



Full wwPDB EM Validation Report ⓘ

Feb 27, 2024 – 10:00 AM EST

PDB ID : 6V8O
EMDB ID : EMD-21107
Title : RSC core
Authors : Patel, A.B.; Moore, C.M.; Greber, B.J.; Nogales, E.
Deposited on : 2019-12-11
Resolution : 3.07 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:

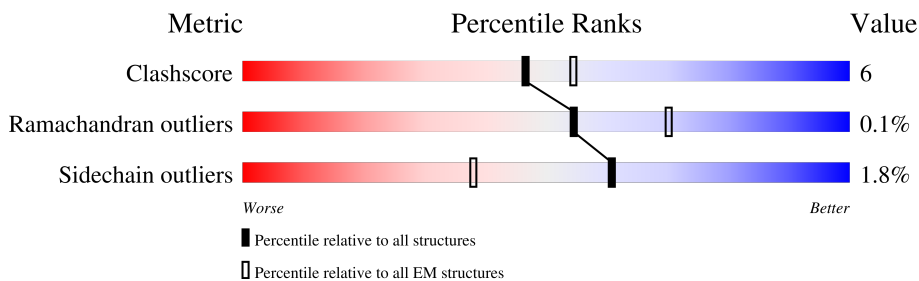
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.07 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	78	
2	D	180	
3	E	435	
4	F	889	
5	G	885	
6	H	625	
7	I	557	
7	J	557	

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Mol	Chain	Length	Quality of chain
7	K	557	
7	L	557	
8	M	483	
9	N	581	
10	O	502	
11	Q	426	
12	R	1359	
13	S	883	
14	2	28	
15	3	19	
15	4	19	
16	5	14	
17	6	15	
18	7	49	

2 Entry composition i

There are 19 unique types of molecules in this entry. The entry contains 25103 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 High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	60	493	301	92	96	4	0	0

- Molecule 2 is a protein called Chromatin structure-remodeling complex protein RSC14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	100	772	490	132	148	2	0	0

- Molecule 3 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	120	978	610	166	200	2	0	0

- Molecule 4 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	67	536	346	94	95	1	0	0

- Molecule 5 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	53	422	270	71	79	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	767	SER	THR	conflict	UNP Q06639

- Molecule 6 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1083	696	175	205	7		

- Molecule 7 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	293	Total	C	N	O	S	0	0
			2416	1537	423	448	8		
7	J	115	Total	C	N	O	S	0	0
			924	579	149	190	6		
7	K	109	Total	C	N	O	S	0	0
			878	554	139	179	6		
7	L	298	Total	C	N	O	S	0	0
			2445	1557	428	452	8		

- Molecule 8 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	310	Total	C	N	O	S	0	0
			2474	1558	414	496	6		

- Molecule 9 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	412	Total	C	N	O	S	0	0
			3275	2105	540	612	18		

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	384	Total	C	N	O	S	0	0
			3145	2025	529	581	10		

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	264	Total	C	N	O	S	0	0
			2137	1349	362	418	8		

- Molecule 12 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R	262	2126	1339	378	407	2	0	0

- Molecule 13 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S	34	278	182	41	54	1	0	0

- Molecule 14 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	2	28	140	84	28	28	0	0

- Molecule 15 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	3	19	95	57	19	19	0	0
15	4	19	95	57	19	19	0	0

- Molecule 16 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	5	14	70	42	14	14	0	0

- Molecule 17 is a protein called Unknown Protein.

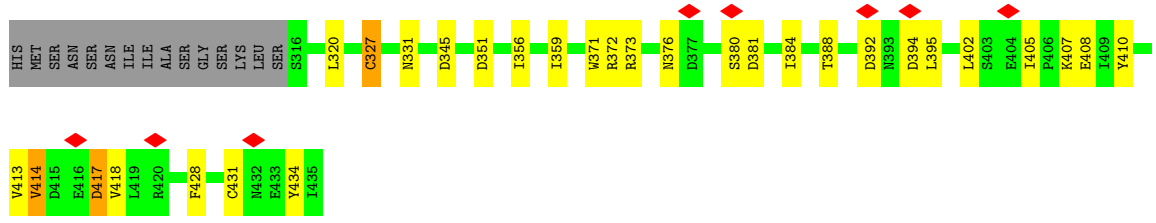
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	6	15	75	45	15	15	0	0

- Molecule 18 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	7	49	245	147	49	49	0	0

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

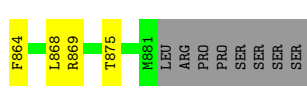
Mol	Chain	Residues	Atoms		AltConf
19	I	1	Total 1	Zn 1	0



• Molecule 4: Chromatin structure-remodeling complex subunit RSC2

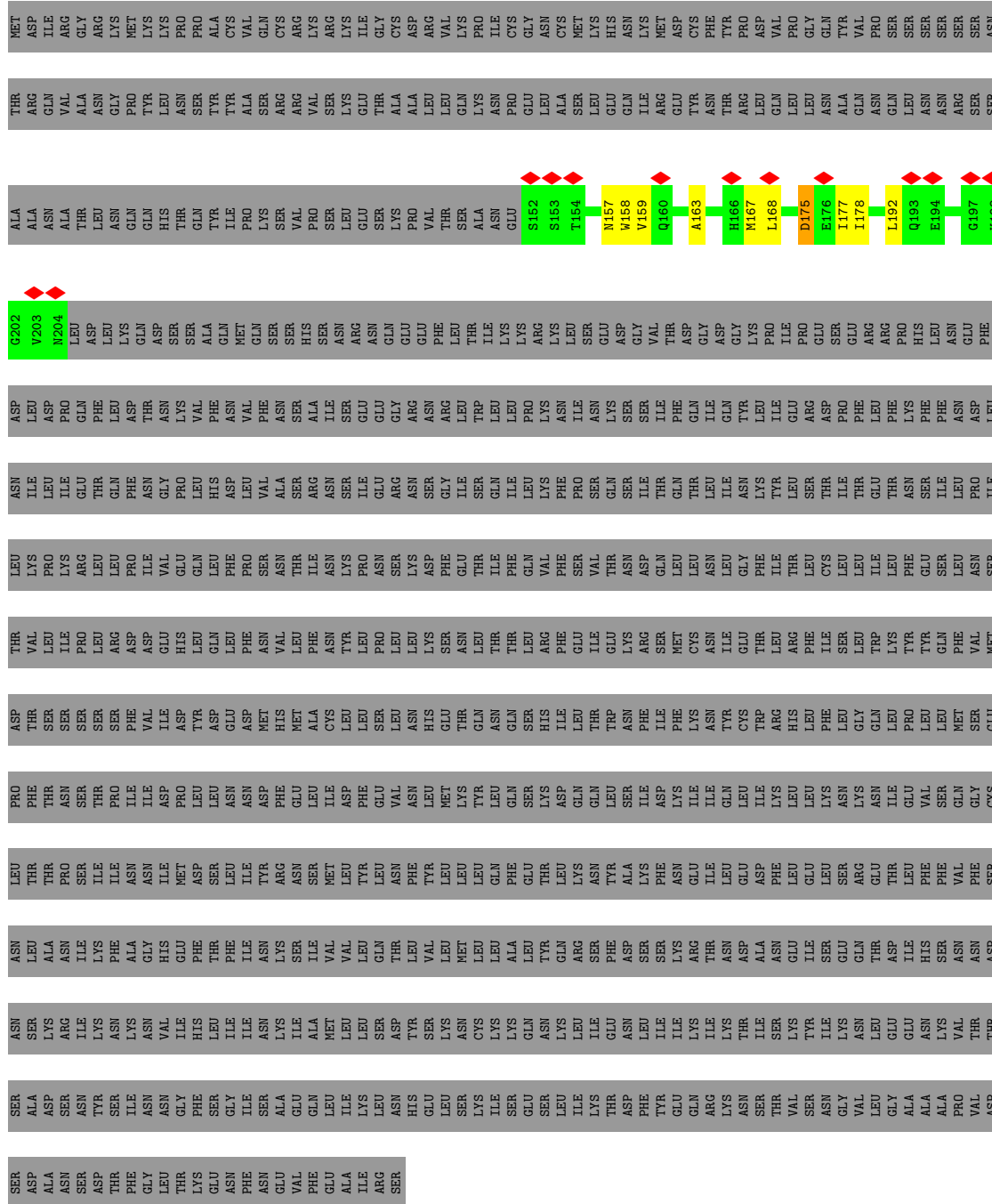
Chain F: 6% 92%

MET	MET	PRO	PRO	ASP	ASP	ASN	ASN	SER	SER	ILE	ILE	ALA	GLY	SER	SER	LEU	SER	S316
ASN	PRO	VAL	SER	PHE	ASN	THR	THR	LEU	LEU	LEU	LEU	VAL	GLN	THR	THR	ALA	ALA	L320
LEU	LYS	GLU	GLY	TYR	PRO	PRO	GLN	LEU	VAL	ASP	ASP	PRO	GLY	THR	THR	ASP	GLN	C327
LYS	THR	ARG	THR	SER	VAL	VAL	LYS	GLY	ARG	GLY	THR	THR	ASP	THR	ASP	GLY	GLY	M331
SER	THR	THR	PRO	PRO	HIS	HIS	GLY	THR	THR	PRO	ARG	HIS	GLN	VAL	GLN	VAL	VAL	D345
ASP	LEU	PHE	GLU	ARG	LEU	PRO	ASP	PRO	ARG	ILE	ILE	ILE	ILE	GLN	ASP	ASP	ASP	D351
ASP	PRO	GLU	ILE	ILE	SER	ASN	THR	PHE	THR	THR	THR	THR	THR	GLY	GLY	GLY	GLY	I356
GLN	ASN	ASP	PRO	GLN	PRO	ILE	THR	THR	THR	TRP	TRP	TRP	TRP	ALA	ASP	ASP	ASP	I359
SER	ASN	VAL	VAL	VAL	TYR	GLY	ASN	PRO	ASP	GLY	GLY	GLY	GLY	VAL	VAL	VAL	VAL	M371
GLU	ALA	THR	ILE	THR	ASP	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	R372
GLY	TYR	ALA	ALA	VAL	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	R373
SER	ASN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	M376
GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	D377
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	S380
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	D381
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	I384
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	T388
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	D392
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	M393
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	D394
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	L395
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	L402
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	S403
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	E404
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	I405
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	K407
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	E408
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	I409
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	Y410



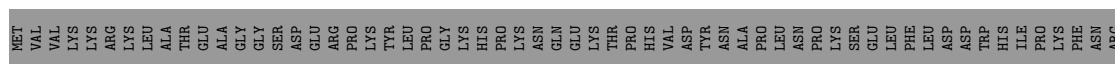
• Molecule 5: Chromatin structure-remodeling complex protein RSC3

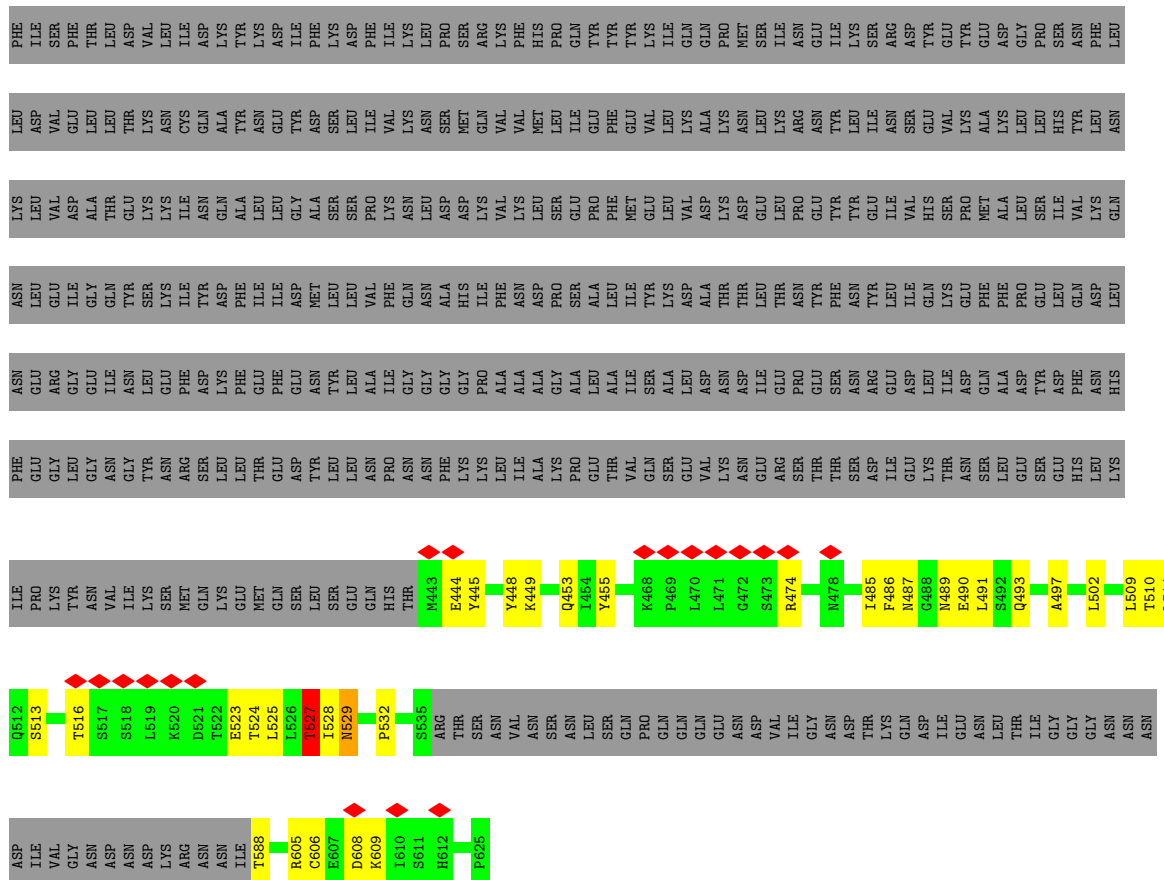
Chain G: 5% 94%



• Molecule 6: Chromatin structure-remodeling complex subunit RSC4

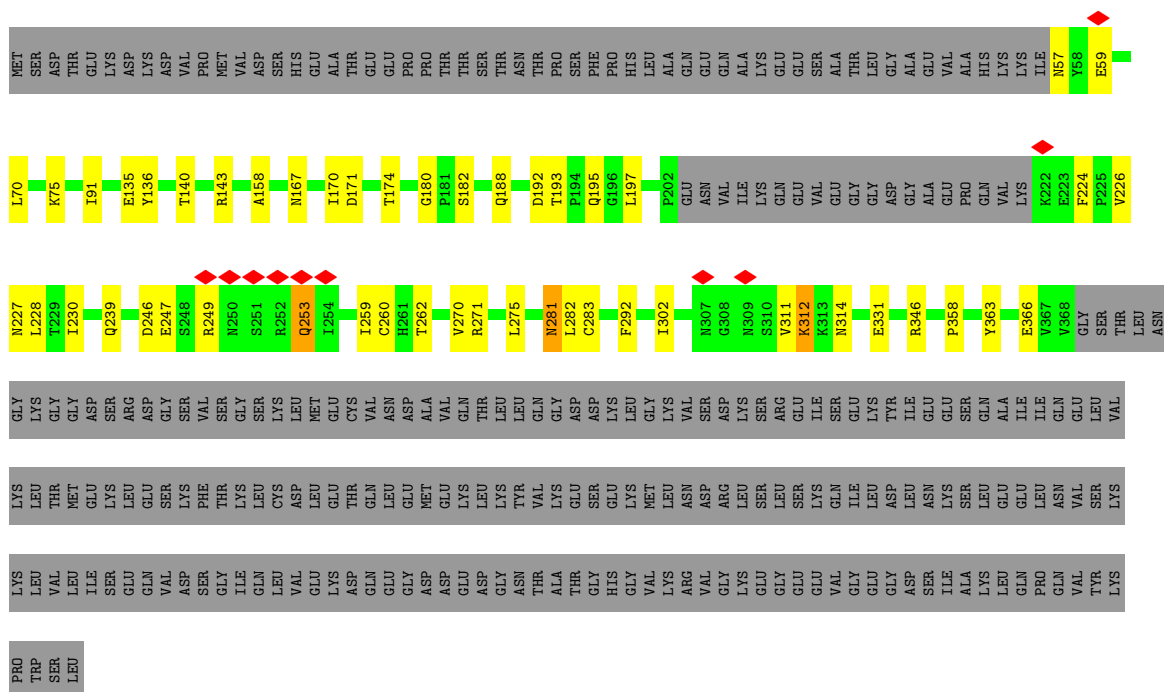
Chain H: 16% 5% 79%

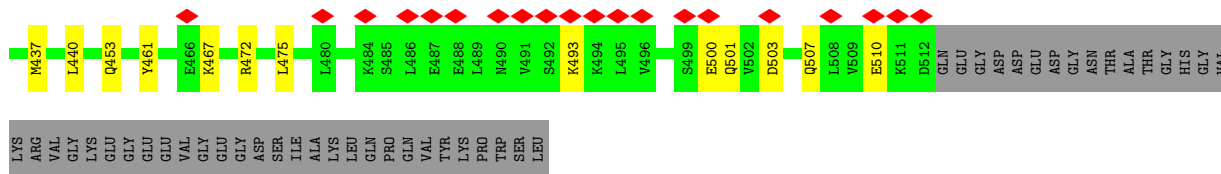




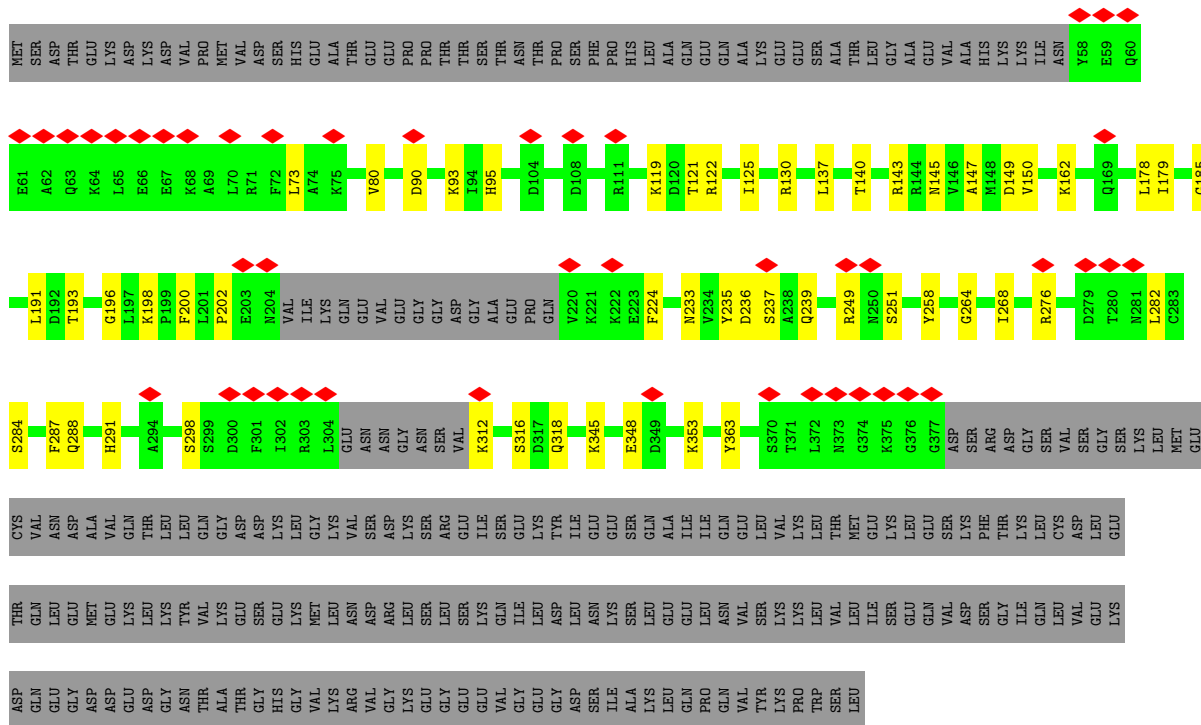
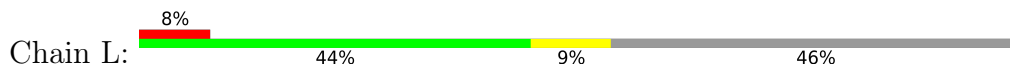
● Molecule 7: Chromatin structure-remodeling complex protein RSC8

Chain I: 44% 8% 47%

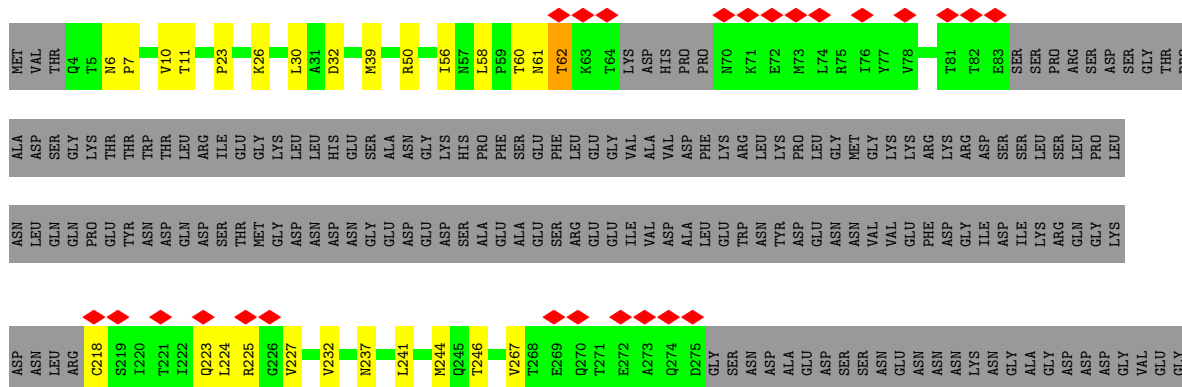




• Molecule 7: Chromatin structure-remodeling complex protein RSC8

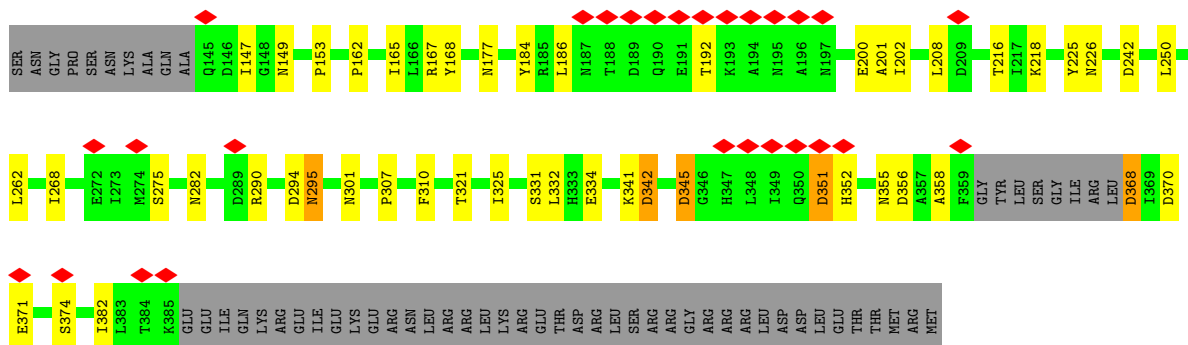
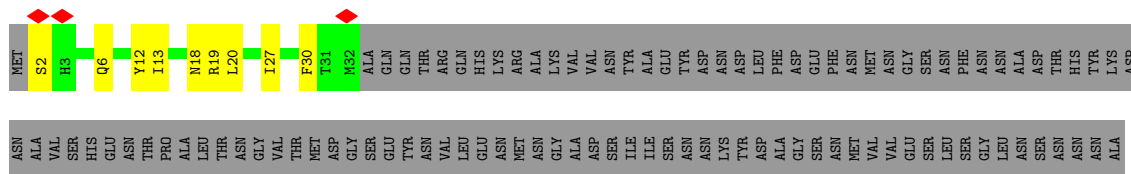


• Molecule 8: Chromatin structure-remodeling complex protein RSC6

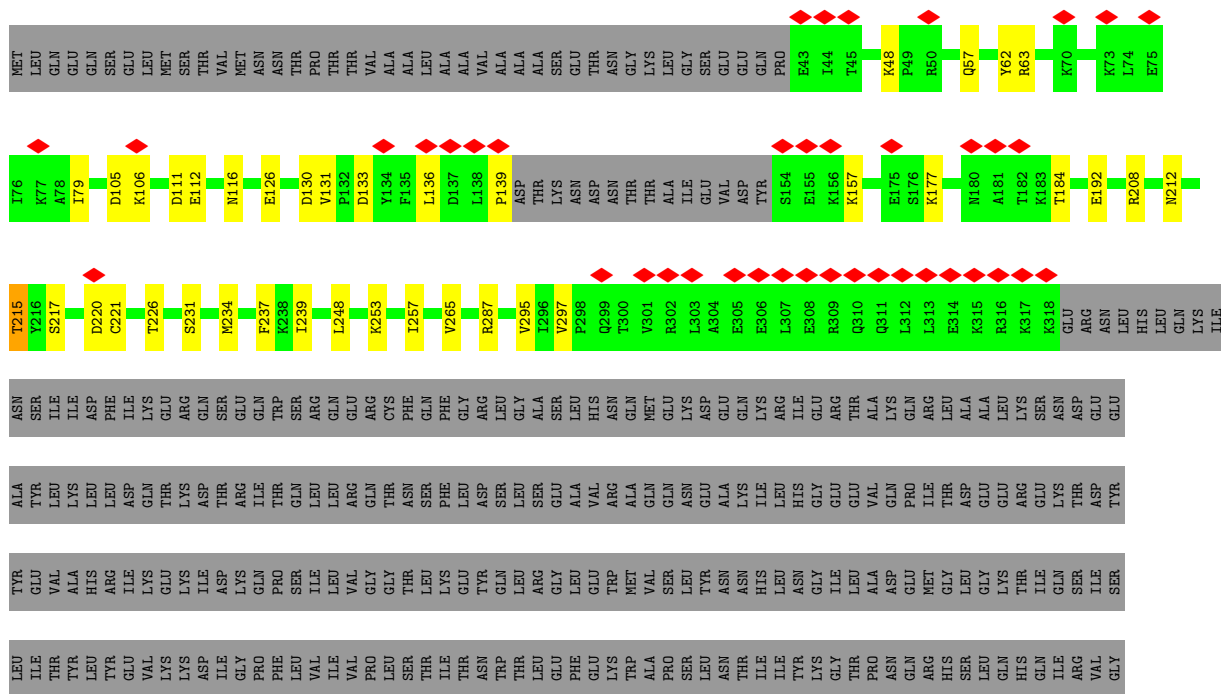


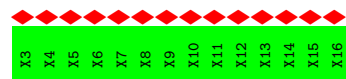


• Molecule 11: Chromatin structure-remodeling complex subunit SFH1

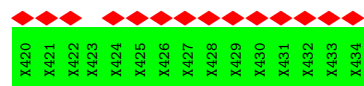
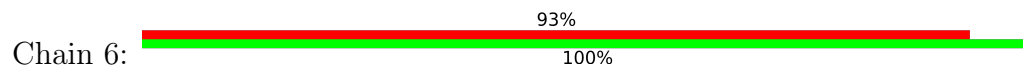


• Molecule 12: Nuclear protein STH1/NPS1

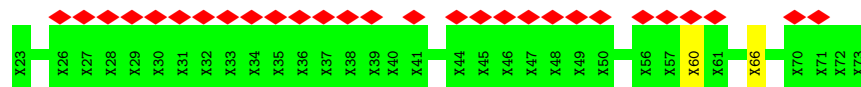




• Molecule 17: Unknown Protein



• Molecule 18: Unknown Protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1920066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	414.432, 414.432, 414.432	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.439, 1.439, 1.439	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	C	0.24	0/495	0.36	0/662
2	D	0.27	0/786	0.38	0/1062
3	E	0.28	0/997	0.44	0/1356
4	F	0.27	0/551	0.41	0/748
5	G	0.26	0/431	0.43	0/584
6	H	0.29	0/1108	0.48	0/1497
7	I	0.32	0/2474	0.41	0/3343
7	J	0.30	0/926	0.40	0/1233
7	K	0.27	0/879	0.39	0/1172
7	L	0.29	0/2502	0.40	0/3376
8	M	0.28	0/2515	0.42	0/3423
9	N	0.30	0/3334	0.42	0/4515
10	O	0.30	0/3216	0.42	1/4358 (0.0%)
11	Q	0.27	0/2181	0.45	0/2964
12	R	0.27	0/2154	0.40	0/2897
13	S	0.26	0/281	0.35	0/378
All	All	0.29	0/24830	0.42	1/33568 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	231	VAL	C-N-CA	5.36	135.09	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	493	0	507	6	0
2	D	772	0	754	11	0
3	E	978	0	935	24	0
4	F	536	0	533	14	0
5	G	422	0	423	10	0
6	H	1083	0	1062	22	0
7	I	2416	0	2358	35	0
7	J	924	0	976	10	0
7	K	878	0	930	14	0
7	L	2445	0	2402	47	0
8	M	2474	0	2465	51	0
9	N	3275	0	3373	51	0
10	O	3145	0	3168	50	0
11	Q	2137	0	2069	39	0
12	R	2126	0	2205	34	0
13	S	278	0	287	6	0
14	2	140	0	34	1	0
15	3	95	0	21	0	0
15	4	95	0	21	1	0
16	5	70	0	16	0	0
17	6	75	0	17	0	0
18	7	245	0	63	2	0
19	I	1	0	0	0	0
All	All	25103	0	24619	323	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 6.

All (323) 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)
11:Q:282:ASN:OD1	11:Q:295:ASN:ND2	2.20	0.75
9:N:217:GLU:OE1	12:R:287:ARG:NH1	2.21	0.74
2:D:96:GLN:NE2	15:4:15:UNK:O	2.22	0.72
4:F:813:LEU:HD11	10:O:183:ILE:HD12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:268:ILE:HD11	10:O:232:LEU:HD22	1.73	0.70
7:I:136:TYR:O	7:I:167:ASN:ND2	2.26	0.69
9:N:345:SER:HA	9:N:348:ILE:HD11	1.75	0.68
10:O:35:PHE:O	10:O:73:LEU:N	2.26	0.68
12:R:231:SER:HB3	12:R:234:MET:HG2	1.75	0.68
7:I:135:GLU:OE2	11:Q:19:ARG:NH2	2.27	0.68
9:N:220:HIS:NE2	10:O:296:GLU:O	2.27	0.68
1:C:20:THR:HG22	10:O:275:ALA:H	1.58	0.68
3:E:376:ASN:ND2	3:E:381:ASP:O	2.27	0.67
7:L:178:LEU:HD21	11:Q:325:ILE:HD11	1.76	0.67
8:M:218:CYS:SG	18:7:60:UNK:N	2.68	0.67
8:M:456:ARG:NH2	10:O:262:THR:O	2.28	0.66
10:O:126:PHE:HB2	12:R:226:THR:HG22	1.78	0.66
11:Q:18:ASN:ND2	11:Q:177:ASN:O	2.29	0.66
6:H:527:THR:C	6:H:529:ASN:H	1.97	0.66
9:N:55:THR:O	9:N:64:ASN:ND2	2.28	0.65
7:L:363:TYR:OH	12:R:116:ASN:ND2	2.29	0.65
10:O:401:TYR:OH	12:R:48:LYS:NZ	2.21	0.65
10:O:33:GLU:HG3	10:O:106:LEU:HD11	1.79	0.65
4:F:813:LEU:HD22	7:L:276:ARG:HH21	1.62	0.65
7:J:426:GLN:NE2	8:M:26:LYS:O	2.30	0.64
11:Q:184:TYR:OH	11:Q:242:ASP:OD1	2.15	0.64
3:E:392:ASP:HB3	7:I:226:VAL:HB	1.80	0.64
7:K:501:GLN:HG2	8:M:244:MET:HB3	1.79	0.63
10:O:430:ARG:NH2	12:R:130:ASP:OD1	2.31	0.63
10:O:41:GLU:OE2	10:O:50:SER:OG	2.16	0.62
4:F:875:THR:HG22	12:R:221:CYS:HB3	1.81	0.62
6:H:449:LYS:O	6:H:516:THR:OG1	2.16	0.61
7:I:260:CYS:HB2	7:I:283:CYS:SG	2.40	0.61
3:E:405:ILE:HD11	7:L:162:LYS:HD3	1.82	0.61
9:N:296:LEU:HD21	9:N:309:LEU:HG	1.83	0.61
7:I:282:LEU:HD21	7:I:292:PHE:HB3	1.83	0.61
7:L:95:HIS:O	7:L:95:HIS:ND1	2.34	0.61
2:D:64:HIS:HD2	2:D:66:TYR:H	1.47	0.60
8:M:463:ASN:HA	8:M:468:ARG:HH21	1.66	0.60
7:L:237:SER:OG	7:L:249:ARG:NH1	2.35	0.60
7:I:312:LYS:H	7:I:312:LYS:HD3	1.66	0.60
7:L:288:GLN:HB2	7:L:291:HIS:CE1	2.37	0.60
11:Q:368:ASP:OD1	11:Q:368:ASP:N	2.35	0.59
11:Q:351:ASP:OD1	11:Q:351:ASP:N	2.35	0.59
9:N:75:THR:HG1	11:Q:12:TYR:HH	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:239:GLN:OE1	7:I:346:ARG:NH1	2.35	0.59
8:M:378:GLN:OE1	8:M:380:GLN:NE2	2.36	0.59
10:O:170:THR:HG22	10:O:172:LEU:H	1.68	0.59
11:Q:2:SER:N	11:Q:6:GLN:OE1	2.35	0.58
3:E:408:GLU:N	3:E:408:GLU:OE1	2.35	0.58
10:O:167:ASP:OD2	10:O:182:LYS:NZ	2.36	0.58
4:F:852:ASP:OD1	4:F:853:VAL:N	2.36	0.57
7:J:434:LYS:NZ	7:J:438:GLU:OE2	2.37	0.57
9:N:574:TYR:O	9:N:578:THR:OG1	2.21	0.57
7:I:271:ARG:HD2	7:I:281:ASN:HD22	1.68	0.57
1:C:33:ARG:NH2	8:M:441:GLU:OE2	2.36	0.56
3:E:380:SER:HB2	8:M:464:ASN:HA	1.85	0.56
7:I:57:ASN:N	7:I:59:GLU:OE1	2.38	0.56
10:O:266:THR:HG23	10:O:267:ARG:HG3	1.87	0.56
6:H:527:THR:O	6:H:529:ASN:N	2.33	0.56
9:N:156:GLN:OE1	12:R:287:ARG:NH2	2.38	0.56
8:M:227:VAL:HG12	9:N:361:ILE:HD12	1.88	0.55
6:H:489:ASN:O	6:H:490:GLU:HG2	2.06	0.55
7:I:226:VAL:HG13	7:I:228:LEU:HG	1.88	0.55
3:E:372:ARG:HB2	7:I:188:GLN:HB2	1.89	0.55
4:F:814:PRO:O	7:L:276:ARG:NH2	2.39	0.55
6:H:513:SER:O	6:H:588:THR:HA	2.07	0.55
11:Q:202:ILE:HG12	11:Q:226:ASN:HB2	1.87	0.55
7:L:179:ILE:HD11	11:Q:321:THR:HA	1.89	0.55
12:R:111:ASP:OD1	12:R:111:ASP:N	2.38	0.55
4:F:813:LEU:HD23	4:F:814:PRO:HD2	1.90	0.54
7:L:268:ILE:HD12	10:O:233:PRO:HD2	1.88	0.54
10:O:198:ARG:NH2	10:O:199:THR:O	2.41	0.54
7:L:251:SER:OG	12:R:57:GLN:NE2	2.41	0.54
12:R:105:ASP:OD1	12:R:106:LYS:N	2.40	0.54
12:R:253:LYS:HE3	12:R:257:ILE:HD11	1.90	0.54
6:H:448:TYR:HA	6:H:493:GLN:HE21	1.73	0.54
7:I:302:ILE:HD11	12:R:239:ILE:HG12	1.89	0.54
10:O:35:PHE:HB2	10:O:36:PRO:HD2	1.89	0.54
7:L:193:THR:OG1	7:L:196:GLY:O	2.26	0.54
2:D:98:GLU:OE2	9:N:41:ARG:NH2	2.29	0.54
7:L:191:LEU:HG	7:L:200:PHE:HB2	1.90	0.54
7:I:363:TYR:HA	7:I:366:GLU:HG2	1.91	0.53
10:O:167:ASP:HB3	10:O:173:ASP:HB3	1.89	0.53
7:J:430:GLN:NE2	7:K:425:SER:OG	2.41	0.53
7:J:458:LYS:NZ	7:K:453:GLN:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:80:VAL:HG21	7:L:130:ARG:HG2	1.91	0.53
3:E:431:CYS:HA	3:E:434:TYR:HD2	1.72	0.53
8:M:451:ASN:OD1	8:M:451:ASN:N	2.42	0.53
9:N:170:GLN:HG3	12:R:295:VAL:HG12	1.90	0.53
8:M:225:ARG:HB3	18:7:66:UNK:HA	1.90	0.53
8:M:267:VAL:HG22	8:M:314:LYS:HE3	1.89	0.53
3:E:327:CYS:SG	7:L:145:ASN:ND2	2.82	0.52
5:G:159:VAL:HG11	13:S:208:VAL:HG21	1.91	0.52
6:H:453:GLN:HA	6:H:486:PHE:O	2.09	0.52
7:I:70:LEU:O	7:I:75:LYS:NZ	2.39	0.52
7:L:233:ASN:ND2	12:R:126:GLU:OE2	2.42	0.52
8:M:456:ARG:NH1	12:R:192:GLU:OE2	2.42	0.52
11:Q:342:ASP:N	11:Q:342:ASP:OD1	2.42	0.52
4:F:798:ILE:HD11	10:O:192:SER:HB2	1.92	0.52
7:I:91:ILE:HD12	7:L:185:GLY:HA2	1.91	0.52
10:O:491:ARG:HG2	14:2:358:UNK:HA	1.91	0.52
3:E:402:LEU:HD12	3:E:405:ILE:HD13	1.92	0.52
7:L:235:TYR:O	10:O:446:ARG:NH1	2.41	0.52
11:Q:147:ILE:HD11	11:Q:167:ARG:HB3	1.90	0.52
8:M:351:LEU:HD11	8:M:368:LEU:HD11	1.90	0.52
3:E:380:SER:OG	8:M:463:ASN:ND2	2.43	0.52
6:H:497:ALA:HB3	10:O:229:ASN:HA	1.92	0.52
7:K:433:VAL:HG21	8:M:32:ASP:HB3	1.90	0.52
8:M:466:ASN:OD1	8:M:466:ASN:N	2.42	0.52
9:N:250:LEU:HB2	9:N:262:ILE:HG21	1.92	0.51
11:Q:358:ALA:H	11:Q:371:GLU:HB2	1.75	0.51
12:R:62:TYR:HB2	12:R:79:ILE:HG21	1.91	0.51
11:Q:268:ILE:HD13	11:Q:341:LYS:HG2	1.93	0.51
3:E:417:ASP:N	3:E:417:ASP:OD1	2.42	0.51
11:Q:200:GLU:HG3	11:Q:201:ALA:H	1.76	0.51
10:O:122:LYS:HG3	12:R:226:THR:HG21	1.93	0.51
9:N:255:ASP:OD1	9:N:256:ARG:N	2.44	0.51
8:M:60:THR:O	8:M:61:ASN:ND2	2.44	0.51
9:N:285:ASP:OD1	9:N:285:ASP:N	2.36	0.51
11:Q:345:ASP:OD1	11:Q:345:ASP:N	2.43	0.50
7:L:348:GLU:HB3	10:O:457:LYS:HE3	1.92	0.50
5:G:175:ASP:OD1	5:G:175:ASP:N	2.43	0.50
10:O:270:HIS:HD2	10:O:272:ASN:HB2	1.77	0.50
7:I:249:ARG:NH2	7:I:253:GLN:HE21	2.09	0.50
11:Q:275:SER:O	11:Q:301:ASN:ND2	2.41	0.50
6:H:511:LEU:HD23	6:H:525:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:147:ALA:HB1	11:Q:355:ASN:HD22	1.76	0.49
4:F:869:ARG:H	7:L:318:GLN:NE2	2.09	0.49
7:I:358:PRO:HB2	7:L:224:PHE:HB2	1.95	0.49
5:G:163:ALA:HB1	13:S:194:ALA:HB1	1.94	0.49
11:Q:153:PRO:HB3	11:Q:168:TYR:CE1	2.47	0.49
2:D:66:TYR:OH	7:I:331:GLU:OE2	2.20	0.49
7:K:440:LEU:HD13	8:M:39:MET:HE2	1.93	0.49
7:L:236:ASP:OD2	7:L:239:GLN:NE2	2.45	0.49
7:L:284:SER:HB2	10:O:181:ILE:HD11	1.95	0.49
7:I:192:ASP:OD1	7:I:193:THR:N	2.45	0.49
8:M:454:ALA:HB1	8:M:460:ILE:HG21	1.93	0.49
9:N:75:THR:OG1	11:Q:12:TYR:OH	2.20	0.49
11:Q:208:LEU:O	11:Q:218:LYS:HA	2.13	0.49
7:L:282:LEU:HD22	7:L:291:HIS:CD2	2.48	0.49
7:J:419:GLU:O	7:J:422:ILE:HG12	2.13	0.49
3:E:345:ASP:O	11:Q:149:ASN:ND2	2.45	0.49
11:Q:30:PHE:HA	11:Q:216:THR:O	2.11	0.49
11:Q:294:ASP:OD1	11:Q:295:ASN:N	2.46	0.49
2:D:62:ALA:HB3	2:D:71:VAL:HG23	1.94	0.48
7:I:249:ARG:HH21	7:I:253:GLN:HE21	1.61	0.48
8:M:308:PRO:HB3	8:M:329:HIS:CD2	2.48	0.48
12:R:217:SER:OG	12:R:220:ASP:OD1	2.32	0.48
3:E:331:ASN:HD21	7:L:137:LEU:HA	1.78	0.48
5:G:167:MET:HE1	5:G:177:ILE:HA	1.95	0.48
7:L:140:THR:HG22	7:L:143:ARG:HH22	1.79	0.48
7:J:467:LYS:NZ	8:M:62:THR:O	2.42	0.48
11:Q:202:ILE:HB	11:Q:225:TYR:HB3	1.96	0.48
9:N:191:ILE:HD12	9:N:218:LEU:HD21	1.96	0.47
8:M:237:ASN:ND2	8:M:321:LYS:O	2.47	0.47
8:M:23:PRO:HB2	8:M:26:LYS:HG2	1.97	0.47
9:N:115:ILE:HA	9:N:120:LEU:HD12	1.96	0.47
11:Q:307:PRO:HB3	11:Q:332:LEU:HD23	1.97	0.47
9:N:341:PRO:HD3	9:N:553:ILE:HD11	1.95	0.47
9:N:68:PHE:CZ	11:Q:13:ILE:HD11	2.49	0.47
10:O:198:ARG:HD3	10:O:203:ASP:OD1	2.14	0.47
2:D:64:HIS:CD2	2:D:66:TYR:H	2.29	0.47
7:L:258:TYR:OH	10:O:173:ASP:OD1	2.33	0.47
6:H:444:GLU:HG2	6:H:445:TYR:H	1.80	0.47
10:O:427:LYS:HZ1	12:R:133:ASP:HA	1.80	0.47
5:G:175:ASP:O	5:G:178:ILE:HG22	2.15	0.47
7:L:147:ALA:HB3	11:Q:371:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:298:SER:HB3	10:O:390:LEU:HG	1.98	0.46
3:E:372:ARG:HH12	7:I:227:ASN:HD21	1.62	0.46
7:K:493:LYS:HE2	7:K:510:GLU:HG2	1.97	0.46
12:R:215:THR:HG21	12:R:237:PHE:H	1.79	0.46
2:D:64:HIS:HD2	2:D:66:TYR:HB2	1.81	0.46
3:E:331:ASN:ND2	7:L:137:LEU:HA	2.31	0.46
9:N:279:SER:OG	9:N:280:ALA:N	2.48	0.46
7:I:311:VAL:HB	7:I:314:ASN:HD22	1.79	0.46
8:M:444:LEU:HD13	12:R:177:LYS:HG2	1.98	0.46
11:Q:331:SER:O	11:Q:334:GLU:HB2	2.15	0.46
6:H:524:THR:HG23	6:H:605:ARG:HB3	1.97	0.46
8:M:335:VAL:O	8:M:338:THR:OG1	2.31	0.46
1:C:44:GLU:HB2	12:R:157:LYS:HD3	1.98	0.46
5:G:192:LEU:HD11	13:S:209:LEU:HD22	1.97	0.46
7:I:246:ASP:OD1	7:I:247:GLU:N	2.49	0.46
7:J:472:ARG:HH22	7:K:467:LYS:HB2	1.81	0.46
10:O:55:ILE:O	10:O:59:SER:N	2.48	0.46
11:Q:162:PRO:O	11:Q:165:ILE:HB	2.16	0.46
4:F:818:TRP:HA	7:L:287:PHE:CD2	2.51	0.45
6:H:527:THR:C	6:H:529:ASN:N	2.68	0.45
9:N:561:LEU:HD21	9:N:571:LEU:HD12	1.98	0.45
6:H:490:GLU:HG3	7:L:264:GLY:O	2.15	0.45
8:M:309:GLU:N	8:M:312:GLU:OE1	2.47	0.45
3:E:414:VAL:HG22	3:E:418:VAL:HB	1.98	0.45
7:J:482:LEU:HD11	7:K:507:GLN:HA	1.99	0.45
8:M:452:GLU:HA	8:M:455:ALA:HB3	1.98	0.45
7:L:150:VAL:HG11	11:Q:310:PHE:CE1	2.51	0.45
2:D:123:ASP:OD2	6:H:474:ARG:NH2	2.50	0.45
8:M:227:VAL:HG13	8:M:346:LEU:HD12	1.99	0.45
10:O:466:SER:OG	12:R:112:GLU:OE2	2.29	0.45
7:I:171:ASP:O	7:I:174:THR:HG22	2.17	0.45
2:D:85:HIS:O	12:R:208:ARG:NH1	2.48	0.45
8:M:372:VAL:HG12	8:M:375:ILE:HB	1.98	0.45
9:N:59:HIS:O	9:N:59:HIS:ND1	2.49	0.45
9:N:234:ALA:HB3	9:N:235:PRO:HD3	1.99	0.45
11:Q:20:LEU:HA	11:Q:27:ILE:HD12	1.99	0.45
6:H:525:LEU:O	6:H:532:PRO:HD2	2.16	0.45
7:L:353:LYS:HD2	7:L:353:LYS:HA	1.86	0.44
9:N:77:ARG:NH1	13:S:198:LEU:H	2.15	0.44
10:O:173:ASP:OD1	10:O:173:ASP:N	2.48	0.44
3:E:392:ASP:OD2	3:E:395:LEU:HD13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:500:GLU:OE1	8:M:246:THR:OG1	2.33	0.44
8:M:447:ASP:HB3	10:O:270:HIS:CD2	2.52	0.44
10:O:257:PRO:HG2	12:R:248:LEU:O	2.18	0.44
8:M:30:LEU:HD23	8:M:30:LEU:HA	1.85	0.44
6:H:608:ASP:O	6:H:609:LYS:HG2	2.16	0.44
7:I:180:GLY:HA3	7:L:198:LYS:HE3	2.00	0.44
8:M:372:VAL:HG13	8:M:375:ILE:HD12	1.99	0.44
2:D:64:HIS:CD2	2:D:66:TYR:HB2	2.52	0.44
3:E:388:THR:HG23	7:I:230:ILE:HB	1.99	0.44
3:E:371:TRP:CD2	7:L:202:PRO:HG3	2.53	0.44
3:E:372:ARG:HH22	7:I:227:ASN:HD21	1.64	0.44
7:K:433:VAL:O	7:K:437:MET:HG2	2.17	0.44
10:O:202:MET:HG3	10:O:204:LEU:HD11	2.00	0.44
7:I:281:ASN:OD1	7:I:281:ASN:N	2.50	0.43
8:M:50:ARG:HA	8:M:50:ARG:HD3	1.78	0.43
3:E:394:ASP:HB2	3:E:428:PHE:HE1	1.84	0.43
8:M:458:SER:O	8:M:458:SER:OG	2.35	0.43
1:C:36:ILE:HD13	1:C:36:ILE:HA	1.89	0.43
5:G:158:TRP:CD1	9:N:74:GLU:HG3	2.54	0.43
9:N:539:ASN:OD1	9:N:577:ASN:ND2	2.51	0.43
9:N:542:ASP:OD1	9:N:542:ASP:N	2.50	0.43
9:N:338:ALA:O	9:N:342:ASN:ND2	2.52	0.43
7:I:135:GLU:HG2	7:I:136:TYR:H	1.84	0.43
7:I:140:THR:HG23	7:I:143:ARG:HH21	1.83	0.43
6:H:491:LEU:HD23	6:H:491:LEU:HA	1.90	0.43
7:J:479:ILE:HD11	7:K:475:LEU:HD21	2.01	0.43
8:M:378:GLN:HG2	8:M:380:GLN:HG3	2.00	0.43
8:M:332:LEU:HD23	9:N:565:PRO:HB3	2.00	0.43
10:O:51:TYR:CE2	10:O:55:ILE:HD11	2.53	0.43
6:H:523:GLU:HG2	6:H:606:CYS:SG	2.59	0.43
9:N:132:LEU:N	9:N:133:PRO:HD2	2.33	0.43
9:N:85:MET:SD	9:N:103:LYS:HB3	2.59	0.42
10:O:44:PRO:HA	10:O:47:ILE:HG13	2.00	0.42
11:Q:356:ASP:O	11:Q:374:SER:N	2.37	0.42
5:G:178:ILE:HD12	13:S:226:LEU:HD23	2.01	0.42
9:N:166:ARG:HG3	9:N:167:ASN:N	2.34	0.42
10:O:433:ARG:NH1	10:O:441:PRO:HB3	2.34	0.42
3:E:320:LEU:HB3	7:L:73:LEU:HD11	2.02	0.42
7:L:121:THR:O	7:L:125:ILE:HG13	2.20	0.42
9:N:328:LYS:HE2	9:N:328:LYS:HB3	1.87	0.42
7:I:158:ALA:HB2	11:Q:186:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:10:VAL:HG22	8:M:11:THR:H	1.84	0.42
9:N:126:LEU:O	9:N:129:THR:OG1	2.26	0.42
11:Q:20:LEU:HD23	11:Q:27:ILE:HG21	2.01	0.42
11:Q:358:ALA:H	11:Q:371:GLU:CB	2.32	0.42
5:G:168:LEU:HD23	5:G:168:LEU:HA	1.93	0.42
7:I:260:CYS:SG	7:I:262:THR:OG1	2.76	0.42
10:O:427:LYS:NZ	12:R:133:ASP:HA	2.34	0.42
12:R:212:ASN:OD1	12:R:212:ASN:N	2.48	0.42
7:L:119:LYS:HG3	7:L:122:ARG:NH2	2.34	0.42
8:M:7:PRO:HB2	10:O:282:LEU:HB3	2.02	0.42
10:O:13:PHE:CE1	10:O:134:GLU:HB3	2.55	0.42
3:E:407:LYS:HA	3:E:410:TYR:CZ	2.55	0.42
4:F:808:ASP:OD1	4:F:809:PRO:HD2	2.19	0.42
7:I:195:GLN:C	7:I:197:LEU:H	2.23	0.42
10:O:119:LEU:HD23	10:O:119:LEU:HA	1.91	0.42
1:C:61:SER:O	1:C:65:MET:HG2	2.20	0.41
4:F:818:TRP:HA	7:L:287:PHE:HD2	1.85	0.41
9:N:165:LEU:HD23	9:N:165:LEU:HA	1.79	0.41
2:D:110:HIS:NE2	2:D:115:CYS:SG	2.93	0.41
7:L:287:PHE:HA	12:R:63:ARG:HH21	1.85	0.41
9:N:298:LEU:HD12	9:N:304:LEU:HD23	2.01	0.41
4:F:862:GLY:HA3	4:F:864:PHE:CE2	2.56	0.41
7:K:472:ARG:NH2	7:K:503:ASP:OD2	2.37	0.41
10:O:222:PRO:HG2	10:O:226:PHE:CE2	2.55	0.41
10:O:270:HIS:ND1	10:O:271:PRO:HD2	2.34	0.41
12:R:136:LEU:C	12:R:139:PRO:HD2	2.40	0.41
12:R:248:LEU:HA	12:R:248:LEU:HD23	1.85	0.41
8:M:340:ASN:HD21	9:N:516:GLU:HG3	1.86	0.41
8:M:405:LEU:HD12	8:M:405:LEU:HA	1.92	0.41
9:N:275:ALA:HB2	9:N:318:PRO:O	2.20	0.41
9:N:335:ILE:O	9:N:339:THR:OG1	2.24	0.41
9:N:361:ILE:HA	9:N:512:ASN:HD21	1.85	0.41
10:O:37:ALA:HB3	10:O:73:LEU:HB2	2.02	0.41
9:N:561:LEU:HD22	9:N:568:THR:HA	2.03	0.41
9:N:274:LYS:HB2	9:N:277:GLU:HB3	2.02	0.41
10:O:239:ASN:ND2	10:O:482:ASN:O	2.53	0.41
1:C:52:ILE:O	1:C:57:ARG:NH2	2.54	0.41
5:G:157:ASN:ND2	13:S:203:PHE:O	2.46	0.41
6:H:455:TYR:CD2	6:H:485:ILE:HG12	2.56	0.41
6:H:502:LEU:HD11	6:H:509:LEU:HD11	2.03	0.41
7:K:461:TYR:HE2	8:M:56:ILE:HG22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:493:LYS:HG3	7:K:510:GLU:HG2	2.02	0.41
8:M:223:GLN:HG3	8:M:224:LEU:H	1.86	0.41
8:M:422:LEU:HD12	8:M:426:PRO:HA	2.03	0.41
8:M:451:ASN:O	12:R:184:THR:HG21	2.21	0.41
9:N:289:LEU:O	9:N:293:VAL:HG23	2.21	0.41
9:N:549:PHE:CZ	9:N:553:ILE:HD12	2.56	0.41
10:O:43:ASN:HD21	10:O:46:LYS:HD2	1.86	0.41
10:O:449:TYR:HH	12:R:126:GLU:CD	2.24	0.41
11:Q:356:ASP:N	11:Q:374:SER:HA	2.35	0.41
3:E:373:ARG:HH22	7:I:182:SER:HA	1.86	0.41
9:N:128:LYS:O	9:N:132:LEU:HG	2.22	0.41
9:N:131:ILE:O	9:N:134:LEU:HB3	2.21	0.41
8:M:6:ASN:HA	8:M:7:PRO:HD3	1.86	0.40
9:N:565:PRO:N	9:N:566:PRO:HD2	2.36	0.40
4:F:868:LEU:HD23	4:F:868:LEU:HA	1.94	0.40
6:H:487:ASN:ND2	6:H:490:GLU:OE2	2.43	0.40
6:H:489:ASN:OD1	6:H:489:ASN:N	2.54	0.40
7:J:418:SER:O	7:J:422:ILE:HG23	2.21	0.40
7:L:90:ASP:HB3	7:L:93:LYS:HB2	2.02	0.40
8:M:338:THR:O	8:M:342:LEU:HG	2.21	0.40
8:M:365:ALA:O	8:M:367:THR:HG23	2.21	0.40
11:Q:290:ARG:HG2	11:Q:382:ILE:HG12	2.04	0.40
4:F:807:GLY:O	7:L:316:SER:HB2	2.21	0.40
7:L:149:ASP:OD1	7:L:149:ASP:N	2.54	0.40
8:M:307:LYS:HA	8:M:308:PRO:HD3	1.96	0.40
7:I:259:ILE:HD12	9:N:43:GLN:HG2	2.03	0.40
7:L:312:LYS:N	7:L:345:LYS:HZ2	2.19	0.40
8:M:316:ASP:OD1	8:M:316:ASP:N	2.53	0.40
9:N:135:GLU:HG3	9:N:190:PHE:CD1	2.57	0.40
9:N:223:LEU:HD23	9:N:223:LEU:HA	1.82	0.40
9:N:263:LEU:HD23	9:N:263:LEU:HA	1.88	0.40
10:O:427:LYS:NZ	12:R:131:VAL:O	2.52	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	C	58/78 (74%)	56 (97%)	2 (3%)	0	100	100
2	D	96/180 (53%)	90 (94%)	6 (6%)	0	100	100
3	E	118/435 (27%)	108 (92%)	10 (8%)	0	100	100
4	F	63/889 (7%)	56 (89%)	7 (11%)	0	100	100
5	G	51/885 (6%)	49 (96%)	2 (4%)	0	100	100
6	H	127/625 (20%)	114 (90%)	10 (8%)	3 (2%)	6	25
7	I	289/557 (52%)	274 (95%)	15 (5%)	0	100	100
7	J	113/557 (20%)	109 (96%)	4 (4%)	0	100	100
7	K	105/557 (19%)	101 (96%)	4 (4%)	0	100	100
7	L	292/557 (52%)	278 (95%)	14 (5%)	0	100	100
8	M	302/483 (62%)	281 (93%)	21 (7%)	0	100	100
9	N	408/581 (70%)	380 (93%)	28 (7%)	0	100	100
10	O	376/502 (75%)	352 (94%)	24 (6%)	0	100	100
11	Q	258/426 (61%)	224 (87%)	34 (13%)	0	100	100
12	R	258/1359 (19%)	236 (92%)	22 (8%)	0	100	100
13	S	32/883 (4%)	32 (100%)	0	0	100	100
All	All	2946/9554 (31%)	2740 (93%)	203 (7%)	3 (0%)	54	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	H	528	ILE
6	H	529	ASN
6	H	527	THR

5.3.2 Protein sidechains [i](#)

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	C	58/75 (77%)	58 (100%)	0	100	100
2	D	82/151 (54%)	82 (100%)	0	100	100
3	E	113/388 (29%)	105 (93%)	8 (7%)	14	43
4	F	60/810 (7%)	60 (100%)	0	100	100
5	G	48/832 (6%)	47 (98%)	1 (2%)	53	77
6	H	126/578 (22%)	124 (98%)	2 (2%)	62	83
7	I	268/500 (54%)	261 (97%)	7 (3%)	46	72
7	J	111/500 (22%)	110 (99%)	1 (1%)	78	90
7	K	106/500 (21%)	106 (100%)	0	100	100
7	L	270/500 (54%)	270 (100%)	0	100	100
8	M	286/435 (66%)	281 (98%)	5 (2%)	60	82
9	N	374/521 (72%)	366 (98%)	8 (2%)	53	77
10	O	358/462 (78%)	354 (99%)	4 (1%)	73	88
11	Q	243/384 (63%)	233 (96%)	10 (4%)	30	62
12	R	240/1228 (20%)	237 (99%)	3 (1%)	69	86
13	S	33/824 (4%)	32 (97%)	1 (3%)	41	70
All	All	2776/8688 (32%)	2726 (98%)	50 (2%)	61	80

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	327	CYS
3	E	351	ASP
3	E	356	ILE
3	E	359	ILE
3	E	384	ILE
3	E	413	VAL
3	E	414	VAL
3	E	417	ASP
5	G	175	ASP
6	H	510	THR
6	H	527	THR
7	I	170	ILE
7	I	224	PHE
7	I	253	GLN
7	I	270	VAL
7	I	275	LEU

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Mol	Chain	Res	Type
7	I	281	ASN
7	I	312	LYS
7	J	459	LEU
8	M	58	LEU
8	M	62	THR
8	M	232	VAL
8	M	241	LEU
8	M	466	ASN
9	N	79	VAL
9	N	91	SER
9	N	104	TYR
9	N	123	LEU
9	N	166	ARG
9	N	170	GLN
9	N	195	PHE
9	N	578	THR
10	O	88	ILE
10	O	208	ILE
10	O	274	TYR
10	O	279	THR
11	Q	192	THR
11	Q	250	LEU
11	Q	262	LEU
11	Q	295	ASN
11	Q	342	ASP
11	Q	345	ASP
11	Q	351	ASP
11	Q	352	HIS
11	Q	368	ASP
11	Q	370	ASP
12	R	215	THR
12	R	265	VAL
12	R	297	VAL
13	S	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	64	HIS
2	D	108	HIS
3	E	331	ASN
3	E	432	ASN

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Mol	Chain	Res	Type
5	G	180	HIS
6	H	493	GLN
6	H	506	GLN
6	H	601	HIS
7	I	60	GLN
7	I	63	GLN
7	I	227	ASN
7	I	314	ASN
7	K	426	GLN
7	K	501	GLN
7	L	145	ASN
7	L	291	HIS
7	L	318	GLN
8	M	61	ASN
8	M	233	GLN
8	M	340	ASN
8	M	378	GLN
8	M	380	GLN
9	N	43	GLN
9	N	512	ASN
9	N	559	HIS
9	N	577	ASN
10	O	18	GLN
10	O	22	ASN
10	O	97	HIS
10	O	270	HIS
10	O	484	ASN
11	Q	3	HIS
11	Q	15	ASN
11	Q	158	GLN
11	Q	164	ASN
11	Q	261	GLN
12	R	57	GLN
12	R	72	ASN
12	R	116	ASN
12	R	123	GLN
12	R	270	HIS
12	R	290	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
18	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	57:UNK	C	60:UNK	N	4.98

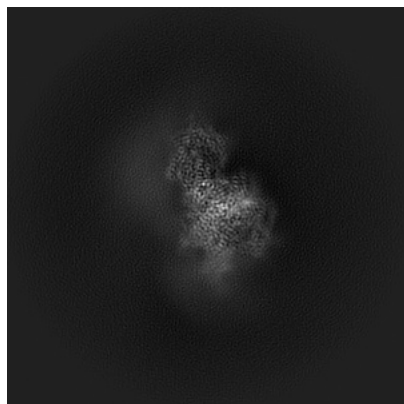
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21107. These allow visual inspection of the internal detail of the map and identification of artifacts.

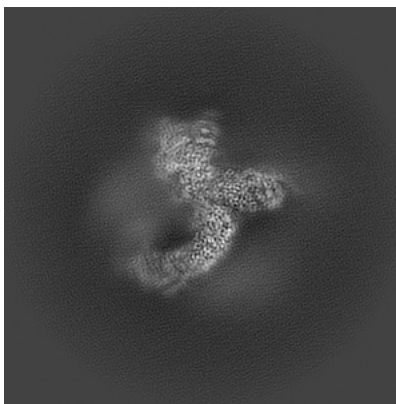
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

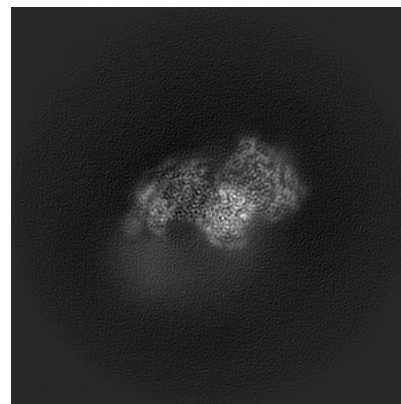
6.1.1 Primary map



X

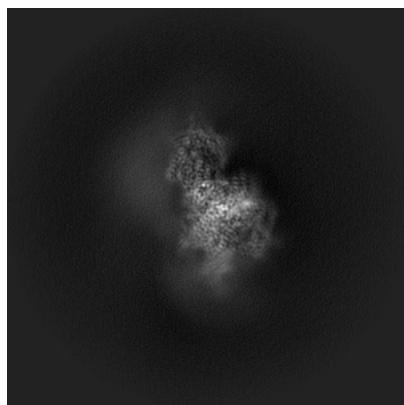


Y

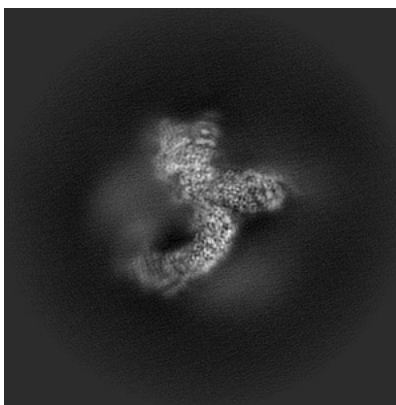


Z

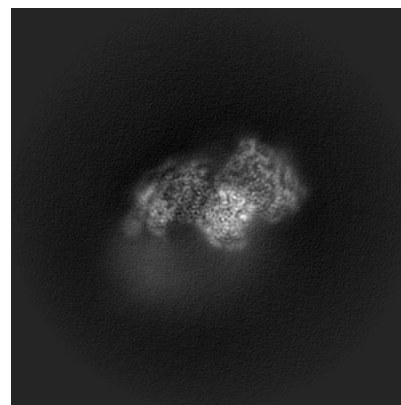
6.1.2 Raw map



X



Y

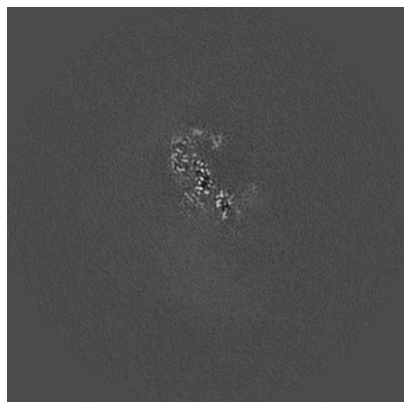


Z

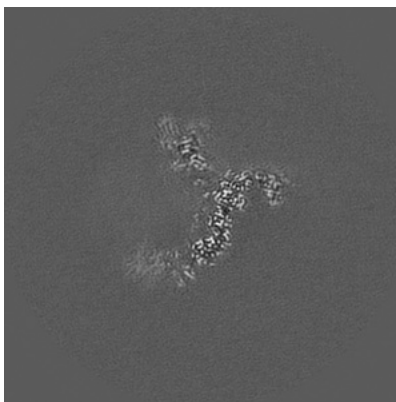
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

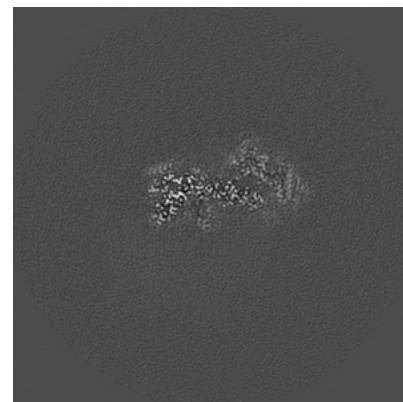
6.2.1 Primary map



X Index: 144

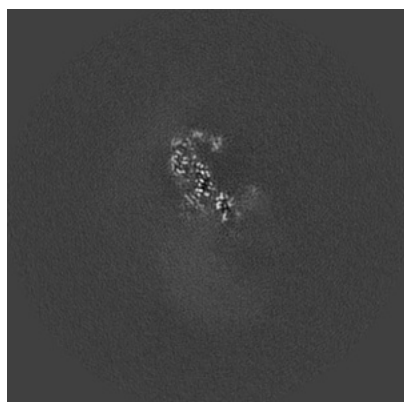


Y Index: 144

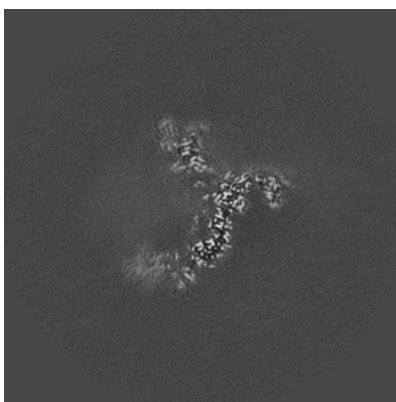


Z Index: 144

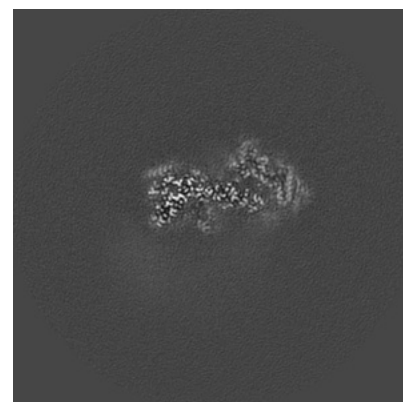
6.2.2 Raw map



X Index: 144



Y Index: 144

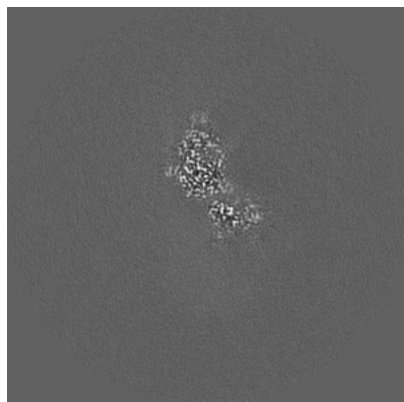


Z Index: 144

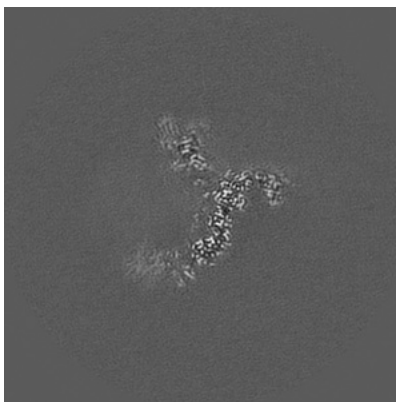
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

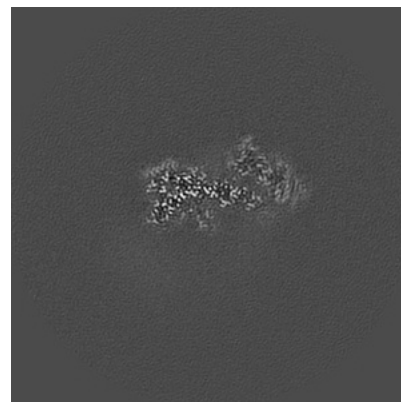
6.3.1 Primary map



X Index: 159

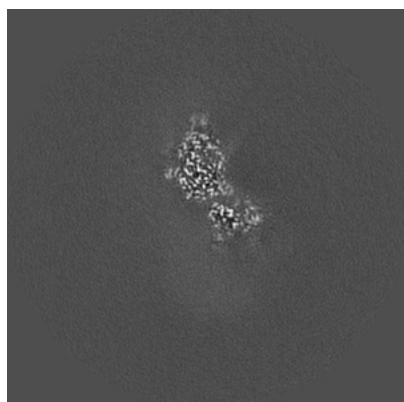


Y Index: 144

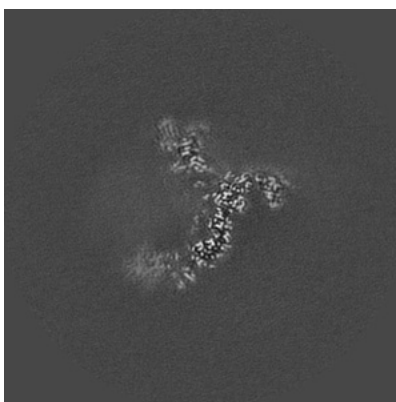


Z Index: 145

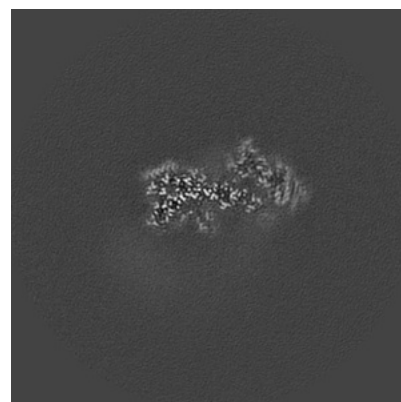
6.3.2 Raw map



X Index: 159



Y Index: 144

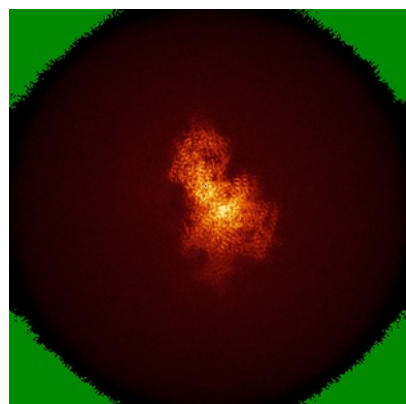


Z Index: 145

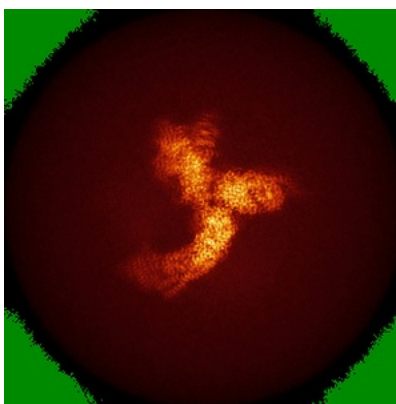
The images above show the largest variance slices of the map in three orthogonal directions.

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

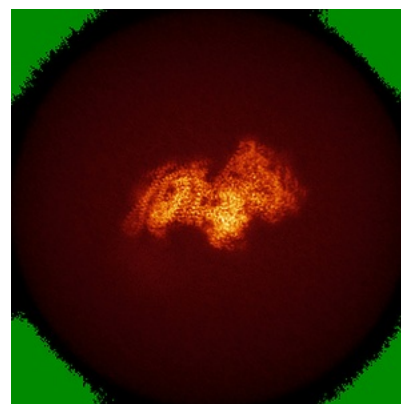
6.4.1 Primary map



X

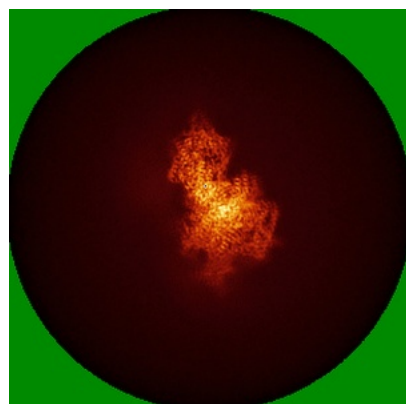


Y

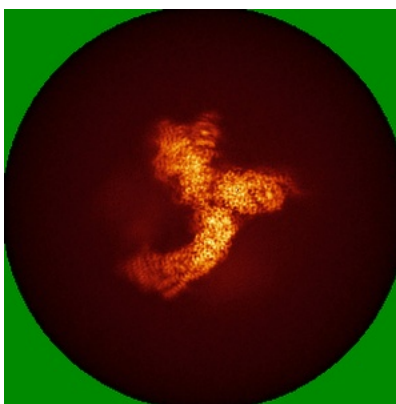


Z

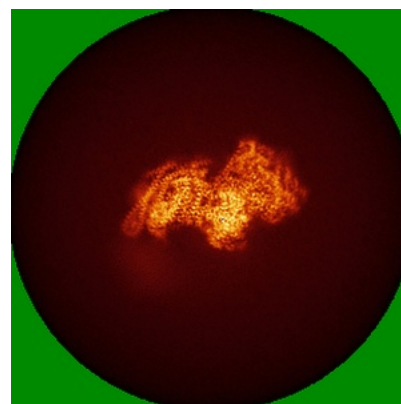
6.4.2 Raw map



X



Y

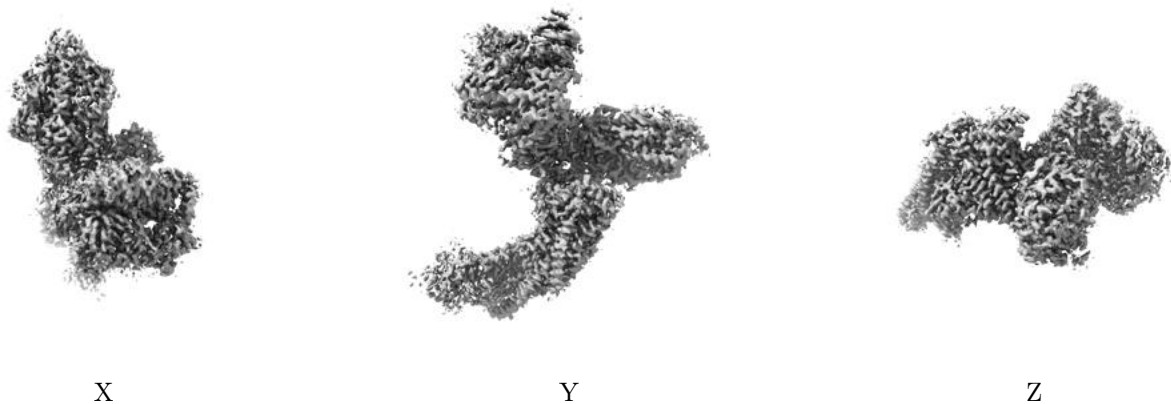


Z

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.

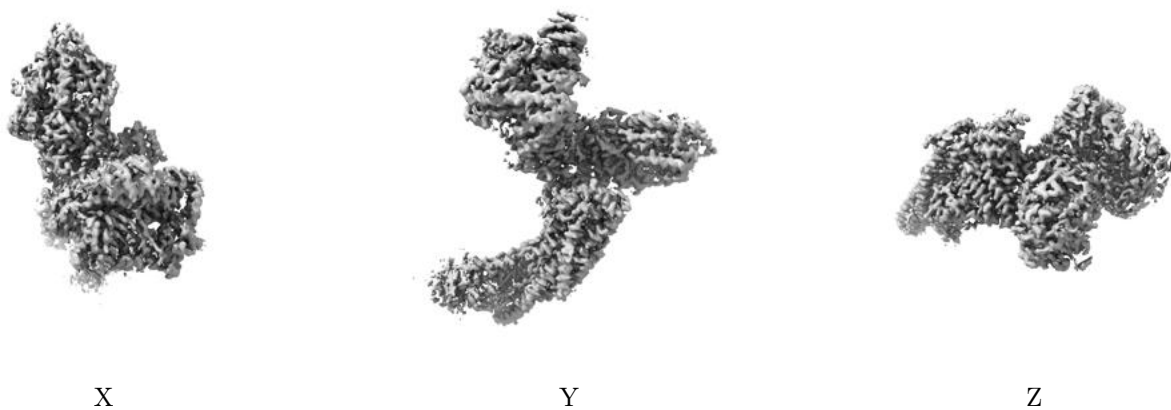
6.5 Orthogonal surface views [i](#)

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.

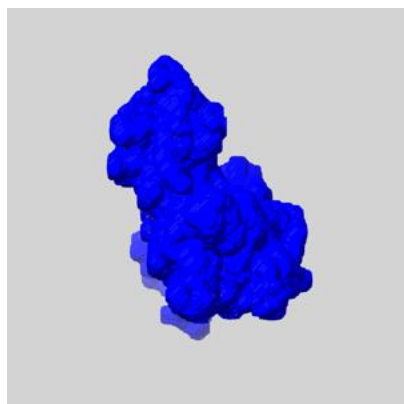
6.6 Mask visualisation [i](#)

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

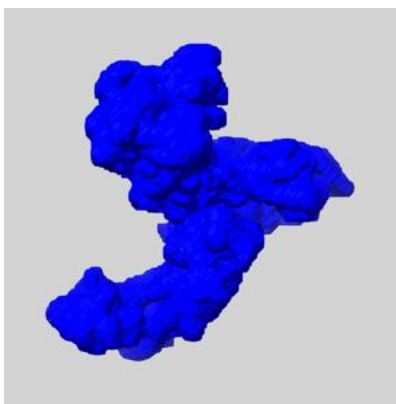
A mask typically either:

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

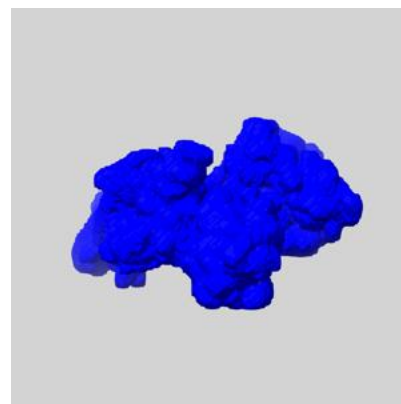
6.6.1 emd_21107_msk_1.map [i](#)



X



Y

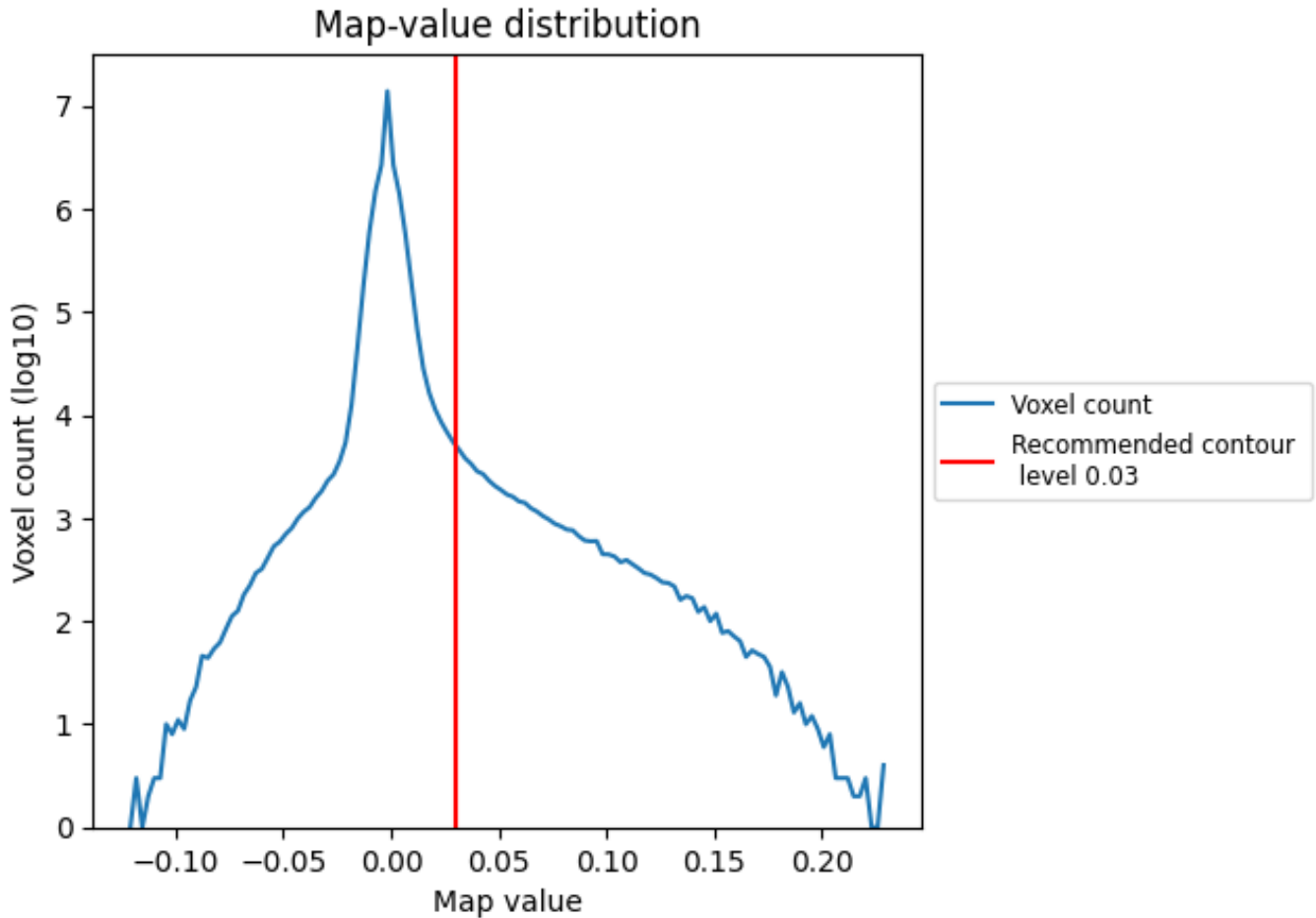


Z

7 Map analysis [i](#)

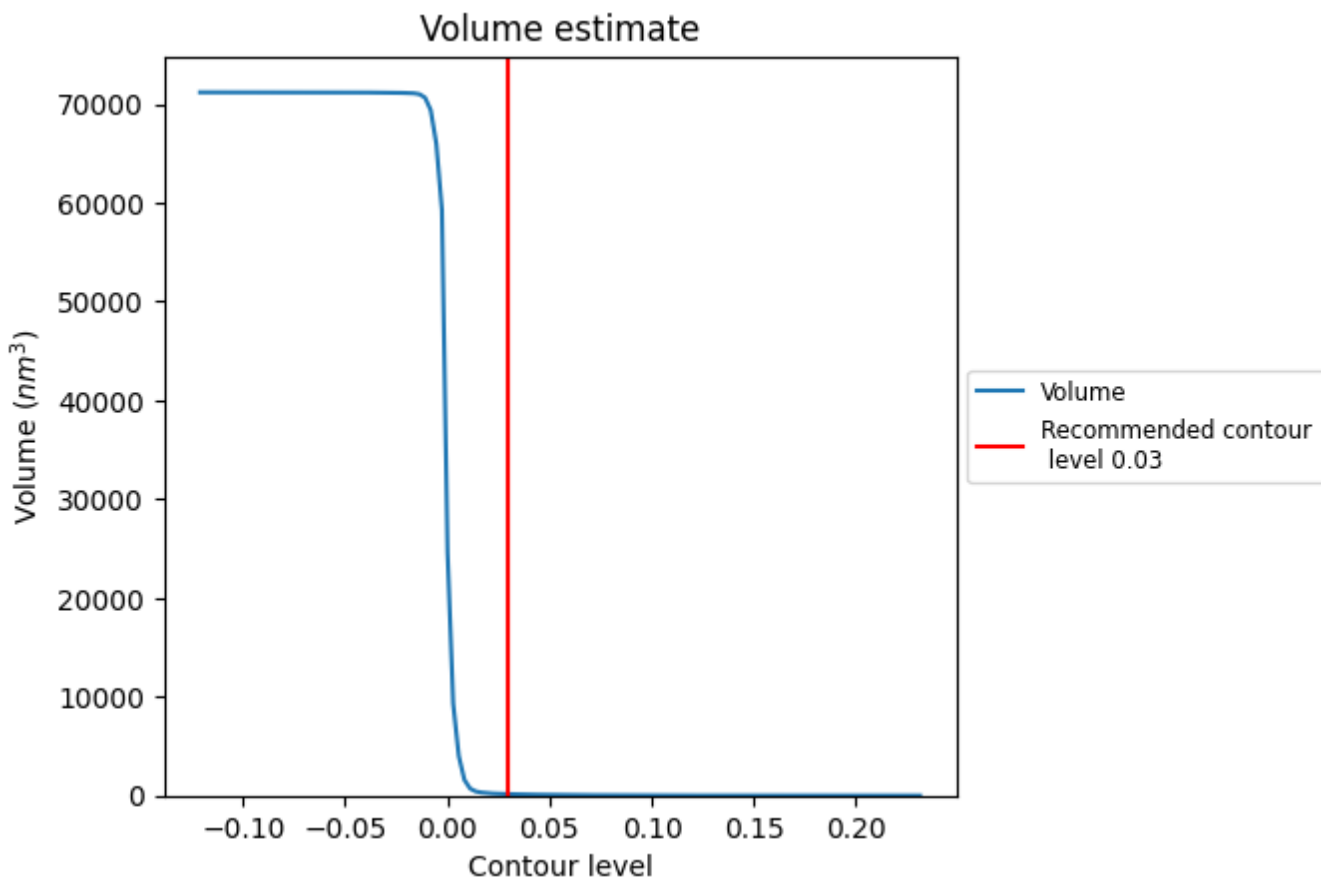
This section contains the results of statistical analysis of the map.

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.

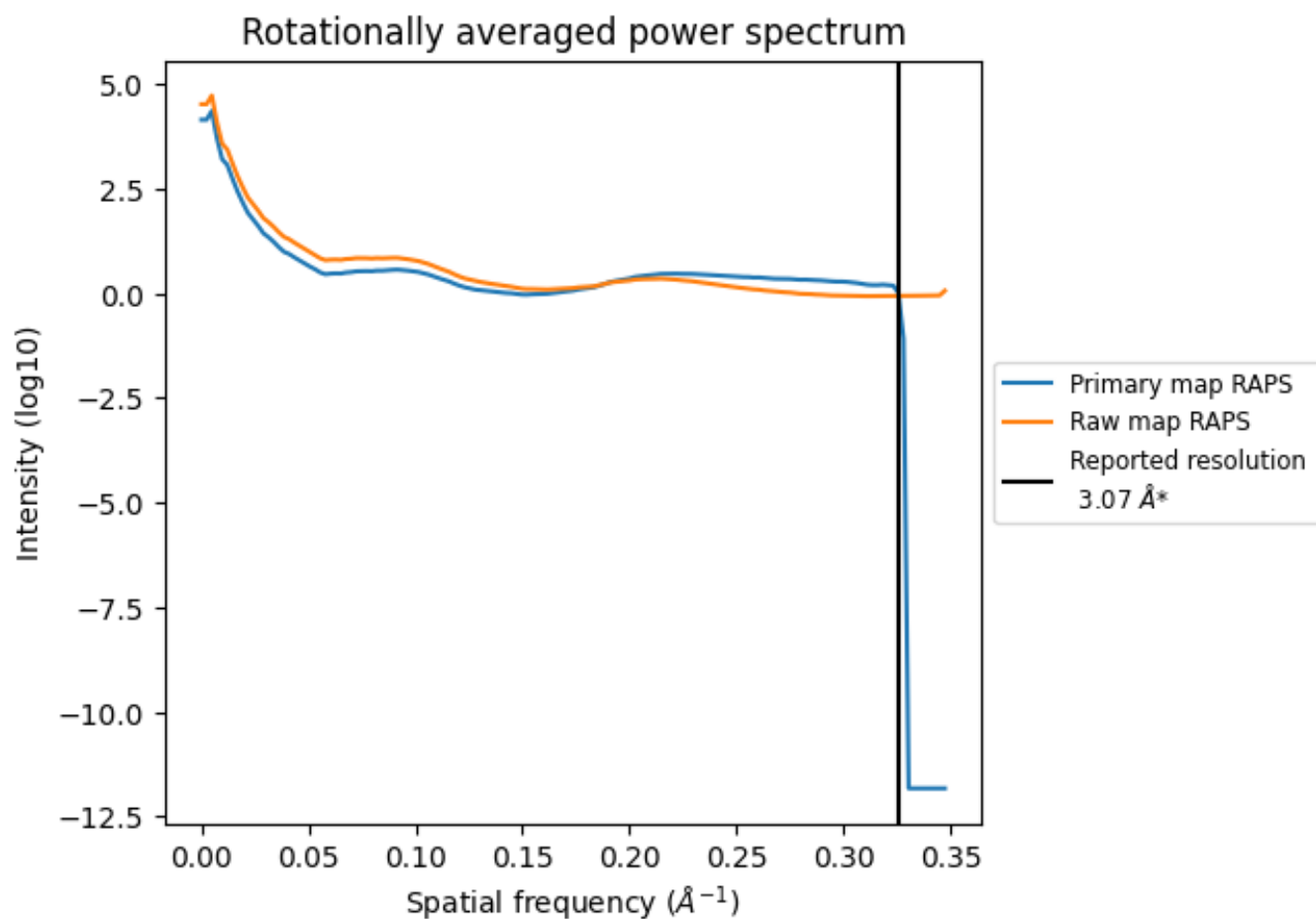
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm^3 ; this corresponds to an approximate mass of 132 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 [i](#)

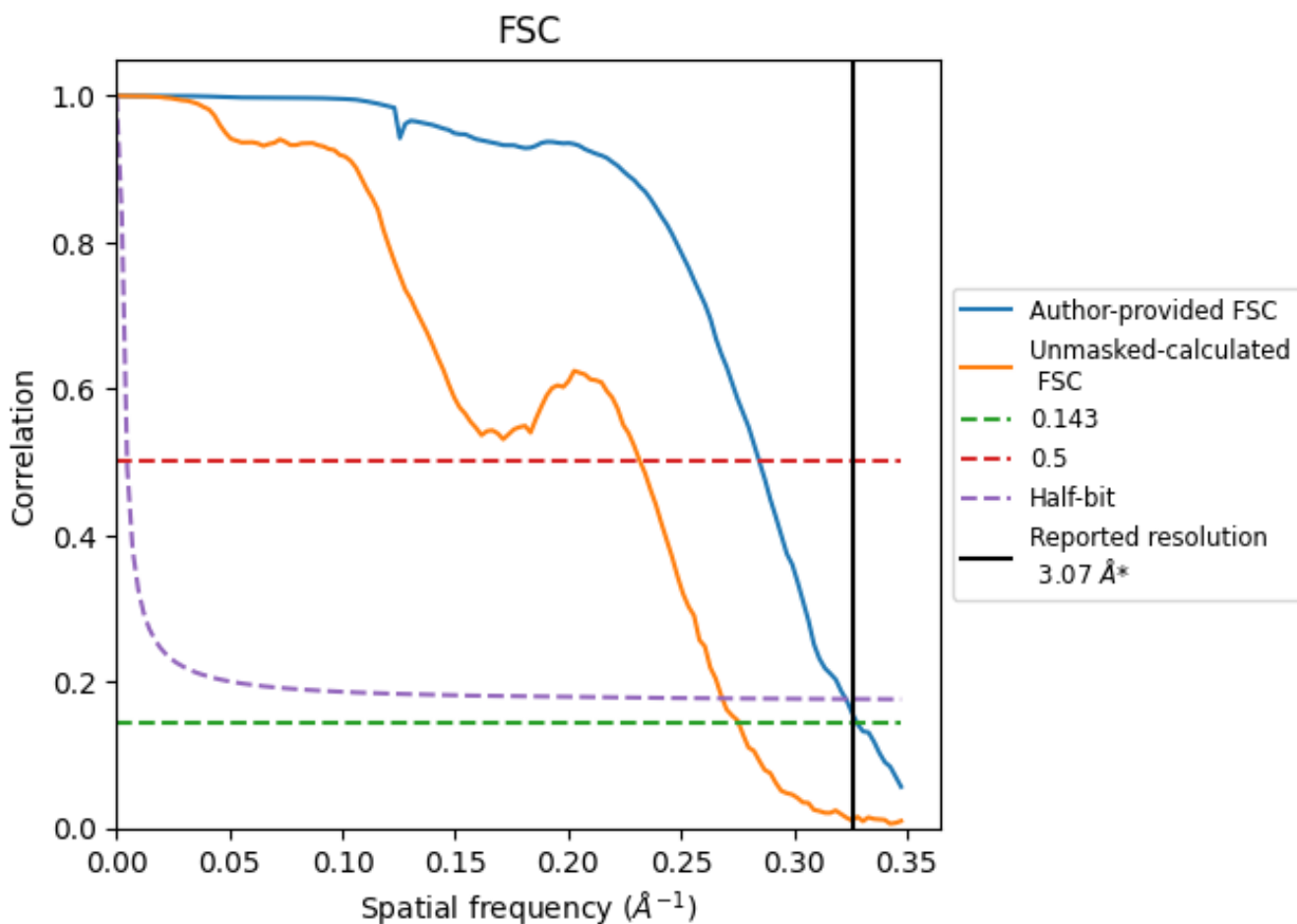


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

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 0.326 Å⁻¹

8.2 Resolution estimates [i](#)

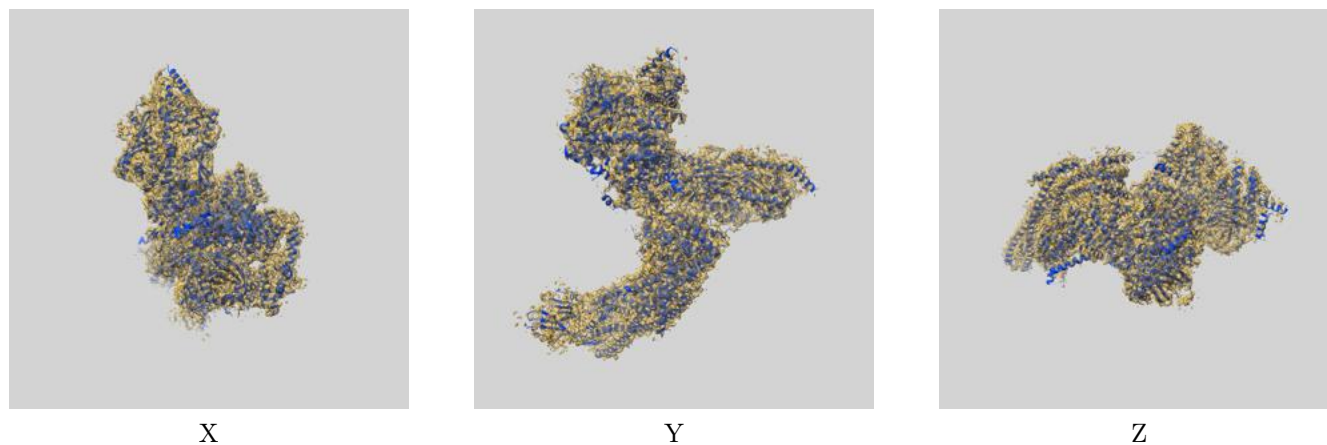
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.05	3.51	3.10
Unmasked-calculated*	3.63	4.31	3.73

*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 3.63 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

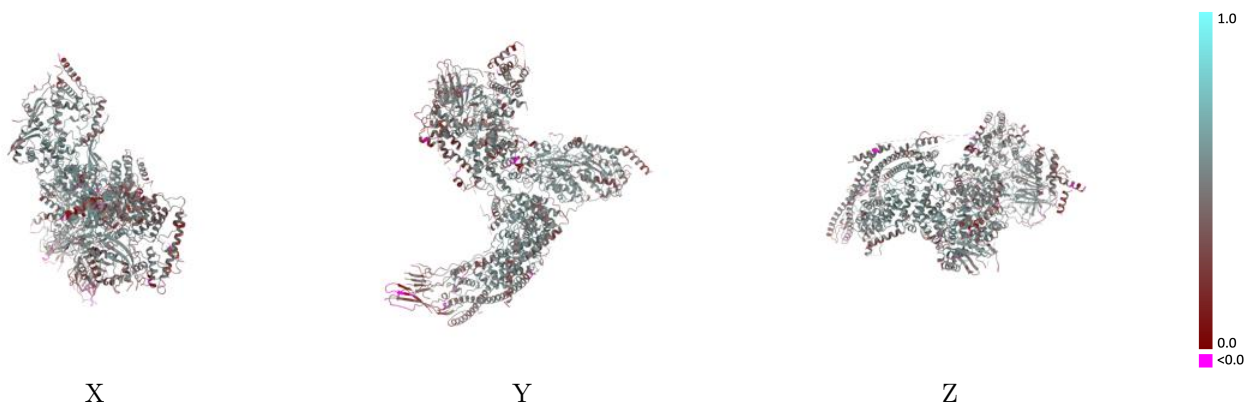
This section contains information regarding the fit between EMDB map EMD-21107 and PDB model 6V8O. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



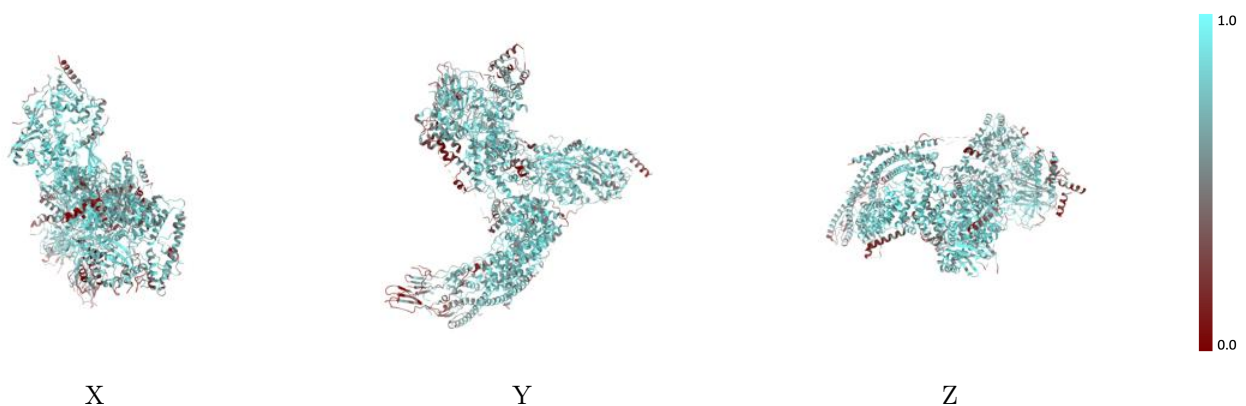
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



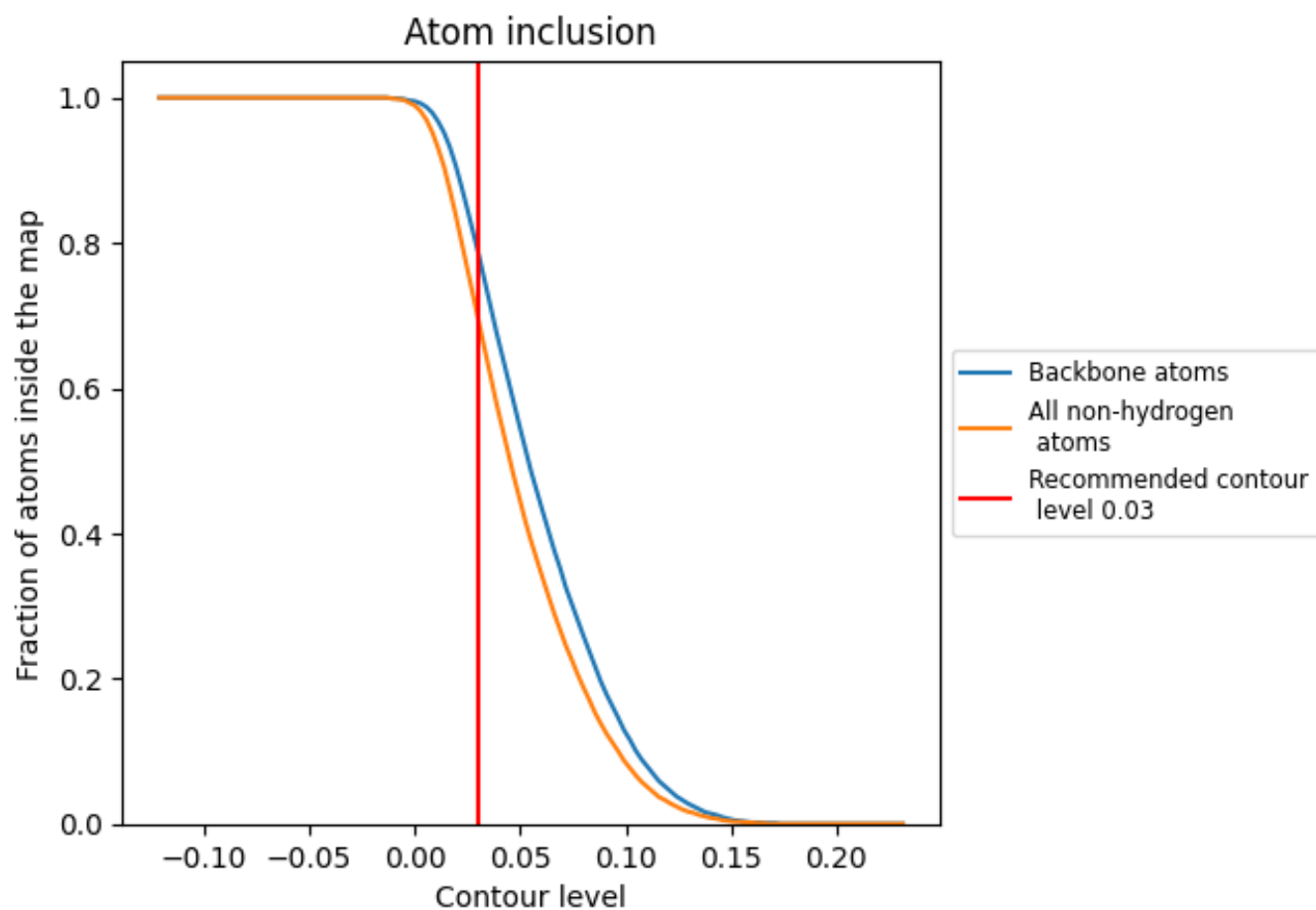
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 79% of all backbone atoms, 70% 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	 0.6970	 0.4610
2	 0.7290	 0.4070
3	 0.3370	 0.3100
4	 0.2320	 0.3290
5	 0.0290	 0.3260
6	 0.1330	 0.2050
7	 0.3800	 0.2310
C	 0.7310	 0.4690
D	 0.5730	 0.3970
E	 0.7350	 0.4600
F	 0.6760	 0.4780
G	 0.4860	 0.4360
H	 0.6530	 0.4340
I	 0.8270	 0.5300
J	 0.6490	 0.4340
K	 0.5760	 0.3920
L	 0.6970	 0.4570
M	 0.6470	 0.4410
N	 0.8150	 0.5190
O	 0.7010	 0.4490
Q	 0.7220	 0.4640
R	 0.6910	 0.4630
S	 0.5180	 0.4750

