Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 01:32 PM JST

PDB ID	:	7X3W / pdb_00007x3w
EMDB ID	:	EMD-32995
Title	:	Cryo-EM structure of ISW1-N1 nucleosome
Authors	:	Lifei, L.; Kangjing, C.; Chen, Z.
Deposited on	:	2022-03-01
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

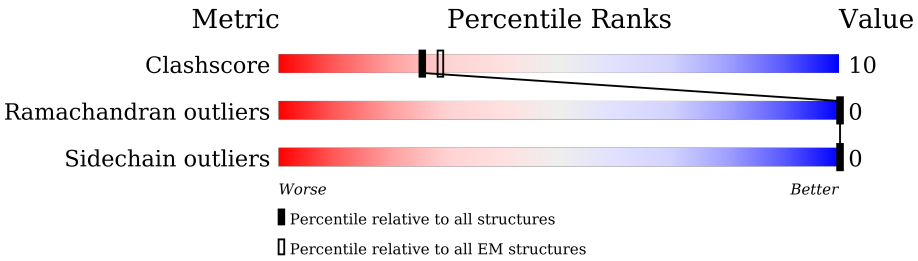
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

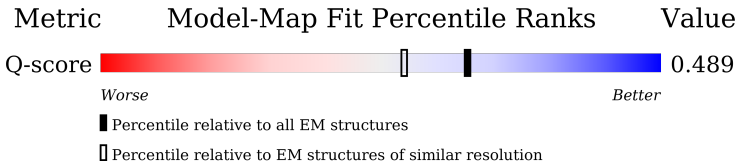
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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 <=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	63% 10% 28%
1	E	136	60% 10% 30%
2	B	103	7% 71% 15% 15%
2	F	103	70% 8% 22%

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Mol	Chain	Length	Quality of chain
3	C	130	77% 5% 18%
3	G	130	76% 6% 18%
4	D	126	59% 15% 26%
4	H	126	60% 13% 26%
5	I	147	61% 38%
6	J	146	71% 29%
7	K	1062	18% 28% 20% 53%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BEF	K	1202	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 16134 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
			Total	C	N	O	S		
1	A	98	801	506	153	139	3	0	0
1	E	95	779	492	148	136	3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	88	707	445	143	118	1	0	0
2	F	80	632	398	122	111	1	0	0

- Molecule 3 is a protein called Histone H2A.

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

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	93	717	450	128	137	2	0	0
4	H	93	725	456	130	137	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	146	2978	1414	542	876	146	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	146	3008	1424	562	876	146	0	0

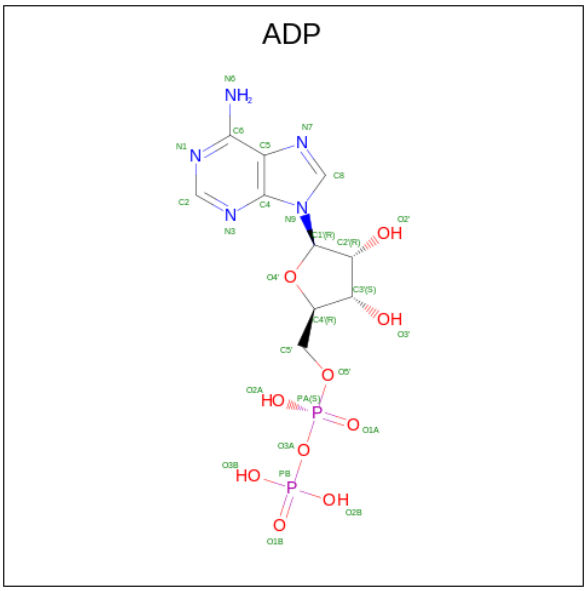
- Molecule 7 is a protein called ISWI chromatin-remodeling complex ATPase ISW1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	504	4129	2639	709	768	13	0	0

There is a discrepancy between the modelled and reference sequences:

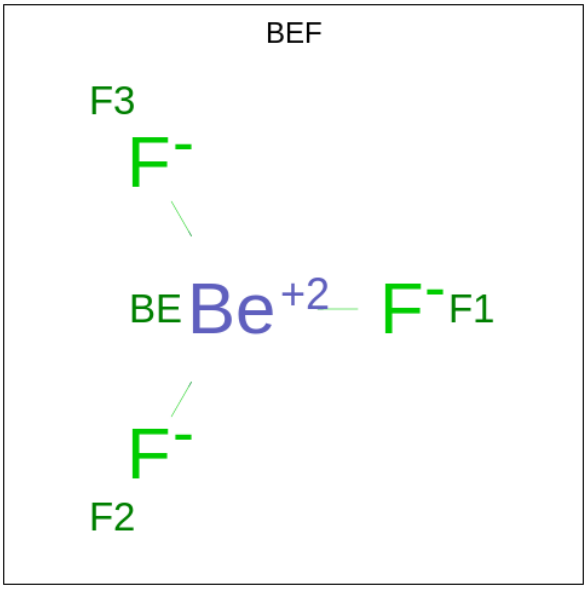
Chain	Residue	Modelled	Actual	Comment	Reference
K	68	MET	-	initiating methionine	UNP P38144

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
9	K	1	4	1	3	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

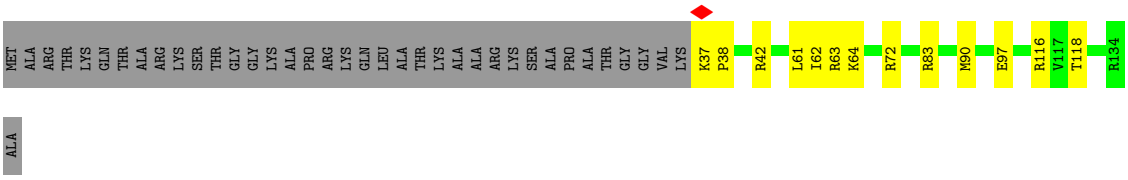
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	K	1	1	1	0

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.

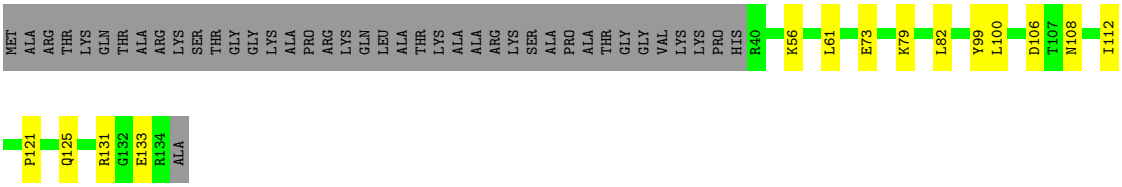
• Molecule 1: Histone H3

Chain A:



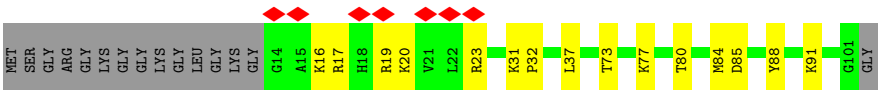
• Molecule 1: Histone H3

Chain E:



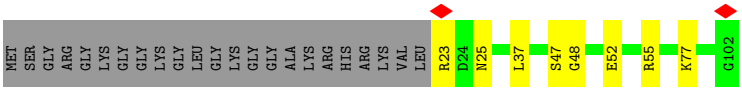
• Molecule 2: Histone H4

Chain B:



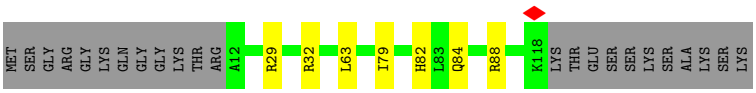
• Molecule 2: Histone H4

Chain F:



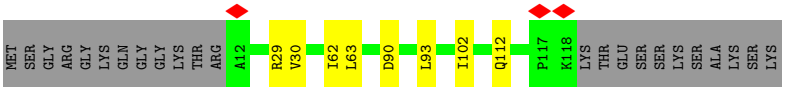
• Molecule 3: Histone H2A

Chain C:



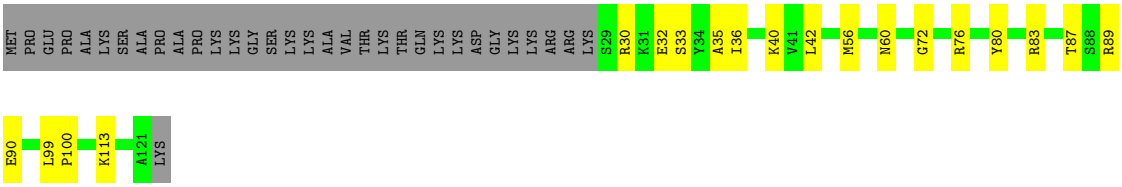
• Molecule 3: Histone H2A

Chain G:



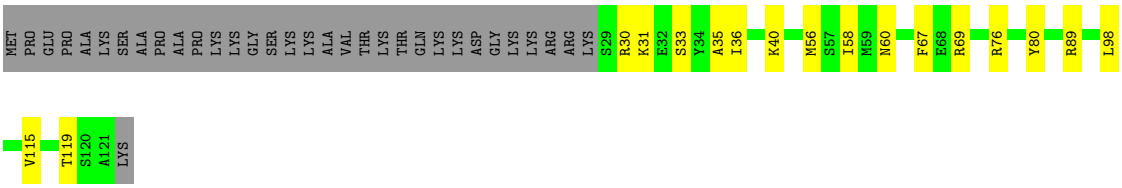
• Molecule 4: Histone H2B 1.1

Chain D:



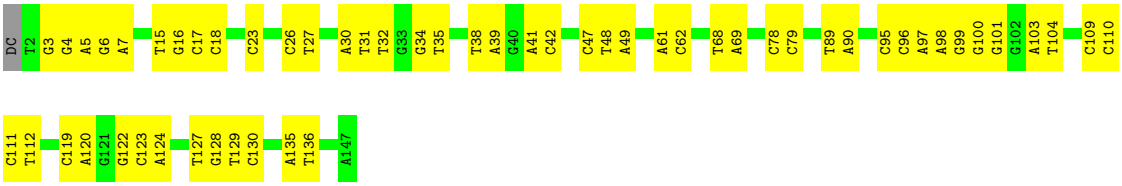
• Molecule 4: Histone H2B 1.1

Chain H:



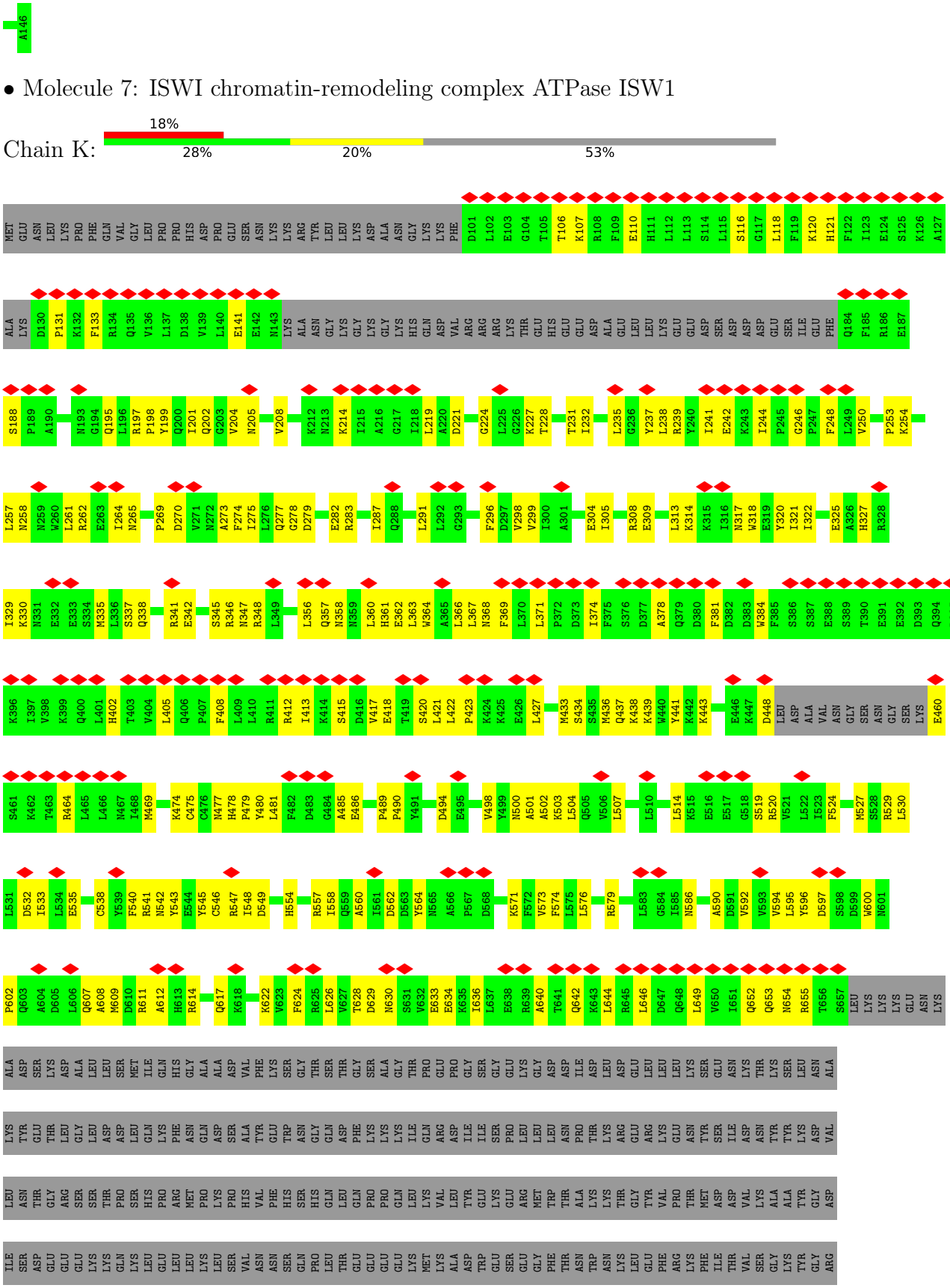
• Molecule 5: DNA (146-MER)

Chain I:



• Molecule 6: DNA (146-MER)

Chain J:


A146
• Molecule 7: ISWI chromatin-remodeling complex ATPase ISW1
Chain K:
18%
28%
20%
53%

ASN SER ILE GLN ALA ILE ALA ARG GLU LEU ALA PRO GLY LYS THR LEU GLU GLU VAL ARG ALA TYR ALA LYS ALA PHE TRP SER ASN ILE GLU ARG ILE GLU ASP TYR GLU LYS TYR LEU LYS ILE ILE GLU ASN GLU GLU GLU LYS ILE LYS ARG VAL LYS MET GLN GLN GLU ALA LEU

ARG ARG LYS LEU SER GLU TYR LYS ASN PRO PHE PHE ASP LEU LYS LEU LEU LYS HIS PRO PRO SER SER ASN ASN LYS ARG THR TYR SER GLU GLU GLU ASP ARG PHE ILE LEU LEU MET LEU PHE LYS TYR GLY LEU ASP ARG ASP ASP VAL TYR GLU LEU VAL ARG ASP GLU ILE ARG ASP

CYS PRO LEU PHE GLU LEU ASP PHE TYR PHE ARG SER ARG THR PRO VAL GLU LEU ALA ARG ARG GLY ASN THR LEU LEU GLN CYS LEU GLU LYS GLU PHE ASN ALA GLY ILE VAL LEU ASP ASP ALA THR LYS ASP ARG MET LYS LYS GLU ASP GLU ASN GLY LYS ARG ILE ARG GLU GLU

PHE ALA ASP GLN THR ALA ASN GLU LYS GLU ASN VAL ASP GLY VAL GLU SER LYS LYS ALA LYS ILE GLU ASP THR SER ASN VAL GLY THR GLU GLN LEU VAL ALA GLU LYS ILE PRO GLU ASN GLU THR THR HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69755	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.076	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	389.69998, 389.69998, 389.69998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.45	0/813	0.45	0/1093
1	E	0.46	0/789	0.50	0/1059
2	B	0.46	0/715	0.50	0/955
2	F	0.48	0/639	0.47	0/855
3	C	0.42	0/821	0.41	0/1112
3	G	0.41	0/825	0.43	0/1116
4	D	0.44	0/728	0.43	0/983
4	H	0.42	0/736	0.43	0/991
5	I	0.44	0/3337	0.46	0/5144
6	J	0.45	0/3377	0.45	0/5214
7	K	0.18	0/4207	0.43	0/5678
All	All	0.40	0/16987	0.45	0/24200

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	A	801	0	831	13	0
1	E	779	0	815	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	707	0	760	15	0
2	F	632	0	665	6	0
3	C	811	0	849	9	0
3	G	815	0	860	7	0
4	D	717	0	723	19	0
4	H	725	0	745	13	0
5	I	2978	0	1639	45	0
6	J	3008	0	1639	32	0
7	K	4129	0	4167	173	0
8	K	27	0	12	7	0
9	K	4	0	0	4	0
10	K	1	0	0	0	0
All	All	16134	0	13705	305	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (305) 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:314:LYS:NZ	7:K:342:GLU:O	2.10	0.83
5:I:99:DG:H2"	5:I:100:DG:C8	2.18	0.78
7:K:507:LEU:HD21	7:K:626:LEU:HD11	1.66	0.78
1:A:72:ARG:HD3	7:K:464:ARG:HH12	1.51	0.75
7:K:202:GLN:OE1	7:K:412:ARG:NH1	2.22	0.72
3:C:32:ARG:NH2	4:D:32:GLU:OE2	2.22	0.72
4:D:30:ARG:HH22	5:I:122:DG:H21	1.38	0.71
7:K:614:ARG:NH2	8:K:1201:ADP:O2B	2.20	0.71
7:K:195:GLN:NE2	8:K:1201:ADP:N1	2.41	0.69
7:K:371:LEU:HB3	7:K:374:ILE:HD12	1.75	0.68
7:K:443:LYS:HD3	7:K:460:GLU:HG2	1.73	0.68
7:K:614:ARG:NH2	9:K:1202:BEF:F2	2.17	0.68
7:K:600:TRP:HE1	7:K:636:ILE:HG12	1.58	0.68
5:I:135:DA:H2"	5:I:136:DT:H5"	1.75	0.67
7:K:413:ILE:HG22	7:K:415:SER:H	1.59	0.67
7:K:418:GLU:HB3	7:K:421:LEU:H	1.58	0.67
7:K:594:VAL:HG12	7:K:624:PHE:HB2	1.77	0.67
7:K:237:TYR:HD2	7:K:238:LEU:HD22	1.60	0.66
7:K:434:SER:HB3	7:K:437:GLN:HG2	1.77	0.66
7:K:633:GLU:HA	7:K:636:ILE:HD12	1.78	0.66
7:K:548:ILE:HD11	7:K:560:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:LYS:HB3	1:E:82:LEU:HD21	1.78	0.65
7:K:607:GLN:O	7:K:611:ARG:NH2	2.29	0.65
7:K:338:GLN:HA	7:K:341:ARG:HE	1.62	0.65
7:K:535:GLU:OE1	7:K:547:ARG:NH1	2.27	0.64
7:K:362:GLU:O	7:K:366:LEU:HD12	1.97	0.64
7:K:254:LYS:HA	7:K:257:LEU:HD13	1.79	0.63
7:K:248:PHE:HB2	7:K:298:VAL:HG22	1.81	0.63
7:K:546:CYS:HB3	7:K:560:ALA:HB1	1.80	0.63
7:K:547:ARG:NE	7:K:549:ASP:OD2	2.31	0.63
6:J:134:DC:H2"	6:J:135:DC:H5'	1.81	0.62
4:D:87:THR:N	4:D:90:GLU:OE1	2.24	0.62
7:K:277:GLN:HG3	7:K:554:HIS:CE1	2.34	0.62
6:J:50:DT:H2'	6:J:51:DT:H71	1.81	0.61
7:K:356:LEU:HD23	7:K:363:LEU:HD13	1.81	0.61
7:K:480:TYR:HA	7:K:485:ALA:HB3	1.81	0.61
7:K:361:HIS:HA	7:K:364:TRP:NE1	2.15	0.61
7:K:614:ARG:NH2	9:K:1202:BEF:F3	2.23	0.61
5:I:129:DT:H2"	5:I:130:DC:C5	2.37	0.60
7:K:361:HIS:HA	7:K:364:TRP:CD1	2.37	0.60
4:D:35:ALA:HA	4:D:56:MET:HE3	1.84	0.60
1:A:72:ARG:HD3	7:K:464:ARG:NH1	2.15	0.60
7:K:433:MET:HE1	7:K:438:LYS:HA	1.82	0.60
4:D:30:ARG:NH2	5:I:122:DG:H21	1.98	0.60
5:I:109:DC:H2"	5:I:110:DC:C5	2.36	0.60
7:K:434:SER:H	7:K:437:GLN:HE21	1.48	0.59
4:D:83:ARG:HG2	4:D:83:ARG:HH11	1.66	0.59
6:J:53:DG:H2'	6:J:54:DC:C6	2.38	0.59
6:J:62:DA:H1'	6:J:63:DC:H5'	1.85	0.59
7:K:287:ILE:HA	7:K:291:LEU:HB2	1.84	0.59
7:K:327:HIS:HA	7:K:330:LYS:NZ	2.17	0.58
7:K:224:GLY:N	9:K:1202:BEF:F2	2.25	0.58
1:A:42:ARG:HH21	6:J:69:DG:P	2.27	0.58
6:J:20:DC:H2"	6:J:21:DA:C8	2.38	0.58
5:I:96:DC:H2"	5:I:97:DA:H5"	1.85	0.58
7:K:227:LYS:NZ	8:K:1201:ADP:O1B	2.35	0.58
7:K:520:ARG:NE	7:K:571:LYS:O	2.36	0.58
6:J:123:DC:H2"	6:J:124:DG:C8	2.39	0.58
7:K:317:ASN:HB3	7:K:346:ARG:HH12	1.69	0.57
5:I:17:DC:H2"	5:I:18:DC:C5	2.39	0.57
7:K:228:THR:OG1	8:K:1201:ADP:O3B	2.12	0.57
7:K:338:GLN:HA	7:K:341:ARG:NE	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:TYR:OH	1:E:133:GLU:OE2	2.20	0.56
5:I:4:DG:H2"	5:I:5:DA:C8	2.40	0.56
7:K:246:GLY:H	7:K:248:PHE:HE2	1.53	0.56
7:K:325:GLU:O	7:K:327:HIS:N	2.39	0.56
5:I:95:DC:P	7:K:335:MET:H	2.29	0.56
7:K:278:GLY:O	7:K:283:ARG:NH1	2.39	0.56
7:K:514:LEU:HB3	7:K:519:SER:HB2	1.88	0.56
7:K:652:GLN:OE1	7:K:655:ARG:NH2	2.39	0.56
8:K:1201:ADP:O2B	9:K:1202:BEF:F3	2.14	0.56
2:B:16:LYS:HE3	2:B:19:ARG:HD3	1.88	0.56
7:K:564:TYR:CE1	7:K:574:PHE:HB2	2.41	0.55
7:K:422:LEU:HD12	7:K:423:PRO:HD2	1.88	0.55
2:B:17:ARG:NH2	7:K:486:GLU:OE2	2.40	0.55
7:K:356:LEU:HD22	7:K:363:LEU:HB2	1.89	0.54
7:K:364:TRP:HA	7:K:367:LEU:HB3	1.89	0.54
7:K:320:TYR:CE1	7:K:347:ASN:HB2	2.43	0.54
5:I:98:DA:H5"	7:K:600:TRP:CE3	2.42	0.54
7:K:405:LEU:HA	7:K:408:PHE:HB3	1.90	0.54
7:K:592:VAL:HG12	7:K:622:LYS:HB2	1.90	0.54
5:I:123:DC:H2"	5:I:124:DA:C8	2.44	0.53
6:J:12:DA:H2'	6:J:13:DT:H71	1.89	0.53
5:I:48:DT:H2"	5:I:49:DA:C8	2.44	0.53
7:K:262:ARG:NH2	7:K:562:ASP:OD2	2.42	0.53
1:E:73:GLU:OE1	2:F:23:ARG:N	2.41	0.53
4:H:31:LYS:HE2	4:H:31:LYS:HA	1.91	0.53
5:I:6:DG:H2"	5:I:7:DA:C8	2.43	0.53
5:I:89:DT:H2"	5:I:90:DA:C8	2.44	0.53
7:K:364:TRP:HB3	7:K:381:PHE:CD2	2.44	0.52
7:K:443:LYS:HA	7:K:448:ASP:HB2	1.91	0.52
7:K:360:LEU:O	7:K:364:TRP:HD1	1.93	0.52
7:K:345:SER:OG	7:K:347:ASN:O	2.24	0.52
1:E:106:ASP:OD1	1:E:131:ARG:NH2	2.38	0.52
1:E:121:PRO:O	1:E:125:GLN:HG3	2.08	0.52
7:K:524:PHE:CD2	7:K:608:ALA:HB1	2.44	0.52
5:I:95:DC:OP1	7:K:335:MET:N	2.43	0.52
2:B:16:LYS:O	2:B:19:ARG:NH2	2.41	0.51
7:K:649:LEU:O	7:K:653:GLN:HG2	2.10	0.51
7:K:538:CYS:O	7:K:542:ASN:N	2.43	0.51
1:A:72:ARG:HH11	7:K:464:ARG:HH12	1.58	0.51
7:K:273:ALA:HA	7:K:298:VAL:O	2.10	0.51
7:K:504:LEU:HD23	7:K:507:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:321:ILE:HG13	7:K:321:ILE:O	2.11	0.51
7:K:602:PRO:HB2	7:K:644:LEU:HD21	1.91	0.51
7:K:131:PRO:HG2	7:K:133:PHE:HD2	1.76	0.51
7:K:291:LEU:HD11	7:K:299:VAL:HG21	1.92	0.50
2:B:20:LYS:HD2	2:B:20:LYS:C	2.37	0.50
4:H:69:ARG:HB3	4:H:98:LEU:HD21	1.93	0.50
5:I:3:DG:H2'	5:I:4:DG:C8	2.46	0.50
6:J:94:DG:H2"	6:J:95:DG:O5'	2.10	0.50
7:K:221:ASP:OD1	7:K:412:ARG:NH2	2.44	0.50
5:I:119:DC:H2"	5:I:120:DA:N7	2.26	0.50
6:J:53:DG:OP1	7:K:474:LYS:NZ	2.27	0.50
6:J:56:DG:OP2	7:K:557:ARG:NH2	2.45	0.50
6:J:52:DG:H2"	6:J:53:DG:H8	1.77	0.49
5:I:15:DT:H2"	5:I:16:DG:C8	2.48	0.49
6:J:126:DC:H2"	6:J:127:DC:O5'	2.12	0.49
7:K:321:ILE:HG12	7:K:348:ARG:HG2	1.94	0.49
7:K:357:GLN:OE1	7:K:358:ASN:HB2	2.12	0.49
7:K:361:HIS:HA	7:K:364:TRP:HE1	1.76	0.49
7:K:258:ASN:ND2	7:K:558:ILE:HG12	2.28	0.49
7:K:341:ARG:HB3	7:K:369:PHE:HE1	1.76	0.49
7:K:548:ILE:HB	7:K:576:LEU:HD13	1.95	0.49
6:J:53:DG:H2'	6:J:54:DC:H6	1.76	0.49
7:K:545:TYR:HB3	7:K:573:VAL:HG23	1.95	0.49
3:C:32:ARG:HG2	3:C:32:ARG:HH11	1.78	0.49
7:K:481:LEU:HD22	7:K:529:ARG:HD3	1.93	0.49
7:K:118:LEU:HD11	7:K:384:TRP:HH2	1.77	0.48
7:K:503:LYS:HD2	7:K:596:TYR:CZ	2.49	0.48
4:H:35:ALA:HA	4:H:56:MET:HE1	1.94	0.48
6:J:54:DC:H2"	6:J:55:DG:C8	2.48	0.48
7:K:434:SER:HB2	7:K:502:ALA:HB2	1.94	0.48
7:K:478:HIS:NE2	7:K:480:TYR:HD2	2.11	0.48
3:G:102:ILE:HG23	4:H:58:ILE:HD13	1.96	0.48
2:B:20:LYS:NZ	2:B:23:ARG:HD2	2.29	0.48
7:K:413:ILE:HD11	7:K:655:ARG:NE	2.28	0.48
7:K:237:TYR:CD1	7:K:241:ILE:HD13	2.48	0.48
5:I:68:DT:H2"	5:I:69:DA:N7	2.29	0.48
6:J:49:DC:H2"	6:J:50:DT:H72	1.96	0.48
7:K:199:TYR:CD1	7:K:417:VAL:HG11	2.49	0.48
7:K:242:GLU:O	7:K:244:ILE:HG13	2.14	0.48
7:K:480:TYR:OH	7:K:500:ASN:OD1	2.32	0.47
6:J:60:DA:H2"	6:J:61:DA:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:364:TRP:CZ3	7:K:378:ALA:HA	2.49	0.47
1:A:42:ARG:NH2	6:J:69:DG:OP1	2.46	0.47
4:H:33:SER:HB2	4:H:60:ASN:ND2	2.28	0.47
4:H:36:ILE:O	4:H:40:LYS:HG3	2.15	0.47
7:K:227:LYS:O	7:K:231:THR:HG23	2.15	0.47
7:K:257:LEU:HD23	7:K:275:ILE:HG23	1.96	0.47
7:K:548:ILE:HD12	7:K:557:ARG:HA	1.96	0.47
3:C:84:GLN:HE21	3:C:88:ARG:HG3	1.80	0.47
5:I:128:DG:H2"	5:I:129:DT:C6	2.50	0.47
3:C:63:LEU:HD22	4:D:42:LEU:HD13	1.97	0.47
7:K:279:ASP:HB2	7:K:282:GLU:OE1	2.15	0.47
7:K:262:ARG:HH22	7:K:562:ASP:CG	2.23	0.47
2:B:77:LYS:HZ1	4:D:89:ARG:CZ	2.27	0.46
5:I:100:DG:H2"	5:I:101:DG:C8	2.51	0.46
1:E:56:LYS:HE3	1:E:56:LYS:HB2	1.63	0.46
7:K:221:ASP:OD2	7:K:412:ARG:N	2.48	0.46
7:K:418:GLU:C	7:K:420:SER:H	2.22	0.46
2:F:47:SER:OG	2:F:48:GLY:N	2.49	0.46
5:I:23:DC:H6	5:I:23:DC:H5'	1.80	0.46
5:I:97:DA:H2"	5:I:98:DA:H5'	1.97	0.46
7:K:595:LEU:HD11	7:K:609:MET:SD	2.56	0.46
4:D:36:ILE:O	4:D:40:LYS:HG3	2.16	0.46
1:E:108:ASN:O	1:E:112:ILE:HG13	2.16	0.46
1:A:83:ARG:O	2:B:80:THR:HA	2.16	0.46
7:K:586:ASN:CG	7:K:614:ARG:HE	2.24	0.46
7:K:586:ASN:ND2	8:K:1201:ADP:H4'	2.31	0.46
3:C:32:ARG:HD3	6:J:30:DG:OP2	2.15	0.46
7:K:188:SER:HB2	7:K:201:ILE:HD11	1.98	0.46
7:K:313:LEU:HD22	7:K:318:TRP:HZ2	1.81	0.46
5:I:78:DC:H2"	5:I:79:DC:C5	2.50	0.46
4:D:72:GLY:O	4:D:76:ARG:HG3	2.16	0.45
7:K:498:VAL:HG23	7:K:504:LEU:HB3	1.98	0.45
7:K:530:LEU:HD11	7:K:596:TYR:CE2	2.51	0.45
7:K:478:HIS:NE2	7:K:480:TYR:HB2	2.31	0.45
7:K:541:ARG:NH2	7:K:543:TYR:OH	2.40	0.45
5:I:99:DG:H2"	5:I:100:DG:H8	1.76	0.45
3:C:63:LEU:HD23	3:C:63:LEU:HA	1.83	0.45
3:C:32:ARG:HG2	3:C:32:ARG:NH1	2.31	0.45
7:K:494:ASP:HA	7:K:540:PHE:CE1	2.52	0.45
7:K:437:GLN:OE1	7:K:479:PRO:HG3	2.17	0.45
6:J:3:DA:H2"	6:J:4:DG:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:341:ARG:CZ	7:K:369:PHE:HZ	2.28	0.45
7:K:250:VAL:HA	7:K:322:ILE:HB	1.98	0.45
2:B:84:MET:HE2	2:B:88:TYR:CZ	2.52	0.45
7:K:329:ILE:HD12	7:K:337:SER:HB3	1.97	0.45
7:K:364:TRP:HE3	7:K:368:ASN:HD21	1.58	0.45
4:D:83:ARG:HG2	4:D:83:ARG:NH1	2.31	0.45
7:K:121:HIS:CE1	7:K:384:TRP:HE1	2.35	0.45
7:K:586:ASN:HB2	7:K:614:ARG:HH11	1.82	0.44
2:F:77:LYS:HE3	4:H:89:ARG:CZ	2.47	0.44
5:I:38:DT:H2"	5:I:39:DA:N7	2.32	0.44
7:K:642:GLN:O	7:K:646:LEU:HG	2.18	0.44
6:J:89:DT:H2"	6:J:90:DA:C8	2.52	0.44
1:A:64:LYS:HE3	1:A:90:MET:HE1	2.00	0.44
5:I:103:DA:H2'	5:I:104:DT:H71	1.98	0.44
7:K:413:ILE:HD11	7:K:655:ARG:CZ	2.47	0.44
7:K:107:LYS:HD2	7:K:214:LYS:HZ2	1.82	0.44
1:A:83:ARG:HD3	6:J:50:DT:H4'	2.00	0.44
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.53	0.44
4:H:115:VAL:O	4:H:119:THR:HG23	2.18	0.44
1:E:61:LEU:HD12	2:F:37:LEU:HD23	2.00	0.44
6:J:81:DC:H2"	6:J:82:DG:C8	2.52	0.44
7:K:278:GLY:HA3	7:K:282:GLU:HB2	2.00	0.44
3:C:29:ARG:NH1	4:D:33:SER:O	2.51	0.43
7:K:327:HIS:O	7:K:330:LYS:HD3	2.18	0.43
7:K:436:MET:HE2	7:K:500:ASN:HB3	1.99	0.43
3:G:112:GLN:HA	3:G:112:GLN:OE1	2.17	0.43
6:J:57:DT:H4'	7:K:308:ARG:NH2	2.32	0.43
5:I:6:DG:H2"	5:I:7:DA:H8	1.82	0.43
7:K:317:ASN:HB3	7:K:346:ARG:NH1	2.33	0.43
7:K:427:LEU:HD22	7:K:624:PHE:HE1	1.81	0.43
7:K:402:HIS:ND1	7:K:654:ASN:HA	2.33	0.43
7:K:478:HIS:CD2	7:K:480:TYR:H	2.36	0.43
3:G:30:VAL:HG13	4:H:67:PHE:HE1	1.83	0.43
3:G:62:ILE:HG12	3:G:93:LEU:HD13	2.00	0.43
3:G:90:ASP:OD2	3:G:90:ASP:C	2.62	0.43
5:I:111:DC:H2"	5:I:112:DT:H72	2.01	0.43
7:K:204:VAL:O	7:K:208:VAL:HG13	2.18	0.43
7:K:418:GLU:HG3	7:K:421:LEU:HD13	2.01	0.43
5:I:98:DA:H5"	7:K:600:TRP:CZ3	2.53	0.43
6:J:16:DC:H2"	6:J:17:DT:C6	2.54	0.43
7:K:520:ARG:HB3	7:K:590:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:111:DC:H2"	6:J:112:DG:C8	2.54	0.43
5:I:30:DA:C8	5:I:31:DT:H72	2.54	0.43
5:I:41:DA:H1'	5:I:42:DC:H5'	2.01	0.43
7:K:611:ARG:NE	7:K:611:ARG:HA	2.33	0.43
7:K:640:ALA:O	7:K:644:LEU:HG	2.18	0.43
2:F:52:GLU:OE1	2:F:55:ARG:NH1	2.52	0.42
6:J:54:DC:H1'	7:K:579:ARG:HH21	1.84	0.42
2:B:73:THR:OG1	2:B:85:ASP:OD2	2.28	0.42
7:K:116:SER:C	7:K:118:LEU:H	2.26	0.42
1:E:100:LEU:HD23	1:E:100:LEU:HA	1.90	0.42
5:I:4:DG:H2"	5:I:5:DA:H8	1.81	0.42
5:I:17:DC:H2"	5:I:18:DC:C6	2.55	0.42
5:I:31:DT:C2'	5:I:32:DT:H71	2.49	0.42
5:I:127:DT:H2"	5:I:128:DG:C8	2.55	0.42
7:K:197:ARG:HB3	7:K:198:PRO:HD2	2.01	0.42
7:K:274:PHE:CE2	7:K:296:PHE:HB3	2.55	0.42
5:I:98:DA:H1'	7:K:469:MET:HE1	2.00	0.42
7:K:629:ASP:OD1	7:K:630:ASN:N	2.52	0.42
7:K:630:ASN:N	7:K:634:GLU:OE2	2.47	0.42
7:K:106:THR:O	7:K:110:GLU:HG3	2.20	0.42
7:K:219:LEU:HD21	7:K:227:LYS:HB2	2.01	0.42
6:J:94:DG:H2"	6:J:95:DG:C5'	2.50	0.42
7:K:205:ASN:HA	7:K:208:VAL:HG22	2.01	0.42
7:K:227:LYS:HG2	8:K:1201:ADP:O1B	2.19	0.42
7:K:532:ASP:HA	7:K:547:ARG:HH12	1.83	0.42
5:I:26:DC:H2"	5:I:27:DT:H71	2.02	0.42
7:K:529:ARG:O	7:K:533:ILE:HG13	2.20	0.42
4:H:33:SER:HB2	4:H:60:ASN:HD21	1.84	0.42
7:K:118:LEU:HD21	7:K:384:TRP:CH2	2.55	0.42
7:K:305:ILE:O	7:K:309:GLU:HG2	2.19	0.42
7:K:433:MET:SD	7:K:437:GLN:HG3	2.60	0.42
7:K:441:TYR:HD1	7:K:475:CYS:SG	2.43	0.42
1:A:37:LYS:HA	1:A:38:PRO:HD3	1.96	0.42
4:H:30:ARG:NH2	6:J:122:DG:H21	2.17	0.42
5:I:34:DG:H2'	5:I:35:DT:C6	2.54	0.42
7:K:118:LEU:HD11	7:K:384:TRP:CH2	2.55	0.42
7:K:612:ALA:O	7:K:617:GLN:NE2	2.52	0.42
1:A:116:ARG:NH1	1:A:118:THR:O	2.53	0.41
5:I:47:DC:H2"	5:I:48:DT:H71	2.02	0.41
7:K:232:ILE:O	7:K:235:LEU:HG	2.19	0.41
7:K:318:TRP:HB2	7:K:345:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:341:ARG:HB3	7:K:369:PHE:CE1	2.53	0.41
5:I:34:DG:H2"	5:I:35:DT:H5'	2.01	0.41
6:J:65:DC:H2"	6:J:66:DG:C8	2.56	0.41
7:K:520:ARG:HH21	7:K:571:LYS:HB2	1.85	0.41
1:E:73:GLU:OE2	2:F:25:ASN:HB2	2.20	0.41
7:K:131:PRO:HG2	7:K:133:PHE:CD2	2.55	0.41
7:K:433:MET:HB2	7:K:628:THR:CG2	2.51	0.41
7:K:439:LYS:O	7:K:443:LYS:HG3	2.19	0.41
1:A:61:LEU:HD12	2:B:37:LEU:HD23	2.01	0.41
2:B:88:TYR:CE1	4:D:80:TYR:CZ	3.08	0.41
6:J:27:DC:H2"	6:J:28:DT:C5	2.54	0.41
7:K:261:LEU:HA	7:K:264:ILE:HG22	2.02	0.41
5:I:61:DA:H1'	5:I:62:DC:H5'	2.03	0.41
7:K:304:GLU:OE1	7:K:304:GLU:N	2.42	0.41
7:K:489:PRO:HD2	7:K:490:PRO:HD2	2.02	0.41
7:K:501:ALA:HB3	7:K:504:LEU:HD12	2.02	0.41
7:K:239:ARG:NH2	7:K:270:ASP:HB3	2.35	0.41
2:B:31:LYS:HB3	2:B:32:PRO:HD3	2.03	0.41
2:B:88:TYR:CD1	4:D:80:TYR:CZ	3.08	0.41
4:D:113:LYS:HB3	4:D:113:LYS:HE3	1.90	0.41
2:B:91:LYS:NZ	4:D:76:ARG:NH2	2.69	0.41
4:D:99:LEU:HA	4:D:100:PRO:HD3	1.83	0.41
3:G:29:ARG:NH1	4:H:33:SER:O	2.54	0.41
7:K:235:LEU:HD11	7:K:264:ILE:HD11	2.03	0.41
7:K:527:MET:HB2	7:K:530:LEU:CB	2.51	0.41
2:B:77:LYS:NZ	4:D:89:ARG:CZ	2.83	0.40
3:G:63:LEU:HD23	3:G:63:LEU:HA	1.82	0.40
7:K:477:ASN:OD1	7:K:597:ASP:HB3	2.21	0.40
1:A:62:ILE:HG13	1:A:97:GLU:OE2	2.21	0.40
4:H:76:ARG:NH1	4:H:80:TYR:OH	2.54	0.40
7:K:532:ASP:OD1	7:K:547:ARG:NH1	2.53	0.40
1:A:63:ARG:NH2	6:J:60:DA:H5"	2.36	0.40
7:K:253:PRO:O	7:K:257:LEU:HD12	2.21	0.40
4:D:33:SER:HB2	4:D:60:ASN:ND2	2.36	0.40
5:I:26:DC:H2"	5:I:27:DT:C7	2.52	0.40
5:I:129:DT:H2'	5:I:129:DT:OP2	2.21	0.40
7:K:120:LYS:NZ	7:K:141:GLU:HG3	2.36	0.40
7:K:265:ASN:O	7:K:269:PRO:HG3	2.22	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	96/136 (71%)	93 (97%)	3 (3%)	0	100	100
1	E	93/136 (68%)	88 (95%)	5 (5%)	0	100	100
2	B	86/103 (84%)	81 (94%)	5 (6%)	0	100	100
2	F	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
3	C	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	G	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
4	D	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
4	H	91/126 (72%)	88 (97%)	3 (3%)	0	100	100
7	K	496/1062 (47%)	453 (91%)	43 (9%)	0	100	100
All	All	1241/2052 (60%)	1173 (94%)	68 (6%)	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	84/111 (76%)	84 (100%)	0	100	100
1	E	82/111 (74%)	82 (100%)	0	100	100
2	B	72/79 (91%)	72 (100%)	0	100	100
2	F	64/79 (81%)	64 (100%)	0	100	100
3	C	81/102 (79%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	82/102 (80%)	82 (100%)	0	100	100
4	D	77/106 (73%)	77 (100%)	0	100	100
4	H	79/106 (74%)	79 (100%)	0	100	100
7	K	459/959 (48%)	459 (100%)	0	100	100
All	All	1080/1755 (62%)	1080 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	75	HIS
4	D	60	ASN
1	E	76	GLN
3	G	24	GLN
4	H	92	GLN
7	K	111	HIS
7	K	258	ASN
7	K	272	ASN
7	K	437	GLN
7	K	526	GLN
7	K	554	HIS
7	K	642	GLN
7	K	648	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	BEF	K	1202	-	0,3,3	-	-	-		
8	ADP	K	1201	10	27,29,29	1.37	4 (14%)	42,45,45	1.99	11 (26%)

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
8	ADP	K	1201	10	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	1201	ADP	C5-C4	4.55	1.47	1.39
8	K	1201	ADP	C5-C6	2.62	1.48	1.41
8	K	1201	ADP	C8-N7	2.42	1.36	1.31
8	K	1201	ADP	C5-N7	-2.12	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	1201	ADP	C5-C4-N3	-5.82	119.16	126.75
8	K	1201	ADP	N3-C4-N9	4.68	134.79	127.08
8	K	1201	ADP	PA-O3A-PB	-4.29	118.10	132.83
8	K	1201	ADP	C2-N3-C4	3.74	120.59	111.75
8	K	1201	ADP	N3-C2-N1	-3.20	123.59	128.60
8	K	1201	ADP	C4-C5-N7	-3.10	106.84	110.62
8	K	1201	ADP	C4-N9-C8	2.86	108.82	105.73
8	K	1201	ADP	C5-N7-C8	2.62	107.23	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	1201	ADP	C3'-C2'-C1'	2.34	105.87	101.43
8	K	1201	ADP	C6-C5-N7	2.21	136.14	132.02
8	K	1201	ADP	N9-C8-N7	-2.09	111.06	113.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	K	1201	ADP	O4'-C4'-C5'-O5'
8	K	1201	ADP	C3'-C4'-C5'-O5'
8	K	1201	ADP	C5'-O5'-PA-O1A

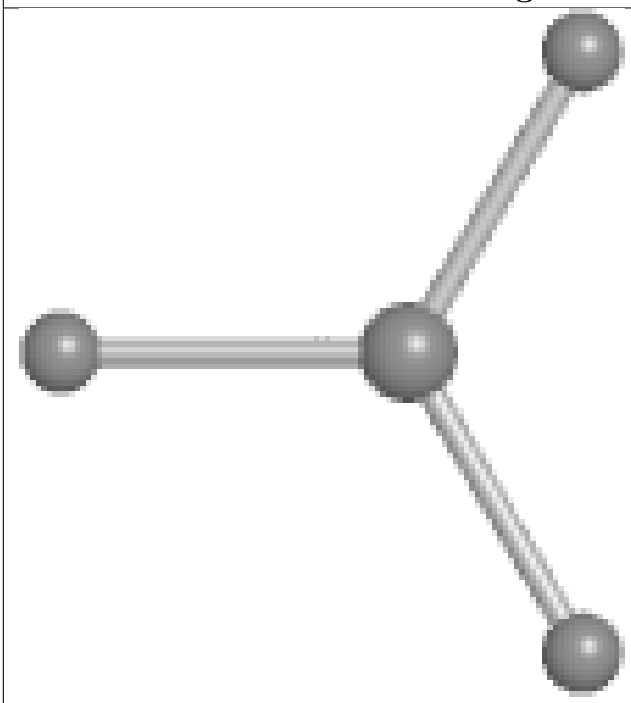
There are no ring outliers.

2 monomers are involved in 10 short contacts:

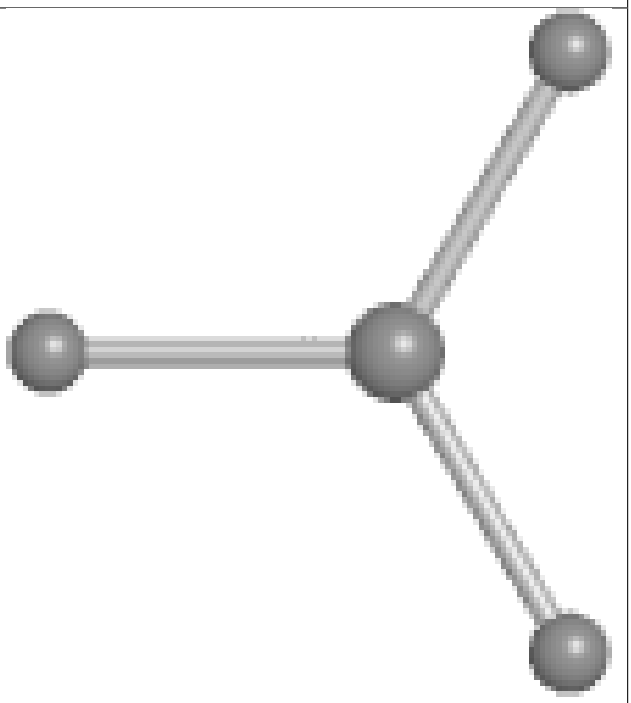
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	1202	BEF	4	0
8	K	1201	ADP	7	0

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 then 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.

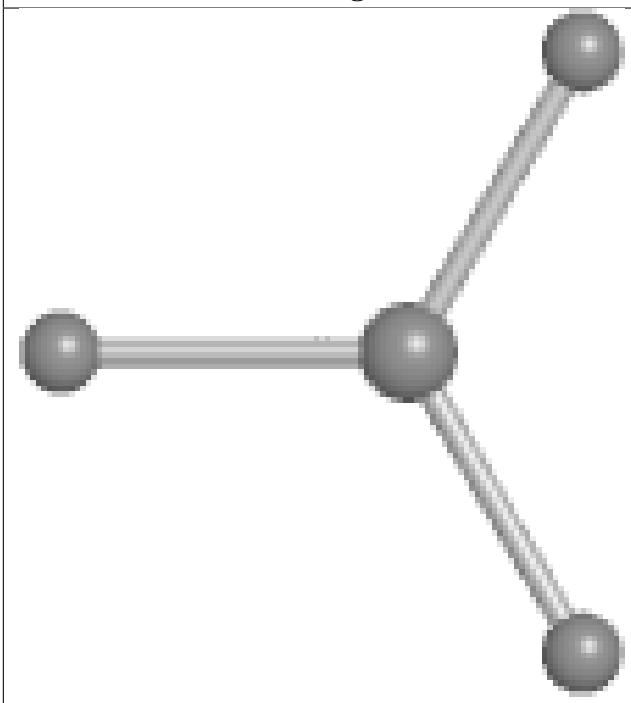
Ligand BEF K 1202



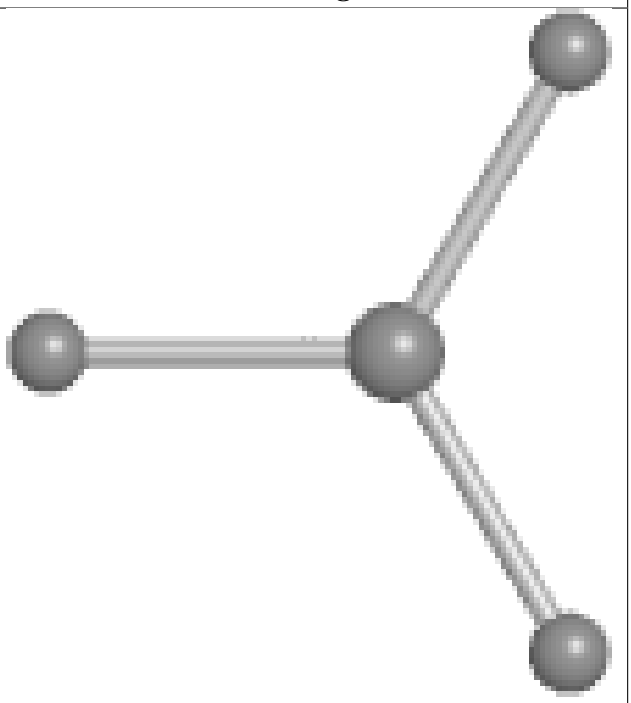
Bond lengths



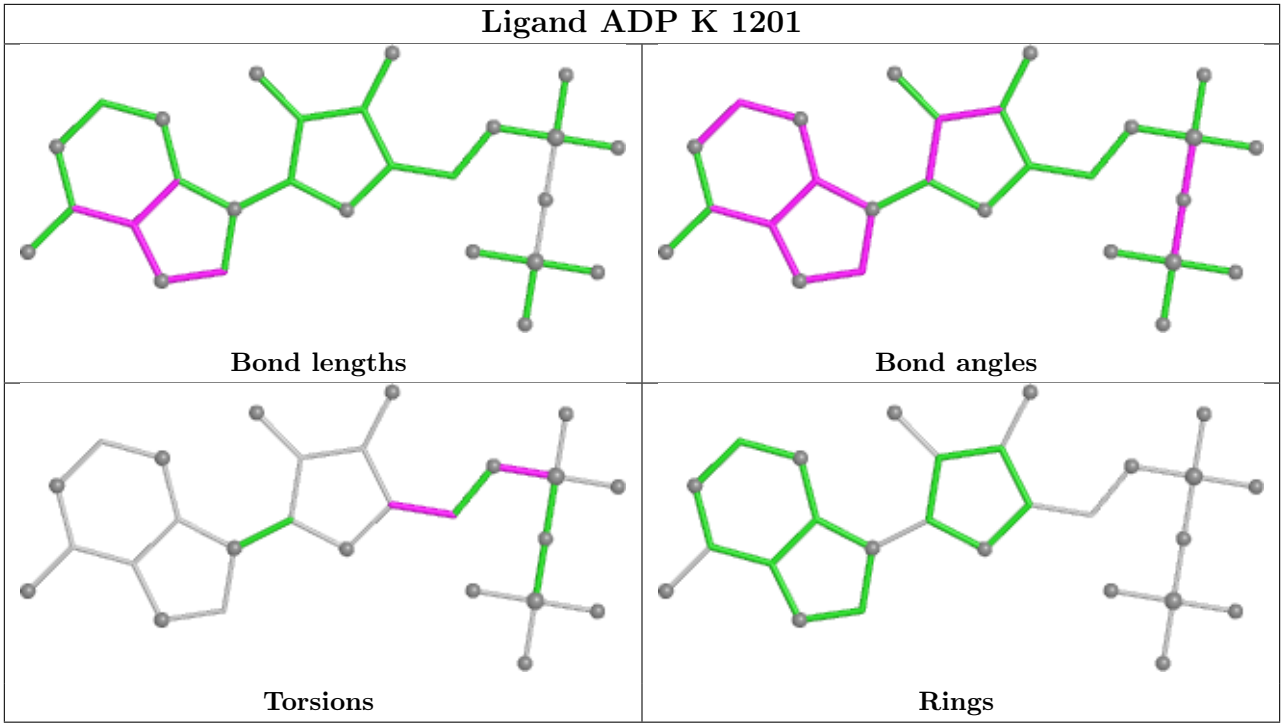
Bond angles



Torsions



Rings



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.

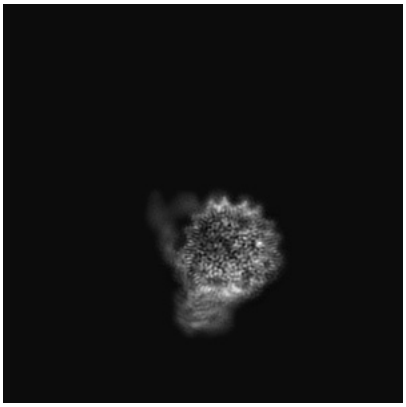
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32995. These allow visual inspection of the internal detail of the map and identification of artifacts.

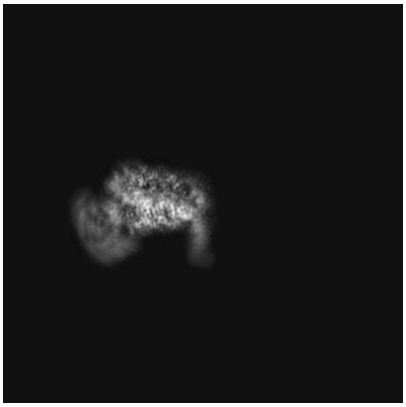
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

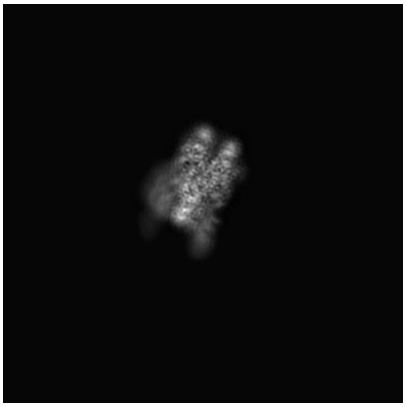
6.1.1 Primary map



X



Y

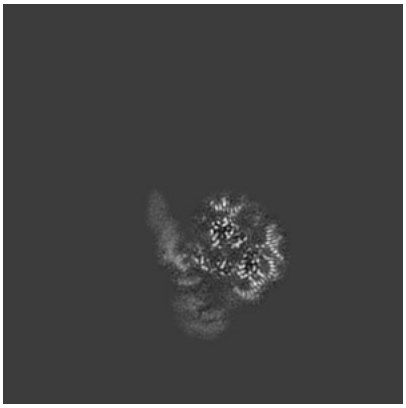


Z

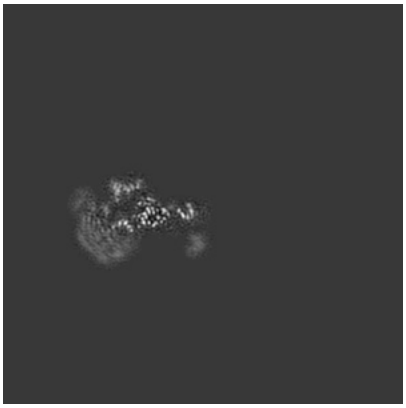
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

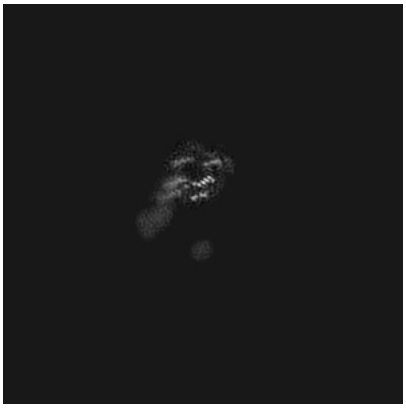
6.2.1 Primary map



X Index: 180



Y Index: 180

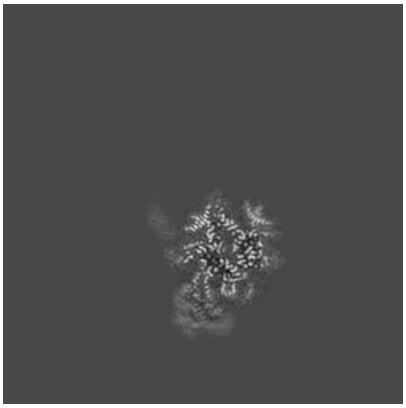


Z Index: 180

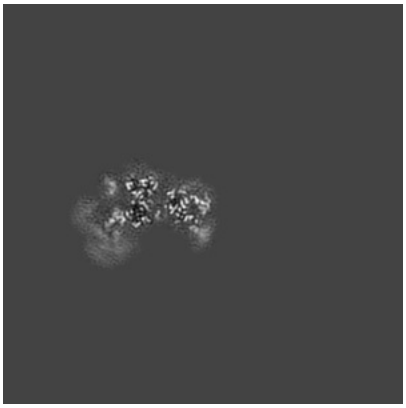
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

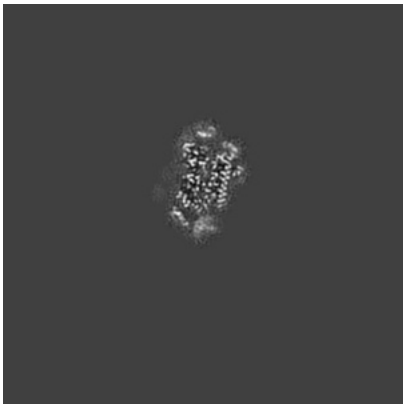
6.3.1 Primary map



X Index: 168



Y Index: 198

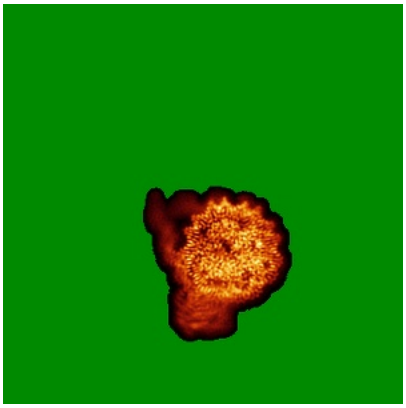


Z Index: 124

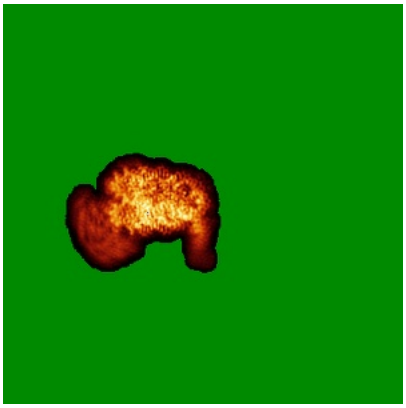
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

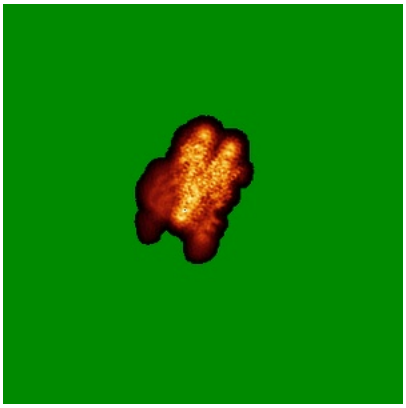
6.4.1 Primary map



X



Y

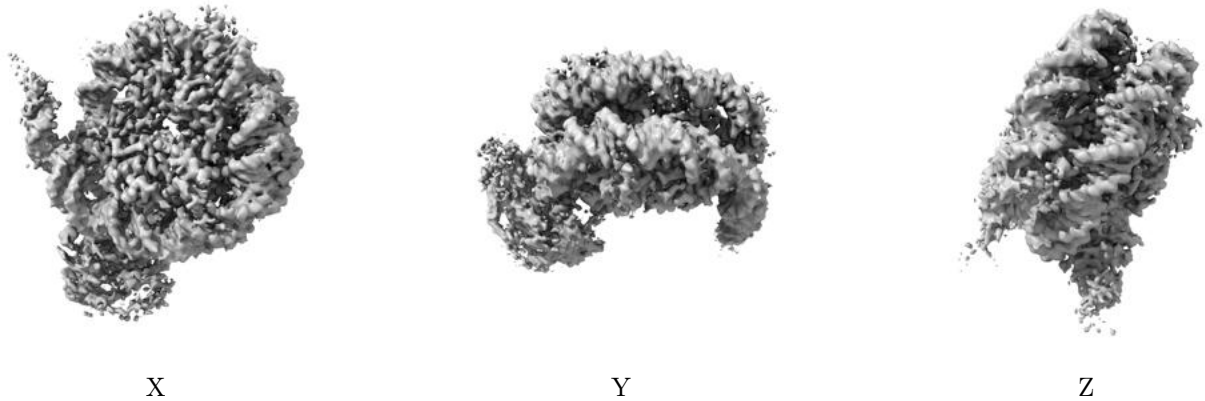


Z

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 (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

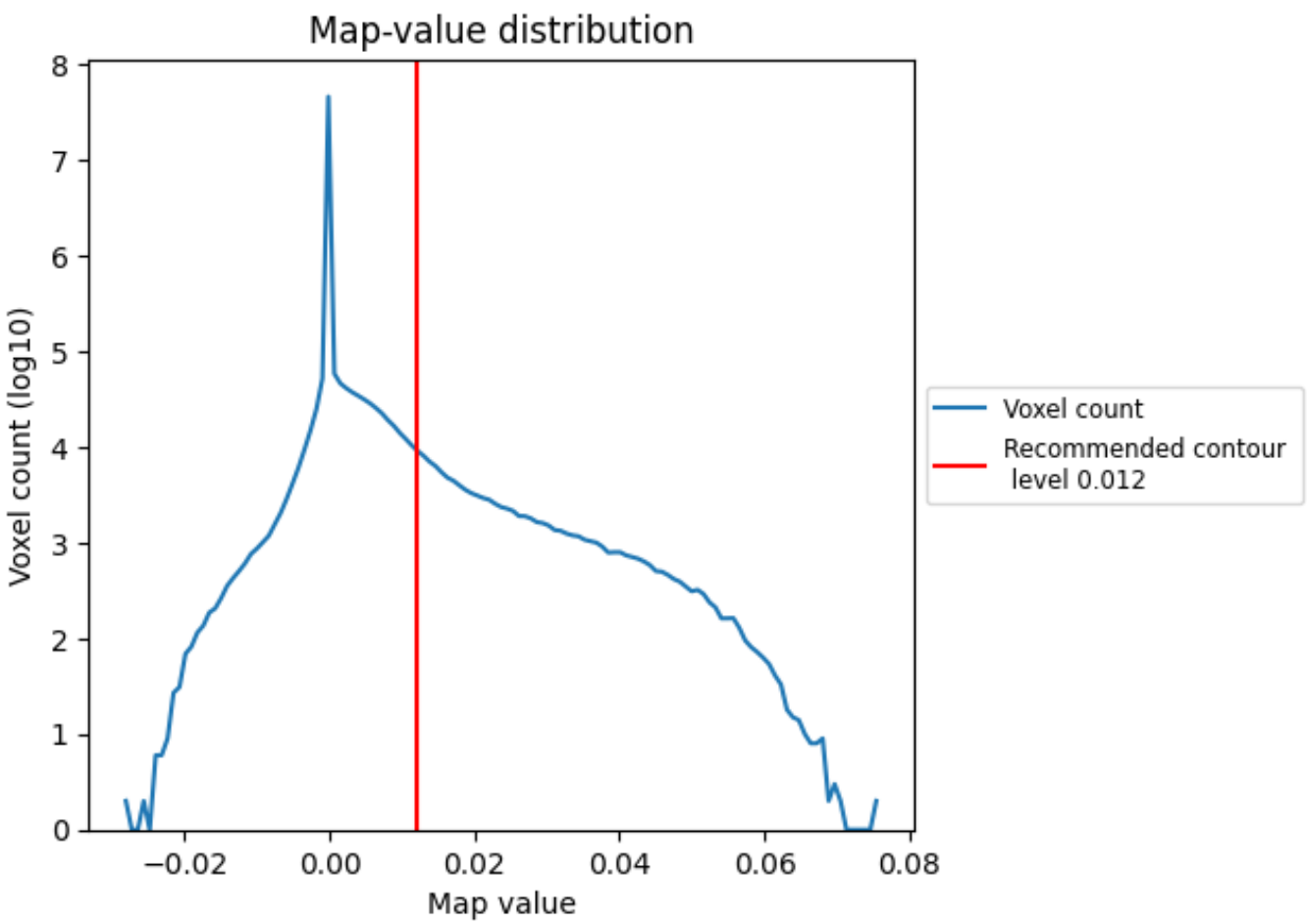
6.6 Mask visualisation (i)

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

7 Map analysis (i)

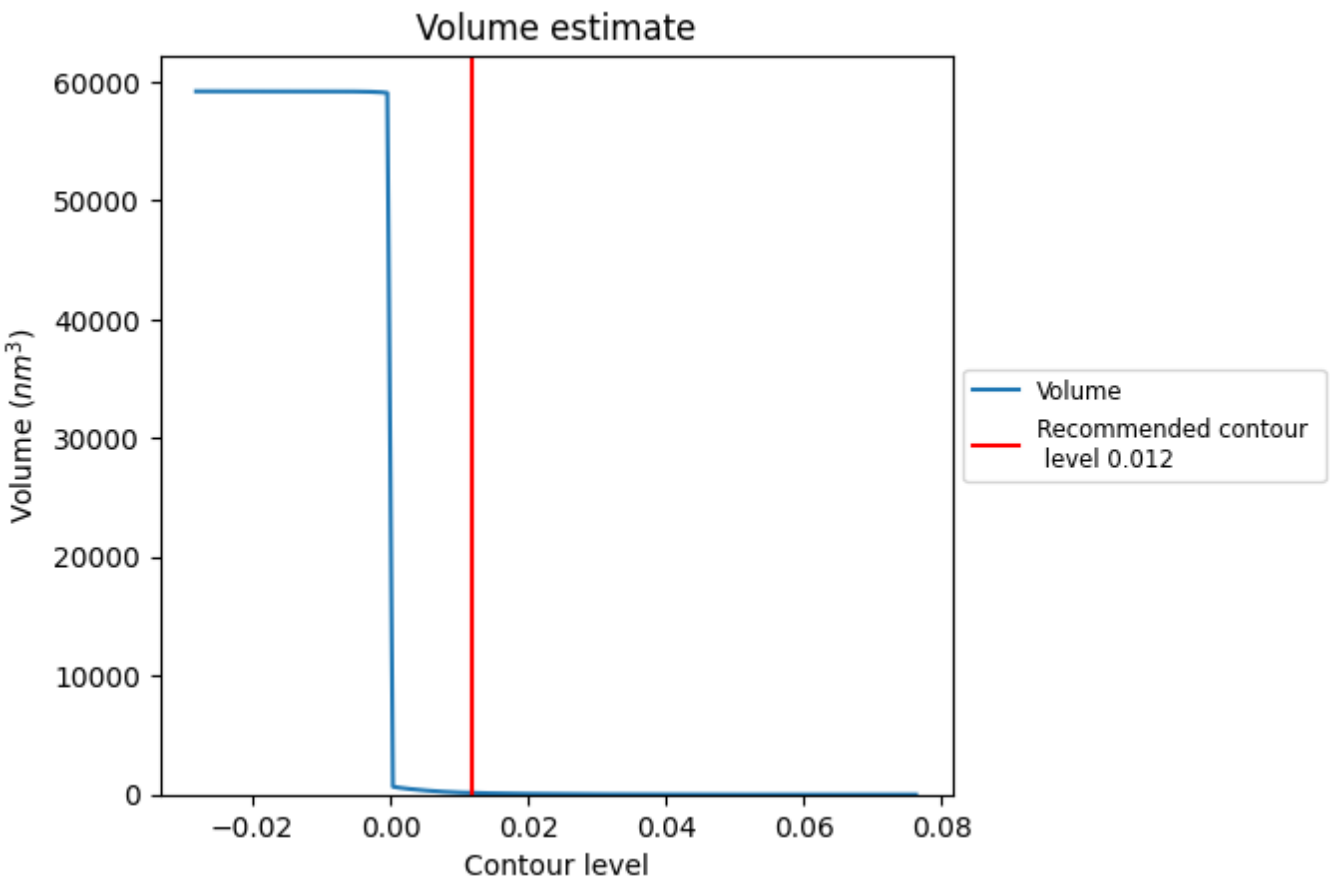
This section contains the results of statistical analysis of the map.

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.

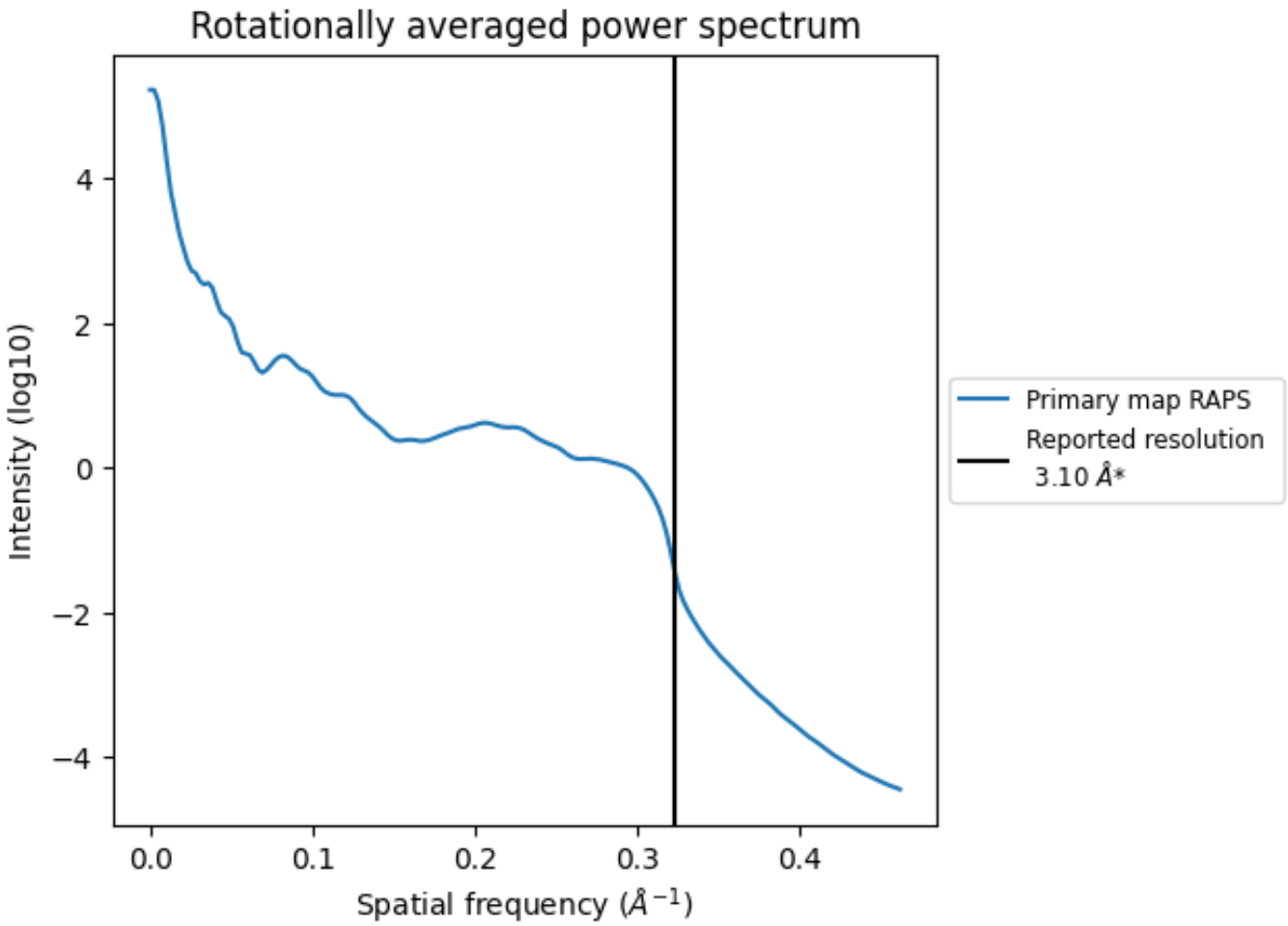
7.2 Volume estimate (i)



The volume at the recommended contour level is 137 nm^3; this corresponds to an approximate mass of 123 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 0.323 Å^{-1}

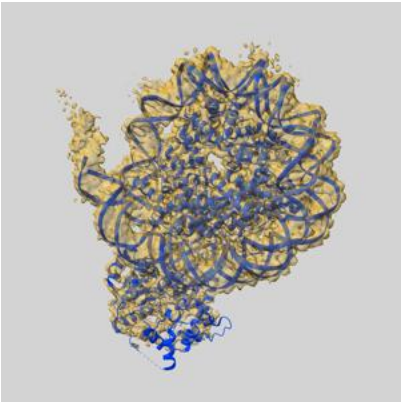
8 Fourier-Shell correlation (i)

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

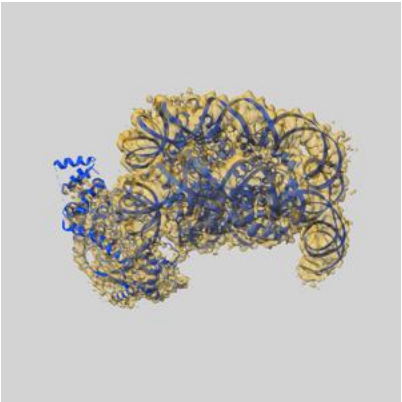
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32995 and PDB model 7X3W. Per-residue inclusion information can be found in section 3 on page 7.

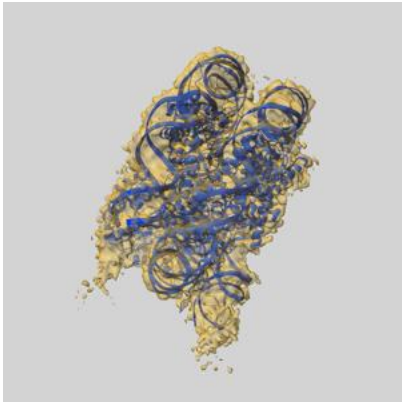
9.1 Map-model overlay (i)



X



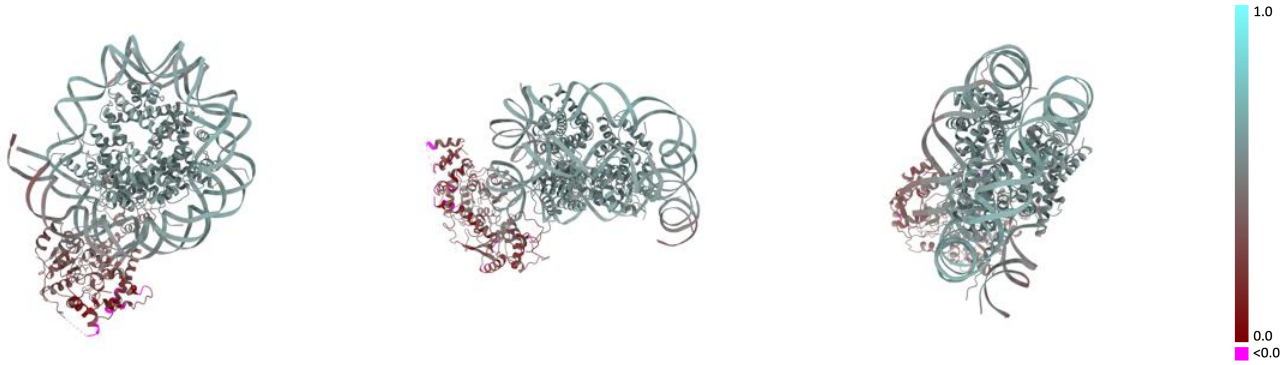
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

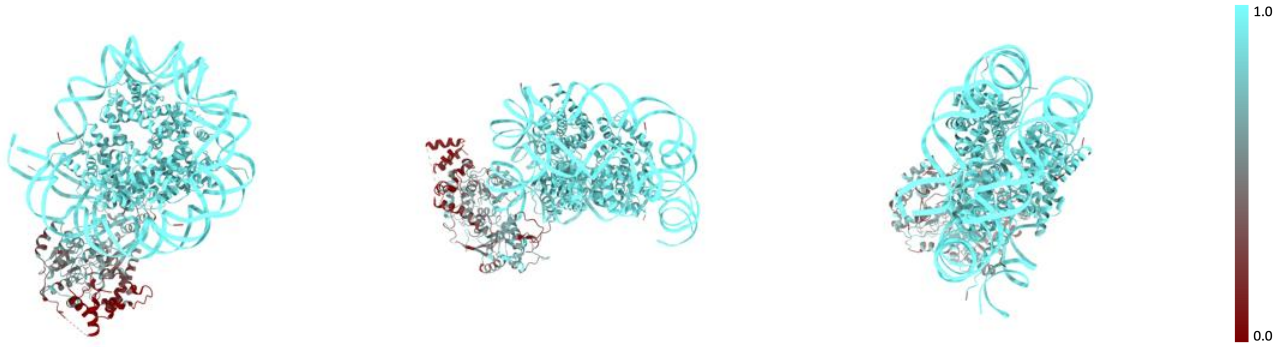
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

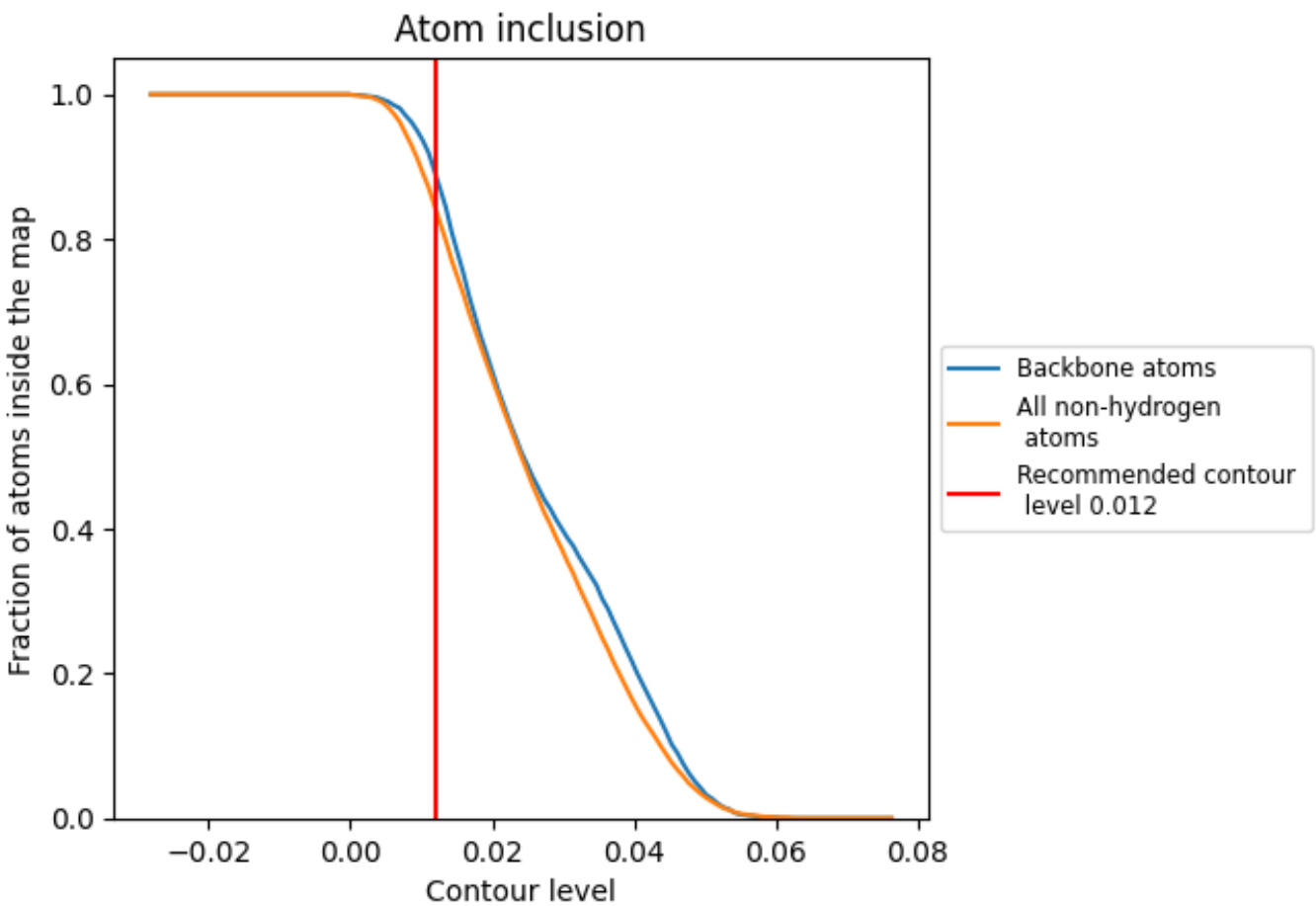
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8410	0.4890
A	0.9330	0.5700
B	0.9000	0.5500
C	0.9400	0.5690
D	0.9600	0.5640
E	0.9570	0.5780
F	0.9670	0.5820
G	0.9200	0.5660
H	0.9560	0.5620
I	0.9910	0.5540
J	0.9930	0.5550
K	0.4750	0.2810