



Full wwPDB EM Validation Report ⓘ

Aug 28, 2023 – 10:20 AM JST

PDB ID : 8J6S
EMDB ID : EMD-36013
Title : Cryo-EM structure of the single CAF-1 bound right-handed Di-tetrasome
Authors : Liu, C.P.; Yu, Z.Y.; Xu, R.M.
Deposited on : 2023-04-26
Resolution : 3.80 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.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

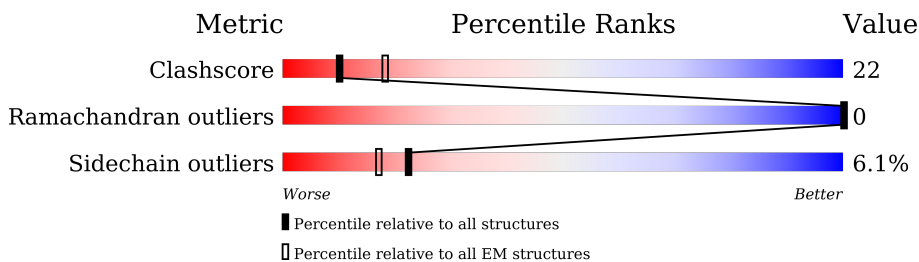
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.






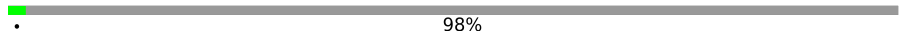
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	136	
1	C	136	
1	E	136	
1	G	136	
2	B	103	
2	D	103	
2	F	103	
2	H	103	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	147	
4	J	147	
5	L	559	
6	K	956	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10030 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	75	484	304	95	83	2	0	0
1	E	90	663	416	127	116	4	0	0
1	C	88	676	428	127	117	4	0	0
1	A	76	568	362	103	99	4	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	H	71	468	299	88	81	0	0
2	F	74	482	302	98	82	0	0
2	D	73	571	360	113	97	1	0
2	B	69	510	321	103	86	0	0

- Molecule 3 is a DNA chain called Widom 601 DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	I	99	2009	955	359	596	99	0	0

- Molecule 4 is a DNA chain called Widom 601 DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	J	98	2031	959	388	586	98	0	0

- Molecule 5 is a protein called Chromatin assembly factor 1 subunit B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	L	302	1494	890	302	302	0	0

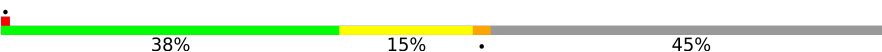
- Molecule 6 is a protein called Chromatin assembly factor 1 subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	K	15	74	44	15	15	0	0

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

Chain G: 

MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY LYS LYS PRO ARG LYS GLN LEU VAL THR THR ALA ALA ARG LYS SER ALA PRO THR THR THR THR VAL LYS LYS HIS ARG TYR ARG PRO GLY THR VAL VAL ALA LEU ARG GLU ILE ARG ARG TYR LYS SER THR E59

R63 D81 A95 Y99 L100 E105 D106 T107 N108 L109 C110 A111 I112 H113 R116 V117 T118 I119 M120 P121 K122 D123 S124 I124 Q125 L126 A127 R128 T129 I130 R131 G132 E133 ARG ALA

- Molecule 1: Histone H3.1

Chain E: 

MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY LYS LYS PRO ARG LYS GLN LEU VAL THR THR ALA ALA ARG LYS SER ALA PRO THR THR THR THR VAL LYS LYS HIS ARG TYR ARG PRO GLY T45 Y46 A47 L48 R49 E50 I51 R52 R53 T58 L62 R63 R64

L65 P66 F67 Q68 R69 L70 W71 R72 E73 I74 F84 Q85 S86 S87 Q93 C96 E97 L100 V101 V101 F104 E105 D106 T107 M108 L109 C110 H113 R116 V117 T118 I119 M120 P121 K122 D123 I124 L126 I130 R134 ALA

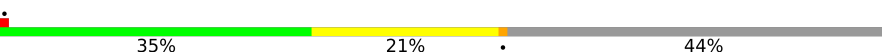
- Molecule 1: Histone H3.1

Chain C: 

MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY LYS LYS PRO ARG LYS GLN LEU VAL THR THR ALA ALA ARG LYS SER ALA PRO THR THR THR THR VAL LYS LYS HIS ARG TYR ARG PRO GLY THR VAL A47 L48 I51 Y54 L61 T62 R63 R64 P66

F67 Q68 R69 E73 I74 D77 R83 F84 Q85 S86 S87 V89 L92 L100 V101 F104 T107 M108 H113 I119 R120 K122 D123 I124 R128 R129 I130 R134 ALA

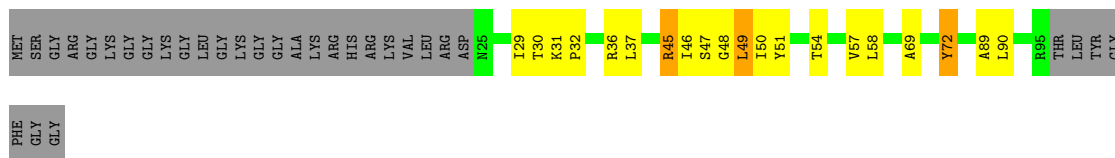
- Molecule 1: Histone H3.1

Chain A: 

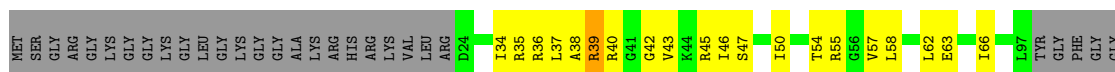
MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY LYS LYS PRO ARG LYS GLN LEU VAL THR THR ALA ALA ARG LYS SER ALA PRO THR THR THR THR VAL LYS LYS HIS ARG TYR ARG PRO GLY THR VAL VAL ALA LEU ARG GLU ILE ARG ARG TYR LYS SER THR E59



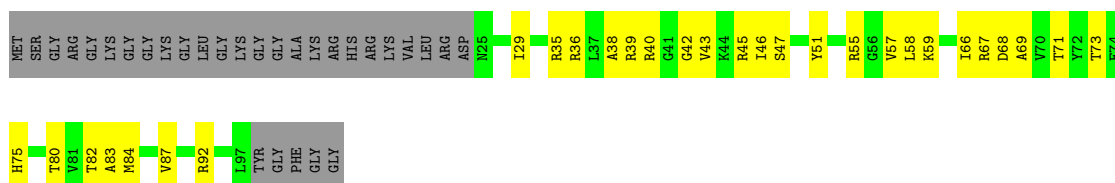
• Molecule 2: Histone H4



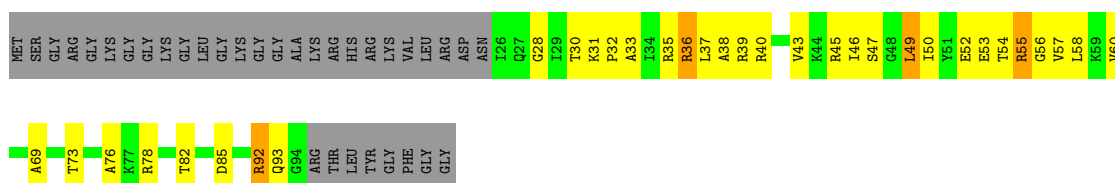
• Molecule 2: Histone H4



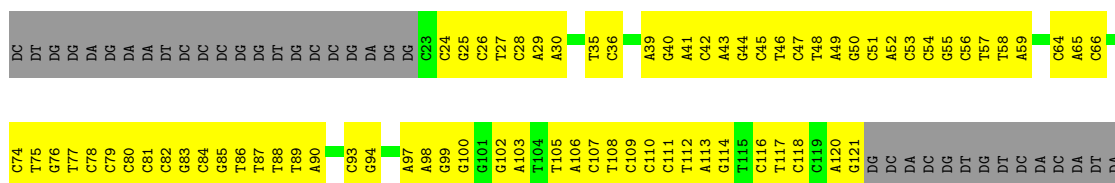
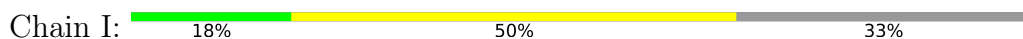
• Molecule 2: Histone H4



• Molecule 2: Histone H4



• Molecule 3: Widom 601 DNA (147-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67319	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.445	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/574	0.67	0/775
1	C	0.32	0/684	0.67	1/922 (0.1%)
1	E	0.31	0/669	0.72	1/903 (0.1%)
1	G	0.27	0/488	0.64	1/667 (0.1%)
2	B	0.27	0/513	0.75	0/691
2	D	0.30	0/576	0.62	0/774
2	F	0.27	0/485	0.59	0/660
2	H	0.25	0/473	0.60	0/645
3	I	0.53	0/2248	0.96	0/3462
4	J	0.51	0/2283	0.89	0/3527
5	L	0.25	0/1486	0.46	0/2058
6	K	0.22	0/72	0.49	0/97
All	All	0.40	0/10551	0.77	3/15181 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	65	LEU	CA-CB-CG	5.57	128.10	115.30
1	C	66	PRO	CA-N-CD	-5.49	103.82	111.50
1	G	121	PRO	CA-N-CD	-5.23	104.18	111.50

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	568	0	564	45	0
1	C	676	0	671	35	0
1	E	663	0	642	50	0
1	G	484	0	413	33	0
2	B	510	0	530	34	0
2	D	571	0	611	31	0
2	F	482	0	421	30	0
2	H	468	0	412	21	0
3	I	2009	0	1112	83	0
4	J	2031	0	1099	100	0
5	L	1494	0	672	12	0
6	K	74	0	35	0	0
All	All	10030	0	7182	362	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 22.

All (362) 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)
1:A:63:ARG:NH2	4:J:33:DA:H5''	1.11	1.43
1:A:63:ARG:NH2	4:J:33:DA:C5'	1.91	1.31
1:A:63:ARG:HH21	4:J:33:DA:C5'	1.55	1.13
1:C:85:GLN:HE21	1:C:87:SER:H	1.14	0.93
1:E:118:THR:OG1	2:F:45:ARG:HD2	1.69	0.91
3:I:56:DC:O2	4:J:92:DG:N2	2.07	0.88
3:I:66:DC:O2	4:J:82:DG:N2	2.10	0.83
3:I:56:DC:N3	4:J:92:DG:N1	2.28	0.81
2:B:46:ILE:HD11	2:B:50:ILE:HD13	1.65	0.79
1:G:121:PRO:HD2	1:G:122:LYS:H	1.50	0.77
1:C:66:PRO:HD2	1:C:67:PHE:H	1.52	0.74
1:C:74:ILE:HD11	2:D:59:LYS:HE3	1.71	0.73
5:L:69:VAL:HA	5:L:85:GLY:HA2	1.70	0.73
3:I:80:DC:H42	4:J:68:DG:H22	1.36	0.72
4:J:75:DC:H2'	4:J:76:DG:C8	2.24	0.72
2:D:45:ARG:HD3	4:J:55:DG:H5'	1.70	0.72
1:E:118:THR:HG23	2:F:45:ARG:HG2	1.72	0.71
3:I:81:DC:H42	4:J:67:DG:H1	1.37	0.71
1:A:63:ARG:NH2	4:J:33:DA:H5'	2.01	0.71
3:I:118:DC:H3'	1:A:65:LEU:CD2	2.21	0.70
2:H:30:THR:OG1	3:I:36:DC:OP1	2.10	0.69
2:F:36:ARG:NH2	4:J:87:DT:OP1	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:ARG:HH22	4:J:117:DA:H4'	1.57	0.69
4:J:113:DA:H2'	4:J:114:DC:C6	2.28	0.69
2:D:80:THR:OG1	4:J:75:DC:OP1	2.11	0.69
1:A:121:PRO:HG3	2:B:49:LEU:HB2	1.75	0.69
4:J:86:DG:H2'	4:J:87:DT:C6	2.29	0.68
3:I:51:DC:H2''	3:I:52:DA:C8	2.28	0.68
1:A:63:ARG:CZ	4:J:33:DA:H5''	2.15	0.67
3:I:50:DG:N2	4:J:99:DT:O2	2.28	0.67
1:E:108:ASN:ND2	2:F:42:GLY:O	2.28	0.66
1:C:85:GLN:NE2	1:C:87:SER:H	1.90	0.66
5:L:288:THR:HA	5:L:323:SER:HA	1.77	0.66
1:G:130:ILE:HG21	1:E:130:ILE:CG2	2.25	0.66
2:H:36:ARG:NH2	3:I:35:DT:OP2	2.28	0.66
1:E:108:ASN:HD21	2:F:43:VAL:HA	1.60	0.66
3:I:97:DA:H2''	3:I:98:DA:N7	2.11	0.66
4:J:52:DG:H2''	4:J:53:DG:C8	2.31	0.66
3:I:40:DG:N2	4:J:109:DT:O2	2.29	0.65
4:J:123:DC:H2''	4:J:124:DG:H5'	1.78	0.65
1:C:108:ASN:HD21	2:D:43:VAL:HA	1.62	0.65
1:A:70:LEU:O	1:A:74:ILE:HG12	1.96	0.65
3:I:111:DC:H2'	3:I:112:DT:H71	1.79	0.65
1:G:130:ILE:HG21	1:E:130:ILE:HG23	1.79	0.64
3:I:80:DC:N4	4:J:68:DG:H22	1.96	0.64
2:F:54:THR:HA	2:F:57:VAL:HG12	1.79	0.64
3:I:66:DC:N3	4:J:82:DG:N1	2.41	0.64
2:B:52:GLU:HA	2:B:55:ARG:HB2	1.80	0.63
1:A:64:LYS:O	1:A:67:PHE:N	2.32	0.63
3:I:114:DG:N2	4:J:35:DT:O2	2.32	0.62
4:J:120:DG:H2''	4:J:121:DA:H5''	1.82	0.62
1:G:100:LEU:HD22	2:H:37:LEU:HD21	1.82	0.62
3:I:76:DG:H22	4:J:73:DA:H2	1.47	0.62
2:B:50:ILE:O	2:B:54:THR:HG23	2.00	0.61
3:I:118:DC:H3'	1:A:65:LEU:HD21	1.83	0.61
4:J:90:DA:H2''	4:J:91:DA:C8	2.36	0.60
2:B:76:ALA:HB1	2:B:78:ARG:HE	1.66	0.60
1:G:124:ILE:HD12	2:H:50:ILE:HD12	1.84	0.60
5:L:362:ALA:HA	5:L:372:PHE:HA	1.83	0.59
2:B:54:THR:HA	2:B:57:VAL:HG22	1.84	0.59
1:E:65:LEU:HD23	1:E:66:PRO:HD3	1.84	0.59
3:I:24:DC:H2'	3:I:25:DG:C8	2.37	0.59
1:E:108:ASN:ND2	2:F:43:VAL:HA	2.16	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:HIS:CE1	1:E:116:ARG:HH22	2.21	0.58
1:G:116:ARG:NH1	1:G:123:ASP:OD1	2.36	0.58
4:J:121:DA:H2'	4:J:122:DG:C8	2.38	0.58
2:F:35:ARG:NH2	3:I:56:DC:OP2	2.36	0.58
3:I:29:DA:N6	4:J:120:DG:O6	2.36	0.58
4:J:111:DC:H2''	4:J:112:DG:C8	2.38	0.58
2:B:35:ARG:O	2:B:39:ARG:HG2	2.03	0.58
4:J:68:DG:H2'	4:J:69:DG:C8	2.39	0.58
1:A:125:GLN:NE2	2:B:53:GLU:OE1	2.31	0.58
4:J:66:DG:H2''	4:J:67:DG:C8	2.39	0.57
1:G:99:TYR:OH	1:G:128:ARG:NH2	2.37	0.57
1:A:85:GLN:HE22	2:B:82:THR:HA	1.69	0.57
2:D:82:THR:HG23	2:D:84:MET:H	1.70	0.57
3:I:111:DC:H2''	3:I:112:DT:H5'	1.86	0.56
1:A:116:ARG:NH1	1:A:118:THR:O	2.38	0.56
1:A:124:ILE:O	1:A:128:ARG:HG3	2.05	0.56
4:J:87:DT:H2'	4:J:88:DT:H71	1.88	0.56
1:G:118:THR:HA	2:H:45:ARG:HB3	1.85	0.56
2:H:47:SER:OG	2:H:48:GLY:N	2.37	0.56
2:B:33:ALA:HA	2:B:36:ARG:NH1	2.20	0.56
4:J:62:DA:H1'	4:J:63:DC:C2	2.40	0.56
1:E:74:ILE:HD13	2:F:66:ILE:HD12	1.86	0.56
3:I:25:DG:H1	4:J:123:DC:H42	1.52	0.56
3:I:118:DC:O5'	1:A:65:LEU:HD21	2.05	0.56
1:G:106:ASP:OD1	1:G:107:THR:N	2.38	0.56
1:E:85:GLN:OE1	1:E:87:SER:N	2.25	0.56
1:E:85:GLN:OE1	1:E:86:SER:N	2.39	0.56
1:C:61:LEU:HD12	2:D:36:ARG:HB3	1.87	0.56
4:J:116:DA:H1'	4:J:117:DA:H5'	1.86	0.56
1:E:69:ARG:O	1:E:73:GLU:HG3	2.05	0.56
1:A:97:GLU:HG2	2:B:37:LEU:HD21	1.87	0.56
1:E:96:CYS:SG	2:F:58:LEU:HD11	2.45	0.56
2:D:38:ALA:HB3	2:D:46:ILE:HD11	1.87	0.56
1:A:119:ILE:HG21	2:B:50:ILE:HD12	1.87	0.56
2:F:39:ARG:HA	2:F:43:VAL:HG22	1.89	0.55
3:I:90:DA:N1	4:J:59:DA:N6	2.54	0.55
4:J:117:DA:H2''	4:J:118:DT:H72	1.89	0.55
1:C:51:ILE:HG13	2:D:39:ARG:HG3	1.88	0.55
2:D:69:ALA:O	2:D:73:THR:HG23	2.07	0.55
4:J:109:DT:O4	4:J:110:DA:N6	2.40	0.55
1:C:130:ILE:HD12	1:A:106:ASP:OD2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:102:DA:H2''	4:J:103:DG:C8	2.42	0.55
1:C:68:GLN:HG2	1:C:89:VAL:HG11	1.89	0.54
3:I:89:DT:H1'	3:I:90:DA:H5'	1.90	0.54
1:G:106:ASP:HB2	1:E:130:ILE:HD12	1.89	0.54
1:C:69:ARG:O	1:C:73:GLU:HG2	2.08	0.54
3:I:27:DT:H2''	3:I:28:DC:H5'	1.88	0.54
4:J:75:DC:H2''	4:J:76:DG:O5'	2.08	0.54
1:E:74:ILE:HD11	2:F:63:GLU:HA	1.89	0.53
1:E:63:ARG:HD3	3:I:66:DC:OP1	2.08	0.53
2:H:29:ILE:HD13	2:H:58:LEU:HD23	1.91	0.53
2:F:39:ARG:HH11	2:F:39:ARG:HG2	1.73	0.53
3:I:78:DC:H2''	3:I:79:DC:C6	2.43	0.53
2:D:29:ILE:HG13	2:D:58:LEU:HD23	1.89	0.53
5:L:59:LEU:O	5:L:116:LYS:N	2.41	0.53
1:C:101:VAL:HG21	2:D:40:ARG:HD2	1.90	0.53
1:G:113:HIS:HE1	1:E:116:ARG:HH22	1.54	0.53
1:E:116:ARG:NH2	1:E:123:ASP:OD1	2.41	0.53
3:I:24:DC:N4	3:I:25:DG:O6	2.42	0.53
5:L:90:ILE:O	5:L:125:LEU:N	2.36	0.53
4:J:57:DT:H2''	4:J:58:DT:C5	2.43	0.53
1:E:93:GLN:NE2	1:E:97:GLU:OE2	2.40	0.53
3:I:78:DC:H2''	3:I:79:DC:C5	2.44	0.53
1:C:48:LEU:HA	1:C:51:ILE:HD12	1.91	0.53
2:B:56:GLY:O	2:B:60:VAL:HG23	2.09	0.53
5:L:324:GLU:O	5:L:349:LEU:N	2.37	0.53
2:H:45:ARG:NH1	4:J:107:DT:H4'	2.25	0.52
1:C:108:ASN:ND2	2:D:42:GLY:O	2.42	0.52
1:G:126:LEU:HD22	1:E:113:HIS:HB3	1.91	0.52
1:A:85:GLN:OE1	1:A:85:GLN:N	2.40	0.52
4:J:105:DT:H2''	4:J:106:DG:N7	2.25	0.52
2:D:67:ARG:O	2:D:71:THR:HG23	2.09	0.52
1:A:61:LEU:HD11	2:B:40:ARG:HH21	1.74	0.52
4:J:82:DG:H2''	4:J:83:DT:C6	2.45	0.52
3:I:56:DC:N4	4:J:92:DG:O6	2.42	0.52
1:C:85:GLN:HE21	1:C:87:SER:N	1.96	0.52
3:I:74:DC:H2''	3:I:75:DT:C5	2.45	0.52
3:I:29:DA:H2''	3:I:30:DA:C8	2.44	0.52
3:I:85:DG:H1'	3:I:86:DT:C4	2.45	0.52
1:E:104:PHE:HA	1:E:107:THR:HG22	1.92	0.51
3:I:109:DC:H2''	3:I:110:DC:H5'	1.92	0.51
1:G:95:ALA:HB1	2:H:90:LEU:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:CYS:SG	1:G:126:LEU:HD23	2.50	0.51
1:G:116:ARG:HD3	1:G:120:MET:SD	2.51	0.51
4:J:96:DT:H2''	4:J:97:DG:N7	2.25	0.51
1:A:69:ARG:NH2	2:B:28:GLY:H	2.07	0.51
1:A:110:CYS:SG	1:A:126:LEU:HD22	2.51	0.51
2:D:84:MET:HE1	2:D:87:VAL:HG11	1.93	0.51
3:I:57:DT:H2''	3:I:58:DT:C5	2.46	0.50
1:A:121:PRO:O	1:A:125:GLN:NE2	2.43	0.50
4:J:93:DC:H2''	4:J:94:DG:C8	2.46	0.50
1:C:47:ALA:O	1:C:51:ILE:HD12	2.12	0.50
1:A:100:LEU:HD11	2:B:58:LEU:HD22	1.93	0.50
1:C:61:LEU:HD23	2:D:40:ARG:NH2	2.26	0.50
3:I:53:DC:H2''	3:I:54:DC:C5	2.47	0.50
4:J:60:DA:H2''	4:J:61:DA:C8	2.47	0.50
3:I:93:DC:H2''	3:I:94:DG:N7	2.27	0.50
3:I:40:DG:H2''	3:I:41:DA:N7	2.26	0.50
1:G:130:ILE:HG21	1:E:130:ILE:HG21	1.93	0.49
2:H:49:LEU:HD12	2:H:49:LEU:H	1.78	0.49
3:I:75:DT:N3	3:I:76:DG:O6	2.45	0.49
1:C:104:PHE:HA	1:C:107:THR:HG22	1.94	0.49
4:J:55:DG:H2''	4:J:56:DG:C8	2.47	0.49
3:I:76:DG:H1'	3:I:77:DT:H5'	1.93	0.49
4:J:37:DG:H2''	4:J:38:DG:C8	2.46	0.49
5:L:293:CYS:HA	5:L:319:PHE:HA	1.95	0.49
2:B:92:ARG:NH2	2:B:93:GLN:HB2	2.26	0.49
1:C:66:PRO:HD2	1:C:67:PHE:N	2.24	0.49
3:I:49:DA:H2''	3:I:50:DG:C8	2.47	0.49
1:C:63:ARG:HA	1:C:63:ARG:NH1	2.28	0.49
1:G:100:LEU:HD22	2:H:37:LEU:CD2	2.43	0.49
3:I:97:DA:H5'	2:D:45:ARG:HH21	1.77	0.49
1:C:119:ILE:O	2:D:47:SER:HB2	2.13	0.49
1:G:126:LEU:HD22	1:E:113:HIS:CB	2.43	0.48
3:I:84:DC:H2''	3:I:85:DG:C8	2.48	0.48
1:A:70:LEU:HA	1:A:73:GLU:HG3	1.93	0.48
1:C:92:LEU:HD11	2:D:66:ILE:HG12	1.95	0.48
5:L:9:ALA:HB1	5:L:13:LYS:H	1.78	0.48
1:E:110:CYS:SG	1:E:126:LEU:HD13	2.54	0.48
3:I:45:DC:H2'	3:I:46:DT:H71	1.95	0.48
1:G:121:PRO:CD	1:G:122:LYS:H	2.24	0.48
1:A:110:CYS:O	1:A:113:HIS:HB3	2.13	0.48
4:J:93:DC:H2''	4:J:94:DG:N7	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HH22	4:J:33:DA:C5'	2.09	0.48
2:B:32:PRO:HD2	2:B:33:ALA:H	1.79	0.48
2:B:52:GLU:OE1	2:B:52:GLU:N	2.41	0.48
4:J:75:DC:H2'	4:J:76:DG:H8	1.75	0.48
1:C:54:TYR:CZ	2:D:36:ARG:HG2	2.48	0.48
2:D:45:ARG:HG3	4:J:55:DG:OP1	2.14	0.48
1:E:108:ASN:HD22	2:F:43:VAL:HG12	1.78	0.48
3:I:106:DA:H2''	3:I:107:DC:C6	2.48	0.48
1:E:70:LEU:HA	1:E:73:GLU:OE2	2.14	0.47
1:E:97:GLU:OE1	2:F:37:LEU:HD21	2.14	0.47
2:D:35:ARG:NH1	4:J:55:DG:OP2	2.47	0.47
2:B:36:ARG:HA	2:B:39:ARG:HG2	1.96	0.47
2:H:30:THR:HG21	3:I:35:DT:H5''	1.96	0.47
2:H:31:LYS:HE2	2:H:51:TYR:CZ	2.49	0.47
1:E:47:ALA:O	1:E:51:ILE:HG12	2.14	0.47
1:A:119:ILE:O	2:B:47:SER:HB3	2.13	0.47
2:B:49:LEU:H	2:B:49:LEU:HD12	1.78	0.47
1:G:126:LEU:HD21	1:E:110:CYS:HA	1.95	0.47
1:E:120:MET:CE	1:E:121:PRO:HD2	2.45	0.47
1:C:83:ARG:HA	1:C:83:ARG:HD2	1.54	0.47
1:A:96:CYS:SG	2:B:58:LEU:HD11	2.54	0.47
1:A:122:LYS:HA	1:A:125:GLN:OE1	2.14	0.47
1:E:58:THR:HG22	1:E:58:THR:O	2.14	0.47
1:A:61:LEU:HD11	2:B:40:ARG:NH2	2.29	0.47
4:J:44:DA:H2'	4:J:45:DT:H71	1.96	0.47
4:J:107:DT:H2''	4:J:108:DC:C4	2.49	0.47
2:D:45:ARG:CD	4:J:55:DG:H5'	2.43	0.47
4:J:75:DC:H4'	4:J:76:DG:OP1	2.15	0.47
3:I:47:DC:H2'	3:I:48:DT:H71	1.96	0.47
1:A:108:ASN:HB2	2:B:43:VAL:HG12	1.95	0.47
3:I:99:DG:H2''	3:I:100:DG:C8	2.50	0.47
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.80	0.46
4:J:54:DC:H2''	4:J:55:DG:C8	2.50	0.46
2:F:35:ARG:HD3	2:F:39:ARG:HH21	1.80	0.46
1:C:74:ILE:CD1	2:D:59:LYS:HE3	2.44	0.46
4:J:99:DT:H2''	4:J:100:DA:C8	2.49	0.46
1:G:63:ARG:NH1	4:J:118:DT:OP1	2.49	0.46
2:B:30:THR:OG1	2:B:32:PRO:HD2	2.15	0.46
3:I:118:DC:H3'	1:A:65:LEU:HD22	1.95	0.46
3:I:39:DA:H61	4:J:110:DA:N6	2.14	0.46
4:J:99:DT:H2''	4:J:100:DA:H8	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:ALA:HB1	1:E:130:ILE:HD11	1.98	0.46
2:H:69:ALA:HA	2:H:72:TYR:CD2	2.51	0.46
3:I:39:DA:N6	4:J:110:DA:N1	2.64	0.46
2:D:83:ALA:O	2:D:87:VAL:HG12	2.16	0.46
2:H:46:ILE:HD11	2:H:50:ILE:HG21	1.98	0.46
4:J:101:DG:H2''	4:J:102:DA:H8	1.80	0.46
1:E:62:ILE:HD11	2:F:37:LEU:HD11	1.97	0.46
1:G:121:PRO:HD2	1:G:122:LYS:N	2.25	0.45
1:E:97:GLU:OE1	1:E:97:GLU:HA	2.16	0.45
3:I:44:DG:H2''	3:I:45:DC:H5	1.81	0.45
2:B:69:ALA:O	2:B:73:THR:OG1	2.27	0.45
2:B:38:ALA:HB1	2:B:43:VAL:HG21	1.97	0.45
1:G:130:ILE:HG12	1:E:106:ASP:HB3	1.99	0.45
1:E:63:ARG:NH2	4:J:86:DG:O3'	2.50	0.45
3:I:79:DC:H4'	3:I:80:DC:OP1	2.14	0.45
4:J:29:DG:H2''	4:J:30:DG:C8	2.51	0.45
3:I:108:DT:O5'	2:B:45:ARG:NH1	2.43	0.45
3:I:102:DG:H2''	3:I:103:DA:C8	2.51	0.45
1:A:63:ARG:HA	1:A:64:LYS:NZ	2.32	0.45
4:J:102:DA:H2''	4:J:103:DG:H5'	1.99	0.45
2:H:36:ARG:HH22	3:I:35:DT:P	2.40	0.45
3:I:86:DT:H2''	3:I:87:DT:OP2	2.16	0.45
4:J:88:DT:H2''	4:J:89:DT:H71	1.99	0.45
5:L:292:ARG:O	5:L:320:ALA:N	2.38	0.45
2:F:50:ILE:O	2:F:54:THR:HG22	2.18	0.44
1:A:67:PHE:CD1	1:A:70:LEU:HD21	2.52	0.44
3:I:82:DC:C2	3:I:83:DG:N7	2.85	0.44
4:J:71:DA:H1'	4:J:72:DC:C6	2.52	0.44
4:J:98:DC:H2''	4:J:99:DT:C5	2.51	0.44
1:E:65:LEU:HD21	3:I:65:DA:H2'	1.98	0.44
2:F:47:SER:O	2:F:50:ILE:HG22	2.17	0.44
3:I:58:DT:H2''	3:I:59:DA:C8	2.53	0.44
1:C:65:LEU:HD23	4:J:65:DC:OP2	2.17	0.44
4:J:65:DC:C2	4:J:66:DG:N7	2.86	0.44
2:H:46:ILE:HD12	2:H:47:SER:H	1.83	0.44
2:F:35:ARG:HD3	2:F:39:ARG:NH2	2.33	0.44
3:I:49:DA:N1	4:J:100:DA:C6	2.86	0.44
4:J:51:DT:H2''	4:J:52:DG:C8	2.53	0.44
4:J:91:DA:N6	4:J:92:DG:O6	2.51	0.44
3:I:44:DG:H2''	3:I:45:DC:C5	2.52	0.44
1:C:63:ARG:NH2	4:J:65:DC:OP1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ILE:HG23	1:A:106:ASP:OD2	2.18	0.44
1:A:67:PHE:O	1:A:71:VAL:HG12	2.18	0.44
2:H:72:TYR:HE2	2:H:89:ALA:HB2	1.82	0.44
2:F:62:LEU:HA	2:F:62:LEU:HD23	1.73	0.44
1:C:121:PRO:O	1:C:124:ILE:N	2.50	0.44
4:J:94:DG:H2''	4:J:95:DG:N7	2.33	0.44
2:F:38:ALA:HB3	2:F:46:ILE:HD11	2.00	0.43
5:L:132:VAL:HA	5:L:148:SER:HA	1.99	0.43
1:E:100:LEU:HD11	2:F:58:LEU:HD22	2.00	0.43
2:D:51:TYR:O	2:D:55:ARG:HG3	2.18	0.43
3:I:26:DC:H2''	3:I:27:DT:H5''	2.00	0.43
1:C:108:ASN:ND2	2:D:43:VAL:HA	2.32	0.43
3:I:54:DC:H1'	3:I:55:DG:C5	2.53	0.43
1:A:66:PRO:O	1:A:69:ARG:HG3	2.18	0.43
4:J:87:DT:C2'	4:J:88:DT:H71	2.48	0.43
3:I:112:DT:O4	3:I:113:DA:N6	2.51	0.43
2:B:37:LEU:HD23	2:B:37:LEU:HA	1.86	0.43
4:J:66:DG:C5	4:J:67:DG:C6	3.06	0.43
4:J:86:DG:H2'	4:J:87:DT:H71	2.00	0.43
1:A:65:LEU:N	1:A:66:PRO:HD2	2.33	0.43
4:J:124:DG:H1'	4:J:125:DG:H5'	1.99	0.43
2:F:37:LEU:HD23	2:F:37:LEU:HA	1.87	0.43
4:J:62:DA:H2''	4:J:63:DC:C5	2.53	0.43
1:E:119:ILE:HG22	1:E:120:MET:H	1.83	0.43
1:E:107:THR:OG1	1:E:123:ASP:HB3	2.19	0.43
4:J:101:DG:H2''	4:J:102:DA:C8	2.54	0.43
4:J:121:DA:H2'	4:J:122:DG:H8	1.83	0.43
3:I:116:DC:H1'	3:I:117:DT:H5'	2.00	0.43
4:J:50:DT:H2''	4:J:51:DT:C5	2.54	0.42
4:J:33:DA:H2''	4:J:34:DC:C5	2.54	0.42
4:J:49:DC:H2''	4:J:50:DT:H5'	2.00	0.42
1:G:113:HIS:CE1	1:E:116:ARG:HH12	2.37	0.42
1:E:50:GLU:OE2	2:F:39:ARG:HG2	2.18	0.42
3:I:86:DT:H6	3:I:86:DT:H2'	1.63	0.42
1:E:72:ARG:NH1	1:E:84:PHE:HB2	2.34	0.42
2:F:39:ARG:HG2	2:F:39:ARG:NH1	2.34	0.42
1:C:63:ARG:HA	1:C:63:ARG:HH11	1.85	0.42
4:J:123:DC:N4	4:J:124:DG:O6	2.53	0.42
5:L:349:LEU:HA	5:L:365:SER:HA	2.01	0.42
3:I:54:DC:H1'	3:I:55:DG:N7	2.35	0.42
3:I:88:DT:H2''	3:I:89:DT:H71	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:LEU:HD12	2:D:58:LEU:HA	1.68	0.42
1:A:68:GLN:HA	1:A:71:VAL:HG12	2.00	0.42
1:G:118:THR:HG22	2:H:45:ARG:CG	2.49	0.42
1:G:120:MET:HB3	1:G:121:PRO:HD3	2.00	0.42
2:D:38:ALA:O	2:D:43:VAL:HG12	2.19	0.42
3:I:82:DC:H2''	3:I:83:DG:H8	1.83	0.42
1:E:97:GLU:O	1:E:101:VAL:HG23	2.19	0.42
1:E:118:THR:HG23	2:F:45:ARG:CG	2.44	0.42
1:E:121:PRO:O	1:E:125:GLN:HG2	2.19	0.42
3:I:84:DC:H2''	3:I:85:DG:H8	1.84	0.42
1:G:106:ASP:OD2	1:G:131:ARG:NH2	2.52	0.42
4:J:43:DA:H2''	4:J:44:DA:C8	2.55	0.42
2:H:54:THR:HA	2:H:57:VAL:HG12	2.02	0.42
3:I:105:DT:H2''	3:I:106:DA:C8	2.54	0.42
2:B:52:GLU:HA	2:B:55:ARG:HE	1.85	0.42
1:G:109:LEU:HA	1:G:112:ILE:HG22	2.02	0.41
3:I:118:DC:OP2	1:A:65:LEU:HD11	2.20	0.41
2:B:31:LYS:HE2	2:B:55:ARG:NH2	2.35	0.41
2:F:58:LEU:HA	2:F:58:LEU:HD12	1.64	0.41
1:E:100:LEU:HA	1:E:100:LEU:HD23	1.76	0.41
4:J:65:DC:C2	4:J:66:DG:C8	3.09	0.41
2:H:30:THR:OG1	2:H:32:PRO:HD2	2.20	0.41
1:E:120:MET:O	1:E:123:ASP:HB2	2.21	0.41
2:F:39:ARG:HD3	2:F:43:VAL:HG23	2.01	0.41
3:I:117:DT:H4'	3:I:118:DC:H5'	2.03	0.41
2:D:92:ARG:NH2	5:L:129:LEU:O	2.53	0.41
3:I:107:DC:H2''	3:I:108:DT:C5	2.56	0.41
1:C:68:GLN:HE22	1:C:72:ARG:HH21	1.68	0.41
2:B:53:GLU:O	2:B:57:VAL:HG13	2.19	0.41
4:J:83:DT:H6	4:J:83:DT:H2'	1.72	0.41
4:J:83:DT:H4'	4:J:84:DG:OP1	2.20	0.41
4:J:117:DA:H2''	4:J:118:DT:C7	2.50	0.41
1:C:74:ILE:HD13	1:C:74:ILE:HA	1.78	0.41
3:I:64:DC:H1'	3:I:65:DA:C8	2.56	0.41
3:I:83:DG:H1'	3:I:84:DC:H5'	2.02	0.41
3:I:106:DA:H2''	3:I:107:DC:C5	2.56	0.41
3:I:112:DT:H6	3:I:112:DT:H2'	1.77	0.41
1:C:61:LEU:HD13	1:C:61:LEU:HA	1.93	0.41
2:D:68:ASP:OD1	2:D:68:ASP:N	2.53	0.41
4:J:55:DG:H2''	4:J:56:DG:H8	1.86	0.41
1:A:63:ARG:HH21	4:J:33:DA:H5''	0.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:89:DT:H6	4:J:89:DT:H2'	1.67	0.41
1:G:105:GLU:O	1:G:109:LEU:HG	2.21	0.40
1:G:121:PRO:CD	1:G:122:LYS:N	2.84	0.40
4:J:81:DC:H2''	4:J:82:DG:C8	2.55	0.40
2:F:34:ILE:HG21	2:F:54:THR:HG21	2.03	0.40
3:I:120:DA:H2''	3:I:121:DG:H8	1.86	0.40
1:C:128:ARG:NH1	2:D:57:VAL:HG23	2.36	0.40
2:B:73:THR:H	2:B:73:THR:HG1	1.68	0.40
1:E:68:GLN:HE22	1:E:72:ARG:CZ	2.34	0.40
3:I:42:DC:H2''	3:I:43:DA:N7	2.36	0.40
1:A:67:PHE:HD1	1:A:70:LEU:HD21	1.87	0.40
1:C:113:HIS:ND1	1:A:126:LEU:HD13	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	74/136 (54%)	69 (93%)	5 (7%)	0	100	100
1	C	86/136 (63%)	81 (94%)	5 (6%)	0	100	100
1	E	88/136 (65%)	85 (97%)	3 (3%)	0	100	100
1	G	73/136 (54%)	70 (96%)	3 (4%)	0	100	100
2	B	67/103 (65%)	64 (96%)	3 (4%)	0	100	100
2	D	71/103 (69%)	69 (97%)	2 (3%)	0	100	100
2	F	72/103 (70%)	70 (97%)	2 (3%)	0	100	100
2	H	69/103 (67%)	68 (99%)	1 (1%)	0	100	100
5	L	286/559 (51%)	277 (97%)	9 (3%)	0	100	100
6	K	11/956 (1%)	9 (82%)	2 (18%)	0	100	100
All	All	897/2471 (36%)	862 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	54/111 (49%)	53 (98%)	1 (2%)	57	76
1	C	65/111 (59%)	62 (95%)	3 (5%)	27	56
1	E	60/111 (54%)	55 (92%)	5 (8%)	11	40
1	G	31/111 (28%)	29 (94%)	2 (6%)	17	48
2	B	47/79 (60%)	42 (89%)	5 (11%)	6	30
2	D	58/79 (73%)	57 (98%)	1 (2%)	60	78
2	F	31/79 (39%)	28 (90%)	3 (10%)	8	33
2	H	32/79 (40%)	29 (91%)	3 (9%)	8	35
All	All	378/760 (50%)	355 (94%)	23 (6%)	22	50

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	99	TYR
1	G	120	MET
2	H	45	ARG
2	H	49	LEU
2	H	72	TYR
1	E	65	LEU
1	E	84	PHE
1	E	85	GLN
1	E	87	SER
1	E	113	HIS
2	F	39	ARG
2	F	40	ARG
2	F	55	ARG
1	C	77	ASP
1	C	100	LEU
1	C	123	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	75	HIS
1	A	67	PHE
2	B	36	ARG
2	B	49	LEU
2	B	55	ARG
2	B	85	ASP
2	B	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	113	HIS
1	E	108	ASN
1	C	68	GLN
1	C	85	GLN
1	C	108	ASN
1	C	113	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

There are no chain breaks in this entry.

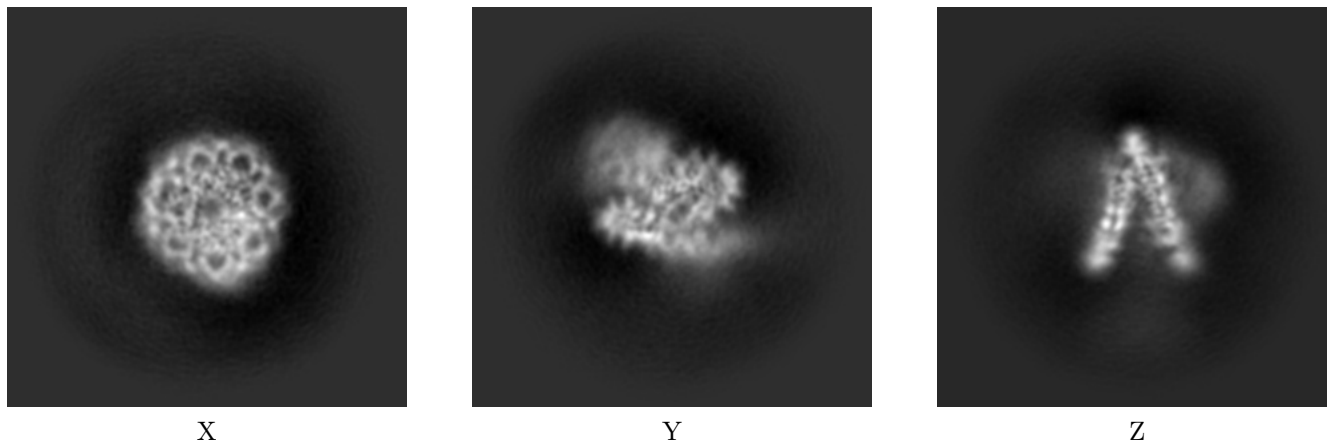
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36013. These allow visual inspection of the internal detail of the map and identification of artifacts.

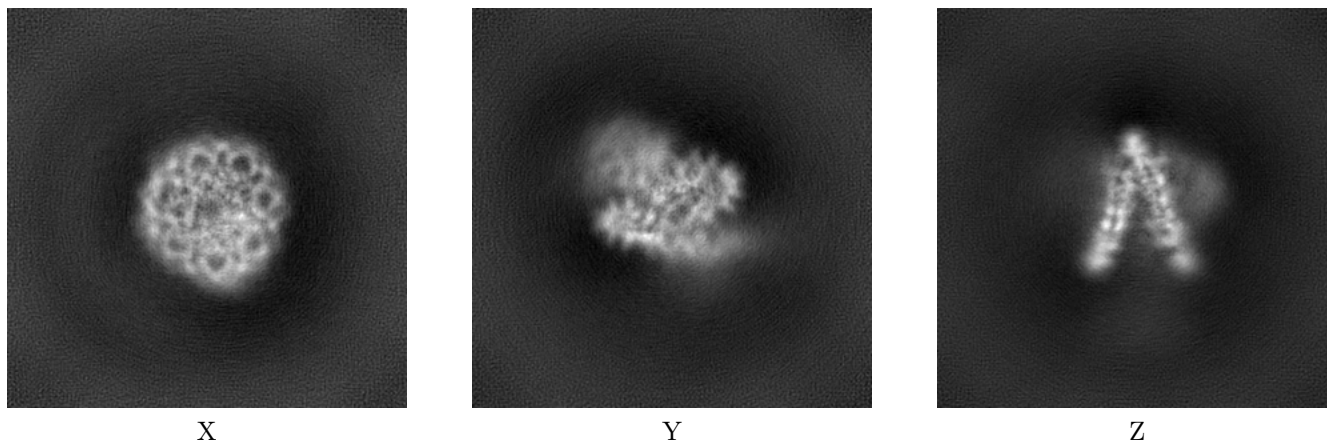
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



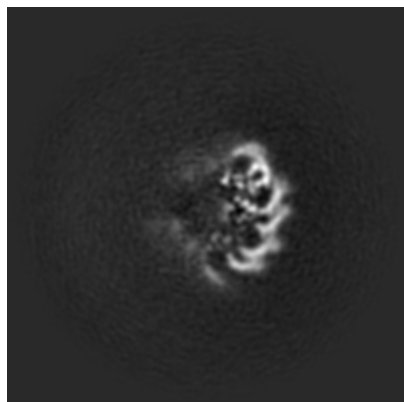
6.1.2 Raw map



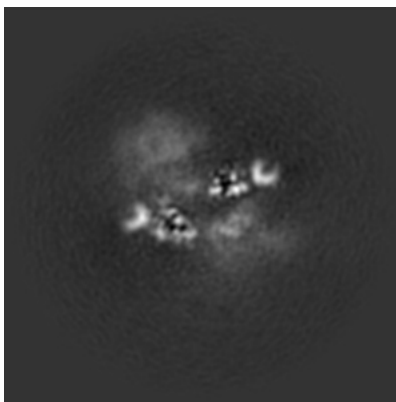
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

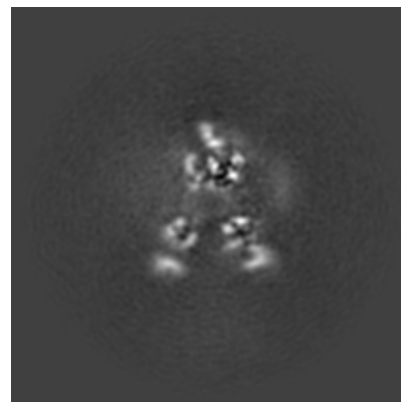
6.2.1 Primary map



X Index: 128

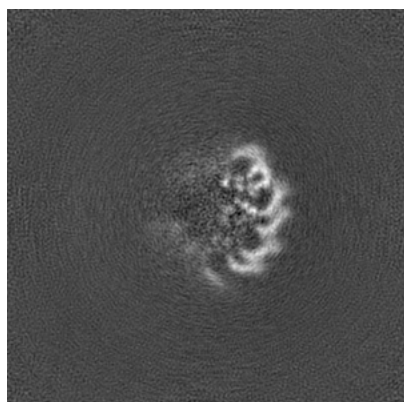


Y Index: 128

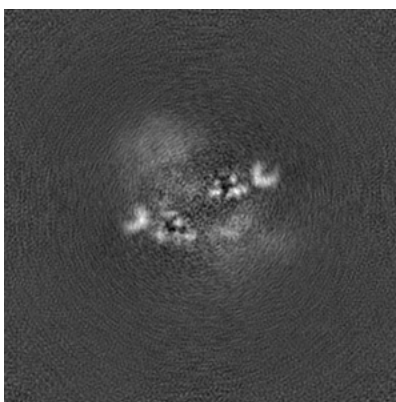


Z Index: 128

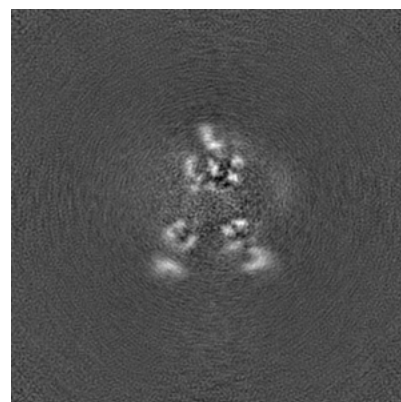
6.2.2 Raw map



X Index: 128



Y Index: 128

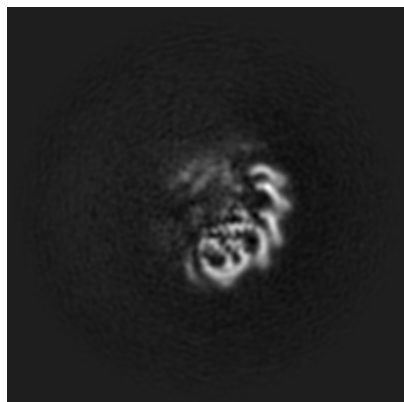


Z Index: 128

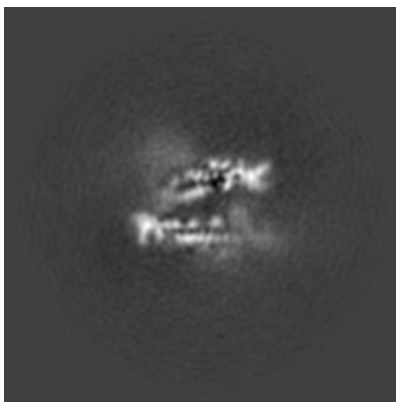
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

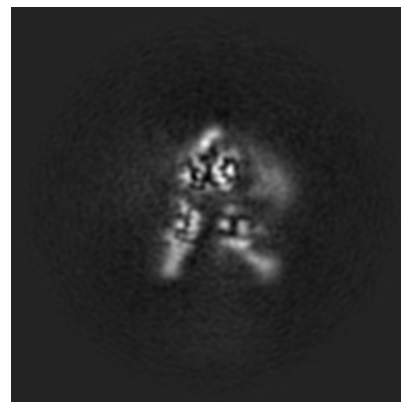
6.3.1 Primary map



X Index: 123

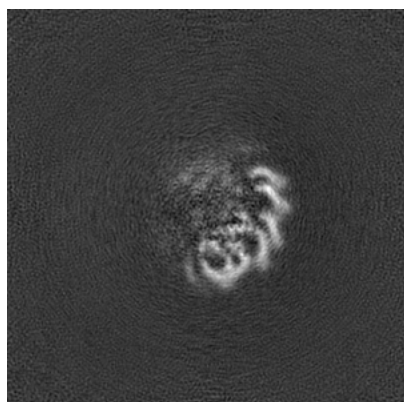


Y Index: 116

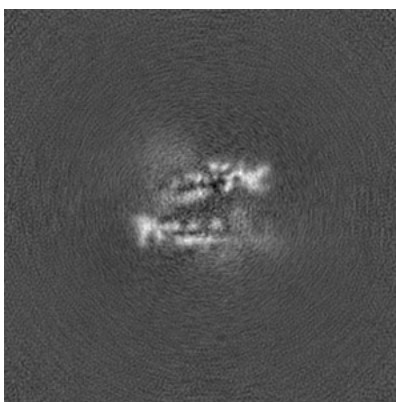


Z Index: 121

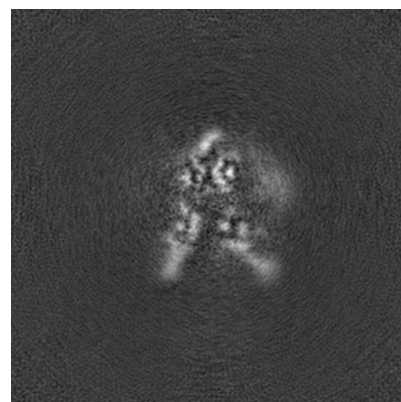
6.3.2 Raw map



X Index: 123



Y Index: 116

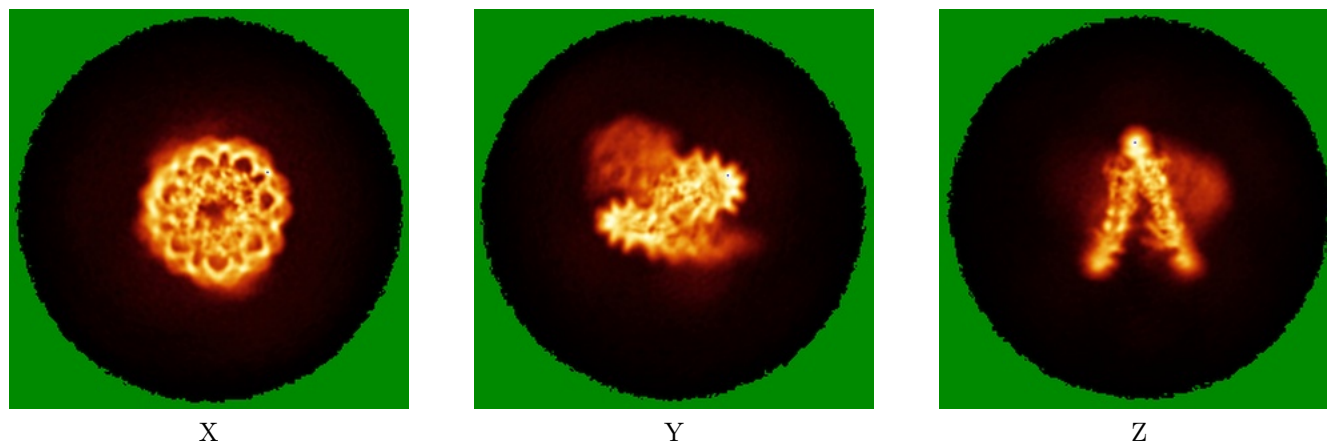


Z Index: 121

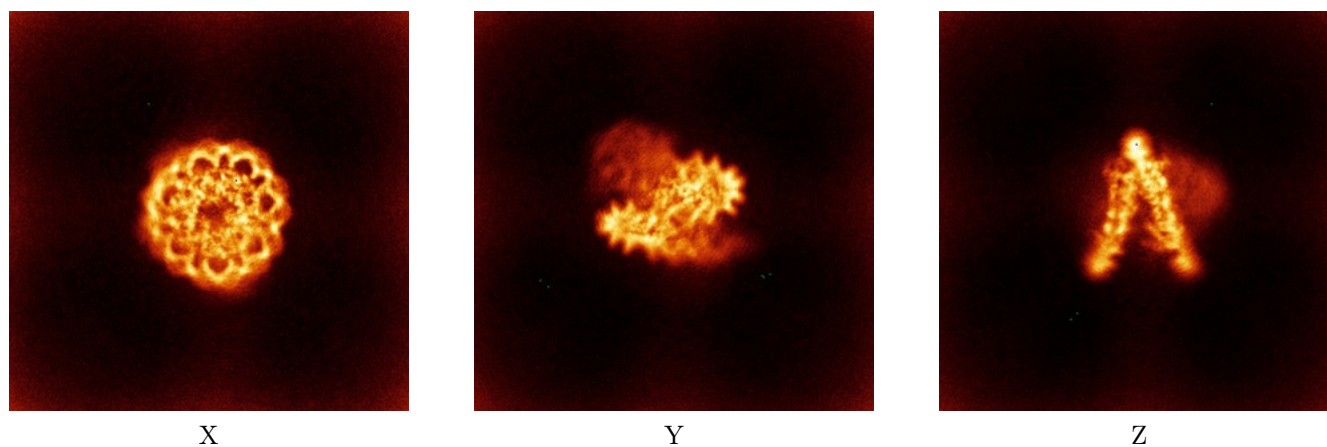
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



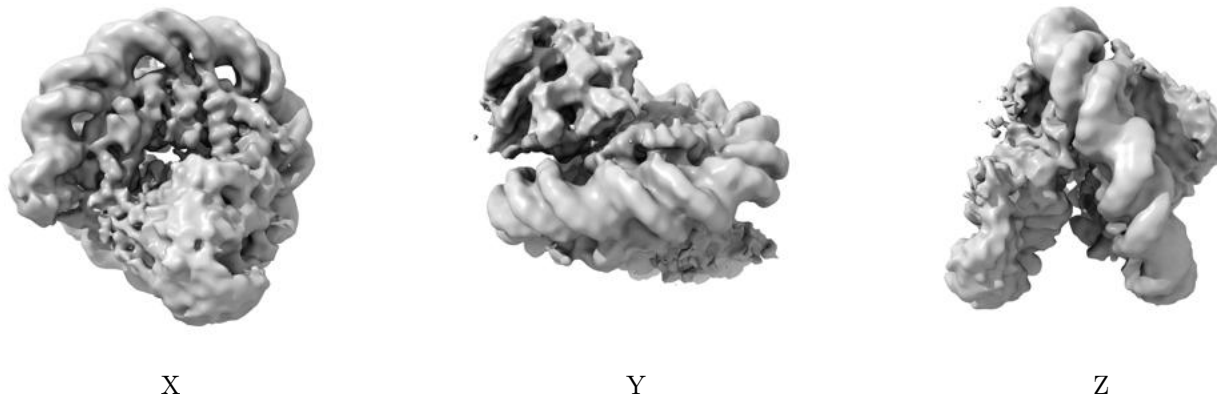
6.4.2 Raw map



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.

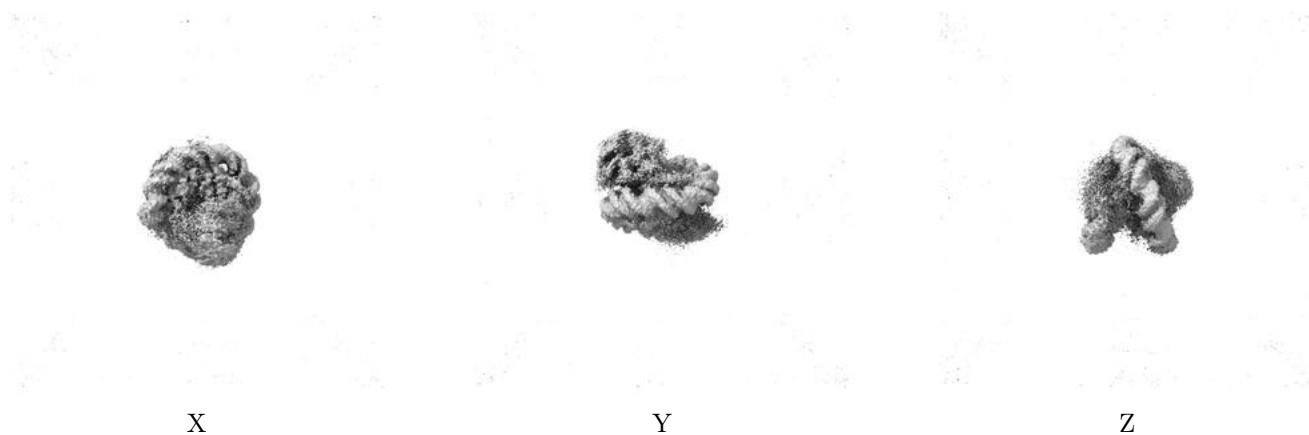
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

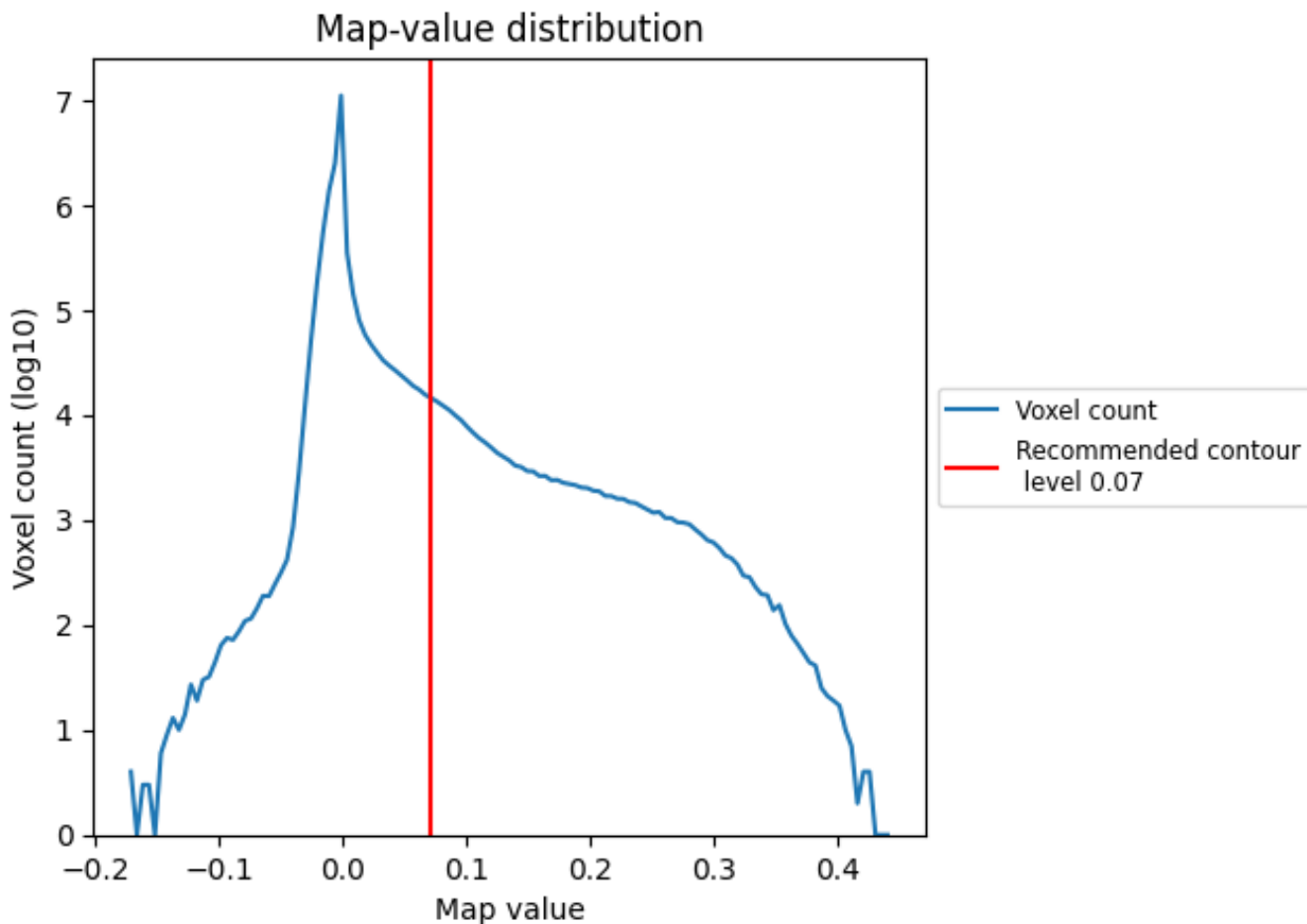
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

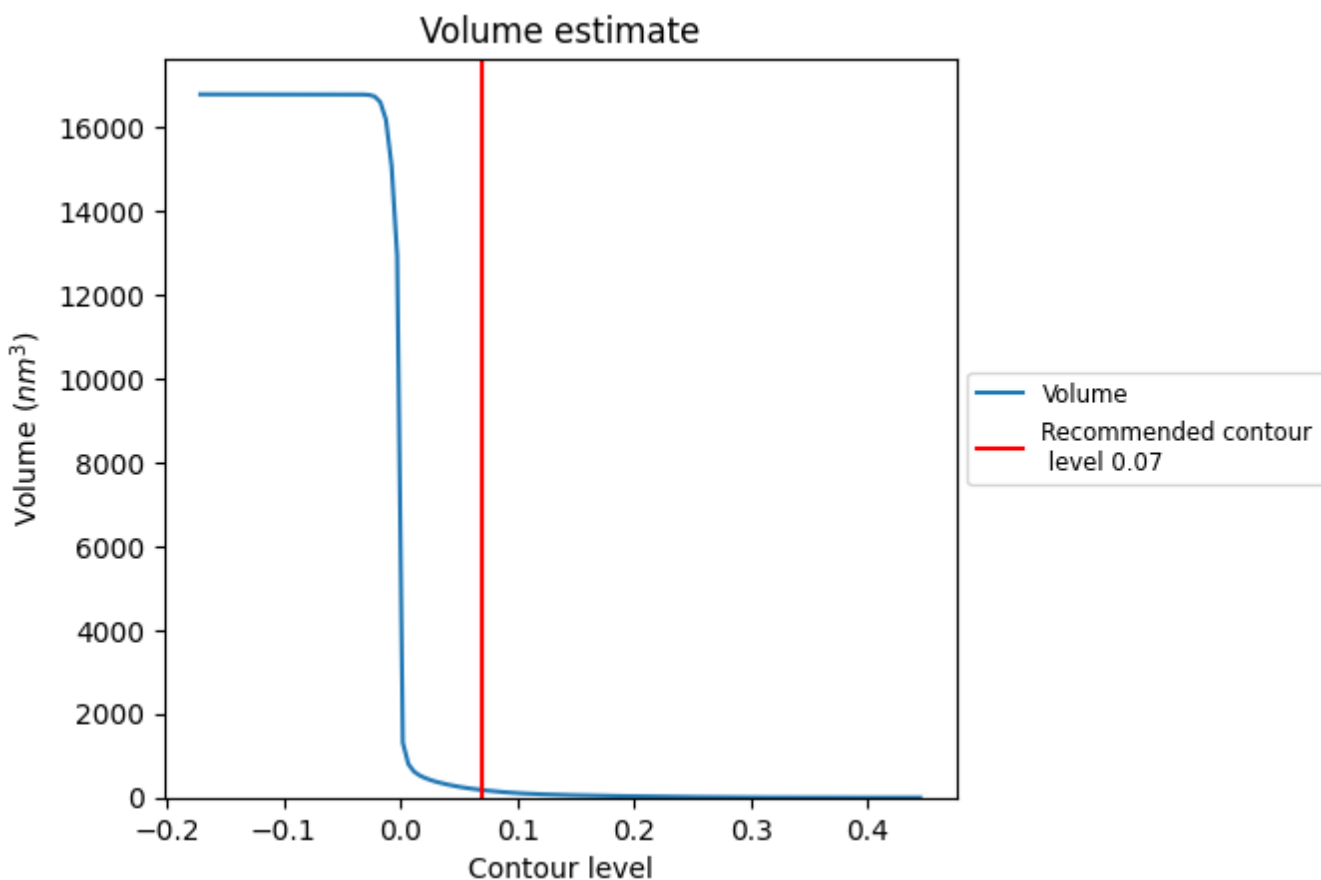
This section contains the results of statistical analysis of the map.

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.

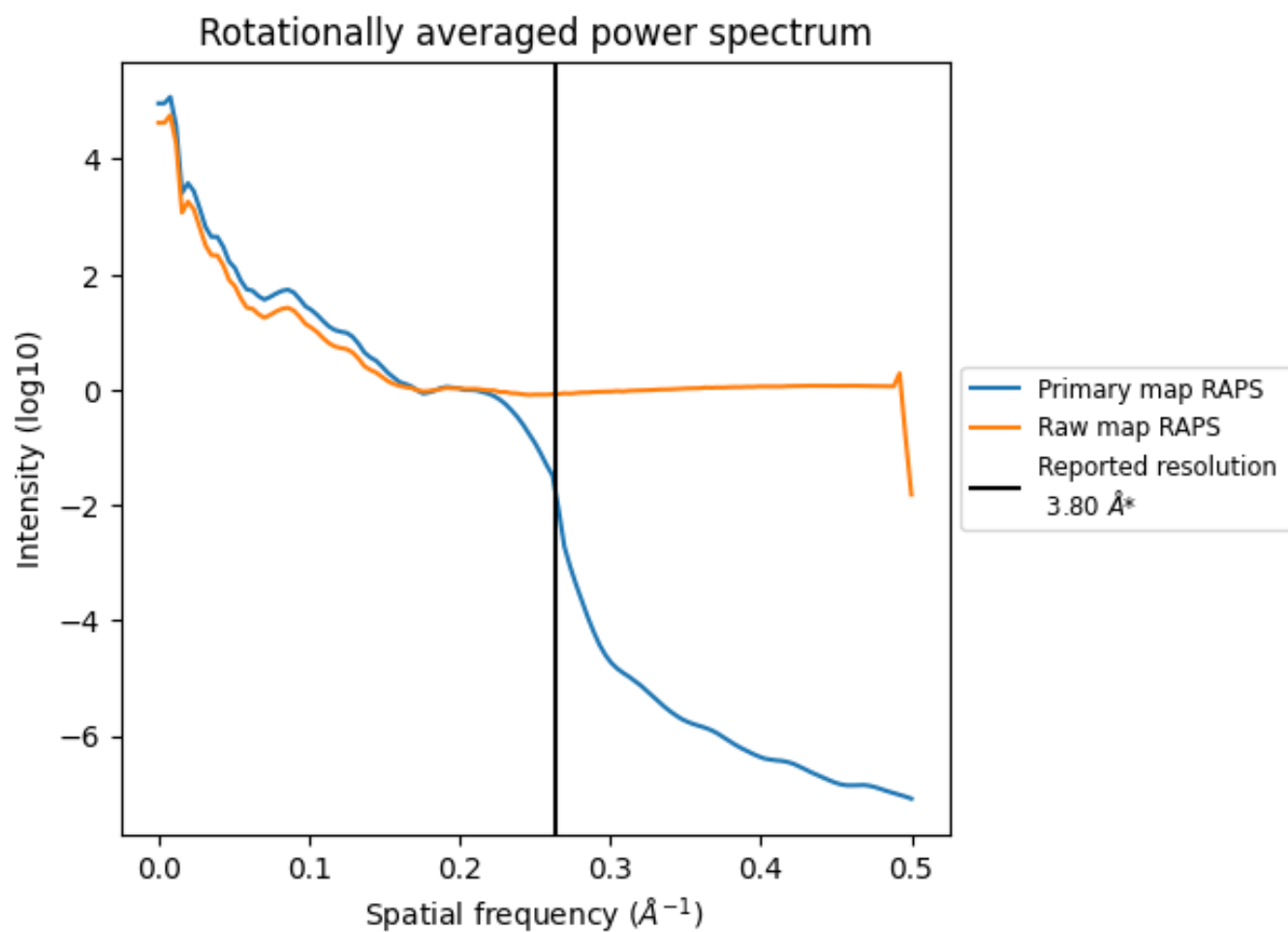
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 162 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 [\(i\)](#)

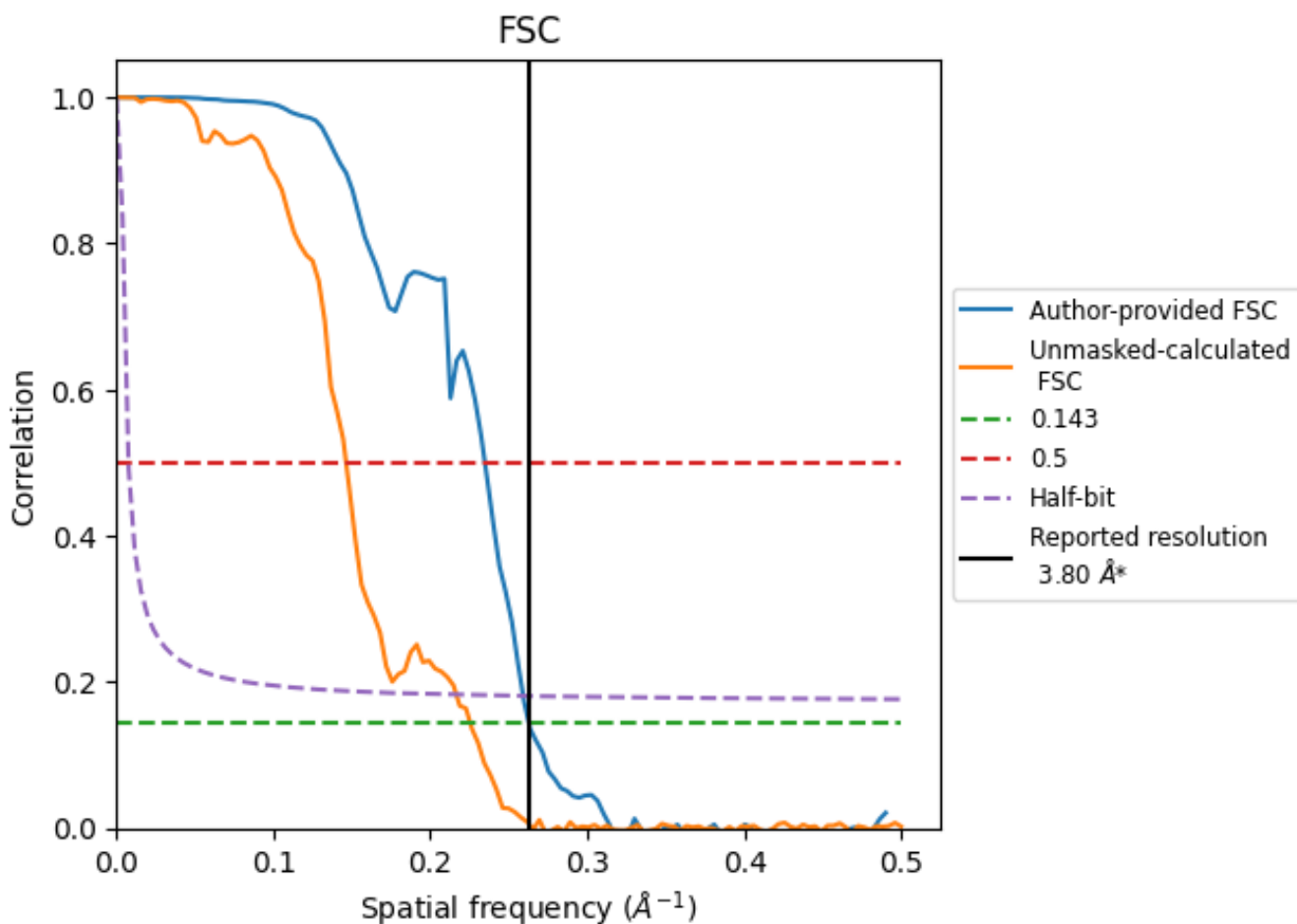


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

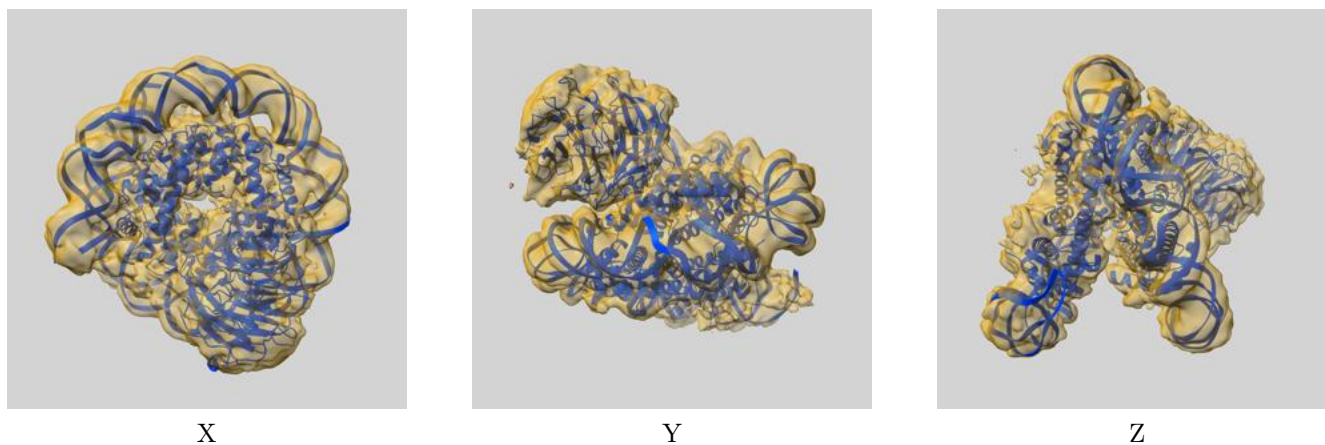
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.26	3.86
Unmasked-calculated*	4.43	6.83	4.62

*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 4.43 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36013 and PDB model 8J6S. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



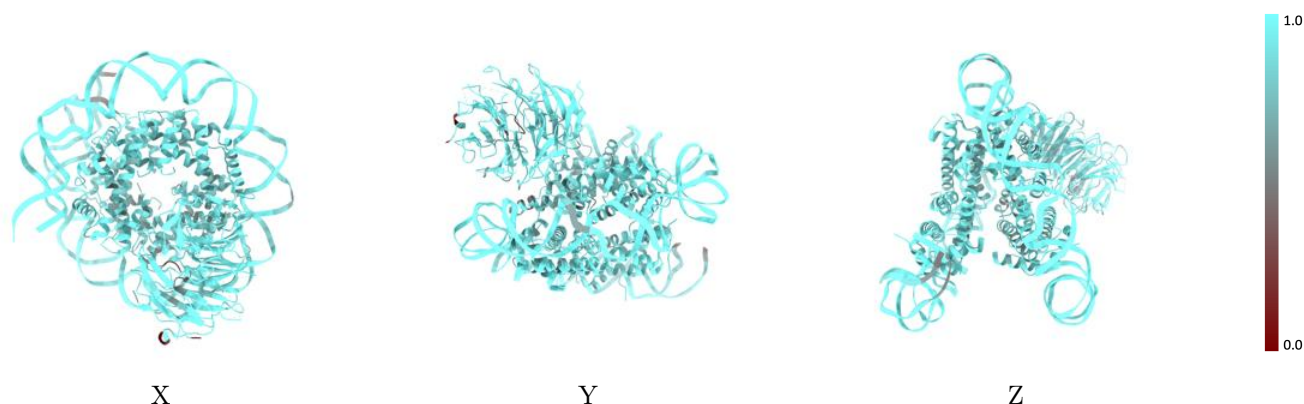
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



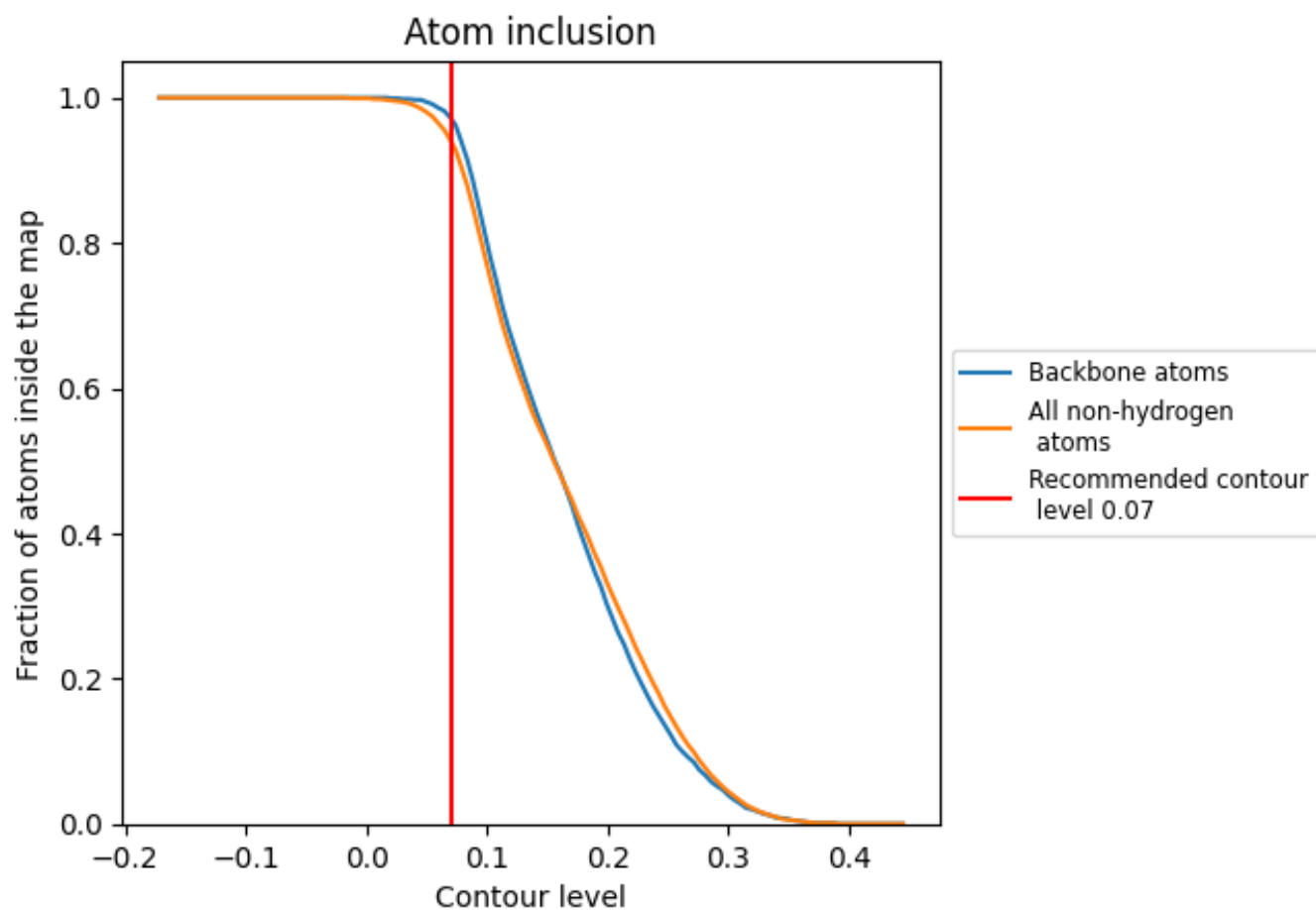
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.3010
A	 0.9260	 0.3220
B	 0.9220	 0.3020
C	 0.9070	 0.3680
D	 0.9230	 0.3780
E	 0.8910	 0.3380
F	 0.9570	 0.3600
G	 0.9370	 0.3000
H	 0.9560	 0.2890
I	 0.9680	 0.2800
J	 0.9600	 0.2830
K	 0.7160	 0.1980
L	 0.9360	 0.2620

