Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 01:16 pm GMT

PDB ID	:	7QXS
EMDB ID	:	EMD-14197
Title	:	Cryo-EM structure of human telomerase-DNA-TPP1-POT1 complex (with POT1 side chains)
Authors	:	Sekne, Z.; Ghanim, G.E.; van Roon, A.M.M.; Nguyen, T.H.D.
Deposited on	:	2022-01-27
Resolution	:	3.90 Å(reported)
Based on initial models	:	7BG9, 1XJV

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:

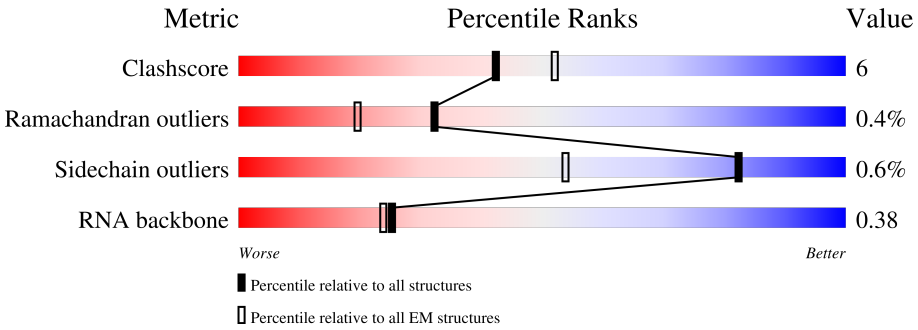
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1132	69% 15% 16%
2	B	451	29% 21% 5% 43%
3	L	130	15% 58% 5% 37%
4	M	166	16% 52% 46%
5	N	30	13% 63% 7% 27%
6	O	458	22% 74%
7	P	634	20% 37% 60%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17820 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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	951	7626	4892	1418	1280	36	0	0

- Molecule 2 is a RNA chain called RNA (256-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	256	5431	2420	947	1808	256	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	L	82	643	403	128	112	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	90	699	440	123	134	2	0	0

- Molecule 5 is a DNA chain called Telomeric DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	N	22	461	220	86	134	21	0	0

- Molecule 6 is a protein called Adrenocortical dysplasia homolog (Mouse), isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	O	120	955	603	171	177	4	0	0

- Molecule 7 is a protein called Protection of telomeres protein 1.

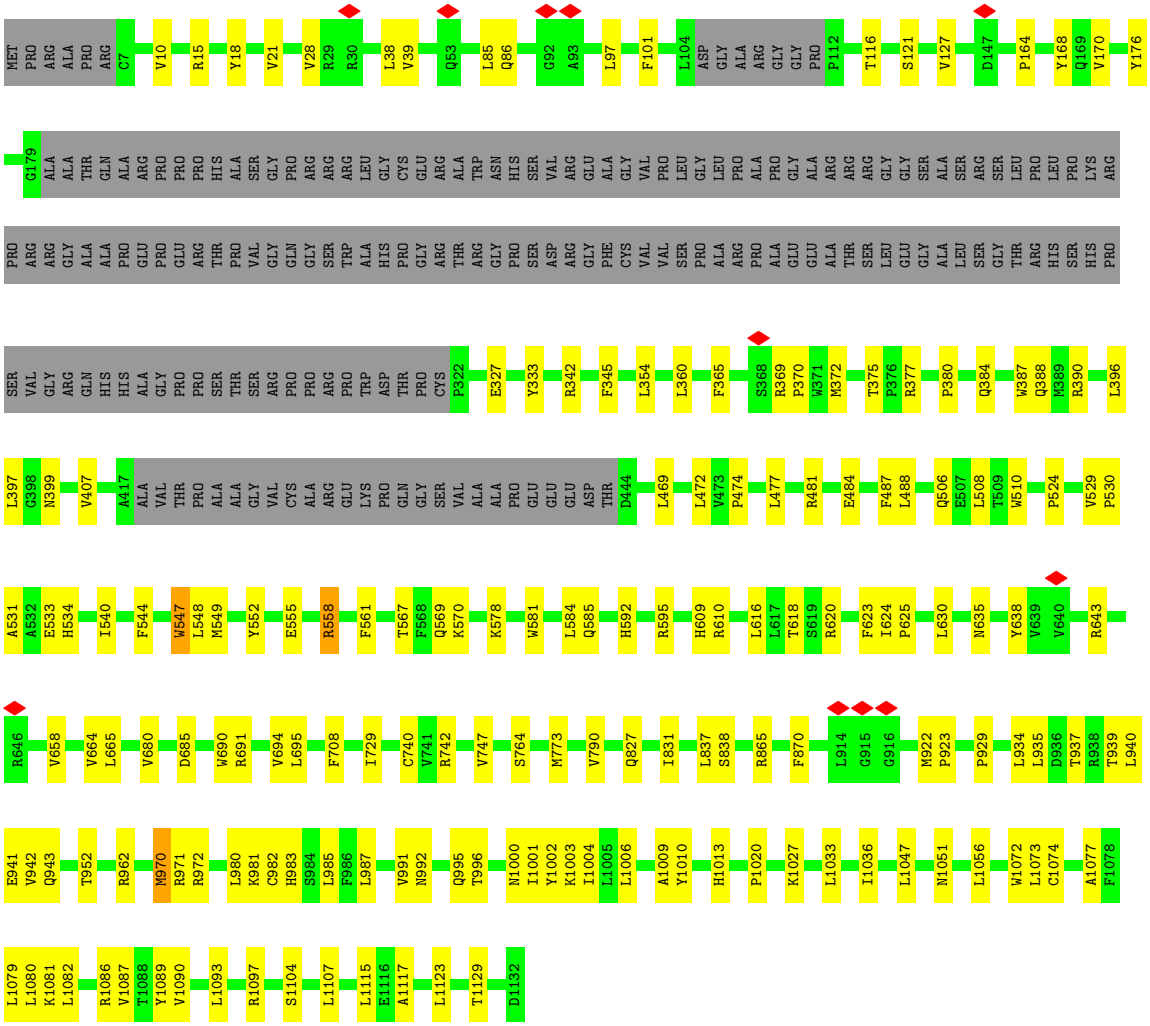
Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	251	Total	C	N	O	S	0	0
			2005	1299	337	364	5		

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.

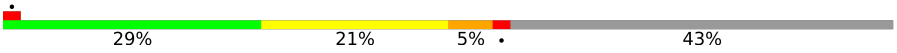
• Molecule 1: Telomerase reverse transcriptase

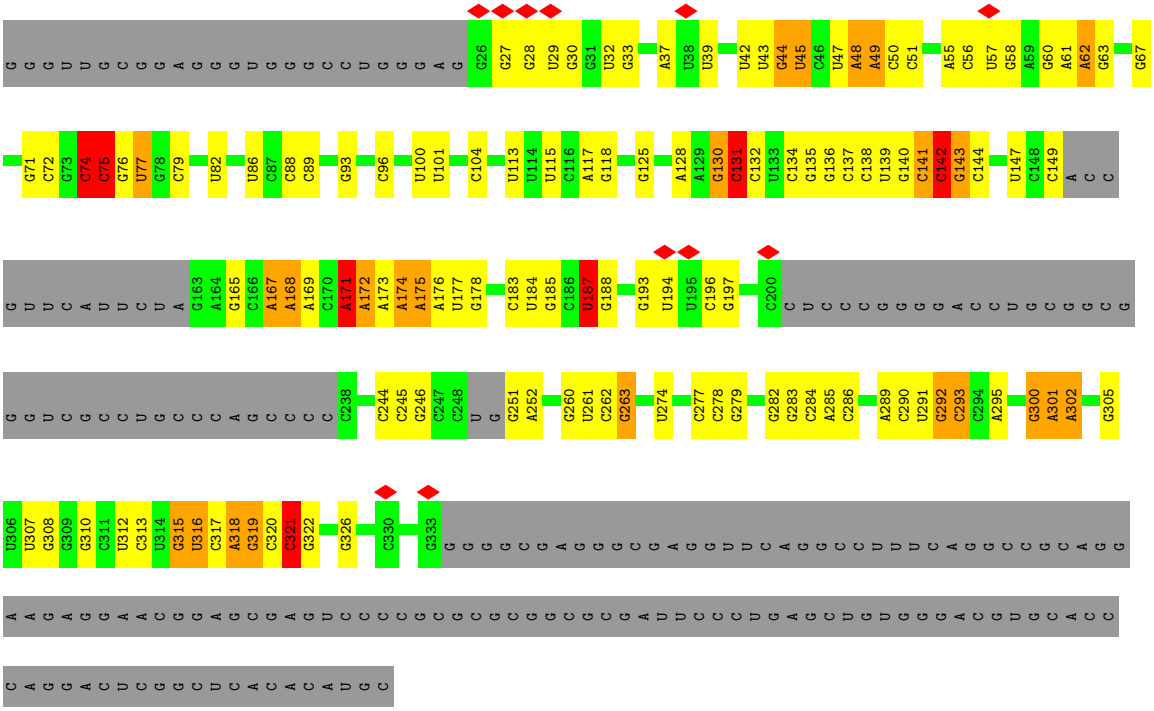
Chain A:



• Molecule 2: RNA (256-MER)

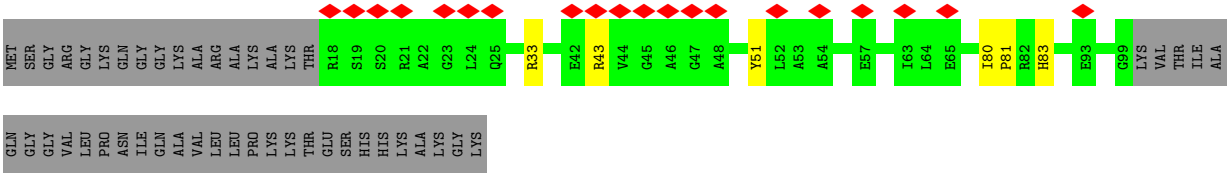
Chain B:





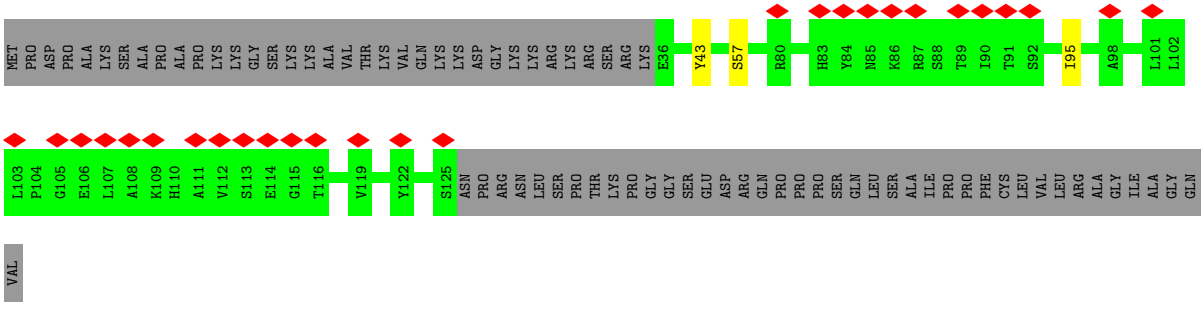
• Molecule 3: Histone H2A

Chain L:



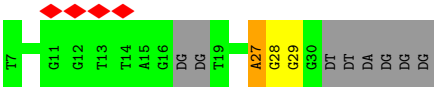
• Molecule 4: Histone H2B

Chain M:



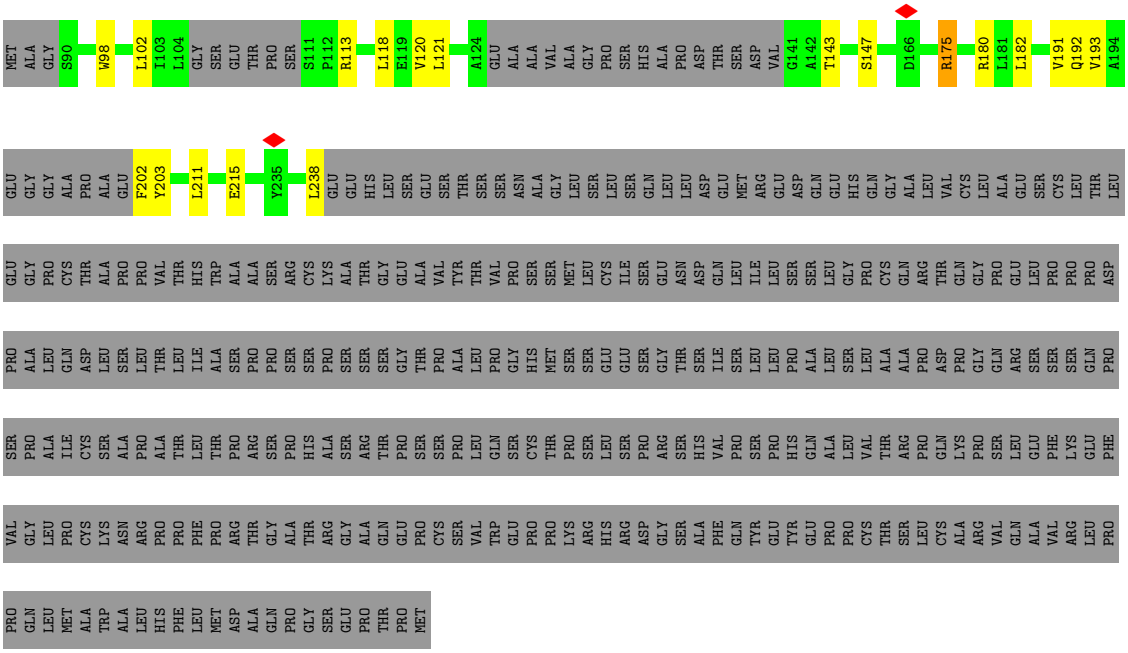
• Molecule 5: Telomeric DNA

Chain N:



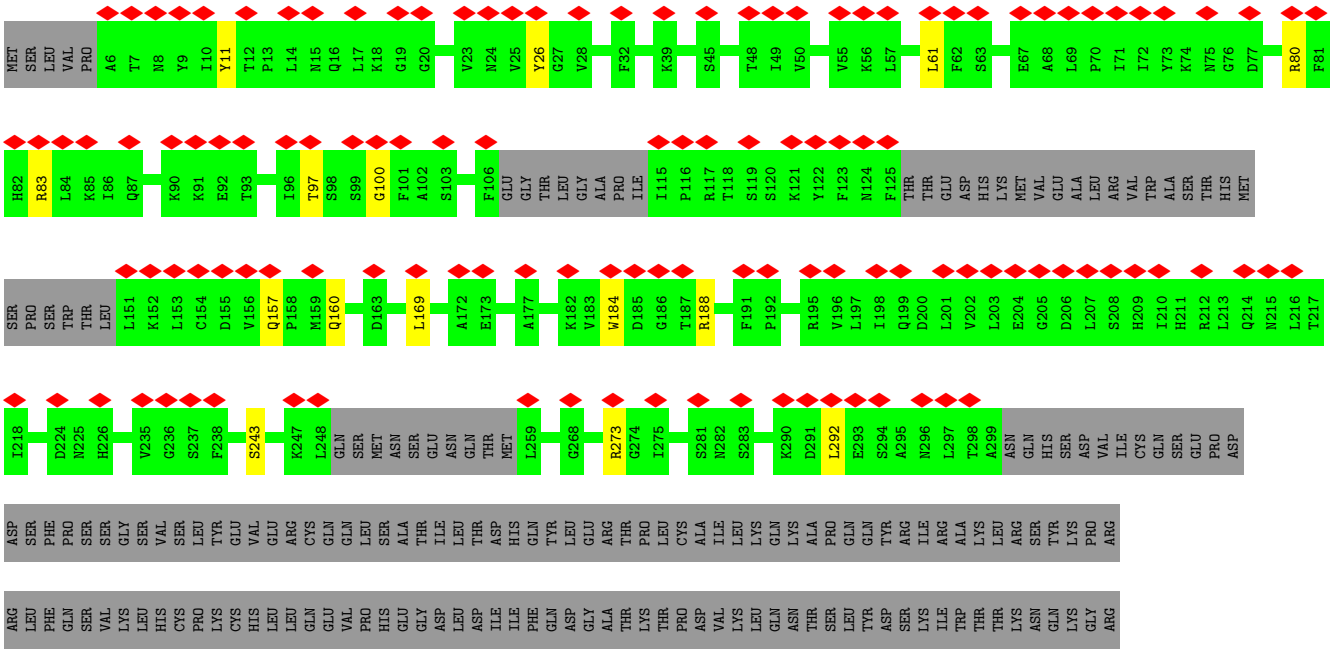
• Molecule 6: Adrenocortical dysplasia homolog (Mouse), isoform CRA_a

Chain O:



• Molecule 7: Protection of telomeres protein 1

Chain P:



LYS VAL ALA VAL HIS PHE VAL LYS ASN ASN GLY ILE LEU PRO LEU SER ASN GLU CYS LEU LEU LEU ILE GLU GLY GLY THR LEU SER GLU ILE CYS LYS LEU SER ASN LYS PHE ASN SER VAL ILE PRO VAL ARG SER GLY HIS GLU ASP LEU GLU LEU LEU ASP LEU SER ALA PRO PHE

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

GLY VAL LEU GLU ALA TYR LEU MET ASP SER ASP LYS PHE PHE GLN ILE PRO ALA SER GLU VAL LEU MET ASP ASP LEU GLN LYS SER VAL ASP MET ILE MET ASP MET PHE CYS PRO PRO GLY ILE LYS ILE ASP ALA TYR PRO TRP LEU GLU CYS PHE ILE LYS SER TYR ASN VAL

THR ASN GLY THR ASP ASN GLN ILE CYS TYR GLN ILE PHE ASP THR THR VAL ALA GLU ASP VAL ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	192871	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45871	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	305.2, 305.2, 305.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.66	5/7810 (0.1%)	0.81	1/10584 (0.0%)
2	B	0.41	0/6055	0.91	14/9426 (0.1%)
3	L	0.52	0/650	0.71	0/874
4	M	0.50	0/710	0.60	0/957
5	N	0.41	0/517	0.89	0/798
6	O	0.34	0/968	0.63	1/1307 (0.1%)
7	P	0.36	0/2048	0.57	2/2774 (0.1%)
All	All	0.53	5/18758 (0.0%)	0.81	18/26720 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
5	N	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	638	TYR	CE1-CZ	10.15	1.51	1.38
1	A	638	TYR	CG-CD1	7.25	1.48	1.39
1	A	638	TYR	CG-CD2	7.20	1.48	1.39
1	A	638	TYR	CE2-CZ	7.02	1.47	1.38
1	A	547	TRP	CD2-CE2	5.52	1.48	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	142	C	C2'-C3'-O3'	8.95	129.19	109.50
7	P	188	ARG	NE-CZ-NH2	8.30	124.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	P	188	ARG	NE-CZ-NH1	-7.73	116.44	120.30
2	B	131	C	C5'-C4'-O4'	7.07	117.58	109.10
2	B	174	A	C2'-C3'-O3'	6.97	124.85	113.70
2	B	131	C	C1'-O4'-C4'	-6.13	105.00	109.90
6	O	175	ARG	NE-CZ-NH2	6.09	123.35	120.30
2	B	319	G	N9-C1'-C2'	-6.05	105.35	112.00
2	B	74	C	C1'-O4'-C4'	-5.94	105.15	109.90
2	B	187	U	C2'-C3'-O3'	5.87	123.09	113.70
2	B	292	G	C2'-C3'-O3'	5.65	122.75	113.70
2	B	321	C	C4'-C3'-O3'	5.65	124.31	113.00
2	B	315	G	C2'-C3'-O3'	5.57	122.61	113.70
2	B	75	C	N1-C1'-C2'	5.54	121.21	114.00
2	B	171	A	C2'-C3'-O3'	5.54	122.56	113.70
2	B	131	C	O4'-C1'-N1	5.22	112.38	108.20
2	B	300	G	C4'-C3'-O3'	5.06	123.12	113.00
1	A	742	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	75	C	Sidechain
5	N	27	DA	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	7626	0	7871	131	0
2	B	5431	0	2767	65	0
3	L	643	0	680	8	0
4	M	699	0	712	5	0
5	N	461	0	253	2	0
6	O	955	0	962	13	0
7	P	2005	0	2033	21	0
All	All	17820	0	15278	213	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 6.

All (213) 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)
7:P:184:TRP:CZ3	7:P:292:LEU:HD22	1.85	1.10
1:A:1072:TRP:HE1	1:A:1104:SER:HG	1.07	0.97
6:O:192:GLN:HB2	6:O:203:TYR:CD2	2.06	0.89
7:P:184:TRP:CE3	7:P:292:LEU:HD22	2.08	0.88
2:B:302:A:N7	4:M:57:SER:HB2	1.94	0.82
7:P:26:TYR:HE1	7:P:80:ARG:HG3	1.45	0.80
1:A:375:THR:OG1	2:B:284:C:H3'	1.82	0.80
7:P:26:TYR:CE1	7:P:80:ARG:HG3	2.18	0.77
1:A:831:ILE:HD13	1:A:838:SER:HB3	1.67	0.74
1:A:506:GLN:OE1	2:B:305:G:H4'	1.88	0.72
7:P:61:LEU:HA	7:P:97:THR:HG23	1.72	0.72
1:A:375:THR:HG1	2:B:284:C:H3'	1.54	0.69
2:B:115:U:C2	2:B:175:A:C2	2.80	0.69
1:A:581:TRP:CE3	1:A:584:LEU:HD23	2.27	0.69
1:A:1086:ARG:O	1:A:1090:VAL:HG23	1.92	0.68
2:B:244:C:H5"	3:L:43:ARG:NH2	2.09	0.68
2:B:244:C:H5"	3:L:43:ARG:CZ	2.24	0.68
7:P:83:ARG:HH11	7:P:100:GLY:HA3	1.60	0.67
1:A:665:LEU:HD21	1:A:729:ILE:HD12	1.77	0.65
1:A:981:LYS:HE3	1:A:1004:ILE:HG12	1.78	0.64
7:P:184:TRP:CH2	7:P:292:LEU:HB3	2.32	0.64
1:A:569:GLN:HE22	1:A:952:THR:HA	1.64	0.63
7:P:184:TRP:CZ3	7:P:292:LEU:CD2	2.73	0.63
1:A:472:LEU:HD21	1:A:552:TYR:OH	1.98	0.63
1:A:943:GLN:OE1	1:A:1003:LYS:NZ	2.32	0.62
1:A:658:VAL:HG13	1:A:837:LEU:HD11	1.80	0.62
1:A:474:PRO:HD2	1:A:477:LEU:HD12	1.82	0.61
1:A:1082:LEU:O	1:A:1093:LEU:HD21	2.00	0.61
1:A:127:VAL:HG22	1:A:170:VAL:HG23	1.83	0.61
1:A:620:ARG:CZ	2:B:47:U:C5	2.83	0.61
1:A:481:ARG:NH2	2:B:183:C:OP2	2.34	0.61
1:A:922:MET:HG2	1:A:923:PRO:HD2	1.81	0.61
7:P:169:LEU:CD1	7:P:184:TRP:CD1	2.84	0.60
1:A:581:TRP:HE1	1:A:585:GLN:HE21	1.50	0.60
1:A:1006:LEU:HA	1:A:1077:ALA:HB1	1.83	0.60
1:A:1080:LEU:HD21	1:A:1123:LEU:HG	1.84	0.60
1:A:1010:TYR:CE1	1:A:1081:LYS:HD3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:157:GLN:H	7:P:160:GLN:HE21	1.50	0.60
1:A:980:LEU:HD21	5:N:27:DA:N3	2.16	0.60
1:A:544:PHE:O	1:A:547:TRP:HB3	2.03	0.59
1:A:399:ASN:HB3	1:A:472:LEU:HA	1.86	0.58
7:P:169:LEU:HD11	7:P:184:TRP:CD1	2.37	0.58
3:L:80:ILE:HG22	3:L:83:HIS:CE1	2.38	0.58
1:A:1013:HIS:CD2	1:A:1089:TYR:OH	2.57	0.58
1:A:690:TRP:HE1	1:A:991:VAL:HG13	1.69	0.58
1:A:530:PRO:HB3	2:B:318:A:H61	1.70	0.57
1:A:865:ARG:HD3	1:A:870:PHE:CE1	2.39	0.57
2:B:140:G:H2'	2:B:141:C:C5'	2.34	0.57
1:A:15:ARG:HA	1:A:21:VAL:HG21	1.85	0.57
7:P:169:LEU:HD21	7:P:184:TRP:HE1	1.70	0.57
1:A:943:GLN:HA	1:A:1000:ASN:ND2	2.21	0.56
1:A:529:VAL:HG13	1:A:533:GLU:HB3	1.86	0.56
7:P:11:TYR:CZ	7:P:26:TYR:OH	2.51	0.56
1:A:1033:LEU:HA	1:A:1036:ILE:HD12	1.88	0.55
1:A:1010:TYR:CZ	1:A:1081:LYS:HD3	2.42	0.55
6:O:102:LEU:HD22	6:O:113:ARG:NH1	2.22	0.54
7:P:11:TYR:CE2	7:P:26:TYR:OH	2.53	0.54
1:A:694:VAL:HG12	1:A:940:LEU:HD23	1.88	0.54
2:B:71:G:H2'	2:B:72:C:C6	2.43	0.54
1:A:101:PHE:CD2	1:A:121:SER:HB2	2.44	0.53
3:L:80:ILE:HG12	3:L:81:PRO:HD2	1.91	0.53
6:O:120:VAL:HG13	6:O:120:VAL:O	2.09	0.53
1:A:635:ASN:ND2	2:B:48:A:N3	2.54	0.52
6:O:180:ARG:HG2	6:O:215:GLU:HG2	1.91	0.52
1:A:680:VAL:HG12	1:A:685:ASP:CG	2.30	0.52
1:A:992:ASN:HB2	1:A:996:THR:HB	1.90	0.52
1:A:510:TRP:O	2:B:313:C:O2'	2.26	0.52
1:A:708:PHE:CZ	1:A:937:THR:HA	2.45	0.52
7:P:169:LEU:HG	7:P:184:TRP:CD1	2.45	0.52
1:A:691:ARG:O	1:A:695:LEU:HG	2.09	0.52
6:O:193:VAL:HG21	6:O:238:LEU:HD21	1.92	0.52
1:A:971:ARG:O	1:A:972:ARG:C	2.48	0.51
1:A:168:TYR:CD1	1:A:773:MET:HG2	2.46	0.51
1:A:1051:ASN:HD22	1:A:1056:LEU:HD11	1.76	0.51
2:B:321:C:N4	3:L:33:ARG:NH2	2.59	0.51
1:A:922:MET:HG2	1:A:923:PRO:CD	2.40	0.51
2:B:184:U:C5	2:B:185:G:C8	2.99	0.51
1:A:922:MET:CG	1:A:923:PRO:CD	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:LYS:NZ	2:B:312:U:OP1	2.25	0.51
2:B:171:A:C2	2:B:172:A:C4	2.99	0.50
2:B:100:U:C4	2:B:101:U:C5	2.99	0.50
1:A:387:TRP:HH2	2:B:290:C:C6	2.29	0.50
7:P:184:TRP:HH2	7:P:292:LEU:HB3	1.75	0.50
1:A:592:HIS:HA	1:A:595:ARG:HE	1.77	0.50
1:A:342:ARG:HD3	1:A:558:ARG:HD3	1.94	0.50
1:A:620:ARG:CZ	2:B:48:A:C5	2.95	0.50
1:A:665:LEU:HD21	1:A:729:ILE:CD1	2.43	0.49
1:A:623:PHE:O	1:A:624:ILE:CG2	2.60	0.49
2:B:77:U:H5"	2:B:77:U:C6	2.48	0.49
1:A:942:VAL:O	1:A:1000:ASN:ND2	2.34	0.49
2:B:263:G:C5	2:B:295:A:C2	3.01	0.49
1:A:943:GLN:HA	1:A:1000:ASN:CG	2.33	0.48
2:B:143:G:H2'	2:B:144:C:C6	2.47	0.48
6:O:120:VAL:HG21	6:O:175:ARG:HG2	1.95	0.48
2:B:96:C:H1'	2:B:168:A:C4	2.47	0.48
2:B:140:G:H2'	2:B:141:C:H5"	1.95	0.48
2:B:136:G:H2'	2:B:137:C:O4'	2.14	0.48
1:A:941:GLU:HB3	1:A:996:THR:HG21	1.95	0.48
2:B:130:G:H2'	2:B:131:C:H5'	1.95	0.48
1:A:624:ILE:HG13	1:A:624:ILE:O	2.14	0.48
1:A:399:ASN:HB3	1:A:472:LEU:CA	2.44	0.47
1:A:1080:LEU:CD2	1:A:1123:LEU:HG	2.44	0.47
7:P:11:TYR:CG	7:P:26:TYR:CE2	3.02	0.47
1:A:1006:LEU:HD12	1:A:1077:ALA:O	2.14	0.47
2:B:302:A:C8	4:M:57:SER:HB2	2.49	0.47
1:A:390:ARG:NH1	2:B:290:C:OP2	2.48	0.47
1:A:690:TRP:NE1	1:A:991:VAL:HG13	2.30	0.47
1:A:86:GLN:HB2	1:A:116:THR:HG23	1.97	0.47
1:A:534:HIS:NE2	2:B:315:G:H4'	2.30	0.47
2:B:251:G:H3'	2:B:252:A:C8	2.49	0.46
1:A:85:LEU:CD2	1:A:97:LEU:HD23	2.45	0.46
6:O:118:LEU:HD11	6:O:147:SER:HB2	1.98	0.46
2:B:117:A:C6	2:B:118:G:C5	3.03	0.46
1:A:922:MET:CG	1:A:923:PRO:HD2	2.45	0.46
1:A:995:GLN:HE22	1:A:1117:ALA:HB3	1.81	0.46
1:A:609:HIS:HA	1:A:616:LEU:HD22	1.97	0.46
1:A:1006:LEU:CA	1:A:1077:ALA:HB1	2.45	0.46
5:N:28:DG:C6	5:N:29:DG:C6	3.03	0.46
1:A:1001:ILE:HG23	1:A:1073:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ARG:HH12	2:B:283:G:H3'	1.81	0.46
2:B:115:U:O2	2:B:175:A:N3	2.49	0.46
1:A:831:ILE:HD13	1:A:838:SER:CB	2.42	0.45
2:B:172:A:C2	2:B:173:A:C5	3.05	0.45
1:A:747:VAL:CG1	1:A:790:VAL:HB	2.46	0.45
1:A:327:GLU:N	1:A:327:GLU:OE1	2.48	0.45
1:A:658:VAL:HG13	1:A:837:LEU:CD1	2.44	0.45
1:A:970:MET:O	1:A:971:ARG:C	2.54	0.45
1:A:1107:LEU:HD13	1:A:1115:LEU:HD12	1.99	0.45
7:P:243:SER:HB3	7:P:273:ARG:HG2	1.99	0.45
1:A:548:LEU:HD12	1:A:552:TYR:CB	2.47	0.45
1:A:623:PHE:O	1:A:624:ILE:HG23	2.16	0.45
2:B:316:U:C2	4:M:43:TYR:CE2	3.04	0.45
1:A:508:LEU:HD21	1:A:549:MET:CB	2.47	0.45
2:B:293:C:C6	2:B:293:C:H5"	2.52	0.45
1:A:1006:LEU:O	1:A:1009:ALA:HB3	2.16	0.45
3:L:80:ILE:CG1	3:L:81:PRO:HD2	2.47	0.45
1:A:15:ARG:CZ	2:B:62:A:C8	3.00	0.44
1:A:345:PHE:CZ	1:A:555:GLU:HG3	2.52	0.44
1:A:360:LEU:HD22	1:A:397:LEU:HD21	1.98	0.44
1:A:354:LEU:HD12	2:B:289:A:H5"	2.00	0.44
1:A:569:GLN:NE2	1:A:952:THR:HA	2.29	0.44
1:A:10:VAL:HG13	1:A:790:VAL:HG22	1.99	0.44
1:A:981:LYS:O	1:A:983:HIS:N	2.50	0.44
1:A:1086:ARG:O	1:A:1090:VAL:CG2	2.62	0.44
6:O:182:LEU:HD23	6:O:211:LEU:HB3	1.98	0.44
2:B:113:U:C2	2:B:178:G:C2	3.06	0.44
1:A:85:LEU:HD21	1:A:97:LEU:HD23	2.00	0.44
1:A:740:CYS:N	1:A:764:SER:O	2.48	0.44
1:A:929:PRO:HA	1:A:934:LEU:HD23	1.98	0.44
1:A:365:PHE:CE1	1:A:540:ILE:HG23	2.53	0.44
1:A:1002:TYR:HB2	1:A:1073:LEU:HD22	2.00	0.44
1:A:1082:LEU:C	1:A:1093:LEU:HD21	2.38	0.44
1:A:407:VAL:HG11	2:B:187:U:C2	2.53	0.43
6:O:102:LEU:HB2	6:O:113:ARG:HH12	1.83	0.43
2:B:316:U:C2	4:M:43:TYR:HE2	2.36	0.43
7:P:169:LEU:CD2	7:P:184:TRP:HE1	2.31	0.43
1:A:28:VAL:HG21	1:A:38:LEU:HD22	1.99	0.43
1:A:531:ALA:HA	2:B:301:A:C6	2.54	0.43
1:A:690:TRP:O	1:A:694:VAL:HG13	2.18	0.43
2:B:88:C:H2'	2:B:89:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:C:H4'	2:B:143:G:H5'	2.01	0.43
2:B:244:C:C2	2:B:326:G:N2	2.87	0.43
1:A:558:ARG:O	1:A:578:LYS:HD2	2.18	0.43
6:O:98:TRP:CE3	6:O:113:ARG:HD3	2.53	0.43
2:B:72:C:C4	2:B:74:C:C4	3.06	0.43
1:A:384:GLN:HG3	2:B:291:U:O2'	2.19	0.43
1:A:375:THR:HA	2:B:285:A:H5'	2.01	0.42
1:A:38:LEU:HG	1:A:39:VAL:HG23	2.00	0.42
1:A:561:PHE:N	1:A:578:LYS:HG3	2.34	0.42
2:B:44:G:H4'	2:B:45:U:H5'	2.01	0.42
2:B:244:C:OP2	3:L:43:ARG:NH2	2.43	0.42
6:O:102:LEU:HD22	6:O:113:ARG:HH12	1.82	0.42
1:A:1006:LEU:HD13	1:A:1077:ALA:HA	2.00	0.42
1:A:987:LEU:HD13	1:A:1047:LEU:HA	2.02	0.42
3:L:51:TYR:HB3	4:M:95:ILE:HD11	2.01	0.42
6:O:191:VAL:HG22	6:O:202:PHE:CD1	2.55	0.42
1:A:484:GLU:O	1:A:488:LEU:HG	2.20	0.42
1:A:680:VAL:HB	1:A:685:ASP:HB3	2.01	0.42
6:O:121:LEU:HD12	6:O:143:THR:HG22	2.01	0.42
1:A:369:ARG:HH21	1:A:370:PRO:HD2	1.85	0.42
1:A:623:PHE:CD2	1:A:630:LEU:HD13	2.55	0.42
2:B:50:C:H2'	2:B:51:C:C6	2.54	0.42
1:A:983:HIS:CD2	1:A:985:LEU:H	2.38	0.42
1:A:1079:LEU:HD11	1:A:1097:ARG:HG2	2.00	0.42
2:B:48:A:O2'	2:B:49:A:OP2	2.34	0.42
1:A:377:ARG:HH11	2:B:284:C:H5	1.67	0.42
1:A:664:VAL:HG23	1:A:665:LEU:HD12	2.02	0.42
2:B:136:G:H2'	2:B:137:C:C6	2.55	0.42
1:A:531:ALA:HA	2:B:301:A:N1	2.35	0.41
7:P:184:TRP:HZ3	7:P:292:LEU:HA	1.85	0.41
1:A:396:LEU:HD12	1:A:472:LEU:O	2.21	0.41
1:A:548:LEU:HD12	1:A:552:TYR:HB3	2.01	0.41
2:B:167:A:H2'	2:B:168:A:C5	2.56	0.41
1:A:127:VAL:CG2	1:A:170:VAL:HG23	2.49	0.41
7:P:169:LEU:CG	7:P:184:TRP:CD1	3.04	0.41
1:A:610:ARG:HH21	1:A:618:THR:HG21	1.85	0.41
2:B:76:G:H2'	2:B:77:U:C5'	2.50	0.41
1:A:747:VAL:HG12	1:A:790:VAL:HB	2.03	0.41
1:A:827:GLN:HE22	1:A:831:ILE:C	2.23	0.41
1:A:935:LEU:CD2	1:A:942:VAL:HG12	2.51	0.41
1:A:939:THR:HB	1:A:941:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:G:C2	2:B:137:C:C2	3.09	0.41
1:A:567:THR:HG23	1:A:625:PRO:O	2.20	0.41
1:A:740:CYS:SG	1:A:764:SER:O	2.79	0.40
2:B:137:C:H2'	2:B:138:C:C6	2.57	0.40
1:A:372:MET:HG2	1:A:380:PRO:HD3	2.03	0.40
2:B:32:U:H2'	2:B:33:G:C8	2.57	0.40
2:B:67:G:C2	2:B:143:G:C2	3.09	0.40
1:A:388:GLN:HE22	1:A:524:PRO:HD3	1.85	0.40
1:A:469:LEU:HD11	1:A:487:PHE:HE2	1.86	0.40
1:A:581:TRP:CZ3	1:A:584:LEU:CD2	3.04	0.40
2:B:76:G:H2'	2:B:77:U:C4'	2.52	0.40
2:B:115:U:O2	2:B:175:A:C2	2.75	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	943/1132 (83%)	876 (93%)	61 (6%)	6 (1%)	22 57
3	L	80/130 (62%)	79 (99%)	1 (1%)	0	100 100
4	M	88/166 (53%)	83 (94%)	5 (6%)	0	100 100
6	O	112/458 (24%)	110 (98%)	2 (2%)	0	100 100
7	P	243/634 (38%)	236 (97%)	7 (3%)	0	100 100
All	All	1466/2520 (58%)	1384 (94%)	76 (5%)	6 (0%)	32 65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	CYS
1	A	164	PRO

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Mol	Chain	Res	Type
1	A	1087	VAL
1	A	643	ARG
1	A	570	LYS
1	A	1020	PRO

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	824/958 (86%)	816 (99%)	8 (1%)	73 81
3	L	64/99 (65%)	64 (100%)	0	100 100
4	M	77/140 (55%)	77 (100%)	0	100 100
6	O	106/390 (27%)	106 (100%)	0	100 100
7	P	226/576 (39%)	226 (100%)	0	100 100
All	All	1297/2163 (60%)	1289 (99%)	8 (1%)	82 88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	176	TYR
1	A	333	TYR
1	A	558	ARG
1	A	962	ARG
1	A	970	MET
1	A	1074	CYS
1	A	1129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	86	GLN

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Mol	Chain	Res	Type
1	A	388	GLN
1	A	666	ASN
1	A	700	GLN
1	A	969	ASN
1	A	983	HIS
1	A	1013	HIS
4	M	64	ASN
7	P	8	ASN
7	P	24	ASN
7	P	160	GLN
7	P	264	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	252/451 (55%)	74 (29%)	21 (8%)

All (74) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	27	G
2	B	28	G
2	B	29	U
2	B	30	G
2	B	37	A
2	B	39	U
2	B	43	U
2	B	45	U
2	B	48	A
2	B	49	A
2	B	55	A
2	B	56	C
2	B	57	U
2	B	58	G
2	B	60	G
2	B	61	A
2	B	62	A
2	B	63	G
2	B	74	C
2	B	75	C
2	B	77	U

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Mol	Chain	Res	Type
2	B	79	C
2	B	82	U
2	B	86	U
2	B	93	G
2	B	104	C
2	B	125	G
2	B	128	A
2	B	131	C
2	B	132	C
2	B	134	C
2	B	135	G
2	B	139	U
2	B	141	C
2	B	142	C
2	B	143	G
2	B	147	U
2	B	149	C
2	B	165	G
2	B	167	A
2	B	168	A
2	B	169	A
2	B	172	A
2	B	175	A
2	B	177	U
2	B	187	U
2	B	188	G
2	B	193	G
2	B	194	U
2	B	196	C
2	B	197	G
2	B	246	G
2	B	260	G
2	B	261	U
2	B	262	C
2	B	263	G
2	B	274	U
2	B	277	C
2	B	278	C
2	B	279	G
2	B	282	G
2	B	286	C
2	B	292	G

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Mol	Chain	Res	Type
2	B	293	C
2	B	301	A
2	B	302	A
2	B	308	G
2	B	310	G
2	B	316	U
2	B	317	C
2	B	318	A
2	B	319	G
2	B	320	C
2	B	322	G

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	42	U
2	B	44	G
2	B	60	G
2	B	74	C
2	B	130	G
2	B	142	C
2	B	167	A
2	B	171	A
2	B	174	A
2	B	176	A
2	B	187	U
2	B	245	C
2	B	260	G
2	B	261	U
2	B	262	C
2	B	282	G
2	B	292	G
2	B	300	G
2	B	307	U
2	B	319	G
2	B	321	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

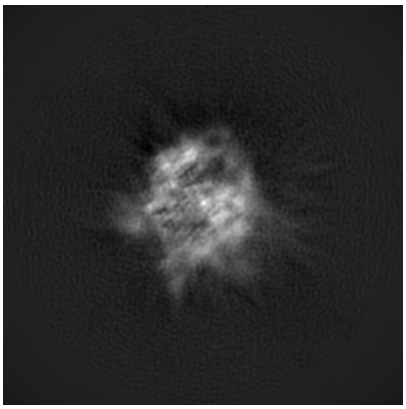
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14197. These allow visual inspection of the internal detail of the map and identification of artifacts.

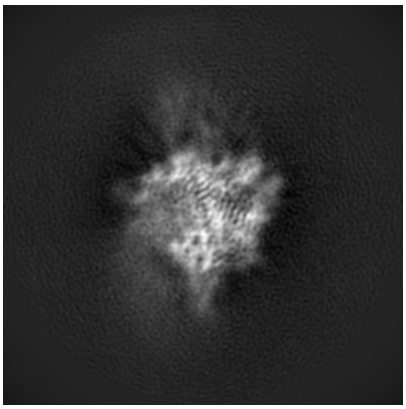
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

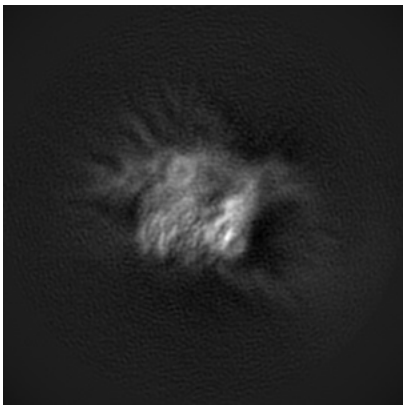
6.1.1 Primary map



X

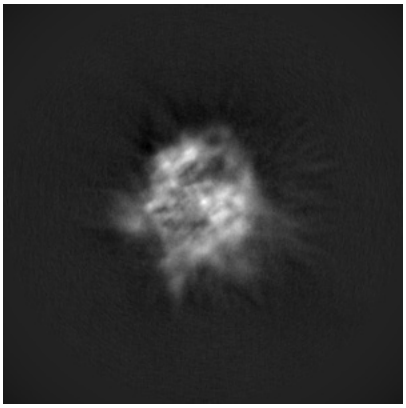


Y

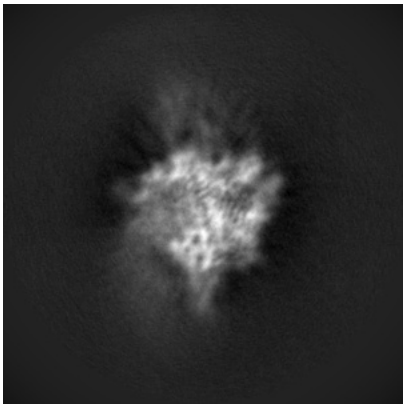


Z

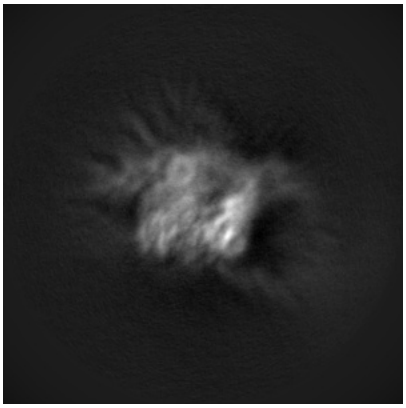
6.1.2 Raw map



X



Y

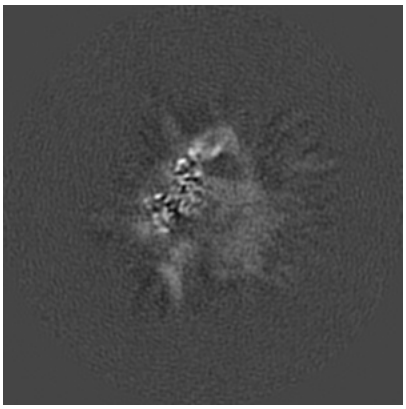


Z

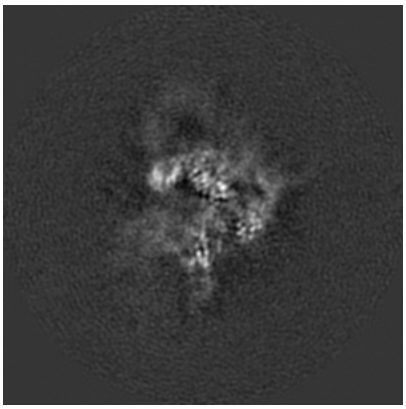
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

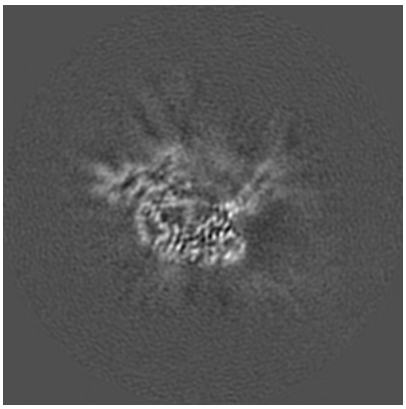
6.2.1 Primary map



X Index: 140

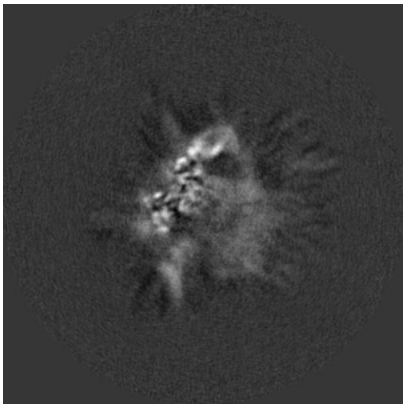


Y Index: 140

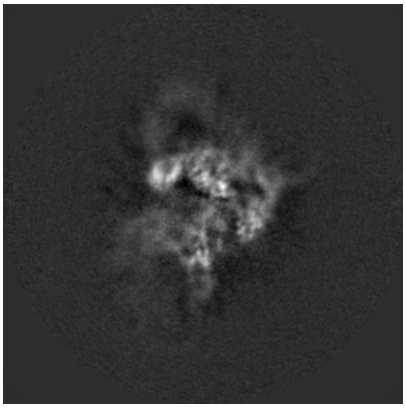


Z Index: 140

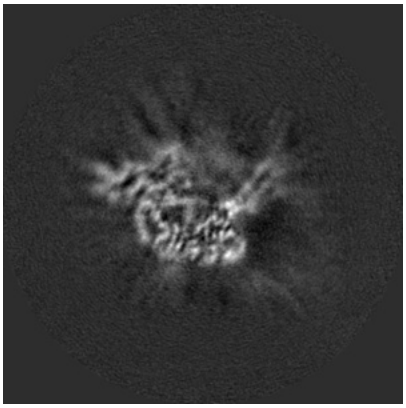
6.2.2 Raw map



X Index: 140



Y Index: 140

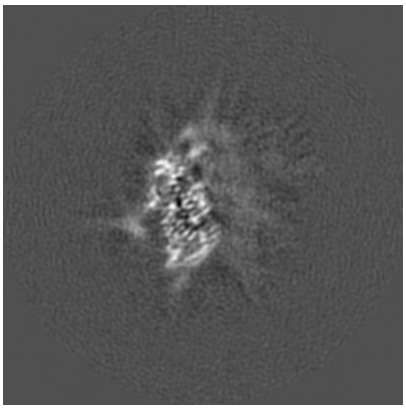


Z Index: 140

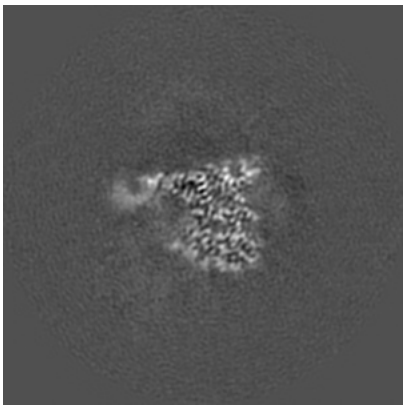
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

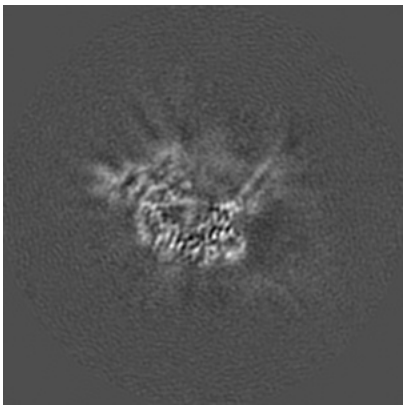
6.3.1 Primary map



X Index: 157

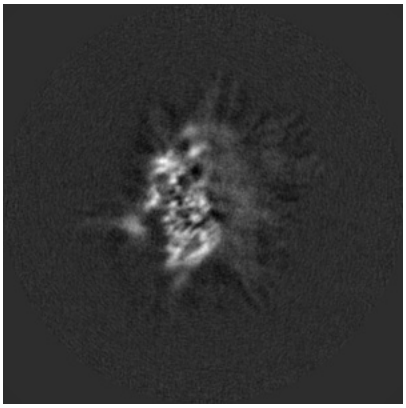


Y Index: 119

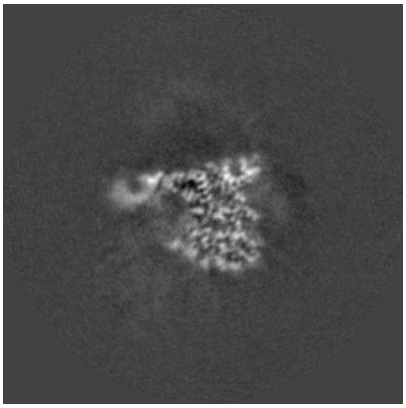


Z Index: 141

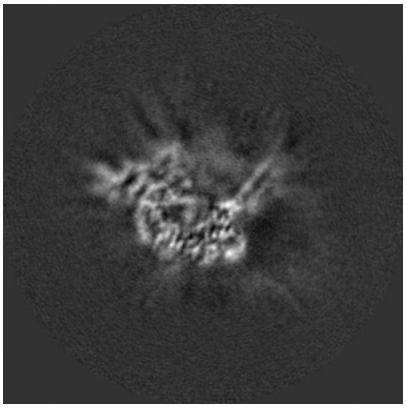
6.3.2 Raw map



X Index: 158



Y Index: 119

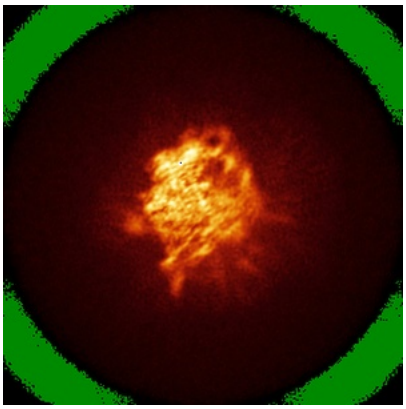


Z Index: 141

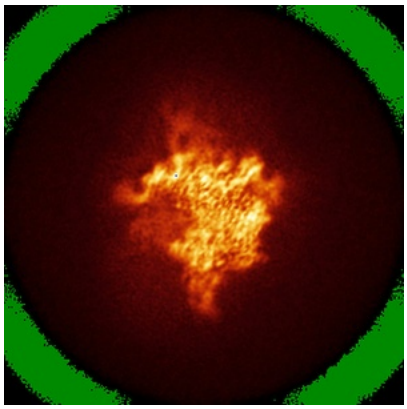
The images above show the largest variance slices of the map in three orthogonal directions.

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

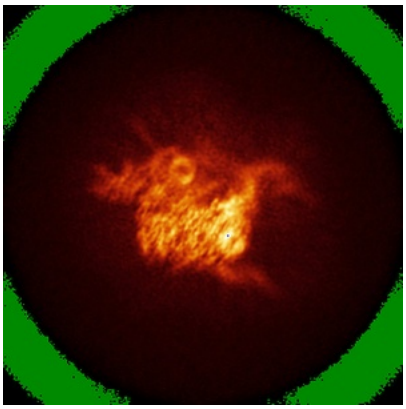
6.4.1 Primary map



X

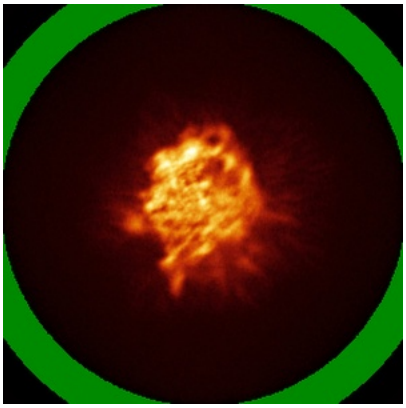


Y

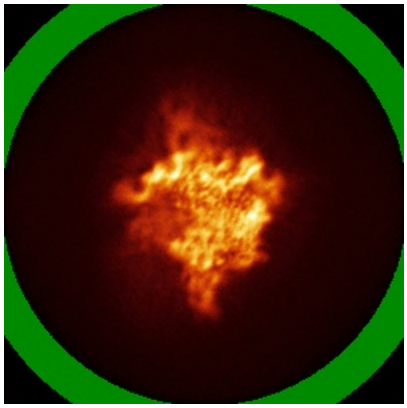


Z

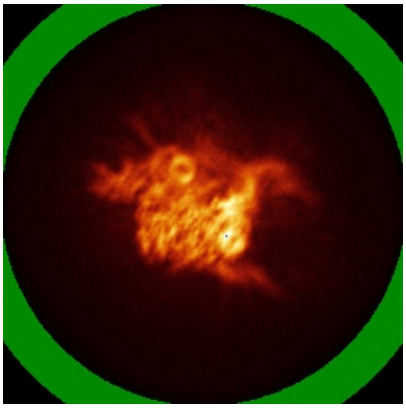
6.4.2 Raw map



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 0.009. 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.

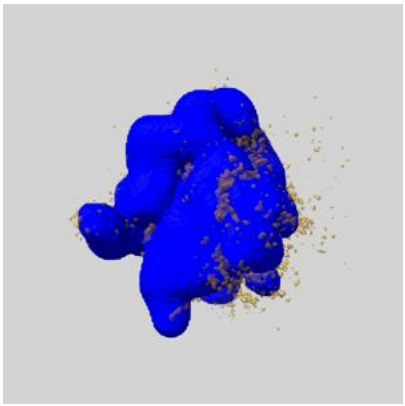
6.6 Mask visualisation (i)

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

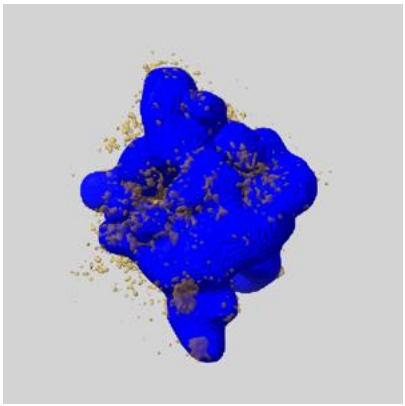
A mask typically either:

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

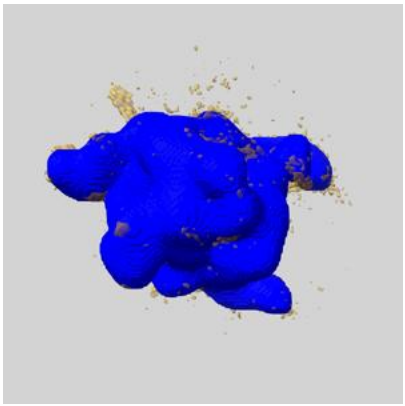
6.6.1 emd_14197_msk_1.map (i)



X



Y

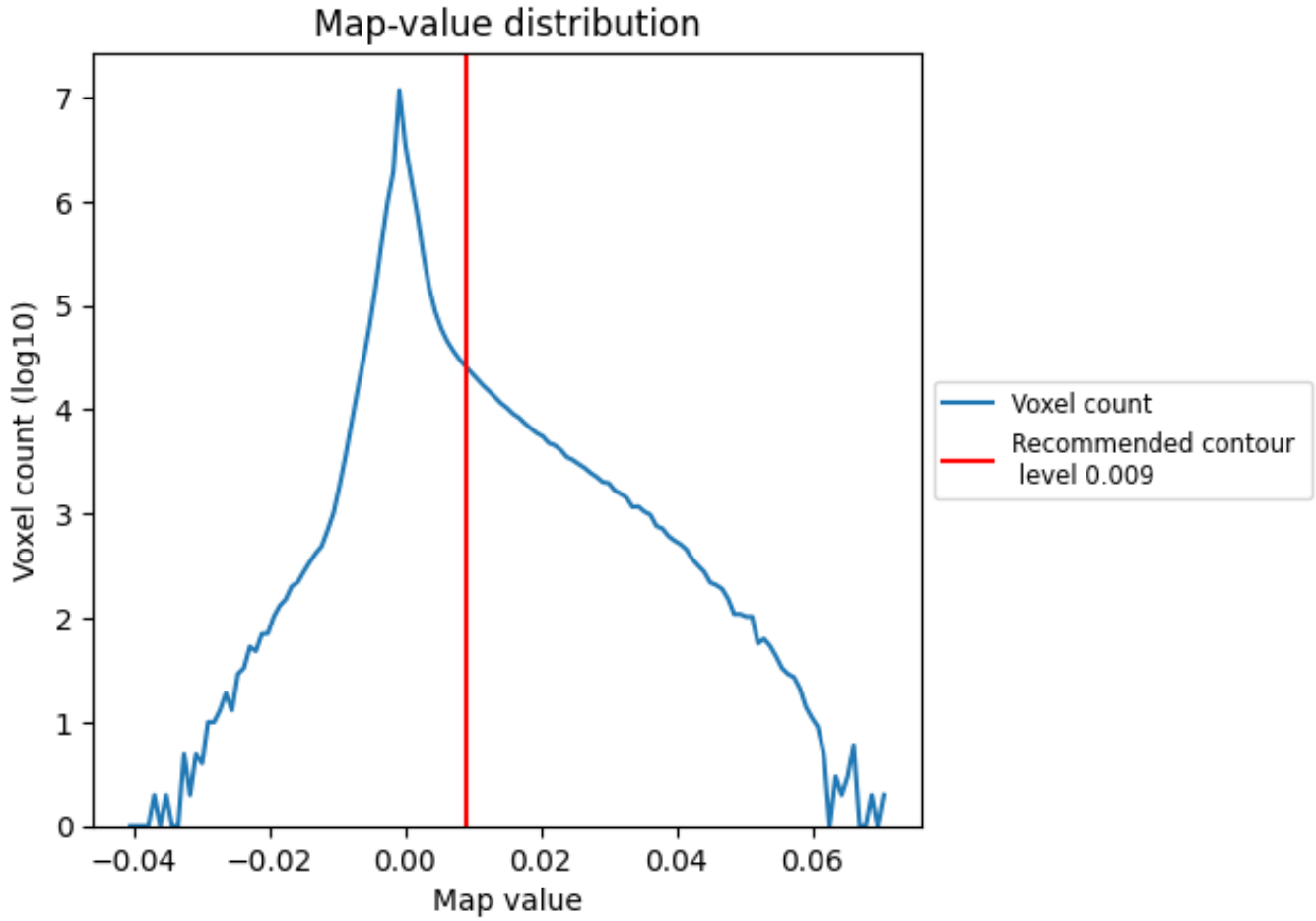


Z

7 Map analysis

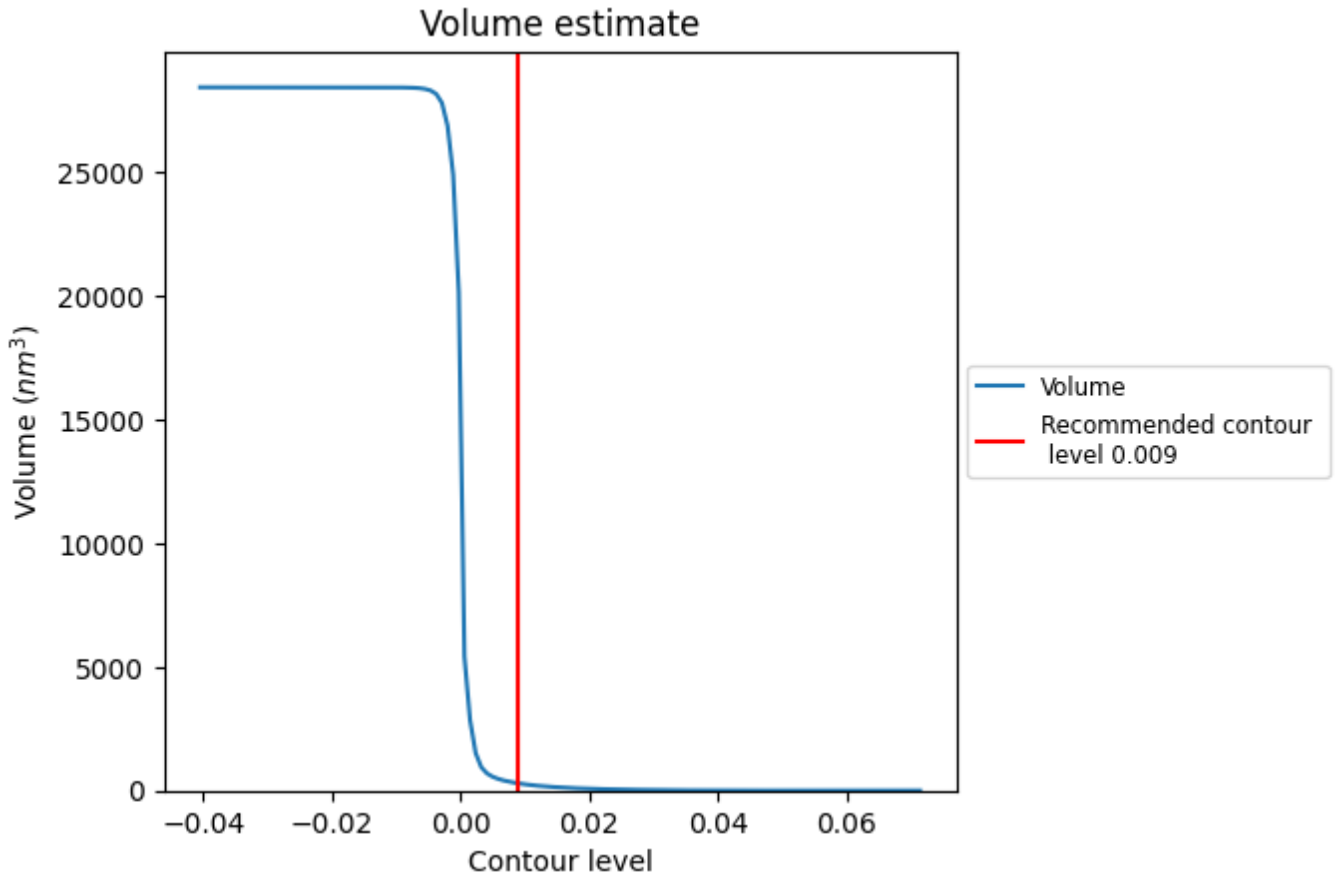
This section contains the results of statistical analysis of the map.

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.

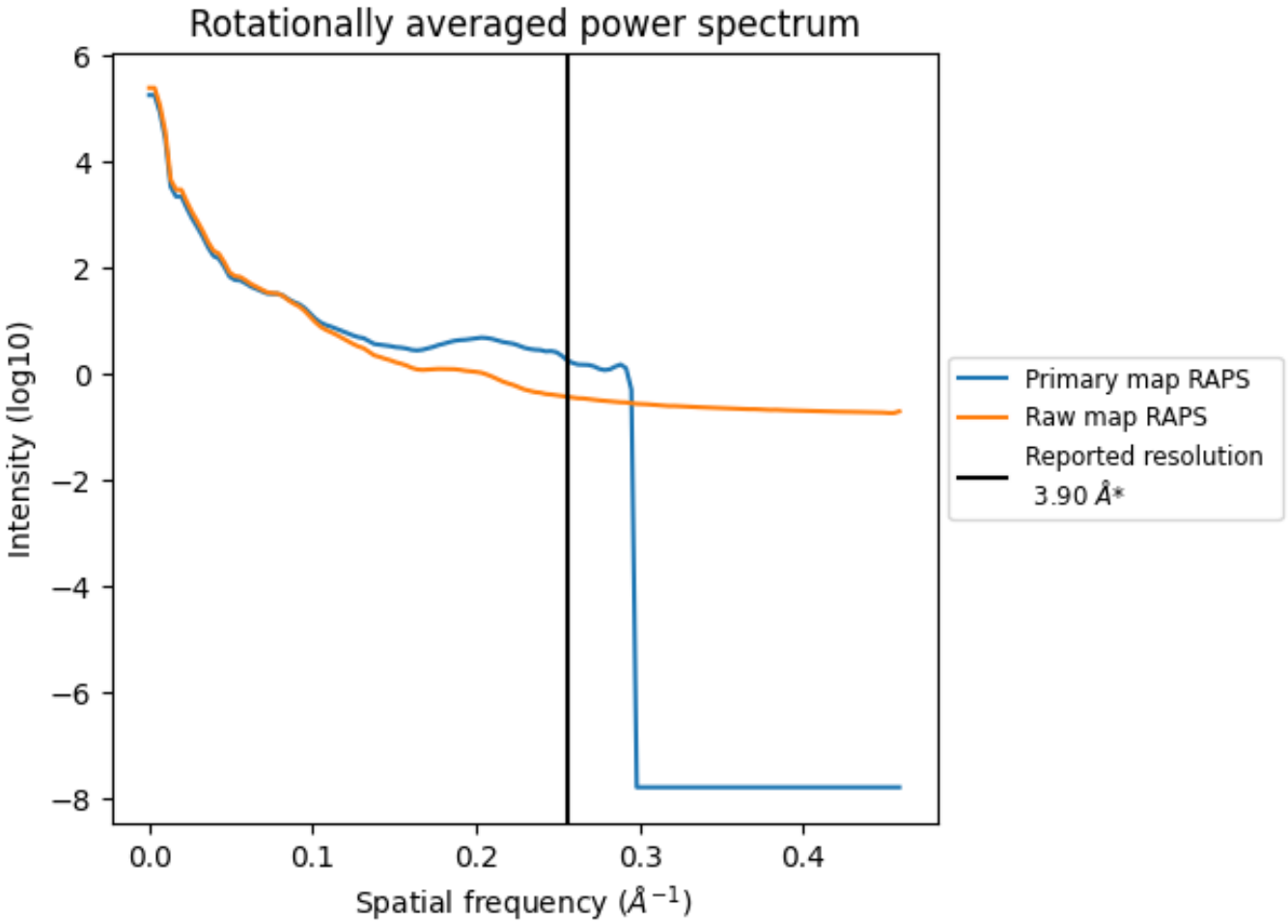
7.2 Volume estimate



The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 263 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)

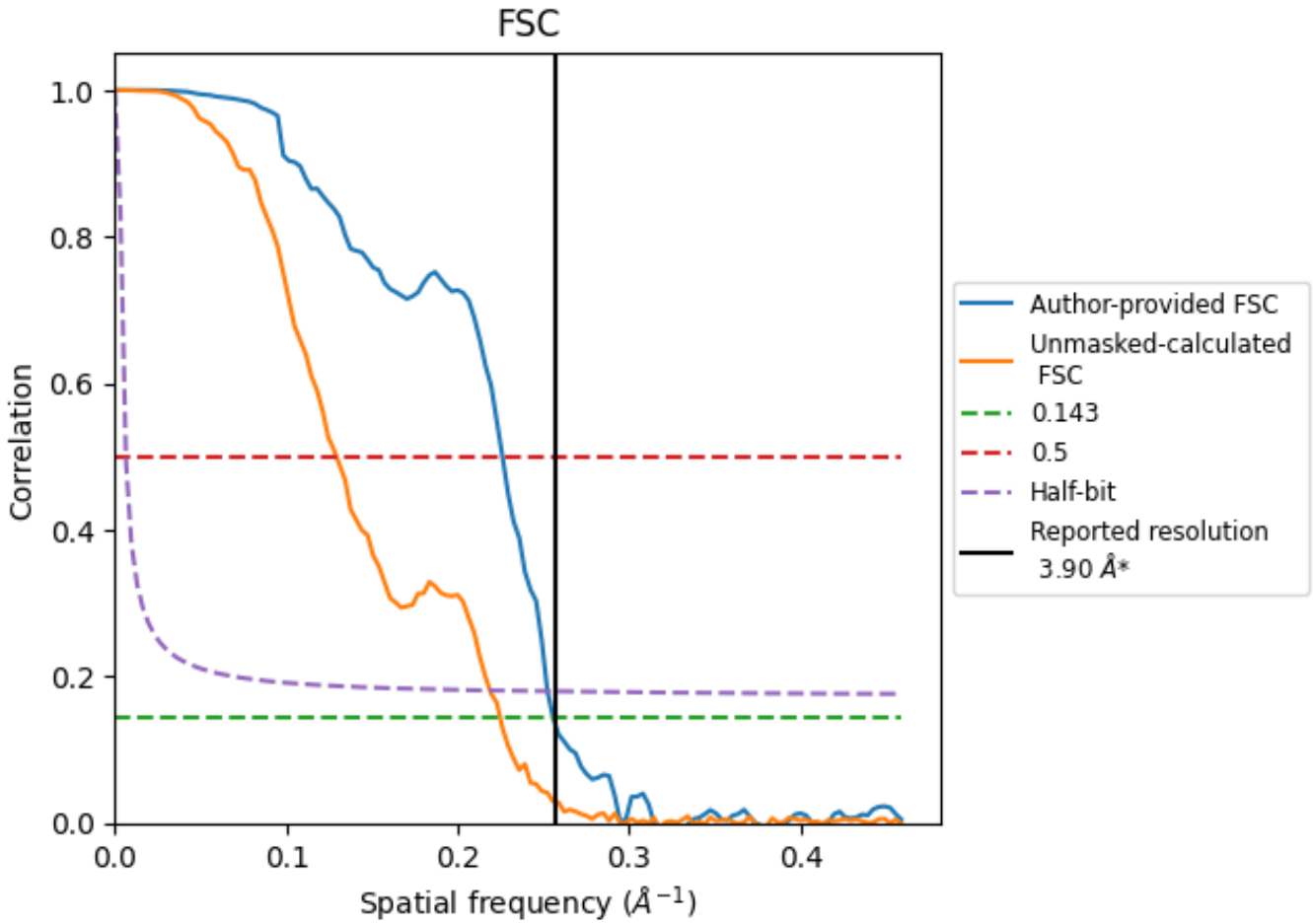


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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)

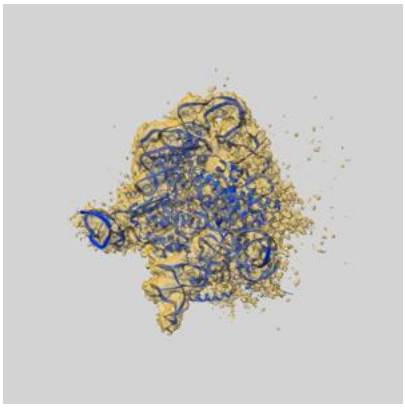
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.42	3.96
Unmasked-calculated*	4.45	7.74	4.57

*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 4.45 differs from the reported value 3.9 by more than 10 %

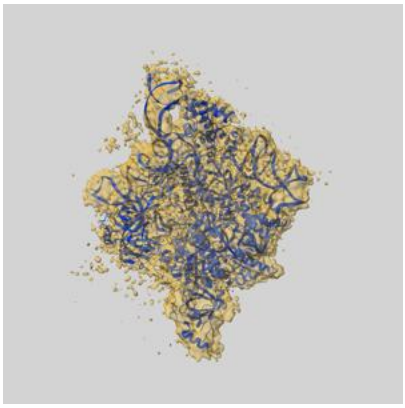
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14197 and PDB model 7QXS. Per-residue inclusion information can be found in section 3 on page 5.

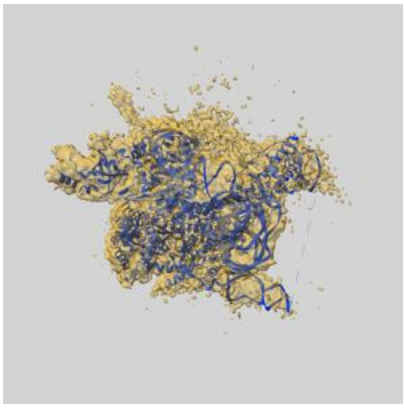
9.1 Map-model overlay



X



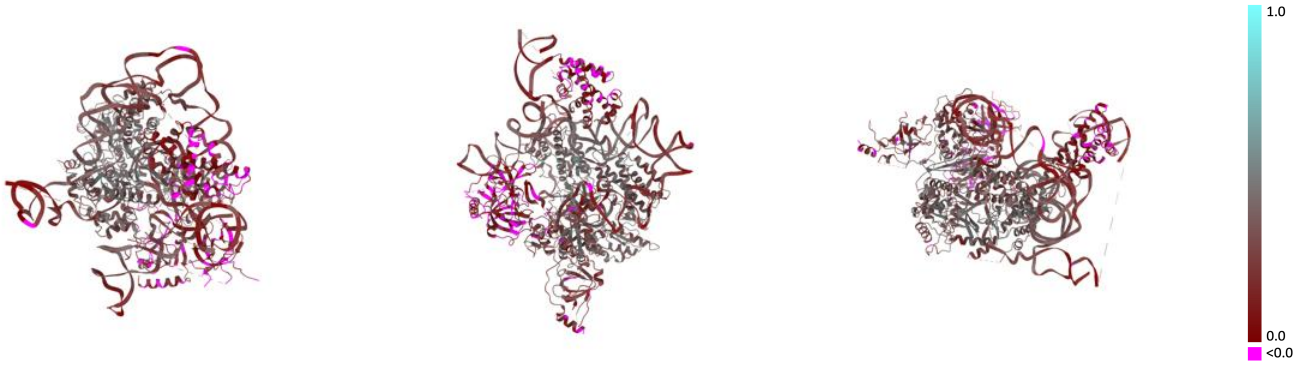
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

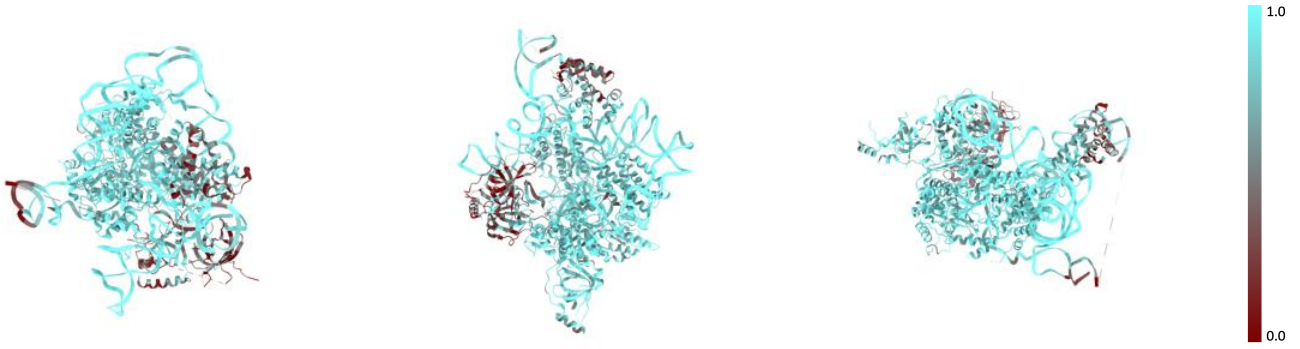
9.2 Q-score mapped to coordinate model (i)



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.

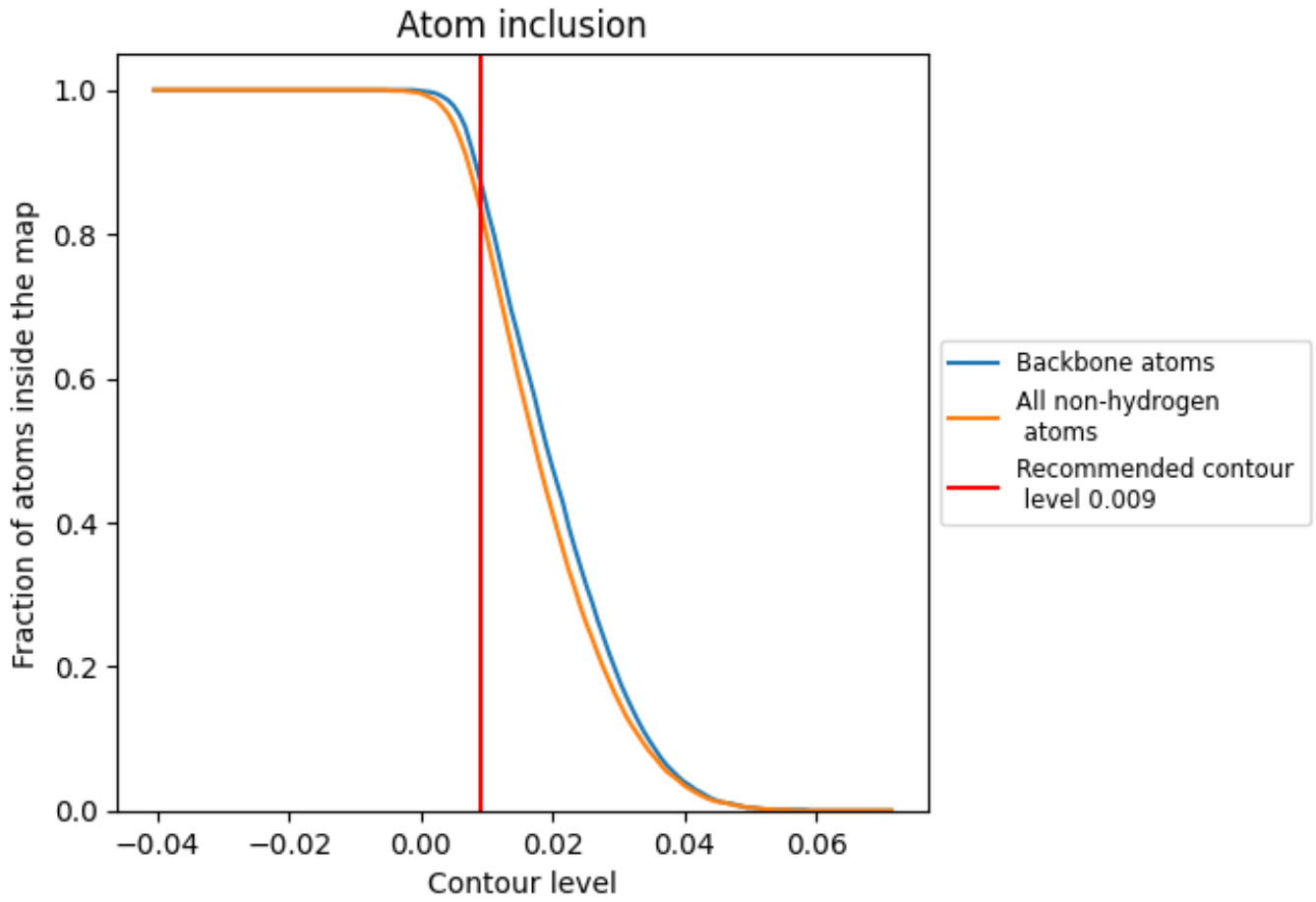
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.2690
A	0.9200	0.3590
B	0.9240	0.2570
L	0.6290	0.1010
M	0.6050	0.1160
N	0.7640	0.2490
O	0.8570	0.2450
P	0.4240	0.0850