



Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 10:23 am BST

PDB ID : 7OOB / pdb_00007oob
EMDB ID : EMD-13009
Title : Pol II-CSB-CSA-DDB1-UVSSA-ADPBeF3 (Structure2)
Authors : Kokic, G.; Cramer, P.
Deposited on : 2021-05-27
Resolution : 2.70 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.dev133
Mogul : 1.8.4, 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 EMD 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

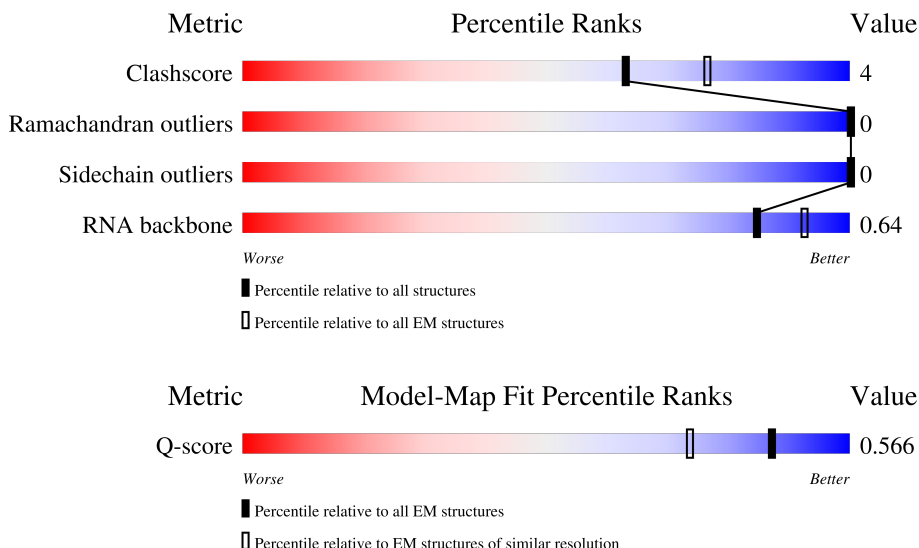
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



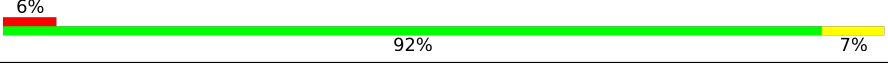
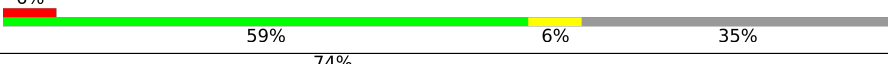
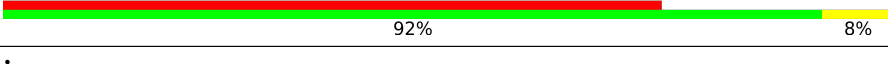
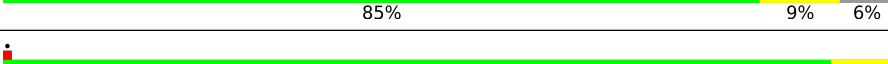
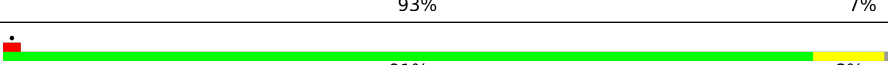
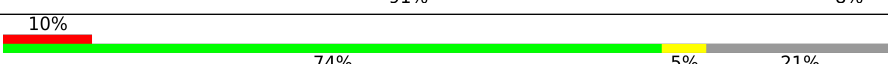
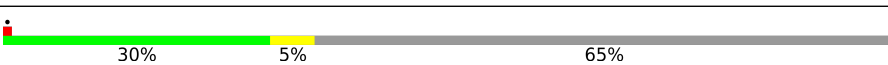
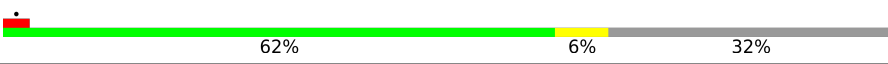
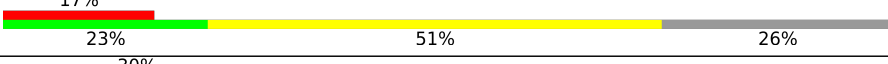
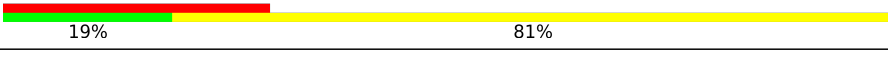
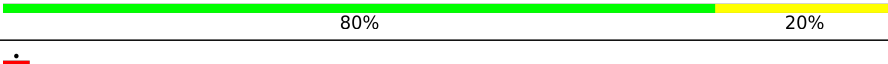
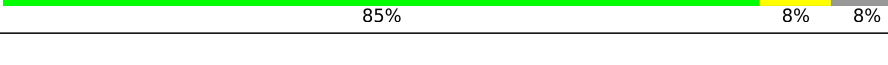
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	1970	
2	B	1174	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	b	1496	
14	d	1143	
15	N	47	
16	T	47	
17	P	10	
18	a	396	

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 90756 atoms, of which 44495 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1412	Total	C	H	N	O	S	0	0
			22494	7033	11315	2002	2074	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1131	Total	C	H	N	O	S	0	0
			18140	5727	9088	1592	1669	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	260	Total	C	H	N	O	S	0	0
			4120	1309	2031	359	415	6		

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	126	Total	C	H	N	O	S	0	0
			2046	642	1016	175	209	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3457	1089	1737	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	82	Total	C	H	N	O	S	0	0
			1341	418	684	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2709	875	1358	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	148	Total	C	H	N	O	S	0	0
			2333	750	1147	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			1828	587	879	169	182	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	67	Total	C	H	N	O	S	0	0
			1086	345	553	90	92	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			781	241	393	75	66	6		

- Molecule 13 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	b	520	Total	C	H	N	O	S	0	0
			8561	2746	4302	746	746	21		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-2	SER	-	expression tag	UNP Q03468
b	-1	ASN	-	expression tag	UNP Q03468
b	0	ALA	-	expression tag	UNP Q03468

- Molecule 14 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	d	781	Total	C	H	N	O	S	0	0
			12317	3919	6153	1038	1173	34		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-2	SER	-	expression tag	UNP Q16531
d	-1	ASN	-	expression tag	UNP Q16531
d	0	ALA	-	expression tag	UNP Q16531

- Molecule 15 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	35	Total	C	N	O	P	0	0
			727	344	142	206	35		

- Molecule 16 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 17 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	P	10	Total	C	H	N	O	P	0	0
			329	98	109	45	67	10		

- Molecule 18 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	a	365	Total	C	H	N	O	S	0	0
			5626	1775	2777	507	548	19		

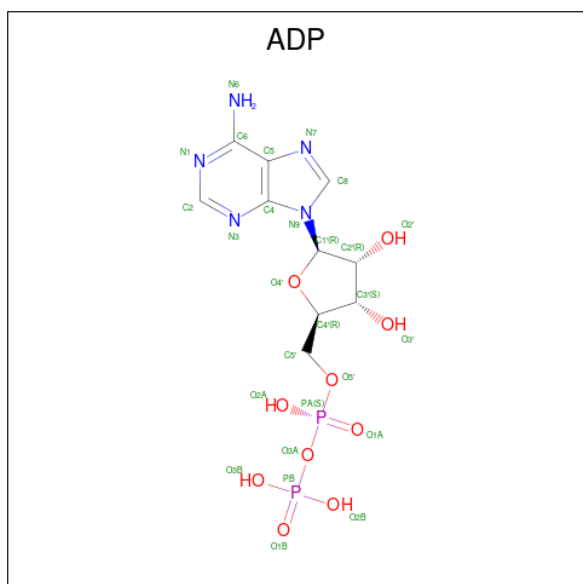
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	
19	C	1	Total	Zn	0
			1	1	
19	I	2	Total	Zn	0
			2	2	
19	J	1	Total	Zn	0
			1	1	
19	L	1	Total	Zn	0
			1	1	

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

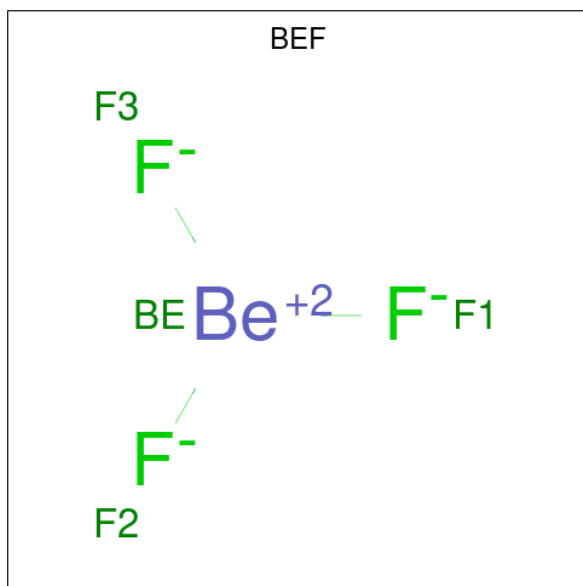
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Mg	0
			1	1	
20	b	1	Total	Mg	0
			1	1	

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



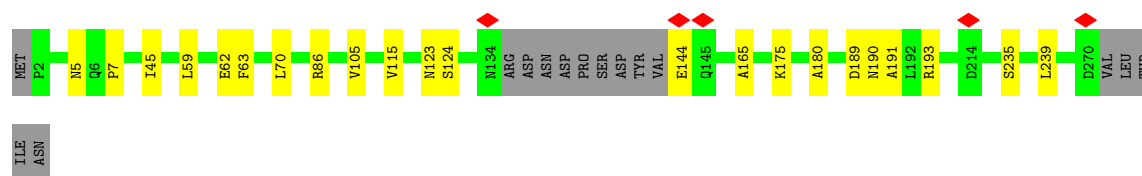
Mol	Chain	Residues	Atoms						AltConf
21	b	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

- Molecule 22 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).

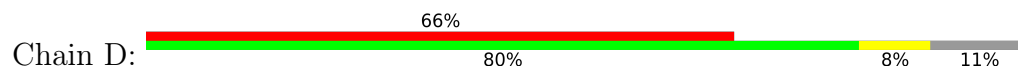
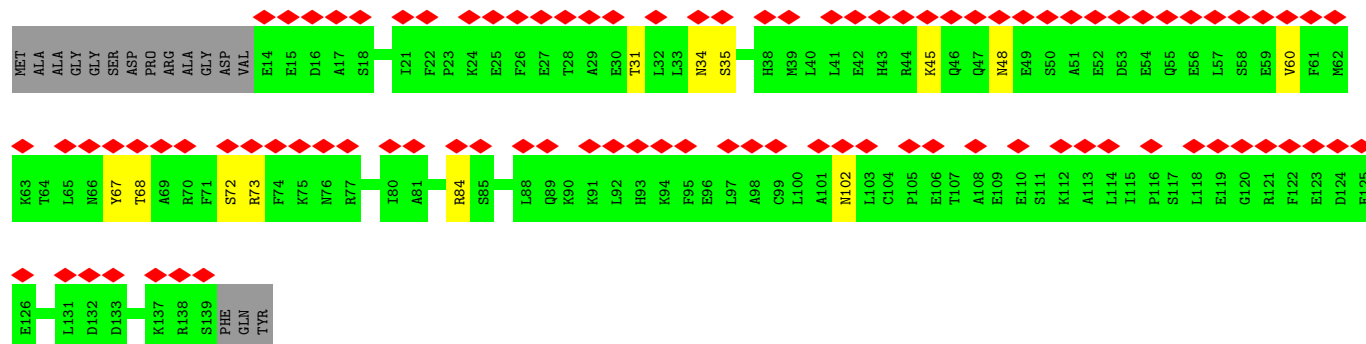


Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
22	b	1	4	1	3	0

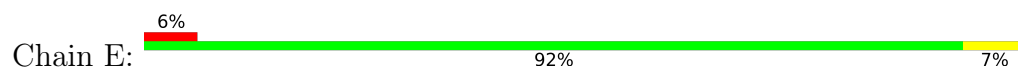




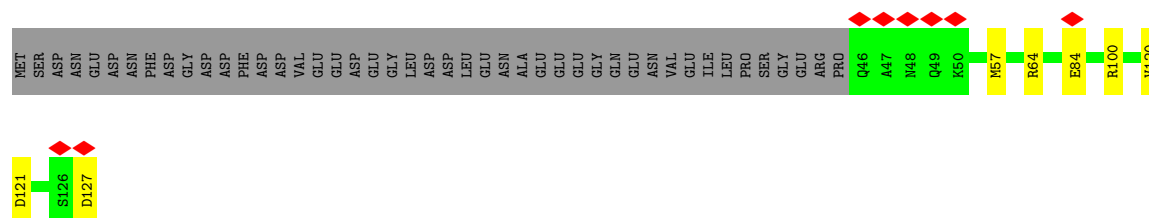
• Molecule 4: RPOL4c domain-containing protein



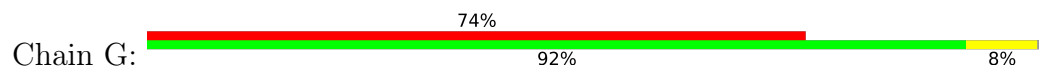
• Molecule 5: DNA-directed RNA polymerase II subunit E

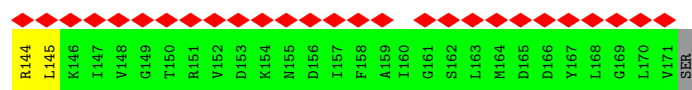


• Molecule 6: DNA-directed RNA polymerase II subunit F

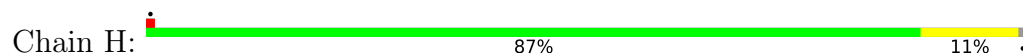


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

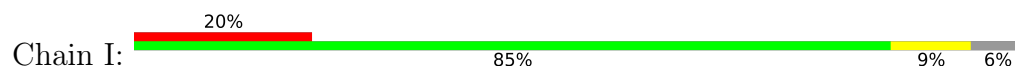
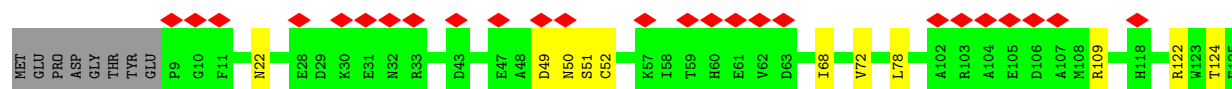




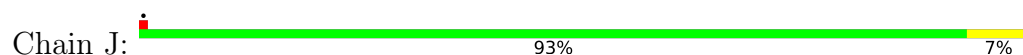
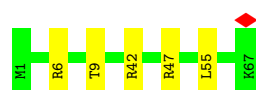
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



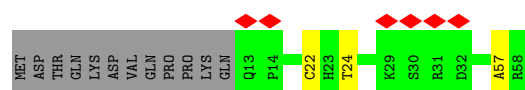
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



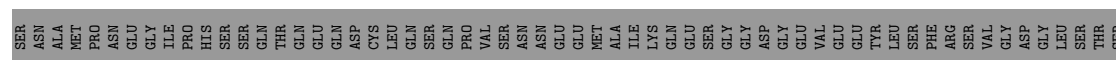
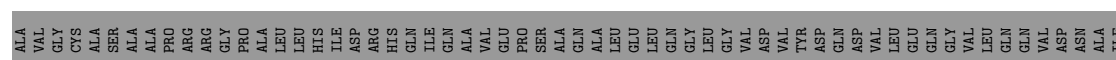
- Molecule 11: RNA_pol_L_2 domain-containing protein



- Molecule 12: RNA polymerase II subunit K



- Molecule 13: DNA excision repair protein ERCC-6

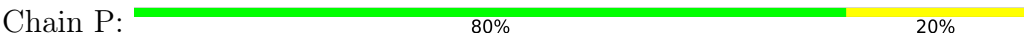




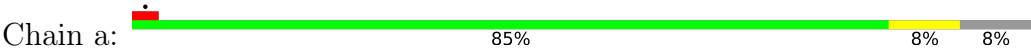
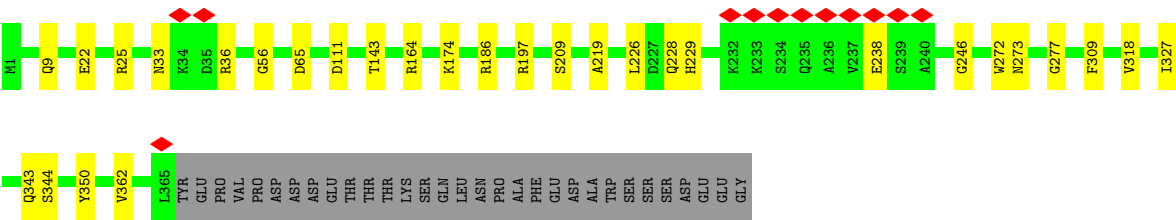
[illegible]

Chain N:

Chain T:



● Molecule 18: DNA excision repair protein ERCC-8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, ADP, ZN, 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	0.23	0/11382	0.41	0/15368
2	B	0.23	0/9233	0.39	0/12463
3	C	0.26	0/2132	0.41	0/2896
4	D	0.18	0/1043	0.32	0/1400
5	E	0.20	0/1751	0.35	0/2366
6	F	0.22	0/667	0.35	0/901
7	G	0.19	0/1382	0.39	0/1874
8	H	0.22	0/1207	0.37	0/1628
9	I	0.18	0/972	0.40	0/1316
10	J	0.23	0/542	0.37	0/730
11	K	0.21	0/939	0.34	0/1271
12	L	0.23	0/394	0.42	0/524
13	b	0.28	0/4362	0.49	0/5890
14	d	0.26	0/6271	0.46	1/8470 (0.0%)
15	N	0.20	0/817	0.34	0/1258
16	T	0.25	0/1056	0.44	0/1624
17	P	0.24	0/247	0.31	0/384
18	a	0.26	0/2908	0.46	0/3939
All	All	0.24	0/47305	0.41	1/64302 (0.0%)

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
1	A	0	1
13	b	0	1
14	d	0	1
18	a	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
14	d	929	SER	N-CA-C	5.22	121.91	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
18	a	174	LYS	Peptide
13	b	493	PHE	Peptide
14	d	884	ILE	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	11179	11315	11313	87	0
2	B	9052	9088	9087	57	0
3	C	2089	2031	2031	15	0
4	D	1030	1016	1016	9	0
5	E	1720	1737	1737	11	0
6	F	657	684	684	5	0
7	G	1351	1358	1358	10	0
8	H	1186	1147	1147	9	0
9	I	949	879	879	8	0
10	J	533	553	553	5	0
11	K	920	942	942	7	0
12	L	388	393	393	2	0
13	b	4259	4302	4302	46	0
14	d	6164	6153	6165	43	0
15	N	727	0	394	30	0
16	T	947	0	532	65	0
17	P	220	109	109	1	0
18	a	2849	2777	2778	18	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
20	A	1	0	0	0	0
20	b	1	0	0	0	0
21	b	27	11	12	2	0
22	b	4	0	0	1	0
All	All	46261	44495	45432	387	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 4.

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:CYS:SG	1:A:184:CYS:HB3	1.83	1.17
16:T:12:DT:H2''	16:T:13:DT:H5''	1.48	0.92
13:b:964:THR:HG1	13:b:967:THR:HG1	1.16	0.89
16:T:8:DC:H2'	16:T:9:DT:H71	1.56	0.87
1:A:338:SER:OG	1:A:341:GLN:OE1	1.92	0.87
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.57	0.86
15:N:44:DA:H2''	15:N:45:DG:H5''	1.56	0.86
15:N:7:DG:H2''	15:N:8:DA:H5''	1.57	0.85
2:B:565:THR:OG1	2:B:610:ARG:O	1.95	0.84
13:b:679:GLN:OE1	13:b:939:SER:OG	1.98	0.82
16:T:42:DA:H2''	16:T:43:DA:H5''	1.62	0.81
16:T:3:DC:H2'	16:T:4:DT:H71	1.62	0.80
16:T:7:DG:H2''	16:T:8:DC:H5''	1.64	0.79
16:T:11:DC:H2'	16:T:12:DT:H71	1.64	0.79
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.16	0.79
9:I:68:ILE:O	9:I:122:ARG:NH1	2.17	0.78
16:T:32:DC:H3'	16:T:33:DT:H5''	1.62	0.78
1:A:114:CYS:SG	1:A:184:CYS:CB	2.68	0.78
18:a:143:THR:OG1	18:a:164:ARG:NH1	2.19	0.76
14:d:102:THR:OG1	14:d:1065:VAL:O	2.04	0.75
2:B:357:CYS:SG	2:B:361:LYS:NZ	2.58	0.75
15:N:1:DC:H2''	15:N:2:DT:H5'	1.67	0.75
13:b:711:ILE:O	13:b:985:ARG:NH2	2.20	0.74
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.21	0.74
1:A:374:SER:OG	1:A:376:ASP:OD1	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:GLY:O	2:B:361:LYS:NZ	2.20	0.74
15:N:10:DC:H2''	15:N:11:DT:H71	1.68	0.74
13:b:717:SER:O	13:b:994:ARG:NH1	2.21	0.73
1:A:538:VAL:HG12	1:A:539:GLN:H	1.53	0.72
1:A:70:ARG:NH2	1:A:75:ALA:O	2.21	0.72
1:A:413:TYR:OH	1:A:450:MET:O	2.08	0.71
3:C:180:ALA:O	10:J:42:ARG:NH2	2.23	0.71
14:d:134:ARG:NH1	14:d:164:VAL:O	2.22	0.71
16:T:8:DC:H5''	16:T:8:DC:H6	1.55	0.71
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.64	0.71
1:A:576:GLN:O	1:A:590:GLN:NE2	2.23	0.71
2:B:198:GLU:OE2	2:B:388:TYR:OH	2.09	0.70
1:A:549:THR:O	1:A:589:LYS:NZ	2.24	0.70
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.24	0.69
8:H:92:MET:HE2	8:H:143:LEU:HD22	1.74	0.69
14:d:226:PHE:O	14:d:241:ASN:ND2	2.26	0.69
2:B:957:THR:OG1	2:B:959:GLU:O	2.11	0.69
1:A:321:GLU:OE1	1:A:341:GLN:NE2	2.26	0.69
16:T:34:DA:H1'	16:T:35:DT:H5'	1.75	0.69
16:T:16:DC:H2''	16:T:17:DC:H5'	1.74	0.68
16:T:6:DT:H2'	16:T:7:DG:C8	2.27	0.68
18:a:22:GLU:OE2	18:a:25:ARG:NH2	2.27	0.68
14:d:111:ARG:NH2	18:a:197:ARG:O	2.26	0.68
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.76	0.68
1:A:332:SER:HB3	16:T:29:DT:H5''	1.75	0.67
2:B:551:GLU:OE2	2:B:578:LYS:NZ	2.27	0.67
2:B:591:ARG:HE	2:B:603:MET:HE2	1.60	0.67
16:T:24:DC:H2'	16:T:25:DT:C6	2.31	0.66
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.29	0.66
2:B:329:GLY:O	2:B:335:ARG:NE	2.29	0.66
1:A:1198:GLU:OE1	1:A:1198:GLU:N	2.29	0.66
4:D:67:TYR:OH	7:G:86:ASP:O	2.13	0.65
1:A:413:TYR:O	1:A:415:GLY:N	2.30	0.65
1:A:373:LEU:O	1:A:485:ASN:ND2	2.30	0.64
16:T:42:DA:H2''	16:T:43:DA:C5'	2.28	0.64
16:T:7:DG:H2''	16:T:8:DC:C5'	2.26	0.64
2:B:1104:ARG:NH1	2:B:1109:GLU:OE2	2.31	0.63
14:d:381:ALA:O	14:d:385:GLY:N	2.31	0.63
16:T:20:DT:H2'	16:T:21:DC:C6	2.33	0.63
16:T:16:DC:H2'	16:T:17:DC:C6	2.33	0.63
18:a:228:GLN:HE21	18:a:229:HIS:CE1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:42:DA:H4'	16:T:43:DA:OP1	1.98	0.62
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.35	0.62
3:C:190:ASN:O	3:C:193:ARG:NH1	2.33	0.62
1:A:507:GLN:N	2:B:1105:GLU:OE2	2.33	0.62
2:B:347:MET:HE1	2:B:365:LEU:HD22	1.82	0.62
1:A:1311:LEU:HD12	1:A:1332:GLN:HG3	1.82	0.61
1:A:41:ILE:HD12	1:A:255:VAL:HG11	1.81	0.61
1:A:358:ARG:NH1	16:T:22:DC:OP1	2.34	0.61
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.82	0.61
2:B:210:LYS:NZ	2:B:212:ASP:O	2.33	0.61
9:I:50:ASN:O	9:I:51:SER:OG	2.16	0.61
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.14	0.61
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.18	0.60
8:H:71:ASP:OD2	8:H:142:TYR:OH	2.19	0.60
13:b:964:THR:OG1	13:b:967:THR:OG1	2.04	0.60
1:A:808:PRO:HG2	2:B:675:LEU:HD12	1.83	0.60
2:B:927:ARG:NH1	2:B:1057:ASP:OD1	2.33	0.60
21:b:1501:ADP:O1B	22:b:1502:BEF:F1	2.10	0.60
16:T:9:DT:H2''	16:T:10:DC:C6	2.36	0.60
15:N:10:DC:C2'	15:N:11:DT:H71	2.32	0.60
14:d:1080:ARG:NH1	18:a:344:SER:O	2.34	0.60
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.34	0.60
2:B:794:VAL:HG12	2:B:967:ILE:HG22	1.83	0.60
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.34	0.59
18:a:36:ARG:NH1	18:a:350:TYR:OH	2.36	0.59
5:E:134:GLU:OE2	5:E:181:ARG:NH2	2.36	0.58
13:b:575:THR:OG1	16:T:39:DA:OP1	2.20	0.58
8:H:102:ASP:OD2	8:H:110:THR:OG1	2.21	0.58
1:A:521:VAL:HG13	1:A:535:MET:HE1	1.84	0.58
13:b:635:ILE:O	13:b:640:TRP:NE1	2.35	0.58
2:B:847:LYS:NZ	2:B:864:ASP:OD2	2.22	0.58
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.86	0.58
14:d:130:MET:HE2	14:d:169:PHE:HZ	1.68	0.58
18:a:56:GLY:O	18:a:343:GLN:NE2	2.37	0.57
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.86	0.57
14:d:47:GLU:OE1	14:d:47:GLU:N	2.38	0.57
2:B:501:LEU:HD12	2:B:505:LEU:CD1	2.33	0.57
2:B:413:LYS:O	2:B:417:ILE:HD12	2.04	0.56
16:T:5:DC:H2''	16:T:6:DT:O4'	2.05	0.56
1:A:1180:ASN:ND2	1:A:1183:SER:OG	2.38	0.56
15:N:43:DG:H2''	15:N:44:DA:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:510:TYR:OH	13:b:536:LEU:O	2.23	0.56
1:A:421:ARG:NH1	1:A:444:TYR:OH	2.39	0.56
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.39	0.56
5:E:120:ASP:OD1	5:E:121:MET:N	2.38	0.56
16:T:34:DA:H2''	16:T:35:DT:H5'	1.87	0.56
16:T:7:DG:H4'	16:T:8:DC:OP1	2.04	0.56
13:b:747:LYS:NZ	13:b:946:GLU:OE1	2.40	0.56
13:b:975:ARG:NE	15:N:16:DT:OP1	2.36	0.55
13:b:869:ASP:OD1	13:b:884:LYS:NZ	2.38	0.55
1:A:54:LEU:O	1:A:61:ARG:NH2	2.40	0.55
18:a:186:ARG:NH1	18:a:238:GLU:O	2.40	0.55
14:d:196:SER:O	14:d:200:LYS:N	2.39	0.55
13:b:538:LYS:N	21:b:1501:ADP:O2B	2.39	0.55
1:A:904:GLN:NE2	1:A:981:CYS:O	2.37	0.55
15:N:6:DT:H2''	15:N:7:DG:C8	2.42	0.55
13:b:840:LYS:NZ	13:b:969:GLU:OE2	2.40	0.55
16:T:15:DT:H2''	16:T:16:DC:C6	2.42	0.55
2:B:602:SER:OG	2:B:620:ARG:NH1	2.41	0.54
5:E:78:GLU:OE1	5:E:78:GLU:N	2.41	0.54
13:b:859:LEU:N	13:b:928:ARG:O	2.41	0.54
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.41	0.54
6:F:84:GLU:OE2	6:F:84:GLU:N	2.40	0.54
16:T:19:DA:H2'	16:T:20:DT:C6	2.43	0.54
16:T:44:DC:H2'	16:T:45:DT:H72	1.88	0.54
3:C:59:LEU:HD13	3:C:63:PHE:CD1	2.42	0.54
13:b:693:PHE:CD2	13:b:696:LYS:HB2	2.42	0.54
15:N:44:DA:C2'	15:N:45:DG:H5''	2.34	0.54
16:T:45:DT:H2''	16:T:46:DA:O5'	2.08	0.54
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.90	0.54
4:D:31:THR:O	4:D:84:ARG:NH2	2.40	0.54
14:d:308:THR:O	14:d:383:LYS:NZ	2.39	0.54
14:d:130:MET:HE1	14:d:195:VAL:HG11	1.90	0.53
16:T:29:DT:C2'	16:T:30:DG:H4'	2.38	0.53
1:A:108:ARG:NH2	1:A:191:ILE:O	2.41	0.53
9:I:109:ARG:HE	9:I:124:THR:HG21	1.73	0.53
1:A:413:TYR:O	1:A:449:HIS:ND1	2.41	0.53
14:d:213:GLU:OE2	14:d:236:SER:N	2.42	0.53
16:T:12:DT:C2'	16:T:13:DT:H5''	2.30	0.53
2:B:959:GLU:O	2:B:961:ILE:N	2.40	0.53
14:d:119:GLY:O	14:d:134:ARG:NH2	2.35	0.53
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:3:DC:H2''	16:T:4:DT:O5'	2.09	0.52
16:T:24:DC:H2'	16:T:25:DT:H6	1.73	0.52
3:C:86:ARG:HD3	11:K:11:LEU:HD11	1.91	0.52
1:A:865:ILE:HD13	1:A:1092:ALA:HB3	1.91	0.52
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.42	0.52
1:A:862:ARG:NH1	2:B:1088:GLU:OE2	2.42	0.52
13:b:682:LEU:HD12	13:b:708:SER:HA	1.91	0.52
13:b:693:PHE:HD1	18:a:219:ALA:HB2	1.75	0.52
1:A:889:LEU:O	1:A:890:ARG:NH1	2.42	0.52
8:H:136:GLU:O	8:H:139:SER:OG	2.27	0.51
1:A:951:GLU:OE2	1:A:954:ARG:NH2	2.44	0.51
3:C:7:PRO:O	11:K:104:ARG:NH1	2.43	0.51
15:N:14:DT:H72	16:T:34:DA:H2	1.75	0.51
13:b:915:ARG:NH2	16:T:37:DA:H4'	2.26	0.51
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.43	0.51
16:T:34:DA:H1'	16:T:35:DT:C5'	2.41	0.51
13:b:549:LEU:HD23	13:b:566:LEU:HD13	1.92	0.50
13:b:857:ARG:NH1	13:b:901:TYR:O	2.40	0.50
14:d:755:SER:O	14:d:758:THR:N	2.45	0.50
5:E:141:GLU:N	5:E:141:GLU:OE1	2.45	0.50
14:d:289:GLU:N	14:d:289:GLU:OE1	2.44	0.50
16:T:34:DA:H2''	16:T:35:DT:C5'	2.41	0.50
7:G:23:LEU:CD1	7:G:54:ILE:HG21	2.42	0.50
2:B:312:GLN:NE2	9:I:22:ASN:OD1	2.46	0.49
13:b:534:MET:SD	13:b:534:MET:N	2.86	0.49
2:B:812:ARG:NH2	2:B:900:GLU:OE2	2.45	0.49
13:b:549:LEU:HD11	13:b:554:ILE:HD11	1.93	0.49
1:A:114:CYS:HG	1:A:184:CYS:CB	2.21	0.49
15:N:8:DA:H2'	15:N:9:DT:H71	1.94	0.49
18:a:33:ASN:HB2	18:a:362:VAL:HG22	1.94	0.49
13:b:521:LEU:HD21	13:b:528:GLY:HA3	1.94	0.49
5:E:209:VAL:O	5:E:210:GLN:NE2	2.44	0.49
5:E:114:ALA:O	5:E:117:SER:OG	2.26	0.49
1:A:481:THR:O	1:A:483:ARG:NE	2.46	0.49
14:d:1109:VAL:HG12	14:d:1109:VAL:O	2.13	0.49
16:T:8:DC:H5''	16:T:8:DC:C6	2.41	0.49
13:b:633:ASP:OD1	13:b:634:ASP:N	2.46	0.48
9:I:72:VAL:HG22	9:I:78:LEU:HD11	1.95	0.48
13:b:922:ASN:OD1	13:b:950:ARG:NE	2.34	0.48
1:A:728:THR:H	1:A:736:THR:HG21	1.79	0.48
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:244:LYS:HZ1	14:d:296:THR:HG22	1.77	0.48
1:A:455:ILE:HG23	1:A:520:MET:HE1	1.96	0.48
4:D:34:ASN:OD1	4:D:35:SER:N	2.46	0.48
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.29	0.48
2:B:1035:ARG:NH1	2:B:1036:LYS:O	2.47	0.48
1:A:1357:THR:O	5:E:142:HIS:NE2	2.45	0.48
3:C:70:LEU:O	10:J:6:ARG:NE	2.40	0.48
14:d:1081:LYS:HE2	14:d:1083:GLU:OE2	2.13	0.48
1:A:523:ARG:NH1	6:F:127:ASP:OD2	2.47	0.48
1:A:1229:GLU:OE1	1:A:1229:GLU:N	2.45	0.48
4:D:68:THR:O	4:D:72:SER:OG	2.21	0.48
14:d:986:ASP:OD1	14:d:986:ASP:N	2.47	0.48
15:N:32:DG:H2''	15:N:33:DA:C8	2.49	0.48
18:a:318:VAL:O	18:a:327:ILE:N	2.46	0.48
2:B:777:ASN:O	10:J:47:ARG:NH1	2.40	0.48
9:I:50:ASN:ND2	9:I:52:CYS:O	2.46	0.47
14:d:1081:LYS:HG2	14:d:1083:GLU:OE2	2.13	0.47
16:T:20:DT:H2'	16:T:21:DC:H6	1.78	0.47
1:A:1471:PHE:O	6:F:64:ARG:NH1	2.47	0.47
14:d:930:VAL:HG22	14:d:948:ASP:HB3	1.96	0.47
16:T:41:DC:H2''	16:T:42:DA:C8	2.49	0.47
2:B:905:ASP:N	2:B:922:ARG:O	2.46	0.47
13:b:800:ILE:HD13	16:T:35:DT:O4'	2.13	0.47
9:I:109:ARG:NE	9:I:124:THR:HG21	2.29	0.47
1:A:98:GLY:HA3	1:A:1440:MET:HE3	1.97	0.47
15:N:39:DA:H2''	15:N:40:DG:C8	2.50	0.47
16:T:30:DG:N3	16:T:30:DG:H2'	2.28	0.47
15:N:7:DG:C2'	15:N:8:DA:H5''	2.37	0.47
15:N:44:DA:H2''	15:N:45:DG:C8	2.50	0.47
18:a:65:ASP:OD1	18:a:65:ASP:N	2.48	0.47
16:T:17:DC:H2''	16:T:18:DC:O5'	2.15	0.47
16:T:34:DA:C1'	16:T:35:DT:H5'	2.45	0.47
1:A:1297:THR:HG23	1:A:1297:THR:O	2.15	0.47
3:C:144:GLU:OE1	3:C:144:GLU:N	2.48	0.47
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.48	0.46
16:T:29:DT:C3'	16:T:30:DG:H4'	2.45	0.46
13:b:667:THR:HG22	13:b:669:HIS:H	1.80	0.46
15:N:3:DA:H1'	15:N:4:DG:H5'	1.96	0.46
1:A:1433:GLU:OE1	16:T:17:DC:H4'	2.14	0.46
2:B:438:ARG:NH2	2:B:442:ASP:OD1	2.48	0.46
3:C:175:LYS:NZ	12:L:57:ALA:O	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:VAL:CG1	1:A:831:LEU:HD22	2.46	0.46
14:d:18:CYS:SG	14:d:315:THR:HG23	2.56	0.46
4:D:60:VAL:HG11	7:G:44:PHE:CE2	2.51	0.46
16:T:32:DC:H3'	16:T:33:DT:C5'	2.42	0.46
1:A:1166:LEU:O	1:A:1170:THR:OG1	2.13	0.46
4:D:73:ARG:NE	4:D:102:ASN:O	2.47	0.46
13:b:784:GLU:OE2	13:b:793:MET:HG2	2.16	0.46
16:T:43:DA:H2''	16:T:44:DC:C6	2.51	0.46
16:T:44:DC:H2'	16:T:45:DT:C7	2.46	0.46
1:A:78:MET:O	2:B:1072:ARG:NH2	2.49	0.45
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.52	0.45
1:A:1478:GLU:N	1:A:1478:GLU:OE1	2.49	0.45
2:B:294:ASP:OD1	2:B:379:ARG:NH2	2.48	0.45
7:G:18:PHE:HA	7:G:22:LEU:HD13	1.97	0.45
15:N:45:DG:H2''	15:N:46:DC:O5'	2.16	0.45
1:A:844:ARG:NH2	2:B:501:LEU:HD13	2.31	0.45
1:A:321:GLU:OE1	1:A:321:GLU:N	2.50	0.45
3:C:189:ASP:O	3:C:191:ALA:N	2.48	0.45
7:G:54:ILE:HG23	7:G:54:ILE:O	2.16	0.45
15:N:1:DC:C2	15:N:2:DT:H72	2.52	0.45
16:T:4:DT:H2''	16:T:5:DC:C6	2.51	0.45
13:b:883:LEU:HD11	13:b:897:LEU:HD22	1.99	0.45
14:d:38:ARG:NE	14:d:54:GLU:OE2	2.38	0.45
18:a:226:LEU:HD23	18:a:272:TRP:CD2	2.51	0.45
5:E:112:PRO:HB3	16:T:7:DG:H5'	1.98	0.45
8:H:88:PHE:CD1	8:H:144:LEU:HD12	2.51	0.45
15:N:41:DC:H2''	15:N:42:DA:C8	2.52	0.45
15:N:44:DA:H2''	15:N:45:DG:H8	1.82	0.45
2:B:15:ASP:OD1	2:B:15:ASP:N	2.47	0.45
2:B:629:GLU:N	2:B:632:LYS:O	2.41	0.45
7:G:144:ARG:C	7:G:145:LEU:HD12	2.42	0.45
13:b:924:THR:O	13:b:953:GLN:NE2	2.47	0.45
16:T:23:DT:H2'	16:T:24:DC:H6	1.82	0.45
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.80	0.44
1:A:823:VAL:HG11	1:A:831:LEU:HD22	1.99	0.44
16:T:23:DT:H2'	16:T:24:DC:C6	2.52	0.44
16:T:29:DT:H2''	16:T:30:DG:H4'	1.99	0.44
13:b:808:HIS:O	13:b:810:ASP:N	2.49	0.44
16:T:19:DA:H2'	16:T:20:DT:H6	1.82	0.44
1:A:896:LEU:O	1:A:1396:ARG:NH1	2.50	0.44
1:A:1189:ASP:OD2	1:A:1258:ARG:NE	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:929:SER:O	14:d:930:VAL:HG13	2.18	0.44
16:T:11:DC:H2''	16:T:12:DT:O5'	2.16	0.44
1:A:499:ASP:OD1	17:P:10:A:H4'	2.18	0.44
13:b:670:ARG:HH22	13:b:694:PRO:HD3	1.83	0.44
15:N:6:DT:H2''	15:N:7:DG:H8	1.81	0.44
13:b:859:LEU:HD12	13:b:910:PHE:HB3	1.99	0.44
13:b:1386:SER:OG	18:a:111:ASP:OD2	2.19	0.44
14:d:19:VAL:HG22	14:d:64:MET:HE3	2.00	0.44
12:L:22:CYS:SG	12:L:24:THR:OG1	2.72	0.44
14:d:125:ASP:OD2	14:d:129:ARG:NE	2.43	0.44
1:A:467:MET:SD	1:A:524:MET:HB3	2.58	0.44
2:B:887:TYR:O	2:B:888:THR:HG22	2.17	0.44
16:T:17:DC:H2'	16:T:18:DC:C6	2.53	0.44
2:B:84:TYR:HE1	2:B:132:VAL:HG22	1.83	0.43
13:b:709:VAL:HB	13:b:710:PRO:HD3	2.00	0.43
13:b:1395:ALA:O	13:b:1399:LEU:HD23	2.18	0.43
16:T:34:DA:H2''	16:T:35:DT:O5'	2.18	0.43
18:a:273:ASN:O	18:a:277:GLY:N	2.50	0.43
1:A:260:VAL:O	1:A:342:ARG:NH1	2.44	0.43
1:A:883:ILE:HD11	1:A:1424:THR:HA	1.99	0.43
13:b:549:LEU:HD23	13:b:566:LEU:CD1	2.48	0.43
14:d:963:ASP:OD1	14:d:963:ASP:N	2.50	0.43
1:A:410:ASN:OD1	1:A:449:HIS:NE2	2.46	0.43
3:C:5:ASN:OD1	11:K:52:LYS:NZ	2.51	0.43
15:N:32:DG:H2''	15:N:33:DA:H8	1.82	0.43
1:A:937:ASP:OD1	1:A:938:LEU:N	2.50	0.43
15:N:39:DA:H2''	15:N:40:DG:H8	1.82	0.43
8:H:71:ASP:OD1	8:H:72:ASP:N	2.52	0.43
14:d:1002:GLU:HG3	14:d:1036:MET:SD	2.59	0.43
2:B:256:ILE:HD11	2:B:373:LEU:HD21	2.00	0.43
14:d:6:VAL:O	14:d:1091:GLY:N	2.45	0.43
1:A:863:ARG:HB3	1:A:1414:ILE:HG22	2.01	0.43
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.33	0.43
4:D:45:LYS:O	4:D:48:ASN:N	2.51	0.43
14:d:1051:LEU:HB2	14:d:1089:ILE:HD13	2.00	0.43
3:C:123:ASN:OD1	3:C:124:SER:N	2.51	0.43
1:A:94:VAL:HG21	1:A:311:GLN:HA	2.01	0.43
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.54	0.43
16:T:12:DT:H2''	16:T:13:DT:C6	2.54	0.43
2:B:628:VAL:HG12	2:B:629:GLU:O	2.18	0.42
4:D:68:THR:O	4:D:72:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:654:PRO:HA	13:b:659:THR:HG21	2.00	0.42
14:d:196:SER:OG	14:d:203:ASN:OD1	2.37	0.42
15:N:43:DG:H2''	15:N:44:DA:H8	1.83	0.42
1:A:255:VAL:HG23	1:A:280:LEU:HD22	2.01	0.42
2:B:850:ASP:OD1	2:B:850:ASP:N	2.53	0.42
15:N:8:DA:C2'	15:N:9:DT:H71	2.49	0.42
16:T:25:DT:H2''	16:T:26:DC:H6	1.84	0.42
15:N:14:DT:H72	16:T:34:DA:C2	2.53	0.42
1:A:695:ASP:OD1	1:A:695:ASP:N	2.52	0.42
9:I:49:ASP:OD1	9:I:49:ASP:N	2.49	0.42
1:A:413:TYR:HB3	1:A:414:PRO:HD3	2.02	0.42
1:A:595:ILE:HD11	1:A:675:VAL:HG11	2.02	0.42
13:b:831:GLN:O	13:b:837:ARG:NH2	2.52	0.42
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.52	0.42
2:B:1091:ARG:NH2	2:B:1092:ASP:OD1	2.53	0.42
16:T:44:DC:H2''	16:T:45:DT:C6	2.54	0.42
2:B:761:THR:H	2:B:764:MET:HE3	1.85	0.42
13:b:651:ILE:O	13:b:687:SER:OG	2.31	0.42
2:B:967:ILE:HG21	2:B:1048:TYR:OH	2.19	0.42
8:H:49:PRO:O	8:H:147:LYS:NZ	2.49	0.42
14:d:272:LEU:HB3	14:d:314:LEU:HD11	2.02	0.42
14:d:884:ILE:HG22	14:d:885:ASN:H	1.83	0.42
1:A:381:PRO:HG2	1:A:384:ILE:HD12	2.01	0.41
14:d:282:MET:HE2	14:d:305:LEU:HD11	2.01	0.41
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.02	0.41
14:d:907:ASN:OD1	14:d:947:ARG:NH2	2.54	0.41
16:T:3:DC:H2''	16:T:4:DT:C5'	2.50	0.41
1:A:86:GLY:C	1:A:255:VAL:HG12	2.46	0.41
5:E:110:MET:HG2	5:E:114:ALA:HB3	2.03	0.41
5:E:127:LEU:HD23	5:E:127:LEU:H	1.86	0.41
16:T:34:DA:C2'	16:T:35:DT:H5'	2.49	0.41
13:b:678:MET:HE2	13:b:685:LEU:HB2	2.03	0.41
13:b:549:LEU:CD1	13:b:554:ILE:HD11	2.51	0.41
15:N:33:DA:H2''	15:N:34:DG:O5'	2.19	0.41
15:N:45:DG:H1'	15:N:46:DC:H5'	2.01	0.41
3:C:235:SER:OG	3:C:239:LEU:O	2.37	0.41
14:d:218:MET:HB3	14:d:232:ILE:HB	2.02	0.41
6:F:57:MET:HE1	6:F:120:VAL:HG13	2.02	0.41
8:H:51:ASP:N	8:H:54:ASP:OD2	2.45	0.41
13:b:766:CYS:N	13:b:963:LEU:O	2.53	0.41
14:d:8:THR:OG1	14:d:1036:MET:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:41:DC:H2''	15:N:42:DA:N7	2.36	0.41
1:A:349:ARG:NH2	2:B:1070:LEU:HD21	2.36	0.41
1:A:848:ILE:HG21	2:B:496:ALA:HB1	2.03	0.41
1:A:883:ILE:O	1:A:883:ILE:HG22	2.20	0.41
2:B:899:SER:OG	11:K:1:MET:HE2	2.21	0.41
14:d:72:GLU:OE1	14:d:103:ARG:NH2	2.50	0.41
14:d:275:ASP:OD1	14:d:279:ARG:N	2.54	0.41
15:N:4:DG:C2'	15:N:5:DT:H72	2.50	0.41
2:B:292:PHE:HD1	2:B:298:MET:HE1	1.86	0.41
2:B:864:ASP:OD1	2:B:865:VAL:N	2.51	0.41
14:d:207:TRP:CB	14:d:242:GLY:HA2	2.52	0.41
16:T:30:DG:H3'	16:T:31:DG:C4'	2.51	0.41
8:H:7:GLU:OE2	8:H:57:ARG:NH1	2.54	0.40
16:T:31:DG:H2''	16:T:32:DC:O4'	2.20	0.40
18:a:309:PHE:CD1	18:a:318:VAL:HG22	2.56	0.40
2:B:733:MET:HE1	2:B:1054:MET:HE2	2.02	0.40
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.03	0.40
6:F:100:ARG:NH2	6:F:121:ASP:O	2.52	0.40
7:G:30:LEU:HD22	7:G:70:VAL:HG21	2.03	0.40
1:A:883:ILE:HD11	1:A:1424:THR:HG22	2.02	0.40
13:b:575:THR:HA	13:b:578:MET:HE2	2.03	0.40
14:d:929:SER:HB2	14:d:952:ASN:HB2	2.04	0.40
14:d:1005:ASN:ND2	18:a:9:GLN:O	2.46	0.40
18:a:209:SER:OG	18:a:246:GLY:O	2.32	0.40
13:b:497:PHE:HB2	13:b:519:TRP:CE2	2.56	0.40
14:d:1058:LEU:O	14:d:1062:ILE:N	2.53	0.40
1:A:286:ILE:HD12	1:A:309:LEU:HD23	2.04	0.40
1:A:1212:LEU:HD11	1:A:1289:GLU:HB2	2.03	0.40
2:B:735:VAL:HG21	10:J:55:LEU:HD13	2.02	0.40
2:B:962:THR:O	10:J:9:THR:HG23	2.21	0.40
3:C:45:ILE:HG22	3:C:165:ALA:HB1	2.04	0.40
7:G:11:ILE:HD13	7:G:33:GLU:OE1	2.21	0.40
7:G:23:LEU:HD12	7:G:54:ILE:HG21	2.04	0.40
13:b:640:TRP:O	13:b:667:THR:OG1	2.25	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	1402/1970 (71%)	1365 (97%)	37 (3%)	0	100	100
2	B	1123/1174 (96%)	1076 (96%)	47 (4%)	0	100	100
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
13	b	512/1496 (34%)	477 (93%)	35 (7%)	0	100	100
14	d	765/1143 (67%)	721 (94%)	44 (6%)	0	100	100
18	a	363/396 (92%)	343 (94%)	20 (6%)	0	100	100
All	All	5484/7622 (72%)	5263 (96%)	221 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1242/1749 (71%)	1242 (100%)	0	100	100
2	B	992/1027 (97%)	992 (100%)	0	100	100
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	116/126 (92%)	116 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	b	466/1299 (36%)	466 (100%)	0	100	100
14	d	686/1001 (68%)	686 (100%)	0	100	100
18	a	320/348 (92%)	320 (100%)	0	100	100
All	All	4910/6718 (73%)	4910 (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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	735	GLN
1	A	792	ASN
1	A	1077	ASN
1	A	1078	GLN
2	B	227	ASN
2	B	319	ASN
2	B	1160	GLN
4	D	38	HIS
4	D	43	HIS
7	G	60	GLN
8	H	29	HIS
11	K	36	ASN
13	b	616	HIS
13	b	723	GLN

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Mol	Chain	Res	Type
13	b	777	GLN
13	b	852	HIS
14	d	163	HIS
18	a	169	GLN
18	a	228	GLN
18	a	229	HIS
18	a	326	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	P	9	G

There are no RNA pucker outliers to report.

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 12 ligands modelled in this entry, 10 are 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
22	BEF	b	1502	-	0,3,3	-	-	-	-	-
21	ADP	b	1501	20	27,29,29	1.26	4 (14%)	42,45,45	1.96	12 (28%)

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
21	ADP	b	1501	20	-	2/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1501	ADP	C5-C4	3.76	1.46	1.39
21	b	1501	ADP	C5-N7	-2.37	1.34	1.39
21	b	1501	ADP	C4-N9	-2.36	1.32	1.37
21	b	1501	ADP	C8-N7	2.11	1.35	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1501	ADP	C5-C4-N3	-5.38	119.73	126.75
21	b	1501	ADP	N3-C4-N9	4.87	135.11	127.08
21	b	1501	ADP	C4-N9-C8	3.88	109.93	105.73
21	b	1501	ADP	C2-N3-C4	3.86	120.86	111.75
21	b	1501	ADP	N3-C2-N1	-3.83	122.61	128.60
21	b	1501	ADP	N9-C8-N7	-2.73	110.17	113.91
21	b	1501	ADP	PA-O3A-PB	-2.46	124.40	132.83
21	b	1501	ADP	C5-N7-C8	2.41	106.93	103.51
21	b	1501	ADP	C4-C5-N7	-2.31	107.81	110.62
21	b	1501	ADP	C5-C6-N6	-2.29	118.45	123.43
21	b	1501	ADP	C6-C5-N7	2.07	135.89	132.02
21	b	1501	ADP	N6-C6-N1	2.04	122.83	118.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

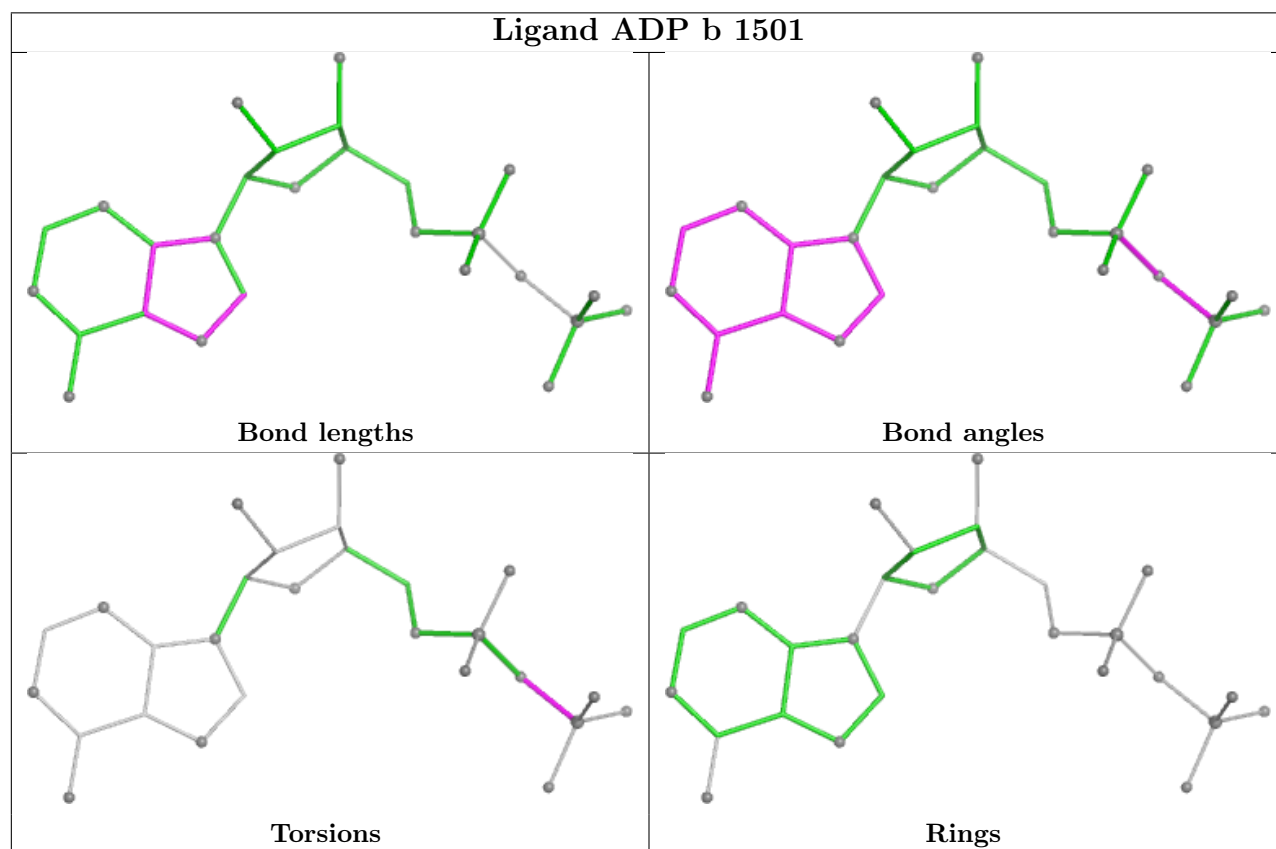
Mol	Chain	Res	Type	Atoms
21	b	1501	ADP	PA-O3A-PB-O1B
21	b	1501	ADP	PA-O3A-PB-O3B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	1502	BEF	1	0
21	b	1501	ADP	2	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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

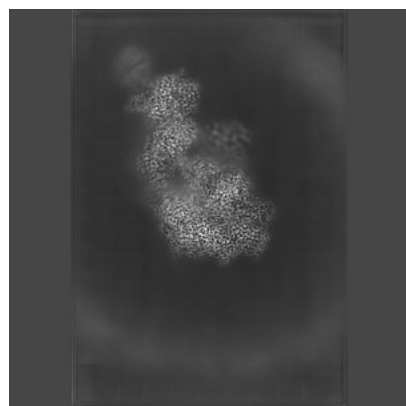
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13009. These allow visual inspection of the internal detail of the map and identification of artifacts.

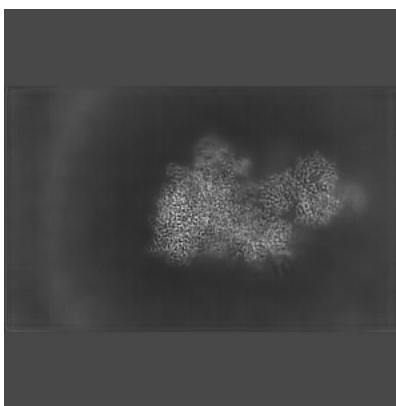
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

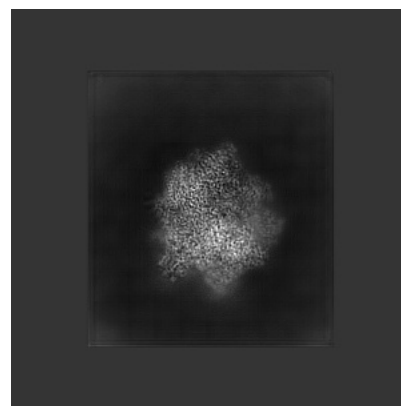
6.1.1 Primary map



X

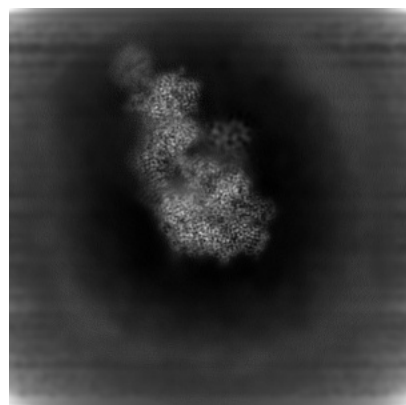


Y

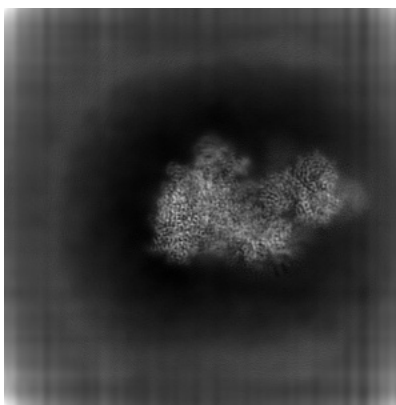


Z

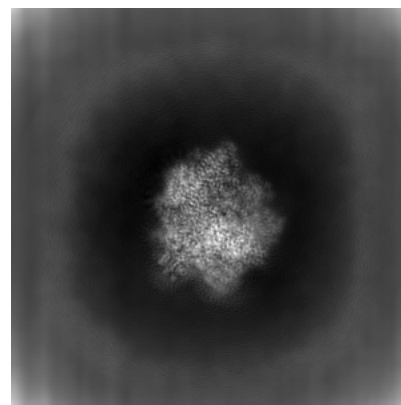
6.1.2 Raw map



X



Y

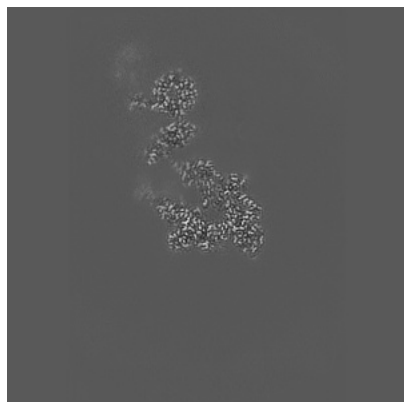


Z

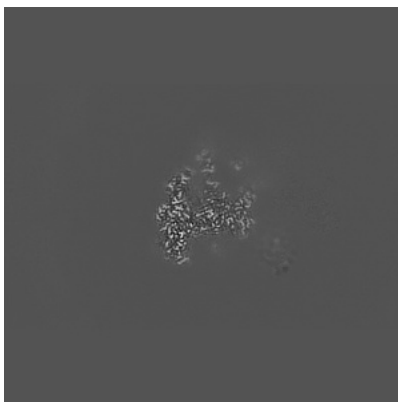
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

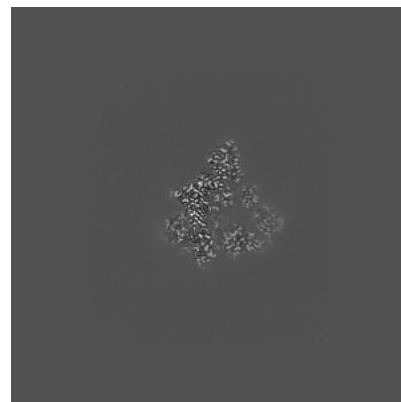
6.2.1 Primary map



X Index: 200

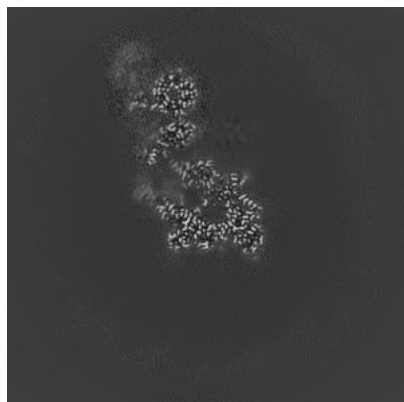


Y Index: 200

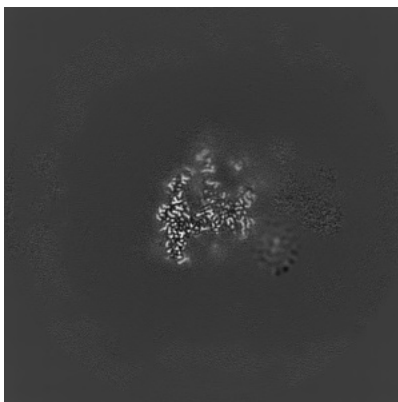


Z Index: 200

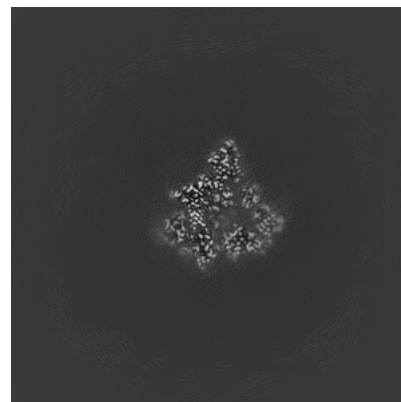
6.2.2 Raw map



X Index: 200



Y Index: 200

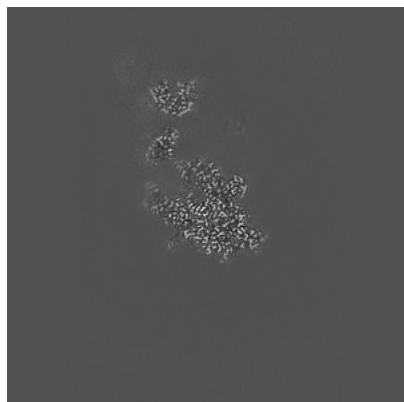


Z Index: 200

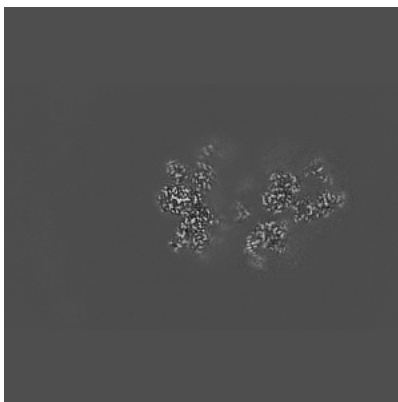
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

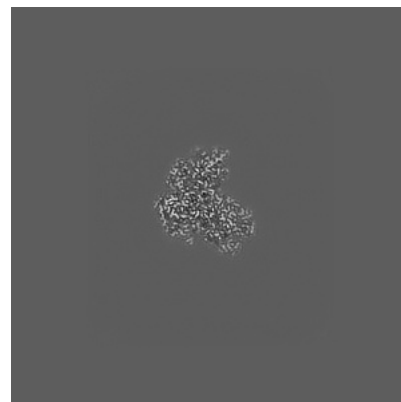
6.3.1 Primary map



X Index: 191

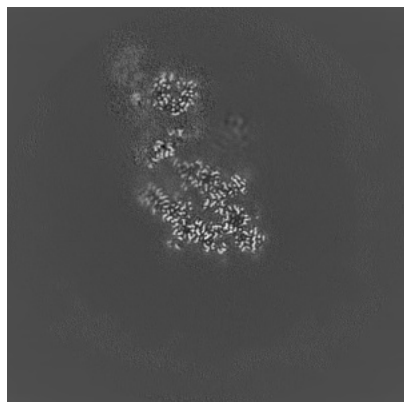


Y Index: 172

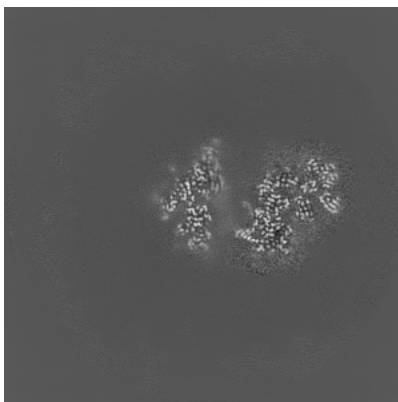


Z Index: 174

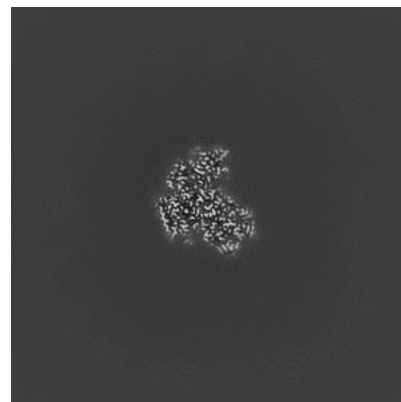
6.3.2 Raw map



X Index: 195



Y Index: 164

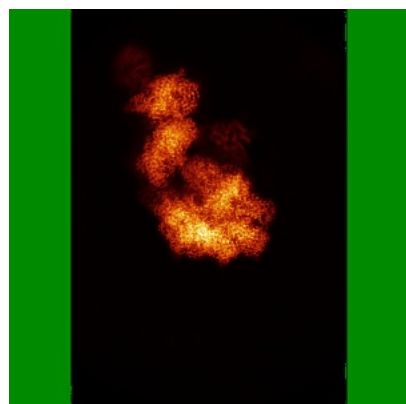


Z Index: 173

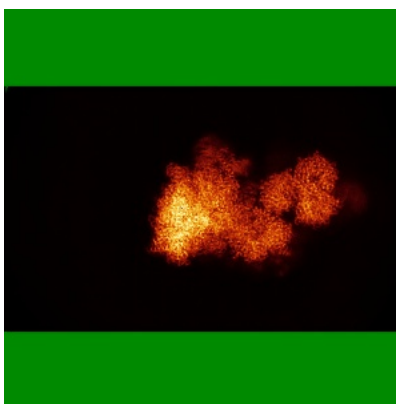
The images above show the largest variance slices of the map in three orthogonal directions.

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

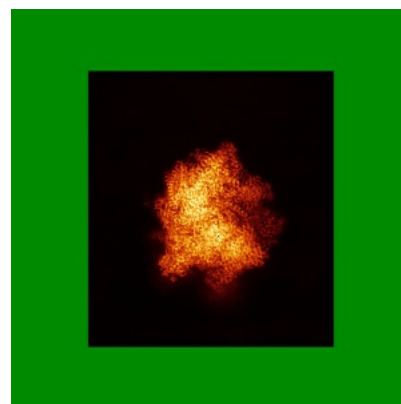
6.4.1 Primary map



X

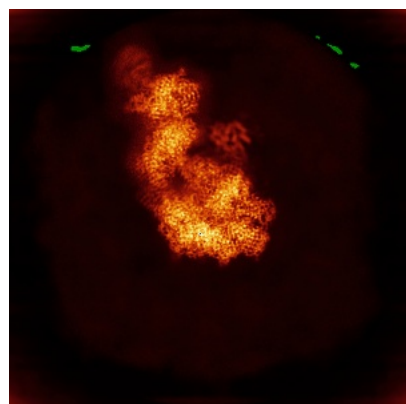


Y

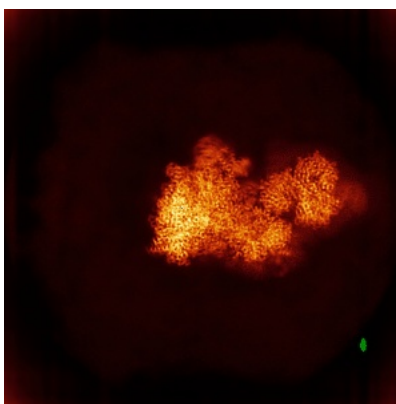


Z

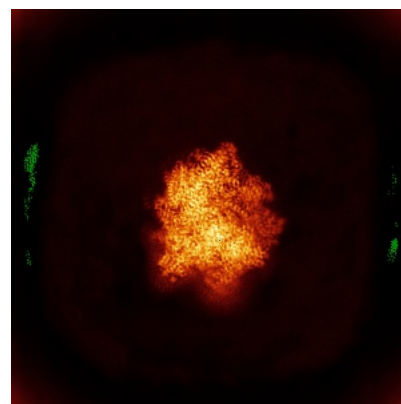
6.4.2 Raw map



X



Y

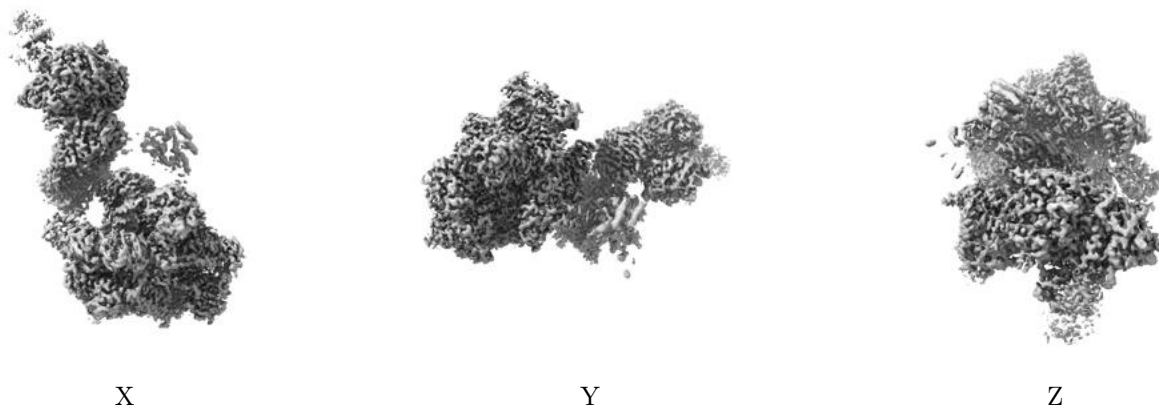


Z

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.

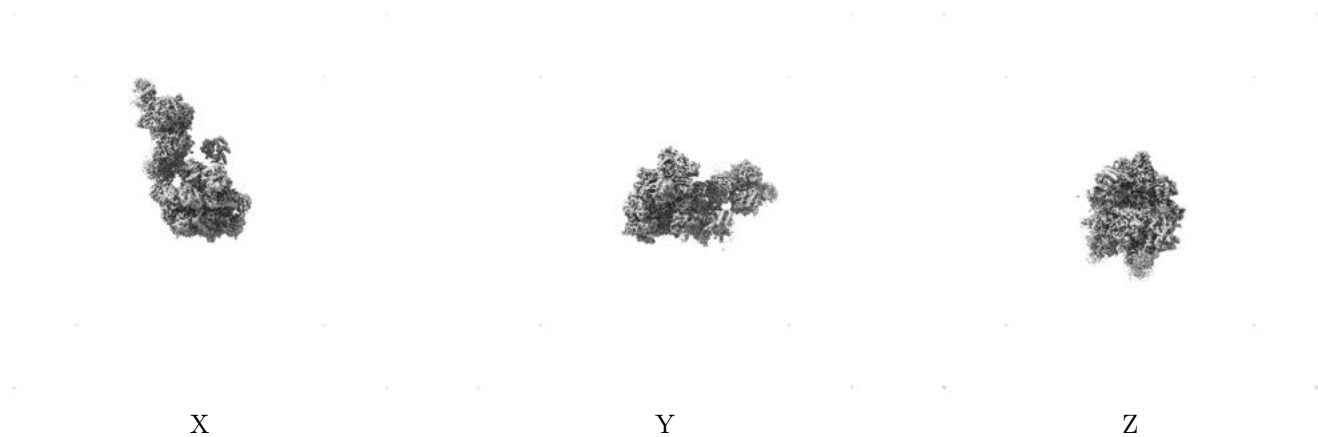
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

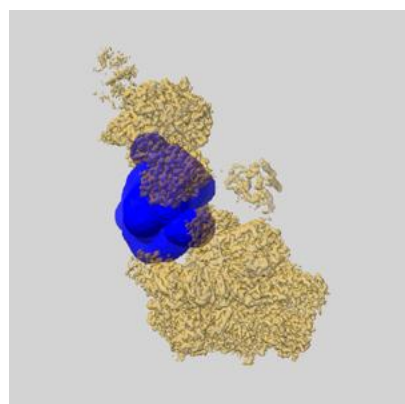
6.6 Mask visualisation [i](#)

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

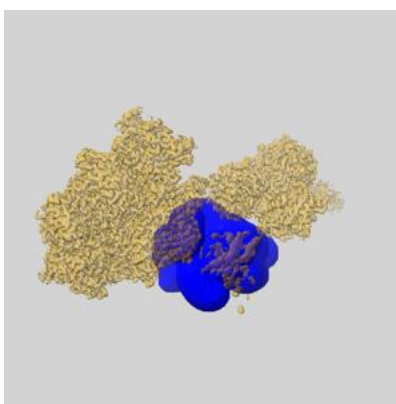
A mask typically either:

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

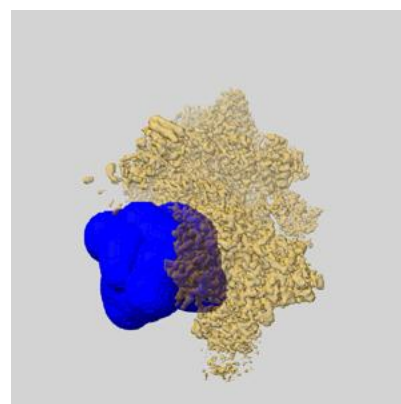
6.6.1 emd_13009_msk_4.map [i](#)



X

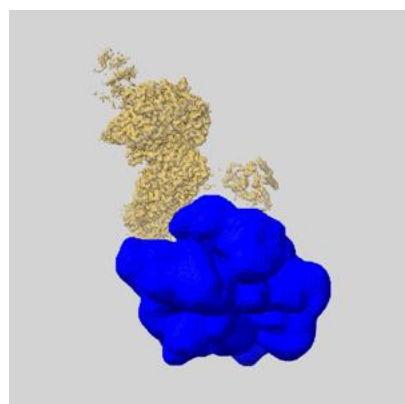


Y

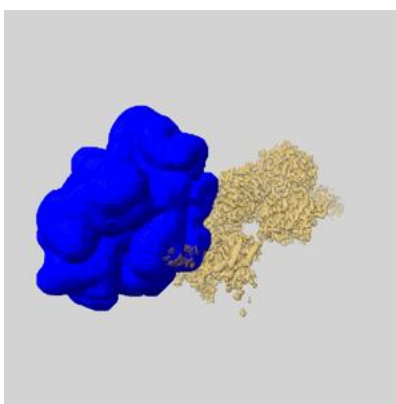


Z

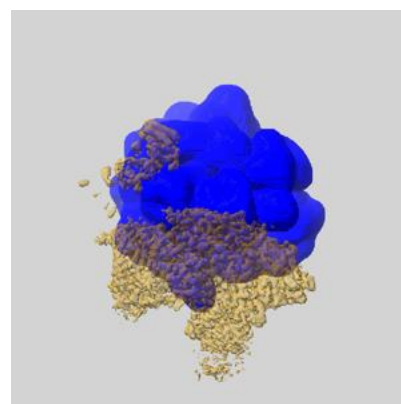
6.6.2 emd_13009_msk_3.map [i](#)



X

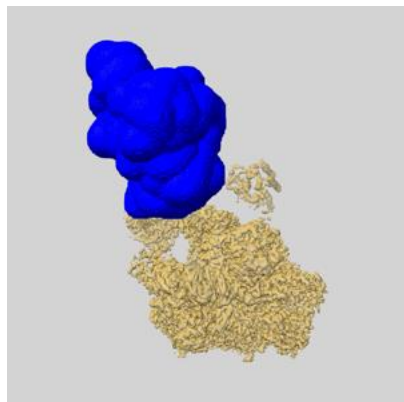


Y

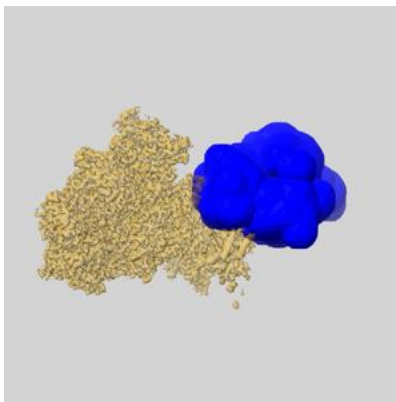


Z

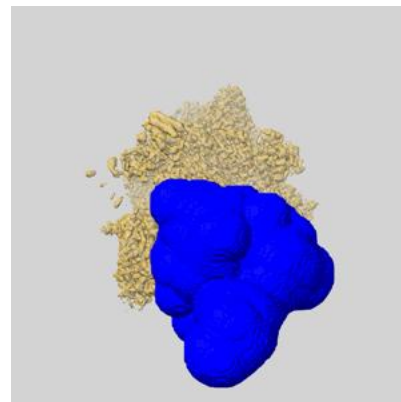
6.6.3 emd_13009_msk_2.map [i](#)



X

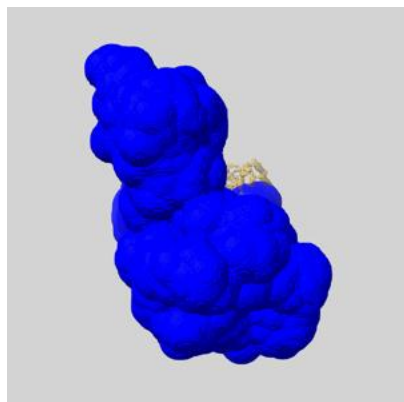


Y

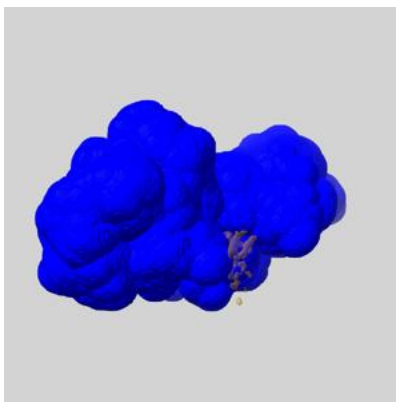


Z

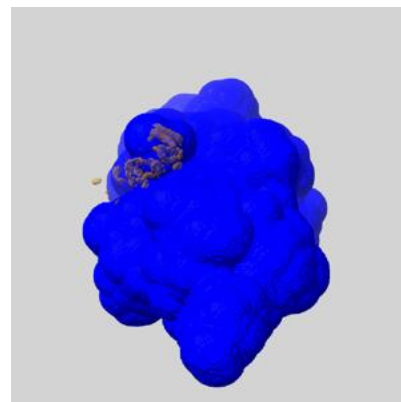
6.6.4 emd_13009_msk_1.map [i](#)



X



Y

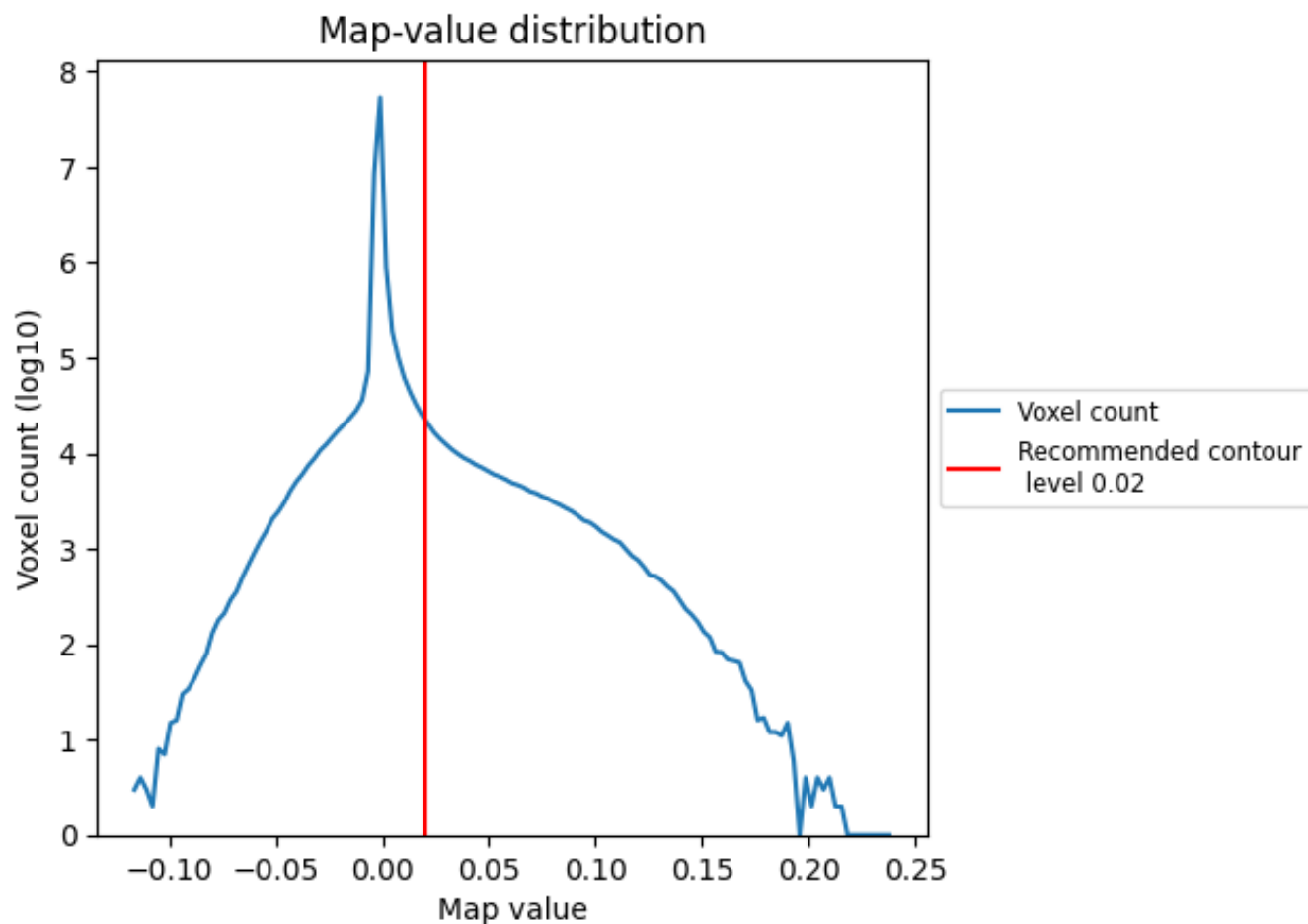


Z

7 Map analysis [i](#)

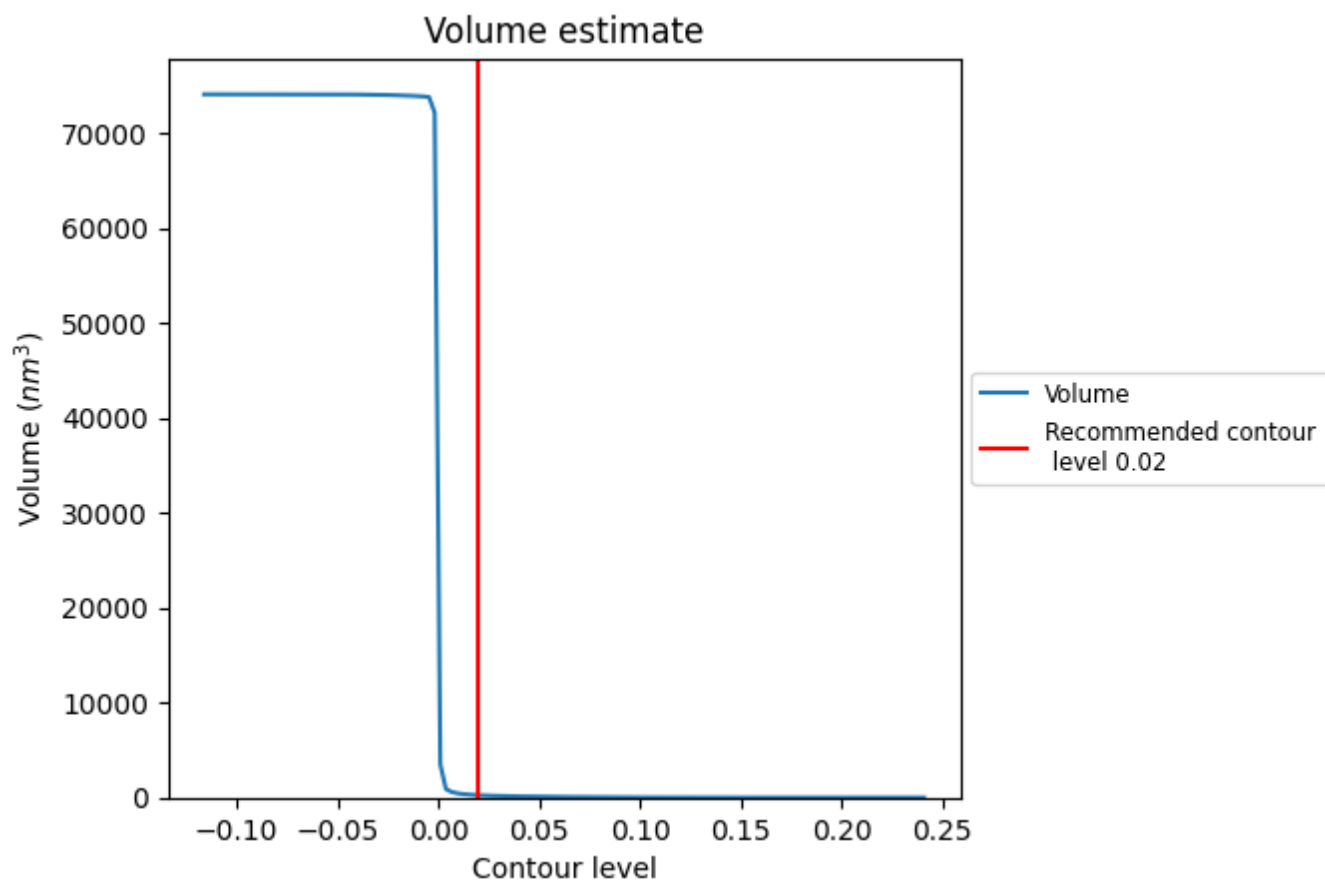
This section contains the results of statistical analysis of the map.

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.

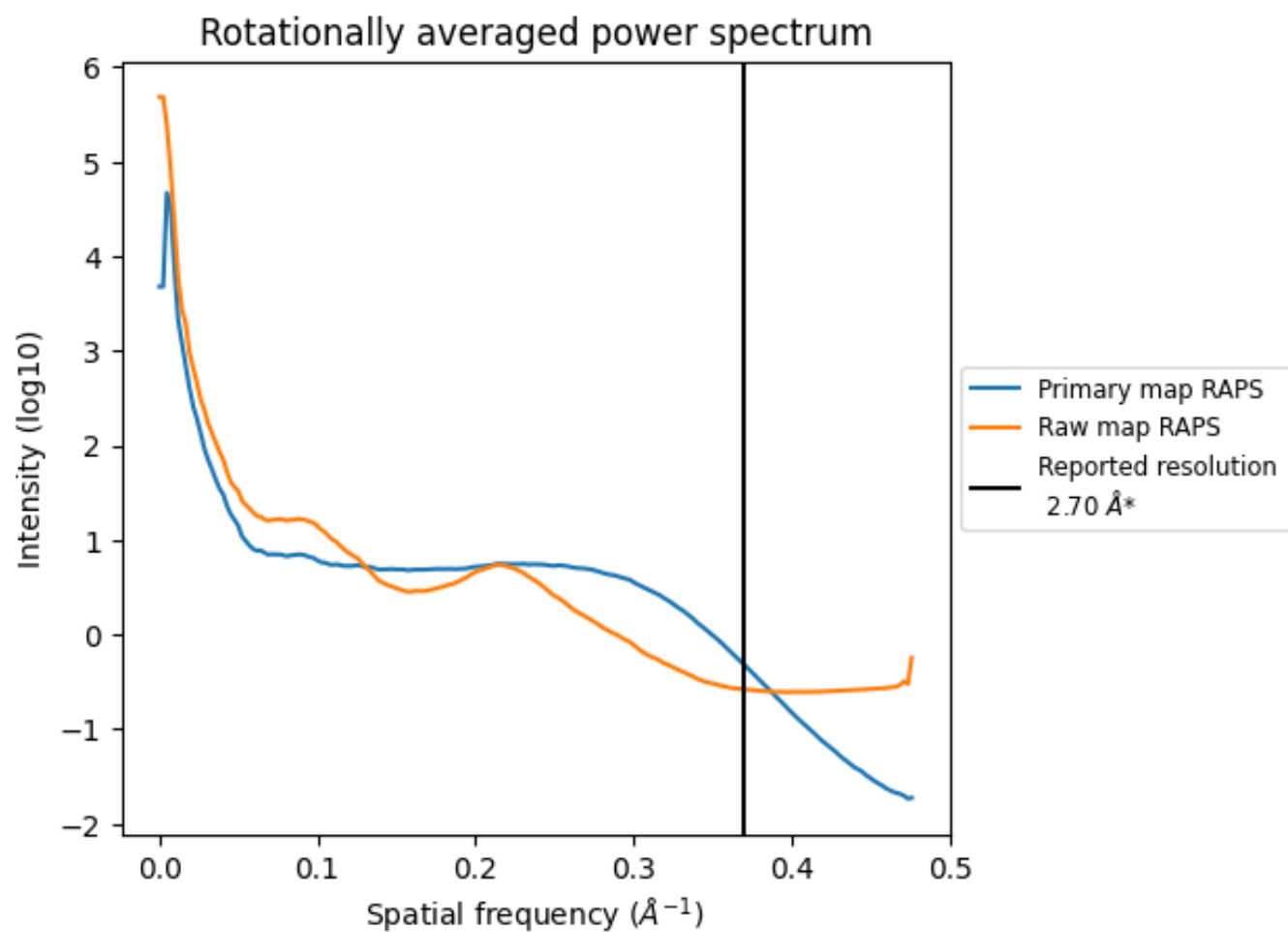
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm^3 ; this corresponds to an approximate mass of 223 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 ⓘ

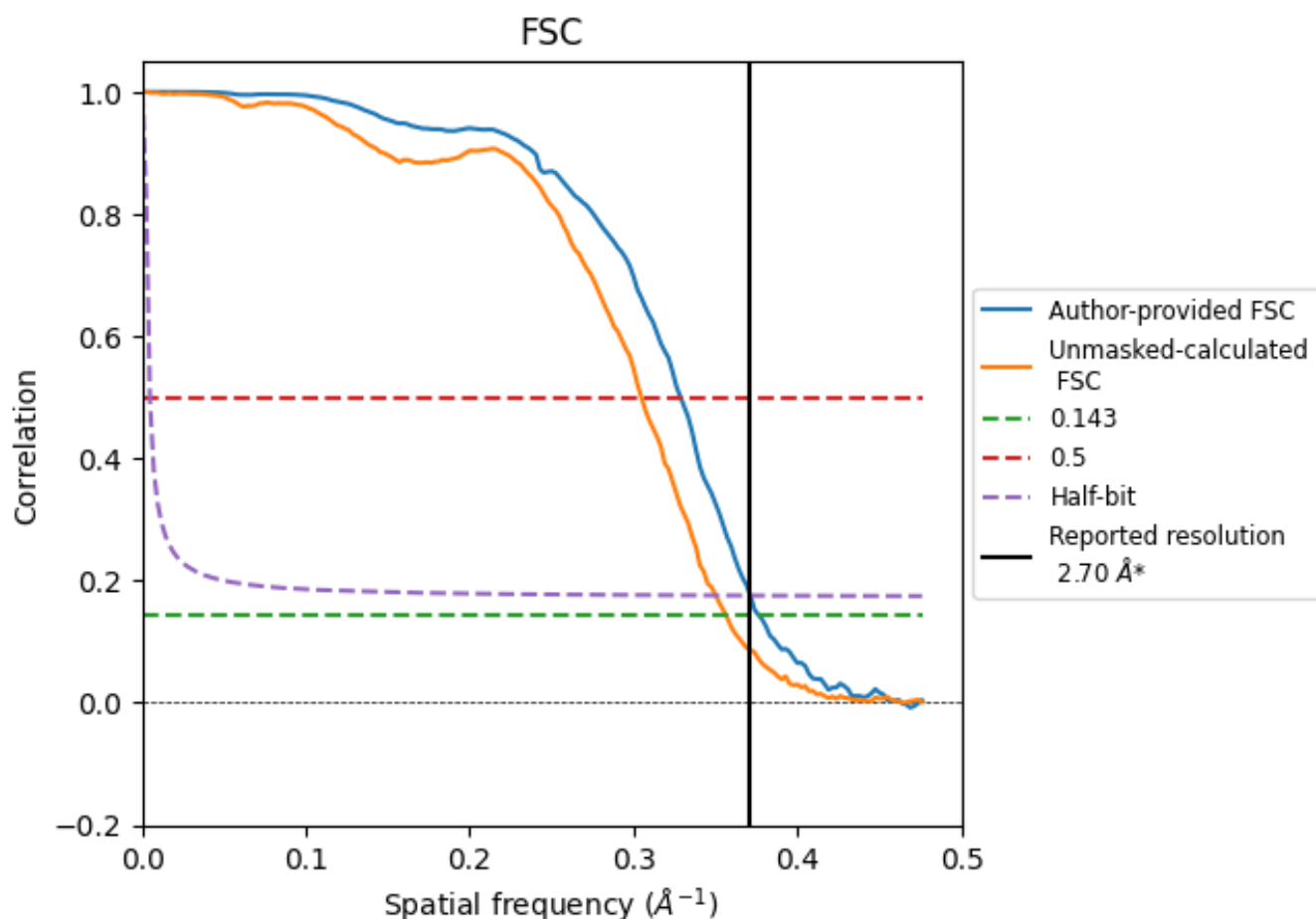


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

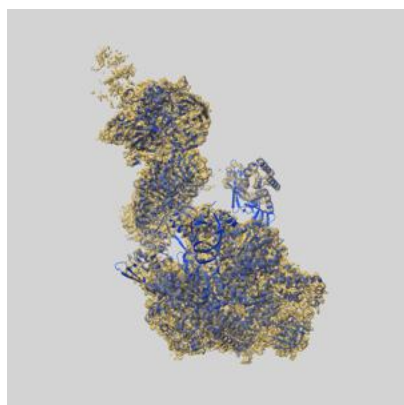
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.66	3.04	2.69
Unmasked-calculated*	2.81	3.28	2.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

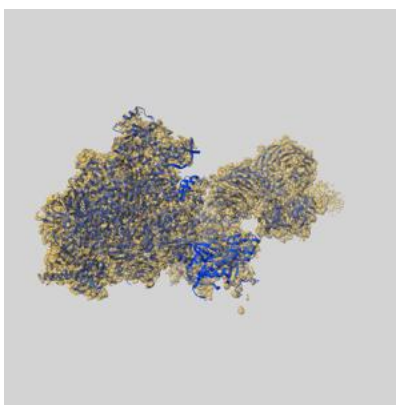
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13009 and PDB model 7OOB. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

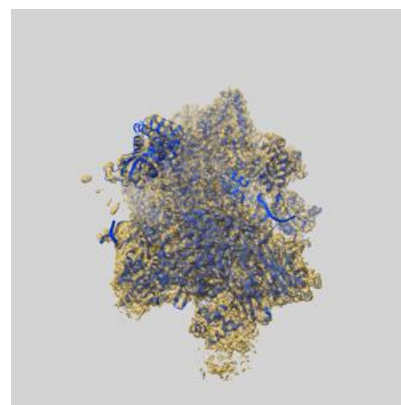
9.1 Map-model overlay [i](#)



X



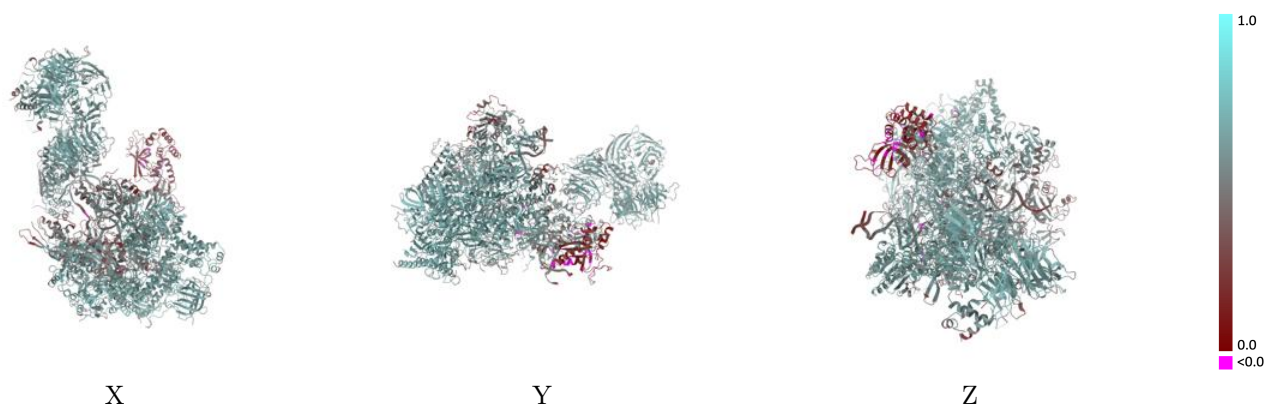
Y



Z

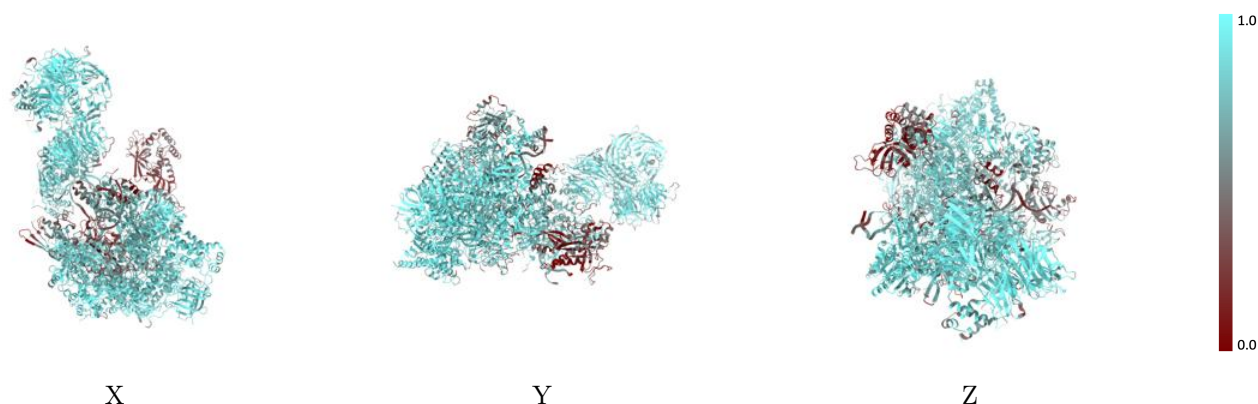
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



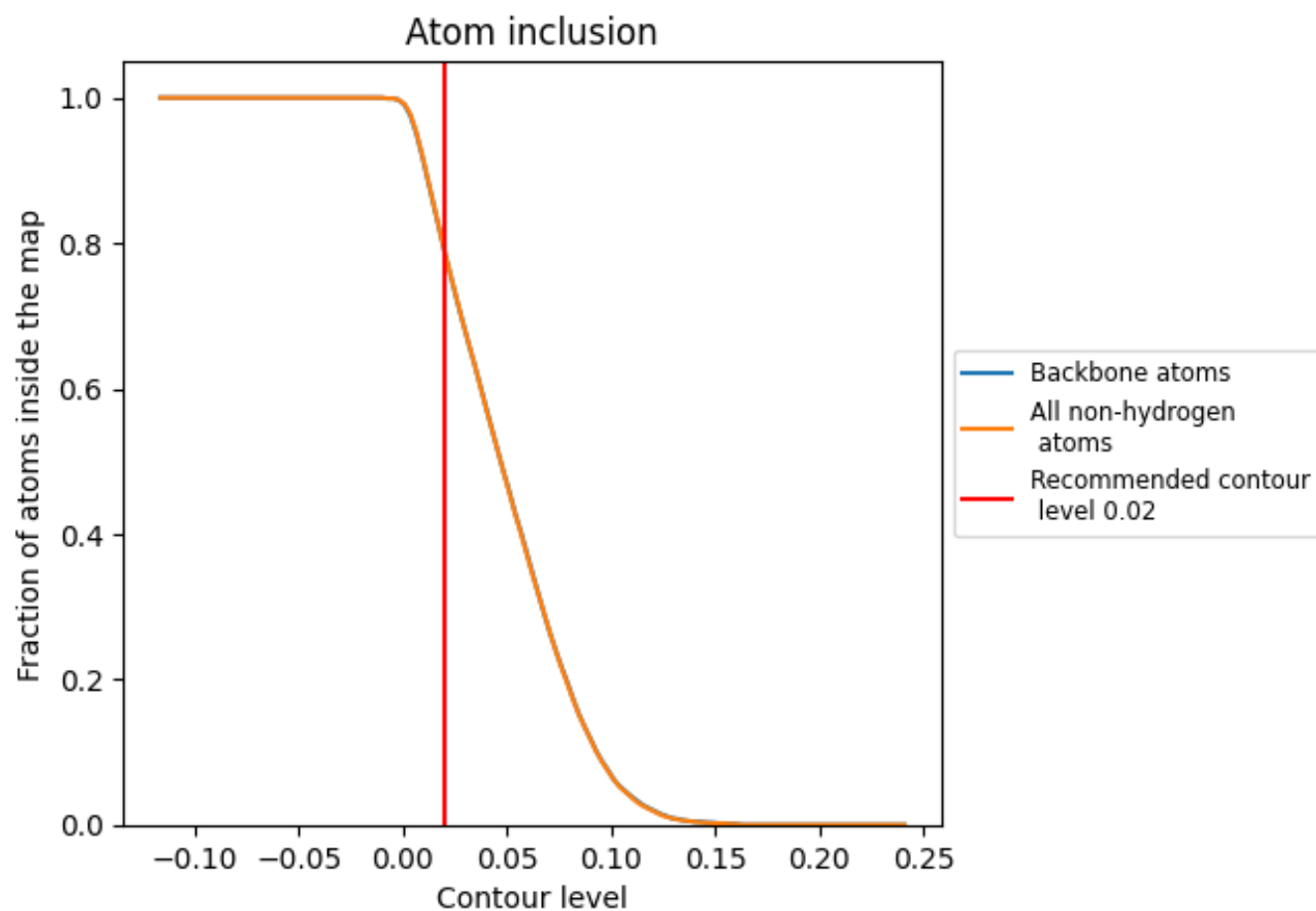
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.5660
A	 0.7980	 0.5810
B	 0.8190	 0.5900
C	 0.8980	 0.6280
D	 0.2350	 0.1820
E	 0.7920	 0.5690
F	 0.8510	 0.6030
G	 0.2930	 0.2910
H	 0.8820	 0.6130
I	 0.6810	 0.5050
J	 0.9230	 0.6540
K	 0.9060	 0.6290
L	 0.7180	 0.5180
N	 0.5750	 0.4840
P	 0.9500	 0.6530
T	 0.6470	 0.4900
a	 0.8700	 0.5970
b	 0.8640	 0.5760
d	 0.8650	 0.5880

