



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:06 AM UTC

PDB ID : 6M4H / pdb_00006m4h
EMDB ID : EMD-30078
Title : Structural mechanism of nucleosome dynamics governed by human histone variants H2A.B and H2A.Z.2.2
Authors : Zhou, M.; Dai, L.C.; Li, C.M.; Shi, L.X.; Huang, Y.; Guo, Z.Q.
Deposited on : 2020-03-07
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

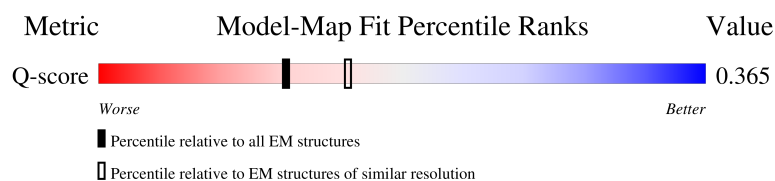
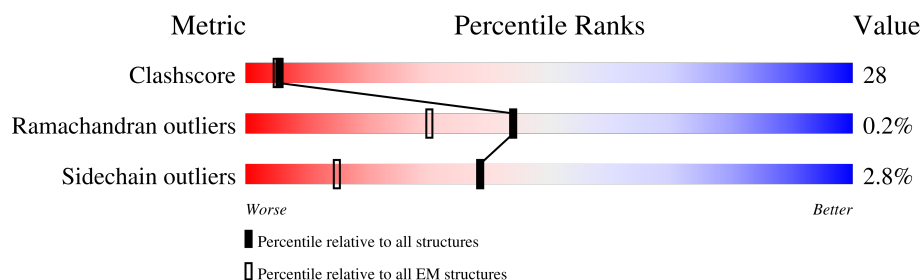
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	I	147	
2	J	147	
3	A	136	
3	E	136	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	103	
4	F	103	
5	C	115	
5	G	115	
6	D	126	
6	H	126	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9420 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 DNA chain called DNA (103-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	103	Total	C	N	O	P	0	0
			2132	1006	406	617	103		

- Molecule 2 is a DNA chain called DNA (103-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	103	Total	C	N	O	P	0	0
			2090	993	375	619	103		

- Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	74	Total	C	N	O	S	0	0
			599	381	110	104	4		
3	E	74	Total	C	N	O	S	0	0
			599	381	110	104	4		

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	76	Total	C	N	O	S	0	0
			610	387	118	104	1		
4	F	76	Total	C	N	O	S	0	0
			610	387	118	104	1		

- Molecule 5 is a protein called Histone H2A-Bbd type 2/3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	90	Total	C	N	O	S	0	0
			705	439	128	137	1		
5	G	90	Total	C	N	O	S	0	0
			705	439	128	137	1		

- Molecule 6 is a protein called Histone H2B type 2-E.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	88	Total	C	N	O	S	0	0
			685	433	121	129	2		
6	H	88	Total	C	N	O	S	0	0
			685	433	121	129	2		

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

L60 L61 R63 Q68 R69 L70 R72 K79 L82 R83 Q83 C96 E97 V101 G102 L103 F104 E105 D106 T107 H113 R116 V117 T118 T119 M120 P121 K122 D123 T124 R128 R133 ARG ALA

• Molecule 4: Histone H4

Chain B:  50% 23% 26%

MET SER GLY ARG LYS GLY GLY LYS LEU LEU GLY GLY GLY GLY GLY LYS LYS ARG HIS ARG LYS VAL LEU LEU ASP Y25 R35 R36 R37 Q42 T46 S47 Q48 E53 V57 L62 V65 I66 R67 D68 A69 T73 E74 H75 R78 K79 T80 V81 T82 D85

R92 Q93 G94 R95 L96 Y98 G99 F100 GLY GLY

• Molecule 4: Histone H4

Chain F:  53% 19% 26%

MET SER GLY ARG LYS GLY GLY LYS LEU LEU GLY GLY GLY GLY GLY LYS LYS ARG HIS ARG LYS VAL LEU LEU ASP Y25 R35 R36 R37 I50 E53 V57 L62 V65 D68 A69 V70 T71 Y72 T73 E74 H75 R78 K79 T80 V81 T82 D85 R92 Q93

G94 R95 F100 GLY GLY

• Molecule 5: Histone H2A-Bbd type 2/3

Chain C:  8% 46% 30% 22%

MET PRO ARG ARG ARG ARG ARG ARG GLY SER SER GLY GLY ALA GLY GLY GLY ARG ARG ARG THR CYS S20 R21 L27 S28 F29 S30 V34 R39 E40 G41 H42 Y43 A44 A45 Q46 L47 S48 R49 T50 A51 P52 V53 Y54 L55 V58 I59 E60 Y61 L62 K65 V66 L69 A70 G71

N72 Q75 N76 R80 D94 R95 L96 L97 S98 M102 T103 T104 T105 T106 V109 ALA PRO GLY GLU ASP

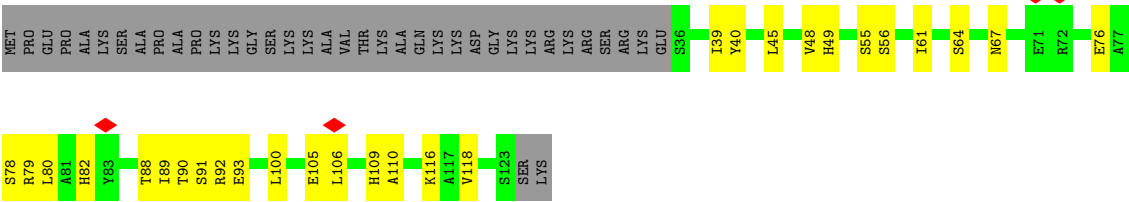
• Molecule 5: Histone H2A-Bbd type 2/3

Chain G:  9% 48% 28% 22%

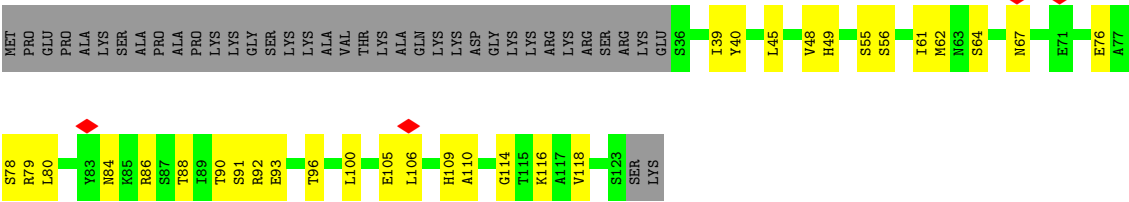
MET PRO ARG ARG ARG ARG ARG ARG GLY SER SER GLY GLY ALA GLY GLY GLY ARG ARG ARG THR CYS S20 R21 A25 E26 L27 S28 F29 E40 G41 H42 Y43 A44 A45 Q46 L47 S48 R49 V53 Y54 V58 I59 E60 Y61 L62 T63 A64 K65 V66 G71 Q75 H76 S77 G78 E79

R80 L86 R95 L96 L97 S98 F101 M102 T103 T104 T105 T106 V109 ALA PRO GLY GLU ASP

• Molecule 6: Histone H2B type 2-E



● Molecule 6: Histone H2B type 2-E



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38472	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.689	Depositor
Minimum map value	-0.726	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	249.59999, 249.59999, 249.59999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	I	0.43	0/2396	0.53	0/3701
2	J	0.43	0/2339	0.50	0/3602
3	A	0.27	0/606	0.59	0/813
3	E	0.26	0/606	0.59	0/813
4	B	0.25	0/617	0.56	0/827
4	F	0.25	0/617	0.56	0/827
5	C	0.33	0/713	0.65	0/968
5	G	0.37	0/713	0.67	0/968
6	D	0.22	0/696	0.57	0/938
6	H	0.21	0/696	0.57	0/938
All	All	0.36	0/9999	0.56	0/14395

There are no bond length outliers.

There are no bond angle outliers.

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	I	2132	0	1152	164	0
2	J	2090	0	1156	172	0
3	A	599	0	630	23	0
3	E	599	0	630	28	0
4	B	610	0	653	29	0
4	F	610	0	653	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	705	0	717	59	0
5	G	705	0	717	49	0
6	D	685	0	703	33	0
6	H	685	0	703	40	0
All	All	9420	0	7714	467	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 28.

All (467) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:31:DT:OP1	5:C:20:SER:CA	1.77	1.32
1:I:31:DA:C5'	5:G:20:SER:HA	1.63	1.29
1:I:40:DA:OP1	6:H:88:THR:HG22	1.25	1.25
1:I:31:DA:H5'	5:G:20:SER:CA	1.68	1.24
2:J:31:DT:H5'	5:C:20:SER:HA	1.25	1.11
2:J:31:DT:OP1	5:C:20:SER:HA	1.40	1.08
2:J:31:DT:OP1	5:C:20:SER:OG	1.73	1.06
5:C:65:LYS:CE	5:C:96:LEU:HD21	1.86	1.05
5:C:65:LYS:HE2	5:C:96:LEU:HD21	1.10	1.05
2:J:31:DT:OP1	5:C:20:SER:CB	2.05	1.05
2:J:31:DT:H5'	5:C:20:SER:CA	1.86	1.05
1:I:81:DC:OP2	4:B:48:GLY:N	1.88	1.05
5:C:58:VAL:HG23	6:D:110:ALA:HB1	1.34	1.04
5:G:65:LYS:HE2	5:G:96:LEU:HD21	1.42	1.01
2:J:40:DG:OP1	6:D:88:THR:HG22	1.60	1.01
2:J:91:DA:OP2	3:E:69:ARG:NH2	1.97	0.96
1:I:40:DA:OP1	6:H:88:THR:CG2	2.13	0.96
1:I:113:DA:OP2	5:C:39:ARG:NH2	1.97	0.95
2:J:31:DT:C5'	5:C:20:SER:HA	1.98	0.94
5:G:58:VAL:HG23	6:H:110:ALA:HB1	1.46	0.94
5:C:65:LYS:HE2	5:C:96:LEU:CD2	1.98	0.93
5:G:65:LYS:CE	5:G:96:LEU:HD21	2.00	0.92
1:I:25:DG:N2	2:J:123:DC:O2	2.06	0.88
2:J:31:DT:OP1	5:C:20:SER:C	2.18	0.86
1:I:31:DA:H5'	5:G:20:SER:HA	0.88	0.85
1:I:91:DA:OP2	3:A:69:ARG:NH2	2.09	0.84
1:I:109:DT:H2''	1:I:110:DA:N7	1.92	0.84
1:I:31:DA:C5'	5:G:20:SER:CA	2.40	0.83
1:I:25:DG:N1	2:J:123:DC:N3	2.26	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:DG:N1	2:J:28:DC:N3	2.27	0.82
1:I:120:DG:N2	2:J:28:DC:O2	2.13	0.81
2:J:31:DT:P	5:C:20:SER:HA	2.21	0.80
2:J:31:DT:OP1	5:C:21:ARG:N	2.14	0.79
1:I:29:DG:N2	2:J:119:DC:O2	2.16	0.79
5:C:69:LEU:HD11	5:C:96:LEU:HD23	1.66	0.78
6:D:76:GLU:OE1	6:D:79:ARG:NH2	2.17	0.78
6:H:76:GLU:OE1	6:H:79:ARG:NH2	2.17	0.77
1:I:111:DC:N4	2:J:37:DG:O6	2.18	0.77
1:I:29:DG:N1	2:J:119:DC:N3	2.32	0.76
1:I:81:DC:OP2	4:B:48:GLY:CA	2.33	0.76
1:I:28:DT:O4	2:J:119:DC:N4	2.21	0.74
2:J:31:DT:H2'	2:J:32:DT:C6	2.23	0.73
2:J:37:DG:N2	2:J:38:DT:O4	2.20	0.73
5:C:58:VAL:CG2	6:D:110:ALA:HB1	2.14	0.73
5:C:27:LEU:HD22	5:C:60:GLU:OE1	1.90	0.72
5:G:66:VAL:HG11	6:H:62:MET:HE1	1.72	0.72
2:J:31:DT:P	5:C:21:ARG:H	2.14	0.71
3:E:97:GLU:O	3:E:101:VAL:HG23	1.90	0.71
1:I:111:DC:N3	2:J:37:DG:C6	2.58	0.71
3:A:97:GLU:O	3:A:101:VAL:HG23	1.91	0.70
1:I:116:DA:H2''	1:I:117:DA:C8	2.26	0.70
1:I:101:DG:H1'	1:I:102:DA:N7	2.05	0.70
2:J:101:DG:OP1	3:E:83:ARG:NH1	2.25	0.69
1:I:82:DG:H5'	1:I:82:DG:C8	2.28	0.69
1:I:82:DG:P	4:B:35:ARG:HH12	2.16	0.69
5:C:65:LYS:HZ1	5:C:96:LEU:HD11	1.58	0.69
1:I:111:DC:N3	2:J:37:DG:C5	2.61	0.68
2:J:36:DC:H2''	2:J:37:DG:H5''	1.76	0.68
1:I:40:DA:OP2	6:H:86:ARG:HD2	1.94	0.68
5:G:65:LYS:HE2	5:G:96:LEU:CD2	2.20	0.68
1:I:31:DA:H5'	5:G:20:SER:N	2.10	0.67
1:I:40:DA:P	6:H:88:THR:HG22	2.33	0.67
1:I:46:DC:H2''	1:I:47:DC:H2'	1.76	0.67
1:I:42:DT:H2''	1:I:43:DA:H5''	1.76	0.66
2:J:86:DT:H2'	2:J:87:DT:C6	2.31	0.66
5:C:51:ALA:HB3	5:C:52:PRO:HD3	1.78	0.66
5:G:53:VAL:HG23	6:H:118:VAL:HG12	1.77	0.66
5:C:69:LEU:HD13	5:C:94:ASP:OD2	1.95	0.66
1:I:113:DA:P	5:C:39:ARG:NH2	2.69	0.65
5:G:58:VAL:CG2	6:H:110:ALA:HB1	2.22	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:112:DT:OP2	5:G:49:ARG:HB2	1.96	0.65
5:G:106:ILE:HG23	6:H:61:ILE:HD13	1.79	0.65
4:F:74:GLU:O	6:H:92:ARG:NH2	2.29	0.65
5:G:65:LYS:NZ	5:G:96:LEU:HD21	2.12	0.64
4:B:74:GLU:O	6:D:92:ARG:NH2	2.31	0.64
5:G:29:PHE:HE2	5:G:59:ILE:HG22	1.63	0.64
1:I:103:DG:N2	2:J:46:DT:O2	2.31	0.64
4:B:53:GLU:OE1	4:B:53:GLU:HA	1.98	0.64
2:J:121:DG:H2''	2:J:122:DG:C8	2.33	0.64
5:G:71:GLY:HA3	6:H:49:HIS:CD2	2.32	0.64
3:E:121:PRO:HB3	4:F:53:GLU:HG2	1.80	0.63
1:I:36:DA:H2''	1:I:37:DG:H5''	1.80	0.63
5:C:65:LYS:NZ	5:C:96:LEU:HD11	2.13	0.63
2:J:36:DC:H1'	2:J:37:DG:O4'	1.99	0.63
2:J:30:DA:H2'	2:J:31:DT:H71	1.80	0.63
1:I:81:DC:OP2	4:B:48:GLY:HA3	1.98	0.63
4:F:53:GLU:OE1	4:F:53:GLU:HA	1.98	0.63
4:B:73:THR:HG21	4:B:81:VAL:HG22	1.80	0.62
2:J:86:DT:H2''	2:J:87:DT:H5'	1.80	0.62
6:H:90:THR:HG22	6:H:91:SER:H	1.65	0.62
5:G:75:GLN:C	5:G:77:SER:H	2.07	0.61
4:F:73:THR:HG21	4:F:81:VAL:HG22	1.80	0.61
1:I:53:DG:H2'	1:I:54:DC:C6	2.36	0.61
6:D:90:THR:HG22	6:D:91:SER:H	1.65	0.61
5:G:48:SER:HB3	6:H:90:THR:HA	1.82	0.61
3:A:103:LEU:O	3:A:107:THR:HG23	2.01	0.60
2:J:46:DT:H2''	2:J:47:DC:C6	2.36	0.60
4:B:92:ARG:NH2	6:D:100:LEU:O	2.34	0.60
3:E:103:LEU:O	3:E:107:THR:HG23	2.01	0.60
1:I:29:DG:H2''	1:I:30:DG:C8	2.36	0.60
1:I:49:DC:H2''	1:I:50:DT:H72	1.84	0.59
1:I:120:DG:O6	2:J:28:DC:N4	2.34	0.59
1:I:82:DG:OP1	4:B:46:ILE:N	2.29	0.59
4:B:69:ALA:O	4:B:73:THR:HG23	2.04	0.58
5:C:53:VAL:HG23	6:D:118:VAL:HG12	1.84	0.58
1:I:104:DC:H2'	1:I:105:DT:C6	2.39	0.58
2:J:33:DG:H2''	2:J:34:DG:C8	2.39	0.58
5:G:27:LEU:HD22	5:G:60:GLU:OE1	2.04	0.58
4:F:69:ALA:O	4:F:73:THR:HG23	2.04	0.58
1:I:85:DC:H2''	1:I:86:DG:C8	2.38	0.58
5:C:58:VAL:HG23	6:D:110:ALA:CB	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:DA:H8	1:I:71:DA:H5''	1.69	0.57
2:J:33:DG:C2	2:J:34:DG:C6	2.92	0.57
2:J:33:DG:H8	2:J:33:DG:H5''	1.69	0.57
1:I:74:DG:H1'	1:I:75:DC:H5'	1.87	0.56
1:I:89:DT:H4'	1:I:90:DA:OP1	2.05	0.56
1:I:91:DA:H5'	1:I:91:DA:C8	2.40	0.56
5:C:69:LEU:HD13	5:C:94:ASP:CG	2.29	0.56
1:I:49:DC:O2	2:J:100:DG:N2	2.38	0.56
2:J:64:DC:H2''	2:J:65:DA:C8	2.40	0.56
2:J:60:DA:H2''	2:J:61:DA:H8	1.71	0.56
1:I:31:DA:H5''	5:G:20:SER:CA	2.32	0.56
5:C:51:ALA:N	5:C:52:PRO:HD2	2.20	0.56
2:J:70:DC:H2''	2:J:71:DG:N7	2.21	0.56
2:J:106:DA:H2''	2:J:107:DC:H5''	1.87	0.56
1:I:46:DC:H1'	1:I:47:DC:H5'	1.86	0.55
1:I:118:DT:H2'	1:I:119:DT:H72	1.88	0.55
2:J:39:DA:H5''	5:C:46:ARG:NH1	2.20	0.55
5:C:71:GLY:HA3	6:D:49:HIS:CD2	2.41	0.55
1:I:88:DT:H2''	1:I:89:DT:H71	1.88	0.55
1:I:81:DC:H5'	1:I:81:DC:C6	2.40	0.55
1:I:85:DC:H2''	1:I:86:DG:H8	1.72	0.55
1:I:102:DA:H2''	1:I:103:DG:H5''	1.89	0.55
1:I:38:DG:H1'	1:I:39:DG:OP2	2.06	0.55
5:G:43:TYR:HB3	6:H:78:SER:OG	2.06	0.55
6:H:45:LEU:HA	6:H:48:VAL:HG12	1.89	0.55
2:J:85:DG:H2'	2:J:86:DT:H71	1.89	0.55
5:C:29:PHE:HE2	5:C:59:ILE:HG22	1.71	0.55
1:I:109:DT:H2''	1:I:110:DA:C5	2.41	0.55
2:J:91:DA:OP2	3:E:69:ARG:CZ	2.55	0.55
6:D:45:LEU:HA	6:D:48:VAL:HG12	1.89	0.54
1:I:29:DG:O6	2:J:119:DC:N4	2.40	0.54
3:A:108:ASN:ND2	4:B:42:GLY:O	2.39	0.54
1:I:113:DA:H2''	1:I:114:DC:H5''	1.88	0.54
2:J:120:DA:H2'	2:J:121:DG:C8	2.43	0.54
1:I:105:DT:H2''	1:I:106:DG:C8	2.43	0.54
2:J:61:DA:C4	2:J:62:DC:C5	2.95	0.54
2:J:112:DT:P	5:G:49:ARG:HB2	2.47	0.54
2:J:62:DC:H2''	2:J:63:DG:C8	2.43	0.54
5:G:102:ASN:OD1	5:G:102:ASN:N	2.34	0.54
1:I:49:DC:H2''	1:I:50:DT:C7	2.37	0.54
2:J:61:DA:H2''	2:J:62:DC:H6	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:71:DG:O3'	3:A:120:MET:HE1	2.08	0.53
5:C:71:GLY:HA3	6:D:49:HIS:NE2	2.24	0.53
2:J:87:DT:H2''	2:J:88:DT:C6	2.43	0.53
4:B:68:ASP:OD2	4:B:92:ARG:NH1	2.42	0.53
3:E:61:LEU:HD12	4:F:37:LEU:HD23	1.91	0.53
1:I:55:DG:H2''	1:I:56:DG:C8	2.44	0.53
4:F:68:ASP:OD2	4:F:92:ARG:NH1	2.42	0.53
1:I:29:DG:O6	2:J:118:DC:N4	2.42	0.52
1:I:79:DT:H2''	1:I:80:DA:C8	2.43	0.52
2:J:29:DA:H2''	2:J:30:DA:C8	2.44	0.52
1:I:62:DA:H1'	1:I:63:DC:H5'	1.90	0.52
1:I:84:DG:H2''	1:I:85:DC:C6	2.45	0.52
1:I:105:DT:H2''	1:I:106:DG:H8	1.73	0.52
2:J:95:DC:H2'	2:J:96:DC:C6	2.45	0.52
1:I:31:DA:H5''	5:G:21:ARG:N	2.25	0.52
1:I:73:DA:H1'	1:I:74:DG:H5'	1.91	0.52
4:B:98:TYR:HE2	5:G:101:PHE:HE1	1.56	0.52
5:C:51:ALA:N	5:C:52:PRO:CD	2.71	0.52
1:I:82:DG:OP2	4:B:35:ARG:NH2	2.37	0.52
2:J:98:DA:H2''	2:J:99:DG:C8	2.45	0.52
2:J:89:DT:H4'	2:J:90:DA:OP1	2.09	0.52
6:D:105:GLU:HG2	6:D:109:HIS:CD2	2.45	0.52
1:I:25:DG:O6	2:J:123:DC:N4	2.41	0.52
3:E:68:GLN:HE21	3:E:72:ARG:HH21	1.58	0.52
2:J:82:DC:H2''	2:J:83:DG:C8	2.45	0.51
2:J:82:DC:H2''	2:J:83:DG:H8	1.75	0.51
1:I:108:DC:H2''	1:I:109:DT:H71	1.92	0.51
2:J:77:DT:H1'	2:J:78:DC:H5'	1.91	0.51
2:J:81:DC:H5'	2:J:81:DC:C6	2.45	0.51
1:I:31:DA:C5'	5:G:20:SER:N	2.72	0.51
1:I:90:DA:C8	1:I:91:DA:C5	2.98	0.51
2:J:94:DG:H2''	2:J:95:DC:H5''	1.92	0.51
5:C:97:LEU:HA	6:D:106:LEU:HD11	1.93	0.51
4:F:75:HIS:O	6:H:92:ARG:NH1	2.25	0.51
6:H:105:GLU:HG2	6:H:109:HIS:CD2	2.45	0.51
5:C:102:ASN:OD1	5:C:102:ASN:N	2.35	0.51
1:I:86:DG:H2'	1:I:87:DT:C6	2.46	0.50
5:C:69:LEU:CD1	5:C:94:ASP:OD2	2.59	0.50
2:J:103:DA:H1'	2:J:104:DT:H5'	1.93	0.50
1:I:71:DA:H5'	3:E:116:ARG:HG2	1.92	0.50
1:I:111:DC:H2'	1:I:112:DG:C5	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:31:DT:H5'	5:C:20:SER:C	2.37	0.50
2:J:72:DC:P	3:A:120:MET:HE1	2.52	0.50
2:J:116:DC:H1'	2:J:117:DT:C6	2.46	0.50
4:B:75:HIS:NE2	6:D:93:GLU:HG3	2.27	0.50
3:E:128:ARG:HH11	4:F:57:VAL:HG22	1.75	0.50
1:I:55:DG:H2''	1:I:56:DG:H8	1.76	0.50
1:I:47:DC:H1'	1:I:48:DC:C5	2.46	0.50
5:C:43:TYR:HB3	6:D:78:SER:OG	2.12	0.50
5:G:29:PHE:CD1	6:H:40:TYR:HB3	2.46	0.50
1:I:119:DT:C4	2:J:28:DC:N4	2.80	0.50
2:J:28:DC:H2''	2:J:29:DA:C8	2.47	0.50
3:A:68:GLN:HE21	3:A:72:ARG:HH21	1.58	0.50
2:J:37:DG:N3	2:J:37:DG:H5'	2.27	0.50
2:J:43:DA:C6	2:J:44:DG:C6	3.00	0.50
5:C:51:ALA:H	5:C:52:PRO:HD2	1.77	0.50
5:G:75:GLN:C	5:G:77:SER:N	2.70	0.50
6:D:105:GLU:HG2	6:D:109:HIS:HD2	1.77	0.49
1:I:79:DT:H2''	1:I:80:DA:N7	2.27	0.49
1:I:116:DA:H2''	1:I:117:DA:H8	1.77	0.49
6:H:105:GLU:HG2	6:H:109:HIS:HD2	1.77	0.49
2:J:31:DT:H5'	5:C:20:SER:N	2.28	0.49
2:J:74:DC:H4'	2:J:75:DT:OP1	2.11	0.49
2:J:109:DC:H2''	2:J:110:DC:C5	2.48	0.49
5:C:29:PHE:CD1	6:D:40:TYR:HB3	2.47	0.49
2:J:39:DA:C6	2:J:40:DG:C6	3.01	0.49
2:J:76:DG:H2''	2:J:77:DT:C2	2.48	0.49
2:J:91:DA:C5	2:J:92:DC:C4	3.01	0.49
1:I:91:DA:H1'	1:I:92:DG:H5''	1.95	0.49
2:J:115:DT:H2''	2:J:116:DC:H5'	1.95	0.48
3:E:97:GLU:HG2	4:F:37:LEU:HD21	1.94	0.48
2:J:63:DG:C4	2:J:64:DC:C5	3.01	0.48
5:C:48:SER:HB3	6:D:90:THR:HA	1.94	0.48
2:J:82:DC:P	4:F:35:ARG:HH12	2.37	0.48
5:G:46:ARG:O	6:H:88:THR:HA	2.12	0.48
1:I:52:DG:C4	1:I:53:DG:C8	3.01	0.48
1:I:80:DA:H4'	1:I:81:DC:OP1	2.14	0.48
2:J:52:DA:C4	2:J:53:DC:C5	3.01	0.48
1:I:40:DA:H2''	1:I:41:DG:C8	2.48	0.48
1:I:40:DA:H2''	1:I:41:DG:H8	1.79	0.48
1:I:47:DC:H1'	1:I:48:DC:C4	2.49	0.48
1:I:111:DC:C2	2:J:37:DG:C5	3.01	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:98:TYR:CE2	5:G:104:THR:HG21	2.48	0.48
5:C:42:HIS:CD2	5:G:45:GLN:HE21	2.32	0.48
4:F:75:HIS:CE1	6:H:84:ASN:ND2	2.82	0.48
1:I:110:DA:H1'	1:I:111:DC:O5'	2.13	0.48
2:J:84:DC:C2	2:J:85:DG:C5	3.02	0.48
1:I:51:DT:C2	1:I:52:DG:C8	3.02	0.47
1:I:71:DA:OP1	3:E:117:VAL:HB	2.14	0.47
1:I:91:DA:OP2	3:A:69:ARG:CZ	2.62	0.47
3:A:61:LEU:HD12	4:B:37:LEU:HD23	1.96	0.47
1:I:98:DC:H2''	1:I:99:DT:C5	2.49	0.47
2:J:42:DC:C2	2:J:43:DA:N7	2.83	0.47
2:J:36:DC:C2'	2:J:37:DG:H5''	2.44	0.47
2:J:55:DG:H2'	2:J:55:DG:OP2	2.15	0.47
1:I:40:DA:OP2	6:H:86:ARG:CD	2.63	0.47
1:I:60:DA:H2''	1:I:61:DA:H8	1.79	0.47
1:I:112:DG:N1	2:J:37:DG:H8	2.13	0.47
2:J:53:DC:C2	2:J:54:DC:C4	3.03	0.47
2:J:94:DG:C4	2:J:95:DC:C5	3.03	0.47
1:I:71:DA:H5''	1:I:71:DA:C8	2.48	0.47
1:I:71:DA:OP1	3:E:118:THR:N	2.43	0.47
1:I:75:DC:H2''	1:I:76:DG:C8	2.50	0.47
2:J:65:DA:C8	2:J:65:DA:H5'	2.50	0.47
2:J:102:DG:C5	2:J:103:DA:C5	3.03	0.47
5:G:54:TYR:CE1	6:H:114:GLY:C	2.93	0.47
1:I:94:DG:C4	1:I:95:DG:C8	3.03	0.47
5:C:44:ALA:HB2	6:D:89:ILE:HG13	1.97	0.47
1:I:82:DG:C2	2:J:67:DG:N2	2.83	0.47
3:E:83:ARG:O	4:F:80:THR:HA	2.15	0.47
2:J:93:DC:C2	2:J:94:DG:C8	3.03	0.46
5:C:61:TYR:CZ	6:D:109:HIS:HB3	2.50	0.46
3:E:128:ARG:NH1	4:F:57:VAL:HG22	2.30	0.46
5:G:66:VAL:CG1	6:H:62:MET:HE1	2.43	0.46
1:I:99:DT:O2	2:J:50:DG:N2	2.48	0.46
3:E:62:ILE:O	3:E:93:GLN:NE2	2.48	0.46
2:J:71:DG:H8	2:J:71:DG:H5''	1.79	0.46
5:G:54:TYR:CD1	6:H:114:GLY:C	2.93	0.46
1:I:59:DA:P	1:I:59:DA:H8	2.38	0.46
1:I:78:DG:H2''	1:I:79:DT:H5''	1.97	0.46
2:J:107:DC:H1'	2:J:108:DT:H5'	1.97	0.46
5:C:27:LEU:CD2	5:C:60:GLU:OE1	2.63	0.46
5:C:103:THR:HB	4:F:94:GLY:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:DA:H2''	1:I:60:DA:C8	2.51	0.46
2:J:40:DG:H2''	2:J:41:DA:H8	1.81	0.46
5:C:30:SER:HB2	6:D:40:TYR:CZ	2.50	0.46
5:G:79:GLU:OE1	5:G:86:LEU:HD11	2.16	0.46
2:J:59:DA:H8	2:J:59:DA:OP2	1.99	0.46
2:J:40:DG:C2	2:J:41:DA:C5	3.04	0.46
3:A:62:ILE:O	3:A:93:GLN:NE2	2.48	0.46
3:A:68:GLN:HA	3:A:71:VAL:HG22	1.97	0.46
2:J:33:DG:H5''	2:J:33:DG:C8	2.48	0.46
1:I:25:DG:N2	2:J:123:DC:C2	2.80	0.45
1:I:25:DG:H1'	1:I:26:DC:H5'	1.98	0.45
2:J:58:DT:H1'	2:J:59:DA:C8	2.51	0.45
3:A:123:ASP:OD1	3:E:113:HIS:NE2	2.49	0.45
4:F:94:GLY:O	4:F:95:ARG:HD2	2.17	0.45
1:I:35:DT:C4	1:I:36:DA:N6	2.84	0.45
1:I:100:DA:H2''	1:I:101:DG:C8	2.51	0.45
1:I:101:DG:H1'	1:I:102:DA:C8	2.50	0.45
2:J:102:DG:H2''	2:J:103:DA:H8	1.80	0.45
2:J:117:DT:H1'	2:J:118:DC:C6	2.51	0.45
3:A:79:LYS:HD3	3:A:82:LEU:HD21	1.98	0.45
2:J:37:DG:H2'	2:J:38:DT:C2	2.51	0.45
2:J:71:DG:H5''	2:J:71:DG:C8	2.52	0.45
3:E:79:LYS:HD3	3:E:82:LEU:HD21	1.98	0.45
2:J:102:DG:H2''	2:J:103:DA:C8	2.51	0.45
1:I:24:DT:O4	2:J:123:DC:N4	2.49	0.45
3:E:124:ILE:HD11	4:F:50:ILE:HG23	1.97	0.45
5:G:62:LEU:O	5:G:66:VAL:HG12	2.17	0.45
1:I:81:DC:P	4:B:48:GLY:H	2.38	0.45
2:J:121:DG:H2''	2:J:122:DG:H8	1.81	0.45
4:B:94:GLY:O	4:B:95:ARG:HD2	2.16	0.45
1:I:118:DT:O4	2:J:29:DA:N6	2.50	0.45
2:J:49:DA:H4'	2:J:50:DG:H5'	1.98	0.45
2:J:51:DC:P	3:A:72:ARG:HH22	2.40	0.45
2:J:51:DC:H2''	2:J:52:DA:H8	1.82	0.45
2:J:53:DC:N3	2:J:54:DC:N4	2.65	0.45
3:E:68:GLN:HE21	3:E:72:ARG:HE	1.65	0.45
1:I:39:DG:H2''	1:I:40:DA:C8	2.52	0.45
1:I:111:DC:H2''	1:I:112:DG:H5'	1.98	0.45
1:I:118:DT:H2'	1:I:119:DT:C7	2.46	0.45
1:I:90:DA:C8	1:I:91:DA:C6	3.05	0.45
3:E:68:GLN:HA	3:E:71:VAL:HG22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:DA:H2''	1:I:61:DA:C8	2.52	0.44
1:I:84:DG:H2''	1:I:85:DC:H6	1.82	0.44
1:I:93:DC:H2''	1:I:94:DG:H8	1.82	0.44
1:I:49:DC:OP2	1:I:49:DC:H2'	2.18	0.44
1:I:52:DG:H2''	1:I:53:DG:H8	1.83	0.44
3:E:107:THR:HG21	3:E:124:ILE:HG12	1.99	0.44
4:B:73:THR:HG22	4:B:85:ASP:OD2	2.17	0.44
5:G:95:ARG:HA	5:G:98:SER:OG	2.18	0.44
2:J:38:DT:H2''	2:J:39:DA:N7	2.33	0.44
3:A:97:GLU:HG2	4:B:37:LEU:HD21	1.98	0.44
6:H:76:GLU:O	6:H:80:LEU:HD13	2.18	0.44
1:I:67:DG:OP2	1:I:67:DG:H2'	2.18	0.44
6:D:76:GLU:O	6:D:80:LEU:HD13	2.18	0.44
4:F:92:ARG:NH2	6:H:100:LEU:O	2.50	0.44
2:J:25:DG:H5'	2:J:25:DG:C8	2.52	0.44
2:J:89:DT:H2''	2:J:90:DA:O5'	2.18	0.44
3:A:107:THR:HG21	3:A:124:ILE:HG12	1.99	0.44
5:C:95:ARG:HA	5:C:98:SER:OG	2.18	0.44
1:I:88:DT:H2''	1:I:89:DT:C7	2.46	0.44
5:C:62:LEU:O	5:C:66:VAL:HG12	2.17	0.44
1:I:31:DA:H5''	5:G:20:SER:C	2.42	0.44
1:I:89:DT:H2''	1:I:90:DA:O5'	2.18	0.44
2:J:71:DG:C2	2:J:72:DC:C2	3.06	0.44
2:J:102:DG:C6	2:J:103:DA:C6	3.06	0.44
1:I:115:DC:H2''	1:I:116:DA:H5''	2.00	0.43
2:J:39:DA:H5''	5:C:46:ARG:HH11	1.82	0.43
2:J:42:DC:N3	2:J:43:DA:N6	2.65	0.43
3:E:63:ARG:HA	3:E:63:ARG:HD3	1.87	0.43
1:I:32:DG:H2''	1:I:33:DA:H8	1.84	0.43
1:I:107:DT:H2''	1:I:108:DC:C6	2.54	0.43
1:I:110:DA:N6	2:J:37:DG:N2	2.67	0.43
2:J:46:DT:H2''	2:J:47:DC:C5	2.54	0.43
3:A:68:GLN:HE21	3:A:72:ARG:HE	1.65	0.43
5:G:48:SER:CB	6:H:90:THR:HA	2.48	0.43
1:I:61:DA:H2''	1:I:62:DA:H8	1.82	0.43
1:I:100:DA:C8	1:I:100:DA:H5'	2.54	0.43
1:I:102:DA:C6	1:I:103:DG:C6	3.06	0.43
1:I:119:DT:H2''	1:I:120:DG:C8	2.53	0.43
2:J:32:DT:H2''	2:J:33:DG:C8	2.53	0.43
4:B:75:HIS:O	6:D:92:ARG:NH1	2.28	0.43
6:H:39:ILE:N	6:H:39:ILE:HD12	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:128:ARG:HH11	4:B:57:VAL:HG22	1.84	0.43
4:F:73:THR:HG22	4:F:85:ASP:OD2	2.17	0.43
5:G:28:SER:H	5:G:60:GLU:CD	2.26	0.43
6:H:64:SER:HA	6:H:67:ASN:ND2	2.34	0.43
1:I:109:DT:C2	1:I:110:DA:C6	3.07	0.43
2:J:60:DA:H2''	2:J:61:DA:C8	2.52	0.43
1:I:26:DC:N4	2:J:121:DG:O6	2.52	0.43
2:J:83:DG:C4	2:J:84:DC:C5	3.06	0.43
6:D:39:ILE:HD12	6:D:39:ILE:N	2.34	0.43
6:H:90:THR:HG22	6:H:91:SER:N	2.33	0.43
2:J:55:DG:OP2	2:J:55:DG:H8	2.02	0.43
2:J:85:DG:C5	2:J:86:DT:C4	3.07	0.43
1:I:65:DC:H1'	1:I:66:DG:H5'	1.99	0.43
1:I:95:DG:H2'	1:I:96:DT:C6	2.54	0.43
2:J:32:DT:O2	2:J:33:DG:N7	2.52	0.43
3:A:75:ALA:HB2	4:B:66:ILE:HG21	2.01	0.43
5:C:106:ILE:HG23	6:D:61:ILE:HD13	2.01	0.42
4:F:75:HIS:NE2	6:H:93:GLU:HG3	2.33	0.42
1:I:91:DA:C4	1:I:92:DG:C5	3.06	0.42
4:F:78:ARG:NH1	4:F:82:THR:HG23	2.35	0.42
1:I:43:DA:C2'	1:I:44:DA:H8	2.32	0.42
1:I:112:DG:H1'	1:I:113:DA:C8	2.54	0.42
2:J:84:DC:H2''	2:J:85:DG:C8	2.54	0.42
2:J:120:DA:H2''	2:J:121:DG:OP1	2.20	0.42
1:I:102:DA:C4	1:I:103:DG:C5	3.08	0.42
3:A:113:HIS:NE2	3:E:123:ASP:OD1	2.52	0.42
5:C:65:LYS:NZ	5:C:96:LEU:HD21	2.30	0.42
6:D:64:SER:HA	6:D:67:ASN:ND2	2.34	0.42
3:E:96:CYS:SG	4:F:62:LEU:HD21	2.59	0.42
1:I:35:DT:H2''	1:I:36:DA:O5'	2.19	0.42
2:J:113:DA:H2''	2:J:114:DG:H8	1.85	0.42
4:B:95:ARG:NH1	5:G:103:THR:HA	2.35	0.42
5:G:58:VAL:HG23	6:H:110:ALA:CB	2.31	0.42
1:I:71:DA:O3'	3:E:120:MET:HE1	2.19	0.42
2:J:76:DG:H2''	2:J:77:DT:O2	2.19	0.42
4:B:78:ARG:NH1	4:B:82:THR:HG23	2.35	0.42
5:C:50:THR:O	6:D:91:SER:HB2	2.18	0.42
5:G:53:VAL:CG2	6:H:118:VAL:HG12	2.48	0.42
1:I:31:DA:H2''	1:I:32:DG:C8	2.55	0.42
1:I:71:DA:C2	2:J:77:DT:H72	2.54	0.42
2:J:39:DA:H1'	2:J:40:DG:O4'	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:54:TYR:CE1	6:H:114:GLY:HA3	2.55	0.42
2:J:39:DA:C4	2:J:40:DG:C5	3.08	0.42
2:J:40:DG:P	6:D:88:THR:HG22	2.57	0.42
2:J:53:DC:C2	2:J:54:DC:C5	3.08	0.42
1:I:41:DG:H2'	1:I:42:DT:H71	2.00	0.42
2:J:99:DG:H2'	2:J:99:DG:OP2	2.19	0.42
2:J:41:DA:C5	2:J:42:DC:C4	3.08	0.42
2:J:43:DA:C4	2:J:44:DG:N7	2.88	0.42
2:J:71:DG:C4	2:J:72:DC:C5	3.07	0.42
5:C:46:ARG:O	6:D:88:THR:HA	2.20	0.42
1:I:40:DA:H5'	6:H:86:ARG:CZ	2.49	0.41
1:I:91:DA:C5	1:I:92:DG:C6	3.08	0.41
2:J:33:DG:H2''	2:J:34:DG:H8	1.83	0.41
4:B:96:THR:O	5:G:104:THR:HA	2.20	0.41
2:J:79:DC:H4'	2:J:80:DC:OP1	2.20	0.41
2:J:112:DT:C2	2:J:113:DA:N7	2.89	0.41
2:J:62:DC:C2	2:J:63:DG:N7	2.89	0.41
2:J:108:DT:H2''	2:J:109:DC:C5	2.56	0.41
6:H:55:SER:OG	6:H:56:SER:N	2.53	0.41
1:I:59:DA:H2''	1:I:60:DA:H8	1.85	0.41
1:I:81:DC:H5'	1:I:81:DC:H6	1.85	0.41
2:J:103:DA:C2	2:J:104:DT:C2	3.08	0.41
2:J:119:DC:H2'	2:J:120:DA:C8	2.56	0.41
5:C:51:ALA:CB	5:C:52:PRO:HD3	2.48	0.41
6:D:55:SER:OG	6:D:56:SER:N	2.53	0.41
1:I:92:DG:H5'	1:I:92:DG:H8	1.86	0.41
3:A:96:CYS:SG	4:B:62:LEU:HD21	2.60	0.41
5:C:49:ARG:HD2	5:C:49:ARG:HA	1.69	0.41
1:I:123:DC:H2''	1:I:124:DG:C8	2.56	0.41
2:J:39:DA:C5	2:J:40:DG:C6	3.09	0.41
2:J:117:DT:H4'	2:J:118:DC:H5'	2.02	0.41
1:I:110:DA:N6	2:J:37:DG:H22	2.19	0.41
5:C:55:LEU:HA	5:C:58:VAL:HG12	2.02	0.41
6:D:82:HIS:NE2	5:G:41:GLY:HA2	2.35	0.41
4:F:71:THR:HG22	6:H:96:THR:HG23	2.03	0.41
2:J:52:DA:H2''	2:J:53:DC:H6	1.86	0.41
2:J:69:DA:H1'	2:J:70:DC:H5'	2.03	0.41
1:I:38:DG:H2''	1:I:39:DG:C8	2.56	0.41
1:I:94:DG:C6	1:I:95:DG:C6	3.09	0.41
1:I:105:DT:OP2	1:I:105:DT:H2'	2.21	0.41
1:I:112:DG:N1	2:J:37:DG:C8	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:112:DG:C2	2:J:37:DG:H8	2.39	0.41
1:I:117:DA:H8	1:I:117:DA:OP2	2.04	0.41
1:I:120:DG:N2	2:J:28:DC:C2	2.85	0.41
3:A:116:ARG:NH1	3:A:118:THR:O	2.54	0.41
4:B:78:ARG:NH1	4:B:80:THR:O	2.54	0.41
5:G:97:LEU:HA	6:H:106:LEU:HD11	2.02	0.41
1:I:112:DG:H2''	1:I:113:DA:OP2	2.20	0.41
2:J:75:DT:H2''	2:J:76:DG:C8	2.56	0.41
2:J:92:DC:C2	2:J:93:DC:C5	3.09	0.41
3:A:106:ASP:OD2	3:A:131:ARG:NH2	2.51	0.41
3:E:101:VAL:O	3:E:105:GLU:HG3	2.21	0.41
4:F:78:ARG:NH1	4:F:80:THR:O	2.54	0.41
2:J:74:DC:H1'	2:J:75:DT:C6	2.57	0.40
5:G:29:PHE:HZ	5:G:63:THR:HG21	1.85	0.40
1:I:29:DG:C2	1:I:30:DG:C6	3.09	0.40
1:I:112:DG:C6	1:I:113:DA:C6	3.10	0.40
2:J:90:DA:C2	2:J:91:DA:C6	3.10	0.40
2:J:99:DG:H2''	2:J:100:DG:C8	2.57	0.40
5:C:30:SER:O	5:C:34:VAL:HG23	2.22	0.40
2:J:47:DC:H1'	2:J:48:DT:C5	2.56	0.40
2:J:110:DC:H2''	2:J:111:DC:C5	2.56	0.40
1:I:112:DG:C4	1:I:113:DA:C5	3.09	0.40
2:J:64:DC:H2''	2:J:65:DA:H8	1.81	0.40
2:J:83:DG:H2''	2:J:84:DC:OP2	2.21	0.40
2:J:103:DA:C4	2:J:104:DT:C5	3.09	0.40
6:D:90:THR:HG22	6:D:91:SER:N	2.33	0.40
3:E:116:ARG:NH1	3:E:118:THR:O	2.54	0.40
2:J:81:DC:H6	2:J:81:DC:H2'	1.60	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	
3	A	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
3	E	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
4	B	74/103 (72%)	72 (97%)	2 (3%)	0	100	100
4	F	74/103 (72%)	72 (97%)	2 (3%)	0	100	100
5	C	88/115 (76%)	81 (92%)	6 (7%)	1 (1%)	11	43
5	G	88/115 (76%)	82 (93%)	6 (7%)	0	100	100
6	D	86/126 (68%)	85 (99%)	1 (1%)	0	100	100
6	H	86/126 (68%)	85 (99%)	1 (1%)	0	100	100
All	All	640/960 (67%)	619 (97%)	20 (3%)	1 (0%)	44	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	52	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	64/111 (58%)	63 (98%)	1 (2%)	55	69
3	E	64/111 (58%)	63 (98%)	1 (2%)	55	69
4	B	63/79 (80%)	61 (97%)	2 (3%)	34	56
4	F	63/79 (80%)	61 (97%)	2 (3%)	34	56
5	C	79/96 (82%)	75 (95%)	4 (5%)	21	46
5	G	79/96 (82%)	75 (95%)	4 (5%)	21	46
6	D	75/106 (71%)	74 (99%)	1 (1%)	61	71
6	H	75/106 (71%)	74 (99%)	1 (1%)	61	71
All	All	562/784 (72%)	546 (97%)	16 (3%)	38	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	101	VAL
4	B	53	GLU
4	B	65	VAL
5	C	49	ARG
5	C	102	ASN
5	C	104	THR
5	C	109	VAL
6	D	116	LYS
3	E	101	VAL
4	F	53	GLU
4	F	65	VAL
5	G	48	SER
5	G	102	ASN
5	G	104	THR
5	G	109	VAL
6	H	116	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	85	GLN
4	B	75	HIS
5	C	45	GLN
5	C	72	ASN
5	C	75	GLN
5	C	92	HIS
6	D	84	ASN
6	D	109	HIS
3	E	68	GLN
3	E	85	GLN
4	F	75	HIS
5	G	45	GLN
5	G	72	ASN
5	G	92	HIS
6	H	84	ASN
6	H	109	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

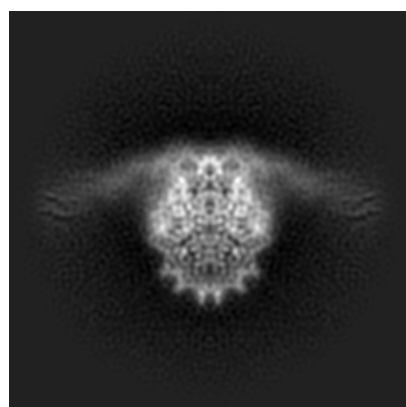
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30078. These allow visual inspection of the internal detail of the map and identification of artifacts.

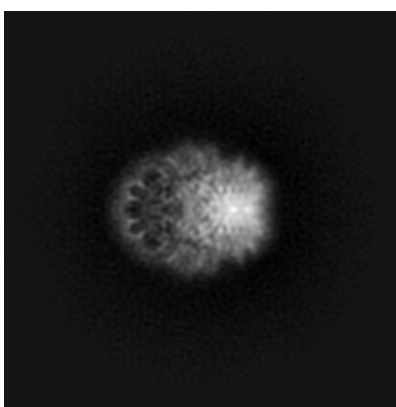
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

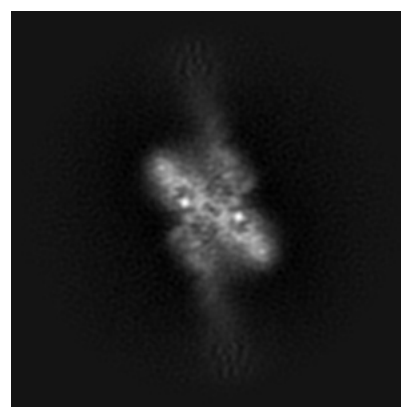
6.1.1 Primary map



X



Y

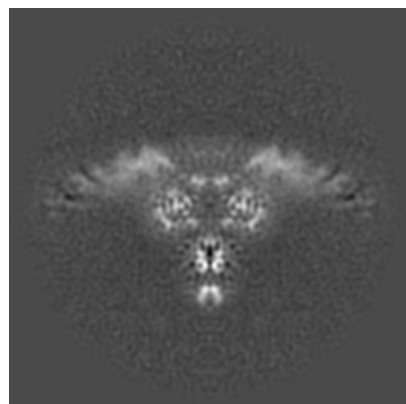


Z

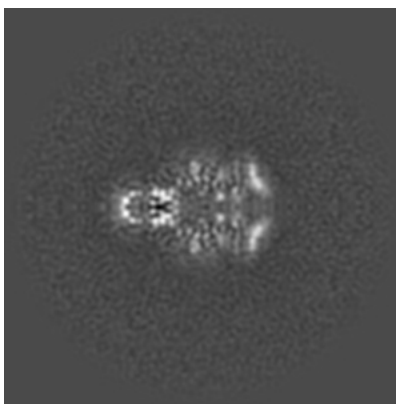
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

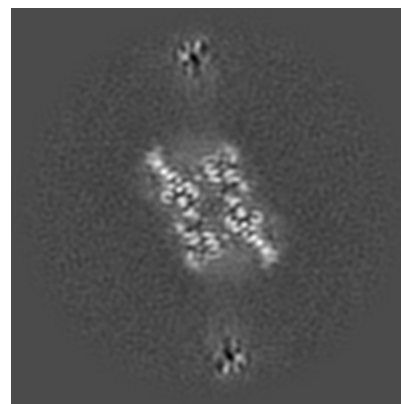
6.2.1 Primary map



X Index: 120



Y Index: 120

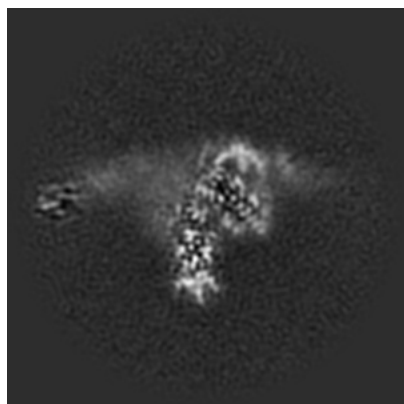


Z Index: 120

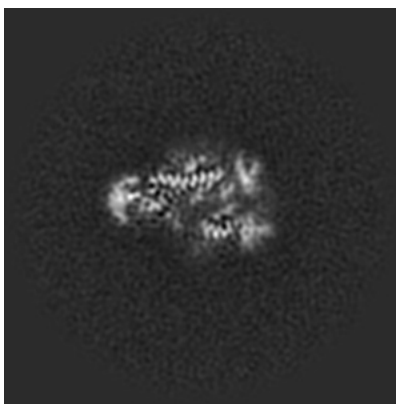
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

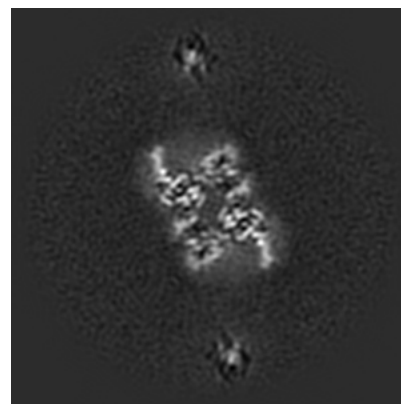
6.3.1 Primary map



X Index: 128



Y Index: 115

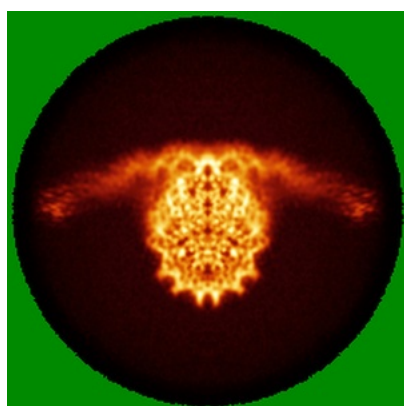


Z Index: 118

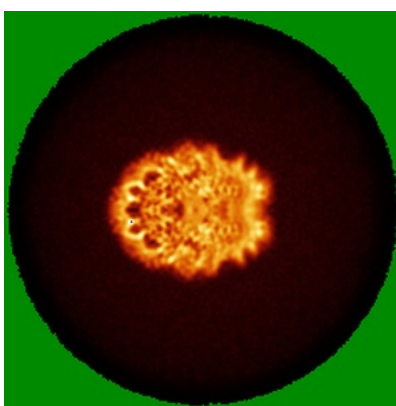
The images above show the largest variance slices of the map in three orthogonal directions.

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

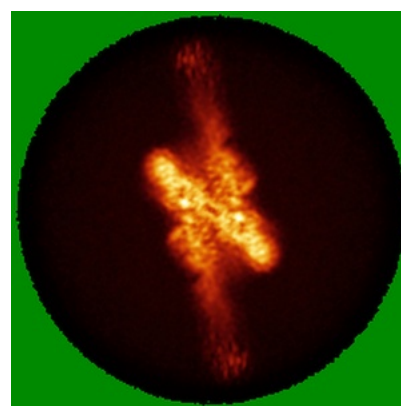
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

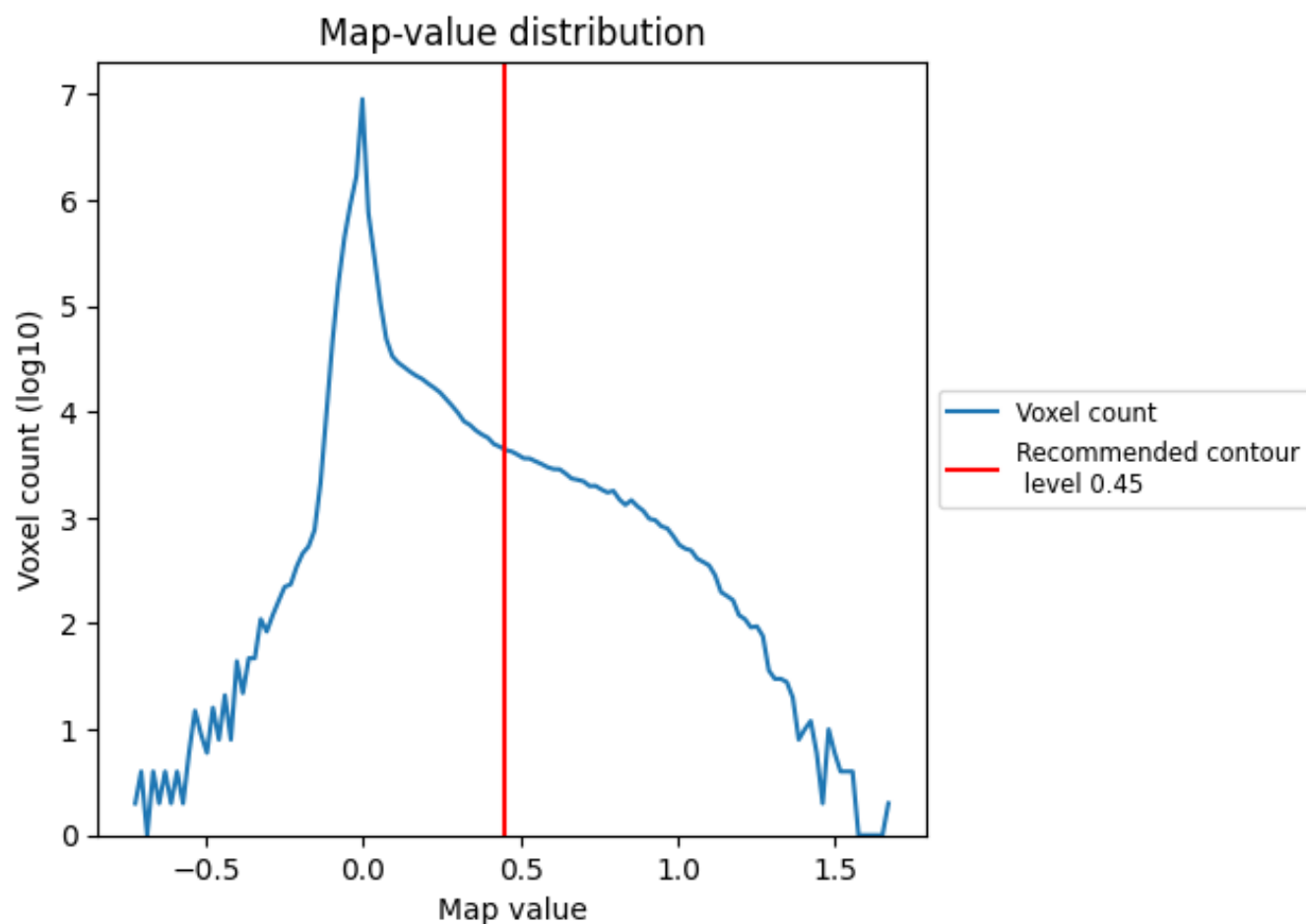
6.6 Mask visualisation

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

7 Map analysis [i](#)

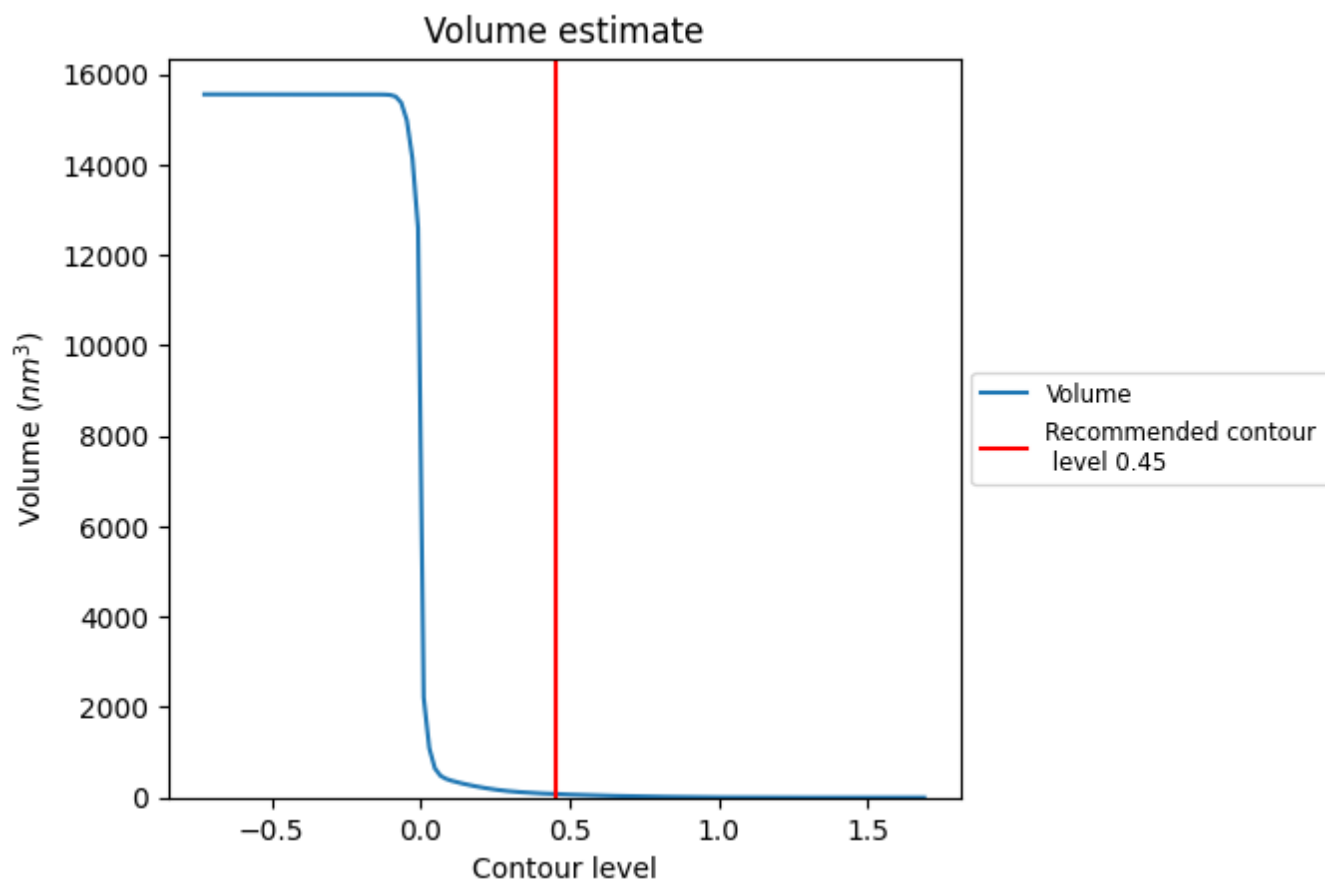
This section contains the results of statistical analysis of the map.

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.

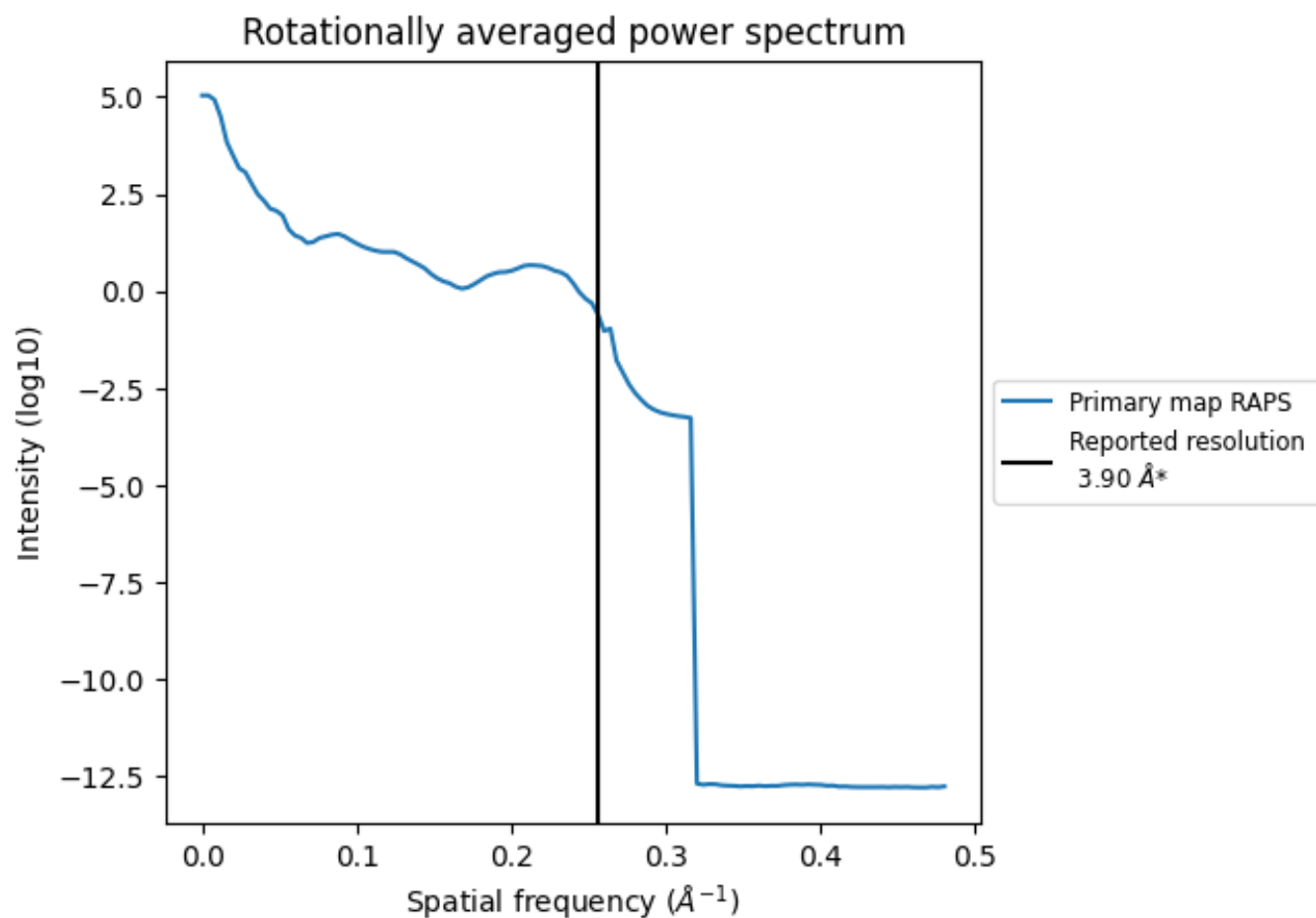
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm³; this corresponds to an approximate mass of 71 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 0.256 Å⁻¹

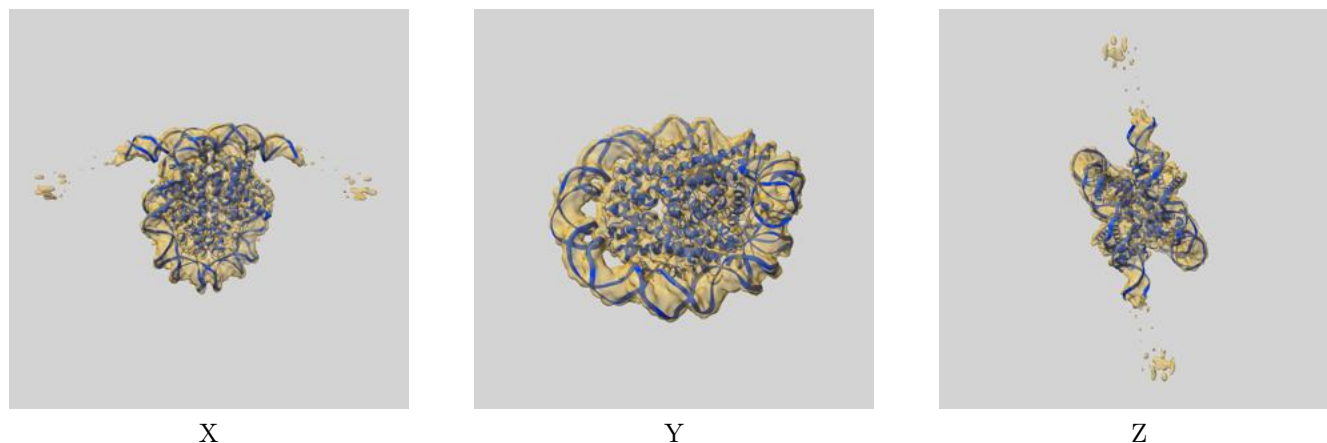
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

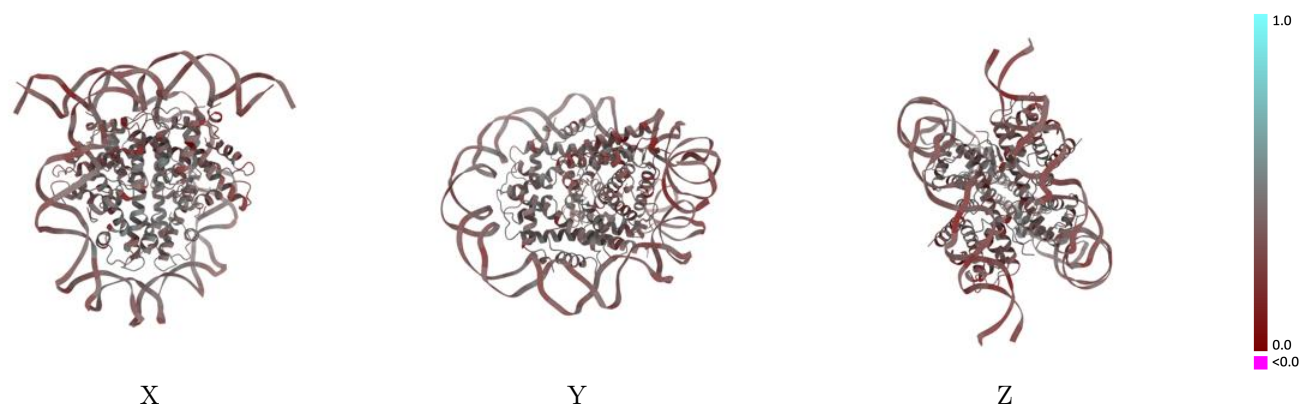
This section contains information regarding the fit between EMDB map EMD-30078 and PDB model 6M4H. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.45 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](#)

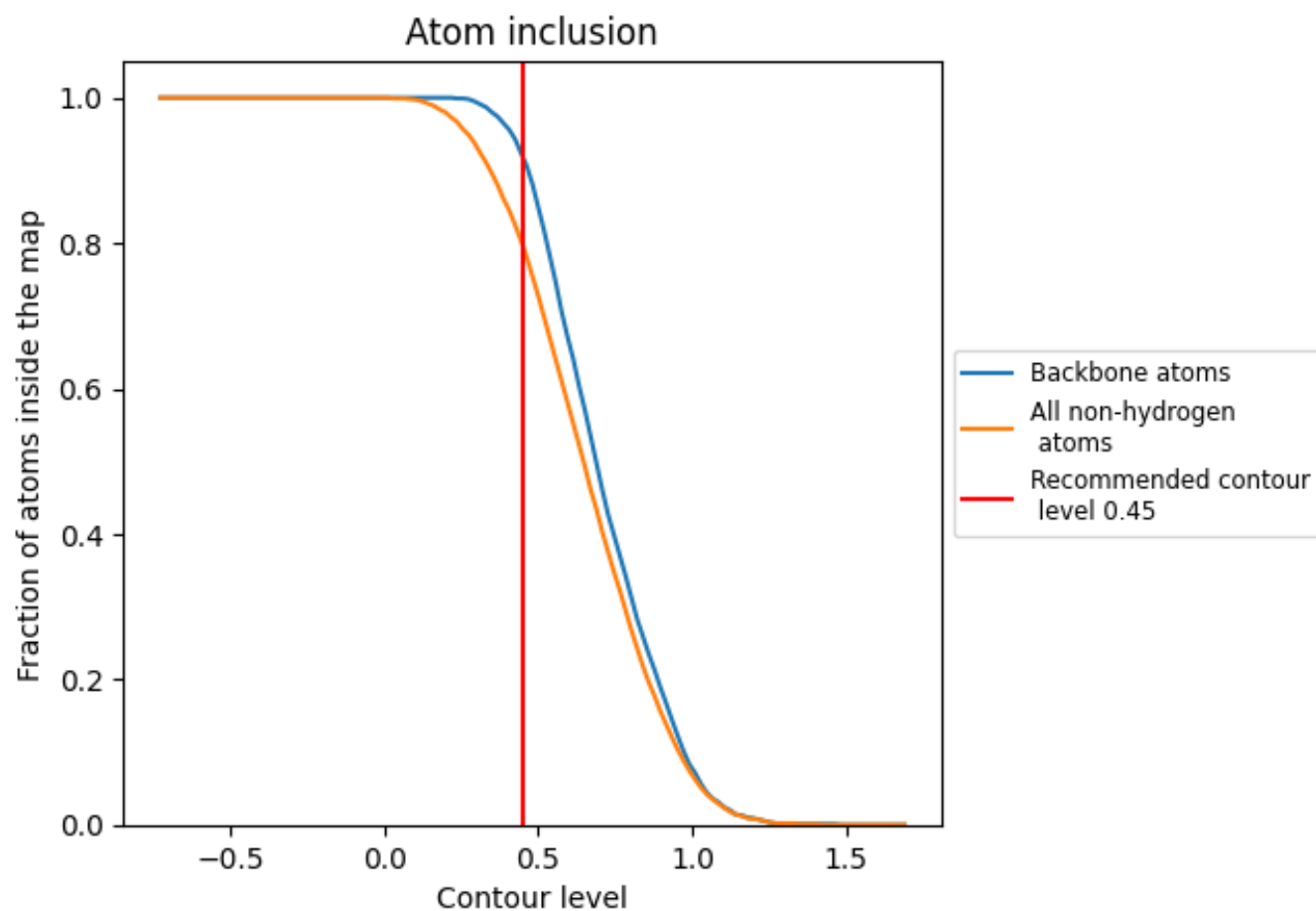


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 80% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7970	0.3650
A	0.7560	0.4150
B	0.7250	0.4130
C	0.6360	0.3480
D	0.6540	0.3460
E	0.7590	0.4170
F	0.7360	0.4130
G	0.6300	0.3440
H	0.6550	0.3450
I	0.9150	0.3470
J	0.9330	0.3520

1.0

0.0

<0.0