



Full wwPDB EM Validation Report ⓘ

Jun 29, 2024 – 10:35 am BST

PDB ID : 8QP9
EMDB ID : EMD-18545
Title : Cryo-EM Structure of Pre-B+AMPPNP Complex (core part)
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on : 2023-09-30
Resolution : 4.10 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:

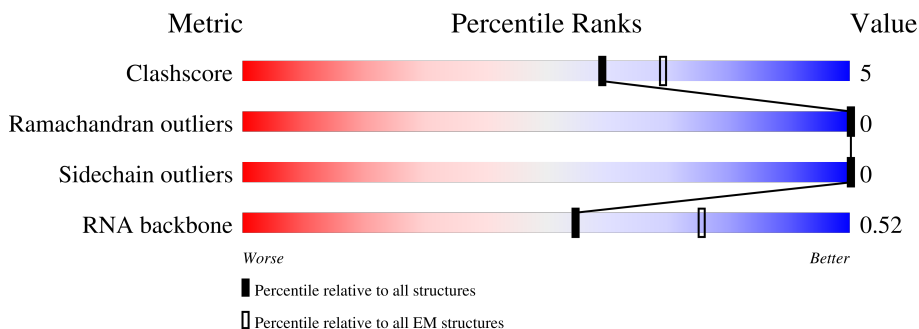
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 4.10 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	7	793	98%
2	B	2136	95%
3	C	972	78% (10% yellow, 12% grey)
4	D	142	96% (19% red, 5% orange)
5	J	683	94% (5% orange, 6% green)
6	L	499	90% (7% orange, 10% green)
7	R	480	78% (13% orange, 20% green)

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Mol	Chain	Length	Quality of chain
8	S	800	<p>5% 7% 93%</p>
9	U	565	<p>5% 77% 19%</p>
10	X	155	<p>12% 16% 83%</p>
11	G	820	<p>12% 88%</p>
12	6	106	<p>23% 17% 16% 65%</p>
13	5	117	<p>11% 27% 29% 39%</p>
14	4	144	<p>31% 21% 24% 8% 47%</p>
15	A	2335	<p>16% 80% 18%</p>
16	N	941	<p>16% 84%</p>

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 25123 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 Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	7	13	65	39	13	13	0	0

- Molecule 2 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	109	614	384	114	114	2	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	852	4924	3109	911	894	10	0	0

- Molecule 4 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	141	738	453	143	142	0	0

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	J	42	216	132	42	42	0	0

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	L	50	251	151	50	50	0	0

- Molecule 7 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	R	106	531	319	106	106	0	0

- Molecule 8 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	S	59	294	176	59	59	0	0

- Molecule 9 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	U	456	2308	1396	456	456	0	0

- Molecule 10 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	X	26	130	78	26	26	0	0

- Molecule 11 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	101	503	301	101	101	0	0

- Molecule 12 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	6	37	795	355	148	255	37	0	0

- Molecule 13 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	5	71	1496	672	257	497	70	0	0

- Molecule 14 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	4	76	1617	723	286	532	76	0	0

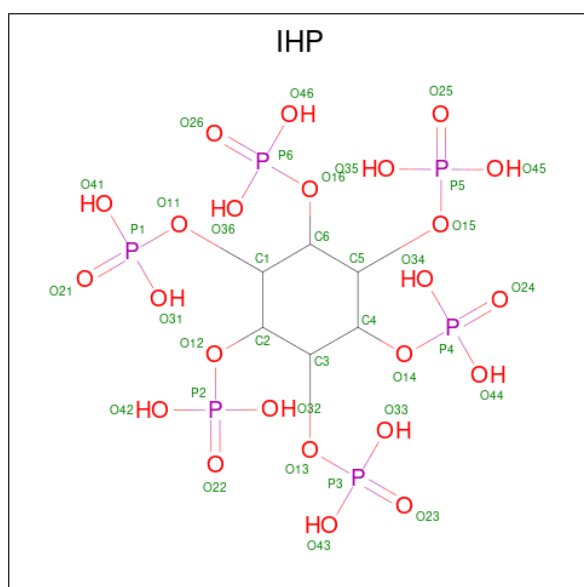
- Molecule 15 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	A	1916	9845	5994	1930	1919	2	0	0

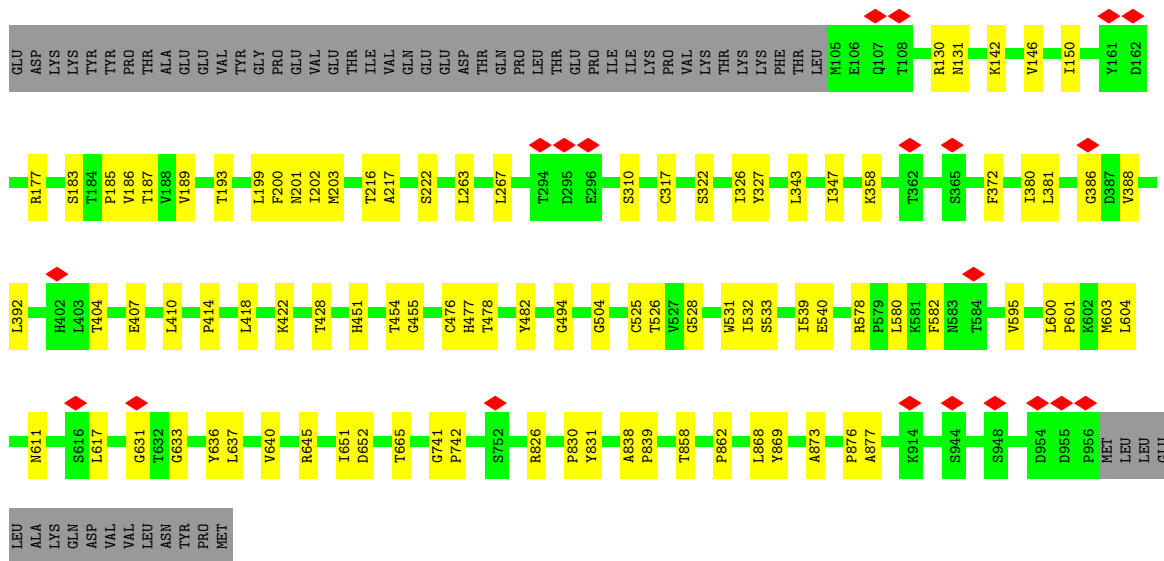
- Molecule 16 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	N	152	760	456	152	152	0	0

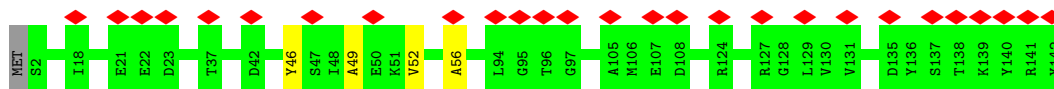
- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



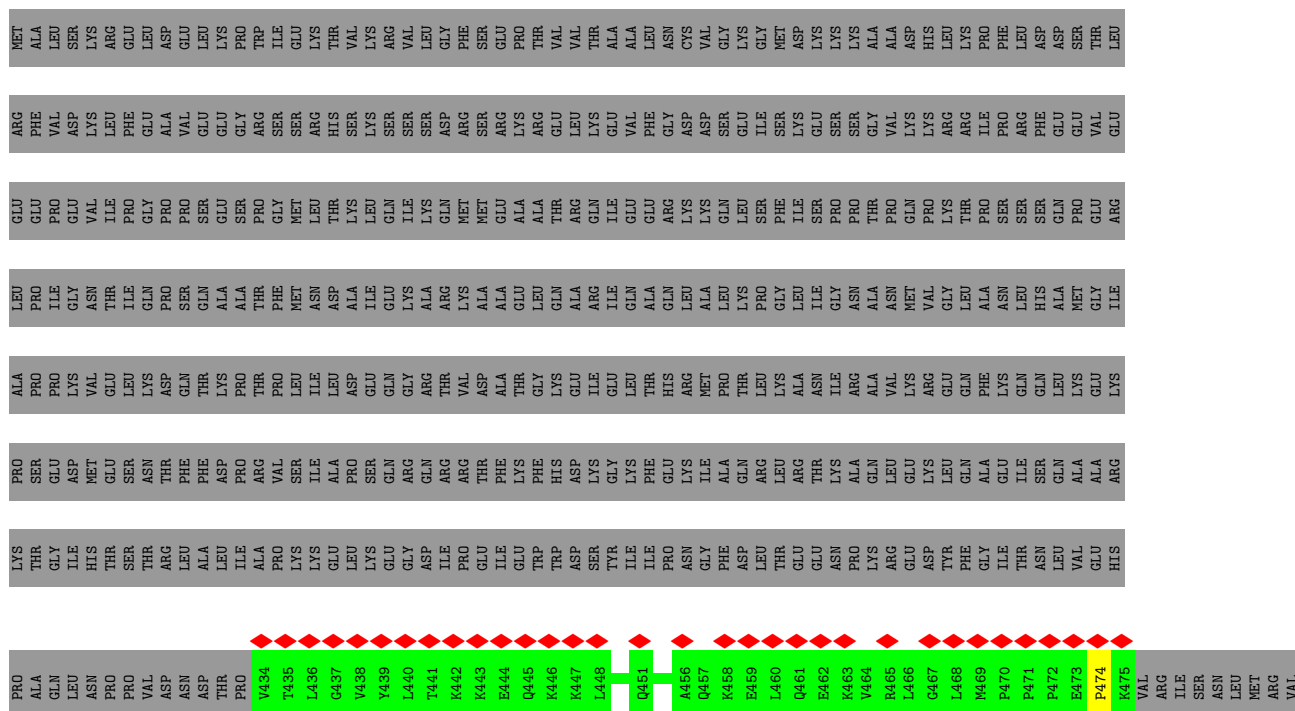
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	A	1	36	6	24	6	0

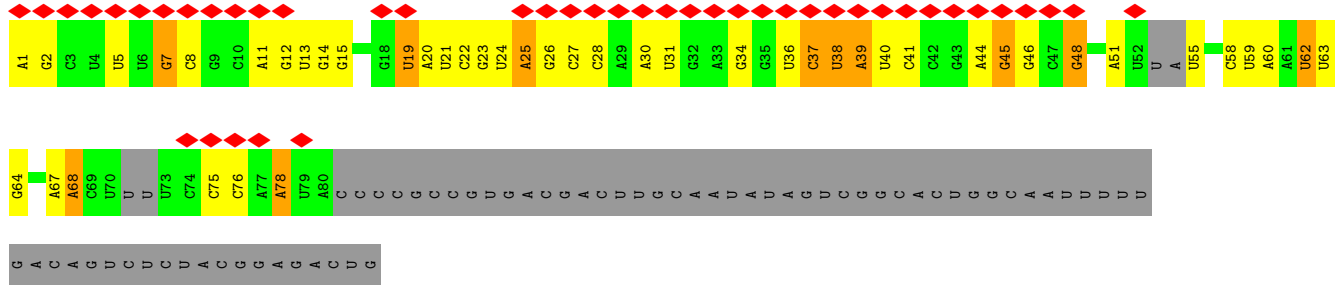


• Molecule 4: Thioredoxin-like protein 4A

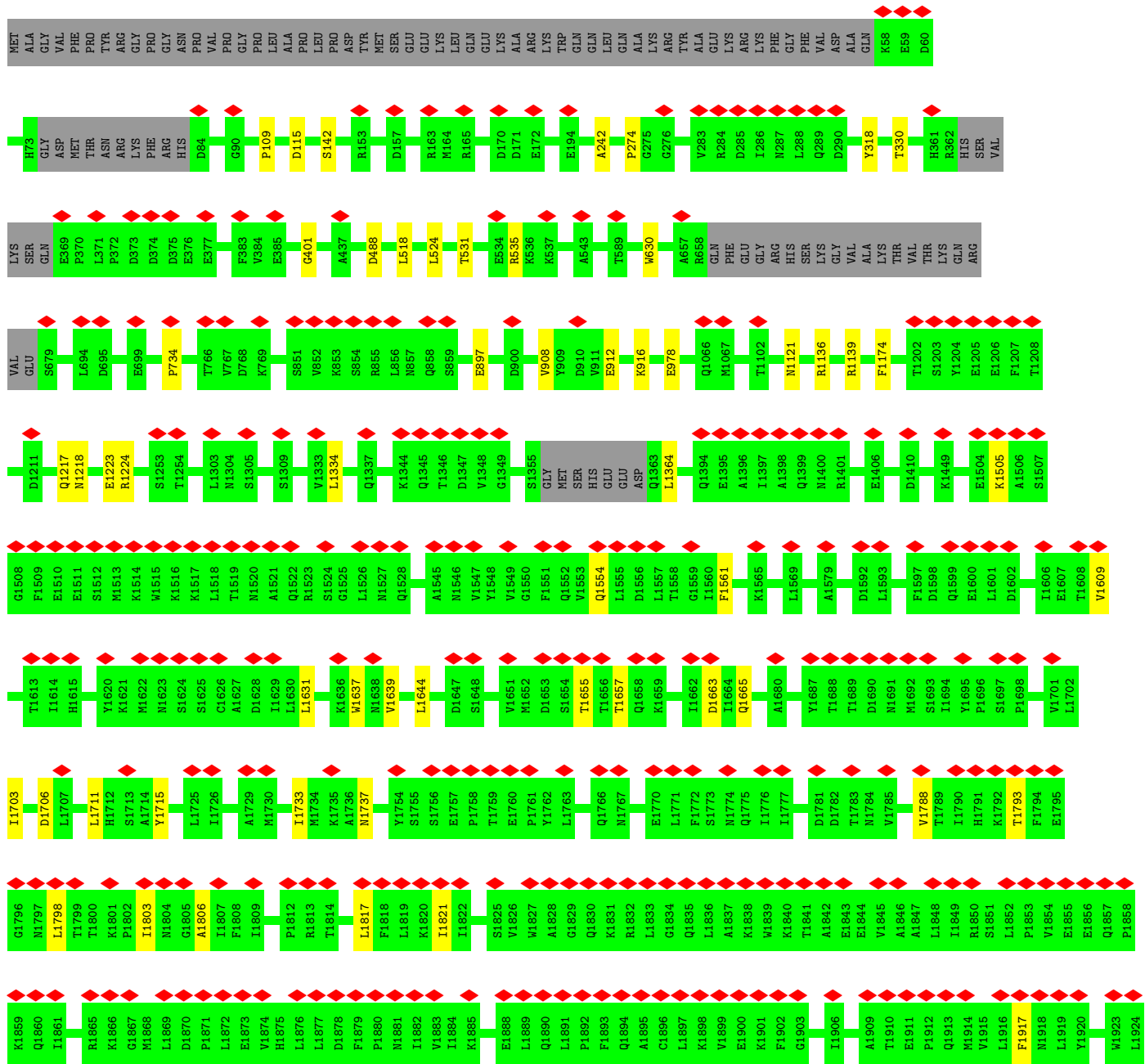
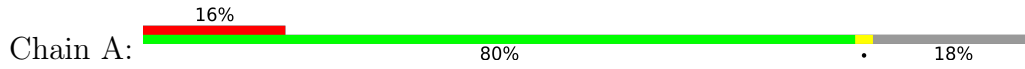


• Molecule 5: U4/U6 small nuclear ribonucleoprotein Prp3





● Molecule 15: Pre-mRNA-processing-splicing factor 8



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

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

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

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

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

ALA GLY ARG ILE LYS ASN THR PHE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53422	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.043	Depositor
Map size (Å)	648.0, 648.0, 648.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: IHP

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	7	0.22	0/64	0.31	0/88
2	B	0.24	0/620	0.35	0/857
3	C	0.25	0/5017	0.44	0/6973
4	D	0.24	0/747	0.41	0/1041
5	J	0.23	0/219	0.35	0/307
6	L	0.23	0/253	0.43	0/352
7	R	0.24	0/534	0.46	0/745
8	S	0.24	0/295	0.38	0/410
9	U	0.24	0/2330	0.43	0/3268
10	X	0.22	0/130	0.46	0/180
11	G	0.23	0/502	0.40	0/698
12	6	0.13	0/889	0.68	0/1382
13	5	0.17	0/1669	0.75	2/2594 (0.1%)
14	4	0.14	0/1805	0.69	0/2805
15	A	0.23	0/9965	0.40	0/13971
16	N	0.24	0/763	0.38	0/1061
All	All	0.23	0/25802	0.48	2/36732 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	23	C	C2-N1-C1'	5.77	125.15	118.80
13	5	23	C	N1-C2-O2	5.27	122.06	118.90

There are no chirality outliers.

There are no planarity outliers.

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	7	65	0	28	0	0
2	B	614	0	384	3	0
3	C	4924	0	3387	50	0
4	D	738	0	361	2	0
5	J	216	0	108	1	0
6	L	251	0	128	2	0
7	R	531	0	253	7	0
8	S	294	0	138	2	0
9	U	2308	0	1104	11	0
10	X	130	0	64	1	0
11	G	503	0	224	4	0
12	6	795	0	402	13	0
13	5	1496	0	759	18	0
14	4	1617	0	819	23	0
15	A	9845	0	4904	33	0
16	N	760	0	367	3	0
17	A	36	0	6	0	0
All	All	25123	0	13436	156	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 5.

All (156) 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)
3:C:525:CYS:SG	3:C:526:THR:N	2.60	0.75
3:C:386:GLY:HA2	15:A:401:GLY:HA3	1.70	0.74
14:4:64:G:H22	14:4:67:A:H5'	1.54	0.70
3:C:451:HIS:O	3:C:578:ARG:NH1	2.25	0.67
15:A:142:SER:HA	15:A:242:ALA:HB2	1.78	0.66
12:6:69:A:N6	14:4:5:U:O4	2.30	0.64
3:C:187:THR:N	3:C:533:SER:O	2.32	0.62
13:5:71:C:O2'	13:5:73:C:N4	2.30	0.61
16:N:78:TYR:HA	16:N:84:TYR:HA	1.81	0.61
13:5:74:U:H2'	13:5:75:G:C8	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:VAL:HG13	2:B:312:PHE:HA	1.81	0.61
14:4:22:C:H2'	14:4:23:G:C8	2.35	0.61
15:A:1136:ARG:HA	15:A:1139:ARG:HD3	1.83	0.60
3:C:645:ARG:NH2	15:A:318:TYR:O	2.35	0.59
3:C:603:MET:HB2	3:C:651:ILE:HD11	1.85	0.59
3:C:830:PRO:HG2	3:C:877:ALA:HB3	1.83	0.59
6:L:353:LYS:O	14:4:58:C:N4	2.34	0.59
3:C:310:SER:HA	3:C:317:CYS:HA	1.85	0.58
13:5:76:A:H2'	13:5:77:G:H8	1.69	0.58
3:C:150:ILE:HD11	3:C:186:VAL:HG21	1.86	0.58
15:A:1334:LEU:HA	15:A:1364:LEU:HA	1.85	0.57
3:C:476:CYS:SG	3:C:477:HIS:N	2.78	0.57
14:4:24:U:O2'	14:4:48:G:N2	2.31	0.57
15:A:1217:GLN:HA	15:A:1224:ARG:HA	1.85	0.56
3:C:839:PRO:HA	3:C:868:LEU:HA	1.88	0.56
11:G:348:ALA:O	11:G:352:TRP:N	2.39	0.56
14:4:13:U:H2'	14:4:14:G:H8	1.69	0.56
3:C:478:THR:HA	3:C:494:GLY:HA3	1.88	0.56
15:A:897:GLU:O	15:A:908:VAL:N	2.35	0.55
15:A:1788:VAL:HA	15:A:1803:ILE:H	1.70	0.55
3:C:636:TYR:O	3:C:640:VAL:HG23	2.08	0.54
8:S:721:THR:O	8:S:725:ALA:N	2.32	0.54
3:C:388:VAL:O	3:C:392:LEU:CB	2.56	0.54
15:A:1733:ILE:O	15:A:1737:ASN:N	2.41	0.53
3:C:217:ALA:HA	3:C:580:LEU:HD21	1.91	0.53
12:6:74:U:H2'	12:6:75:G:H8	1.73	0.52
9:U:429:LYS:O	9:U:440:LYS:N	2.40	0.52
9:U:135:ALA:HA	9:U:142:TYR:HA	1.89	0.52
9:U:520:LEU:HA	9:U:527:TRP:HA	1.92	0.52
3:C:600:LEU:HD23	15:A:1121:ASN:HA	1.91	0.52
13:5:47:A:O2'	13:5:48:A:O5'	2.23	0.51
3:C:404:THR:HG23	3:C:407:GLU:H	1.76	0.50
3:C:131:ASN:HB3	3:C:222:SER:HA	1.92	0.50
3:C:410:LEU:HD23	3:C:414:PRO:HB2	1.93	0.50
3:C:177:ARG:NH1	15:A:330:THR:O	2.45	0.50
3:C:831:TYR:HA	3:C:876:PRO:HA	1.94	0.49
13:5:12:U:H3	13:5:65:G:H1	1.59	0.49
14:4:59:U:H2'	14:4:60:A:C8	2.48	0.49
3:C:631:GLY:HA3	3:C:637:LEU:HD11	1.95	0.49
3:C:862:PRO:HA	3:C:869:TYR:HA	1.94	0.49
14:4:7:G:H2'	14:4:8:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1639:VAL:N	15:A:1655:THR:O	2.46	0.49
7:R:446:TYR:HA	7:R:451:PRO:HB3	1.94	0.49
9:U:457:ARG:O	9:U:468:ASN:N	2.45	0.49
13:5:66:A:O2'	13:5:67:A:H8	1.96	0.48
3:C:347:ILE:HG22	3:C:358:LYS:HA	1.95	0.48
12:6:33:G:H22	14:4:76:C:H2'	1.78	0.48
3:C:142:LYS:O	3:C:146:VAL:HG23	2.14	0.48
3:C:858:THR:H	3:C:873:ALA:HA	1.78	0.48
3:C:200:PHE:HB3	3:C:202:ILE:HG13	1.96	0.48
3:C:531:TRP:HA	3:C:540:GLU:HA	1.95	0.48
3:C:601:PRO:HA	3:C:604:LEU:HG	1.95	0.48
15:A:1637:TRP:N	15:A:1657:THR:O	2.47	0.48
9:U:430:GLU:HA	9:U:439:LEU:HA	1.96	0.48
14:4:19:U:O2'	14:4:20:A:O4'	2.30	0.48
9:U:460:LYS:HA	9:U:465:VAL:HA	1.95	0.48
14:4:11:A:H2'	14:4:12:G:H8	1.78	0.48
3:C:322:SER:O	3:C:326:ILE:HG12	2.14	0.47
12:6:55:C:H2'	12:6:56:A:C8	2.49	0.47
4:D:52:VAL:O	4:D:56:ALA:N	2.47	0.47
2:B:303:GLU:O	2:B:307:VAL:HG23	2.15	0.47
9:U:125:SER:N	9:U:142:TYR:O	2.47	0.47
11:G:283:SER:HA	15:A:274:PRO:HB3	1.97	0.47
6:L:376:ASN:O	15:A:1505:LYS:N	2.38	0.46
12:6:32:U:O2	14:4:78:A:N6	2.48	0.46
15:A:115:ASP:HA	15:A:488:ASP:HA	1.97	0.46
15:A:518:LEU:HA	15:A:524:LEU:HA	1.97	0.46
15:A:1644:LEU:HA	15:A:1715:TYR:HA	1.97	0.46
16:N:255:LEU:O	16:N:259:SER:N	2.40	0.46
4:D:46:TYR:HA	4:D:49:ALA:HB2	1.98	0.46
12:6:58:G:N3	14:4:55:U:N3	2.56	0.46
13:5:63:A:H2'	13:5:64:G:C8	2.51	0.46
14:4:64:G:N2	14:4:67:A:H5'	2.28	0.46
3:C:532:ILE:N	3:C:539:ILE:O	2.40	0.46
3:C:504:GLY:H	3:C:528:GLY:HA2	1.81	0.46
15:A:1793:THR:H	15:A:1798:LEU:HA	1.81	0.46
12:6:48:A:H5''	12:6:49:G:H21	1.80	0.45
14:4:37:C:O2'	14:4:38:U:H5'	2.16	0.45
15:A:1665:GLN:N	15:A:1703:ILE:O	2.46	0.45
13:5:23:C:H5''	13:5:24:G:H2'	1.99	0.45
7:R:387:ASP:N	14:4:68:A:N1	2.64	0.45
3:C:189:VAL:HA	3:C:199:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1817:LEU:O	15:A:1917:PHE:N	2.50	0.45
7:R:383:ILE:N	7:R:427:VAL:O	2.34	0.44
13:5:12:U:H2'	13:5:13:C:C6	2.52	0.44
13:5:75:G:H2'	13:5:76:A:O4'	2.17	0.44
15:A:531:THR:O	15:A:535:ARG:N	2.46	0.44
15:A:1663:ASP:O	15:A:1703:ILE:N	2.47	0.44
14:4:39:A:H4'	14:4:40:U:H5''	1.98	0.44
3:C:263:LEU:HD23	3:C:267:LEU:HD12	1.98	0.44
3:C:611:ASN:HA	3:C:617:LEU:HD23	1.99	0.44
7:R:382:ARG:HA	7:R:428:SER:HA	2.00	0.44
11:G:242:ASP:O	11:G:246:GLU:N	2.46	0.44
12:6:60:C:H2'	12:6:61:C:C6	2.52	0.44
14:4:11:A:H2'	14:4:12:G:C8	2.51	0.44
12:6:60:C:H42	14:4:15:G:H1	1.66	0.44
3:C:183:SER:O	3:C:482:TYR:OH	2.25	0.44
3:C:633:GLY:O	3:C:637:LEU:HD13	2.18	0.44
14:4:45:G:H2'	14:4:46:G:C8	2.52	0.43
14:4:62:U:H2'	14:4:63:U:C6	2.53	0.43
3:C:185:PRO:HA	3:C:203:MET:HA	1.99	0.43
3:C:193:THR:HA	3:C:428:THR:HB	2.00	0.43
12:6:59:G:H2'	12:6:60:C:C6	2.53	0.43
7:R:385:CYS:O	7:R:425:GLY:N	2.41	0.43
15:A:1609:VAL:HA	15:A:1631:LEU:HA	2.01	0.43
3:C:454:THR:HG22	3:C:455:GLY:N	2.33	0.43
12:6:53:A:H2'	12:6:54:G:C8	2.54	0.43
13:5:17:U:H2'	13:5:18:C:C6	2.53	0.43
3:C:130:ARG:O	3:C:201:ASN:N	2.43	0.42
3:C:380:ILE:HG13	3:C:381:LEU:HD12	2.02	0.42
15:A:1928:SER:O	15:A:1932:ALA:N	2.44	0.42
13:5:53:U:H2'	13:5:54:U:C6	2.54	0.42
14:4:27:C:H2'	14:4:28:C:C6	2.55	0.42
15:A:1554:GLN:HA	15:A:1561:PHE:HA	2.00	0.42
3:C:216:THR:HG21	3:C:582:PHE:HA	2.01	0.42
3:C:327:TYR:OH	3:C:372:PHE:O	2.37	0.42
13:5:63:A:H2'	13:5:64:G:H8	1.84	0.42
14:4:24:U:H5''	14:4:25:A:O5'	2.19	0.42
15:A:1706:ASP:N	15:A:1711:LEU:O	2.42	0.42
15:A:1806:ALA:HA	15:A:1821:ILE:HA	2.01	0.42
3:C:343:LEU:HD11	3:C:372:PHE:HB2	2.02	0.41
9:U:213:SER:N	9:U:221:TYR:O	2.53	0.41
13:5:47:A:O2'	13:5:48:A:H8	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:418:LEU:HD21	3:C:422:LYS:HZ2	1.84	0.41
3:C:665:THR:O	3:C:826:ARG:N	2.53	0.41
3:C:741:GLY:HA2	3:C:742:PRO:HD3	1.86	0.41
9:U:431:TYR:N	9:U:438:PHE:O	2.42	0.41
15:A:912:GLU:O	15:A:916:LYS:N	2.40	0.41
2:B:290:LEU:HD23	2:B:290:LEU:HA	1.91	0.41
8:S:733:PHE:O	10:X:141:MET:N	2.37	0.41
3:C:595:VAL:HG22	3:C:652:ASP:O	2.20	0.41
3:C:838:ALA:O	3:C:869:TYR:N	2.54	0.41
7:R:408:LEU:N	7:R:428:SER:O	2.53	0.41
13:5:29:A:H2'	13:5:30:A:C8	2.56	0.41
13:5:47:A:HO2'	13:5:48:A:P	2.43	0.41
15:A:1218:ASN:N	15:A:1223:GLU:O	2.54	0.41
5:J:474:PRO:O	12:6:56:A:O2'	2.39	0.41
11:G:271:LYS:O	13:5:45:C:N4	2.46	0.40
15:A:978:GLU:O	15:A:1174:PHE:N	2.54	0.40
7:R:414:ARG:HA	7:R:421:THR:HA	2.04	0.40
9:U:266:PRO:HA	9:U:267:PRO:HD3	1.96	0.40
12:6:50:A:H2'	12:6:51:U:C6	2.57	0.40
9:U:214:ARG:HA	9:U:220:THR:HA	2.03	0.40
13:5:76:A:H2'	13:5:77:G:C8	2.54	0.40
15:A:109:PRO:HD3	15:A:630:TRP:CZ2	2.57	0.40
15:A:734:PRO:HB2	16:N:149:LEU:HA	2.02	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	7	11/793 (1%)	11 (100%)	0	0	100	100
2	B	107/2136 (5%)	104 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	850/972 (87%)	822 (97%)	28 (3%)	0	100	100
4	D	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
5	J	40/683 (6%)	40 (100%)	0	0	100	100
6	L	48/499 (10%)	42 (88%)	6 (12%)	0	100	100
7	R	104/480 (22%)	99 (95%)	5 (5%)	0	100	100
8	S	57/800 (7%)	56 (98%)	1 (2%)	0	100	100
9	U	454/565 (80%)	433 (95%)	21 (5%)	0	100	100
10	X	24/155 (16%)	24 (100%)	0	0	100	100
11	G	97/820 (12%)	92 (95%)	5 (5%)	0	100	100
15	A	1906/2335 (82%)	1858 (98%)	48 (2%)	0	100	100
16	N	146/941 (16%)	143 (98%)	3 (2%)	0	100	100
All	All	3983/11321 (35%)	3861 (97%)	122 (3%)	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	
2	B	20/1908 (1%)	20 (100%)	0	100	100
3	C	221/866 (26%)	221 (100%)	0	100	100
4	D	10/130 (8%)	10 (100%)	0	100	100
5	J	4/599 (1%)	4 (100%)	0	100	100
6	L	3/424 (1%)	3 (100%)	0	100	100
7	R	4/369 (1%)	4 (100%)	0	100	100
8	S	2/681 (0%)	2 (100%)	0	100	100
9	U	23/511 (4%)	23 (100%)	0	100	100
10	X	1/144 (1%)	1 (100%)	0	100	100
11	G	1/721 (0%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	A	127/2108 (6%)	127 (100%)	0	100	100
16	N	6/792 (1%)	6 (100%)	0	100	100
All	All	422/9253 (5%)	422 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	6	35/106 (33%)	4 (11%)	0
13	5	69/117 (58%)	20 (28%)	2 (2%)
14	4	74/144 (51%)	22 (29%)	1 (1%)
All	All	178/367 (48%)	46 (25%)	3 (1%)

All (46) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	6	36	A
12	6	49	G
12	6	59	G
12	6	77	C
13	5	4	C
13	5	7	U
13	5	21	A
13	5	23	C
13	5	25	C
13	5	28	A
13	5	36	C
13	5	37	G
13	5	38	C
13	5	47	A
13	5	48	A
13	5	57	G
13	5	58	U
13	5	59	G
13	5	67	A
13	5	69	A

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Mol	Chain	Res	Type
13	5	70	A
13	5	71	C
13	5	72	U
13	5	78	U
14	4	2	G
14	4	7	G
14	4	19	U
14	4	21	U
14	4	25	A
14	4	26	G
14	4	30	A
14	4	31	U
14	4	34	G
14	4	36	U
14	4	37	C
14	4	38	U
14	4	39	A
14	4	41	C
14	4	44	A
14	4	45	G
14	4	48	G
14	4	51	A
14	4	62	U
14	4	68	A
14	4	75	C
14	4	78	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	5	57	G
13	5	58	U
14	4	1	A

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

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	IHP	A	2401	-	36,36,36	0.68	0	54,60,60	0.95	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	IHP	A	2401	-	-	7/30/54/54	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

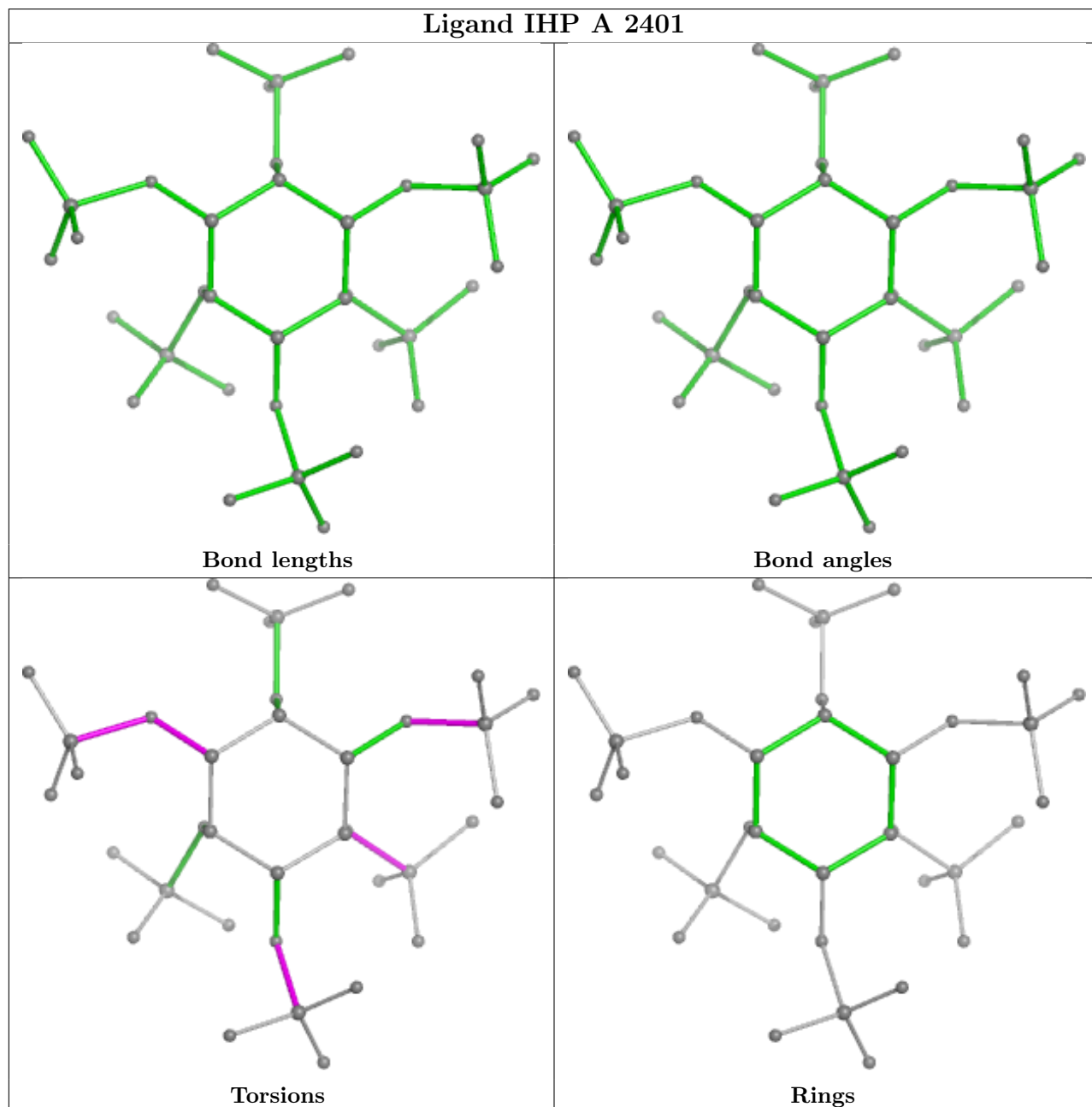
Mol	Chain	Res	Type	Atoms
17	A	2401	IHP	C3-C4-O14-P4
17	A	2401	IHP	C5-C4-O14-P4
17	A	2401	IHP	C6-O16-P6-O26
17	A	2401	IHP	C1-O11-P1-O31
17	A	2401	IHP	C2-O12-P2-O42
17	A	2401	IHP	C4-O14-P4-O44
17	A	2401	IHP	C6-O16-P6-O36

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

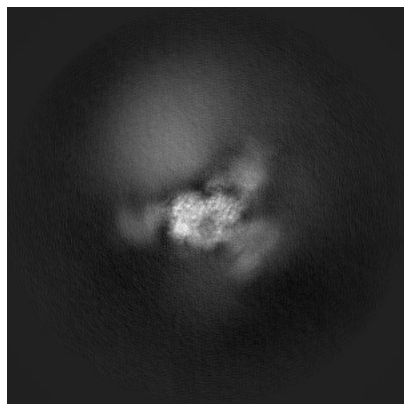
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18545. These allow visual inspection of the internal detail of the map and identification of artifacts.

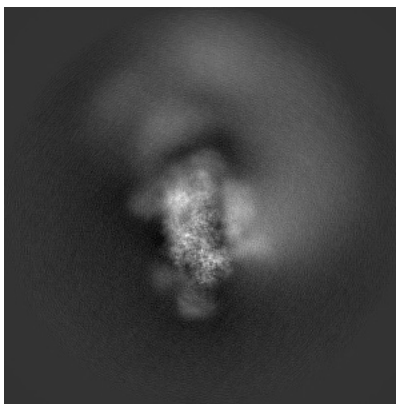
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

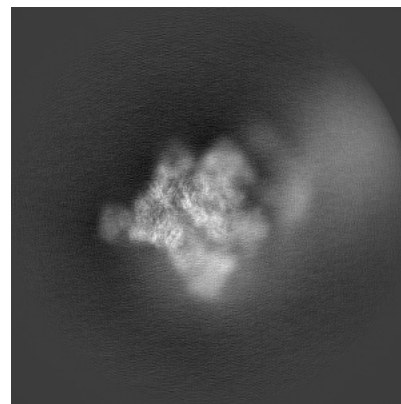
6.1.1 Primary map



X

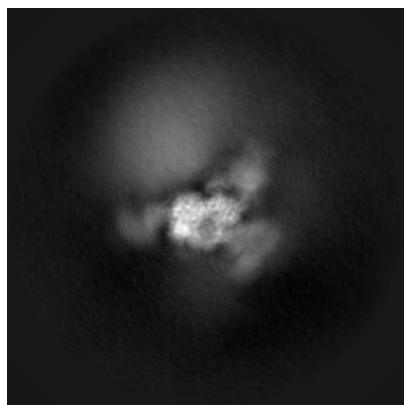


Y

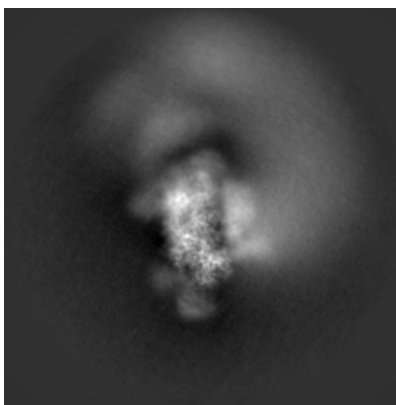


Z

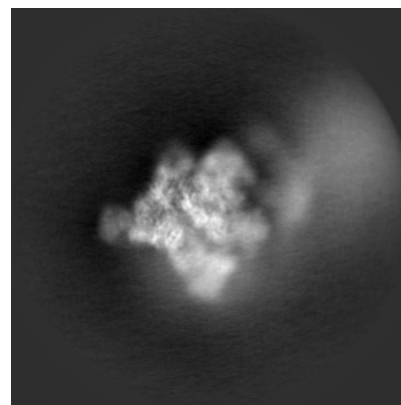
6.1.2 Raw map



X



Y

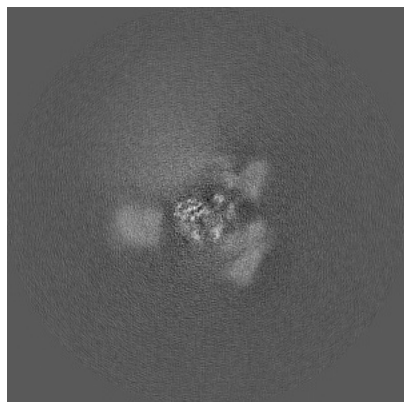


Z

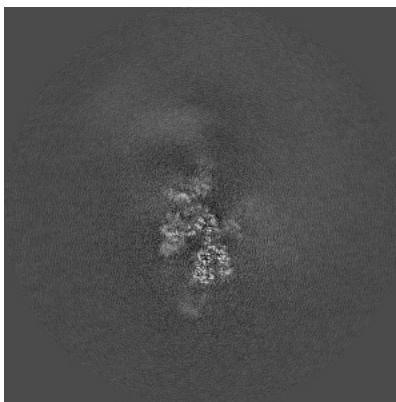
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

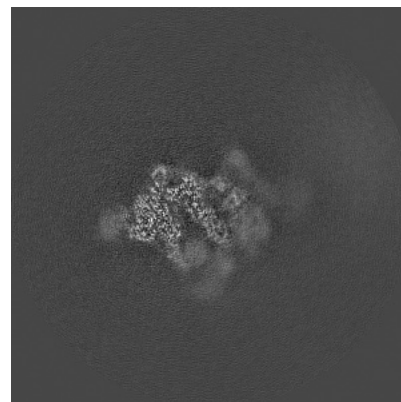
6.2.1 Primary map



X Index: 240

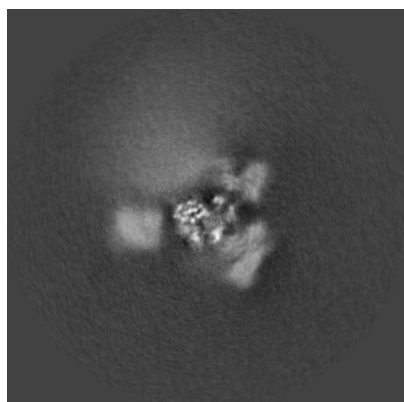


Y Index: 240

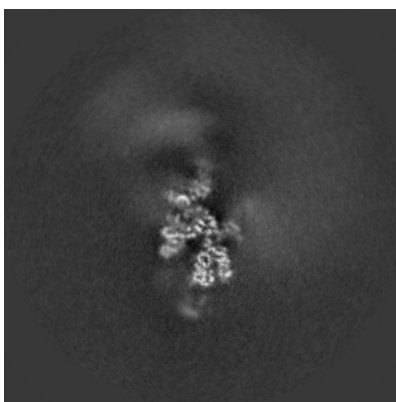


Z Index: 240

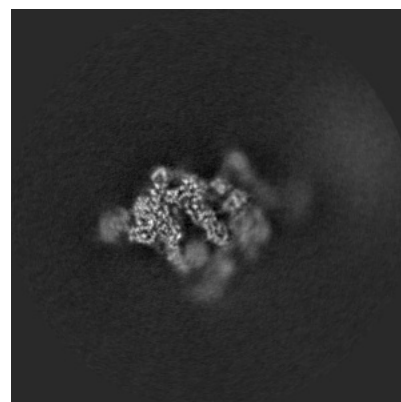
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

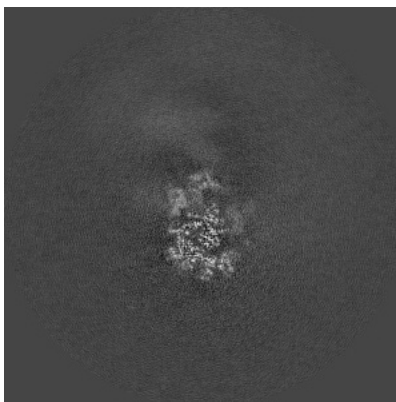
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

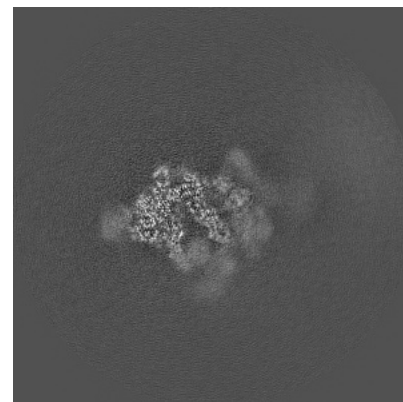
6.3.1 Primary map



X Index: 186

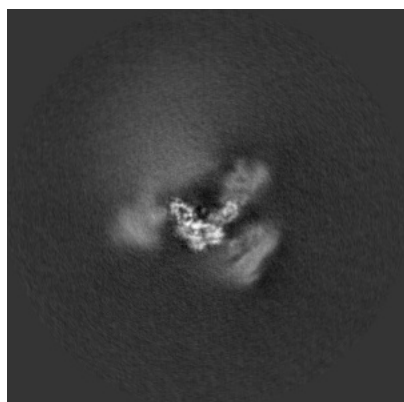


Y Index: 254

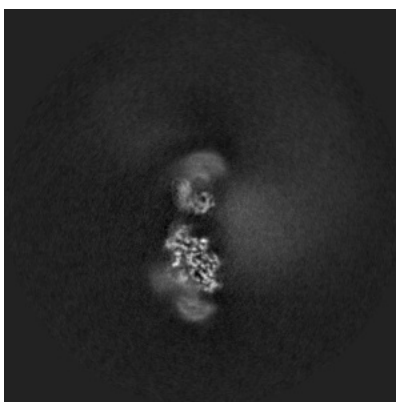


Z Index: 239

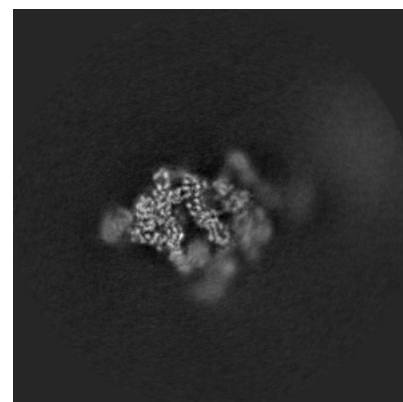
6.3.2 Raw map



X Index: 249



Y Index: 207

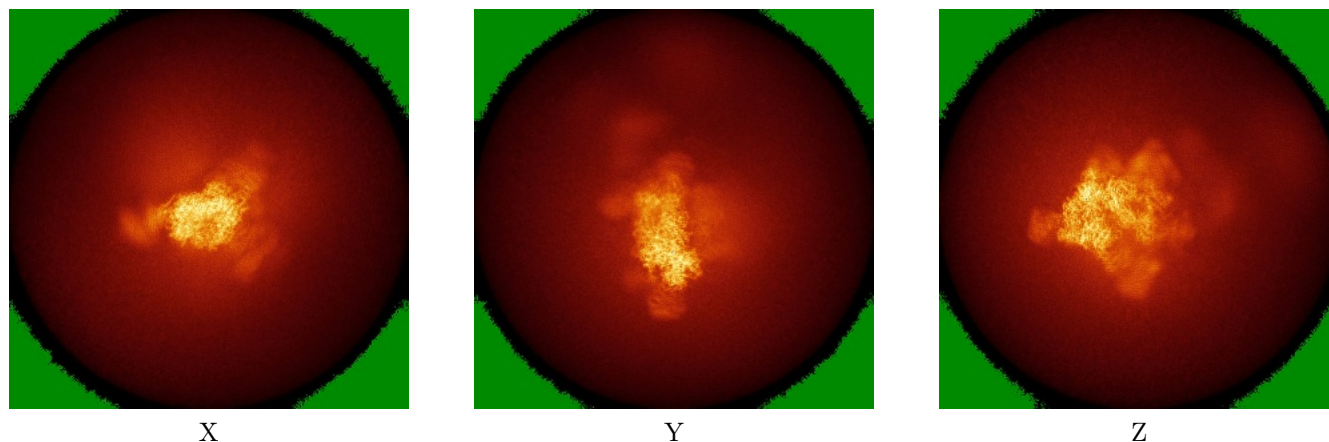


Z Index: 238

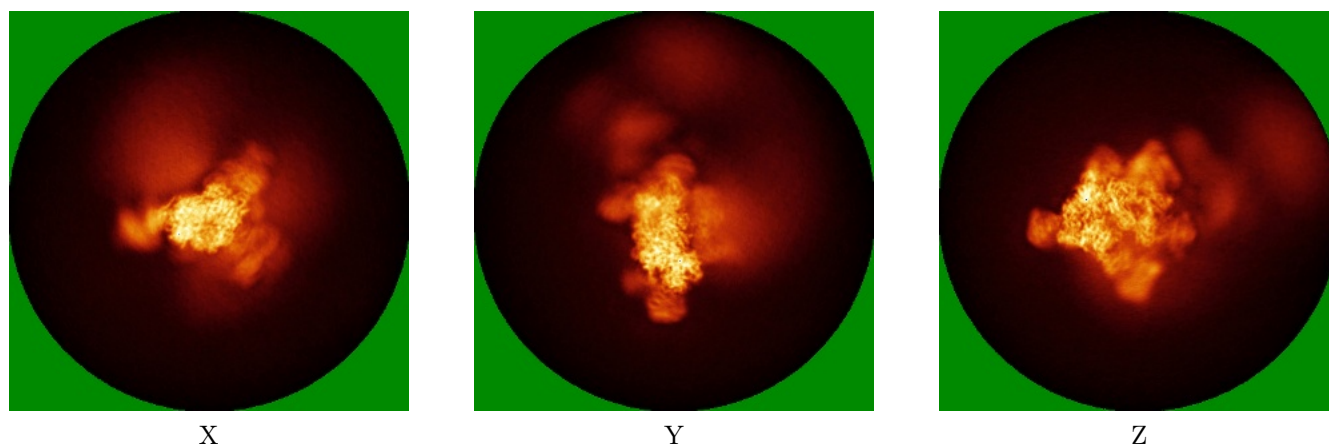
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



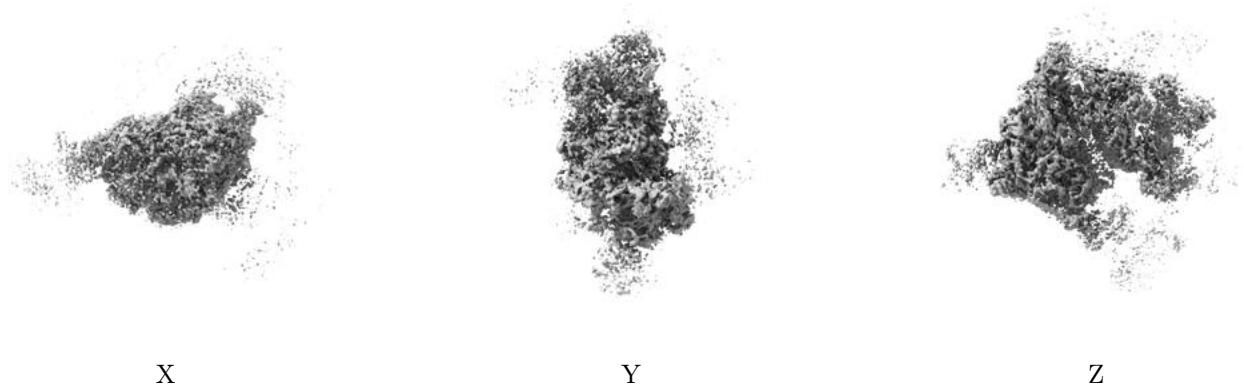
6.4.2 Raw map



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.

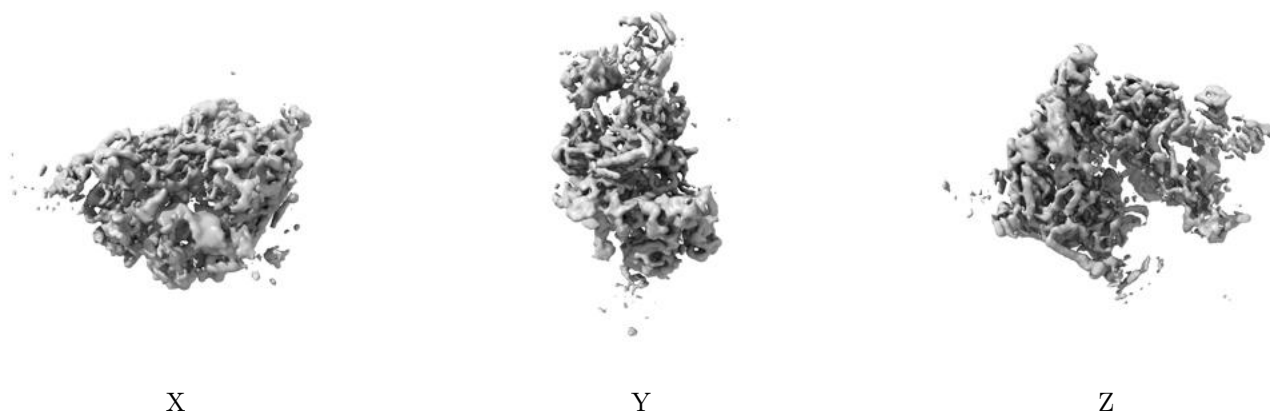
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.043. 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.

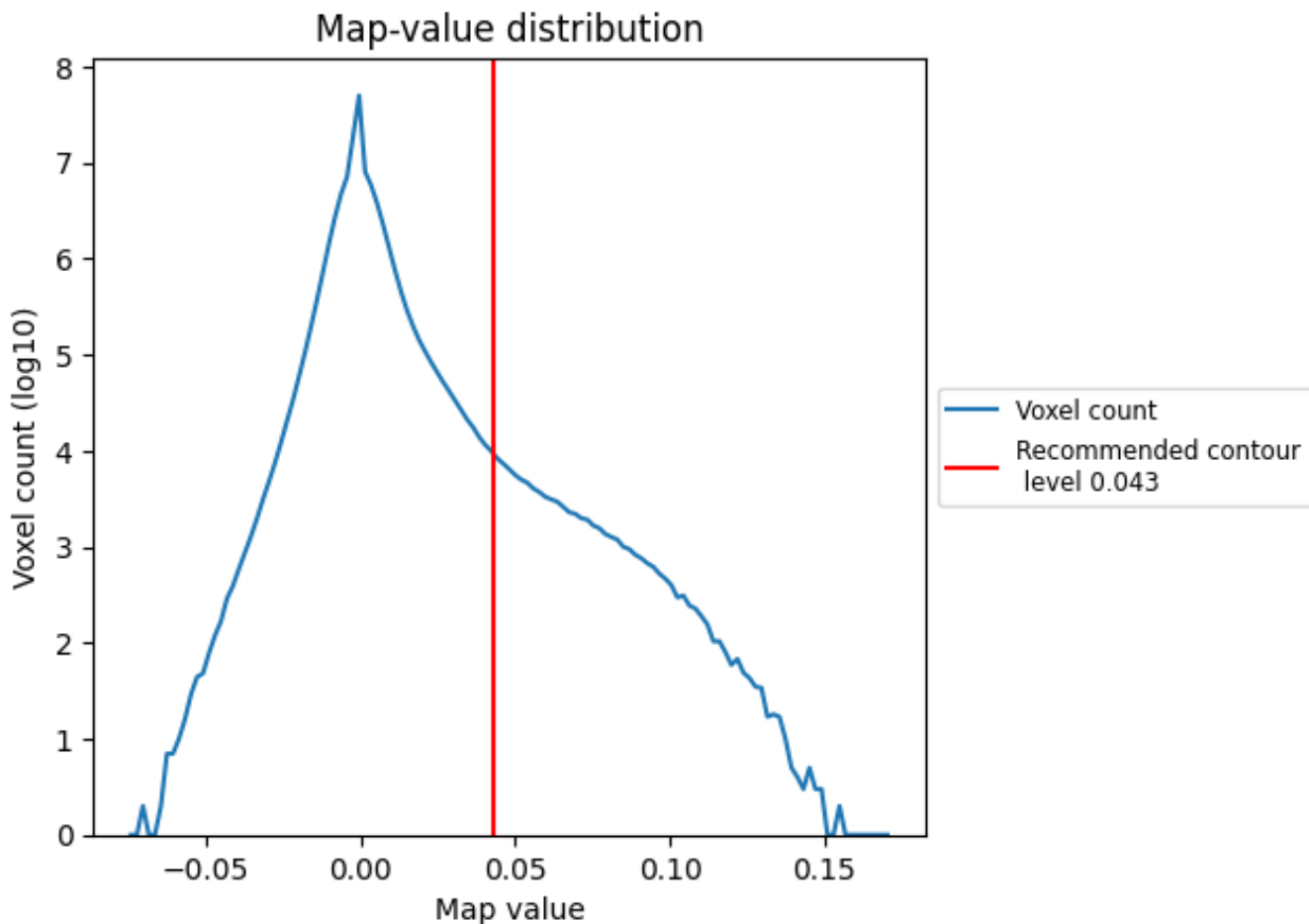
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

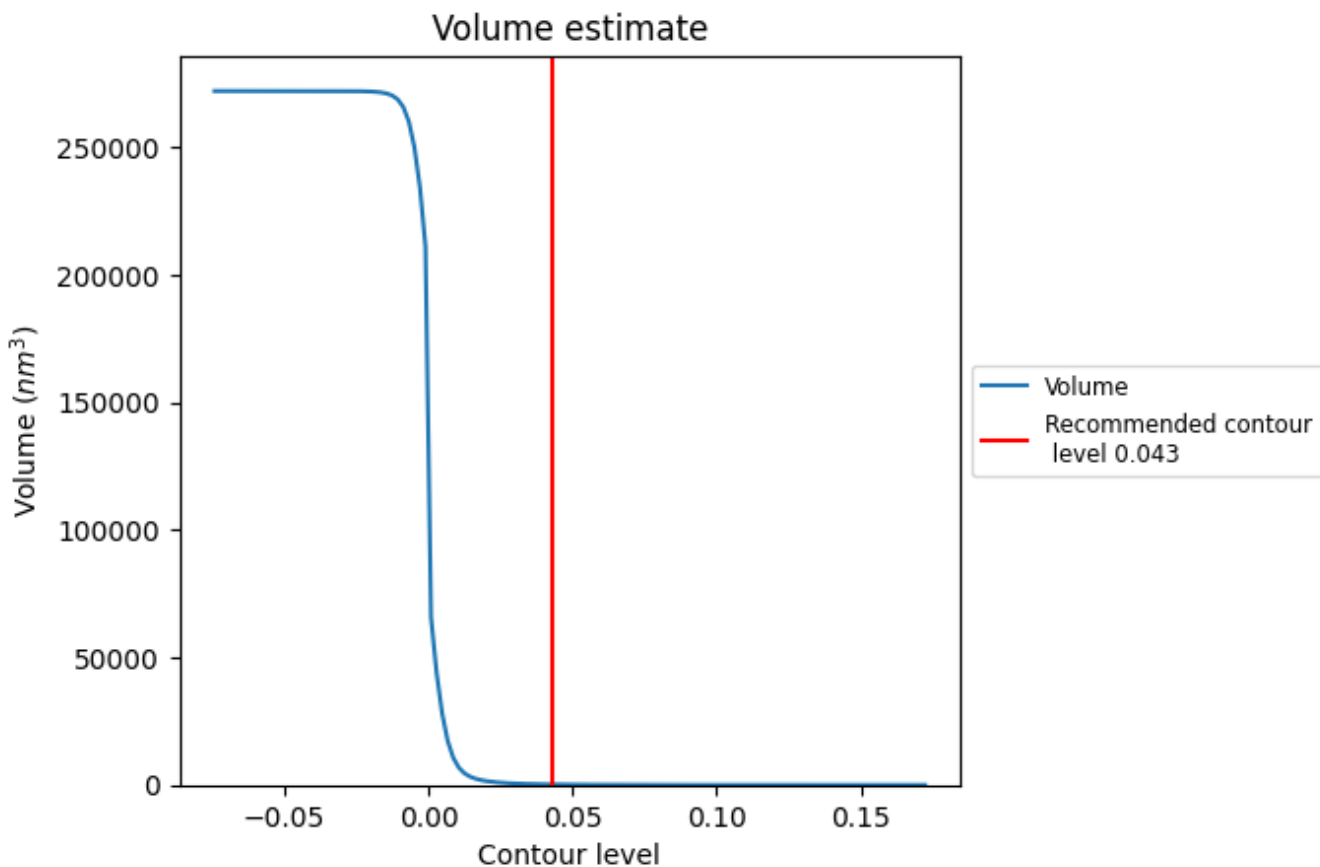
This section contains the results of statistical analysis of the map.

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.

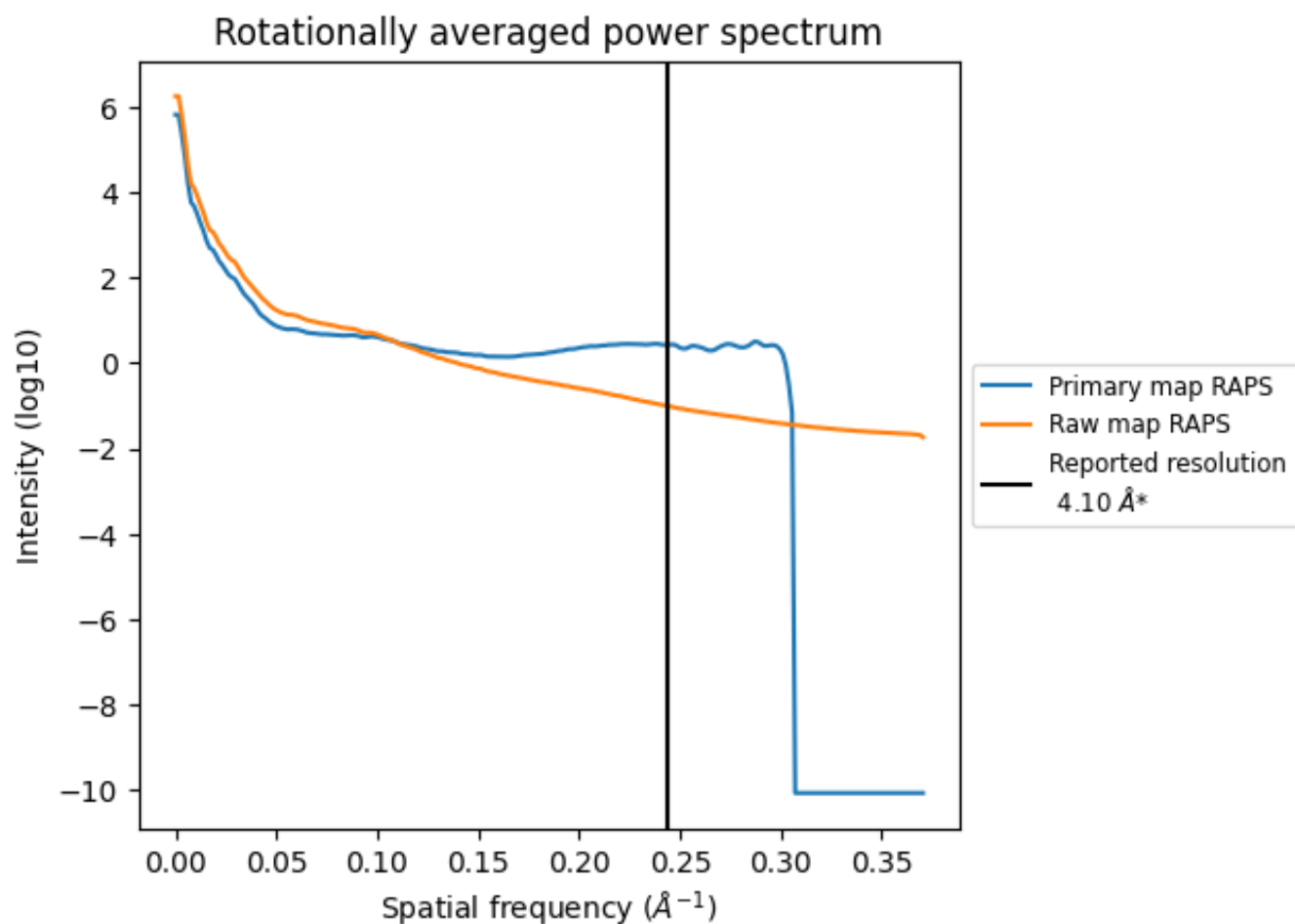
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 214 nm³; this corresponds to an approximate mass of 194 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](#)

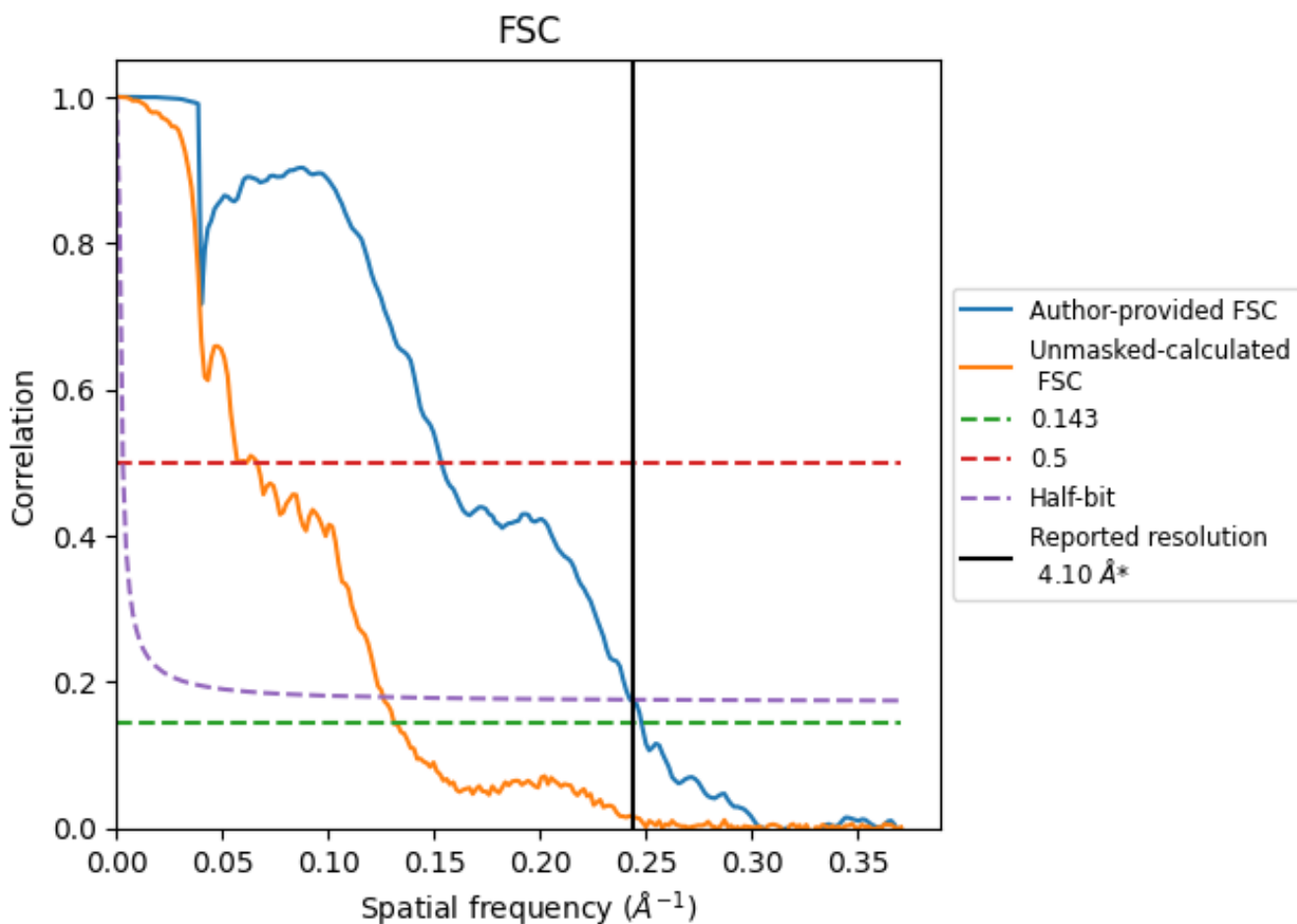


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

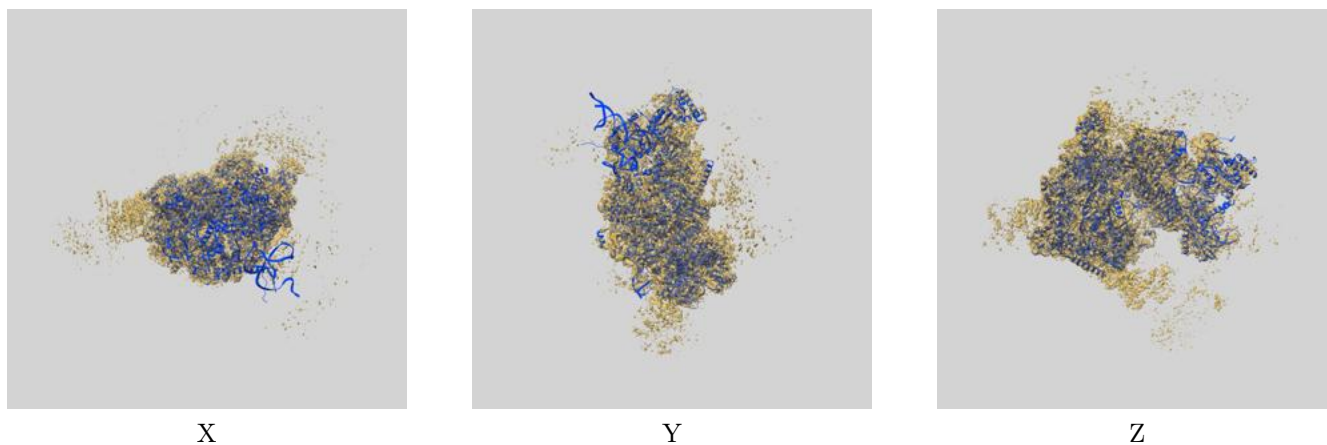
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.03	6.52	4.12
Unmasked-calculated*	7.63	16.26	7.94

*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 7.63 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

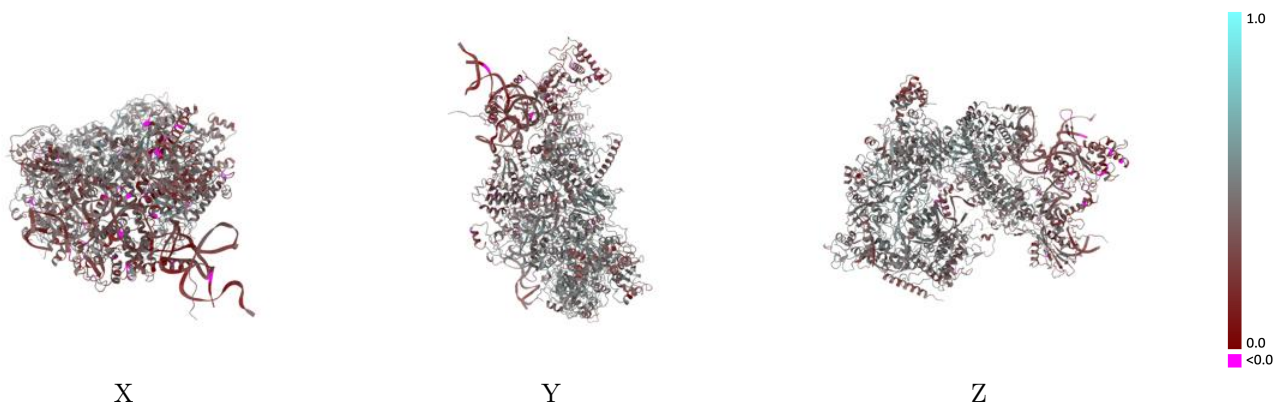
This section contains information regarding the fit between EMDB map EMD-18545 and PDB model 8QP9. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



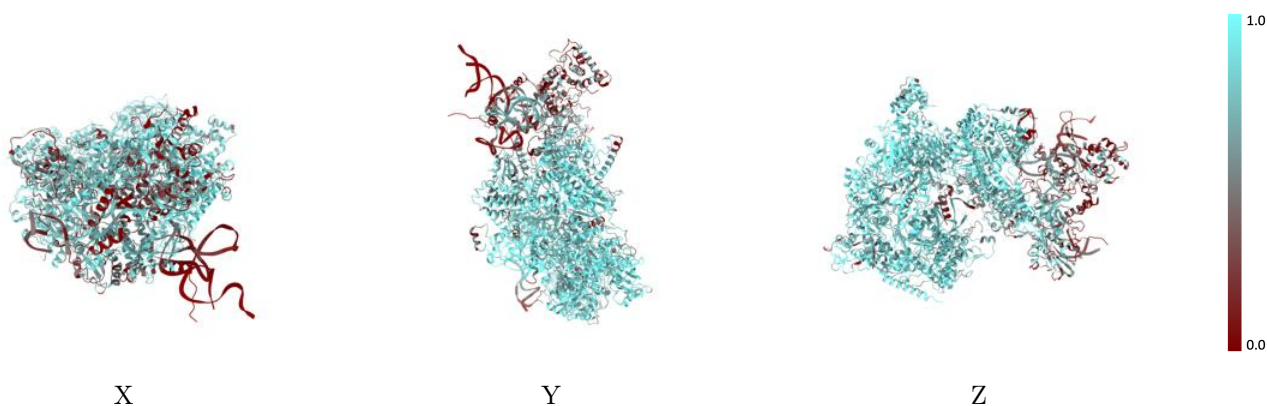
The images above show the 3D surface view of the map at the recommended contour level 0.043 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



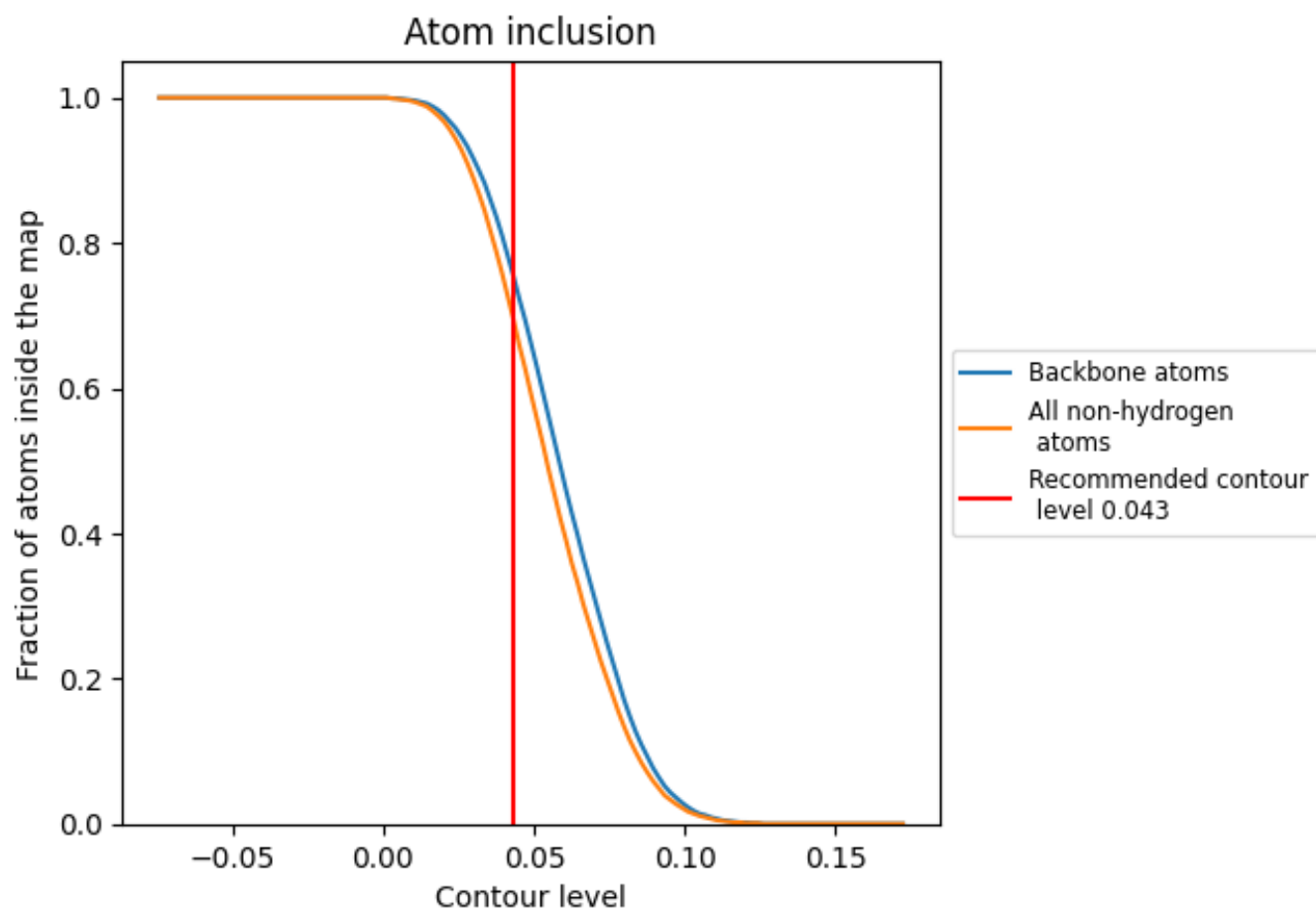
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.043).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.043) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.4080
4	 0.3350	 0.2610
5	 0.7330	 0.3590
6	 0.3470	 0.2560
7	 0.6610	 0.3630
A	 0.7230	 0.4240
B	 0.7810	 0.3670
C	 0.8320	 0.4730
D	 0.6780	 0.4050
G	 0.7280	 0.4230
J	 0.2320	 0.2460
L	 0.2790	 0.3600
N	 0.6800	 0.3830
R	 0.4010	 0.3040
S	 0.3030	 0.3270
U	 0.8750	 0.4650
X	 0.2690	 0.3730

