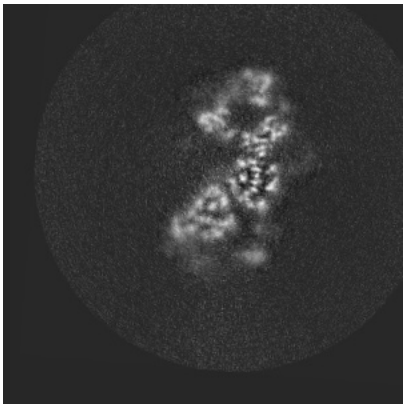


Y Index: 192

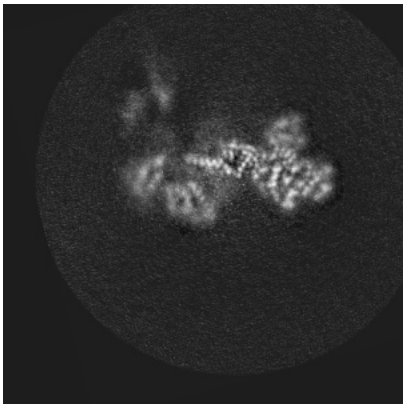


Z Index: 192

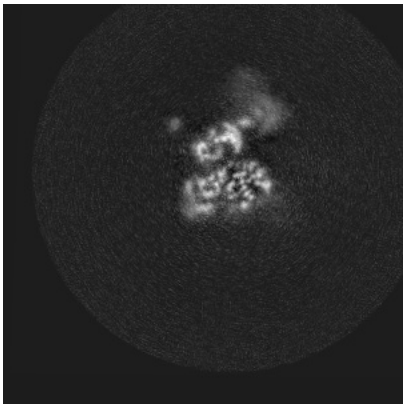
6.2.2 Raw map



X Index: 192



Y Index: 192

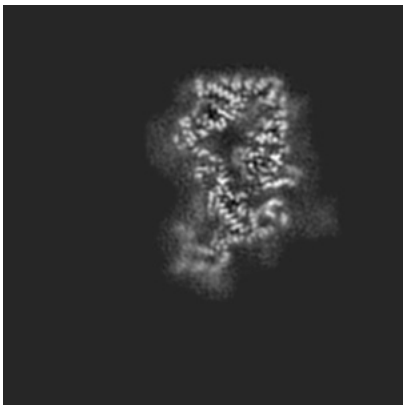


Z Index: 192

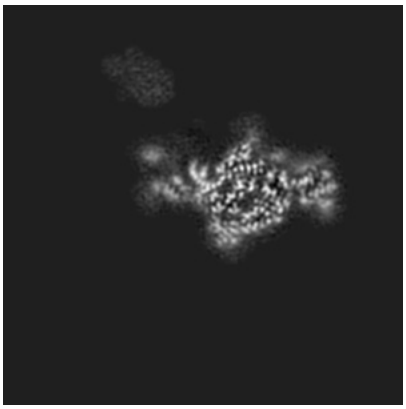
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

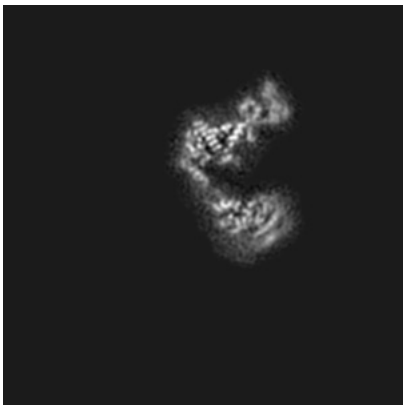
6.3.1 Primary map



X Index: 218

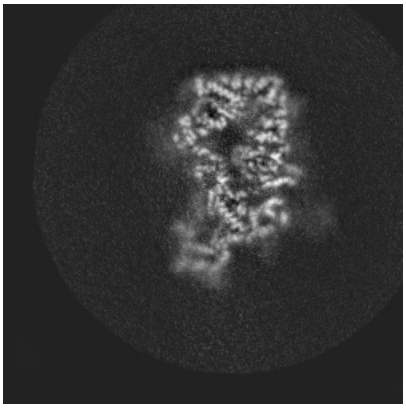


Y Index: 253

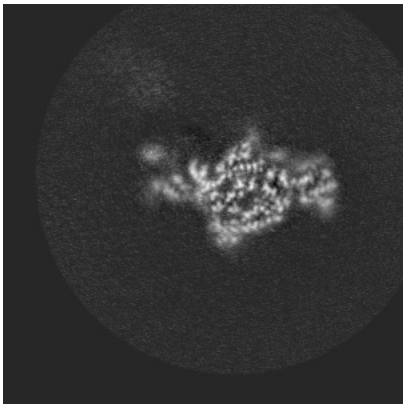


Z Index: 259

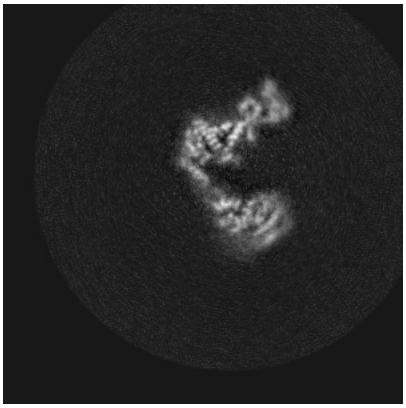
6.3.2 Raw map



X Index: 218



Y Index: 253

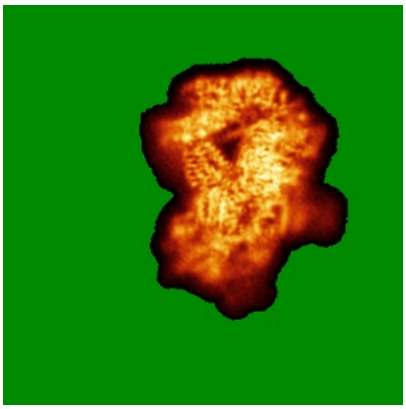


Z Index: 259

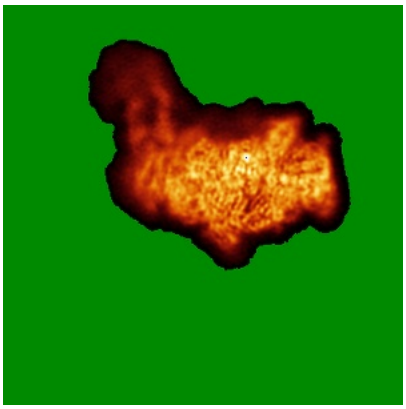
The images above show the largest variance slices of the map in three orthogonal directions.

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

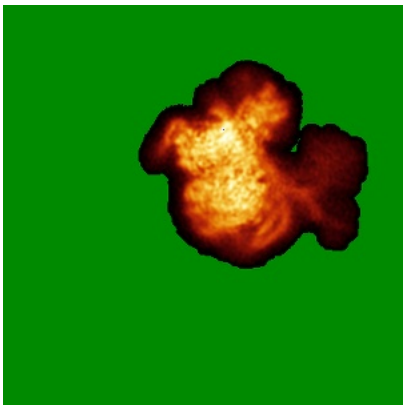
6.4.1 Primary map



X

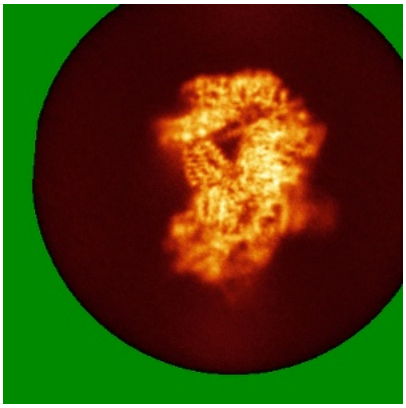


Y

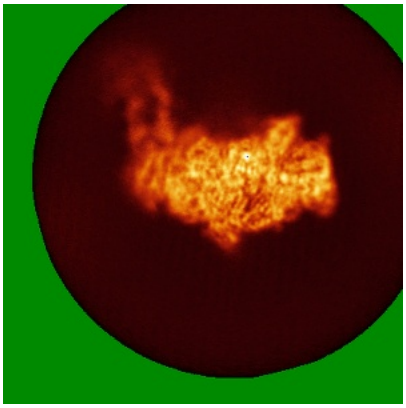


Z

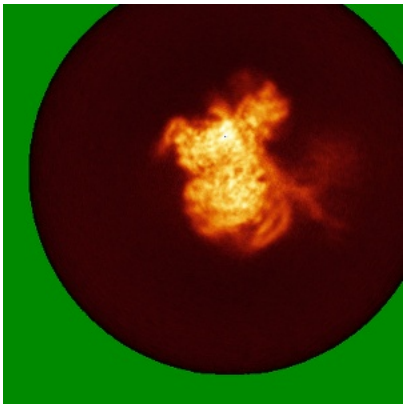
6.4.2 Raw map



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.

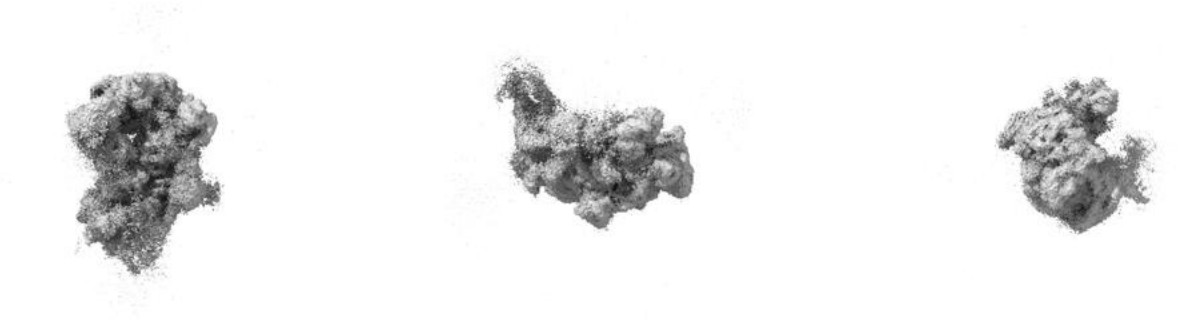
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

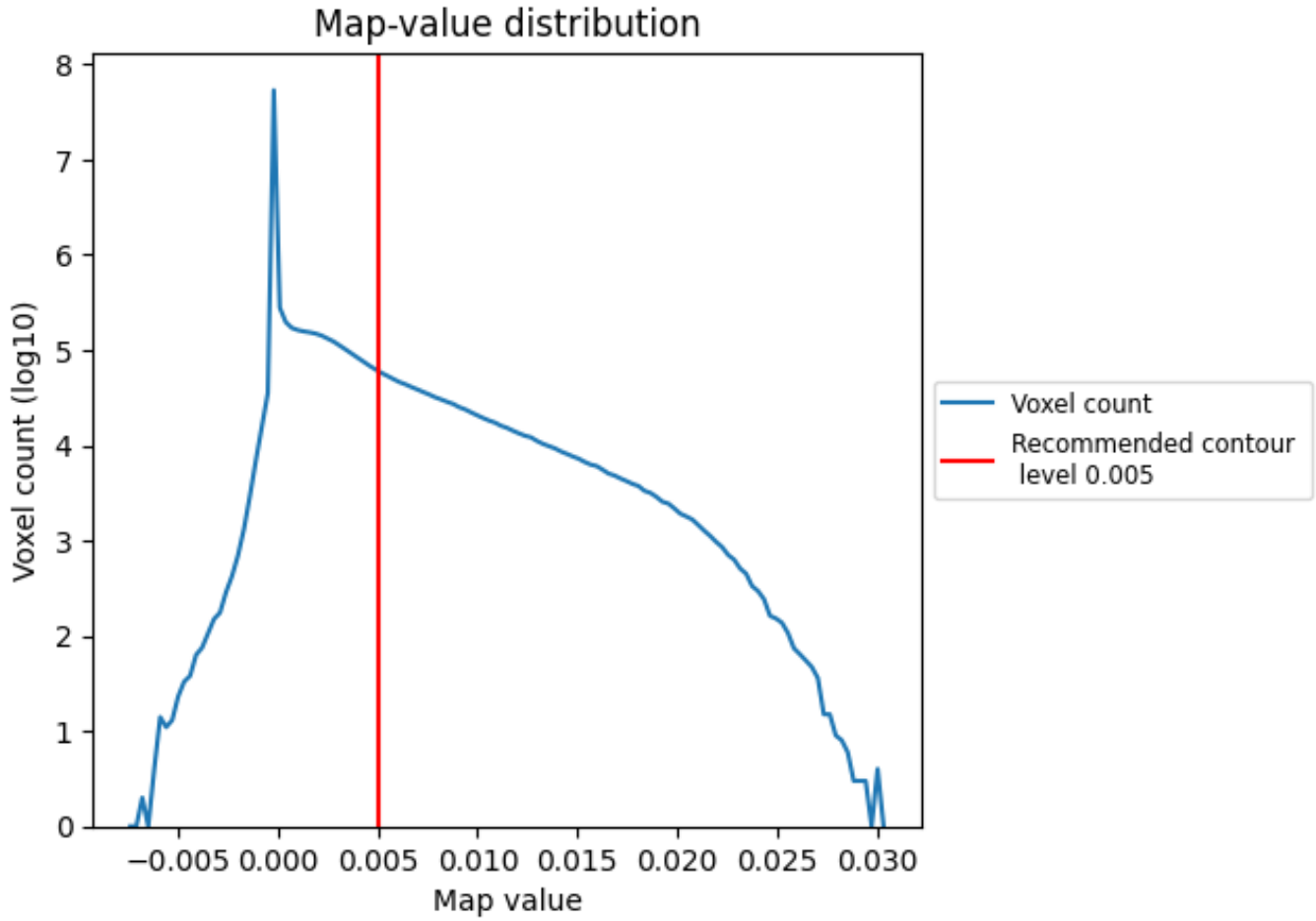
6.6 Mask visualisation (i)

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

7 Map analysis

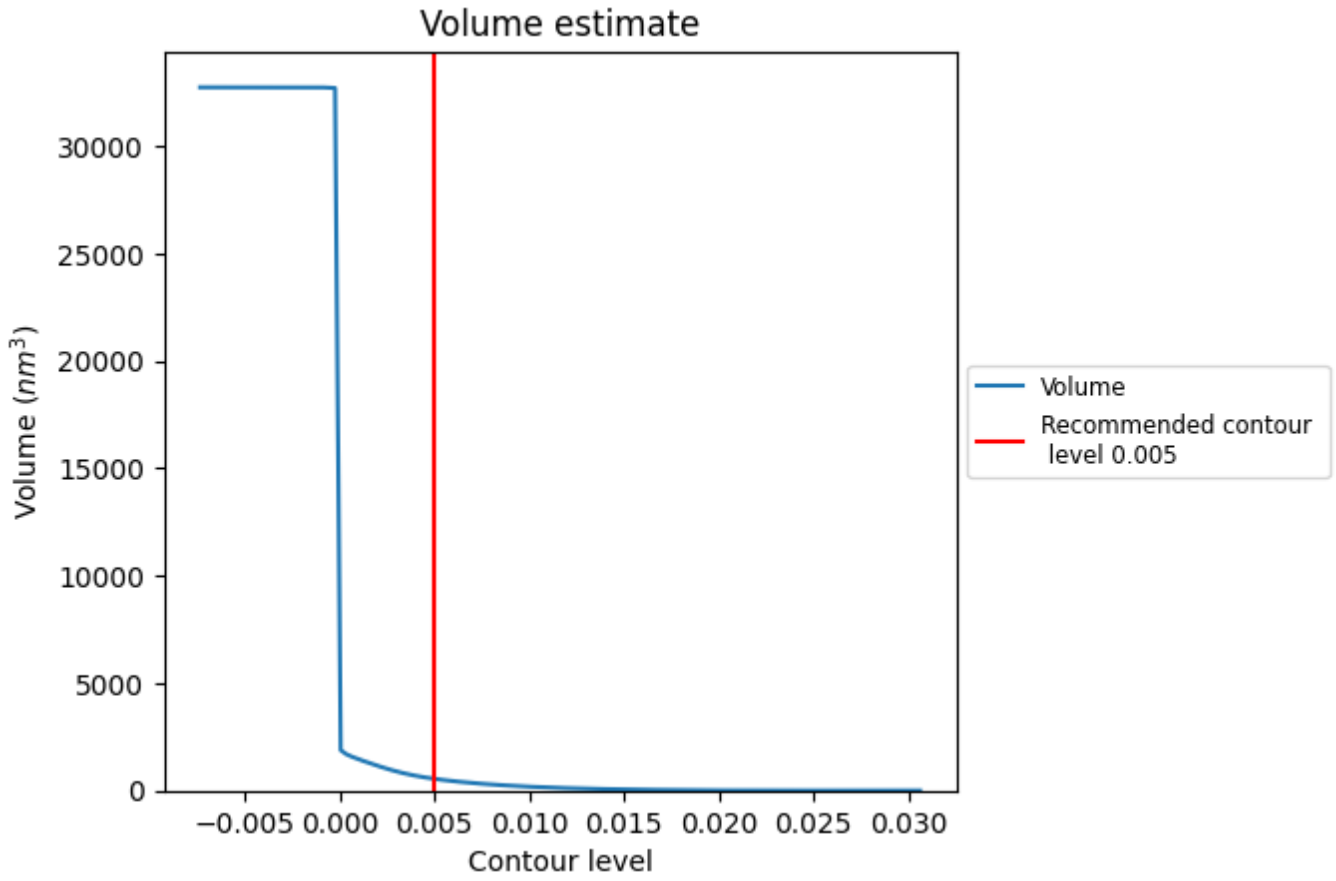
This section contains the results of statistical analysis of the map.

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.

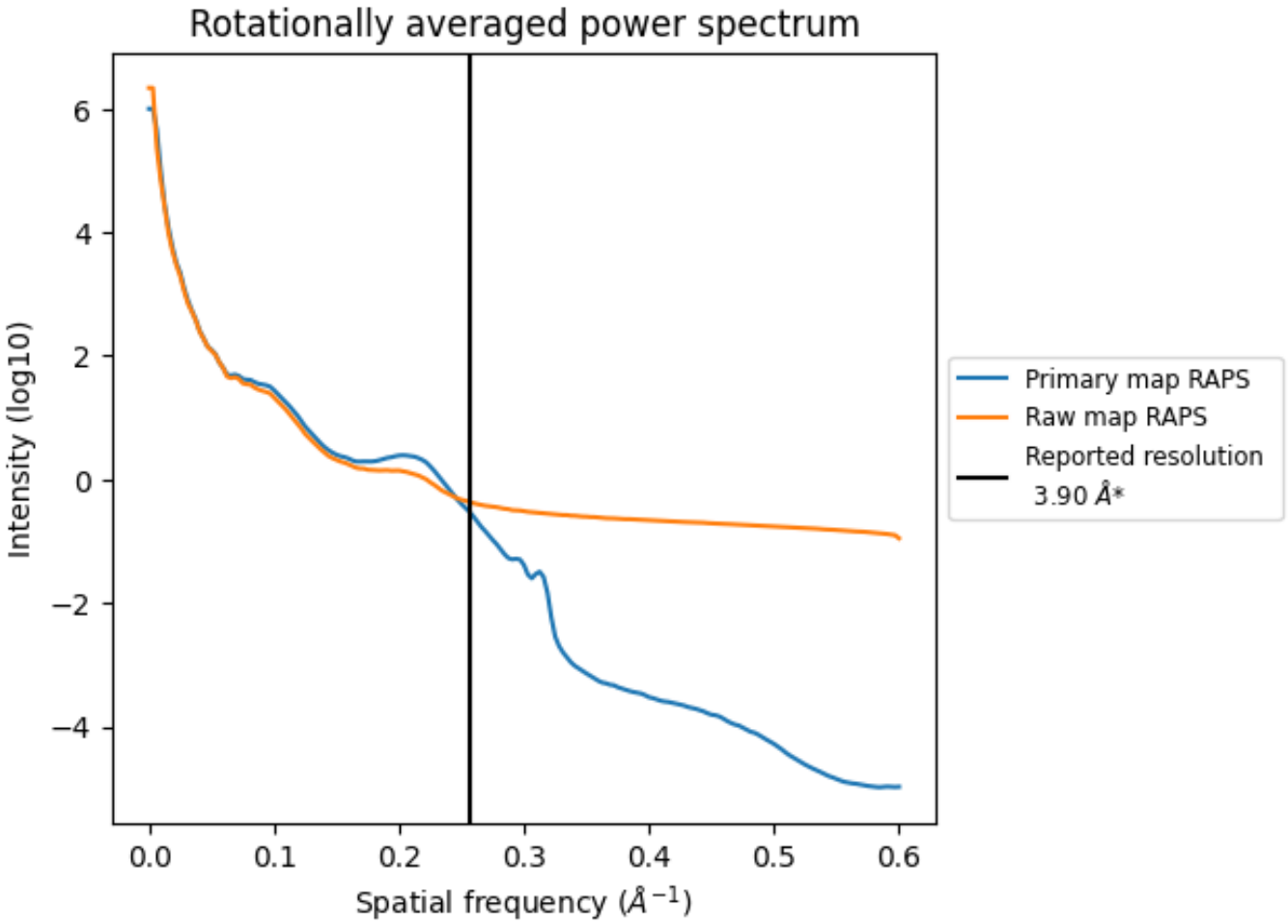
7.2 Volume estimate



The volume at the recommended contour level is 546 nm^3; this corresponds to an approximate mass of 493 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)

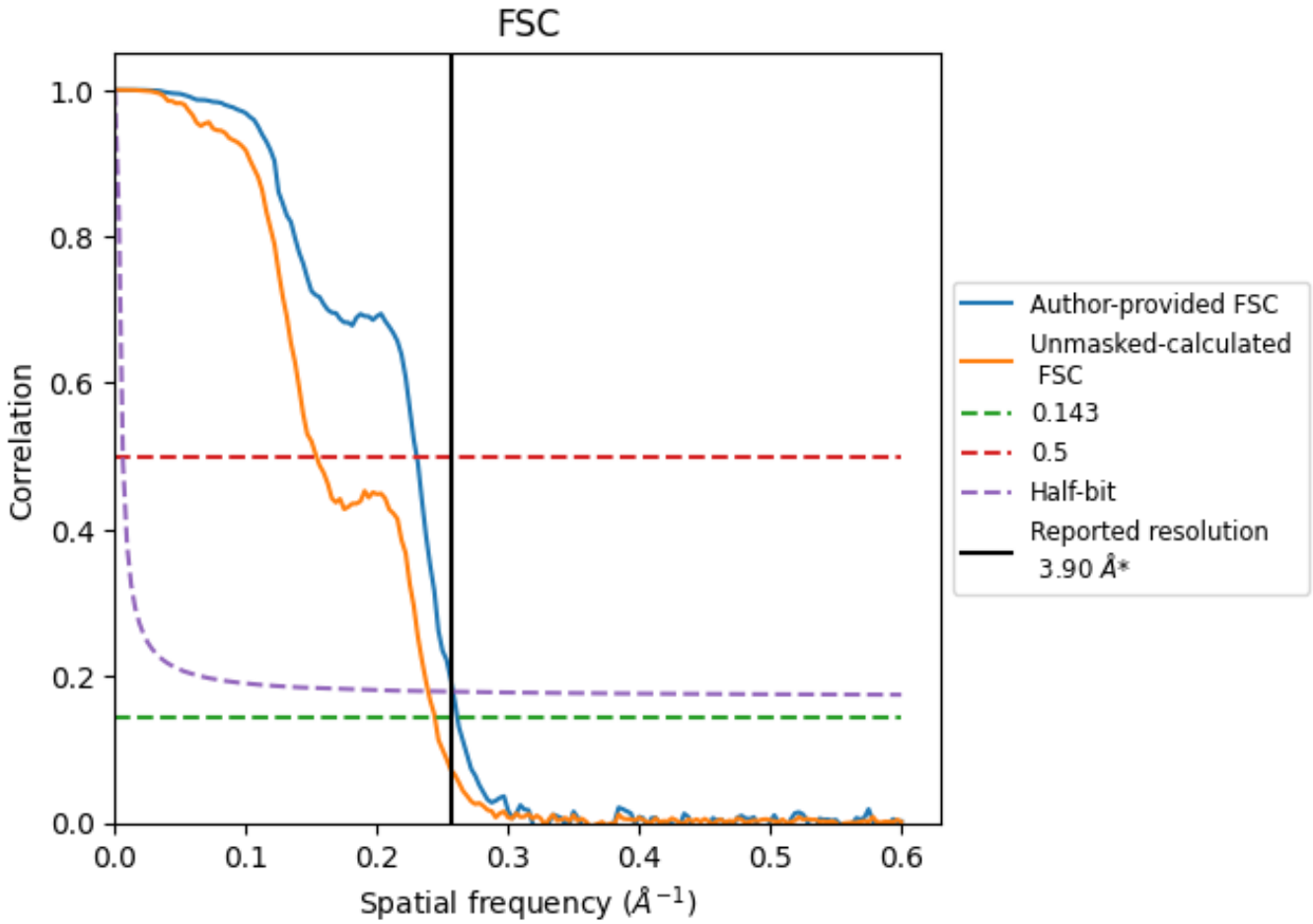


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

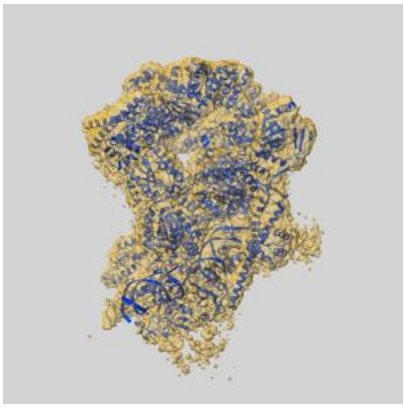
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.82	4.34	3.87
Unmasked-calculated*	4.09	6.50	4.18

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

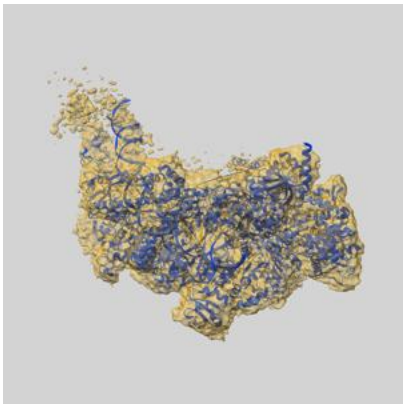
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27997 and PDB model 8EBT. Per-residue inclusion information can be found in section 3 on page 7.

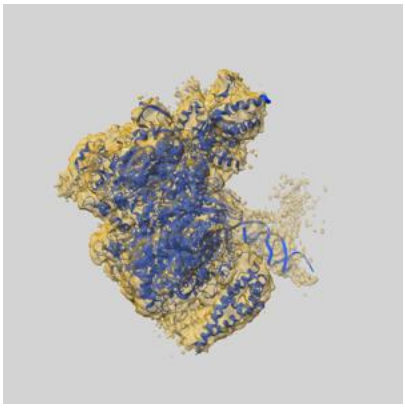
9.1 Map-model overlay



X



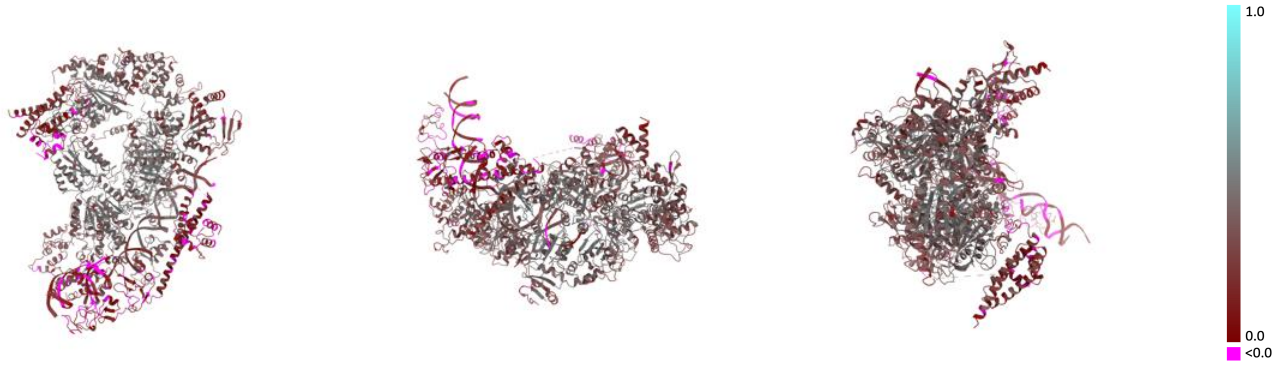
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

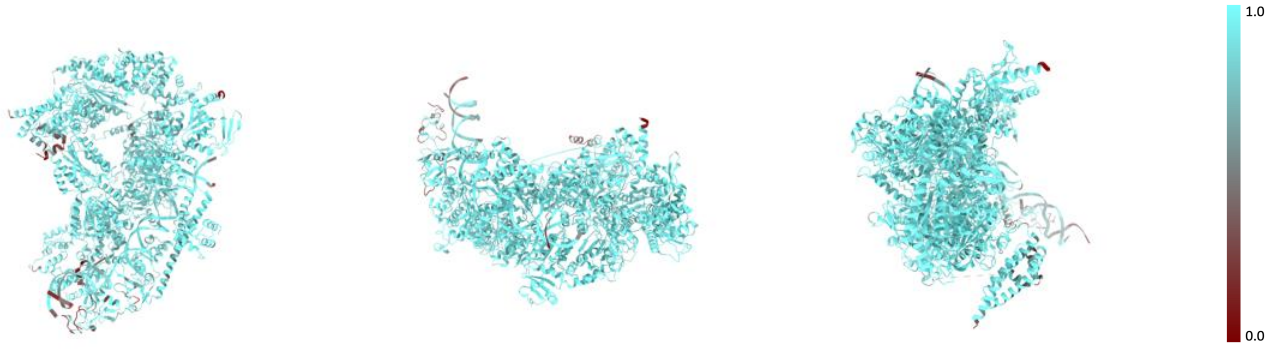
9.2 Q-score mapped to coordinate model (i)



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.

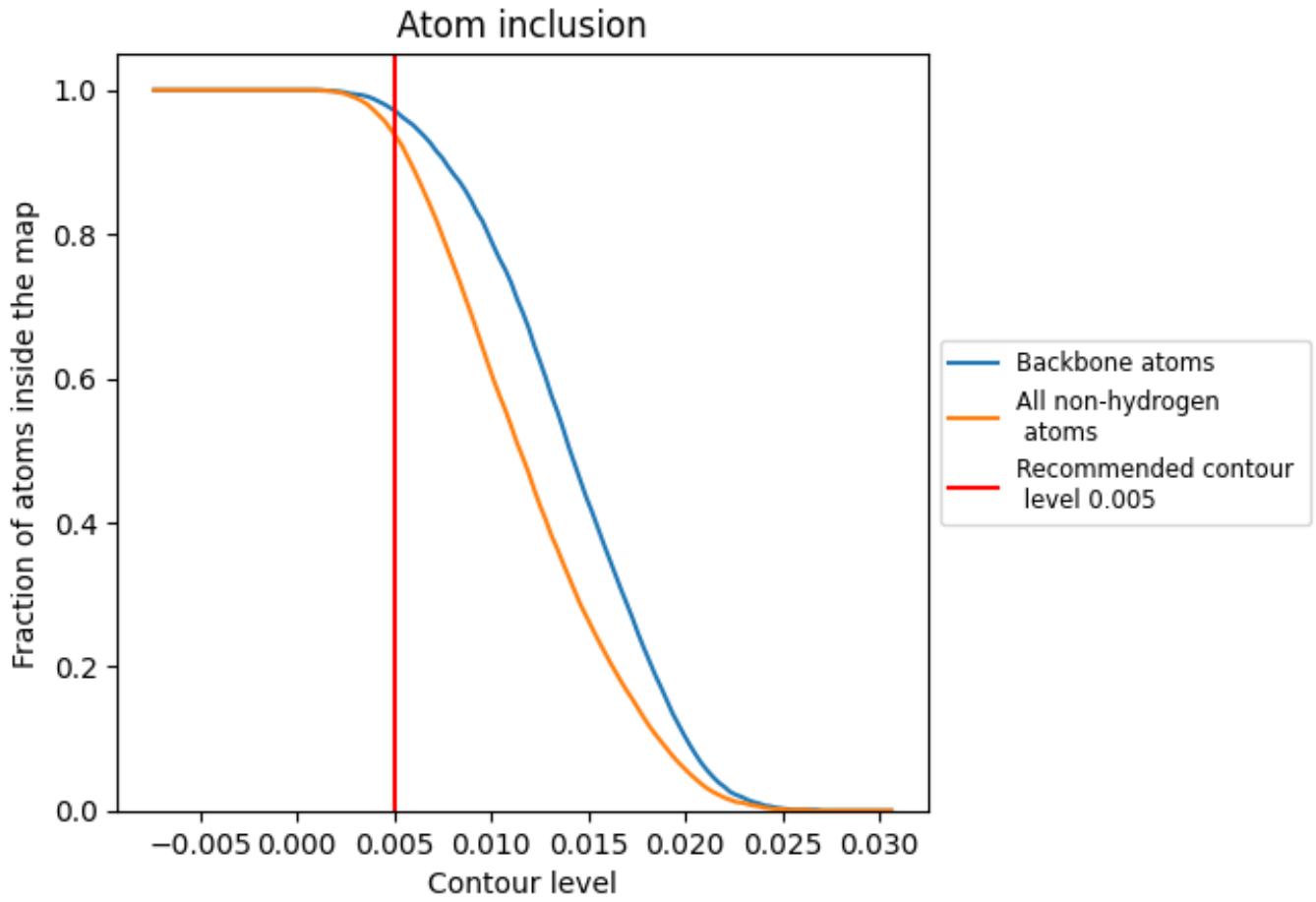
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.3040
A	0.9820	0.3980
B	0.9730	0.3110
C	0.8570	0.1780
D	0.9610	0.3340
E	0.9640	0.3710
F	0.9730	0.3900
G	0.9620	0.3230
H	0.7940	0.1130
J	0.9280	0.0820
K	0.9440	0.2690
L	0.8800	0.2060
M	0.8070	0.2000