



Full wwPDB EM Validation Report ⓘ

Apr 6, 2024 – 12:55 PM EDT

PDB ID : 8UHG
EMDB ID : EMD-42280
Title : Structure of paused transcription complex Pol II-DSIF-NELF - poised post-translocated
Authors : Vos, S.M.; Su, B.G.
Deposited on : 2023-10-09
Resolution : 2.70 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:

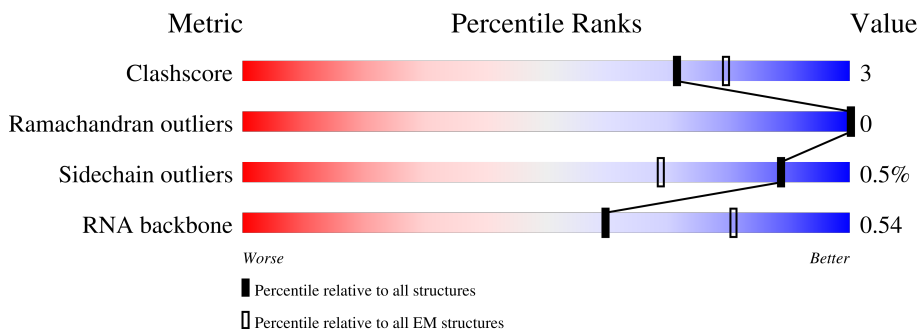
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

1 Overall quality at a glance

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

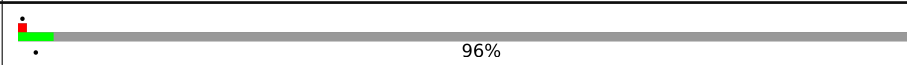


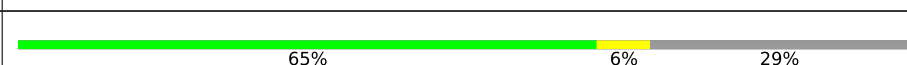
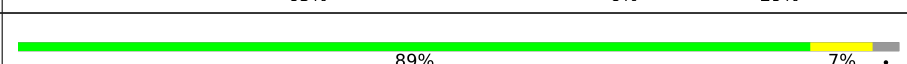
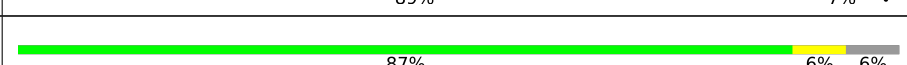
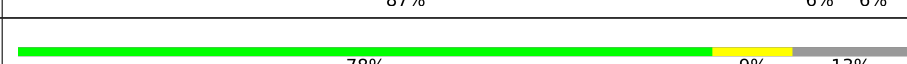
The reported resolution of this entry is 2.70 Å.

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.






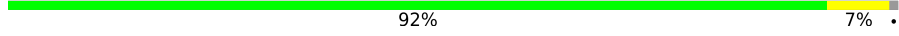


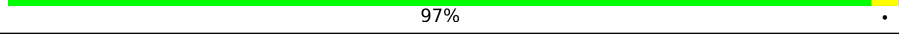



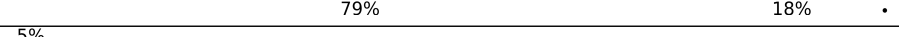


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	380	 96%
2	V	554	 56% 85% 14%
3	W	590	 26% 79% 10% 11%
4	A	1970	 65% 6% 29%
5	B	1174	 89% 7%
6	C	271	 87% 6% 6%
7	D	142	 78% 9% 13%

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Mol	Chain	Length	Quality of chain
8	E	210	 89% 10%
9	F	127	 58% 39%
10	G	171	 87% 13%
11	H	150	 92% 7%
12	I	125	 82% 9% 9%
13	J	67	 90% 9%
14	K	115	 97%
15	L	58	 64% 10% 24%
16	N	50	 50% 46%
17	P	16	 38% 38% 12% 6% 6%
18	T	38	 79% 18%
19	U	528	 5% 31% 6% 63%
20	Z	1087	 6% 23% 75%

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 89307 atoms, of which 44423 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 Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	X	15	283	85	159	23	16	0	0

- Molecule 2 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	V	550	8912	2825	4501	751	811	24	0	0

- Molecule 3 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	W	526	8362	2673	4183	698	784	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	A	1399	22303	6976	11208	1985	2064	70	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	B	1136	18193	5739	9117	1597	1676	64	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	C	254	4031	1282	1993	348	402	6	0	0

- Molecule 7 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	D	124	2016	632	1004	173	203	4	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	E	207	3438	1083	1729	298	320	8	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	F	77	1271	397	653	105	111	5	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	G	171	2710	875	1358	219	250	8	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	H	148	2333	750	1147	194	237	5	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	I	114	1789	571	861	166	180	11	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	J	66	1064	339	540	88	91	6	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	K	115	1863	593	942	152	174	2	0	0

- Molecule 15 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	L	44	752	231	379	72	64	6	0	0

- Molecule 16 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
16	N	27	856	263	305	97	164	27	0	0

- Molecule 17 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
17	P	15	474	141	158	50	110	15	0	0

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
18	T	38	1207	371	425	148	225	38	0	0

- Molecule 19 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	U	196	3054	953	1556	253	284	8	0	0

- Molecule 20 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	Z	274	4387	1373	2205	393	405	11	0	0

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total 2	Zn 2	0
21	B	1	Total 1	Zn 1	0
21	C	1	Total 1	Zn 1	0
21	I	2	Total 2	Zn 2	0
21	J	1	Total 1	Zn 1	0
21	L	1	Total 1	Zn 1	0

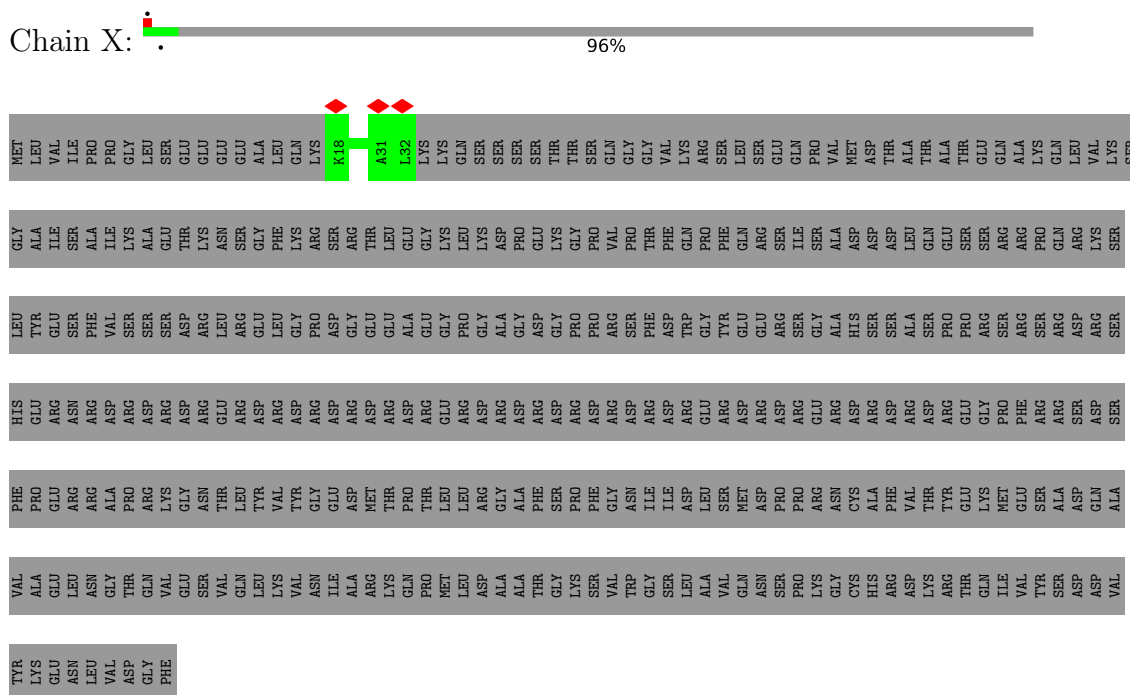
- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total 1	Mg 1	0

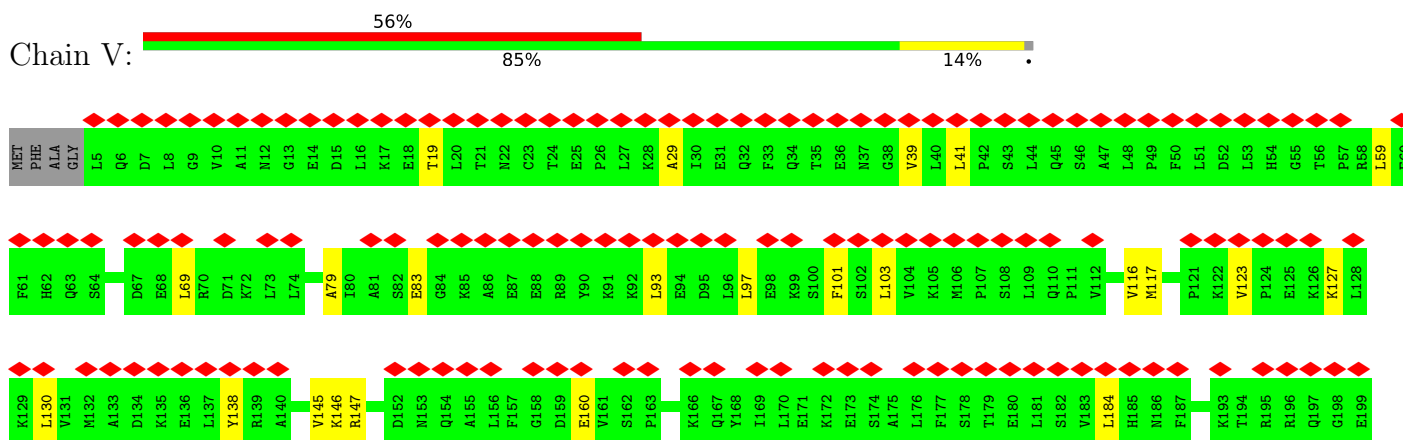
3 Residue-property plots

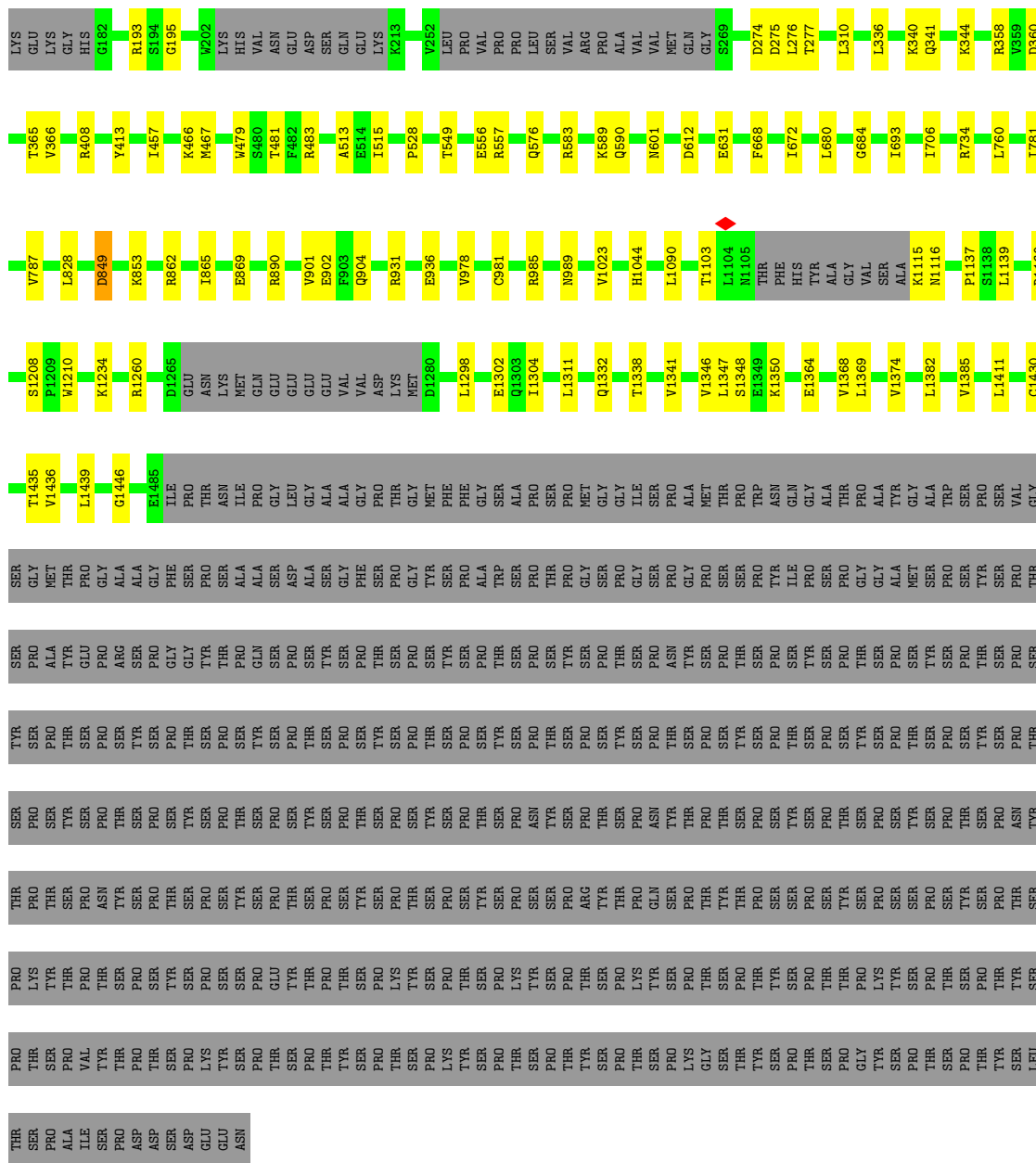
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Negative elongation factor E

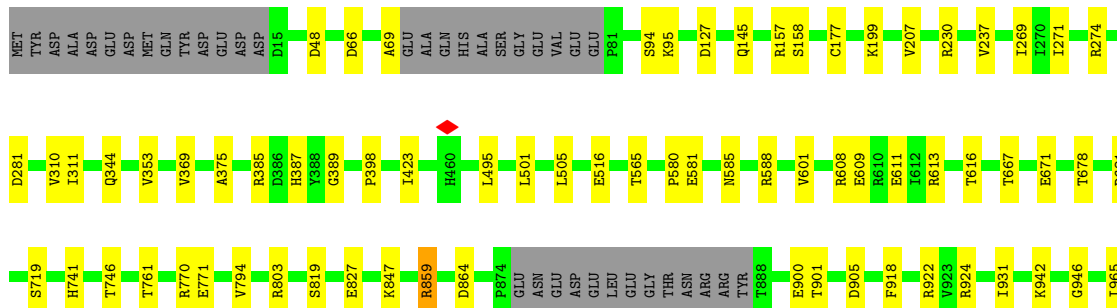
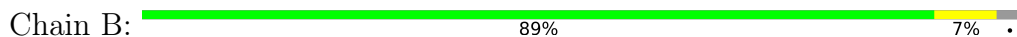


- Molecule 2: Negative elongation factor B





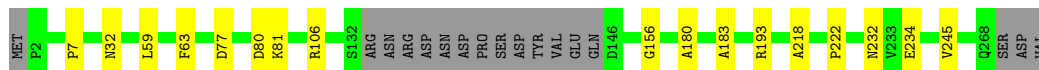
- Molecule 5: DNA-directed RNA polymerase subunit beta





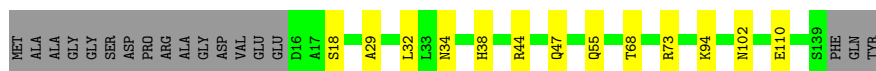
- Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C: 87% 6% 6%



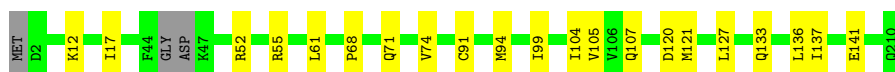
- Molecule 7: RNA polymerase Rpb4/RPC9 core domain-containing protein

Chain D: 78% 9% 13%



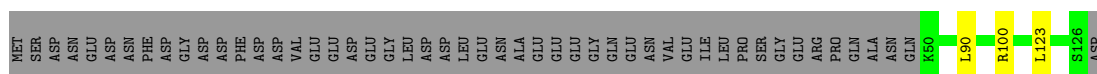
- Molecule 8: DNA-directed RNA polymerase II subunit E

Chain E: 89% 10%



- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 58% 39%



- Molecule 10: DNA-directed RNA polymerase subunit

Chain G: 87% 13%



- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 92% 7%



- Molecule 12: DNA-directed RNA polymerase II subunit RPB9

Chain I: 82% 9% 9%



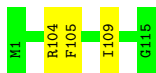
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 90% 9%



- Molecule 14: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 97%



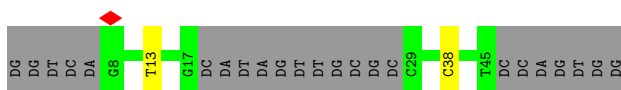
- Molecule 15: RNA polymerase II subunit K

Chain L: 64% 10% 24%



- Molecule 16: Non-template DNA

Chain N: 50% 46%



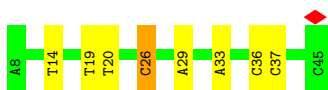
- Molecule 17: RNA

Chain P: 38% 38% 12% 6% 6%



- Molecule 18: Template DNA

Chain T: 79% 18%



- Molecule 19: Negative elongation factor A

Chain U: 5% 31% 6% 63%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90283	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.739	Depositor
Minimum map value	-0.921	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	X	0.28	0/124	0.47	0/159
2	V	0.33	0/4496	0.66	1/6074 (0.0%)
3	W	0.31	0/4261	0.57	0/5777
4	A	0.29	0/11294	0.62	1/15241 (0.0%)
5	B	0.29	0/9257	0.61	0/12493
6	C	0.28	0/2081	0.60	0/2828
7	D	0.29	0/1025	0.58	0/1376
8	E	0.30	0/1739	0.62	0/2347
9	F	0.30	0/628	0.61	0/848
10	G	0.31	0/1383	0.60	0/1874
11	H	0.28	0/1207	0.63	0/1628
12	I	0.30	0/949	0.62	0/1284
13	J	0.30	0/533	0.66	0/719
14	K	0.31	0/940	0.55	0/1271
15	L	0.29	0/378	0.72	0/500
16	N	0.94	0/615	1.12	1/944 (0.1%)
17	P	0.41	0/351	1.40	9/544 (1.7%)
18	T	0.93	2/878 (0.2%)	1.14	5/1353 (0.4%)
19	U	0.32	0/1521	0.62	1/2063 (0.0%)
20	Z	0.27	0/2214	0.61	0/2979
All	All	0.34	2/45874 (0.0%)	0.65	18/62302 (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
12	I	0	1
20	Z	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	36	DC	C1'-N1	6.62	1.57	1.49
18	T	26	DC	C1'-N1	5.03	1.55	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	9	C	C2-N1-C1'	12.22	132.25	118.80
17	P	9	C	C6-N1-C1'	-9.11	109.86	120.80
17	P	9	C	N1-C2-O2	8.12	123.78	118.90
2	V	262	PHE	CB-CG-CD1	7.37	125.95	120.80
17	P	9	C	O4'-C1'-N1	7.10	113.88	108.20
17	P	9	C	C5-C6-N1	6.63	124.32	121.00
18	T	26	DC	O4'-C4'-C3'	-6.46	101.92	104.50
17	P	9	C	N3-C2-O2	-6.20	117.56	121.90
17	P	9	C	C6-N1-C2	-6.07	117.87	120.30
18	T	37	DC	O4'-C1'-N1	-6.05	103.76	108.00
18	T	29	DA	O5'-P-OP1	5.98	117.88	110.70
17	P	4	U	C5-C6-N1	5.80	125.60	122.70
16	N	13	DT	O4'-C1'-N1	5.63	111.94	108.00
17	P	6	U	P-O3'-C3'	5.61	126.43	119.70
4	A	100	LEU	CA-CB-CG	5.46	127.86	115.30
18	T	36	DC	C2-N1-C1'	5.25	124.58	118.80
19	U	56	LEU	CA-CB-CG	5.13	127.10	115.30
18	T	36	DC	N1-C2-O2	5.02	121.91	118.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	I	103	ARG	Peptide
20	Z	711	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	X	124	159	159	0	0
2	V	4411	4501	4501	58	0
3	W	4179	4183	4181	45	0
4	A	11095	11208	11207	73	0
5	B	9076	9117	9116	57	0
6	C	2038	1993	1989	13	0
7	D	1012	1004	1004	10	0
8	E	1709	1729	1729	14	0
9	F	618	653	653	3	0
10	G	1352	1358	1358	15	0
11	H	1186	1147	1147	5	0
12	I	928	861	859	7	0
13	J	524	540	540	6	0
14	K	921	942	942	3	0
15	L	373	379	378	6	0
16	N	551	305	307	1	0
17	P	316	158	158	2	0
18	T	782	425	427	4	0
19	U	1498	1556	1556	19	0
20	Z	2182	2205	2205	14	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	A	1	0	0	0	0
All	All	44884	44423	44416	308	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 3.

All (308) 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)
5:B:237:VAL:HG21	5:B:369:VAL:HG12	1.67	0.76
7:D:73:ARG:NE	7:D:102:ASN:O	2.19	0.75
2:V:79:ALA:O	2:V:83:GLU:N	2.22	0.72
2:V:138:TYR:OH	2:V:160:GLU:OE1	2.10	0.70
3:W:481:HIS:O	3:W:489:GLN:NE2	2.25	0.70
3:W:101:LEU:O	3:W:104:THR:OG1	2.09	0.69
5:B:864:ASP:OD1	20:Z:725:LYS:NZ	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:57:LEU:O	19:U:60:THR:OG1	2.06	0.69
3:W:322:PRO:O	3:W:375:ARG:NH1	2.25	0.69
4:A:341:GLN:OE1	4:A:344:LYS:NZ	2.26	0.69
6:C:77:ASP:O	6:C:81:LYS:NZ	2.26	0.68
4:A:576:GLN:O	4:A:590:GLN:NE2	2.26	0.68
7:D:18:SER:OG	10:G:83:GLU:OE1	2.10	0.68
4:A:193:ARG:NH1	4:A:195:GLY:O	2.28	0.67
15:L:15:MET:SD	15:L:15:MET:N	2.67	0.67
11:H:128:ASP:OD1	11:H:131:ASN:ND2	2.27	0.67
4:A:97:VAL:HG23	4:A:100:LEU:HD23	1.77	0.67
5:B:611:GLU:OE1	5:B:613:ARG:NH1	2.28	0.67
15:L:22:CYS:SG	15:L:24:THR:OG1	2.52	0.66
4:A:734:ARG:NH1	12:I:108:MET:SD	2.69	0.66
2:V:494:SER:OG	2:V:501:HIS:ND1	2.27	0.65
3:W:321:ASP:OD1	3:W:375:ARG:NH2	2.29	0.65
19:U:24:TRP:O	19:U:55:LYS:NZ	2.30	0.65
2:V:490:PHE:O	2:V:494:SER:N	2.30	0.65
4:A:513:ALA:HB2	9:F:90:LEU:HD21	1.78	0.65
4:A:931:ARG:NH1	4:A:936:GLU:OE1	2.29	0.65
5:B:608:ARG:NH1	5:B:609:GLU:OE2	2.30	0.64
3:W:198:LEU:HD22	19:U:92:MET:HE2	1.78	0.64
4:A:27:SER:OG	4:A:29:ASP:OD1	2.09	0.64
7:D:34:ASN:OD1	7:D:73:ARG:NH1	2.32	0.63
20:Z:427:GLU:OE2	20:Z:469:ARG:NH2	2.32	0.63
7:D:73:ARG:NH2	10:G:86:ASP:OD2	2.32	0.62
4:A:467:MET:SD	4:A:467:MET:N	2.73	0.62
19:U:68:VAL:HG13	19:U:75:LEU:HD12	1.81	0.62
5:B:771:GLU:O	13:J:55:LEU:HD21	2.00	0.61
2:V:466:THR:HG22	2:V:507:LEU:HD22	1.83	0.61
5:B:387:HIS:NE2	5:B:671:GLU:OE2	2.33	0.61
10:G:38:CYS:SG	10:G:39:THR:N	2.74	0.61
2:V:147:ARG:NH1	2:V:206:ARG:O	2.33	0.61
2:V:505:LEU:HD22	2:V:544:LEU:HD22	1.83	0.61
6:C:193:ARG:NH2	6:C:218:ALA:O	2.33	0.61
5:B:847:LYS:NZ	5:B:864:ASP:OD2	2.34	0.60
2:V:405:ASN:ND2	2:V:439:ASN:O	2.34	0.60
8:E:55:ARG:NH2	8:E:107:GLN:OE1	2.35	0.60
4:A:90:LEU:HD22	4:A:310:LEU:HD21	1.84	0.59
3:W:236:HIS:HB3	19:U:58:LEU:HD11	1.85	0.59
4:A:1364:GLU:O	4:A:1368:VAL:HG12	2.03	0.58
2:V:97:LEU:HD22	2:V:117:MET:CE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:12:LYS:NZ	8:E:136:LEU:O	2.29	0.58
4:A:668:PHE:CZ	4:A:672:ILE:HD11	2.39	0.58
9:F:100:ARG:NH2	9:F:123:LEU:O	2.37	0.58
16:N:38:DC:N4	18:T:14:DT:O4	2.36	0.58
4:A:1234:LYS:NZ	4:A:1298:LEU:O	2.37	0.57
4:A:693:ILE:HD13	4:A:828:LEU:HD21	1.85	0.57
11:H:106:THR:OG1	11:H:107:GLU:OE1	2.15	0.57
19:U:14:HIS:O	19:U:18:GLY:N	2.37	0.57
4:A:22:GLN:NE2	4:A:1446:GLY:O	2.38	0.57
3:W:123:LEU:O	3:W:127:PHE:N	2.38	0.56
2:V:426:LEU:HD21	2:V:456:ALA:HB2	1.87	0.56
8:E:141:GLU:N	8:E:141:GLU:OE1	2.39	0.56
15:L:25:GLU:N	15:L:25:GLU:OE1	2.38	0.55
2:V:97:LEU:HD11	2:V:127:LYS:CD	2.37	0.55
5:B:127:ASP:OD2	5:B:145:GLN:NE2	2.40	0.55
3:W:264:GLU:OE1	3:W:267:ARG:NH1	2.40	0.55
3:W:281:LEU:HD13	3:W:293:CYS:SG	2.47	0.54
4:A:481:THR:OG1	4:A:483:ARG:NH1	2.39	0.54
4:A:1311:LEU:HD22	4:A:1332:GLN:HG3	1.88	0.54
4:A:631:GLU:OE1	11:H:95:LYS:NZ	2.33	0.54
4:A:904:GLN:OE1	4:A:1044:HIS:NE2	2.41	0.54
7:D:110:GLU:OE2	10:G:144:ARG:NH1	2.41	0.54
5:B:581:GLU:OE1	12:I:74:GLN:NE2	2.41	0.54
2:V:19:THR:HG22	2:V:29:ALA:HB1	1.88	0.54
7:D:29:ALA:O	7:D:94:LYS:NZ	2.37	0.54
4:A:869:GLU:N	4:A:869:GLU:OE1	2.41	0.53
5:B:900:GLU:N	5:B:900:GLU:OE1	2.41	0.53
5:B:48:ASP:OD1	5:B:158:SER:OG	2.26	0.53
4:A:849:ASP:OD2	4:A:853:LYS:NZ	2.40	0.53
5:B:94:SER:OG	5:B:95:LYS:N	2.40	0.53
4:A:100:LEU:HD12	4:A:101:VAL:N	2.24	0.53
4:A:275:ASP:OD1	4:A:276:LEU:N	2.42	0.53
4:A:902:GLU:OE1	4:A:985:ARG:NH2	2.42	0.53
6:C:106:ARG:NH1	6:C:156:GLY:O	2.42	0.53
4:A:680:LEU:O	4:A:684:GLY:N	2.41	0.53
5:B:1035:ARG:NH1	5:B:1036:LYS:O	2.42	0.53
5:B:1117:HIS:HB3	5:B:1146:ILE:HD11	1.91	0.53
4:A:1374:VAL:HG11	4:A:1411:LEU:HD11	1.90	0.53
2:V:117:MET:SD	2:V:123:VAL:HG11	2.48	0.52
15:L:24:THR:OG1	15:L:38:GLU:OE2	2.27	0.52
4:A:340:LYS:HG3	4:A:1436:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:457:ILE:HD11	4:A:515:ILE:HD12	1.91	0.52
4:A:601:ASN:ND2	4:A:989:ASN:OD1	2.42	0.52
2:V:551:LEU:HD12	2:V:554:ARG:HB3	1.91	0.52
3:W:62:ILE:HD11	3:W:83:LEU:HD21	1.91	0.52
5:B:501:LEU:HD12	5:B:505:LEU:HD12	1.90	0.52
10:G:22:LEU:O	10:G:25:THR:HG22	2.10	0.52
4:A:853:LYS:HE2	4:A:1103:THR:HG22	1.92	0.52
5:B:585:ASN:OD1	5:B:588:ARG:NH2	2.43	0.52
2:V:97:LEU:HD22	2:V:117:MET:HE1	1.91	0.52
4:A:340:LYS:CG	4:A:1436:VAL:HG21	2.40	0.52
5:B:344:GLN:NE2	5:B:353:VAL:O	2.43	0.51
2:V:342:LEU:HD12	2:V:420:MET:CG	2.40	0.51
2:V:313:THR:O	2:V:317:SER:OG	2.23	0.51
4:A:706:ILE:HD11	4:A:787:VAL:HG21	1.92	0.51
4:A:583:ARG:NH1	6:C:222:PRO:O	2.43	0.51
5:B:207:VAL:HG11	5:B:375:ALA:CB	2.41	0.51
5:B:794:VAL:O	5:B:946:GLY:N	2.42	0.51
2:V:223:ARG:NH2	2:V:300:ASP:OD1	2.44	0.51
4:A:365:THR:OG1	4:A:366:VAL:N	2.44	0.51
11:H:8:ASP:OD2	11:H:32:SER:OG	2.19	0.51
20:Z:424:ASP:HB2	20:Z:440:ILE:HD12	1.93	0.50
17:P:5:U:O2'	17:P:6:U:O5'	2.23	0.50
2:V:184:LEU:HD23	8:E:68:PRO:CG	2.42	0.50
2:V:463:HIS:O	2:V:466:THR:OG1	2.24	0.50
4:A:668:PHE:CE1	4:A:672:ILE:HD11	2.45	0.50
19:U:177:GLU:O	19:U:181:LYS:NZ	2.29	0.50
19:U:29:ILE:O	19:U:33:LEU:N	2.44	0.50
2:V:263:THR:OG1	2:V:304:ILE:HD13	2.11	0.50
2:V:495:PRO:HB3	2:V:530:THR:HG21	1.93	0.50
3:W:59:GLU:OE1	3:W:61:SER:OG	2.27	0.50
3:W:341:LEU:O	3:W:394:HIS:ND1	2.43	0.50
2:V:101:PHE:CE2	2:V:130:LEU:HD23	2.47	0.50
5:B:1109:GLU:OE1	5:B:1109:GLU:N	2.45	0.50
5:B:1032:PHE:O	6:C:32:ASN:ND2	2.45	0.49
2:V:97:LEU:HD11	2:V:127:LYS:HE3	1.92	0.49
2:V:117:MET:HB2	2:V:145:VAL:HG22	1.94	0.49
2:V:205:THR:O	2:V:209:GLY:N	2.44	0.49
3:W:57:ILE:HD13	3:W:83:LEU:HD13	1.95	0.49
5:B:269:ILE:HG12	5:B:369:VAL:HG11	1.93	0.49
5:B:1079:SER:OG	5:B:1080:ARG:N	2.45	0.49
5:B:681:ASP:N	5:B:681:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:486:PHE:CZ	2:V:507:LEU:HD23	2.47	0.49
3:W:235:GLU:HB3	19:U:58:LEU:HD13	1.94	0.49
5:B:310:VAL:HG23	5:B:311:ILE:HD12	1.94	0.49
7:D:38:HIS:HB2	7:D:68:THR:HG22	1.94	0.49
2:V:342:LEU:HD12	2:V:420:MET:HG2	1.95	0.49
2:V:505:LEU:HB2	2:V:540:LEU:HD23	1.94	0.49
6:C:183:ALA:HB3	6:C:232:ASN:HB3	1.95	0.49
5:B:1054:MET:O	5:B:1058:LYS:NZ	2.46	0.49
3:W:455:LEU:HD22	3:W:469:VAL:HG22	1.95	0.48
5:B:794:VAL:HG13	5:B:965:ILE:HG23	1.94	0.48
4:A:133:SER:O	4:A:140:ARG:NH2	2.46	0.48
6:C:59:LEU:HD13	6:C:63:PHE:CD2	2.48	0.48
7:D:55:GLN:HB3	10:G:32:THR:HG22	1.95	0.48
3:W:367:VAL:HG22	19:U:148:ALA:N	2.29	0.48
15:L:53:VAL:HG23	20:Z:737:HIS:NE2	2.28	0.48
2:V:272:GLU:OE1	2:V:279:ARG:NH2	2.43	0.48
3:W:50:LYS:HE2	3:W:65:THR:HG21	1.95	0.48
2:V:97:LEU:HD11	2:V:127:LYS:HD2	1.95	0.48
2:V:101:PHE:CZ	2:V:130:LEU:HD23	2.48	0.48
3:W:50:LYS:CE	3:W:65:THR:HG21	2.44	0.48
2:V:370:ILE:HG23	2:V:371:THR:HG23	1.95	0.48
4:A:1160:ARG:NH2	4:A:1350:LYS:O	2.46	0.48
20:Z:440:ILE:HG23	20:Z:450:ILE:HD11	1.95	0.48
2:V:514:ARG:O	2:V:514:ARG:NE	2.47	0.48
4:A:1347:LEU:HB3	8:E:137:ILE:HD13	1.95	0.48
5:B:741:HIS:O	5:B:922:ARG:NH2	2.47	0.48
5:B:678:THR:OG1	5:B:681:ASP:OD1	2.31	0.48
3:W:207:THR:O	3:W:211:THR:HG23	2.14	0.48
3:W:470:LEU:O	3:W:474:VAL:HG13	2.14	0.48
10:G:10:GLU:HB3	10:G:67:LEU:HD11	1.95	0.48
3:W:56:TYR:HD2	3:W:62:ILE:HD13	1.78	0.47
2:V:69:LEU:HD22	3:W:101:LEU:HD12	1.97	0.47
3:W:246:SER:HB3	3:W:283:LEU:HD21	1.95	0.47
4:A:862:ARG:NH2	18:T:26:DC:O3'	2.42	0.47
19:U:48:LEU:O	19:U:53:LYS:NZ	2.47	0.47
19:U:89:TRP:HA	19:U:92:MET:HE3	1.96	0.47
10:G:151:ARG:HB2	20:Z:491:LEU:HD11	1.95	0.47
20:Z:561:LEU:HD23	20:Z:635:MET:HG3	1.95	0.47
3:W:93:THR:O	3:W:97:LEU:HD13	2.14	0.47
4:A:862:ARG:HA	4:A:865:ILE:HG22	1.96	0.47
2:V:39:VAL:HG12	2:V:41:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:513:ALA:CB	9:F:90:LEU:HD21	2.45	0.47
4:A:556:GLU:OE1	4:A:557:ARG:N	2.48	0.47
4:A:853:LYS:CE	4:A:1103:THR:HG22	2.45	0.47
4:A:904:GLN:NE2	4:A:981:CYS:O	2.45	0.47
3:W:306:ASN:N	3:W:306:ASN:OD1	2.46	0.47
3:W:497:LEU:HD22	3:W:533:PHE:HD2	1.79	0.46
20:Z:450:ILE:HG21	20:Z:468:LEU:HD11	1.98	0.46
4:A:528:PRO:HG2	4:A:1090:LEU:HD11	1.97	0.46
7:D:32:LEU:HD11	10:G:4:HIS:HB2	1.98	0.46
10:G:123:SER:OG	10:G:125:PRO:O	2.27	0.46
4:A:466:LYS:HD2	4:A:1090:LEU:HD13	1.97	0.46
4:A:274:ASP:O	4:A:277:THR:OG1	2.33	0.46
4:A:760:LEU:HD11	4:A:781:ILE:HG21	1.96	0.46
4:A:1368:VAL:HG13	4:A:1369:LEU:HG	1.97	0.46
12:I:83:ASP:OD2	12:I:84:HIS:NE2	2.49	0.46
20:Z:543:ASP:N	20:Z:543:ASP:OD1	2.49	0.46
3:W:509:VAL:HG13	3:W:510:LEU:HD12	1.97	0.46
2:V:466:THR:OG1	2:V:506:ARG:NH2	2.49	0.46
10:G:93:ASN:OD1	10:G:94:LYS:N	2.48	0.46
3:W:62:ILE:HD11	3:W:83:LEU:CD2	2.46	0.45
4:A:275:ASP:HB2	4:A:336:LEU:HD12	1.98	0.45
3:W:281:LEU:HD11	3:W:297:GLY:HA3	1.98	0.45
4:A:1139:LEU:HD13	4:A:1346:VAL:HG21	1.99	0.45
5:B:271:ILE:CD1	5:B:311:ILE:HD13	2.47	0.45
5:B:608:ARG:O	12:I:69:ILE:HD12	2.17	0.45
3:W:534:VAL:HG21	3:W:557:LEU:HD13	1.98	0.45
4:A:1304:ILE:HG23	4:A:1338:THR:OG1	2.15	0.45
10:G:41:LYS:O	10:G:78:ARG:NH1	2.49	0.45
2:V:368:GLU:OE2	2:V:413:LYS:NZ	2.50	0.45
4:A:62:GLN:O	4:A:84:HIS:N	2.49	0.45
4:A:97:VAL:HG23	4:A:100:LEU:CD2	2.45	0.45
5:B:803:ARG:NH1	13:J:9:THR:O	2.50	0.45
2:V:59:LEU:HD13	3:W:55:ASP:HB3	1.99	0.45
2:V:243:MET:SD	2:V:246:HIS:ND1	2.87	0.45
2:V:97:LEU:HD21	2:V:127:LYS:HE3	1.98	0.45
4:A:360:ASP:OD1	5:B:1062:ARG:NE	2.43	0.45
10:G:82:GLY:N	10:G:147:ILE:O	2.47	0.45
4:A:1348:SER:HB3	8:E:136:LEU:HD13	1.97	0.45
6:C:180:ALA:O	13:J:42:ARG:NH2	2.50	0.45
2:V:97:LEU:HD13	2:V:117:MET:HE3	2.00	0.44
2:V:469:LEU:HD23	2:V:507:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:476:PHE:HB3	2:V:515:VAL:HG22	1.99	0.44
2:V:502:ARG:HD2	2:V:540:LEU:HD22	1.99	0.44
3:W:497:LEU:HD23	3:W:500:MET:HE3	1.99	0.44
4:A:408:ARG:NH1	4:A:413:TYR:O	2.51	0.44
5:B:385:ARG:HE	5:B:495:LEU:HD13	1.80	0.44
2:V:451:THR:HG21	2:V:456:ALA:HB3	2.00	0.44
4:A:1115:LYS:NZ	4:A:1116:ASN:O	2.44	0.44
11:H:34:SER:OG	11:H:35:PHE:N	2.50	0.44
2:V:97:LEU:HD22	2:V:117:MET:HE3	1.99	0.44
4:A:1302:GLU:OE1	4:A:1302:GLU:N	2.45	0.44
3:W:468:GLN:O	3:W:472:LEU:N	2.49	0.44
4:A:358:ARG:O	5:B:1111:SER:OG	2.25	0.44
2:V:449:VAL:O	2:V:492:THR:HG21	2.17	0.44
6:C:245:VAL:HG11	14:K:105:PHE:CZ	2.52	0.44
8:E:71:GLN:HB2	8:E:99:ILE:HD12	1.99	0.44
13:J:65:LEU:HD13	13:J:65:LEU:O	2.18	0.44
18:T:19:DT:H2'	18:T:20:DT:H71	2.00	0.44
4:A:865:ILE:O	4:A:869:GLU:N	2.50	0.43
5:B:770:ARG:NH2	5:B:771:GLU:OE2	2.51	0.43
4:A:84:HIS:HD1	5:B:1127:ILE:HG22	1.83	0.43
5:B:389:GLY:HA2	5:B:667:THR:HG23	1.99	0.43
13:J:65:LEU:HD11	15:L:45:TYR:HB2	2.00	0.43
2:V:97:LEU:HD11	2:V:127:LYS:CE	2.48	0.43
5:B:516:GLU:N	5:B:516:GLU:OE1	2.51	0.43
5:B:761:THR:HG23	5:B:1000:THR:HA	2.01	0.43
5:B:905:ASP:OD2	5:B:924:ARG:NH1	2.50	0.43
8:E:94:MET:HE1	8:E:127:LEU:HD11	2.00	0.43
4:A:479:TRP:CD1	5:B:931:ILE:HD12	2.54	0.43
4:A:1210:TRP:O	4:A:1260:ARG:NH1	2.51	0.43
5:B:274:ARG:NH2	5:B:281:ASP:OD1	2.51	0.43
20:Z:513:VAL:HG21	20:Z:518:LEU:HD21	2.00	0.43
4:A:74:CYS:SG	4:A:84:HIS:CE1	3.12	0.43
5:B:207:VAL:HG11	5:B:375:ALA:HB2	2.01	0.43
3:W:314:PHE:HB2	3:W:359:ILE:HD11	2.01	0.43
5:B:157:ARG:NH2	5:B:177:CYS:O	2.52	0.43
19:U:21:ASP:OD1	19:U:22:GLU:N	2.51	0.43
3:W:202:SER:HB2	19:U:120:ILE:HD11	2.00	0.42
2:V:429:VAL:O	2:V:433:THR:OG1	2.33	0.42
3:W:57:ILE:HD13	3:W:83:LEU:HB3	2.00	0.42
4:A:1208:SER:O	4:A:1260:ARG:NH1	2.52	0.42
5:B:988:LYS:O	5:B:992:ASN:ND2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1068:GLN:N	5:B:1073:GLN:O	2.45	0.42
6:C:80:ASP:OD1	6:C:81:LYS:N	2.51	0.42
4:A:1382:LEU:HA	4:A:1385:VAL:HG12	2.01	0.42
2:V:69:LEU:CD2	3:W:101:LEU:HD12	2.50	0.42
6:C:7:PRO:O	14:K:104:ARG:NH1	2.48	0.42
12:I:17:CYS:SG	12:I:18:GLN:N	2.93	0.42
20:Z:561:LEU:HD21	20:Z:636:PHE:HA	1.99	0.42
4:A:901:VAL:HB	4:A:978:VAL:HG22	2.00	0.42
4:A:1435:THR:OG1	4:A:1436:VAL:N	2.52	0.42
19:U:34:THR:O	19:U:37:VAL:N	2.52	0.42
5:B:69:ALA:HB2	5:B:423:ILE:HG22	2.02	0.42
5:B:565:THR:HG21	5:B:580:PRO:HG3	2.01	0.42
5:B:230:ARG:NH2	5:B:398:PRO:O	2.52	0.42
2:V:457:PHE:O	2:V:499:ASN:ND2	2.53	0.42
3:W:261:ILE:O	3:W:265:VAL:HG23	2.19	0.42
3:W:370:TRP:CD1	19:U:152:LEU:HD13	2.54	0.42
5:B:859:ARG:NH1	5:B:901:THR:OG1	2.53	0.42
20:Z:604:ASP:OD1	20:Z:605:GLY:N	2.52	0.42
5:B:746:THR:HG21	18:T:33:DA:OP1	2.20	0.41
12:I:69:ILE:HG22	12:I:71:ASP:H	1.84	0.41
8:E:104:ILE:HG22	8:E:105:VAL:O	2.20	0.41
8:E:133:GLN:HA	8:E:136:LEU:HD12	2.02	0.41
12:I:69:ILE:O	12:I:72:VAL:HG22	2.20	0.41
2:V:251:GLY:O	2:V:255:THR:HG22	2.19	0.41
8:E:17:ILE:HD12	8:E:74:VAL:HG11	2.02	0.41
2:V:103:LEU:HD13	3:W:100:TRP:HH2	1.86	0.41
4:A:549:THR:O	4:A:589:LYS:NZ	2.48	0.41
5:B:601:VAL:HG22	5:B:616:THR:HG23	2.02	0.41
8:E:61:LEU:HD11	8:E:71:GLN:HB3	2.02	0.41
2:V:486:PHE:HZ	2:V:507:LEU:HD23	1.86	0.41
5:B:819:SER:OG	5:B:827:GLU:OE1	2.22	0.41
20:Z:554:GLU:OE2	20:Z:559:GLN:NE2	2.54	0.41
3:W:314:PHE:O	3:W:318:THR:OG1	2.23	0.41
3:W:477:PHE:CZ	3:W:497:LEU:HD21	2.55	0.41
14:K:105:PHE:CD2	14:K:109:ILE:HD11	2.56	0.41
4:A:1137:PRO:HB2	4:A:1341:VAL:HG13	2.01	0.41
6:C:234:GLU:OE2	13:J:12:LYS:NZ	2.52	0.41
19:U:171:SER:OG	19:U:175:ARG:NH2	2.54	0.41
5:B:942:LYS:NZ	17:P:16:G:O3'	2.54	0.41
7:D:44:ARG:NH1	7:D:47:GLN:OE1	2.54	0.41
8:E:120:ASP:OD1	8:E:121:MET:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:184:LEU:HD23	8:E:68:PRO:HG3	2.02	0.41
4:A:890:ARG:CZ	4:A:1023:VAL:HG12	2.50	0.41
5:B:66:ASP:OD1	5:B:66:ASP:N	2.54	0.41
19:U:102:ASP:OD1	19:U:102:ASP:N	2.54	0.41
2:V:93:LEU:HD22	2:V:116:VAL:HG22	2.03	0.41
3:W:411:LEU:HD23	19:U:178:LEU:HB3	2.02	0.41
10:G:1:MET:N	10:G:78:ARG:O	2.54	0.41
6:C:59:LEU:HD13	6:C:63:PHE:CE2	2.55	0.40
10:G:152:VAL:HG22	10:G:157:ILE:HG12	2.02	0.40
2:V:338:LEU:HD21	2:V:374:LEU:HD13	2.04	0.40
4:A:1430:CYS:O	4:A:1435:THR:HG22	2.21	0.40
5:B:859:ARG:NH1	20:Z:735:GLU:OE2	2.55	0.40
3:W:209:LEU:HD23	3:W:212:ILE:HD12	2.04	0.40
3:W:497:LEU:HD23	3:W:500:MET:CE	2.52	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	X	13/380 (3%)	13 (100%)	0	0	100	100
2	V	548/554 (99%)	531 (97%)	17 (3%)	0	100	100
3	W	512/590 (87%)	492 (96%)	20 (4%)	0	100	100
4	A	1387/1970 (70%)	1339 (96%)	48 (4%)	0	100	100
5	B	1130/1174 (96%)	1077 (95%)	53 (5%)	0	100	100
6	C	250/271 (92%)	241 (96%)	9 (4%)	0	100	100
7	D	122/142 (86%)	115 (94%)	7 (6%)	0	100	100
8	E	203/210 (97%)	196 (97%)	7 (3%)	0	100	100
9	F	75/127 (59%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
11	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
12	I	112/125 (90%)	105 (94%)	7 (6%)	0	100	100
13	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
14	K	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
15	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
19	U	192/528 (36%)	189 (98%)	3 (2%)	0	100	100
20	Z	266/1087 (24%)	260 (98%)	6 (2%)	0	100	100
All	All	5344/7719 (69%)	5153 (96%)	191 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	13/331 (4%)	13 (100%)	0	100	100
2	V	493/495 (100%)	490 (99%)	3 (1%)	86	95
3	W	466/513 (91%)	464 (100%)	2 (0%)	91	97
4	A	1232/1749 (70%)	1228 (100%)	4 (0%)	92	98
5	B	994/1027 (97%)	989 (100%)	5 (0%)	88	96
6	C	231/248 (93%)	231 (100%)	0	100	100
7	D	114/126 (90%)	114 (100%)	0	100	100
8	E	190/192 (99%)	188 (99%)	2 (1%)	73	90
9	F	67/111 (60%)	67 (100%)	0	100	100
10	G	152/152 (100%)	151 (99%)	1 (1%)	84	94
11	H	129/131 (98%)	128 (99%)	1 (1%)	81	93
12	I	103/112 (92%)	102 (99%)	1 (1%)	76	91
13	J	55/56 (98%)	54 (98%)	1 (2%)	59	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	K	104/104 (100%)	104 (100%)	0	100	100
15	L	41/55 (74%)	40 (98%)	1 (2%)	49	77
19	U	167/451 (37%)	164 (98%)	3 (2%)	59	83
20	Z	244/940 (26%)	244 (100%)	0	100	100
All	All	4795/6793 (71%)	4771 (100%)	24 (0%)	89	96

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	146	LYS
2	V	262	PHE
2	V	533	SER
3	W	59	GLU
3	W	278	GLN
4	A	103	THR
4	A	612	ASP
4	A	849	ASP
4	A	1439	LEU
5	B	199	LYS
5	B	719	SER
5	B	859	ARG
5	B	918	PHE
5	B	1080	ARG
8	E	52	ARG
8	E	91	CYS
10	G	39	THR
11	H	124	ARG
12	I	41	ASN
13	J	47	ARG
15	L	15	MET
19	U	28	SER
19	U	56	LEU
19	U	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
11	H	131	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	P	14/16 (87%)	7 (50%)	1 (7%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	P	5	U
17	P	6	U
17	P	7	G
17	P	8	G
17	P	9	C
17	P	10	A
17	P	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	P	6	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

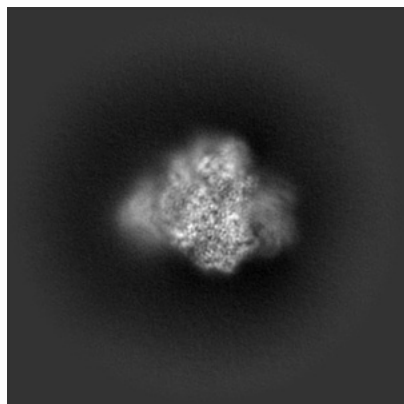
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42280. These allow visual inspection of the internal detail of the map and identification of artifacts.

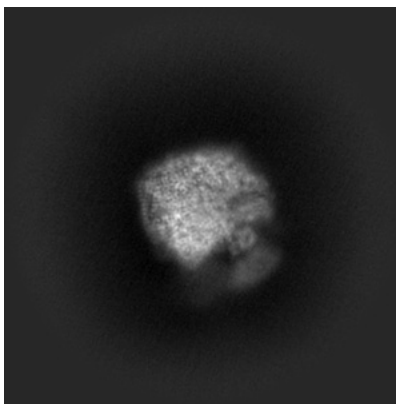
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

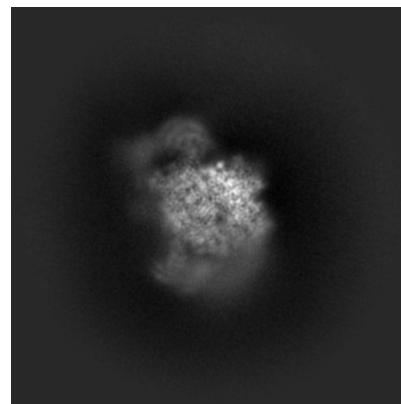
6.1.1 Primary map



X

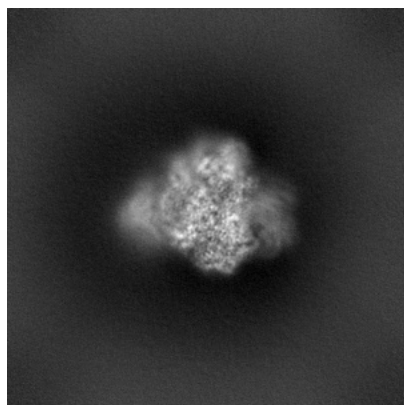


Y

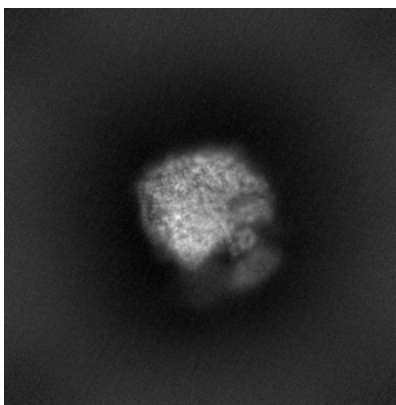


Z

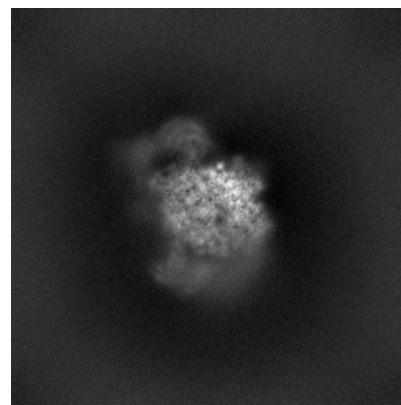
6.1.2 Raw map



X



Y

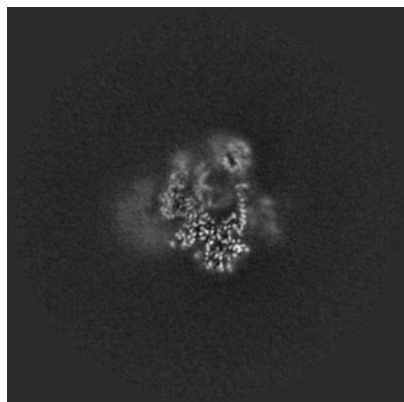


Z

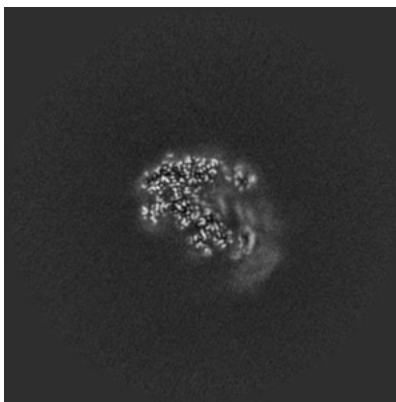
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

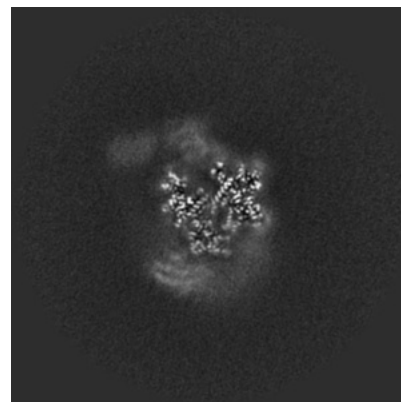
6.2.1 Primary map



X Index: 256



Y Index: 256

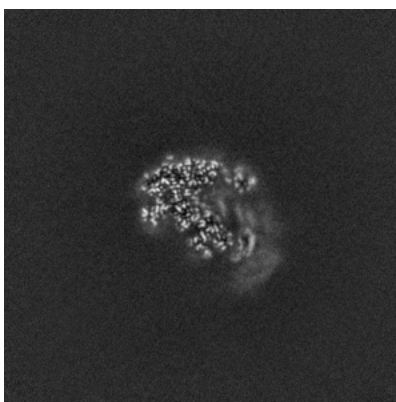


Z Index: 256

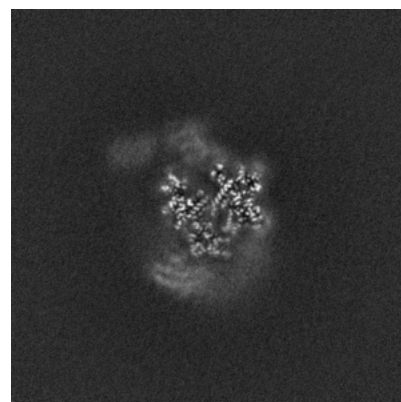
6.2.2 Raw map



X Index: 256



Y Index: 256

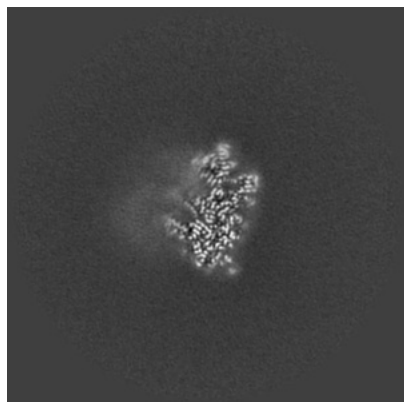


Z Index: 256

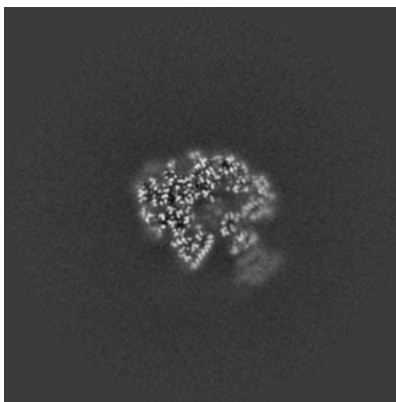
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

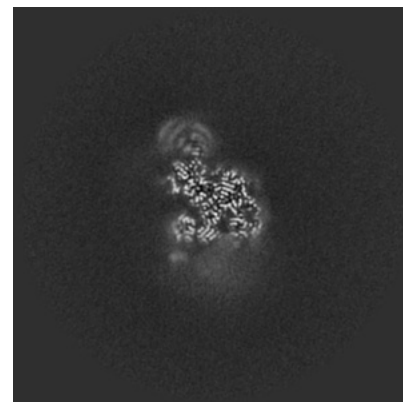
6.3.1 Primary map



X Index: 289

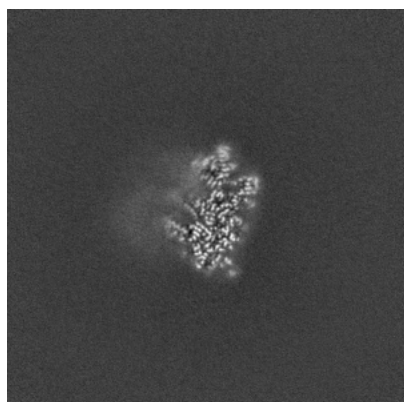


Y Index: 281

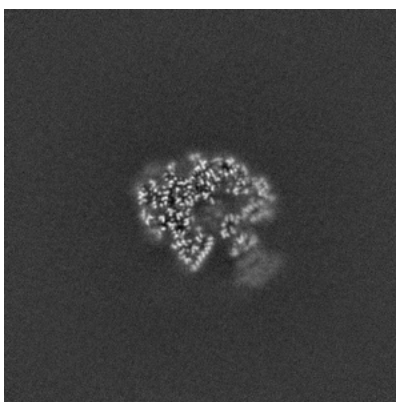


Z Index: 220

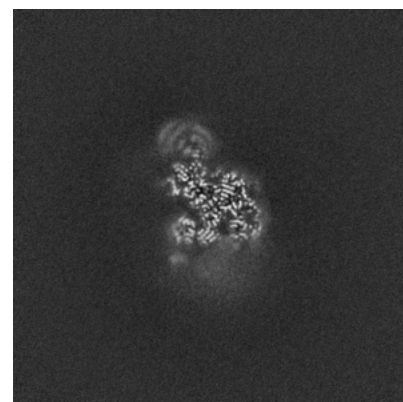
6.3.2 Raw map



X Index: 289



Y Index: 281

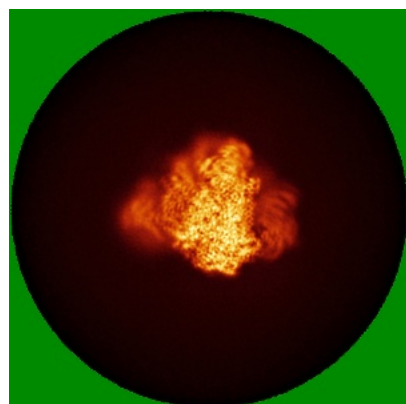


Z Index: 220

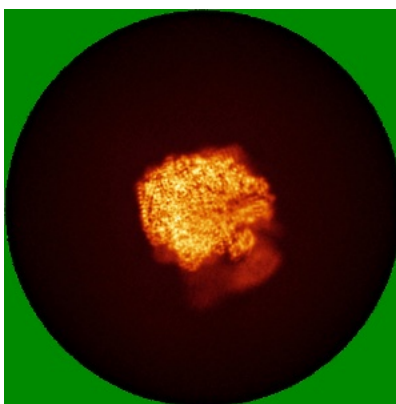
The images above show the largest variance slices of the map in three orthogonal directions.

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

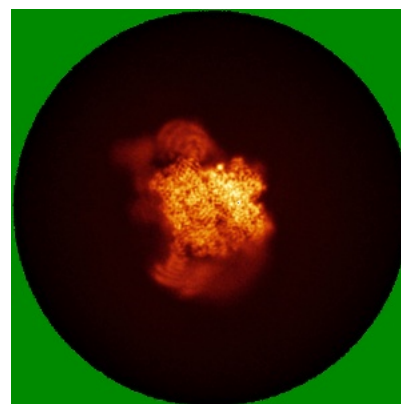
6.4.1 Primary map



X

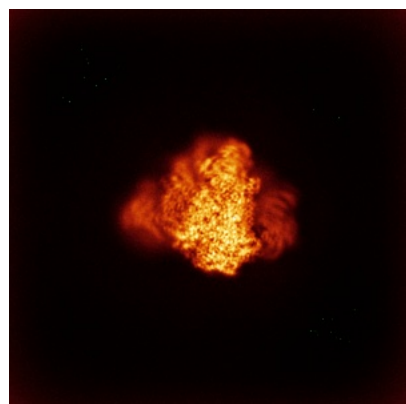


Y

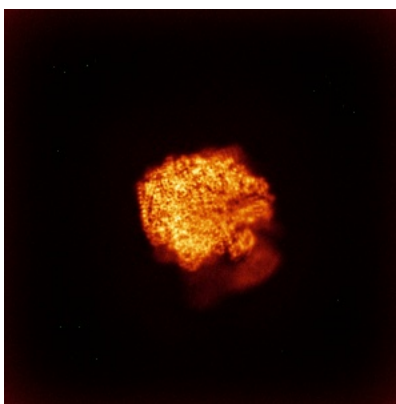


Z

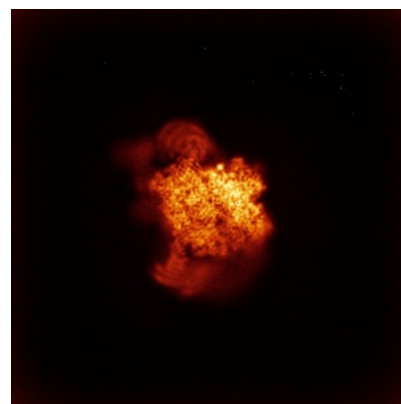
6.4.2 Raw map



X



Y

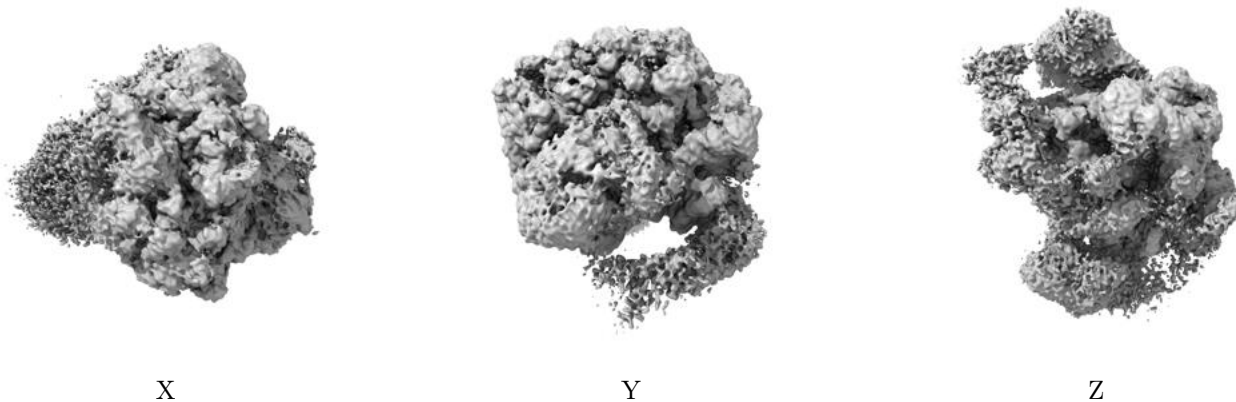


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

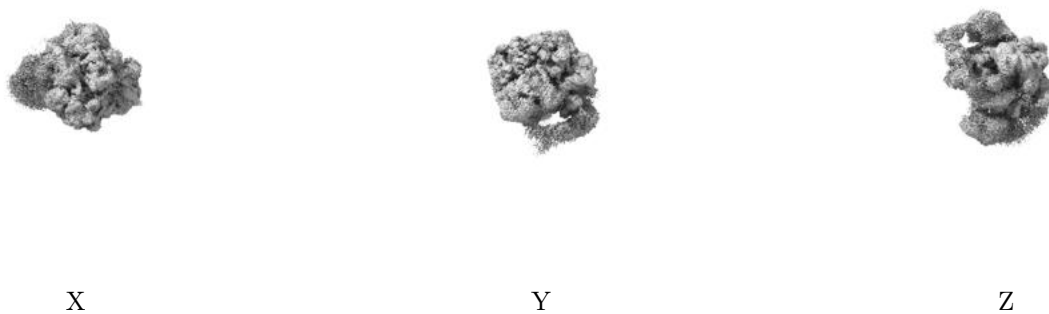
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

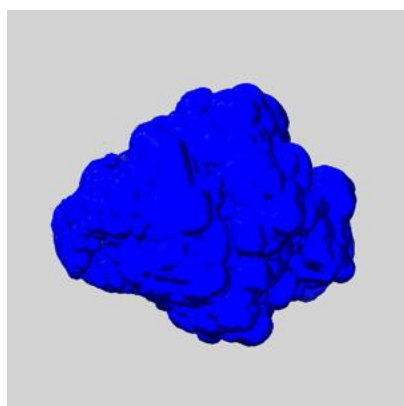
6.6 Mask visualisation [i](#)

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

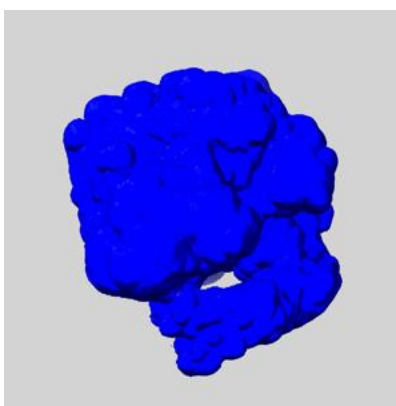
A mask typically either:

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

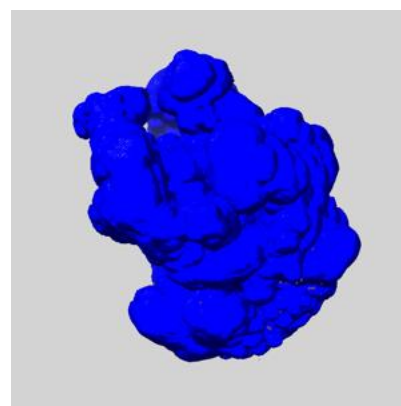
6.6.1 emd_42280_msk_1.map [i](#)



X



Y

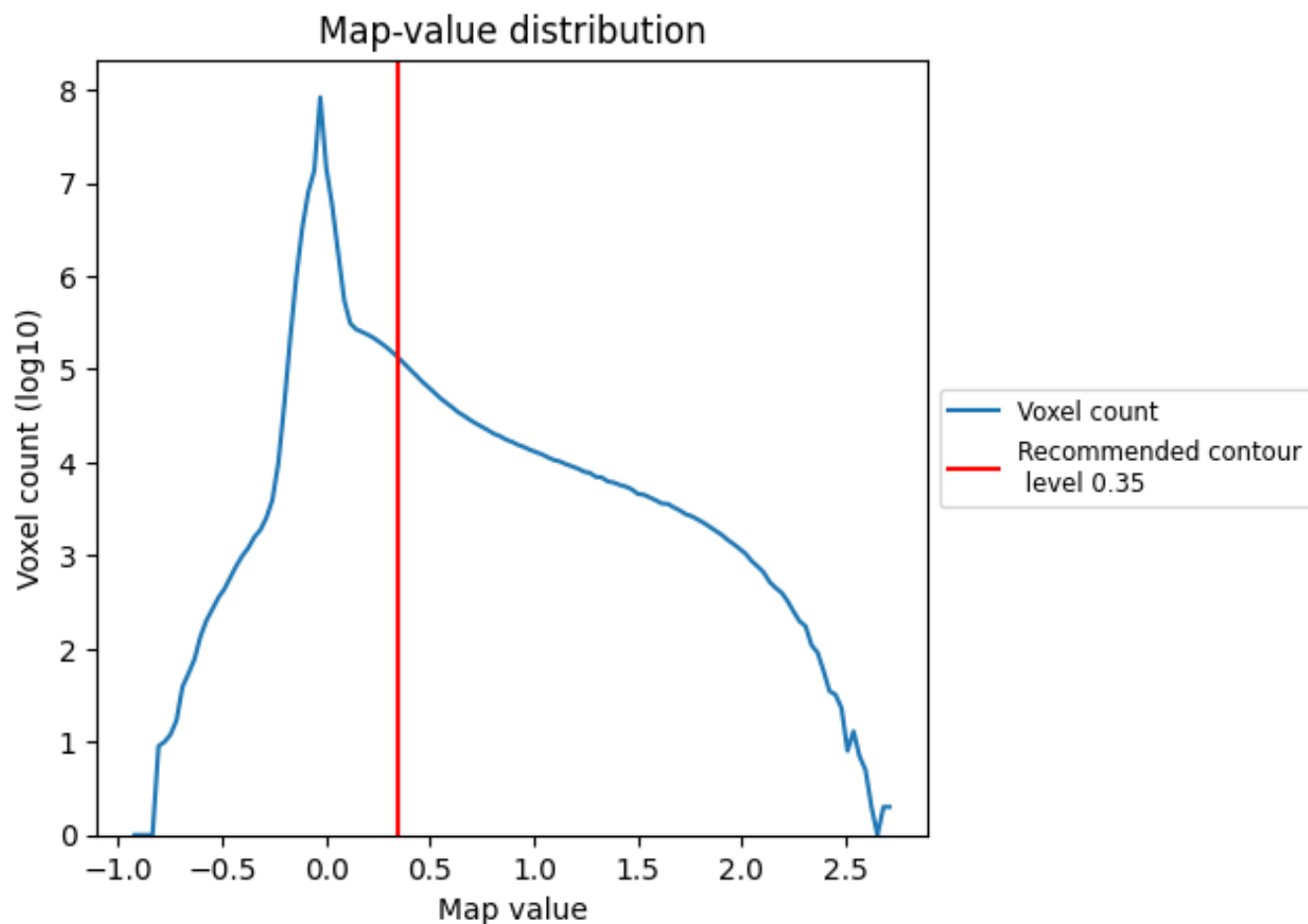


Z

7 Map analysis [i](#)

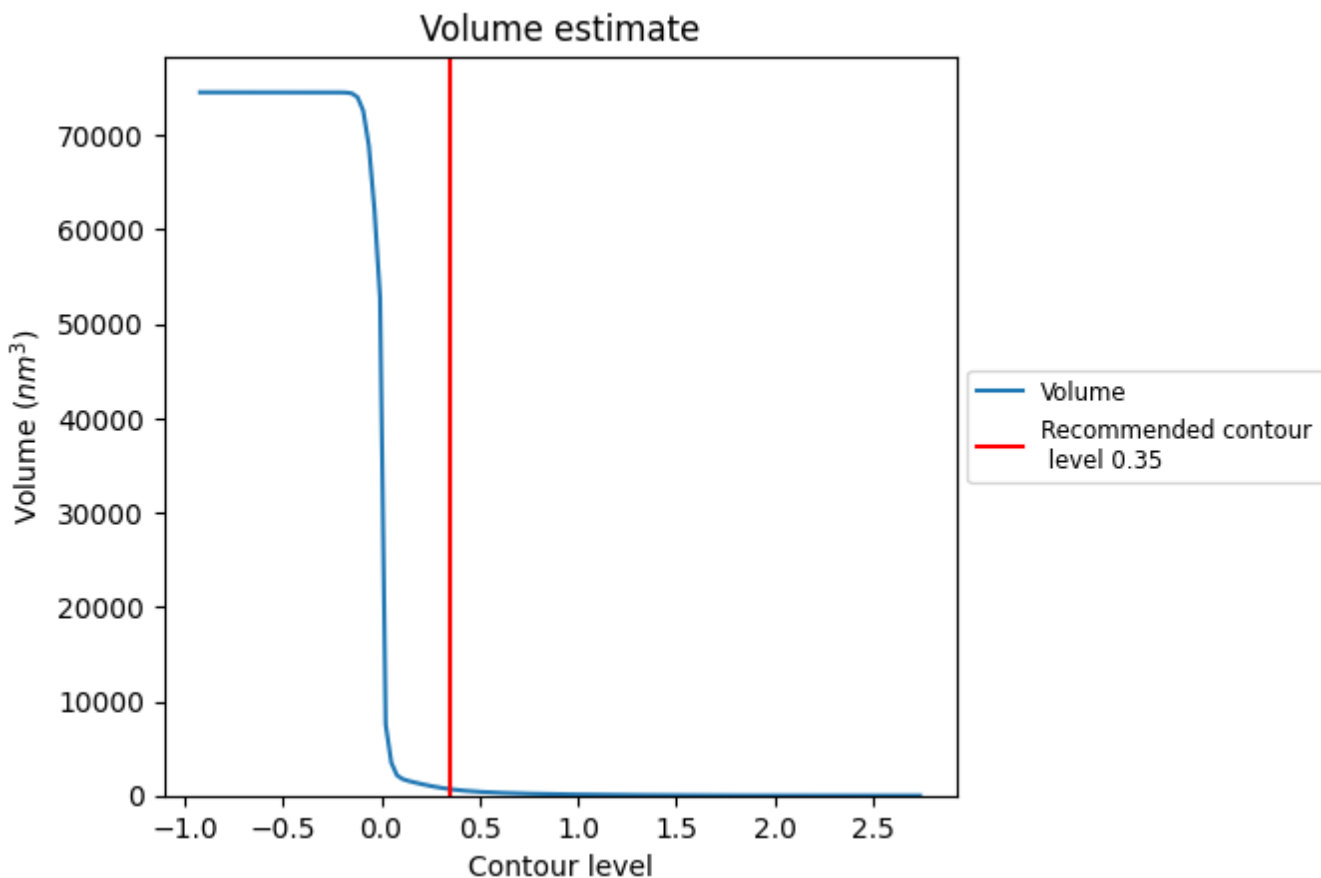
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

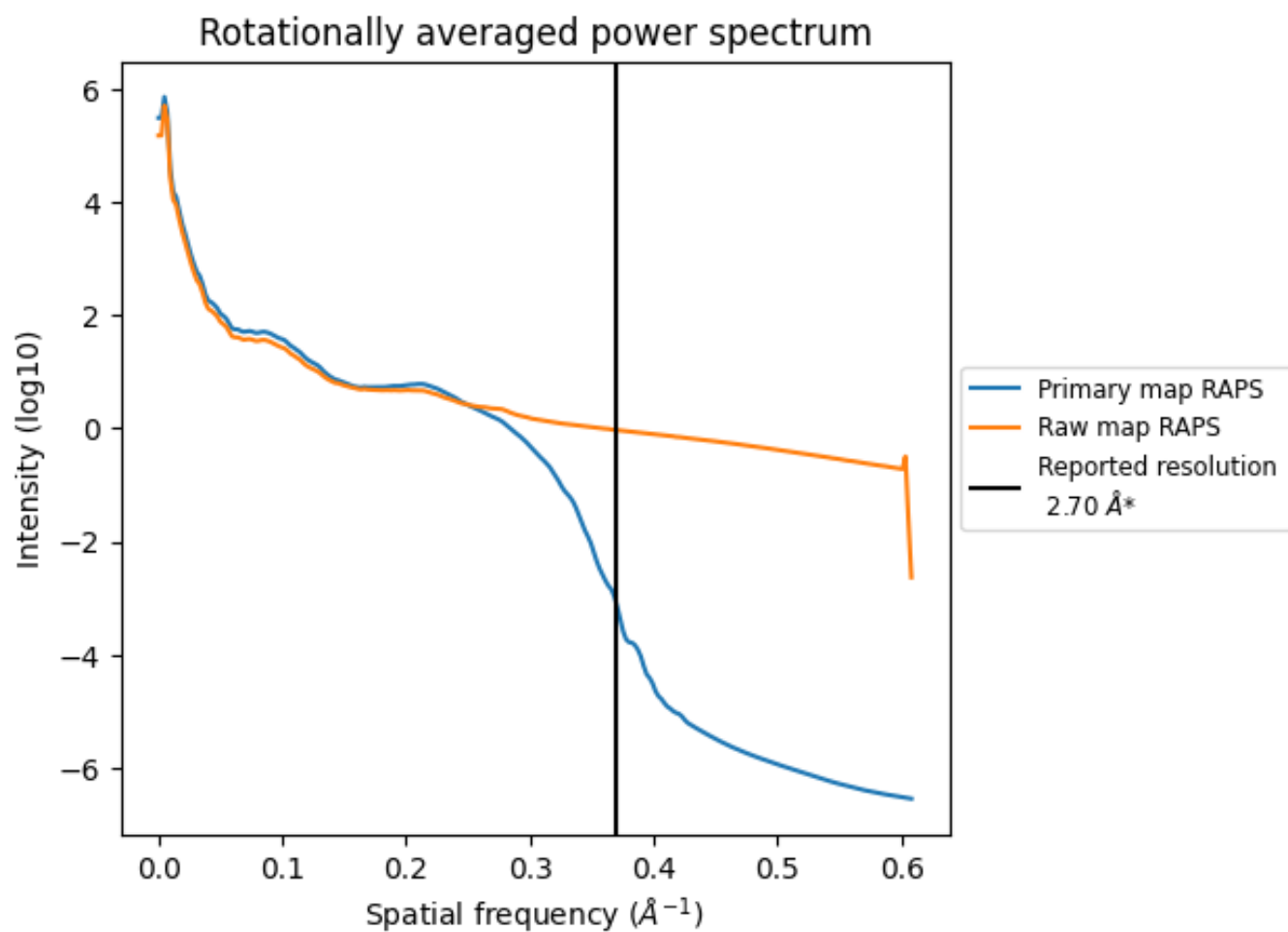
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 683 nm³; this corresponds to an approximate mass of 617 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](#)

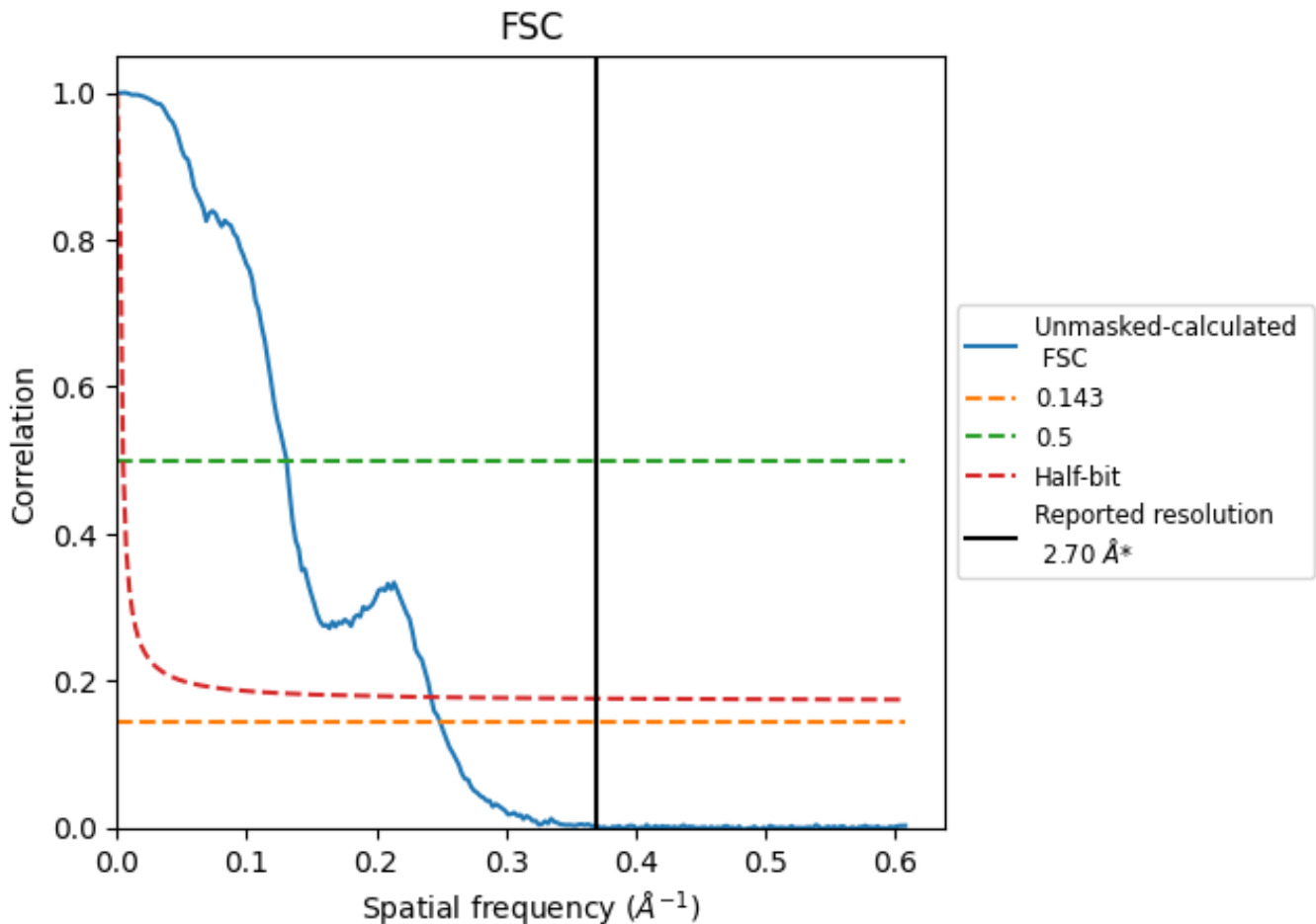


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

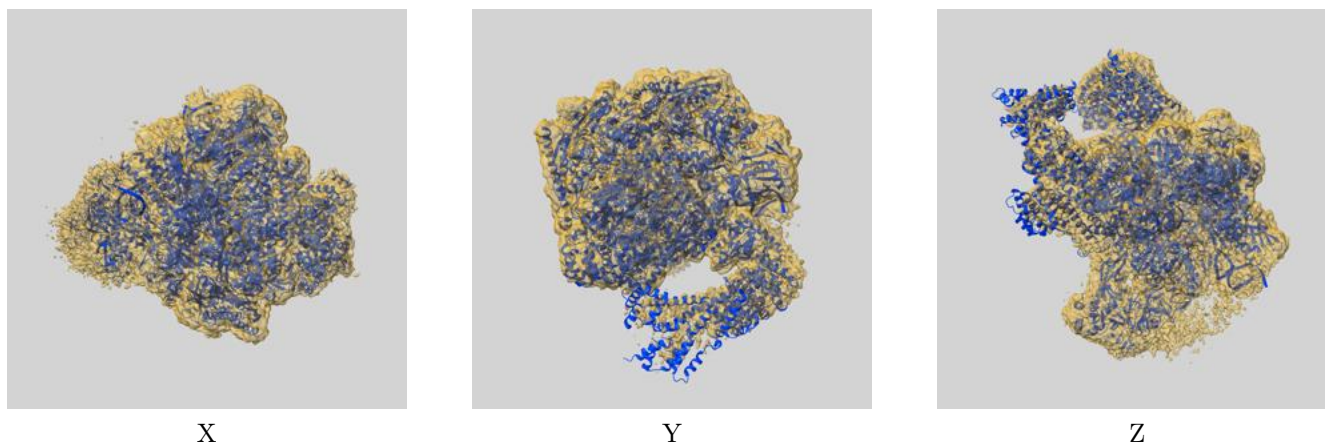
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.65	4.13

*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 4.01 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

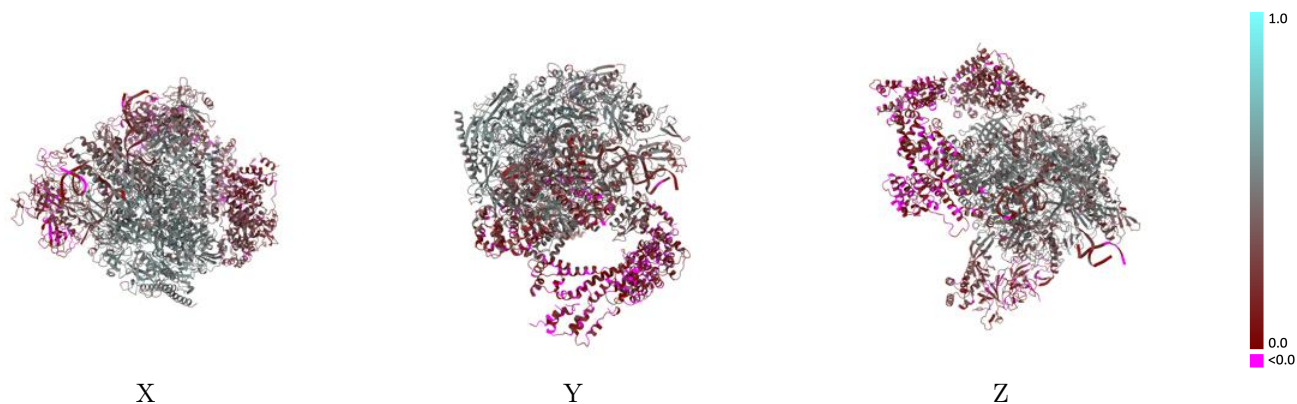
This section contains information regarding the fit between EMDB map EMD-42280 and PDB model 8UHG. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



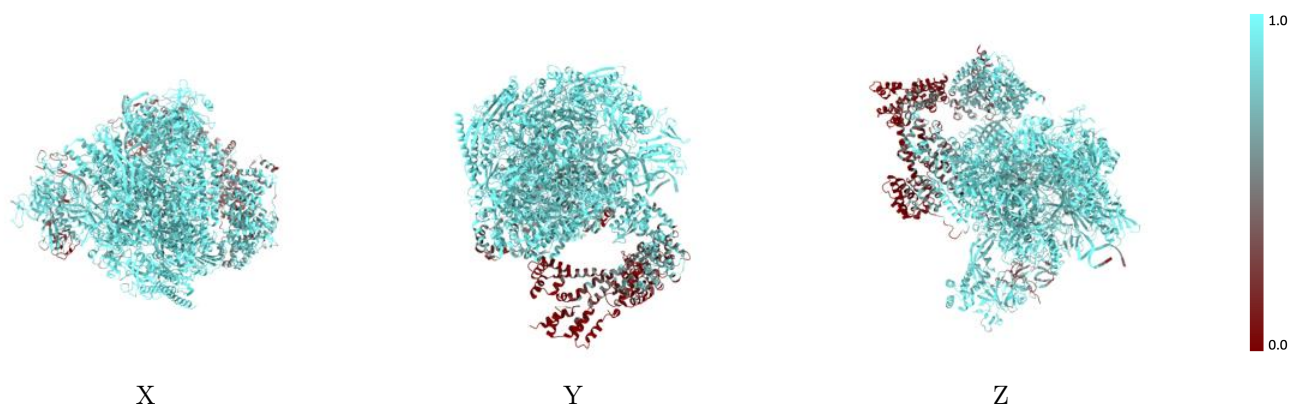
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



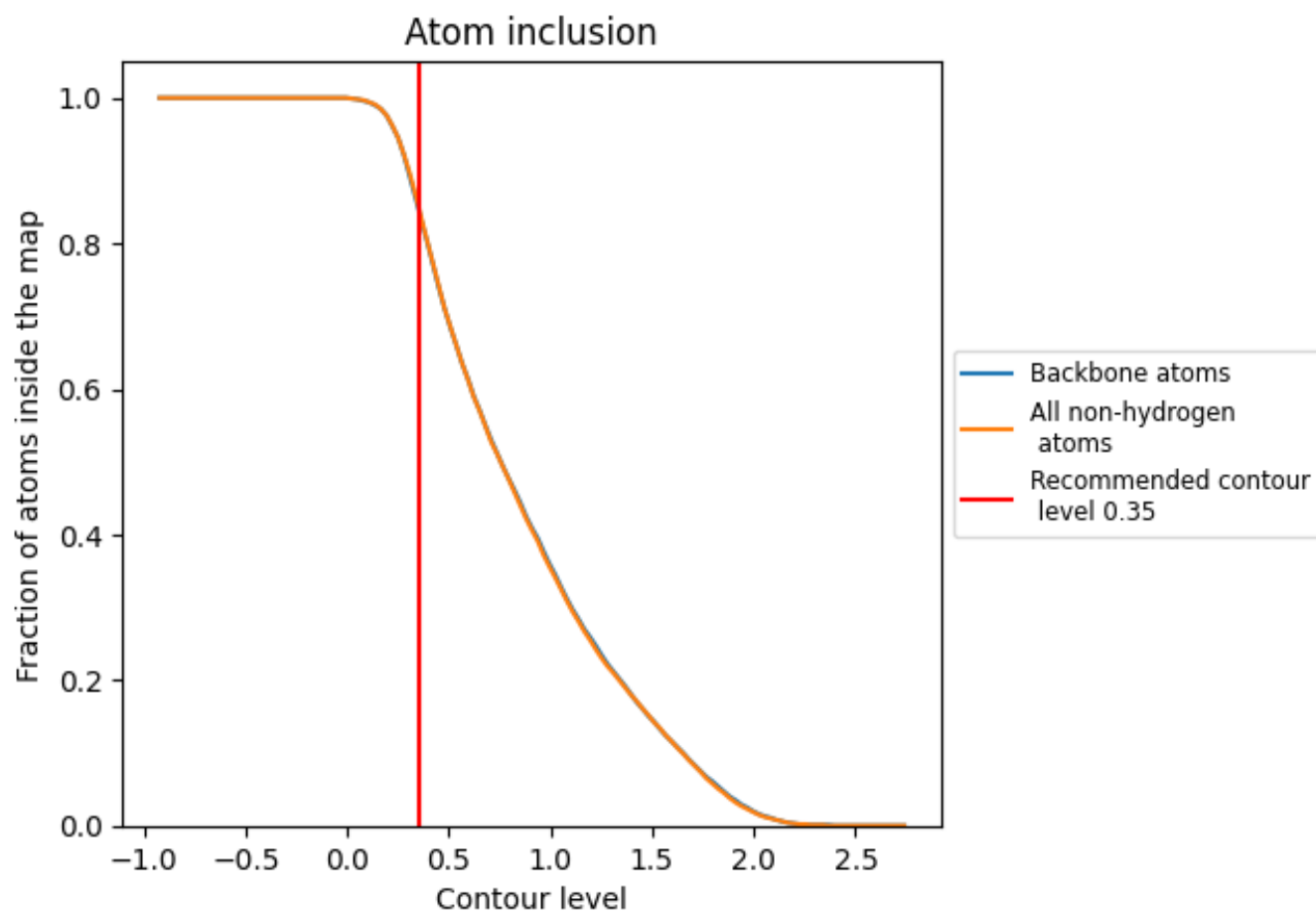
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.3530
A	 0.9580	 0.4470
B	 0.9660	 0.4720
C	 0.9850	 0.5020
D	 0.9690	 0.2100
E	 0.9640	 0.4140
F	 0.9870	 0.4910
G	 0.9670	 0.2600
H	 0.9730	 0.4830
I	 0.9800	 0.4170
J	 0.9790	 0.5150
K	 0.9780	 0.5030
L	 0.9890	 0.4710
N	 0.8730	 0.1520
P	 0.9620	 0.3350
T	 0.9140	 0.2540
U	 0.7430	 0.1840
V	 0.3890	 0.0780
W	 0.6280	 0.1790
X	 0.7900	 0.1130
Z	 0.6690	 0.1580

