



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:01 AM UTC

PDB ID : 6IFK / pdb_00006ifk
EMDB ID : EMD-9653
Title : Cryo-EM structure of type III-A Csm-CTR1 complex, AMPPNP bound
Authors : You, L.; Ma, J.; Wang, J.; Zhang, X.; Wang, Y.
Deposited on : 2018-09-20
Resolution : 3.20 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

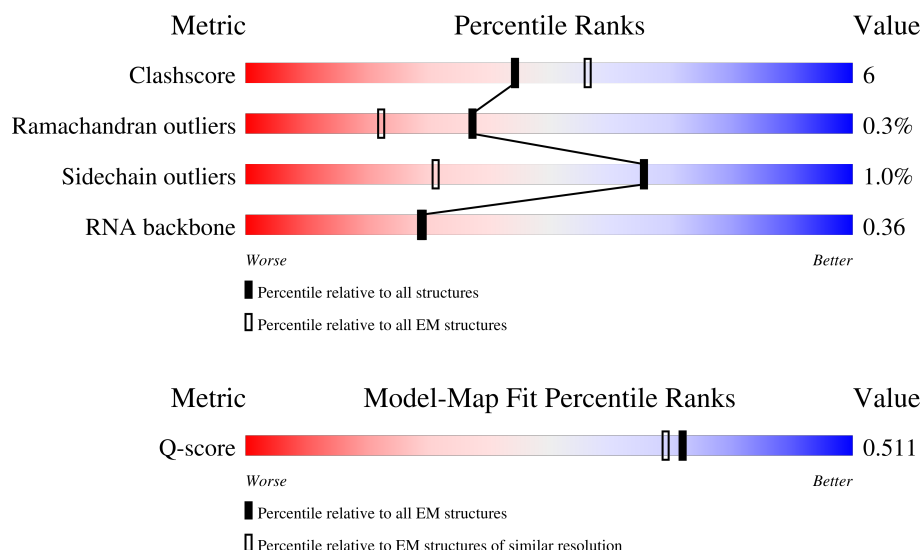
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	758	
2	C	126	
2	D	126	

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Mol	Chain	Length	Quality of chain
3	E	220	
3	F	220	
3	G	220	
4	B	299	
5	H	357	
6	N	34	
7	J	42	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19448 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 Type III-A CRISPR-associated protein Csm1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	734	Total	C	N	O	S	0	0
			5812	3728	977	1091	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASN	ASP	engineered mutation	UNP A0A2U2M0F3

- Molecule 2 is a protein called Type III-A CRISPR-associated protein Csm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	121	Total	C	N	O	S	0	0
			995	642	166	185	2		
2	C	121	Total	C	N	O	S	0	0
			995	642	166	185	2		

- Molecule 3 is a protein called Type III-A CRISPR-associated RAMP protein Csm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	217	Total	C	N	O	S	0	0
			1695	1075	291	327	2		
3	F	216	Total	C	N	O	S	0	0
			1697	1075	290	330	2		
3	E	207	Total	C	N	O	S	0	0
			1626	1033	279	312	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	33	ASN	ASP	engineered mutation	UNP A0A2U2M035
F	33	ASN	ASP	engineered mutation	UNP A0A2U2M035
E	33	ASN	ASP	engineered mutation	UNP A0A2U2M035

- Molecule 4 is a protein called Type III-A CRISPR-associated RAMP protein Csm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	295	Total	C	N	O	S	0	0
			2347	1500	386	456	5		

- Molecule 5 is a protein called Type III-A CRISPR-associated RAMP protein Csm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	345	Total	C	N	O	S	0	0
			2786	1792	478	510	6		

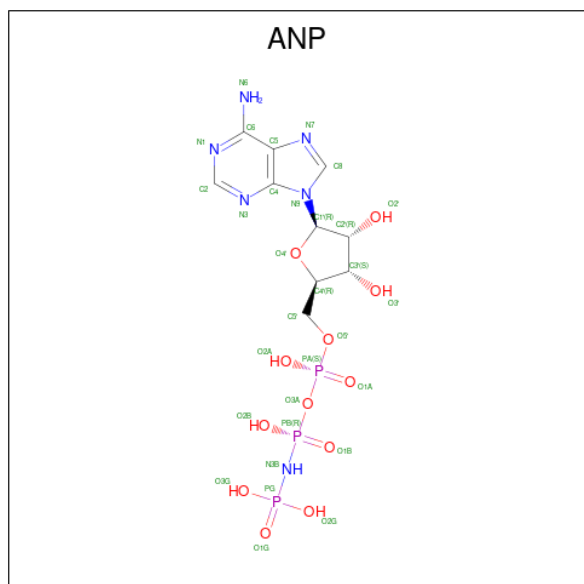
- Molecule 6 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	34	Total	C	N	O	P	0	0
			715	321	123	237	34		

- Molecule 7 is a RNA chain called CTR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	33	Total	C	N	O	P	0	0
			715	320	139	223	33		

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

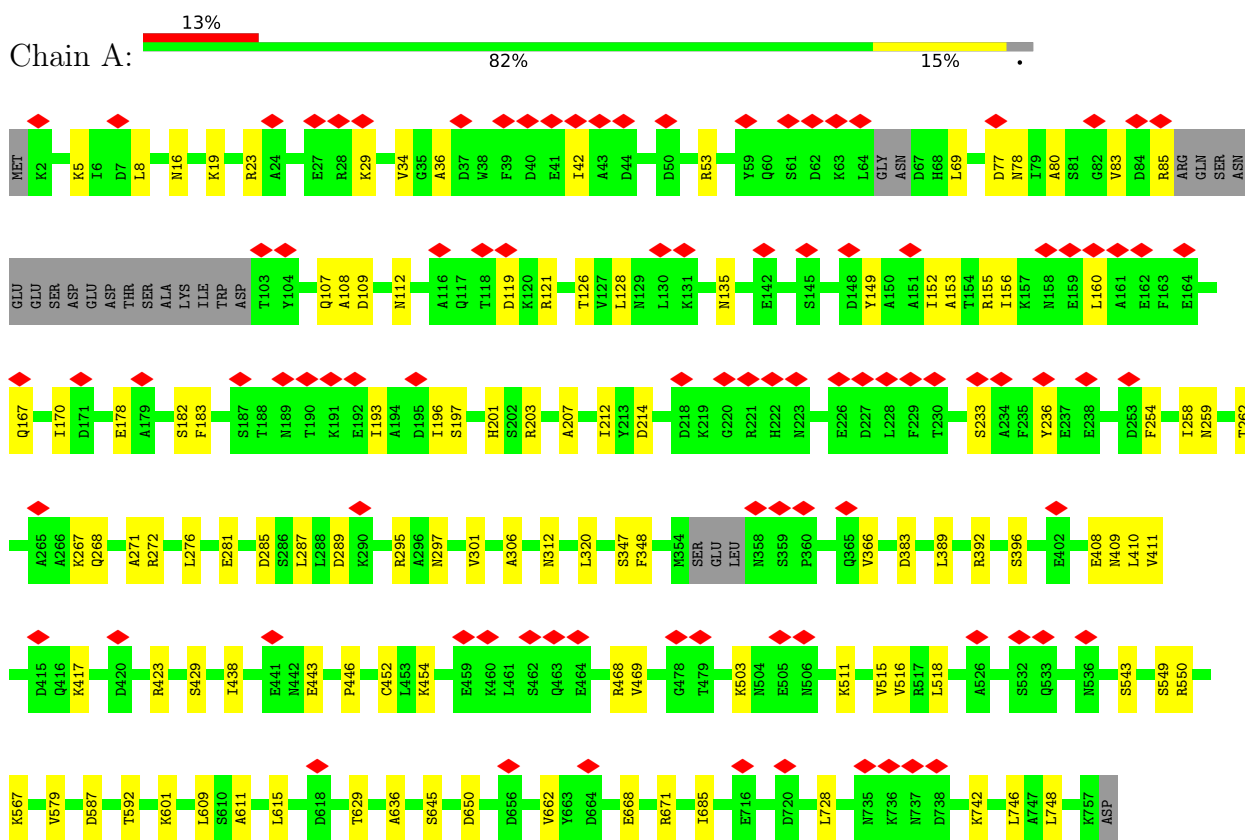
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Zn	0
			1	1	

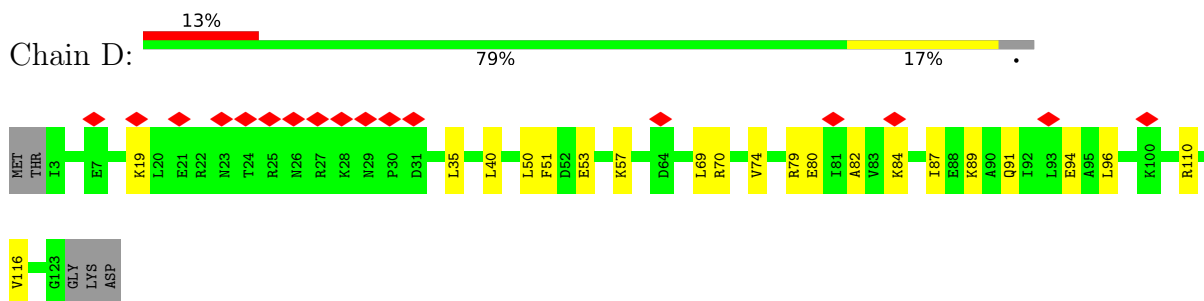
3 Residue-property plots

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

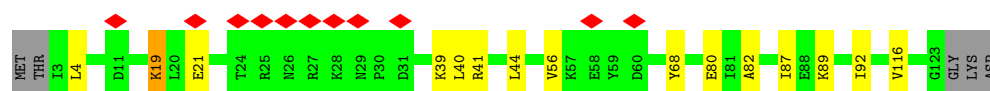
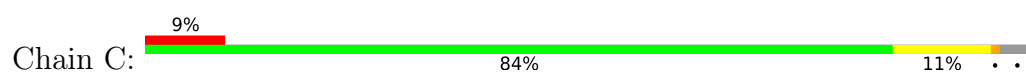
- Molecule 1: Type III-A CRISPR-associated protein Csm1



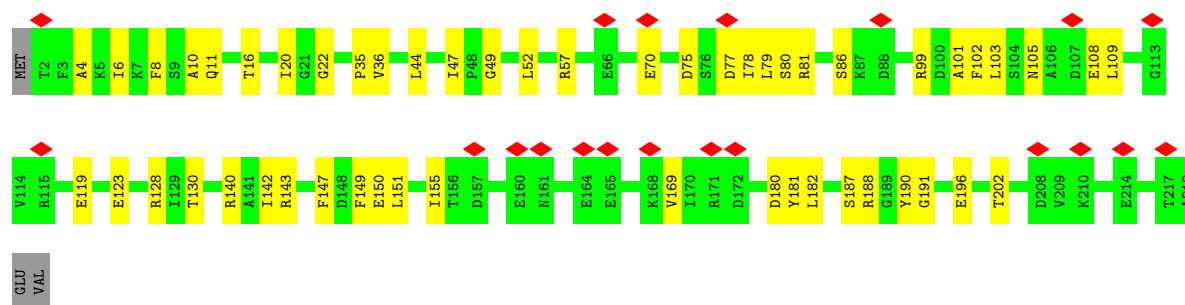
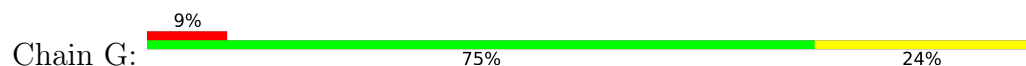
- Molecule 2: Type III-A CRISPR-associated protein Csm2



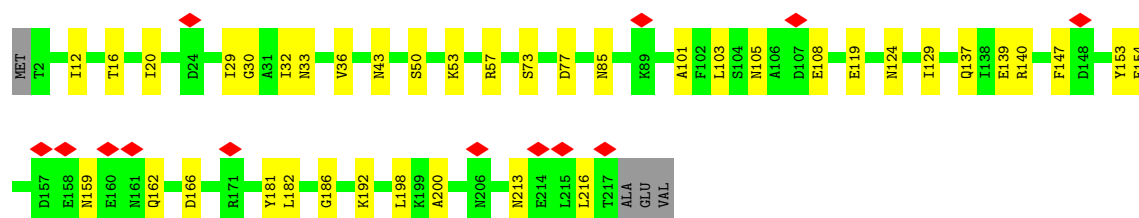
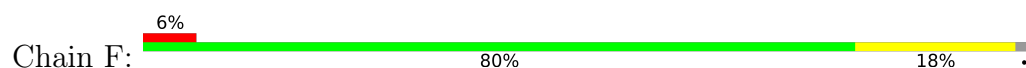
- Molecule 2: Type III-A CRISPR-associated protein Csm2



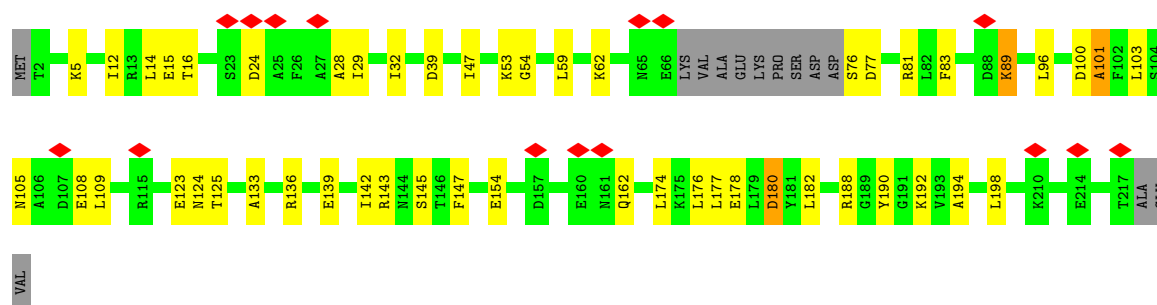
- Molecule 3: Type III-A CRISPR-associated RAMP protein Csm3



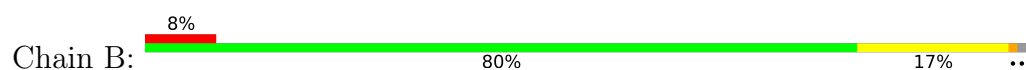
- Molecule 3: Type III-A CRISPR-associated RAMP protein Csm3

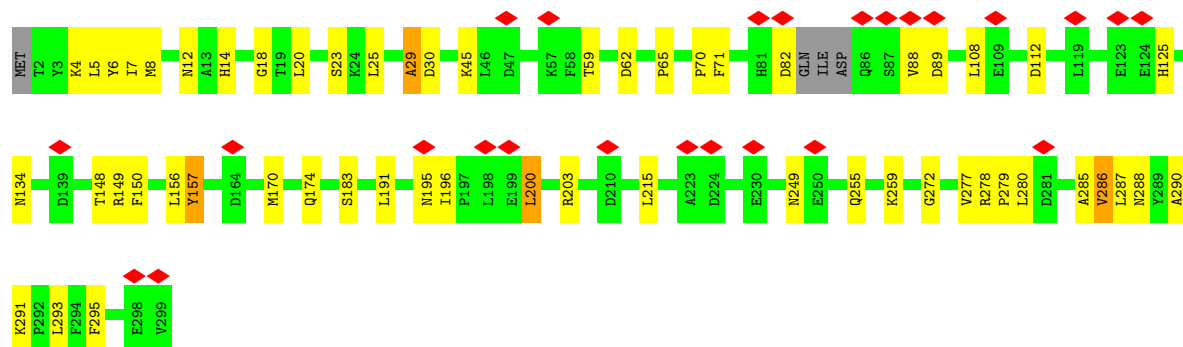


- Molecule 3: Type III-A CRISPR-associated RAMP protein Csm3

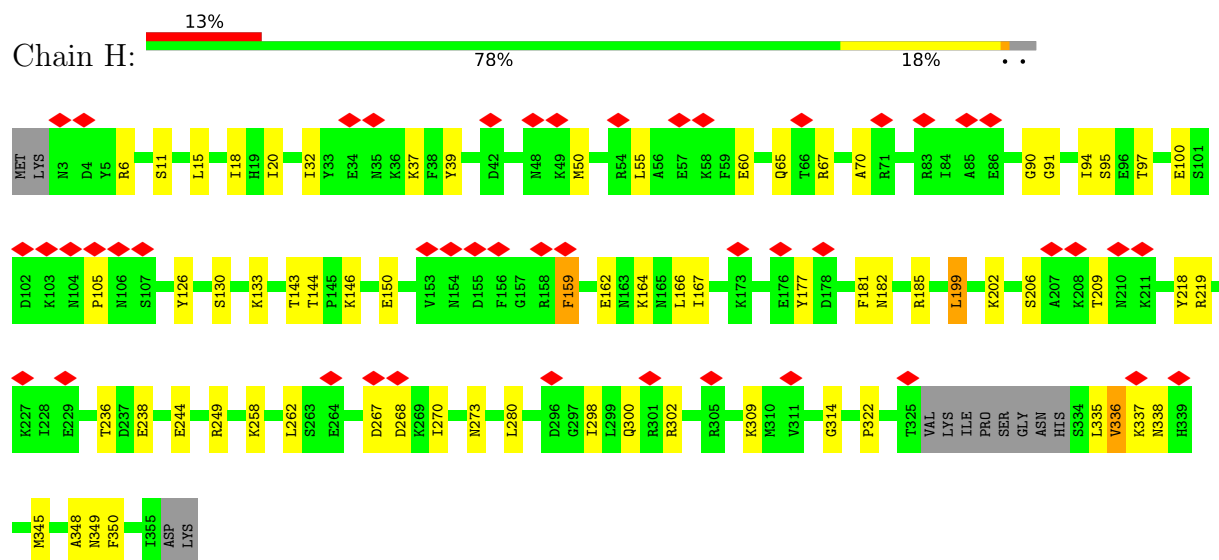


- Molecule 4: Type III-A CRISPR-associated RAMP protein Csm4





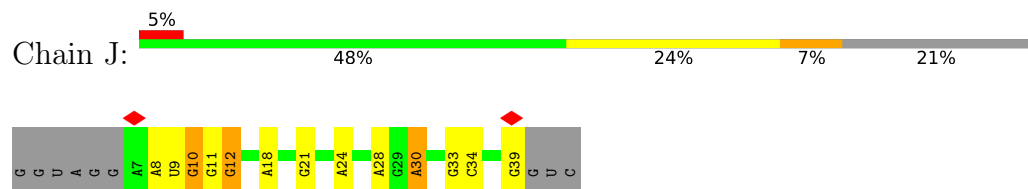
- Molecule 5: Type III-A CRISPR-associated RAMP protein Csm5



- Molecule 6: crRNA



- Molecule 7: CTR1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61538	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.394	Depositor
Minimum map value	-0.218	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.065	Depositor
Map size ($\text{\AA}$)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, 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	0.36	0/5932	0.60	0/8007
2	C	0.38	0/1009	0.60	0/1358
2	D	0.32	0/1009	0.57	0/1358
3	E	0.45	0/1649	0.76	2/2218 (0.1%)
3	F	0.43	0/1722	0.72	0/2318
3	G	0.44	0/1720	0.70	0/2316
4	B	0.40	0/2398	0.69	1/3239 (0.0%)
5	H	0.38	0/2850	0.77	2/3836 (0.1%)
6	N	0.55	0/797	0.62	2/1237 (0.2%)
7	J	0.41	0/803	0.44	0/1251
All	All	0.40	0/19889	0.66	7/27138 (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
3	E	0	2
4	B	0	1
5	H	0	4
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	336	VAL	N-CA-C	10.08	120.90	110.62
5	H	199	LEU	CA-CB-CG	6.56	139.25	116.30
6	N	9	G	O4'-C1'-N9	5.06	115.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	143	ARG	CA-C-N	5.05	131.19	121.54
3	E	143	ARG	C-N-CA	5.05	131.19	121.54
6	N	21	G	O4'-C1'-N9	5.04	115.76	108.20
4	B	157	TYR	CA-CB-CG	5.01	122.92	113.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	286	VAL	Peptide
3	E	101	ALA	Peptide
3	E	28	ALA	Peptide
5	H	105	PRO	Peptide
5	H	159	PHE	Peptide
5	H	20	ILE	Peptide
5	H	90	GLY	Peptide

5.2 Too-close contacts

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	5812	0	5549	62	0
2	C	995	0	1012	10	0
2	D	995	0	1012	13	0
3	E	1626	0	1641	34	0
3	F	1697	0	1710	25	0
3	G	1695	0	1709	38	0
4	B	2347	0	2284	39	0
5	H	2786	0	2783	37	0
6	N	715	0	366	21	0
7	J	715	0	358	4	0
8	A	62	0	26	4	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0
All	All	19448	0	18450	242	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 6.

All (242) 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)
5:H:267:ASP:OD2	5:H:337:LYS:NZ	2.19	0.72
4:B:29:ALA:H	4:B:62:ASP:HB3	1.57	0.70
1:A:411:VAL:HG21	1:A:423:ARG:HD2	1.72	0.69
5:H:336:VAL:HG22	5:H:338:ASN:OD1	1.95	0.67
5:H:273:ASN:O	5:H:349:ASN:ND2	2.26	0.67
1:A:268:GLN:HE21	1:A:272:ARG:HH21	1.43	0.66
5:H:70:ALA:HB2	7:J:10:G:H5'	1.77	0.65
3:G:8:PHE:HB2	3:G:151:LEU:HB3	1.78	0.65
5:H:6:ARG:NH2	5:H:244:GLU:OE2	2.31	0.64
2:D:80:GLU:HG2	2:D:82:ALA:H	1.63	0.63
5:H:18:ILE:HD11	5:H:348:ALA:HB2	1.81	0.63
4:B:71:PHE:O	4:B:157:TYR:OH	2.17	0.62
3:E:89:LYS:HE3	4:B:249:ASN:HB2	1.81	0.62
4:B:4:LYS:HD2	4:B:195:ASN:HA	1.82	0.62
4:B:88:VAL:HG12	4:B:89:ASP:N	2.13	0.61
3:F:12:ILE:HB	3:F:147:PHE:HB2	1.82	0.61
3:E:100:ASP:OD2	4:B:12:ASN:ND2	2.34	0.61
3:F:159:ASN:HB2	3:F:162:GLN:HB2	1.83	0.61
1:A:516:VAL:HG21	1:A:592:THR:HG21	1.83	0.60
3:G:86:SER:OG	6:N:17:G:N2	2.29	0.60
4:B:174:GLN:HE21	4:B:191:LEU:HB3	1.66	0.60
1:A:503:LYS:HE3	1:A:511:LYS:HB2	1.83	0.60
3:E:109:LEU:HD13	3:E:142:ILE:HD11	1.83	0.60
1:A:396:SER:HB2	4:B:280:LEU:HB2	1.83	0.59
3:E:123:GLU:HA	6:N:15:U:H5''	1.84	0.59
3:E:47:ILE:HB	3:E:101:ALA:HB3	1.84	0.59
3:G:77:ASP:HA	3:G:80:SER:HB2	1.85	0.58
5:H:97:THR:HG23	5:H:322:PRO:HD3	1.83	0.58
1:A:36:ALA:HB1	1:A:53:ARG:HD2	1.86	0.58
1:A:549:SER:HA	8:A:801:ANP:HN62	1.67	0.58
1:A:77:ASP:OD1	1:A:201:HIS:NE2	2.34	0.58
3:G:130:THR:HB	5:H:302:ARG:HD2	1.84	0.58
1:A:8:LEU:HD13	1:A:69:LEU:HB3	1.86	0.58
3:G:128:ARG:NH2	6:N:26:A:OP2	2.36	0.58
3:E:81:ARG:NH1	3:E:162:GLN:OE1	2.37	0.58
3:G:187:SER:HA	5:H:185:ARG:HA	1.86	0.57
1:A:109:ASP:OD2	1:A:121:ARG:NH2	2.37	0.57
2:D:51:PHE:HZ	2:D:110:ARG:HH21	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASN:ND2	1:A:347:SER:OG	2.37	0.57
3:F:198:LEU:HB3	3:F:216:LEU:HD23	1.87	0.56
3:E:53:LYS:NZ	4:B:183:SER:OG	2.39	0.56
1:A:636:ALA:HB2	1:A:645:SER:HB2	1.87	0.56
1:A:108:ALA:HB1	1:A:112:ASN:HD22	1.71	0.56
4:B:25:LEU:HD21	4:B:125:HIS:HE1	1.71	0.56
1:A:78:ASN:ND2	1:A:85:ARG:O	2.39	0.55
3:E:178:GLU:HG2	3:E:194:ALA:HA	1.88	0.55
3:F:105:ASN:HB2	3:F:108:GLU:HB3	1.88	0.55
1:A:178:GLU:OE2	1:A:203:ARG:NH1	2.39	0.55
3:G:57:ARG:NH2	6:N:19:U:OP1	2.40	0.55
1:A:668:GLU:OE1	1:A:671:ARG:NH1	2.40	0.54
5:H:219:ARG:HH11	5:H:345:MET:HE2	1.72	0.54
3:G:16:THR:H	3:G:143:ARG:HG3	1.73	0.54
3:E:39:ASP:OD1	4:B:149:ARG:NE	2.37	0.54
3:E:188:ARG:NH1	6:N:13:U:OP2	2.40	0.54
4:B:88:VAL:CG1	4:B:89:ASP:N	2.71	0.53
3:G:99:ARG:HD2	3:F:192:LYS:HD2	1.89	0.53
3:F:53:LYS:HD3	3:E:188:ARG:HG2	1.90	0.53
1:A:128:LEU:HD21	1:A:183:PHE:HE2	1.74	0.53
2:D:50:LEU:HD12	2:D:69:LEU:HD13	1.90	0.53
1:A:267:LYS:HB3	1:A:429:SER:HB2	1.89	0.53
5:H:143:THR:O	5:H:249:ARG:NH1	2.42	0.53
4:B:5:LEU:HD23	4:B:196:ILE:HG12	1.90	0.53
5:H:150:GLU:HG3	5:H:166:LEU:HD21	1.91	0.53
1:A:167:GLN:HA	1:A:170:ILE:HB	1.91	0.52
1:A:207:ALA:O	1:A:297:ASN:ND2	2.42	0.52
5:H:262:LEU:HD12	5:H:270:ILE:HD12	1.90	0.52
4:B:287:LEU:N	6:N:1:A:OP2	2.39	0.52
3:E:124:ASN:ND2	6:N:15:U:O2	2.42	0.52
4:B:134:ASN:HD22	6:N:9:G:H21	1.55	0.52
3:G:70:GLU:HA	3:F:129:ILE:HG12	1.91	0.52
3:G:140:ARG:NH2	5:H:126:TYR:OH	2.43	0.52
3:E:101:ALA:HB1	3:E:147:PHE:HB3	1.92	0.52
3:F:101:ALA:HB1	3:F:147:PHE:HB3	1.90	0.51
3:E:125:THR:OG1	6:N:13:U:O2	2.23	0.51
3:G:47:ILE:HB	3:G:101:ALA:HB3	1.92	0.51
3:G:188:ARG:NH1	6:N:25:U:OP2	2.43	0.51
3:E:54:GLY:HA3	6:N:8:C:H5'	1.92	0.51
3:G:105:ASN:HB2	3:G:108:GLU:HB3	1.93	0.51
3:F:124:ASN:HD22	6:N:21:G:H21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ILE:HG23	1:A:748:LEU:HD22	1.91	0.51
5:H:15:LEU:HD22	5:H:335:LEU:HD22	1.92	0.51
8:A:802:ANP:O2A	8:A:802:ANP:N3B	2.44	0.50
3:E:16:THR:HG23	3:E:192:LYS:HE2	1.93	0.50
3:E:105:ASN:HB2	3:E:108:GLU:HB3	1.93	0.50
3:F:119:GLU:OE2	3:F:140:ARG:NH1	2.44	0.50
2:D:40:LEU:HG	2:D:116:VAL:HG22	1.94	0.50
3:E:53:LYS:HE3	3:E:83:PHE:HD1	1.77	0.50
4:B:30:ASP:OD2	4:B:288:ASN:ND2	2.45	0.50
4:B:278:ARG:HD3	4:B:285:ALA:HA	1.94	0.50
1:A:408:GLU:OE1	1:A:409:ASN:ND2	2.44	0.50
2:D:91:GLN:HB2	2:D:94:GLU:HB2	1.94	0.49
1:A:193:ILE:HG13	1:A:196:ILE:HD13	1.94	0.49
3:E:177:LEU:HD22	3:E:182:LEU:HB2	1.94	0.49
1:A:178:GLU:O	1:A:182:SER:OG	2.29	0.49
3:G:109:LEU:HD13	3:G:142:ILE:HD11	1.94	0.49
3:E:174:LEU:HD13	3:E:198:LEU:HD11	1.94	0.49
4:B:134:ASN:ND2	6:N:9:G:N3	2.61	0.49
1:A:446:PRO:HA	1:A:452:CYS:HA	1.95	0.49
5:H:162:GLU:HG2	5:H:164:LYS:H	1.78	0.49
2:D:110:ARG:HD2	2:C:68:TYR:CD1	2.48	0.49
1:A:80:ALA:O	1:A:543:SER:OG	2.31	0.49
4:B:149:ARG:NH1	4:B:150:PHE:O	2.46	0.49
1:A:16:ASN:HB3	1:A:19:LYS:HD2	1.95	0.48
1:A:650:ASP:O	1:A:742:LYS:NZ	2.45	0.48
5:H:300:GLN:HG3	5:H:309:LYS:HD3	1.95	0.48
3:G:123:GLU:OE2	3:G:190:TYR:OH	2.22	0.48
4:B:288:ASN:H	6:N:1:A:P	2.35	0.48
2:D:84:LYS:HD2	2:D:87:ILE:HD11	1.94	0.48
3:F:154:GLU:OE1	3:E:62:LYS:NZ	2.45	0.48
3:E:5:LYS:HG2	3:E:154:GLU:HG2	1.95	0.48
1:A:287:LEU:HD21	1:A:320:LEU:HD23	1.95	0.48
1:A:518:LEU:HD23	1:A:609:LEU:HD13	1.96	0.48
2:C:40:LEU:HG	2:C:116:VAL:HG22	1.94	0.48
2:C:44:LEU:HD21	3:F:30:GLY:HA3	1.94	0.48
1:A:389:LEU:HD22	1:A:392:ARG:HD3	1.94	0.48
3:G:6:ILE:HG22	3:G:202:THR:HG22	1.95	0.48
3:G:180:ASP:OD1	5:H:185:ARG:NH1	2.47	0.48
3:F:20:ILE:H	3:F:36:VAL:HG23	1.77	0.48
3:E:32:ILE:HG21	3:E:139:GLU:HB2	1.95	0.48
2:C:80:GLU:HG2	2:C:82:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:236:THR:HG22	5:H:238:GLU:H	1.78	0.48
2:D:35:LEU:HD11	2:D:40:LEU:HB2	1.95	0.48
1:A:258:ILE:HG13	1:A:262:THR:HG21	1.96	0.47
3:F:153:TYR:OH	3:F:166:ASP:OD2	2.28	0.47
5:H:258:LYS:HA	5:H:262:LEU:HB2	1.97	0.47
1:A:567:LYS:HB3	1:A:587:ASP:HB3	1.96	0.47
2:C:56:VAL:HG22	3:F:43:ASN:HB3	1.96	0.47
4:B:255:GLN:HE21	4:B:279:PRO:HA	1.80	0.47
3:F:57:ARG:NH1	6:N:13:U:OP1	2.48	0.47
3:E:133:ALA:O	7:J:28:A:O2'	2.26	0.47
3:G:52:LEU:HD23	3:G:182:LEU:HD21	1.96	0.47
1:A:126:THR:OG1	1:A:135:ASN:ND2	2.47	0.47
1:A:348:PHE:HB3	1:A:366:VAL:HG21	1.97	0.47
1:A:281:GLU:OE2	1:A:295:ARG:NH1	2.48	0.47
1:A:233:SER:HA	1:A:236:TYR:HB3	1.97	0.47
3:G:77:ASP:O	3:G:81:ARG:NH1	2.47	0.47
3:F:32:ILE:HG21	3:F:139:GLU:HB2	1.96	0.47
3:E:15:GLU:HB3	3:E:192:LYS:HE3	1.97	0.47
3:E:176:LEU:O	3:E:180:ASP:N	2.48	0.47
1:A:662:VAL:HG11	1:A:746:LEU:HD12	1.97	0.46
4:B:6:TYR:HB3	4:B:191:LEU:HD11	1.96	0.46
1:A:152:ILE:O	1:A:155:ARG:HB3	2.15	0.46
3:F:33:ASN:HD22	3:F:137:GLN:H	1.62	0.46
3:F:200:ALA:H	3:F:213:ASN:HD21	1.61	0.46
4:B:286:VAL:HG13	6:N:1:A:H3'	1.96	0.46
3:G:11:GLN:HB2	3:G:196:GLU:HB2	1.98	0.46
3:G:102:PHE:HE2	3:F:16:THR:HG22	1.80	0.46
3:G:181:TYR:HB2	3:G:191:GLY:HA3	1.96	0.46
5:H:159:PHE:HB3	5:H:298:ILE:HG23	1.96	0.46
1:A:301:VAL:HG23	1:A:306:ALA:HB2	1.98	0.46
2:C:87:ILE:HG22	2:C:92:ILE:HD12	1.97	0.46
1:A:259:ASN:O	1:A:262:THR:OG1	2.29	0.46
5:H:268:ASP:N	5:H:268:ASP:OD1	2.48	0.46
3:G:75:ASP:HB3	3:G:79:LEU:HB2	1.97	0.46
3:G:4:ALA:HB3	3:G:155:ILE:HB	1.98	0.46
1:A:410:LEU:HB3	1:A:417:LYS:HD2	1.97	0.46
1:A:153:ALA:O	1:A:156:ILE:HB	2.16	0.46
1:A:515:VAL:HG12	1:A:629:THR:HG21	1.98	0.45
3:G:44:LEU:HD12	3:G:103:LEU:HB3	1.98	0.45
3:G:99:ARG:HB2	3:G:150:GLU:HB2	1.98	0.45
4:B:8:MET:HG3	4:B:156:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:ARG:NH2	7:J:12:G:O5'	2.49	0.45
4:B:108:LEU:HD21	4:B:200:LEU:HD23	1.97	0.45
8:A:802:ANP:O1G	8:A:802:ANP:O2B	2.34	0.45
2:D:19:LYS:HE2	2:D:89:LYS:HG3	1.98	0.45
4:B:272:GLY:HA3	4:B:291:LYS:HA	1.97	0.45
3:F:73:SER:HA	3:F:85:ASN:HD21	1.81	0.45
4:B:70:PRO:HG2	4:B:108:LEU:HD12	1.97	0.45
1:A:518:LEU:HG	1:A:611:ALA:HB2	1.99	0.44
3:E:136:ARG:NH2	6:N:13:U:O2'	2.50	0.44
4:B:23:SER:OG	4:B:148:THR:OG1	2.28	0.44
1:A:285:ASP:OD1	1:A:295:ARG:NH2	2.51	0.44
3:G:20:ILE:H	3:G:36:VAL:HG23	1.83	0.44
4:B:112:ASP:OD2	4:B:203:ARG:NH2	2.46	0.44
3:G:86:SER:HB2	6:N:18:C:H1'	1.99	0.44
2:D:53:GLU:OE1	2:D:57:LYS:NZ	2.44	0.44
4:B:18:GLY:HA2	6:N:3:G:C8	2.53	0.44
3:G:188:ARG:HB3	5:H:130:SER:HB3	2.00	0.44
6:N:16:A:H2'	6:N:17:G:C8	2.53	0.44
4:B:59:THR:HG21	4:B:293:LEU:HD13	1.99	0.43
3:G:78:ILE:HD11	3:G:169:VAL:HG21	1.99	0.43
8:A:801:ANP:O1G	8:A:801:ANP:O2B	2.36	0.43
4:B:6:TYR:HD2	4:B:170:MET:HE2	1.83	0.43
5:H:65:GLN:HG3	5:H:67:ARG:HB2	2.00	0.43
3:G:49:GLY:HA2	3:G:52:LEU:HD12	1.99	0.43
3:F:50:SER:HB3	3:E:188:ARG:HB3	2.00	0.43
1:A:29:LYS:HE3	1:A:34:VAL:HA	2.00	0.43
1:A:196:ILE:HG12	1:A:543:SER:HB3	2.01	0.43
2:C:19:LYS:HE2	2:C:89:LYS:HG3	2.01	0.43
2:C:21:GLU:OE1	2:C:89:LYS:NZ	2.49	0.43
3:G:52:LEU:HD13	3:G:149:PHE:HE1	1.83	0.43
1:A:5:LYS:NZ	1:A:214:ASP:OD1	2.52	0.43
3:G:101:ALA:HB1	3:G:147:PHE:HB3	2.01	0.43
3:G:119:GLU:OE2	3:G:140:ARG:NE	2.52	0.43
5:H:11:SER:O	5:H:350:PHE:HA	2.19	0.43
5:H:133:LYS:NZ	5:H:181:PHE:O	2.51	0.43
5:H:37:LYS:NZ	5:H:95:SER:OG	2.49	0.42
5:H:32:ILE:HD12	5:H:39:TYR:HD2	1.84	0.42
5:H:144:THR:HG22	5:H:146:LYS:HG2	2.00	0.42
5:H:167:ILE:HD13	5:H:181:PHE:HE2	1.83	0.42
3:E:59:LEU:HD13	3:E:176:LEU:HB3	2.01	0.42
4:B:259:LYS:HD3	4:B:290:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:177:TYR:OH	5:H:182:ASN:ND2	2.44	0.42
1:A:119:ASP:N	1:A:119:ASP:OD1	2.52	0.42
3:G:22:GLY:N	3:G:35:PRO:O	2.49	0.42
1:A:289:ASP:OD2	1:A:468:ARG:NH2	2.53	0.42
3:G:10:ALA:HB3	3:G:149:PHE:HD2	1.83	0.42
1:A:518:LEU:HD13	1:A:579:VAL:HB	2.00	0.42
5:H:206:SER:OG	5:H:209:THR:O	2.38	0.42
1:A:254:PHE:HD2	1:A:276:LEU:HD11	1.85	0.42
5:H:50:MET:HE3	5:H:50:MET:HB3	1.85	0.42
4:B:82:ASP:OD1	4:B:82:ASP:N	2.51	0.42
2:C:41:ARG:HH12	3:F:29:ILE:HG22	1.85	0.41
3:E:136:ARG:HD3	7:J:30:A:C6	2.55	0.41
1:A:443:GLU:HB3	1:A:454:LYS:HD2	2.01	0.41
3:E:96:LEU:HD23	3:E:96:LEU:HA	1.88	0.41
4:B:25:LEU:HD21	4:B:125:HIS:CE1	2.54	0.41
6:N:16:A:H2'	6:N:17:G:H8	1.85	0.41
3:F:181:TYR:CG	3:F:186:GLY:HA3	2.55	0.41
2:D:70:ARG:HA	2:D:96:LEU:HD13	2.01	0.41
1:A:267:LYS:O	1:A:271:ALA:HB3	2.21	0.41
5:H:94:ILE:HD11	5:H:199:LEU:HD23	2.02	0.41
1:A:383:ASP:OD1	1:A:383:ASP:N	2.52	0.41
1:A:121:ARG:NH1	1:A:601:LYS:O	2.54	0.41
1:A:410:LEU:HD22	1:A:417:LYS:HG3	2.03	0.41
2:C:39:LYS:HA	2:C:39:LYS:HD2	1.94	0.41
3:E:14:LEU:HD12	3:E:145:SER:HB2	2.02	0.41
3:E:76:SER:OG	3:E:77:ASP:N	2.54	0.41
4:B:215:LEU:HD11	4:B:295:PHE:HB2	2.02	0.41
4:B:14:HIS:CE1	4:B:20:LEU:HD12	2.56	0.41
4:B:255:GLN:H	4:B:277:VAL:HB	1.86	0.41
5:H:97:THR:HB	5:H:100:GLU:HG3	2.02	0.41
3:E:24:ASP:OD1	3:E:24:ASP:N	2.40	0.40
1:A:23:ARG:HG2	1:A:149:TYR:HE2	1.86	0.40
1:A:42:ILE:H	1:A:42:ILE:HG13	1.74	0.40
1:A:203:ARG:NE	1:A:550:ARG:HH21	2.19	0.40
3:G:8:PHE:CD2	3:G:151:LEU:HD22	2.56	0.40
5:H:280:LEU:HD12	5:H:280:LEU:HA	1.88	0.40
2:D:74:VAL:HG11	5:H:60:GLU:HG3	2.03	0.40
4:B:65:PRO:HG2	4:B:71:PHE:HD2	1.87	0.40
1:A:107:GLN:HE22	1:A:197:SER:HB3	1.86	0.40
3:F:77:ASP:OD1	3:F:77:ASP:N	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/758 (96%)	661 (91%)	64 (9%)	1 (0%)	48	79
2	C	119/126 (94%)	109 (92%)	10 (8%)	0	100	100
2	D	119/126 (94%)	107 (90%)	12 (10%)	0	100	100
3	E	203/220 (92%)	186 (92%)	15 (7%)	2 (1%)	12	45
3	F	214/220 (97%)	195 (91%)	19 (9%)	0	100	100
3	G	215/220 (98%)	186 (86%)	29 (14%)	0	100	100
4	B	291/299 (97%)	252 (87%)	38 (13%)	1 (0%)	36	68
5	H	341/357 (96%)	286 (84%)	52 (15%)	3 (1%)	14	47
All	All	2228/2326 (96%)	1982 (89%)	239 (11%)	7 (0%)	37	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	29	ALA
3	E	29	ILE
3	E	89	LYS
5	H	202	LYS
1	A	83	VAL
5	H	91	GLY
5	H	314	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	585/651 (90%)	579 (99%)	6 (1%)	68	80
2	C	105/112 (94%)	103 (98%)	2 (2%)	50	73
2	D	105/112 (94%)	105 (100%)	0	100	100
3	E	175/188 (93%)	171 (98%)	4 (2%)	44	70
3	F	184/188 (98%)	182 (99%)	2 (1%)	65	79
3	G	182/188 (97%)	182 (100%)	0	100	100
4	B	257/263 (98%)	254 (99%)	3 (1%)	63	79
5	H	295/312 (95%)	293 (99%)	2 (1%)	76	83
All	All	1888/2014 (94%)	1869 (99%)	19 (1%)	65	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	LEU
1	A	212	ILE
1	A	438	ILE
1	A	469	VAL
1	A	615	LEU
1	A	728	LEU
2	C	4	LEU
2	C	19	LYS
3	F	103	LEU
3	F	182	LEU
3	E	12	ILE
3	E	103	LEU
3	E	180	ASP
3	E	190	TYR
4	B	7	ILE
4	B	45	LYS
4	B	200	LEU
5	H	55	LEU
5	H	218	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	16	ASN
1	A	107	GLN

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Mol	Chain	Res	Type
1	A	135	ASN
1	A	252	GLN
1	A	263	ASN
1	A	268	GLN
1	A	312	ASN
1	A	322	GLN
1	A	328	ASN
1	A	365	GLN
1	A	414	HIS
1	A	416	GLN
1	A	427	GLN
1	A	436	HIS
1	A	497	ASN
1	A	561	ASN
1	A	639	ASN
1	A	675	ASN
1	A	699	ASN
2	D	42	ASN
2	C	23	ASN
3	G	159	ASN
3	F	33	ASN
3	F	85	ASN
3	F	124	ASN
3	F	197	ASN
3	F	213	ASN
3	E	33	ASN
3	E	65	ASN
4	B	67	GLN
4	B	125	HIS
4	B	134	ASN
4	B	161	ASN
4	B	167	ASN
4	B	174	GLN
4	B	246	HIS
4	B	284	HIS
4	B	288	ASN
5	H	72	ASN
5	H	104	ASN
5	H	115	ASN
5	H	148	ASN
5	H	151	ASN
5	H	294	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	N	33/34 (97%)	7 (21%)	1 (3%)
7	J	32/42 (76%)	12 (37%)	1 (3%)
All	All	65/76 (85%)	19 (29%)	2 (3%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	N	2	C
6	N	3	G
6	N	8	C
6	N	9	G
6	N	15	U
6	N	21	G
6	N	23	U
7	J	8	A
7	J	9	U
7	J	10	G
7	J	11	G
7	J	12	G
7	J	18	A
7	J	21	G
7	J	24	A
7	J	30	A
7	J	33	G
7	J	34	C
7	J	39	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	N	13	U
7	J	9	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 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	ANP	A	801	9	33,33,33	0.94	3 (9%)	45,52,52	0.66	0
8	ANP	A	802	-	33,33,33	1.00	4 (12%)	45,52,52	0.56	0

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	ANP	A	801	9	-	12/18/38/38	0/3/3/3
8	ANP	A	802	-	-	7/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	802	ANP	PB-O3A	-2.94	1.55	1.59
8	A	801	ANP	PB-O3A	-2.86	1.55	1.59
8	A	802	ANP	PG-O1G	2.49	1.50	1.46
8	A	802	ANP	PG-N3B	2.35	1.69	1.63
8	A	802	ANP	PB-O1B	2.31	1.49	1.46
8	A	801	ANP	PA-O3A	-2.04	1.57	1.59
8	A	801	ANP	PG-N3B	2.01	1.68	1.63

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

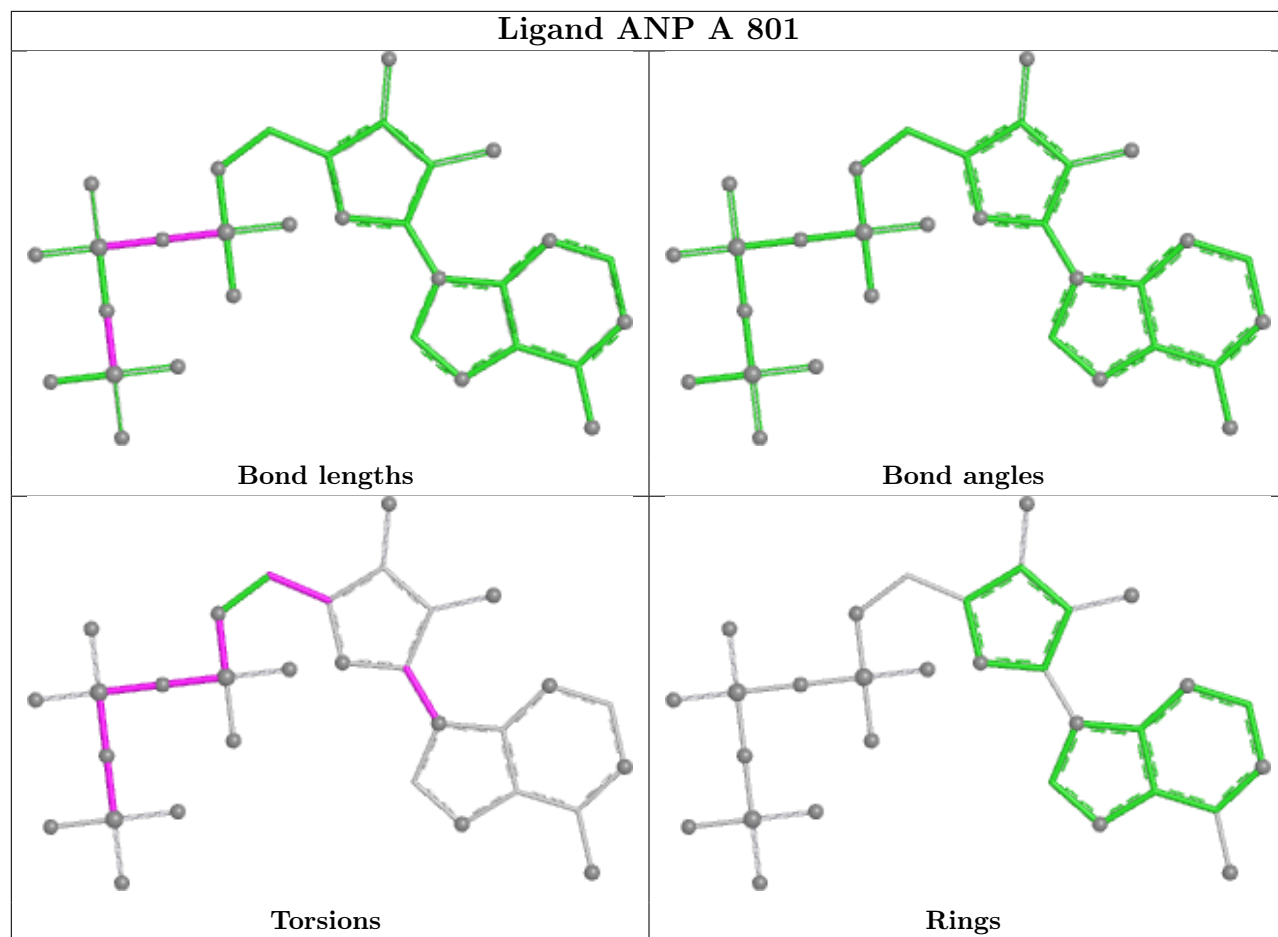
Mol	Chain	Res	Type	Atoms
8	A	801	ANP	PB-N3B-PG-O1G
8	A	801	ANP	PG-N3B-PB-O1B
8	A	801	ANP	PA-O3A-PB-O2B
8	A	802	ANP	PB-N3B-PG-O1G
8	A	802	ANP	PG-N3B-PB-O1B
8	A	802	ANP	PA-O3A-PB-O2B
8	A	802	ANP	C5'-O5'-PA-O1A
8	A	802	ANP	C5'-O5'-PA-O2A
8	A	802	ANP	C5'-O5'-PA-O3A
8	A	801	ANP	O4'-C4'-C5'-O5'
8	A	801	ANP	C2'-C1'-N9-C8
8	A	801	ANP	PB-O3A-PA-O1A
8	A	801	ANP	C3'-C4'-C5'-O5'
8	A	801	ANP	PG-N3B-PB-O3A
8	A	801	ANP	C5'-O5'-PA-O1A
8	A	801	ANP	C2'-C1'-N9-C4
8	A	801	ANP	PB-O3A-PA-O2A
8	A	801	ANP	O4'-C1'-N9-C8
8	A	802	ANP	PG-N3B-PB-O3A

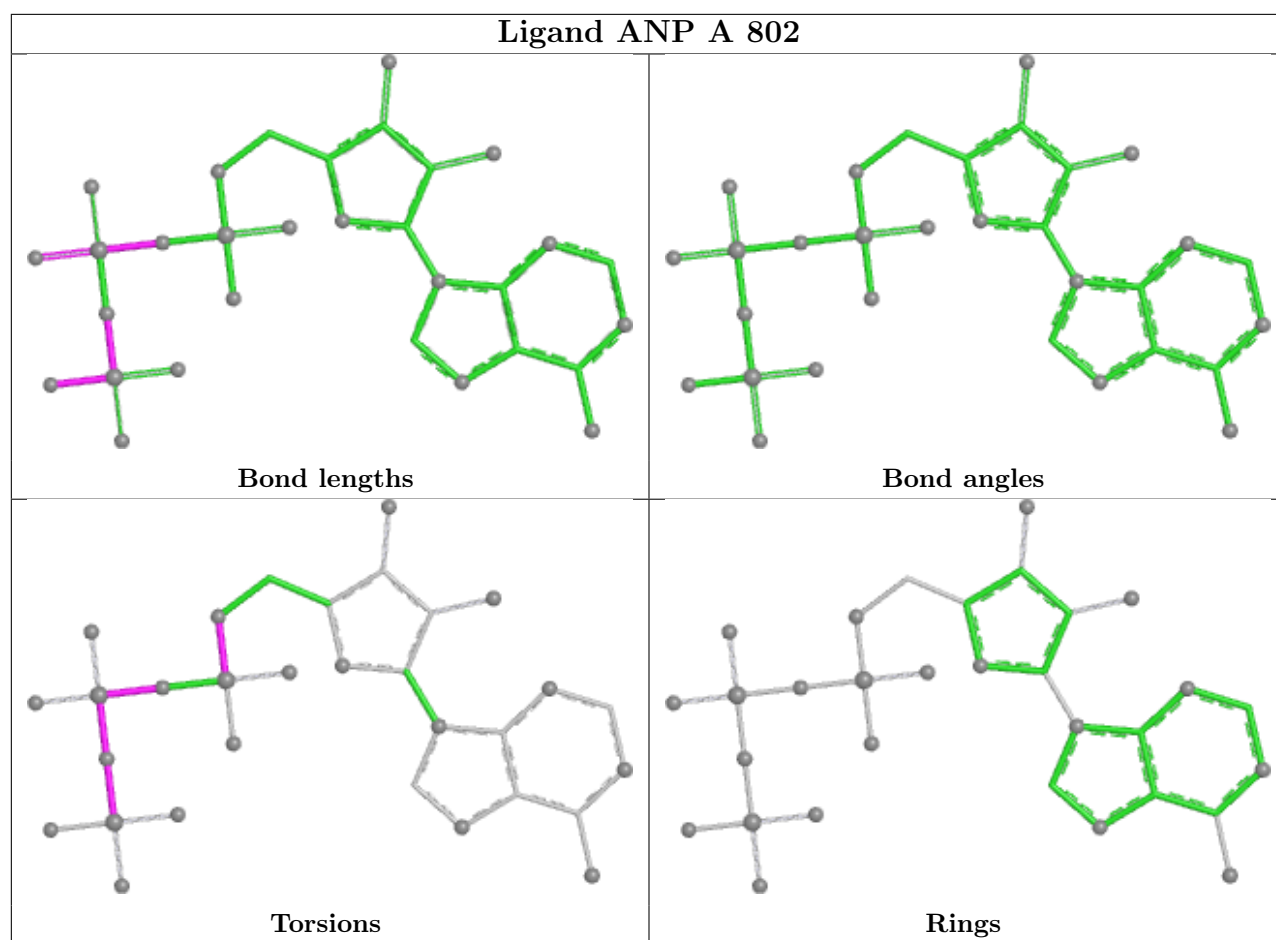
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	801	ANP	2	0
8	A	802	ANP	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

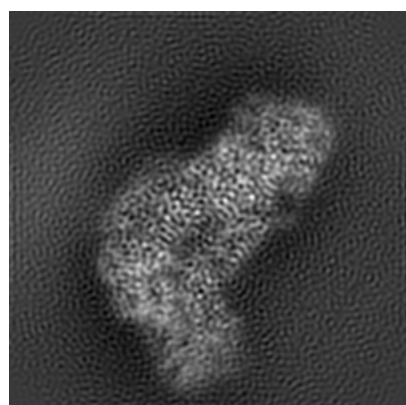
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9653. These allow visual inspection of the internal detail of the map and identification of artifacts.

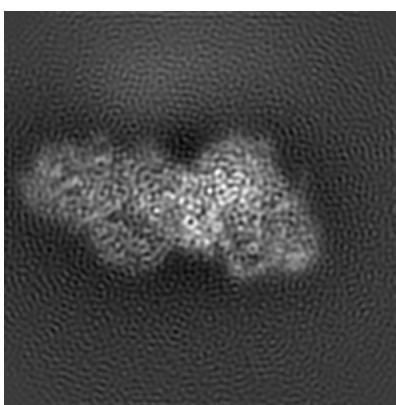
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

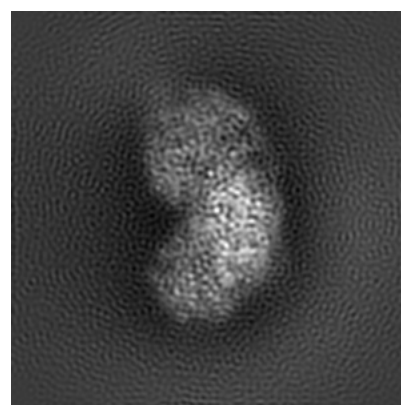
6.1.1 Primary map



X



Y

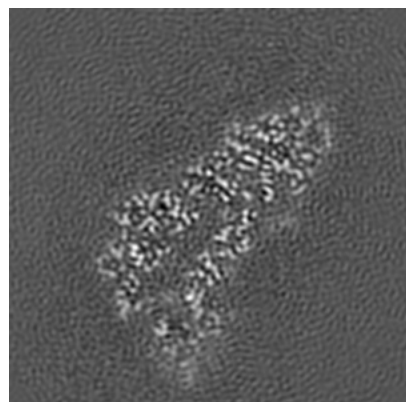


Z

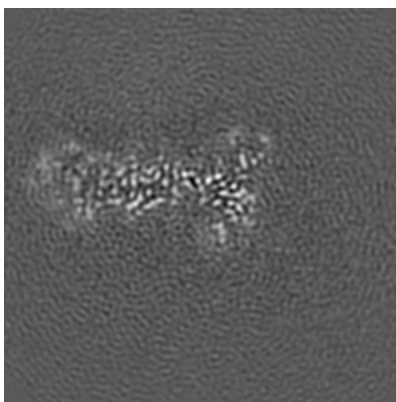
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

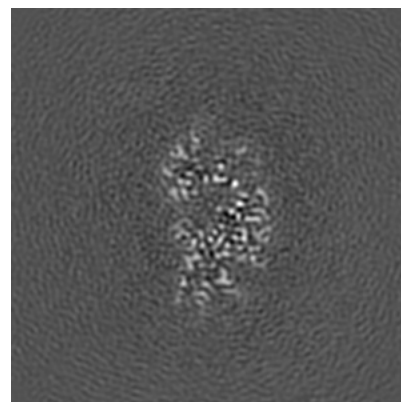
6.2.1 Primary map



X Index: 100



Y Index: 100

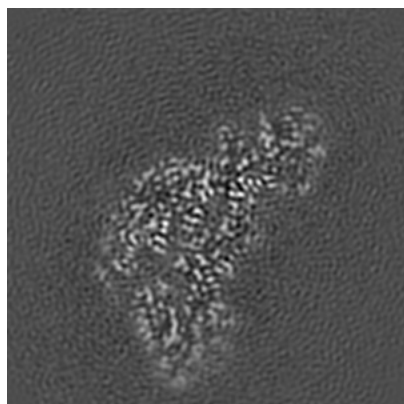


Z Index: 100

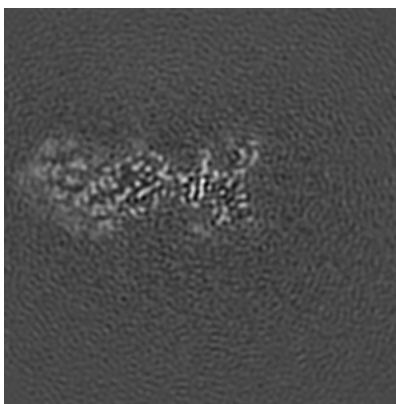
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

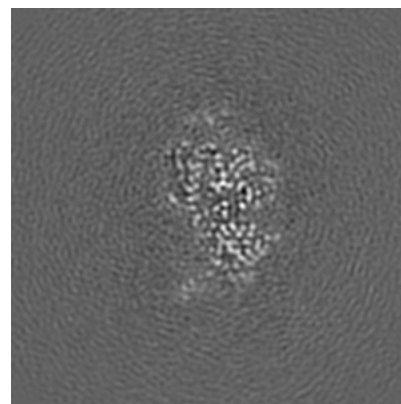
6.3.1 Primary map



X Index: 106



Y Index: 94

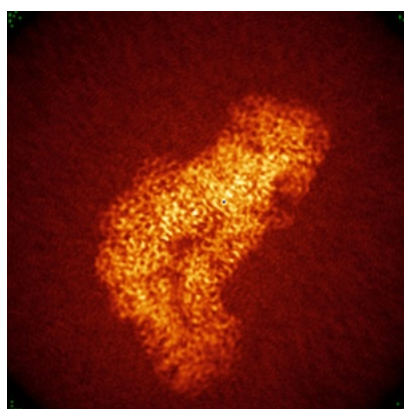


Z Index: 107

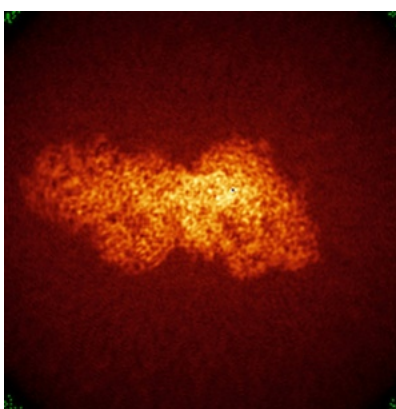
The images above show the largest variance slices of the map in three orthogonal directions.

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

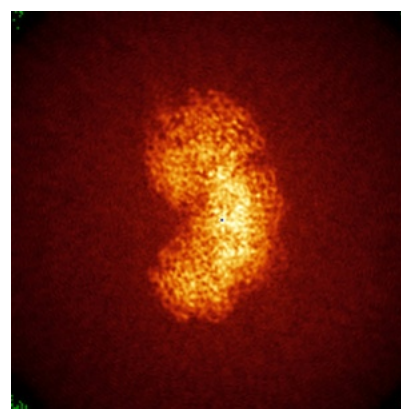
6.4.1 Primary map



X



Y

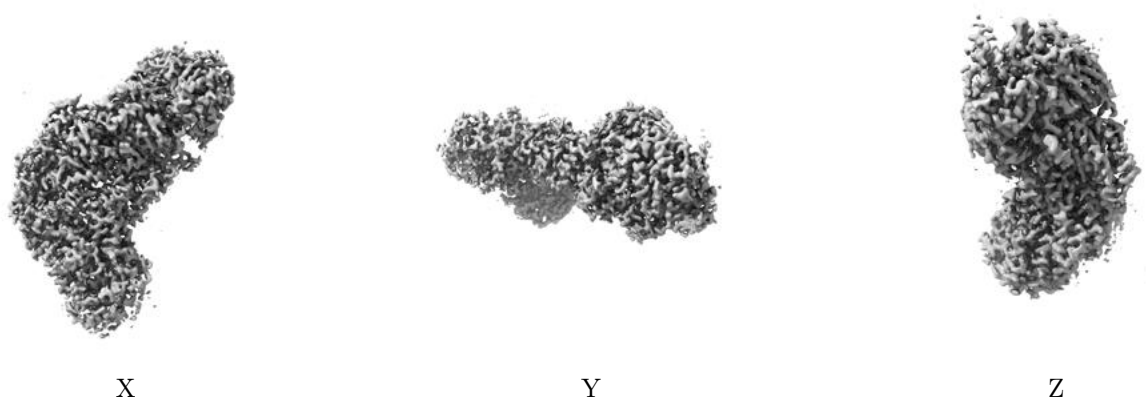


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

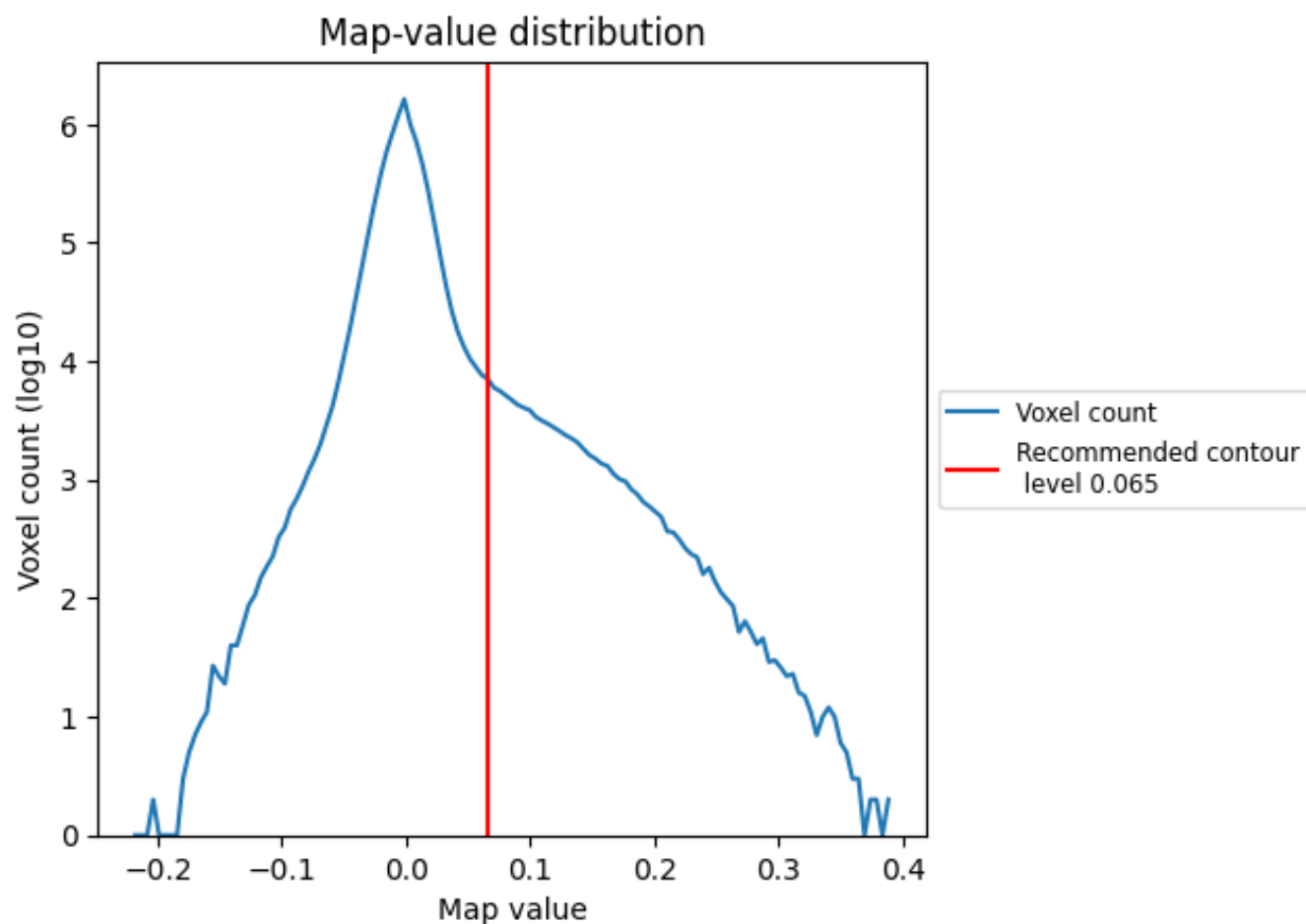
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

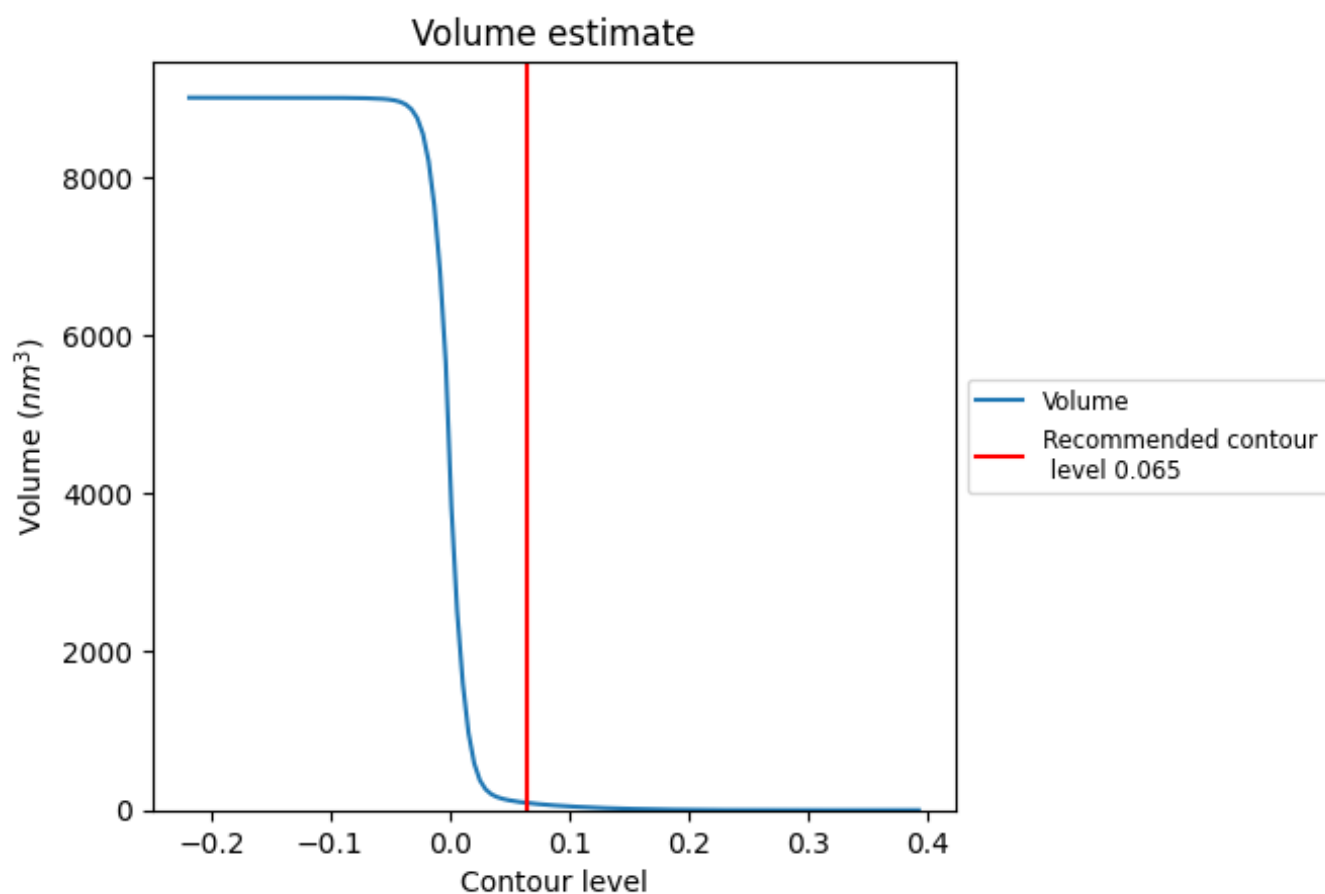
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

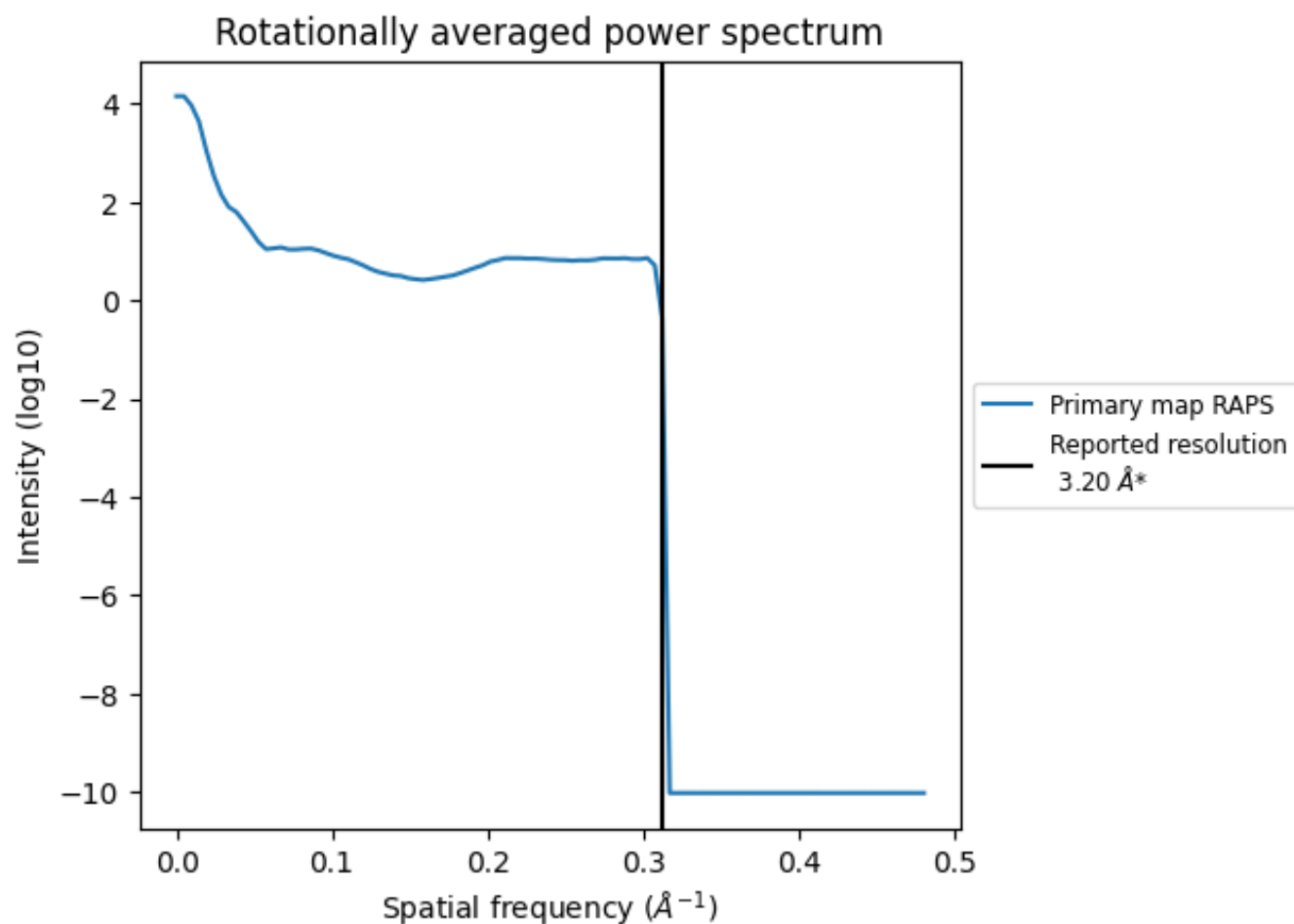
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm³; this corresponds to an approximate mass of 83 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 0.312 Å⁻¹

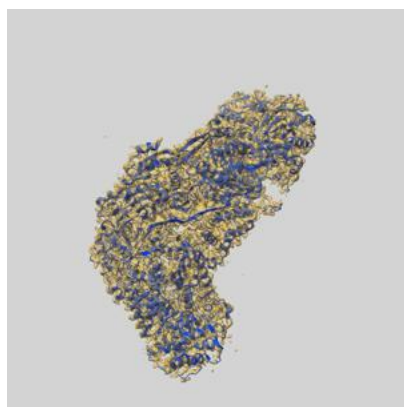
8 Fourier-Shell correlation ⓘ

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

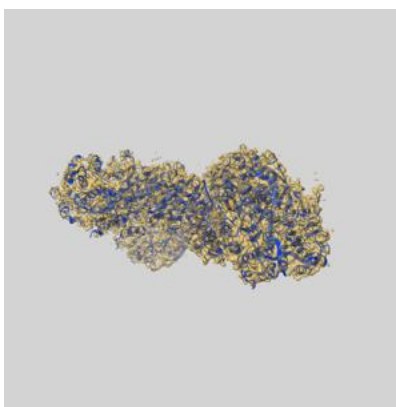
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9653 and PDB model 6IFK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

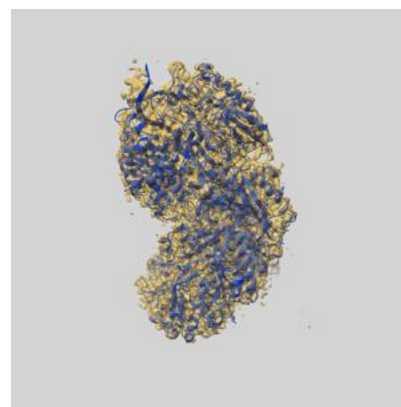
9.1 Map-model overlay [i](#)



X



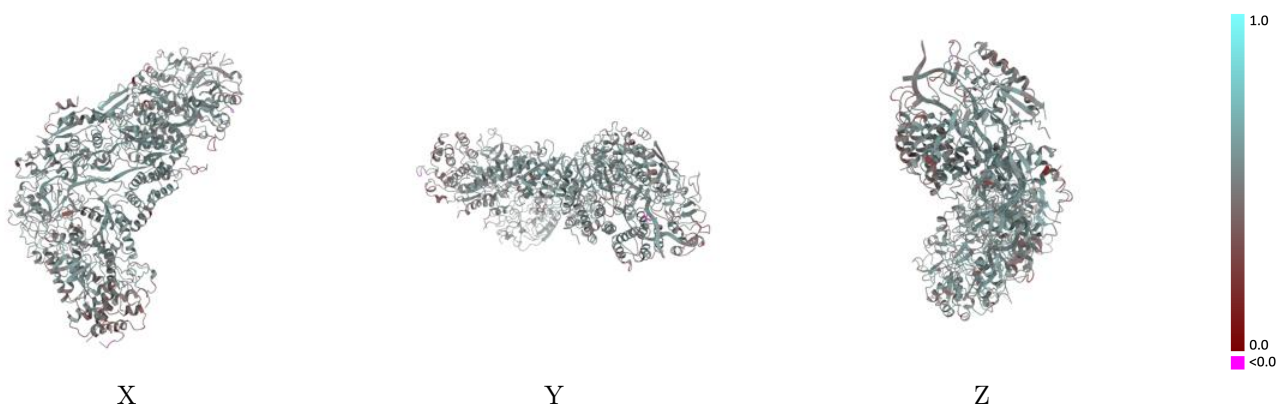
Y



Z

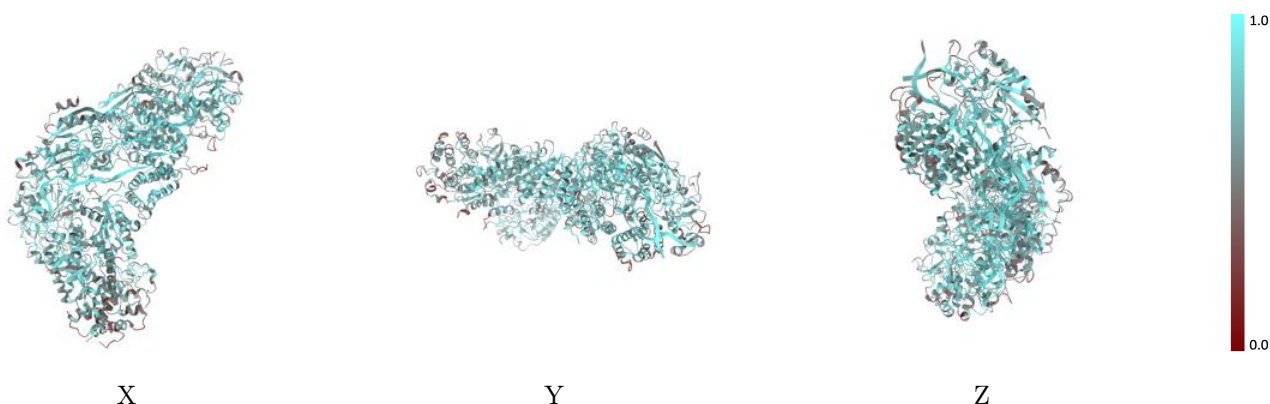
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



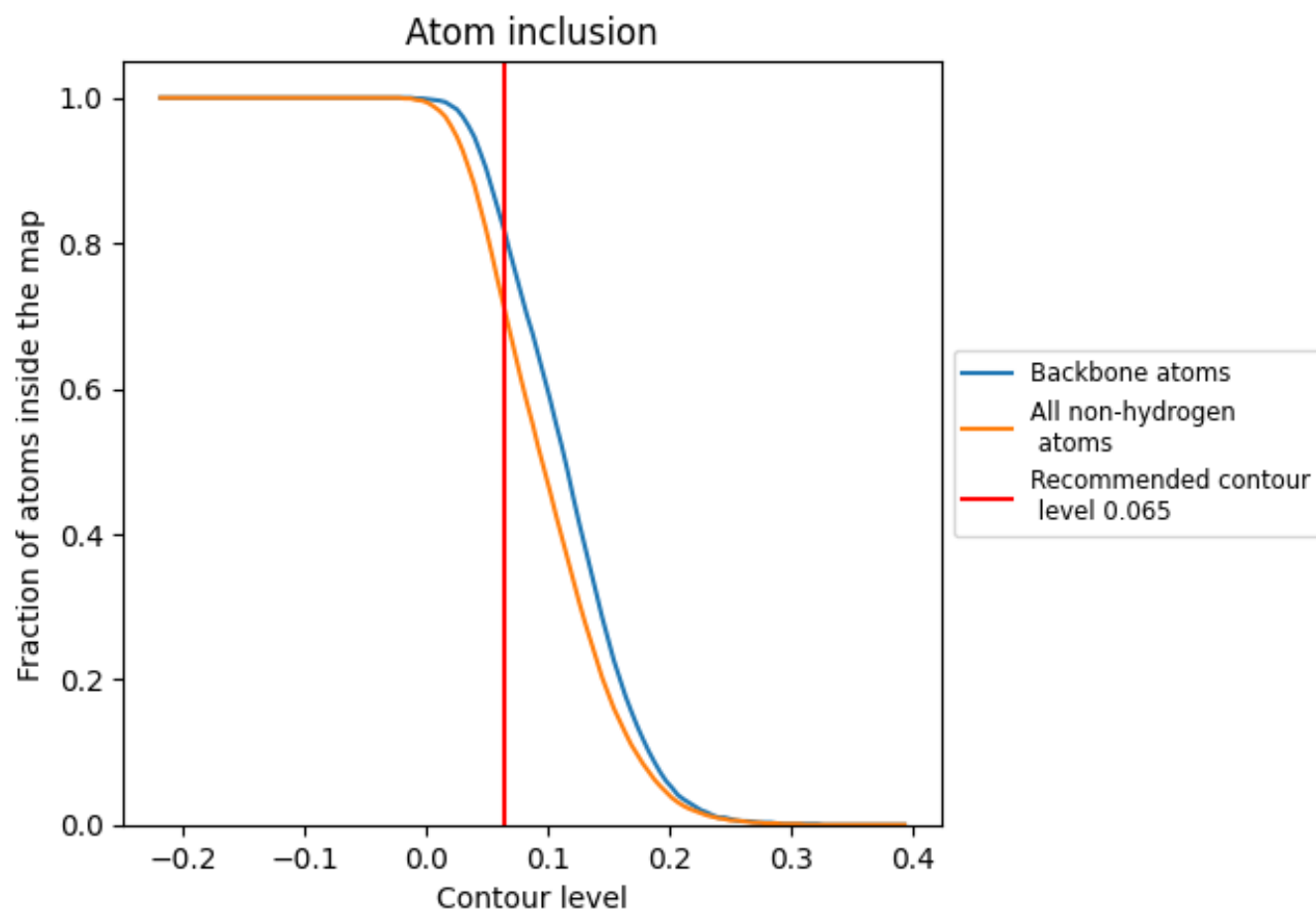
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 71% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7060	0.5110
A	0.6740	0.5010
B	0.7090	0.5050
C	0.7090	0.5140
D	0.6590	0.4960
E	0.7290	0.5290
F	0.7470	0.5320
G	0.7140	0.5220
H	0.6540	0.4890
J	0.8380	0.5420
N	0.9200	0.5720

1.0

0.0

<0.0