



## Full wwPDB EM Validation Report ⓘ

Nov 12, 2025 – 04:17 PM JST

PDB ID : 9J8W / pdb\_00009j8w  
EMDB ID : EMD-61243  
Title : Cryo-EM structure of NCP-UV-DDB complex containing CPD  
Authors : Matsumoto, S.; Takizawa, Y.; Ogasawara, M.; Hashimoto, K.; Negishi, L.; Xu, W.; Tachibana, H.; Yamamoto, J.; Iwai, S.; Sugasawa, K.; Kurumizaka, H.  
Deposited on : 2024-08-21  
Resolution : 3.38 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](mailto: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.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

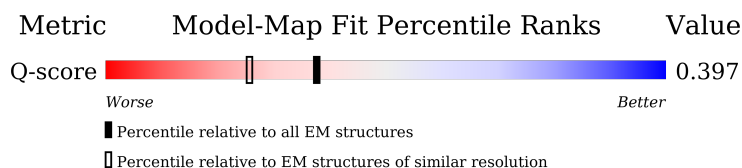
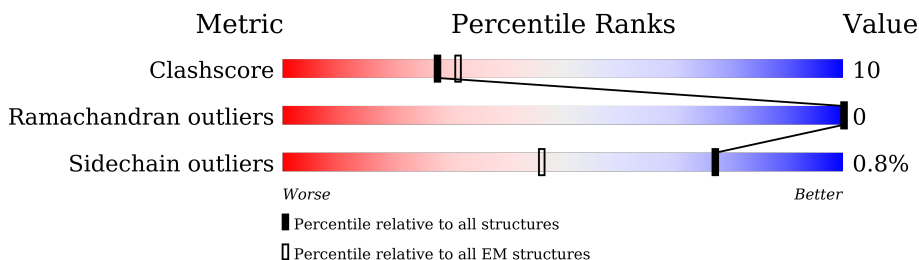
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*





The reported resolution of this entry is 3.38 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14261 ( 2.88 - 3.88 )

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  $\geq 3$ , 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	136	
1	E	136	
2	B	103	
2	F	103	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	C	130	
3	G	130	
4	D	126	
4	H	126	
5	I	145	
6	J	144	
7	L	427	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27957 atoms, of which 12800 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 Histone H3.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	101	Total	C	H	N	O	S	0	0
			1708	525	876	161	142	4		
1	E	101	Total	C	H	N	O	S	0	0
			1708	525	876	161	142	4		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	86	Total	C	H	N	O	S	0	0
			1434	436	740	140	117	1		
2	F	82	Total	C	H	N	O	S	0	0
			1348	412	695	127	113	1		

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	117	Total	C	H	N	O		0	0
			1878	571	969	181	157			
3	G	117	Total	C	H	N	O		0	0
			1878	571	969	181	157			

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	97	Total	C	H	N	O	S	0	0
			1559	480	793	142	142	2		
4	H	97	Total	C	H	N	O	S	0	0
			1560	480	794	142	142	2		

- Molecule 5 is a DNA chain called Human alpha-satellite DNA (145-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	145	Total	C	H	N	O	P	0	0
			4611	1421	1641	535	870	144		

- Molecule 6 is a DNA chain called Human alpha-satellite DNA (145-MER) with CPD at position 95.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	144	Total	C	H	N	O	P	0	0
			4607	1420	1640	536	867	144		

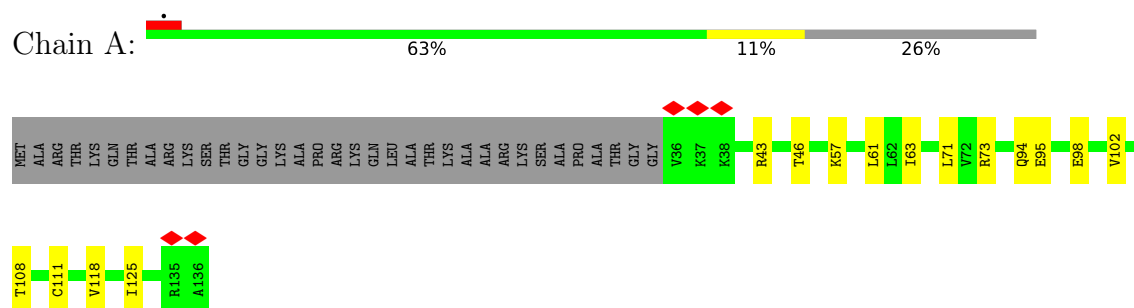
- Molecule 7 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	361	Total	C	H	N	O	S	0	0
			5666	1815	2807	515	513	16		

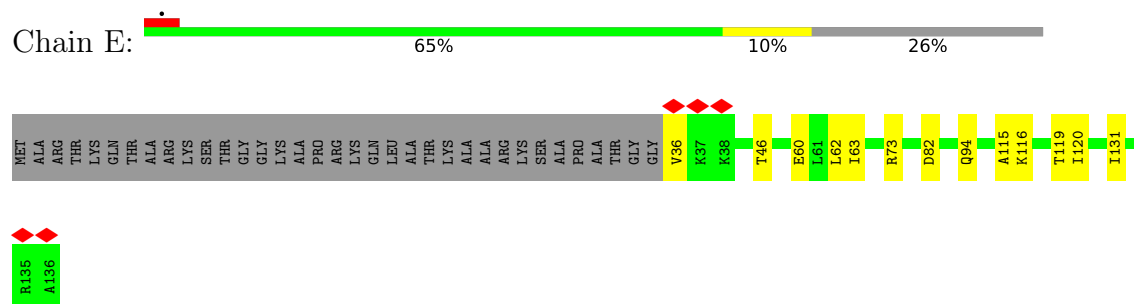
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

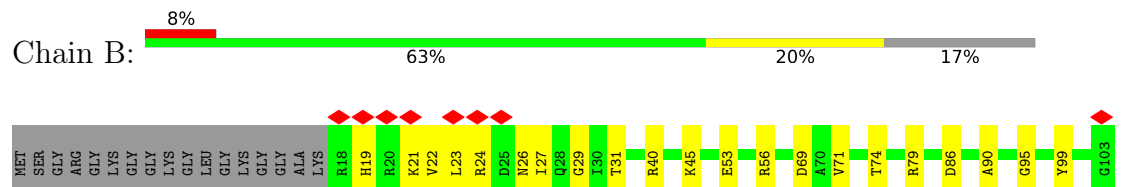
#### • Molecule 1: Histone H3.1



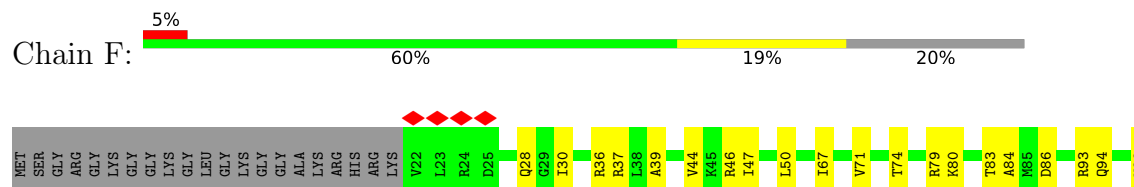
#### • Molecule 1: Histone H3.1



#### • Molecule 2: Histone H4

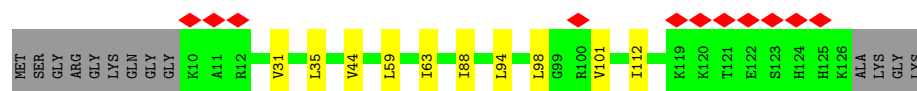
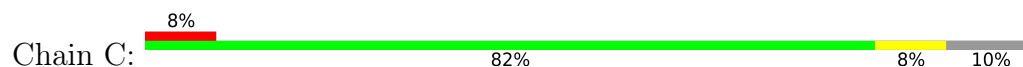


#### • Molecule 2: Histone H4

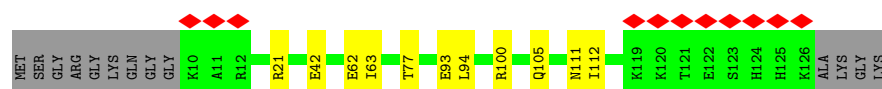
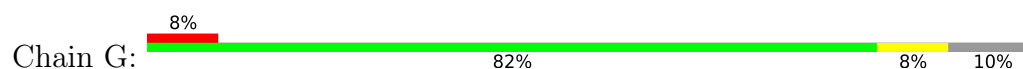




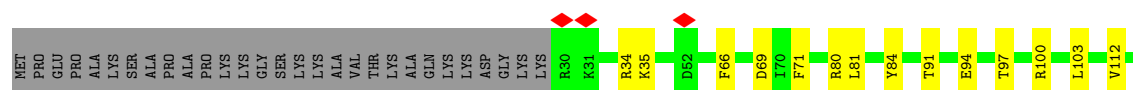
• Molecule 3: Histone H2A type 1-B/E



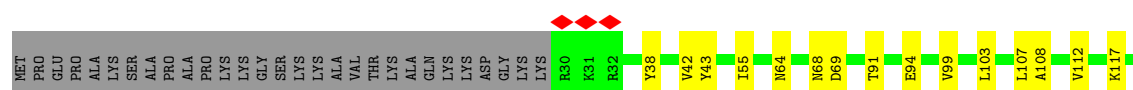
• Molecule 3: Histone H2A type 1-B/E



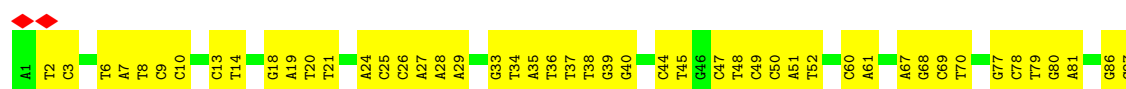
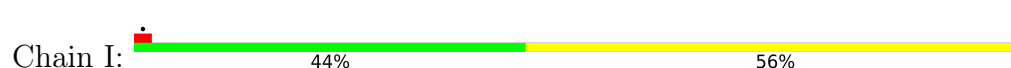
• Molecule 4: Histone H2B type 1-J



• Molecule 4: Histone H2B type 1-J

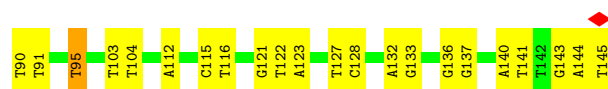


• Molecule 5: Human alpha-satellite DNA (145-MER)

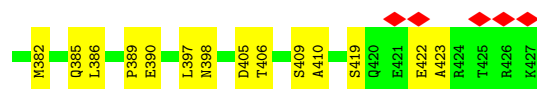
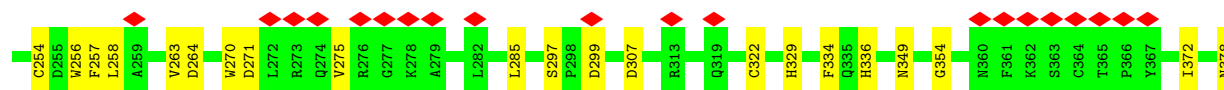
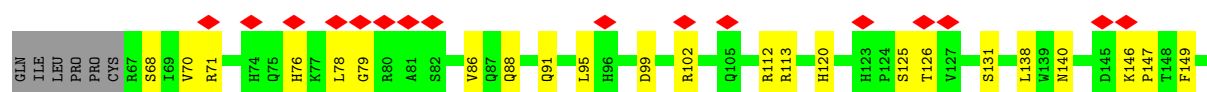
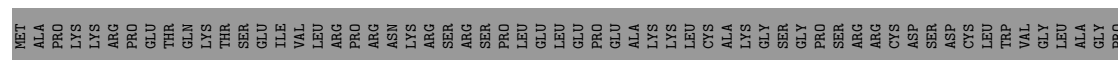




- Molecule 6: Human alpha-satellite DNA (145-MER) with CPD at position 95



- Molecule 7: DNA damage-binding protein 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.53	Depositor
Minimum defocus (nm)	10000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.211	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: TTD

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	0.20	0/844	0.32	0/1130
1	E	0.18	0/844	0.28	0/1130
2	B	0.21	0/702	0.34	0/937
2	F	0.20	0/660	0.32	0/883
3	C	0.18	0/921	0.28	0/1239
3	G	0.17	0/921	0.26	0/1239
4	D	0.18	0/777	0.27	0/1040
4	H	0.18	0/777	0.26	0/1040
5	I	0.26	0/3331	0.51	0/5140
6	J	0.27	0/3283	0.49	0/5062
7	L	0.26	0/2938	0.49	4/3987 (0.1%)
All	All	0.23	0/15998	0.43	4/22827 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	L	201	ASN	N-CA-C	-9.50	101.89	112.72
7	L	202	ILE	CB-CA-C	6.46	119.14	110.42
7	L	202	ILE	N-CA-CB	-5.63	104.16	111.82
7	L	199	THR	N-CA-C	5.50	122.51	110.80

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	A	832	876	878	13	0
1	E	832	876	878	13	0
2	B	694	740	742	15	0
2	F	653	695	696	19	0
3	C	909	969	973	12	0
3	G	909	969	973	11	0
4	D	766	793	797	10	0
4	H	766	794	797	9	0
5	I	2970	1641	1641	76	0
6	J	2967	1640	1640	58	0
7	L	2859	2807	2822	65	0
All	All	15157	12800	12837	263	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 10.

All (263) 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)
7:L:349:ASN:ND2	7:L:378:ASN:OD1	2.13	0.82
7:L:329:HIS:NE2	7:L:354:GLY:O	2.12	0.80
7:L:271:ASP:OD1	7:L:275:VAL:HG13	1.83	0.79
7:L:382:MET:SD	7:L:385:GLN:NE2	2.57	0.77
5:I:91:DT:H2'	5:I:92:DT:H71	1.66	0.77
7:L:125:SER:OG	7:L:140:ASN:OD1	2.02	0.76
2:B:99:TYR:OH	4:H:69:ASP:OD2	2.01	0.76
1:A:71:LEU:HD11	2:B:27:ILE:HG22	1.67	0.75
1:A:108:THR:HG21	1:A:125:ILE:HD13	1.69	0.74
1:E:82:ASP:OD2	2:F:80:LYS:NZ	2.19	0.74
1:A:63:ILE:O	1:A:94:GLN:NE2	2.21	0.73
5:I:141:DT:H2'	5:I:142:DT:H71	1.72	0.72
4:D:69:ASP:OD2	2:F:99:TYR:OH	2.08	0.71
5:I:24:DA:N1	6:J:121:DG:O6	2.22	0.71
7:L:397:LEU:O	7:L:398:ASN:ND2	2.24	0.71
7:L:208:ASP:OD2	7:L:250:LEU:N	2.25	0.68
7:L:206:SER:OG	7:L:248:VAL:HG22	1.95	0.67
4:H:91:THR:OG1	4:H:94:GLU:OE1	2.13	0.66
2:F:79:ARG:NH2	2:F:86:ASP:OD2	2.29	0.66
1:E:46:THR:OG1	6:J:143:DG:OP1	2.10	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:63:DG:H2'	6:J:64:DT:H72	1.79	0.65
3:C:101:VAL:HG11	2:F:99:TYR:CE2	2.33	0.64
1:E:82:ASP:O	2:F:80:LYS:NZ	2.30	0.64
7:L:194:PHE:HB3	7:L:228:LEU:HD22	1.79	0.64
6:J:50:DC:N4	6:J:51:DA:H62	1.97	0.63
4:D:35:LYS:N	6:J:123:DA:OP1	2.31	0.63
3:C:63:ILE:HD11	3:C:88:ILE:HG13	1.82	0.62
7:L:113:ARG:NH1	7:L:336:HIS:O	2.32	0.62
5:I:89:DT:H2''	5:I:90:DT:H71	1.82	0.62
1:A:43:ARG:O	1:A:46:THR:HG22	1.99	0.62
7:L:389:PRO:O	7:L:390:GLU:HB2	1.99	0.61
3:C:63:ILE:HD11	3:C:88:ILE:CG1	2.31	0.61
4:H:99:VAL:HG13	4:H:103:LEU:HD12	1.82	0.60
7:L:271:ASP:O	7:L:275:VAL:HG22	2.02	0.60
6:J:144:DA:N3	6:J:145:DT:O3'	2.35	0.60
6:J:103:DT:H2'	6:J:104:DT:H71	1.83	0.60
7:L:76:HIS:CD2	7:L:86:VAL:HG21	2.37	0.60
5:I:69:DC:H2'	5:I:70:DT:H71	1.84	0.59
6:J:63:DG:C2'	6:J:64:DT:H72	2.32	0.59
6:J:95:TTD:OP1	7:L:155:ALA:HA	2.02	0.59
7:L:297:SER:OG	7:L:299:ASP:OD1	2.17	0.59
5:I:78:DC:H2'	5:I:79:DT:H72	1.84	0.59
2:B:79:ARG:NH2	2:B:86:ASP:OD2	2.36	0.59
7:L:138:LEU:HD12	7:L:186:PHE:CD2	2.39	0.58
3:G:42:GLU:OE1	3:G:42:GLU:N	2.34	0.58
2:B:31:THR:HG21	5:I:60:DC:OP2	2.04	0.57
2:B:24:ARG:O	2:B:26:ASN:ND2	2.37	0.57
3:G:93:GLU:N	3:G:93:GLU:OE1	2.37	0.57
2:F:39:ALA:O	2:F:44:VAL:HG22	2.05	0.56
2:F:36:ARG:NH1	5:I:81:DA:OP2	2.39	0.56
6:J:103:DT:C2'	6:J:104:DT:H71	2.36	0.56
7:L:209:VAL:HG23	7:L:216:VAL:HG22	1.86	0.55
1:E:62:LEU:O	2:F:37:ARG:NH1	2.39	0.55
1:A:108:THR:HG21	1:A:125:ILE:CD1	2.37	0.55
2:B:40:ARG:NH1	2:B:45:LYS:O	2.39	0.55
3:C:112:ILE:N	3:C:112:ILE:HD12	2.22	0.55
6:J:89:DT:H2'	6:J:90:DT:H72	1.89	0.55
7:L:254:CYS:SG	7:L:256:TRP:NE1	2.78	0.55
2:F:39:ALA:HB1	2:F:44:VAL:HG21	1.89	0.55
7:L:271:ASP:OD1	7:L:271:ASP:O	2.25	0.54
2:F:94:GLN:N	2:F:94:GLN:OE1	2.41	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:142:DT:H4'	5:I:143:DG:OP1	2.07	0.54
1:E:120:ILE:HD11	2:F:47:ILE:HD12	1.89	0.54
5:I:103:DT:H2'	5:I:104:DT:H71	1.89	0.54
7:L:112:ARG:NH1	7:L:154:GLY:O	2.41	0.54
5:I:89:DT:C2'	5:I:90:DT:H71	2.37	0.53
7:L:264:ASP:OD1	7:L:264:ASP:O	2.27	0.53
7:L:68:SER:OG	7:L:71:ARG:NH1	2.42	0.53
5:I:13:DC:H2'	5:I:14:DT:H72	1.91	0.53
1:A:108:THR:CG2	1:A:125:ILE:HD13	2.36	0.52
7:L:307:ASP:OD1	7:L:307:ASP:C	2.52	0.52
1:E:36:VAL:HG13	1:E:36:VAL:O	2.09	0.52
7:L:227:LEU:C	7:L:227:LEU:HD23	2.34	0.52
5:I:47:DC:H2'	5:I:48:DT:H72	1.90	0.52
7:L:99:ASP:OD1	7:L:102:ARG:NH2	2.43	0.52
7:L:215:MET:HE2	7:L:227:LEU:HD21	1.90	0.52
3:C:98:LEU:HD11	4:D:66:PHE:CE1	2.45	0.52
5:I:70:DT:O2	6:J:77:DG:N2	2.43	0.52
4:D:91:THR:OG1	4:D:94:GLU:OE1	2.19	0.51
7:L:398:ASN:ND2	7:L:409:SER:OG	2.42	0.51
7:L:76:HIS:O	7:L:79:GLY:N	2.38	0.51
4:D:100:ARG:HH21	4:D:112:VAL:HG21	1.75	0.51
1:E:60:GLU:N	1:E:60:GLU:OE1	2.43	0.51
5:I:112:DA:C2	6:J:35:DA:C2	2.98	0.51
2:B:19:HIS:ND1	2:B:19:HIS:O	2.44	0.51
7:L:220:ASP:OD2	7:L:224:ASN:ND2	2.43	0.51
7:L:422:GLU:OE1	7:L:423:ALA:N	2.39	0.51
4:H:108:ALA:O	4:H:112:VAL:HG23	2.10	0.50
6:J:61:DA:C6	6:J:62:DT:H73	2.46	0.50
1:A:95:GLU:OE2	3:G:105:GLN:N	2.42	0.50
7:L:88:GLN:C	7:L:88:GLN:CD	2.79	0.50
3:C:98:LEU:HD11	4:D:66:PHE:HE1	1.75	0.50
7:L:257:PHE:HA	7:L:271:ASP:HA	1.94	0.50
1:E:119:THR:HG22	2:F:46:ARG:HB3	1.92	0.50
7:L:126:THR:HG23	7:L:138:LEU:HD21	1.94	0.50
7:L:168:ASN:OD1	7:L:168:ASN:C	2.55	0.50
4:H:38:TYR:O	4:H:42:VAL:HG23	2.12	0.50
7:L:168:ASN:OD1	7:L:170:ASN:N	2.42	0.49
3:G:62:GLU:OE2	4:H:107:LEU:HD11	2.13	0.49
7:L:397:LEU:HB2	7:L:410:ALA:HB3	1.94	0.49
3:C:31:VAL:HG22	4:D:71:PHE:HE2	1.77	0.49
6:J:39:DG:H2''	6:J:40:DG:C8	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:91:GLN:O	7:L:95:LEU:HG	2.12	0.49
7:L:249:ALA:O	7:L:258:LEU:HD12	2.11	0.49
4:H:64:ASN:O	4:H:68:ASN:ND2	2.46	0.49
3:C:35:LEU:HB3	3:C:44:VAL:HG21	1.95	0.49
5:I:20:DT:H2'	5:I:21:DT:H71	1.95	0.48
3:G:111:ASN:OD1	3:G:111:ASN:C	2.56	0.48
6:J:115:DC:H2'	6:J:116:DT:H71	1.94	0.48
5:I:61:DA:C2	6:J:86:DG:N2	2.82	0.48
5:I:104:DT:H2'	5:I:105:DT:C6	2.48	0.48
5:I:6:DT:C2	5:I:7:DA:C8	3.02	0.48
2:B:71:VAL:HA	2:B:74:THR:HG22	1.96	0.48
5:I:87:DC:H2''	5:I:88:DC:C6	2.49	0.48
5:I:33:DG:H2'	5:I:34:DT:C6	2.49	0.47
5:I:94:DA:H2'	5:I:95:DT:C6	2.50	0.47
3:C:63:ILE:HD13	3:C:94:LEU:HD22	1.97	0.47
6:J:72:DA:H2''	6:J:73:DA:C8	2.50	0.47
2:F:67:ILE:O	2:F:71:VAL:HG23	2.15	0.47
5:I:13:DC:C2'	5:I:14:DT:H72	2.45	0.47
5:I:127:DT:H4'	5:I:128:DC:OP1	2.14	0.47
5:I:51:DA:H2''	5:I:52:DT:H71	1.97	0.47
7:L:275:VAL:HG23	7:L:275:VAL:O	2.14	0.47
4:D:80:ARG:O	4:D:84:TYR:CD1	2.68	0.46
5:I:140:DA:C2	6:J:7:DA:C2	3.04	0.46
5:I:86:DG:N2	6:J:61:DA:C2	2.83	0.46
6:J:41:DA:H2''	6:J:42:DA:H8	1.80	0.46
5:I:38:DT:H4'	5:I:39:DG:OP1	2.15	0.46
5:I:90:DT:C2'	5:I:91:DT:H72	2.46	0.46
6:J:62:DT:H2'	6:J:63:DG:C8	2.50	0.46
7:L:270:TRP:HB3	7:L:275:VAL:HG21	1.97	0.46
7:L:159:ILE:H	7:L:159:ILE:HD12	1.80	0.46
7:L:263:VAL:HG12	7:L:263:VAL:O	2.16	0.46
1:A:57:LYS:HB2	1:A:57:LYS:NZ	2.31	0.46
5:I:9:DC:H4'	5:I:10:DC:OP1	2.15	0.46
5:I:20:DT:C2'	5:I:21:DT:H71	2.46	0.46
7:L:406:THR:HG23	7:L:419:SER:HB2	1.98	0.46
7:L:385:GLN:C	7:L:386:LEU:HD22	2.41	0.45
1:A:111:CYS:SG	1:E:131:ILE:HD11	2.56	0.45
2:F:28:GLN:HA	2:F:28:GLN:OE1	2.16	0.45
5:I:18:DG:H1'	5:I:19:DA:C8	2.51	0.45
5:I:47:DC:H2''	5:I:48:DT:C6	2.51	0.45
7:L:120:HIS:NE2	7:L:169:THR:HG21	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LYS:O	2:B:23:LEU:N	2.49	0.45
2:F:93:ARG:HH11	2:F:93:ARG:HG2	1.81	0.45
5:I:44:DC:H2''	5:I:45:DT:O5'	2.16	0.45
6:J:83:DC:H4'	6:J:84:DA:OP1	2.17	0.45
7:L:149:PHE:CD1	7:L:149:PHE:C	2.95	0.45
6:J:72:DA:H2''	6:J:73:DA:C5'	2.47	0.45
5:I:50:DC:O2	7:L:334:PHE:CE1	2.69	0.45
2:B:22:VAL:HG23	2:B:22:VAL:O	2.17	0.44
3:C:59:LEU:HD21	4:D:103:LEU:HD21	2.00	0.44
5:I:37:DT:H2''	5:I:38:DT:H72	1.99	0.44
6:J:80:DG:H2''	6:J:81:DA:H8	1.82	0.44
3:C:63:ILE:HD11	3:C:88:ILE:HG12	2.00	0.44
5:I:26:DC:H1'	5:I:27:DA:C5	2.52	0.44
5:I:51:DA:O4'	7:L:334:PHE:HE1	2.00	0.44
6:J:71:DG:C2	6:J:72:DA:C5	3.06	0.44
7:L:160:THR:HG22	7:L:175:SER:O	2.17	0.44
5:I:26:DC:O3'	5:I:27:DA:C8	2.70	0.44
5:I:37:DT:H2''	5:I:38:DT:C7	2.47	0.44
5:I:92:DT:C2	5:I:93:DG:C8	3.06	0.44
7:L:236:TRP:O	7:L:237:ASN:CB	2.66	0.44
5:I:67:DA:H2''	5:I:68:DG:C8	2.52	0.44
6:J:127:DT:H2''	6:J:128:DC:C6	2.53	0.44
7:L:131:SER:O	7:L:159:ILE:HD12	2.18	0.44
7:L:203:TRP:CZ2	7:L:221:ASN:ND2	2.85	0.43
6:J:41:DA:H2'	6:J:41:DA:N3	2.34	0.43
7:L:209:VAL:HG23	7:L:216:VAL:CG2	2.48	0.43
3:C:63:ILE:HD12	3:C:94:LEU:HD13	2.00	0.43
1:E:73:ARG:NH1	6:J:50:DC:OP1	2.40	0.43
5:I:103:DT:C5	5:I:104:DT:H73	2.53	0.43
5:I:35:DA:C2	6:J:112:DA:C2	3.07	0.43
5:I:102:DG:H2'	5:I:103:DT:H71	1.99	0.43
6:J:9:DC:C2'	6:J:10:DC:O4'	2.66	0.43
7:L:389:PRO:O	7:L:390:GLU:CB	2.64	0.43
4:H:43:TYR:CE1	4:H:55:ILE:HG22	2.54	0.43
7:L:146:LYS:O	7:L:147:PRO:C	2.62	0.43
6:J:20:DT:H2''	6:J:21:DT:C2	2.53	0.43
2:F:30:ILE:N	2:F:30:ILE:HD12	2.33	0.43
7:L:221:ASN:O	7:L:221:ASN:OD1	2.37	0.43
5:I:24:DA:C2	5:I:25:DC:C4	3.07	0.42
5:I:48:DT:H1'	5:I:49:DC:C5	2.53	0.42
6:J:95:TTD:H72	6:J:95:TTD:H5A1	1.86	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:140:DA:C8	6:J:141:DT:H72	2.54	0.42
6:J:52:DT:O2	6:J:52:DT:C2'	2.66	0.42
1:A:61:LEU:HD23	1:A:98:GLU:CD	2.44	0.42
5:I:116:DT:C6	5:I:117:DT:H72	2.54	0.42
5:I:119:DT:H4'	5:I:120:DG:OP1	2.19	0.42
5:I:129:DT:H4'	5:I:130:DG:OP1	2.19	0.42
6:J:38:DT:H2''	6:J:39:DG:C8	2.54	0.42
6:J:89:DT:H2''	6:J:90:DT:C6	2.55	0.42
6:J:95:TTD:O2	6:J:95:TTD:O4'	2.37	0.42
7:L:76:HIS:O	7:L:78:LEU:N	2.52	0.42
7:L:184:GLN:HA	7:L:191:LEU:HD22	2.02	0.42
7:L:190:ILE:O	7:L:190:ILE:HG23	2.18	0.42
5:I:19:DA:H2''	5:I:20:DT:H5'	2.01	0.42
5:I:24:DA:C6	6:J:121:DG:O6	2.73	0.42
6:J:90:DT:C2'	6:J:91:DT:H71	2.49	0.42
6:J:22:DC:H2'	6:J:23:DT:H71	2.01	0.42
3:G:21:ARG:NH2	6:J:31:DG:OP1	2.52	0.42
7:L:405:ASP:OD1	7:L:406:THR:N	2.53	0.42
2:B:24:ARG:NH2	2:B:53:GLU:OE2	2.52	0.42
5:I:39:DG:H2''	5:I:40:DG:C8	2.55	0.42
6:J:59:DG:H2''	6:J:60:DC:C6	2.55	0.42
5:I:7:DA:C8	5:I:8:DT:H72	2.55	0.42
5:I:99:DG:N2	6:J:48:DT:O2	2.53	0.42
5:I:114:DA:H2''	5:I:115:DC:O5'	2.20	0.42
1:A:73:ARG:NH2	5:I:50:DC:OP1	2.47	0.41
3:G:63:ILE:HD13	3:G:94:LEU:HD13	2.02	0.41
6:J:4:DA:C2	6:J:5:DA:C6	3.08	0.41
1:E:63:ILE:O	1:E:94:GLN:NE2	2.54	0.41
2:F:50:LEU:HD23	2:F:50:LEU:N	2.35	0.41
1:A:118:VAL:O	1:A:118:VAL:HG12	2.20	0.41
3:G:77:THR:O	3:G:77:THR:HG22	2.19	0.41
5:I:35:DA:C2'	5:I:36:DT:H71	2.50	0.41
6:J:9:DC:H2''	6:J:10:DC:O4'	2.19	0.41
5:I:49:DC:H1'	5:I:50:DC:C6	2.55	0.41
5:I:140:DA:C4'	5:I:141:DT:OP1	2.68	0.41
6:J:72:DA:H2''	6:J:73:DA:H5'	2.01	0.41
7:L:372:ILE:H	7:L:372:ILE:HD12	1.86	0.41
2:B:95:GLY:O	3:G:100:ARG:NH2	2.53	0.41
4:D:81:LEU:HD13	4:D:97:THR:HB	2.02	0.41
5:I:88:DC:H1'	5:I:89:DT:C5	2.56	0.41
7:L:235:LEU:O	7:L:236:TRP:HE3	2.03	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:63:ILE:CD1	3:G:94:LEU:HD13	2.51	0.41
5:I:137:DG:H2''	5:I:138:DA:C8	2.56	0.41
5:I:143:DG:C2	5:I:144:DA:N1	2.88	0.41
6:J:41:DA:C2'	6:J:42:DA:H8	2.33	0.41
6:J:95:TTD:H73	7:L:200:ILE:HG23	2.03	0.41
4:H:117:LYS:O	4:H:120:THR:HG22	2.20	0.41
5:I:25:DC:H4'	5:I:26:DC:OP1	2.20	0.41
5:I:143:DG:C2	6:J:4:DA:C2	3.09	0.41
5:I:90:DT:H2''	5:I:91:DT:C7	2.51	0.41
6:J:3:DC:H2'	6:J:4:DA:C8	2.56	0.41
6:J:10:DC:N4	6:J:11:DA:H62	2.19	0.41
6:J:122:DT:H71	6:J:123:DA:N7	2.36	0.41
1:A:98:GLU:O	1:A:102:VAL:HG23	2.21	0.40
2:B:27:ILE:HD12	2:B:56:ARG:HB3	2.03	0.40
5:I:2:DT:H2''	5:I:3:DC:C6	2.56	0.40
5:I:28:DA:H2''	5:I:29:DA:H8	1.85	0.40
6:J:56:DA:H4'	6:J:56:DA:OP1	2.20	0.40
6:J:132:DA:C6	6:J:133:DG:C6	3.08	0.40
2:B:69:ASP:HB2	2:B:90:ALA:HB1	2.02	0.40
1:E:120:ILE:HG13	1:E:120:ILE:O	2.21	0.40
5:I:140:DA:H2'	5:I:141:DT:H72	2.03	0.40
6:J:37:DT:H2''	6:J:38:DT:C6	2.55	0.40
1:E:115:ALA:C	1:E:116:LYS:HG2	2.46	0.40
2:F:83:THR:HG22	2:F:84:ALA:N	2.36	0.40
5:I:50:DC:H2'	5:I:51:DA:C8	2.56	0.40
5:I:79:DT:H4'	5:I:80:DG:OP1	2.21	0.40
6:J:136:DG:H2''	6:J:137:DG:O4'	2.22	0.40
7:L:70:VAL:HG22	7:L:70:VAL:O	2.21	0.40
5:I:19:DA:H2'	5:I:20:DT:H72	2.04	0.40
5:I:44:DC:H4'	5:I:45:DT:OP1	2.21	0.40
5:I:88:DC:H2''	5:I:89:DT:C7	2.51	0.40
2:B:26:ASN:O	2:B:29:GLY:N	2.38	0.40
2:F:71:VAL:HA	2:F:74:THR:HG22	2.03	0.40
3:G:111:ASN:OD1	3:G:112:ILE:N	2.54	0.40
5:I:77:DG:H2''	5:I:78:DC:C6	2.56	0.40
5:I:124:DG:C6	5:I:125:DA:C6	3.10	0.40
6:J:53:DC:N3	6:J:54:DA:N1	2.70	0.40
7:L:285:LEU:HD12	7:L:285:LEU:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	99/136 (73%)	97 (98%)	2 (2%)	0	100	100
1	E	99/136 (73%)	96 (97%)	3 (3%)	0	100	100
2	B	84/103 (82%)	75 (89%)	9 (11%)	0	100	100
2	F	80/103 (78%)	77 (96%)	3 (4%)	0	100	100
3	C	115/130 (88%)	107 (93%)	8 (7%)	0	100	100
3	G	115/130 (88%)	111 (96%)	4 (4%)	0	100	100
4	D	95/126 (75%)	91 (96%)	4 (4%)	0	100	100
4	H	95/126 (75%)	93 (98%)	2 (2%)	0	100	100
7	L	359/427 (84%)	318 (89%)	41 (11%)	0	100	100
All	All	1141/1417 (80%)	1065 (93%)	76 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/111 (79%)	88 (100%)	0	100	100
1	E	88/111 (79%)	88 (100%)	0	100	100
2	B	71/79 (90%)	71 (100%)	0	100	100
2	F	67/79 (85%)	67 (100%)	0	100	100
3	C	93/100 (93%)	93 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	93/100 (93%)	93 (100%)	0	100	100
4	D	83/105 (79%)	81 (98%)	2 (2%)	44	67
4	H	83/105 (79%)	83 (100%)	0	100	100
7	L	313/371 (84%)	307 (98%)	6 (2%)	52	72
All	All	979/1161 (84%)	971 (99%)	8 (1%)	77	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	34	ARG
4	D	124	SER
7	L	177	MET
7	L	197	SER
7	L	198	ASP
7	L	200	ILE
7	L	202	ILE
7	L	322	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
2	B	26	ASN
4	D	85	ASN
3	G	32	HIS
4	H	50	HIS
7	L	76	HIS
7	L	336	HIS
7	L	398	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	TTD	J	95	6	42,45,46	3.39	18 (42%)	62,74,77	2.24	21 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TTD	J	95	6	-	12/22/109/110	0/5/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	95	TTD	C5-C6	-7.56	1.46	1.55
6	J	95	TTD	C5T-C6T	-7.52	1.46	1.55
6	J	95	TTD	C2-N3	6.77	1.50	1.38
6	J	95	TTD	C2-N1	6.53	1.49	1.36
6	J	95	TTD	C2T-N3T	6.49	1.49	1.38
6	J	95	TTD	C2'-C3R	-6.39	1.38	1.52
6	J	95	TTD	C2T-N1T	6.35	1.49	1.36
6	J	95	TTD	C4-N3	6.05	1.46	1.37
6	J	95	TTD	C4T-N3T	5.48	1.46	1.37
6	J	95	TTD	C2'-C1'	-3.31	1.43	1.52
6	J	95	TTD	C6-N1	3.19	1.51	1.46
6	J	95	TTD	PB-O3R	3.16	1.68	1.60
6	J	95	TTD	PB-O5R	2.81	1.70	1.59
6	J	95	TTD	C3'-C4'	-2.80	1.45	1.53
6	J	95	TTD	O2-C2	-2.40	1.18	1.23
6	J	95	TTD	C6T-C6	2.26	1.63	1.56
6	J	95	TTD	O4-C4	-2.18	1.19	1.22
6	J	95	TTD	O2T-C2T	-2.15	1.19	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	95	TTD	C4-N3-C2	-5.30	118.53	126.67
6	J	95	TTD	O4R-C1R-N1T	5.17	114.77	108.65
6	J	95	TTD	C2'-C1'-N1	-4.71	109.22	115.59
6	J	95	TTD	C4T-N3T-C2T	-4.52	119.72	126.67
6	J	95	TTD	C5-C4-N3	4.26	119.77	116.06
6	J	95	TTD	C5T-C4T-N3T	4.17	119.69	116.06
6	J	95	TTD	O4'-C1'-N1	3.92	113.30	108.65
6	J	95	TTD	N3-C2-N1	3.91	120.75	116.69
6	J	95	TTD	N3T-C2T-N1T	3.70	120.53	116.69
6	J	95	TTD	O4-C4-C5	-3.42	120.15	122.88
6	J	95	TTD	C5-C5T-C6T	3.21	92.36	88.38
6	J	95	TTD	C5T-C6T-N1T	3.16	120.04	115.61
6	J	95	TTD	C6-C5-C4	3.13	123.41	114.50
6	J	95	TTD	O4T-C4T-C5T	-2.90	120.56	122.88
6	J	95	TTD	O4P-PB-O3R	2.74	117.60	106.78
6	J	95	TTD	C4'-O4R-C1R	-2.53	103.33	109.45
6	J	95	TTD	O2T-C2T-N1T	-2.42	119.73	123.49
6	J	95	TTD	PB-O5R-C5R	-2.33	108.05	121.68
6	J	95	TTD	O4P-PB-O5R	2.25	118.22	107.75
6	J	95	TTD	C5'-C4R-C3R	-2.05	109.85	114.53
6	J	95	TTD	O4R-C1R-C2R	-2.01	102.45	106.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	95	TTD	C4R-C3R-O3R-PB
6	J	95	TTD	O4'-C1'-N1-C2
6	J	95	TTD	O4'-C1'-N1-C6
6	J	95	TTD	O4R-C4'-C5R-O5R
6	J	95	TTD	C2R-C1R-N1T-C6T
6	J	95	TTD	O4R-C1R-N1T-C2T
6	J	95	TTD	C2R-C1R-N1T-C2T
6	J	95	TTD	C3'-C4'-C5R-O5R
6	J	95	TTD	O4R-C1R-N1T-C6T
6	J	95	TTD	C2'-C3R-O3R-PB
6	J	95	TTD	O4'-C4R-C5'-O5'
6	J	95	TTD	C4'-C5R-O5R-PB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	95	TTD	4	0

## 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](#)

There are no chain breaks in this entry.

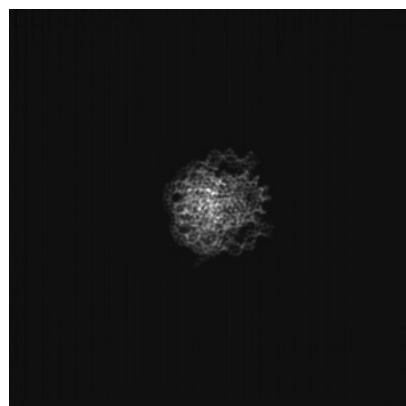
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61243. These allow visual inspection of the internal detail of the map and identification of artifacts.

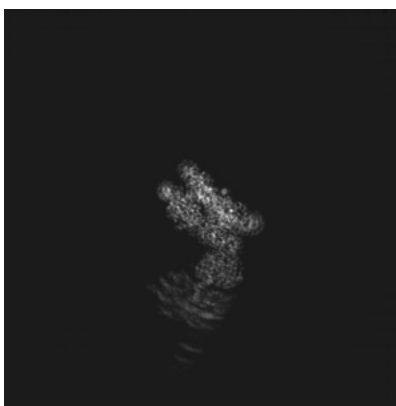
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

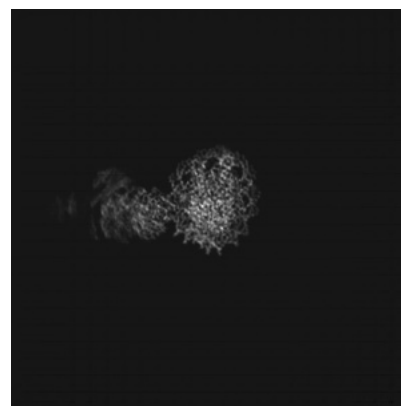
#### 6.1.1 Primary map



X

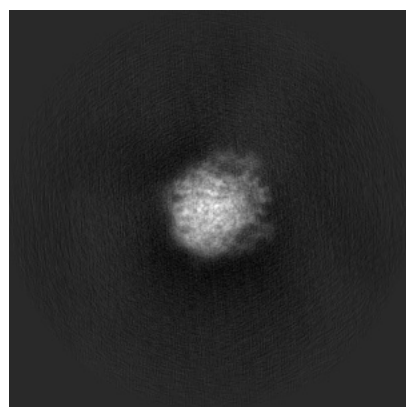


Y

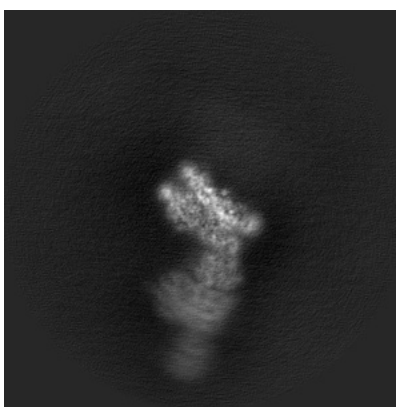


Z

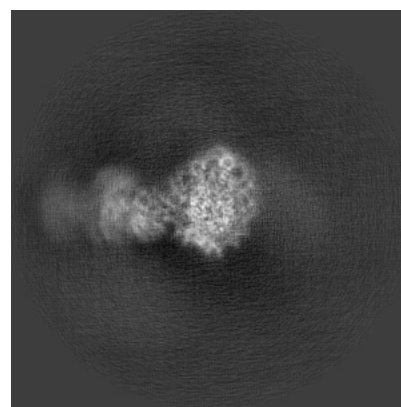
#### 6.1.2 Raw map



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: 180

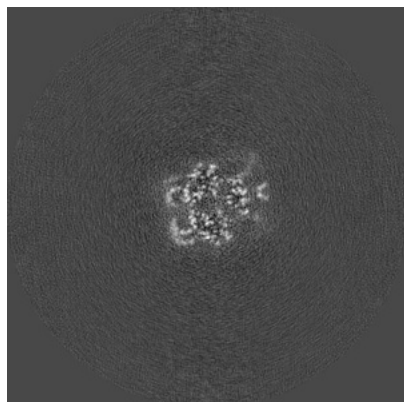


Y Index: 180

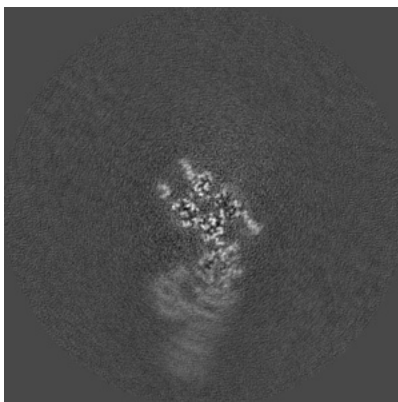


Z Index: 180

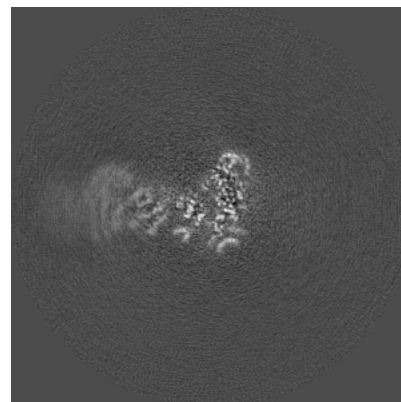
### 6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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: 178



Y Index: 182

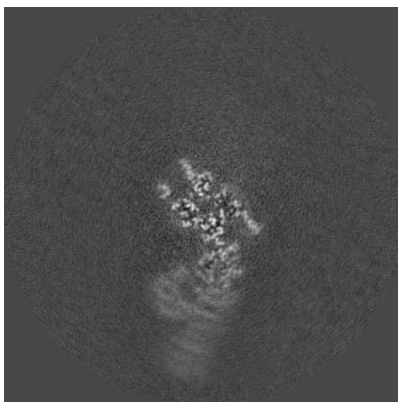


Z Index: 188

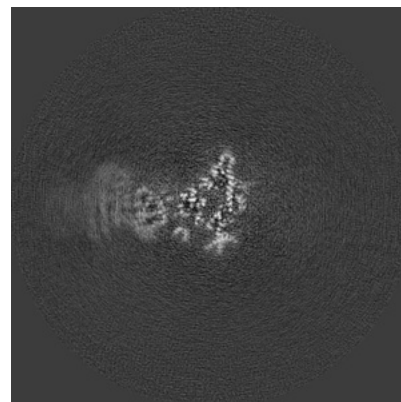
### 6.3.2 Raw map



X Index: 172



Y Index: 180

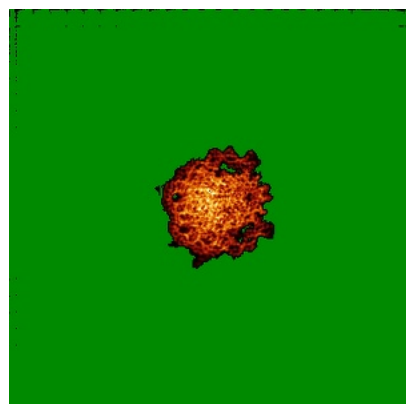


Z Index: 184

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

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

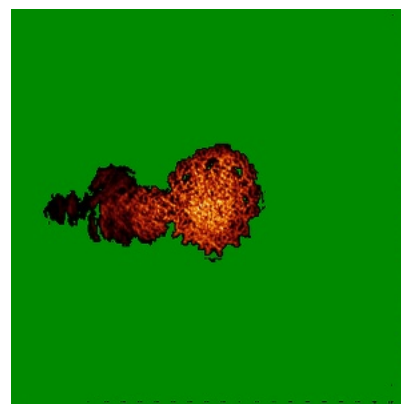
### 6.4.1 Primary map



X

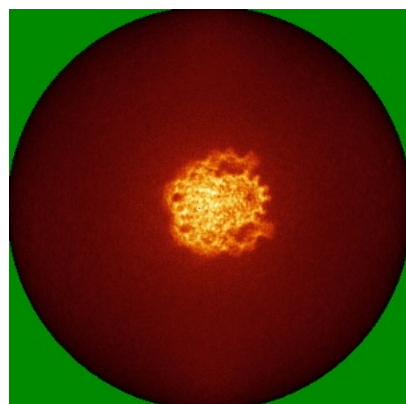


Y

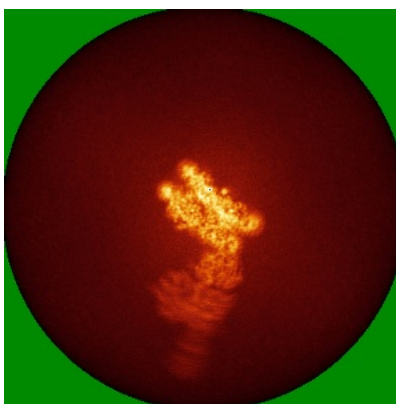


Z

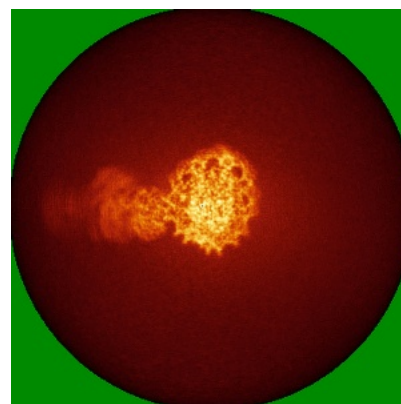
### 6.4.2 Raw map



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.

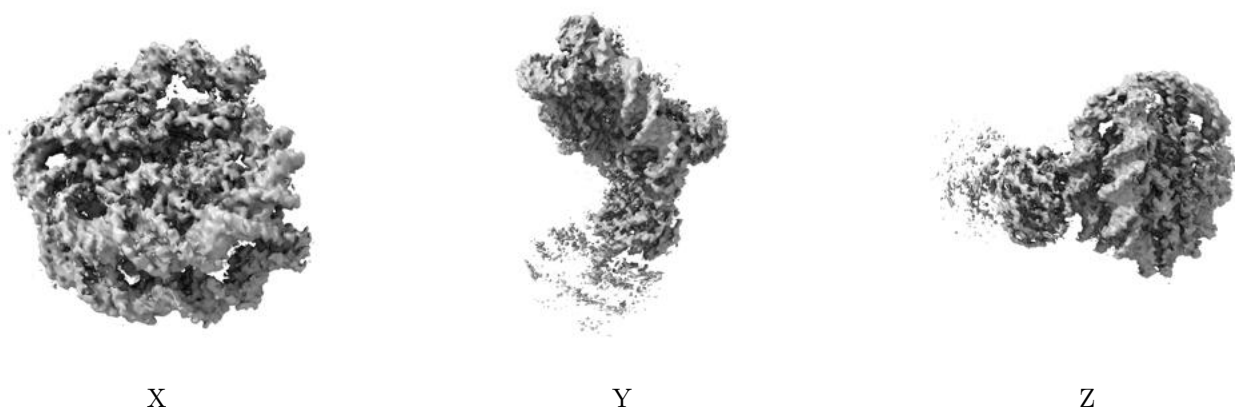
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

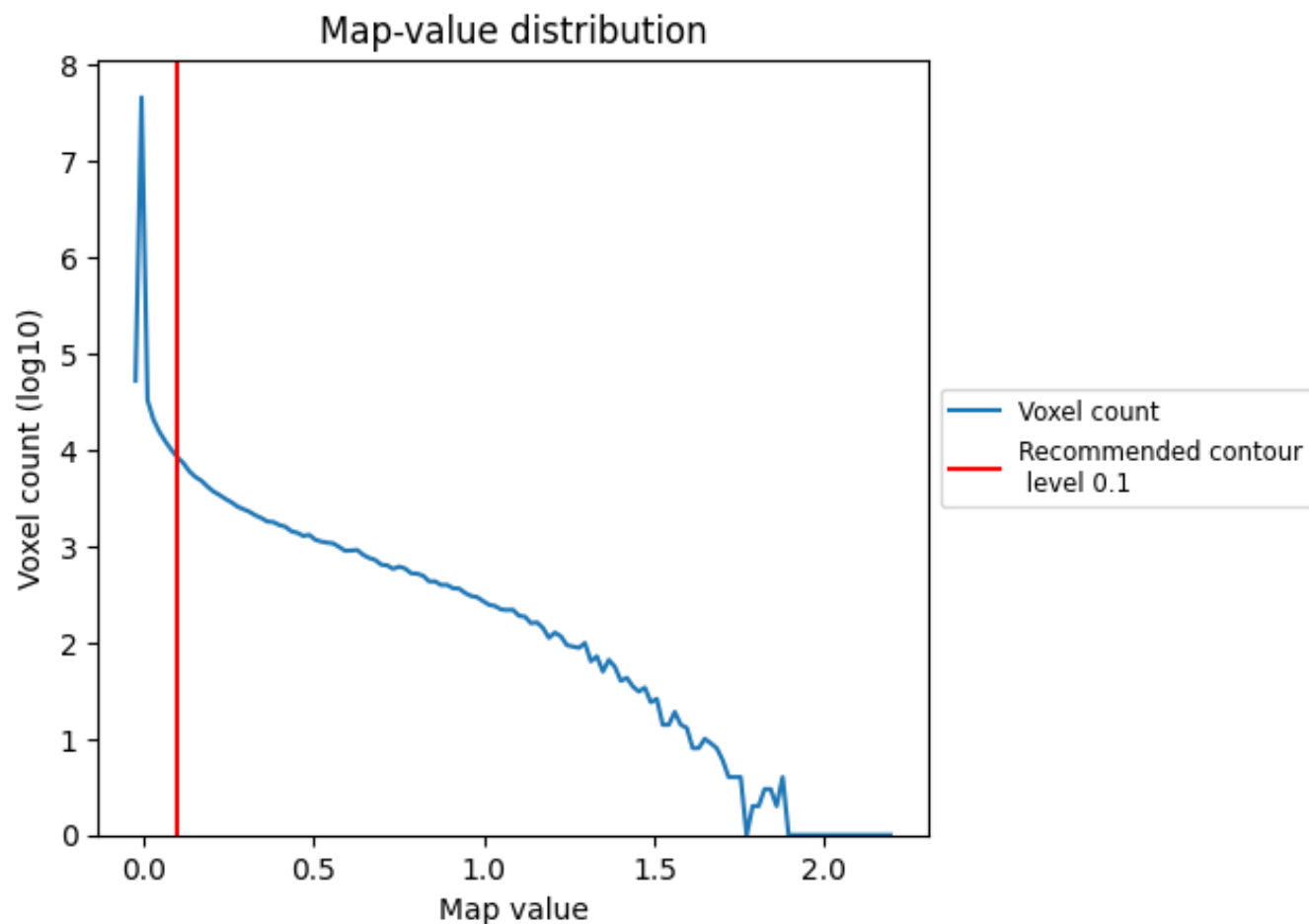
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

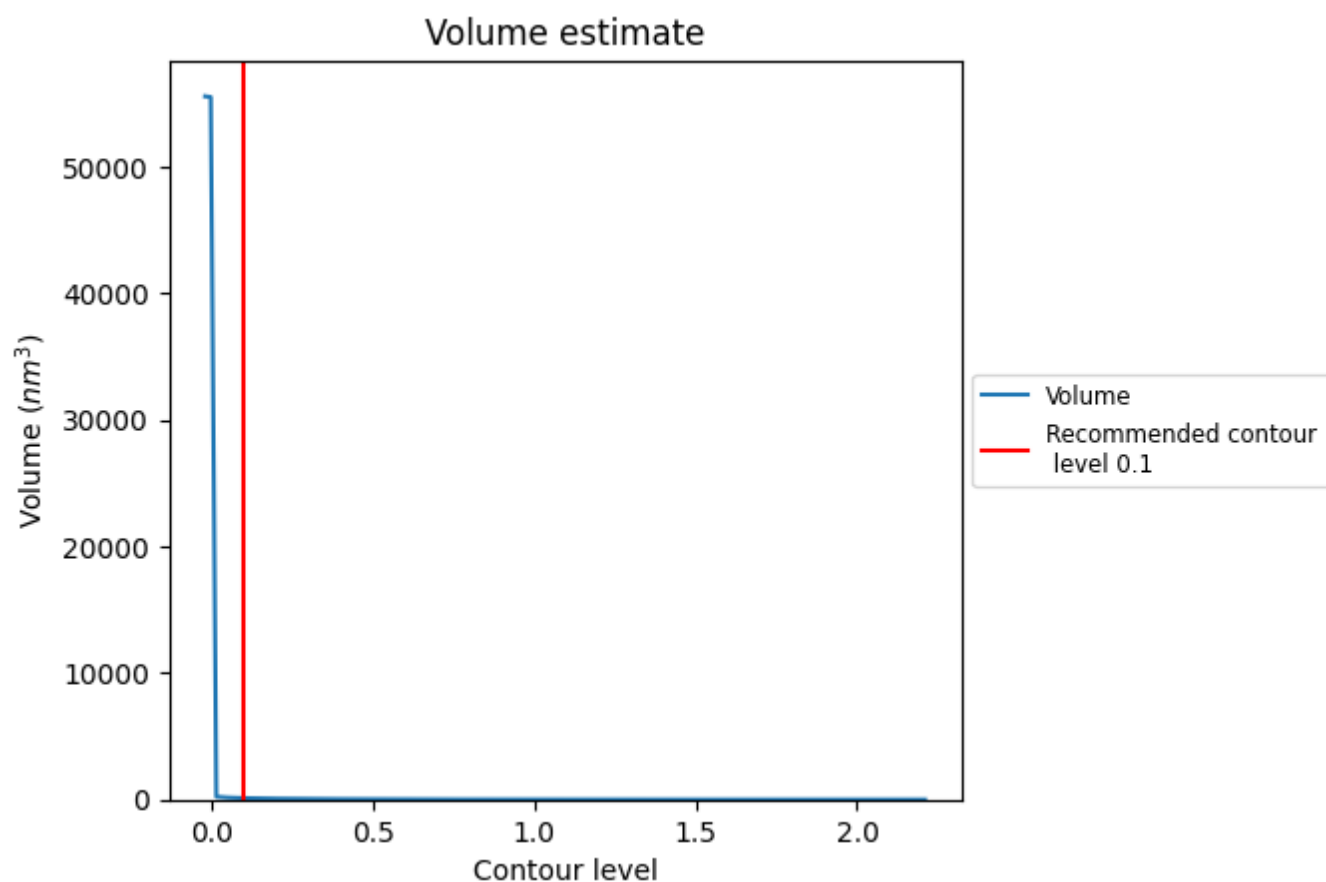
This section contains the results of statistical analysis of the map.

### 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.

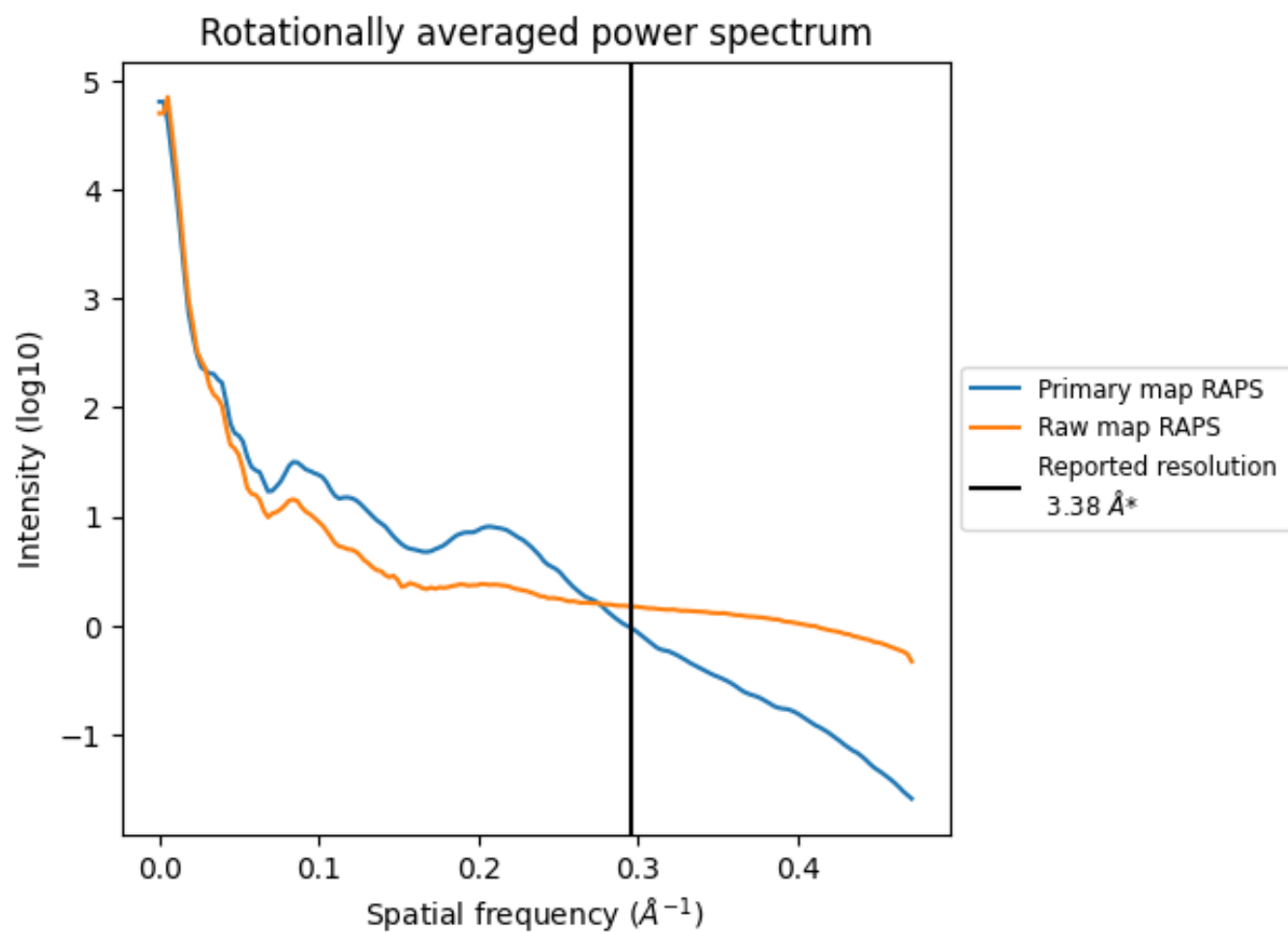
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm<sup>3</sup>; this corresponds to an approximate mass of 103 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 ⓘ

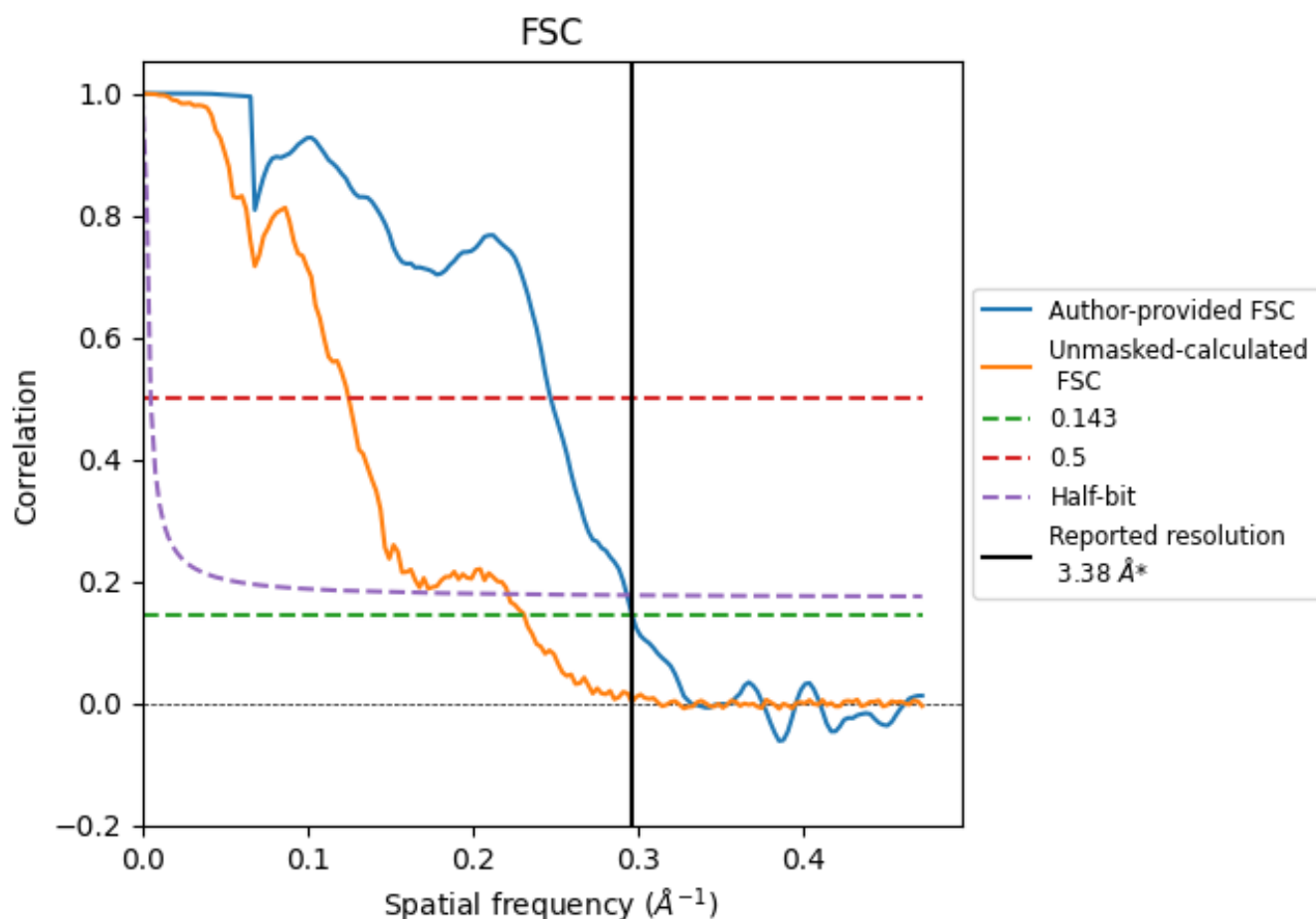


\*Reported resolution corresponds to spatial frequency of 0.296 Å<sup>-1</sup>

## 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  $0.296 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	3.37	4.05	3.41
Unmasked-calculated*	4.33	8.01	4.52

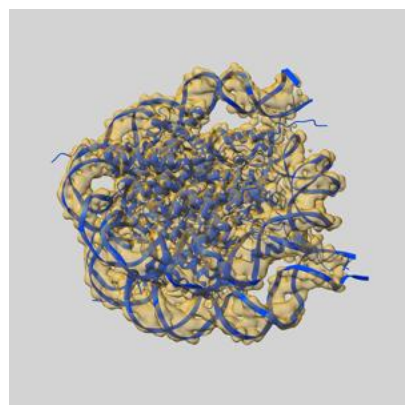
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.33 differs from the reported value 3.38 by more than 10 %



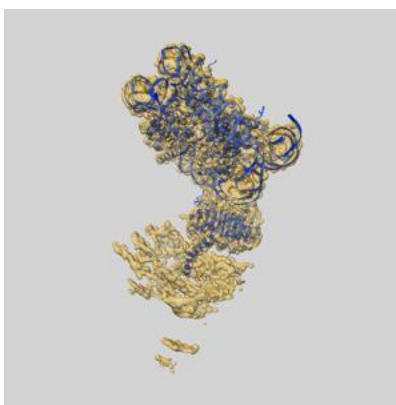
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61243 and PDB model 9J8W. Per-residue inclusion information can be found in section [3](#) on page [6](#).

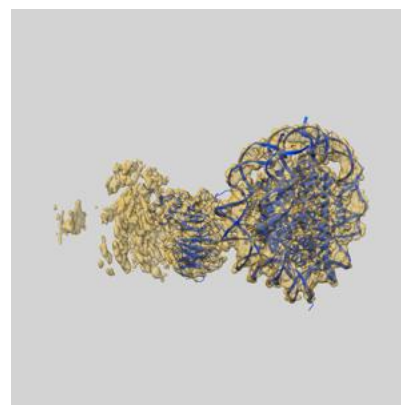
### 9.1 Map-model overlay [i](#)



X



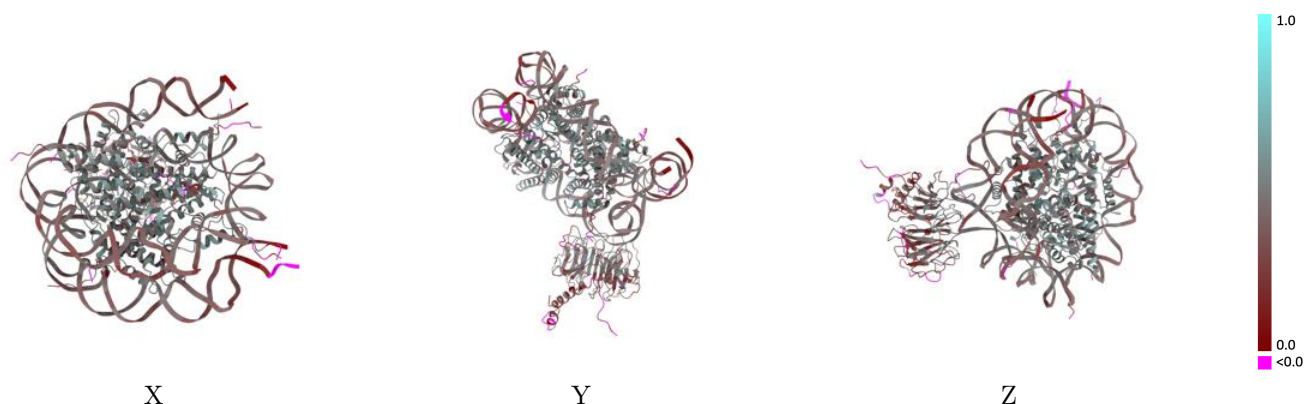
Y



Z

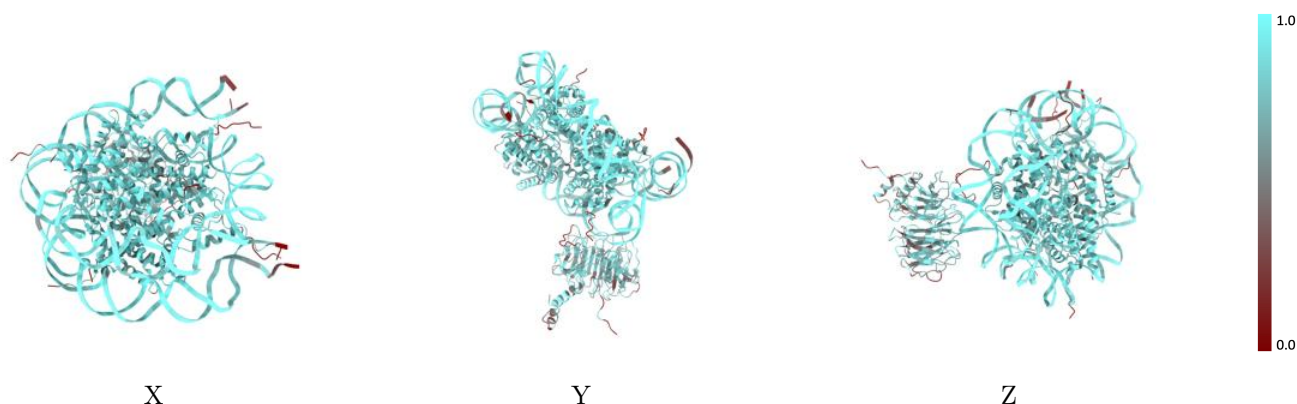
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



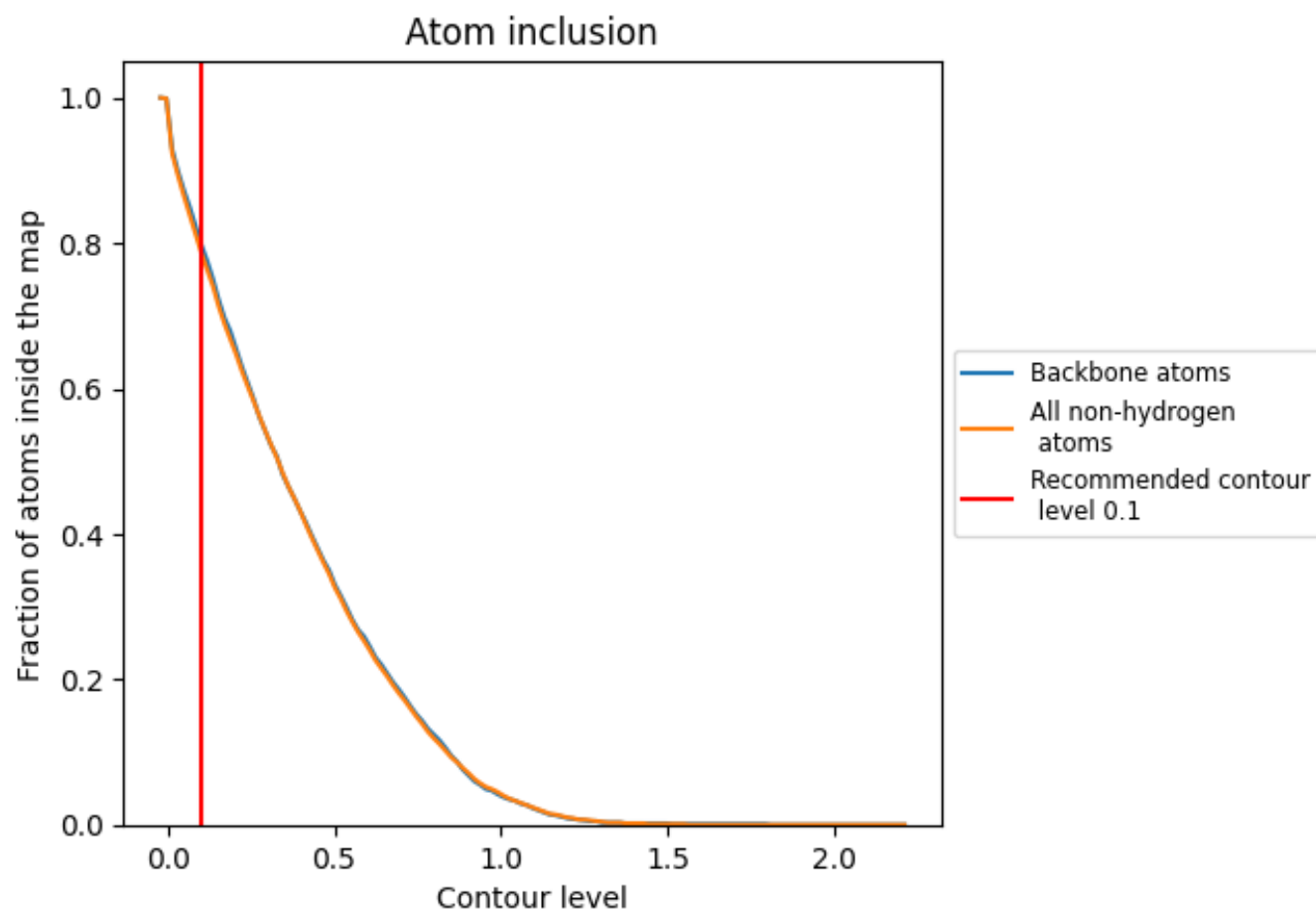
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.3970
A	 0.8350	 0.4760
B	 0.8010	 0.4410
C	 0.7830	 0.4490
D	 0.8260	 0.4580
E	 0.8220	 0.4730
F	 0.8440	 0.4740
G	 0.7720	 0.4430
H	 0.8200	 0.4590
I	 0.8640	 0.3660
J	 0.8590	 0.3660
L	 0.6650	 0.3210

