



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:11 PM UTC

PDB ID : 9G9I / pdb_00009g9i
EMDB ID : EMD-51153
Title : CryoEM structure of Enterococcus italicus Csm-crRNA-CTR2 complex bound to pNppA3 and AMPNPP
Authors : Jungfer, K.; Jinek, M.
Deposited on : 2024-07-25
Resolution : 3.31 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

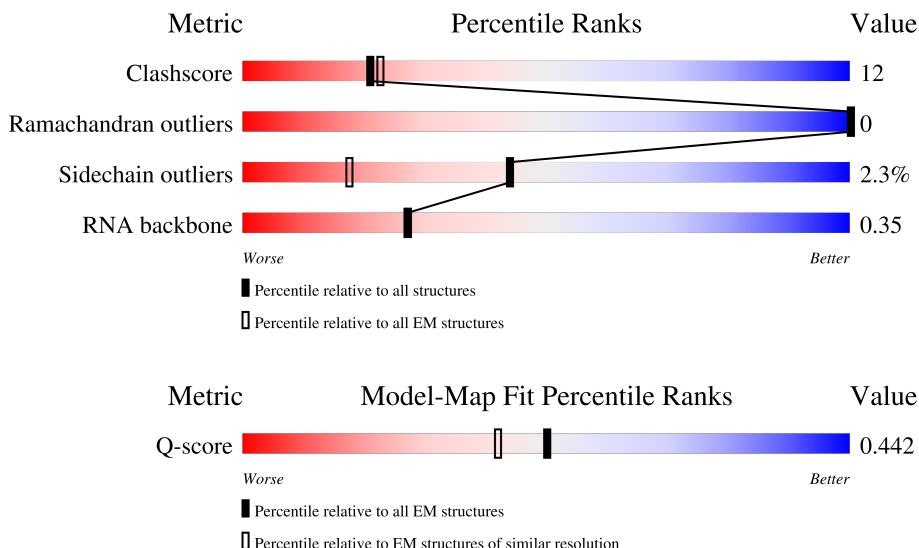
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.31 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	14550 (2.81 - 3.81)

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	774	
2	B	140	
2	C	140	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	214	66% 24% 9%
3	E	214	8% 71% 28%
3	F	214	10% 56% 29% 14%
4	G	307	68% 28%
5	R	45	11% 29% 16% 44%
6	H	379	58% 53% 23% 24%
7	T	47	15% 19% 64%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17927 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 CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	720	5763	3678	952	1109	24	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP E6LHV7
A	-17	HIS	-	expression tag	UNP E6LHV7
A	-16	HIS	-	expression tag	UNP E6LHV7
A	-15	HIS	-	expression tag	UNP E6LHV7
A	-14	HIS	-	expression tag	UNP E6LHV7
A	-13	HIS	-	expression tag	UNP E6LHV7
A	-12	HIS	-	expression tag	UNP E6LHV7
A	-11	HIS	-	expression tag	UNP E6LHV7
A	-10	HIS	-	expression tag	UNP E6LHV7
A	-9	HIS	-	expression tag	UNP E6LHV7
A	-8	HIS	-	expression tag	UNP E6LHV7
A	-7	LEU	-	expression tag	UNP E6LHV7
A	-6	GLU	-	expression tag	UNP E6LHV7
A	-5	VAL	-	expression tag	UNP E6LHV7
A	-4	LEU	-	expression tag	UNP E6LHV7
A	-3	PHE	-	expression tag	UNP E6LHV7
A	-2	GLN	-	expression tag	UNP E6LHV7
A	-1	GLY	-	expression tag	UNP E6LHV7
A	0	PRO	-	expression tag	UNP E6LHV7
A	1	SER	-	expression tag	UNP E6LHV7

- Molecule 2 is a protein called CRISPR system Cms protein Csm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	111	932	606	152	173	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	114	Total	C	N	O	S	0	0
			958	623	158	176	1		

- Molecule 3 is a protein called CRISPR system Cms endoribonuclease Csm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	194	Total	C	N	O	S	0	0
			1508	951	267	287	3		
3	E	213	Total	C	N	O	S	0	0
			1643	1034	292	313	4		
3	F	184	Total	C	N	O	S	0	0
			1426	899	253	271	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	ALA	ASP	engineered mutation	UNP E6LHV5
E	32	ALA	ASP	engineered mutation	UNP E6LHV5
F	32	ALA	ASP	engineered mutation	UNP E6LHV5

- Molecule 4 is a protein called CRISPR system Cms protein Csm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	297	Total	C	N	O	S	0	0
			2349	1515	385	444	5		

- Molecule 5 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	25	Total	C	N	O	P	0	0
			533	240	102	167	24		

- Molecule 6 is a protein called CRISPR system Cms protein Csm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	289	Total	C	N	O	S	0	0
			2346	1516	404	419	7		

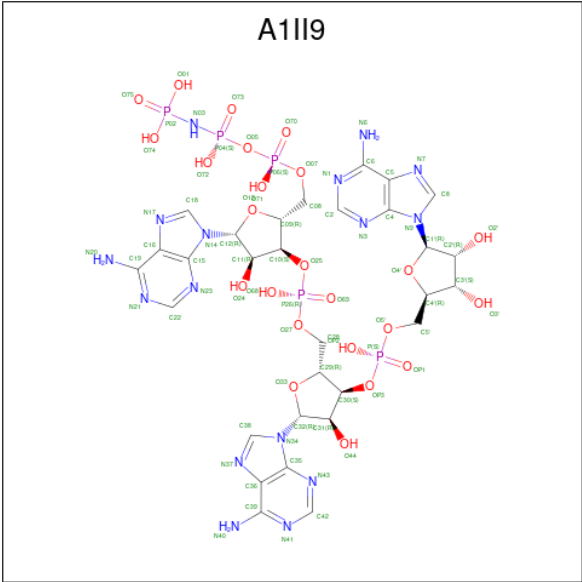
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	350	LEU	-	expression tag	UNP E6LHV3
H	351	GLU	-	expression tag	UNP E6LHV3
H	352	VAL	-	expression tag	UNP E6LHV3
H	353	LEU	-	expression tag	UNP E6LHV3
H	354	PHE	-	expression tag	UNP E6LHV3
H	355	GLN	-	expression tag	UNP E6LHV3
H	356	GLY	-	expression tag	UNP E6LHV3
H	357	PRO	-	expression tag	UNP E6LHV3
H	358	GLY	-	expression tag	UNP E6LHV3
H	359	GLY	-	expression tag	UNP E6LHV3
H	360	GLY	-	expression tag	UNP E6LHV3
H	361	TRP	-	expression tag	UNP E6LHV3
H	362	SER	-	expression tag	UNP E6LHV3
H	363	HIS	-	expression tag	UNP E6LHV3
H	364	PRO	-	expression tag	UNP E6LHV3
H	365	GLN	-	expression tag	UNP E6LHV3
H	366	PHE	-	expression tag	UNP E6LHV3
H	367	GLU	-	expression tag	UNP E6LHV3
H	368	LYS	-	expression tag	UNP E6LHV3
H	369	GLY	-	expression tag	UNP E6LHV3
H	370	GLY	-	expression tag	UNP E6LHV3
H	371	GLY	-	expression tag	UNP E6LHV3
H	372	TRP	-	expression tag	UNP E6LHV3
H	373	SER	-	expression tag	UNP E6LHV3
H	374	HIS	-	expression tag	UNP E6LHV3
H	375	PRO	-	expression tag	UNP E6LHV3
H	376	GLN	-	expression tag	UNP E6LHV3
H	377	PHE	-	expression tag	UNP E6LHV3
H	378	GLU	-	expression tag	UNP E6LHV3
H	379	LYS	-	expression tag	UNP E6LHV3

- Molecule 7 is a RNA chain called CTR.

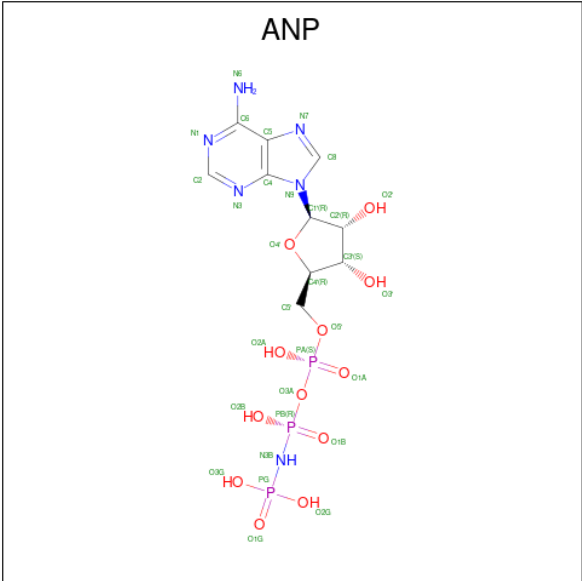
Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	17	Total	C	N	O	P	0	0
			361	161	62	121	17		

- Molecule 8 is adenosine-5'-[(beta,gamma)-imido]triphosphate-adenosine-monophosphate-a denosine-monophosphate (CCD ID: A1II9) (formula: C₃₀H₄₁N₁₆O₂₄P₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			75	30	16	24	5	

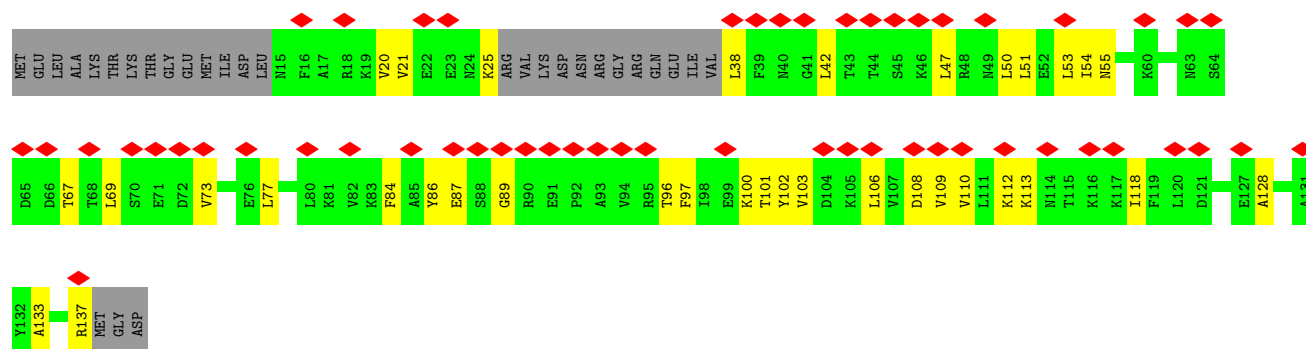
- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



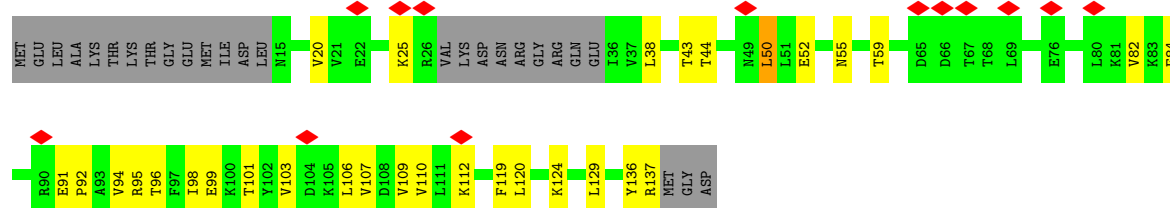
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

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

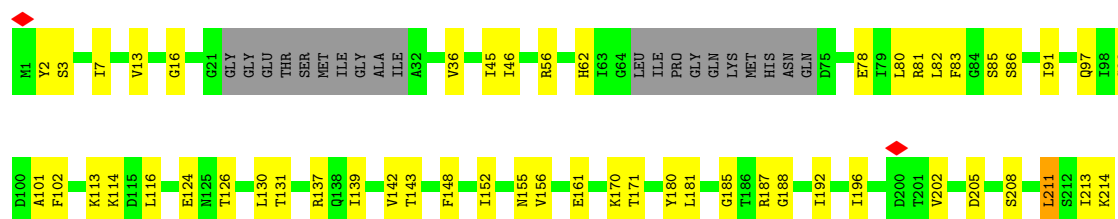
Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Mg	0
			2	2	



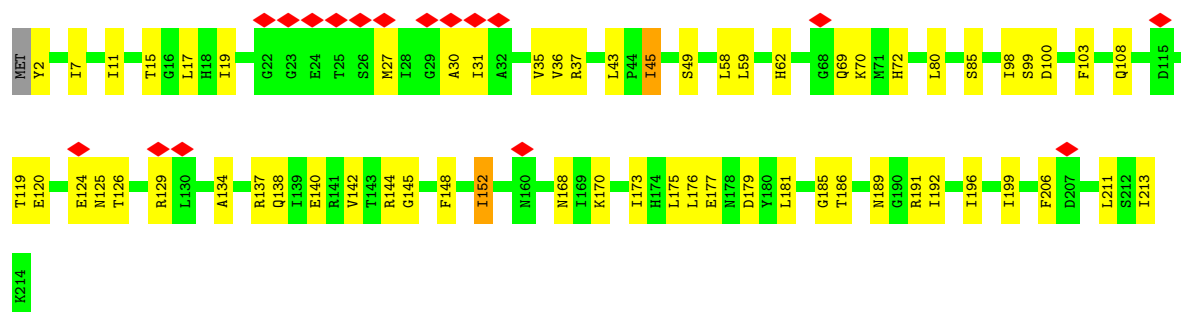
- Molecule 2: CRISPR system Cms protein Csm2



- Molecule 3: CRISPR system Cms endoribonuclease Csm3

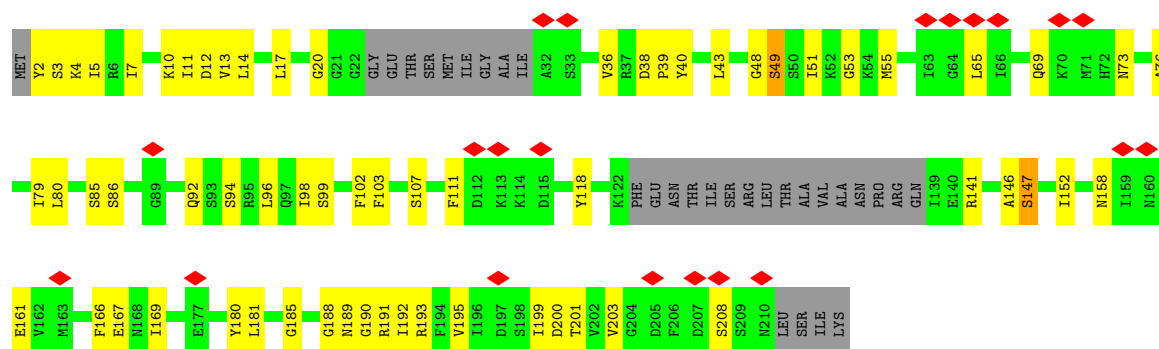


- Molecule 3: CRISPR system Cms endoribonuclease Csm3



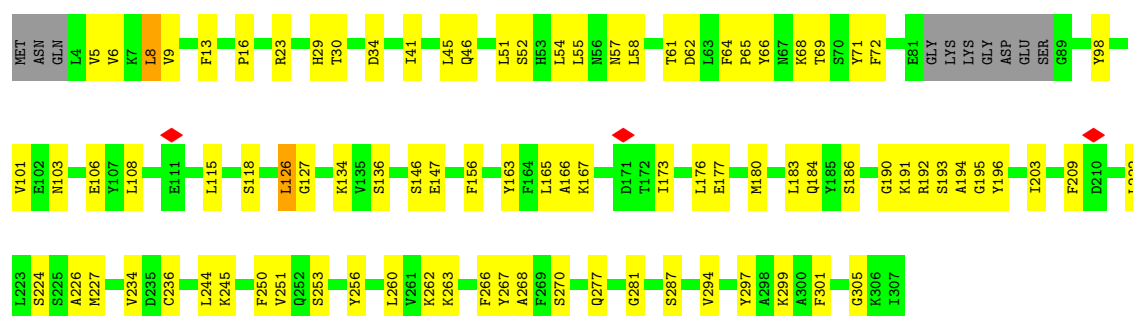
- Molecule 3: CRISPR system Cms endoribonuclease Csm3





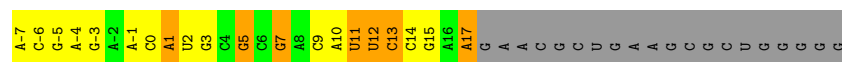
• Molecule 4: CRISPR system Cms protein Csm4

Chain G: 68% 28%



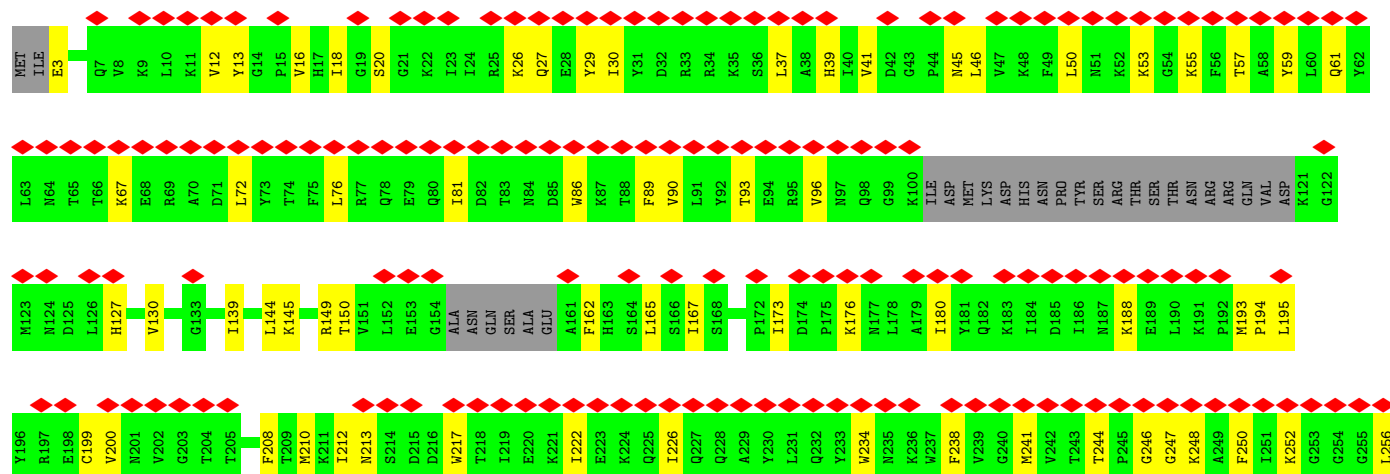
• Molecule 5: crRNA

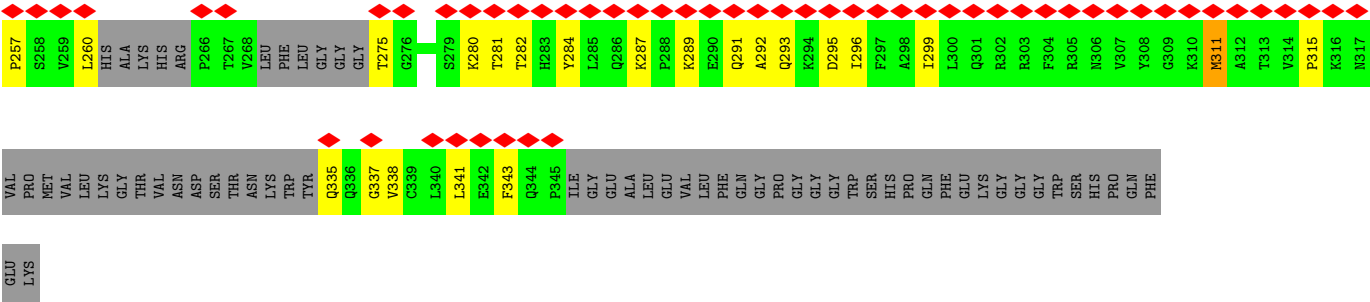
Chain R: 11% 29% 16% 44%



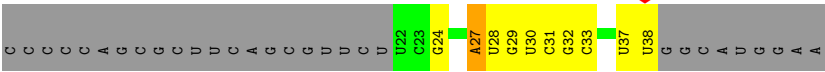
• Molecule 6: CRISPR system Cms protein Csm5

Chain H: 58% 53% 23% 24%





● Molecule 7: CTR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67.12	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.568	Depositor
Minimum map value	-0.344	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.071	Depositor
Map size ($\text{\AA}$)	312.0, 312.0, 312.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.65, 0.65, 0.65	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: MG, A1II9, ANP

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	0.28	0/5870	0.48	2/7917 (0.0%)
2	B	0.23	0/974	0.45	0/1310
2	C	0.21	0/948	0.39	0/1275
3	D	0.15	0/1530	0.35	0/2056
3	E	0.22	0/1669	0.39	0/2246
3	F	0.29	0/1448	0.45	0/1944
4	G	0.26	0/2397	0.45	2/3230 (0.1%)
5	R	0.64	0/597	0.94	0/929
6	H	0.16	0/2395	0.34	0/3223
7	T	0.71	0/402	0.87	0/624
All	All	0.28	0/18230	0.47	4/24754 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ASP	N-CA-C	-7.21	105.01	113.88
4	G	8	LEU	CA-C-N	-5.28	116.64	123.19
4	G	8	LEU	C-N-CA	-5.28	116.64	123.19
1	A	496	ASP	N-CA-C	-5.13	106.14	114.09

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	5763	0	5756	128	0
2	B	958	0	980	26	0
2	C	932	0	947	26	0
3	D	1508	0	1527	37	0
3	E	1643	0	1663	50	0
3	F	1426	0	1433	50	0
4	G	2349	0	2351	65	0
5	R	533	0	274	15	0
6	H	2346	0	2398	57	0
7	T	361	0	183	5	0
8	A	75	0	0	0	0
9	A	31	0	13	1	0
10	A	2	0	0	0	0
All	All	17927	0	17525	417	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 12.

All (417) 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)
4:G:68:LYS:HG2	4:G:69:THR:HG23	1.43	0.99
4:G:8:LEU:HD11	4:G:163:TYR:HD2	1.28	0.98
1:A:441:VAL:HG11	1:A:467:LYS:HG2	1.56	0.87
3:E:43:LEU:HD11	3:E:108:GLN:HE21	1.43	0.83
3:F:85:SER:HB3	3:F:92:GLN:H	1.46	0.81
4:G:8:LEU:HD11	4:G:163:TYR:CD2	2.16	0.77
2:B:109:VAL:HA	2:B:112:LYS:HD2	1.67	0.74
2:B:110:VAL:HG21	2:B:119:PHE:HB2	1.70	0.73
3:E:45:ILE:HD11	3:E:100:ASP:HB3	1.71	0.73
2:B:98:ILE:HG23	2:B:103:VAL:HG23	1.72	0.72
4:G:245:LYS:HG3	4:G:270:SER:HB2	1.70	0.72
6:H:144:LEU:HB3	6:H:167:ILE:HG21	1.72	0.71
4:G:45:LEU:HG	4:G:51:LEU:HD21	1.72	0.71
3:D:130:LEU:HG	3:D:131:THR:HG23	1.73	0.70
3:F:188:GLY:HA2	3:F:191:ARG:HH12	1.54	0.70
3:F:5:ILE:HA	3:F:201:THR:HA	1.74	0.70
2:C:128:ALA:HA	2:B:82:VAL:HG21	1.72	0.69
1:A:7:LEU:HD23	1:A:74:VAL:HB	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:65:PRO:HB3	4:G:126:LEU:HG	1.74	0.69
3:D:99:SER:HA	4:G:195:GLY:HA2	1.74	0.69
2:C:50:LEU:O	2:C:54:ILE:HD12	1.92	0.68
1:A:705:ILE:HG12	2:B:124:LYS:HG2	1.75	0.68
3:E:124:GLU:HA	5:R:13:C:H5''	1.76	0.67
3:E:37:ARG:HH12	3:E:119:THR:HG21	1.59	0.67
1:A:266:ASN:HA	1:A:630:SER:HB3	1.76	0.66
1:A:318:PRO:HB2	1:A:320:THR:HG23	1.76	0.66
1:A:129:TYR:HB3	1:A:142:PRO:HB2	1.77	0.65
1:A:224:GLU:HG3	1:A:320:THR:HB	1.79	0.65
3:E:185:GLY:HA2	3:E:189:ASN:H	1.61	0.65
6:H:165:LEU:HA	6:H:212:ILE:HG22	1.79	0.64
3:F:200:ASP:HA	3:F:208:SER:HB2	1.79	0.64
3:F:51:ILE:O	3:F:55:MET:HG3	1.98	0.63
1:A:580:TYR:CZ	1:A:582:GLY:HA3	2.34	0.63
3:E:15:THR:HG22	3:F:102:PHE:HZ	1.62	0.63
3:E:137:ARG:HD3	7:T:27:A:C6	2.34	0.63
4:G:190:GLY:HA2	5:R:-4:A:H5''	1.81	0.63
3:D:46:ILE:HB	3:D:101:ALA:HB3	1.81	0.62
1:A:139:TYR:HB3	1:A:566:GLU:HG2	1.80	0.62
1:A:441:VAL:CG1	1:A:467:LYS:HG2	2.28	0.62
6:H:292:ALA:O	6:H:296:ILE:HG22	2.00	0.62
3:E:59:LEU:HD21	3:E:168:ASN:HB3	1.81	0.62
3:E:176:LEU:HD11	3:E:181:LEU:HD13	1.81	0.62
1:A:628:PRO:HB2	1:A:631:LYS:HB2	1.81	0.62
4:G:191:LYS:HG3	4:G:194:ALA:HB3	1.82	0.62
6:H:12:VAL:HG11	6:H:200:VAL:HG13	1.81	0.62
4:G:34:ASP:HA	4:G:297:TYR:HB3	1.82	0.61
1:A:388:LEU:HD11	4:G:234:VAL:HA	1.82	0.61
6:H:234:TRP:HD1	6:H:238:PHE:HB3	1.64	0.61
1:A:528:ARG:HB2	1:A:636:THR:HG22	1.83	0.61
2:C:110:VAL:HG22	2:C:118:ILE:HG22	1.81	0.61
3:E:43:LEU:HD11	3:E:108:GLN:NE2	2.16	0.60
3:F:7:ILE:HG22	3:F:199:ILE:HA	1.84	0.60
1:A:442:VAL:HG12	1:A:454:ARG:HD2	1.84	0.60
3:D:124:GLU:HA	5:R:7:G:H5''	1.83	0.60
2:B:106:LEU:O	2:B:110:VAL:HG12	2.02	0.59
1:A:287:LEU:O	1:A:291:VAL:HG23	2.01	0.59
2:C:89:GLY:HA2	6:H:67:LYS:HG3	1.84	0.59
2:C:109:VAL:HG23	2:C:112:LYS:HE2	1.84	0.59
2:C:25:LYS:HA	2:C:38:LEU:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:39:HIS:HB3	6:H:90:VAL:HG11	1.85	0.58
1:A:221:TYR:HA	1:A:320:THR:HG22	1.85	0.58
6:H:96:VAL:HG22	6:H:180:ILE:HD12	1.84	0.58
4:G:244:LEU:HD21	4:G:267:TYR:HB3	1.86	0.58
2:C:69:LEU:H	2:C:69:LEU:HD12	1.69	0.58
6:H:53:LYS:HG2	6:H:55:LYS:HD3	1.85	0.58
1:A:124:LYS:HB2	1:A:613:LYS:HD3	1.85	0.58
1:A:434:LEU:HA	1:A:458:VAL:HG11	1.85	0.57
3:D:208:SER:HA	3:D:211:LEU:HD23	1.86	0.57
3:F:98:ILE:HD13	3:F:152:ILE:HG12	1.87	0.57
3:D:102:PHE:HZ	4:G:16:PRO:HD3	1.70	0.57
1:A:629:ILE:HD12	1:A:629:ILE:H	1.71	0.56
2:C:50:LEU:HD21	2:C:87:GLU:HG3	1.88	0.56
3:E:30:ALA:HB1	3:E:138:GLN:HE22	1.71	0.56
1:A:129:TYR:HA	1:A:144:ASP:HA	1.88	0.56
7:T:28:U:H2'	7:T:29:G:H8	1.72	0.55
3:D:181:LEU:HD22	3:D:192:ILE:HD13	1.87	0.55
1:A:115:ILE:HD12	1:A:115:ILE:H	1.71	0.55
3:F:180:TYR:CG	3:F:185:GLY:HA3	2.41	0.55
4:G:236:CYS:HA	4:G:277:GLN:HB3	1.88	0.55
1:A:14:HIS:CE1	1:A:211:THR:HG21	2.41	0.55
1:A:116:PHE:HA	1:A:119:VAL:HB	1.88	0.55
1:A:464:ALA:O	1:A:468:ILE:HG22	2.06	0.55
3:F:166:PHE:HA	3:F:169:ILE:HD12	1.88	0.54
4:G:58:LEU:HD21	4:G:176:LEU:HD13	1.88	0.54
1:A:22:ARG:HD2	1:A:154:TYR:CZ	2.43	0.54
1:A:617:SER:HB3	1:A:648:LYS:O	2.06	0.54
3:D:196:ILE:HG13	3:D:213:ILE:HB	1.89	0.54
3:D:3:SER:HB2	3:D:156:VAL:HB	1.88	0.54
2:B:95:ARG:O	2:B:99:GLU:HG2	2.07	0.54
6:H:57:THR:O	6:H:61:GLN:HG2	2.07	0.54
4:G:167:LYS:HB2	4:G:301:PHE:HE2	1.71	0.54
3:D:180:TYR:CG	3:D:185:GLY:HA3	2.43	0.54
4:G:281:GLY:HA3	4:G:299:LYS:HA	1.90	0.54
6:H:30:ILE:HG13	6:H:39:HIS:HB2	1.89	0.54
3:D:130:LEU:HD22	3:E:70:LYS:HA	1.90	0.53
1:A:528:ARG:HD2	1:A:636:THR:HB	1.89	0.53
6:H:29:TYR:HA	6:H:41:VAL:HG23	1.89	0.53
6:H:188:LYS:HG2	6:H:244:THR:HB	1.91	0.53
3:E:186:THR:HG21	3:F:94:SER:HB2	1.90	0.53
1:A:527:LEU:HB3	1:A:588:LEU:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:103:PHE:HE1	3:F:146:ALA:HB1	1.74	0.53
6:H:193:MET:SD	6:H:194:PRO:HD2	2.49	0.53
4:G:222:LEU:HD11	4:G:226:ALA:HB3	1.90	0.53
3:F:65:LEU:HD22	3:F:69:GLN:HE22	1.73	0.52
3:F:86:SER:HB2	5:R:10:A:HI'	1.90	0.52
1:A:264:ILE:HD11	1:A:283:LEU:HG	1.92	0.52
6:H:149:ARG:HA	6:H:162:PHE:HE2	1.74	0.52
1:A:139:TYR:HD2	1:A:566:GLU:HG3	1.74	0.52
7:T:30:U:H2'	7:T:31:C:C6	2.45	0.52
3:E:98:ILE:HG23	3:E:152:ILE:HG22	1.91	0.52
4:G:29:HIS:ND1	4:G:30:THR:HG23	2.24	0.52
3:D:187:ARG:HB3	3:E:49:SER:HB3	1.91	0.52
2:B:43:THR:HG22	2:B:137:ARG:HH12	1.75	0.51
3:E:80:LEU:HB3	3:E:85:SER:HB2	1.91	0.51
1:A:154:TYR:HE1	1:A:190:ILE:HD12	1.74	0.51
1:A:498:ASP:HA	1:A:577:SER:HA	1.92	0.51
3:E:43:LEU:HD13	3:E:103:PHE:HB3	1.92	0.51
1:A:692:LEU:HD22	1:A:744:ILE:HG23	1.92	0.51
3:E:173:ILE:O	3:E:177:GLU:HG3	2.11	0.51
3:E:176:LEU:HG	3:E:192:ILE:HD11	1.92	0.51
1:A:255:LEU:HG	1:A:350:ILE:HG13	1.91	0.51
1:A:256:ASP:HB2	1:A:378:LEU:HD21	1.93	0.51
1:A:567:LEU:HD12	1:A:581:SER:HB3	1.93	0.51
4:G:13:PHE:HB2	4:G:156:PHE:HD2	1.76	0.51
1:A:525:GLY:HA3	1:A:592:TRP:HA	1.93	0.51
1:A:257:MET:HG2	1:A:348:VAL:HG22	1.92	0.50
3:E:144:ARG:HD3	3:F:38:ASP:OD2	2.11	0.50
3:F:4:LYS:HB2	3:F:203:VAL:HG12	1.93	0.50
4:G:251:VAL:HG11	4:G:256:TYR:CG	2.47	0.50
3:D:86:SER:HA	3:D:91:ILE:HD13	1.94	0.50
3:E:58:LEU:HD22	3:F:2:TYR:HE2	1.77	0.50
1:A:733:ASN:HB3	1:A:736:GLN:HB2	1.94	0.50
1:A:635:GLU:O	1:A:639:LEU:HG	2.12	0.50
3:D:7:ILE:HB	3:D:152:ILE:HG12	1.93	0.50
3:E:7:ILE:HG13	3:E:199:ILE:HG23	1.94	0.50
4:G:61:THR:HA	4:G:224:SER:HB3	1.93	0.50
6:H:81:ILE:HG23	6:H:86:TRP:HE1	1.77	0.50
6:H:18:ILE:HD13	6:H:139:ILE:HG12	1.94	0.49
6:H:248:LYS:O	6:H:252:LYS:HG2	2.12	0.49
6:H:250:PHE:HZ	6:H:335:GLN:HB2	1.77	0.49
1:A:310:GLY:HA2	1:A:580:TYR:OH	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:120:GLU:HB3	3:F:39:PRO:HG2	1.94	0.49
4:G:136:SER:O	4:G:146:SER:HA	2.12	0.49
3:D:2:TYR:OH	3:D:155:ASN:HB3	2.12	0.49
3:D:170:LYS:HG3	3:D:214:LYS:H	1.76	0.49
1:A:62:LYS:H	1:A:62:LYS:HD2	1.78	0.49
3:E:179:ASP:HB2	3:F:4:LYS:HE3	1.94	0.49
4:G:183:LEU:HA	4:G:186:SER:HB3	1.95	0.49
6:H:311:MET:HE1	6:H:315:PRO:HG3	1.93	0.49
3:E:145:GLY:HA3	3:F:40:TYR:CD1	2.47	0.49
1:A:368:SER:HB2	1:A:539:ILE:HG23	1.93	0.49
1:A:225:MET:HE2	1:A:225:MET:N	2.28	0.48
3:D:126:THR:OG1	3:D:137:ARG:NH1	2.46	0.48
5:R:14:C:H2'	5:R:15:G:C8	2.47	0.48
2:B:110:VAL:CG2	2:B:119:PHE:HB2	2.43	0.48
3:E:15:THR:HG22	3:F:102:PHE:CZ	2.47	0.48
2:C:109:VAL:HA	2:C:112:LYS:HG3	1.95	0.48
3:F:73:ASN:ND2	3:F:86:SER:HB3	2.29	0.48
3:D:97:GLN:HG2	4:G:193:SER:HA	1.95	0.48
2:B:91:GLU:HB2	2:B:94:VAL:HG23	1.95	0.48
1:A:206:ASP:OD1	1:A:557:ARG:HD3	2.14	0.48
1:A:528:ARG:HA	1:A:586:LEU:O	2.13	0.48
3:F:53:GLY:HA3	5:R:12:U:H5'	1.95	0.48
3:F:7:ILE:HG13	3:F:152:ILE:HB	1.96	0.48
1:A:165:LEU:HD12	1:A:169:LEU:HD12	1.95	0.47
2:C:21:VAL:HG13	2:C:38:LEU:HD21	1.95	0.47
3:E:7:ILE:HB	3:E:152:ILE:HG12	1.96	0.47
4:G:41:ILE:HG23	4:G:51:LEU:HD11	1.96	0.47
6:H:241:MET:O	6:H:247:GLY:HA3	2.14	0.47
1:A:80:ILE:HD11	1:A:241:THR:HG22	1.95	0.47
4:G:227:MET:HA	4:G:227:MET:HE3	1.96	0.47
1:A:705:ILE:CG1	2:B:124:LYS:HG2	2.44	0.47
2:C:51:LEU:O	2:C:55:ASN:HB2	2.14	0.47
3:F:7:ILE:HG22	3:F:199:ILE:HG12	1.96	0.47
6:H:193:MET:HE3	6:H:195:LEU:HG	1.97	0.47
1:A:267:ILE:HA	4:G:23:ARG:HH22	1.78	0.47
3:E:196:ILE:HG21	3:E:199:ILE:HD11	1.95	0.47
4:G:180:MET:O	4:G:184:GLN:HG3	2.15	0.47
4:G:263:LYS:HD3	4:G:294:VAL:HG11	1.95	0.47
5:R:2:U:H2'	5:R:3:G:H8	1.78	0.47
6:H:3:GLU:HA	6:H:213:ASN:HA	1.96	0.47
1:A:356:THR:HG22	1:A:359:ASP:CG	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:THR:OG1	2:C:103:VAL:HG13	2.14	0.47
3:D:81:ARG:NH1	3:D:161:GLU:HB3	2.30	0.47
3:E:129:ARG:HB2	3:F:69:GLN:HB2	1.97	0.47
3:D:113:LYS:O	3:D:114:LYS:HG2	2.15	0.47
4:G:297:TYR:CZ	4:G:299:LYS:HB2	2.50	0.47
1:A:576:ILE:HD13	1:A:588:LEU:HD21	1.96	0.47
1:A:64:LEU:HB3	1:A:235:PHE:CZ	2.49	0.46
6:H:127:HIS:HE2	6:H:195:LEU:HD22	1.80	0.46
2:C:108:ASP:O	2:C:112:LYS:HG3	2.15	0.46
1:A:291:VAL:HG11	1:A:305:LEU:HD22	1.97	0.46
2:C:50:LEU:O	2:C:53:LEU:HG	2.15	0.46
2:C:133:ALA:HB1	2:C:137:ARG:HH21	1.81	0.46
3:F:14:LEU:HD11	3:F:193:ARG:HG3	1.97	0.46
1:A:499:PHE:CD2	1:A:575:ARG:HA	2.49	0.46
1:A:529:ALA:HB3	1:A:586:LEU:HB3	1.98	0.46
2:B:55:ASN:O	2:B:59:THR:HG23	2.15	0.46
3:D:80:LEU:HB3	3:D:85:SER:HB2	1.98	0.46
5:R:17:A:OP2	6:H:145:LYS:HE2	2.16	0.46
7:T:37:U:H2'	7:T:38:U:O4'	2.16	0.46
3:F:107:SER:HB2	3:F:147:SER:OG	2.16	0.46
6:H:76:LEU:HD13	6:H:86:TRP:CG	2.51	0.46
6:H:46:LEU:HD11	6:H:72:LEU:HD21	1.97	0.46
1:A:714:LEU:HB3	1:A:724:THR:HB	1.97	0.46
3:F:13:VAL:HA	3:F:192:ILE:HG22	1.97	0.46
3:F:49:SER:HB2	5:R:13:C:OP1	2.16	0.46
4:G:5:VAL:HB	4:G:173:ILE:HG13	1.98	0.46
3:F:76:ALA:HB3	3:F:79:ILE:HD12	1.97	0.45
1:A:236:SER:HB3	1:A:237:PRO:HD3	1.98	0.45
1:A:248:ASP:HA	1:A:356:THR:HA	1.99	0.45
1:A:402:THR:HA	4:G:262:LYS:HG3	1.98	0.45
1:A:740:LEU:O	1:A:744:ILE:HG13	2.16	0.45
2:C:102:TYR:O	2:C:106:LEU:HD22	2.15	0.45
3:E:19:ILE:HB	3:E:36:VAL:HG12	1.98	0.45
3:F:51:ILE:HG12	3:F:181:LEU:HD21	1.97	0.45
4:G:6:VAL:HA	4:G:166:ALA:O	2.17	0.45
4:G:9:VAL:HG11	4:G:180:MET:HE2	1.98	0.45
1:A:206:ASP:OD2	1:A:554:THR:HG23	2.17	0.45
1:A:247:GLU:O	1:A:249:VAL:HG23	2.16	0.45
1:A:298:LEU:HD13	1:A:317:LEU:HD22	1.99	0.45
2:C:97:PHE:O	2:C:101:THR:HG23	2.16	0.45
1:A:222:LEU:HD21	1:A:244:PHE:HE1	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HA	1:A:30:LYS:HD2	1.77	0.45
1:A:214:ILE:HG23	1:A:250:PHE:CE1	2.52	0.45
2:B:50:LEU:HD13	2:B:84:PHE:HE1	1.81	0.45
3:F:43:LEU:HD22	3:F:103:PHE:HD2	1.80	0.45
1:A:526:VAL:HG22	1:A:589:ILE:HG12	1.97	0.45
3:F:10:LYS:HG2	3:F:147:SER:HB2	1.98	0.45
6:H:45:ASN:HB3	6:H:89:PHE:HB2	1.99	0.45
1:A:118:VAL:HB	1:A:546:TYR:HD2	1.82	0.45
1:A:184:GLU:HB2	1:A:205:TYR:CZ	2.52	0.45
1:A:571:LEU:HD12	1:A:576:ILE:HG21	1.99	0.45
3:E:15:THR:HG23	3:E:191:ARG:HB2	1.98	0.45
3:E:142:VAL:HG11	3:E:148:PHE:HZ	1.81	0.45
1:A:658:LYS:HB3	1:A:660:PHE:CE2	2.52	0.45
3:D:16:GLY:HA2	3:D:142:VAL:O	2.17	0.45
3:D:188:GLY:HA2	3:E:99:SER:HA	1.98	0.45
3:E:125:ASN:HD22	3:E:134:ALA:HB1	1.81	0.45
6:H:50:LEU:HD21	6:H:59:TYR:HB2	1.99	0.45
1:A:644:LYS:O	1:A:648:LYS:HG2	2.16	0.45
2:B:101:THR:HB	2:B:129:LEU:HD11	1.98	0.45
4:G:108:LEU:HD13	4:G:305:GLY:HA3	1.97	0.45
1:A:496:ASP:O	1:A:497:TYR:C	2.60	0.44
1:A:508:LYS:HD3	1:A:508:LYS:HA	1.87	0.44
1:A:586:LEU:HD21	1:A:588:LEU:HD13	1.98	0.44
3:D:62:HIS:HA	3:E:2:TYR:HB2	1.99	0.44
4:G:64:PHE:HB2	4:G:163:TYR:CE1	2.53	0.44
2:B:92:PRO:O	2:B:96:THR:HG22	2.17	0.44
3:F:80:LEU:HD11	3:F:85:SER:HB2	2.00	0.44
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.85	0.44
6:H:26:LYS:HA	6:H:29:TYR:CZ	2.53	0.44
6:H:53:LYS:HE3	6:H:55:LYS:HD3	1.99	0.44
3:F:17:LEU:HA	3:F:190:GLY:HA2	1.99	0.44
3:F:65:LEU:HB3	3:F:69:GLN:HE21	1.81	0.44
1:A:9:TYR:CE2	1:A:179:LEU:HD22	2.53	0.44
1:A:186:LEU:HB3	1:A:187:TRP:CD1	2.51	0.44
1:A:622:MET:HE1	1:A:749:TYR:CZ	2.52	0.44
1:A:747:LEU:O	1:A:751:ILE:HG22	2.17	0.44
3:F:11:ILE:O	3:F:147:SER:HA	2.16	0.44
1:A:250:PHE:HB2	1:A:355:CYS:SG	2.57	0.44
2:B:106:LEU:HA	2:B:109:VAL:HG12	1.99	0.44
4:G:54:LEU:HD11	4:G:58:LEU:HD22	1.99	0.44
1:A:180:LEU:HD11	1:A:303:ALA:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:C	1:A:239:GLU:H	2.25	0.44
2:C:20:VAL:HG11	2:C:101:THR:HG22	2.00	0.44
2:C:38:LEU:HD13	2:C:137:ARG:NH2	2.33	0.44
3:D:7:ILE:HD13	3:D:213:ILE:HD11	1.98	0.44
3:E:170:LYS:HG2	3:E:213:ILE:HA	1.99	0.44
6:H:20:SER:HB2	6:H:130:VAL:HA	2.00	0.44
1:A:676:PRO:HA	1:A:679:GLU:HG2	1.99	0.44
2:C:109:VAL:O	2:C:113:LYS:HG2	2.17	0.44
1:A:260:ILE:HG23	1:A:283:LEU:HD12	2.00	0.44
3:E:170:LYS:HE3	3:E:170:LYS:HB3	1.75	0.44
3:F:180:TYR:CD1	3:F:185:GLY:HA3	2.53	0.44
6:H:210:MET:HE3	6:H:212:ILE:HD13	2.00	0.44
6:H:289:LYS:O	6:H:293:GLN:HG2	2.18	0.44
1:A:222:LEU:HD13	1:A:230:TYR:HD1	1.82	0.43
2:B:96:THR:HA	2:B:99:GLU:CG	2.48	0.43
4:G:297:TYR:CE2	4:G:299:LYS:HB2	2.53	0.43
6:H:16:VAL:HB	6:H:337:GLY:HA2	2.00	0.43
1:A:285:THR:HG21	1:A:456:LEU:HD13	1.99	0.43
1:A:674:MET:HE2	1:A:746:TYR:CE1	2.54	0.43
2:B:120:LEU:HD23	2:B:120:LEU:HA	1.85	0.43
3:D:7:ILE:HG21	3:D:213:ILE:HD12	1.99	0.43
3:E:17:LEU:HD21	3:E:181:LEU:HB3	2.00	0.43
3:F:20:GLY:HA2	3:F:36:VAL:N	2.33	0.43
2:B:52:GLU:HA	2:B:55:ASN:ND2	2.33	0.43
3:D:116:LEU:HD21	3:D:143:THR:HG21	2.01	0.43
3:E:181:LEU:HD12	3:E:181:LEU:HA	1.89	0.43
1:A:209:LYS:HE2	1:A:303:ALA:HA	2.00	0.43
1:A:493:TRP:CD1	1:A:561:MET:HE1	2.54	0.43
4:G:115:LEU:HD23	4:G:115:LEU:H	1.83	0.43
6:H:217:TRP:HB3	6:H:222:ILE:HD11	2.00	0.43
1:A:153:GLN:H	1:A:153:GLN:HG3	1.59	0.43
2:B:25:LYS:HD2	2:B:136:TYR:HD2	1.84	0.43
3:F:7:ILE:CG2	3:F:199:ILE:HG12	2.49	0.43
6:H:150:THR:OG1	6:H:280:LYS:HB3	2.19	0.43
6:H:257:PRO:HB2	6:H:260:LEU:HG	2.00	0.43
1:A:115:ILE:HA	1:A:201:ASP:HB3	1.99	0.43
3:D:62:HIS:CE1	3:D:171:THR:HG21	2.53	0.43
3:E:206:PHE:HE2	3:E:211:LEU:HD11	1.83	0.43
4:G:72:PHE:HB3	4:G:98:TYR:HB3	2.00	0.43
4:G:103:ASN:O	4:G:106:GLU:HB3	2.18	0.43
1:A:526:VAL:HG12	1:A:636:THR:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:THR:O	2:C:100:LYS:HG2	2.19	0.43
3:D:13:VAL:O	3:D:13:VAL:HG23	2.19	0.43
4:G:66:TYR:HB2	4:G:71:TYR:HD1	1.84	0.43
6:H:144:LEU:HD22	6:H:208:PHE:CE2	2.54	0.43
1:A:409:LEU:HD11	4:G:23:ARG:HE	1.84	0.43
1:A:278:SER:HB2	1:A:427:ILE:HG23	2.01	0.42
1:A:310:GLY:HA2	1:A:580:TYR:HH	1.84	0.42
4:G:287:SER:HB3	4:G:294:VAL:HB	2.01	0.42
6:H:144:LEU:HD22	6:H:208:PHE:HE2	1.83	0.42
3:E:62:HIS:HB2	3:E:175:LEU:HD11	2.01	0.42
4:G:6:VAL:HG22	4:G:165:LEU:HD23	2.01	0.42
3:E:31:ILE:HA	3:E:138:GLN:HB2	2.01	0.42
3:F:111:PHE:HD2	3:F:118:TYR:HD1	1.65	0.42
4:G:127:GLY:HA2	4:G:156:PHE:HA	2.01	0.42
6:H:76:LEU:HB3	6:H:86:TRP:CE2	2.54	0.42
6:H:275:THR:HG22	6:H:337:GLY:HA3	2.01	0.42
1:A:205:TYR:HD2	1:A:557:ARG:HH11	1.66	0.42
1:A:442:VAL:HG13	1:A:450:LEU:HD12	2.01	0.42
6:H:238:PHE:HE2	6:H:256:LEU:HD13	1.84	0.42
1:A:161:MET:HG2	1:A:182:TRP:CZ2	2.55	0.42
1:A:602:LEU:HD12	1:A:602:LEU:HA	1.82	0.42
3:F:96:LEU:HA	3:F:96:LEU:HD12	1.78	0.42
4:G:180:MET:HE3	4:G:180:MET:HB3	1.86	0.42
3:D:78:GLU:OE2	3:D:78:GLU:HA	2.20	0.42
4:G:52:SER:HA	4:G:55:LEU:HD12	2.01	0.42
4:G:250:PHE:CZ	4:G:262:LYS:HG2	2.55	0.42
1:A:642:LEU:O	1:A:645:ARG:HG2	2.19	0.42
1:A:735:GLN:HA	1:A:735:GLN:OE1	2.20	0.42
4:G:8:LEU:HA	4:G:8:LEU:HD12	1.81	0.42
4:G:134:LYS:HB3	5:R:1:A:OP2	2.19	0.42
6:H:287:LYS:HB2	6:H:292:ALA:HB2	2.02	0.42
6:H:341:LEU:HD22	6:H:343:PHE:HE1	1.84	0.42
1:A:388:LEU:CD1	4:G:234:VAL:HA	2.50	0.42
1:A:440:PHE:HB2	1:A:477:TYR:HB2	2.01	0.42
1:A:523:ARG:HB3	1:A:622:MET:HG2	2.00	0.42
3:E:72:HIS:CE1	5:R:5:G:H4'	2.55	0.42
3:E:185:GLY:HA2	3:E:189:ASN:N	2.31	0.42
1:A:288:GLU:HG3	1:A:492:LEU:HD21	2.02	0.41
1:A:622:MET:HE2	1:A:622:MET:HB3	1.91	0.41
1:A:12:LEU:HD12	1:A:208:SER:HB3	2.02	0.41
2:B:52:GLU:HA	2:B:55:ASN:HD21	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:205:ASP:OD1	3:D:205:ASP:N	2.52	0.41
3:F:158:ASN:HB3	3:F:161:GLU:HB2	2.02	0.41
4:G:192:ARG:HA	4:G:196:TYR:O	2.20	0.41
1:A:32:THR:O	1:A:36:ILE:HG12	2.20	0.41
2:B:20:VAL:HG11	2:B:101:THR:HG22	2.02	0.41
2:B:38:LEU:HA	2:B:38:LEU:HD12	1.86	0.41
4:G:147:GLU:O	4:G:147:GLU:HG3	2.19	0.41
6:H:37:LEU:HD21	6:H:93:THR:OG1	2.20	0.41
6:H:256:LEU:HD12	6:H:257:PRO:HD2	2.02	0.41
6:H:281:THR:HG22	6:H:284:TYR:H	1.85	0.41
1:A:146:LYS:H	1:A:146:LYS:HD2	1.85	0.41
1:A:281:PHE:HD1	1:A:494:MET:HE1	1.86	0.41
3:D:36:VAL:HG23	3:D:45:ILE:HG13	2.01	0.41
3:D:56:ARG:HH11	3:D:83:PHE:HB2	1.84	0.41
3:E:145:GLY:HA3	3:F:40:TYR:CE1	2.56	0.41
3:F:48:GLY:O	3:F:98:ILE:HG21	2.20	0.41
4:G:183:LEU:HD12	4:G:186:SER:HB3	2.02	0.41
1:A:163:ASP:OD1	1:A:163:ASP:C	2.63	0.41
2:B:107:VAL:HA	2:B:110:VAL:HG12	2.02	0.41
3:E:126:THR:HB	5:R:11:U:H1'	2.03	0.41
4:G:266:PHE:CE2	4:G:268:ALA:HB2	2.55	0.41
1:A:514:TYR:CD2	1:A:590:GLY:HA2	2.56	0.41
1:A:623:TYR:CD1	1:A:632:MET:HG3	2.56	0.41
4:G:177:GLU:HG2	4:G:203:ILE:HD13	2.03	0.41
4:G:287:SER:HB3	4:G:294:VAL:H	1.84	0.41
1:A:694:LYS:HG3	1:A:713:LEU:HD11	2.03	0.41
3:F:10:LYS:O	3:F:195:VAL:HG22	2.21	0.41
1:A:280:SER:HA	9:A:802:ANP:HN62	1.85	0.41
1:A:669:ILE:HG22	1:A:670:LEU:HD23	2.03	0.41
2:B:25:LYS:HE2	2:B:25:LYS:HB3	1.86	0.41
3:D:2:TYR:HB2	4:G:46:GLN:O	2.20	0.41
3:F:55:MET:HE2	3:F:55:MET:HB3	1.98	0.41
5:R:2:U:H2'	5:R:3:G:C8	2.55	0.41
1:A:12:LEU:HD23	1:A:179:LEU:HD23	2.02	0.41
1:A:503:ASN:OD1	1:A:503:ASN:C	2.63	0.41
1:A:618:ALA:O	1:A:651:VAL:HA	2.21	0.41
2:C:42:LEU:HD22	2:C:137:ARG:NH2	2.36	0.41
2:C:106:LEU:HA	2:C:109:VAL:HG12	2.02	0.41
3:D:130:LEU:HB3	3:E:69:GLN:O	2.20	0.41
4:G:62:ASP:HB2	4:G:64:PHE:CE1	2.55	0.41
6:H:13:TYR:HB2	6:H:338:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:176:LYS:HE2	6:H:176:LYS:HB3	1.84	0.41
6:H:291:GLN:OE1	6:H:291:GLN:HA	2.19	0.41
1:A:133:PHE:HB3	1:A:153:GLN:NE2	2.36	0.41
1:A:576:ILE:HD11	1:A:595:VAL:HA	2.02	0.41
3:D:181:LEU:HD12	3:D:181:LEU:HA	1.79	0.41
4:G:266:PHE:HE2	4:G:268:ALA:HB2	1.86	0.41
4:G:58:LEU:HD12	4:G:58:LEU:HA	1.88	0.40
6:H:30:ILE:HD11	6:H:90:VAL:HG21	2.03	0.40
7:T:31:C:H2'	7:T:32:G:O4'	2.21	0.40
1:A:6:GLU:HG2	1:A:49:LEU:HD23	2.02	0.40
1:A:18:LYS:O	1:A:22:ARG:HG3	2.20	0.40
2:C:73:VAL:O	2:C:77:LEU:HG	2.20	0.40
3:D:142:VAL:HG11	3:D:148:PHE:CZ	2.57	0.40
6:H:226:ILE:HD13	6:H:341:LEU:HD13	2.02	0.40
6:H:295:ASP:O	6:H:299:ILE:HG12	2.21	0.40
1:A:234:LEU:HD12	1:A:235:PHE:N	2.37	0.40
1:A:723:LEU:O	1:A:723:LEU:HD12	2.22	0.40
2:C:86:TYR:CE2	6:H:27:GLN:HG2	2.57	0.40
2:B:55:ASN:HB2	3:E:27:MET:HA	2.03	0.40
3:F:141:ARG:HD2	3:F:189:ASN:HB2	2.03	0.40
4:G:101:VAL:HG21	4:G:209:PHE:CZ	2.57	0.40
4:G:253:SER:HB3	5:R:-7:A:C8	2.57	0.40
1:A:161:MET:HG2	1:A:182:TRP:HZ2	1.87	0.40
2:C:84:PHE:HD1	2:C:84:PHE:HA	1.77	0.40
3:E:11:ILE:HG23	3:E:148:PHE:HB2	2.02	0.40
3:E:35:VAL:HG22	3:E:140:GLU:OE1	2.21	0.40
5:R:9:C:H2'	5:R:10:A:C8	2.57	0.40
6:H:188:LYS:HA	6:H:246:GLY:H	1.87	0.40
6:H:241:MET:HE3	6:H:241:MET:HA	2.03	0.40
3:F:20:GLY:HA2	3:F:36:VAL:H	1.86	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	710/774 (92%)	679 (96%)	31 (4%)	0	100	100
2	B	110/140 (79%)	110 (100%)	0	0	100	100
2	C	107/140 (76%)	105 (98%)	2 (2%)	0	100	100
3	D	188/214 (88%)	180 (96%)	8 (4%)	0	100	100
3	E	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
3	F	178/214 (83%)	173 (97%)	5 (3%)	0	100	100
4	G	293/307 (95%)	287 (98%)	6 (2%)	0	100	100
6	H	277/379 (73%)	273 (99%)	4 (1%)	0	100	100
All	All	2074/2382 (87%)	2009 (97%)	65 (3%)	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	642/688 (93%)	623 (97%)	19 (3%)	36	61
2	B	106/128 (83%)	104 (98%)	2 (2%)	50	68
2	C	103/128 (80%)	101 (98%)	2 (2%)	50	68
3	D	165/180 (92%)	161 (98%)	4 (2%)	43	65
3	E	179/180 (99%)	177 (99%)	2 (1%)	65	74
3	F	155/180 (86%)	149 (96%)	6 (4%)	28	56
4	G	254/262 (97%)	250 (98%)	4 (2%)	55	71
6	H	256/330 (78%)	252 (98%)	4 (2%)	55	71
All	All	1860/2076 (90%)	1817 (98%)	43 (2%)	44	66

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	180	LEU
1	A	192	SER
1	A	196	THR
1	A	202	VAL
1	A	228	VAL
1	A	234	LEU
1	A	258	SER
1	A	307	TYR
1	A	355	CYS
1	A	409	LEU
1	A	412	ASP
1	A	421	CYS
1	A	492	LEU
1	A	537	THR
1	A	588	LEU
1	A	634	SER
1	A	642	LEU
1	A	651	VAL
2	C	47	LEU
2	C	67	THR
2	B	44	THR
2	B	50	LEU
3	D	82	LEU
3	D	139	ILE
3	D	202	VAL
3	D	211	LEU
3	E	45	ILE
3	E	152	ILE
3	F	3	SER
3	F	12	ASP
3	F	49	SER
3	F	99	SER
3	F	147	SER
3	F	167	GLU
4	G	57	ASN
4	G	118	SER
4	G	126	LEU
4	G	260	LEU
6	H	173	ILE
6	H	199	CYS
6	H	282	THR
6	H	311	MET

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	24	ASN
1	A	42	ASN
1	A	153	GLN
1	A	181	GLN
1	A	226	ASN
1	A	229	ASN
1	A	304	ASN
1	A	395	ASN
1	A	569	ASN
1	A	732	GLN
1	A	750	GLN
3	E	108	GLN
3	E	138	GLN
3	E	174	HIS
3	E	178	ASN
3	F	69	GLN
3	F	73	ASN
3	F	174	HIS
4	G	47	GLN
4	G	292	HIS
6	H	51	ASN
6	H	235	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	24/45 (53%)	9 (37%)	4 (16%)
7	T	16/47 (34%)	3 (18%)	0
All	All	40/92 (43%)	12 (30%)	4 (10%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	R	-6	C
5	R	-5	G
5	R	-3	G
5	R	-1	A
5	R	0	C
5	R	7	G
5	R	12	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	13	C
5	R	17	A
7	T	24	G
7	T	27	A
7	T	33	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	R	-1	A
5	R	1	A
5	R	5	G
5	R	11	U

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 4 ligands modelled in this entry, 2 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	$\# Z > 2$
8	A1II9	A	801	10	83,83,83	3.49	35 (42%)	119,130,130	2.24	32 (26%)
9	ANP	A	802	-	33,33,33	1.12	5 (15%)	45,52,52	0.88	2 (4%)

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	A1II9	A	801	10	-	26/48/100/100	0/9/9/9
9	ANP	A	802	-	-	5/18/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	801	A1II9	C11-C10	-10.68	1.29	1.53
8	A	801	A1II9	C31-C32	-9.08	1.25	1.53
8	A	801	A1II9	C2'-C1'	-8.89	1.25	1.53
8	A	801	A1II9	C3'-C4'	-8.82	1.30	1.53
8	A	801	A1II9	O4'-C1'	8.43	1.61	1.42
8	A	801	A1II9	C30-C29	-8.39	1.31	1.52
8	A	801	A1II9	O33-C32	7.93	1.60	1.42
8	A	801	A1II9	C31-C30	7.42	1.69	1.53
8	A	801	A1II9	C2'-C3'	6.01	1.69	1.53
8	A	801	A1II9	P06-O05	5.69	1.65	1.59
8	A	801	A1II9	P04-O05	5.12	1.65	1.59
8	A	801	A1II9	C39-N40	4.90	1.46	1.34
8	A	801	A1II9	C19-N20	4.79	1.46	1.34
8	A	801	A1II9	C6-N6	4.78	1.46	1.34
8	A	801	A1II9	O13-C09	4.40	1.54	1.45
8	A	801	A1II9	O13-C12	-4.38	1.31	1.42
8	A	801	A1II9	O4'-C4'	4.01	1.53	1.45
8	A	801	A1II9	O33-C29	3.93	1.53	1.45
8	A	801	A1II9	P04-O73	3.50	1.51	1.46
8	A	801	A1II9	P02-O75	3.37	1.51	1.46
8	A	801	A1II9	C11-C12	3.24	1.63	1.53
9	A	802	ANP	PG-O1G	3.22	1.51	1.46
8	A	801	A1II9	P04-N03	3.11	1.71	1.63
9	A	802	ANP	PB-O1B	3.00	1.50	1.46
8	A	801	A1II9	P02-N03	2.98	1.71	1.63
8	A	801	A1II9	C38-N34	-2.74	1.32	1.37
8	A	801	A1II9	C8-N9	-2.72	1.32	1.37
8	A	801	A1II9	C18-N14	-2.69	1.33	1.37
8	A	801	A1II9	P-OP3	2.64	1.67	1.59
8	A	801	A1II9	P26-O25	2.60	1.67	1.59
8	A	801	A1II9	P02-O01	-2.37	1.50	1.56
8	A	801	A1II9	C16-N17	-2.31	1.34	1.39
9	A	802	ANP	PB-O2B	-2.29	1.50	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	801	A1II9	C5-N7	-2.26	1.35	1.39
9	A	802	ANP	PG-O3G	-2.24	1.50	1.56
8	A	801	A1II9	C36-N37	-2.22	1.35	1.39
9	A	802	ANP	PG-O2G	-2.16	1.51	1.56
8	A	801	A1II9	P02-O74	-2.06	1.51	1.56
8	A	801	A1II9	C5'-C4'	2.03	1.57	1.51
8	A	801	A1II9	C28-C29	2.02	1.57	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801	A1II9	O13-C12-N14	-10.73	87.49	108.09
8	A	801	A1II9	C11-C12-N14	8.09	133.41	113.30
8	A	801	A1II9	C5-C4-N3	-5.76	118.78	126.72
8	A	801	A1II9	N43-C42-N41	-4.77	121.36	128.58
8	A	801	A1II9	N23-C22-N21	-4.58	121.64	128.58
8	A	801	A1II9	N3-C2-N1	-4.53	121.73	128.58
8	A	801	A1II9	N3-C4-N9	4.21	134.33	127.17
8	A	801	A1II9	C16-C15-N23	-4.15	121.00	126.72
8	A	801	A1II9	C36-C35-N43	-4.04	121.16	126.72
9	A	802	ANP	O2B-PB-O1B	4.02	118.49	109.87
8	A	801	A1II9	C2-N3-C4	3.83	121.18	111.83
8	A	801	A1II9	C3'-C2'-C1'	3.70	108.46	101.46
8	A	801	A1II9	N9-C8-N7	-3.62	108.80	113.94
8	A	801	A1II9	C4-C5-N7	-3.46	106.62	110.58
8	A	801	A1II9	C5-N7-C8	3.42	108.82	103.45
8	A	801	A1II9	C29-O33-C32	-3.24	102.32	109.47
8	A	801	A1II9	N43-C35-N34	3.17	132.56	127.17
8	A	801	A1II9	C22-N23-C15	3.11	119.43	111.83
8	A	801	A1II9	N34-C38-N37	-3.08	109.57	113.94
8	A	801	A1II9	C42-N43-C35	3.08	119.35	111.83
8	A	801	A1II9	N14-C18-N17	-2.98	109.70	113.94
8	A	801	A1II9	C4-N9-C8	2.98	108.87	105.74
8	A	801	A1II9	C35-N34-C38	2.95	108.84	105.74
8	A	801	A1II9	N23-C15-N14	2.92	132.14	127.17
8	A	801	A1II9	C15-C16-N17	-2.88	107.29	110.58
8	A	801	A1II9	C16-N17-C18	2.75	107.77	103.45
8	A	801	A1II9	C36-N37-C38	2.58	107.50	103.45
8	A	801	A1II9	C15-N14-C18	2.52	108.38	105.74
8	A	801	A1II9	C35-C36-N37	-2.42	107.81	110.58
8	A	801	A1II9	C2'-C3'-C4'	2.42	107.28	102.61
8	A	801	A1II9	C31-C30-C29	2.36	107.37	103.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801	A1II9	C42-N41-C39	2.27	122.46	118.73
9	A	802	ANP	O2G-PG-O1G	-2.19	107.95	113.45
8	A	801	A1II9	C30-C31-C32	2.15	104.61	99.89

There are no chirality outliers.

All (31) torsion outliers are listed below:

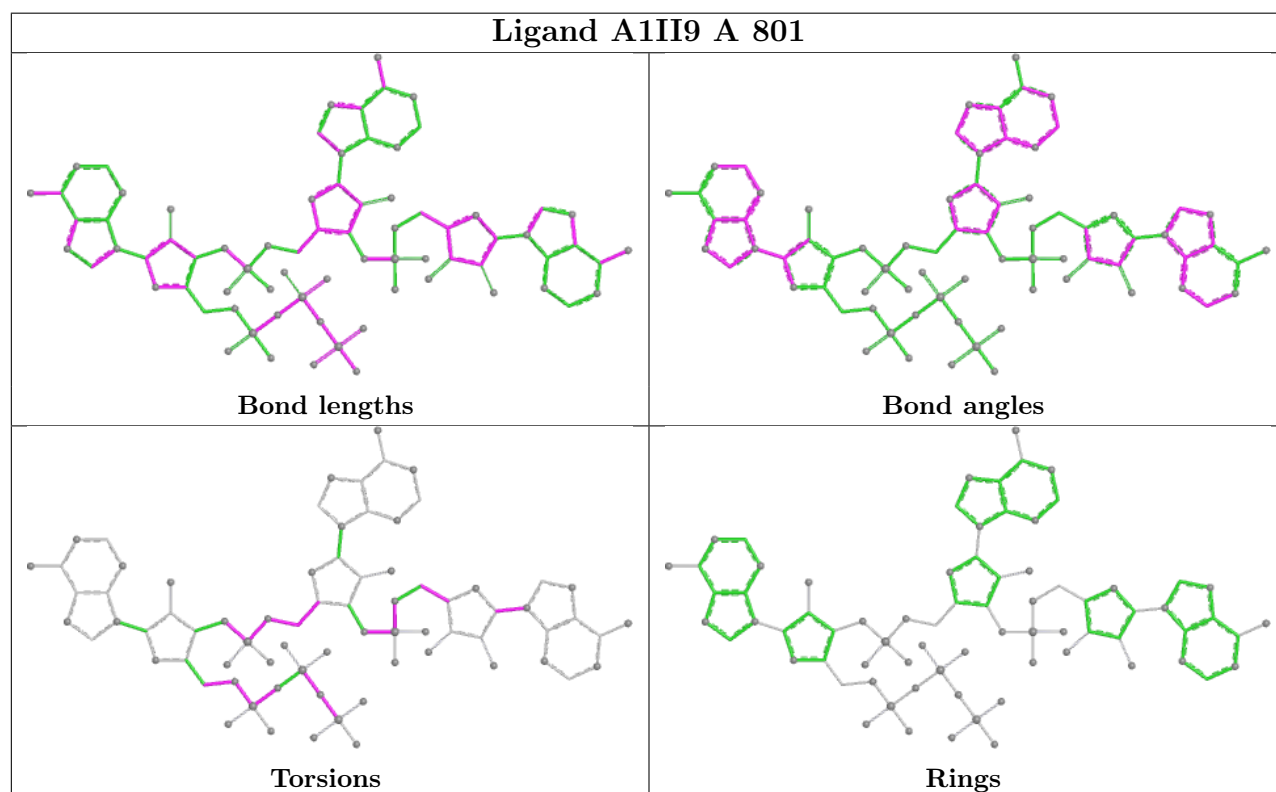
Mol	Chain	Res	Type	Atoms
8	A	801	A1II9	P04-N03-P02-O75
8	A	801	A1II9	P02-N03-P04-O73
8	A	801	A1II9	C08-O07-P06-O70
8	A	801	A1II9	C08-O07-P06-O05
8	A	801	A1II9	C10-O25-P26-O69
8	A	801	A1II9	C10-O25-P26-O27
8	A	801	A1II9	C28-O27-P26-O25
8	A	801	A1II9	C28-O27-P26-O69
8	A	801	A1II9	C28-O27-P26-O68
8	A	801	A1II9	C30-OP3-P-O5'
8	A	801	A1II9	C5'-O5'-P-OP3
8	A	801	A1II9	C5'-O5'-P-OP1
8	A	801	A1II9	C5'-O5'-P-OP2
8	A	801	A1II9	O4'-C4'-C5'-O5'
9	A	802	ANP	PB-N3B-PG-O1G
8	A	801	A1II9	C3'-C4'-C5'-O5'
8	A	801	A1II9	C09-C08-O07-P06
8	A	801	A1II9	O27-C28-C29-O33
8	A	801	A1II9	O27-C28-C29-C30
8	A	801	A1II9	C2'-C1'-N9-C8
9	A	802	ANP	C2'-C1'-N9-C8
8	A	801	A1II9	C10-O25-P26-O68
9	A	802	ANP	PG-N3B-PB-O3A
9	A	802	ANP	C5'-O5'-PA-O2A
8	A	801	A1II9	C29-C28-O27-P26
8	A	801	A1II9	P04-O05-P06-O71
8	A	801	A1II9	P04-O05-P06-O70
8	A	801	A1II9	O4'-C1'-N9-C8
8	A	801	A1II9	C30-OP3-P-OP1
8	A	801	A1II9	C30-OP3-P-OP2
9	A	802	ANP	O4'-C1'-N9-C8

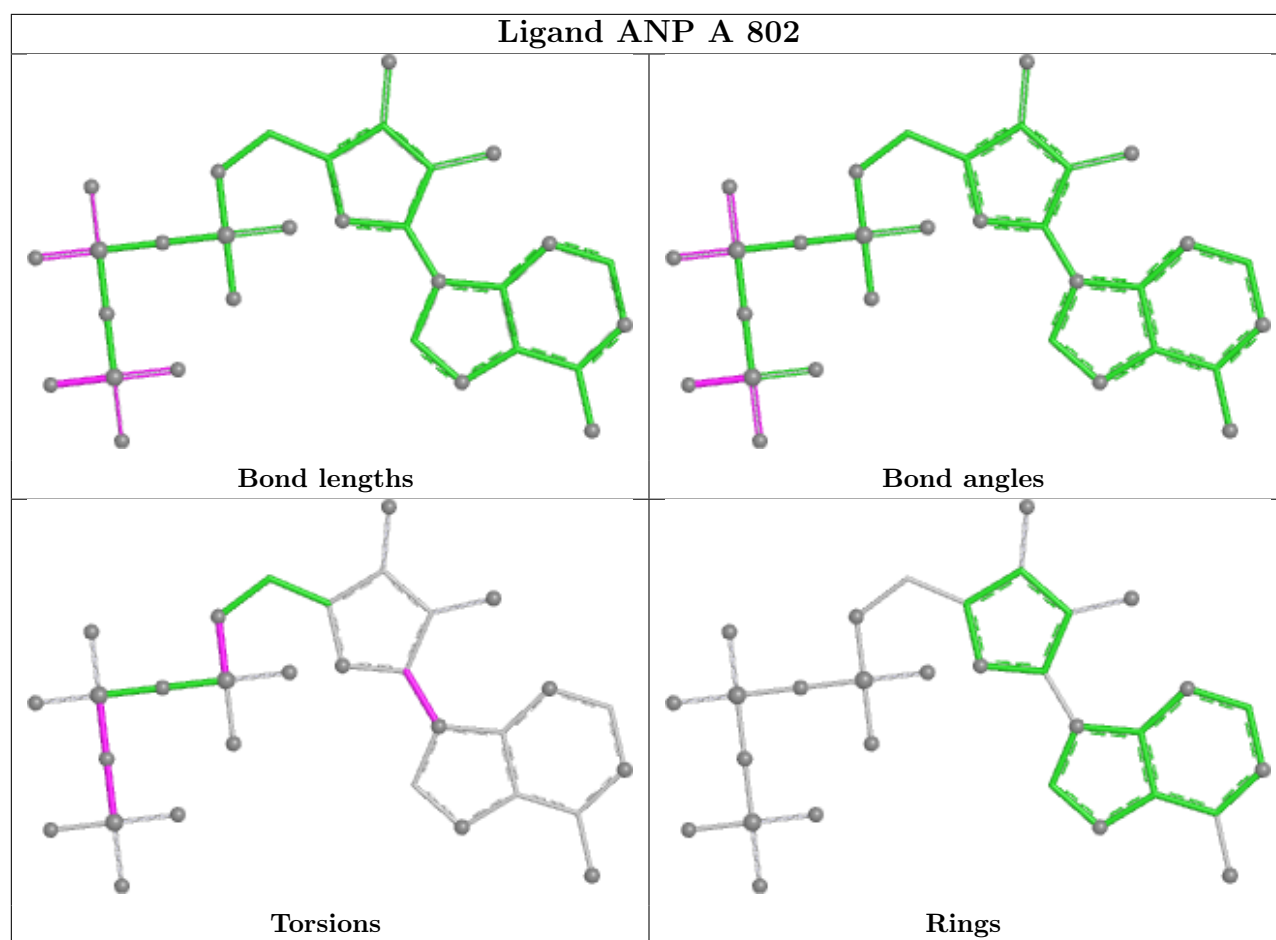
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	802	ANP	1	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

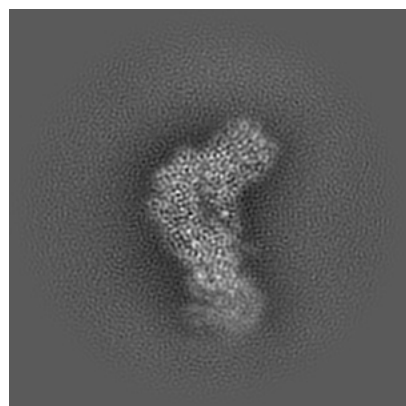
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51153. These allow visual inspection of the internal detail of the map and identification of artifacts.

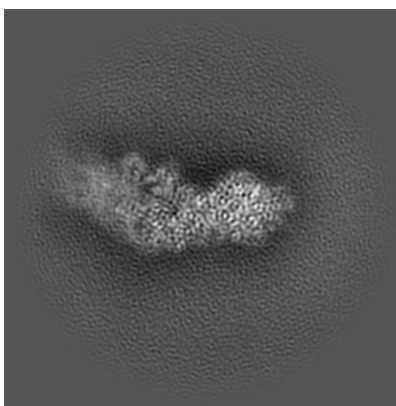
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

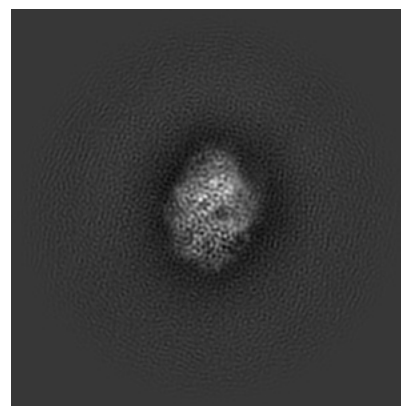
6.1.1 Primary map



X

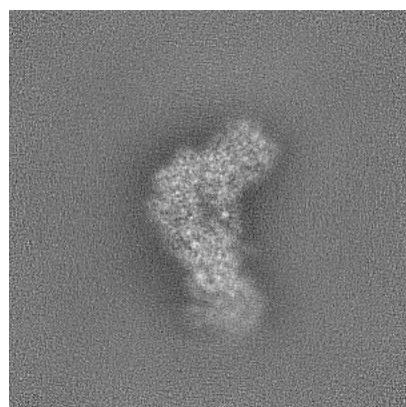


Y

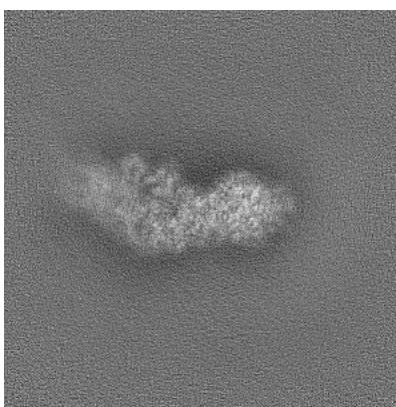


Z

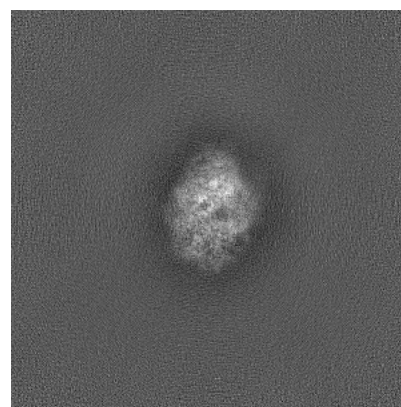
6.1.2 Raw map



X



Y

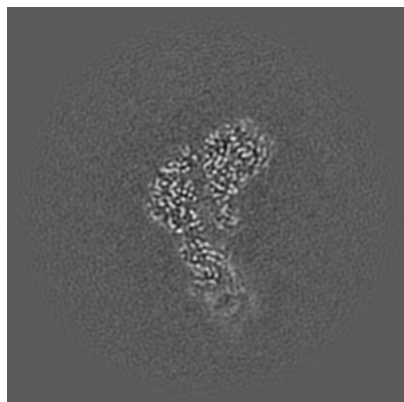


Z

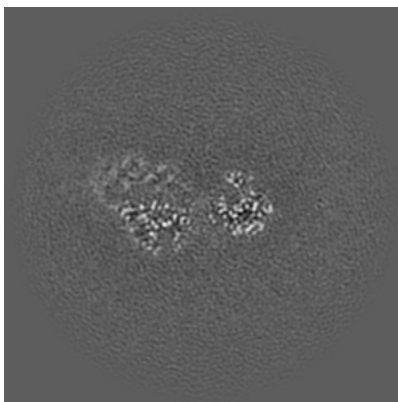
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

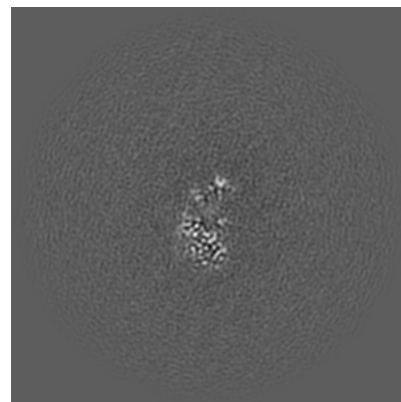
6.2.1 Primary map



X Index: 240

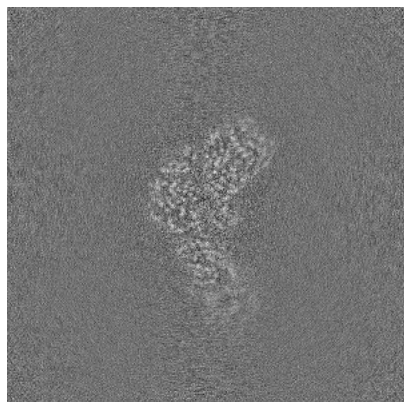


Y Index: 240

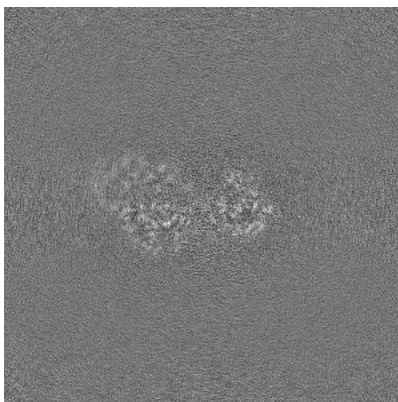


Z Index: 240

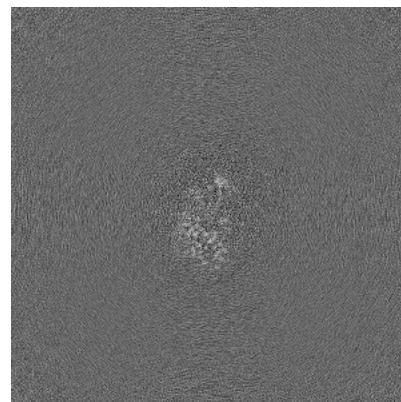
6.2.2 Raw map



X Index: 240



Y Index: 240

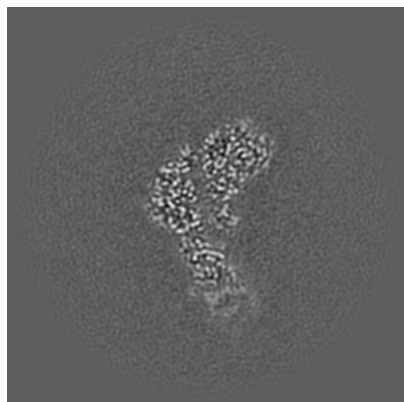


Z Index: 240

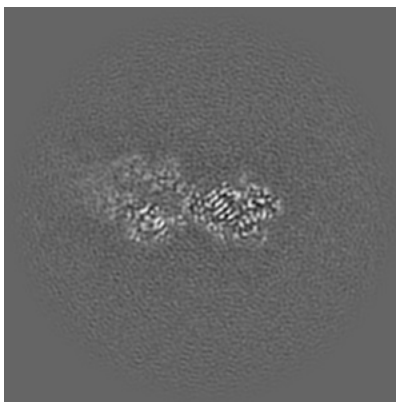
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

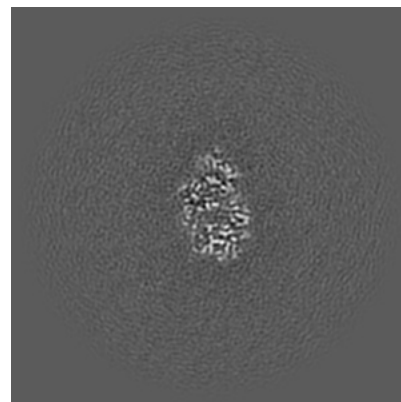
6.3.1 Primary map



X Index: 239

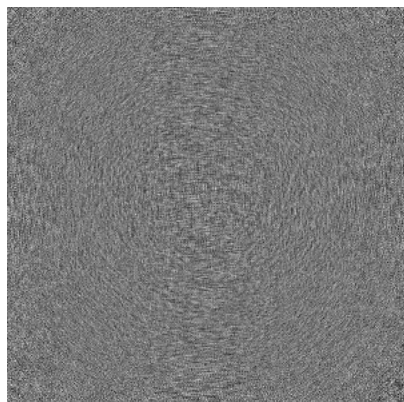


Y Index: 253

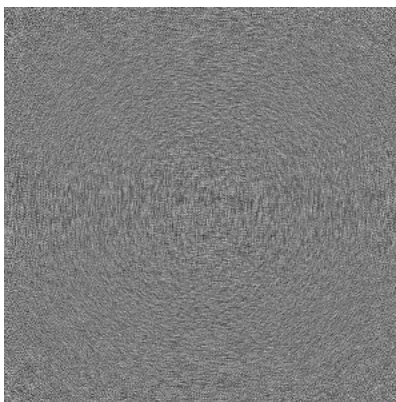


Z Index: 284

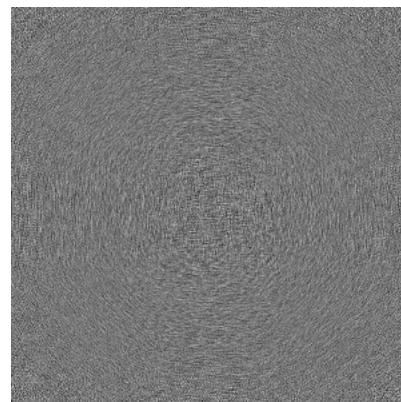
6.3.2 Raw map



X Index: 0



Y Index: 0

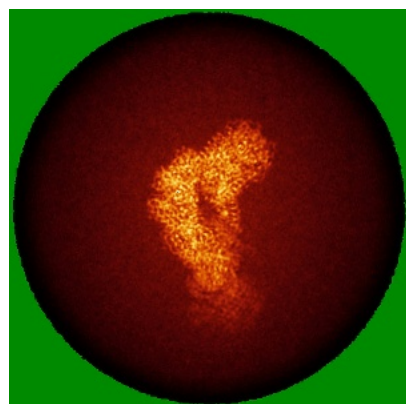


Z Index: 0

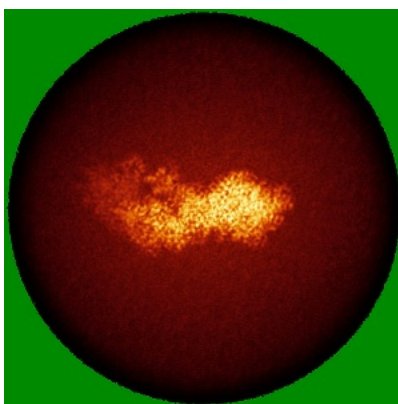
The images above show the largest variance slices of the map in three orthogonal directions.

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

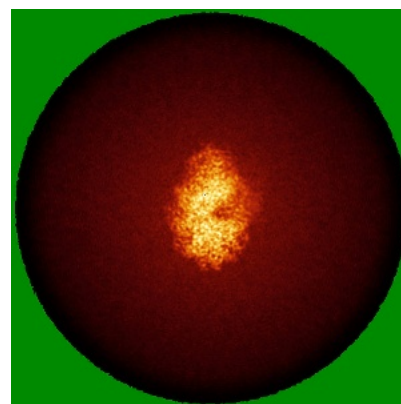
6.4.1 Primary map



X

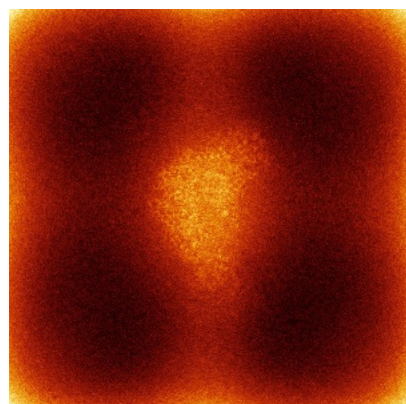


Y

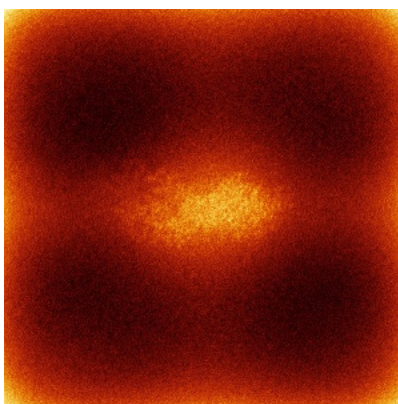


Z

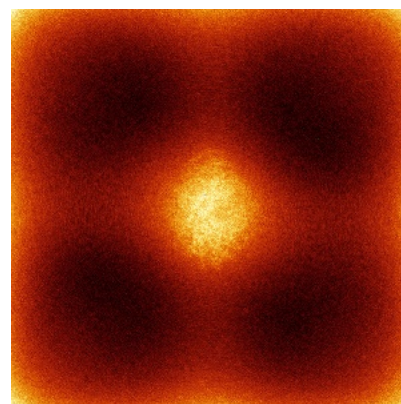
6.4.2 Raw map



X



Y

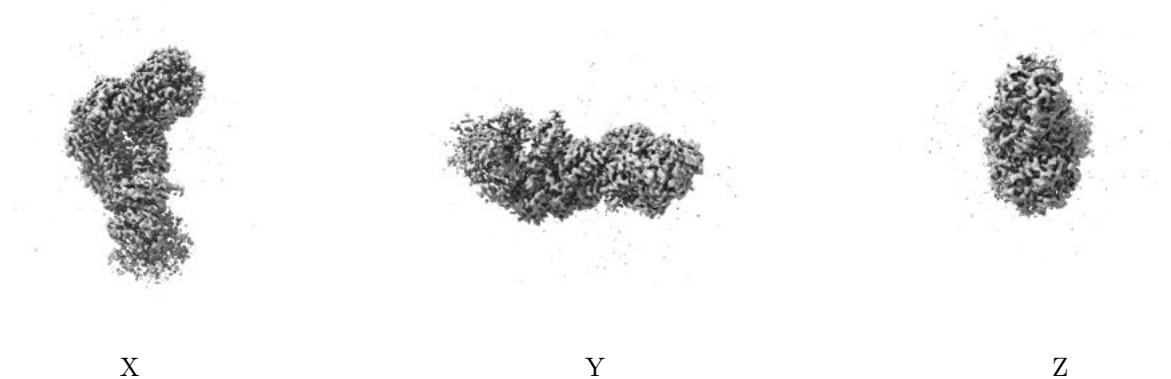


Z

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.

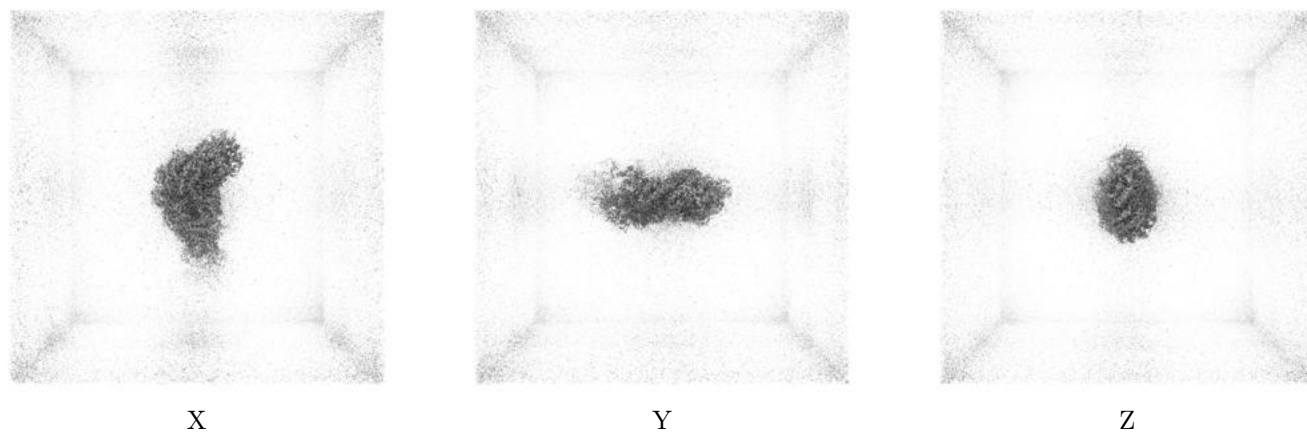
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.071. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

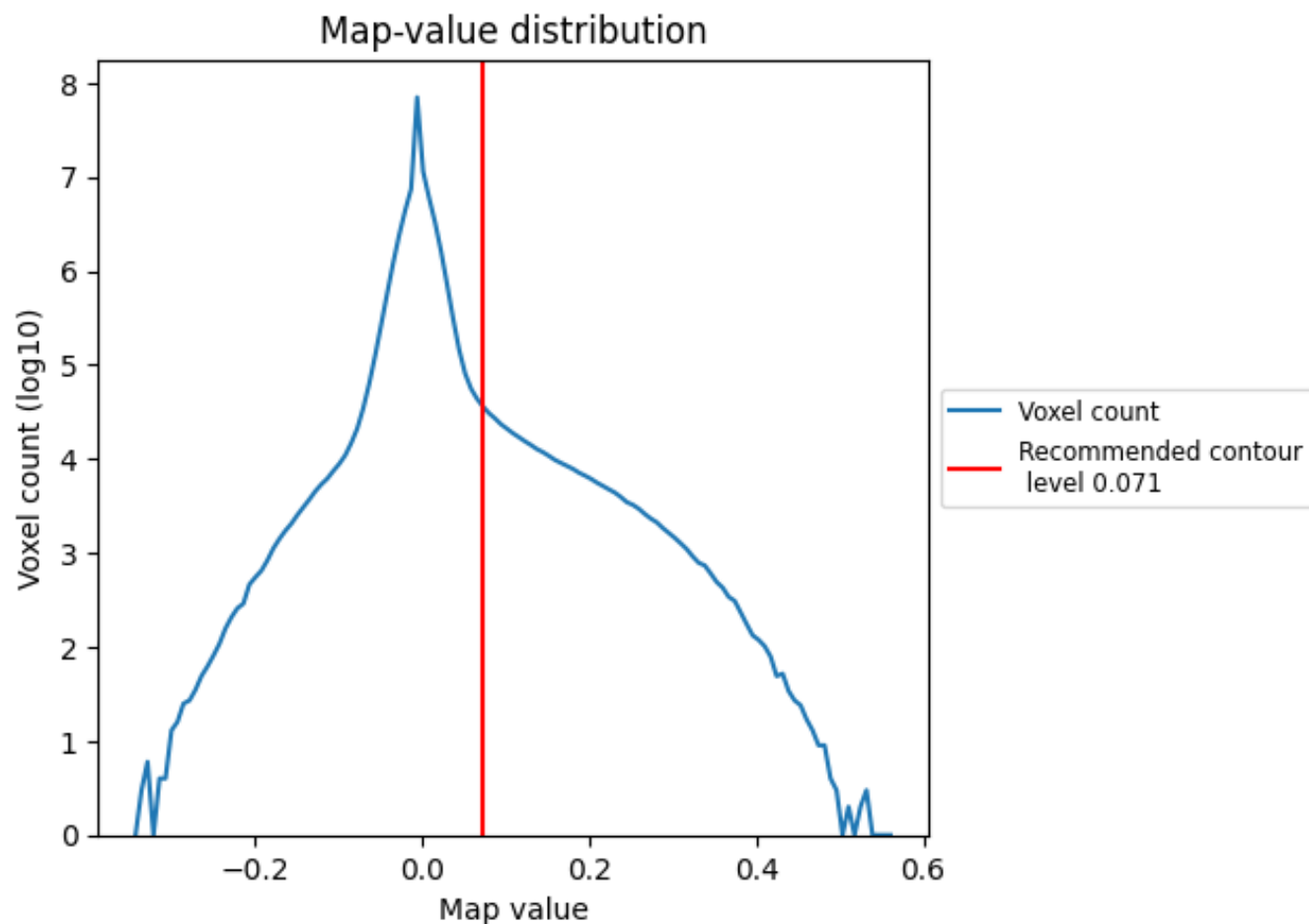
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

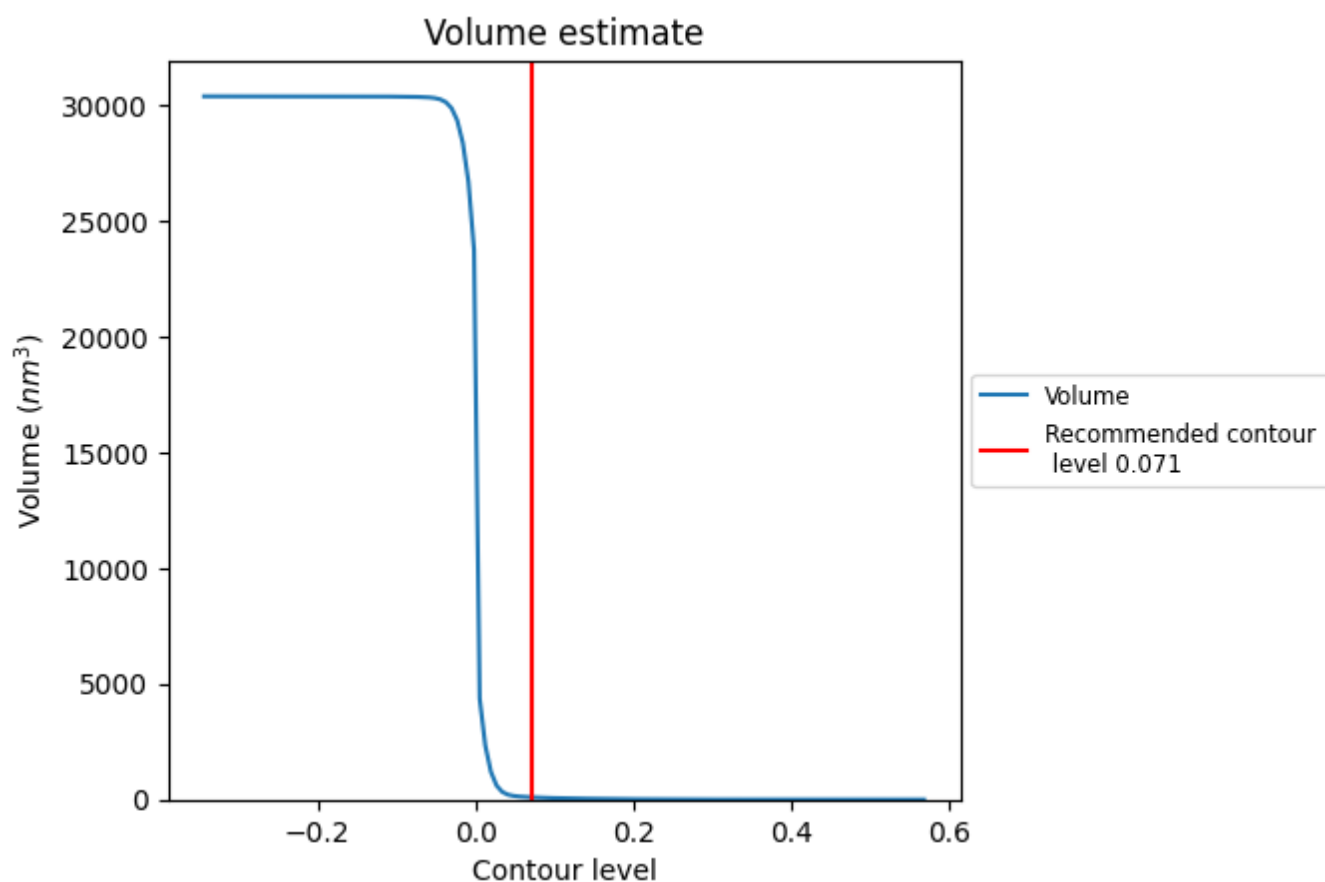
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

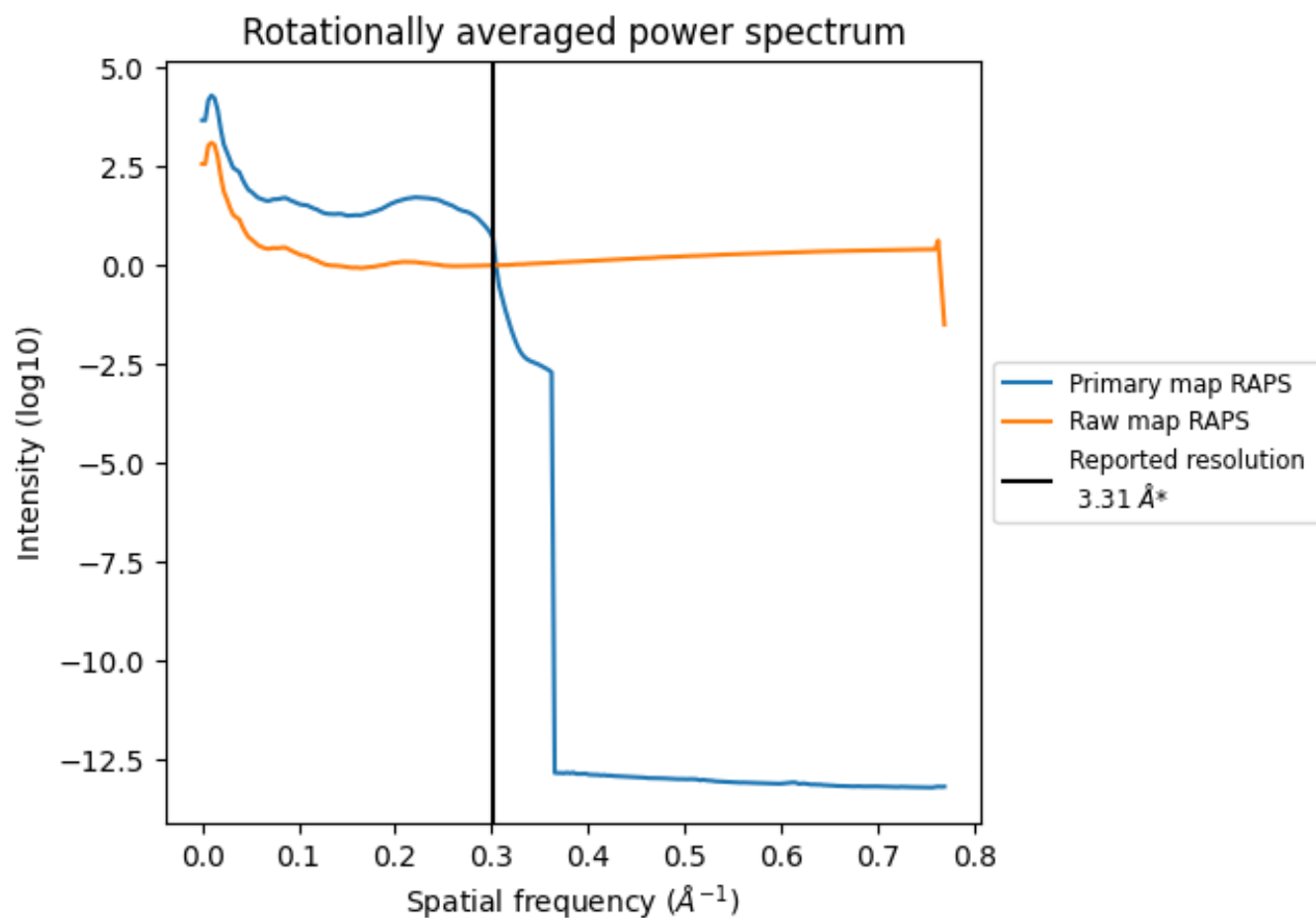
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 89 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 ⓘ

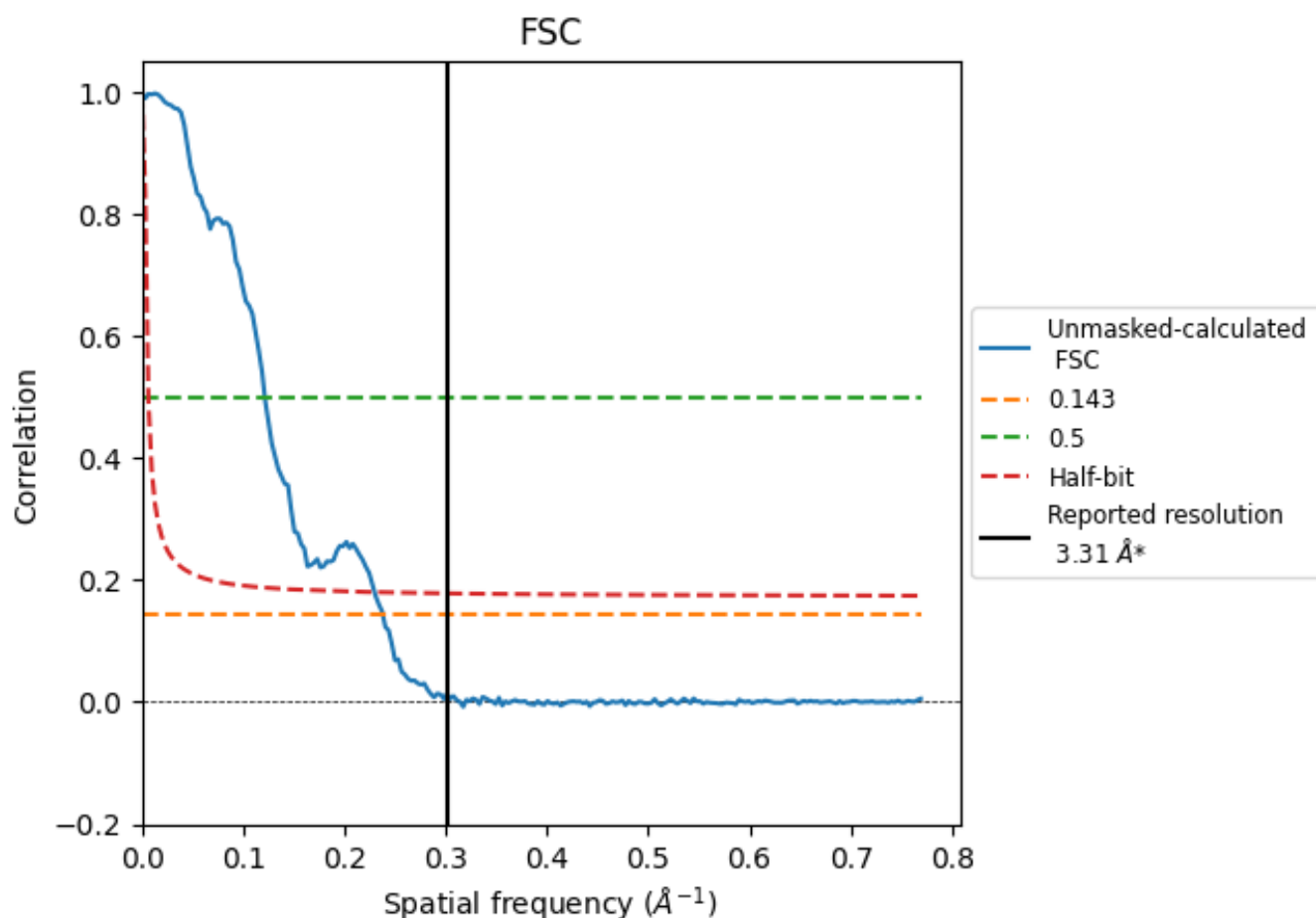


*Reported resolution corresponds to spatial frequency of 0.302 $\text{\AA}^{-1}$

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 $0.302 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

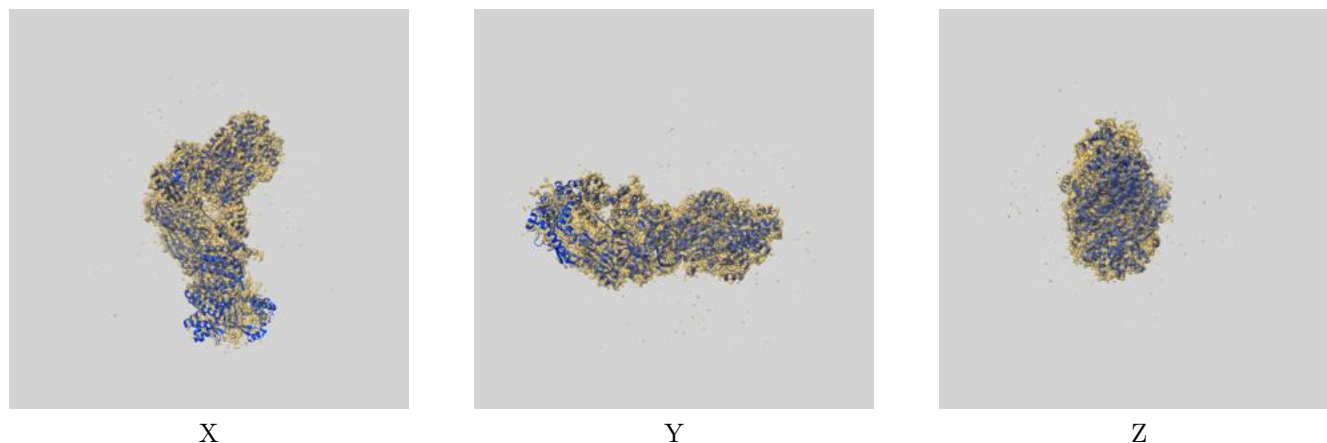
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.21	8.24	4.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.31 by more than 10 %

9 Map-model fit [i](#)

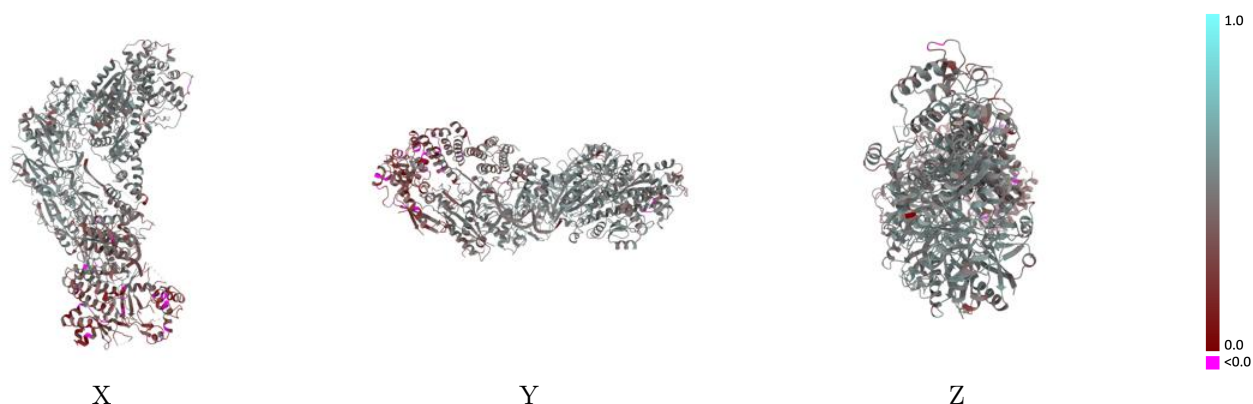
This section contains information regarding the fit between EMDB map EMD-51153 and PDB model 9G9I. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



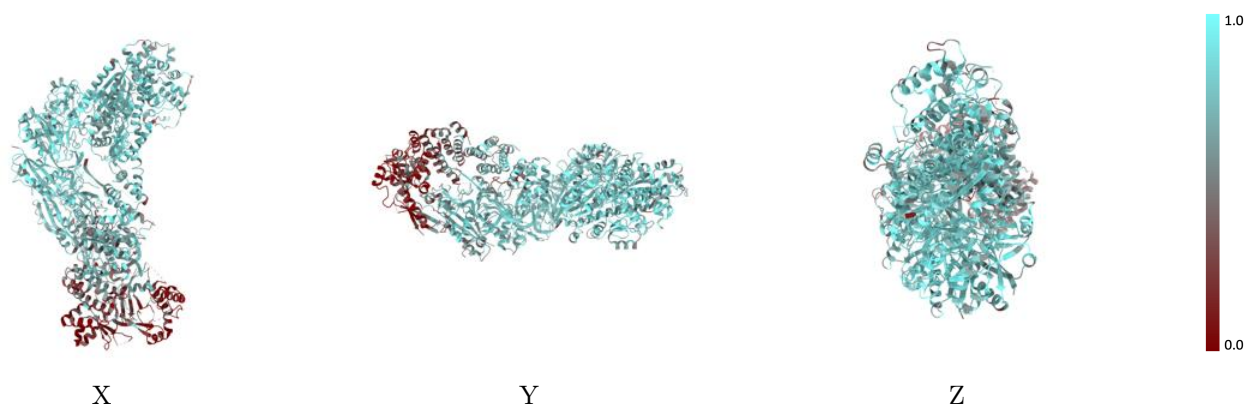
The images above show the 3D surface view of the map at the recommended contour level 0.071 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



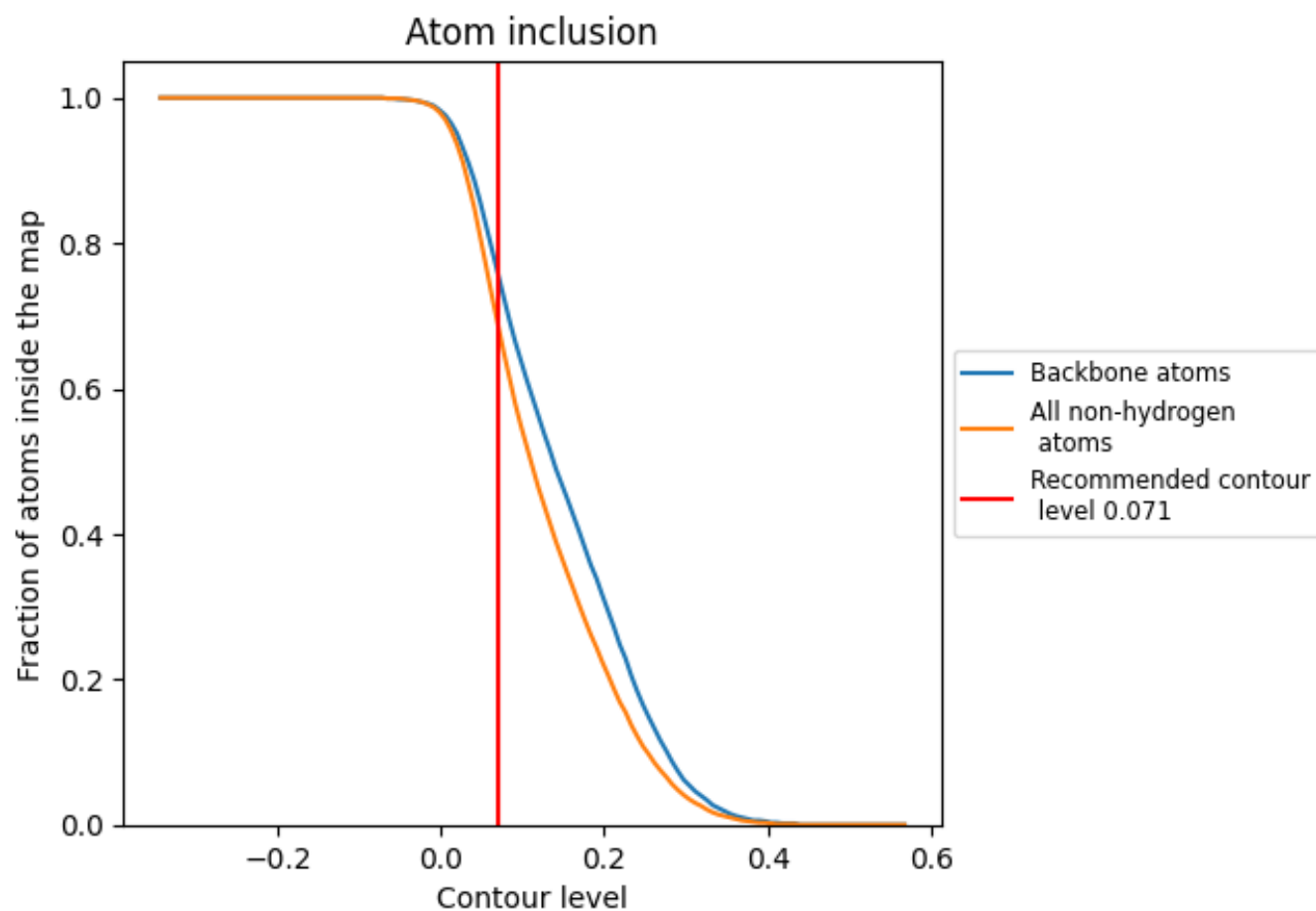
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.071).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.071) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.4420
A	0.7790	0.4820
B	0.6410	0.3880
C	0.4270	0.3300
D	0.8200	0.5150
E	0.7580	0.4850
F	0.7000	0.4480
G	0.8060	0.5050
H	0.2380	0.2680
R	0.8740	0.4660
T	0.6760	0.3670

1.0
0.0
<0.0