



Full wwPDB EM Validation Report ⓘ

Apr 6, 2025 – 12:56 AM JST

PDB ID : 9JNX / pdb_00009jnx
EMDB ID : EMD-61630
Title : Structure of isw1-nucleosome complex in ADP*+ state
Authors : Sia, Y.; Pan, H.; Chen, Z.
Deposited on : 2024-09-24
Resolution : 3.00 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

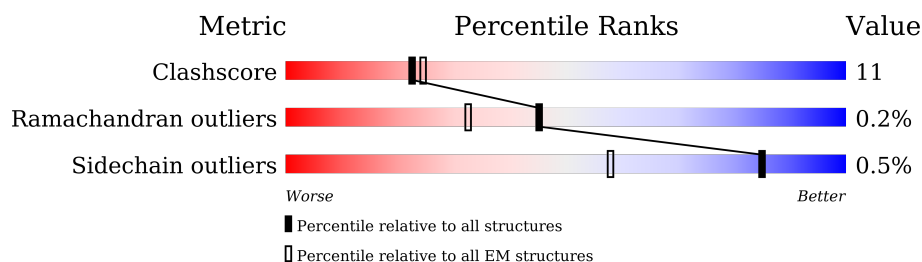
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	122	
4	H	122	

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Mol	Chain	Length	Quality of chain
5	I	146	<div><div></div><div>46%</div><div>54%</div></div>
6	J	146	<div><div></div><div>50%</div><div>50%</div></div>
7	K	1061	<div><div></div><div>7%</div><div>34%</div><div>20%</div><div>45%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16809 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			779	492	148	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	88	Total	C	N	O	S	0	0
			707	445	143	118	1		
2	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			811	510	158	143		
3	G	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 7 is a protein called ISWI chromatin-remodeling complex ATPase ISW1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	579	Total	C	N	O	S	0	0
			4766	3046	815	892	13		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	K	1	Total	Mg	0
			1	1	

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

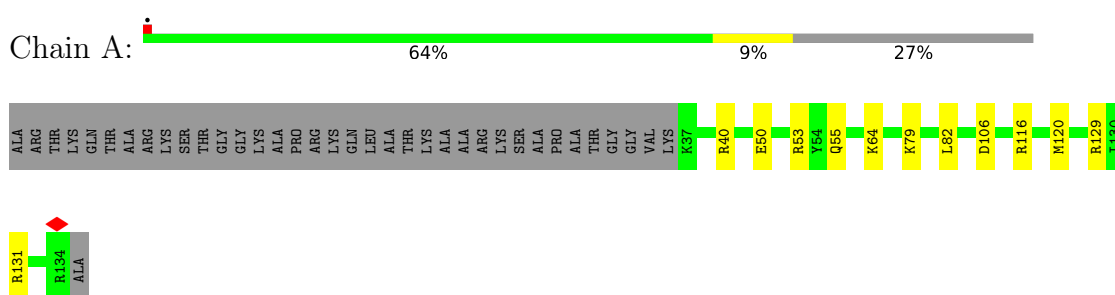


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	K	1	27	10	5	10	2	0

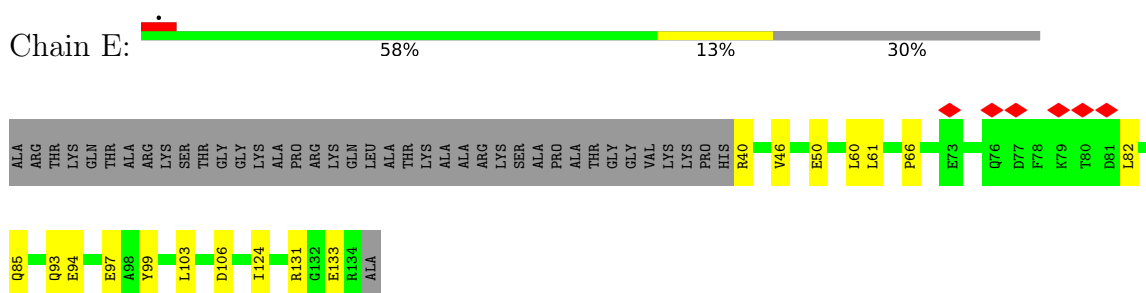
3 Residue-property plots

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

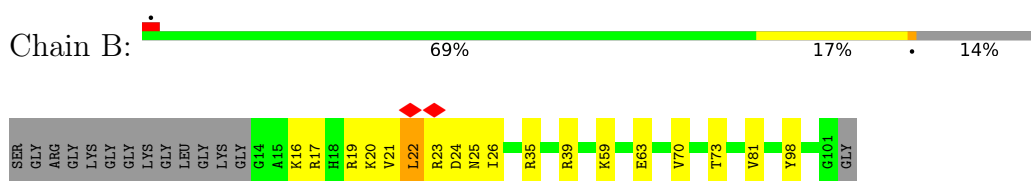
• Molecule 1: Histone H3



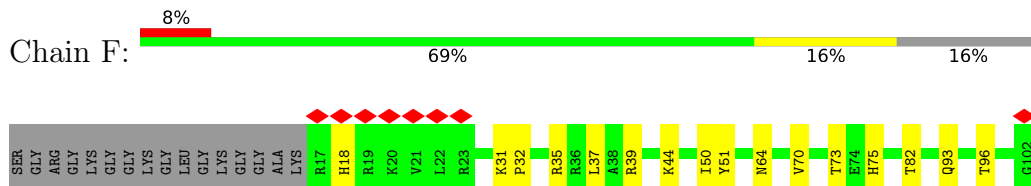
• Molecule 1: Histone H3



• Molecule 2: Histone H4



• Molecule 2: Histone H4



• Molecule 3: Histone H2A

Chain C:  74% 9% 17%

SER GLY ARG GLY LYS GLN GLY LYS THR ARG A12 T16 L51 E61 E62 L63 E64 I78 E92 R95 V100 Q104 Q112 L115 K118 LYS THR GLU SER SER LYS SER ALA LYS SER LYS

• Molecule 3: Histone H2A

Chain G:  68% 15% 17%

SER GLY ARG GLY LYS GLN GLY LYS THR ARG A12 K15 R20 R29 V40 H31 R35 Y39 R42 V43 G44 L63 E64 L65 R77 I78 I79 H82 A86 V87 R88 E91 E92 L93 N94 N110 K118 LYS THR GLU SER SER LYS SER ALA LYS

SER LYS

• Molecule 4: Histone H2B

Chain D:  67% 9% 24%

ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS VAL THR LYS THR GLN LYS LYS ASP GLY LYS ARG ARG LYS R29 R30 L42 T51 E73 R76 T87 E90 I91 E102 K105 H106 A121 LYS

• Molecule 4: Histone H2B

Chain H:  66% 11% 24%

ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS VAL THR LYS THR GLN LYS LYS ASP GLY LYS ARG ARG LYS T29 E32 L42 D48 K54 D65 E68 E73 R76 T85 I86 T87 S88 R89 E90 T93 A121 LYS

• Molecule 5: DNA (146-MER)

Chain I:  46% 54%

T2 C3 G4 C12 G13 C21 C26 T27 C28 A29 A30 T31 C36 C37 T38 A39 G40 A41 T46 C47 T48 A52 C53 T57 T58 A59 A60 A61 A65 C66 C67 T68 A69 G76 T77 C78 C79 C82 C83 T87 T88 T89 A90 A91 C92 C93 C94 C95

A98 G99 G100 G101 A102 A103 A106 C107 T108 C109 C110 C111 T112 T113 G114 T115 T116 T117 C118 C119 A120 G121 C122 C123 A124 T127 G128 T129 C130 A131 A135 T136 T137 T138 A139 C140 A141 T142 C143 C144 T147

• Molecule 6: DNA (146-MER)

Chain J:  50% 50%

A1 G5 A6 T7 G8 T9 A10 T11 A12 T13 A14 T15 C16 T17 C20 A21 T28 G29 G30 A31 G32 A33 C34 T35 A36 T42 A43 C48 C49 T50 T51 G52 G53 C54 G55 G56 T57 T58 A59 A60 C65 G66 G67 G68 G69 G70 A71 C72 C77 G78 T79 A80 C81

G82 T83 T88 T89 A90 A91 G92 C93 G94 G95 T96 G97 C98 T99 A100 C111 G112 A113 T119 G120 A121 G122 C123 G124 T128 C129 G130 G131 A139 T140 T143 C144 G145 A146

• Molecule 7: ISWI chromatin-remodeling complex ATPase ISW1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93305	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.333	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.063	Depositor
Map size (\AA)	346.4, 346.4, 346.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.35	0/813	0.45	0/1093
1	E	0.33	0/789	0.42	0/1059
2	B	0.34	0/715	0.48	0/955
2	F	0.35	0/680	0.48	0/912
3	C	0.33	0/821	0.45	0/1112
3	G	0.32	0/825	0.46	0/1116
4	D	0.34	0/729	0.44	0/985
4	H	0.35	0/737	0.45	0/993
5	I	0.66	0/3333	0.96	0/5137
6	J	0.67	0/3381	0.92	0/5221
7	K	0.30	0/4855	0.48	0/6543
All	All	0.48	0/17678	0.70	0/25126

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
7	K	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	22	LEU	Peptide
7	K	545	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	801	0	831	7	0
1	E	779	0	815	12	0
2	B	707	0	760	14	0
2	F	672	0	698	13	0
3	C	811	0	849	12	0
3	G	815	0	860	13	0
4	D	718	0	725	8	0
4	H	726	0	747	11	0
5	I	2975	0	1639	67	0
6	J	3011	0	1639	61	0
7	K	4766	0	4801	162	0
8	K	1	0	0	0	0
9	K	27	0	12	0	0
All	All	16809	0	14376	346	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 11.

All (346) 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:K:531:LEU:HD11	7:K:575:LEU:HB3	1.53	0.89
5:I:113:DA:H2'	5:I:114:DG:C8	2.17	0.80
7:K:398:VAL:O	7:K:402:HIS:ND1	2.16	0.76
5:I:117:DT:H2''	5:I:118:DC:H5''	1.67	0.75
5:I:12:DC:H2'	5:I:13:DG:C8	2.23	0.73
3:G:77:ARG:NH1	5:I:21:DG:OP1	2.22	0.72
3:C:63:LEU:HD21	4:D:42:LEU:HB2	1.72	0.72
7:K:222:GLU:OE2	7:K:411:ARG:NH2	2.23	0.72
7:K:744:GLU:OE2	7:K:747:GLY:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:GLU:OE1	7:K:769:ARG:NH2	2.24	0.71
1:A:40:ARG:NH2	5:I:83:DG:N3	2.38	0.71
5:I:68:DT:H2''	5:I:69:DA:C8	2.26	0.70
1:A:106:ASP:OD2	1:A:131:ARG:NH2	2.22	0.69
6:J:81:DC:H2'	6:J:82:DG:C8	2.26	0.69
5:I:98:DA:H2'	5:I:99:DG:C8	2.28	0.68
7:K:184:GLN:O	7:K:205:ASN:ND2	2.26	0.68
1:E:103:LEU:HA	1:E:131:ARG:HH22	1.58	0.68
5:I:130:DC:H2''	5:I:131:DA:N7	2.09	0.67
6:J:10:DA:H2''	6:J:11:DT:H5'	1.77	0.67
5:I:94:DG:H2''	5:I:95:DC:H5''	1.75	0.66
7:K:585:ILE:O	7:K:614:ARG:NH2	2.28	0.66
7:K:493:THR:HG22	7:K:540:PHE:HB2	1.78	0.66
7:K:257:LEU:HD11	7:K:302:SER:HB3	1.78	0.65
1:E:106:ASP:OD2	1:E:131:ARG:NH2	2.29	0.65
5:I:99:DG:H2'	5:I:100:DG:C8	2.31	0.65
7:K:122:PHE:O	7:K:125:SER:OG	2.14	0.65
3:G:42:ARG:HB2	4:H:85:THR:HG22	1.79	0.65
5:I:135:DA:H2''	5:I:136:DT:H5''	1.79	0.64
7:K:209:SER:O	7:K:213:ASN:ND2	2.30	0.64
5:I:47:DC:H2''	5:I:48:DT:H71	1.79	0.64
7:K:89:ARG:HH22	7:K:245:PRO:HD2	1.62	0.63
7:K:358:ASN:OD1	7:K:359:ASN:N	2.31	0.63
5:I:52:DA:H2''	5:I:53:DC:H5''	1.82	0.62
7:K:524:PHE:CE1	7:K:576:LEU:HD22	2.34	0.62
2:B:19:ARG:HD3	2:B:19:ARG:H	1.65	0.62
7:K:524:PHE:HE1	7:K:576:LEU:HD22	1.65	0.62
5:I:78:DC:H2''	5:I:79:DC:C6	2.35	0.61
7:K:655:ARG:HA	7:K:658:LEU:HB2	1.82	0.61
7:K:359:ASN:OD1	7:K:360:LEU:N	2.33	0.60
6:J:120:DG:H2''	6:J:121:DA:C8	2.36	0.60
7:K:498:VAL:HA	7:K:504:LEU:HD22	1.83	0.60
6:J:130:DG:H2''	6:J:131:DG:C8	2.36	0.60
7:K:535:GLU:HG2	7:K:545:TYR:CZ	2.36	0.60
7:K:126:LYS:NZ	7:K:374:ILE:O	2.31	0.60
7:K:424:LYS:HA	7:K:621:VAL:HG23	1.83	0.60
7:K:503:LYS:NZ	7:K:633:GLU:OE2	2.31	0.60
7:K:196:LEU:HD22	7:K:201:ILE:HG13	1.84	0.59
7:K:417:VAL:N	7:K:418:GLU:OE2	2.35	0.59
7:K:358:ASN:HB2	7:K:643:LYS:HD3	1.82	0.59
7:K:477:ASN:ND2	7:K:597:ASP:OD2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:514:LEU:O	7:K:518:GLY:N	2.34	0.59
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.85	0.58
7:K:345:SER:OG	7:K:348:ARG:NH1	2.34	0.58
7:K:420:SER:O	7:K:421:LEU:C	2.41	0.58
3:C:112:GLN:HB2	3:C:115:LEU:HD13	1.83	0.58
7:K:548:ILE:HD11	7:K:557:ARG:HD3	1.84	0.58
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.18	0.58
5:I:127:DT:H2'	5:I:128:DG:C8	2.38	0.58
6:J:10:DA:H2'	6:J:11:DT:H71	1.85	0.58
7:K:425:LYS:HE3	7:K:620:GLN:HE22	1.69	0.57
7:K:627:VAL:HG21	7:K:637:LEU:HD22	1.85	0.57
5:I:120:DA:H2''	5:I:121:DG:C8	2.38	0.57
5:I:82:DC:H2''	5:I:83:DG:C8	2.39	0.57
5:I:87:DT:H2''	5:I:88:DT:H71	1.86	0.57
7:K:332:GLU:OE1	7:K:341:ARG:NH2	2.38	0.57
7:K:564:TYR:CE2	7:K:574:PHE:HB2	2.39	0.57
7:K:514:LEU:HA	7:K:517:GLU:HB3	1.87	0.56
6:J:50:DT:H2'	6:J:51:DT:C6	2.39	0.56
5:I:99:DG:OP2	7:K:639:ARG:NH1	2.37	0.56
6:J:79:DT:H2''	6:J:80:DA:C8	2.40	0.56
7:K:382:ASP:O	7:K:386:SER:N	2.38	0.56
7:K:541:ARG:HB3	7:K:543:TYR:HE1	1.69	0.56
7:K:120:LYS:NZ	7:K:124:GLU:OE1	2.38	0.56
3:G:88:ARG:NH1	3:G:94:ASN:OD1	2.39	0.56
6:J:111:DC:H2''	6:J:112:DG:C8	2.40	0.56
6:J:54:DC:H2''	6:J:55:DG:H5'	1.88	0.56
6:J:57:DT:OP2	7:K:254:LYS:NZ	2.37	0.56
7:K:185:PHE:HB3	7:K:205:ASN:ND2	2.21	0.56
7:K:426:GLU:HA	7:K:623:VAL:HB	1.87	0.56
7:K:249:LEU:HD23	7:K:321:ILE:HD12	1.88	0.55
7:K:523:ILE:HD12	7:K:523:ILE:H	1.71	0.55
5:I:92:DC:H2''	5:I:93:DC:H5''	1.87	0.55
5:I:121:DG:H2''	5:I:122:DG:C8	2.41	0.55
7:K:121:HIS:O	7:K:124:GLU:HG2	2.06	0.55
5:I:65:DA:H2'	5:I:66:DC:C6	2.41	0.55
7:K:239:ARG:HG3	7:K:245:PRO:HA	1.89	0.55
5:I:116:DC:H2'	5:I:117:DT:C6	2.42	0.55
6:J:112:DG:H2''	6:J:113:DA:H8	1.71	0.54
7:K:630:ASN:O	7:K:745:TRP:NE1	2.40	0.54
6:J:5:DG:H2''	6:J:6:DA:C8	2.42	0.54
2:B:59:LYS:O	2:B:63:GLU:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:494:ASP:OD1	7:K:496:HIS:ND1	2.39	0.54
5:I:3:DC:H2''	5:I:4:DG:C8	2.43	0.54
5:I:106:DA:H2''	5:I:107:DC:H5''	1.90	0.54
7:K:418:GLU:OE1	7:K:418:GLU:N	2.41	0.54
7:K:715:SER:O	7:K:719:THR:HG23	2.08	0.54
6:J:7:DT:H2''	6:J:8:DG:C8	2.42	0.54
7:K:539:TYR:HB2	7:K:545:TYR:OH	2.07	0.54
3:G:31:HIS:CD2	3:G:35:ARG:HE	2.24	0.53
5:I:110:DC:H2''	5:I:111:DC:C5	2.44	0.53
7:K:240:TYR:OH	7:K:270:ASP:OD1	2.27	0.53
7:K:357:GLN:N	7:K:362:GLU:OE2	2.41	0.53
7:K:398:VAL:HG23	7:K:399:LYS:HD2	1.89	0.53
6:J:66:DG:H2''	6:J:67:DG:O5'	2.09	0.52
3:G:63:LEU:HD13	4:H:42:LEU:HB2	1.92	0.52
7:K:496:HIS:HA	7:K:499:TYR:HE1	1.75	0.52
2:B:20:LYS:HG3	2:B:22:LEU:H	1.75	0.52
4:D:73:GLU:OE2	4:D:76:ARG:NH2	2.43	0.52
5:I:67:DG:H2''	5:I:68:DT:H71	1.92	0.52
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.24	0.52
5:I:98:DA:H2''	5:I:99:DG:OP1	2.09	0.52
7:K:102:LEU:HA	7:K:105:THR:HB	1.92	0.52
6:J:59:DA:H2''	6:J:60:DA:H5''	1.91	0.52
7:K:630:ASN:OD1	7:K:745:TRP:NE1	2.40	0.52
6:J:139:DA:H1'	6:J:140:DT:H5'	1.92	0.51
1:E:60:LEU:HD21	1:E:94:GLU:HG2	1.91	0.51
7:K:416:ASP:N	7:K:418:GLU:OE2	2.42	0.51
7:K:316:ILE:HB	7:K:318:TRP:CE2	2.45	0.51
7:K:108:ARG:NE	7:K:373:ASP:OD2	2.44	0.51
6:J:99:DT:H2''	6:J:100:DA:N7	2.26	0.51
5:I:121:DG:H2''	5:I:122:DG:N7	2.26	0.51
3:C:78:ILE:HD11	4:D:51:ILE:HD12	1.92	0.51
5:I:109:DC:H2''	5:I:110:DC:C5	2.46	0.51
6:J:8:DG:H2'	6:J:9:DT:H71	1.93	0.51
5:I:120:DA:H2''	5:I:121:DG:N7	2.26	0.51
6:J:51:DT:H2''	6:J:52:DG:H8	1.76	0.51
7:K:222:GLU:HG3	7:K:414:LYS:HB2	1.93	0.51
6:J:54:DC:OP1	7:K:577:THR:HG21	2.11	0.50
7:K:290:LYS:O	7:K:294:CYS:N	2.44	0.50
5:I:40:DG:H2''	5:I:41:DA:C8	2.46	0.50
7:K:331:ASN:HB3	7:K:334:SER:OG	2.12	0.50
7:K:648:GLN:HA	7:K:652:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:239:ARG:NH1	7:K:270:ASP:O	2.34	0.50
7:K:524:PHE:HA	7:K:576:LEU:O	2.12	0.50
5:I:46:DT:H2''	5:I:47:DC:C6	2.47	0.50
7:K:395:ASP:O	7:K:399:LYS:HD3	2.11	0.50
5:I:141:DA:H2''	5:I:142:DT:OP2	2.12	0.50
5:I:142:DT:H1'	5:I:143:DC:OP2	2.12	0.50
7:K:86:ASN:O	7:K:86:ASN:ND2	2.45	0.50
7:K:248:PHE:HE1	7:K:320:TYR:HD2	1.60	0.50
2:F:70:VAL:HA	2:F:73:THR:HG22	1.94	0.49
2:F:35:ARG:O	2:F:39:ARG:HG2	2.12	0.49
7:K:473:ARG:O	7:K:477:ASN:HB2	2.12	0.49
7:K:84:GLU:OE2	7:K:88:LYS:NZ	2.46	0.49
4:D:30:ARG:HG3	5:I:124:DA:H4'	1.95	0.49
6:J:112:DG:H2''	6:J:113:DA:C8	2.46	0.49
7:K:382:ASP:HB3	7:K:387:SER:HB2	1.95	0.49
4:D:106:HIS:NE2	7:K:766:PRO:O	2.46	0.48
7:K:639:ARG:O	7:K:642:GLN:HG2	2.13	0.48
5:I:98:DA:H2'	5:I:99:DG:H8	1.76	0.48
6:J:93:DC:H2''	6:J:94:DG:C8	2.48	0.48
1:E:66:PRO:HD3	6:J:91:DA:H5''	1.96	0.48
5:I:57:DT:H2''	5:I:58:DT:C6	2.49	0.48
5:I:114:DG:H2'	5:I:115:DT:H71	1.95	0.48
6:J:35:DT:H2''	6:J:36:DA:C8	2.49	0.48
7:K:302:SER:O	7:K:306:ILE:HG12	2.13	0.48
7:K:619:LYS:O	7:K:620:GLN:HG2	2.13	0.48
4:D:87:THR:OG1	4:D:90:GLU:OE1	2.20	0.48
7:K:617:GLN:NE2	7:K:620:GLN:O	2.47	0.48
7:K:538:CYS:SG	7:K:543:TYR:HB2	2.54	0.48
1:A:79:LYS:O	1:A:82:LEU:HD23	2.14	0.48
1:E:40:ARG:NH2	6:J:83:DT:O2	2.46	0.48
6:J:128:DT:H2''	6:J:129:DC:C5	2.48	0.48
2:B:70:VAL:HA	2:B:73:THR:HG22	1.96	0.48
6:J:49:DC:H2'	6:J:50:DT:H71	1.96	0.48
6:J:71:DA:H4'	6:J:72:DC:OP1	2.14	0.48
7:K:385:PHE:CZ	7:K:731:LEU:HD21	2.48	0.48
4:D:102:GLU:HB2	7:K:769:ARG:HD3	1.95	0.47
6:J:119:DT:H2''	6:J:120:DG:N7	2.28	0.47
6:J:16:DC:H2''	6:J:17:DT:C5	2.48	0.47
7:K:417:VAL:C	7:K:418:GLU:CD	2.73	0.47
5:I:111:DC:H2''	5:I:112:DT:C7	2.44	0.47
7:K:337:SER:O	7:K:341:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:357:GLN:HG2	7:K:603:GLN:HG3	1.96	0.47
7:K:330:LYS:NZ	7:K:357:GLN:OE1	2.30	0.47
7:K:521:VAL:HG23	7:K:573:VAL:HG23	1.96	0.47
2:B:17:ARG:HG3	7:K:536:ASP:OD2	2.15	0.47
6:J:32:DG:H2''	6:J:33:DA:O5'	2.13	0.47
6:J:68:DG:H2''	6:J:69:DG:C8	2.50	0.47
7:K:113:LEU:HD11	7:K:120:LYS:HB3	1.97	0.47
7:K:415:SER:C	7:K:418:GLU:OE1	2.53	0.47
2:F:75:HIS:O	4:H:89:ARG:NH1	2.40	0.47
7:K:94:ASP:N	7:K:94:ASP:OD1	2.44	0.47
2:B:35:ARG:O	2:B:39:ARG:HG2	2.15	0.47
5:I:130:DC:H2''	5:I:131:DA:C8	2.50	0.47
2:B:20:LYS:HG3	2:B:21:VAL:N	2.29	0.47
7:K:198:PRO:HA	7:K:201:ILE:HD12	1.97	0.46
5:I:136:DT:H2''	5:I:137:DA:H5''	1.98	0.46
6:J:123:DC:H2''	6:J:124:DG:C8	2.51	0.46
7:K:493:THR:HG22	7:K:493:THR:O	2.15	0.46
3:C:100:VAL:HG22	2:F:96:THR:HB	1.98	0.46
1:A:55:GLN:NE2	3:G:110:ASN:H	2.14	0.46
6:J:66:DG:H4'	6:J:67:DG:OP1	2.16	0.46
7:K:585:ILE:HG22	7:K:587:LEU:HG	1.97	0.46
2:B:16:LYS:HE3	7:K:532:ASP:OD1	2.15	0.46
7:K:642:GLN:HB2	7:K:726:TYR:OH	2.15	0.46
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.50	0.46
5:I:89:DT:H2''	5:I:90:DA:C8	2.51	0.46
5:I:95:DC:P	7:K:328:ARG:HH21	2.39	0.46
6:J:15:DT:H2''	6:J:16:DC:C6	2.51	0.46
6:J:89:DT:H2''	6:J:90:DA:C8	2.51	0.46
7:K:263:GLU:OE1	7:K:263:GLU:N	2.49	0.46
1:A:116:ARG:NH1	1:A:120:MET:SD	2.89	0.45
7:K:418:GLU:N	7:K:418:GLU:CD	2.69	0.45
7:K:544:GLU:N	7:K:544:GLU:OE2	2.49	0.45
7:K:496:HIS:HA	7:K:499:TYR:CE1	2.50	0.45
6:J:59:DA:H2''	6:J:60:DA:C8	2.51	0.45
7:K:373:ASP:OD1	7:K:374:ILE:HG13	2.16	0.45
4:H:54:LYS:HB3	4:H:54:LYS:HE3	1.75	0.45
6:J:20:DC:H2''	6:J:21:DA:H8	1.80	0.45
7:K:92:LEU:HG	7:K:317:ASN:HB2	1.99	0.45
7:K:106:THR:HG22	7:K:136:VAL:HG13	1.98	0.45
7:K:522:LEU:HD11	7:K:590:ALA:HB3	1.97	0.45
3:C:104:GLN:OE1	3:C:104:GLN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:VAL:O	1:E:50:GLU:HG3	2.15	0.45
1:E:93:GLN:O	1:E:97:GLU:HG3	2.16	0.45
5:I:30:DA:H2'	5:I:31:DT:H71	1.98	0.45
6:J:121:DA:H2''	6:J:122:DG:C8	2.52	0.45
2:B:17:ARG:HG2	7:K:533:ILE:HG12	1.99	0.45
5:I:111:DC:H2''	5:I:112:DT:H71	1.98	0.45
6:J:65:DC:H2''	6:J:66:DG:C8	2.52	0.45
7:K:261:LEU:HD12	7:K:262:ARG:N	2.31	0.45
2:B:73:THR:HG21	2:B:81:VAL:HG22	1.98	0.45
5:I:141:DA:H2'	5:I:142:DT:H71	1.98	0.45
6:J:88:DT:H2''	6:J:89:DT:C6	2.52	0.45
7:K:185:PHE:HZ	7:K:189:PRO:HB3	1.82	0.45
7:K:320:TYR:HE1	7:K:347:ASN:ND2	2.15	0.45
7:K:249:LEU:HB2	7:K:318:TRP:CZ3	2.52	0.44
5:I:60:DA:H2''	5:I:61:DA:C8	2.52	0.44
2:B:24:ASP:OD1	2:B:25:ASN:N	2.50	0.44
3:C:115:LEU:HD23	2:F:44:LYS:HB2	2.00	0.44
5:I:36:DC:H2''	5:I:37:DG:C8	2.52	0.44
7:K:417:VAL:N	7:K:418:GLU:CD	2.71	0.44
7:K:468:ILE:HG22	7:K:471:GLN:HE21	1.83	0.44
2:F:64:ASN:HB3	2:F:93:GLN:HE22	1.82	0.44
5:I:39:DA:H5''	5:I:39:DA:H8	1.83	0.44
7:K:729:LEU:HD12	7:K:729:LEU:HA	1.90	0.44
4:H:48:ASP:OD1	4:H:48:ASP:N	2.46	0.44
7:K:437:GLN:HE21	7:K:476:CYS:HA	1.83	0.44
7:K:598:SER:OG	7:K:625:ARG:NH1	2.50	0.44
3:C:92:GLU:HA	3:C:92:GLU:OE2	2.18	0.44
6:J:77:DC:H2''	6:J:78:DG:C8	2.53	0.44
7:K:242:GLU:OE1	7:K:244:ILE:HG13	2.18	0.44
4:H:73:GLU:OE2	4:H:76:ARG:NH2	2.50	0.44
5:I:113:DA:H2'	5:I:114:DG:H8	1.76	0.44
6:J:119:DT:H2''	6:J:120:DG:C8	2.53	0.44
7:K:347:ASN:OD1	7:K:348:ARG:N	2.50	0.44
7:K:711:LEU:HD12	7:K:714:LYS:HE3	1.99	0.44
1:E:85:GLN:NE2	2:F:82:THR:HG22	2.32	0.43
6:J:71:DA:H2''	6:J:72:DC:O5'	2.18	0.43
3:C:51:LEU:HD12	4:D:91:ILE:HD12	1.99	0.43
6:J:57:DT:H5'	6:J:57:DT:C6	2.53	0.43
7:K:235:LEU:HD23	7:K:235:LEU:HA	1.87	0.43
5:I:12:DC:H2'	5:I:13:DG:H8	1.79	0.43
1:E:82:LEU:HD23	1:E:82:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:117:GLY:O	7:K:120:LYS:HG2	2.17	0.43
7:K:296:PHE:CD2	7:K:299:VAL:HG13	2.54	0.43
5:I:29:DA:H2''	5:I:30:DA:C8	2.54	0.43
7:K:744:GLU:HA	7:K:748:GLN:HB2	2.01	0.43
6:J:28:DT:H2''	6:J:29:DG:C8	2.53	0.43
7:K:523:ILE:HA	7:K:594:VAL:O	2.19	0.43
7:K:617:GLN:HE22	7:K:620:GLN:H	1.66	0.43
3:C:16:THR:HA	6:J:30:DG:H5''	2.00	0.43
7:K:183:PHE:CE2	7:K:185:PHE:HB2	2.54	0.43
7:K:393:ASP:N	7:K:393:ASP:OD1	2.51	0.43
3:G:91:GLU:HG2	3:G:92:GLU:N	2.34	0.43
5:I:67:DG:H2''	5:I:68:DT:C7	2.49	0.43
7:K:108:ARG:NH1	7:K:214:LYS:O	2.51	0.43
7:K:603:GLN:O	7:K:607:GLN:HG2	2.19	0.43
2:F:31:LYS:HB3	2:F:32:PRO:HD3	2.01	0.42
5:I:66:DC:H2''	5:I:67:DG:C8	2.53	0.42
5:I:76:DG:H5'	5:I:76:DG:C8	2.54	0.42
7:K:220:ALA:HA	7:K:352:THR:O	2.19	0.42
7:K:319:GLU:CD	7:K:346:ARG:HE	2.22	0.42
7:K:580:ALA:O	7:K:611:ARG:NH2	2.51	0.42
2:F:75:HIS:HB2	4:H:93:THR:HG21	2.01	0.42
5:I:40:DG:H4'	5:I:41:DA:OP1	2.18	0.42
7:K:509:LYS:HB2	7:K:509:LYS:HE3	1.90	0.42
3:C:95:LYS:HE3	3:C:95:LYS:HB2	1.66	0.42
7:K:494:ASP:OD1	7:K:494:ASP:N	2.53	0.42
7:K:563:ASP:OD1	7:K:564:TYR:N	2.52	0.42
3:G:44:GLY:HA2	6:J:112:DG:H5'	2.02	0.42
2:F:18:HIS:O	2:F:18:HIS:ND1	2.52	0.42
5:I:26:DC:H2''	5:I:27:DT:H71	2.02	0.42
5:I:116:DC:C6	5:I:117:DT:H72	2.54	0.42
6:J:48:DC:H2''	6:J:49:DC:H6	1.85	0.42
7:K:557:ARG:O	7:K:561:ILE:HG12	2.19	0.42
7:K:560:ALA:HA	7:K:563:ASP:OD2	2.20	0.42
5:I:102:DG:H2''	5:I:103:DA:C8	2.55	0.42
6:J:11:DT:C2	6:J:12:DA:N7	2.88	0.42
7:K:540:PHE:CD2	7:K:541:ARG:HG2	2.55	0.42
3:G:29:ARG:NH2	4:H:32:GLU:OE1	2.52	0.42
7:K:250:VAL:HB	7:K:300:ILE:HG12	2.00	0.42
7:K:576:LEU:HD23	7:K:577:THR:O	2.20	0.42
7:K:579:ARG:NH2	7:K:601:ASN:OD1	2.52	0.42
7:K:118:LEU:HD21	7:K:384:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:65:DA:H2''	5:I:66:DC:O5'	2.20	0.41
5:I:139:DA:H1'	5:I:140:DC:H5'	2.01	0.41
6:J:49:DC:H2'	6:J:50:DT:H6	1.85	0.41
7:K:308:ARG:HA	7:K:308:ARG:HD3	1.87	0.41
7:K:318:TRP:HB3	7:K:321:ILE:HD11	2.02	0.41
7:K:508:ASP:OD1	7:K:537:TYR:OH	2.38	0.41
3:G:15:LYS:HB2	3:G:20:ARG:NH2	2.36	0.41
6:J:82:DG:H2'	6:J:83:DT:H71	2.02	0.41
7:K:424:LYS:HG2	7:K:621:VAL:HG21	2.02	0.41
4:H:87:THR:HG22	4:H:90:GLU:OE1	2.21	0.41
6:J:123:DC:H2''	6:J:124:DG:H8	1.85	0.41
7:K:83:PRO:HB3	7:K:295:ASP:OD1	2.20	0.41
3:G:65:LEU:HB3	3:G:86:ALA:HB1	2.02	0.41
6:J:16:DC:H2''	6:J:17:DT:C6	2.55	0.41
1:A:64:LYS:HB3	1:A:64:LYS:HE2	1.59	0.41
6:J:93:DC:H2''	6:J:94:DG:H8	1.85	0.41
7:K:298:VAL:HG12	7:K:300:ILE:HG13	2.03	0.41
7:K:434:SER:HB3	7:K:437:GLN:HB2	2.01	0.41
1:E:124:ILE:HD12	2:F:50:ILE:HD11	2.02	0.41
6:J:42:DT:O4	6:J:43:DA:N6	2.54	0.41
7:K:109:PHE:HE1	7:K:123:ILE:HG13	1.86	0.41
5:I:76:DG:H5'	5:I:76:DG:H8	1.86	0.41
6:J:12:DA:C2'	6:J:13:DT:H71	2.50	0.41
5:I:143:DC:H2''	5:I:144:DC:C6	2.56	0.41
7:K:268:THR:O	7:K:271:VAL:HG12	2.21	0.41
3:C:64:GLU:OE1	7:K:771:ARG:NH1	2.51	0.41
2:F:31:LYS:HG3	2:F:51:TYR:CZ	2.56	0.41
7:K:135:GLN:OE1	7:K:135:GLN:N	2.54	0.41
7:K:219:LEU:HD23	7:K:221:ASP:H	1.85	0.41
7:K:329:ILE:HG23	7:K:329:ILE:O	2.20	0.41
7:K:364:TRP:CH2	7:K:378:ALA:HB2	2.56	0.41
7:K:489:PRO:CD	7:K:490:PRO:HD2	2.51	0.41
5:I:59:DA:H2''	5:I:60:DA:C8	2.56	0.41
7:K:613:HIS:CD2	7:K:621:VAL:HG21	2.56	0.41
2:B:24:ASP:CG	2:B:26:ILE:HG22	2.42	0.40
6:J:9:DT:H2''	6:J:10:DA:C8	2.56	0.40
6:J:143:DT:H2''	6:J:144:DC:C6	2.56	0.40
7:K:648:GLN:O	7:K:652:GLN:HB2	2.21	0.40
5:I:77:DT:H2''	5:I:78:DC:C6	2.57	0.40
5:I:123:DC:H2''	5:I:124:DA:C8	2.57	0.40
6:J:48:DC:H2''	6:J:49:DC:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:58:DT:H6	6:J:58:DT:H2'	1.75	0.40
7:K:356:LEU:O	7:K:356:LEU:HD23	2.22	0.40
2:B:23:ARG:H	2:B:23:ARG:HG3	1.50	0.40
7:K:118:LEU:HD21	7:K:384:TRP:HZ2	1.87	0.40
1:A:50:GLU:HA	1:A:53:ARG:HG2	2.04	0.40
3:G:39:TYR:OH	4:H:68:GLU:OE2	2.36	0.40
7:K:419:THR:OG1	7:K:420:SER:N	2.50	0.40
7:K:509:LYS:HD2	7:K:708:LEU:HB3	2.03	0.40
7:K:601:ASN:HA	7:K:602:PRO:HD3	1.98	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	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
1	E	93/135 (69%)	91 (98%)	2 (2%)	0	100	100
2	B	86/102 (84%)	79 (92%)	7 (8%)	0	100	100
2	F	84/102 (82%)	80 (95%)	4 (5%)	0	100	100
3	C	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
3	G	105/129 (81%)	104 (99%)	1 (1%)	0	100	100
4	D	91/122 (75%)	85 (93%)	6 (7%)	0	100	100
4	H	91/122 (75%)	89 (98%)	2 (2%)	0	100	100
7	K	567/1061 (53%)	495 (87%)	70 (12%)	2 (0%)	30	66
All	All	1318/2037 (65%)	1220 (93%)	96 (7%)	2 (0%)	45	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	418	GLU
7	K	420	SER

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	84/110 (76%)	83 (99%)	1 (1%)	67	86
1	E	82/110 (74%)	82 (100%)	0	100	100
2	B	72/78 (92%)	72 (100%)	0	100	100
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	82/101 (81%)	82 (100%)	0	100	100
4	D	77/102 (76%)	76 (99%)	1 (1%)	65	85
4	H	79/102 (78%)	79 (100%)	0	100	100
7	K	530/958 (55%)	526 (99%)	4 (1%)	79	90
All	All	1154/1740 (66%)	1148 (100%)	6 (0%)	85	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
4	D	105	LYS
7	K	86	ASN
7	K	420	SER
7	K	655	ARG
7	K	714	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
7	K	613	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
9	ADP	K	1202	8	24,29,29	0.92	1 (4%)	29,45,45	1.37	3 (10%)

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
9	ADP	K	1202	8	-	7/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	1202	ADP	C5-C4	2.44	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	1202	ADP	PA-O3A-PB	-3.50	120.81	132.83
9	K	1202	ADP	N3-C2-N1	-2.90	124.15	128.68
9	K	1202	ADP	C4-C5-N7	-2.81	106.47	109.40

There are no chirality outliers.

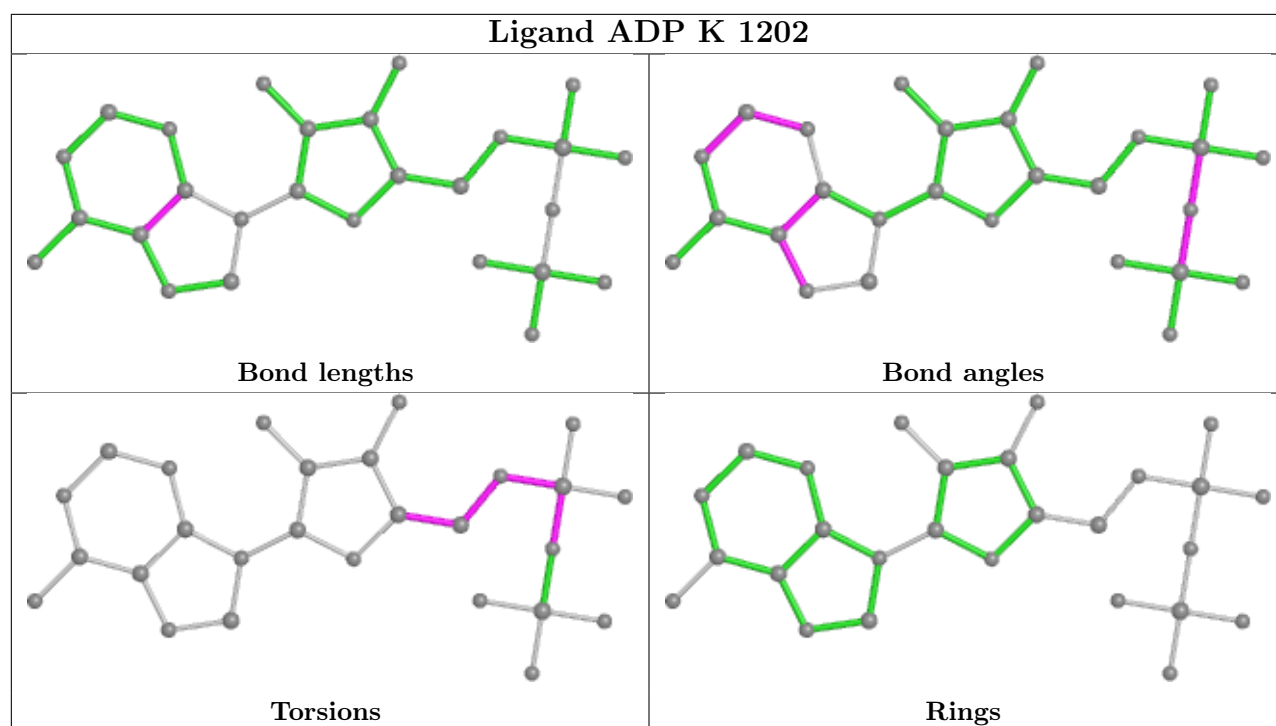
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	1202	ADP	PB-O3A-PA-O5'
9	K	1202	ADP	C5'-O5'-PA-O2A
9	K	1202	ADP	O4'-C4'-C5'-O5'
9	K	1202	ADP	C3'-C4'-C5'-O5'
9	K	1202	ADP	C5'-O5'-PA-O3A
9	K	1202	ADP	C5'-O5'-PA-O1A
9	K	1202	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

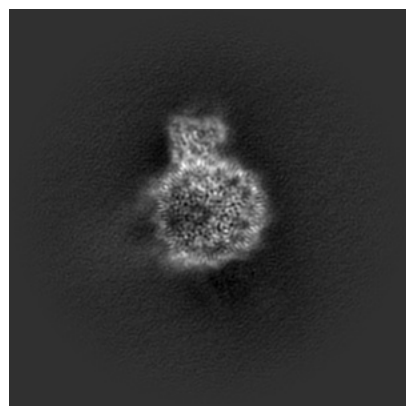
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61630. These allow visual inspection of the internal detail of the map and identification of artifacts.

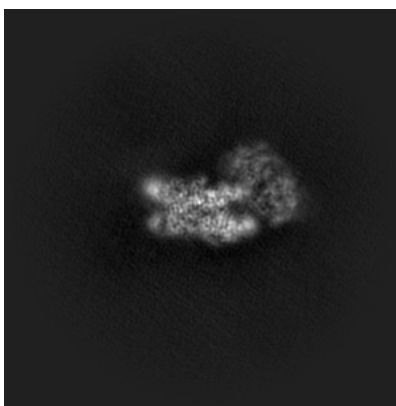
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

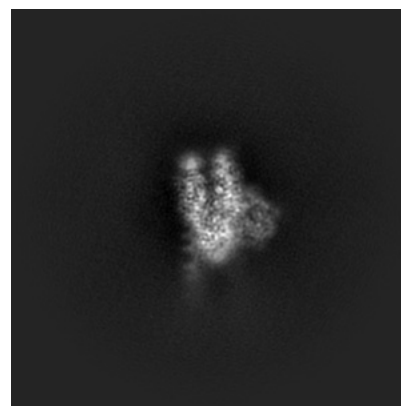
6.1.1 Primary map



X

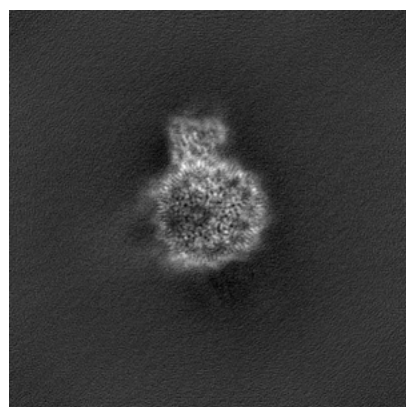


Y

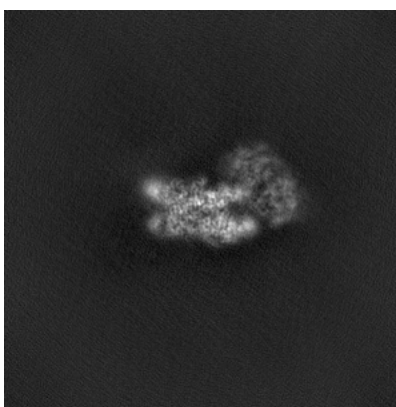


Z

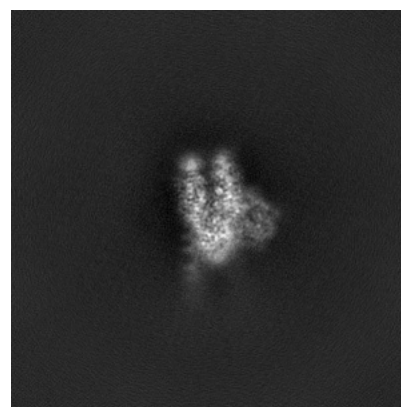
6.1.2 Raw map



X



Y

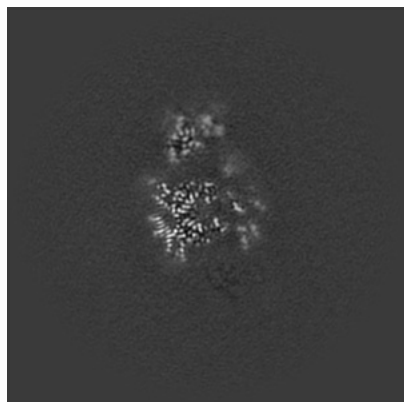


Z

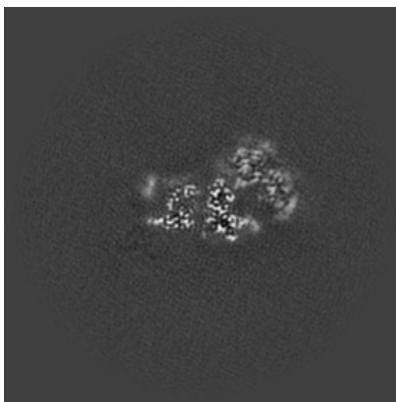
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

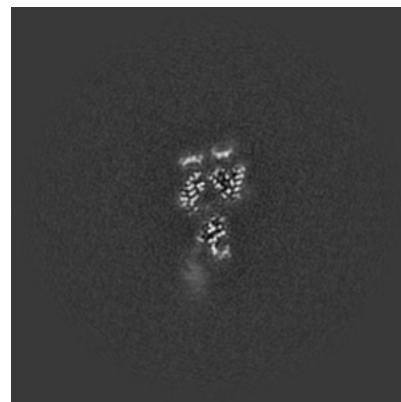
6.2.1 Primary map



X Index: 160

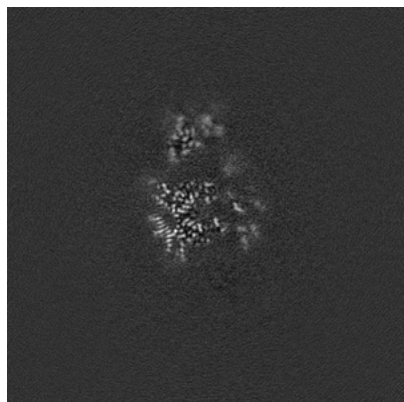


Y Index: 160

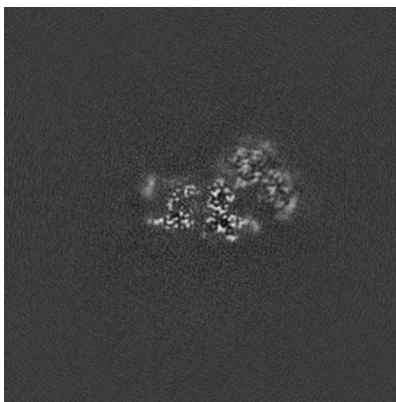


Z Index: 160

6.2.2 Raw map



X Index: 160



Y Index: 160

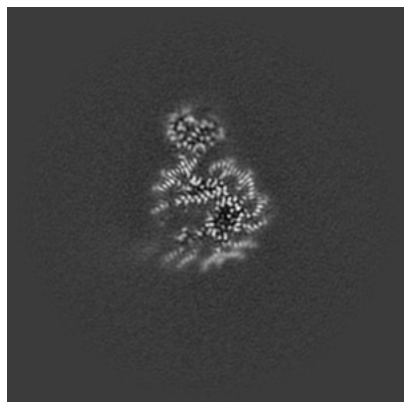


Z Index: 160

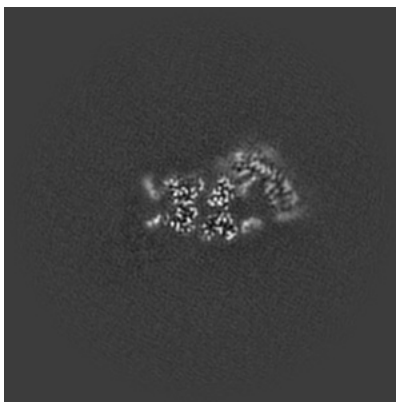
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

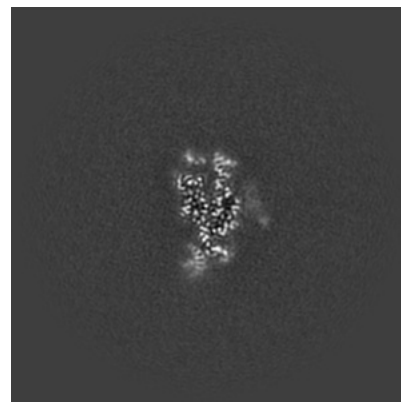
6.3.1 Primary map



X Index: 172

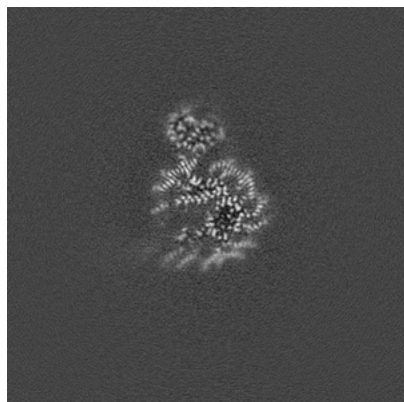


Y Index: 164

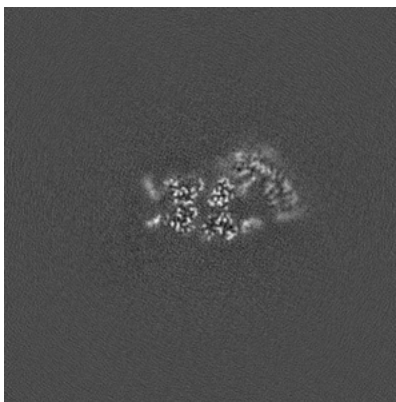


Z Index: 174

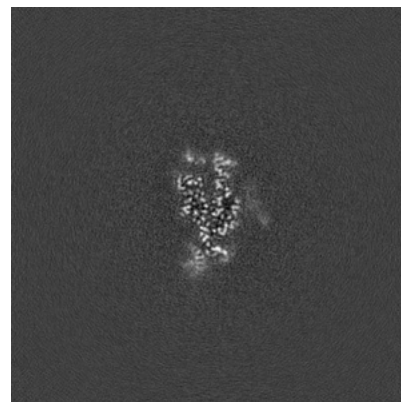
6.3.2 Raw map



X Index: 172



Y Index: 164

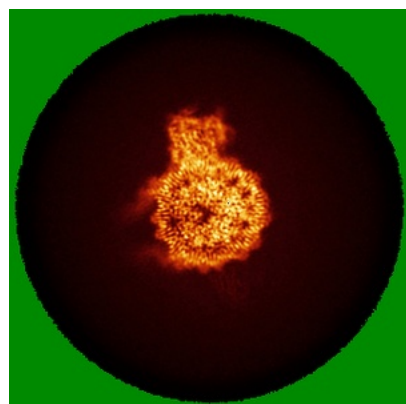


Z Index: 174

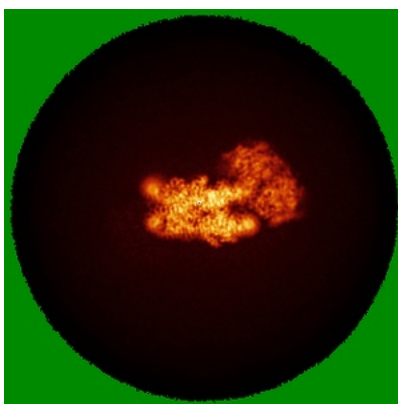
The images above show the largest variance slices of the map in three orthogonal directions.

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

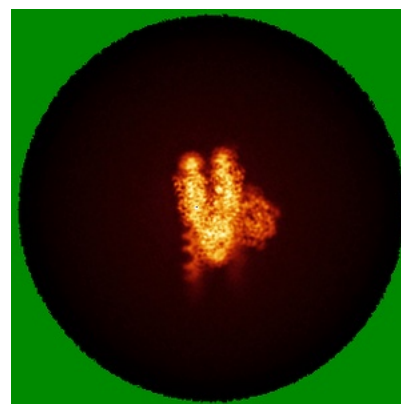
6.4.1 Primary map



X

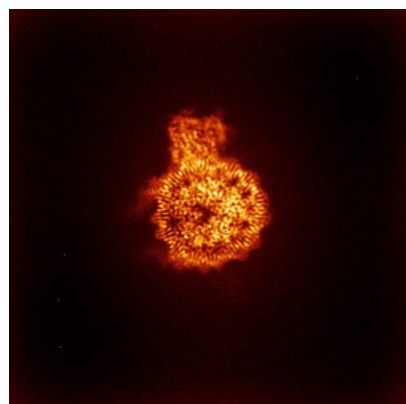


Y

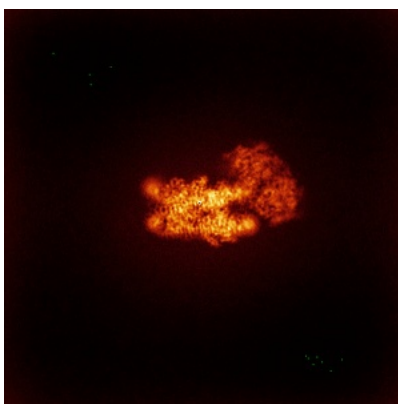


Z

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.

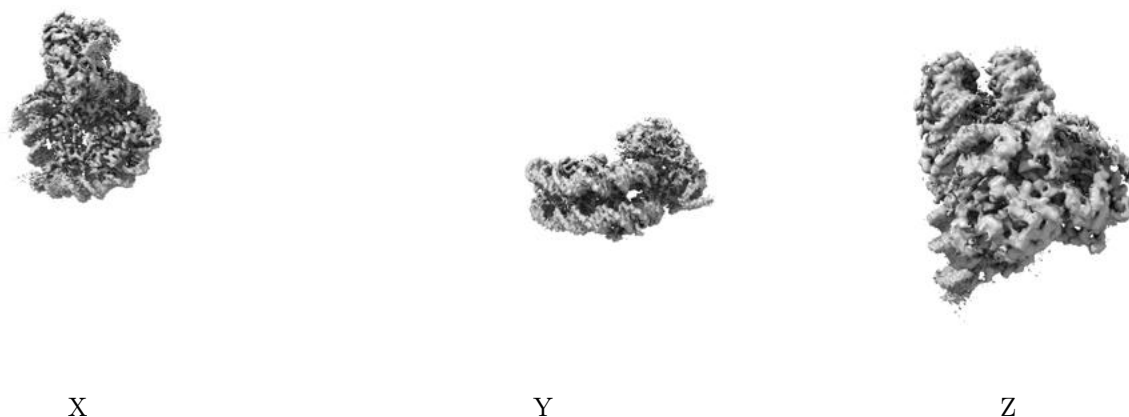
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.063. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

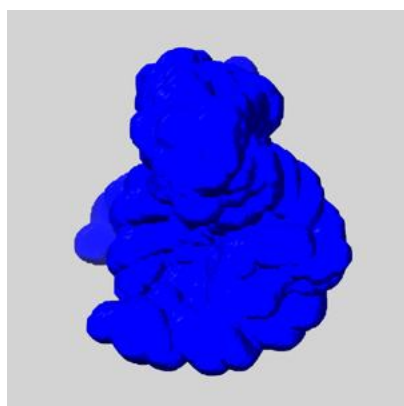
6.6 Mask visualisation [i](#)

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

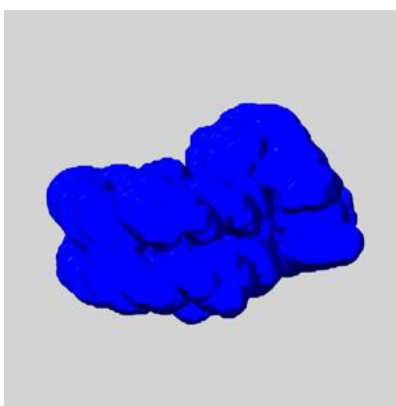
A mask typically either:

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

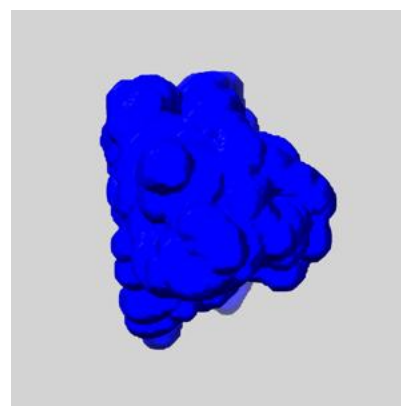
6.6.1 emd_61630_msk_1.map [i](#)



X



Y

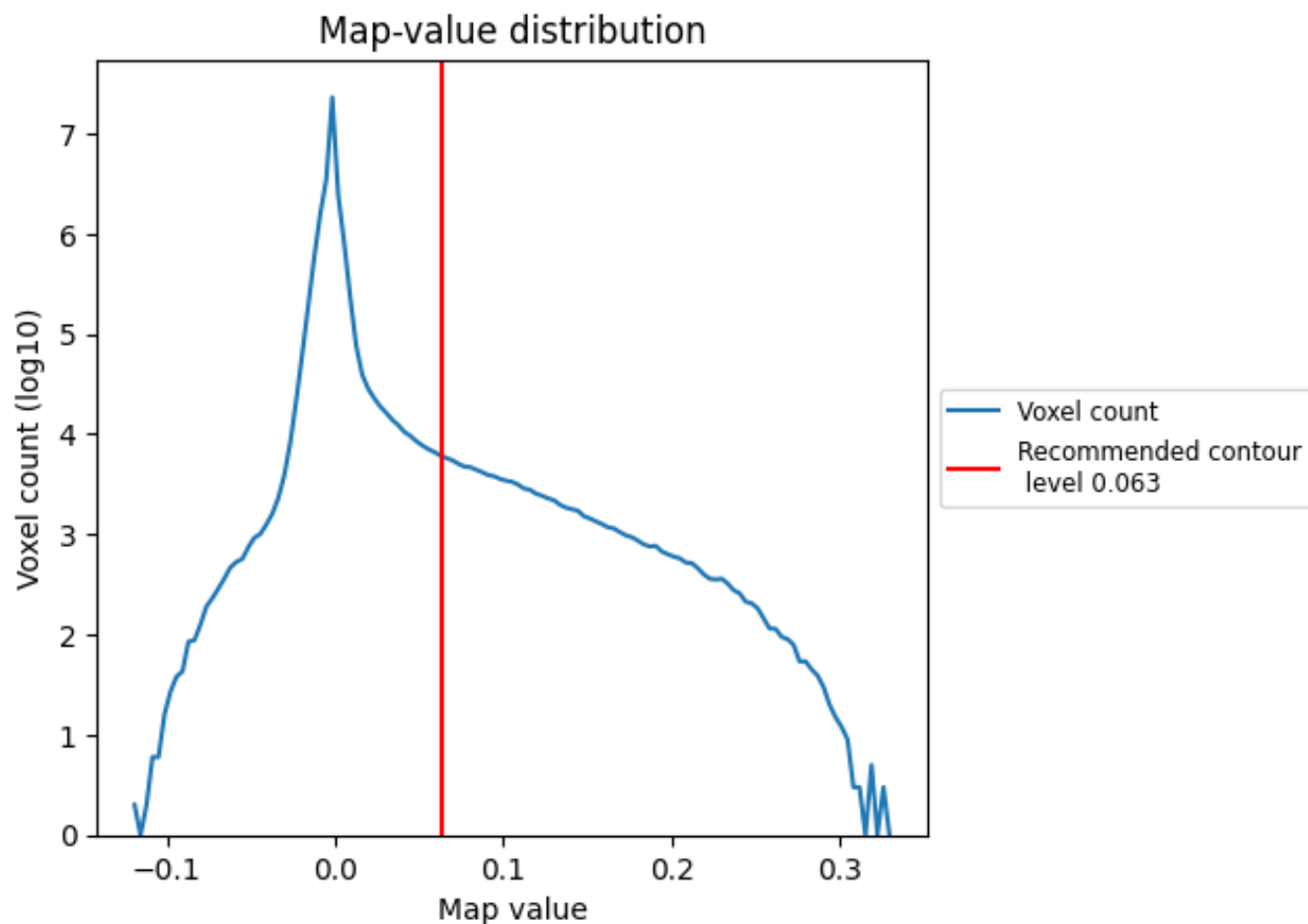


Z

7 Map analysis [i](#)

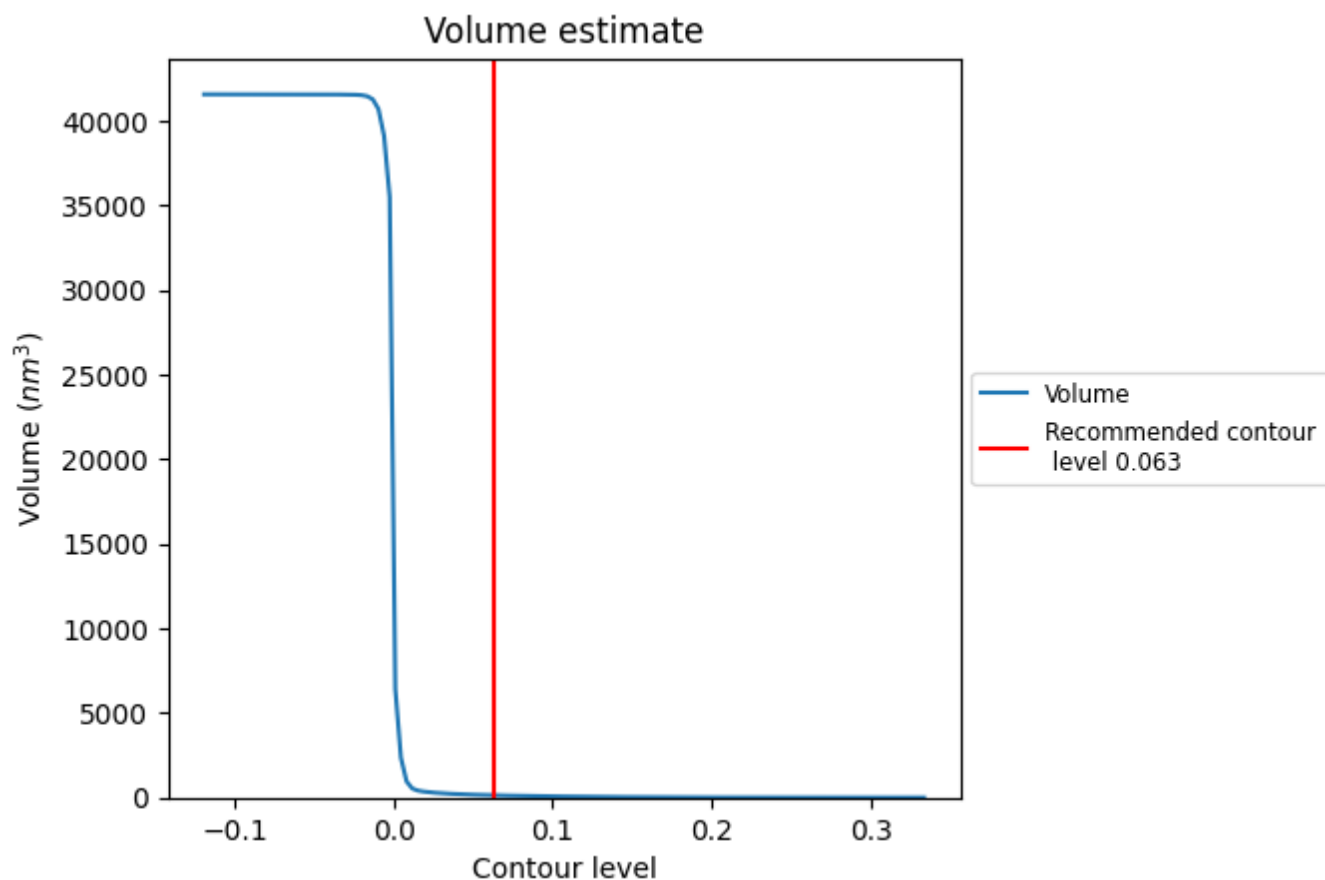
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

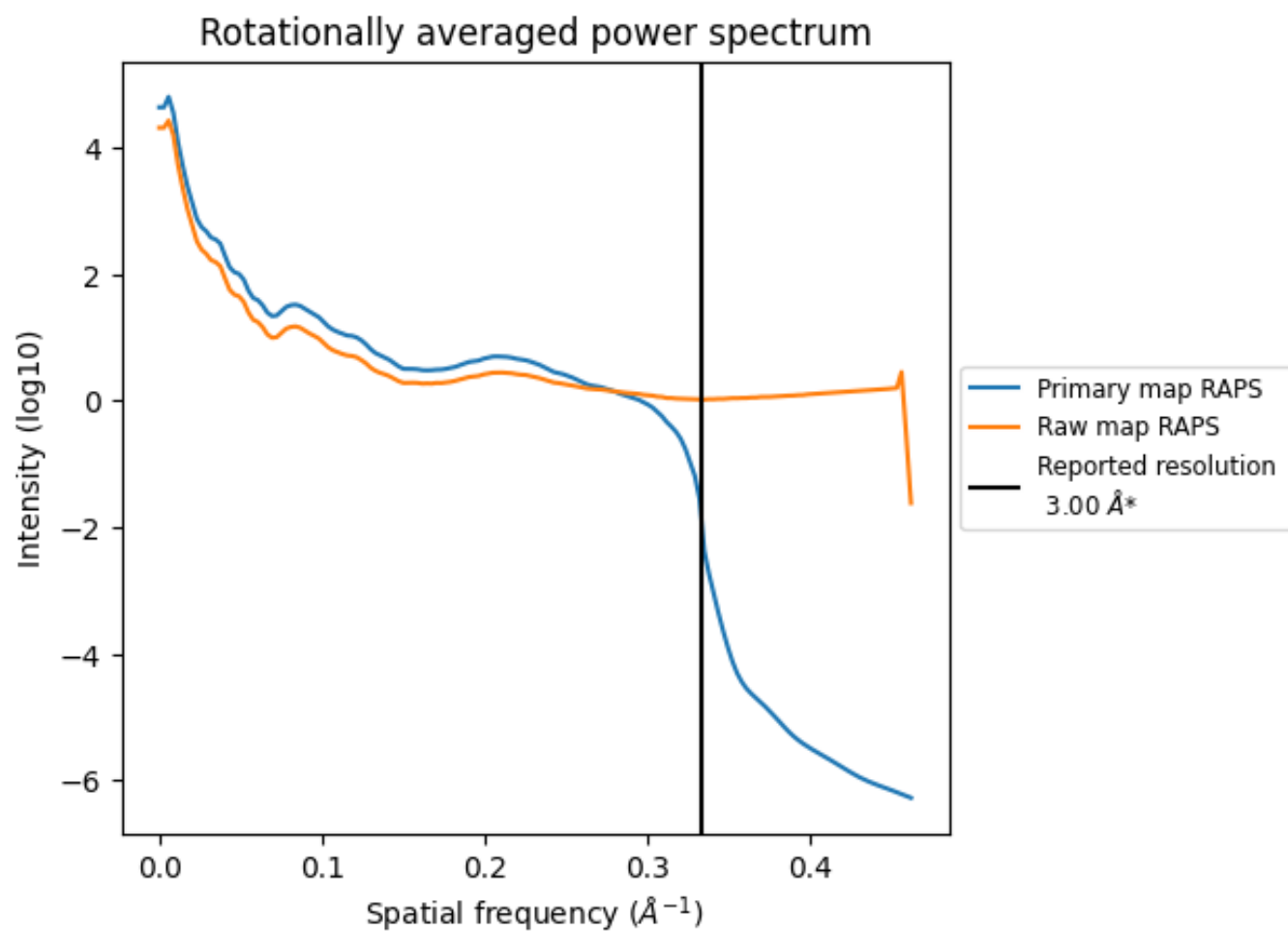
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 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 ⓘ

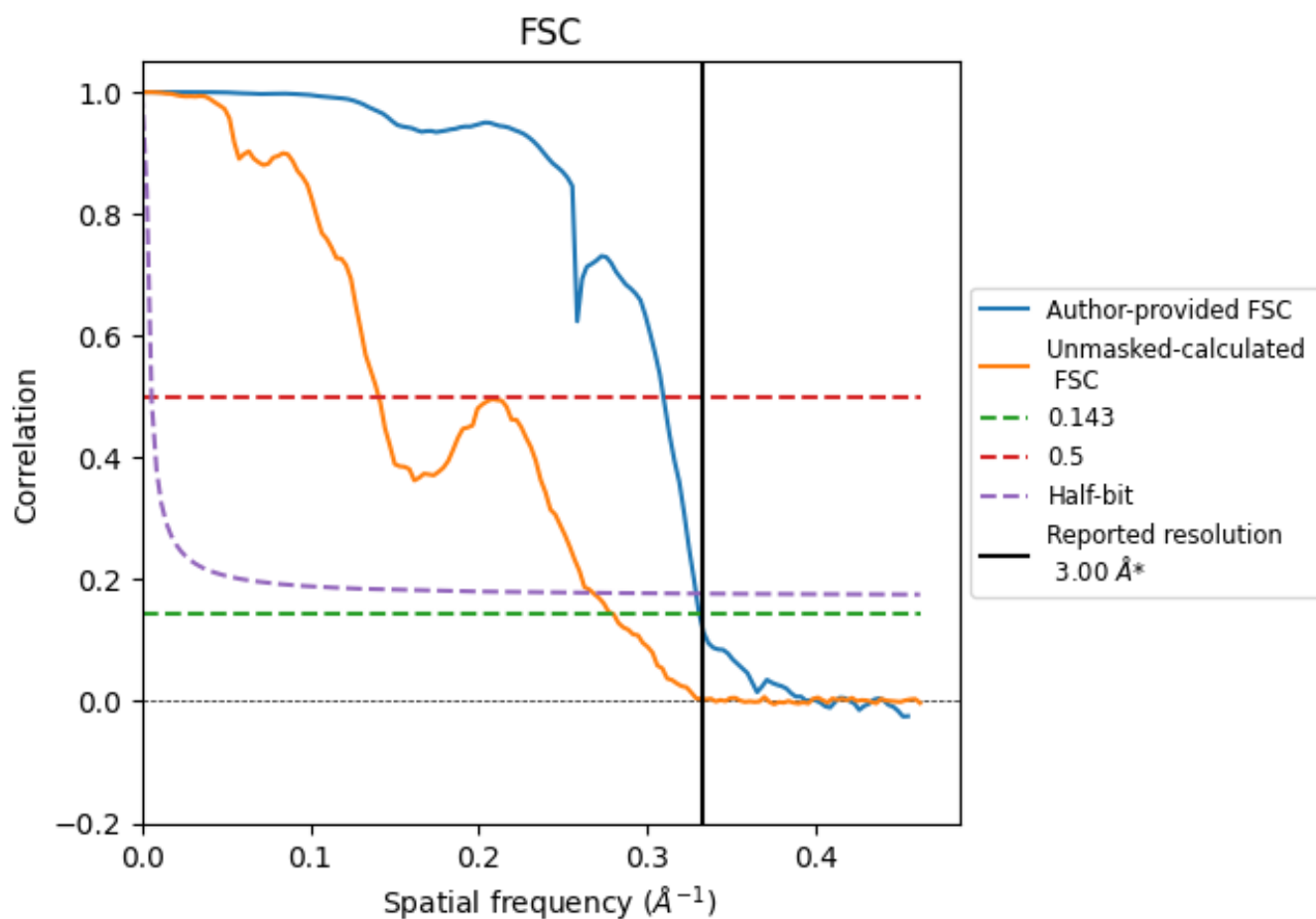


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

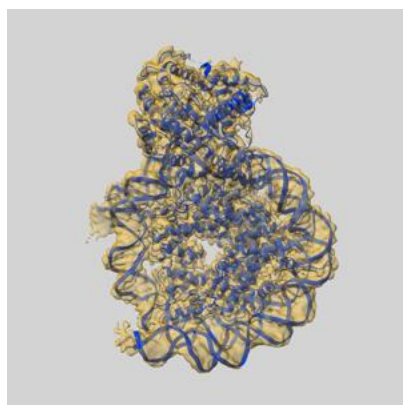
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.23	3.04
Unmasked-calculated*	3.57	7.12	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 3.0 by more than 10 %

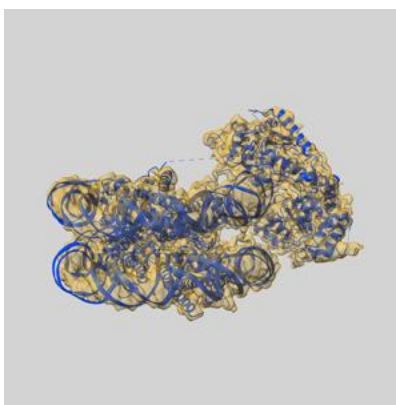
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61630 and PDB model 9JNX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

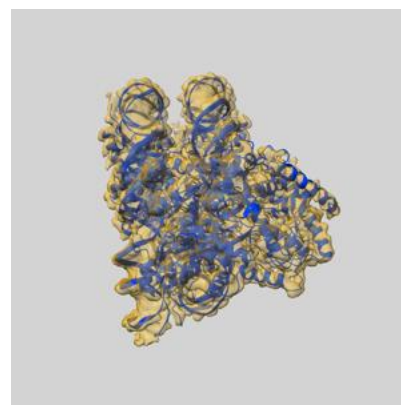
9.1 Map-model overlay [i](#)



X



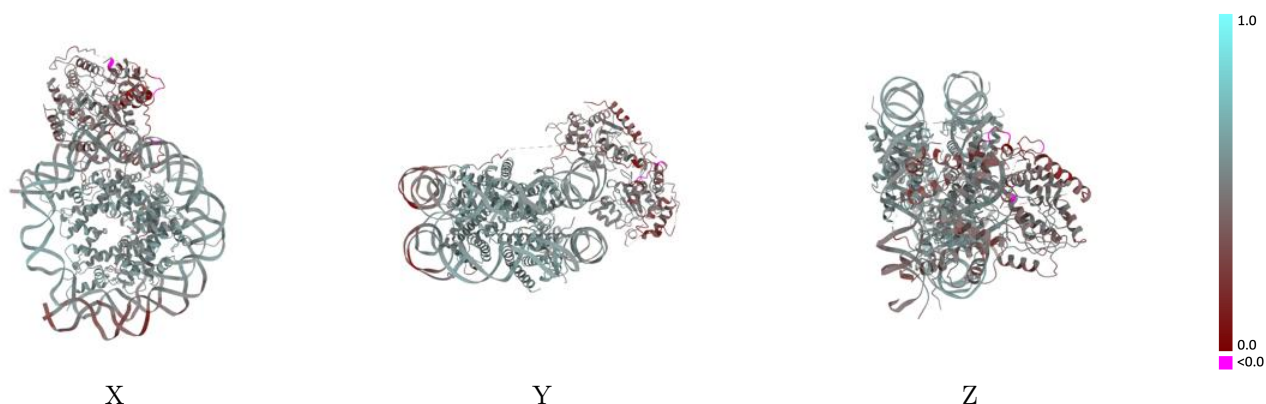
Y



Z

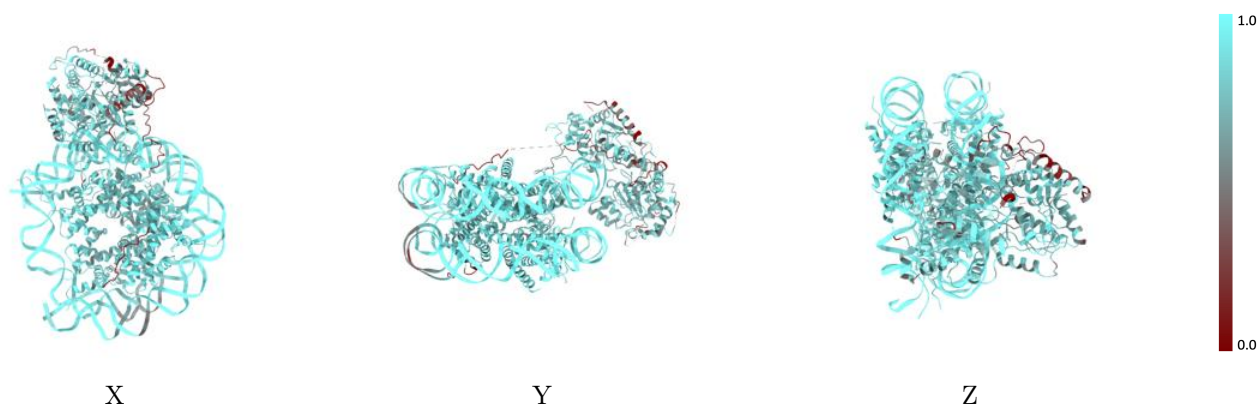
The images above show the 3D surface view of the map at the recommended contour level 0.063 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



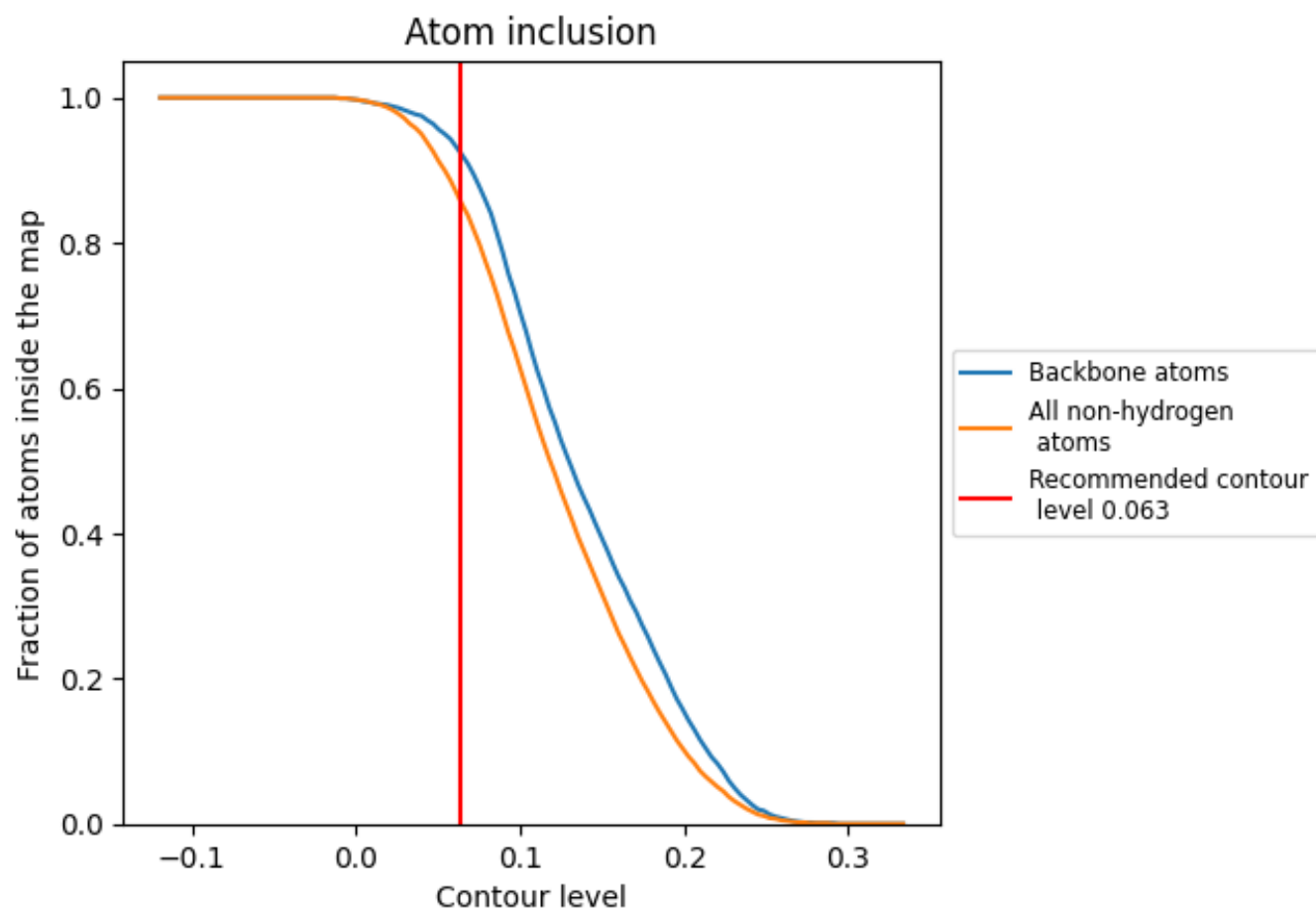
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.063).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.063) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8610	<div><div></div></div> 0.4970
A	<div><div></div></div> 0.9080	<div><div></div></div> 0.5570
B	<div><div></div></div> 0.9110	<div><div></div></div> 0.5570
C	<div><div></div></div> 0.9110	<div><div></div></div> 0.5650
D	<div><div></div></div> 0.9230	<div><div></div></div> 0.5520
E	<div><div></div></div> 0.8750	<div><div></div></div> 0.5580
F	<div><div></div></div> 0.8570	<div><div></div></div> 0.5430
G	<div><div></div></div> 0.9210	<div><div></div></div> 0.5640
H	<div><div></div></div> 0.9210	<div><div></div></div> 0.5500
I	<div><div></div></div> 0.9430	<div><div></div></div> 0.5120
J	<div><div></div></div> 0.9370	<div><div></div></div> 0.5070
K	<div><div></div></div> 0.7080	<div><div></div></div> 0.4060

1.0

0.0

<0.0