Full wwPDB EM Validation Report (i)

Apr 20, 2024 – 07:52 pm BST

PDB ID	:	6YBS
EMDB ID	:	EMD-10772
Title	:	Structure of a human 48S translational initiation complex - head
Authors	:	Brito Querido, J.; Sokabe, M.; Kraatz, S.; Gordiyenko, Y.; Skehel, M.; Fraser, C.; Ramakrishnan, V.
Deposited on	:	2020-03-17
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

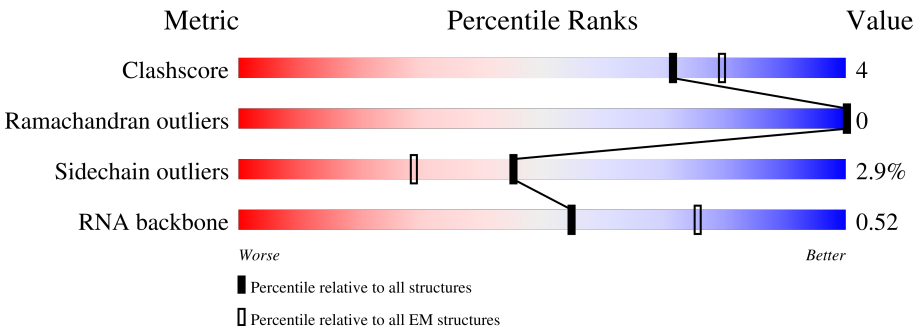
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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 <=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	548	6%, 64%, 34%
2	c	317	96%
3	n	69	91%, 9%
4	X	135	51%, 6%, 42%
5	h	119	87%, 13%
6	o	320	23%, 76%
7	a	165	59%, 40%

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Mol	Chain	Length	Quality of chain
8	m	132	84% 8% 8%
9	i	56	89% 11%
10	b	145	74% 24%
11	Z	243	83% 10% 7%
12	d	145	96%
13	e	125	50% 47%
14	f	152	91% 7%
15	V	204	79% 10% 10%
16	k	156	31% 66%
17	Y	146	87% 10%
18	A	1869	18% 8% 73%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 28732 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 Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	x	360	2317	1421	435	453	8	0	0

- Molecule 2 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	313	2436	1535	424	465	12	0	0

- Molecule 3 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	n	63	498	302	101	93	2	0	0

- Molecule 4 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	78	641	403	127	109	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	h	103	817	511	155	147	4	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	o	77	616	389	111	116	0	0

- Molecule 7 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	a	99	834	544	149	135	6	0	0

- Molecule 8 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	m	122	950	596	168	177	9	0	0

- Molecule 9 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	50	419	262	85	67	5	0	0

- Molecule 10 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	b	110	913	580	168	158	7	0	0

- Molecule 11 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Z	227	1765	1125	317	315	8	0	0

- Molecule 12 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	d	142	1105	692	213	197	3	0	0

- Molecule 13 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	e	66	523	338	93	91	1	0	0

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	f	142	1176	737	239	199	1	0	0

- Molecule 15 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	V	184	1461	914	276	264	7	0	0

- Molecule 16 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	k	53	435	276	82	70	7	0	0

- Molecule 17 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Y	141	1124	715	212	194	3	0	0

- Molecule 18 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	A	501	10672	4764	1893	3514	501	0	0

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
19	f	1	1	1	0
19	A	28	28	28	0

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

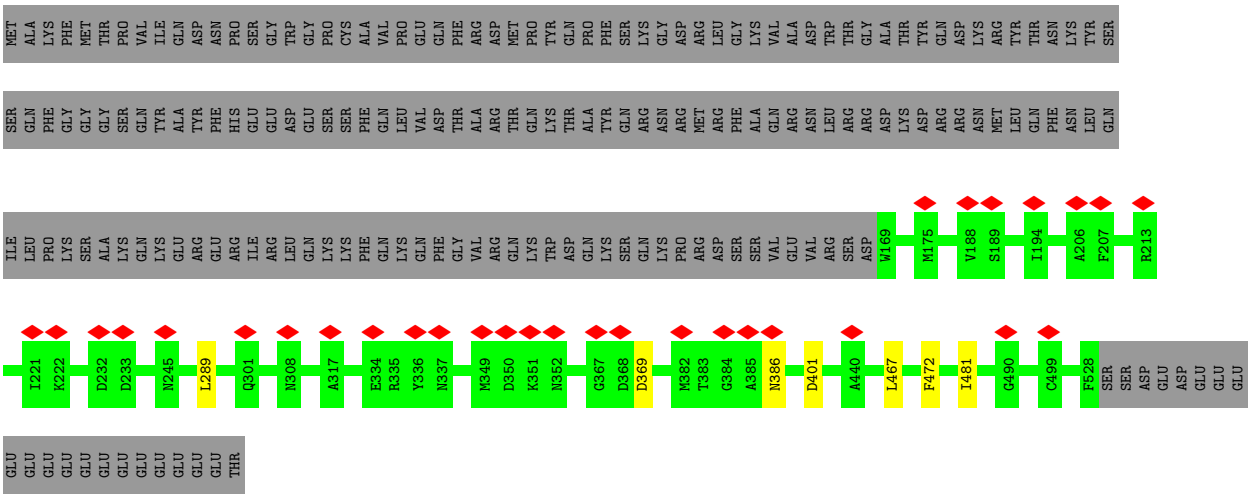
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	k	1	1	1	0

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.

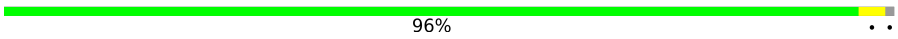
• Molecule 1: Eukaryotic translation initiation factor 3 subunit D

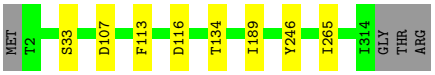
Chain x:



• Molecule 2: Receptor of activated protein C kinase 1

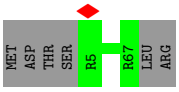
Chain c:





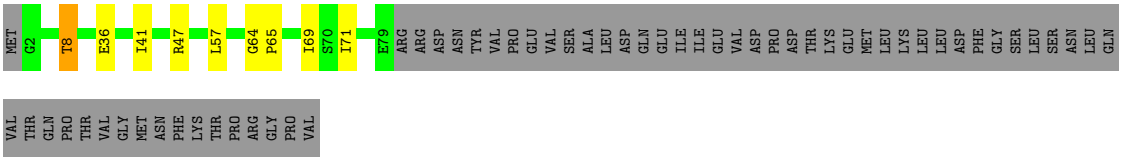
• Molecule 3: 40S ribosomal protein S28

Chain n:



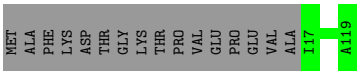
• Molecule 4: 40S ribosomal protein S17

Chain X:



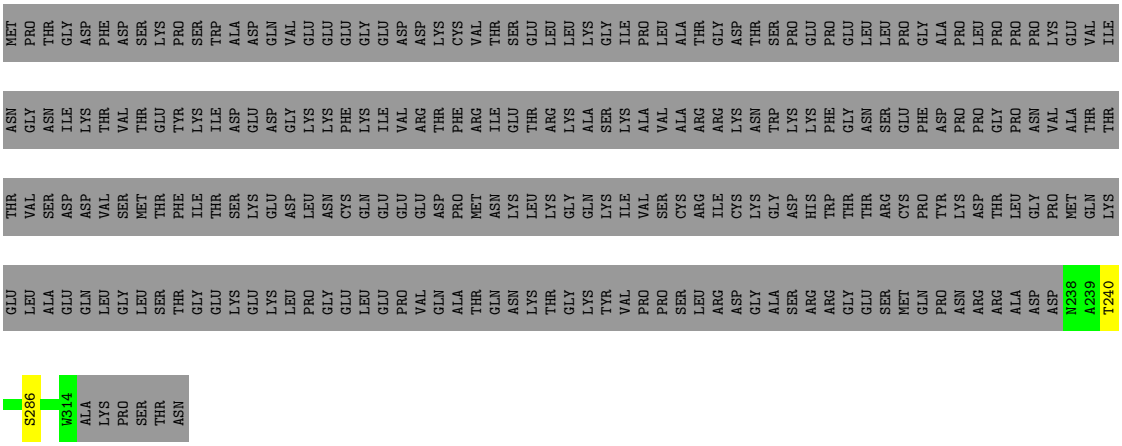
• Molecule 5: 40S ribosomal protein S20

Chain h: 87% 13%



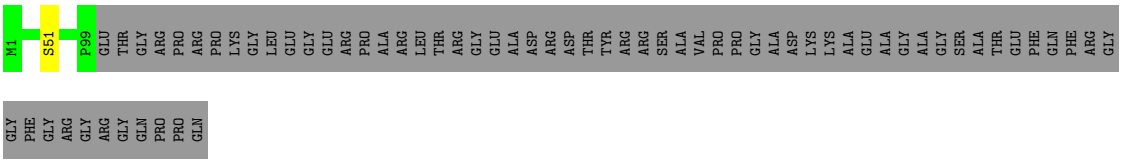
• Molecule 6: Eukaryotic translation initiation factor 3 subunit G

Chain o: 23% 76%



• Molecule 7: 40S ribosomal protein S10

Chain a: 59% 40%



• Molecule 8: 40S ribosomal protein S12

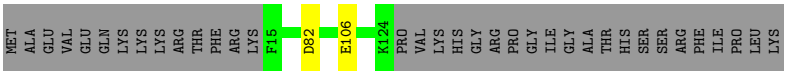
Chain m: 84% 8% 8%

• Molecule 9: 40S ribosomal protein S29

Chain i: 89% 11%

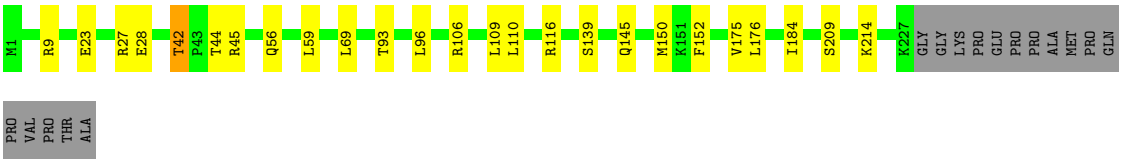
- Molecule 10: 40S ribosomal protein S15

Chain b:



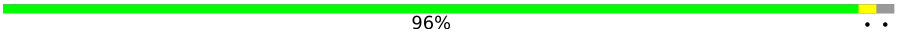
- Molecule 11: 40S ribosomal protein S3

Chain Z:



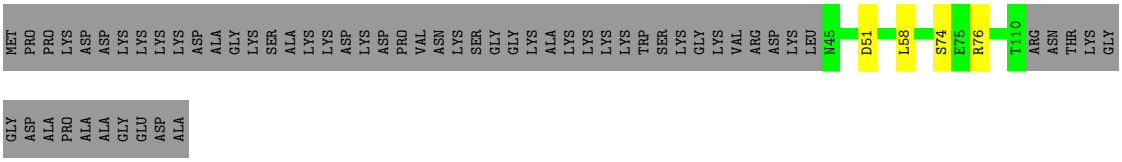
- Molecule 12: 40S ribosomal protein S19

Chain d:



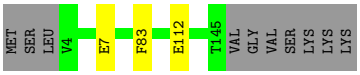
- Molecule 13: 40S ribosomal protein S25

Chain e:



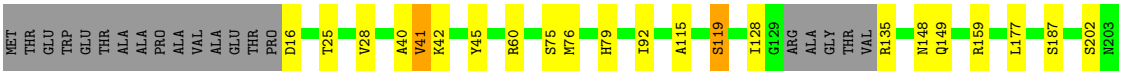
- Molecule 14: 40S ribosomal protein S18

Chain f:



- Molecule 15: 40S ribosomal protein S5

Chain V:



R204

- Molecule 16: Ubiquitin-40S ribosomal protein S27a

Chain k: 31% • 66%

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

ILE GLN LYS GLU SER THR LEU HIS LEU VAL LEU ARG LEU ARG GLY GLY ALA LYS LYS ARG LYS LYS LYS SER TYR THR THR PRO LYS LYS ASN LYS **H93** V102 L103 **K107** VAL ASP GLU ASN GLY LYS **I114** Y140 C144 **N151** LYS PRO GLU ASP LYS

- Molecule 17: 40S ribosomal protein S16

Chain Y: 87% 10% •

MET PRO SER LYS GLY **P6** **L7** Q8 R27 L31 **I32** K33 L58 R62 V93 Q97 K105 D116 **R117** T118 **L119** L120 V121 Q142 **R146**

- Molecule 18: 18S rRNA

Chain A: 18% 8% • 73%

U A C C U G G U U G A U C C U G C C A G U A G C A U A U G U C U C A A A G A U U A A G C C A U G C

A G U A C G C A C G G C C G G U A C A G U G A A A C U G C G A A U G G C U C A U A A A U C A G U U A U G G U OMU C C PSU U

OMU G G G U C G C U U C G C U C U C U C C U A C U U U G G G A U A A C U G U G G U A A2M U U C U A G A2M G C U A A U A OMC A U G C C G

A C G G G C G C U G A C C C C C U U C U G G C C G G G G G G G G A A U G C C G U G G C C A U U U A U C A G A U C A A A A C C A A C C C G

G U C A C C C C U C U C C C G G G C C C C C G G G G G G G G C C G G G G G C C G G C U U U G G G U G A C U C U A G A U

A A C C U C G G C C C G A U G G C A C G C C C C C C C C C G G G C G G A C G A C C C A U U U C G A A C G U C U G C C C U A

U C A A C U U U C G A U G G U A G G U C G G C C C U A C C A U G G G U G A C C A A C G G G U G G G U G A A C U C U A A G G

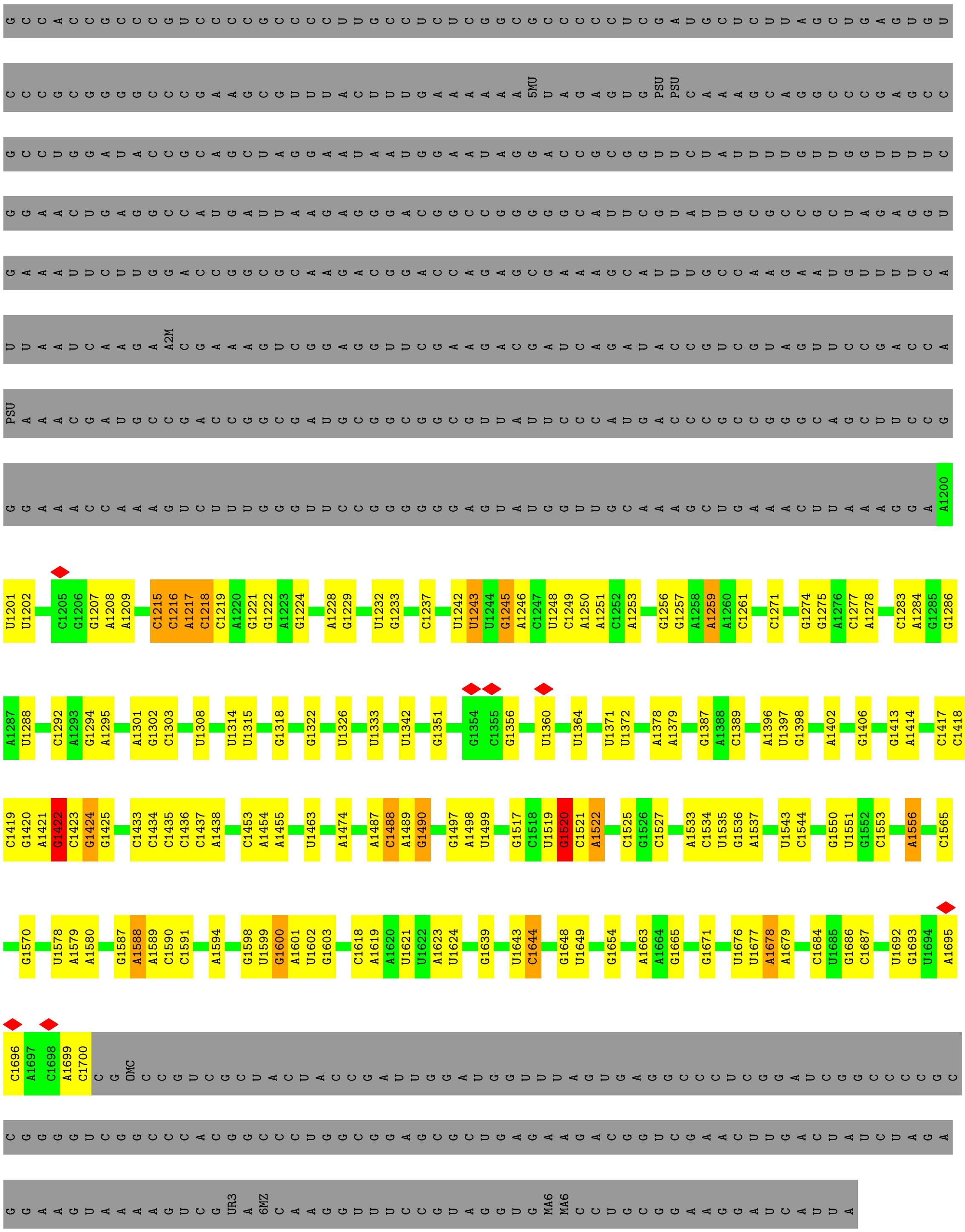
G U U C C G A U U C C G G A G G A G G G G A G G C C C G G A C G G C U A A C C A C A A U C C A A G G G A A G G G G G C A G G C A G G G

C G C A2M A A U U A C C C A C U C C C G A C C C C G G G G G A OMG G U A G U G A OMC G A A A A A U A A C C A A U U A C C A G G G A C U C U

U U C G A G G C C U G U A A U U G G G A A G G U C C C U U U A A A U C C C A A U U G G G A G G G A U C C A U U G G G A G

G G C A A G U C U G G PSU G C C A G C A G G C U C C C A A U A OMG C G U A U A U U A A G C G G A G G G A U C C A U U G G G A C

U G C A G U U A2M A A A A G C U C G U A G U U G C G G G C C G G G C C G G G C U C C C G C G A G G G C U G G C G A


A1200
U1201 U1202 C1205 G1206 G1207 A1208 A1209 C1215 C1216 A1217 C1218 C1219 A1220 G1221 G1222 A1223 G1224 A1228 G1229 U1232 G1233 C1237 U1242 U1243 U1244 G1245 A1246 C1247 U1248 C1249 A1250 A1251 C1252 A1253 G1256 G1257 A1258 A1259 A1260 C1261 C1271 G1274 G1275 A1276 C1277 A1278 C1283 A1284 G1285 G1286
A1287 U1288 C1292 A1293 G1294 A1295 A1301 G1302 C1303 U1308 U1314 U1315 G1318 G1322 U1326 U1333 U1342 G1351 G1354 C1355 G1356 U1360 U1364 U1371 U1372 A1378 A1379 G1387 A1388 C1389 A1396 U1397 G1398 A1402 G1406 G1413 A1414 C1417 C1418
C1419 G1420 A1421 G1422 C1423 G1424 G1425 C1433 C1434 C1435 C1436 C1437 A1438 C1453 A1454 A1455 U1463 A1474 A1487 C1488 A1489 G1490 G1497 A1498 U1499 G1517 C1518 U1519 G1520 C1521 A1522 C1525 G1526 C1527 A1533 C1534 U1535 G1536 A1537 U1543 C1544 G1550 U1551 G1552 C1553 A1556 C1565
G1570 U1578 A1579 A1580 G1587 A1588 A1589 C1590 C1591 A1594 G1598 U1599 G1600 A1601 U1602 G1603 C1618 A1619 A1620 U1621 U1622 A1623 U1624 G1639 U1643 C1644 G1648 U1649 G1654 A1663 A1664 G1665 G1671 U1676 U1677 A1678 A1679 C1684 U1685 G1686 C1687 U1692 G1693 U1694 A1695
C1696 A1697 C1698 A1699 C1700

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144882	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 ($e^-/Å^2$)	107	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.408	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	537.0, 537.0, 537.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	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: MG, 5MC, A2M, PSU, JMH, ZN

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	0/2346	0.60	1/3213 (0.0%)
2	c	0.33	0/2493	0.62	1/3394 (0.0%)
3	n	0.36	0/500	0.60	0/669
4	X	0.35	0/648	0.54	0/863
5	h	0.36	0/827	0.62	0/1110
6	o	0.36	0/628	0.68	0/846
7	a	0.35	0/859	0.51	0/1159
8	m	0.33	0/960	0.61	0/1286
9	i	0.40	0/429	0.52	0/568
10	b	0.38	0/929	0.58	1/1241 (0.1%)
11	Z	0.34	0/1793	0.56	0/2414
12	d	0.37	0/1123	0.49	0/1504
13	e	0.34	0/529	0.58	0/712
14	f	0.33	0/1194	0.56	0/1599
15	V	0.33	0/1481	0.59	1/1988 (0.1%)
16	k	0.33	0/444	0.64	0/588
17	Y	0.37	0/1142	0.59	0/1528
18	A	0.66	1/11830 (0.0%)	1.14	76/18435 (0.4%)
All	All	0.49	1/30155 (0.0%)	0.87	80/43117 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1556	A	N9-C4	5.38	1.41	1.37

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1453	C	C2-N1-C1'	10.14	129.96	118.80
18	A	1520	G	C2-N3-C4	9.82	116.81	111.90

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1453	C	N1-C2-O2	9.69	124.72	118.90
18	A	1520	G	N3-C4-C5	-9.50	123.85	128.60
18	A	1578	U	N3-C2-O2	-9.03	115.88	122.20
18	A	1578	U	N1-C2-O2	9.02	129.11	122.80
18	A	1271	C	N1-C2-O2	8.94	124.27	118.90
18	A	1600	G	N3-C4-C5	-8.22	124.49	128.60
18	A	1600	G	C2-N3-C4	8.04	115.92	111.90
18	A	1261	C	N1-C2-O2	7.82	123.59	118.90
1	x	481	ILE	CG1-CB-CG2	-7.64	94.59	111.40
18	A	1600	G	P-O3'-C3'	7.60	128.81	119.70
18	A	1591	C	N1-C2-O2	7.59	123.45	118.90
18	A	1453	C	C5-C6-N1	7.44	124.72	121.00
18	A	1578	U	C2-N1-C1'	7.42	126.60	117.70
18	A	1565	C	C2-N1-C1'	7.26	126.79	118.80
18	A	1520	G	N3-C4-N9	7.17	130.31	126.00
18	A	1271	C	N3-C2-O2	-7.15	116.89	121.90
18	A	1422	G	N3-C4-N9	7.09	130.25	126.00
18	A	1520	G	C4-N9-C1'	7.04	135.66	126.50
18	A	1453	C	C6-N1-C1'	-7.00	112.40	120.80
18	A	1696	C	N1-C2-O2	6.99	123.09	118.90
18	A	1600	G	N3-C4-N9	6.91	130.15	126.00
18	A	1453	C	N3-C2-O2	-6.84	117.11	121.90
2	c	189	ILE	CG1-CB-CG2	-6.79	96.47	111.40
18	A	1216	C	N1-C2-O2	6.75	122.95	118.90
18	A	1453	C	C6-N1-C2	-6.64	117.64	120.30
18	A	1696	C	N3-C2-O2	-6.63	117.26	121.90
15	V	177	LEU	CA-CB-CG	6.63	130.54	115.30
18	A	1218	C	C5-C6-N1	6.63	124.31	121.00
18	A	1422	G	C4-N9-C1'	6.58	135.05	126.50
18	A	1591	C	N3-C2-O2	-6.55	117.31	121.90
18	A	1261	C	C2-N1-C1'	6.46	125.91	118.80
18	A	1389	C	C2-N1-C1'	6.45	125.89	118.80
18	A	1556	A	C2-N3-C4	6.38	113.79	110.60
18	A	1261	C	N3-C2-O2	-6.30	117.49	121.90
18	A	1237	C	C6-N1-C2	-6.26	117.80	120.30
18	A	1590	C	C6-N1-C2	-6.26	117.80	120.30
18	A	1389	C	C6-N1-C2	-6.17	117.83	120.30
18	A	1520	G	C8-N9-C4	-6.11	103.95	106.40
18	A	1649	U	N1-C2-O2	6.09	127.06	122.80
18	A	1422	G	C8-N9-C1'	-6.07	119.11	127.00
18	A	1261	C	C6-N1-C2	-6.04	117.88	120.30
18	A	1333	U	N3-C2-O2	-6.04	117.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1271	C	C2-N1-C1'	5.93	125.32	118.80
18	A	1422	G	N3-C4-C5	-5.87	125.67	128.60
18	A	1590	C	N1-C2-O2	5.84	122.41	118.90
18	A	1333	U	N1-C2-O2	5.78	126.85	122.80
18	A	1687	C	C2-N1-C1'	5.73	125.11	118.80
18	A	1237	C	C5-C6-N1	5.73	123.87	121.00
18	A	1591	C	C6-N1-C2	-5.69	118.03	120.30
18	A	1565	C	C6-N1-C2	-5.66	118.04	120.30
18	A	1216	C	N3-C2-O2	-5.63	117.96	121.90
18	A	1271	C	C6-N1-C2	-5.61	118.06	120.30
18	A	1215	C	O4'-C1'-N1	-5.54	103.77	108.20
18	A	1684	C	N1-C2-O2	5.53	122.22	118.90
18	A	1218	C	C6-N1-C2	-5.52	118.09	120.30
18	A	1649	U	N3-C2-O2	-5.50	118.35	122.20
18	A	1649	U	C2-N1-C1'	5.43	124.21	117.70
18	A	1315	U	N3-C2-O2	-5.37	118.44	122.20
18	A	1259	A	C2-N3-C4	5.35	113.28	110.60
18	A	1556	A	N3-C4-N9	5.29	131.63	127.40
18	A	1525	C	C6-N1-C2	-5.29	118.19	120.30
18	A	1315	U	C2-N1-C1'	5.28	124.04	117.70
18	A	1565	C	N1-C2-O2	5.27	122.06	118.90
18	A	1261	C	C5-C6-N1	5.25	123.63	121.00
18	A	1292	C	N1-C2-O2	5.22	122.03	118.90
18	A	1590	C	C5-C6-N1	5.21	123.60	121.00
18	A	1590	C	N3-C2-O2	-5.20	118.26	121.90
18	A	1522	A	C2-N3-C4	5.19	113.19	110.60
18	A	1553	C	N1-C2-O2	5.18	122.00	118.90
18	A	1565	C	C5-C6-N1	5.14	123.57	121.00
18	A	1520	G	C8-N9-C1'	-5.14	120.32	127.00
18	A	1578	U	C6-N1-C1'	-5.11	114.05	121.20
18	A	1249	C	C6-N1-C2	-5.09	118.26	120.30
18	A	1364	U	N3-C2-O2	-5.07	118.65	122.20
10	b	82	ASP	CB-CG-OD1	5.07	122.86	118.30
18	A	1517	G	N9-C1'-C2'	-5.06	106.44	112.00
18	A	1314	U	C2-N1-C1'	5.04	123.75	117.70
18	A	1389	C	C5-C6-N1	5.03	123.51	121.00

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	x	2317	0	1733	0	0
2	c	2436	0	2393	0	0
3	n	498	0	525	0	0
4	X	641	0	694	5	0
5	h	817	0	882	0	0
6	o	616	0	600	0	0
7	a	834	0	861	0	0
8	m	950	0	987	0	0
9	i	419	0	415	0	0
10	b	913	0	951	0	0
11	Z	1765	0	1865	15	0
12	d	1105	0	1138	0	0
13	e	523	0	573	0	0
14	f	1176	0	1233	0	0
15	V	1461	0	1511	11	0
16	k	435	0	434	0	0
17	Y	1124	0	1193	8	0
18	A	10672	0	5391	35	0
19	A	28	0	0	0	0
19	f	1	0	0	0	0
20	k	1	0	0	0	0
All	All	28732	0	23379	66	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 4.

All (66) 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)
18:A:1351:G:H1	18:A:1360:U:H3	1.11	0.92
18:A:1488:C:O2'	18:A:1490:G:OP2	2.14	0.66
11:Z:116:ARG:NH2	11:Z:150:MET:SD	2.75	0.59
18:A:1396:A:O2'	18:A:1398:G:N7	2.34	0.58
11:Z:42:THR:HG22	11:Z:45:ARG:H	1.67	0.58
17:Y:58:LEU:HB3	17:Y:62:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:115:ALA:O	15:V:119:SER:HB3	2.05	0.56
17:Y:93:VAL:HG21	17:Y:120:LEU:HD21	1.88	0.55
17:Y:97:GLN:HB2	17:Y:105:LYS:HG3	1.89	0.54
18:A:1277:C:H2'	18:A:1278:A:H8	1.73	0.54
15:V:159:ARG:NH1	18:A:1535:U:O4	2.42	0.53
18:A:1228:A:H2'	18:A:1229:G:C8	2.44	0.52
17:Y:142:GLN:NE2	18:A:1527:C:OP1	2.43	0.52
4:X:36:GLU:OE1	4:X:47:ARG:NH1	2.44	0.51
17:Y:8:GLN:HG3	17:Y:27:ARG:HH21	1.77	0.49
15:V:16:ASP:N	15:V:16:ASP:OD1	2.46	0.48
18:A:1245:G:H2'	18:A:1246:A:C8	2.49	0.48
18:A:1643:U:H2'	18:A:1644:C:C6	2.49	0.48
17:Y:31:LEU:HD11	17:Y:33:LYS:HE2	1.95	0.48
11:Z:176:LEU:HD13	18:A:1499:U:H4'	1.96	0.47
15:V:75:SER:O	15:V:75:SER:OG	2.32	0.47
18:A:1413:G:H2'	18:A:1414:A:H8	1.80	0.47
18:A:1360:U:O2'	18:A:1379:A:OP2	2.28	0.47
11:Z:28:GLU:HG2	11:Z:69:LEU:HD21	1.97	0.47
15:V:76:MET:HG2	15:V:92:ILE:HD11	1.96	0.46
18:A:1422:G:O2'	18:A:1424:G:OP2	2.33	0.46
18:A:1536:G:H2'	18:A:1537:A:C8	2.49	0.46
11:Z:209:SER:O	11:Z:209:SER:OG	2.33	0.46
18:A:1217:A:H2'	18:A:1218:C:C6	2.51	0.45
11:Z:93:THR:HG21	11:Z:96:LEU:HD12	1.98	0.45
18:A:1228:A:H2'	18:A:1229:G:H8	1.81	0.45
18:A:1232:U:H2'	18:A:1233:G:C8	2.52	0.45
18:A:1221:G:O2'	18:A:1676:U:O2	2.29	0.45
18:A:1424:G:H2'	18:A:1425:G:H8	1.81	0.45
11:Z:9:ARG:NH2	18:A:1551:U:OP1	2.50	0.44
18:A:1351:G:O6	18:A:1360:U:O4	2.35	0.44
18:A:1588:A:H2'	18:A:1589:A:C8	2.52	0.44
18:A:1678:A2M:HM'3	18:A:1678:A2M:H1'	1.80	0.44
15:V:40:ALA:HB1	15:V:45:TYR:CG	2.53	0.44
15:V:28:VAL:O	15:V:42:LYS:NZ	2.50	0.43
17:Y:121:VAL:HG13	18:A:1474:A:H5"	2.01	0.43
18:A:1413:G:H2'	18:A:1414:A:C8	2.53	0.43
18:A:1550:G:H3'	18:A:1579:A:H61	1.82	0.43
18:A:1536:G:H2'	18:A:1537:A:H8	1.83	0.43
4:X:8:THR:HG21	18:A:1387:G:H21	1.83	0.43
15:V:25:THR:OG1	15:V:41:VAL:O	2.36	0.43
18:A:1221:G:H2'	18:A:1222:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:56:GLN:HE22	11:Z:59:LEU:HD23	1.84	0.42
15:V:148:ASN:ND2	18:A:1677:U:OP1	2.52	0.42
18:A:1692:U:H2'	18:A:1693:G:C8	2.55	0.42
17:Y:116:ASP:OD1	17:Y:118:THR:OG1	2.38	0.42
11:Z:110:LEU:HD23	11:Z:110:LEU:HA	1.92	0.42
18:A:1520:G:H2'	18:A:1520:G:N3	2.35	0.42
11:Z:214:LYS:HE3	11:Z:214:LYS:HB3	1.91	0.41
18:A:1277:C:H2'	18:A:1278:A:C8	2.54	0.41
11:Z:23:GLU:OE2	11:Z:27:ARG:NE	2.47	0.41
4:X:41:ILE:HD12	4:X:47:ARG:HG2	2.03	0.41
15:V:128:ILE:O	15:V:135:ARG:NH2	2.47	0.41
11:Z:106:ARG:HG3	11:Z:175:VAL:HG22	2.03	0.41
15:V:60:ARG:HD2	18:A:1679:A:H2'	2.02	0.41
18:A:1201:U:H2'	18:A:1202:U:C6	2.56	0.41
11:Z:109:LEU:HD12	11:Z:184:ILE:HD11	2.03	0.40
4:X:57:LEU:HD13	4:X:69:ILE:HD11	2.03	0.40
4:X:64:GLY:HA2	4:X:65:PRO:HD3	1.91	0.40
11:Z:145:GLN:HE21	11:Z:145:GLN:HB3	1.64	0.40
11:Z:150:MET:HE3	11:Z:152:PHE:HZ	1.85	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	358/548 (65%)	328 (92%)	30 (8%)	0	100	100
2	c	311/317 (98%)	294 (94%)	17 (6%)	0	100	100
3	n	61/69 (88%)	57 (93%)	4 (7%)	0	100	100
4	X	76/135 (56%)	73 (96%)	3 (4%)	0	100	100
5	h	101/119 (85%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	o	75/320 (23%)	73 (97%)	2 (3%)	0	100	100
7	a	97/165 (59%)	93 (96%)	4 (4%)	0	100	100
8	m	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
9	i	48/56 (86%)	45 (94%)	3 (6%)	0	100	100
10	b	108/145 (74%)	105 (97%)	3 (3%)	0	100	100
11	Z	225/243 (93%)	219 (97%)	6 (3%)	0	100	100
12	d	140/145 (97%)	133 (95%)	7 (5%)	0	100	100
13	e	64/125 (51%)	60 (94%)	4 (6%)	0	100	100
14	f	140/152 (92%)	136 (97%)	4 (3%)	0	100	100
15	V	180/204 (88%)	169 (94%)	11 (6%)	0	100	100
16	k	49/156 (31%)	42 (86%)	7 (14%)	0	100	100
17	Y	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
All	All	2292/3177 (72%)	2171 (95%)	121 (5%)	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	152/494 (31%)	146 (96%)	6 (4%)	32	65
2	c	272/275 (99%)	265 (97%)	7 (3%)	46	74
3	n	56/62 (90%)	56 (100%)	0	100	100
4	X	69/122 (57%)	67 (97%)	2 (3%)	42	72
5	h	94/107 (88%)	94 (100%)	0	100	100
6	o	64/277 (23%)	62 (97%)	2 (3%)	40	70
7	a	90/136 (66%)	89 (99%)	1 (1%)	73	89
8	m	104/108 (96%)	93 (89%)	11 (11%)	6	26
9	i	44/49 (90%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	b	100/130 (77%)	99 (99%)	1 (1%)	76	90
11	Z	190/202 (94%)	187 (98%)	3 (2%)	62	84
12	d	112/115 (97%)	109 (97%)	3 (3%)	44	74
13	e	58/103 (56%)	54 (93%)	4 (7%)	15	45
14	f	123/132 (93%)	120 (98%)	3 (2%)	49	76
15	V	156/170 (92%)	150 (96%)	6 (4%)	33	66
16	k	47/140 (34%)	43 (92%)	4 (8%)	10	37
17	Y	117/121 (97%)	117 (100%)	0	100	100
All	All	1848/2743 (67%)	1795 (97%)	53 (3%)	45	72

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	289	LEU
1	x	369	ASP
1	x	386	ASN
1	x	401	ASP
1	x	467	LEU
1	x	472	PHE
2	c	33	SER
2	c	107	ASP
2	c	113	PHE
2	c	116	ASP
2	c	134	THR
2	c	246	TYR
2	c	265	ILE
4	X	8	THR
4	X	71	ILE
6	o	240	THR
6	o	286	SER
7	a	51	SER
8	m	12	MET
8	m	62	VAL
8	m	66	GLU
8	m	74	ILE
8	m	91	LEU
8	m	92	CYS
8	m	94	ILE
8	m	117	GLU

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Mol	Chain	Res	Type
8	m	124	ILE
8	m	127	TYR
8	m	132	LYS
10	b	106	GLU
11	Z	42	THR
11	Z	44	THR
11	Z	139	SER
12	d	34	VAL
12	d	96	SER
12	d	130	ASP
13	e	51	ASP
13	e	58	LEU
13	e	74	SER
13	e	76	ARG
14	f	7	GLU
14	f	83	PHE
14	f	112	GLU
15	V	41	VAL
15	V	79	HIS
15	V	119	SER
15	V	149	GLN
15	V	187	SER
15	V	202	SER
16	k	102	VAL
16	k	103	LEU
16	k	140	TYR
16	k	144	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	x	305	ASN
1	x	312	ASN
1	x	429	ASN
2	c	51	ASN
2	c	159	ASN
2	c	162	ASN
4	X	31	ASN
5	h	92	HIS
7	a	50	GLN
8	m	82	ASN
9	i	16	GLN

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Mol	Chain	Res	Type
9	i	26	ASN
9	i	45	GLN
10	b	41	GLN
10	b	103	ASN
10	b	114	HIS
11	Z	56	GLN
11	Z	145	GLN
12	d	85	ASN
13	e	46	ASN
13	e	106	GLN
14	f	72	GLN
14	f	105	ASN
15	V	36	GLN
15	V	82	ASN
15	V	148	ASN
15	V	165	ASN
15	V	179	ASN
17	Y	11	GLN
17	Y	35	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	A	499/1869 (26%)	97 (19%)	10 (2%)

All (97) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	A	1207	G
18	A	1208	A
18	A	1209	A
18	A	1215	C
18	A	1216	C
18	A	1217	A
18	A	1224	G
18	A	1242	U
18	A	1243	PSU
18	A	1245	G
18	A	1248	U
18	A	1250	A
18	A	1251	A

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Mol	Chain	Res	Type
18	A	1253	A
18	A	1256	G
18	A	1257	G
18	A	1259	A
18	A	1274	G
18	A	1275	G
18	A	1283	C
18	A	1284	A
18	A	1286	G
18	A	1288	U
18	A	1294	G
18	A	1295	A
18	A	1301	A
18	A	1302	G
18	A	1303	C
18	A	1308	U
18	A	1318	G
18	A	1322	G
18	A	1326	U
18	A	1342	U
18	A	1356	G
18	A	1371	U
18	A	1372	U
18	A	1378	A
18	A	1397	U
18	A	1402	A
18	A	1406	G
18	A	1417	C
18	A	1418	C
18	A	1419	C
18	A	1420	G
18	A	1421	A
18	A	1422	G
18	A	1423	C
18	A	1424	G
18	A	1433	C
18	A	1435	C
18	A	1436	C
18	A	1437	C
18	A	1438	A
18	A	1454	A
18	A	1455	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	A	1463	U
18	A	1487	A
18	A	1488	C
18	A	1489	A
18	A	1490	G
18	A	1497	G
18	A	1498	A
18	A	1519	U
18	A	1520	G
18	A	1521	C
18	A	1522	A
18	A	1533	A
18	A	1534	C
18	A	1543	U
18	A	1544	C
18	A	1556	A
18	A	1570	G
18	A	1580	A
18	A	1587	G
18	A	1588	A
18	A	1594	A
18	A	1598	G
18	A	1599	U
18	A	1600	G
18	A	1601	A
18	A	1602	U
18	A	1618	C
18	A	1619	A
18	A	1621	U
18	A	1623	A
18	A	1624	U
18	A	1639	G
18	A	1644	C
18	A	1648	G
18	A	1654	G
18	A	1663	A
18	A	1665	G
18	A	1671	G
18	A	1686	G
18	A	1695	A
18	A	1699	A
18	A	1700	C

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	A	1250	A
18	A	1434	C
18	A	1519	U
18	A	1520	G
18	A	1521	C
18	A	1598	G
18	A	1599	U
18	A	1600	G
18	A	1601	A
18	A	1603	G

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

4 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
18	PSU	A	1243	18	18,21,22	1.07	2 (11%)	22,30,33	0.68	0
18	5MC	A	1374	18	18,22,23	0.40	0	26,32,35	0.55	0
18	JMH	A	1219	19,18	18,22,23	0.68	1 (5%)	21,32,35	0.64	0
18	A2M	A	1678	18	18,25,26	0.60	0	18,36,39	0.82	1 (5%)

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
18	PSU	A	1243	18	-	0/7/25/26	0/2/2/2
18	5MC	A	1374	18	-	0/7/25/26	0/2/2/2
18	JMH	A	1219	19,18	-	0/7/25/26	0/2/2/2
18	A2M	A	1678	18	-	0/5/27/28	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1243	PSU	C6-C5	3.23	1.39	1.35
18	A	1219	JMH	C5-C4	-2.25	1.37	1.42
18	A	1243	PSU	O4'-C1'	-2.10	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1678	A2M	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1678	A2M	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 30 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.

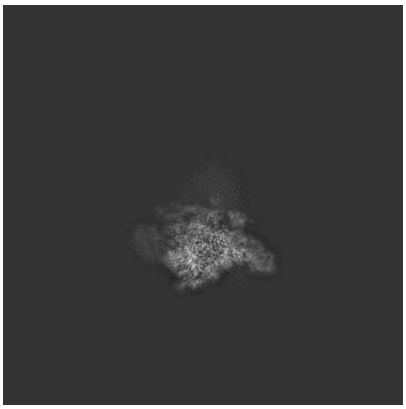
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10772. These allow visual inspection of the internal detail of the map and identification of artifacts.

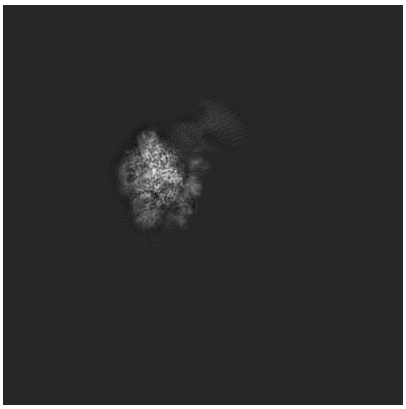
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

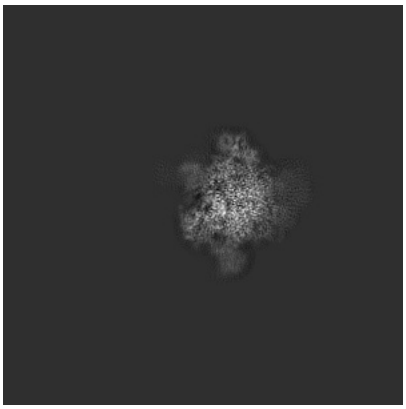
6.1.1 Primary map



X

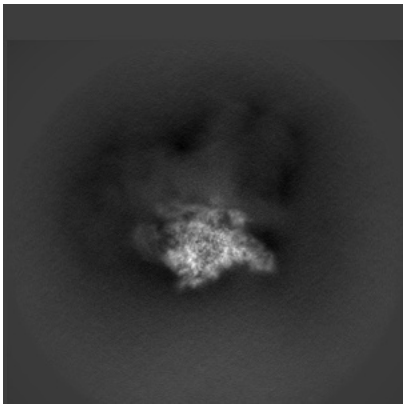


Y

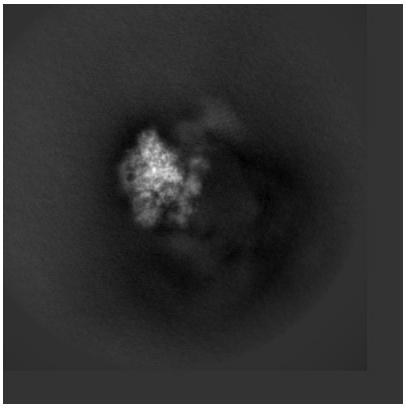


Z

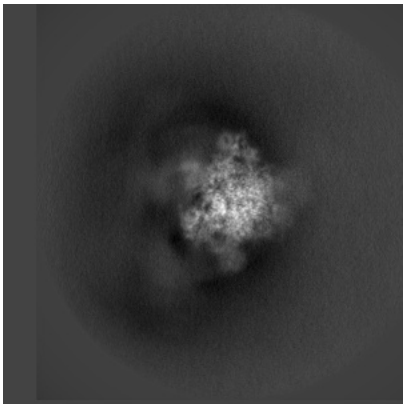
6.1.2 Raw map



X



Y

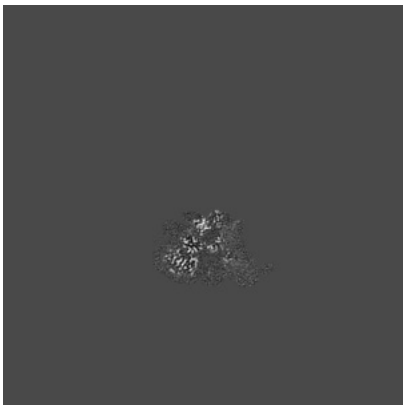


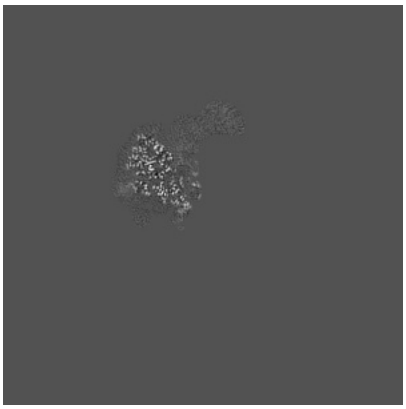
Z

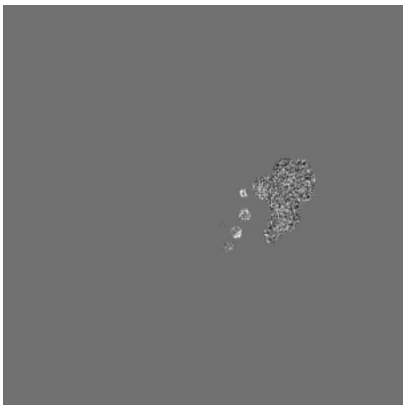
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

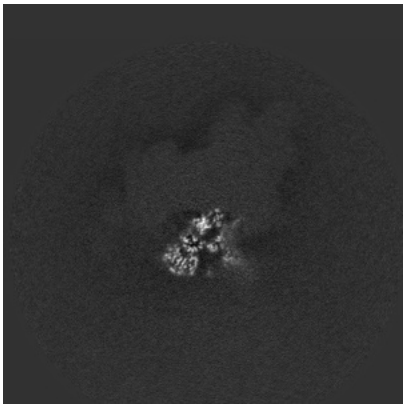
6.2.1 Primary map

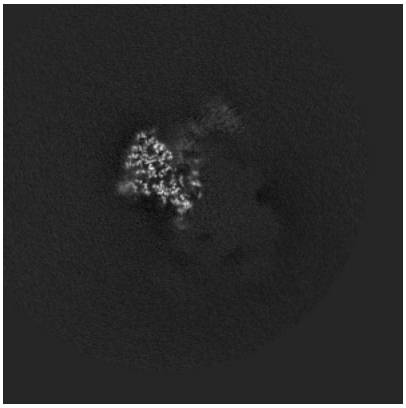

X Index: 250

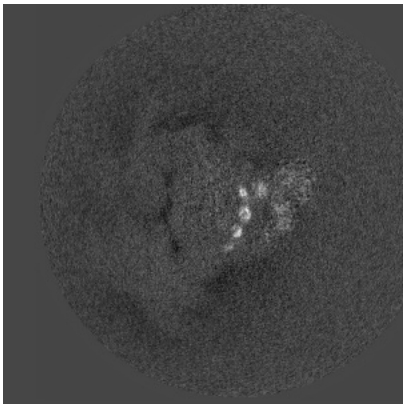

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250


Y Index: 250


Z Index: 250

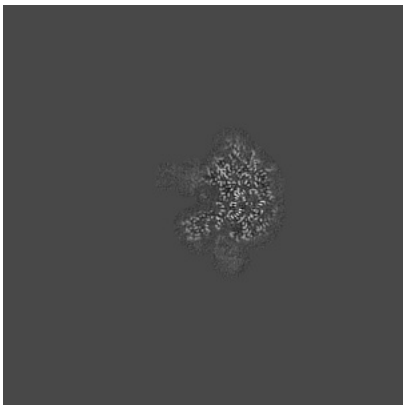
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

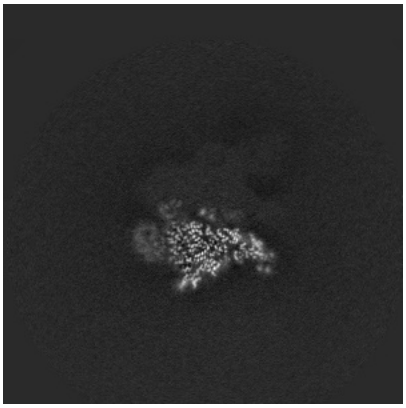
6.3.1 Primary map

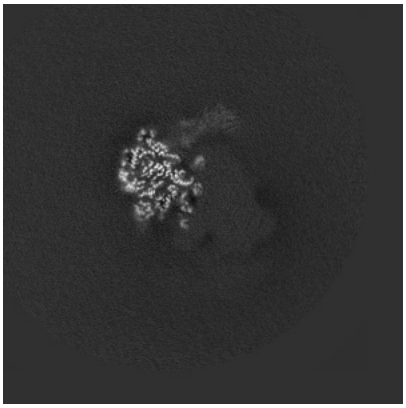
X Index: 288

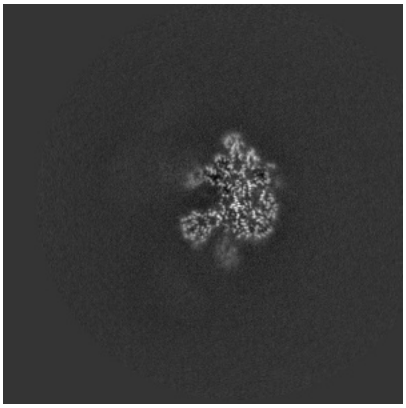
Y Index: 240


Z Index: 190

6.3.2 Raw map


X Index: 288

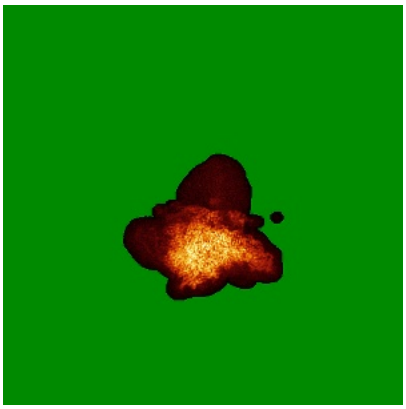

Y Index: 240


Z Index: 187

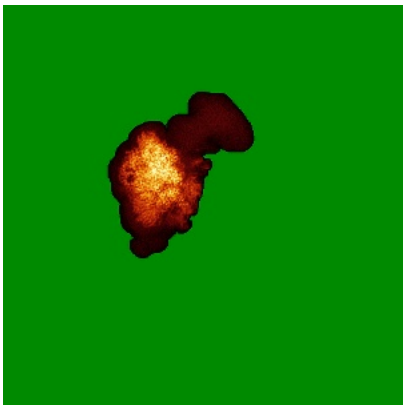
The images above show the largest variance slices of the map in three orthogonal directions.

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

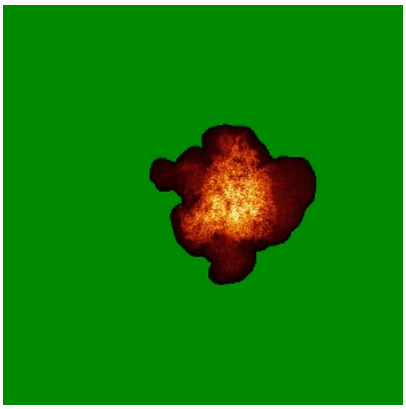
6.4.1 Primary map



X

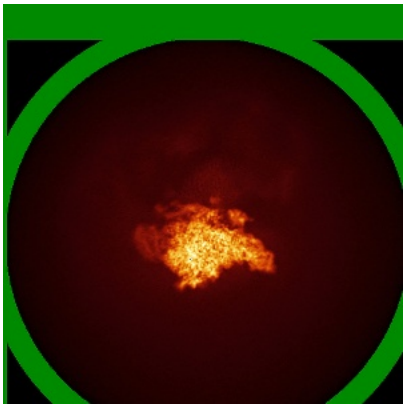


Y

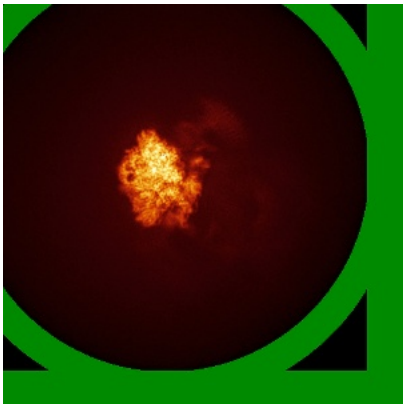


Z

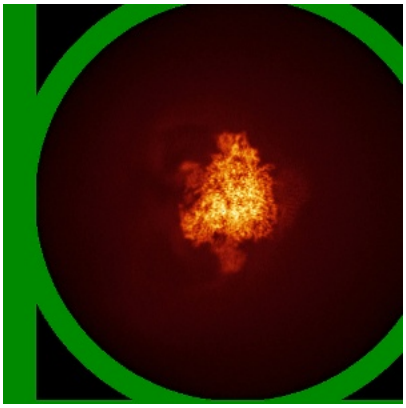
6.4.2 Raw map



X



Y

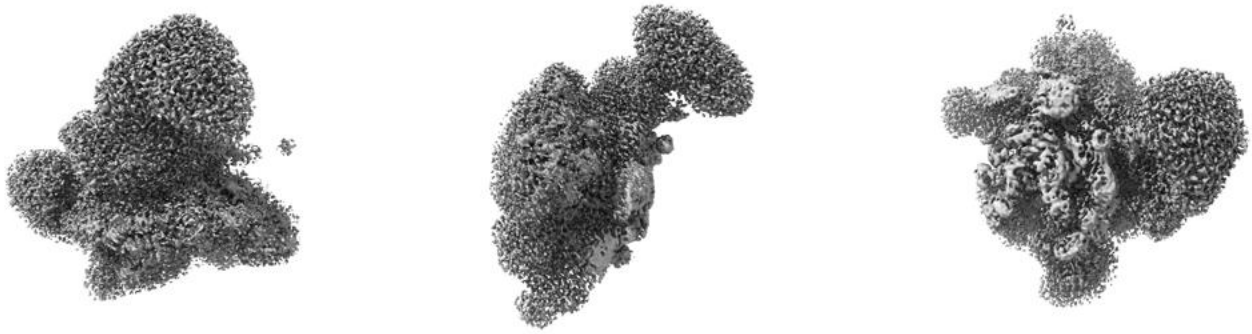


Z

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 0.02. 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.

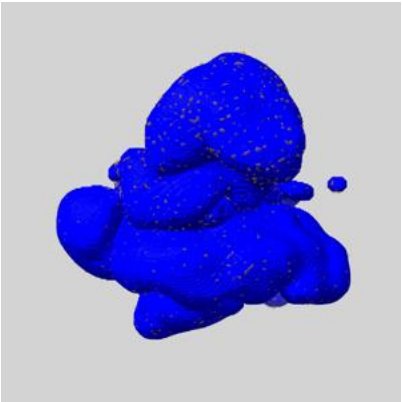
6.6 Mask visualisation (i)

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

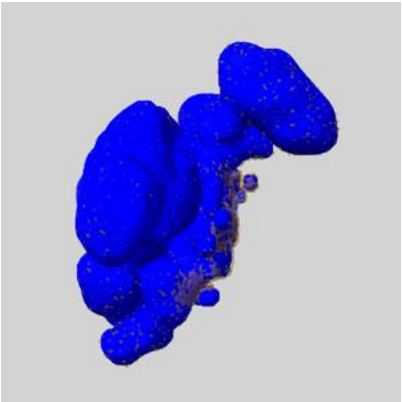
A mask typically either:

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

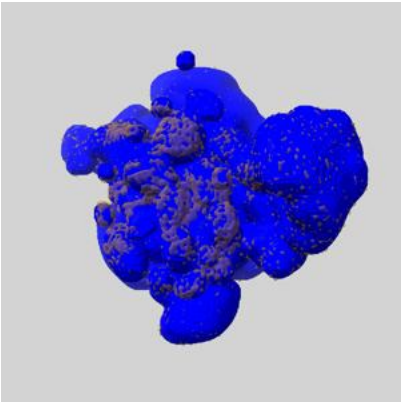
6.6.1 emd_10772_msk_1.map (i)



X



Y

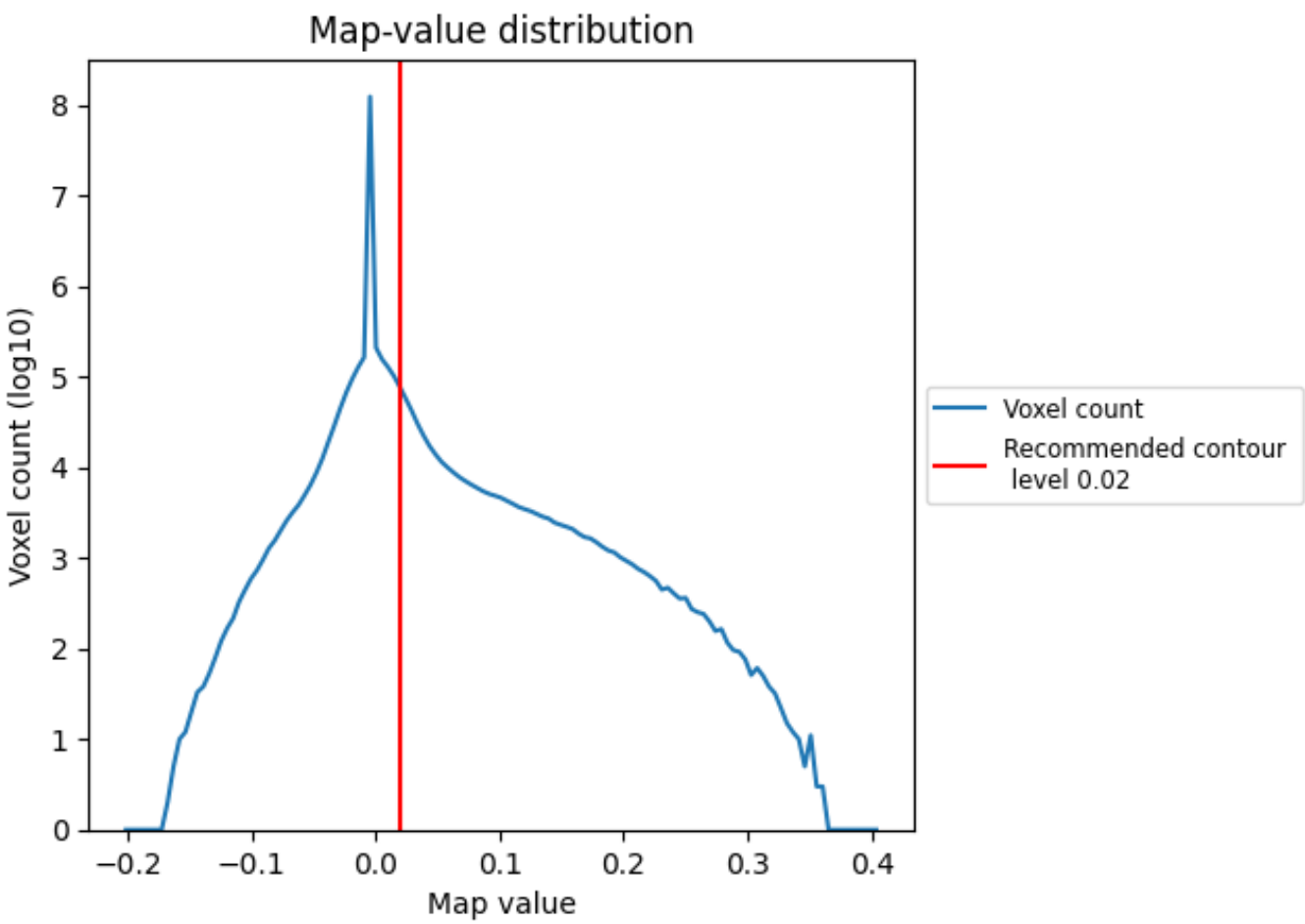


Z

7 Map analysis (i)

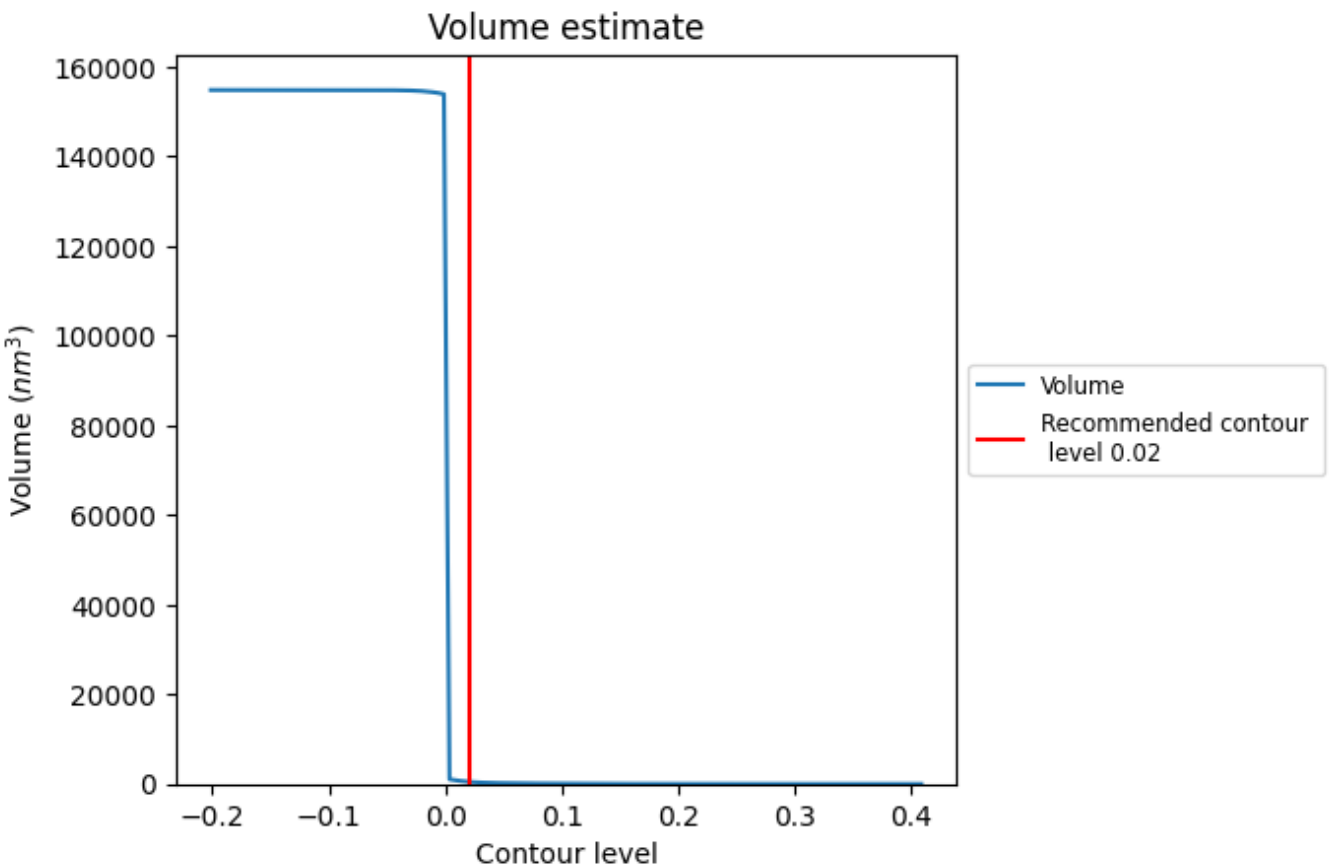
This section contains the results of statistical analysis of the map.

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.

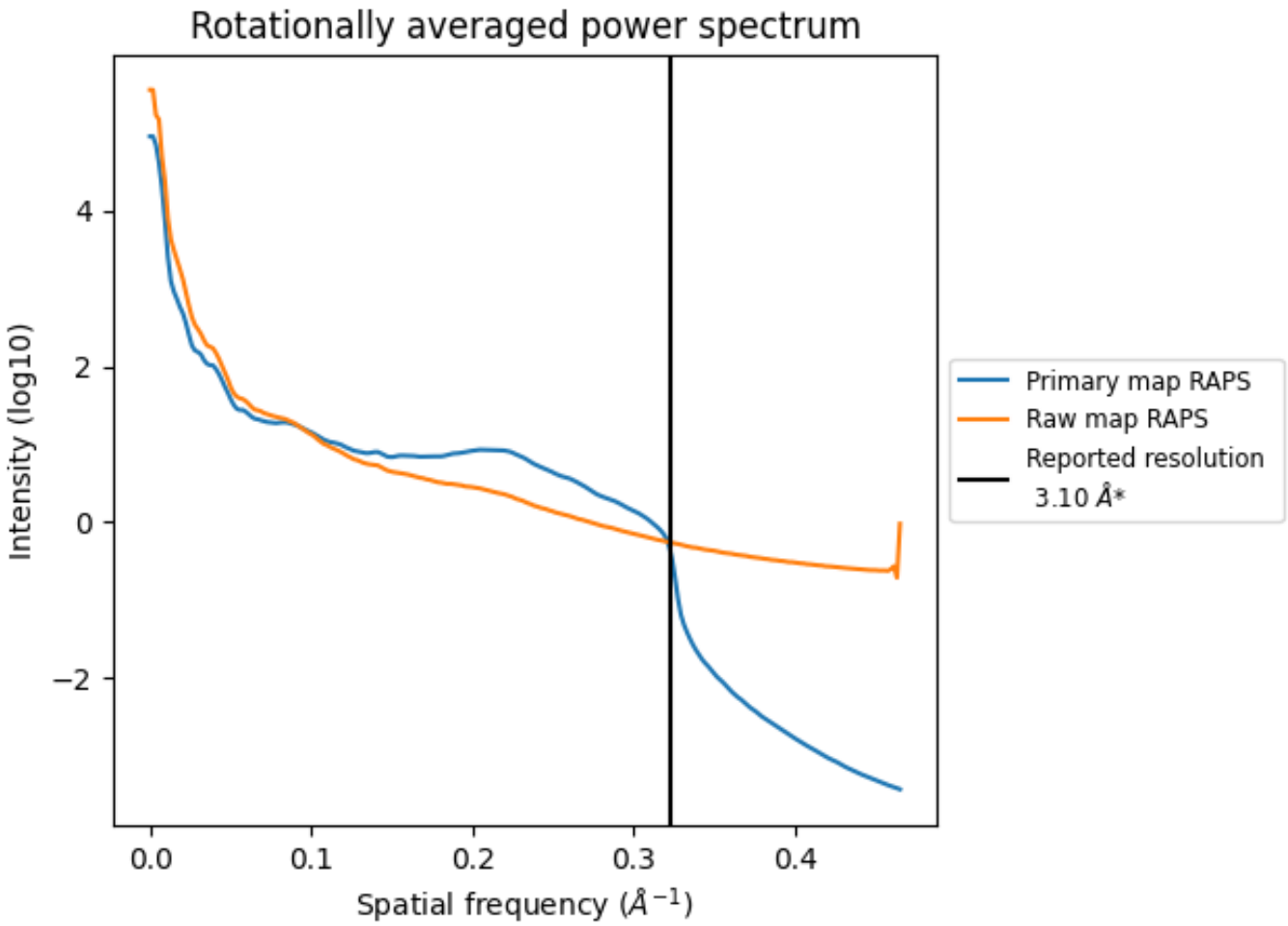
7.2 Volume estimate (i)



The volume at the recommended contour level is 483 nm^3; this corresponds to an approximate mass of 436 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)

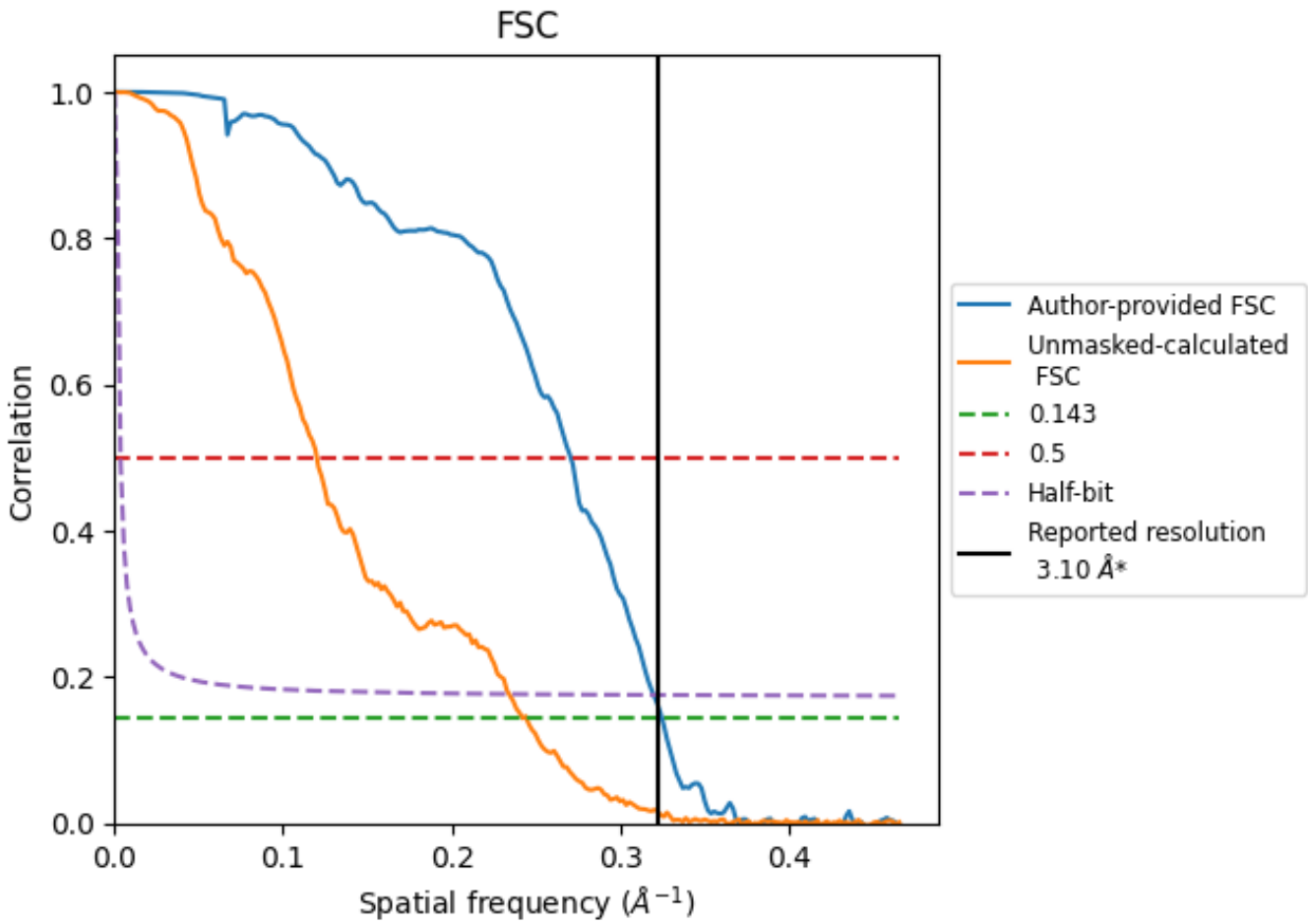


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

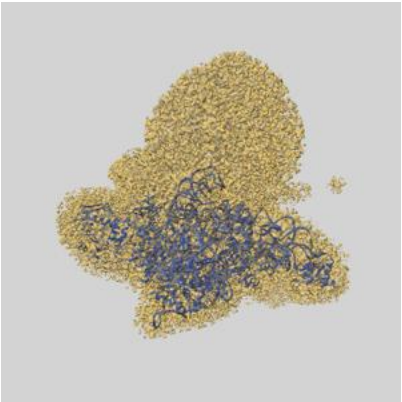
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.70	3.13
Unmasked-calculated*	4.13	8.33	4.27

*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 4.13 differs from the reported value 3.1 by more than 10 %

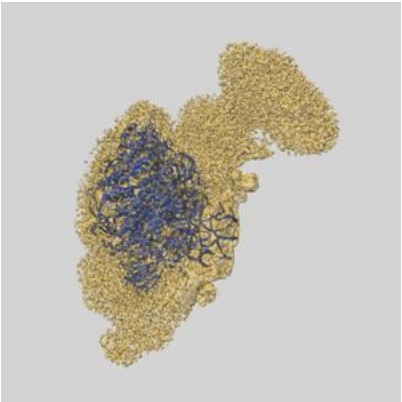
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10772 and PDB model 6YBS. Per-residue inclusion information can be found in section 3 on page 7.

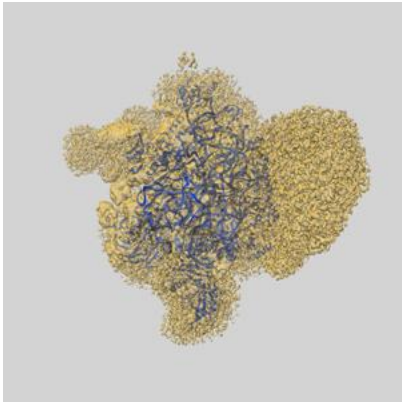
9.1 Map-model overlay (i)



X



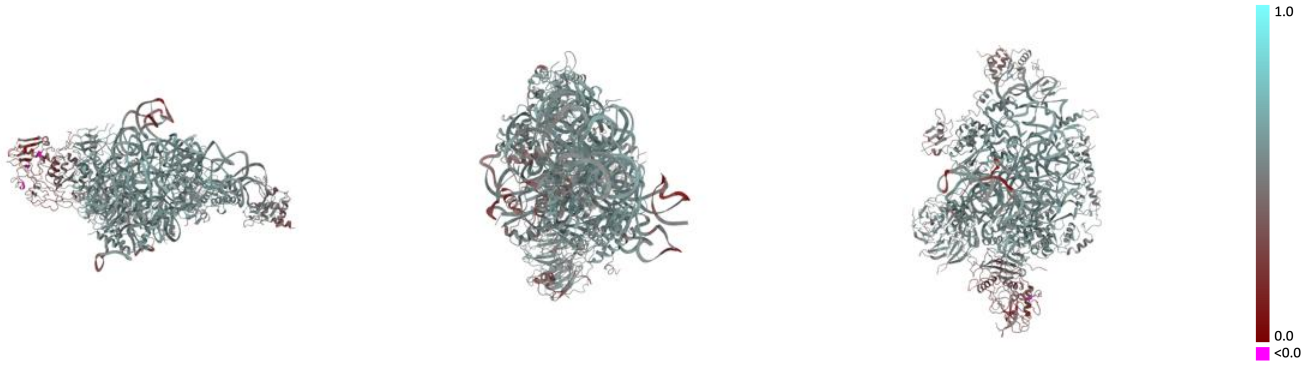
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

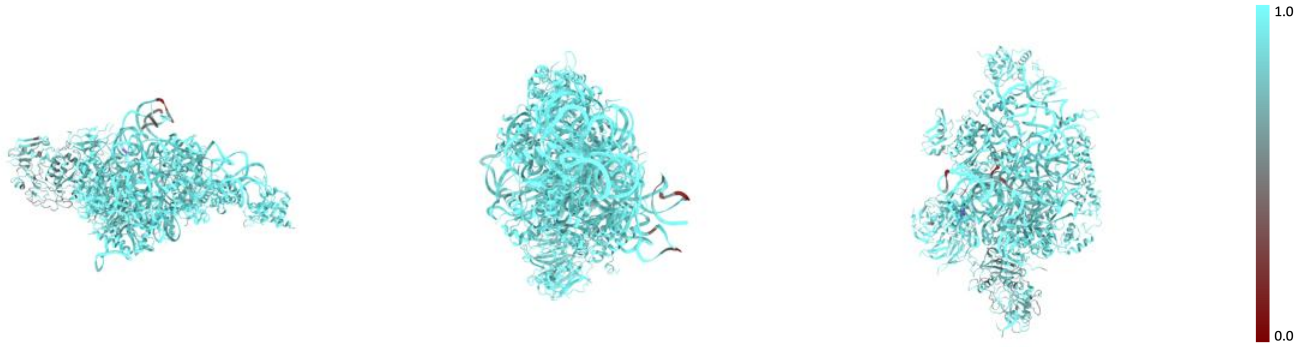
9.2 Q-score mapped to coordinate model (i)



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.

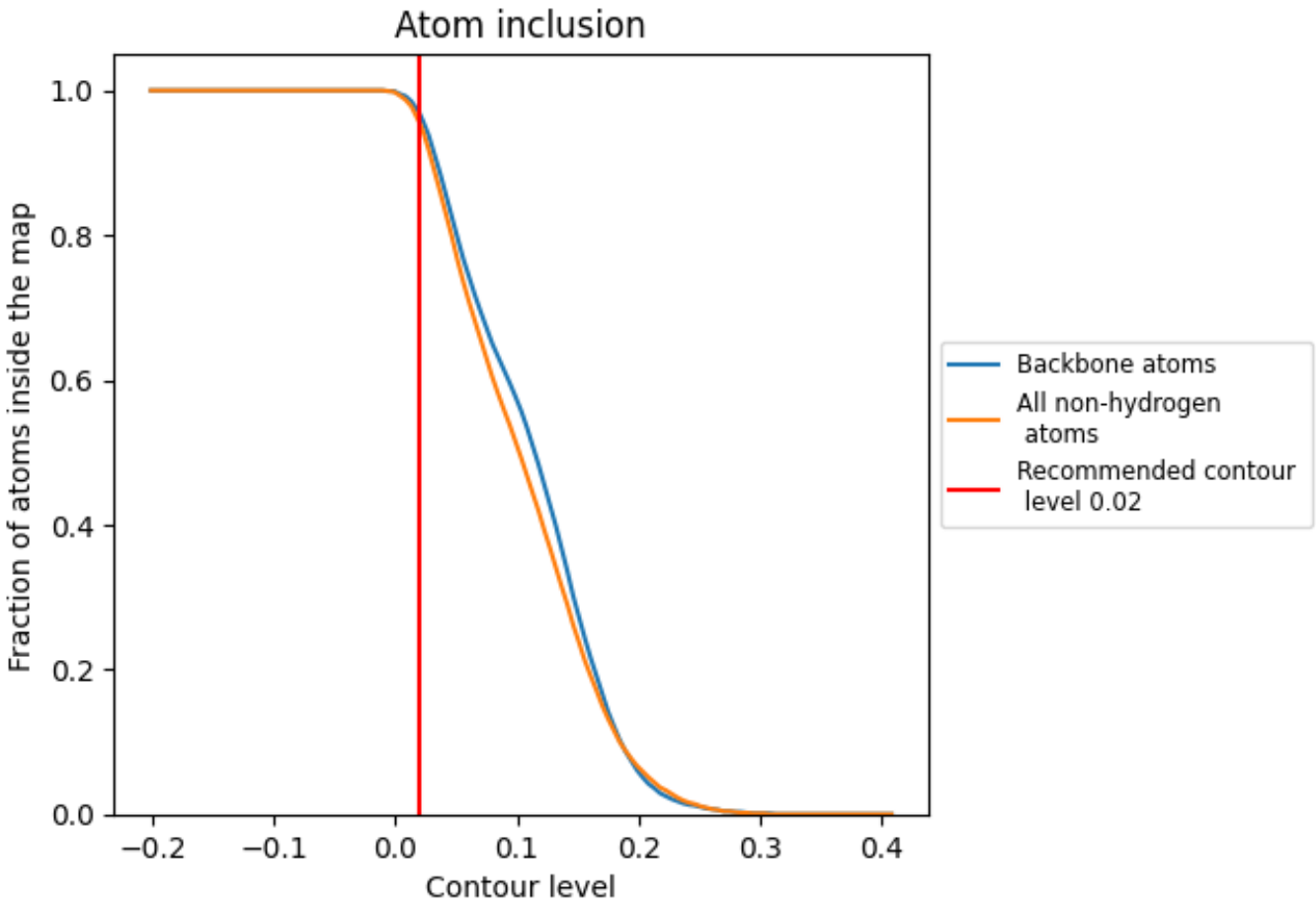
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9550	0.5290
A	0.9780	0.5500
V	0.9690	0.5590
X	0.9680	0.5450
Y	0.9760	0.5780
Z	0.9540	0.5530
a	0.9700	0.5610
b	0.9830	0.5620
c	0.9780	0.5340
d	0.9890	0.5750
e	0.9770	0.5470
f	0.9770	0.5510
h	0.9690	0.5470
i	0.9780	0.5970
k	0.9720	0.4830
m	0.9420	0.4300
n	0.9350	0.5340
o	0.9160	0.4210
x	0.7600	0.3600