



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:59 AM UTC

PDB ID : 7PX3 / pdb_00007px3
EMDB ID : EMD-13690
Title : Structure of U5 snRNP assembly and recycling factor TSSC4 in complex with BRR2 and Jab1 domain of PRPF8
Authors : Bergfort, A.; Kuropka, B.; Ilik, I.A.; Freund, C.; Aktas, T.; Hilal, T.; Weber, G.; Wahl, M.C.
Deposited on : 2021-10-07
Resolution : 3.05 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

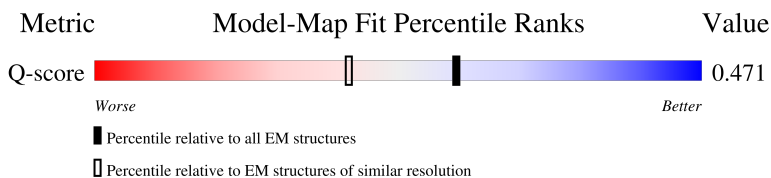
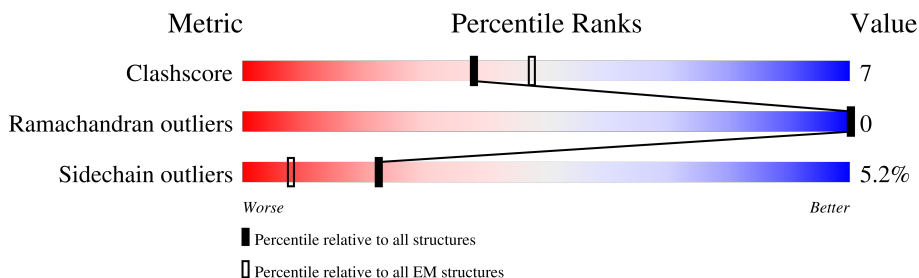
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13971 (2.55 - 3.55)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1747	 76% 20% ..
2	J	263	 78% 16% • 5%
3	T	329	 16% 5% 80%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16430 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 U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1725	Total	C	N	O	S	0	0
			13870	8865	2373	2560	72		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	390	GLY	-	expression tag	UNP O75643
B	391	ALA	-	expression tag	UNP O75643
B	392	GLU	-	expression tag	UNP O75643
B	393	PHE	-	expression tag	UNP O75643

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	250	Total	C	N	O	S	0	0
			2030	1301	350	368	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2058	GLY	-	expression tag	UNP Q6P2Q9
J	2059	PRO	-	expression tag	UNP Q6P2Q9
J	2060	LEU	-	expression tag	UNP Q6P2Q9
J	2061	GLY	-	expression tag	UNP Q6P2Q9
J	2062	SER	-	expression tag	UNP Q6P2Q9
J	2063	MET	-	expression tag	UNP Q6P2Q9

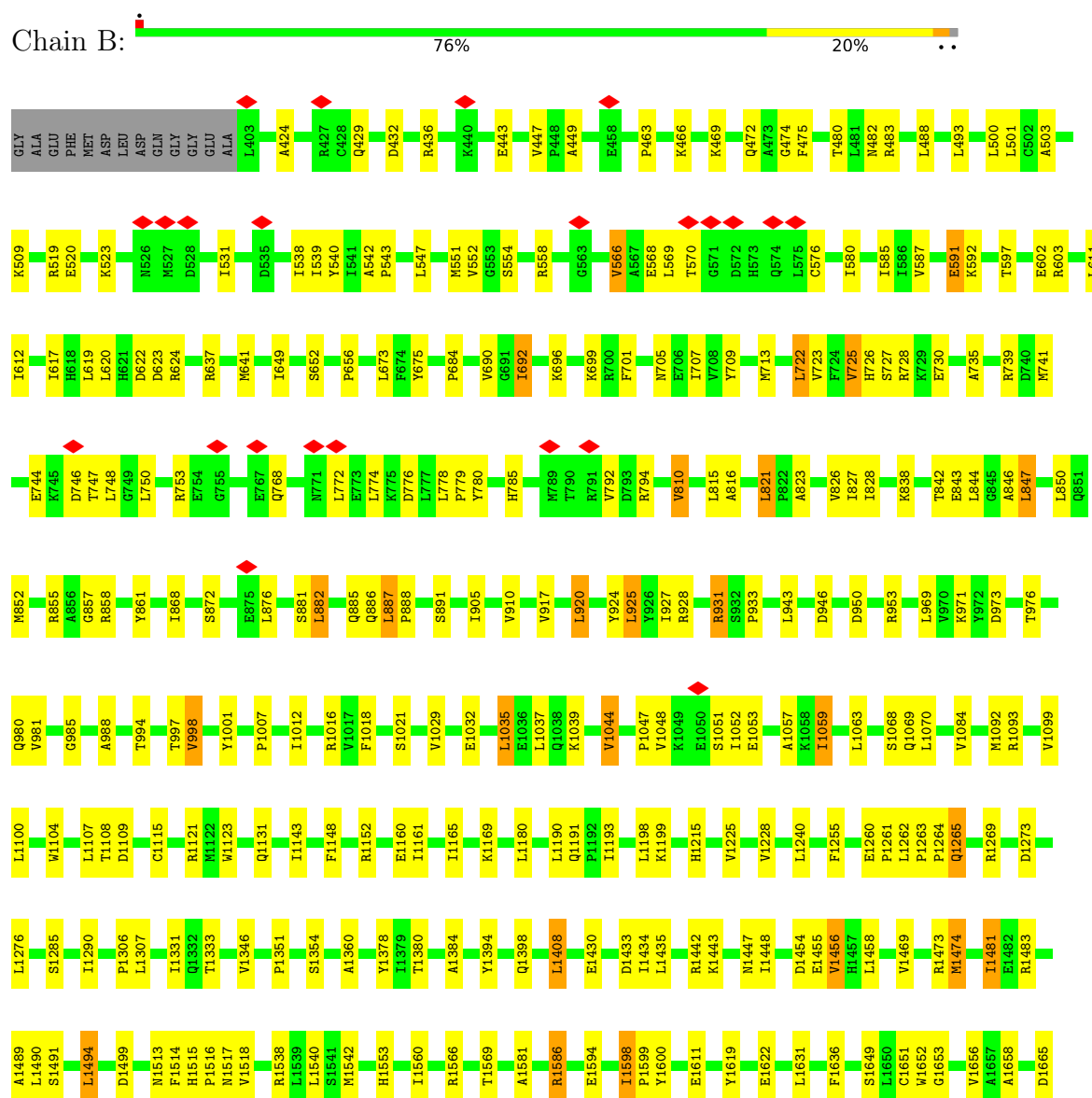
- Molecule 3 is a protein called Protein TSSC4.

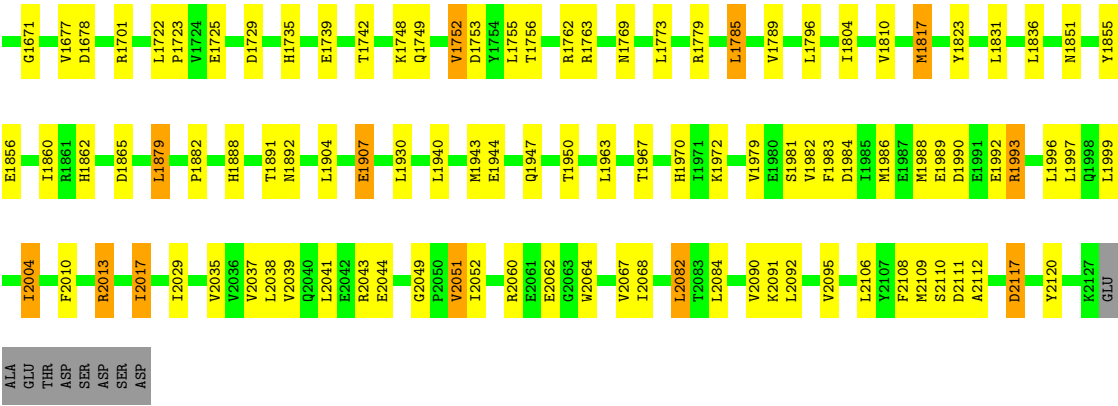
Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	66	Total	C	N	O	S	0	0
			530	332	103	94	1		

3 Residue-property plots

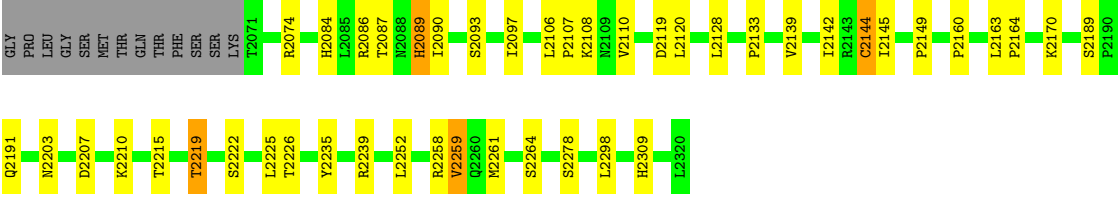
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: U5 small nuclear ribonucleoprotein 200 kDa helicase

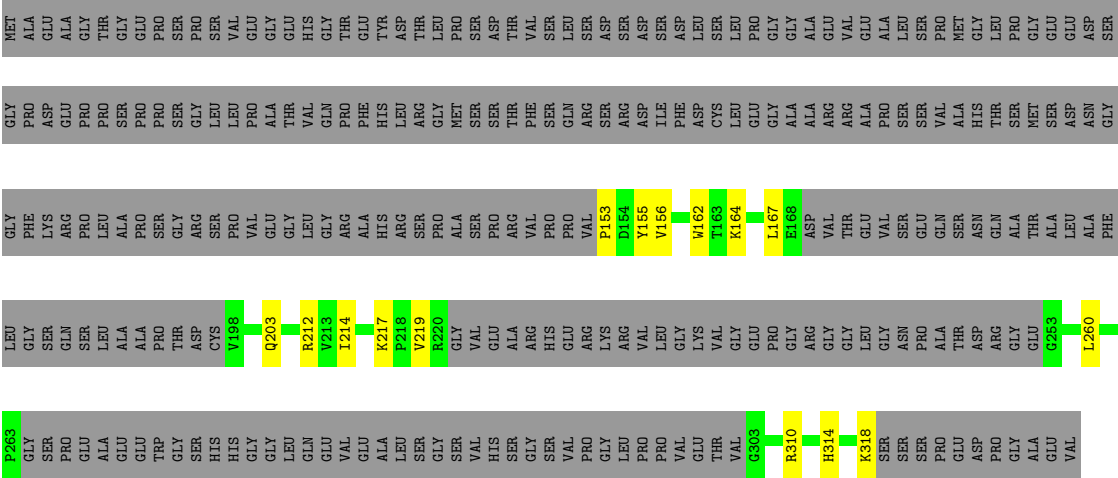




● Molecule 2: Pre-mRNA-processing-splicing factor 8



● Molecule 3: Protein TSSC4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	387973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.916	Depositor
Minimum map value	0.000	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	283.824, 283.824, 283.824	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.876, 0.876, 0.876	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.13	0/14164	0.31	0/19191
2	J	0.15	0/2095	0.33	0/2855
3	T	0.13	0/544	0.38	0/728
All	All	0.13	0/16803	0.31	0/22774

There are no bond length outliers.

There are no bond angle outliers.

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	B	13870	0	14018	214	0
2	J	2030	0	1971	26	0
3	T	530	0	506	11	0
All	All	16430	0	16495	242	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 7.

All (242) 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)
1:B:1598:ILE:HG13	1:B:1599:PRO:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:ILE:HG22	1:B:868:ILE:HB	1.71	0.73
1:B:969:LEU:HD21	1:B:998:VAL:HG11	1.70	0.72
1:B:1456:VAL:HG22	1:B:1491:SER:HB2	1.70	0.72
1:B:713:MET:SD	1:B:753:ARG:NH2	2.66	0.68
1:B:1143:ILE:HG12	1:B:1165:ILE:HD12	1.75	0.68
1:B:971:LYS:HB2	1:B:980:GLN:HB2	1.75	0.68
1:B:539:ILE:HB	1:B:612:ILE:HG22	1.75	0.68
1:B:436:ARG:NH1	1:B:443:GLU:OE2	2.26	0.67
3:T:217:LYS:HD2	3:T:219:VAL:H	1.58	0.67
1:B:1515:HIS:ND1	1:B:1517:ASN:OD1	2.27	0.67
1:B:1538:ARG:NH1	1:B:1665:ASP:OD1	2.30	0.65
1:B:538:ILE:HB	1:B:585:ILE:HG13	1.78	0.65
1:B:1443:LYS:O	1:B:1447:ASN:ND2	2.30	0.65
1:B:713:MET:HE2	1:B:748:LEU:HD13	1.78	0.64
1:B:1671:GLY:HA3	1:B:1860:ILE:HB	1.79	0.64
1:B:1052:ILE:HG13	1:B:1053:GLU:HG2	1.79	0.64
1:B:570:THR:HA	1:B:592:LYS:HG2	1.78	0.63
1:B:1566:ARG:NH1	1:B:1907:GLU:OE1	2.32	0.63
1:B:815:LEU:HD21	1:B:821:LEU:HD11	1.79	0.63
1:B:493:LEU:O	1:B:519:ARG:NH1	2.29	0.62
1:B:1093:ARG:NH2	1:B:1273:ASP:OD1	2.32	0.62
1:B:1035:LEU:HD22	1:B:1039:LYS:HE3	1.81	0.62
1:B:701:PHE:O	1:B:705:ASN:ND2	2.31	0.62
1:B:692:ILE:HG13	1:B:872:SER:HA	1.81	0.62
1:B:552:VAL:HG21	1:B:568:GLU:HB3	1.80	0.61
1:B:858:ARG:HD2	1:B:861:TYR:HB2	1.82	0.61
1:B:1569:THR:HG22	1:B:1619:TYR:HB2	1.82	0.61
2:J:2086:ARG:NH1	2:J:2219:THR:O	2.34	0.61
1:B:1433:ASP:OD1	1:B:1473:ARG:NH2	2.34	0.61
1:B:815:LEU:HD11	1:B:821:LEU:HD21	1.83	0.61
1:B:872:SER:HB3	1:B:876:LEU:HD12	1.82	0.61
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.83	0.60
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.83	0.60
1:B:1940:LEU:HD22	1:B:2109:MET:HE3	1.82	0.60
2:J:2093:SER:OG	2:J:2258:ARG:NH2	2.35	0.59
1:B:705:ASN:HB3	1:B:741:MET:HE1	1.84	0.59
1:B:713:MET:HA	1:B:753:ARG:HH22	1.68	0.59
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.85	0.59
1:B:816:ALA:O	1:B:855:ARG:NH1	2.36	0.58
2:J:2089:HIS:HB3	3:T:164:LYS:HE3	1.84	0.58
1:B:1001:TYR:HH	1:B:1021:SER:HG	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1856:GLU:OE1	1:B:1888:HIS:NE2	2.37	0.57
1:B:1950:THR:OG1	1:B:2060:ARG:NH1	2.37	0.57
1:B:675:TYR:OH	1:B:885:GLN:NE2	2.38	0.57
1:B:1160:GLU:OE1	1:B:1160:GLU:N	2.34	0.57
1:B:543:PRO:HG3	1:B:847:LEU:HD11	1.86	0.57
1:B:2043:ARG:NH2	1:B:2062:GLU:OE2	2.37	0.57
2:J:2235:TYR:OH	2:J:2239:ARG:NH2	2.37	0.56
1:B:969:LEU:HD22	1:B:985:GLY:HA2	1.87	0.56
1:B:1879:LEU:HD13	1:B:1882:PRO:HB3	1.87	0.56
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.88	0.56
1:B:1756:THR:O	1:B:1762:ARG:NH1	2.38	0.56
1:B:637:ARG:HE	1:B:641:MET:HE3	1.71	0.56
2:J:2119:ASP:OD1	2:J:2120:LEU:N	2.39	0.55
1:B:988:ALA:HB2	1:B:998:VAL:HG21	1.88	0.55
1:B:741:MET:HA	1:B:744:GLU:HG3	1.89	0.55
2:J:2108:LYS:HD3	3:T:167:LEU:HA	1.88	0.55
1:B:493:LEU:HD23	1:B:519:ARG:HB2	1.89	0.54
1:B:1983:PHE:HA	1:B:1986:MET:HE2	1.88	0.54
1:B:591:GLU:OE2	1:B:624:ARG:NH2	2.41	0.54
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.90	0.54
1:B:1190:LEU:HD11	1:B:1198:LEU:HD13	1.90	0.53
1:B:1967:THR:H	1:B:1970:HIS:HB2	1.74	0.53
1:B:2082:LEU:HD22	1:B:2090:VAL:HG21	1.90	0.53
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.89	0.53
1:B:1455:GLU:HB3	1:B:1458:LEU:HD13	1.91	0.53
1:B:735:ALA:HB2	1:B:810:VAL:HG11	1.91	0.53
2:J:2163:LEU:HD13	2:J:2164:PRO:HD2	1.91	0.52
1:B:622:ASP:OD1	1:B:623:ASP:N	2.34	0.52
1:B:2010:PHE:HA	1:B:2052:ILE:HD12	1.90	0.52
1:B:2013:ARG:NH1	1:B:2049:GLY:O	2.43	0.52
1:B:1262:LEU:HD12	1:B:1263:PRO:HD2	1.91	0.52
1:B:1394:TYR:O	1:B:1398:GLN:HB3	2.10	0.52
1:B:2051:VAL:HG21	1:B:2112:ALA:HB1	1.92	0.52
1:B:475:PHE:HA	1:B:558:ARG:HH21	1.74	0.52
1:B:846:ALA:HB1	1:B:882:LEU:HD11	1.91	0.52
1:B:2029:ILE:HD12	1:B:2035:VAL:HG22	1.91	0.52
1:B:603:ARG:HB2	1:B:1540:LEU:HD13	1.92	0.52
1:B:774:LEU:HB3	1:B:778:LEU:HG	1.92	0.52
1:B:1131:GLN:OE1	1:B:1276:LEU:N	2.40	0.51
1:B:474:GLY:O	1:B:558:ARG:NE	2.35	0.51
1:B:828:ILE:HD13	1:B:852:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1481:ILE:HG23	1:B:1483:ARG:H	1.76	0.51
1:B:920:LEU:HB3	1:B:953:ARG:HD2	1.94	0.50
1:B:1148:PHE:HE1	1:B:1152:ARG:HD2	1.76	0.50
1:B:1636:PHE:HD2	1:B:1656:VAL:HG21	1.75	0.50
1:B:2038:LEU:HD13	1:B:2091:LYS:HB3	1.92	0.50
1:B:1494:LEU:O	1:B:1513:ASN:ND2	2.41	0.50
2:J:2149:PRO:O	2:J:2160:PRO:HD3	2.11	0.50
2:J:2189:SER:OG	2:J:2191:GLN:OE1	2.29	0.50
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	1.94	0.50
1:B:1265:GLN:HG2	2:J:2298:LEU:HD21	1.92	0.50
1:B:2017:ILE:HG23	1:B:2043:ARG:HB3	1.92	0.50
1:B:429:GLN:O	1:B:886:GLN:NE2	2.35	0.50
1:B:973:ASP:OD2	1:B:976:THR:OG1	2.26	0.49
1:B:1622:GLU:OE2	1:B:1649:SER:OG	2.27	0.49
1:B:723:VAL:HG22	1:B:827:ILE:HD11	1.93	0.49
2:J:2207:ASP:OD2	2:J:2210:LYS:NZ	2.34	0.49
1:B:1879:LEU:HD23	1:B:1892:ASN:HD22	1.76	0.49
1:B:1306:PRO:HA	1:B:1333:THR:HG21	1.95	0.49
1:B:1963:LEU:HD21	1:B:1982:VAL:HG13	1.95	0.49
1:B:482:ASN:OD1	1:B:483:ARG:N	2.40	0.49
1:B:1943:MET:HE1	1:B:2067:VAL:HG21	1.94	0.49
1:B:2117:ASP:N	1:B:2117:ASP:OD1	2.45	0.49
1:B:1180:LEU:O	1:B:1215:HIS:NE2	2.44	0.48
1:B:1600:TYR:HD2	1:B:1631:LEU:HD11	1.79	0.48
1:B:785:HIS:NE2	1:B:794:ARG:HG3	2.28	0.48
1:B:1944:GLU:HA	1:B:1947:GLN:HG2	1.96	0.48
1:B:540:TYR:HB3	1:B:587:VAL:HG22	1.96	0.48
1:B:1836:LEU:HD22	1:B:1930:LEU:HD21	1.95	0.47
1:B:1109:ASP:HB2	1:B:1269:ARG:HH12	1.78	0.47
1:B:1265:GLN:HB3	1:B:1285:SER:HA	1.96	0.47
1:B:1228:VAL:HG21	1:B:1264:PRO:HD2	1.94	0.47
1:B:722:LEU:HB3	1:B:826:VAL:HG12	1.97	0.47
1:B:1990:ASP:HA	1:B:1993:ARG:HD2	1.96	0.47
1:B:2064:TRP:CZ3	1:B:2110:SER:HB2	2.49	0.47
1:B:768:GLN:HG3	1:B:779:PRO:HD3	1.97	0.47
1:B:927:ILE:HG23	1:B:931:ARG:HH21	1.79	0.47
1:B:1059:ILE:HG22	1:B:1084:VAL:HG11	1.97	0.47
1:B:1725:GLU:OE2	1:B:1763:ARG:NH2	2.42	0.47
1:B:1817:MET:HG2	3:T:260:LEU:HB3	1.96	0.47
1:B:1981:SER:OG	1:B:1984:ASP:OD1	2.24	0.47
2:J:2097:ILE:HG12	2:J:2259:VAL:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:ARG:H	1:B:728:ARG:HD2	1.79	0.47
1:B:568:GLU:OE1	1:B:568:GLU:N	2.45	0.47
1:B:1260:GLU:HB3	1:B:1261:PRO:HD3	1.97	0.47
1:B:566:VAL:HB	1:B:585:ILE:HB	1.97	0.46
1:B:725:VAL:HG12	1:B:726:HIS:H	1.80	0.46
1:B:1007:PRO:HG3	1:B:1104:TRP:CE2	2.50	0.46
1:B:597:THR:HG22	1:B:602:GLU:HG3	1.97	0.46
1:B:569:LEU:HD21	1:B:576:CYS:SG	2.55	0.46
1:B:432:ASP:N	1:B:432:ASP:OD1	2.46	0.46
1:B:1069:GLN:HA	1:B:1121:ARG:HH21	1.81	0.46
1:B:1514:PHE:HB3	1:B:1518:VAL:HG11	1.97	0.46
1:B:1989:GLU:HB2	1:B:1992:GLU:HB3	1.97	0.46
2:J:2128:LEU:HD22	2:J:2142:ILE:HG21	1.98	0.46
1:B:1068:SER:HB3	1:B:1123:TRP:HE1	1.81	0.46
1:B:569:LEU:HD22	1:B:580:ILE:HG21	1.96	0.46
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.98	0.46
1:B:1499:ASP:OD2	1:B:1763:ARG:NH1	2.41	0.46
1:B:503:ALA:HB3	1:B:509:LYS:HE3	1.98	0.46
1:B:520:GLU:HA	1:B:523:LYS:HE2	1.97	0.45
1:B:1988:MET:HE2	1:B:1992:GLU:HG3	1.97	0.45
2:J:2090:ILE:HD12	3:T:167:LEU:HD13	1.97	0.45
1:B:1012:ILE:HG12	1:B:1047:PRO:HG2	1.99	0.45
1:B:1161:ILE:O	1:B:1165:ILE:HG12	2.16	0.45
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.47	0.45
2:J:2278:SER:OG	2:J:2309:HIS:NE2	2.38	0.45
1:B:750:LEU:HD22	1:B:780:TYR:CG	2.51	0.45
1:B:2004:ILE:HD12	1:B:2004:ILE:HA	1.84	0.45
3:T:153:PRO:HB2	3:T:156:VAL:HG12	1.99	0.45
1:B:554:SER:O	1:B:558:ARG:HG2	2.17	0.45
1:B:1018:PHE:CE1	1:B:1063:LEU:HD22	2.52	0.45
2:J:2107:PRO:HG2	2:J:2110:VAL:HG22	1.99	0.45
3:T:155:TYR:HA	3:T:162:TRP:CD1	2.51	0.45
1:B:1553:HIS:O	1:B:1701:ARG:NH1	2.50	0.45
2:J:2133:PRO:HD2	2:J:2139:VAL:O	2.17	0.45
1:B:1104:TRP:O	1:B:1108:THR:OG1	2.33	0.44
2:J:2087:THR:HB	3:T:167:LEU:HD23	1.99	0.44
2:J:2219:THR:HG22	2:J:2222:SER:O	2.18	0.44
1:B:619:LEU:HD13	1:B:847:LEU:HD13	1.99	0.44
1:B:2051:VAL:HG11	1:B:2060:ARG:HB2	2.00	0.44
1:B:1430:GLU:O	1:B:1434:ILE:HG23	2.17	0.44
1:B:547:LEU:HD11	1:B:551:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:SER:HB3	1:B:925:LEU:HD23	1.99	0.44
1:B:1594:GLU:O	1:B:1598:ILE:HG12	2.17	0.44
2:J:2144:CYS:SG	2:J:2145:ILE:N	2.89	0.44
1:B:838:LYS:HG3	1:B:842:THR:HG21	2.00	0.44
1:B:1879:LEU:HD23	1:B:1892:ASN:ND2	2.33	0.44
1:B:881:SER:HA	1:B:886:GLN:HB2	1.99	0.44
1:B:1307:LEU:HD23	1:B:1333:THR:HB	1.98	0.44
1:B:1051:SER:HB3	1:B:1057:ALA:HB2	2.00	0.44
1:B:1979:VAL:HG13	1:B:1984:ASP:HB2	1.98	0.44
1:B:1331:ILE:HD11	1:B:1518:VAL:HG13	2.00	0.43
1:B:823:ALA:O	1:B:857:GLY:N	2.41	0.43
1:B:1193:ILE:HG13	1:B:1255:PHE:HE2	1.83	0.43
1:B:1831:LEU:HD21	1:B:1851:ASN:HB3	1.98	0.43
2:J:2225:LEU:HB3	2:J:2261:MET:HE1	2.00	0.43
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	2.00	0.43
1:B:1748:LYS:HE3	1:B:1748:LYS:HB2	1.92	0.43
1:B:611:LEU:HD11	1:B:649:ILE:HD12	1.99	0.43
1:B:994:THR:HG23	1:B:997:THR:H	1.83	0.43
1:B:463:PRO:HD2	1:B:466:LYS:HD2	2.00	0.43
1:B:620:LEU:HD12	1:B:620:LEU:HA	1.86	0.43
1:B:1099:VAL:HG23	1:B:1104:TRP:HE3	1.82	0.43
1:B:1384:ALA:HB1	1:B:1653:GLY:HA2	2.01	0.43
1:B:1434:ILE:HG22	1:B:1823:TYR:CD2	2.54	0.43
1:B:1581:ALA:HA	1:B:1586:ARG:HA	2.01	0.43
1:B:1469:VAL:HG21	1:B:1735:HIS:CG	2.53	0.43
1:B:1722:LEU:HD12	1:B:1723:PRO:HD2	2.00	0.42
1:B:1753:ASP:OD1	3:T:203:GLN:NE2	2.52	0.42
2:J:2278:SER:HG	2:J:2309:HIS:CD2	2.31	0.42
1:B:739:ARG:HG2	1:B:750:LEU:HD21	2.02	0.42
1:B:1032:GLU:H	1:B:1032:GLU:CD	2.28	0.42
1:B:1456:VAL:HG11	1:B:1489:ALA:HB1	2.01	0.42
1:B:1749:GLN:HE21	3:T:214:ILE:HA	1.84	0.42
1:B:723:VAL:HB	1:B:810:VAL:HA	2.01	0.42
1:B:1169:LYS:H	1:B:1169:LYS:HD2	1.83	0.42
1:B:1378:TYR:OH	1:B:1454:ASP:OD2	2.37	0.42
1:B:542:ALA:HB1	1:B:547:LEU:HD23	2.02	0.42
1:B:1408:LEU:HD12	1:B:1408:LEU:HA	1.86	0.42
1:B:1678:ASP:OD1	1:B:1678:ASP:N	2.53	0.42
1:B:2017:ILE:HD13	1:B:2108:PHE:HE2	1.85	0.42
1:B:696:LYS:HB2	1:B:699:LYS:HB3	2.02	0.42
1:B:924:TYR:CZ	1:B:928:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:946:ASP:OD2	1:B:950:ASP:N	2.53	0.42
1:B:1092:MET:HB3	1:B:1115:CYS:SG	2.60	0.42
1:B:463:PRO:HA	1:B:480:THR:HA	2.02	0.41
2:J:2084:HIS:O	2:J:2087:THR:OG1	2.25	0.41
1:B:727:SER:HB2	1:B:730:GLU:HB2	2.02	0.41
1:B:739:ARG:NH2	1:B:776:ASP:OD1	2.43	0.41
1:B:1099:VAL:HG23	1:B:1104:TRP:CE3	2.55	0.41
1:B:1755:LEU:HD23	1:B:1755:LEU:HA	1.94	0.41
1:B:1865:ASP:N	1:B:1865:ASP:OD1	2.54	0.41
1:B:469:LYS:HA	1:B:472:GLN:HG3	2.03	0.41
1:B:1099:VAL:HG21	1:B:1107:LEU:HB3	2.03	0.41
1:B:1290:ILE:N	1:B:1769:ASN:OD1	2.39	0.41
1:B:2060:ARG:NH2	1:B:2111:ASP:OD2	2.54	0.41
1:B:746:ASP:HB2	1:B:748:LEU:HG	2.03	0.41
1:B:887:LEU:HD23	1:B:888:PRO:HD2	2.03	0.41
1:B:1191:GLN:HE21	1:B:1199:LYS:HD3	1.85	0.41
1:B:656:PRO:HD2	1:B:887:LEU:O	2.21	0.41
1:B:905:ILE:HG22	1:B:981:VAL:HG22	2.02	0.41
1:B:2037:VAL:HG11	1:B:2068:ILE:HD11	2.02	0.41
1:B:449:ALA:HB1	1:B:684:PRO:HB2	2.02	0.41
1:B:1044:VAL:HG23	2:J:2074:ARG:HH12	1.85	0.41
1:B:1448:ILE:HD11	1:B:1474:MET:HE2	2.03	0.41
1:B:1538:ARG:HG2	1:B:1542:MET:HE3	2.02	0.41
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	2.03	0.41
1:B:1763:ARG:HD2	1:B:1763:ARG:HA	1.84	0.41
1:B:1970:HIS:CE1	1:B:1997:LEU:HB2	2.55	0.41
1:B:2013:ARG:NH2	1:B:2062:GLU:OE2	2.53	0.41
1:B:2106:LEU:N	1:B:2120:TYR:O	2.52	0.41
1:B:424:ALA:HB3	1:B:888:PRO:HG2	2.03	0.41
2:J:2107:PRO:HA	2:J:2264:SER:O	2.21	0.41
1:B:1651:CYS:HG	1:B:1652:TRP:CD1	2.38	0.40
1:B:1749:GLN:O	1:B:1752:VAL:HG12	2.21	0.40
1:B:1907:GLU:H	1:B:1907:GLU:HG2	1.47	0.40
1:B:2017:ILE:H	1:B:2017:ILE:HG13	1.50	0.40
1:B:1785:LEU:O	1:B:1789:VAL:HG12	2.21	0.40
3:T:217:LYS:HZ1	3:T:219:VAL:HG23	1.86	0.40

There are no symmetry-related clashes.

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	B	1723/1747 (99%)	1686 (98%)	37 (2%)	0	100	100
2	J	248/263 (94%)	242 (98%)	6 (2%)	0	100	100
3	T	58/329 (18%)	53 (91%)	5 (9%)	0	100	100
All	All	2029/2339 (87%)	1981 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	B	1544/1560 (99%)	1462 (95%)	82 (5%)	20	47
2	J	225/236 (95%)	216 (96%)	9 (4%)	28	56
3	T	57/264 (22%)	53 (93%)	4 (7%)	14	38
All	All	1826/2060 (89%)	1731 (95%)	95 (5%)	22	48

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	447	VAL
1	B	488	LEU
1	B	500	LEU
1	B	501	LEU
1	B	531	ILE

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Mol	Chain	Res	Type
1	B	566	VAL
1	B	591	GLU
1	B	673	LEU
1	B	692	ILE
1	B	709	TYR
1	B	722	LEU
1	B	725	VAL
1	B	747	THR
1	B	772	LEU
1	B	792	VAL
1	B	810	VAL
1	B	821	LEU
1	B	843	GLU
1	B	844	LEU
1	B	847	LEU
1	B	850	LEU
1	B	882	LEU
1	B	887	LEU
1	B	910	VAL
1	B	917	VAL
1	B	920	LEU
1	B	925	LEU
1	B	931	ARG
1	B	998	VAL
1	B	1016	ARG
1	B	1029	VAL
1	B	1035	LEU
1	B	1037	LEU
1	B	1044	VAL
1	B	1048	VAL
1	B	1059	ILE
1	B	1070	LEU
1	B	1100	LEU
1	B	1225	VAL
1	B	1240	LEU
1	B	1265	GLN
1	B	1346	VAL
1	B	1380	THR
1	B	1408	LEU
1	B	1435	LEU
1	B	1442	ARG
1	B	1456	VAL

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Mol	Chain	Res	Type
1	B	1474	MET
1	B	1481	ILE
1	B	1494	LEU
1	B	1586	ARG
1	B	1598	ILE
1	B	1611	GLU
1	B	1677	VAL
1	B	1739	GLU
1	B	1742	THR
1	B	1752	VAL
1	B	1773	LEU
1	B	1779	ARG
1	B	1785	LEU
1	B	1796	LEU
1	B	1817	MET
1	B	1862	HIS
1	B	1879	LEU
1	B	1904	LEU
1	B	1907	GLU
1	B	1972	LYS
1	B	1993	ARG
1	B	1996	LEU
1	B	1999	LEU
1	B	2004	ILE
1	B	2013	ARG
1	B	2017	ILE
1	B	2039	VAL
1	B	2041	LEU
1	B	2044	GLU
1	B	2051	VAL
1	B	2082	LEU
1	B	2084	LEU
1	B	2092	LEU
1	B	2095	VAL
1	B	2117	ASP
2	J	2089	HIS
2	J	2144	CYS
2	J	2170	LYS
2	J	2203	ASN
2	J	2215	THR
2	J	2219	THR
2	J	2226	THR

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Mol	Chain	Res	Type
2	J	2252	LEU
2	J	2259	VAL
3	T	212	ARG
3	T	310	ARG
3	T	314	HIS
3	T	318	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	485	GLN
1	B	573	HIS
1	B	584	GLN
1	B	702	GLN
1	B	995	ASN
1	B	1235	HIS
1	B	1447	ASN
1	B	1696	GLN
1	B	1947	GLN
1	B	2012	ASN
2	J	2162	GLN
2	J	2203	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

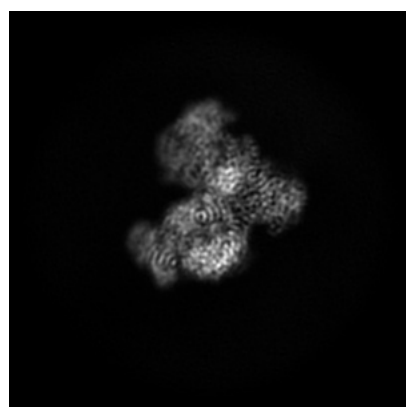
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13690. These allow visual inspection of the internal detail of the map and identification of artifacts.

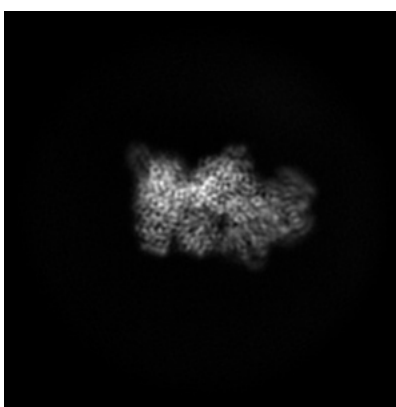
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

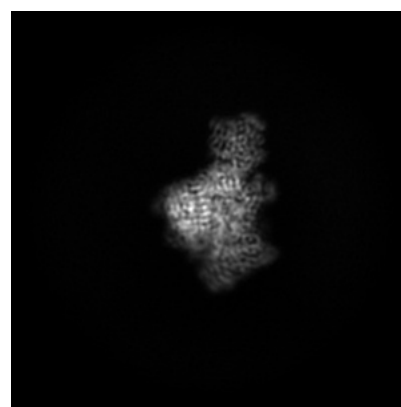
6.1.1 Primary map



X



Y

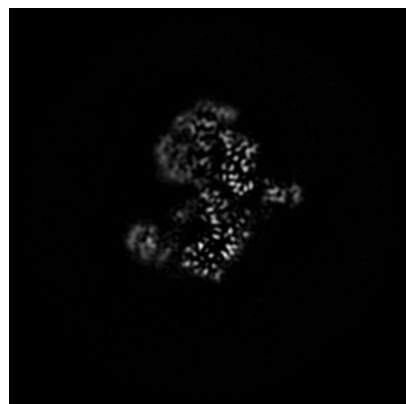


Z

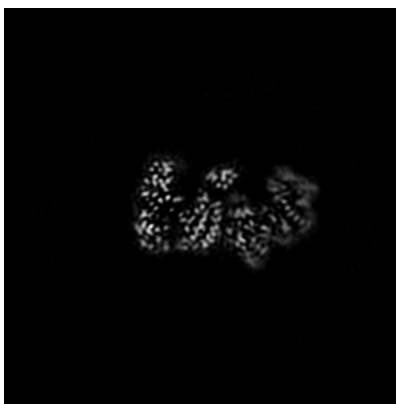
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

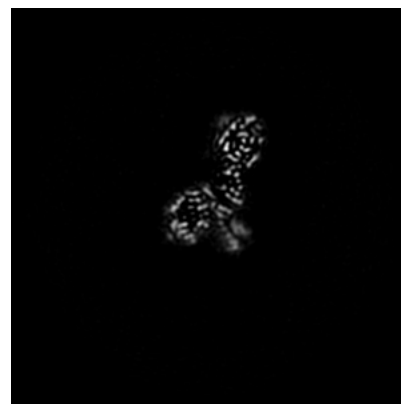
6.2.1 Primary map



X Index: 162



Y Index: 162

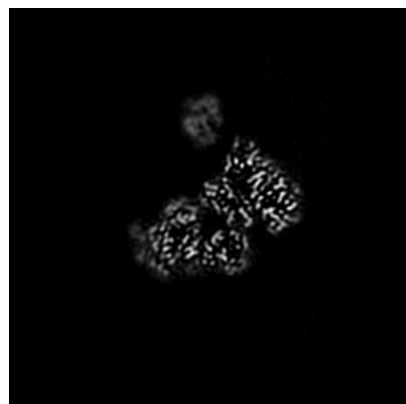


Z Index: 162

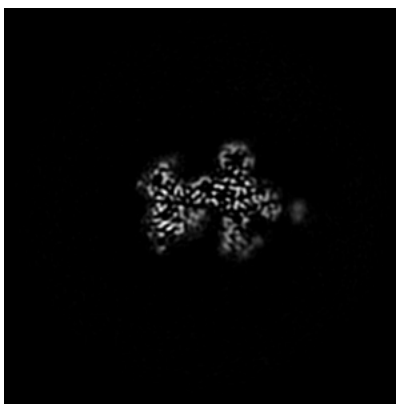
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

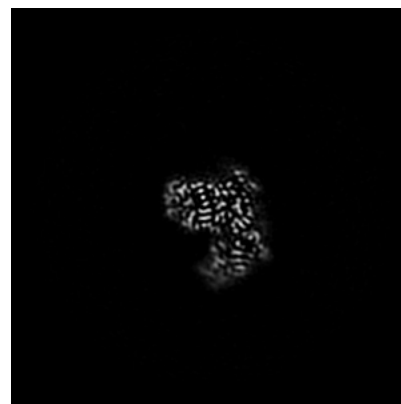
6.3.1 Primary map



X Index: 180



Y Index: 179

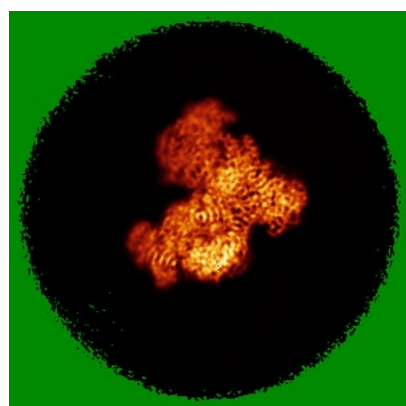


Z Index: 127

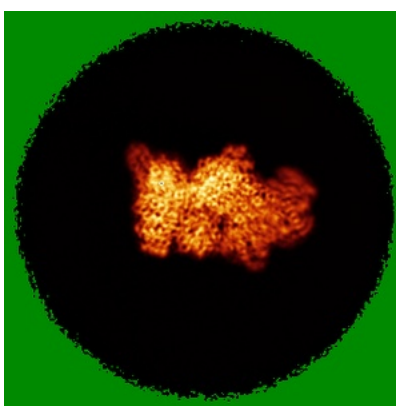
The images above show the largest variance slices of the map in three orthogonal directions.

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

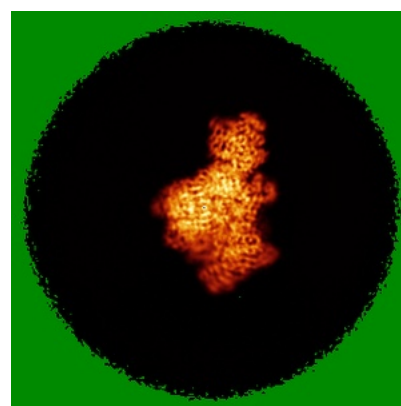
6.4.1 Primary map



X



Y

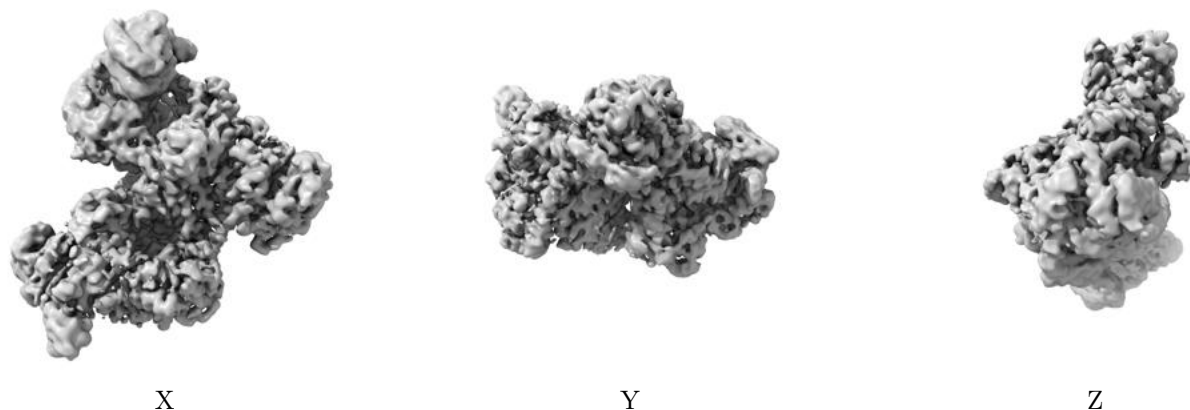


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

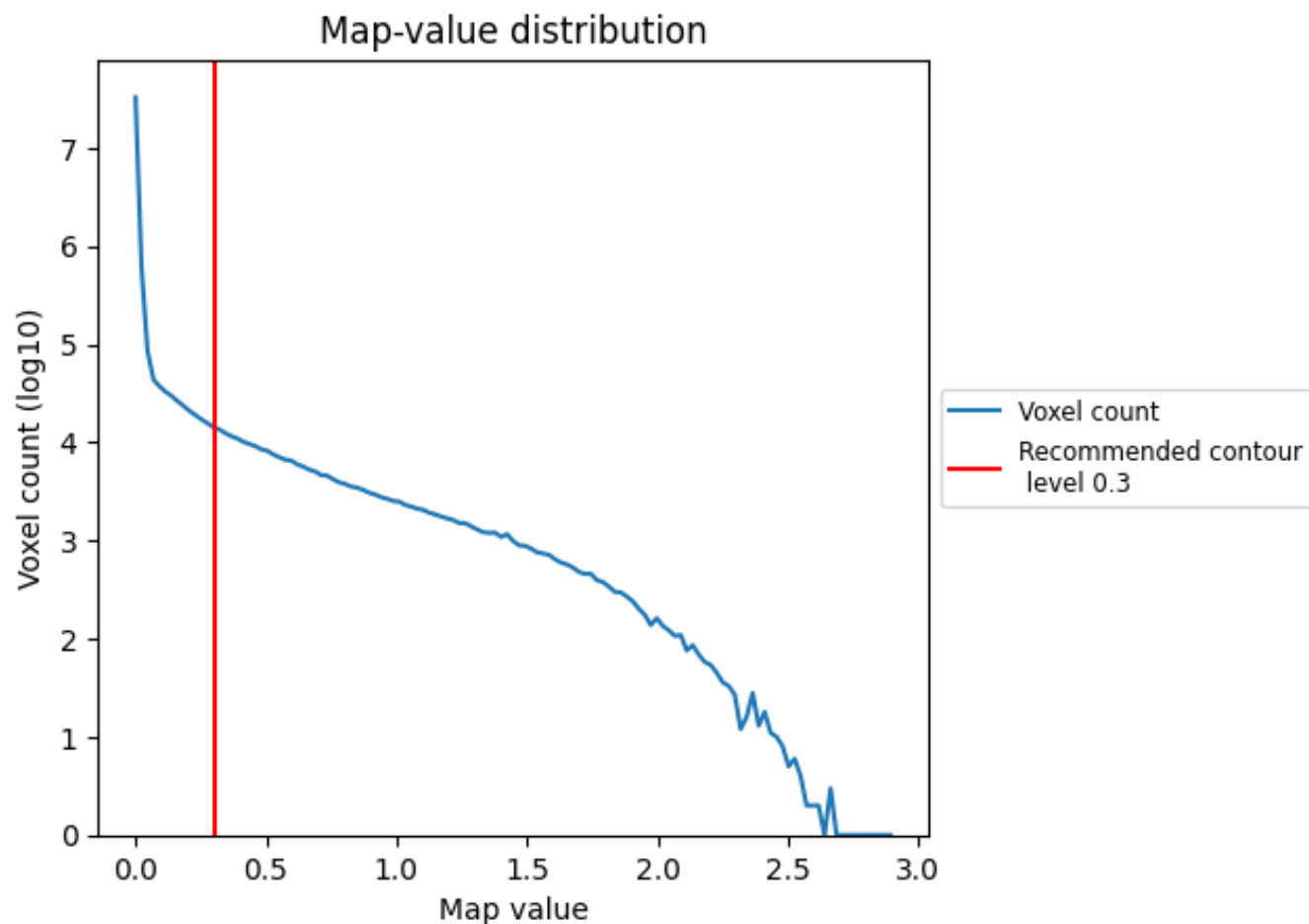
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

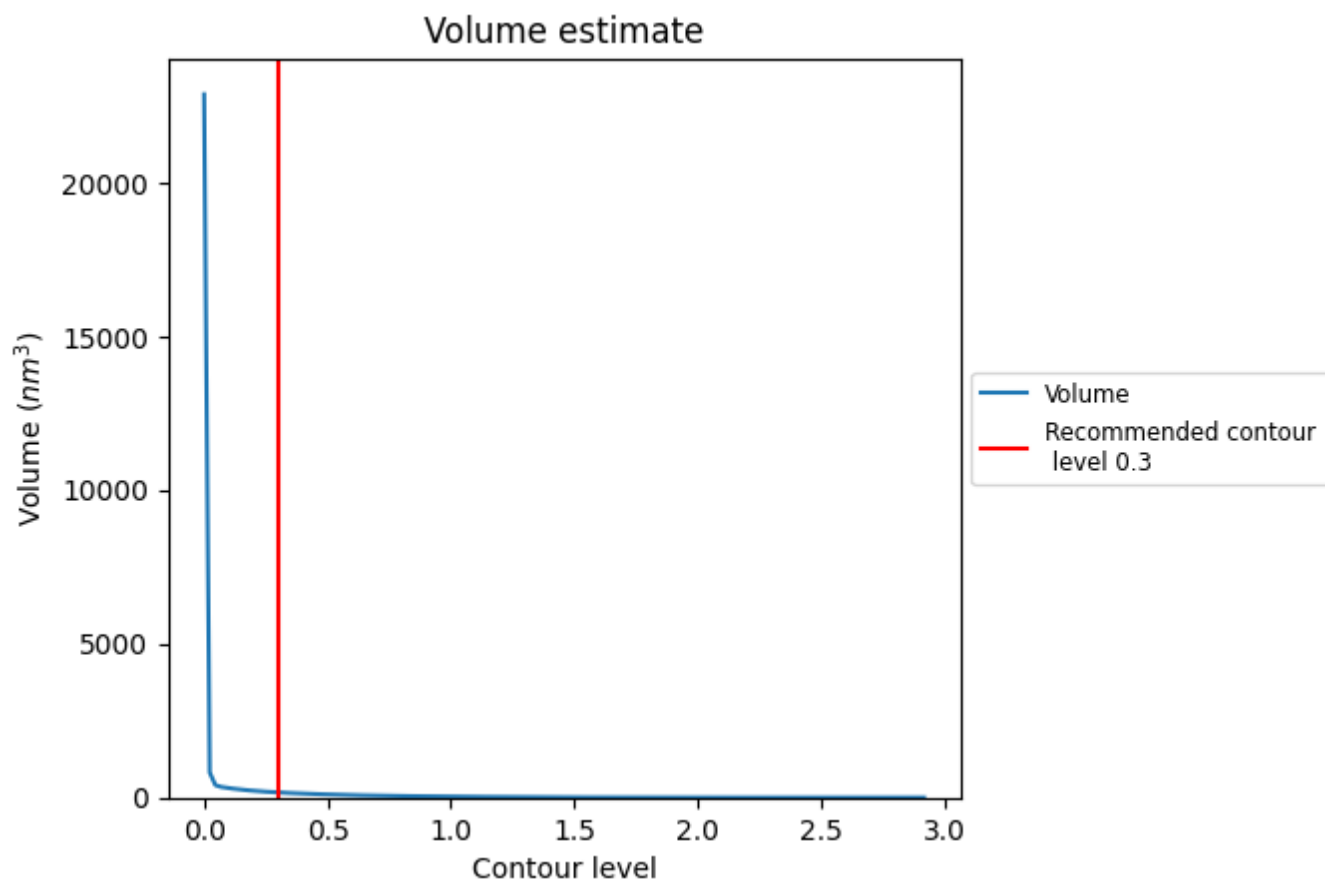
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

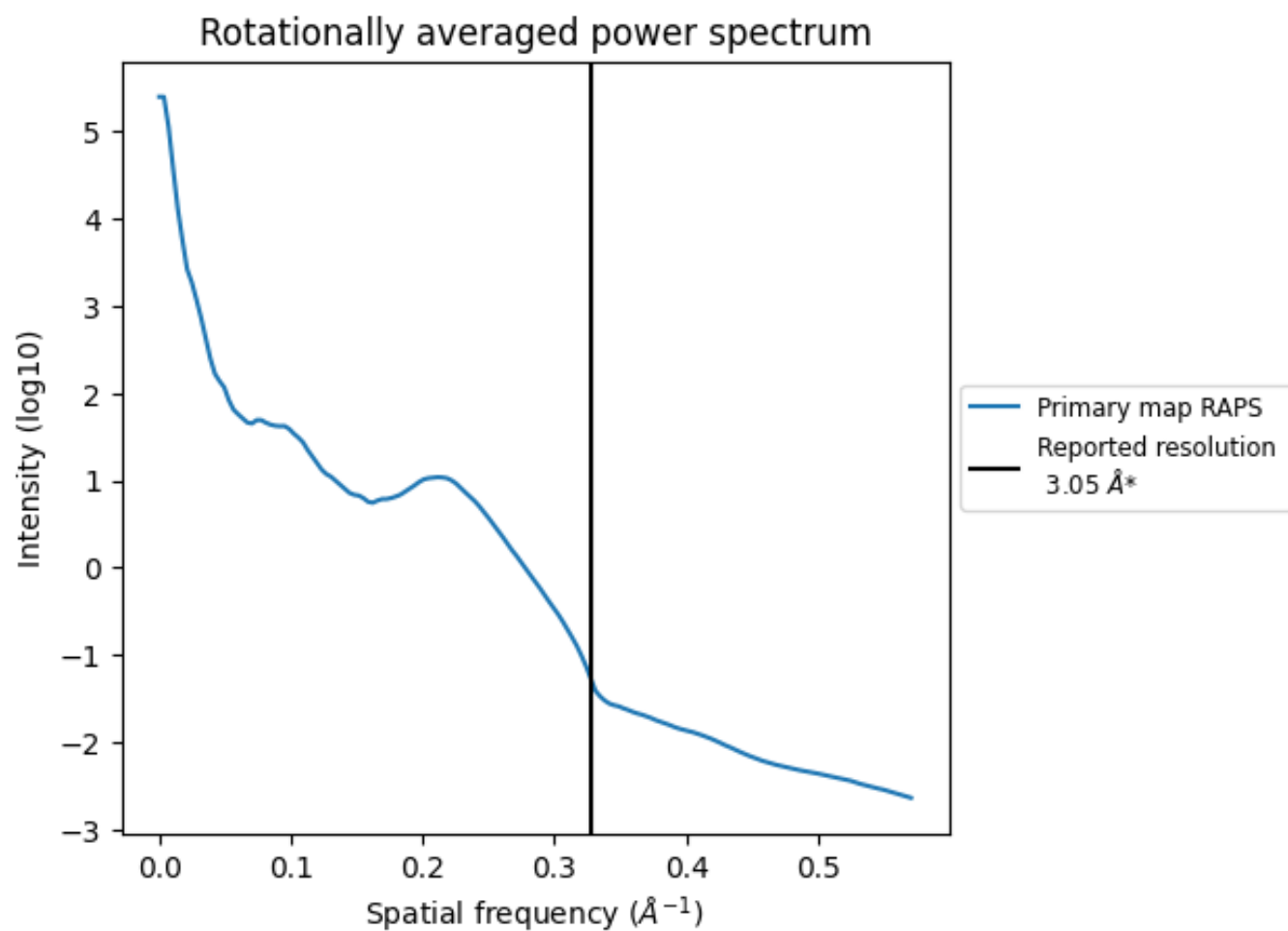
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm^3 ; this corresponds to an approximate mass of 150 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 ⓘ

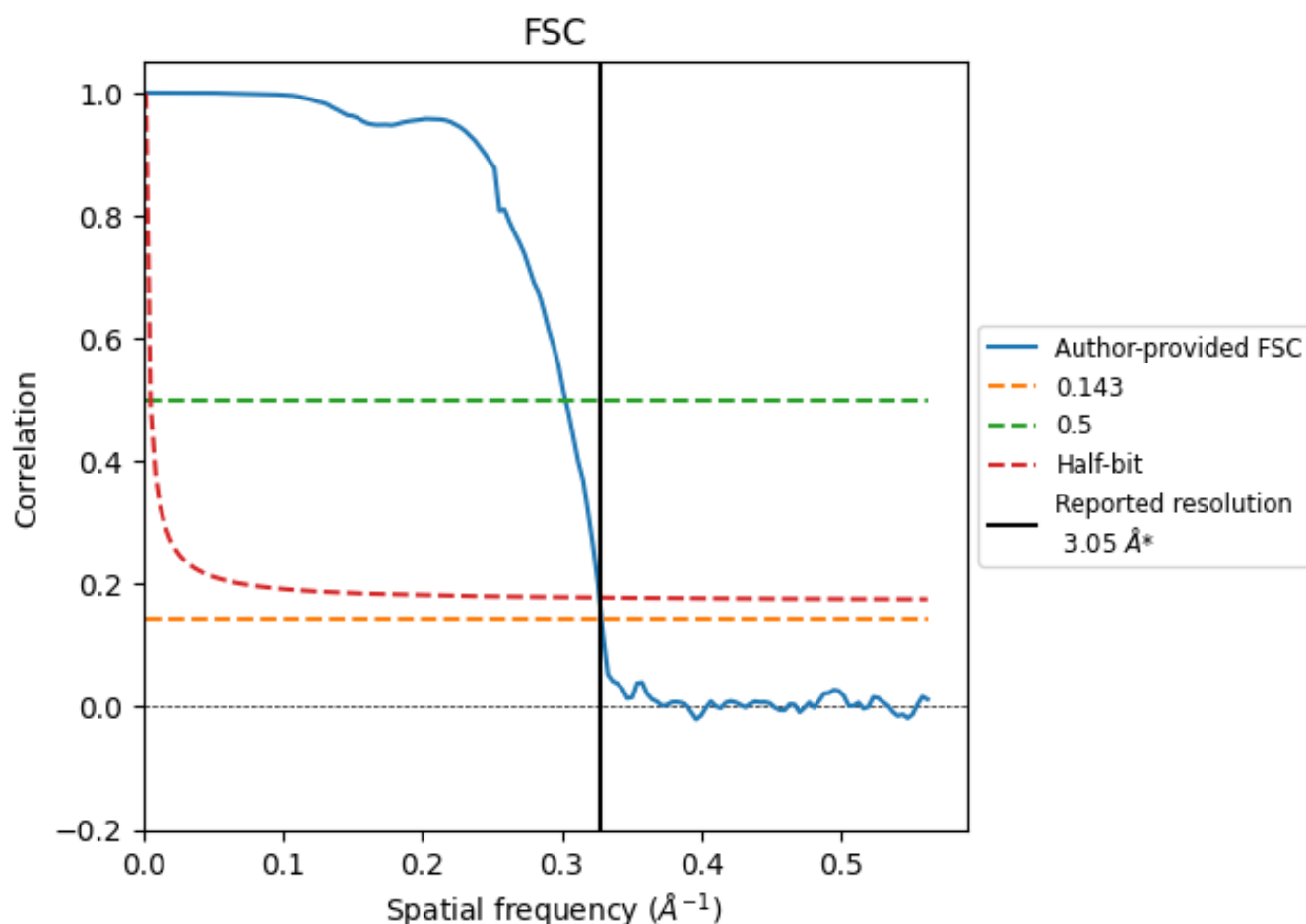


*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

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 0.328 Å⁻¹

8.2 Resolution estimates [i](#)

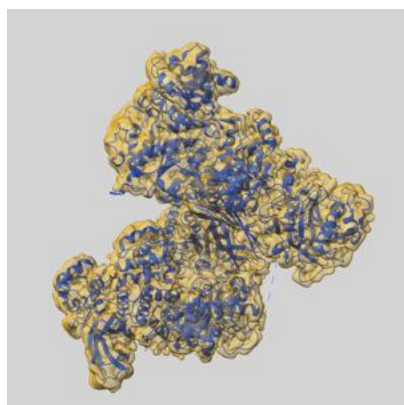
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.05	3.30	3.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

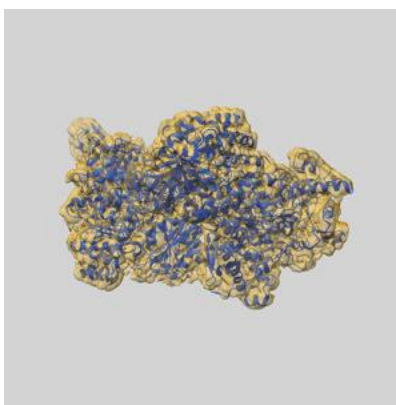
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13690 and PDB model 7PX3. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

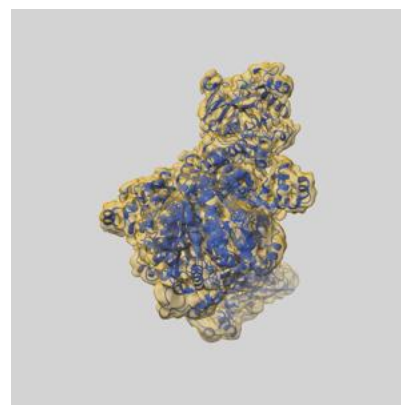
9.1 Map-model overlay [i](#)



X



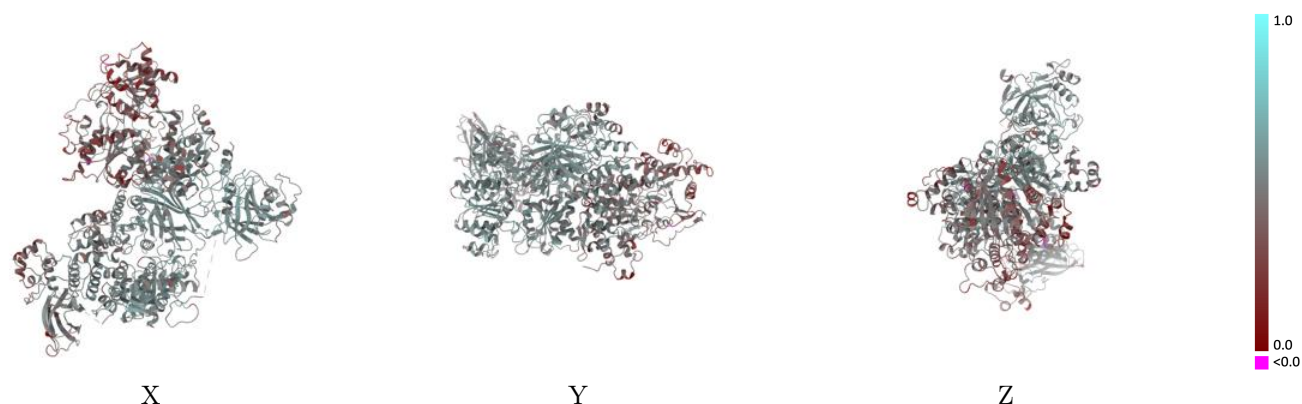
Y



Z

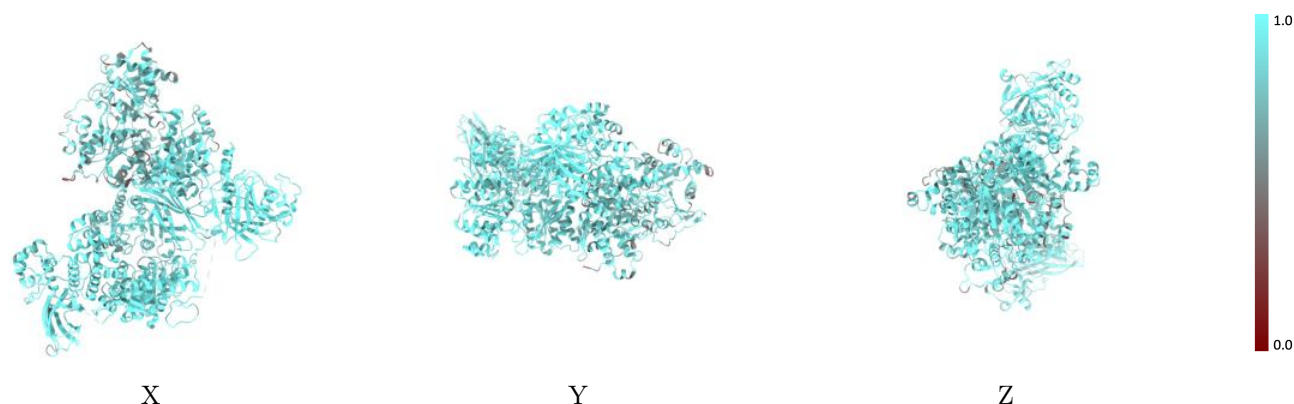
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



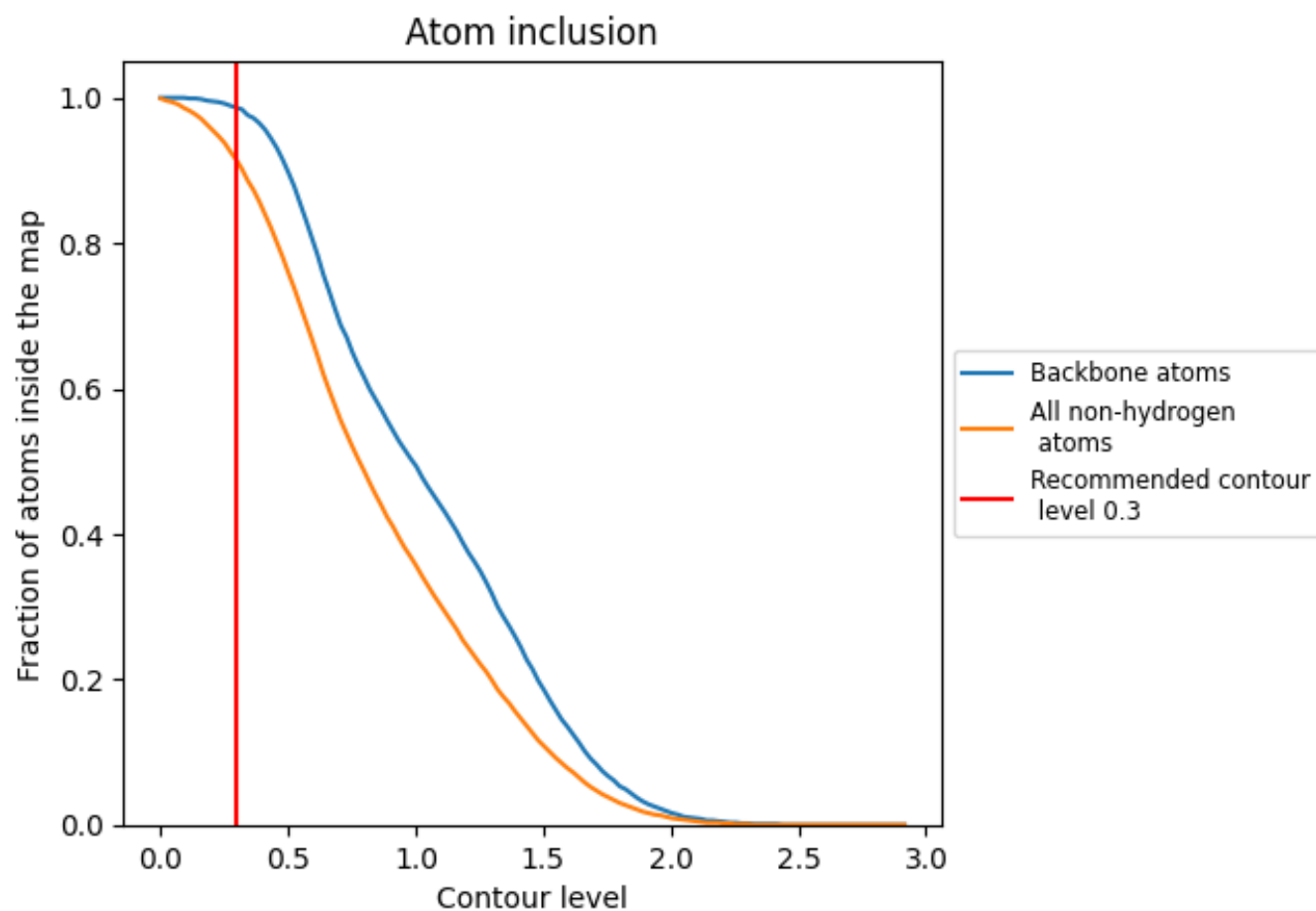
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 91% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.4710
B	0.9060	0.4620
J	0.9580	0.5350
T	0.9260	0.4760

