



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:27 AM UTC

PDB ID : 5GAO / pdb_00005gao
EMDB ID : EMD-8013
Title : Head region of the yeast spliceosomal U4/U6.U5 tri-snRNP
Authors : Nguyen, T.H.D.; Galej, W.P.; Bai, X.C.; Oubridge, C.; Scheres, S.H.W.; Newman, A.J.; Nagai, K.
Deposited on : 2015-12-15
Resolution : 4.20 Å(reported)
Based on initial model : 4BGD

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:

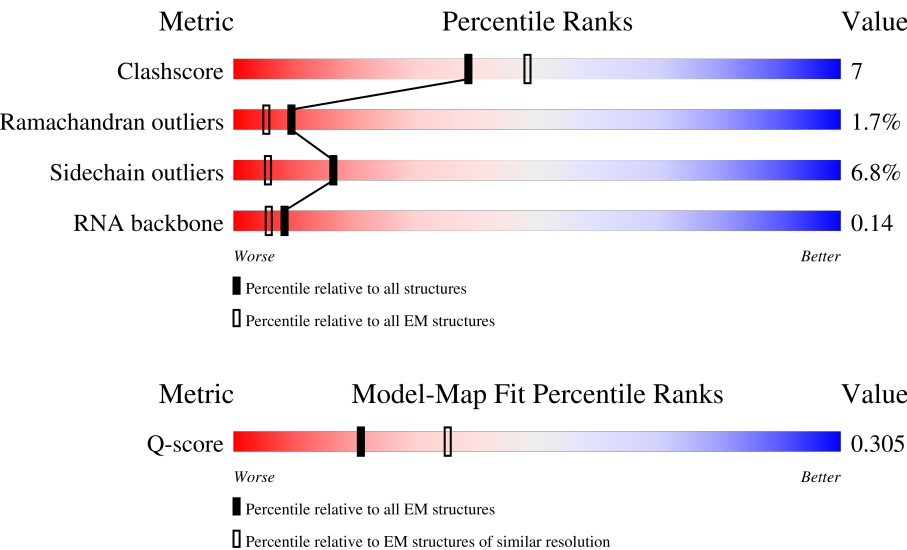
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.20 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	k	196	
2	l	146	
3	m	110	

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Mol	Chain	Length	Quality of chain
4	n	101	
5	p	94	
6	q	86	
7	r	77	
8	E	338	
9	B	2163	
10	V	96	
11	A	267	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 23073 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 Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	k	80	Total	C	N	O	S	0	0
			635	406	115	111	3		

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	91	Total	C	N	O	S	0	0
			720	455	129	134	2		

- Molecule 3 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	m	94	Total	C	N	O	S	0	0
			737	474	140	119	4		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	p	76	Total	C	N	O	S	0	0
			580	382	93	102	3		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	q	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	r	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

- Molecule 8 is a protein called Snu66.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	338	Total	C	N	O		0	0
			1763	1063	352	348			

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	1710	Total	C	N	O	S	1	0
			13690	8772	2283	2579	56		

- Molecule 10 is a RNA chain called Saccharomyces cerevisiae strain UOA_M2 chromosome 5 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	57	Total	C	N	O	P	0	0
			1209	542	212	398	57		

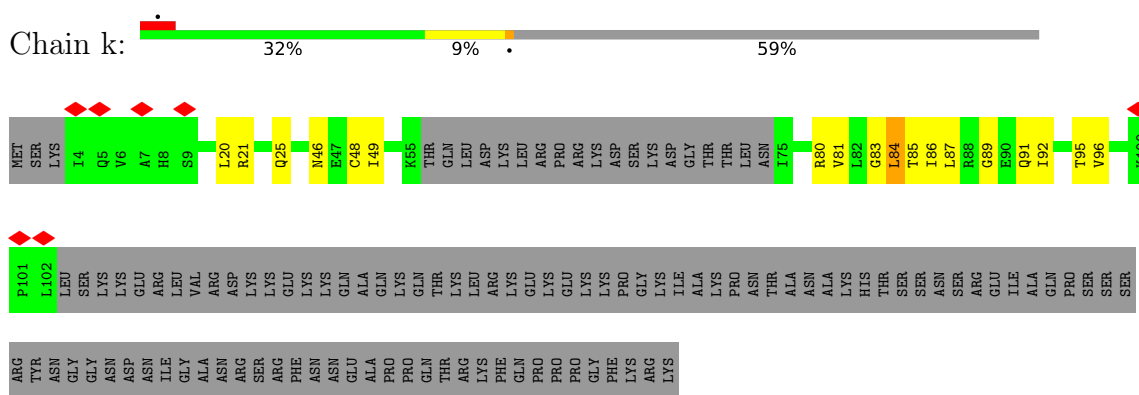
- Molecule 11 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	255	Total	C	N	O	S	0	0
			2015	1300	329	380	6		

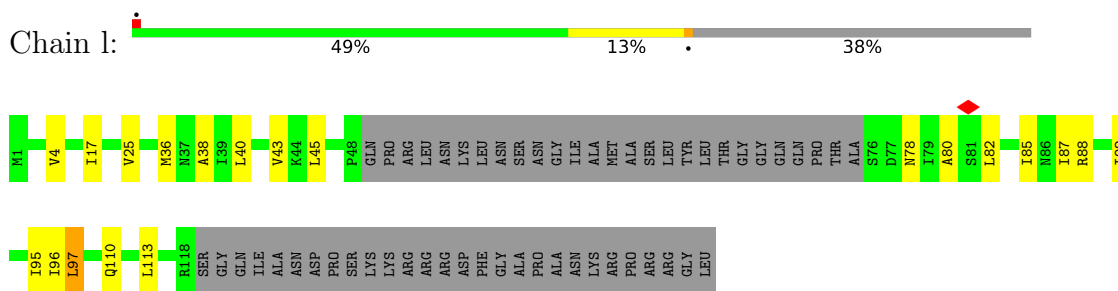
3 Residue-property plots [i](#)

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.

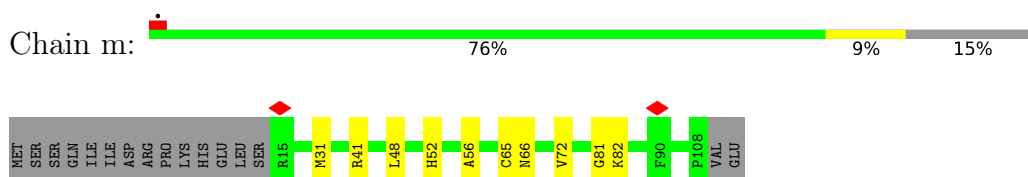
- Molecule 1: Small nuclear ribonucleoprotein-associated protein B



- Molecule 2: Small nuclear ribonucleoprotein Sm D1

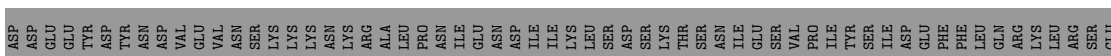


- Molecule 3: Small nuclear ribonucleoprotein Sm D2

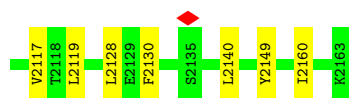


- Molecule 4: Small nuclear ribonucleoprotein Sm D3









- Molecule 10: *Saccharomyces cerevisiae* strain UOA_M2 chromosome 5 sequence

Chain V: 17% 30% 10% 41%



- Molecule 11: Pre-mRNA-splicing factor 8

Chain A: 75% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.073	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.43, 1.43, 1.43	Depositor

5 Model quality

5.1 Standard geometry

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	k	0.66	0/640	0.81	1/860 (0.1%)
2	l	0.67	0/725	0.91	0/980
3	m	0.65	0/749	0.86	0/1009
4	n	0.55	0/634	0.80	0/859
5	p	0.73	0/590	0.91	2/802 (0.2%)
6	q	0.59	0/585	0.82	0/791
7	r	0.58	0/529	0.76	0/711
8	E	0.68	0/1751	0.95	1/2411 (0.0%)
9	B	0.61	0/13989	1.02	18/18966 (0.1%)
10	V	0.44	0/1350	0.87	6/2097 (0.3%)
11	A	0.61	0/2064	0.97	1/2801 (0.0%)
All	All	0.61	0/23606	0.97	29/32287 (0.1%)

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
1	k	0	1
9	B	0	5
All	All	0	6

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	151	G	C2'-C3'-O3'	7.31	120.47	109.50
10	V	83	A	C2'-C3'-O3'	7.30	120.44	109.50
9	B	1297	TRP	N-CA-C	7.24	119.57	109.15
9	B	1785	ASN	CA-C-N	6.27	127.67	119.84
9	B	1785	ASN	C-N-CA	6.27	127.67	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1144	CYS	CA-C-N	6.21	126.12	119.28
9	B	1144	CYS	C-N-CA	6.21	126.12	119.28
9	B	936	VAL	N-CA-CB	6.17	117.77	110.55
9	B	1140	TRP	CA-C-N	6.07	125.56	119.24
9	B	1140	TRP	C-N-CA	6.07	125.56	119.24
9	B	1954	VAL	N-CA-C	5.93	117.38	110.62
10	V	150	G	C4'-C3'-O3'	5.92	118.28	109.40
9	B	1069	ILE	N-CA-C	5.85	121.51	109.34
5	p	45	GLY	N-CA-C	5.82	121.91	111.62
1	k	83	GLY	N-CA-C	5.69	119.50	111.42
10	V	75	U	N1-C1'-C2'	5.65	120.48	112.00
9	B	1104	ASN	N-CA-C	5.65	120.17	112.88
8	E	402	ALA	N-CA-C	5.59	117.06	110.97
9	B	824	LEU	N-CA-C	5.56	118.27	111.82
9	B	2024	ASP	N-CA-C	5.45	117.65	111.11
10	V	143	A	C4'-C3'-O3'	5.38	117.48	109.40
5	p	44	VAL	N-CA-C	5.33	115.83	111.62
9	B	1735	PHE	N-CA-C	5.28	118.85	112.93
9	B	901	VAL	N-CA-CB	5.25	116.69	110.55
9	B	1259	ILE	N-CA-C	-5.21	102.01	108.89
10	V	151	G	C4'-C3'-O3'	-5.16	101.66	109.40
9	B	1287	ASN	N-CA-C	5.11	115.91	108.14
11	A	2204	ALA	N-CA-C	5.09	115.86	107.20
9	B	1089	PHE	N-CA-C	5.04	117.81	109.85

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	B	1200	PRO	Peptide
9	B	1484	TYR	Peptide
9	B	1517	ASN	Peptide
9	B	790	ASP	Peptide
9	B	791	PRO	Peptide
1	k	84	LEU	Peptide

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	k	635	0	681	14	0
2	l	720	0	772	14	0
3	m	737	0	767	2	0
4	n	625	0	647	11	0
5	p	580	0	602	3	0
6	q	573	0	572	6	0
7	r	526	0	555	3	0
8	E	1763	0	1764	3	0
9	B	13690	0	13704	255	0
10	V	1209	0	612	17	0
11	A	2015	0	1970	30	0
All	All	23073	0	22646	333	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 (333) 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)
9:B:1700:ILE:HD11	9:B:1740:LEU:HD13	1.37	1.06
2:l:40:LEU:HD11	2:l:87:ILE:HD11	1.59	0.84
9:B:1208:ALA:HB2	9:B:1218:PHE:CD2	2.23	0.74
9:B:1220:ILE:HD13	9:B:1241:LEU:HD11	1.71	0.72
9:B:1183:ILE:CD1	9:B:1192:VAL:HG11	2.19	0.71
9:B:1224:ALA:HB3	9:B:1264:VAL:HA	1.72	0.71
9:B:632:ILE:HG22	9:B:670:LEU:HD11	1.70	0.71
1:k:96:VAL:HG21	2:l:82:LEU:HD23	1.71	0.71
9:B:1177:ALA:HB2	10:V:99:G:H5"	1.73	0.70
9:B:1085:SER:OG	9:B:1140:TRP:NE1	2.22	0.70
9:B:1001:LEU:HD23	9:B:1015:MET:HE1	1.75	0.69
9:B:1124:PRO:O	9:B:1128:LEU:N	2.23	0.69
9:B:1125:THR:HG21	9:B:1251:ILE:HD11	1.76	0.68
9:B:1294:SER:OG	9:B:1297:TRP:N	2.30	0.65
2:l:45:LEU:HD13	2:l:80:ALA:HB3	1.78	0.65
9:B:1782:ILE:HD11	9:B:1791:VAL:HG21	1.78	0.64
9:B:1880:LEU:HD23	9:B:1927:PHE:CZ	2.31	0.64
9:B:924:VAL:HG12	9:B:998:ALA:HB2	1.79	0.64
9:B:986:LEU:HD21	9:B:1015:MET:HE2	1.80	0.64
6:q:75:CYS:SG	6:q:76:ASN:N	2.71	0.64
9:B:1109:LEU:HD22	9:B:1131:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:2031:LEU:HD23	9:B:2038:LEU:HD23	1.82	0.62
9:B:1291:THR:HG22	9:B:1293:ILE:HD11	1.82	0.62
9:B:804:HIS:CE1	9:B:813:ARG:HB2	2.35	0.62
9:B:1253:TYR:CE1	9:B:1272:PHE:CG	2.87	0.62
11:A:2204:ALA:O	11:A:2229:GLN:NE2	2.34	0.61
9:B:1372:LYS:HB3	9:B:1708:GLY:HA2	1.83	0.61
9:B:1485:GLY:O	9:B:1488:TYR:N	2.34	0.60
9:B:631:LEU:HD22	9:B:654:THR:HG21	1.84	0.60
9:B:1261:PRO:O	9:B:1264:VAL:HG22	2.02	0.59
11:A:2182:VAL:HG23	11:A:2338:GLN:HB3	1.84	0.59
8:E:368:ALA:HB1	9:B:1184:ARG:NH1	2.18	0.59
9:B:499:LEU:HD23	9:B:503:GLN:HB3	1.85	0.59
9:B:1399:ASN:O	9:B:1405:ILE:HD11	2.04	0.58
9:B:1641:TYR:C	9:B:1670:CYS:SG	2.87	0.58
9:B:1396:VAL:HG13	9:B:1445:LEU:HD11	1.84	0.58
9:B:1982:MET:O	9:B:1986:GLY:N	2.36	0.58
9:B:707:PHE:CZ	9:B:902:LEU:HD12	2.38	0.57
9:B:1521:PHE:HD1	9:B:1521:PHE:O	1.88	0.57
9:B:1585:LEU:CD2	9:B:1683:LEU:HD23	2.34	0.57
9:B:2113:ALA:HB2	9:B:2130:PHE:HB3	1.87	0.57
9:B:518:LEU:HD12	9:B:519:ILE:N	2.20	0.57
9:B:740:ILE:HG23	9:B:827:VAL:HG13	1.87	0.56
9:B:1215:VAL:HG21	9:B:1735:PHE:CZ	2.40	0.56
9:B:1582:SER:HB3	9:B:1677:THR:HG21	1.88	0.56
9:B:1876:LEU:HD11	9:B:1982:MET:HE1	1.87	0.56
4:n:68:GLN:HG3	7:r:69:ILE:HD12	1.88	0.56
9:B:2013:VAL:HG13	9:B:2018:ASP:HB2	1.86	0.56
9:B:1682:ILE:HD12	9:B:1722:ILE:CG1	2.36	0.55
10:V:75:U:H2'	10:V:75:U:O2	2.06	0.55
9:B:637:HIS:HB2	9:B:674:LEU:HD12	1.88	0.55
9:B:1080:LEU:HD11	9:B:1084:PHE:CZ	2.41	0.55
9:B:1080:LEU:HD11	9:B:1084:PHE:CE1	2.42	0.55
9:B:1061:ALA:HA	11:A:2395:PHE:CD1	2.42	0.55
1:k:91:GLN:HE22	4:n:24:THR:HG22	1.71	0.55
9:B:1080:LEU:CD1	9:B:1084:PHE:CE1	2.89	0.55
11:A:2227:VAL:HG12	11:A:2374:PHE:CE1	2.42	0.54
9:B:561:ALA:O	9:B:609:PRO:HD3	2.07	0.54
9:B:1629:LEU:HD21	9:B:1644:MET:HE3	1.88	0.54
9:B:593:ARG:HB3	10:V:82:C:OP1	2.06	0.54
1:k:87:LEU:HD12	4:n:71:PHE:HB3	1.90	0.54
9:B:1369:GLY:C	9:B:1512:SER:O	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1704:LEU:O	9:B:1708:GLY:N	2.38	0.54
2:l:45:LEU:HD11	2:l:82:LEU:HD22	1.90	0.54
9:B:1122:GLY:N	9:B:1249:ASP:O	2.41	0.54
2:l:92:ILE:HG21	2:l:95:ILE:HD11	1.88	0.53
9:B:639:LEU:HA	9:B:644:GLY:HA3	1.91	0.53
9:B:774:ASP:HB3	9:B:778:LYS:HB2	1.89	0.53
9:B:933:ASN:O	9:B:936:VAL:HG22	2.08	0.53
1:k:96:VAL:HG22	2:l:85:ILE:HG12	1.91	0.53
9:B:633:ILE:HG21	9:B:636:ILE:HD13	1.90	0.53
9:B:1894:LEU:HD21	9:B:1922:VAL:HA	1.90	0.53
9:B:567:VAL:O	9:B:571:VAL:HG23	2.09	0.53
9:B:1080:LEU:HG	9:B:1084:PHE:CZ	2.44	0.53
1:k:20:LEU:HD23	1:k:95:THR:HB	1.91	0.53
9:B:636:ILE:HG22	9:B:671:SER:HB2	1.91	0.53
9:B:1208:ALA:HA	9:B:1218:PHE:HA	1.91	0.53
9:B:574:PHE:CB	9:B:585:VAL:HG11	2.38	0.52
9:B:1243:LEU:HG	9:B:1252:LEU:HD12	1.91	0.52
9:B:1482:GLY:O	9:B:1483:VAL:HG13	2.09	0.52
2:l:25:VAL:HG13	2:l:43:VAL:HG13	1.90	0.52
11:A:2208:TYR:CE2	11:A:2244:ILE:HD11	2.45	0.52
9:B:508:HIS:O	9:B:512:GLU:N	2.40	0.52
9:B:1032:PHE:CD2	9:B:1080:LEU:HD23	2.44	0.52
9:B:1583:VAL:HG22	9:B:1681:ILE:HB	1.91	0.52
9:B:708:CYS:SG	9:B:709:GLY:N	2.83	0.51
9:B:1521:PHE:CD1	9:B:1521:PHE:C	2.89	0.51
6:q:33:PHE:HB2	10:V:152:A:C2	2.46	0.51
9:B:1682:ILE:HD12	9:B:1722:ILE:HG13	1.93	0.51
8:E:513:ALA:HB3	9:B:1463:LYS:CE	2.41	0.51
9:B:1863:ILE:O	9:B:1867:VAL:HG23	2.11	0.51
9:B:632:ILE:CG2	9:B:670:LEU:HD11	2.40	0.51
9:B:1394:ARG:HB3	9:B:1468:LEU:HD23	1.91	0.51
9:B:1929:LEU:HD21	9:B:1943:PHE:CD1	2.45	0.51
9:B:1139:MET:HE2	9:B:1139:MET:N	2.26	0.51
9:B:1930:LEU:HD22	9:B:1983:LEU:HD21	1.91	0.51
10:V:81:C:C2	10:V:82:C:C6	2.98	0.51
9:B:1585:LEU:HD21	9:B:1683:LEU:HD23	1.92	0.51
7:r:44:MET:HE3	7:r:56:GLN:HB2	1.92	0.50
9:B:1367:PHE:HZ	9:B:1515:LEU:HD11	1.76	0.50
11:A:2197:SER:OG	11:A:2261:THR:HG21	2.11	0.50
9:B:1220:ILE:HD12	9:B:1270:LEU:HB3	1.94	0.50
9:B:594:LEU:CD2	9:B:620:ASN:HD21	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:632:ILE:C	9:B:633:ILE:HD12	2.37	0.50
9:B:1201:LYS:HA	9:B:1302:PHE:CZ	2.47	0.50
9:B:614:ILE:HG21	10:V:81:C:H5'	1.94	0.50
9:B:1986:GLY:O	9:B:1987:VAL:HG13	2.12	0.49
9:B:630:LEU:CD2	9:B:632:ILE:HD11	2.42	0.49
9:B:912:PHE:CE2	9:B:916:LEU:HA	2.47	0.49
9:B:1652:VAL:HA	9:B:1655:LEU:HD12	1.94	0.49
9:B:1459:TRP:CG	9:B:1498:ILE:HD11	2.47	0.49
9:B:503:GLN:O	9:B:507:PHE:N	2.45	0.49
9:B:574:PHE:HB3	9:B:585:VAL:HG11	1.95	0.49
9:B:1477:HIS:N	9:B:1512:SER:OG	2.46	0.49
9:B:1621:ILE:HD12	9:B:1630:ARG:HG3	1.94	0.49
9:B:917:VAL:HG12	9:B:981:LEU:HD21	1.95	0.49
9:B:2103:LEU:HB3	9:B:2113:ALA:HB3	1.94	0.49
9:B:1950:ILE:O	9:B:1954:VAL:HG13	2.12	0.49
9:B:1183:ILE:HG22	9:B:1183:ILE:O	2.13	0.49
9:B:1456:SER:O	9:B:1457:ARG:C	2.56	0.49
9:B:1770:VAL:O	9:B:1774:THR:HG23	2.13	0.49
5:p:58:VAL:HG13	5:p:76:PRO:HA	1.93	0.49
9:B:1368:VAL:O	9:B:1533:TYR:O	2.30	0.49
9:B:1994:LEU:HD13	9:B:2008:CYS:SG	2.53	0.49
9:B:632:ILE:HG12	9:B:668:ILE:HD13	1.94	0.48
9:B:1521:PHE:HD1	9:B:1521:PHE:C	2.21	0.48
8:E:513:ALA:HB3	9:B:1463:LYS:HE3	1.95	0.48
9:B:589:THR:HG23	9:B:589:THR:O	2.12	0.48
9:B:1101:ILE:O	9:B:1105:ALA:N	2.45	0.48
9:B:2044:PHE:O	9:B:2048:TYR:HB2	2.13	0.48
11:A:2194:ILE:HD11	11:A:2293:ILE:HG21	1.94	0.48
6:q:51:LEU:HD11	6:q:81:ILE:HD11	1.96	0.48
9:B:1200:PRO:HG2	9:B:1297:TRP:CD1	2.48	0.48
9:B:527:LYS:HA	9:B:530:ILE:HD12	1.96	0.48
9:B:1179:VAL:HG13	9:B:1183:ILE:HD12	1.96	0.48
10:V:83:A:O2'	10:V:84:G:O5'	2.28	0.48
9:B:1544:LEU:HD13	9:B:1707:VAL:HG12	1.96	0.48
1:k:89:GLY:HA2	1:k:92:ILE:HD12	1.96	0.48
7:r:63:ILE:HB	7:r:68:ILE:HD11	1.95	0.48
9:B:1486:ALA:O	9:B:1490:THR:OG1	2.31	0.48
9:B:483:LEU:HB3	9:B:487:CYS:HB2	1.95	0.48
11:A:2223:THR:HG22	11:A:2224:VAL:O	2.14	0.48
9:B:718:LYS:HE2	9:B:722:MET:HE3	1.96	0.48
11:A:2182:VAL:HG23	11:A:2338:GLN:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:2113:ALA:HB1	9:B:2128:LEU:HB3	1.95	0.47
1:k:91:GLN:NE2	4:n:24:THR:HG22	2.28	0.47
9:B:1751:HIS:HA	9:B:1810:CYS:SG	2.54	0.47
2:l:38:ALA:HB3	2:l:87:ILE:HD12	1.96	0.47
9:B:1546:ILE:HD11	9:B:1707:VAL:HG11	1.96	0.47
9:B:1629:LEU:CD2	9:B:1644:MET:HE3	2.44	0.47
9:B:1215:VAL:HG21	9:B:1735:PHE:HZ	1.79	0.47
9:B:2011:ILE:HG22	9:B:2011:ILE:O	2.14	0.47
11:A:2259:ILE:HD11	11:A:2293:ILE:HD11	1.96	0.47
9:B:631:LEU:HD23	9:B:633:ILE:HD11	1.96	0.47
9:B:634:ASP:CA	9:B:670:LEU:HD12	2.45	0.47
9:B:1782:ILE:HD11	9:B:1791:VAL:CG2	2.45	0.47
10:V:74:U:O2	10:V:74:U:C2'	2.63	0.47
5:p:43:ILE:HD11	5:p:90:ILE:HD12	1.96	0.47
9:B:1011:ASN:O	9:B:1014:SER:N	2.48	0.47
9:B:936:VAL:HG11	9:B:971:GLU:CD	2.40	0.47
9:B:517:MET:SD	9:B:666:ARG:NH2	2.88	0.47
9:B:1438:LEU:O	9:B:1442:SER:N	2.41	0.47
11:A:2311:GLY:HA2	11:A:2329:PHE:CZ	2.50	0.47
10:V:75:U:O2	10:V:75:U:C2'	2.63	0.46
6:q:29:VAL:HG13	6:q:78:VAL:HG13	1.97	0.46
9:B:1147:ARG:NH2	9:B:1157:ILE:HD13	2.30	0.46
2:l:40:LEU:CD1	2:l:87:ILE:HD11	2.38	0.46
1:k:85:THR:HG22	4:n:73:VAL:HA	1.97	0.46
9:B:1396:VAL:HG13	9:B:1445:LEU:CD1	2.44	0.46
2:l:88:ARG:NH1	10:V:147:U:O2'	2.49	0.46
9:B:1201:LYS:HA	9:B:1302:PHE:CE1	2.51	0.46
10:V:79:A:O2'	10:V:80:A:O4'	2.19	0.46
11:A:2228:PRO:HA	11:A:2357:TRP:O	2.16	0.46
9:B:1253:TYR:CZ	9:B:1272:PHE:CB	2.98	0.46
9:B:1786:PRO:HB2	9:B:1791:VAL:HB	1.96	0.46
9:B:1057:LEU:O	9:B:1060:LYS:N	2.49	0.46
9:B:1085:SER:HB2	9:B:1087:LEU:HD13	1.98	0.46
9:B:1812:ASN:HA	9:B:1815:VAL:HG22	1.98	0.46
9:B:644:GLY:N	9:B:645:PRO:HD2	2.31	0.46
9:B:708:CYS:SG	9:B:890:THR:N	2.89	0.46
9:B:1080:LEU:CG	9:B:1084:PHE:CZ	2.99	0.46
9:B:1140:TRP:HE3	9:B:1141:PRO:HD2	1.80	0.45
9:B:592:SER:HB3	10:V:83:A:P	2.55	0.45
9:B:614:ILE:HD11	9:B:1009:TYR:CD2	2.51	0.45
9:B:744:VAL:HG23	9:B:745:HIS:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1075:LYS:O	9:B:1078:VAL:HG12	2.17	0.45
9:B:872:LEU:O	9:B:875:ALA:N	2.49	0.45
9:B:1656:TYR:CE1	9:B:1677:THR:HG22	2.51	0.45
11:A:2329:PHE:O	11:A:2330:GLU:CB	2.65	0.45
11:A:2354:GLY:O	11:A:2355:ASN:CB	2.64	0.45
9:B:480:ILE:HD12	9:B:491:PHE:CD2	2.52	0.45
9:B:1142:THR:HG21	11:A:2389:PRO:HA	1.98	0.45
9:B:2001:ASN:OD1	9:B:2001:ASN:N	2.50	0.45
5:p:44:VAL:HB	5:p:53:VAL:HG13	1.98	0.45
9:B:556:LYS:O	9:B:628:VAL:HA	2.16	0.45
9:B:1157:ILE:HD12	9:B:1158:LYS:N	2.32	0.45
2:l:4:VAL:HG22	2:l:36:MET:CE	2.47	0.45
9:B:1485:GLY:O	9:B:1486:ALA:C	2.60	0.45
9:B:1743:GLU:HB2	9:B:1789:TYR:OH	2.17	0.45
9:B:1981:GLN:NE2	9:B:2149:TYR:O	2.49	0.45
9:B:2113:ALA:HB2	9:B:2130:PHE:CB	2.46	0.45
2:l:43:VAL:HG21	2:l:85:ILE:HG13	1.98	0.44
9:B:708:CYS:SG	9:B:889:ILE:HA	2.57	0.44
9:B:1113:PHE:HZ	9:B:1240:LEU:HD13	1.82	0.44
9:B:1216:MET:O	9:B:1273:THR:HA	2.18	0.44
11:A:2166:LEU:HB3	11:A:2169:ILE:HD11	2.00	0.44
9:B:1095:ASN:O	9:B:1098:ILE:HG22	2.15	0.44
9:B:1745:TYR:O	9:B:1746:LEU:C	2.60	0.44
9:B:1773:PHE:CD2	9:B:1803:LEU:HD21	2.52	0.44
9:B:1939:LEU:HD13	9:B:1947:LEU:HD22	1.99	0.44
11:A:2152:TRP:CG	11:A:2153:ARG:N	2.86	0.44
9:B:634:ASP:HA	9:B:670:LEU:HD12	1.99	0.44
9:B:1194:ASP:O	9:B:1198:ARG:HB2	2.18	0.44
9:B:1432:PRO:HB3	9:B:1454:LEU:HD21	1.99	0.44
11:A:2359:TYR:CD2	11:A:2362:MET:HE3	2.53	0.44
9:B:1426:ASN:HD22	9:B:1442:SER:HB2	1.83	0.44
9:B:1062:PRO:HD3	11:A:2395:PHE:CG	2.53	0.44
9:B:1080:LEU:CD1	9:B:1084:PHE:CZ	3.01	0.44
9:B:1396:VAL:HG21	9:B:1468:LEU:HD13	2.00	0.44
9:B:809:THR:HA	9:B:1092:PHE:CD1	2.53	0.43
9:B:1236:LEU:HD22	9:B:1258:PHE:HB3	2.00	0.43
9:B:1585:LEU:CD1	9:B:1591:CYS:HA	2.48	0.43
1:k:86:ILE:HD11	4:n:10:LEU:HD22	2.00	0.43
4:n:6:ILE:N	4:n:7:PRO:CD	2.81	0.43
9:B:651:VAL:HG11	9:B:683:PHE:CE1	2.54	0.43
9:B:571:VAL:HG21	9:B:587:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:890:THR:OG1	9:B:891:ASP:N	2.51	0.43
9:B:1253:TYR:CD1	9:B:1272:PHE:CD2	3.06	0.43
9:B:931:CYS:SG	9:B:934:ASP:N	2.83	0.43
9:B:2044:PHE:O	9:B:2048:TYR:CB	2.67	0.43
10:V:134:U:C5	10:V:135:A:C8	3.06	0.43
9:B:1853:ALA:HB2	9:B:1863:ILE:HG13	2.01	0.43
6:q:45:THR:HG22	6:q:51:LEU:HD23	1.99	0.43
9:B:726:CYS:O	9:B:730:VAL:HG23	2.17	0.43
11:A:2189:LEU:HD22	11:A:2224:VAL:HG23	2.00	0.43
3:m:56:ALA:HB2	3:m:72:VAL:HG13	2.00	0.43
9:B:978:LEU:CD1	9:B:996:ILE:HD12	2.49	0.43
9:B:1092:PHE:CD1	9:B:1095:ASN:HB3	2.54	0.43
9:B:1139:MET:HE3	9:B:1298:TRP:NE1	2.33	0.43
9:B:1257:LEU:HD22	9:B:1270:LEU:HD12	1.99	0.43
9:B:1704:LEU:HA	9:B:1707:VAL:HG23	2.00	0.43
9:B:1960:VAL:O	9:B:1964:ILE:N	2.52	0.43
9:B:558:VAL:HG21	9:B:612:TRP:CH2	2.54	0.43
9:B:580:PHE:CE2	9:B:581:LEU:HG	2.54	0.43
9:B:1065:ILE:CG1	9:B:1077:ASN:HD21	2.31	0.43
9:B:1571:SER:OG	9:B:1663:VAL:HG21	2.18	0.43
9:B:1867:VAL:HG22	9:B:1964:ILE:HD11	2.01	0.43
9:B:1137:THR:OG1	9:B:1139:MET:HE1	2.19	0.42
9:B:2002:ASN:HA	9:B:2005:LEU:HD12	2.01	0.42
2:l:17:ILE:CG2	2:l:92:ILE:HG23	2.49	0.42
9:B:836:TRP:HA	9:B:836:TRP:CE3	2.54	0.42
9:B:1595:ALA:HB1	9:B:1632:PRO:HB3	2.01	0.42
9:B:562:PRO:HB3	9:B:638:LEU:HD22	2.02	0.42
9:B:1011:ASN:O	9:B:1012:HIS:C	2.62	0.42
9:B:1113:PHE:CZ	9:B:1129:LEU:HD13	2.55	0.42
9:B:1304:ILE:HD12	9:B:1304:ILE:C	2.44	0.42
1:k:46:ASN:O	1:k:84:LEU:HD23	2.19	0.42
1:k:49:ILE:HG23	1:k:80:ARG:O	2.18	0.42
9:B:557:ILE:HD12	9:B:604:VAL:HG22	2.02	0.42
9:B:833:THR:HG22	10:V:77:U:H3'	2.00	0.42
9:B:1819:PHE:HZ	9:B:1863:ILE:HB	1.84	0.42
11:A:2224:VAL:HG11	11:A:2349:PHE:CE2	2.54	0.42
9:B:532:LEU:HD21	9:B:577:ARG:HB3	2.02	0.42
9:B:1453:GLU:O	9:B:1494:ARG:NH1	2.51	0.42
11:A:2165:ARG:HB3	11:A:2300:VAL:HG13	2.00	0.42
9:B:594:LEU:HB2	10:V:83:A:H3'	2.01	0.42
9:B:1095:ASN:O	9:B:1099:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1746:LEU:O	9:B:1747:GLN:C	2.63	0.42
9:B:1781:ARG:O	9:B:1784:VAL:HG22	2.20	0.42
2:l:25:VAL:CG1	2:l:43:VAL:HG22	2.50	0.42
3:m:31:MET:HE1	3:m:65:CYS:SG	2.59	0.42
4:n:81:ALA:HB1	4:n:82:PRO:HA	2.00	0.42
9:B:456:VAL:HG12	9:B:457:LYS:N	2.35	0.42
9:B:613:ASP:HA	9:B:616:THR:HG22	2.02	0.42
9:B:634:ASP:CB	9:B:670:LEU:HD12	2.50	0.42
9:B:1448:THR:O	9:B:1449:PRO:C	2.63	0.42
11:A:2159:ASN:HA	11:A:2162:LEU:HD13	2.00	0.42
6:q:71:ILE:HD12	6:q:71:ILE:C	2.44	0.42
9:B:1584:PHE:CE1	9:B:1666:ILE:HD12	2.55	0.42
11:A:2188:ASN:OD1	11:A:2189:LEU:N	2.53	0.42
9:B:932:ARG:O	9:B:936:VAL:HG13	2.19	0.41
9:B:1156:VAL:HG13	9:B:1183:ILE:CG2	2.51	0.41
9:B:1202:MET:HE1	9:B:1239:PHE:CG	2.55	0.41
9:B:1682:ILE:HD13	9:B:1703:LEU:HD22	2.01	0.41
9:B:2140:LEU:HD11	9:B:2160:ILE:HD11	2.02	0.41
11:A:2204:ALA:O	11:A:2238:ILE:HD11	2.20	0.41
9:B:1202:MET:HE1	9:B:1239:PHE:CD2	2.56	0.41
9:B:1879:MET:HE1	9:B:1975:THR:HB	2.02	0.41
4:n:24:THR:HG23	4:n:68:GLN:O	2.20	0.41
9:B:594:LEU:HD22	9:B:620:ASN:HD21	1.84	0.41
9:B:793:LEU:C	9:B:793:LEU:HD23	2.46	0.41
9:B:1884:SER:HA	9:B:1926:VAL:HG11	2.02	0.41
9:B:1955:VAL:HG21	9:B:2091:TYR:OH	2.20	0.41
9:B:2037:GLN:O	9:B:2041:VAL:HG23	2.19	0.41
9:B:2117:VAL:HG21	9:B:2119:LEU:HD21	2.03	0.41
10:V:81:C:O2	10:V:81:C:H2'	2.20	0.41
1:k:85:THR:HG21	4:n:71:PHE:CE1	2.55	0.41
9:B:1785:ASN:O	9:B:1787:SER:N	2.53	0.41
9:B:1846:THR:C	9:B:1847:LEU:HD23	2.46	0.41
9:B:1880:LEU:HD23	9:B:1927:PHE:CE2	2.55	0.41
9:B:1922:VAL:O	9:B:1926:VAL:HG23	2.20	0.41
9:B:1065:ILE:HG13	9:B:1077:ASN:HD21	1.85	0.41
9:B:1243:LEU:HD22	9:B:1272:PHE:CE2	2.55	0.41
9:B:1533:TYR:HB3	9:B:1535:PHE:CZ	2.56	0.41
9:B:1846:THR:O	9:B:1847:LEU:HD23	2.21	0.41
10:V:135:A:C2	10:V:136:U:C2	3.09	0.41
9:B:1750:ILE:HG21	9:B:1773:PHE:HZ	1.86	0.41
11:A:2188:ASN:CG	11:A:2189:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:898:TYR:O	9:B:901:VAL:HG22	2.21	0.41
9:B:1067:GLU:HB2	9:B:1074:ALA:HB2	2.01	0.41
9:B:1145:PRO:O	9:B:1146:LEU:C	2.64	0.41
9:B:1210:PRO:O	9:B:1785:ASN:ND2	2.43	0.41
9:B:1744:SER:OG	9:B:1746:LEU:N	2.54	0.41
9:B:1939:LEU:CD1	9:B:1947:LEU:HD22	2.51	0.41
11:A:2321:ILE:HG22	11:A:2322:MET:H	1.84	0.41
11:A:2396:SER:O	11:A:2398:LEU:N	2.54	0.41
9:B:770:LEU:O	9:B:772:LYS:N	2.54	0.40
9:B:1087:LEU:HD22	11:A:2395:PHE:CE2	2.55	0.40
9:B:1331:THR:HG23	9:B:1346:LYS:O	2.21	0.40
9:B:1476:ALA:HB1	9:B:1521:PHE:CZ	2.56	0.40
9:B:1631:ALA:HB3	9:B:1632:PRO:HD3	2.02	0.40
9:B:1167:TRP:CD1	9:B:1167:TRP:C	2.98	0.40
9:B:1791:VAL:HG11	9:B:1799:ILE:HG12	2.03	0.40
11:A:2247:LEU:HD11	11:A:2374:PHE:O	2.20	0.40
1:k:85:THR:HG21	4:n:71:PHE:CD1	2.56	0.40
9:B:788:VAL:O	9:B:788:VAL:HG12	2.21	0.40
9:B:808:LEU:HD23	9:B:813:ARG:HA	2.03	0.40
9:B:1454:LEU:C	9:B:1454:LEU:HD23	2.47	0.40
9:B:1500:THR:HG22	9:B:1500:THR:O	2.21	0.40
9:B:1183:ILE:O	9:B:1183:ILE:CG2	2.68	0.40
1:k:21:ARG:N	1:k:96:VAL:O	2.53	0.40
9:B:1145:PRO:HD2	9:B:1167:TRP:CE3	2.57	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	k	76/196 (39%)	67 (88%)	8 (10%)	1 (1%)	9 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	87/146 (60%)	74 (85%)	12 (14%)	1 (1%)	11	45
3	m	92/110 (84%)	80 (87%)	10 (11%)	2 (2%)	5	29
4	n	80/101 (79%)	70 (88%)	10 (12%)	0	100	100
5	p	72/94 (77%)	64 (89%)	8 (11%)	0	100	100
6	q	70/86 (81%)	60 (86%)	10 (14%)	0	100	100
7	r	65/77 (84%)	58 (89%)	6 (9%)	1 (2%)	8	38
8	E	308/338 (91%)	266 (86%)	38 (12%)	4 (1%)	9	41
9	B	1707/2163 (79%)	1499 (88%)	174 (10%)	34 (2%)	6	32
11	A	253/267 (95%)	213 (84%)	34 (13%)	6 (2%)	4	28
All	All	2810/3578 (78%)	2451 (87%)	310 (11%)	49 (2%)	9	35

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	B	448	LEU
9	B	771	THR
9	B	792	SER
9	B	985	GLU
9	B	1370	SER
9	B	1481	GLN
9	B	1483	VAL
11	A	2330	GLU
1	k	81	VAL
9	B	1009	TYR
9	B	1051	LYS
9	B	1069	ILE
9	B	1147	ARG
9	B	1637	VAL
9	B	1697	PRO
11	A	2321	ILE
11	A	2355	ASN
11	A	2398	LEU
8	E	101	ALA
9	B	875	ALA
9	B	1972	ASN
9	B	1991	ASP
11	A	2197	SER
2	l	97	LEU
3	m	66	ASN

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Mol	Chain	Res	Type
8	E	212	ALA
8	E	512	ALA
9	B	928	ASN
9	B	958	PRO
9	B	1024	GLU
9	B	1088	LYS
9	B	1201	LYS
9	B	1296	ASN
9	B	1480	SER
9	B	1485	GLY
9	B	1750	ILE
7	r	59	LEU
8	E	411	ALA
9	B	744	VAL
9	B	1275	GLU
9	B	1317	PHE
9	B	1401	SER
9	B	1185	SER
9	B	1335	GLY
11	A	2388	ARG
9	B	2030	ILE
9	B	1910	PRO
3	m	81	GLY
9	B	1785	ASN

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	k	71/176 (40%)	69 (97%)	2 (3%)	38	59
2	l	85/129 (66%)	80 (94%)	5 (6%)	18	41
3	m	78/103 (76%)	74 (95%)	4 (5%)	21	44
4	n	69/89 (78%)	66 (96%)	3 (4%)	26	48
5	p	65/83 (78%)	59 (91%)	6 (9%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	q	63/77 (82%)	62 (98%)	1 (2%)	55	69
7	r	57/66 (86%)	55 (96%)	2 (4%)	32	53
8	E	20/20 (100%)	19 (95%)	1 (5%)	22	44
9	B	1536/1955 (79%)	1421 (92%)	115 (8%)	12	34
11	A	220/236 (93%)	205 (93%)	15 (7%)	14	37
All	All	2264/2934 (77%)	2110 (93%)	154 (7%)	16	37

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	k	25	GLN
1	k	48	CYS
2	l	78	ASN
2	l	96	ILE
2	l	97	LEU
2	l	110	GLN
2	l	113	LEU
3	m	41	ARG
3	m	48	LEU
3	m	52	HIS
3	m	82	LYS
4	n	20	SER
4	n	43	GLN
4	n	76	ASP
5	p	18	PHE
5	p	77	LEU
5	p	79	LYS
5	p	80	ILE
5	p	81	LEU
5	p	88	THR
6	q	79	LEU
7	r	69	ILE
7	r	71	LEU
8	E	550	GLN
9	B	439	LYS
9	B	453	PHE
9	B	463	ILE
9	B	491	PHE
9	B	505	LYS
9	B	518	LEU

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Mol	Chain	Res	Type
9	B	539	LEU
9	B	566	LEU
9	B	610	GLU
9	B	614	ILE
9	B	645	PRO
9	B	670	LEU
9	B	684	LEU
9	B	717	LYS
9	B	726	CYS
9	B	778	LYS
9	B	782	LYS
9	B	784	GLU
9	B	793	LEU
9	B	815	LEU
9	B	818	ASP
9	B	831	THR
9	B	836	TRP
9	B	864	SER
9	B	870	GLN
9	B	872	LEU
9	B	897	TYR
9	B	901	VAL
9	B	902	LEU
9	B	920	LEU
9	B	921	ASN
9	B	928	ASN
9	B	942	THR
9	B	944	LEU
9	B	948	MET
9	B	978	LEU
9	B	1000	ASP
9	B	1006	SER
9	B	1015	MET
9	B	1016	ASP
9	B	1049	GLU
9	B	1052	ARG
9	B	1054	LEU
9	B	1057	LEU
9	B	1077	ASN
9	B	1085	SER
9	B	1086	GLN
9	B	1088	LYS

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Mol	Chain	Res	Type
9	B	1098	ILE
9	B	1128	LEU
9	B	1131	LEU
9	B	1132	CYS
9	B	1137	THR
9	B	1138	LYS
9	B	1139	MET
9	B	1152	CYS
9	B	1160	LEU
9	B	1179	VAL
9	B	1198	ARG
9	B	1202	MET
9	B	1240	LEU
9	B	1246	THR
9	B	1253	TYR
9	B	1260	THR
9	B	1262	ASP
9	B	1268	PHE
9	B	1270	LEU
9	B	1284	LEU
9	B	1292	LEU
9	B	1312	LYS
9	B	1342	VAL
9	B	1344	GLU
9	B	1370	SER
9	B	1400	PRO
9	B	1453	GLU
9	B	1454	LEU
9	B	1483	VAL
9	B	1490	THR
9	B	1491	LEU
9	B	1493	SER
9	B	1498	ILE
9	B	1513	ASN
9	B	1514	CYS
9	B	1515	LEU
9	B	1519	ARG
9	B	1521	PHE
9	B	1540	ARG
9	B	1541	ILE
9	B	1578	ARG
9	B	1610	LEU

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Mol	Chain	Res	Type
9	B	1612	VAL
9	B	1617	ILE
9	B	1651	ILE
9	B	1680	VAL
9	B	1687	LEU
9	B	1689	ASP
9	B	1696	MET
9	B	1705	GLU
9	B	1707	VAL
9	B	1722	ILE
9	B	1724	THR
9	B	1744	SER
9	B	1847	LEU
9	B	1849	ASN
9	B	1860	PHE
9	B	1887	VAL
9	B	1917	THR
9	B	1928	LEU
9	B	1933	TYR
9	B	1947	LEU
9	B	1975	THR
9	B	1987	VAL
9	B	2000	PHE
9	B	2001	ASN
9	B	2098	SER
11	A	2155	SER
11	A	2164	LEU
11	A	2168	ASN
11	A	2170	TYR
11	A	2188	ASN
11	A	2190	LEU
11	A	2228	PRO
11	A	2238	ILE
11	A	2251	GLU
11	A	2264	GLU
11	A	2306	ASN
11	A	2319	LYS
11	A	2340	LEU
11	A	2356	VAL
11	A	2381	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	33	GLN
1	k	46	ASN
2	l	12	ASN
2	l	14	GLN
2	l	78	ASN
2	l	86	ASN
2	l	110	GLN
2	l	112	GLN
4	n	61	GLN
5	p	86	ASN
6	q	34	ASN
6	q	54	ASN
6	q	77	ASN
9	B	618	ASN
9	B	620	ASN
9	B	621	ASN
9	B	706	GLN
9	B	804	HIS
9	B	805	HIS
9	B	892	GLN
9	B	903	ASN
9	B	904	GLN
9	B	975	HIS
9	B	1102	HIS
9	B	1191	GLN
9	B	1280	ASN
9	B	1309	ASN
9	B	1390	GLN
9	B	1426	ASN
9	B	1513	ASN
9	B	1531	ASN
9	B	1686	ASN
9	B	1727	ASN
9	B	1747	GLN
9	B	1864	GLN
9	B	1916	HIS
9	B	1968	ASN
9	B	2040	GLN
9	B	2069	GLN
9	B	2161	ASN
11	A	2159	ASN
11	A	2237	GLN
11	A	2355	ASN

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Mol	Chain	Res	Type
11	A	2394	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	V	55/96 (57%)	34 (61%)	5 (9%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	V	74	U
10	V	75	U
10	V	78	A
10	V	80	A
10	V	81	C
10	V	83	A
10	V	84	G
10	V	85	A
10	V	86	C
10	V	87	C
10	V	88	G
10	V	89	U
10	V	90	C
10	V	91	U
10	V	94	U
10	V	98	G
10	V	100	U
10	V	101	C
10	V	102	A
10	V	103	A
10	V	129	A
10	V	130	A
10	V	131	G
10	V	132	A
10	V	136	U
10	V	137	G
10	V	138	U
10	V	143	A
10	V	144	A
10	V	145	U
10	V	147	U

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Mol	Chain	Res	Type
10	V	149	U
10	V	151	G
10	V	152	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	V	80	A
10	V	83	A
10	V	88	G
10	V	143	A
10	V	150	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	132:ALA	C	150:ALA	N	37.33
1	E	170:ALA	C	180:ALA	N	34.57
1	E	102:ALA	C	120:ALA	N	31.59
1	E	299:ALA	C	310:ALA	N	27.52
1	E	226:ALA	C	240:ALA	N	26.36
1	E	250:ALA	C	270:ALA	N	25.18
1	E	420:ALA	C	487:ALA	N	24.74
1	E	280:ALA	C	290:ALA	N	24.21
1	E	318:ALA	C	330:ALA	N	14.53
1	E	194:ALA	C	210:ALA	N	14.15
1	E	57:ALA	C	70:ALA	N	11.23
1	E	25:ALA	C	40:ALA	N	8.77
1	E	91:ALA	C	96:ALA	N	7.75
1	E	79:ALA	C	82:ALA	N	5.51

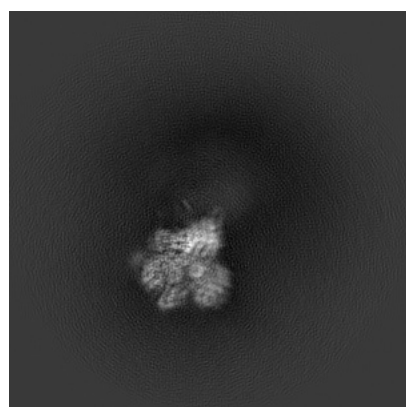
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8013. These allow visual inspection of the internal detail of the map and identification of artifacts.

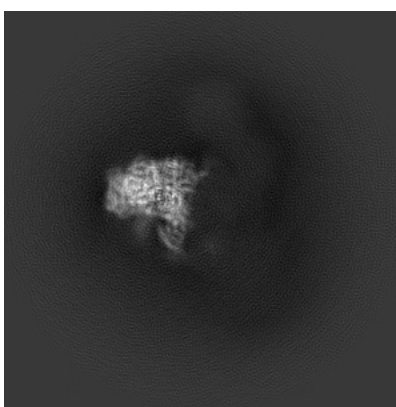
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

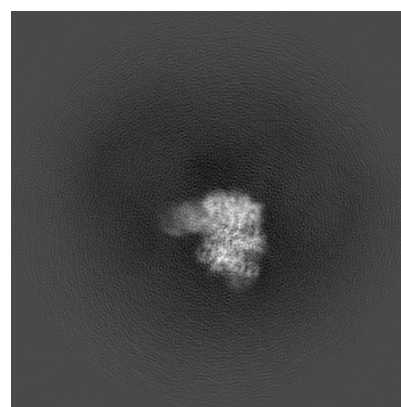
6.1.1 Primary map



X



Y

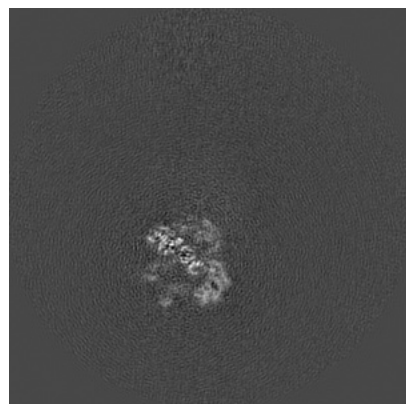


Z

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

6.2 Central slices [i](#)

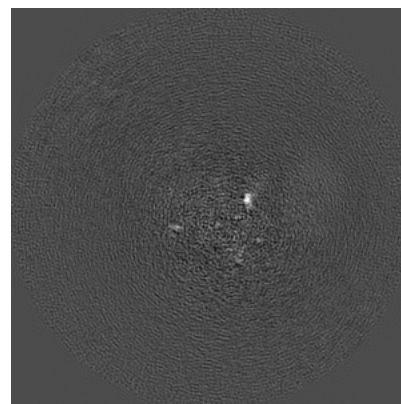
6.2.1 Primary map



X Index: 190



Y Index: 190

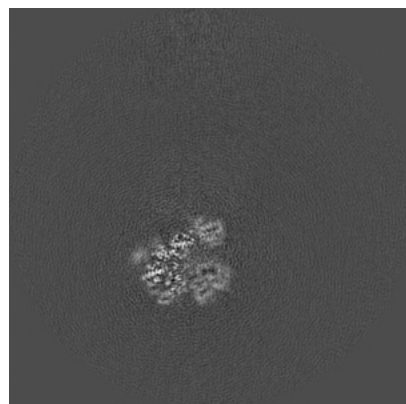


Z Index: 190

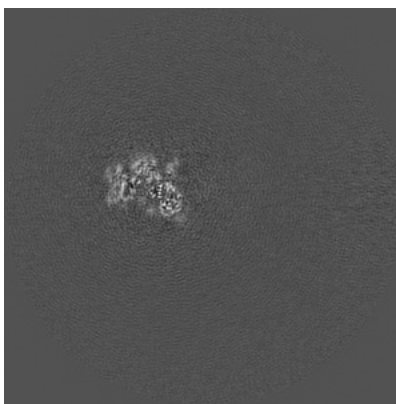
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

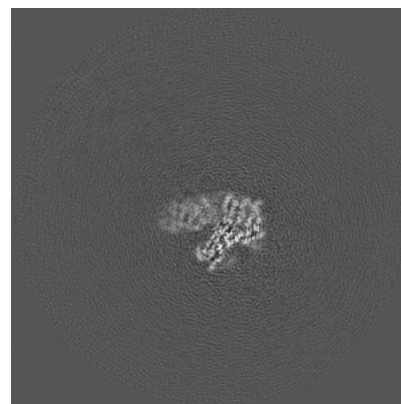
6.3.1 Primary map



X Index: 211



Y Index: 155

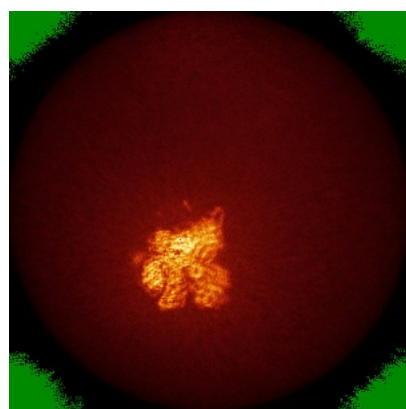


Z Index: 161

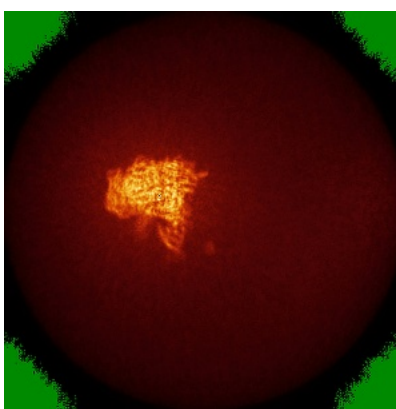
The images above show the largest variance slices of the map in three orthogonal directions.

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

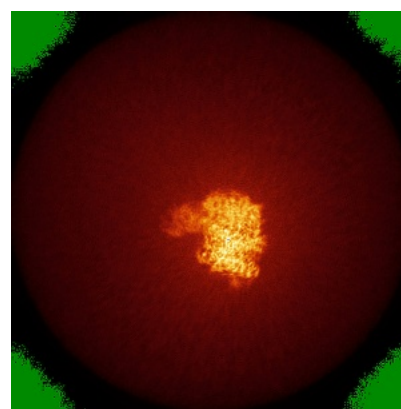
6.4.1 Primary map



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

This section was not generated.

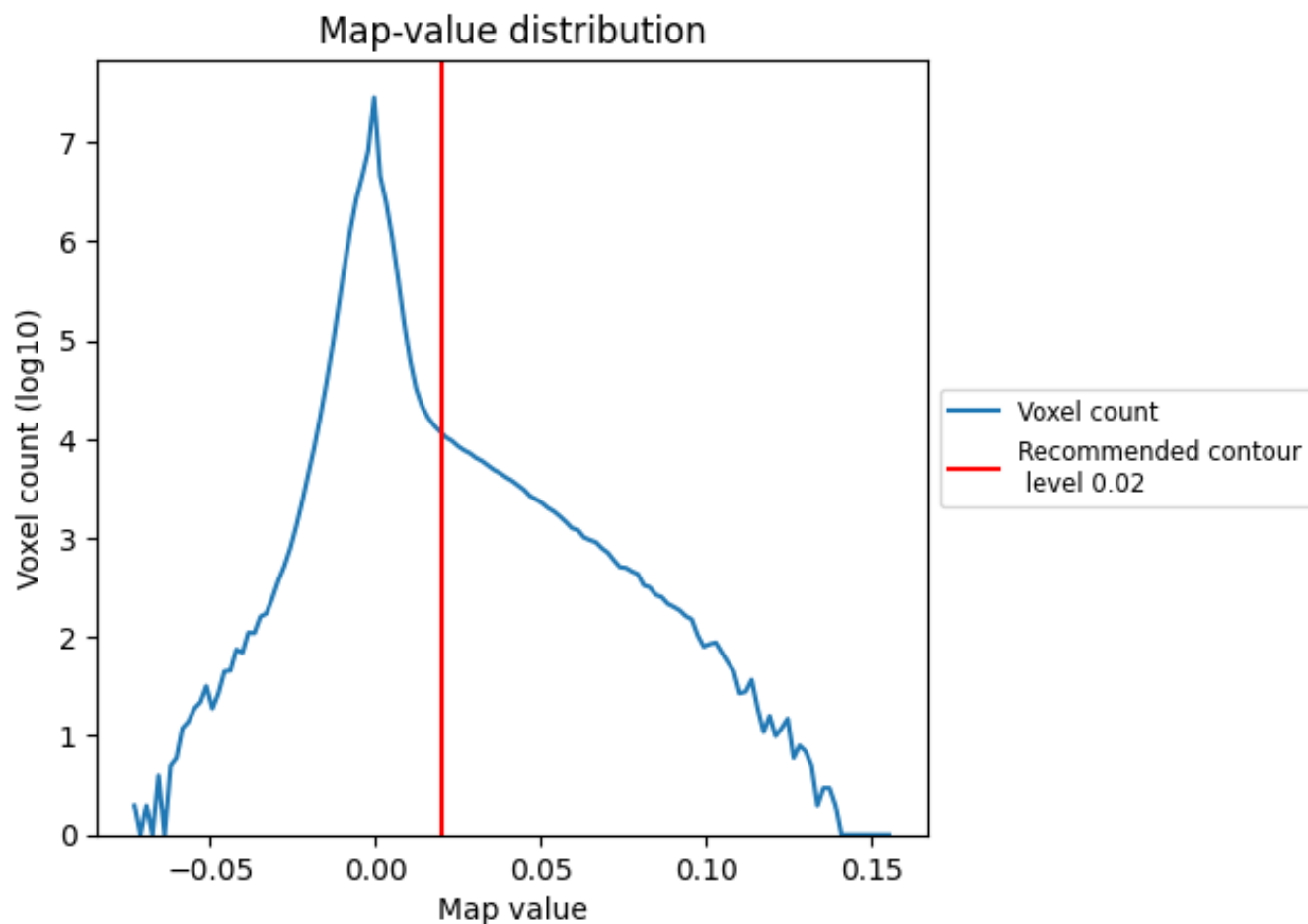
6.6 Mask visualisation

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

7 Map analysis [i](#)

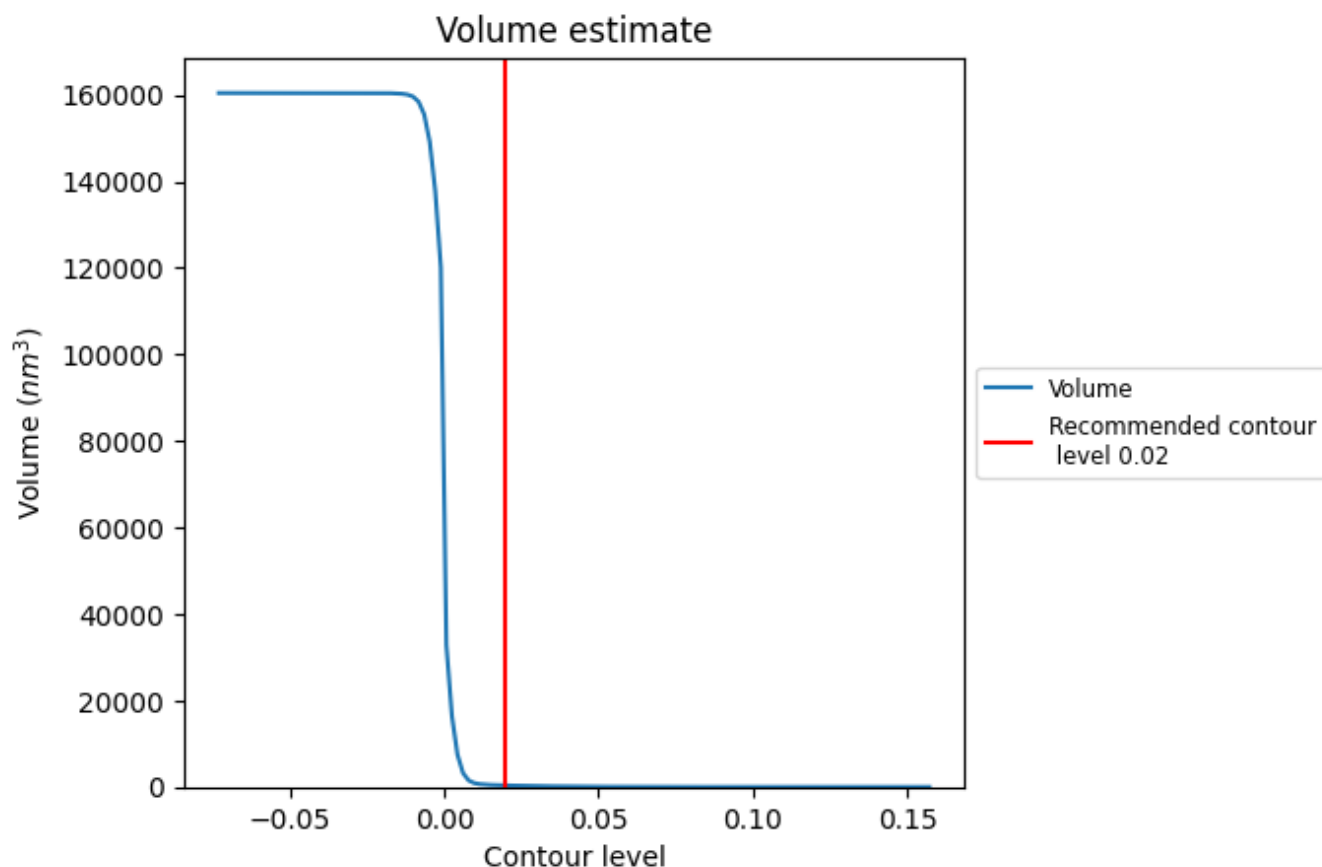
This section contains the results of statistical analysis of the map.

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.

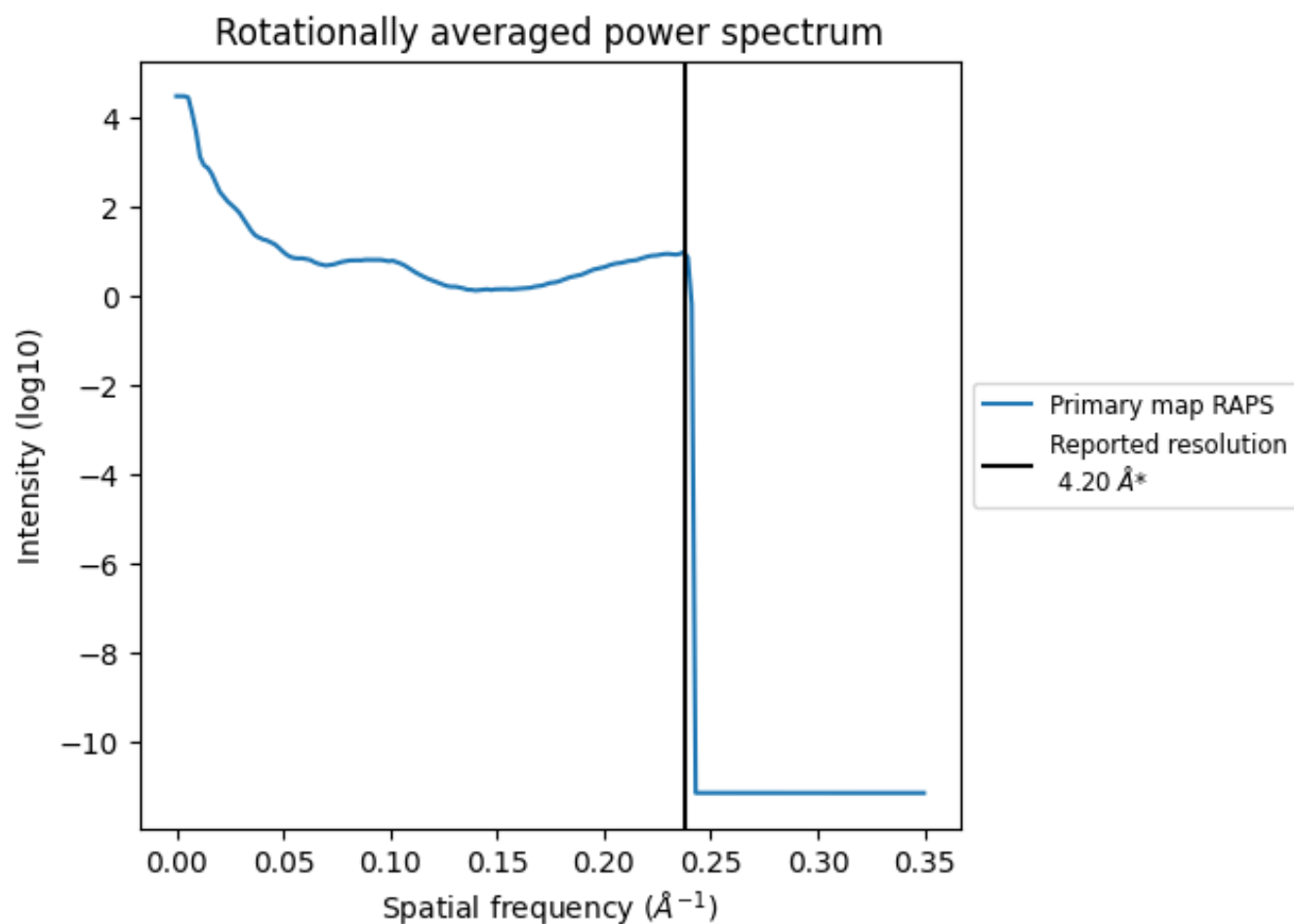
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm³; this corresponds to an approximate mass of 318 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 ⓘ

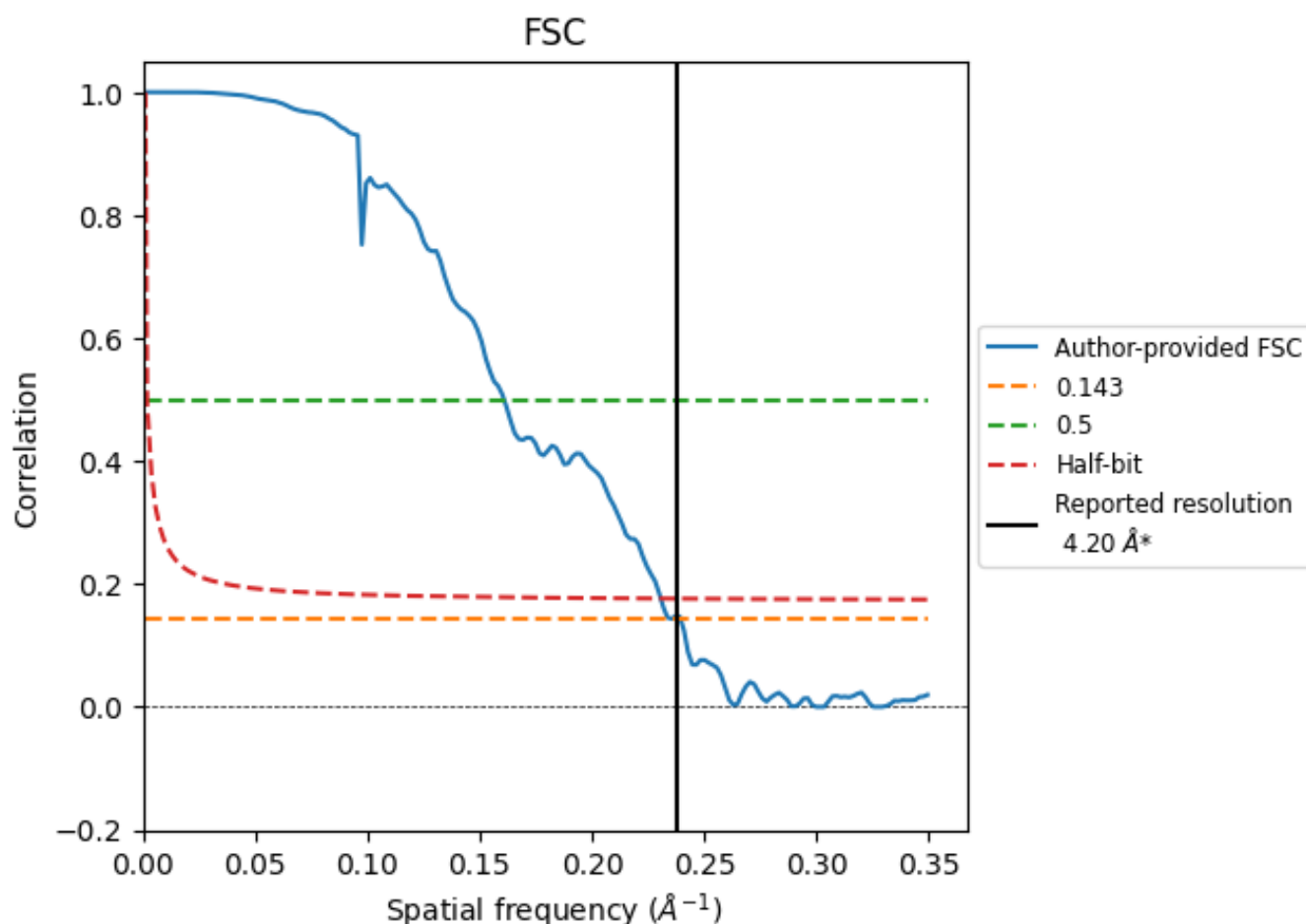


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

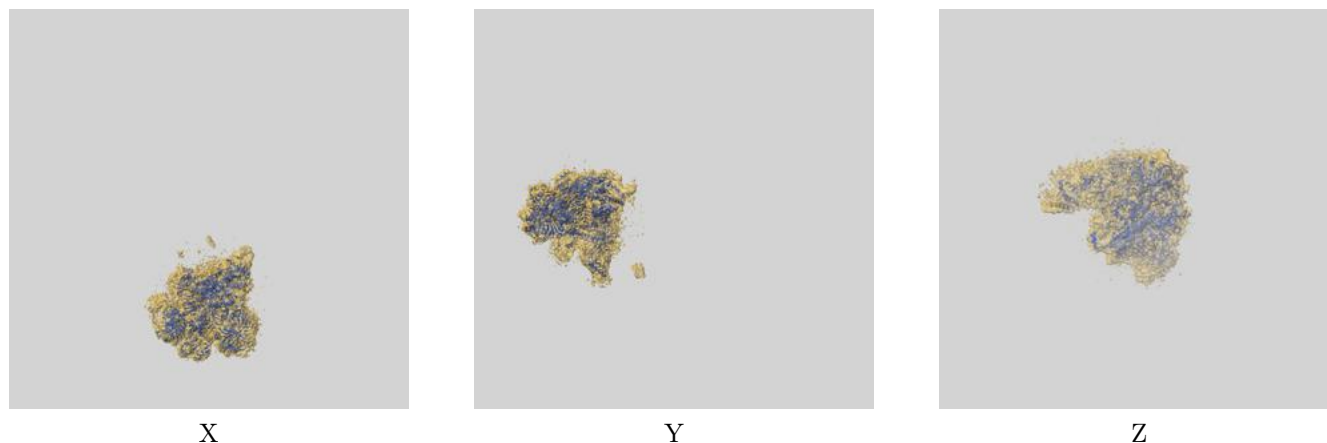
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.22	4.33
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

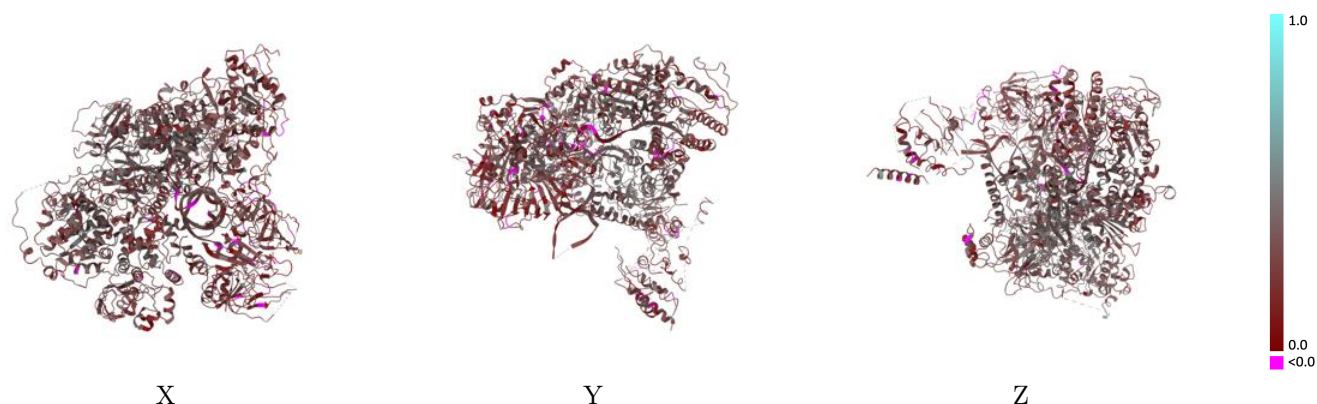
This section contains information regarding the fit between EMDB map EMD-8013 and PDB model 5GAO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



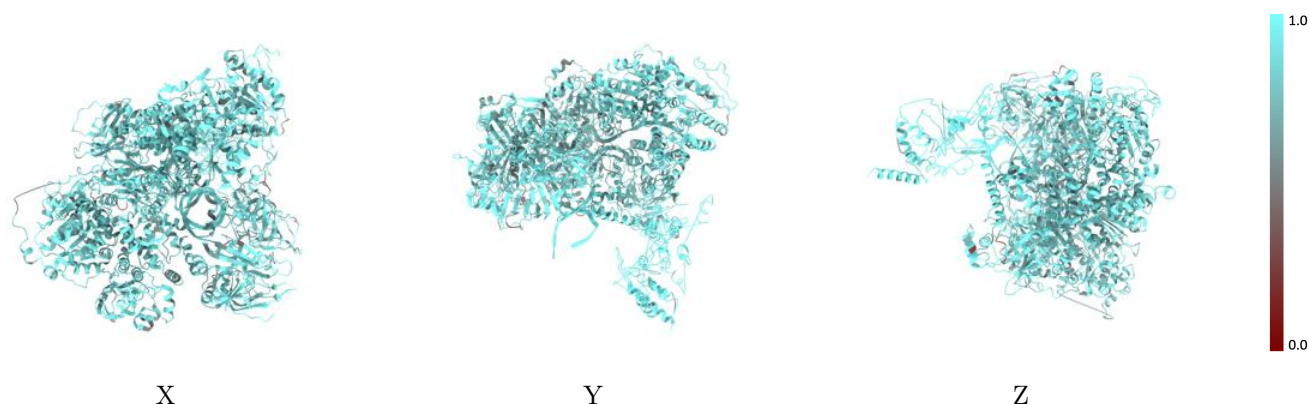
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



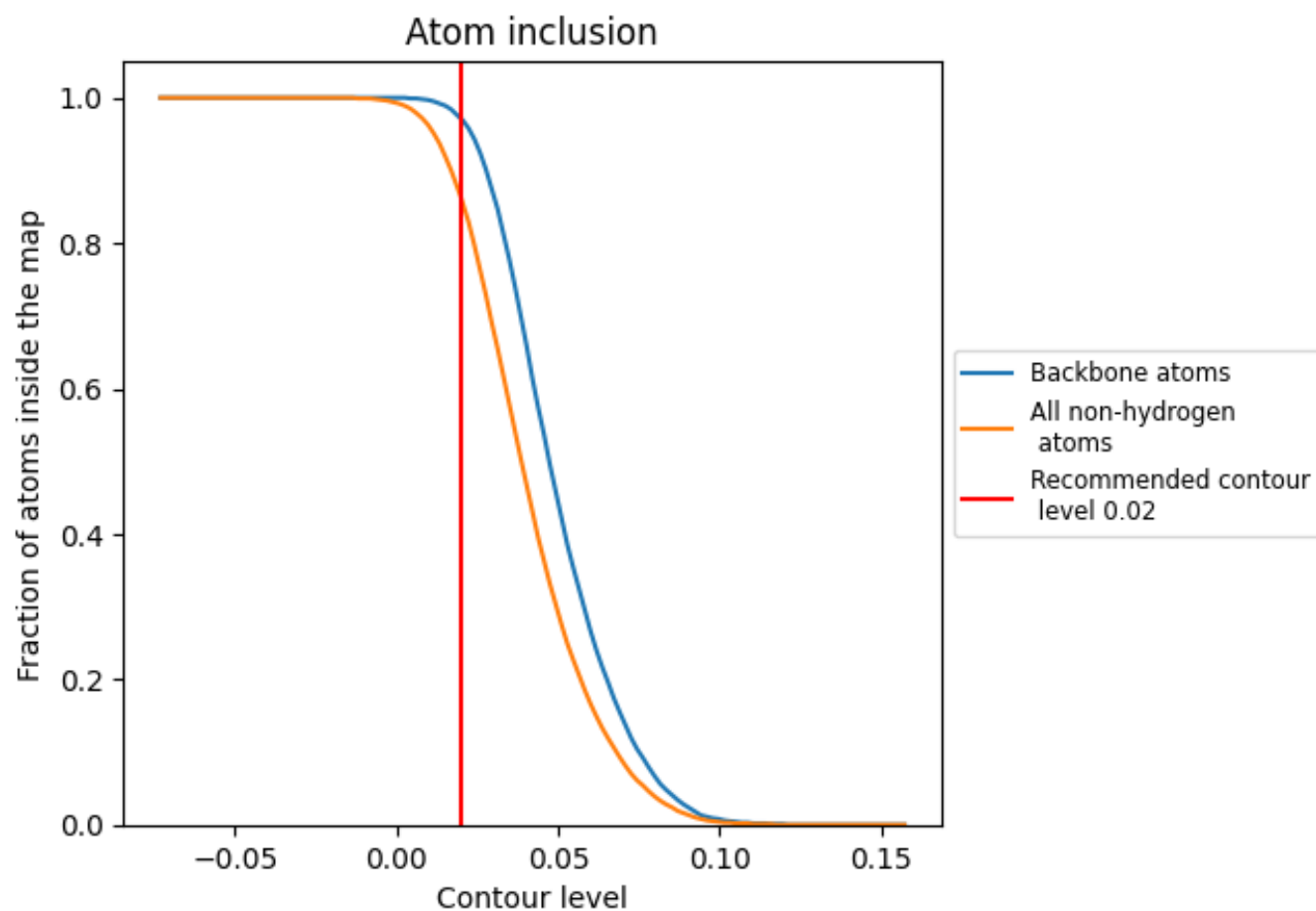
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 86% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.3050
A	0.8800	0.3570
B	0.8630	0.3280
E	0.8810	0.2770
V	0.9240	0.2850
k	0.7790	0.2240
l	0.8110	0.2310
m	0.8350	0.2210
n	0.8240	0.2280
p	0.8560	0.2190
q	0.8680	0.2510
r	0.8420	0.2150

1.0

0.0

<0.0