WORLDWIDE wwPDB

PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

May 17, 2023 – 05:39 pm BST

PDB ID	:	8CAH
EMDB ID	:	EMD-16525
Title	:	Cryo-EM structure of native Otu2-bound ubiquitinated 43S pre-initiation complex
Authors	:	Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2023-01-24
Resolution	:	3.00 Å(reported)

This is a wwPDB EM Validation Summary 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:

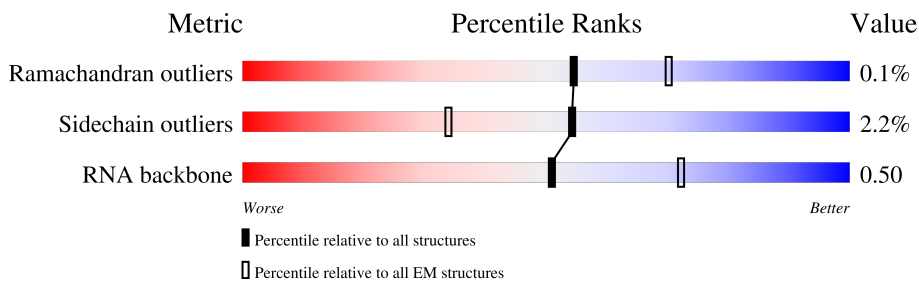|		
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.00 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	Percentile Ranks	Value
Ramachandran outliers		0.1%
Sidechain outliers		2.2%
RNA backbone		0.50

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
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	l	347	95% / 95% ... 5%
2	r	274	19% / 19% ... 81%
3	o	964	5% / 55% ... 45%
4	p	763	19% / 84% ... 15%
5	q	812	· / 78% ... 22%
6	i	153	· / 63% ... 37%
7	m	108	6% / 81% ... 17%
8	j	77	81% / 100%
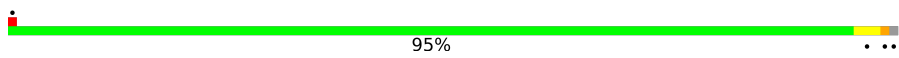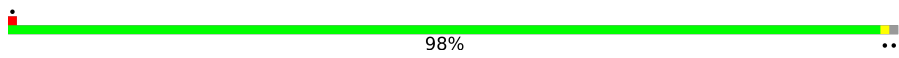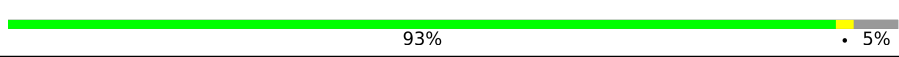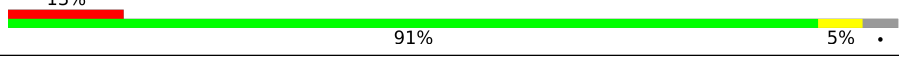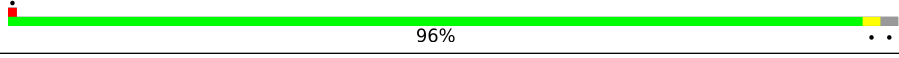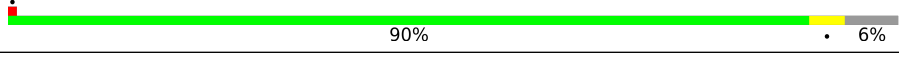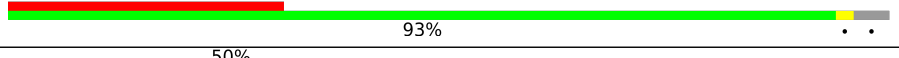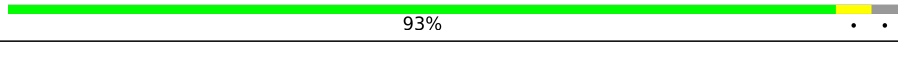
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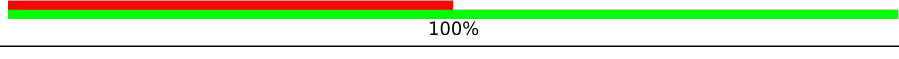| Mol	Chain	Length	Quality of chain
9	2	1800	67% 27%
10	P	252	79% 18%
11	Q	255	85% 11%
12	R	254	83% 15%
13	S	261	97%
14	T	236	94%
15	V	200	93% 6%
16	W	197	90% 7%
17	X	156	90% 9%
18	Y	151	97%
19	Z	137	91% 7%
20	a	87	98%
21	b	130	98%
22	c	145	97%
23	d	135	99%
24	e	119	80% 18%
25	f	82	95%
26	g	63	94% 5%
27	E	142	75% 7% 18%
28	A	240	88% 5% 8%
29	B	225	89% 8%
30	C	105	83% 5% 12%
31	D	143	6% 83% 15%
32	F	143	94% 5%
33	H	136	85% 11%

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Mol	Chain	Length	Quality of chain
34	I	146	95%
35	J	144	98%
36	K	121	81% 17%
37	L	108	8% 74% 24%
38	M	56	93% 5%
39	N	76	13% 91% 5%
40	O	319	96%
41	h	67	90% 6%
42	y	265	29% 70%
42	z	265	43% 55%
43	x	608	31% 93%
44	k	76	50% 100%
45	n	25	72% 28%
46	G	307	84% 16%
47	U	190	93%

2 Entry composition ⓘ

There are 51 unique types of molecules in this entry. The entry contains 95563 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 I.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	l	330	Total 1624	C 964	N 330	O 330	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	r	53	Total 261	C 155	N 53	O 53	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	o	529	Total 2631	C 1573	N 529	O 529	0	0

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	p	646	Total 3201	C 1909	N 646	O 646	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	q	636	Total 3169	C 1897	N 636	O 636	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	i	97	Total 476	C 282	N 97	O 97	0	0

- Molecule 7 is a protein called SUI1 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	m	90	Total 443	C 263	N 90	O 90	0	0

- Molecule 8 is a protein called RNA recognition motif (unknown).

Mol	Chain	Residues	Atoms				AltConf	Trace
8	j	77	Total 385	C 231	N 77	O 77	0	0

- Molecule 9 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	1745	Total 37189	C 16626	N 6587	O 12231	P 1745	0	0

- Molecule 10 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	206	Total 1603	C 1030	N 284	O 287	S 2	0	0

- Molecule 11 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	226	Total 1798	C 1139	N 330	O 325	S 4	0	0

- Molecule 12 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	216	Total 1626	C 1042	N 287	O 295	S 2	0	0

- Molecule 13 is a protein called 40S ribosomal protein S4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	258	Total 2056	C 1308	N 387	O 358	S 3	0	0

- Molecule 14 is a protein called 40S ribosomal protein S6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	228	Total 1815	C 1138	N 351	O 323	S 3	0	0

- Molecule 15 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	187	Total 1476	C 916	N 295	O 263	S 2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	184	Total 1479	C 935	N 285	O 258	S 1	0	0

- Molecule 17 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	142	Total 1142	C 733	N 217	O 189	S 3	0	0

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	150	Total 1192	C 759	N 224	O 207	S 2	0	0

- Molecule 19 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	127	Total 923	C 568	N 185	O 167	S 3	0	0

- Molecule 20 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	87	Total 673	C 415	N 125	O 131	S 2	0	0

- Molecule 21 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	129	Total 1021	C 650	N 188	O 180	S 3	0	0

- Molecule 22 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	144	Total 1121	C 708	N 220	O 191	S 2	0	0

- Molecule 23 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	d	134	Total 1073	C 676	N 208	O 189	0	0

- Molecule 24 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	97	Total 765	C 473	N 160	O 127	S 5	0	0

- Molecule 25 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	81	Total 610	C 382	N 110	O 113	S 5	0	0

- Molecule 26 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	60	Total 472	C 298	N 97	O 76	S 1	0	0

- Molecule 27 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	E	117	Total 916	C 583	N 171	O 155	S 7	0	0

- Molecule 28 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	222	Total 1729	C 1098	N 312	O 313	S 6	0	0

- Molecule 29 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B	206	Total 1605	C 1005	N 299	O 298	S 3	0	0

- Molecule 30 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	92	Total 754	C 489	N 122	O 141	S 2	0	0

- Molecule 31 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D	121	Total 875	C 551	N 153	O 169	S 2	0	0

- Molecule 32 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	F	141	Total 1105	C 708	N 203	O 194	0	0

- Molecule 33 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	121	Total 948	C 596	N 179	O 171	S 2	0	0

- Molecule 34 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	I	145	Total 1188	C 741	N 237	O 208	S 2	0	0

- Molecule 35 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 36 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 37 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	L	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 38 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 39 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N	73	Total	C	N	O	S	0	0
			560	355	106	95	4		

- Molecule 40 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 41 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

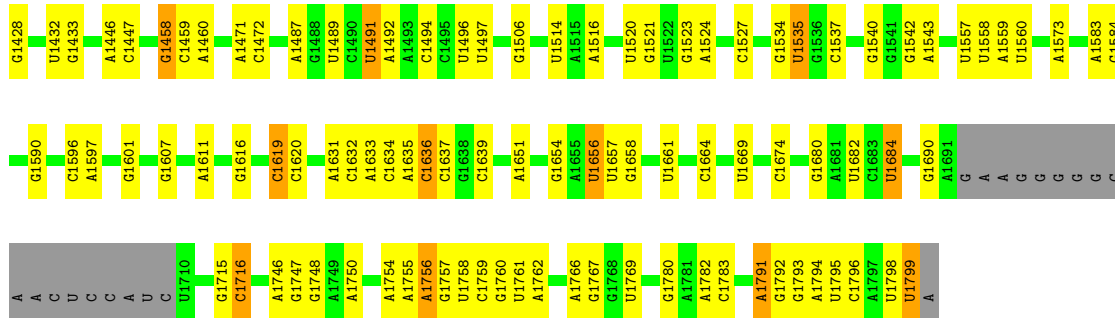- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit J.

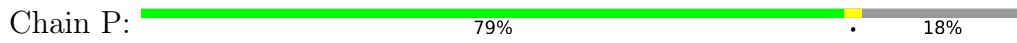| Mol	Chain	Residues	Atoms					AltConf	Trace
42	z	120	Total 896	C 556	N 172	O 166	S 2	0	0
42	y	79	Total 624	C 389	N 113	O 120	S 2	0	0

- Molecule 43 is a protein called RLI1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	582	Total 4607	C 2951	N 795	O 838	S 23	0	0

- Molecule 44 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	k	76	Total 374	C 222	N 76	O 76	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	19	PRO	SER	conflict	UNP P0CH08
k	24	GLU	ASP	conflict	UNP P0CH08
k	28	ALA	SER	conflict	UNP P0CH08

- Molecule 45 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	18	Total 175	C 107	N 48	O 19	S 1	0	0

- Molecule 46 is a protein called OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	G	259	Total 1509	C 917	N 298	O 292	S 2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	178	SER	CYS	conflict	UNP P38747

- Molecule 47 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	U	184	1473	946	263	264	0	0

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
48	2	77	77	77	0
48	S	1	Total 1	Mg 1	0
48	B	1	Total 1	Mg 1	0
48	x	1	Total 1	Mg 1	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
49	M	1	1	1	0
49	N	1	Total 1	Zn 1	0

- Molecule 50 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

Mol	Chain	Residues	Atoms			AltConf
50	x	1	Total	Fe	S	0
			8	4	4	
50	x	1	Total	Fe	S	0
			8	4	4	

- Molecule 51 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					AltConf
51	x	1	Total	C	N	O	P	0
			27	10	5	10	2	
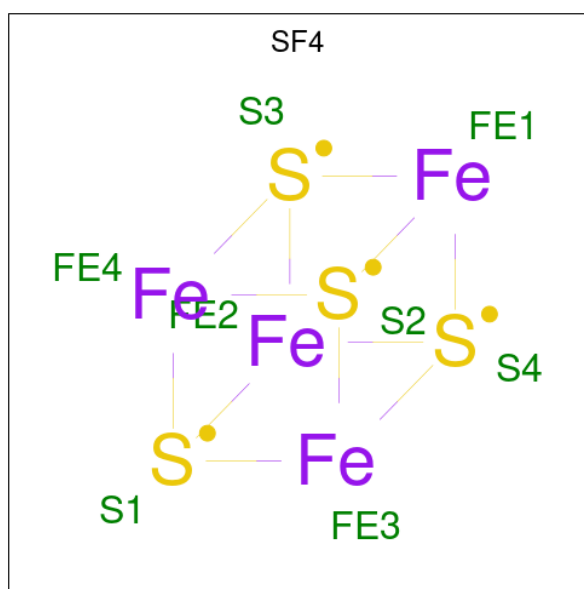
3 Residue-property plots ⓘ

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: Eukaryotic translation initiation factor 3 subunit I

Chain l:

• Molecule 2: Eukaryotic translation initiation factor 3 subunit G

Chain r:

• Molecule 3: Eukaryotic translation initiation factor 3 subunit A

Chain o:

5%

55%   45%

• Molecule 4: Eukaryotic translation initiation factor 3 subunit B

Chain p:

19%

84%   15%

G121 K122 T123 K124 G125 F126 L127 F128 V129 E130 C131 G132 S133 M134 N135 D136 A137 K138 K139 I140 I141 K142 S143 F144 H145 G146 K147 R148 L149 D150 L151 K152 H153 R154 L155 F156 L157 Y158 T159 M160 K161 D162 V163 E164 R165 Y166 N167 S168 ASP ASP PHE ASP THR GLU PHE ARG GLU PRO ASP MET

PRO THR PHE VAL P185 V198 P240 W336 P392 K536 A643 P664 ALA S666 N670 R673 K674 K675 V676 R677 K678 A685 A692 A695 D696 T697 ALA MET ARG D701 L702 I703 L704 H705 Q706 R707 E708 L709 L710 K711 Q712 W713 T714 E715 Y716 K717 E718 K719

I720 G721 Q722 E723 M724 E725 K726 S727 M728 N729 F730 K731 I732 F733 D734 V735 Q736 P737 GLU ASP ALA SER ASP ASP PHE THR ILE GLU ILE VAL GLU VAL LEU GLU GLU THR LYS GLU LYS VAL GLU

• Molecule 5: Eukaryotic translation initiation factor 3 subunit C

Chain q: 78%   22%

MET SER ARG PHE SER SER ASN TYR GLU TYR ASP VAL ALA SER SER SER GLU GLU ASP LEU LEU SER SER SER GLU GLU GLU GLU SER ASP GLN GLU ASP ASP SER SER PHE PHE ASN GLN GLU SER GLU GLU SER GLU SER GLU ALA ASP VAL

ASP SER ASP ASP SER ASP ALA LYS PRO TYR GLY PRO ASP TRP PHE LYS LYS GLU PHE ARG LYS GLN GLN GLY GLY SER ASN LYS PHE LEU LYS SER SER ASN TYR ASP SER SER ASP GLU GLU ASP SER GLU GLU ASP GLY LYS LYS VAL VAL K113 S136 ASP ASP W139 N180

THR GLN GLN ALA ASP LEU LYS ASN K189 A214 LYS PHE ARG ASN ASP PRO GLU SER PHE ASP LYS GLU PRO THR ALA ASP LEU ASP ILE SER ALA ASN GLY PHE THR ILE SER SER GLN GLY ASN ASP GLN ALA VAL Q251 F344 P347 I351 R364 L590 S593

Y637 K641 I645 S655 H658 Y659 D660 K661 L662 S663 E669 T670 E764 E772 E783 I784 T785 K786 L787 E788 E789 A790 M791 V792 K793 L794 ASN LYS GLU TYR LYS ILE ALA LYS GLU ARG LEU ASN PRO PRO SER ASN ARG ARG

• Molecule 6: Eukaryotic translation initiation factor 4C

Chain i: 63%   37%

MET GLY LYS LYS ASN THR LYS GLY GLY LYS LYS GLY ARG ARG GLY LYS LYS ASN ASP S19 D20 G45 I115 ASN GLU THR ASP ASN PHE GLY PHE GLU GLU SER ASP GLU GLU GLU ASP VAL ASN PHE GLU GLY PHE GLY ASN ALA ASP GLU ASP ASP GLU GLU GLY GLY GLU ASP GLU GLU LEU ASP GLU ILE ASP

ASP ILE

• Molecule 7: SUI1 isoform 1

Chain m: 6%   81%   17%

MET SER ILE GLU ASN LEU LYS SER PHE ASP PRO PHE ALA ASP THR GLY ASP ASP E19 T20 A21 T22 E73 R85 G107 F108

• Molecule 8: RNA recognition motif (unknown)

Chain j: 81%   100%

• Molecule 9: 18S ribosomal RNA

Chain 2:

G1428 U1432 G1433 A1446 C1447 G1458 C1459 A1460 A1471 C1472 A1487 G1488 U1489 C1490 U1491 A1492 A1493 C1494 C1495 U1496 U1497 G1506 U1514 A1515 A1516 U1520 U1521 U1522 G1523 A1524 C1527 G1534 U1535 G1536 C1537 G1540 G1541 G1542 A1543 U1557 U1558 A1559 U1560 A1573 A1583 G1584

G1590 C1596 A1597 G1601 G1607 A1611 G1616 C1619 C1620 A1631 C1632 A1633 C1634 A1635 C1636 C1637 G1638 C1639 A1651 G1654 A1655 U1656 U1657 G1658 U1661 C1664 U1669 C1674 G1680 A1681 U1682 C1683 U1684 G1690 A1691 G A A G G G G G C

A A C U C C A U C U1710 G1715 C1716 A1746 G1747 G1748 A1749 A1750 A1754 A1755 A1756 G1757 U1758 C1759 G1760 U1761 A1762 A1766 G1767 U1768 U1769 G1780 A1781 A1782 C1783 A1791 G1792 G1793 A1794 U1795 C1796 A1797 U1798 U1799 A

- Molecule 10: 40S ribosomal protein S0-A

Chain P: 79%   ·   18%

MET S2 D8 H32 R41 P42 D43 R191 D206 P207 GLU GLU VAL GLU GLN GLN VAL ALA GLU GLU ALA THR THR GLU GLU ALA GLY GLU GLU GLU ALA LYS GLU GLU VAL THR GLU GLU GLN ALA GLU ALA THR GLU TRP ALA GLU GLU ASN ALA ASP ASN VAL GLU TRP

- Molecule 11: 40S ribosomal protein S1-A

Chain Q: 85%   ·   11%

MET A2 R8 K13 GLY GLN LYS LYS ARG V20 K55 D59 K94 D108 N148 L184 F205 M229 G233 GLU GLY SER GLY GLU GLU LYS GLY LYS LYS VAL THR GLY PHE LYS ASP GLU VAL LEU GLU THR VAL

- Molecule 12: 40S ribosomal protein S2

Chain R: 83%   ·   15%

MET SER ALA PRO GLU ALA GLN GLN GLN LYS ARG GLY GLY PHE GLY GLY ARG ASN ARG GLY ARG PRO ASN ARG GLY ARG PRO ARG ASN THR GLU GLU LYS G34 V38 L76 Q77 D78 D195 Y222 A249 GLN LYS LYS ARG PHE

- Molecule 13: 40S ribosomal protein S4-B

Chain S: 97%   ··

MET A2 R11 L38 R77 Y182 H197 D212 Q259 GLY LEU

- Molecule 14: 40S ribosomal protein S6-B

Chain T: 94%   · ·

M1 D20 E21 H22 I24 R25 D29 D37 D105 K228 ARG ALA SER SER LEU LYS ALA

- Molecule 15: 40S ribosomal protein S8-A

Chain V: 93%   6%

MET G2 K123 LYS LYS ASN VAL LYS GLU GLU GLU THR VAL ALA K135 K199 LYS

• Molecule 16: 40S ribosomal protein S9-A

Chain W: 90% 7%

MET P2 K37 P67 D94 D103 D151 S152 E153 A167 R168 P169 G185 GLU ALA ALA ASP GLU ALA ASP GLU ALA ASP GLU GLU

• Molecule 17: 40S ribosomal protein S11-A

Chain X: 90% 9%

MET SER THR E4 R67 A145 ALA GLY LYS ALA ASN LYS GLN PHE ALA LYS PHE

• Molecule 18: 40S ribosomal protein S13

Chain Y: 97%

MET G2 K27 K93 P137 K140 N151

• Molecule 19: 40S ribosomal protein S14-A

Chain Z: 91% 7%

MET SER ASN VAL VAL GLN ALA ARG ASP ASN S11 D66 L105 V118 L137

• Molecule 20: 40S ribosomal protein S21-A

Chain a: 98%

M1 K5 L11 R87

• Molecule 21: 40S ribosomal protein S22-A

Chain b: 98%

MET T2 D54 Y130

• Molecule 22: 40S ribosomal protein S23-A

Chain c: 97%

MET G2 P88 F107 L133 S145
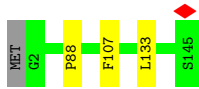
• Molecule 23: 40S ribosomal protein S24-A

Chain d: 99%

MET S2 N34 D135
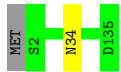
• Molecule 24: 40S ribosomal protein S26-A

Chain e: 80%   18%

MET P2 K19 D52 P98 GLN ARG PRO ARG PHE ASN ARG GLU ASN LYS VAL SER PRO ALA ASP ALA ALA LYS LYS ALA LEU
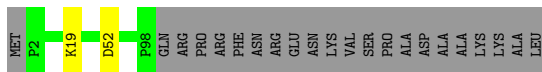
• Molecule 25: 40S ribosomal protein S27-A

Chain f: 95%

MET V2 D34 C56 S78 K82

• Molecule 26: 40S ribosomal protein S30-A

Chain g: 94%   5%

MET A2 L38 T48 S61 VAL GLN
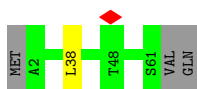
• Molecule 27: RPS15 isoform 1

Chain E: 75%   7%   18%

MET SER GLN ALA VAL ASN ALA LYS LYS ARG VAL PHE K13 K24 L25 L26 E27 M28 M49 K59 L65 N70 E71 K72 M83 V86 G129 ARG ALA GLY ALA THR THR SER ARG PHE ILE PRO LEU LYS

• Molecule 28: 40S ribosomal protein S3

Chain A: 88%   5%   8%

MET VAL ALA L4 Q56 D57 R76 D93 F107 D154 G155 F156 P211 K212 E213 P216 I217 L218 Y225 ARG PRO ALA GLU GLU THR GLU ALA GLN ALA GLU PRO VAL GLU ALA

• Molecule 29: 40S ribosomal protein S5

Chain B:

89%   •   8%

MET SER ASP THR GLU ALA PRO VAL GLU VAL GLN GLU ASP PHE GLU VAL VAL GLU GLU F20 F43 K54 D145 R156 D161 R225

• Molecule 30: 40S ribosomal protein S10-A

Chain C:

83%   5%   12%

M1 L2 K10 L68 N81 L82 I92 GLN GLU ARG ASN THR GLN ARG PRO GLN ARG ARG TYR

• Molecule 31: 40S ribosomal protein S12

6%

Chain D:

83%   •   15%

MET SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU VAL GLU GLU THR VAL VAL VAL GLU GLN THR ALA GLU VAL T23 D39 E68 A69 P82 E83 N84 K85 L88 R108 Q142 Q143

• Molecule 32: 40S ribosomal protein S16-A

Chain F:

94%   5%   •

MET SER A3 S6 K26 G27 L28 L52 L53 D64 E99 R143

• Molecule 33: 40S ribosomal protein S17-A

Chain H:

85%   •   11%

MET G2 L24 Q62 K63 K72 Y84 V85 S94 R95 SER ASN GLY VAL L100 A126 GLN ARG ASP ARG ARG TYR ARG LYS ARG VAL

• Molecule 34: 40S ribosomal protein S18-A

Chain I:

95%   •   ••

MET S2 L3 R40 M73 Y79 A102 R144 R145 A146

• Molecule 35: 40S ribosomal protein S19-A

Chain J:

98%   ••

MET P2 M45 L140 D143 E144

• Molecule 36: 40S ribosomal protein S20

Chain K:

81%   17%

MET SER ASP PHE GLN LYS GLU LYS VAL GLU GLU GLN GLU GLN GLN GLN ILE I20 H48 N49 A119 SER ASN

• Molecule 37: 40S ribosomal protein S25-A

8%

Chain L:

74%   24%

MET PRO PRO LYS GLN GLN LEU SER LYS ALA ALA LYS ALA ALA ALA LEU ALA GLY GLY LYS LYS SER K24 K25 S28 K29 K30 S31 M32 K33 D34 L65 E86 T105 ALA SER GLU
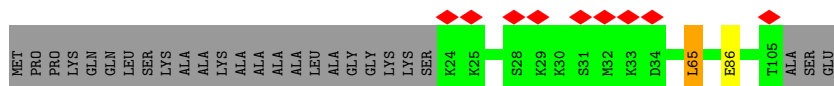
• Molecule 38: RPS29A isoform 1

Chain M:

93%   5%

MET ALA HIS E4 L36 R56
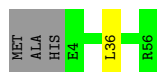
• Molecule 39: 40S ribosomal protein S31

13%

Chain N:

91%   5%

GLY LYS LYS R80 K92 V108 D109 A110 E111 G112 K113 K116 L117 S122 D137 V150 N151 A152
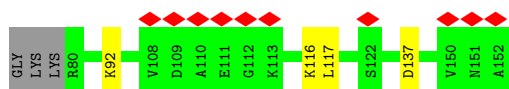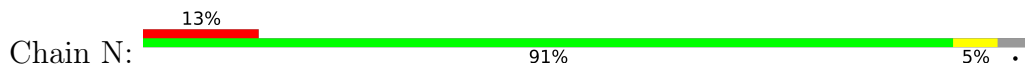
• Molecule 40: Guanine nucleotide-binding protein subunit beta-like protein

Chain O:

96%

MET ALA SER ASN E5 E160 K161 A162 D163 W181 L225 M231 D266 M316 THR ALA ASN

• Molecule 41: 40S ribosomal protein S28-A

Chain h:

90%   6%

MET ASP ASN LYS T5 L9 L33 E58 R64 R67

• Molecule 42: Eukaryotic translation initiation factor 3 subunit J

Chain z:

43%   55%

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

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

• Molecule 42: Eukaryotic translation initiation factor 3 subunit J

Chain y:

• Molecule 43: RLI1 isoform 1

Chain x:

• Molecule 44: 60S ribosomal protein L40-A

Chain k:

• Molecule 45: 60S ribosomal protein L41-A

Chain n:

72%   28%

M1 R18 LYS VAL ARG ALA ARG SER LYS

• Molecule 46: OTU domain-containing protein 2

Chain G:

84%   16%

MET THR GLY MET GLU SER GLY GLU ASN LEU GLU ASN M13 N72 ASN GLU VAL PHE ASP ALA GLU GLN GLU ASP GLU V84 S94 ILE SER ARG ASP GLU LYS GLU GLN GLN ASN VAL PRO VAL GLN GLN GLN GLN GLY GLN THR LYS LYS ARG ARG N120 P193 L196 D197

Q198 D199 M200 E228 S307

• Molecule 47: 40S ribosomal protein S7-A

Chain U:

93%   • •

MET SER ALA P4 L9 L18 L34 D87 R107 R116 D155 D158 S187 GLU THR HIS

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18826	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 $(e^-/Å^2)$	46.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.970	Depositor
Minimum map value	-1.905	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ZN, SF4

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	l	0.25	0/1622	0.49	0/2252
2	r	0.23	0/260	0.40	0/360
3	o	0.23	0/2626	0.33	0/3660
4	p	0.26	0/3197	0.46	0/4452
5	q	0.23	0/3165	0.35	0/4418
6	i	0.32	0/475	0.59	1/658 (0.2%)
7	m	0.25	0/442	0.45	0/613
9	2	0.83	2/41595 (0.0%)	1.15	291/64809 (0.4%)
10	P	0.43	0/1644	0.70	3/2249 (0.1%)
11	Q	0.39	0/1823	0.74	5/2447 (0.2%)
12	R	0.46	0/1656	0.70	3/2251 (0.1%)
13	S	0.47	0/2097	0.71	2/2823 (0.1%)
14	T	0.40	0/1839	0.74	3/2460 (0.1%)
15	V	0.47	0/1501	0.66	0/2006
16	W	0.44	0/1504	0.73	1/2016 (0.0%)
17	X	0.50	0/1168	0.63	0/1575
18	Y	0.47	0/1215	0.74	2/1638 (0.1%)
19	Z	0.42	0/934	0.77	2/1257 (0.2%)
20	a	0.47	0/682	0.76	0/921
21	b	0.47	0/1038	0.67	0/1395
22	c	0.48	0/1139	0.67	1/1518 (0.1%)
23	d	0.47	0/1087	0.67	0/1449
24	e	0.44	0/778	0.68	0/1042
25	f	0.45	0/620	0.80	1/838 (0.1%)
26	g	0.40	0/480	0.74	1/639 (0.2%)
27	E	0.33	0/936	0.89	7/1259 (0.6%)
28	A	0.44	1/1754 (0.1%)	0.79	5/2361 (0.2%)
29	B	0.30	0/1625	0.66	1/2197 (0.0%)
30	C	0.39	0/772	0.81	3/1044 (0.3%)
31	D	0.32	0/883	0.79	2/1199 (0.2%)
32	F	0.35	0/1125	0.65	1/1510 (0.1%)
33	H	0.35	0/957	0.75	0/1283

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	I	0.30	0/1207	0.70	2/1623 (0.1%)
35	J	0.30	0/1130	0.63	1/1517 (0.1%)
36	K	0.34	0/807	0.65	0/1091
37	L	0.28	0/661	0.72	1/888 (0.1%)
38	M	0.33	0/452	0.69	0/600
39	N	0.30	0/571	0.75	1/768 (0.1%)
40	O	0.28	0/2436	0.65	2/3318 (0.1%)
41	h	0.36	0/493	0.82	1/663 (0.2%)
42	y	0.48	0/631	1.00	2/851 (0.2%)
42	z	0.41	0/905	0.94	5/1213 (0.4%)
43	x	0.29	0/4694	0.63	5/6334 (0.1%)
44	k	0.24	0/373	0.48	0/517
45	n	0.34	0/176	0.78	0/225
46	G	0.26	0/1514	0.43	0/2075
47	U	0.39	0/1498	0.77	5/2019 (0.2%)
All	All	0.60	3/100187 (0.0%)	0.91	360/144301 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	p	0	1
21	b	0	1
42	z	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	211	PRO	CG-CD	-10.23	1.16	1.50
9	2	555	A	N7-C5	-5.27	1.36	1.39
9	2	142	G	C2-N3	-5.04	1.28	1.32

The worst 5 of 360 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	1756	A	O5'-P-OP2	-16.64	90.72	105.70
9	2	453	U	N1-C2-O2	13.03	131.92	122.80
9	2	1756	A	O5'-P-OP1	13.02	126.32	110.70
9	2	555	A	N7-C8-N9	12.72	120.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	453	U	C2-N1-C1'	12.53	132.74	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	b	54	ASP	Peptide
4	p	336	TRP	Peptide
42	z	154	ARG	Sidechain

5.2　Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	l	326/347 (94%)	321 (98%)	5 (2%)	0	100	100
2	r	51/274 (19%)	49 (96%)	2 (4%)	0	100	100
3	o	519/964 (54%)	509 (98%)	10 (2%)	0	100	100
4	p	638/763 (84%)	604 (95%)	31 (5%)	3 (0%)	29	68
5	q	628/812 (77%)	601 (96%)	26 (4%)	1 (0%)	47	82
6	i	95/153 (62%)	87 (92%)	8 (8%)	0	100	100
7	m	88/108 (82%)	81 (92%)	5 (6%)	2 (2%)	6	30
10	P	204/252 (81%)	190 (93%)	14 (7%)	0	100	100
11	Q	222/255 (87%)	201 (90%)	21 (10%)	0	100	100
12	R	214/254 (84%)	202 (94%)	12 (6%)	0	100	100
13	S	256/261 (98%)	238 (93%)	18 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	T	226/236 (96%)	217 (96%)	9 (4%)	0	100	100
15	V	183/200 (92%)	176 (96%)	7 (4%)	0	100	100
16	W	182/197 (92%)	172 (94%)	9 (5%)	1 (0%)	29	68
17	X	140/156 (90%)	134 (96%)	6 (4%)	0	100	100
18	Y	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
19	Z	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
20	a	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
21	b	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
22	c	142/145 (98%)	135 (95%)	6 (4%)	1 (1%)	22	60
23	d	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
24	e	95/119 (80%)	88 (93%)	7 (7%)	0	100	100
25	f	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
26	g	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
27	E	115/142 (81%)	110 (96%)	5 (4%)	0	100	100
28	A	220/240 (92%)	208 (94%)	12 (6%)	0	100	100
29	B	204/225 (91%)	194 (95%)	10 (5%)	0	100	100
30	C	90/105 (86%)	81 (90%)	9 (10%)	0	100	100
31	D	119/143 (83%)	103 (87%)	16 (13%)	0	100	100
32	F	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
33	H	117/136 (86%)	111 (95%)	6 (5%)	0	100	100
34	I	143/146 (98%)	137 (96%)	5 (4%)	1 (1%)	22	60
35	J	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
36	K	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
37	L	80/108 (74%)	76 (95%)	4 (5%)	0	100	100
38	M	51/56 (91%)	51 (100%)	0	0	100	100
39	N	71/76 (93%)	60 (84%)	11 (16%)	0	100	100
40	O	310/319 (97%)	293 (94%)	17 (6%)	0	100	100
41	h	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
42	y	77/265 (29%)	71 (92%)	6 (8%)	0	100	100
42	z	118/265 (44%)	109 (92%)	9 (8%)	0	100	100
43	x	578/608 (95%)	549 (95%)	29 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	k	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
45	n	16/25 (64%)	16 (100%)	0	0	100	100
46	G	253/307 (82%)	251 (99%)	2 (1%)	0	100	100
47	U	182/190 (96%)	171 (94%)	11 (6%)	0	100	100
All	All	8220/10188 (81%)	7788 (95%)	423 (5%)	9 (0%)	54	85

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	p	392	PRO
7	m	85	ARG
34	I	102	ALA
4	p	536	LYS
22	c	88	PRO

5.3.2   Protein sidechains ⓘ

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	
10	P	170/210 (81%)	166 (98%)	4 (2%)	49	79
11	Q	200/224 (89%)	194 (97%)	6 (3%)	41	75
12	R	175/205 (85%)	173 (99%)	2 (1%)	73	90
13	S	220/222 (99%)	216 (98%)	4 (2%)	59	85
14	T	189/201 (94%)	185 (98%)	4 (2%)	53	82
15	V	148/161 (92%)	147 (99%)	1 (1%)	84	94
16	W	156/166 (94%)	151 (97%)	5 (3%)	39	74
17	X	126/137 (92%)	125 (99%)	1 (1%)	81	93
18	Y	127/128 (99%)	125 (98%)	2 (2%)	62	86
19	Z	90/105 (86%)	88 (98%)	2 (2%)	52	81
20	a	71/74 (96%)	69 (97%)	2 (3%)	43	77
21	b	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	c	119/120 (99%)	118 (99%)	1 (1%)	81	93
23	d	112/113 (99%)	111 (99%)	1 (1%)	78	92
24	e	82/101 (81%)	80 (98%)	2 (2%)	49	79
25	f	70/71 (99%)	68 (97%)	2 (3%)	42	76
26	g	50/54 (93%)	50 (100%)	0	100	100
27	E	95/118 (80%)	91 (96%)	4 (4%)	30	66
28	A	182/195 (93%)	174 (96%)	8 (4%)	28	65
29	B	172/191 (90%)	168 (98%)	4 (2%)	50	80
30	C	78/98 (80%)	76 (97%)	2 (3%)	46	78
31	D	88/119 (74%)	87 (99%)	1 (1%)	73	90
32	F	117/119 (98%)	111 (95%)	6 (5%)	24	60
33	H	101/124 (82%)	96 (95%)	5 (5%)	24	60
34	I	127/129 (98%)	122 (96%)	5 (4%)	32	69
35	J	115/116 (99%)	114 (99%)	1 (1%)	78	92
36	K	93/114 (82%)	91 (98%)	2 (2%)	52	81
37	L	67/89 (75%)	65 (97%)	2 (3%)	41	75
38	M	47/49 (96%)	46 (98%)	1 (2%)	53	82
39	N	57/66 (86%)	54 (95%)	3 (5%)	22	58
40	O	250/262 (95%)	247 (99%)	3 (1%)	71	90
41	h	55/60 (92%)	53 (96%)	2 (4%)	35	70
42	y	69/221 (31%)	68 (99%)	1 (1%)	67	88
42	z	90/221 (41%)	87 (97%)	3 (3%)	38	73
43	x	516/537 (96%)	506 (98%)	10 (2%)	57	84
45	n	17/23 (74%)	17 (100%)	0	100	100
46	G	62/282 (22%)	62 (100%)	0	100	100
47	U	163/170 (96%)	160 (98%)	3 (2%)	59	85
All	All	4776/5706 (84%)	4671 (98%)	105 (2%)	54	81

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	D	83	GLU
34	I	79	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	x	557	LEU
32	F	26	LYS
33	H	62	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
36	K	36	ASN
42	z	165	ASN
43	x	315	ASN
11	Q	95	ASN
11	Q	92	GLN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	2	1740/1800 (96%)	456 (26%)	16 (0%)

5 of 456 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	2	2	A
9	2	4	C
9	2	17	C
9	2	25	C
9	2	26	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	2	1636	C
9	2	1382	A
9	2	711	U
9	2	1344	A
9	2	640	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 85 ligands modelled in this entry, 82 are monoatomic - leaving 3 for Mogul analysis.

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	$\#|Z| > 2$
50	SF4	x	702	43	0,12,12	-	-	-		
50	SF4	x	701	43	0,12,12	-	-	-		
51	ADP	x	703	43,48	24,29,29	0.93	1 (4%)	29,45,45	1.37	4 (13%)

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
50	SF4	x	702	43	-	-	0/6/5/5
50	SF4	x	701	43	-	-	0/6/5/5
51	ADP	x	703	43,48	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	x	703	ADP	C5-C4	2.44	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	x	703	ADP	C3'-C2'-C1'	3.36	106.04	100.98
51	x	703	ADP	N3-C2-N1	-3.12	123.80	128.68
51	x	703	ADP	C4-C5-N7	-2.55	106.75	109.40
51	x	703	ADP	PA-O3A-PB	-2.09	125.67	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	x	703	ADP	O4'-C4'-C5'-O5'
51	x	703	ADP	C3'-C4'-C5'-O5'

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 then 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.

Ligand ADP x 703

Bond lengths   Bond angles

Torsions   Rings
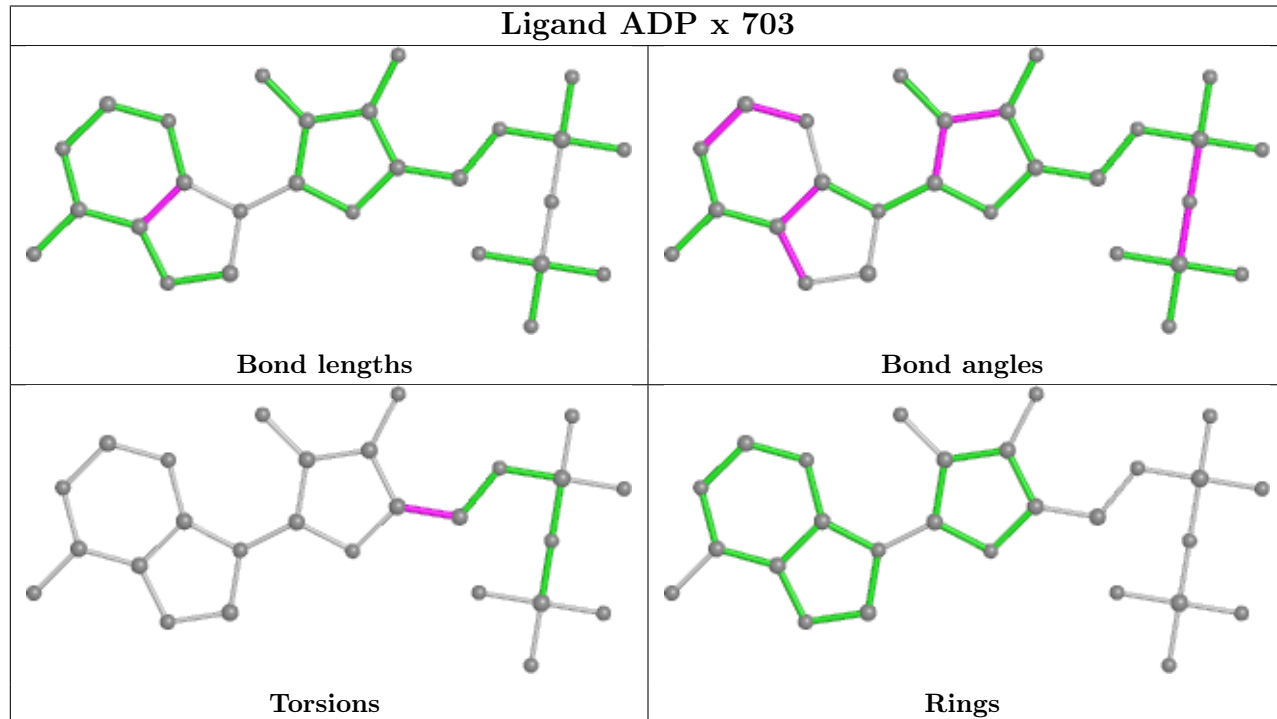
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-16525. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1   Orthogonal projections ⓘ
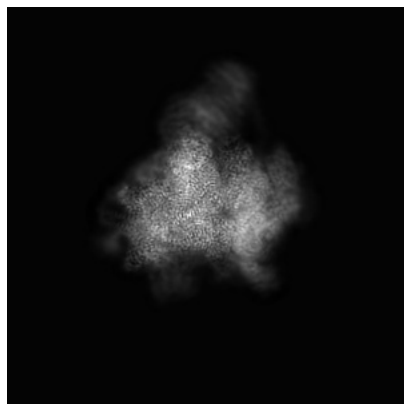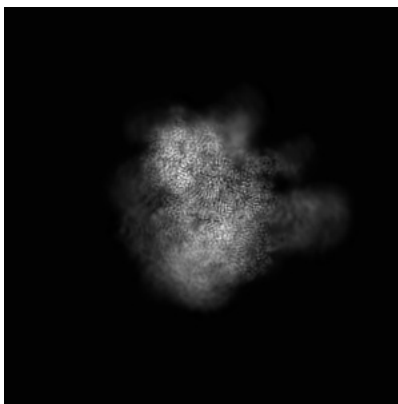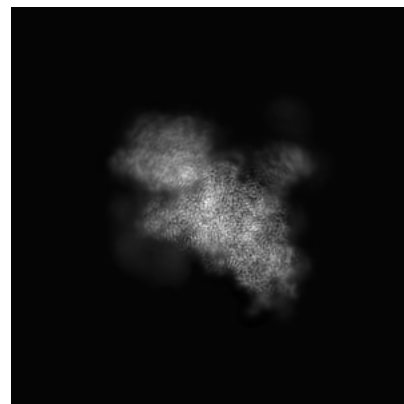
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

X   Y   Z
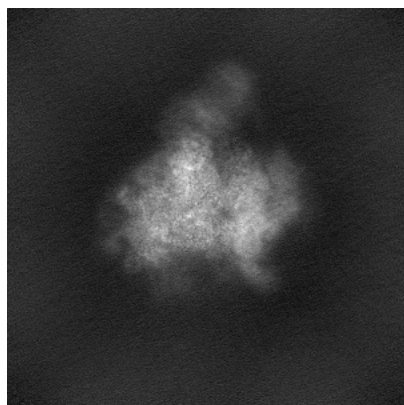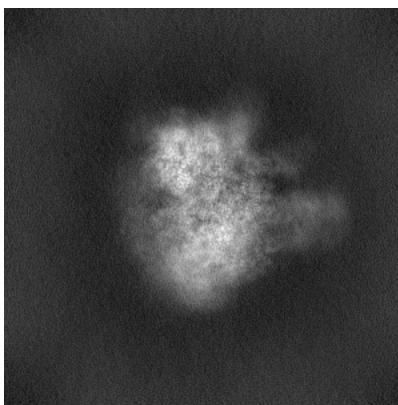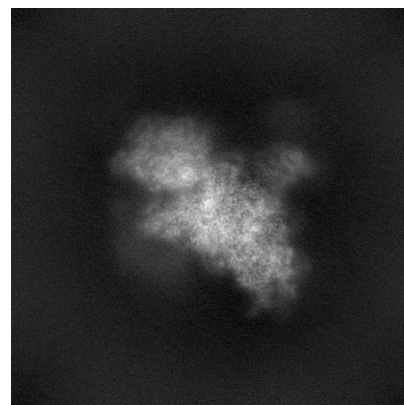
The images above show the map projected \in three orthogonal directions.

6.2 Central slices ⓘ
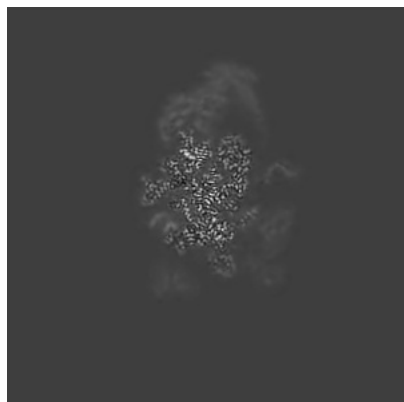
6.2.1 Primary map
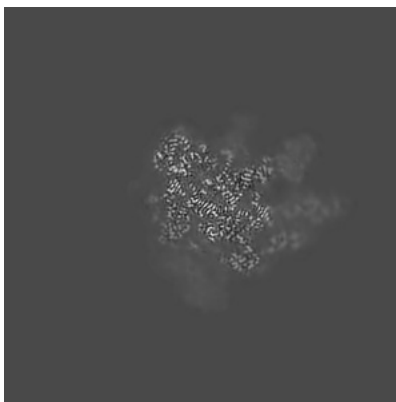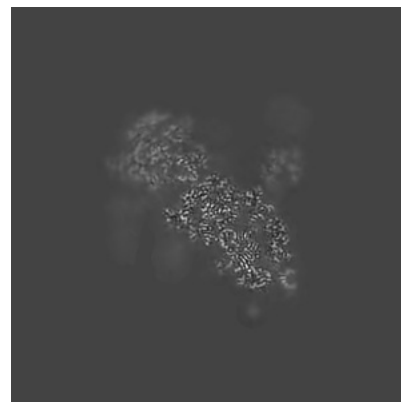
X Index: 210   Y Index: 210   Z Index: 210

6.2.2 Raw map
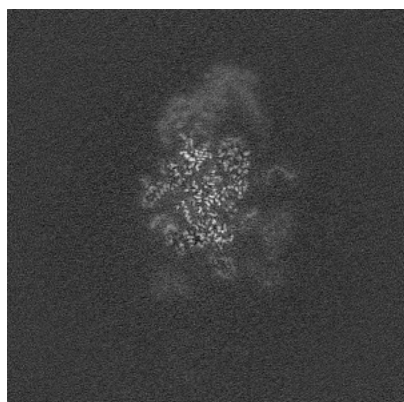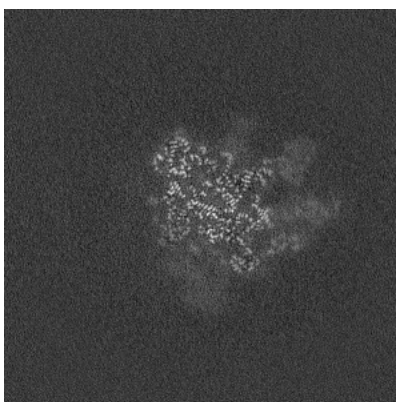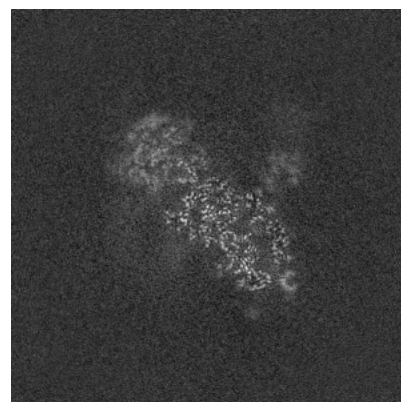
X Index: 210   Y Index: 210   Z Index: 210

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

6.3   Largest variance slices   ⓘ

6.3.1   Primary map
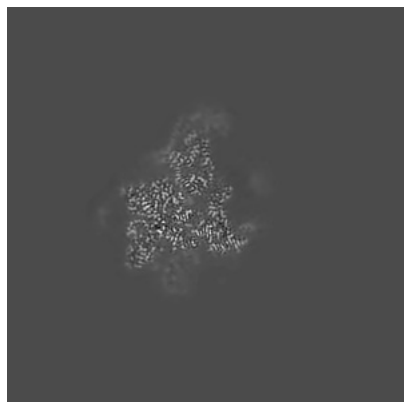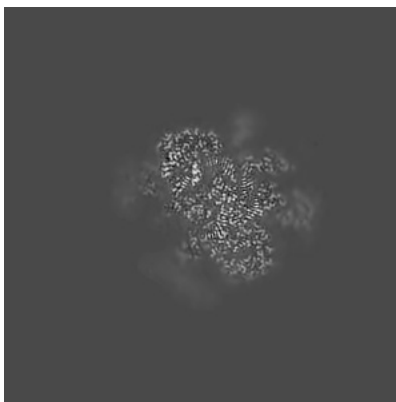
| X Index: 247 | Y Index: 189 | Z Index: 222 |
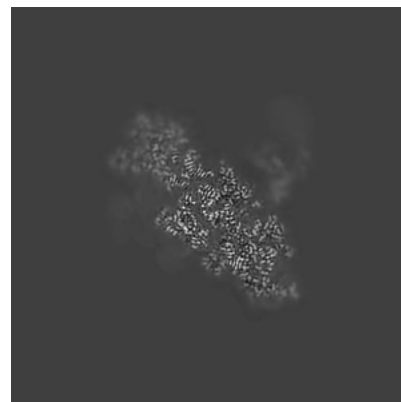
6.3.2   Raw map
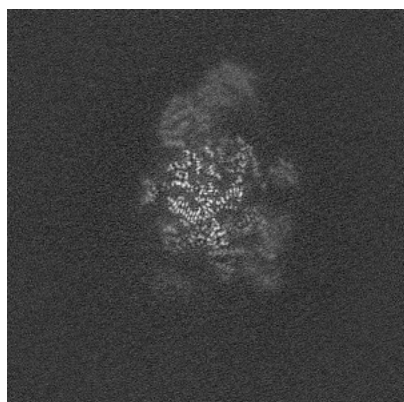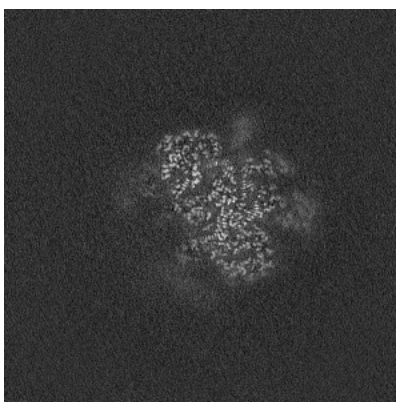
| X Index: 205 | Y Index: 189 | Z Index: 222 |
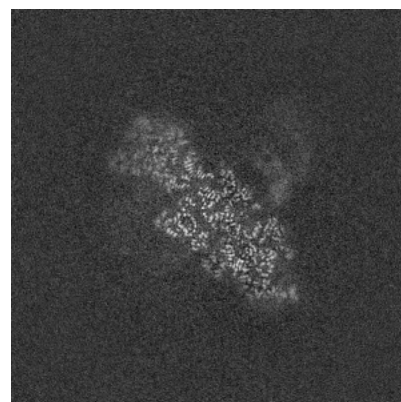
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
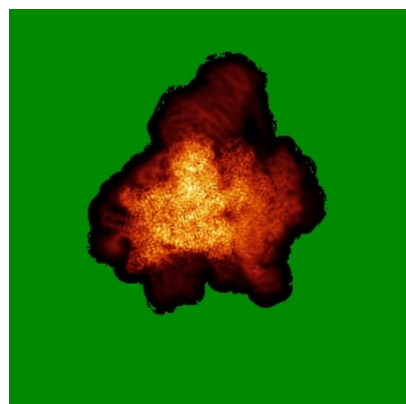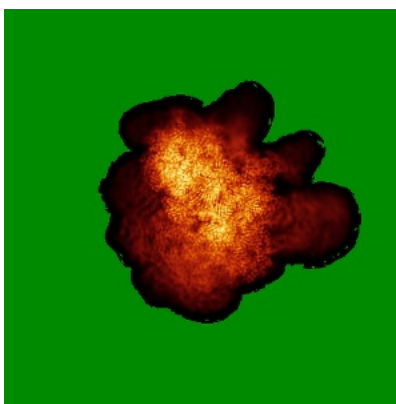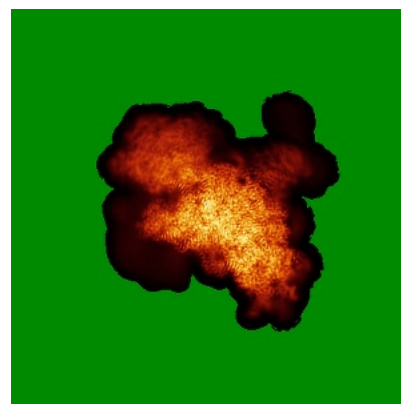
X   Y   Z

6.4.2 Raw map

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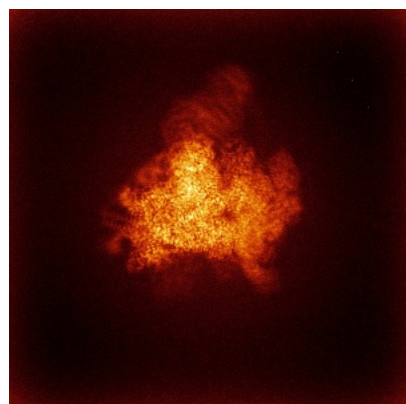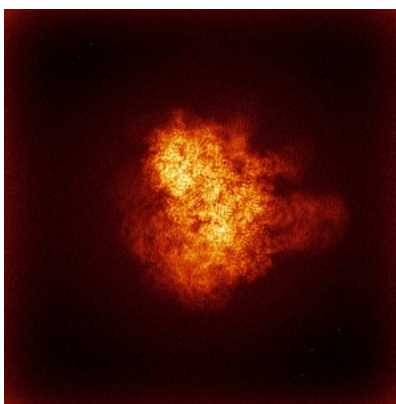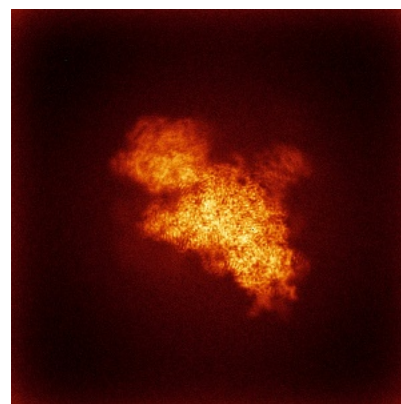
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
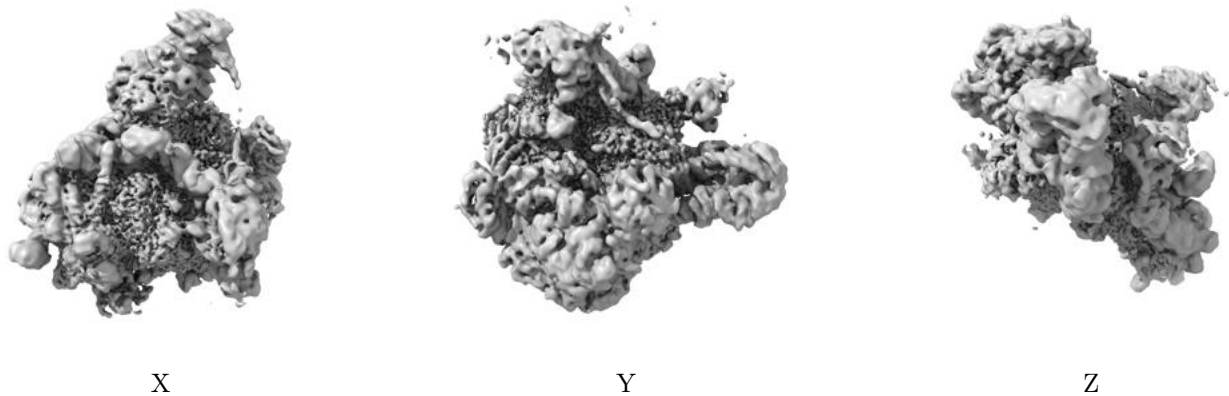
The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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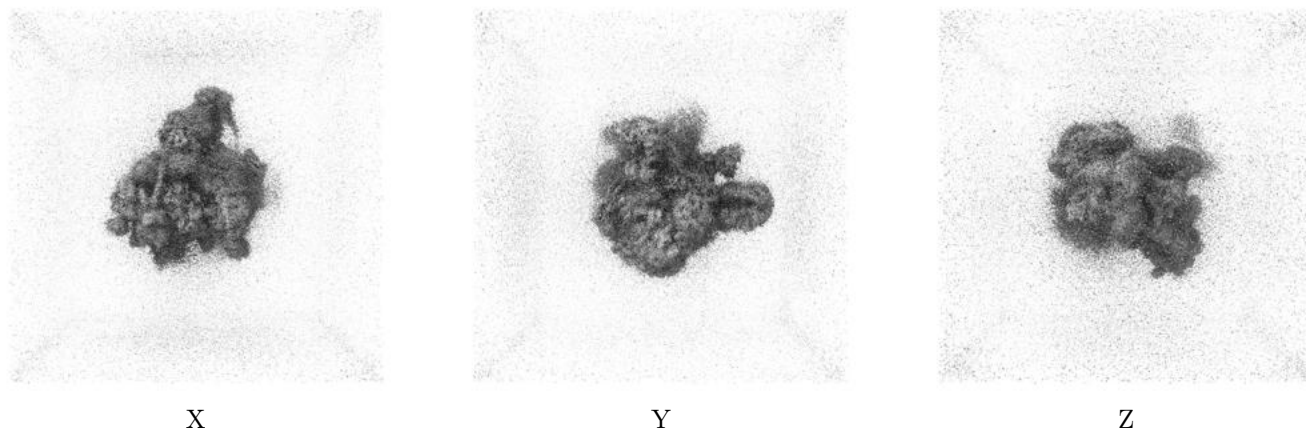
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

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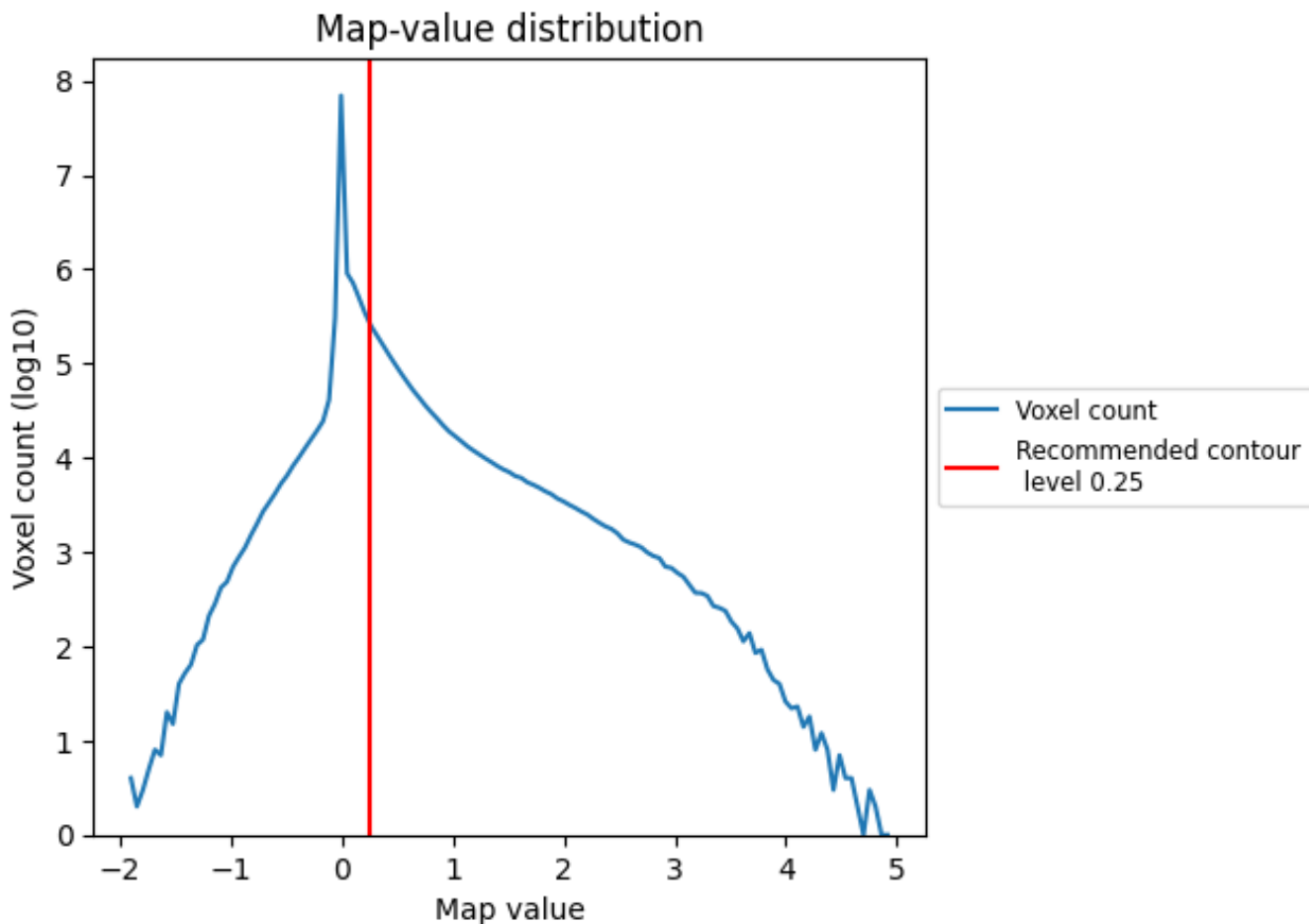
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
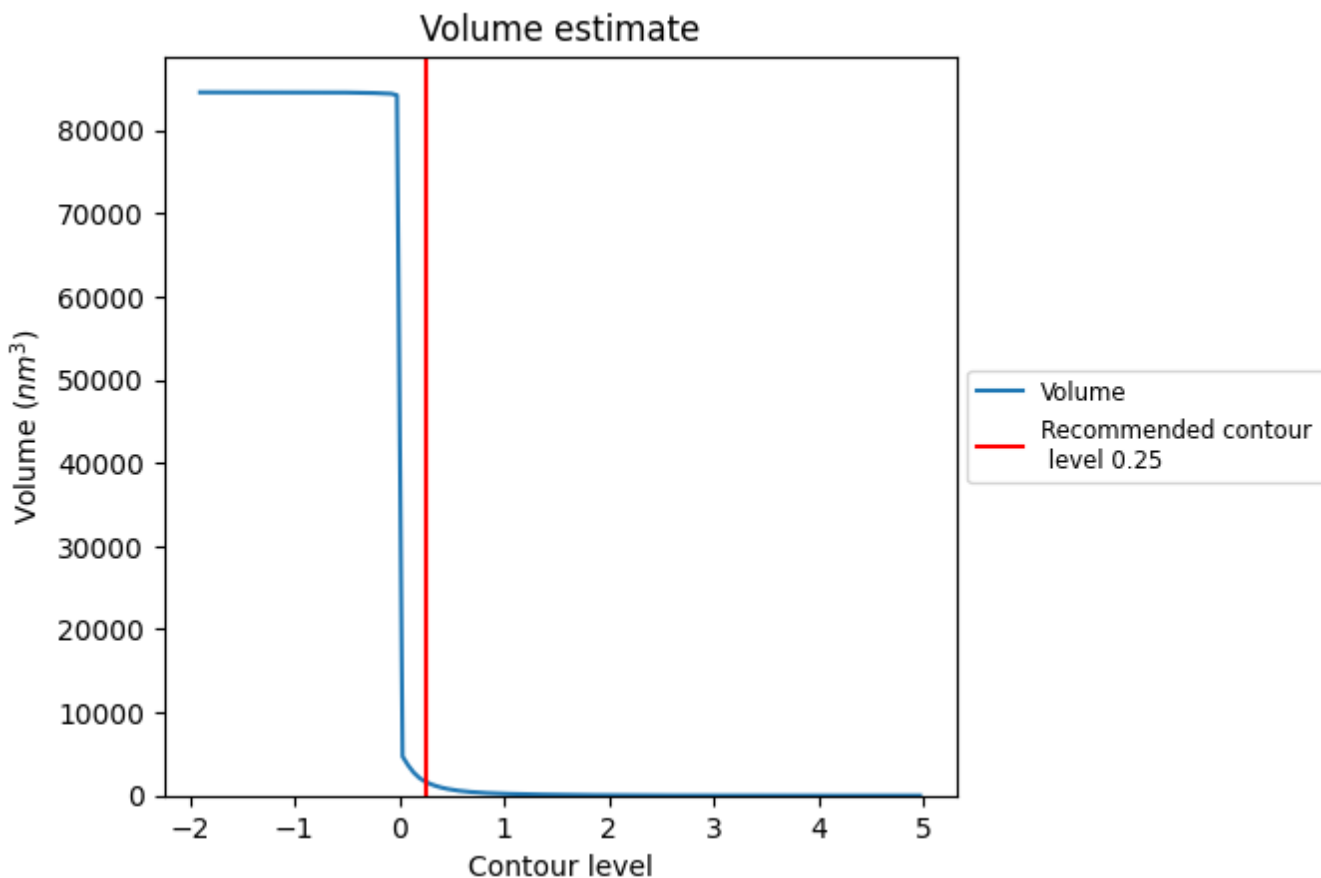
The volume at the recommended contour level is 1650 nm^3; this corresponds to an approximate mass of 1491 kDa.

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 ⓘ
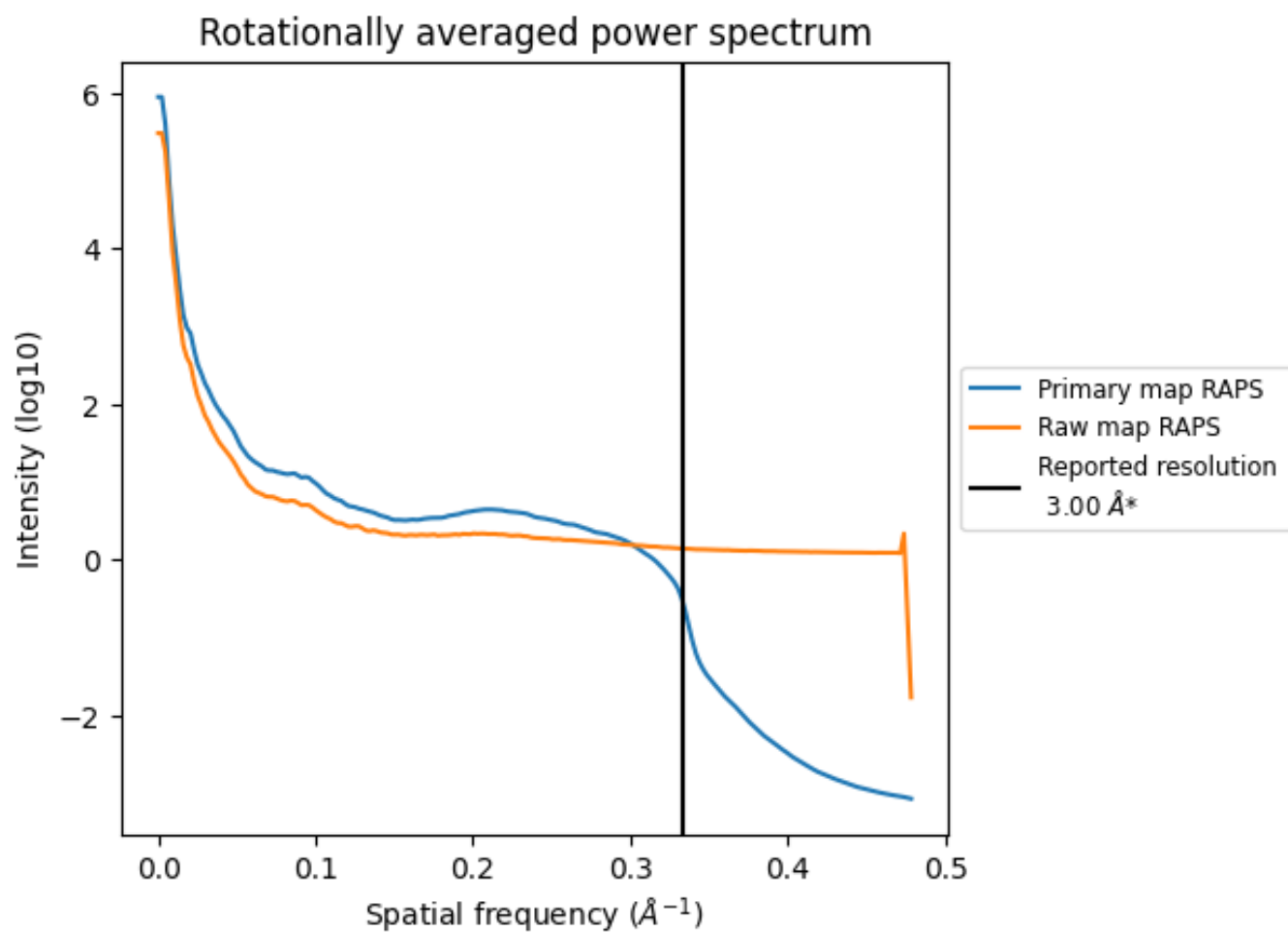
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8   Fourier-Shell correlation ⓘ

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

8.1   FSC ⓘ
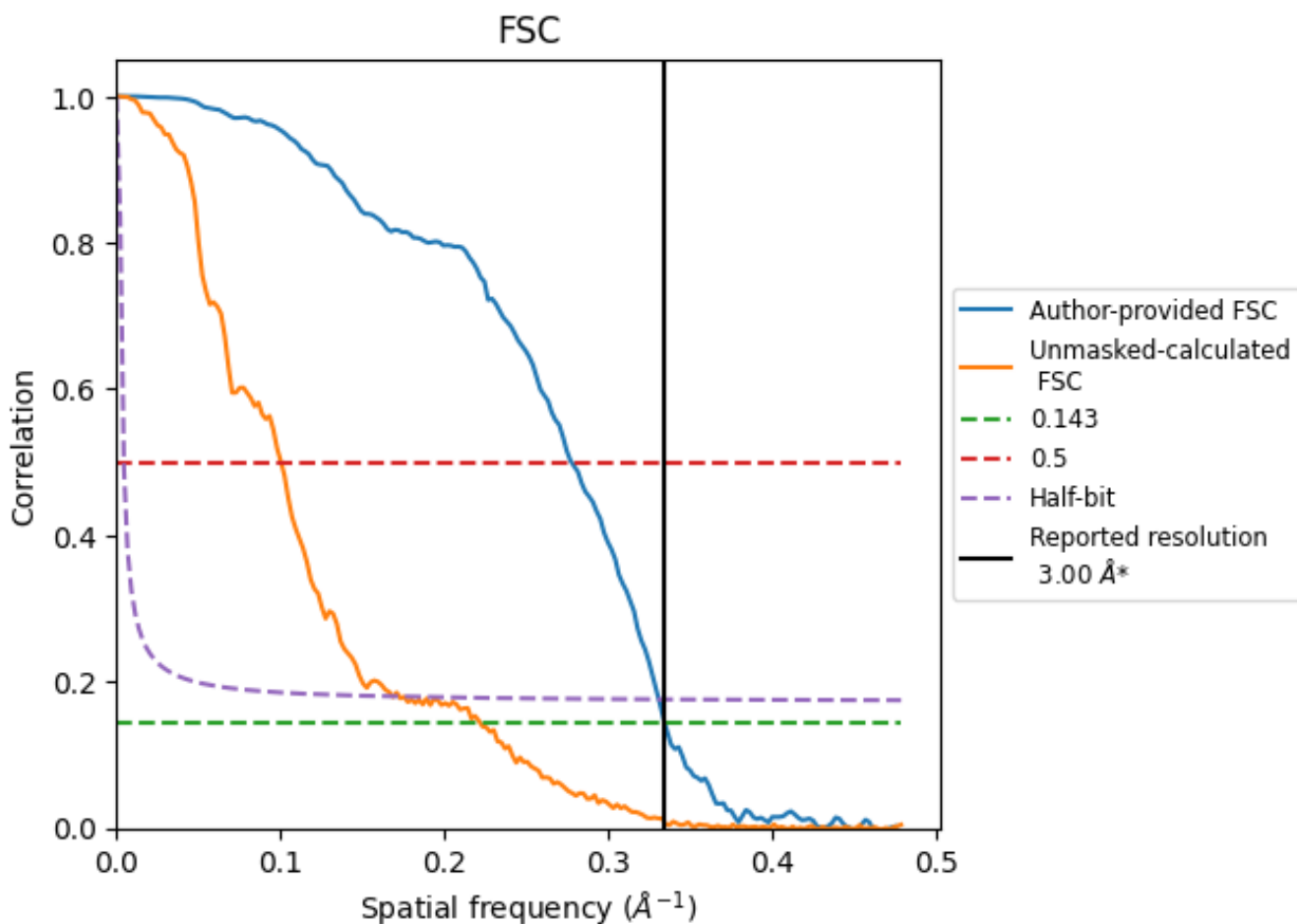
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.60	3.02
Unmasked-calculated*	4.50	9.97	5.94

*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 4.50 differs from the reported value 3.0 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16525 and PDB model 8CAH. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay (i)

| X | Y | Z |
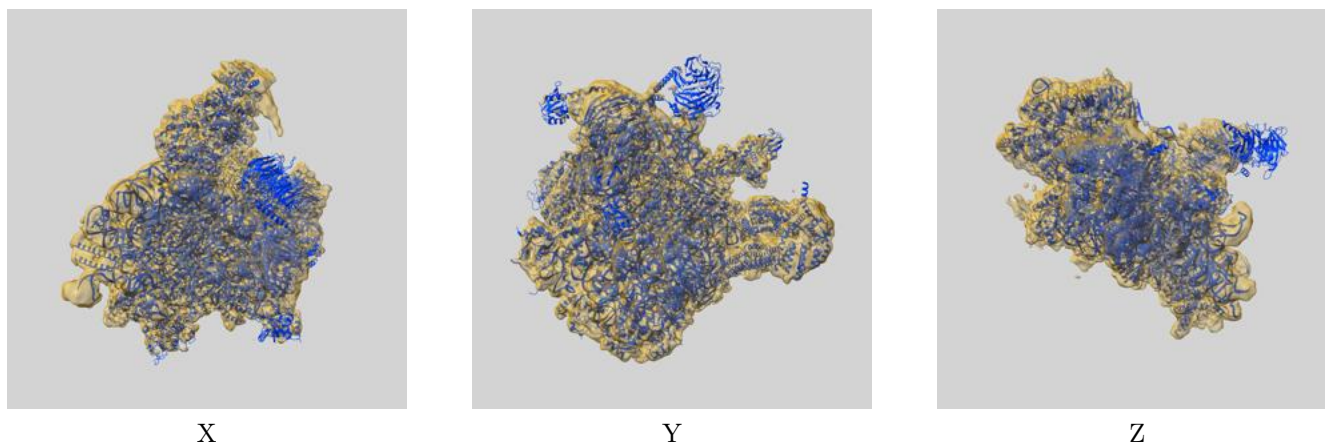
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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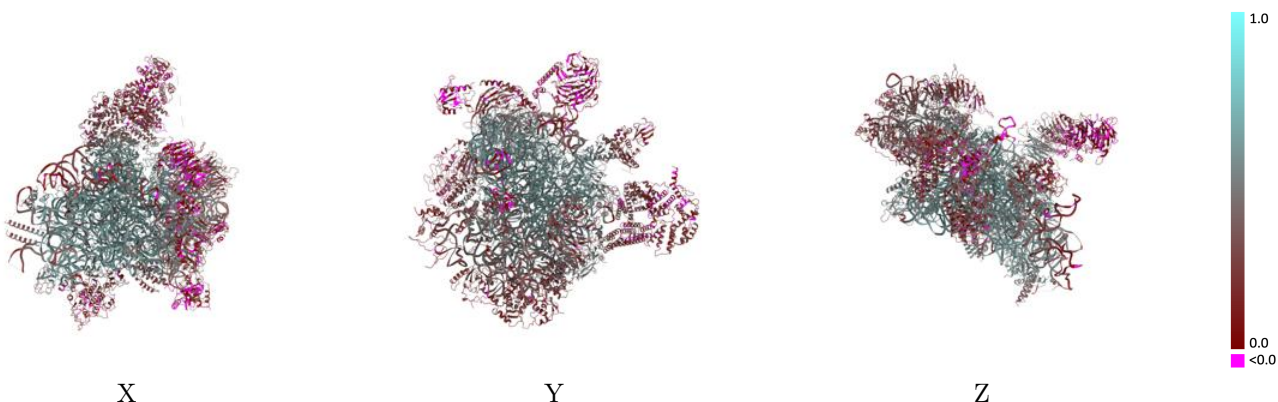
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
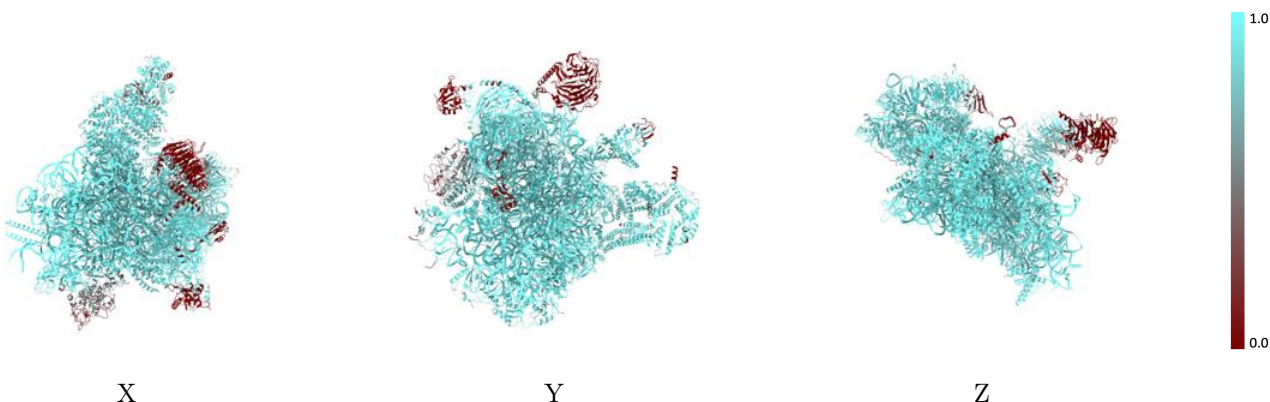
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion ⓘ
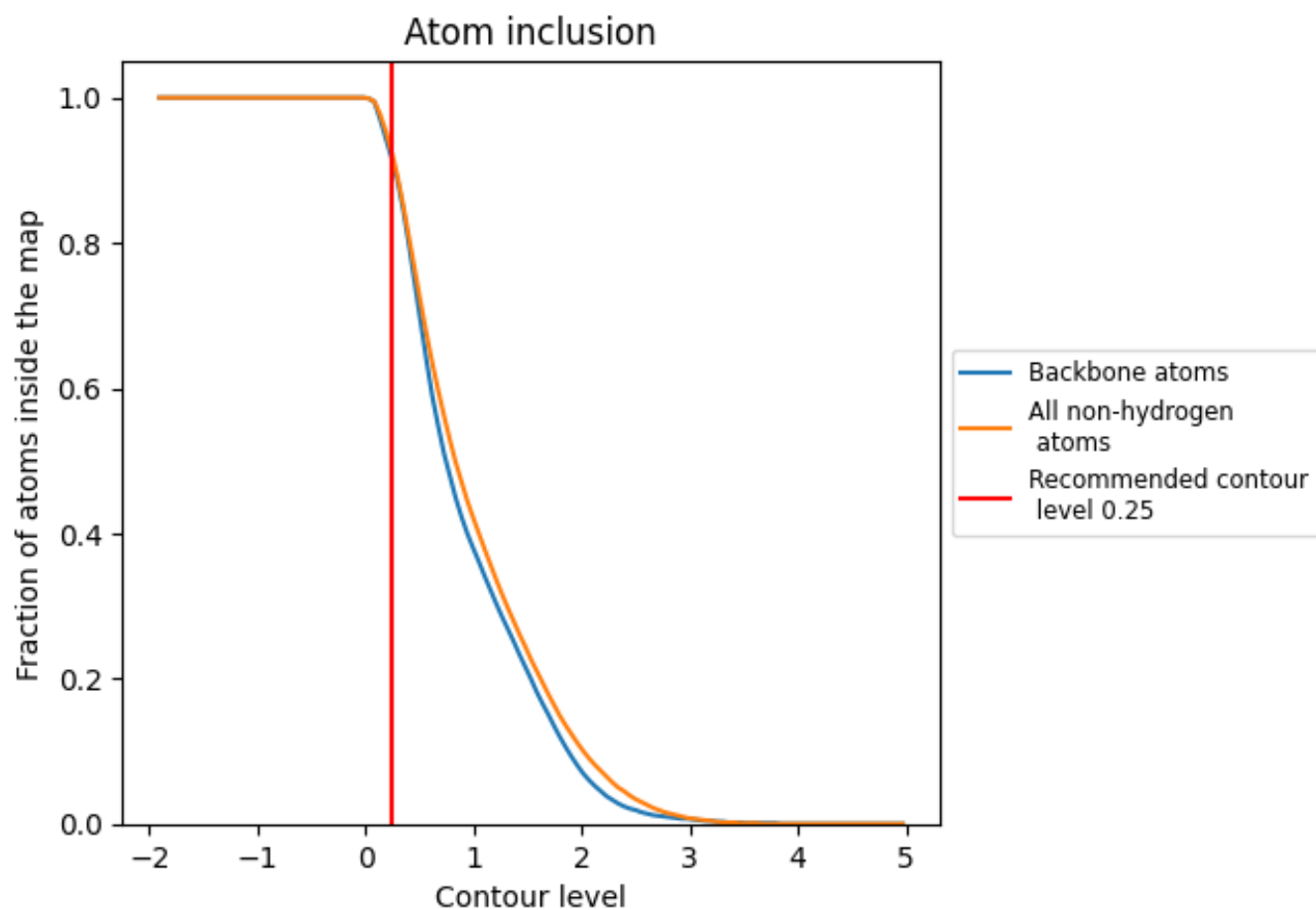
At the recommended contour level, 91% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.4300
2	0.9910	0.5070
A	0.9450	0.4170
B	0.9610	0.3310
C	0.9780	0.3710
D	0.8090	0.1960
E	0.9480	0.2660
F	0.9930	0.3680
G	0.9480	0.3100
H	0.9640	0.4310
I	0.9520	0.2390
J	0.9790	0.2800
K	0.9460	0.3820
L	0.8700	0.1940
M	1.0000	0.4810
N	0.8070	0.1840
O	0.9360	0.2810
P	0.9930	0.5580
Q	0.9810	0.5110
R	0.9940	0.5820
S	0.9960	0.5850
T	0.9830	0.5030
U	0.9770	0.4820
V	0.9940	0.5700
W	0.9820	0.5760
X	0.9870	0.5920
Y	0.9890	0.5620
Z	0.9870	0.5350
a	0.9890	0.5720
b	0.9990	0.6120
c	0.9930	0.5910
d	0.9880	0.5540
e	0.9910	0.5710
f	0.9780	0.5400
g	0.9360	0.4980

1.0

0.0
<0.0

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Chain	Atom inclusion	Q-score
h	0.9370	0.3410
i	0.9500	0.4380
j	0.1950	0.0630
k	0.4920	0.1840
l	0.0110	0.0720
m	0.9320	0.3930
n	1.0000	0.5870
o	0.8920	0.1950
p	0.7640	0.2750
q	0.9420	0.2330
r	0.0000	0.1080
x	0.5460	0.2130
y	0.8360	0.3210
z	0.8890	0.3550