



Full wwPDB EM Validation Report ⓘ

Sep 22, 2026 – 12:35 PM EDT

PDB ID : 9PC8 / pdb_00009pc8
EMDB ID : EMD-71499
Title : Core Mediator of PIC-Med-SWI/SNF
Authors : Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on : 2025-06-27
Resolution : 3.40 Å(reported)
Based on initial model : 8cen

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:

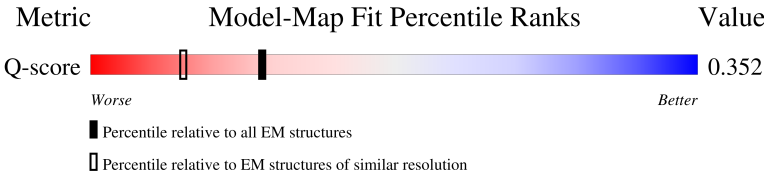
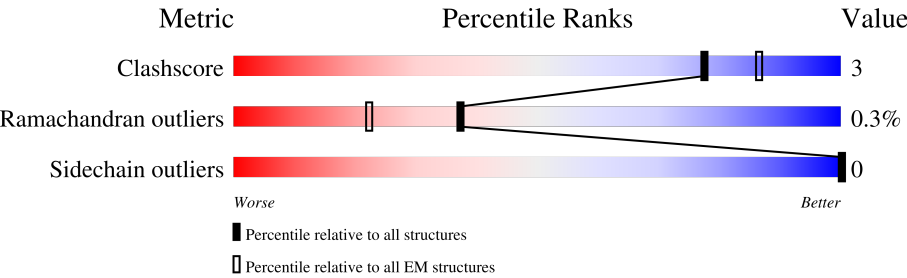
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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.



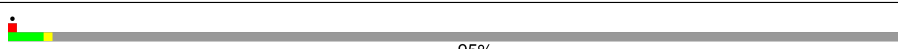
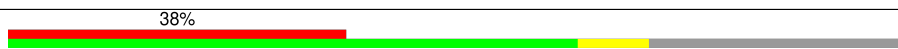
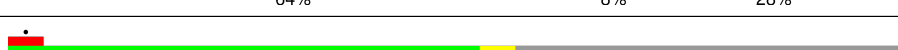
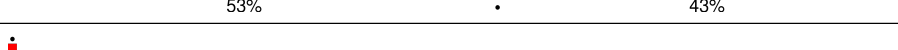
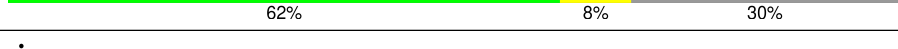
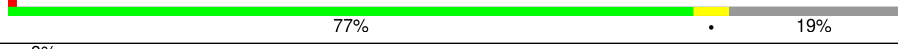
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	f	210	
2	h	284	
3	n	140	
4	o	127	

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Mol	Chain	Length	Quality of chain
5	j	149	
6	d	687	
7	A	1733	
8	p	566	
9	a	295	
10	b	223	
11	c	115	
12	e	307	
13	g	121	
14	i	222	
15	k	157	
16	l	1082	
17	m	220	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 29298 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 Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	h	177	Total	C	N	O	S	0	0
			1441	910	242	284	5		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	n	140	Total	C	N	O	S	0	0
			1124	701	189	228	6		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	o	109	Total	C	N	O	S	0	0
			914	603	141	164	6		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	j	103	Total	C	N	O	S	0	0
			864	539	160	164	1		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	535	Total	C	N	O	S	0	0
			4325	2766	730	816	13		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	A	79	Total	C	N	O	0	0
			575	361	79	135		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	409	Total	C	N	O	S	0	0
			3330	2115	535	669	11		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	157	Total	C	N	O	S	0	0
			1295	822	224	246	3		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	108	Total	C	N	O	S	0	0
			876	546	149	177	4		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	e	248	Total	C	N	O	S	0	0
			1958	1247	325	376	10		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	g	106	Total	C	N	O	S	0	0
			847	528	139	175	5		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	i	185	Total	C	N	O	S	0	0
			1538	989	259	284	6		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	144	Total	C	N	O	S	0	0
			1157	715	204	235	3		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	l	654	Total	C	N	O	S	0	0
			5367	3465	924	954	24		

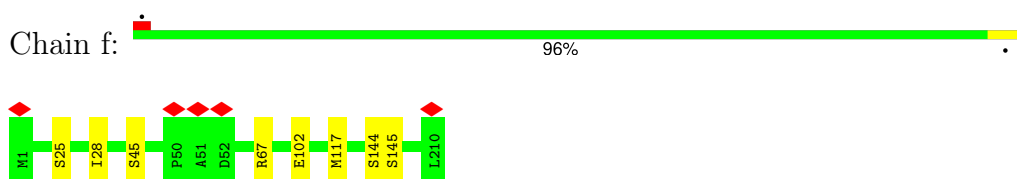
- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	m	83	Total	C	N	O	S	0	0
			671	424	111	135	1		

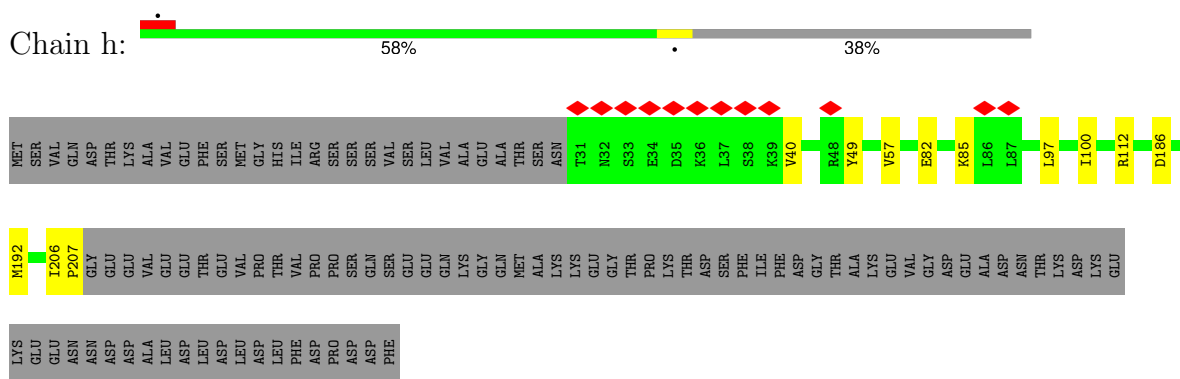
3 Residue-property plots

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.

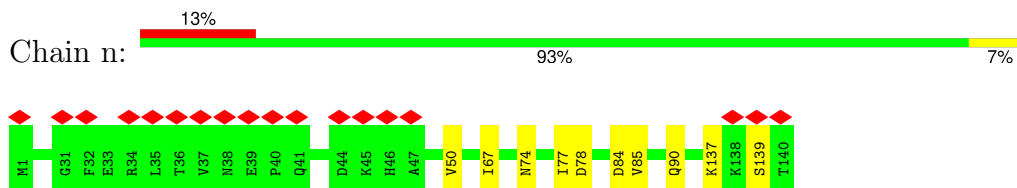
- Molecule 1: Mediator of RNA polymerase II transcription subunit 20



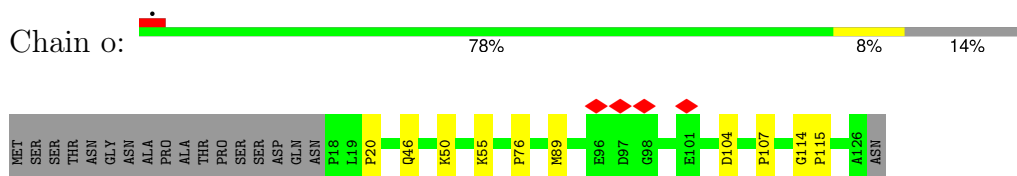
- Molecule 2: Mediator of RNA polymerase II transcription subunit 4



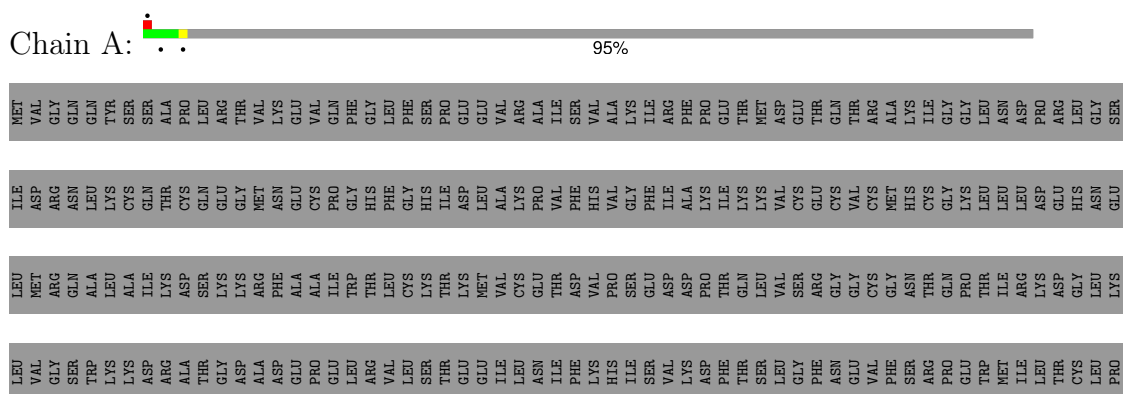
- Molecule 3: Mediator of RNA polymerase II transcription subunit 21



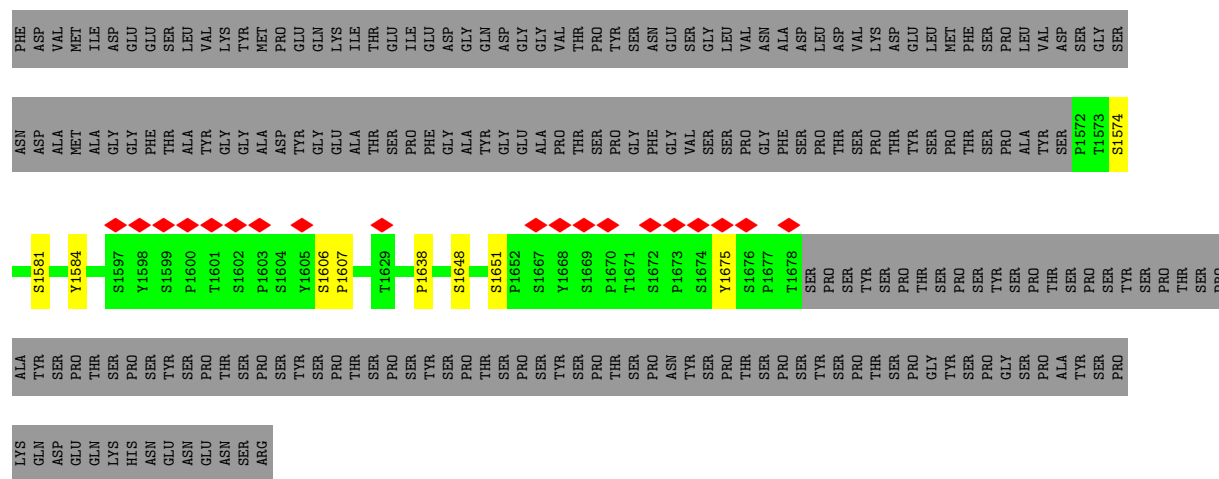
- Molecule 4: Mediator of RNA polymerase II transcription subunit 31

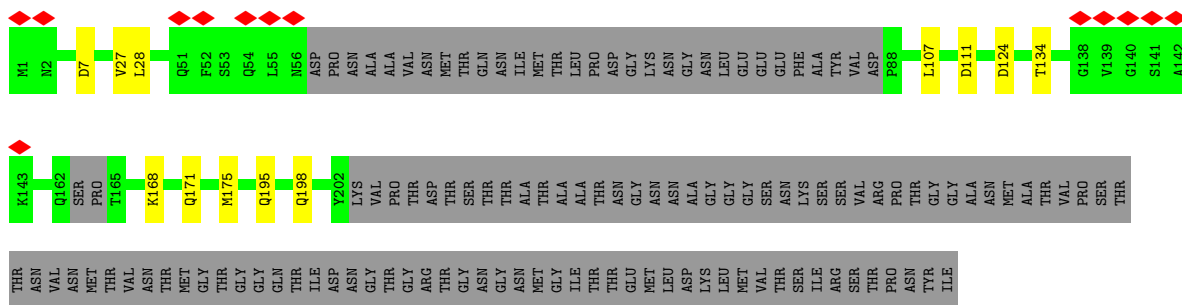


- Molecule 5: Mediator of RNA polymerase II transcription subunit 9

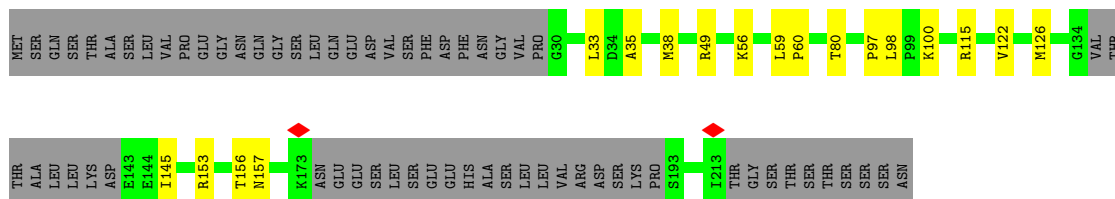




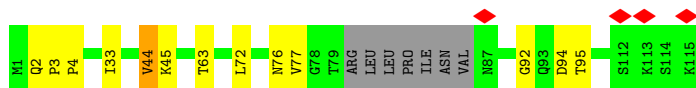
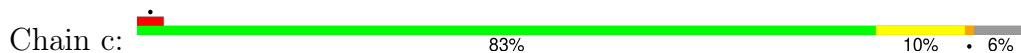




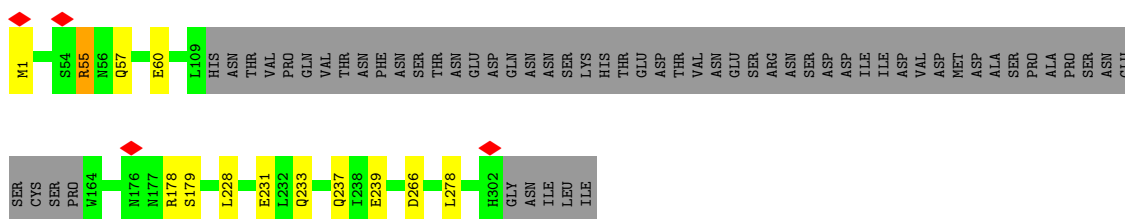
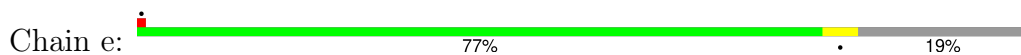
- Molecule 10: Mediator of RNA polymerase II transcription subunit 8



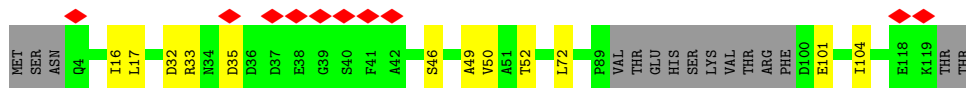
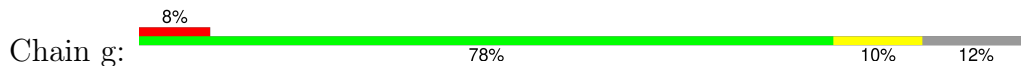
- Molecule 11: Mediator of RNA polymerase II transcription subunit 11



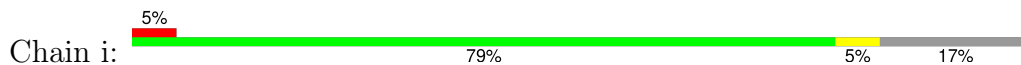
- Molecule 12: Mediator of RNA polymerase II transcription subunit 18

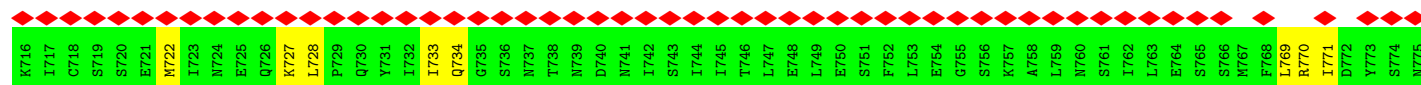


- Molecule 13: Mediator of RNA polymerase II transcription subunit 22



- Molecule 14: Mediator of RNA polymerase II transcription subunit 7





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1482227	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.179	Depositor
Minimum map value	-2.469	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.588	Depositor
Map size ($\text{\AA}$)	537.6, 537.6, 537.6	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	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	f	0.19	0/1635	0.49	0/2215
2	h	0.30	0/1462	0.62	2/1970 (0.1%)
3	n	0.30	0/1135	0.63	0/1526
4	o	0.35	0/941	0.71	3/1282 (0.2%)
5	j	0.37	0/877	0.92	8/1180 (0.7%)
6	d	0.19	0/4389	0.49	3/5901 (0.1%)
7	A	0.23	0/606	0.70	0/848
8	p	0.15	0/3394	0.40	0/4589
9	a	0.19	0/1440	0.46	0/1946
10	b	0.23	0/1320	0.58	3/1785 (0.2%)
11	c	0.42	1/885 (0.1%)	0.80	2/1183 (0.2%)
12	e	0.20	0/1993	0.59	4/2698 (0.1%)
13	g	0.28	0/851	0.65	0/1148
14	i	0.28	0/1569	0.59	0/2117
15	k	0.27	0/1172	0.62	1/1581 (0.1%)
16	l	0.22	0/5460	0.52	0/7373
17	m	0.23	0/684	0.68	3/928 (0.3%)
All	All	0.24	1/29813 (0.0%)	0.57	29/40270 (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
3	n	0	1
6	d	0	1
12	e	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	c	45	LYS	C-N	6.68	1.43	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	55	ARG	CG-CD-NE	13.54	141.78	112.00
10	b	49	ARG	CD-NE-CZ	-9.22	111.49	124.40
11	c	44	VAL	CA-C-N	7.65	132.30	120.97
11	c	44	VAL	C-N-CA	7.65	132.30	120.97
12	e	60	GLU	CA-CB-CG	6.42	126.94	114.10
12	e	55	ARG	CB-CA-C	6.19	122.74	110.42
10	b	49	ARG	CG-CD-NE	6.12	125.47	112.00
4	o	107	PRO	CA-N-CD	-5.91	103.73	112.00
5	j	106	SER	CA-C-N	-5.76	111.34	122.06
5	j	106	SER	C-N-CA	-5.76	111.34	122.06
4	o	104	ASP	N-CA-C	-5.66	107.37	114.56
10	b	49	ARG	N-CA-C	5.63	118.14	111.33
4	o	114	GLY	N-CA-C	5.57	123.70	112.34
5	j	107	GLU	N-CA-CB	5.56	119.19	110.46
15	k	87	ILE	CG1-CB-CG2	-5.46	94.34	110.70
5	j	87	LEU	CA-C-N	5.42	127.86	120.54
5	j	87	LEU	C-N-CA	5.42	127.86	120.54
17	m	34	LEU	CA-C-N	5.30	131.50	121.97
17	m	34	LEU	C-N-CA	5.30	131.50	121.97
2	h	112	ARG	CA-C-N	5.24	131.55	121.54
2	h	112	ARG	C-N-CA	5.24	131.55	121.54
6	d	255	ASN	CA-C-N	5.22	131.52	121.54
6	d	255	ASN	C-N-CA	5.22	131.52	121.54
12	e	57	GLN	CA-CB-CG	5.11	124.32	114.10
17	m	61	ARG	CA-CB-CG	5.10	124.31	114.10
5	j	88	GLU	CA-CB-CG	5.07	124.24	114.10
5	j	107	GLU	CA-C-N	-5.06	114.18	122.79
5	j	107	GLU	C-N-CA	-5.06	114.18	122.79
6	d	255	ASN	N-CA-C	5.00	119.62	111.37

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	d	206	ASP	Peptide
12	e	55	ARG	Peptide,Sidechain
3	n	50	VAL	Peptide

5.2 Too-close contacts ⓘ

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	f	1609	0	1626	5	0
2	h	1441	0	1461	7	0
3	n	1124	0	1147	7	0
4	o	914	0	902	5	0
5	j	864	0	870	9	0
6	d	4325	0	4482	22	0
7	A	575	0	507	5	0
8	p	3330	0	3243	26	0
9	a	1407	0	1385	8	0
10	b	1295	0	1297	12	0
11	c	876	0	885	7	0
12	e	1958	0	1976	6	0
13	g	847	0	858	10	0
14	i	1538	0	1576	8	0
15	k	1157	0	1142	13	0
16	l	5367	0	5607	46	0
17	m	671	0	650	2	0
All	All	29298	0	29614	168	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 3.

All (168) 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)
16:l:89:GLN:HE21	16:l:159:PHE:H	1.39	0.69
11:c:63:THR:HG21	13:g:17:LEU:HD12	1.78	0.66
15:k:122:ARG:HH21	15:k:123:ASP:HB3	1.61	0.65
8:p:167:TYR:O	8:p:171:LEU:HB2	1.99	0.62
15:k:122:ARG:HH11	15:k:147:THR:HG21	1.65	0.61
3:n:74:ASN:HA	3:n:77:ILE:HD12	1.84	0.60
16:l:253:VAL:HG21	16:l:276:ILE:HG21	1.84	0.60
8:p:531:ILE:HB	8:p:538:ILE:HB	1.85	0.59
5:j:145:ARG:O	5:j:149:ARG:NH1	2.36	0.59
14:i:186:ARG:O	14:i:190:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:78:ASP:OD1	14:i:120:ARG:NH2	2.35	0.58
13:g:16:ILE:HG21	13:g:72:LEU:HD11	1.86	0.57
8:p:351:VAL:HA	8:p:558:ILE:HD11	1.86	0.57
16:l:184:LYS:O	16:l:188:ASN:ND2	2.37	0.57
6:d:316:ILE:O	11:c:2:GLN:NE2	2.33	0.57
11:c:33:ILE:HG23	11:c:44:VAL:HG12	1.87	0.56
11:c:72:LEU:O	11:c:76:ASN:ND2	2.38	0.56
16:l:490:GLN:HG2	16:l:502:GLN:HE21	1.70	0.56
15:k:12:GLN:OE1	16:l:152:ARG:NH2	2.39	0.56
1:f:102:GLU:OE2	12:e:1:MET:N	2.38	0.55
8:p:261:ASN:ND2	8:p:325:ILE:O	2.39	0.55
2:h:192:MET:HE3	4:o:20:PRO:HB3	1.88	0.55
16:l:629:LEU:HD11	16:l:692:GLN:HG3	1.89	0.55
16:l:161:VAL:O	16:l:165:LEU:HB2	2.07	0.55
10:b:156:THR:HG21	13:g:32:ASP:HA	1.89	0.54
6:d:120:ASN:HB2	6:d:123:GLU:HG2	1.89	0.54
6:d:503:LEU:HB3	6:d:507:MET:HE1	1.89	0.54
16:l:803:VAL:HG12	16:l:806:GLU:H	1.72	0.54
15:k:60:LEU:HD23	16:l:104:MET:HE2	1.90	0.53
16:l:461:VAL:HG13	16:l:463:ASN:H	1.73	0.53
14:i:11:SER:OG	14:i:12:LEU:N	2.41	0.53
16:l:438:LEU:HG	16:l:460:ILE:HG13	1.91	0.53
13:g:46:SER:HB2	13:g:49:ALA:HB3	1.89	0.53
8:p:297:PRO:HG2	8:p:300:ILE:HD12	1.90	0.53
16:l:414:ARG:NH1	16:l:415:TYR:O	2.43	0.52
2:h:57:VAL:HG23	5:j:87:LEU:HD23	1.92	0.52
6:d:614:ARG:NH1	6:d:636:GLU:OE2	2.43	0.52
3:n:139:SER:HA	16:l:267:ASN:HD21	1.75	0.52
9:a:168:LYS:HA	9:a:171:GLN:HG2	1.93	0.51
6:d:355:ALA:HA	6:d:370:PRO:HA	1.93	0.51
12:e:178:ARG:HE	12:e:179:SER:H	1.57	0.51
8:p:298:PRO:HA	8:p:301:ASP:HB2	1.92	0.51
16:l:505:THR:HA	16:l:560:LYS:HE2	1.93	0.51
6:d:270:ILE:HD11	10:b:145:ILE:HB	1.93	0.51
6:d:446:LYS:NZ	6:d:462:GLU:O	2.42	0.51
16:l:252:THR:HG21	16:l:290:THR:HG21	1.93	0.51
16:l:115:VAL:HA	17:m:141:VAL:HG11	1.93	0.50
6:d:539:ILE:O	6:d:543:ARG:NH2	2.44	0.50
12:e:237:GLN:NE2	12:e:239:GLU:OE2	2.45	0.50
15:k:64:ASN:OD1	15:k:68:ASN:ND2	2.45	0.50
8:p:62:VAL:HB	8:p:80:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:l:158:ASN:ND2	17:m:38:TYR:O	2.45	0.49
6:d:228:LEU:HD22	10:b:33:LEU:HD13	1.94	0.49
6:d:424:ASP:O	6:d:428:GLN:NE2	2.41	0.49
16:l:508:VAL:HG22	16:l:681:GLU:HB2	1.93	0.49
6:d:397:ILE:HD11	6:d:404:ILE:HG23	1.93	0.49
5:j:148:GLN:HG3	14:i:207:GLN:HG3	1.94	0.49
16:l:480:ARG:NH1	16:l:496:SER:O	2.45	0.49
16:l:263:PRO:HD2	16:l:266:LEU:HD12	1.93	0.49
6:d:253:SER:HA	10:b:98:LEU:HD12	1.95	0.49
16:l:641:SER:HB2	16:l:652:GLU:HB2	1.95	0.48
6:d:254:LEU:HD23	10:b:97:PRO:HA	1.95	0.48
7:A:1581:SER:HB2	10:b:115:ARG:HH22	1.78	0.48
11:c:94:ASP:N	11:c:94:ASP:OD1	2.46	0.48
15:k:32:LEU:HD12	15:k:52:ASN:HB3	1.95	0.48
3:n:84:ASP:N	3:n:84:ASP:OD1	2.44	0.48
15:k:21:GLN:OE1	15:k:66:ARG:NH2	2.39	0.48
7:A:1648:SER:HB2	7:A:1651:SER:HB3	1.96	0.48
8:p:78:LYS:NZ	8:p:79:LEU:O	2.44	0.48
6:d:86:LEU:HD13	16:l:209:LEU:HD21	1.94	0.48
8:p:53:ARG:NH1	8:p:66:ASP:OD1	2.47	0.48
6:d:650:SER:HA	6:d:658:VAL:HA	1.95	0.47
16:l:734:GLN:O	16:l:770:ARG:NH1	2.44	0.47
16:l:722:MET:HE2	16:l:727:LYS:HB3	1.96	0.47
8:p:53:ARG:HH12	8:p:64:ASP:HB3	1.79	0.47
8:p:549:ASP:OD1	8:p:554:TRP:NE1	2.46	0.47
14:i:128:LEU:HD21	15:k:136:LEU:HD13	1.96	0.47
16:l:246:LEU:HD21	16:l:274:GLY:H	1.79	0.47
16:l:413:VAL:HB	16:l:427:ILE:HB	1.95	0.47
8:p:105:LEU:O	8:p:109:THR:OG1	2.32	0.46
16:l:273:ASN:O	16:l:275:ARG:NH1	2.48	0.46
16:l:140:GLN:HA	16:l:143:LYS:HD2	1.98	0.46
5:j:90:LEU:H	5:j:90:LEU:HG	1.50	0.46
16:l:92:LEU:HD21	16:l:148:VAL:HG22	1.98	0.46
16:l:113:THR:O	16:l:117:THR:OG1	2.30	0.46
4:o:46:GLN:O	4:o:50:LYS:HB3	2.14	0.46
10:b:153:ARG:O	10:b:157:ASN:ND2	2.48	0.46
13:g:35:ASP:OD1	13:g:35:ASP:N	2.48	0.46
8:p:273:PHE:HB3	8:p:278:ILE:HD12	1.97	0.46
7:A:1675:TYR:HD2	16:l:170:ARG:HD2	1.81	0.46
8:p:45:GLU:HB3	8:p:53:ARG:HB2	1.98	0.46
11:c:92:GLY:O	11:c:95:THR:OG1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:76:PRO:HB2	16:l:212:PRO:HG3	1.98	0.46
6:d:403:TYR:HE2	6:d:473:LYS:HE3	1.80	0.46
9:a:195:GLN:OE1	9:a:198:GLN:NE2	2.41	0.45
8:p:61:ILE:HD12	8:p:128:ASP:HB2	1.99	0.45
16:l:771:ILE:HG23	16:l:778:ILE:HG22	1.99	0.45
12:e:231:GLU:OE1	12:e:233:GLN:NE2	2.47	0.45
16:l:354:GLU:OE1	16:l:358:LYS:NZ	2.48	0.45
10:b:80:THR:HG21	13:g:52:THR:HG21	1.99	0.44
8:p:74:ILE:HG22	8:p:108:LEU:HD22	1.99	0.44
15:k:19:GLN:HA	15:k:22:VAL:HG12	2.00	0.44
3:n:67:ILE:HG13	15:k:128:LYS:HG3	2.00	0.44
8:p:339:SER:HA	8:p:342:LEU:HD12	1.99	0.44
16:l:89:GLN:HB3	16:l:90:VAL:H	1.67	0.44
6:d:23:PRO:HB2	6:d:86:LEU:HD11	1.99	0.44
14:i:161:LEU:HD12	14:i:161:LEU:HA	1.84	0.44
16:l:564:VAL:HG12	16:l:568:MET:HE2	2.00	0.44
1:f:144:SER:OG	1:f:145:SER:N	2.51	0.44
2:h:97:LEU:HA	2:h:100:ILE:HG22	2.00	0.44
8:p:276:ASP:HB2	8:p:320:THR:HG22	1.99	0.44
16:l:728:LEU:HB2	16:l:733:ILE:HD11	1.99	0.44
2:h:186:ASP:N	2:h:186:ASP:OD1	2.50	0.43
2:h:206:ILE:HD12	2:h:207:PRO:HD2	2.00	0.43
5:j:67:PRO:HA	5:j:70:PHE:HB3	1.98	0.43
5:j:108:ASN:OD1	5:j:112:LYS:NZ	2.51	0.43
12:e:266:ASP:OD1	12:e:266:ASP:N	2.49	0.43
16:l:428:THR:OG1	16:l:443:ASP:OD2	2.28	0.43
16:l:423:SER:HG	16:l:444:ASN:HD21	1.62	0.43
8:p:45:GLU:O	8:p:53:ARG:N	2.44	0.43
8:p:134:GLU:H	8:p:161:LYS:HG3	1.84	0.43
10:b:100:LYS:HE2	10:b:100:LYS:HB3	1.81	0.43
8:p:76:ASP:OD1	8:p:76:ASP:N	2.51	0.43
2:h:82:GLU:HA	2:h:85:LYS:HE2	2.00	0.43
3:n:137:LYS:HA	5:j:136:LYS:HE3	2.01	0.43
9:a:124:ASP:OD1	9:a:124:ASP:N	2.51	0.43
15:k:22:VAL:HA	15:k:25:ILE:HG12	2.00	0.43
16:l:161:VAL:O	16:l:165:LEU:CB	2.67	0.43
6:d:276:ASN:HD22	13:g:50:VAL:HG22	1.83	0.43
1:f:25:SER:HA	1:f:28:ILE:HD12	1.99	0.42
8:p:101:SER:OG	8:p:106:ASN:ND2	2.51	0.42
16:l:220:LYS:HE2	16:l:220:LYS:HB2	1.89	0.42
2:h:49:TYR:HD2	5:j:98:LEU:HD21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:35:ALA:HA	10:b:38:MET:HE3	2.01	0.42
11:c:3:PRO:HA	11:c:4:PRO:HD3	1.92	0.42
16:l:424:LYS:O	16:l:444:ASN:ND2	2.49	0.42
8:p:23:PRO:HG2	8:p:115:LYS:HA	2.02	0.42
8:p:95:ASP:OD1	8:p:189:ARG:NH1	2.52	0.42
9:a:107:LEU:HD23	9:a:107:LEU:HA	1.95	0.42
14:i:175:ILE:O	14:i:179:GLU:HG3	2.20	0.42
16:l:769:LEU:HB3	16:l:780:LEU:HD12	2.02	0.42
16:l:708:LEU:HB3	16:l:713:ILE:HB	2.02	0.41
10:b:122:VAL:HG12	10:b:126:MET:HE2	2.02	0.41
9:a:27:VAL:HG13	9:a:28:LEU:HD12	2.01	0.41
6:d:276:ASN:OD1	13:g:33:ARG:NH2	2.54	0.41
9:a:111:ASP:HB3	9:a:134:THR:HA	2.02	0.41
9:a:171:GLN:O	9:a:175:MET:HG2	2.21	0.41
16:l:195:LEU:HD12	16:l:195:LEU:HA	1.90	0.41
14:i:175:ILE:HD12	14:i:175:ILE:HA	1.96	0.41
4:o:115:PRO:HB3	7:A:1638:PRO:HG3	2.02	0.41
6:d:257:ASP:OD1	6:d:258:LYS:N	2.51	0.41
10:b:59:LEU:HA	10:b:60:PRO:HD3	1.88	0.41
6:d:232:VAL:HG12	6:d:233:LYS:HG3	2.02	0.41
13:g:101:GLU:HA	13:g:104:ILE:HD12	2.03	0.41
1:f:45:SER:HB2	1:f:117:MET:HE1	2.03	0.41
12:e:228:LEU:HD21	12:e:278:LEU:HD12	2.03	0.41
4:o:55:LYS:HE2	4:o:89:MET:SD	2.61	0.40
15:k:123:ASP:OD1	15:k:124:SER:N	2.53	0.40
5:j:87:LEU:HG	5:j:91:THR:HG23	2.03	0.40
1:f:67:ARG:HA	1:f:67:ARG:HD3	1.95	0.40
6:d:396:LYS:HG2	6:d:403:TYR:CE1	2.57	0.40
7:A:1606:SER:HA	7:A:1607:PRO:HD3	1.88	0.40
8:p:190:THR:HG22	8:p:198:ILE:HG23	2.03	0.40
15:k:64:ASN:OD1	16:l:97:ARG:NH1	2.54	0.40
9:a:7:ASP:OD1	9:a:7:ASP:N	2.55	0.40
13:g:49:ALA:HA	13:g:52:THR:HG22	2.02	0.40
3:n:85:VAL:HG11	3:n:90:GLN:HE21	1.86	0.40
8:p:113:ASP:OD1	8:p:113:ASP:N	2.52	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	f	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
2	h	175/284 (62%)	164 (94%)	10 (6%)	1 (1%)	21	50
3	n	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
4	o	107/127 (84%)	101 (94%)	6 (6%)	0	100	100
5	j	99/149 (66%)	91 (92%)	7 (7%)	1 (1%)	12	40
6	d	525/687 (76%)	511 (97%)	13 (2%)	1 (0%)	43	71
7	A	73/1733 (4%)	64 (88%)	7 (10%)	2 (3%)	4	20
8	p	405/566 (72%)	385 (95%)	20 (5%)	0	100	100
9	a	163/295 (55%)	153 (94%)	10 (6%)	0	100	100
10	b	151/223 (68%)	145 (96%)	5 (3%)	1 (1%)	18	47
11	c	104/115 (90%)	99 (95%)	4 (4%)	1 (1%)	12	40
12	e	244/307 (80%)	234 (96%)	10 (4%)	0	100	100
13	g	102/121 (84%)	89 (87%)	13 (13%)	0	100	100
14	i	179/222 (81%)	175 (98%)	4 (2%)	0	100	100
15	k	140/157 (89%)	139 (99%)	1 (1%)	0	100	100
16	l	640/1082 (59%)	607 (95%)	32 (5%)	1 (0%)	43	71
17	m	79/220 (36%)	69 (87%)	8 (10%)	2 (2%)	4	21
All	All	3532/6638 (53%)	3348 (95%)	174 (5%)	10 (0%)	37	65

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	h	40	VAL
10	b	56	LYS
11	c	77	VAL
5	j	64	GLU
6	d	256	SER

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Mol	Chain	Res	Type
16	l	646	LYS
7	A	1574	SER
7	A	1584	TYR
17	m	19	PRO
17	m	35	ILE

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	f	178/178 (100%)	178 (100%)	0	100	100
2	h	164/258 (64%)	164 (100%)	0	100	100
3	n	132/132 (100%)	132 (100%)	0	100	100
4	o	102/117 (87%)	102 (100%)	0	100	100
5	j	101/144 (70%)	101 (100%)	0	100	100
6	d	499/642 (78%)	499 (100%)	0	100	100
7	A	79/1520 (5%)	79 (100%)	0	100	100
8	p	390/528 (74%)	390 (100%)	0	100	100
9	a	158/259 (61%)	158 (100%)	0	100	100
10	b	148/207 (72%)	148 (100%)	0	100	100
11	c	101/108 (94%)	101 (100%)	0	100	100
12	e	224/280 (80%)	224 (100%)	0	100	100
13	g	98/113 (87%)	98 (100%)	0	100	100
14	i	175/208 (84%)	175 (100%)	0	100	100
15	k	132/145 (91%)	132 (100%)	0	100	100
16	l	618/1001 (62%)	618 (100%)	0	100	100
17	m	77/195 (40%)	77 (100%)	0	100	100
All	All	3376/6035 (56%)	3376 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	75	ASN
1	f	94	ASN
1	f	141	ASN
2	h	119	ASN
3	n	7	GLN
3	n	29	ASN
5	j	13	GLN
5	j	68	HIS
5	j	123	GLN
6	d	120	ASN
6	d	296	ASN
6	d	310	ASN
6	d	350	HIS
8	p	106	ASN
8	p	118	HIS
8	p	332	ASN
8	p	536	HIS
9	a	10	GLN
9	a	56	ASN
9	a	159	ASN
9	a	201	HIS
10	b	106	HIS
10	b	157	ASN
11	c	51	HIS
11	c	54	GLN
11	c	76	ASN
11	c	93	GLN
11	c	101	GLN
12	e	3	GLN
12	e	4	GLN
12	e	51	ASN
12	e	57	GLN
12	e	258	ASN
12	e	294	GLN
13	g	61	GLN
13	g	68	ASN
13	g	103	GLN
14	i	160	HIS
14	i	181	GLN
15	k	68	ASN
15	k	109	GLN

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Mol	Chain	Res	Type
16	1	89	GLN
16	1	160	HIS
16	1	178	ASN
16	1	188	ASN
16	1	192	ASN
16	1	402	HIS
16	1	502	GLN
16	1	523	GLN
16	1	631	HIS
16	1	787	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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
7	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1652:PRO	C	1667:SER	N	32.61
1	A	1614:PRO	C	1629:THR	N	25.71

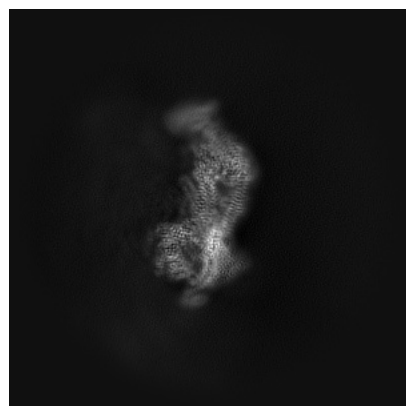
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71499. These allow visual inspection of the internal detail of the map and identification of artifacts.

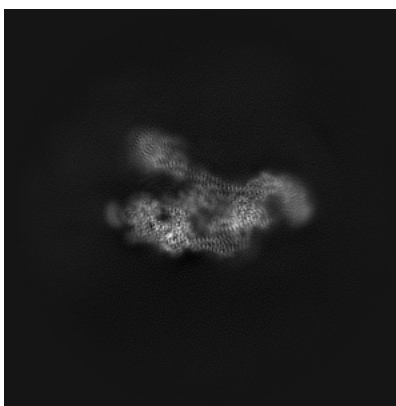
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

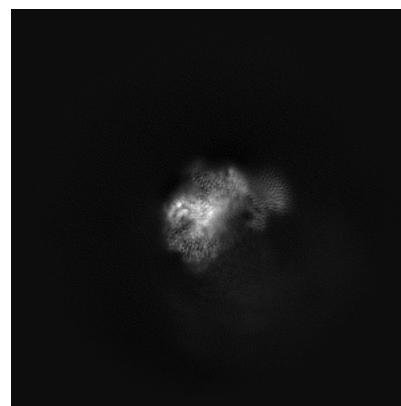
6.1.1 Primary map



X

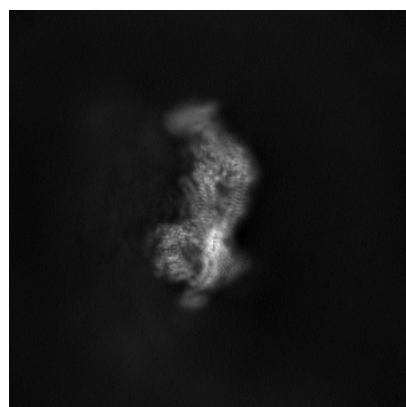


Y

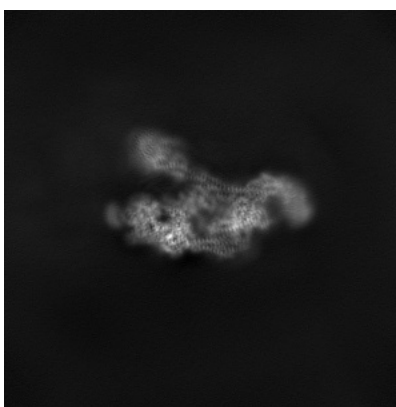


Z

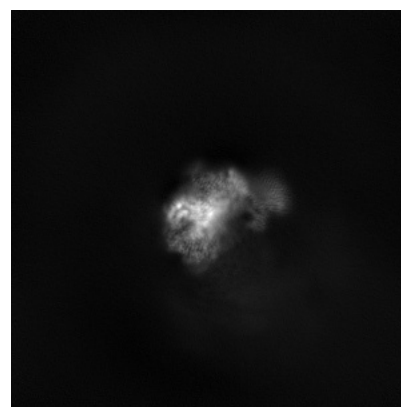
6.1.2 Raw map



X



Y

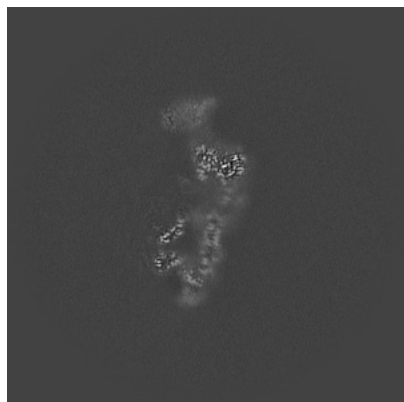


Z

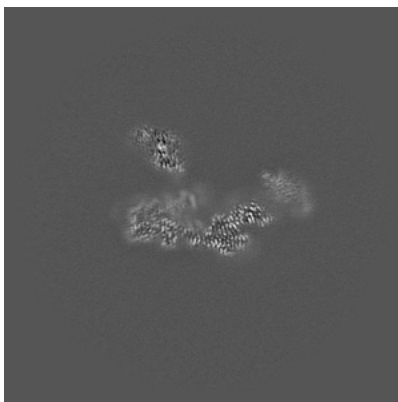
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192

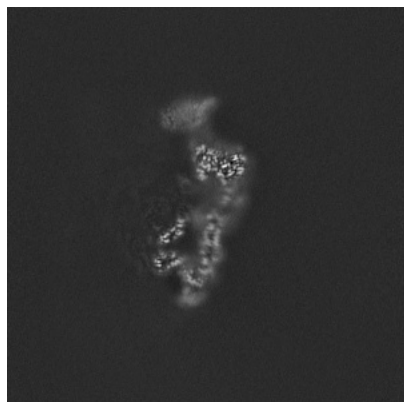


Y Index: 192

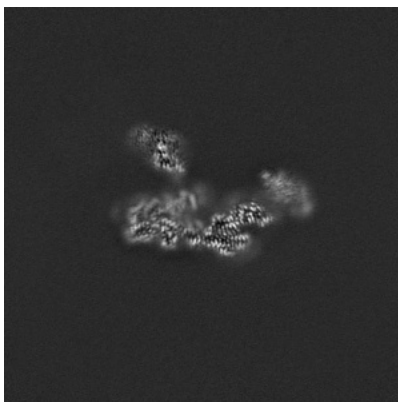


Z Index: 192

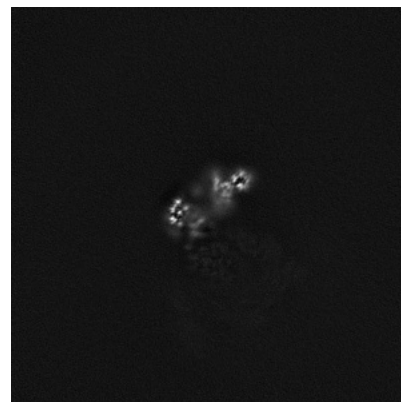
6.2.2 Raw map



X Index: 192



Y Index: 192

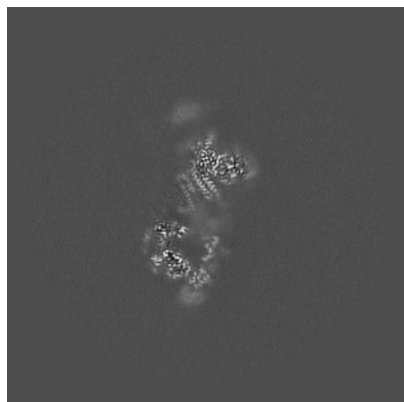


Z Index: 192

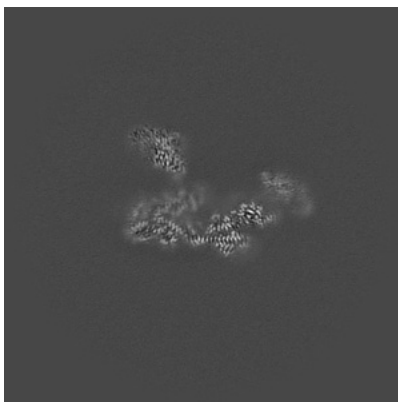
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

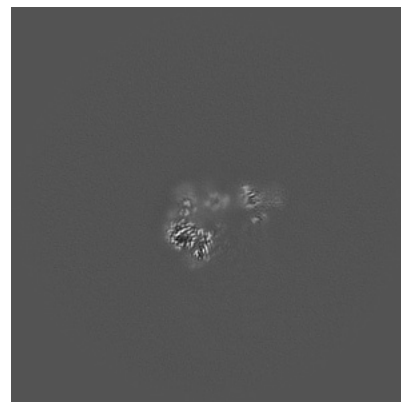
6.3.1 Primary map



X Index: 180

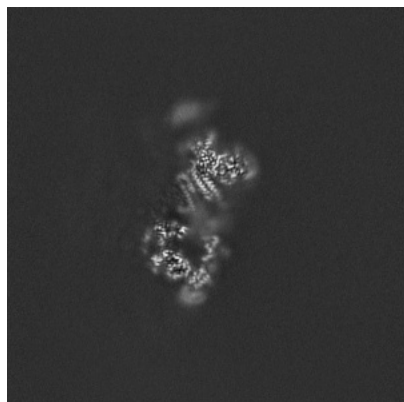


Y Index: 194

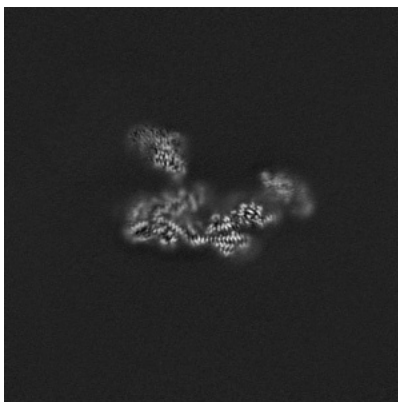


Z Index: 169

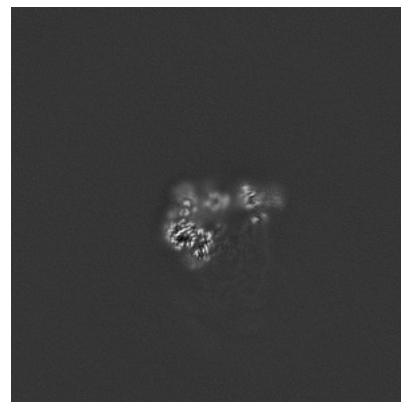
6.3.2 Raw map



X Index: 180



Y Index: 194

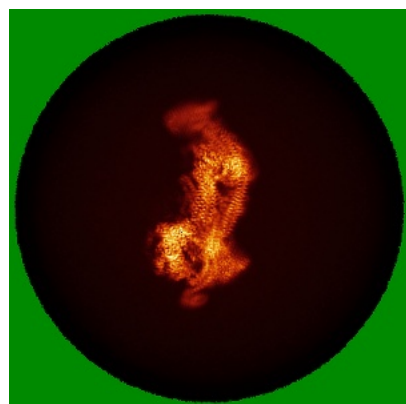


Z Index: 169

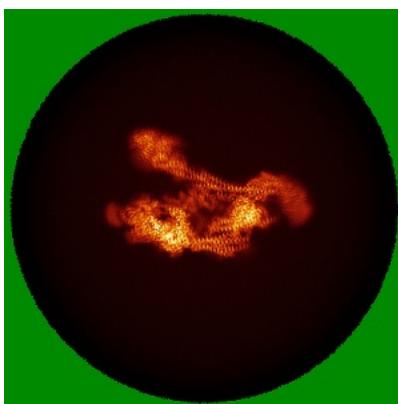
The images above show the largest variance slices of the map in three orthogonal directions.

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

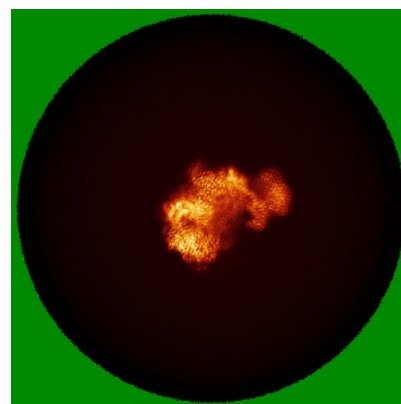
6.4.1 Primary map



X

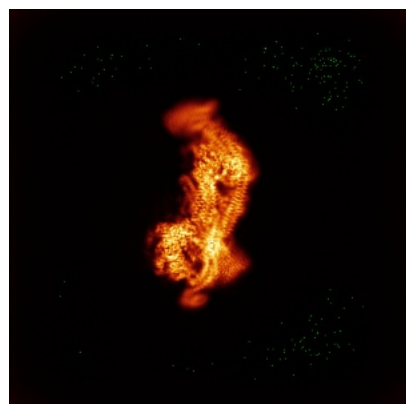


Y

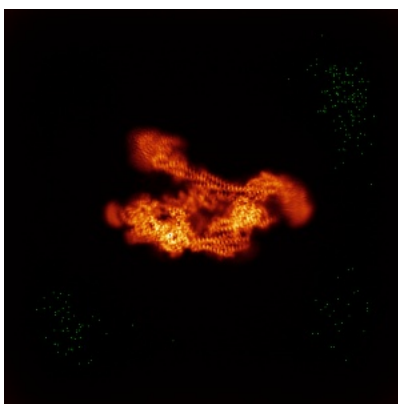


Z

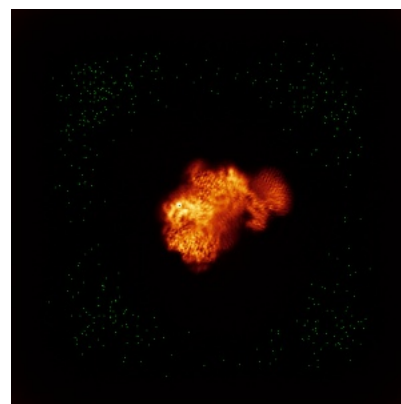
6.4.2 Raw map



X



Y

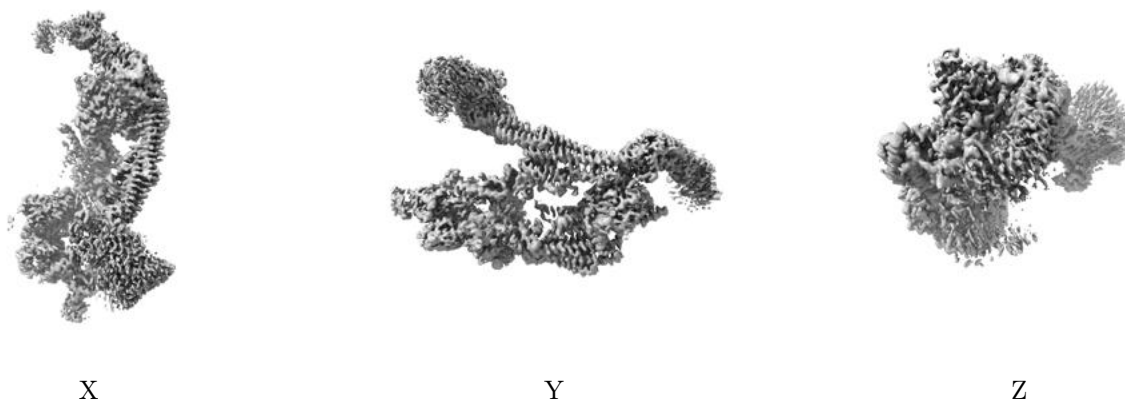


Z

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

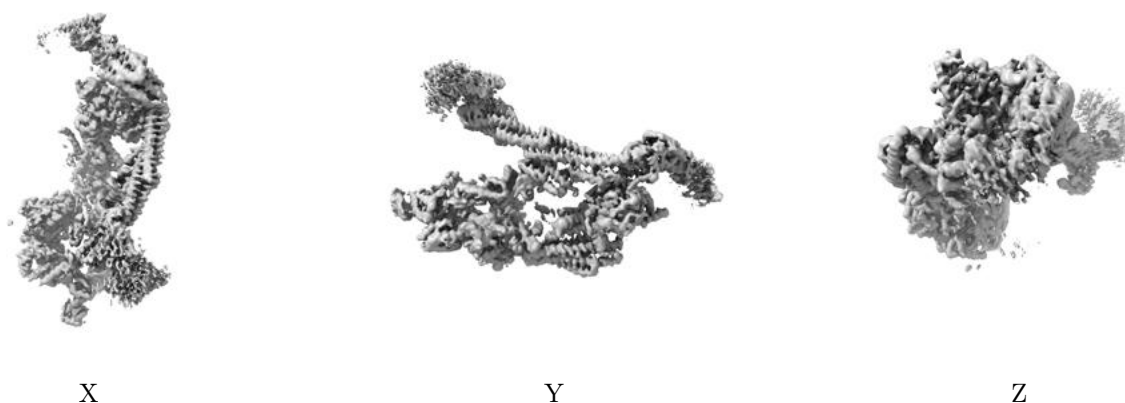
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.588. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

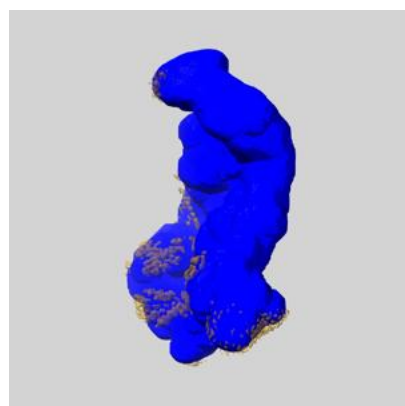
6.6 Mask visualisation [i](#)

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

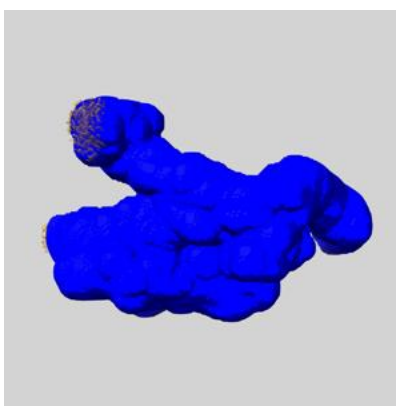
A mask typically either:

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

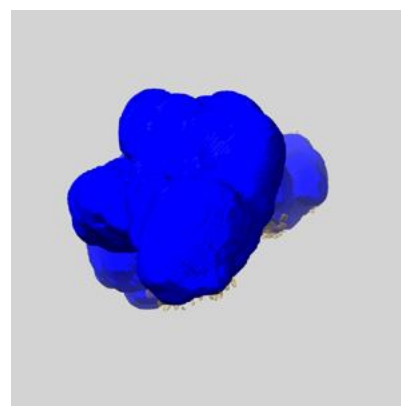
6.6.1 emd_71499_msk_1.map [i](#)



X



Y

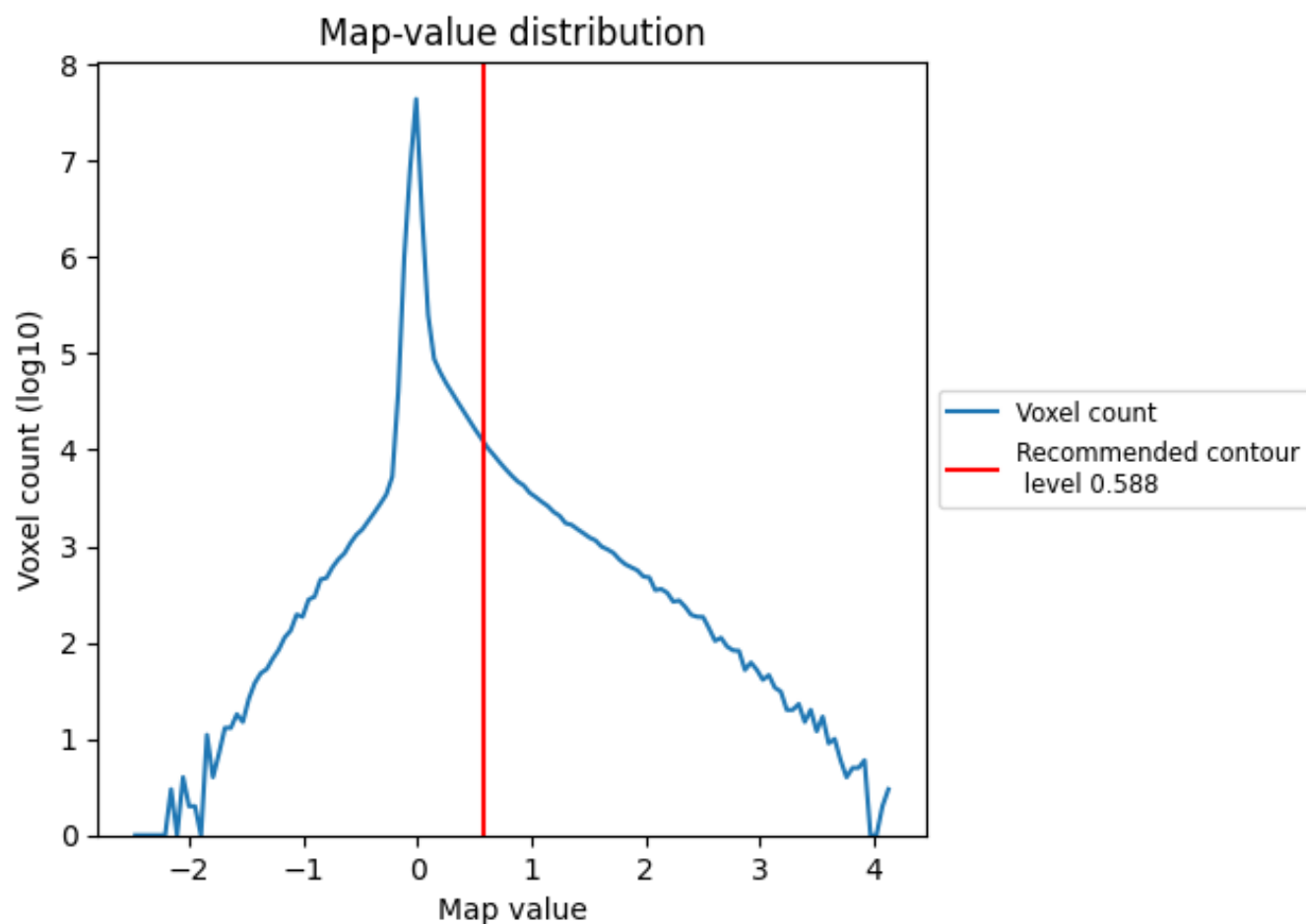


Z

7 Map analysis [i](#)

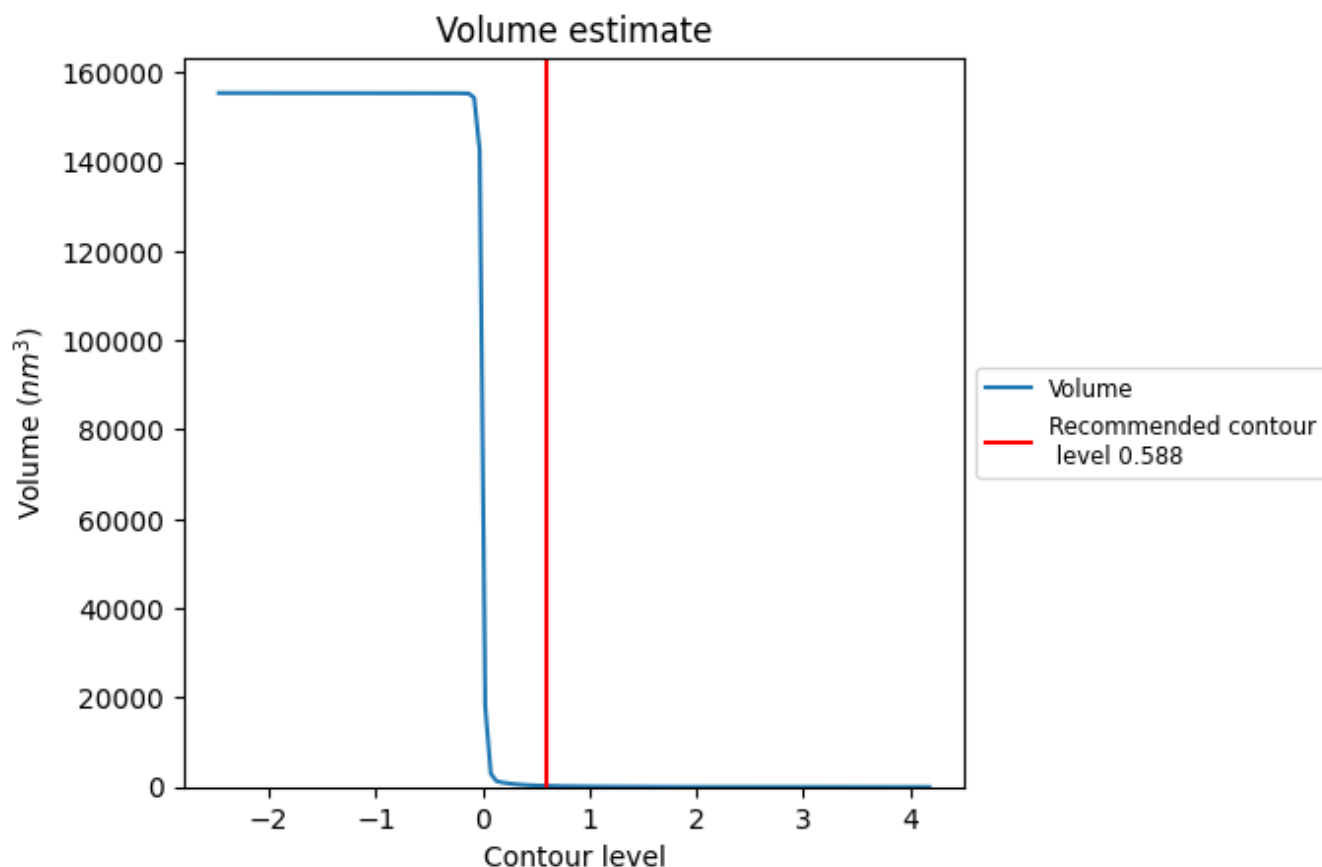
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

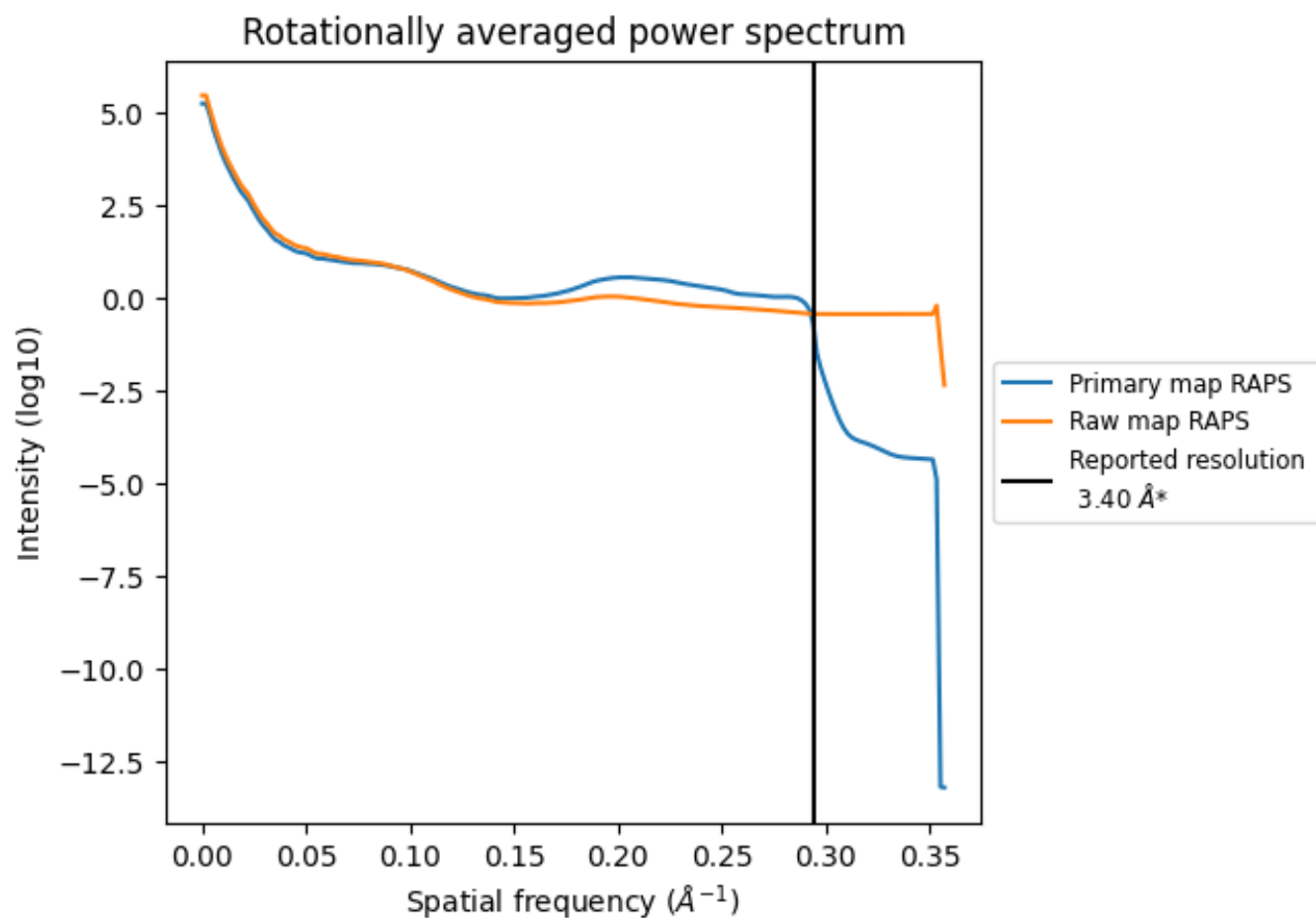
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm³; this corresponds to an approximate mass of 223 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 ⓘ

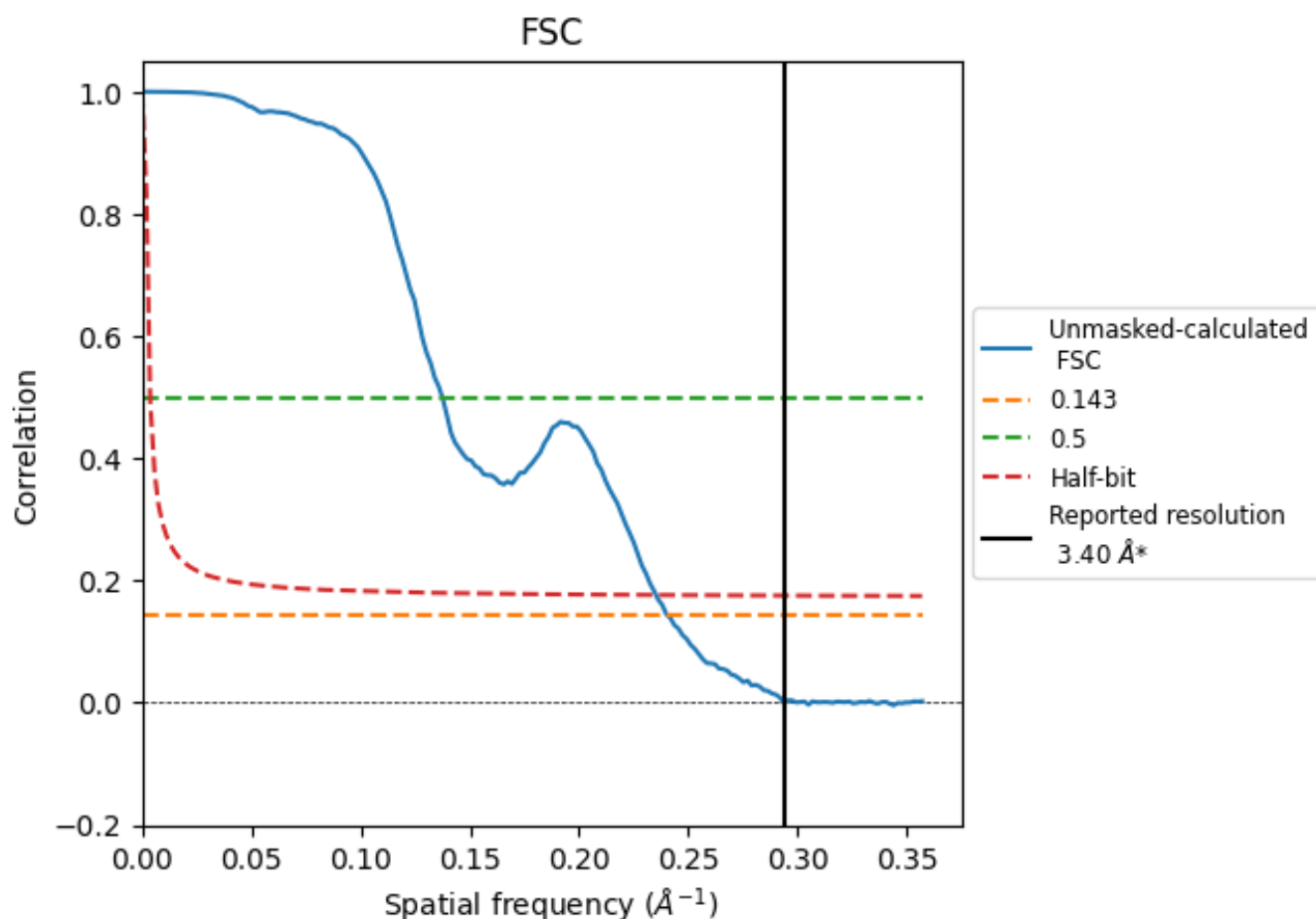


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

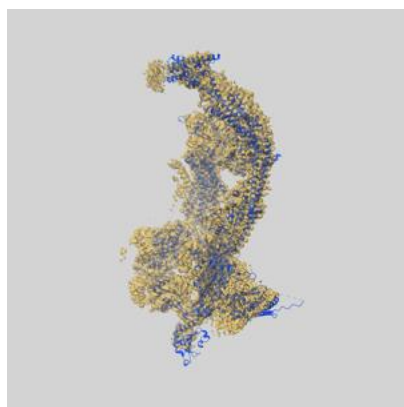
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.28	4.25

*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 4.16 differs from the reported value 3.4 by more than 10 %

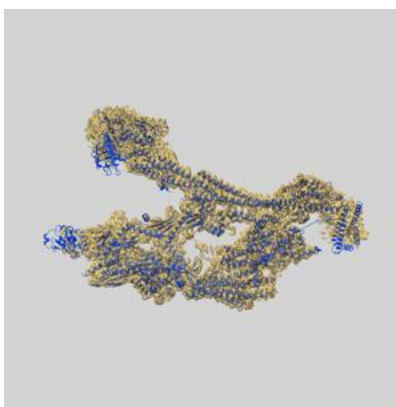
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71499 and PDB model 9PC8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

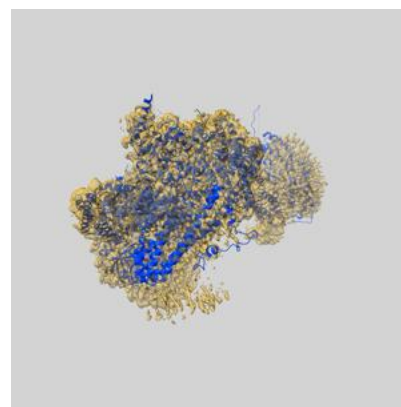
9.1 Map-model overlay [i](#)



X



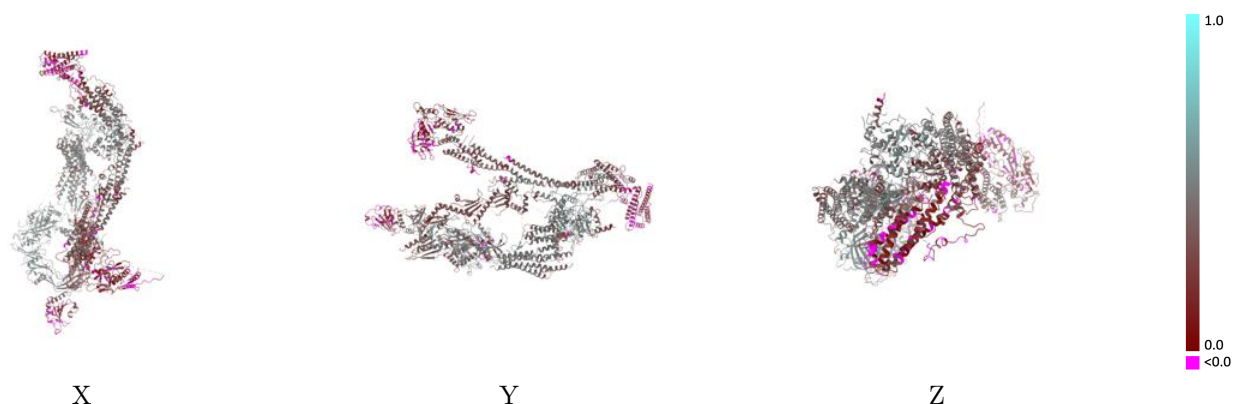
Y



Z

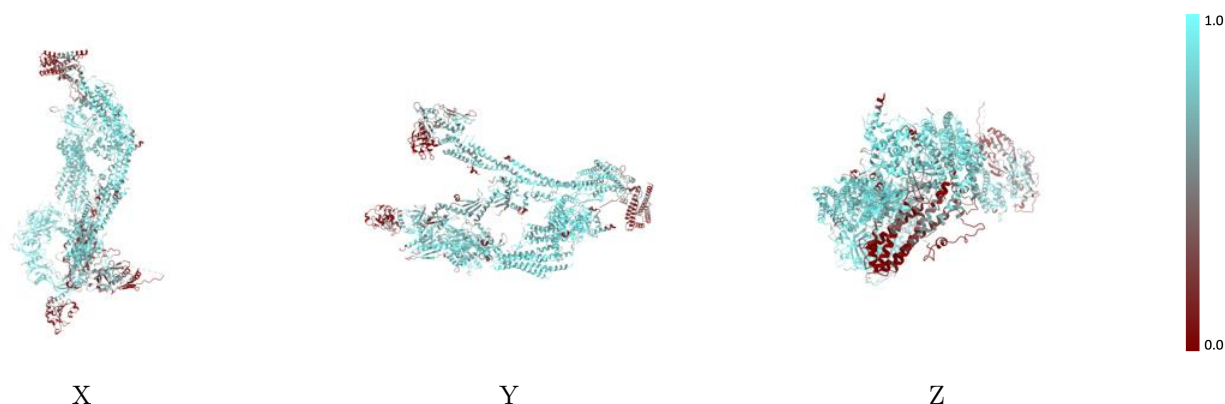
The images above show the 3D surface view of the map at the recommended contour level 0.588 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



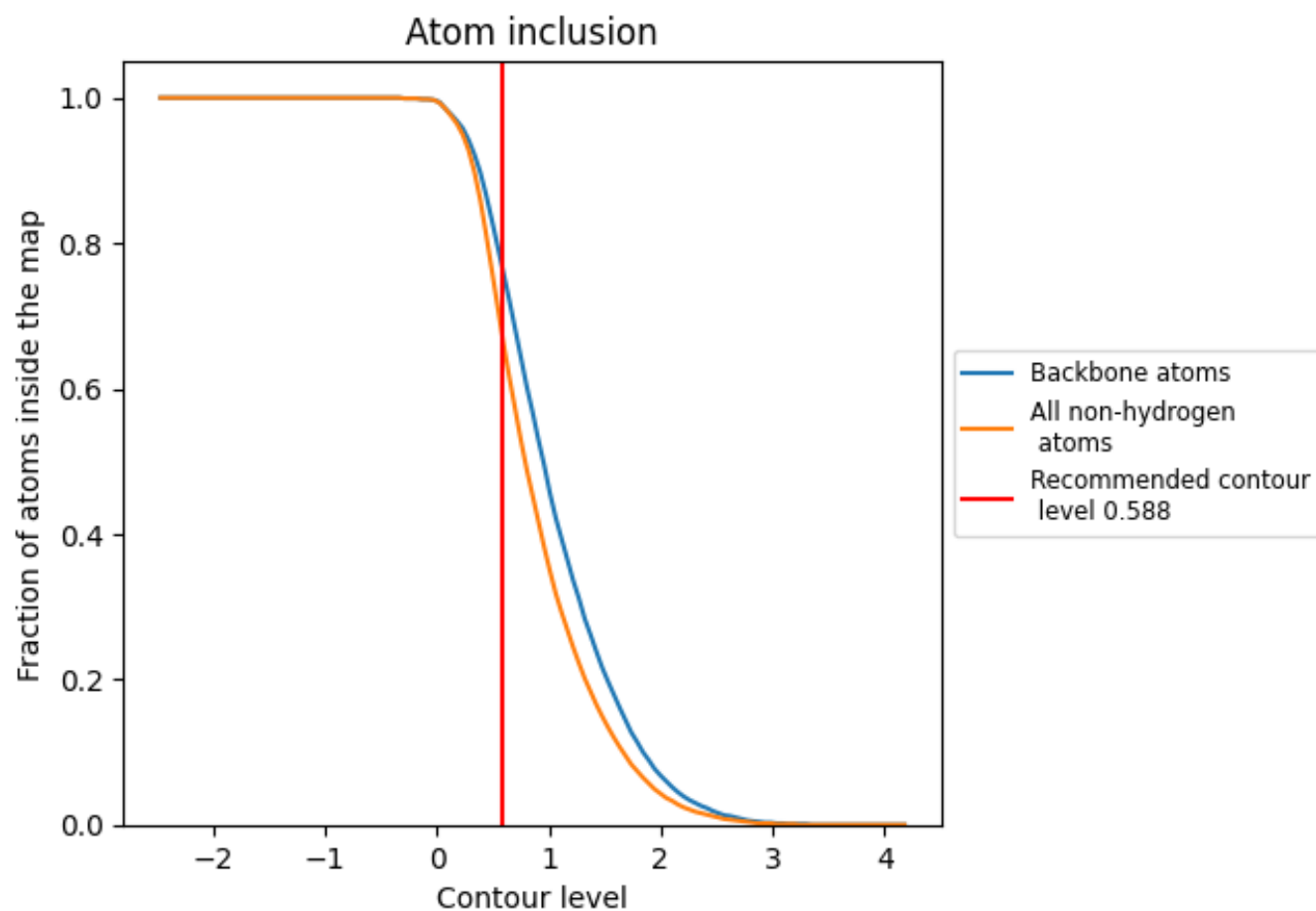
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.588).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.588) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.3520
A	 0.6860	 0.4250
a	 0.8260	 0.4540
b	 0.8480	 0.4490
c	 0.8190	 0.4170
d	 0.7190	 0.3920
e	 0.8910	 0.4990
f	 0.8640	 0.4760
g	 0.7530	 0.3920
h	 0.7680	 0.4000
i	 0.8250	 0.4230
j	 0.7720	 0.3420
k	 0.4310	 0.1860
l	 0.5060	 0.2620
m	 0.3120	 0.1560
n	 0.6880	 0.3510
o	 0.8600	 0.4780
p	 0.3920	 0.1890

