



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 6MZM / pdb_00006mzm
EMDB ID : EMD-9306
Title : Human TFIID bound to promoter DNA and TFIIA
Authors : Patel, A.B.; Louder, R.K.; Greber, B.J.; Grunberg, S.; Luo, J.; Fang, J.; Liu, Y.; Ranish, J.; Hahn, S.; Nogales, E.
Deposited on : 2018-11-05
Resolution : 7.50 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:

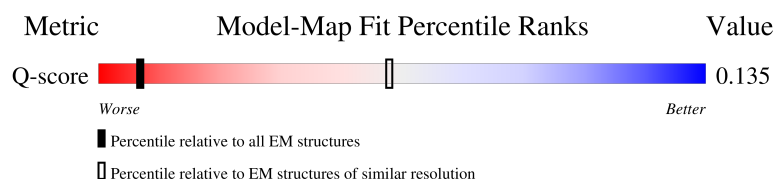
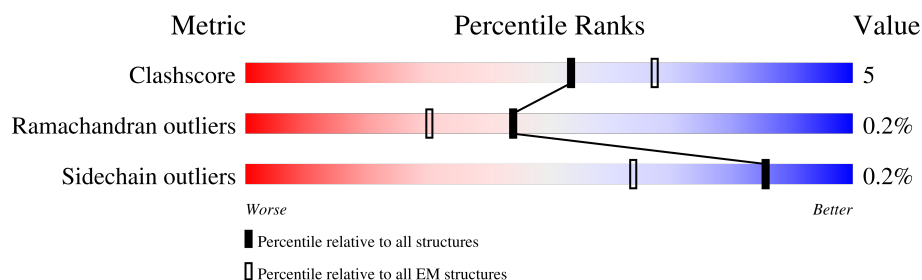
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.50 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.



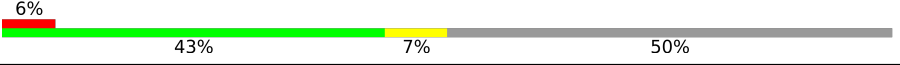
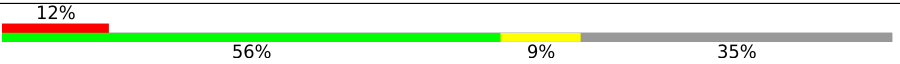
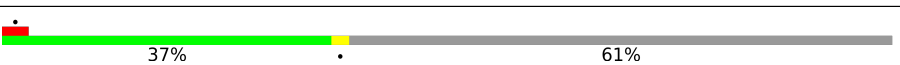
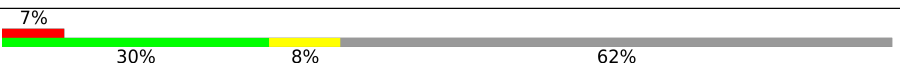
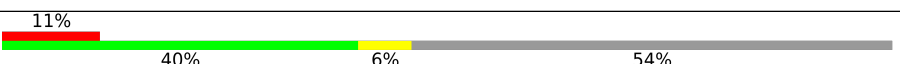
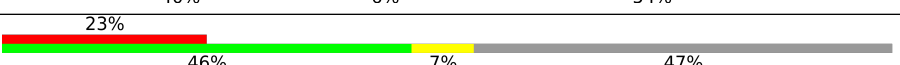
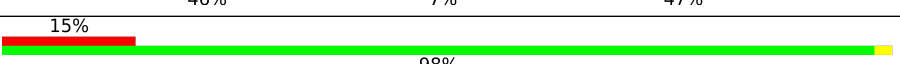
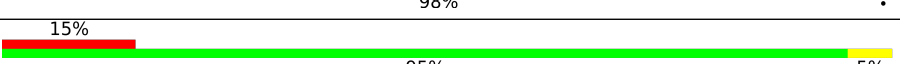
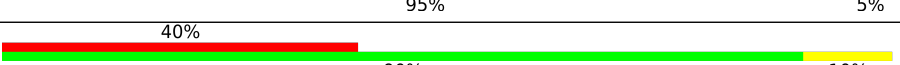
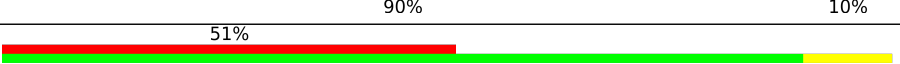
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	436 (7.00 - 8.00)

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	A	496	 22% 80% 10% 10%
2	B	1199	 9% 64% 17% 19%
3	D	1025	 12% 88%
4	G	800	 14% 48% 11% 41%

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Mol	Chain	Length	Quality of chain
5	H	677	
6	I	677	
7	J	349	
8	K	310	
9	L	264	
10	O	218	
11	R	161	
12	T	339	
13	U	80	
14	V	80	
15	W	90	
16	X	97	
17	Z	238	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32243 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 Transcription initiation factor TFIID subunit 1, TAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	445	Total	C	N	O	S	0	0
			3610	2300	642	645	23		

- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 2, TAF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	968	Total	C	N	O	S	0	0
			7832	5031	1322	1421	58		

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4, TAF4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	128	Total	C	N	O	0	0
			816	501	156	159		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5, TAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	473	Total	C	N	O	S	0	0
			3646	2314	638	679	15		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	257	Total	C	N	O	S	0	0
			1943	1230	347	355	11		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	339	Total	C	N	O	S	0	0
			2520	1585	445	474	16		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	123	Total	C	N	O	S	0	0
			998	638	184	172	4		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 8, TAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	202	Total	C	N	O	S	0	0
			1449	906	260	278	5		

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 9, TAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	104	Total	C	N	O	S	0	0
			732	456	129	142	5		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	82	Total	C	N	O	S	0	0
			645	413	102	126	4		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	74	Total	C	N	O	S	0	0
			611	381	107	120	3		

- Molecule 12 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	180	Total	C	N	O	S	0	0
			1429	927	252	243	7		

- Molecule 13 is a DNA chain called SCP DNA (80-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	80	Total	C	N	O	P	0	0
			1626	770	292	484	80		

- Molecule 14 is a DNA chain called SCP DNA (80-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	80	Total	C	N	O	P	0	0
			1654	778	320	476	80		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	90	Total	C	N	O	S	0	0
			749	478	126	141	4		

- Molecule 16 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	97	Total	C	N	O	S	0	0
			793	502	140	149	2		

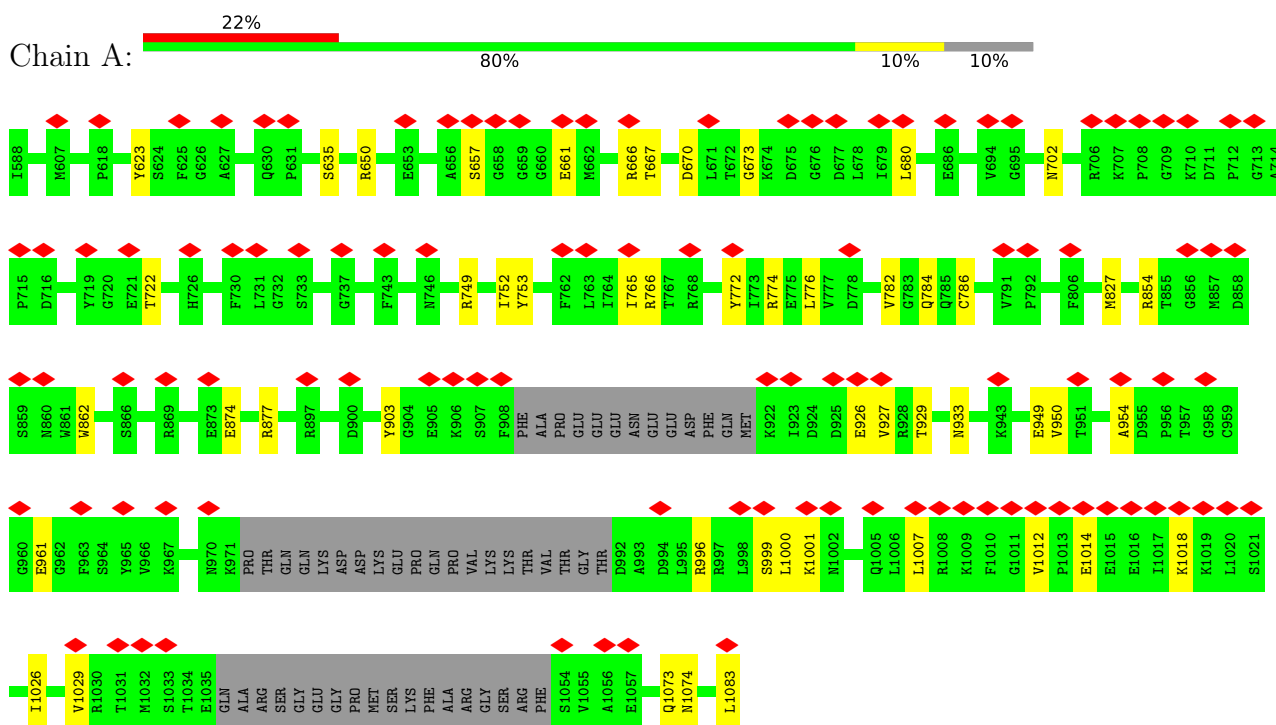
- Molecule 17 is a protein called Unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Z	238	Total	C	N	O	0	0
			1190	714	238	238		

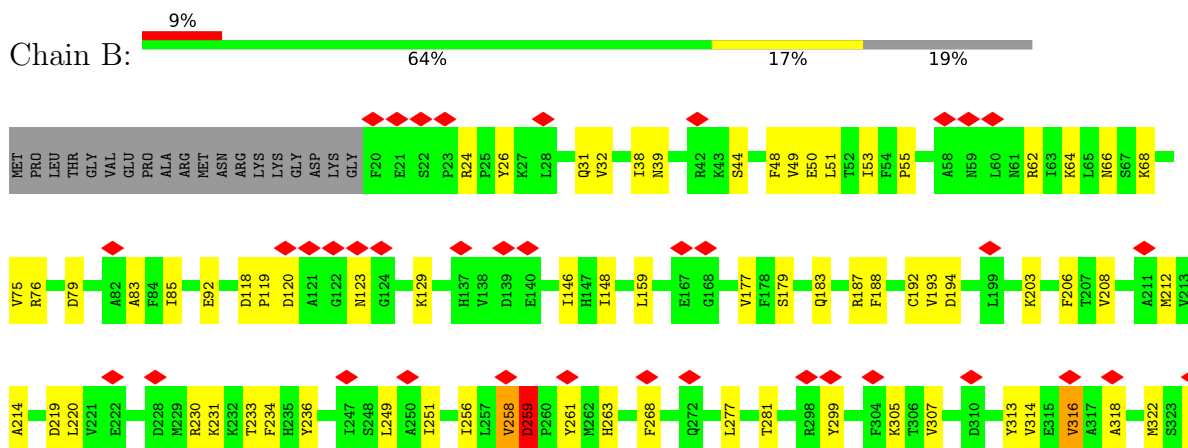
3 Residue-property plots

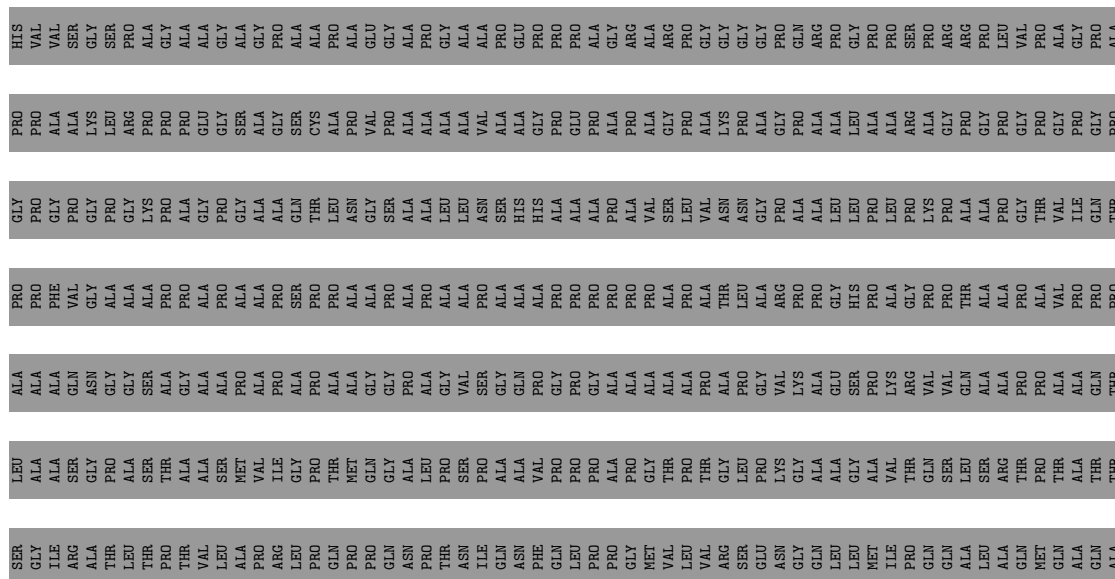
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transcription initiation factor TFIID subunit 1, TAF1

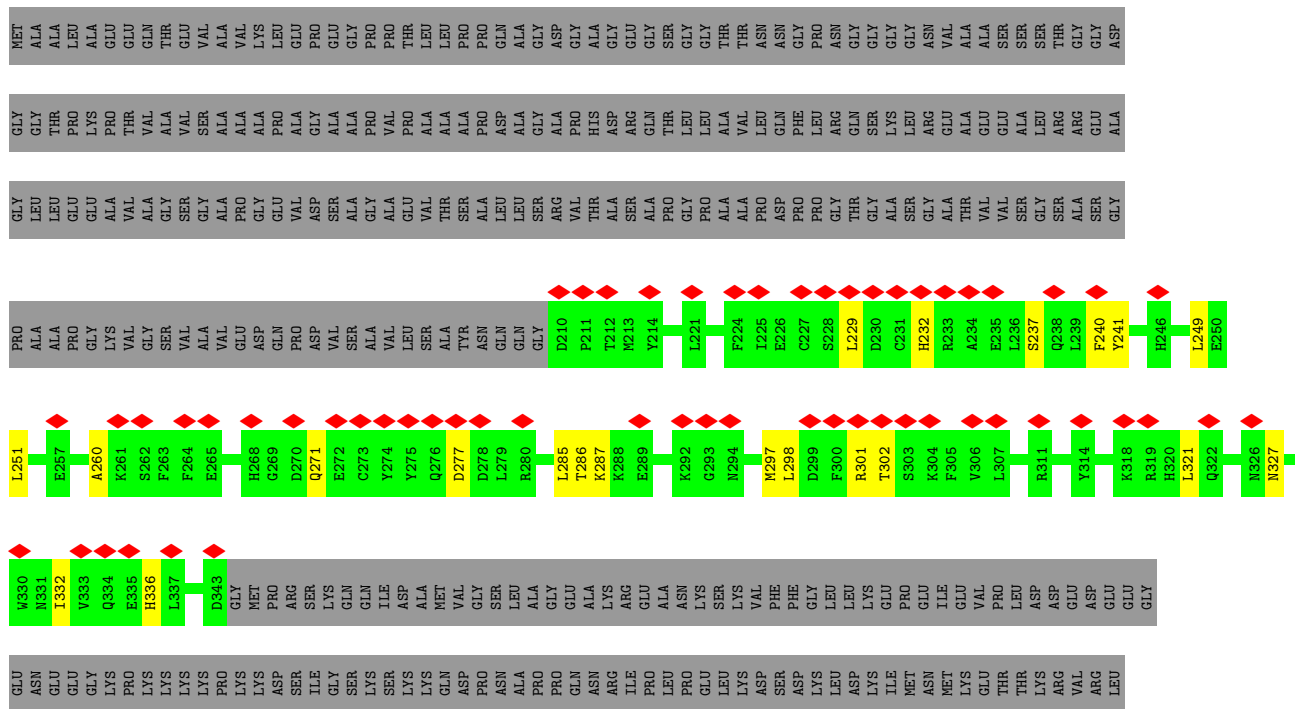


- Molecule 2: Transcription initiation factor TFIID subunit 2, TAF2

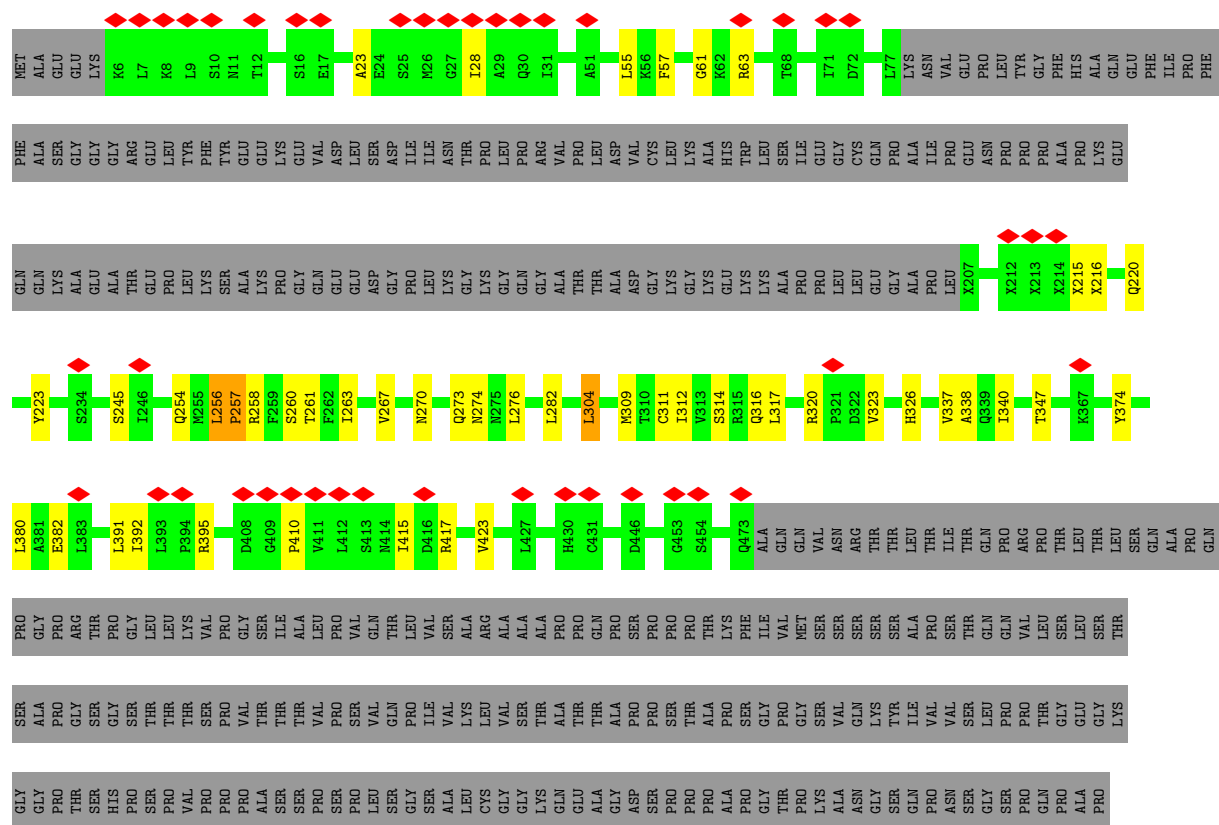




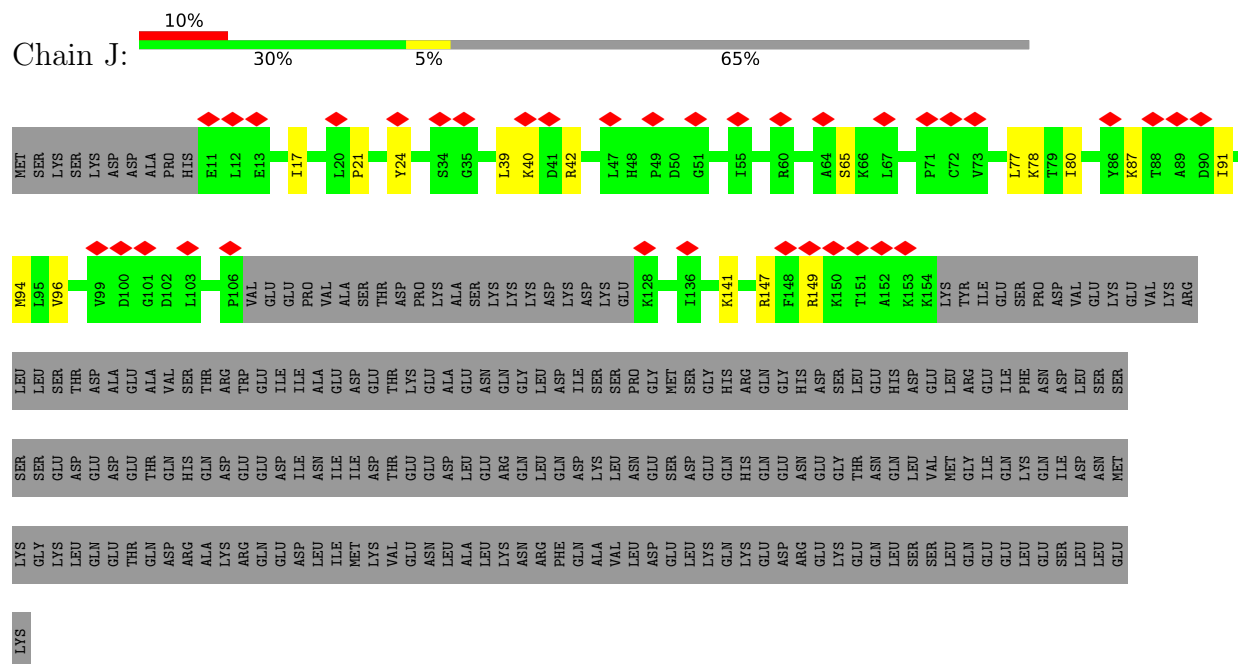
- Molecule 4: Transcription initiation factor TFIID subunit 5, TAF5





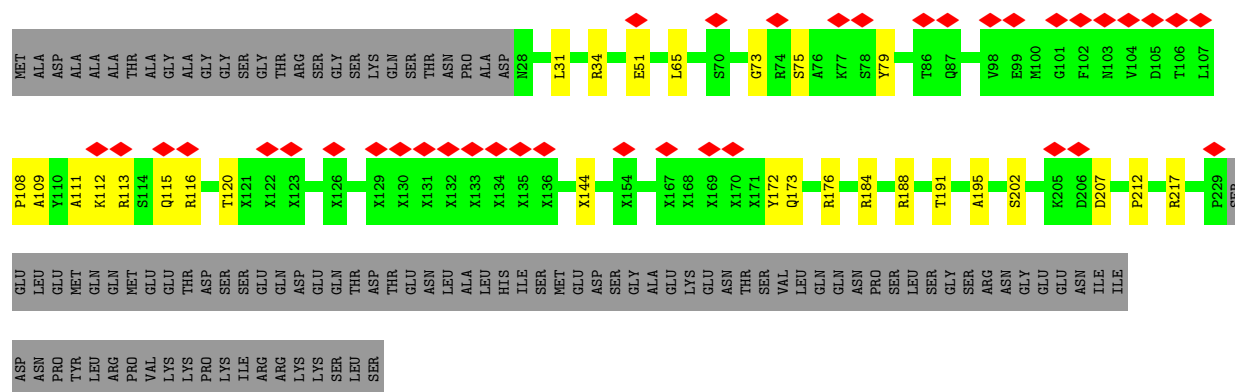


• Molecule 7: Transcription initiation factor TFIID subunit 7

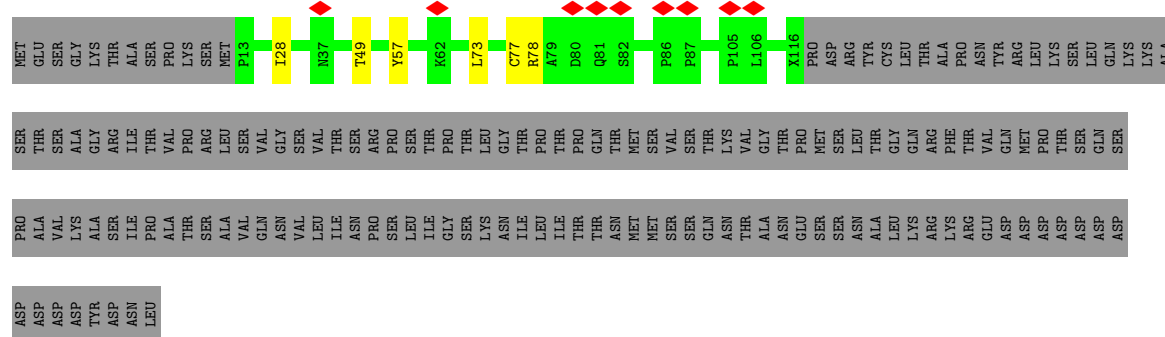


• Molecule 8: Transcription initiation factor TFIID subunit 8, TAF8

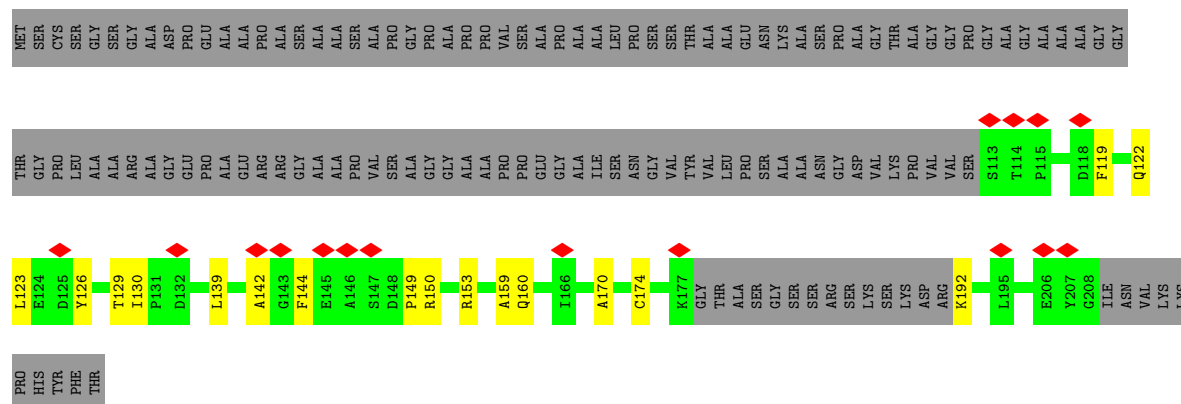




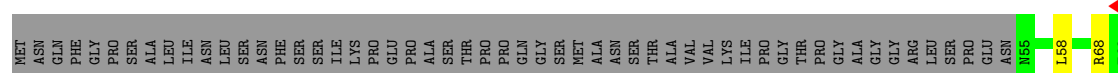
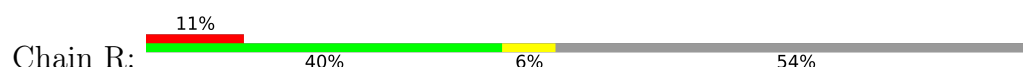
- Molecule 9: Transcription initiation factor TFIID subunit 9, TAF9

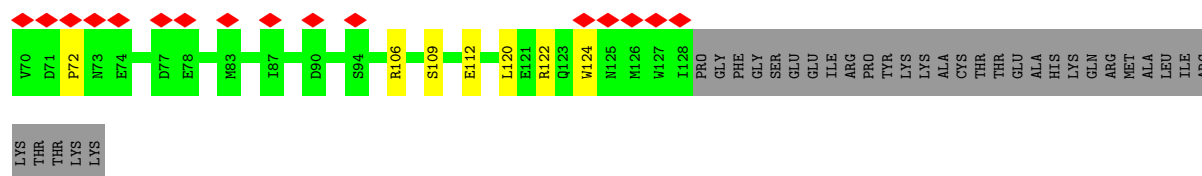


- Molecule 10: Transcription initiation factor TFIID subunit 10

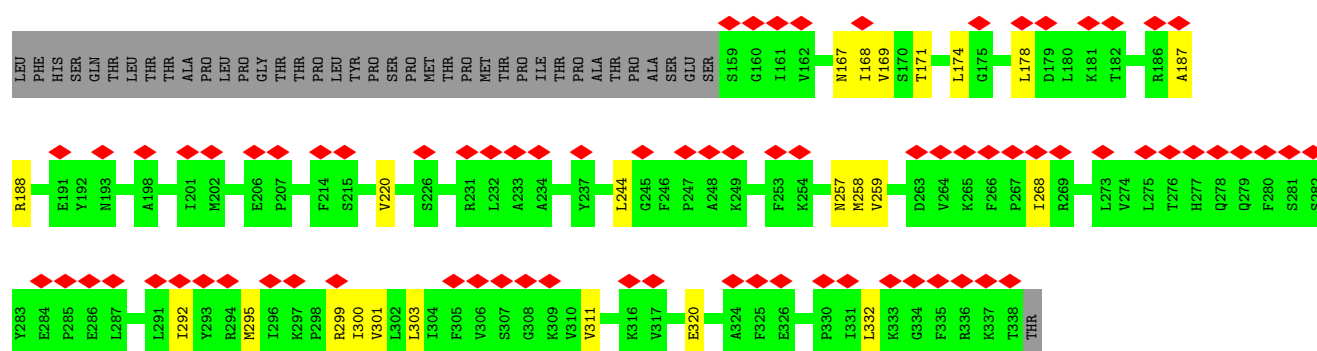


- Molecule 11: Transcription initiation factor TFIID subunit 12

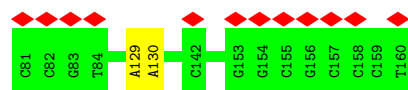




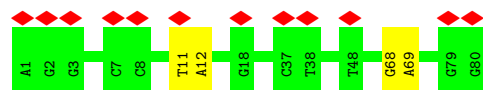
• Molecule 12: TATA-box-binding protein



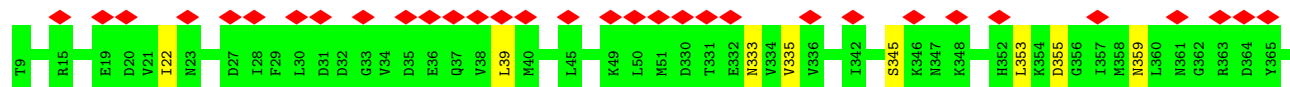
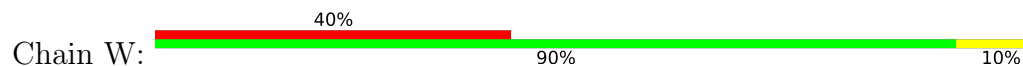
• Molecule 13: SCP DNA (80-MER)



• Molecule 14: SCP DNA (80-MER)

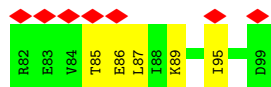
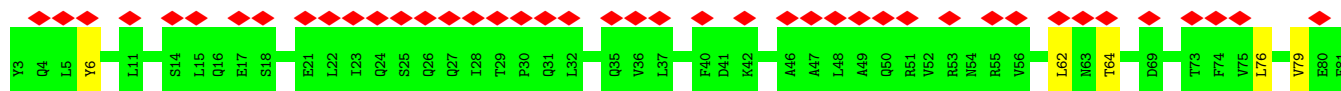
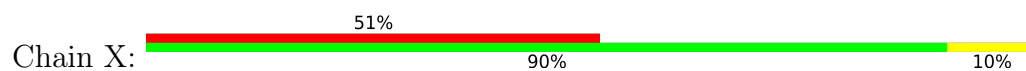


• Molecule 15: Transcription initiation factor IIA subunit 1

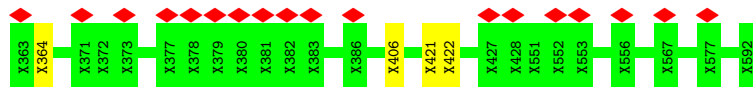
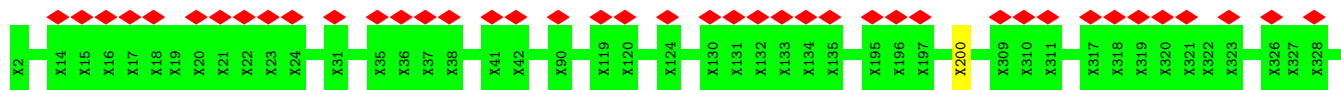




- Molecule 16: Transcription initiation factor IIA subunit 2



- Molecule 17: Unk



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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	A	0.19	0/3694	0.51	3/4967 (0.1%)
2	B	0.24	0/8029	0.66	8/10882 (0.1%)
3	D	0.19	0/821	0.43	0/1124
4	G	0.23	0/3537	0.60	0/4802
5	H	0.29	0/1978	0.65	3/2693 (0.1%)
6	I	0.21	0/2506	0.58	2/3402 (0.1%)
7	J	0.23	0/1017	0.52	0/1370
8	K	0.21	0/1212	0.52	0/1640
9	L	0.19	0/705	0.50	0/955
10	O	0.21	0/657	0.45	0/891
11	R	0.20	0/618	0.51	0/835
12	T	0.22	0/1455	0.51	0/1958
13	U	0.25	0/1819	0.51	0/2802
14	V	0.24	0/1859	0.47	0/2870
15	W	0.28	0/762	0.60	0/1026
16	X	0.25	0/803	0.69	0/1088
All	All	0.23	0/31472	0.58	16/43305 (0.0%)

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	A	0	1
2	B	0	8
4	G	0	3
5	H	0	4
6	I	0	1
8	K	0	3
15	W	0	1
16	X	0	1
17	Z	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	23

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	304	LEU	CA-C-N	7.79	125.15	120.24
6	I	304	LEU	C-N-CA	7.79	125.15	120.24
1	A	657	SER	N-CA-C	6.81	120.83	111.71
5	H	384	GLY	N-CA-C	6.73	118.36	111.56
2	B	765	ASN	CA-C-N	5.55	132.14	121.54
2	B	765	ASN	C-N-CA	5.55	132.14	121.54
1	A	657	SER	CA-C-N	5.50	131.59	121.70
1	A	657	SER	C-N-CA	5.50	131.59	121.70
2	B	258	VAL	CA-C-N	5.48	127.60	120.26
2	B	258	VAL	C-N-CA	5.48	127.60	120.26
2	B	733	PRO	CA-C-N	5.12	131.33	121.54
2	B	733	PRO	C-N-CA	5.12	131.33	121.54
2	B	259	ASP	N-CA-C	5.07	119.64	112.75
5	H	253	TYR	CA-C-N	5.05	131.19	121.54
5	H	253	TYR	C-N-CA	5.05	131.19	121.54
2	B	859	ARG	CB-CG-CD	5.03	122.86	111.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	949	GLU	Peptide
2	B	193	VAL	Peptide
2	B	259	ASP	Peptide
2	B	316	VAL	Peptide
2	B	415	HIS	Peptide
2	B	737	LYS	Peptide
2	B	821	ASN	Peptide
2	B	822	LEU	Peptide
2	B	843	LEU	Peptide
4	G	668	HIS	Peptide
4	G	721	ARG	Peptide
4	G	783	LEU	Peptide
5	H	313	VAL	Peptide
5	H	314	SER	Peptide

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Mol	Chain	Res	Type	Group
5	H	348	THR	Peptide
5	H	441	PRO	Peptide
6	I	256	LEU	Peptide
8	K	113	ARG	Peptide
8	K	144	UNK	Peptide
8	K	217	ARG	Peptide
15	W	345	SER	Peptide
16	X	85	THR	Peptide
17	Z	364	UNK	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	A	3610	0	3640	31	0
2	B	7832	0	7789	124	0
3	D	816	0	632	5	0
4	G	3646	0	3312	51	0
5	H	1943	0	1922	23	0
6	I	2520	0	2422	27	0
7	J	998	0	1055	12	0
8	K	1449	0	1281	20	0
9	L	732	0	624	5	0
10	O	645	0	640	14	0
11	R	611	0	610	9	0
12	T	1429	0	1521	15	0
13	U	1626	0	897	1	0
14	V	1654	0	893	6	0
15	W	749	0	740	5	0
16	X	793	0	801	5	0
17	Z	1190	0	276	4	0
All	All	32243	0	29055	318	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 5.

All (318) 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)
2:B:31:GLN:HA	2:B:50:GLU:O	1.41	1.17
2:B:835:ARG:HH21	8:K:188:ARG:HD2	1.58	0.68
2:B:564:LEU:H	2:B:580:GLN:HB2	1.59	0.68
4:G:718:ARG:HG2	4:G:771:GLY:H	1.59	0.67
4:G:321:LEU:HD22	4:G:327:ASN:HD21	1.60	0.66
2:B:230:ARG:HG3	2:B:231:LYS:HG3	1.77	0.66
1:A:854:ARG:HH12	14:V:68:DG:H21	1.43	0.65
1:A:666:ARG:HG3	1:A:667:THR:HG23	1.77	0.65
6:I:392:ILE:HA	6:I:395:ARG:HB2	1.79	0.65
4:G:586:TYR:HB3	4:G:605:HIS:HB3	1.77	0.65
2:B:206:PHE:O	2:B:233:THR:HA	1.96	0.64
2:B:443:TRP:HE1	2:B:966:ARG:HB2	1.63	0.64
2:B:214:ALA:HB1	2:B:249:LEU:HD11	1.80	0.64
2:B:92:GLU:HG2	2:B:958:ASN:HB3	1.78	0.63
2:B:31:GLN:CA	2:B:50:GLU:O	2.33	0.63
2:B:314:VAL:HG12	2:B:316:VAL:H	1.63	0.63
10:O:130:ILE:HG13	10:O:160:GLN:HE21	1.64	0.62
12:T:257:ASN:ND2	14:V:12:DA:N3	2.43	0.62
4:G:733:ASN:HB3	4:G:761:LEU:HB2	1.81	0.62
4:G:286:THR:HG22	4:G:287:LYS:HG3	1.82	0.62
4:G:472:GLY:HA3	4:G:783:LEU:HD13	1.82	0.62
5:H:324:ASP:HA	5:H:327:TRP:HD1	1.65	0.62
4:G:468:ASN:HA	4:G:786:THR:HG23	1.82	0.61
4:G:546:VAL:HA	4:G:562:SER:HA	1.82	0.61
2:B:678:ARG:NH1	2:B:682:THR:OG1	2.33	0.61
2:B:159:LEU:HD23	2:B:179:SER:HB3	1.82	0.61
4:G:726:LEU:HB2	4:G:738:TRP:HB2	1.83	0.61
10:O:170:ALA:O	10:O:174:CYS:HB2	2.01	0.61
2:B:538:ASN:HD22	2:B:547:GLU:HB2	1.66	0.60
4:G:229:LEU:HB2	4:G:232:HIS:HD2	1.67	0.60
2:B:344:ARG:NH1	2:B:382:MET:SD	2.74	0.60
2:B:838:ASN:HD22	8:K:191:THR:HG23	1.66	0.60
2:B:75:VAL:HG13	2:B:148:ILE:HG12	1.84	0.60
2:B:396:LYS:HD2	2:B:660:VAL:HA	1.83	0.59
2:B:538:ASN:HA	2:B:542:ASN:HD22	1.68	0.59
12:T:187:ALA:HB2	12:T:244:LEU:HD11	1.85	0.58
8:K:73:GLY:HA3	10:O:142:ALA:HB1	1.84	0.58
1:A:635:SER:HB3	7:J:40:LYS:HB2	1.84	0.58
2:B:48:PHE:HA	2:B:148:ILE:O	2.04	0.58
6:I:338:ALA:HB2	6:I:382:GLU:HB3	1.86	0.57
2:B:530:LYS:HG2	2:B:639:LYS:HB3	1.85	0.57
2:B:549:LYS:HG2	2:B:587:LYS:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:65:LEU:HD11	10:O:159:ALA:HB1	1.86	0.57
12:T:303:LEU:HB2	12:T:311:VAL:HB	1.86	0.57
2:B:549:LYS:HE2	2:B:587:LYS:HE2	1.87	0.57
1:A:927:VAL:O	1:A:933:ASN:ND2	2.35	0.56
8:K:191:THR:O	8:K:195:ALA:HB2	2.05	0.56
2:B:32:VAL:HB	2:B:50:GLU:HB2	1.87	0.56
2:B:187:ARG:NH2	2:B:194:ASP:OD1	2.35	0.56
2:B:539:ARG:HG3	2:B:545:GLU:HA	1.88	0.56
12:T:171:THR:HG22	12:T:220:VAL:HG22	1.87	0.56
2:B:371:LYS:NZ	2:B:446:TYR:OH	2.39	0.56
4:G:692:ARG:NH2	4:G:706:GLU:OE1	2.39	0.56
8:K:195:ALA:HB1	8:K:212:PRO:HG2	1.87	0.56
4:G:237:SER:HA	4:G:240:PHE:HD2	1.71	0.56
6:I:215:UNK:O	6:I:254:GLN:NE2	2.38	0.56
2:B:946:ASN:ND2	2:B:986:CYS:SG	2.76	0.56
4:G:240:PHE:HB3	4:G:271:GLN:HE22	1.71	0.56
2:B:530:LYS:HE2	2:B:639:LYS:HD3	1.87	0.55
6:I:323:VAL:HA	6:I:326:HIS:HD2	1.70	0.55
1:A:961:GLU:OE1	7:J:147:ARG:NH1	2.40	0.55
4:G:475:ALA:HB3	4:G:781:VAL:HG11	1.88	0.55
16:X:87:LEU:HD21	16:X:89:LYS:HE3	1.87	0.55
5:H:381:ALA:HA	5:H:388:ILE:HD11	1.87	0.55
9:L:49:THR:OG1	9:L:78:ARG:NH1	2.40	0.55
11:R:106:ARG:HH22	11:R:112:GLU:HB2	1.70	0.55
1:A:996:ARG:HA	1:A:1026:ILE:HD13	1.87	0.55
2:B:550:GLN:HE22	2:B:580:GLN:HG2	1.72	0.55
6:I:260:SER:HB2	6:I:304:LEU:HD21	1.88	0.55
8:K:108:PRO:O	8:K:111:ALA:HB3	2.07	0.55
12:T:169:VAL:HB	12:T:257:ASN:HB3	1.88	0.55
2:B:26:TYR:HB2	2:B:53:ILE:HD11	1.89	0.54
2:B:32:VAL:HG22	2:B:203:LYS:HB3	1.89	0.54
1:A:903:TYR:HE2	1:A:926:GLU:HB3	1.72	0.54
1:A:999:SER:O	1:A:1001:LYS:N	2.41	0.54
2:B:630:ILE:O	2:B:638:ARG:NH1	2.40	0.54
4:G:298:LEU:O	4:G:302:THR:OG1	2.25	0.54
9:L:57:TYR:OH	11:R:122:ARG:NH2	2.37	0.54
2:B:85:ILE:HD11	2:B:129:LYS:HE3	1.89	0.53
2:B:183:GLN:OE1	2:B:361:ARG:NH2	2.41	0.53
2:B:396:LYS:HZ3	2:B:663:GLN:HB2	1.72	0.53
4:G:609:ALA:HB3	4:G:623:PHE:HB2	1.89	0.53
2:B:956:LEU:O	2:B:961:THR:OG1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:684:LEU:HB2	4:G:696:TRP:HB2	1.90	0.53
2:B:208:VAL:HG11	2:B:214:ALA:HB2	1.91	0.53
2:B:24:ARG:NH1	2:B:120:ASP:OD1	2.42	0.52
12:T:168:ILE:HG12	12:T:258:MET:HG2	1.90	0.52
2:B:359:ILE:HG23	2:B:498:VAL:HB	1.90	0.52
4:G:671:PRO:O	4:G:689:THR:OG1	2.27	0.52
6:I:410:PRO:O	6:I:417:ARG:NH2	2.40	0.52
1:A:702:ASN:HB2	1:A:722:THR:HA	1.92	0.52
1:A:680:LEU:HD11	7:J:91:ILE:HD12	1.91	0.52
1:A:753:TYR:OH	1:A:1074:ASN:OD1	2.27	0.52
3:D:892:THR:H	11:R:109:SER:HB2	1.75	0.52
8:K:31:LEU:HD11	8:K:34:ARG:HH21	1.74	0.52
2:B:338:GLU:HG2	2:B:341:LEU:HD12	1.91	0.52
2:B:32:VAL:HA	2:B:203:LYS:O	2.09	0.52
2:B:307:VAL:HB	2:B:324:ILE:HG12	1.92	0.51
2:B:431:LEU:HD13	2:B:976:PHE:HB2	1.92	0.51
11:R:120:LEU:O	11:R:124:TRP:N	2.40	0.51
4:G:470:TYR:HD2	6:I:63:ARG:HH22	1.59	0.51
4:G:476:VAL:HG22	4:G:768:LEU:HD22	1.91	0.51
4:G:564:ASP:HB2	4:G:566:THR:HG22	1.92	0.51
2:B:691:PHE:HD2	2:B:694:VAL:H	1.58	0.51
8:K:51:GLU:OE1	10:O:192:LYS:N	2.43	0.51
4:G:730:SER:OG	4:G:732:ASP:OD1	2.29	0.51
3:D:873:LEU:HD23	11:R:58:LEU:HD13	1.92	0.51
6:I:314:SER:OG	17:Z:200:UNK:O	2.29	0.51
2:B:313:TYR:O	2:B:966:ARG:NH1	2.44	0.51
1:A:784:GLN:H	1:A:1073:GLN:HE22	1.58	0.51
2:B:268:PHE:HB2	2:B:307:VAL:HG22	1.91	0.51
2:B:451:CYS:HA	2:B:454:HIS:HD2	1.76	0.51
2:B:539:ARG:HD3	2:B:546:LEU:HG	1.93	0.51
2:B:38:ILE:HD11	2:B:177:VAL:HG11	1.93	0.50
2:B:212:MET:HE2	2:B:251:ILE:HG22	1.91	0.50
5:H:233:GLY:O	5:H:239:ARG:NH1	2.44	0.50
2:B:219:ASP:O	2:B:236:TYR:HA	2.10	0.50
3:D:912:ASN:HB2	11:R:124:TRP:HH2	1.76	0.50
4:G:332:ILE:HA	4:G:336:HIS:HD2	1.75	0.50
4:G:783:LEU:HD21	4:G:787:ARG:HG3	1.94	0.50
6:I:57:PHE:O	6:I:61:GLY:N	2.41	0.50
12:T:188:ARG:HH11	16:X:64:THR:HG21	1.77	0.50
8:K:172:TYR:OH	8:K:176:ARG:NH1	2.44	0.50
6:I:55:LEU:HD13	9:L:28:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:663:GLN:HA	2:B:666:ILE:HB	1.94	0.50
1:A:752:ILE:HG22	1:A:782:VAL:HG22	1.92	0.49
2:B:118:ASP:O	2:B:123:ASN:ND2	2.44	0.49
4:G:277:ASP:OD1	4:G:649:ARG:NH2	2.45	0.49
4:G:695:LEU:HB3	4:G:705:GLY:H	1.77	0.49
5:H:404:ARG:NH2	5:H:452:PHE:O	2.45	0.49
2:B:599:ASN:HA	2:B:602:LYS:HB2	1.94	0.49
3:D:934:TYR:O	10:O:150:ARG:NH2	2.44	0.49
8:K:112:LYS:HA	8:K:116:ARG:HD2	1.94	0.49
2:B:891:LEU:HA	2:B:894:VAL:HG12	1.95	0.49
12:T:174:LEU:HD12	12:T:178:LEU:HD11	1.94	0.49
2:B:929:MET:HA	2:B:932:LYS:HB2	1.95	0.49
4:G:479:THR:O	4:G:555:ARG:NH2	2.44	0.49
2:B:402:ILE:HD12	2:B:455:LEU:HD12	1.94	0.49
2:B:328:ASN:O	2:B:847:ARG:NH2	2.33	0.48
2:B:597:ARG:NH1	2:B:621:ALA:O	2.44	0.48
1:A:1026:ILE:HA	1:A:1029:VAL:HG12	1.95	0.48
5:H:389:LYS:HG3	5:H:438:LEU:HD11	1.95	0.48
2:B:566:VAL:O	2:B:577:HIS:HA	2.13	0.48
5:H:410:PRO:O	5:H:417:ARG:NH2	2.47	0.48
1:A:996:ARG:HG2	1:A:1026:ILE:HG21	1.95	0.48
2:B:299:TYR:OH	2:B:353:GLN:NE2	2.47	0.48
2:B:539:ARG:NH1	2:B:593:HIS:O	2.37	0.48
5:H:306:PRO:HB3	17:Z:406:UNK:HA	1.95	0.48
2:B:917:ASP:OD1	2:B:923:ARG:NE	2.34	0.47
9:L:57:TYR:HH	11:R:122:ARG:HH21	1.59	0.47
1:A:1014:GLU:O	1:A:1018:LYS:HB2	2.13	0.47
2:B:565:LYS:HA	2:B:578:THR:O	2.14	0.47
4:G:653:LEU:HD12	4:G:663:ARG:HB2	1.95	0.47
12:T:268:ILE:HD13	12:T:332:LEU:HD22	1.96	0.47
2:B:338:GLU:OE2	2:B:847:ARG:NH2	2.48	0.47
2:B:917:ASP:H	2:B:923:ARG:HH21	1.62	0.47
4:G:558:LEU:HB3	4:G:570:TRP:HB2	1.96	0.47
1:A:926:GLU:OE1	7:J:149:ARG:NH1	2.39	0.47
5:H:418:ILE:O	5:H:422:HIS:ND1	2.45	0.47
6:I:258:ARG:HD3	17:Z:422:UNK:HA	1.97	0.47
12:T:300:ILE:HD11	12:T:320:GLU:HB3	1.95	0.47
1:A:670:ASP:O	7:J:78:LYS:NZ	2.37	0.47
2:B:565:LYS:HE3	2:B:577:HIS:HB3	1.97	0.47
2:B:669:LEU:HB3	2:B:678:ARG:HE	1.80	0.47
5:H:387:VAL:HG13	5:H:391:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:411:VAL:HA	5:H:417:ARG:HH21	1.79	0.47
1:A:661:GLU:OE1	2:B:471:GLN:NE2	2.47	0.47
2:B:604:ILE:HG23	2:B:607:MET:HE3	1.97	0.47
1:A:765:ILE:HB	1:A:772:TYR:HB2	1.96	0.47
2:B:366:ASP:HB3	2:B:499:SER:HB2	1.97	0.47
2:B:692:TYR:HE1	2:B:745:GLN:HG2	1.81	0.46
5:H:370:TRP:HZ2	5:H:406:VAL:HG21	1.80	0.46
2:B:259:ASP:HB3	2:B:263:HIS:HA	1.97	0.46
2:B:389:ASN:HB3	2:B:659:VAL:HG21	1.97	0.46
6:I:258:ARG:NH1	17:Z:421:UNK:O	2.48	0.46
7:J:21:PRO:HB2	7:J:24:TYR:HD2	1.80	0.46
2:B:463:ARG:NH1	2:B:514:ASP:O	2.48	0.46
2:B:570:GLU:OE1	2:B:593:HIS:ND1	2.48	0.46
2:B:898:THR:HG21	2:B:907:LEU:HD13	1.98	0.46
1:A:673:GLY:O	1:A:774:ARG:NH1	2.49	0.46
1:A:929:THR:HG22	1:A:954:ALA:HA	1.97	0.46
8:K:109:ALA:O	8:K:112:LYS:HB2	2.15	0.46
8:K:202:SER:HB2	8:K:207:ASP:HB2	1.98	0.46
2:B:51:LEU:HB2	2:B:146:ILE:HB	1.97	0.46
2:B:387:GLY:O	2:B:391:TYR:N	2.46	0.46
4:G:768:LEU:HB3	4:G:769:LEU:H	1.66	0.46
15:W:333:ASN:HA	15:W:359:ASN:O	2.16	0.46
15:W:335:VAL:HB	16:X:95:ILE:HG12	1.97	0.46
2:B:529:VAL:HG22	2:B:559:LYS:HB3	1.97	0.46
2:B:608:ASN:O	2:B:657:ARG:NH2	2.49	0.46
2:B:806:VAL:HG12	2:B:808:PRO:HD3	1.98	0.46
6:I:320:ARG:HD3	6:I:415:ILE:HD13	1.98	0.45
4:G:241:TYR:HD1	4:G:271:GLN:HG3	1.82	0.45
6:I:263:ILE:HG23	6:I:282:LEU:HD22	1.98	0.45
12:T:295:MET:O	12:T:299:ARG:HA	2.17	0.45
16:X:62:LEU:HA	16:X:76:LEU:HD13	1.99	0.45
5:H:370:TRP:O	5:H:374:TYR:HB2	2.17	0.45
1:A:854:ARG:NH2	14:V:69:DA:N3	2.65	0.45
12:T:292:ILE:HG21	14:V:11:DT:H5''	1.98	0.45
2:B:361:ARG:HD2	2:B:367:GLU:HG3	1.98	0.45
6:I:311:CYS:O	6:I:316:GLN:NE2	2.49	0.45
2:B:332:SER:H	2:B:335:ILE:HD12	1.81	0.45
2:B:840:GLU:HG3	2:B:850:ILE:HB	1.99	0.45
4:G:558:LEU:HD23	4:G:572:LEU:HD21	1.98	0.45
5:H:380:LEU:HD23	5:H:383:LEU:HD12	1.98	0.45
10:O:119:PHE:HA	10:O:122:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:ARG:HH22	8:K:184:ARG:HE	1.63	0.45
10:O:139:LEU:HB3	10:O:144:PHE:HB3	1.99	0.45
10:O:149:PRO:HG2	10:O:153:ARG:HH12	1.81	0.45
2:B:206:PHE:HB2	2:B:234:PHE:HB2	1.99	0.44
5:H:403:ILE:HG23	5:H:420:ALA:HB1	1.98	0.44
8:K:120:THR:HA	10:O:129:THR:HG23	1.99	0.44
4:G:730:SER:OG	4:G:734:THR:OG1	2.32	0.44
2:B:26:TYR:HA	2:B:55:PRO:HA	1.99	0.44
2:B:76:ARG:HD2	2:B:79:ASP:HA	1.99	0.44
2:B:259:ASP:O	2:B:261:TYR:N	2.51	0.44
2:B:401:LYS:HB3	2:B:448:MET:HE1	1.99	0.44
8:K:75:SER:O	8:K:79:TYR:HB2	2.16	0.44
15:W:22:ILE:HG23	15:W:39:LEU:HD11	2.00	0.44
1:A:1083:LEU:O	7:J:141:LYS:NZ	2.49	0.44
2:B:50:GLU:HA	2:B:146:ILE:O	2.18	0.44
6:I:276:LEU:HB3	6:I:326:HIS:CE1	2.53	0.44
12:T:167:ASN:HB3	12:T:259:VAL:HB	1.99	0.44
2:B:432:HIS:HB2	2:B:440:THR:HG22	2.00	0.44
5:H:308:VAL:O	5:H:311:CYS:HB2	2.18	0.44
8:K:191:THR:O	8:K:195:ALA:CB	2.65	0.44
4:G:491:ASP:HA	4:G:540:TYR:HB3	1.99	0.44
6:I:380:LEU:HD13	6:I:391:LEU:HD13	1.98	0.44
8:K:115:GLN:HE22	10:O:126:TYR:HB3	1.82	0.44
4:G:651:VAL:HB	4:G:665:PHE:HB2	2.00	0.43
10:O:139:LEU:HA	10:O:142:ALA:HB3	2.00	0.43
5:H:217:SER:OG	5:H:218:VAL:N	2.46	0.43
2:B:458:ARG:O	2:B:462:ASN:ND2	2.51	0.43
6:I:257:PRO:O	6:I:261:THR:N	2.51	0.43
7:J:77:LEU:HG	7:J:87:LYS:HA	2.01	0.43
2:B:820:ASP:HB2	2:B:822:LEU:HD23	2.01	0.43
4:G:461:ILE:HG12	4:G:792:LEU:HB3	2.00	0.43
4:G:735:VAL:HG22	4:G:766:GLN:HE22	1.83	0.43
2:B:76:ARG:HH11	2:B:79:ASP:H	1.66	0.43
2:B:871:PRO:O	2:B:875:LYS:N	2.41	0.43
6:I:216:UNK:HA	6:I:220:GLN:HE21	1.84	0.43
1:A:874:GLU:HA	1:A:877:ARG:HD2	2.01	0.43
2:B:899:LYS:HA	2:B:935:PRO:HB3	2.01	0.43
6:I:263:ILE:O	6:I:267:VAL:N	2.49	0.43
6:I:309:MET:HA	6:I:312:ILE:HD12	2.01	0.43
2:B:39:ASN:HB3	2:B:44:SER:H	1.83	0.43
2:B:64:LYS:HD3	2:B:119:PRO:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:608:VAL:HG12	4:G:624:ALA:HB2	2.00	0.43
7:J:65:SER:HA	7:J:96:VAL:O	2.18	0.43
10:O:123:LEU:HA	10:O:126:TYR:HD2	1.83	0.43
4:G:552:SER:HB3	4:G:557:TYR:HB2	1.99	0.43
4:G:605:HIS:ND1	4:G:629:ASP:OD1	2.52	0.43
2:B:842:LEU:HD23	2:B:842:LEU:HA	1.88	0.42
5:H:305:ILE:HD11	5:H:340:ILE:HG21	2.01	0.42
6:I:223:TYR:HH	6:I:245:SER:HG	1.65	0.42
1:A:650:ARG:HH11	7:J:80:ILE:HD11	1.84	0.42
2:B:926:ILE:O	2:B:930:LEU:HB2	2.19	0.42
15:W:353:LEU:HB2	15:W:370:ALA:HB3	2.00	0.42
2:B:815:GLU:HA	2:B:819:LEU:HD12	2.01	0.42
6:I:274:ASN:HD21	6:I:317:LEU:H	1.67	0.42
2:B:66:ASN:N	2:B:192:CYS:O	2.45	0.42
2:B:83:ALA:HB3	2:B:129:LYS:HB2	2.01	0.42
2:B:530:LYS:HB2	2:B:552:TYR:HE1	1.84	0.42
7:J:39:LEU:HA	7:J:42:ARG:HB2	2.00	0.42
1:A:680:LEU:HD23	1:A:776:LEU:HD22	2.01	0.42
2:B:305:LYS:O	2:B:322:MET:HA	2.20	0.42
2:B:885:ASP:HA	2:B:888:ILE:HG22	2.02	0.42
1:A:749:ARG:HB3	1:A:786:CYS:HB2	2.02	0.42
2:B:49:VAL:HG12	2:B:148:ILE:HB	2.00	0.42
8:K:75:SER:O	8:K:79:TYR:CB	2.68	0.42
1:A:1007:LEU:HD22	1:A:1012:VAL:HG21	2.01	0.42
2:B:802:LEU:HD22	2:B:829:ILE:HG12	2.02	0.42
10:O:126:TYR:O	10:O:153:ARG:NE	2.53	0.42
2:B:719:MET:HE1	2:B:756:ALA:HB3	2.01	0.42
5:H:324:ASP:HA	5:H:327:TRP:CD1	2.50	0.42
6:I:337:VAL:HA	6:I:340:ILE:HD12	2.01	0.42
1:A:623:TYR:HE2	1:A:766:ARG:HE	1.66	0.41
2:B:220:LEU:HD23	2:B:236:TYR:HE1	1.85	0.41
2:B:256:ILE:HD12	2:B:277:LEU:HD12	2.02	0.41
4:G:636:HIS:HA	4:G:677:PHE:HD2	1.85	0.41
11:R:68:ARG:NH1	11:R:72:PRO:O	2.52	0.41
2:B:258:VAL:HG11	2:B:281:THR:HB	2.02	0.41
2:B:891:LEU:HD13	2:B:926:ILE:HD11	2.03	0.41
6:I:23:ALA:HB1	6:I:28:ILE:HD12	2.02	0.41
6:I:270:ASN:HA	6:I:273:GLN:HB2	2.03	0.41
2:B:318:ALA:HB2	2:B:349:SER:HA	2.01	0.41
2:B:710:VAL:HG22	2:B:762:ASP:HA	2.02	0.41
2:B:955:LYS:O	2:B:959:SER:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:355:ASP:O	16:X:6:TYR:OH	2.33	0.41
2:B:735:ILE:HD12	8:K:173:GLN:HE21	1.85	0.41
4:G:716:SER:HB2	4:G:769:LEU:HB2	2.03	0.41
4:G:766:GLN:HE21	4:G:782:HIS:CE1	2.39	0.41
6:I:374:TYR:HD1	6:I:423:VAL:HG13	1.86	0.41
2:B:68:LYS:HD3	2:B:188:PHE:HE1	1.86	0.41
5:H:386:ASP:HA	5:H:389:LYS:HB3	2.02	0.41
13:U:129:DA:H2''	13:U:130:DA:C8	2.55	0.41
2:B:848:HIS:CD2	2:B:886:ILE:HD11	2.56	0.41
4:G:249:LEU:HD22	4:G:301:ARG:HG2	2.03	0.41
5:H:366:GLU:HG2	5:H:367:LYS:H	1.86	0.41
7:J:17:ILE:O	7:J:94:MET:HA	2.20	0.41
12:T:301:VAL:HG11	14:V:11:DT:H4'	2.02	0.41
2:B:848:HIS:HB3	2:B:851:THR:HB	2.02	0.41
2:B:946:ASN:ND2	2:B:984:PRO:O	2.35	0.41
5:H:419:GLY:HA2	5:H:422:HIS:CE1	2.56	0.41
4:G:485:ILE:HG21	4:G:787:ARG:HG2	2.03	0.40
4:G:779:PRO:HA	4:G:791:VAL:HA	2.03	0.40
4:G:251:LEU:HD13	4:G:260:ALA:HA	2.04	0.40
4:G:285:LEU:HD13	4:G:297:MET:HE3	2.02	0.40
9:L:77:CYS:SG	11:R:122:ARG:NH2	2.94	0.40
4:G:594:SER:HB2	4:G:597:GLY:H	1.86	0.40
5:H:278:LEU:HD23	5:H:281:TYR:HD2	1.87	0.40
1:A:827:MET:HE2	1:A:862:TRP:HE1	1.87	0.40
3:D:910:LEU:HD23	3:D:913:LEU:HD12	2.04	0.40
4:G:486:ALA:HA	4:G:492:SER:HA	2.03	0.40
4:G:783:LEU:HD23	4:G:783:LEU:HA	1.80	0.40
5:H:257:PRO:HG3	5:H:300:TYR:CZ	2.56	0.40
12:T:292:ILE:HG12	14:V:11:DT:H5''	2.03	0.40
2:B:62:ARG:HG2	2:B:129:LYS:HG2	2.02	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	A	437/496 (88%)	431 (99%)	4 (1%)	2 (0%)	24	63
2	B	966/1199 (81%)	823 (85%)	143 (15%)	0	100	100
3	D	124/1025 (12%)	118 (95%)	6 (5%)	0	100	100
4	G	429/800 (54%)	382 (89%)	47 (11%)	0	100	100
5	H	255/677 (38%)	237 (93%)	17 (7%)	1 (0%)	30	67
6	I	326/677 (48%)	303 (93%)	21 (6%)	2 (1%)	21	59
7	J	119/349 (34%)	117 (98%)	2 (2%)	0	100	100
8	K	149/310 (48%)	140 (94%)	9 (6%)	0	100	100
9	L	96/264 (36%)	93 (97%)	3 (3%)	0	100	100
10	O	78/218 (36%)	74 (95%)	4 (5%)	0	100	100
11	R	72/161 (45%)	70 (97%)	2 (3%)	0	100	100
12	T	178/339 (52%)	175 (98%)	3 (2%)	0	100	100
15	W	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
16	X	95/97 (98%)	91 (96%)	3 (3%)	1 (1%)	11	46
All	All	3410/6702 (51%)	3139 (92%)	265 (8%)	6 (0%)	44	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	LEU
1	A	950	VAL
16	X	86	GLU
6	I	256	LEU
6	I	257	PRO
5	H	321	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/437 (90%)	393 (100%)	0	100	100
2	B	879/1083 (81%)	878 (100%)	1 (0%)	88	89
3	D	52/771 (7%)	52 (100%)	0	100	100
4	G	367/619 (59%)	366 (100%)	1 (0%)	86	86
5	H	200/574 (35%)	200 (100%)	0	100	100
6	I	252/564 (45%)	251 (100%)	1 (0%)	84	84
7	J	113/322 (35%)	113 (100%)	0	100	100
8	K	132/223 (59%)	132 (100%)	0	100	100
9	L	61/229 (27%)	60 (98%)	1 (2%)	55	70
10	O	71/154 (46%)	71 (100%)	0	100	100
11	R	70/141 (50%)	70 (100%)	0	100	100
12	T	155/293 (53%)	155 (100%)	0	100	100
15	W	84/84 (100%)	84 (100%)	0	100	100
16	X	89/89 (100%)	88 (99%)	1 (1%)	65	76
All	All	2918/5583 (52%)	2913 (100%)	5 (0%)	85	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	343	ARG
4	G	558	LEU
6	I	347	THR
9	L	73	LEU
16	X	79	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	802	HIS
1	A	1073	GLN
2	B	100	GLN
2	B	217	ASN
2	B	227	HIS
2	B	454	HIS
2	B	462	ASN
2	B	471	GLN
2	B	486	GLN

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Mol	Chain	Res	Type
2	B	489	GLN
2	B	538	ASN
2	B	542	ASN
2	B	550	GLN
2	B	792	ASN
2	B	838	ASN
2	B	848	HIS
2	B	924	HIS
2	B	946	ASN
3	D	879	GLN
3	D	904	HIS
4	G	232	HIS
4	G	246	HIS
4	G	271	GLN
4	G	320	HIS
4	G	327	ASN
4	G	331	ASN
4	G	336	HIS
4	G	710	HIS
4	G	733	ASN
4	G	766	GLN
5	H	273	GLN
5	H	398	GLN
6	I	220	GLN
6	I	244	GLN
6	I	326	HIS
6	I	350	ASN
6	I	385	HIS
6	I	430	HIS
8	K	173	GLN
9	L	76	GLN
10	O	160	GLN
11	R	75	GLN
11	R	119	HIS
11	R	125	ASN
12	T	193	ASN
15	W	343	HIS
15	W	352	HIS

5.3.3 RNA ⓘ

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
17	Z	8
15	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	95:UNK	C	119:UNK	N	129.92
1	Z	52:UNK	C	81:UNK	N	114.22
1	Z	143:UNK	C	195:UNK	N	96.41
1	Z	223:UNK	C	309:UNK	N	55.85
1	Z	386:UNK	C	401:UNK	N	34.49
1	Z	328:UNK	C	358:UNK	N	34.04
1	Z	428:UNK	C	551:UNK	N	25.25
1	W	51:MET	C	330:ASP	N	15.43
1	Z	571:UNK	C	573:UNK	N	4.33

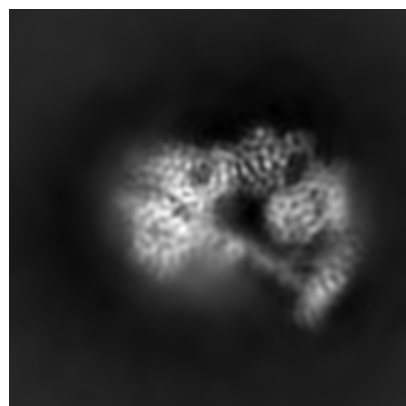
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9306. These allow visual inspection of the internal detail of the map and identification of artifacts.

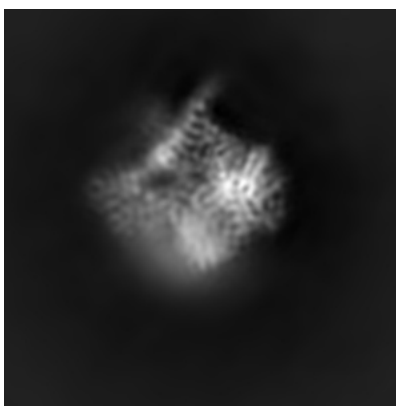
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

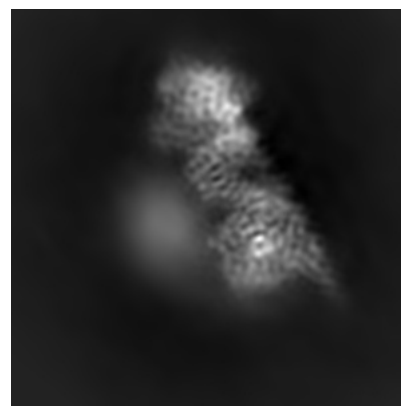
6.1.1 Primary map



X

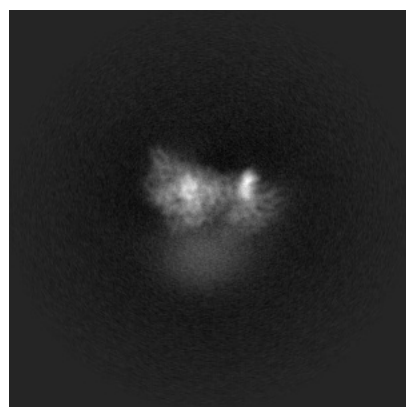


Y

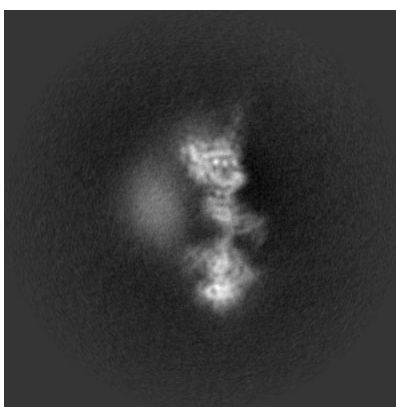


Z

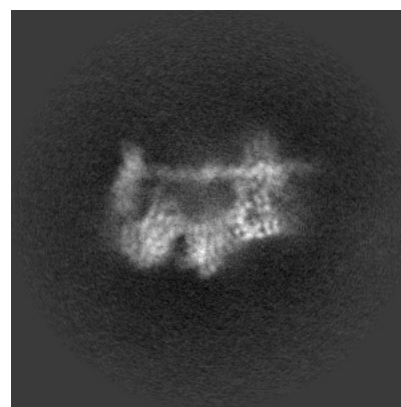
6.1.2 Raw map



X



Y

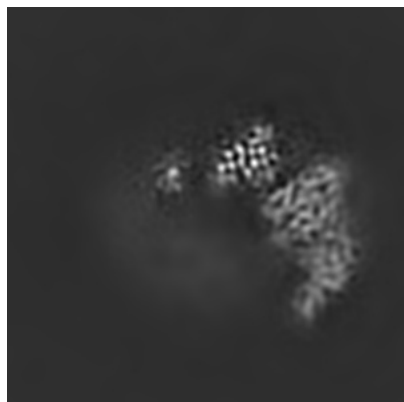


Z

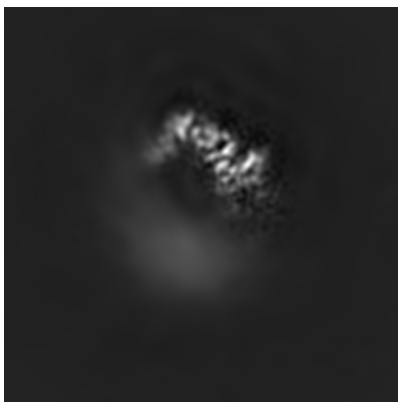
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 144

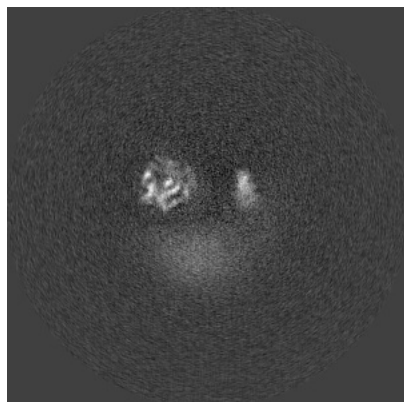


Y Index: 144

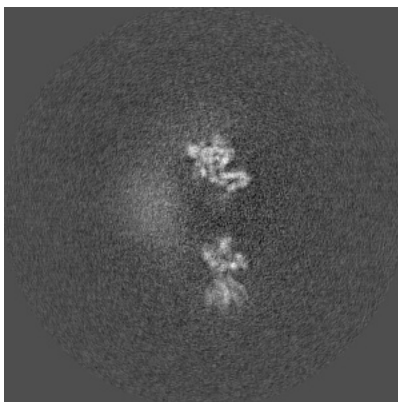


Z Index: 144

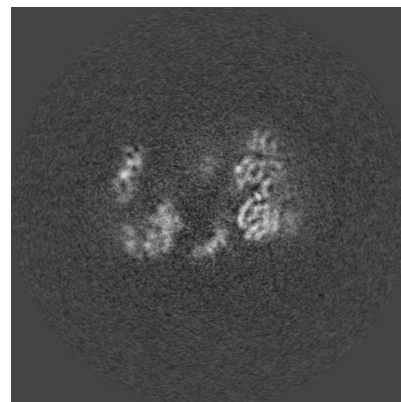
6.2.2 Raw map



X Index: 192



Y Index: 192

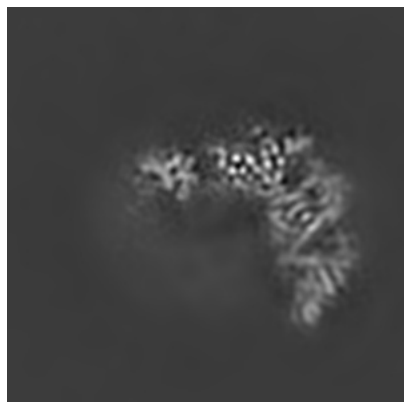


Z Index: 192

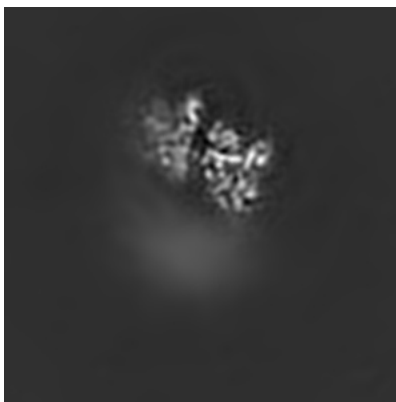
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

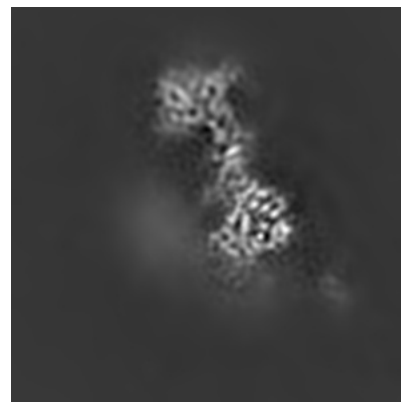
6.3.1 Primary map



X Index: 153

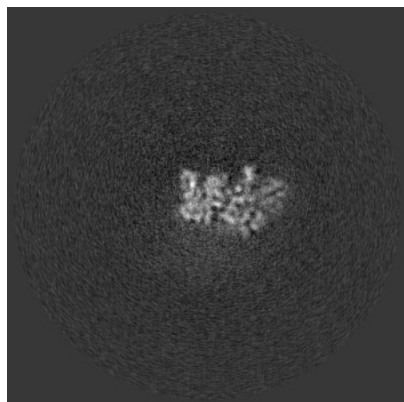


Y Index: 122

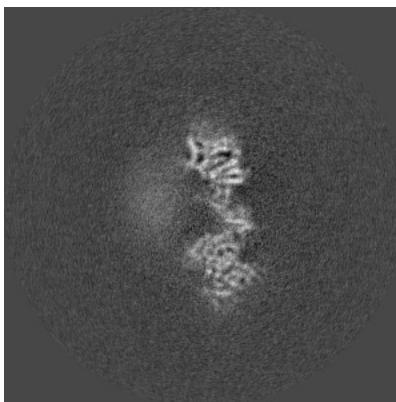


Z Index: 158

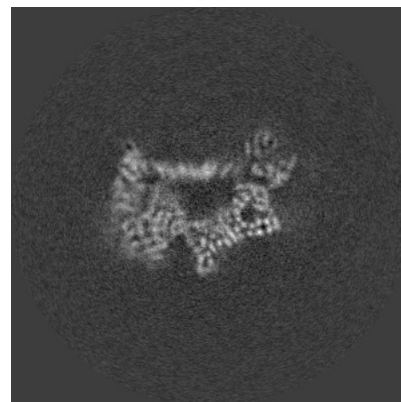
6.3.2 Raw map



X Index: 245



Y Index: 172



Z Index: 213

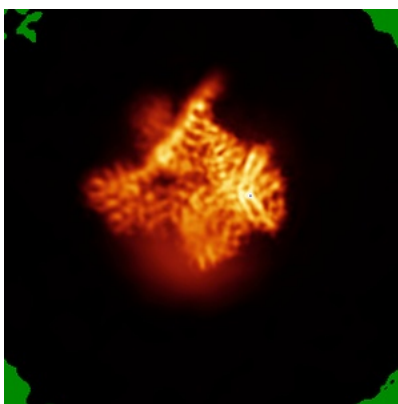
The images above show the largest variance slices of the map in three orthogonal directions.

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

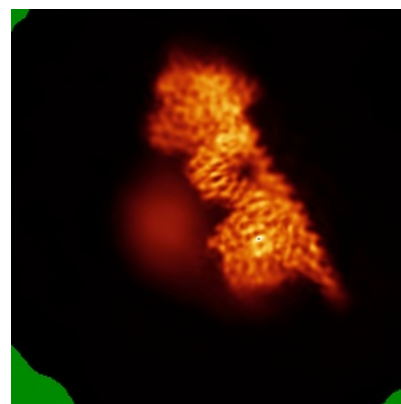
6.4.1 Primary map



X

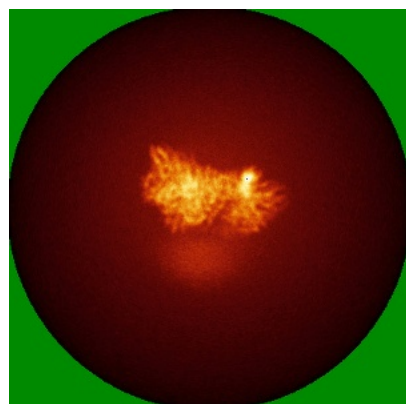


Y

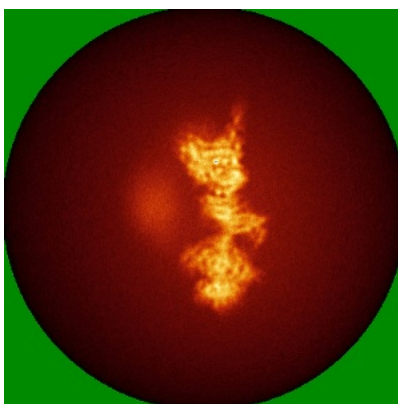


Z

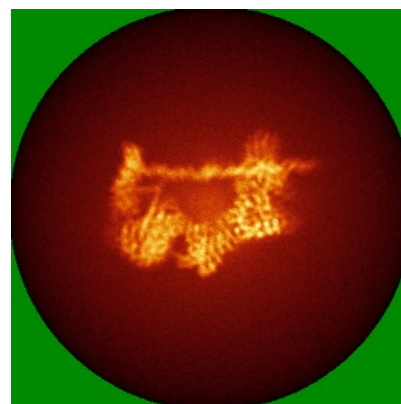
6.4.2 Raw map



X



Y

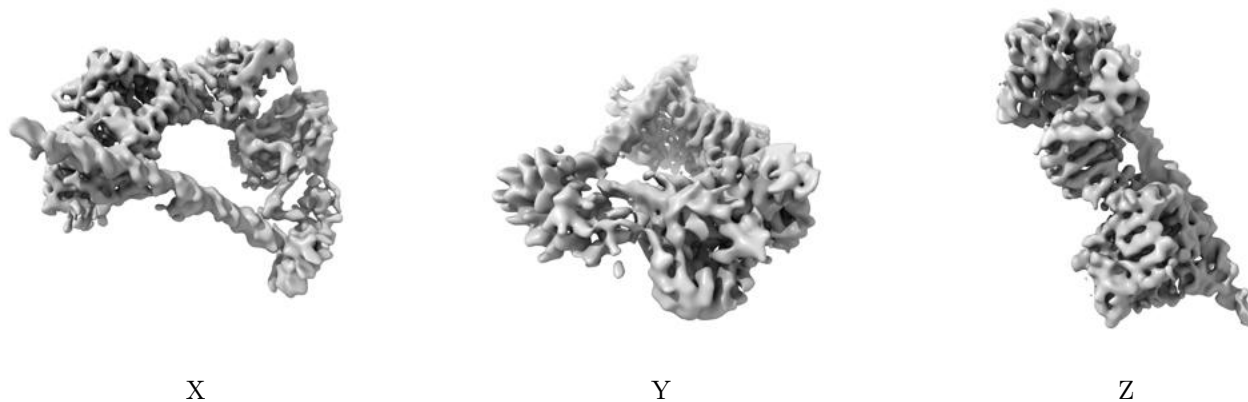


Z

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.

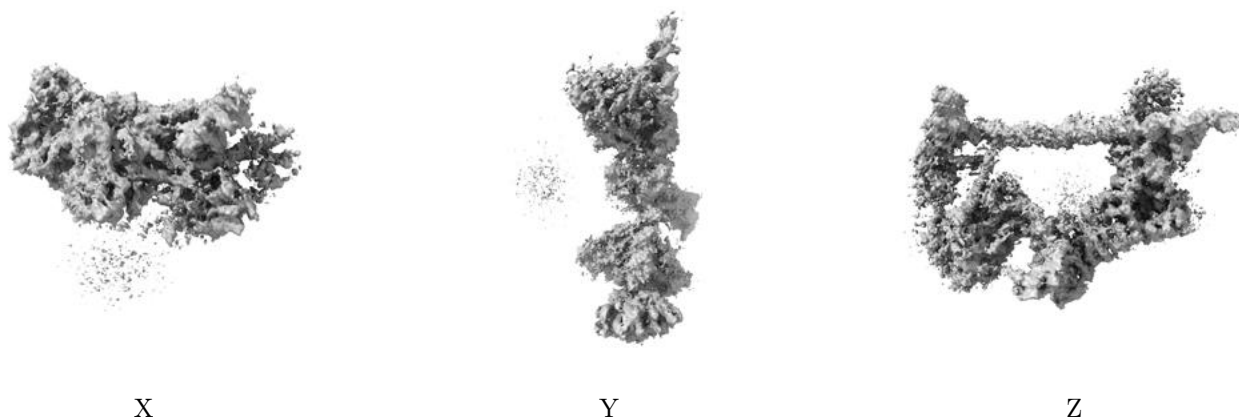
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

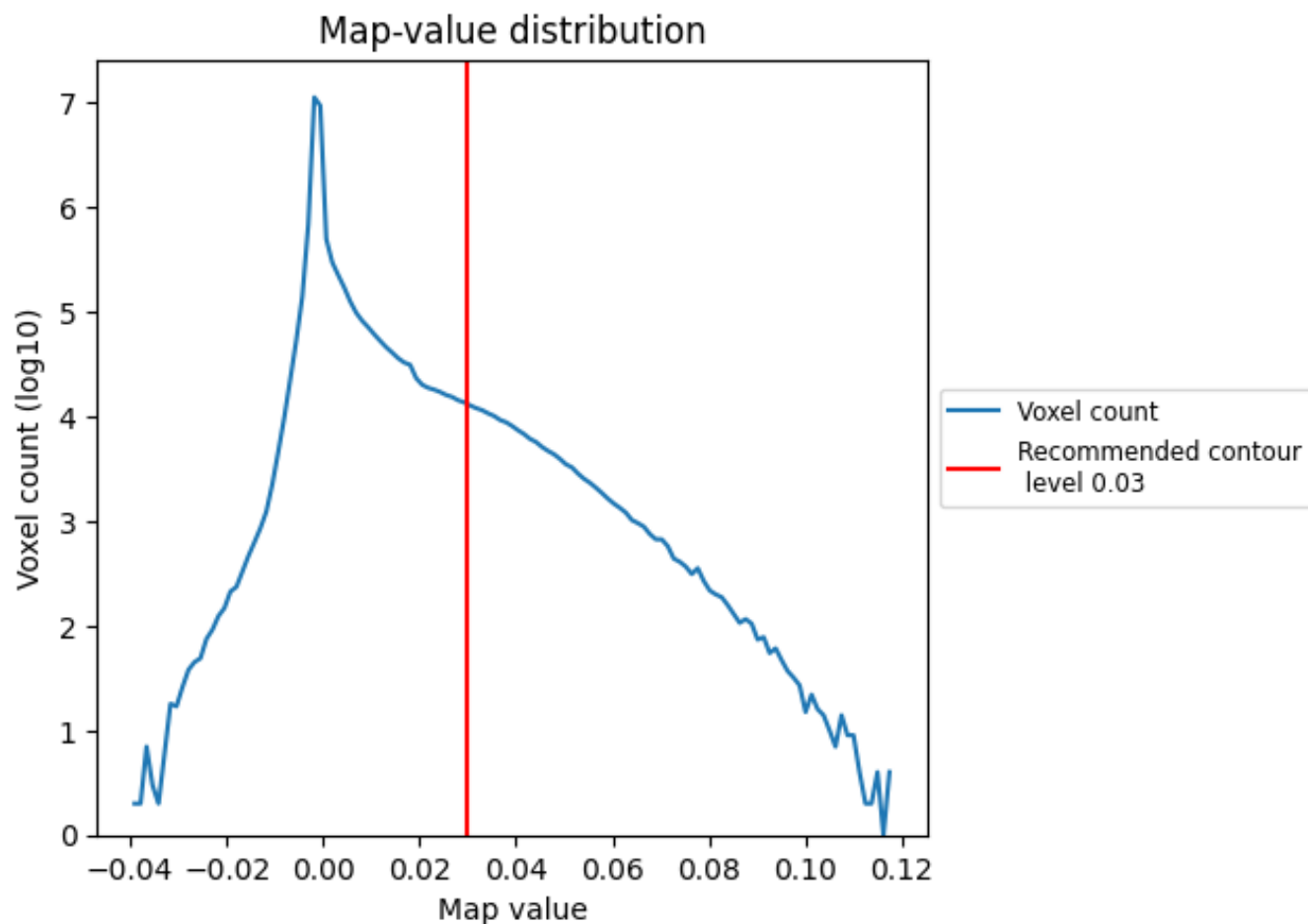
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

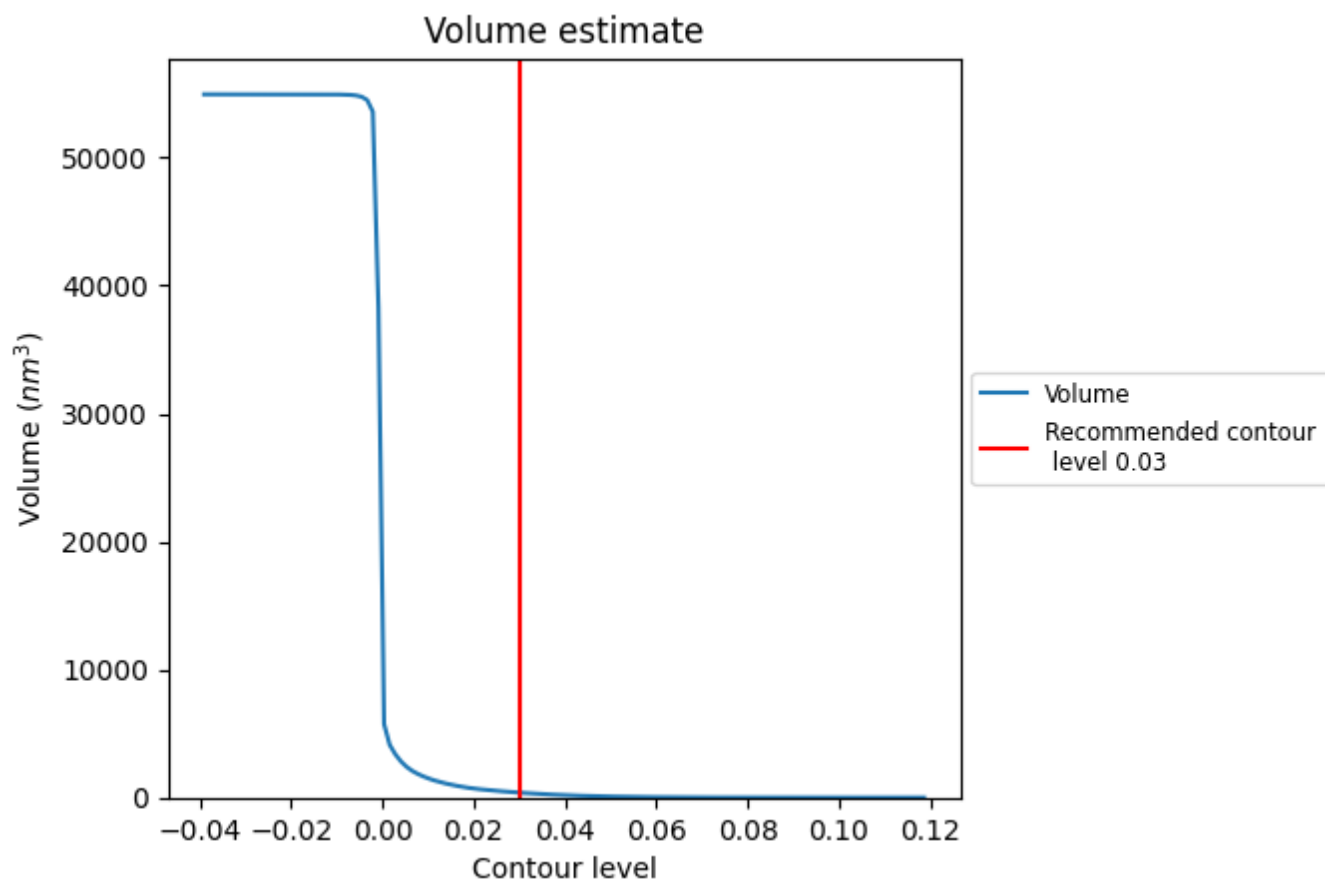
This section contains the results of statistical analysis of the map.

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.

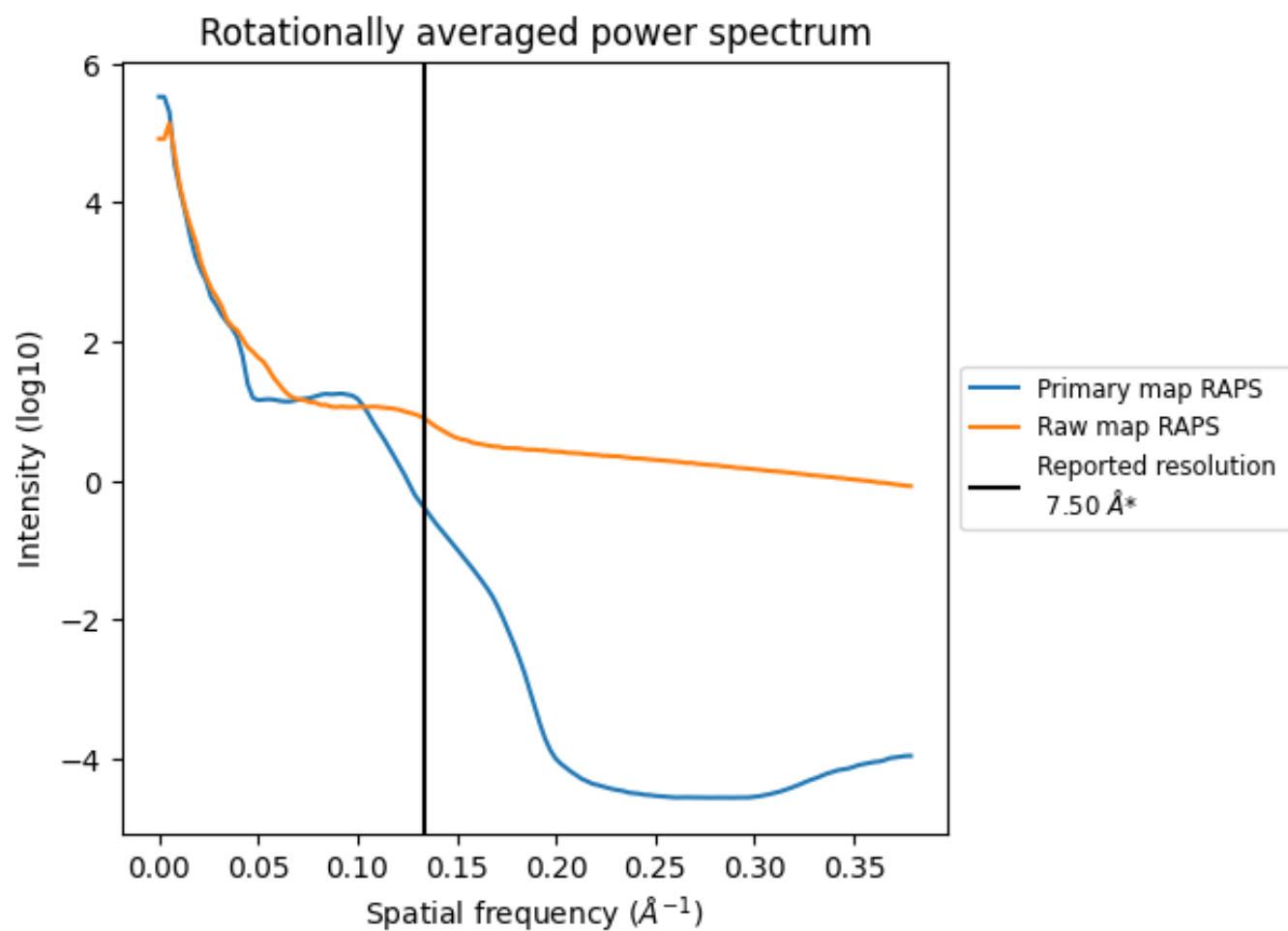
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 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 ⓘ

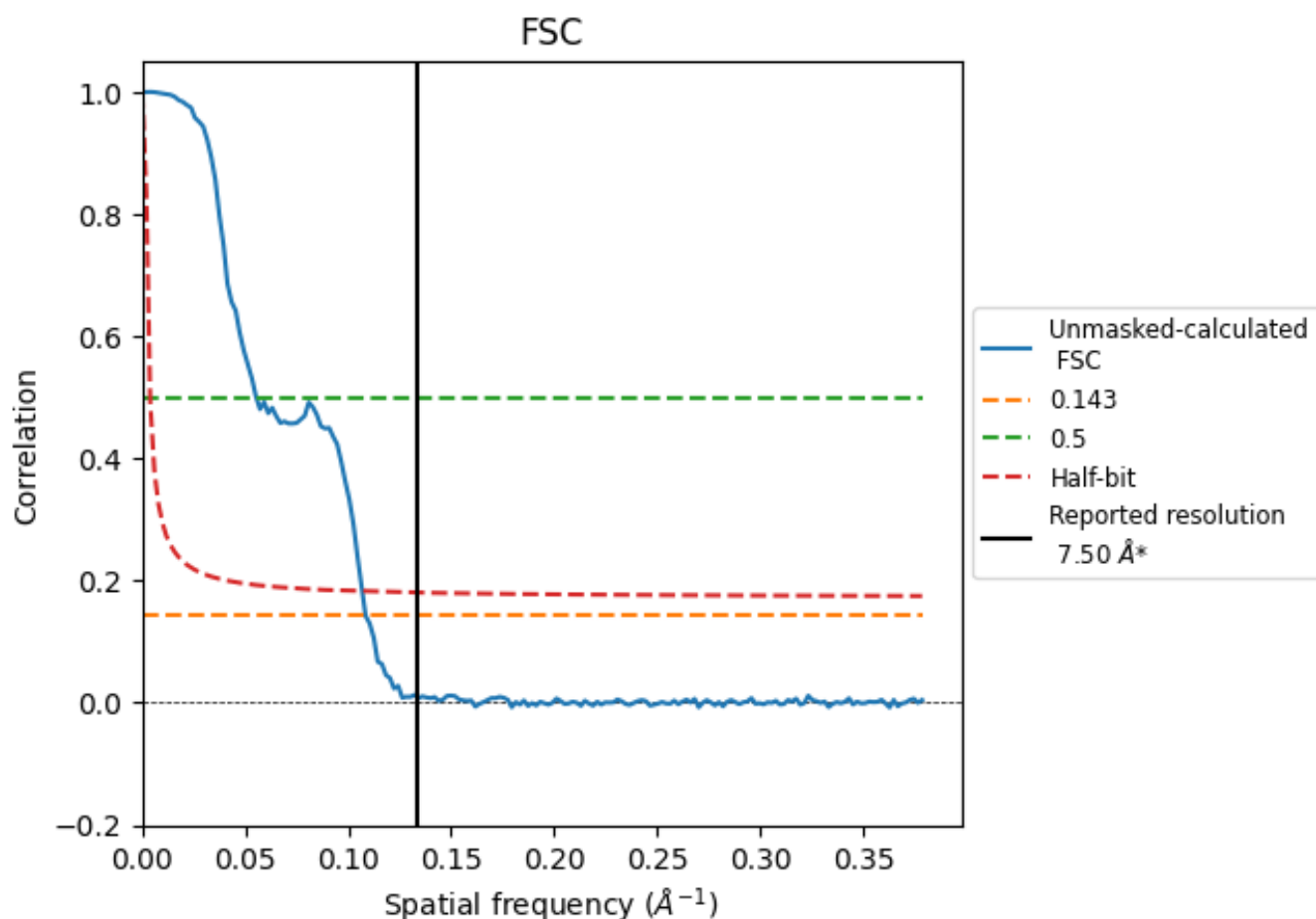


*Reported resolution corresponds to spatial frequency of 0.133 Å⁻¹

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 0.133 Å⁻¹

8.2 Resolution estimates [i](#)

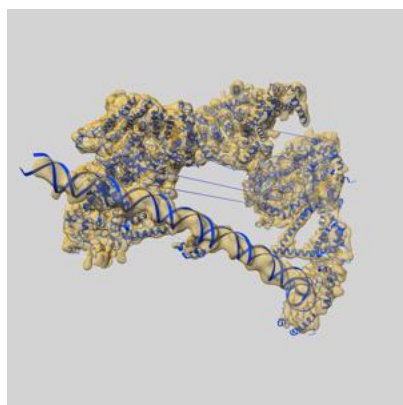
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.22	18.05	9.35

*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 9.22 differs from the reported value 7.5 by more than 10 %

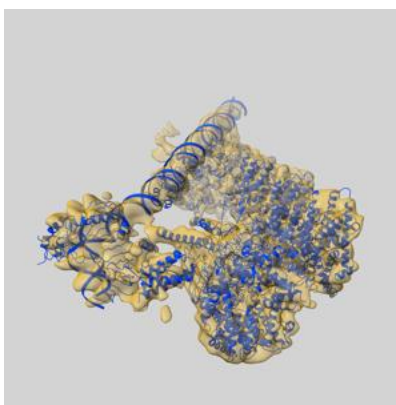
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9306 and PDB model 6MZM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

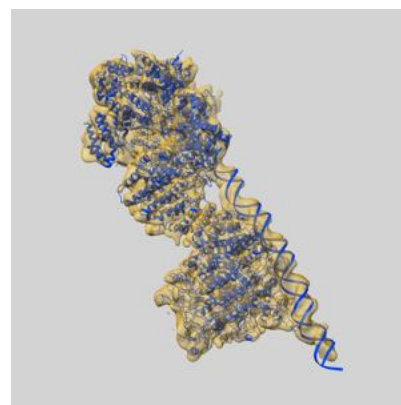
9.1 Map-model overlay [i](#)



X



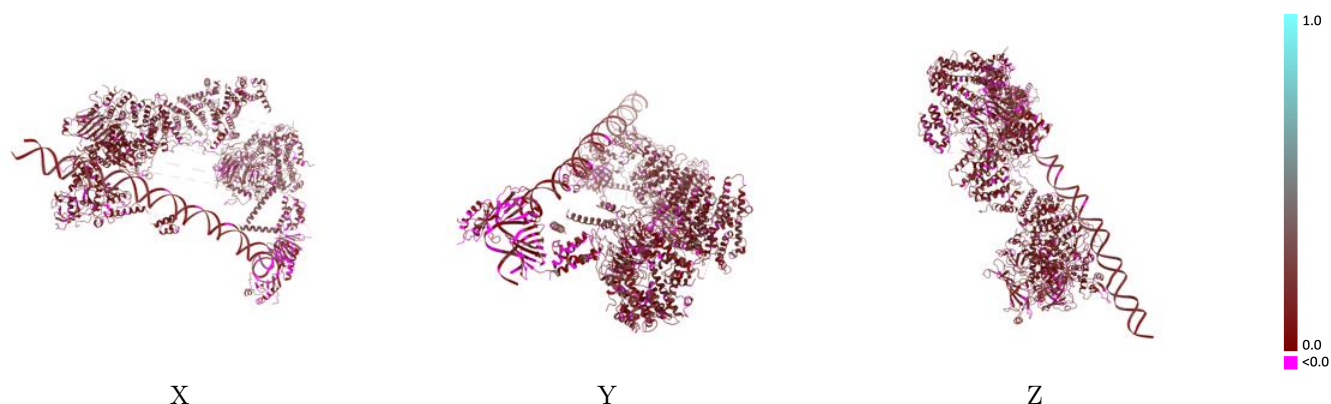
Y



Z

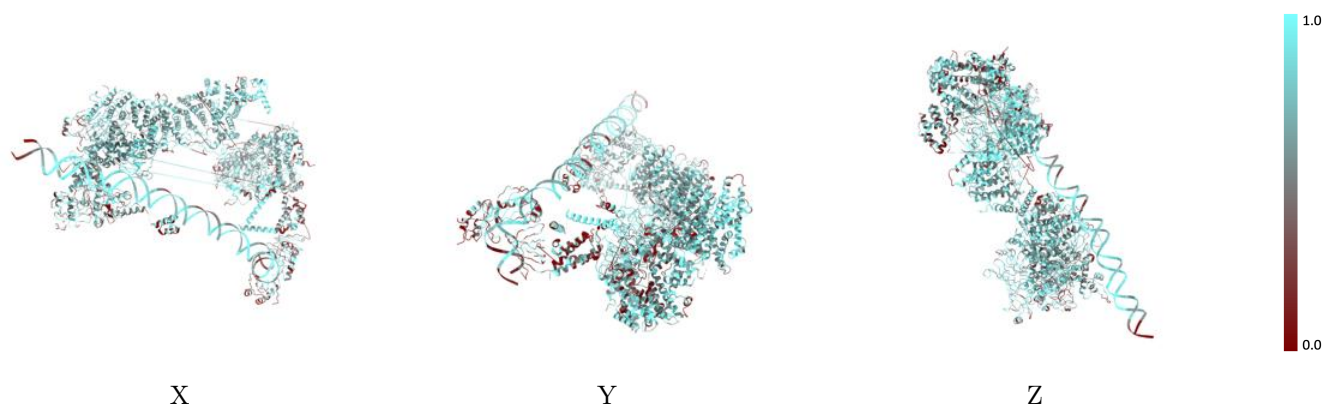
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



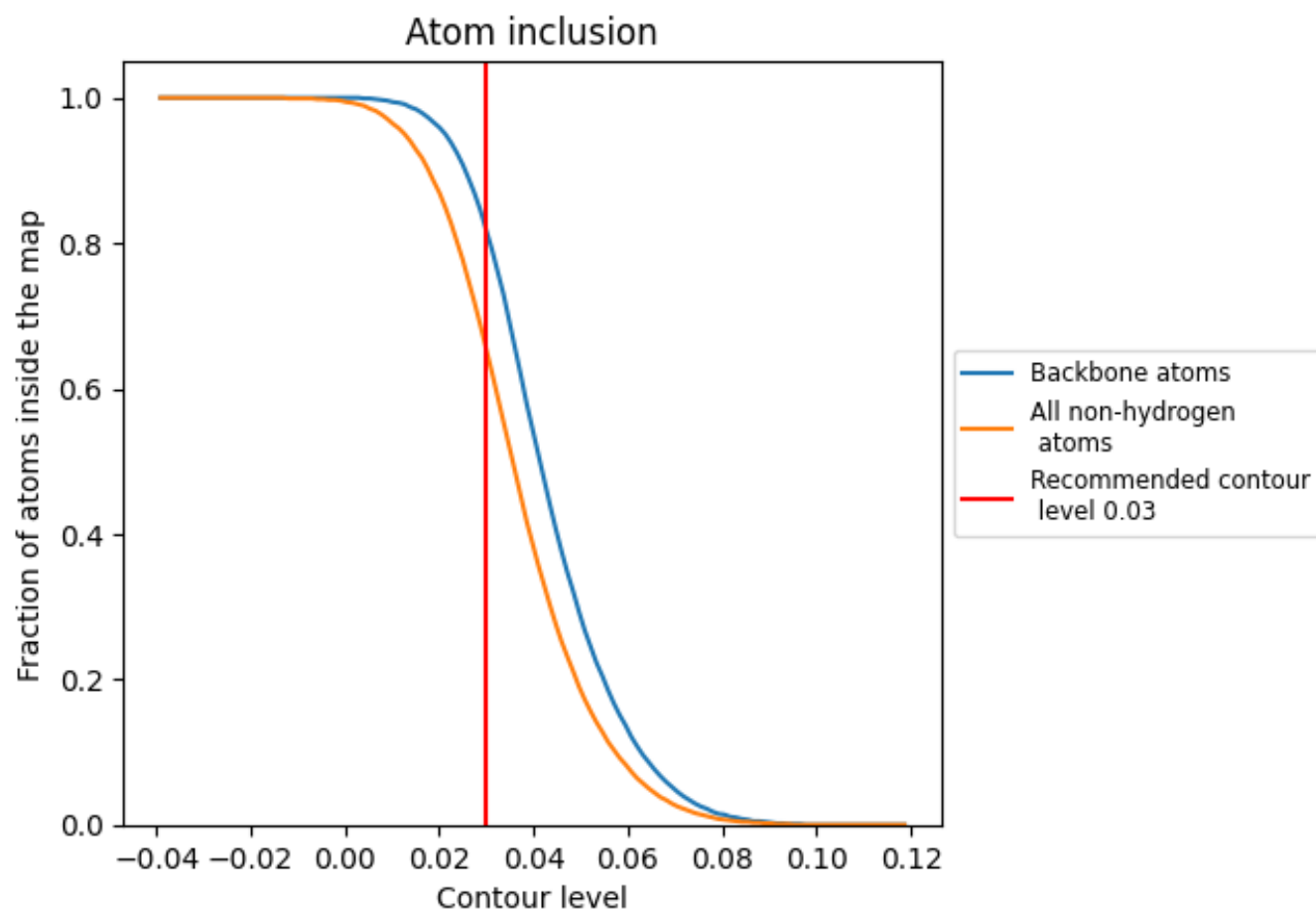
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 65% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6540	 0.1350
A	 0.5890	 0.1280
B	 0.6840	 0.1460
D	 0.7430	 0.1970
G	 0.6550	 0.1160
H	 0.7130	 0.1520
I	 0.7050	 0.1420
J	 0.5950	 0.1050
K	 0.6580	 0.1590
L	 0.7170	 0.1700
O	 0.6510	 0.1420
R	 0.5760	 0.1460
T	 0.4820	 0.0480
U	 0.7070	 0.1370
V	 0.7070	 0.1340
W	 0.5140	 0.0710
X	 0.4370	 0.0390
Z	 0.7250	 0.2280

