Full wwPDB EM Validation Report ⓘ

Feb 15, 2024 – 10:33 AM EST

PDB ID	:	8SYI
EMDB ID	:	EMD-40874
Title	:	Cyanobacterial RNAP-EC
Authors	:	Qayyum, M.Z.; Imashimizu, M.; Leanca, M.; Vishwakarma, R.K.; Bradley Riaz, A.; Yuzenkova, Y.; Murakami, K.S.
Deposited on	:	2023-05-25
Resolution	:	2.94 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

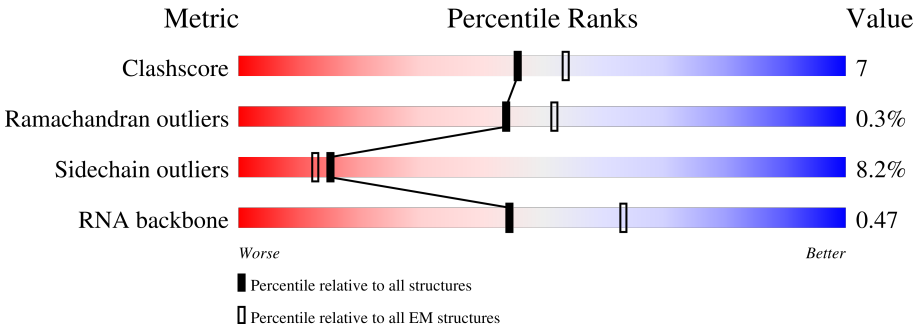
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.94 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
RNA backbone	4643	859

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	309	58% 15% • 27%
1	B	309	59% 13% • 27%
2	C	1100	80% 16% • •
3	D	624	80% 18% • •
4	Z	1318	5% 68% 22% • 7%
5	E	76	75% 8% 17%
6	G	205	• 48% 10% 41%

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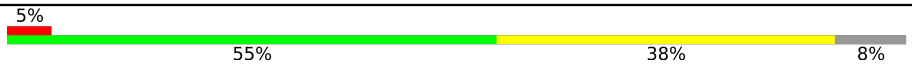
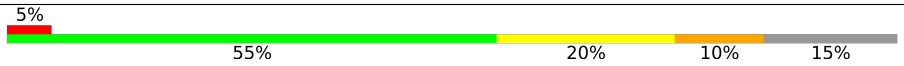
Mol	Chain	Length	Quality of chain
7	N	40	
8	R	20	
9	T	40	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29500 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1730	1081	306	339	4		
1	B	226	Total	C	N	O	S	0	0
			1730	1081	306	339	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1061	Total	C	N	O	S	0	0
			8382	5264	1484	1607	27		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	620	Total	C	N	O	S	0	0
			4961	3127	901	912	21		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	1221	Total	C	N	O	S	0	0
			9357	5827	1658	1850	22		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	63	Total	C	N	O	S	0	0
			510	316	90	102	2		

- Molecule 6 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	120	Total	C	N	O	S	0	0
			957	606	179	169	3		

- Molecule 7 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	37	Total	C	N	O	P	0	0
			745	354	129	225	37		

- Molecule 8 is a RNA chain called RNA (5'-R(P*UP*UP*CP*AP*AP*AP*GP*CP*GP*GP *AP*GP*AP*GP*GP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	17	Total	C	N	O	P	0	0
			370	165	72	116	17		

- Molecule 9 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	37	Total	C	N	O	P	0	0
			755	358	140	221	36		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

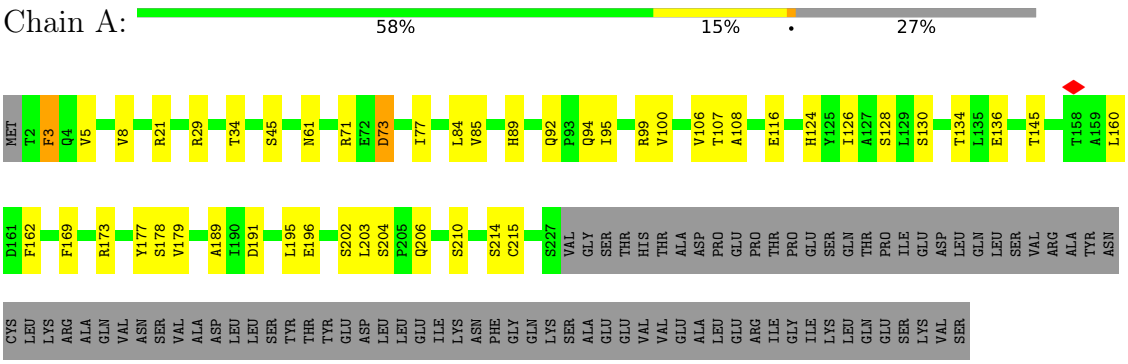
Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Zn	0
			1	1	
11	Z	1	Total	Zn	0
			1	1	

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.

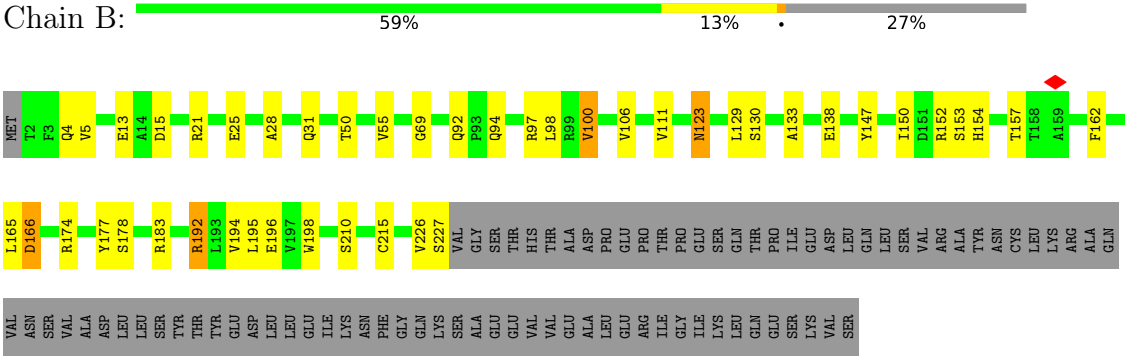
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



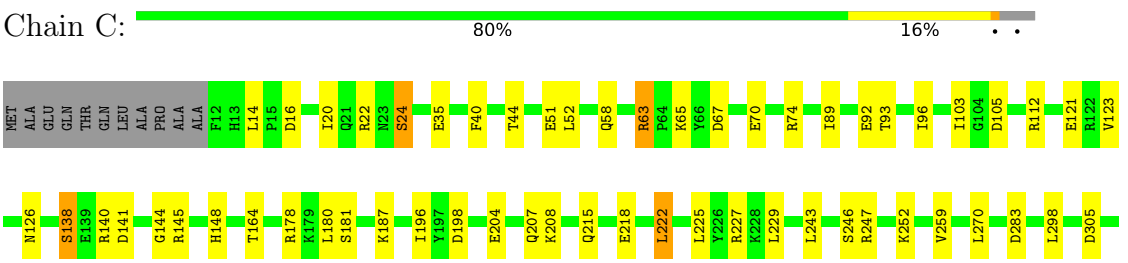
• Molecule 1: DNA-directed RNA polymerase subunit alpha

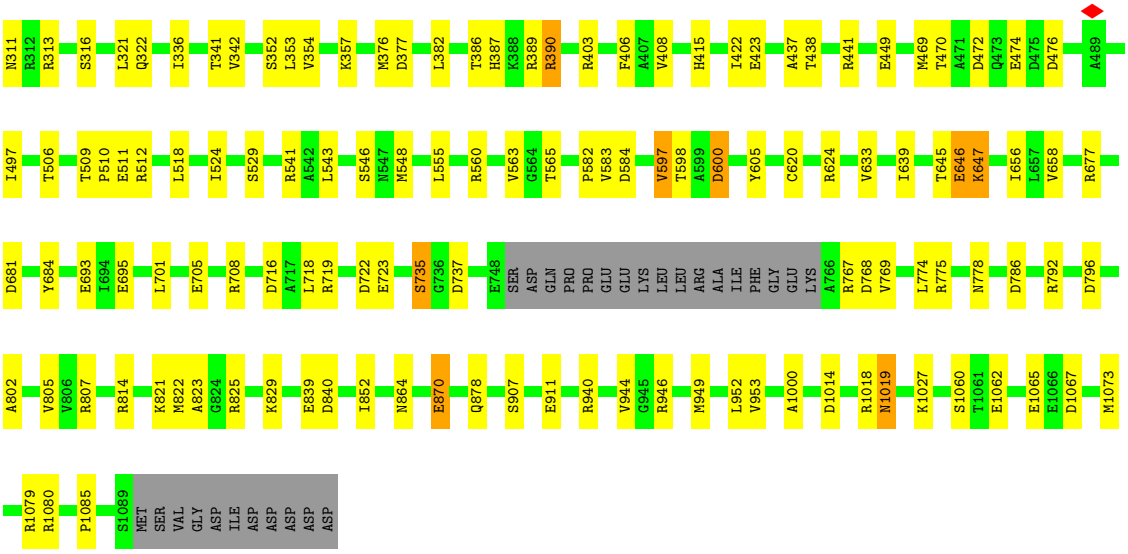
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

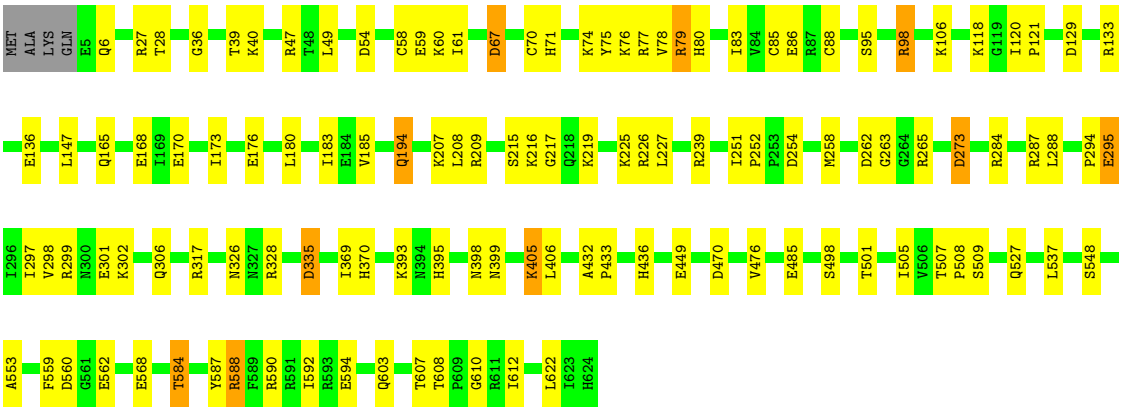
Chain C:





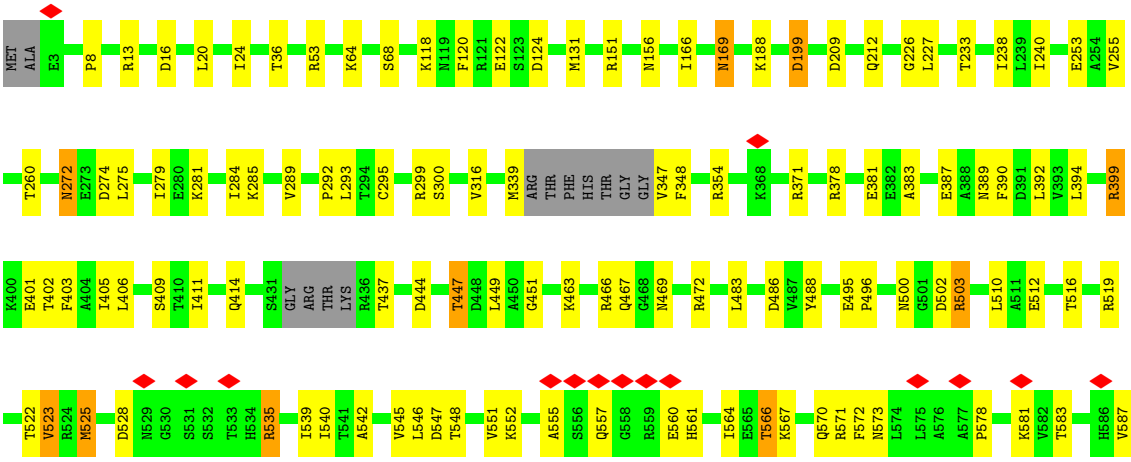
• Molecule 3: DNA-directed RNA polymerase subunit gamma

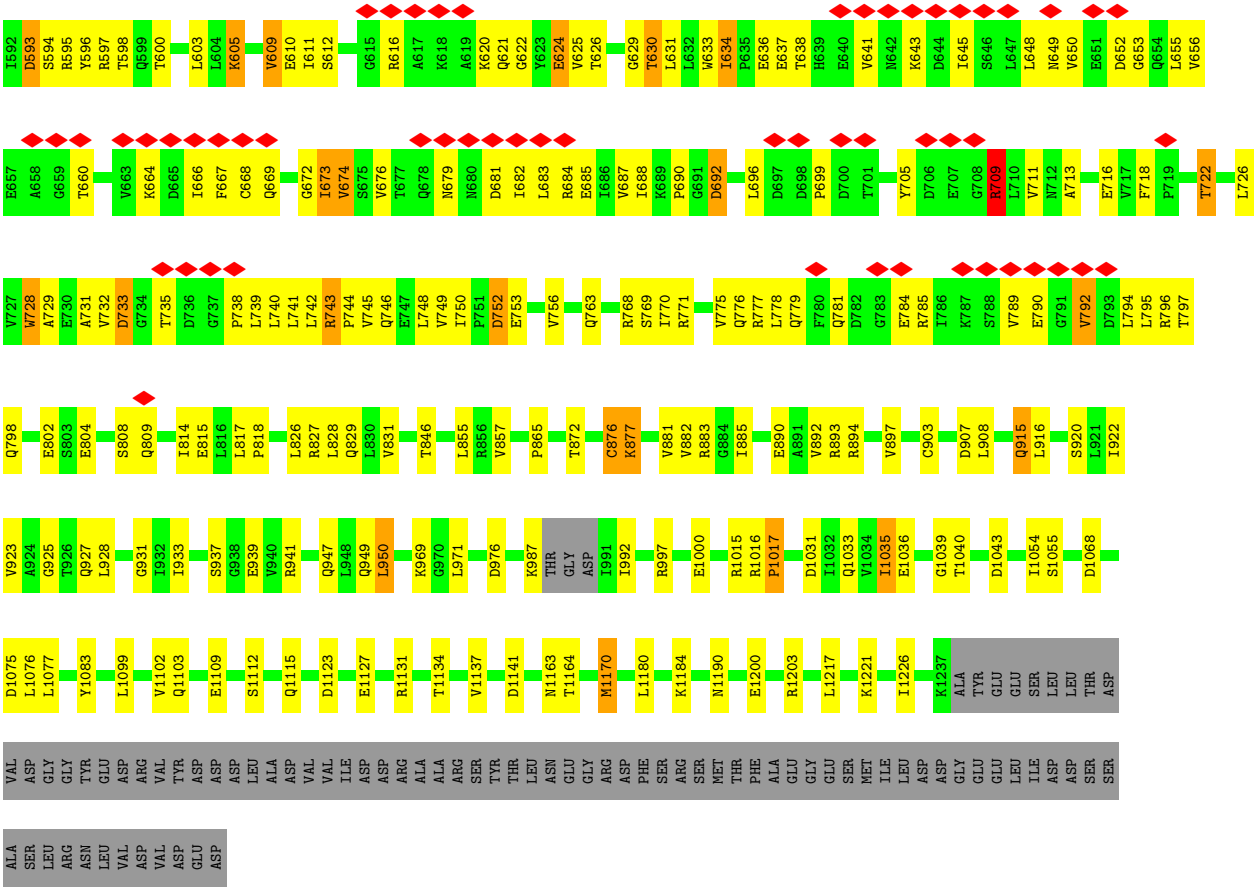
Chain D:



• Molecule 4: DNA-directed RNA polymerase subunit beta'

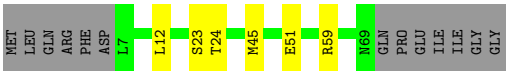
Chain Z:





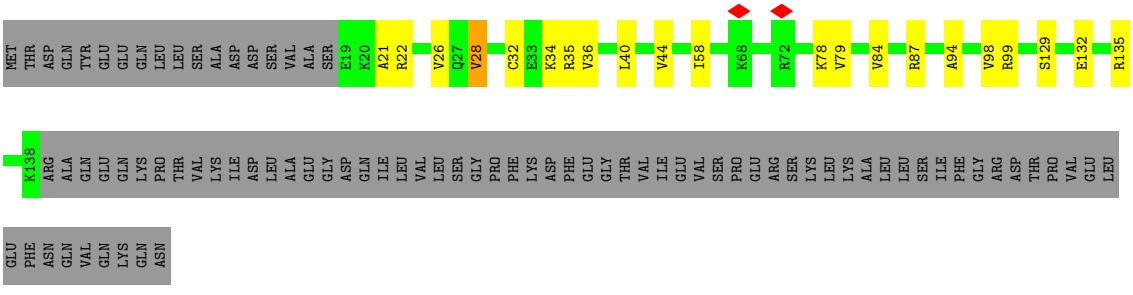
• Molecule 5: DNA-directed RNA polymerase subunit omega

Chain E:



• Molecule 6: Transcription termination/antitermination protein NusG

Chain G:

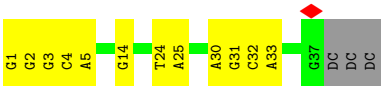


• Molecule 7: DNA (37-MER)

Chain N:

• Molecule 8: RNA (5'-R(P*UP*UP*CP*AP*AP*AP*GP*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3')

• Molecule 9: DNA (37-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	176309	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.035	Depositor
Minimum map value	-0.835	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.183	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	0/1759	0.54	0/2398
1	B	0.27	0/1759	0.55	0/2398
2	C	0.30	0/8541	0.55	1/11567 (0.0%)
3	D	0.29	0/5056	0.54	0/6842
4	Z	0.27	0/9476	0.55	0/12835
5	E	0.29	0/514	0.54	0/691
6	G	0.26	0/976	0.51	0/1317
7	N	0.54	0/831	0.89	0/1277
8	R	0.34	0/415	0.78	0/646
9	T	0.59	0/846	0.88	0/1304
All	All	0.31	0/30173	0.58	1/41275 (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
4	Z	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	584	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	Z	1131	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	1730	0	1710	14	0
1	B	1730	0	1710	17	0
2	C	8382	0	8349	85	0
3	D	4961	0	4991	67	0
4	Z	9357	0	9461	182	0
5	E	510	0	514	2	0
6	G	957	0	987	12	0
7	N	745	0	416	8	0
8	R	370	0	184	2	0
9	T	755	0	416	8	0
10	D	1	0	0	0	0
11	D	1	0	0	0	0
11	Z	1	0	0	0	0
All	All	29500	0	28738	385	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 (385) 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)
4:Z:622:GLY:HA3	4:Z:778:LEU:O	1.50	1.09
4:Z:634:ILE:HB	4:Z:745:VAL:HG22	1.58	0.84
4:Z:551:VAL:HG23	4:Z:826:LEU:HB3	1.61	0.83
3:D:369:ILE:O	3:D:370:HIS:ND1	2.14	0.81
4:Z:451:GLY:HA3	4:Z:483:LEU:O	1.83	0.79
3:D:568:GLU:HB2	3:D:588:ARG:HH21	1.48	0.78
2:C:708:ARG:HD2	2:C:723:GLU:HA	1.69	0.74
4:Z:903:CYS:SG	4:Z:941:ARG:NH2	2.60	0.72
3:D:265:ARG:NH2	9:T:24:DT:OP1	2.23	0.71
4:Z:692:ASP:HB3	4:Z:742:LEU:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:469:MET:HE3	2:C:474:GLU:HB3	1.74	0.70
3:D:118:LYS:O	3:D:317:ARG:NH1	2.24	0.70
2:C:74:ARG:NH1	2:C:796:ASP:OD1	2.25	0.69
1:B:123:ASN:O	1:B:123:ASN:ND2	2.24	0.69
2:C:305:ASP:O	2:C:311:ASN:ND2	2.26	0.69
1:A:73:ASP:OD1	1:A:73:ASP:N	2.20	0.68
2:C:270:LEU:CD1	2:C:283:ASP:OD1	2.42	0.68
6:G:28:VAL:HG21	6:G:36:VAL:HG11	1.76	0.68
3:D:295:GLU:OE2	3:D:299:ARG:NH1	2.27	0.68
4:Z:763:GLN:HA	4:Z:769:SER:HA	1.75	0.67
6:G:58:ILE:HG22	6:G:84:VAL:HG23	1.75	0.67
4:Z:510:LEU:HD11	4:Z:876:CYS:HB3	1.77	0.67
2:C:497:ILE:HG13	2:C:510:PRO:HB3	1.77	0.66
4:Z:631:LEU:HD12	4:Z:748:LEU:HB2	1.76	0.66
4:Z:503:ARG:HH21	4:Z:881:VAL:HG23	1.60	0.66
4:Z:591:LEU:HB2	4:Z:797:THR:HB	1.78	0.66
1:B:166:ASP:N	1:B:166:ASP:OD1	2.29	0.65
1:B:92:GLN:OE1	1:B:94:GLN:NE2	2.30	0.64
3:D:170:GLU:HA	3:D:173:ILE:HG22	1.78	0.64
4:Z:630:THR:HA	4:Z:749:VAL:HG22	1.79	0.64
4:Z:768:ARG:NH1	4:Z:804:GLU:OE2	2.31	0.64
4:Z:399:ARG:NH1	4:Z:401:GLU:OE2	2.23	0.64
4:Z:525:MET:HE3	4:Z:525:MET:H	1.62	0.64
1:A:92:GLN:O	1:A:94:GLN:NE2	2.31	0.64
4:Z:683:LEU:HD23	4:Z:684:ARG:H	1.63	0.63
4:Z:573:ASN:HB2	4:Z:590:GLU:HG2	1.81	0.63
4:Z:769:SER:O	4:Z:804:GLU:N	2.31	0.63
2:C:112:ARG:NH2	2:C:121:GLU:OE2	2.32	0.63
4:Z:776:GLN:HA	4:Z:797:THR:HA	1.81	0.63
3:D:129:ASP:OD2	3:D:226:ARG:NH1	2.32	0.63
3:D:588:ARG:H	3:D:588:ARG:HD3	1.62	0.63
3:D:147:LEU:HD13	3:D:194:GLN:HG2	1.81	0.62
4:Z:688:ILE:HG22	4:Z:690:PRO:HD3	1.81	0.62
4:Z:542:ALA:HB1	4:Z:770:ILE:HD13	1.82	0.62
4:Z:817:LEU:HB3	4:Z:828:LEU:HD23	1.80	0.62
4:Z:392:LEU:N	4:Z:403:PHE:O	2.32	0.62
4:Z:775:VAL:O	4:Z:777:ARG:NH1	2.33	0.61
4:Z:571:ARG:NH2	4:Z:573:ASN:OD1	2.31	0.61
4:Z:814:ILE:HD11	4:Z:831:VAL:HG22	1.82	0.61
4:Z:997:ARG:NH1	4:Z:1000:GLU:OE2	2.34	0.61
2:C:716:ASP:O	2:C:719:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:630:THR:O	4:Z:630:THR:OG1	2.19	0.60
2:C:390:ARG:HH12	2:C:423:GLU:HG2	1.65	0.60
4:Z:634:ILE:HG13	4:Z:743:ARG:HD2	1.82	0.60
4:Z:713:ALA:HA	4:Z:726:LEU:HA	1.83	0.60
2:C:646:GLU:HG3	2:C:647:LYS:H	1.67	0.60
2:C:825:ARG:NH2	2:C:870:GLU:OE2	2.30	0.60
4:Z:598:THR:HG21	4:Z:794:LEU:HD13	1.83	0.60
3:D:77:ARG:HG3	3:D:79:ARG:H	1.65	0.59
3:D:67:ASP:OD1	3:D:67:ASP:N	2.35	0.59
4:Z:827:ARG:NH2	4:Z:829:GLN:OE1	2.35	0.59
7:N:6:DC:H2"	7:N:7:DA:C8	2.37	0.59
4:Z:293:LEU:HG	4:Z:1127:GLU:HG2	1.84	0.59
4:Z:371:ARG:HH21	4:Z:387:GLU:HB2	1.67	0.59
6:G:94:ALA:O	6:G:98:VAL:HG12	2.03	0.59
2:C:259:VAL:HG21	2:C:313:ARG:HD2	1.83	0.58
4:Z:603:LEU:HB2	4:Z:634:ILE:HG23	1.84	0.58
2:C:140:ARG:HH22	4:Z:467:GLN:HE22	1.52	0.58
3:D:288:LEU:HD12	3:D:301:GLU:HG3	1.86	0.57
4:Z:790:GLU:HG3	4:Z:792:VAL:H	1.69	0.57
4:Z:925:GLY:HA2	4:Z:933:ILE:HG23	1.84	0.57
3:D:85:CYS:SG	3:D:86:GLU:N	2.77	0.57
1:A:29:ARG:HH11	1:A:189:ALA:HB1	1.69	0.57
4:Z:609:VAL:HG12	4:Z:629:GLY:HA2	1.86	0.57
3:D:120:ILE:HB	3:D:121:PRO:HD3	1.86	0.57
2:C:658:VAL:HG23	2:C:852:ILE:HG23	1.87	0.57
2:C:821:LYS:HD3	2:C:952:LEU:HD12	1.85	0.57
4:Z:666:ILE:HG22	4:Z:667:PHE:H	1.69	0.57
4:Z:1200:GLU:OE1	4:Z:1203:ARG:NH1	2.38	0.57
2:C:145:ARG:HA	4:Z:467:GLN:HG2	1.87	0.56
4:Z:1035:ILE:HG22	4:Z:1039:GLY:HA2	1.87	0.56
3:D:70:CYS:SG	3:D:71:HIS:N	2.78	0.56
4:Z:542:ALA:HB3	4:Z:831:VAL:HA	1.88	0.56
4:Z:752:ASP:OD1	4:Z:752:ASP:N	2.37	0.56
4:Z:637:GLU:OE1	4:Z:669:GLN:NE2	2.38	0.56
7:N:35:DC:H2"	7:N:36:DT:H5'	1.86	0.56
4:Z:583:THR:OG1	4:Z:809:GLN:O	2.21	0.56
2:C:35:GLU:OE1	2:C:322:GLN:NE2	2.34	0.56
4:Z:199:ASP:OD1	4:Z:199:ASP:N	2.39	0.56
3:D:273:ASP:N	3:D:273:ASP:OD1	2.38	0.55
2:C:140:ARG:NH1	4:Z:467:GLN:OE1	2.39	0.55
2:C:403:ARG:HD2	7:N:27:DG:H3'	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:507:THR:HG22	4:Z:24:ILE:HG13	1.87	0.55
2:C:708:ARG:HH21	2:C:718:LEU:HB3	1.71	0.55
4:Z:629:GLY:HA3	4:Z:750:ILE:H	1.70	0.55
4:Z:729:ALA:HA	4:Z:742:LEU:HD23	1.89	0.54
4:Z:781:GLN:N	4:Z:784:GLU:OE2	2.40	0.54
4:Z:1103:GLN:NE2	4:Z:1134:THR:OG1	2.34	0.54
3:D:399:ASN:OD1	3:D:399:ASN:N	2.41	0.54
4:Z:1017:PRO:HG3	4:Z:1036:GLU:HG2	1.88	0.54
3:D:173:ILE:HD11	3:D:183:ILE:HG12	1.89	0.54
4:Z:525:MET:H	4:Z:525:MET:CE	2.19	0.54
4:Z:645:ILE:HA	4:Z:648:LEU:HD12	1.90	0.54
3:D:568:GLU:HB2	3:D:588:ARG:NH2	2.21	0.54
4:Z:650:VAL:HG23	4:Z:660:THR:HG23	1.90	0.54
4:Z:546:LEU:H	4:Z:827:ARG:HD2	1.72	0.53
4:Z:997:ARG:NH2	4:Z:1109:GLU:OE1	2.41	0.53
3:D:527:GLN:HG2	3:D:553:ALA:HA	1.89	0.53
4:Z:915:GLN:HE21	4:Z:920:SER:HB3	1.72	0.53
4:Z:733:ASP:OD1	4:Z:733:ASP:N	2.31	0.53
4:Z:711:VAL:HG21	4:Z:729:ALA:H	1.73	0.53
1:B:55:VAL:HG12	1:B:165:LEU:HD11	1.89	0.53
2:C:693:GLU:OE2	2:C:807:ARG:NE	2.37	0.53
4:Z:652:ASP:HA	4:Z:674:VAL:HB	1.91	0.53
2:C:16:ASP:OD2	2:C:22:ARG:NH1	2.41	0.53
3:D:432:ALA:HB3	3:D:433:PRO:HD3	1.90	0.53
4:Z:633:TRP:O	4:Z:746:GLN:NE2	2.42	0.53
2:C:229:LEU:HD13	2:C:247:ARG:HH21	1.74	0.53
3:D:95:SER:O	3:D:98:ARG:HB2	2.09	0.53
4:Z:566:THR:HG22	4:Z:570:GLN:HB3	1.91	0.53
4:Z:716:GLU:HG3	4:Z:722:THR:HG23	1.91	0.53
4:Z:733:ASP:HA	4:Z:738:PRO:HA	1.91	0.53
7:N:19:DC:H2"	7:N:20:DT:H5'	1.90	0.53
2:C:792:ARG:NH1	2:C:802:ALA:O	2.43	0.52
1:A:29:ARG:NH2	1:A:191:ASP:OD2	2.43	0.52
4:Z:233:THR:HA	4:Z:238:ILE:HA	1.90	0.52
4:Z:679:ASN:OD1	4:Z:684:ARG:NH1	2.43	0.52
4:Z:743:ARG:NH1	4:Z:744:PRO:HG2	2.25	0.52
1:B:25:GLU:HB3	1:B:192:ARG:HG3	1.92	0.52
4:Z:447:THR:OG1	4:Z:449:LEU:O	2.27	0.52
4:Z:272:ASN:OD1	4:Z:272:ASN:N	2.37	0.52
4:Z:519:ARG:H	4:Z:865:PRO:HB3	1.74	0.51
4:Z:728:TRP:HB2	4:Z:745:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:546:LEU:HB2	4:Z:827:ARG:HG3	1.91	0.51
2:C:722:ASP:O	2:C:723:GLU:HG3	2.10	0.51
3:D:584:THR:O	3:D:584:THR:OG1	2.28	0.51
3:D:587:TYR:HB3	3:D:588:ARG:HH11	1.74	0.51
4:Z:777:ARG:NH1	4:Z:798:GLN:HB3	2.26	0.51
4:Z:776:GLN:HB2	4:Z:795:LEU:HD11	1.93	0.51
4:Z:587:VAL:HG13	4:Z:798:GLN:HG2	1.93	0.51
4:Z:713:ALA:HB2	4:Z:726:LEU:HG	1.92	0.51
2:C:878:GLN:OE1	2:C:946:ARG:NE	2.44	0.50
4:Z:622:GLY:CA	4:Z:778:LEU:O	2.40	0.50
4:Z:732:VAL:HB	4:Z:741:LEU:HD13	1.94	0.50
1:A:106:VAL:HB	1:A:126:ILE:O	2.11	0.50
4:Z:683:LEU:CD2	4:Z:684:ARG:H	2.24	0.50
1:A:61:ASN:N	1:A:61:ASN:OD1	2.45	0.50
4:Z:151:ARG:HB2	4:Z:166:ILE:HB	1.93	0.50
9:T:14:DG:H5'	9:T:14:DG:H8	1.76	0.50
4:Z:818:PRO:HD2	4:Z:827:ARG:HH21	1.76	0.50
4:Z:676:VAL:HG22	4:Z:683:LEU:HD11	1.92	0.50
2:C:509:THR:HG23	2:C:512:ARG:HG3	1.94	0.49
4:Z:1180:LEU:HD22	4:Z:1184:LYS:HD3	1.95	0.49
2:C:656:ILE:HD11	2:C:949:MET:HG3	1.93	0.49
1:B:69:GLY:HA3	1:B:133:ALA:HB2	1.94	0.49
5:E:51:GLU:OE2	5:E:59:ARG:NH1	2.46	0.49
9:T:4:DC:H2'	9:T:5:DA:N7	2.27	0.49
4:Z:390:PHE:H	4:Z:405:ILE:HG12	1.76	0.49
1:B:28:ALA:HB3	1:B:31:GLN:HG3	1.95	0.49
1:B:98:LEU:HD12	1:B:111:VAL:HG22	1.94	0.49
1:B:97:ARG:HD3	1:B:138:GLU:HG3	1.94	0.49
3:D:58:CYS:SG	3:D:59:GLU:N	2.85	0.49
2:C:597:VAL:HG13	2:C:605:TYR:HB2	1.94	0.48
2:C:735:SER:OG	2:C:778:ASN:HA	2.13	0.48
2:C:44:THR:HG22	2:C:51:GLU:HG2	1.95	0.48
4:Z:437:THR:OG1	4:Z:987:LYS:O	2.25	0.48
3:D:74:LYS:HG2	3:D:75:TYR:HD1	1.78	0.48
4:Z:169:ASN:N	4:Z:169:ASN:OD1	2.46	0.48
6:G:26:VAL:HB	6:G:84:VAL:HG12	1.94	0.48
4:Z:389:ASN:HD21	4:Z:406:LEU:HD12	1.77	0.48
4:Z:636:GLU:HA	4:Z:743:ARG:NE	2.29	0.48
4:Z:1170:MET:SD	4:Z:1170:MET:N	2.86	0.48
3:D:294:PRO:HG2	3:D:297:ILE:HD12	1.94	0.48
4:Z:275:LEU:O	4:Z:279:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:611:ILE:HA	4:Z:625:VAL:HA	1.95	0.48
4:Z:1217:LEU:HD22	4:Z:1226:ILE:HD11	1.95	0.48
2:C:1014:ASP:O	2:C:1018:ARG:HG3	2.14	0.48
3:D:287:ARG:NH2	6:G:79:VAL:O	2.46	0.48
4:Z:626:THR:O	4:Z:753:GLU:HG3	2.14	0.48
4:Z:668:CYS:SG	4:Z:669:GLN:N	2.87	0.48
2:C:138:SER:HB2	2:C:148:HIS:CE1	2.49	0.48
2:C:677:ARG:O	2:C:681:ASP:HB2	2.14	0.48
2:C:438:THR:OG1	2:C:524:ILE:O	2.31	0.48
2:C:695:GLU:OE2	2:C:805:VAL:HG22	2.14	0.47
4:Z:444:ASP:OD1	4:Z:444:ASP:N	2.36	0.47
2:C:89:ILE:HG12	2:C:96:ILE:HG12	1.95	0.47
2:C:560:ARG:HG3	2:C:646:GLU:HB3	1.95	0.47
3:D:568:GLU:HA	3:D:588:ARG:HE	1.80	0.47
4:Z:523:VAL:H	4:Z:539:ILE:HD12	1.79	0.47
6:G:129:SER:N	6:G:132:GLU:OE2	2.47	0.47
2:C:778:ASN:OD1	2:C:778:ASN:N	2.47	0.47
4:Z:292:PRO:HG2	4:Z:1127:GLU:HB3	1.95	0.47
4:Z:603:LEU:HD23	4:Z:785:ARG:HG3	1.96	0.47
3:D:76:LYS:O	3:D:80:HIS:ND1	2.48	0.47
4:Z:653:GLY:O	4:Z:735:THR:OG1	2.33	0.47
4:Z:1075:ASP:OD2	4:Z:1076:LEU:N	2.48	0.47
2:C:218:GLU:O	2:C:222:LEU:HD12	2.14	0.47
4:Z:564:ILE:HB	4:Z:572:PHE:HB2	1.96	0.47
2:C:1060:SER:HB2	2:C:1065:GLU:HB3	1.97	0.47
3:D:216:LYS:HG3	3:D:217:GLY:N	2.30	0.47
4:Z:1016:ARG:N	4:Z:1017:PRO:HD2	2.30	0.47
4:Z:673:ILE:O	4:Z:688:ILE:HG12	2.14	0.46
3:D:559:PHE:O	3:D:603:GLN:NE2	2.43	0.46
4:Z:1036:GLU:HB2	4:Z:1040:THR:H	1.80	0.46
9:T:24:DT:H2”	9:T:25:DA:C8	2.50	0.46
2:C:376:MET:HG3	2:C:377:ASP:N	2.28	0.46
2:C:1062:GLU:HG3	2:C:1065:GLU:HB2	1.96	0.46
4:Z:555:ALA:HA	4:Z:560:GLU:HA	1.97	0.46
4:Z:656:VAL:O	4:Z:672:GLY:N	2.43	0.46
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.77	0.46
8:R:7:A:H1’	8:R:8:A:C4	2.51	0.46
4:Z:603:LEU:HD12	4:Z:634:ILE:HD13	1.97	0.46
2:C:382:LEU:O	2:C:386:THR:HG23	2.15	0.46
2:C:529:SER:O	2:C:565:THR:HG21	2.16	0.46
7:N:25:DA:H2”	7:N:26:DT:C2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:36:GLY:HA2	3:D:61:ILE:HG23	1.98	0.46
3:D:75:TYR:HE2	3:D:83:ILE:HD12	1.81	0.46
3:D:498:SER:OG	3:D:501:THR:O	2.27	0.46
1:B:21:ARG:HG3	1:B:196:GLU:HG2	1.98	0.45
4:Z:600:THR:HB	4:Z:789:VAL:HA	1.97	0.45
9:T:30:DA:H2"	9:T:31:DG:C8	2.51	0.45
9:T:32:DC:H2"	9:T:33:DA:C8	2.51	0.45
2:C:225:LEU:HD12	2:C:229:LEU:HG	1.97	0.45
4:Z:620:LYS:HD2	4:Z:620:LYS:HA	1.83	0.45
4:Z:927:GLN:O	4:Z:928:LEU:HD13	2.16	0.45
2:C:389:ARG:NH2	2:C:437:ALA:O	2.49	0.45
4:Z:908:LEU:HD12	4:Z:908:LEU:HA	1.75	0.45
2:C:701:LEU:HD12	2:C:701:LEU:H	1.81	0.45
3:D:326:ASN:HB3	3:D:328:ARG:HG2	1.98	0.45
4:Z:610:GLU:O	4:Z:626:THR:OG1	2.35	0.45
4:Z:907:ASP:HA	4:Z:947:GLN:HG3	1.99	0.45
2:C:510:PRO:HD2	2:C:511:GLU:OE1	2.17	0.45
3:D:40:LYS:HB2	3:D:54:ASP:O	2.16	0.45
4:Z:593:ASP:OD1	4:Z:593:ASP:N	2.49	0.45
2:C:63:ARG:HA	2:C:63:ARG:HD3	1.68	0.45
2:C:1000:ALA:HA	3:D:485:GLU:OE2	2.17	0.45
3:D:393:LYS:HB3	3:D:393:LYS:HE2	1.77	0.45
3:D:537:LEU:HB3	3:D:612:ILE:HG23	1.98	0.45
4:Z:486:ASP:OD1	4:Z:897:VAL:HB	2.16	0.45
4:Z:1054:ILE:HD13	4:Z:1068:ASP:HB2	1.99	0.45
2:C:187:LYS:NZ	2:C:215:GLN:OE1	2.49	0.45
2:C:1019:ASN:ND2	2:C:1085:PRO:HA	2.32	0.45
4:Z:16:ASP:OD1	4:Z:16:ASP:N	2.46	0.45
4:Z:463:LYS:HE2	4:Z:463:LYS:HB2	1.59	0.45
4:Z:557:GLN:HB2	4:Z:561:HIS:HE2	1.82	0.45
4:Z:612:SER:N	4:Z:624:GLU:O	2.48	0.45
2:C:647:LYS:HB3	2:C:647:LYS:HE3	1.72	0.45
2:C:449:GLU:HG2	2:C:470:THR:HG22	1.98	0.45
3:D:147:LEU:HB2	3:D:185:VAL:HG23	1.99	0.45
5:E:23:SER:O	5:E:24:THR:OG1	2.29	0.45
2:C:541:ARG:HA	2:C:541:ARG:HD2	1.85	0.45
4:Z:383:ALA:HB1	4:Z:411:ILE:O	2.17	0.45
4:Z:711:VAL:HG21	4:Z:729:ALA:HB3	1.98	0.45
4:Z:778:LEU:HD23	4:Z:778:LEU:HA	1.77	0.45
6:G:78:LYS:HE2	6:G:78:LYS:HB2	1.79	0.44
1:B:13:GLU:O	1:B:15:ASP:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:GLU:HA	2:C:207:GLN:HB3	1.99	0.44
2:C:103:ILE:HD13	2:C:103:ILE:HA	1.82	0.44
3:D:498:SER:HB3	3:D:505:ILE:HD12	2.00	0.44
3:D:207:LYS:HD2	3:D:207:LYS:O	2.17	0.44
1:A:21:ARG:HG3	1:A:196:GLU:HG2	2.00	0.44
2:C:141:ASP:HB3	2:C:144:GLY:H	1.81	0.44
3:D:262:ASP:OD1	3:D:263:GLY:N	2.50	0.44
4:Z:523:VAL:HG11	4:Z:857:VAL:HB	1.99	0.44
4:Z:641:VAL:HG21	4:Z:664:LYS:H	1.83	0.44
4:Z:808:SER:OG	4:Z:809:GLN:OE1	2.34	0.44
4:Z:927:GLN:HG2	4:Z:931:GLY:HA2	2.00	0.44
4:Z:699:PRO:HD2	4:Z:738:PRO:HB2	1.99	0.44
4:Z:1099:LEU:HD22	4:Z:1134:THR:HB	2.00	0.44
2:C:24:SER:OG	2:C:316:SER:HB2	2.17	0.44
2:C:548:MET:HE3	2:C:823:ALA:HB1	1.98	0.44
4:Z:557:GLN:HB2	4:Z:561:HIS:NE2	2.33	0.44
7:N:16:DT:H2"	7:N:17:DA:C8	2.52	0.44
4:Z:209:ASP:OD2	4:Z:1221:LYS:NZ	2.49	0.44
2:C:940:ARG:HH12	4:Z:131:MET:HE1	1.83	0.43
4:Z:679:ASN:HB3	4:Z:682:ILE:O	2.18	0.43
2:C:180:LEU:HD12	2:C:181:SER:O	2.16	0.43
2:C:907:SER:O	2:C:911:GLU:HG2	2.18	0.43
3:D:98:ARG:HB3	3:D:254:ASP:OD2	2.18	0.43
3:D:219:LYS:HD3	3:D:219:LYS:HA	1.57	0.43
4:Z:240:ILE:HD11	4:Z:1115:GLN:HG3	2.00	0.43
3:D:405:LYS:HG3	3:D:406:LEU:N	2.33	0.43
4:Z:739:LEU:HG	4:Z:740:LEU:H	1.84	0.43
1:A:177:TYR:HB3	1:A:195:LEU:HD12	2.00	0.43
2:C:639:ILE:HD13	2:C:639:ILE:HA	1.83	0.43
3:D:60:LYS:HB3	3:D:60:LYS:HE3	1.85	0.43
9:T:3:DG:H2"	9:T:4:DC:O4'	2.18	0.43
1:B:150:ILE:HD12	1:B:153:SER:HB2	2.01	0.43
2:C:270:LEU:HD13	2:C:283:ASP:OD1	2.17	0.43
2:C:693:GLU:HG3	2:C:807:ARG:HG3	2.00	0.43
4:Z:581:LYS:HA	4:Z:581:LYS:HD3	1.77	0.43
4:Z:733:ASP:HA	4:Z:739:LEU:H	1.83	0.43
2:C:145:ARG:HH21	4:Z:469:ASN:HD21	1.65	0.43
4:Z:578:PRO:O	4:Z:815:GLU:HG2	2.19	0.43
2:C:582:PRO:HD2	2:C:583:VAL:HG23	2.01	0.43
6:G:21:ALA:HB1	6:G:87:ARG:HD3	2.01	0.43
3:D:180:LEU:HD23	3:D:180:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:607:THR:OG1	3:D:608:THR:N	2.50	0.43
4:Z:705:TYR:CZ	4:Z:731:ALA:HB3	2.53	0.43
2:C:541:ARG:HG3	2:C:864:ASN:OD1	2.19	0.43
4:Z:939:GLU:O	4:Z:950:LEU:HB2	2.19	0.42
1:A:89:HIS:ND1	1:A:116:GLU:O	2.43	0.42
3:D:209:ARG:HD3	3:D:227:LEU:HD21	2.01	0.42
1:B:177:TYR:HB3	1:B:195:LEU:HD12	2.02	0.42
3:D:251:ILE:HG12	3:D:252:PRO:HD2	2.01	0.42
4:Z:64:LYS:NZ	4:Z:124:ASP:HB2	2.35	0.42
4:Z:894:ARG:HB3	4:Z:971:LEU:HD12	2.02	0.42
6:G:34:LYS:HE2	6:G:34:LYS:HB2	1.87	0.42
7:N:11:DT:H2"	7:N:12:DG:C8	2.54	0.42
1:B:174:ARG:HB3	1:B:198:TRP:CE3	2.54	0.42
3:D:590:ARG:CZ	3:D:592:ILE:HD11	2.49	0.42
4:Z:226:GLY:HA3	4:Z:289:VAL:O	2.19	0.42
2:C:58:GLN:N	2:C:58:GLN:OE1	2.53	0.42
2:C:357:LYS:HE2	2:C:357:LYS:HB3	1.83	0.42
3:D:77:ARG:HD2	3:D:78:VAL:H	1.85	0.42
3:D:208:LEU:HD12	3:D:208:LEU:HA	1.83	0.42
6:G:32:CYS:SG	6:G:35:ARG:NH1	2.93	0.42
2:C:422:ILE:O	2:C:543:LEU:HD12	2.19	0.42
3:D:369:ILE:O	3:D:370:HIS:CG	2.72	0.42
4:Z:596:TYR:HB3	4:Z:794:LEU:HB3	2.01	0.42
7:N:13:DC:H2'	7:N:14:DT:H71	2.02	0.42
1:A:100:VAL:HG21	1:A:106:VAL:HG13	2.02	0.42
2:C:123:VAL:HG11	2:C:387:HIS:ND1	2.35	0.42
4:Z:118:LYS:HB2	4:Z:118:LYS:HE3	1.48	0.42
2:C:555:LEU:HD22	2:C:684:TYR:HA	2.02	0.42
3:D:165:GLN:HA	3:D:168:GLU:HG2	2.01	0.42
3:D:284:ARG:HE	3:D:284:ARG:HB2	1.58	0.42
2:C:563:VAL:HG12	2:C:563:VAL:O	2.19	0.42
6:G:40:LEU:O	6:G:44:VAL:HG12	2.19	0.42
2:C:767:ARG:HG3	2:C:769:VAL:HG22	2.01	0.41
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.53	0.41
4:Z:587:VAL:HG22	4:Z:798:GLN:HG3	2.02	0.41
4:Z:779:GLN:NE2	4:Z:794:LEU:HD12	2.34	0.41
1:B:226:VAL:HG23	1:B:227:SER:H	1.86	0.41
2:C:353:LEU:HD12	2:C:353:LEU:HA	1.83	0.41
2:C:1079:ARG:HD3	2:C:1079:ARG:HA	1.78	0.41
3:D:335:ASP:OD1	3:D:335:ASP:N	2.53	0.41
3:D:508:PRO:HG2	4:Z:20:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:611:ILE:HG13	4:Z:625:VAL:HG22	2.03	0.41
4:Z:728:TRP:H	4:Z:745:VAL:HG21	1.85	0.41
4:Z:729:ALA:HA	4:Z:742:LEU:CD2	2.49	0.41
1:B:100:VAL:HG11	1:B:106:VAL:HG22	2.02	0.41
4:Z:557:GLN:HB2	4:Z:561:HIS:CE1	2.55	0.41
2:C:336:ILE:HD11	2:C:354:VAL:HG12	2.03	0.41
4:Z:638:THR:HG22	4:Z:687:VAL:HG12	2.02	0.41
4:Z:776:GLN:H	4:Z:776:GLN:HG2	1.69	0.41
3:D:622:LEU:HD12	4:Z:8:PRO:HG3	2.02	0.41
4:Z:285:LYS:HB3	4:Z:285:LYS:HE3	1.91	0.41
4:Z:598:THR:HB	4:Z:633:TRP:CH2	2.56	0.41
4:Z:655:LEU:HD12	4:Z:673:ILE:HG12	2.03	0.41
4:Z:718:PHE:HD1	4:Z:718:PHE:HA	1.80	0.41
4:Z:496:PRO:HG3	4:Z:892:VAL:HG11	2.03	0.41
4:Z:522:THR:OG1	4:Z:539:ILE:O	2.32	0.41
4:Z:855:LEU:HD22	4:Z:857:VAL:HG22	2.03	0.41
8:R:6:C:H1'	8:R:7:A:C8	2.55	0.41
9:T:1:DG:H2"	9:T:2:DG:C8	2.55	0.41
2:C:208:LYS:HE3	2:C:208:LYS:HB2	1.74	0.41
3:D:225:LYS:HB3	3:D:225:LYS:HE2	1.70	0.41
4:Z:394:LEU:H	4:Z:401:GLU:HB2	1.85	0.41
4:Z:488:TYR:OH	4:Z:877:LYS:HD3	2.20	0.41
4:Z:512:GLU:HA	4:Z:872:THR:O	2.21	0.41
4:Z:605:LYS:HG2	4:Z:728:TRP:CH2	2.56	0.41
6:G:22:ARG:HD2	6:G:22:ARG:HA	1.82	0.41
2:C:14:LEU:HD23	2:C:14:LEU:HA	1.81	0.41
2:C:600:ASP:OD1	2:C:600:ASP:N	2.54	0.41
4:Z:156:ASN:O	4:Z:188:LYS:NZ	2.45	0.41
4:Z:500:ASN:HA	4:Z:885:ILE:HD13	2.03	0.41
4:Z:542:ALA:O	4:Z:831:VAL:HG12	2.21	0.41
4:Z:1017:PRO:HG3	4:Z:1036:GLU:HA	2.02	0.41
1:A:29:ARG:HA	1:A:29:ARG:HE	1.87	0.40
3:D:298:VAL:HG12	3:D:302:LYS:HE3	2.03	0.40
4:Z:528:ASP:HB2	4:Z:535:ARG:HH21	1.86	0.40
4:Z:709:ARG:HE	4:Z:709:ARG:HB2	1.78	0.40
1:A:99:ARG:HG3	1:A:136:GLU:HG2	2.02	0.40
2:C:243:LEU:HD12	2:C:243:LEU:HA	1.84	0.40
4:Z:768:ARG:HA	4:Z:768:ARG:HD3	1.92	0.40
1:A:73:ASP:O	1:A:77:ILE:HG13	2.22	0.40
1:A:108:ALA:HB2	1:A:124:HIS:HB3	2.03	0.40
2:C:1062:GLU:OE2	2:C:1065:GLU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:106:LYS:HB3	3:D:106:LYS:HE3	1.71	0.40
3:D:608:THR:HG22	3:D:610:GLY:H	1.86	0.40
4:Z:354:ARG:HE	4:Z:354:ARG:HB3	1.63	0.40
4:Z:495:GLU:OE2	4:Z:496:PRO:HD2	2.22	0.40
4:Z:502:ASP:O	4:Z:882:VAL:HG12	2.22	0.40
4:Z:1077:LEU:HD13	4:Z:1102:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/309 (72%)	212 (95%)	11 (5%)	1 (0%)	34	64
1	B	224/309 (72%)	203 (91%)	21 (9%)	0	100	100
2	C	1057/1100 (96%)	1003 (95%)	53 (5%)	1 (0%)	51	80
3	D	618/624 (99%)	576 (93%)	40 (6%)	2 (0%)	41	69
4	Z	1213/1318 (92%)	1066 (88%)	139 (12%)	8 (1%)	22	52
5	E	61/76 (80%)	57 (93%)	4 (7%)	0	100	100
6	G	118/205 (58%)	114 (97%)	4 (3%)	0	100	100
All	All	3515/3941 (89%)	3231 (92%)	272 (8%)	12 (0%)	44	69

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	398	ASN
4	Z	792	VAL
4	Z	1017	PRO
4	Z	540	ILE
4	Z	916	LEU

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Mol	Chain	Res	Type
4	Z	523	VAL
4	Z	709	ARG
4	Z	284	ILE
4	Z	567	LYS
3	D	215	SER
1	A	3	PHE
2	C	92	GLU

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	188/262 (72%)	160 (85%)	28 (15%)	3 8
1	B	188/262 (72%)	170 (90%)	18 (10%)	8 24
2	C	906/938 (97%)	842 (93%)	64 (7%)	14 38
3	D	536/539 (99%)	505 (94%)	31 (6%)	20 48
4	Z	1012/1093 (93%)	912 (90%)	100 (10%)	8 23
5	E	57/68 (84%)	55 (96%)	2 (4%)	36 67
6	G	102/178 (57%)	99 (97%)	3 (3%)	42 73
All	All	2989/3340 (90%)	2743 (92%)	246 (8%)	15 31

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	5	VAL
1	A	8	VAL
1	A	34	THR
1	A	45	SER
1	A	71	ARG
1	A	73	ASP
1	A	84	LEU
1	A	85	VAL
1	A	95	ILE

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Mol	Chain	Res	Type
1	A	107	THR
1	A	128	SER
1	A	130	SER
1	A	134	THR
1	A	145	THR
1	A	160	LEU
1	A	162	PHE
1	A	169	PHE
1	A	173	ARG
1	A	178	SER
1	A	179	VAL
1	A	202	SER
1	A	203	LEU
1	A	204	SER
1	A	206	GLN
1	A	210	SER
1	A	214	SER
1	A	215	CYS
1	B	4	GLN
1	B	5	VAL
1	B	50	THR
1	B	100	VAL
1	B	123	ASN
1	B	130	SER
1	B	147	TYR
1	B	152	ARG
1	B	154	HIS
1	B	157	THR
1	B	162	PHE
1	B	166	ASP
1	B	178	SER
1	B	183	ARG
1	B	192	ARG
1	B	194	VAL
1	B	210	SER
1	B	215	CYS
2	C	20	ILE
2	C	24	SER
2	C	40	PHE
2	C	52	LEU
2	C	63	ARG
2	C	65	LYS

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Mol	Chain	Res	Type
2	C	67	ASP
2	C	70	GLU
2	C	93	THR
2	C	105	ASP
2	C	126	ASN
2	C	138	SER
2	C	164	THR
2	C	178	ARG
2	C	196	ILE
2	C	198	ASP
2	C	222	LEU
2	C	227	ARG
2	C	246	SER
2	C	252	LYS
2	C	298	LEU
2	C	321	LEU
2	C	341	THR
2	C	342	VAL
2	C	352	SER
2	C	390	ARG
2	C	406	PHE
2	C	408	VAL
2	C	415	HIS
2	C	441	ARG
2	C	472	ASP
2	C	476	ASP
2	C	506	THR
2	C	518	LEU
2	C	546	SER
2	C	597	VAL
2	C	598	THR
2	C	600	ASP
2	C	620	CYS
2	C	624	ARG
2	C	633	VAL
2	C	645	THR
2	C	646	GLU
2	C	647	LYS
2	C	705	GLU
2	C	735	SER
2	C	737	ASP
2	C	768	ASP

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Mol	Chain	Res	Type
2	C	774	LEU
2	C	775	ARG
2	C	786	ASP
2	C	814	ARG
2	C	822	MET
2	C	829	LYS
2	C	839	GLU
2	C	840	ASP
2	C	870	GLU
2	C	944	VAL
2	C	953	VAL
2	C	1019	ASN
2	C	1027	LYS
2	C	1067	ASP
2	C	1073	MET
2	C	1080	ARG
3	D	6	GLN
3	D	27	ARG
3	D	28	THR
3	D	39	THR
3	D	47	ARG
3	D	49	LEU
3	D	67	ASP
3	D	79	ARG
3	D	88	CYS
3	D	98	ARG
3	D	176	GLU
3	D	194	GLN
3	D	239	ARG
3	D	258	MET
3	D	273	ASP
3	D	295	GLU
3	D	306	GLN
3	D	335	ASP
3	D	395	HIS
3	D	405	LYS
3	D	436	HIS
3	D	449	GLU
3	D	470	ASP
3	D	476	VAL
3	D	509	SER
3	D	548	SER

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Mol	Chain	Res	Type
3	D	560	ASP
3	D	562	GLU
3	D	584	THR
3	D	588	ARG
3	D	594	GLU
4	Z	13	ARG
4	Z	36	THR
4	Z	53	ARG
4	Z	68	SER
4	Z	120	PHE
4	Z	122	GLU
4	Z	169	ASN
4	Z	199	ASP
4	Z	212	GLN
4	Z	227	LEU
4	Z	253	GLU
4	Z	255	VAL
4	Z	260	THR
4	Z	272	ASN
4	Z	274	ASP
4	Z	281	LYS
4	Z	295	CYS
4	Z	299	ARG
4	Z	300	SER
4	Z	316	VAL
4	Z	339	MET
4	Z	347	VAL
4	Z	348	PHE
4	Z	378	ARG
4	Z	381	GLU
4	Z	399	ARG
4	Z	402	THR
4	Z	409	SER
4	Z	414	GLN
4	Z	447	THR
4	Z	466	ARG
4	Z	472	ARG
4	Z	503	ARG
4	Z	516	THR
4	Z	525	MET
4	Z	535	ARG
4	Z	545	VAL

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Mol	Chain	Res	Type
4	Z	547	ASP
4	Z	548	THR
4	Z	552	LYS
4	Z	566	THR
4	Z	593	ASP
4	Z	594	SER
4	Z	595	ARG
4	Z	597	ARG
4	Z	605	LYS
4	Z	609	VAL
4	Z	616	ARG
4	Z	621	GLN
4	Z	624	GLU
4	Z	630	THR
4	Z	634	ILE
4	Z	643	LYS
4	Z	649	ASN
4	Z	673	ILE
4	Z	674	VAL
4	Z	681	ASP
4	Z	685	GLU
4	Z	692	ASP
4	Z	696	LEU
4	Z	709	ARG
4	Z	722	THR
4	Z	728	TRP
4	Z	733	ASP
4	Z	743	ARG
4	Z	752	ASP
4	Z	756	VAL
4	Z	771	ARG
4	Z	796	ARG
4	Z	802	GLU
4	Z	846	THR
4	Z	876	CYS
4	Z	877	LYS
4	Z	883	ARG
4	Z	890	GLU
4	Z	893	ARG
4	Z	915	GLN
4	Z	922	ILE
4	Z	923	VAL

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Mol	Chain	Res	Type
4	Z	937	SER
4	Z	949	GLN
4	Z	950	LEU
4	Z	969	LYS
4	Z	976	ASP
4	Z	992	ILE
4	Z	1015	ARG
4	Z	1031	ASP
4	Z	1033	GLN
4	Z	1035	ILE
4	Z	1043	ASP
4	Z	1055	SER
4	Z	1083	TYR
4	Z	1112	SER
4	Z	1123	ASP
4	Z	1137	VAL
4	Z	1141	ASP
4	Z	1163	ASN
4	Z	1164	THR
4	Z	1170	MET
4	Z	1190	ASN
5	E	12	LEU
5	E	45	MET
6	G	28	VAL
6	G	99	ARG
6	G	135	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	667	ASN
3	D	246	ASN
4	Z	557	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	16/20 (80%)	5 (31%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	R	6	C
8	R	7	A
8	R	9	A
8	R	11	C
8	R	12	G

There are no RNA pucker outliers to report.

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

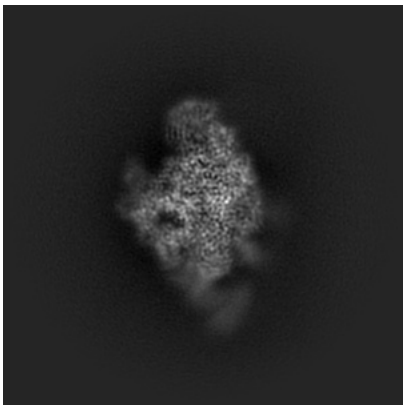
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40874. These allow visual inspection of the internal detail of the map and identification of artifacts.

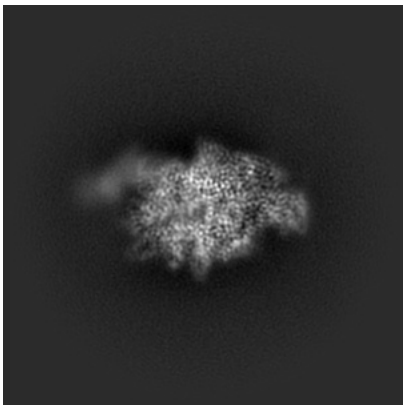
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

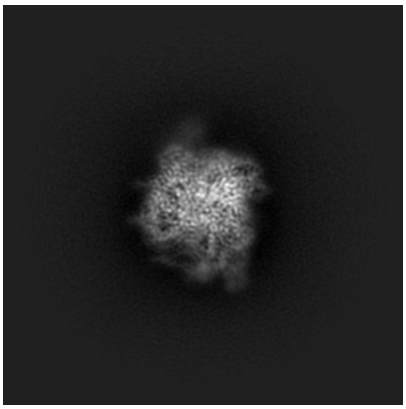
6.1.1 Primary map



X

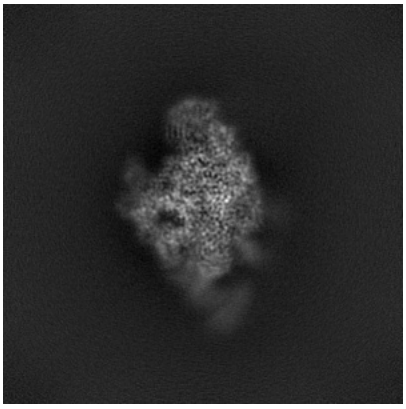


Y

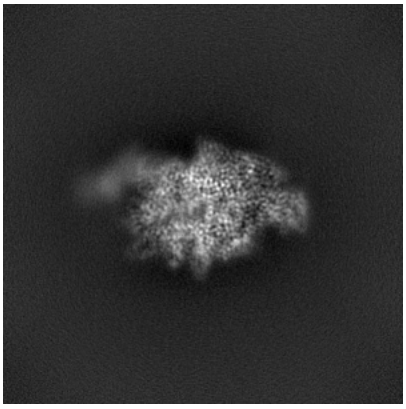


Z

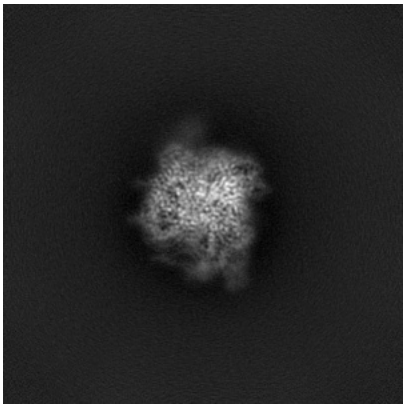
6.1.2 Raw map



X



Y

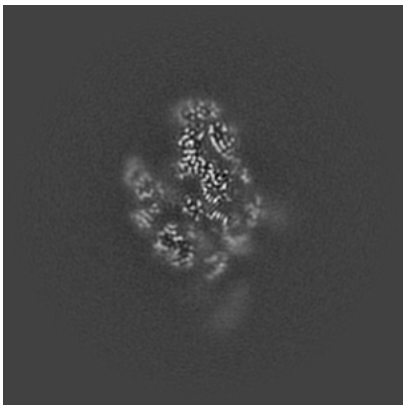


Z

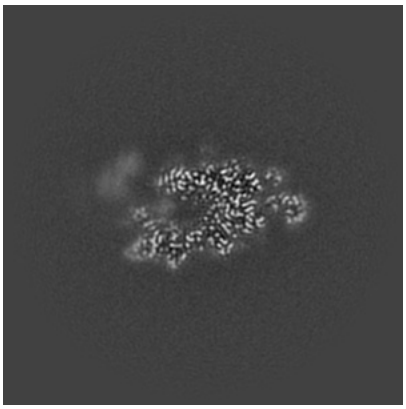
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

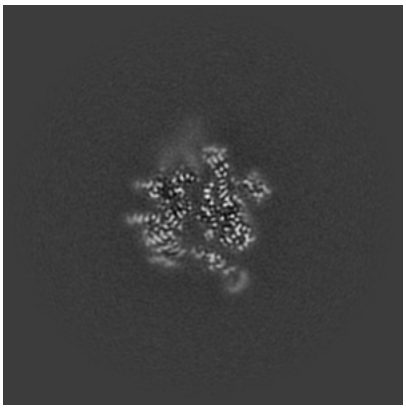
6.2.1 Primary map



X Index: 200

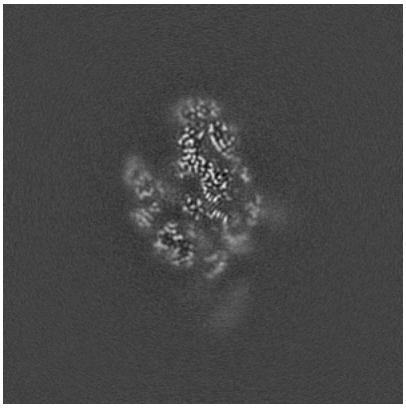


Y Index: 200

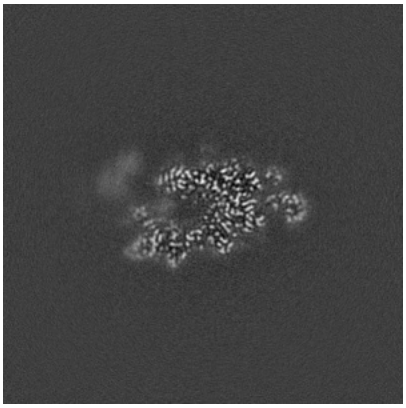


Z Index: 200

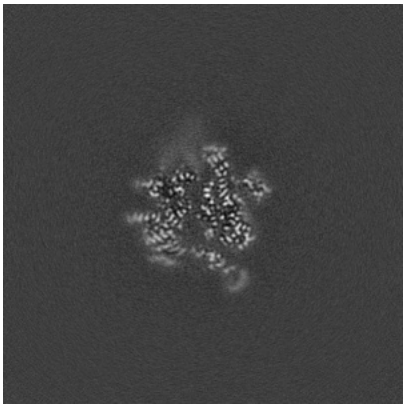
6.2.2 Raw map



X Index: 200



Y Index: 200

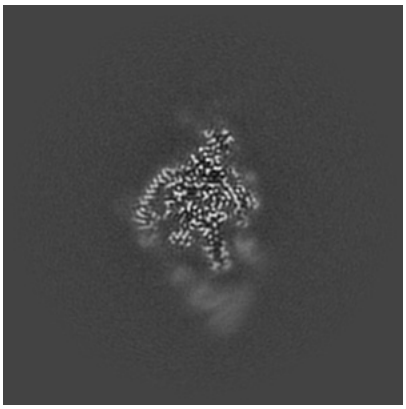


Z Index: 200

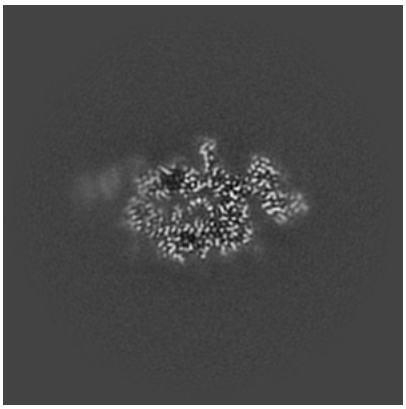
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

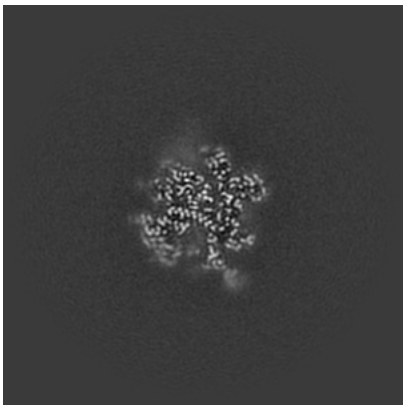
6.3.1 Primary map



X Index: 219

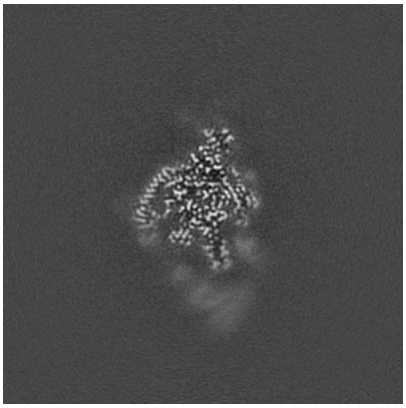


Y Index: 210

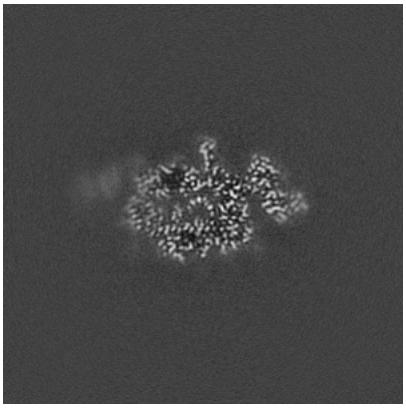


Z Index: 205

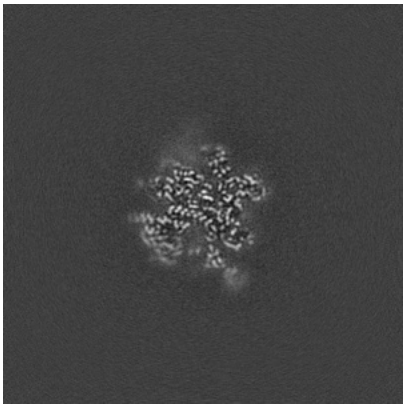
6.3.2 Raw map



X Index: 219



Y Index: 210

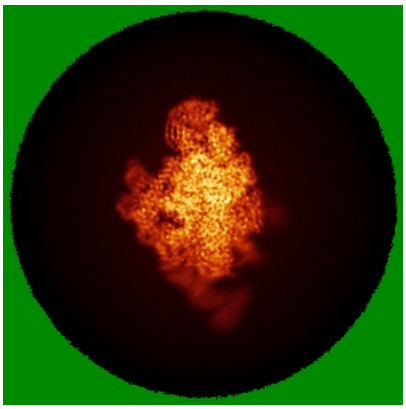


Z Index: 204

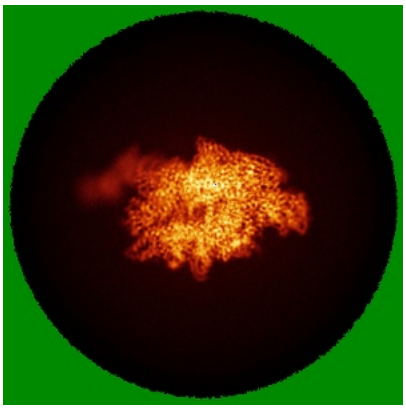
The images above show the largest variance slices of the map in three orthogonal directions.

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

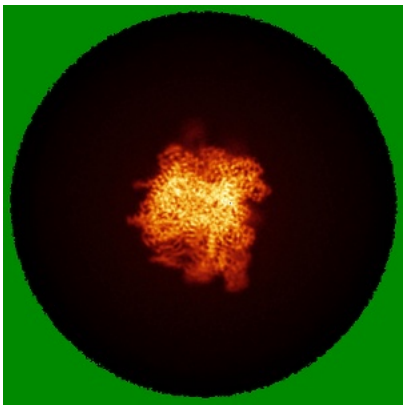
6.4.1 Primary map



X

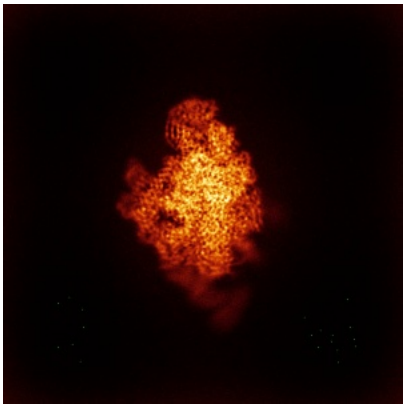


Y

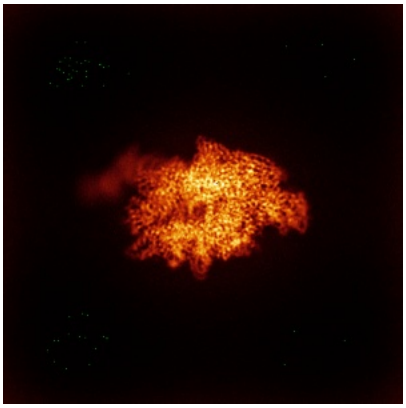


Z

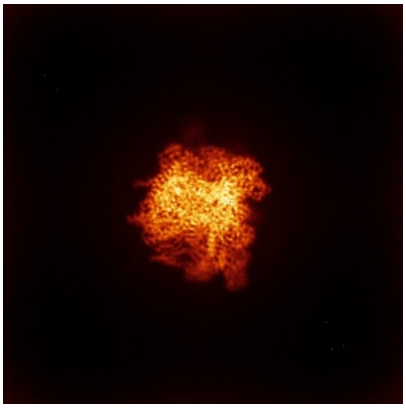
6.4.2 Raw map



X



Y

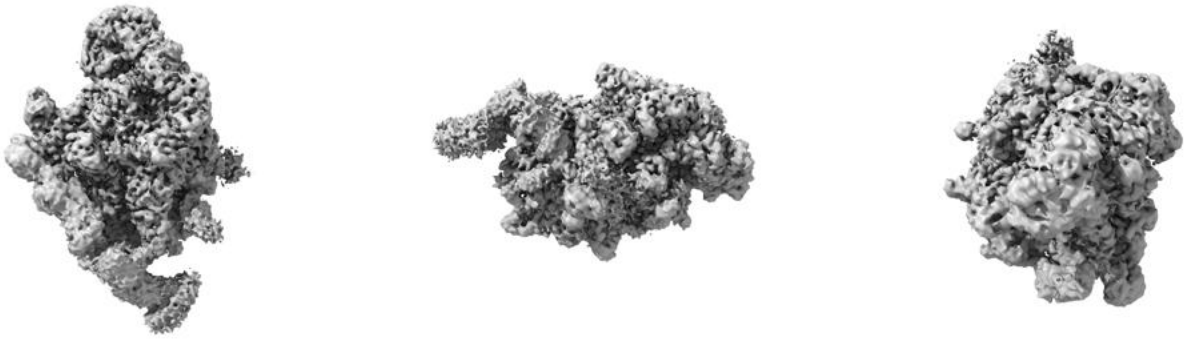


Z

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)

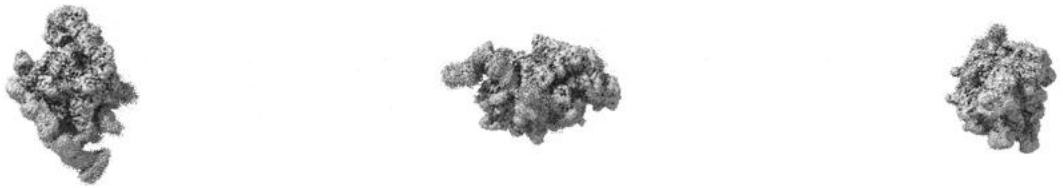
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.183. 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.

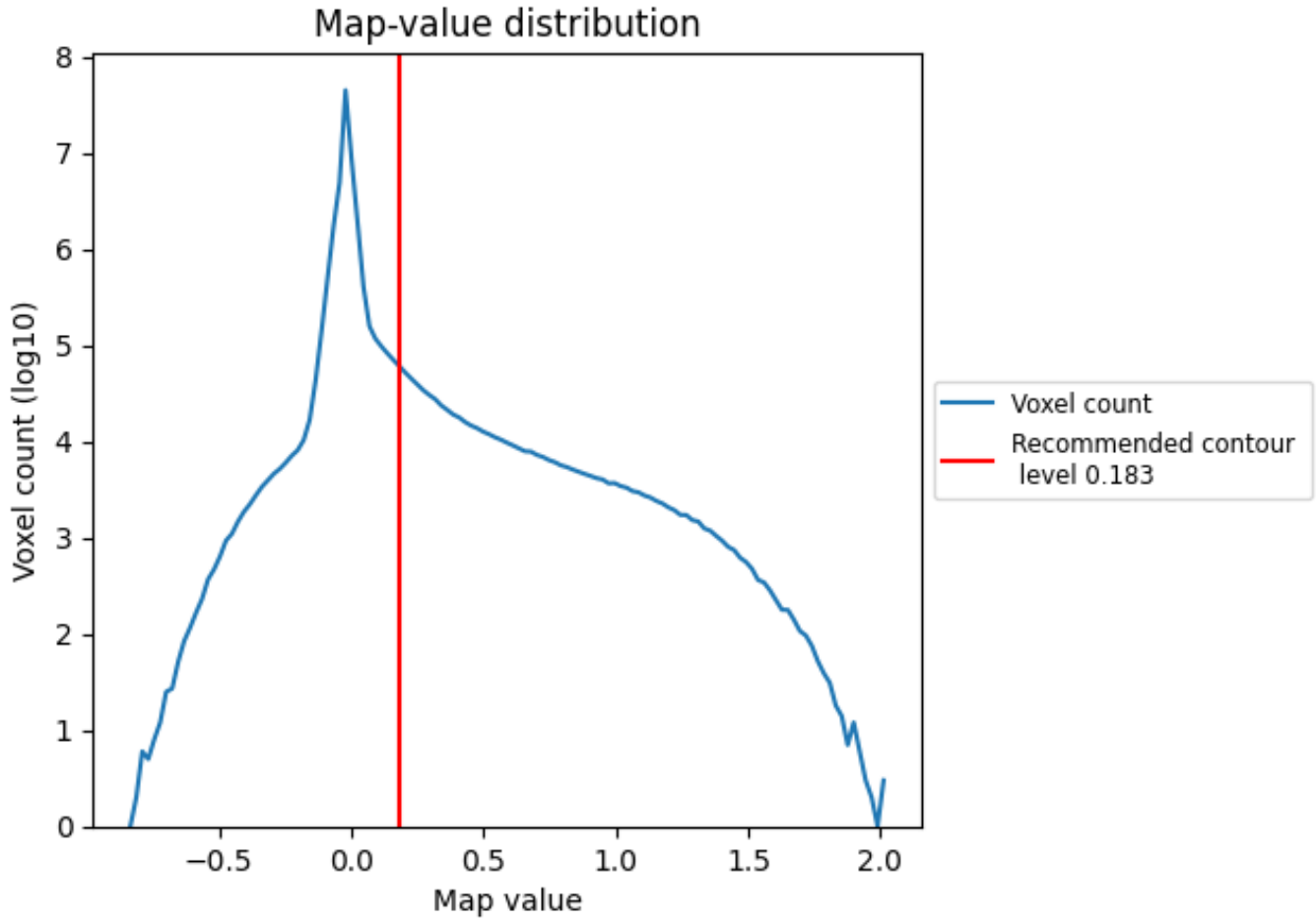
6.6 Mask visualisation (i)

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

7 Map analysis

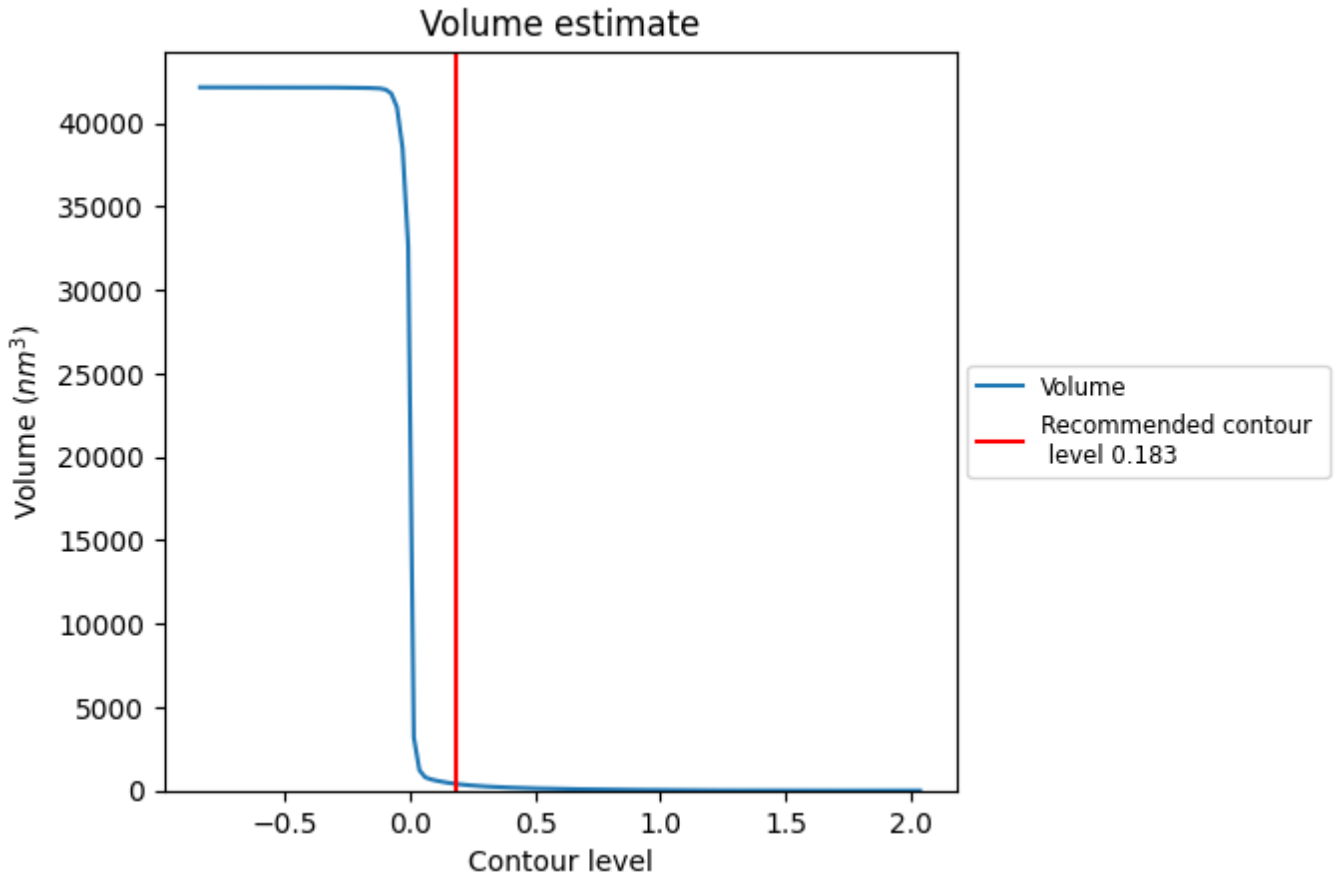
This section contains the results of statistical analysis of the map.

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.

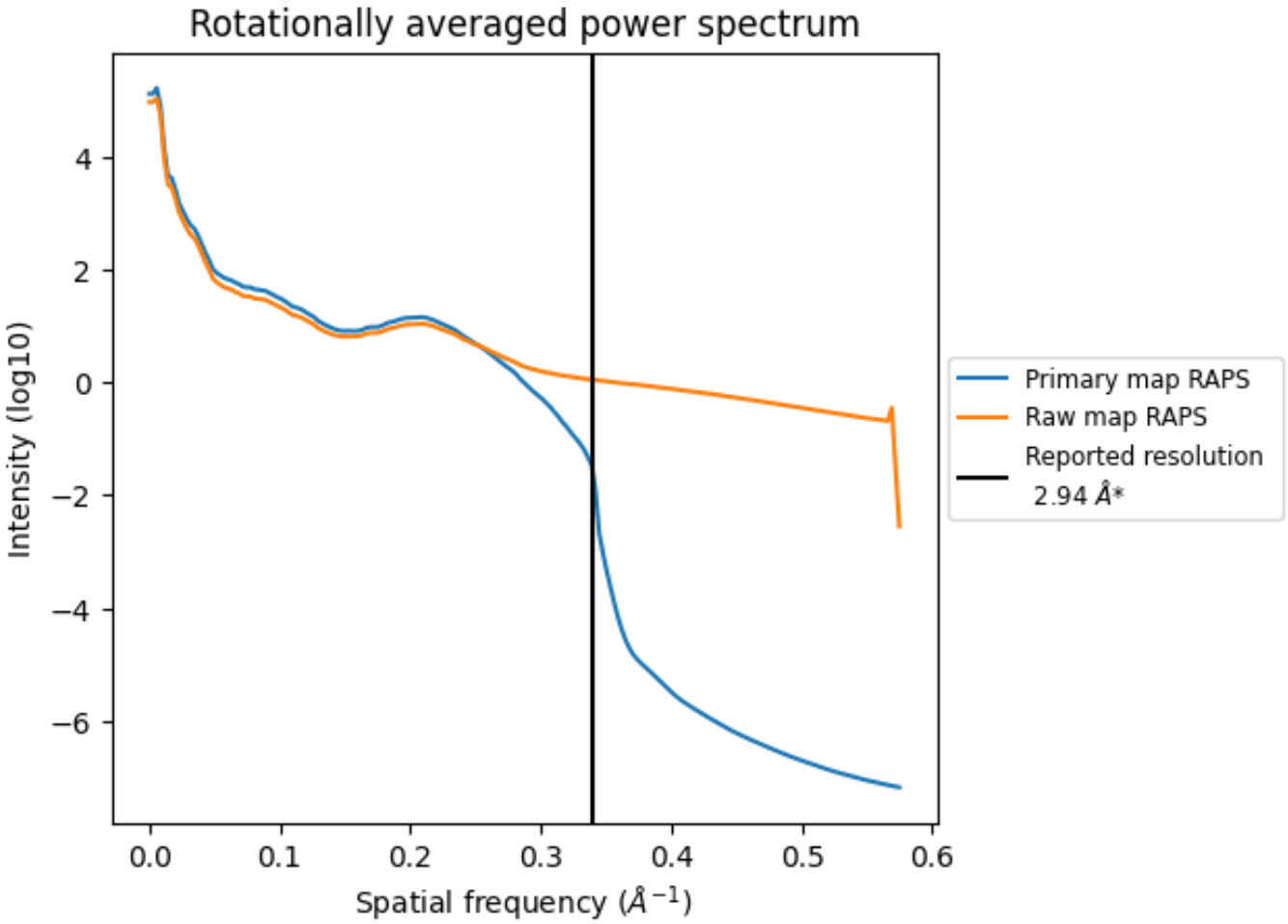
7.2 Volume estimate



The volume at the recommended contour level is 406 nm^3; this corresponds to an approximate mass of 366 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)

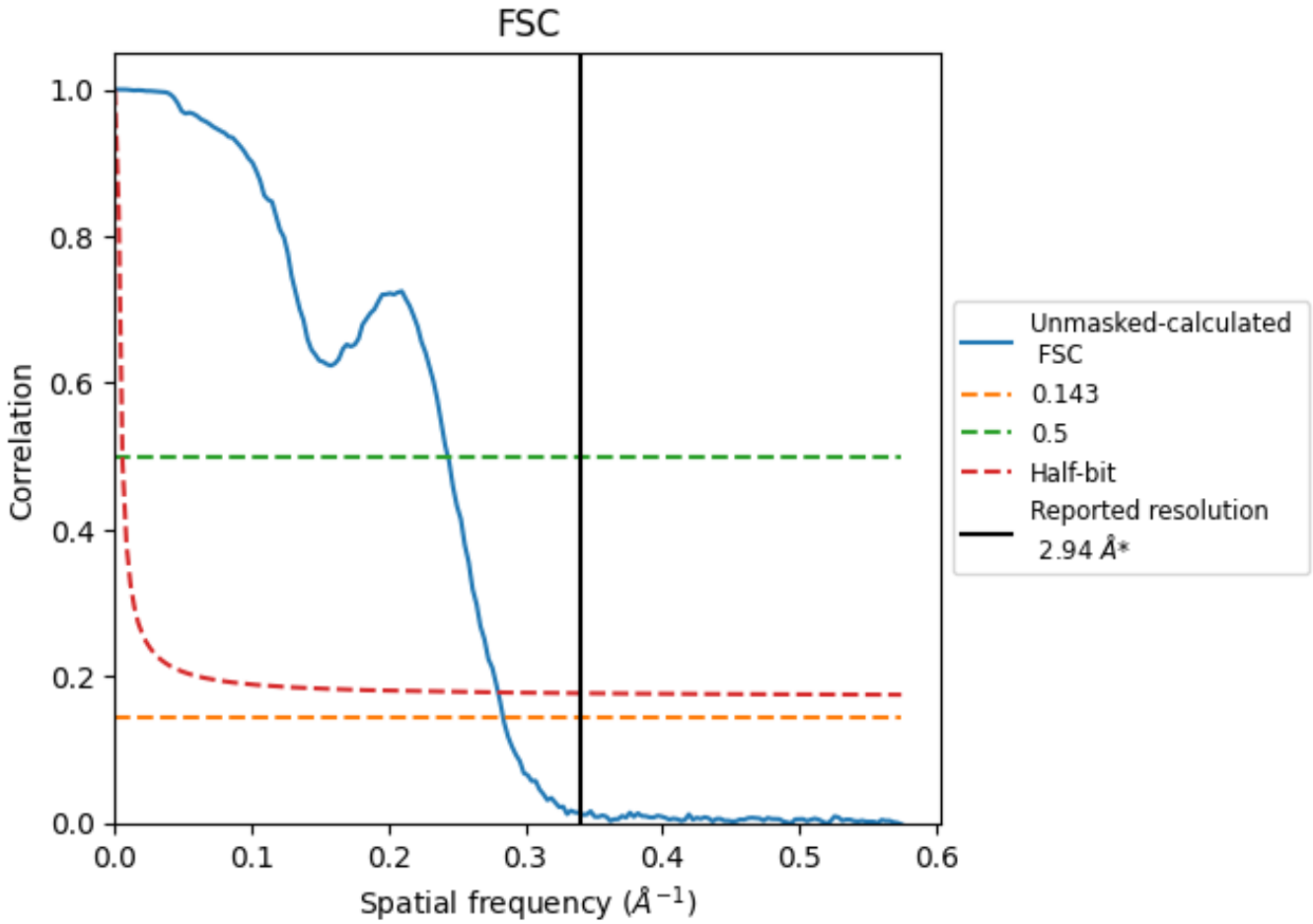


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

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 0.340 Å^{-1}

8.2 Resolution estimates (i)

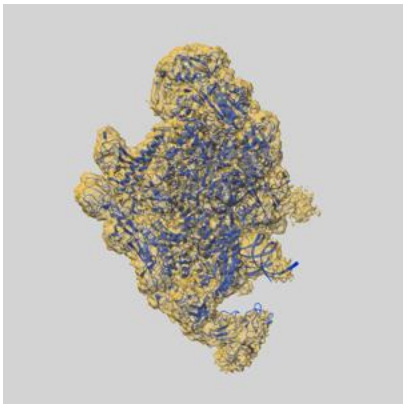
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.52	4.11	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.52 differs from the reported value 2.94 by more than 10 %

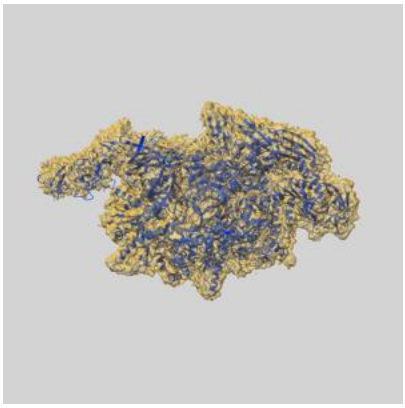
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40874 and PDB model 8SYI. Per-residue inclusion information can be found in section 3 on page 6.

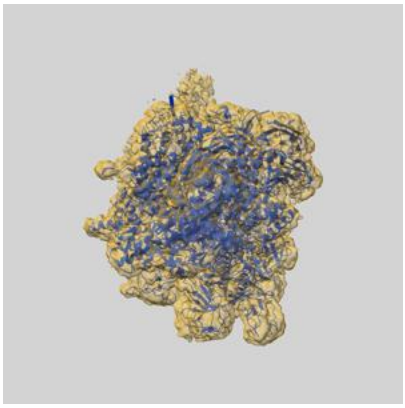
9.1 Map-model overlay



X



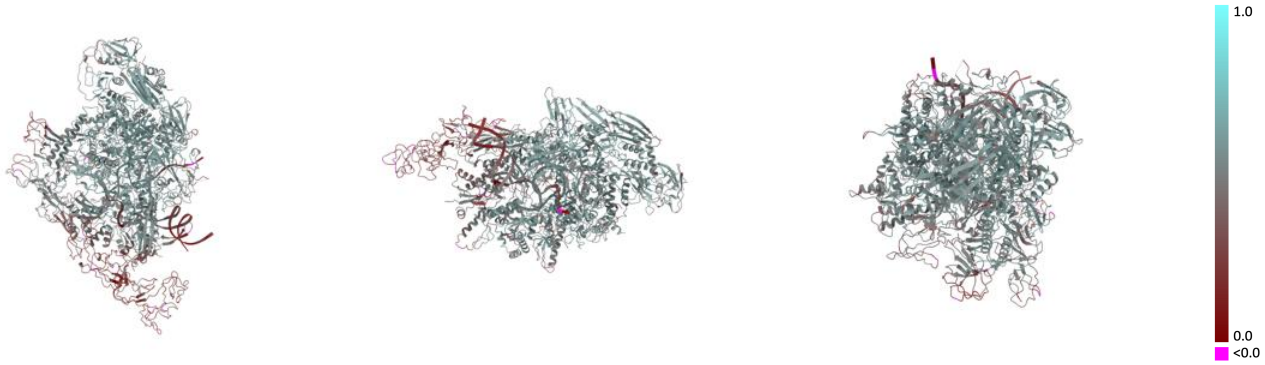
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.183 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

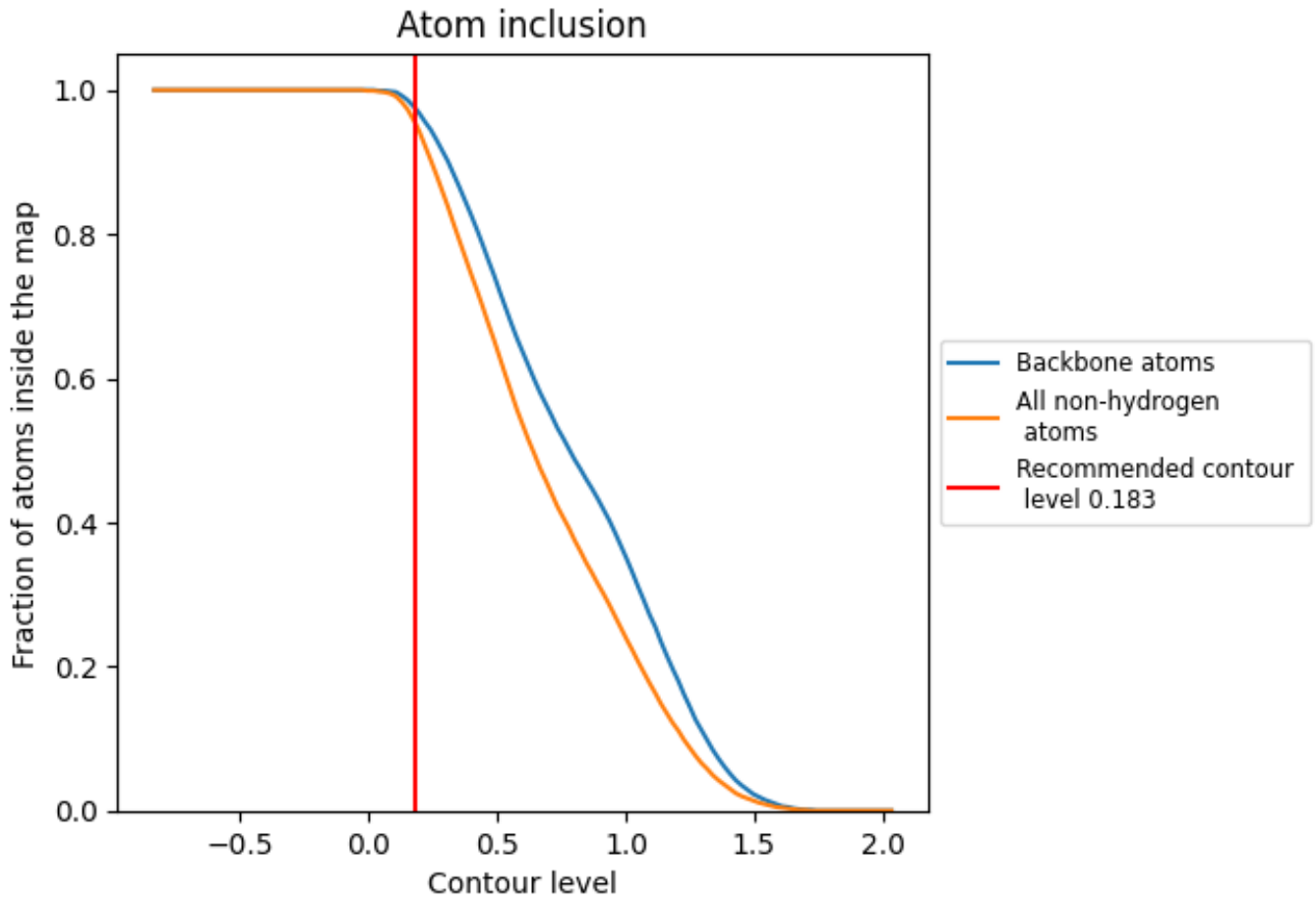
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.183).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.4910
A	0.9820	0.5470
B	0.9860	0.5210
C	0.9790	0.5470
D	0.9780	0.5330
E	0.9760	0.5150
G	0.9340	0.4160
N	0.9260	0.3720
R	0.8860	0.4110
T	0.9400	0.4340
Z	0.9110	0.4270