



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:13 PM UTC

PDB ID : 8PMP / pdb_00008pmp
EMDB ID : EMD-17763
Title : Structure of the human nuclear cap-binding complex bound to ARS2[147-871] and m7GTP
Authors : Dubiez, E.; Pellegrini, E.; Foucher, A.E.; Cusack, S.; Kadlec, J.
Deposited on : 2023-06-29
Resolution : 3.43 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

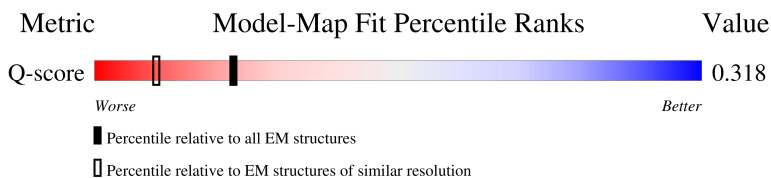
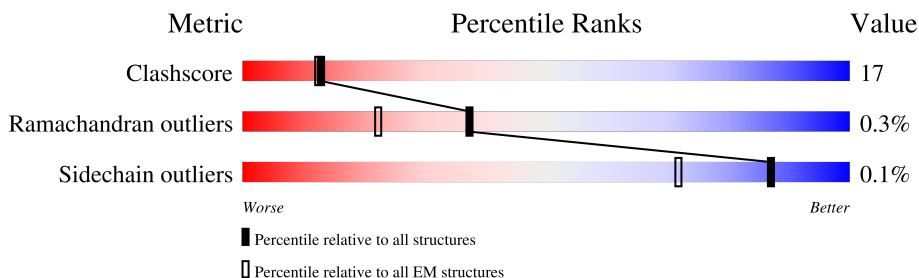
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13927 (2.93 - 3.93)

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	772	6% 76% 20% .
2	B	156	15% 63% 33% ..
3	D	729	97% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7554 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 Nuclear cap-binding protein subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	747	Total	C	N	O	S	0	0
			6112	3932	1037	1105	38		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP Q09161

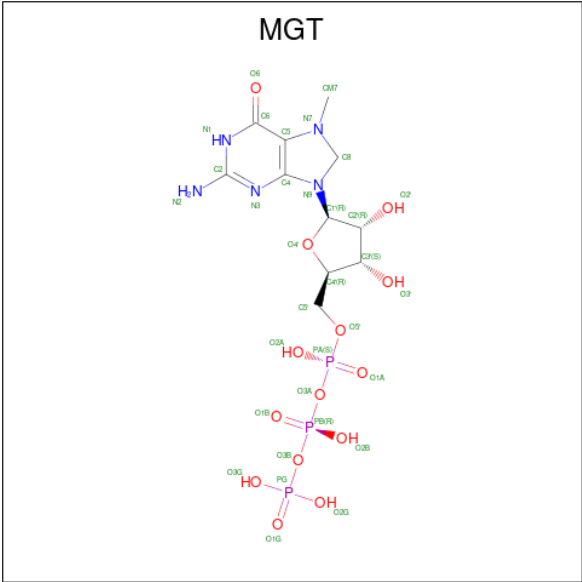
- Molecule 2 is a protein called Nuclear cap-binding protein subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	152	Total	C	N	O	S	0	0
			1237	769	222	240	6		

- Molecule 3 is a protein called Serrate RNA effector molecule homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	21	Total	C	N	O	0	0
			172	108	27	37		

- Molecule 4 is 7N-METHYL-8-HYDROGUANOSINE-5'-TRIPHOSPHATE (CCD ID: MGT) (formula: C₁₁H₂₀N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

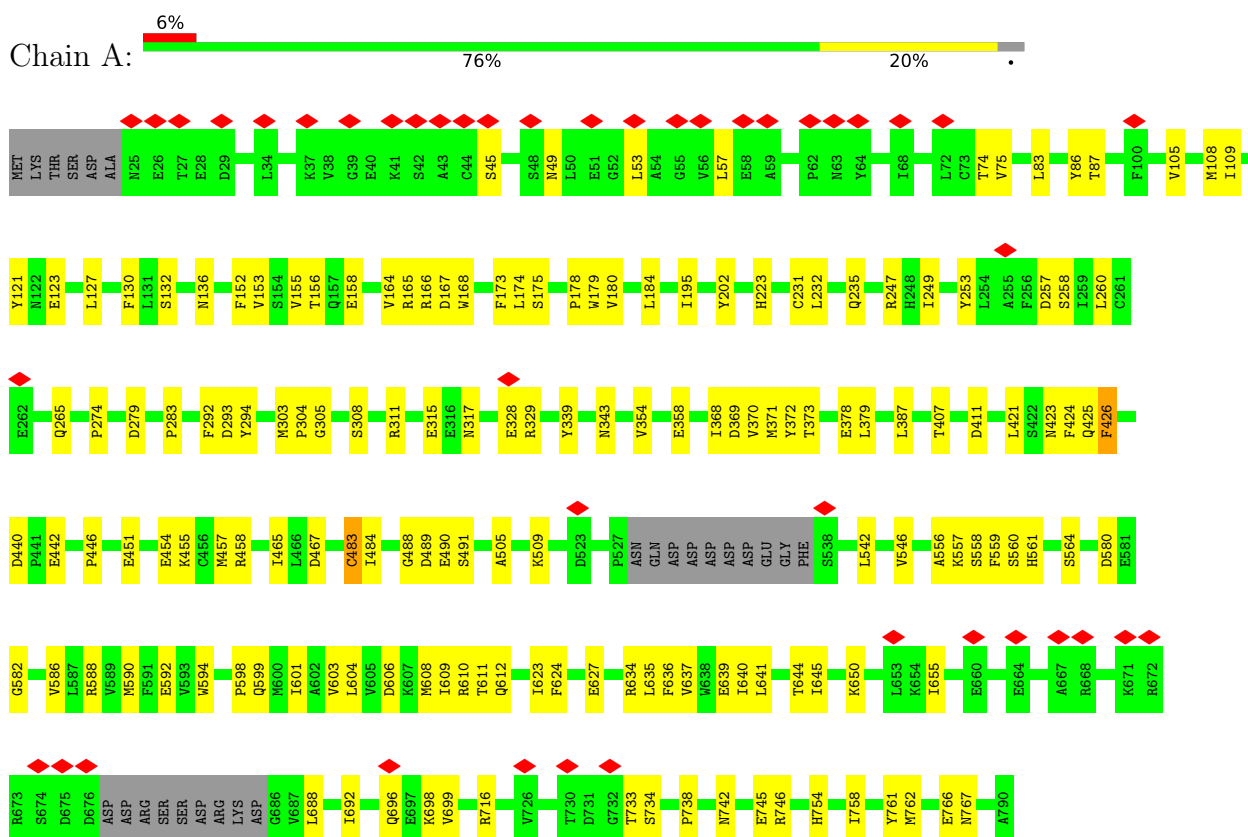


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			33	11	5	14	3	

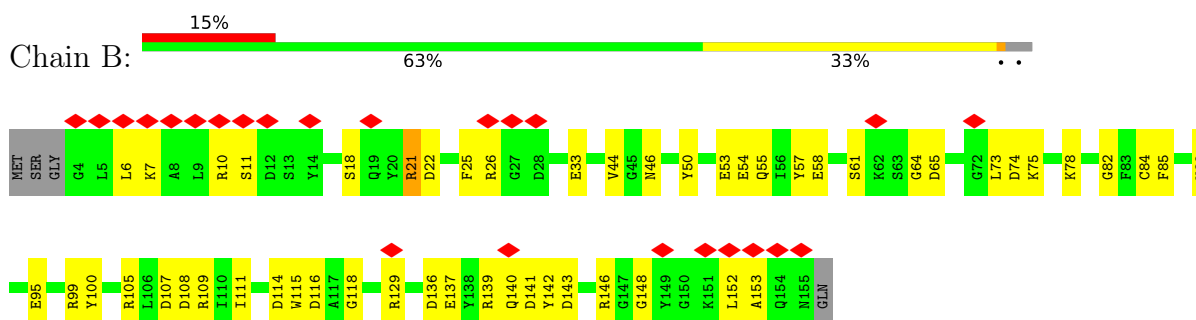
3 Residue-property plots

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: Nuclear cap-binding protein subunit 1



- Molecule 2: Nuclear cap-binding protein subunit 2



- Molecule 3: Serrate RNA effector molecule homolog

97%

A854	Tyr	Ala	Met	Cys	Leu	Asn	Met	Leu	Ser	Leu	Lys	Val
P865	Phe	Phe	Gly	Glu	Val	Gly	Arg	Glu	Gly	Glu	Arg	Met
D866	Asn	Asn	Arg	Tyr	Ser	Ile	Val	Leu	Gly	Gln	Arg	Lys
D867	Gly	Asn	Asp	Asn	Ala	Thr	Ala	Lys	Gly	Glu	Gln	Thr
D869	Val	Phe	Pro	Glu	Glu	His	Ser	Lys	Lys	Glu	Ala	Lys
D869	Arg	Leu	Glu	Asp	Glu	Lys	Glu	Glu	Lys	Glu	Arg	Glu
F870	Pro	Thr	Gln	Glu	Leu	Gln	Gln	Lys	Glu	Glu	Gly	Phe
F871	Val	Ala	Val	Pro	Leu	Ile	Ile	Lys	Pro	Ala	Ala	Leu
	Val	Lys	Glu	Asn	Gly	Arg	Arg	Glu	Lys	Gly	Gln	Ser
	Thr	Arg	Lys	Arg	Ser	Asn	Cys	Glu	Glu	Lys	Asn	Leu
	Gly	Pro	Phe	Cys	Ser	Asp	Arg	Glu	Asp	Pro	Arg	Asp
	Gly	Ala	Val	Gly	Gly	Ile	Phe	Trp	Ser	Gly	Leu	Asp
	Pro	Leu	Thr	Ile	Ala	Lys	Thr	Glu	Glu	Ser	Val	Val
	Pro	Pro	Ser	Ile	Pro	Ala	Arg	Pro	Lys	Pro	Phe	Asp
	Tyr	Glu	Asn	His	Pro	Ala	Arg	Pro	Glu	Ser	Asp	Val
	His	Ile	Thr	Val	Pro	Lys	Thr	Lys	Ala	Lys	Glu	Thr
	Ala	Lys	Gln	Arg	Glu	Lys	Gly	Asp	Lys	Lys	Ser	Glu
	Pro	Pro	Leu	Gly	Pro	Ile	Thr	Val	Lys	Lys	Met	Ala
	Ala	Ala	Leu	Gly	Pro	Ile	Thr	Ala	Ser	Glu	Leu	Val
	Pro	Ala	Gly	Met	Pro	His	Phe	Gly	Ser	Glu	Met	Ala
	Tyr	Gln	Gly	Pro	Lys	Thr	Asp	Leu	Lys	Ala	Arg	Lys
	Gly	Pro	Asp	Pro	Glu	Leu	Arg	Gly	Lys	Ala	Gly	Arg
	Ala	Pro	Lys	Asn	Lys	Thr	Asp	Gly	Arg	Ala	Thr	Arg
	Arg	Pro	Trp	Asn	Gly	Asp	Trp	Cys	Arg	Gly	Trp	Tyr
	Gly	Ala	Leu	Ile	Ile	Thr	Ile	Pro	Asp	Ala	Phe	Asn
	Asn	Gln	Cys	Ser	Ala	Thr	Val	Arg	Arg	Lys	Asn	Tyr
	Tyr	Ile	Pro	His	Gln	Lys	His	Pro	His	Gly	Lys	Lys
	Asp	Leu	Leu	Gly	Ile	Leu	Glu	Leu	Ser	Asp	Leu	Leu
	Phe	Pro	Gly	Val	Val	Ala	Cys	His	Gly	Gly	Leu	Leu
	Arg	Gly	Lys	Glu	Leu	Ala	Trp	Thr	Asp	Arg	Leu	Leu
	Gln	Thr	Phe	Trp	Asp	Pro	Leu	Ser	Phe	Thr	Lys	Gln
	Gly	Pro	Lys	Gln	Glu	Gly	Lys	Leu	Asp	Asn	Ala	Gln
	Tyr	Leu	Pro	Thr	Glu	Thr	Gly	Leu	Glu	Asp	Met	Met
	Pro	His	Arg	Lys	Leu	Thr	Arg	Ala	Glu	Lys	Met	Leu
	Arg	Gln	Lys	Leu	Asp	Ser	Lys	Pro	Ser	Asp	Leu	Ala
	Pro	Thr	His	Leu	Leu	Ser	Thr	Ala	Glu	Asp	Leu	Ala
	Pro	Pro	Ile	Pro	Leu	Pro	Ile	Met	Ser	Gly	Asp	His
	Val	Gln	Met	Glu	Leu	Gln	Arg	Arg	Ser	Lys	Ala	Asp
	Val	Gly	Asn	Glu	Leu	Asn	Val	Arg	Ser	Glu	Val	Glu
	Val	His	Lys	Lys	Val	Asn	Gly	Ala	Glu	Ala	Lys	Val
	Pro	Pro	Lys	Arg	Ser	Thr	Arg	Pro	Glu	Lys	Met	Leu
	Pro	Ala	Glu	Cys	Glu	Lys	Thr	Ala	Leu	Ala	Lys	Leu
	Pro	Thr	Gln	Thr	Val	Lys	Phe	Pro	Glu	Ala	Arg	Thr
	Thr	Arg	Phe	Gly	Glu	Thr	Arg	Ala	Glu	Glu	Thr	Thr
	Arg	Pro	Glu	Ser	Pro	Ile	Val	Val	Glu	Ala	Arg	His
	Val	Ala	Val	Val	Leu	Leu	Val	Val	Leu	Ala	Thr	Pro
	Val	Ala	Val	Pro	Glu	Pro	Pro	Val	Glu	Ala	Arg	Pro
	Val	Ala	Val	Pro	Leu	Thr	Val	Val	Glu	Ala	Arg	Pro
	Val	Ala	Val	Pro	Glu	Thr	Val	Val	Glu	Ala	Arg	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84474	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.13	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.429	Depositor
Minimum map value	-0.218	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	302.04, 302.04, 302.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83900005, 0.83900005, 0.83900005	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: MGT

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	0.15	0/6266	0.35	0/8499
2	B	0.13	0/1257	0.34	0/1677
3	D	0.50	0/176	0.60	0/238
All	All	0.16	0/7699	0.36	0/10414

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	21	ARG	Sidechain

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	6112	0	6091	207	0
2	B	1237	0	1193	120	0
3	D	172	0	149	43	0
4	B	33	0	16	0	0
All	All	7554	0	7449	248	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 17.

All (248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:HB2	2:B:53:GLU:CG	1.34	1.58
1:A:559:PHE:HB2	2:B:53:GLU:CD	1.31	1.47
1:A:559:PHE:CE2	2:B:54:GLU:HA	1.64	1.32
1:A:559:PHE:CB	2:B:53:GLU:CD	2.11	1.24
1:A:610:ARG:HD2	2:B:89:TYR:OH	1.03	1.18
1:A:610:ARG:CD	2:B:89:TYR:OH	1.91	1.18
1:A:561:HIS:NE2	3:D:859:TYR:HA	1.56	1.17
1:A:559:PHE:CZ	2:B:54:GLU:CB	2.28	1.17
1:A:559:PHE:CB	2:B:53:GLU:CG	2.24	1.13
1:A:368:ILE:CG2	2:B:100:TYR:CE2	2.33	1.11
1:A:368:ILE:HG21	2:B:100:TYR:CE2	1.85	1.11
1:A:559:PHE:HB2	2:B:53:GLU:HG3	1.26	1.06
1:A:559:PHE:CZ	2:B:54:GLU:HB3	1.90	1.04
1:A:368:ILE:HG21	2:B:100:TYR:HE2	1.23	1.02
1:A:612:GLN:HG3	3:D:871:PHE:HB2	1.42	1.01
1:A:559:PHE:CE2	2:B:54:GLU:CA	2.45	0.98
1:A:560:SER:N	2:B:53:GLU:OE2	1.94	0.98
1:A:603:VAL:HG22	2:B:57:TYR:CE1	2.01	0.95
1:A:559:PHE:CB	2:B:53:GLU:HG3	1.92	0.95
1:A:558:SER:OG	3:D:857:VAL:HG11	1.69	0.93
1:A:603:VAL:HG22	2:B:57:TYR:CD1	2.04	0.92
1:A:559:PHE:CZ	2:B:54:GLU:HB2	2.04	0.90
2:B:18:SER:O	2:B:21:ARG:NH2	2.06	0.89
1:A:458:ARG:HD3	2:B:58:GLU:HB2	1.55	0.88
1:A:370:VAL:HG22	2:B:100:TYR:HB3	1.52	0.88
1:A:558:SER:OG	3:D:857:VAL:HG21	1.75	0.86
1:A:156:THR:O	1:A:166:ARG:NH1	2.08	0.86
1:A:370:VAL:HG13	2:B:100:TYR:CD2	2.11	0.86
2:B:136:ASP:OD1	2:B:139:ARG:NH1	2.10	0.84
1:A:564:SER:OG	3:D:862:LEU:CD1	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:N	2:B:53:GLU:OE2	2.12	0.83
1:A:603:VAL:CG2	2:B:57:TYR:CD1	2.61	0.83
1:A:370:VAL:HG13	2:B:100:TYR:CG	2.14	0.81
1:A:561:HIS:HA	3:D:862:LEU:HD13	1.63	0.80
1:A:560:SER:N	2:B:53:GLU:CD	2.39	0.80
1:A:610:ARG:HD2	2:B:89:TYR:HH	1.44	0.80
1:A:558:SER:HG	3:D:857:VAL:HG21	1.44	0.79
1:A:557:LYS:HE3	3:D:858:GLU:O	1.83	0.79
1:A:559:PHE:CG	2:B:53:GLU:HG3	2.17	0.78
1:A:158:GLU:O	1:A:166:ARG:NH2	2.17	0.78
1:A:454:GLU:OE1	1:A:634:ARG:NH2	2.16	0.77
1:A:559:PHE:CA	2:B:53:GLU:CD	2.57	0.77
1:A:559:PHE:CE1	2:B:54:GLU:HB3	2.19	0.77
1:A:411:ASP:OD2	1:A:746:ARG:NH1	2.19	0.76
1:A:564:SER:CB	3:D:862:LEU:HD12	2.16	0.76
1:A:560:SER:H	2:B:53:GLU:CD	1.93	0.76
1:A:564:SER:OG	3:D:862:LEU:HD11	1.84	0.75
1:A:559:PHE:HZ	2:B:54:GLU:HB2	1.52	0.74
2:B:114:ASP:OD1	2:B:115:TRP:N	2.20	0.74
1:A:407:THR:N	1:A:745:GLU:OE1	2.19	0.74
1:A:564:SER:HB2	3:D:862:LEU:HD12	1.71	0.72
1:A:370:VAL:HG13	2:B:100:TYR:CB	2.20	0.72
1:A:83:LEU:O	1:A:87:THR:OG1	2.06	0.72
1:A:559:PHE:HB2	2:B:53:GLU:OE1	1.88	0.71
1:A:458:ARG:O	2:B:55:GLN:HB3	1.92	0.70
2:B:73:LEU:HD21	3:D:859:TYR:CG	2.27	0.69
1:A:612:GLN:HG3	3:D:871:PHE:CB	2.20	0.69
2:B:22:ASP:OD1	2:B:25:PHE:N	2.26	0.68
1:A:561:HIS:CE1	3:D:859:TYR:CD2	2.82	0.68
2:B:73:LEU:CD2	3:D:859:TYR:HB2	2.24	0.68
1:A:559:PHE:CE2	2:B:54:GLU:CB	2.76	0.67
1:A:368:ILE:CG2	2:B:100:TYR:HE2	1.87	0.67
1:A:370:VAL:CG2	2:B:100:TYR:HB3	2.23	0.67
1:A:561:HIS:HA	3:D:862:LEU:CD1	2.24	0.67
1:A:627:GLU:N	1:A:627:GLU:OE1	2.27	0.67
1:A:560:SER:OG	3:D:859:TYR:CE2	2.48	0.66
2:B:140:GLN:N	2:B:140:GLN:OE1	2.29	0.66
2:B:78:LYS:CB	3:D:860:ARG:HA	2.25	0.66
1:A:370:VAL:CG1	2:B:100:TYR:CD2	2.78	0.66
1:A:490:GLU:OE2	1:A:490:GLU:N	2.28	0.66
1:A:766:GLU:OE1	1:A:767:ASN:ND2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:CG	2:B:53:GLU:CG	2.78	0.65
1:A:257:ASP:OD1	1:A:258:SER:N	2.29	0.65
1:A:559:PHE:CB	2:B:53:GLU:OE1	2.41	0.65
1:A:559:PHE:HE2	2:B:54:GLU:HA	1.51	0.64
1:A:303:MET:SD	1:A:311:ARG:NH2	2.71	0.63
1:A:564:SER:CB	3:D:862:LEU:CD1	2.74	0.63
1:A:423:ASN:O	2:B:105:ARG:HD3	1.97	0.63
1:A:612:GLN:CG	3:D:871:PHE:HB2	2.25	0.63
1:A:458:ARG:HD2	2:B:58:GLU:HG2	1.81	0.62
2:B:139:ARG:NH2	2:B:148:GLY:O	2.33	0.61
2:B:73:LEU:CD2	3:D:859:TYR:CD1	2.83	0.61
1:A:458:ARG:CD	2:B:58:GLU:CG	2.77	0.61
2:B:78:LYS:HB3	3:D:860:ARG:HA	1.80	0.61
1:A:458:ARG:HD2	2:B:58:GLU:CG	2.30	0.61
1:A:559:PHE:CZ	2:B:54:GLU:CA	2.78	0.61
1:A:603:VAL:CG2	2:B:57:TYR:CG	2.84	0.61
2:B:46:ASN:OD1	2:B:109:ARG:NH1	2.34	0.61
2:B:73:LEU:HD21	3:D:859:TYR:CD1	2.36	0.60
1:A:559:PHE:CD2	2:B:53:GLU:HG3	2.36	0.60
1:A:136:ASN:ND2	1:A:179:TRP:O	2.32	0.60
1:A:458:ARG:CD	2:B:58:GLU:HG2	2.30	0.60
1:A:560:SER:OG	3:D:859:TYR:CD2	2.54	0.60
1:A:560:SER:N	2:B:53:GLU:OE1	2.34	0.59
1:A:588:ARG:O	1:A:592:GLU:HG3	2.03	0.59
1:A:370:VAL:CG1	2:B:100:TYR:CB	2.81	0.59
1:A:328:GLU:OE2	2:B:11:SER:OG	2.18	0.58
1:A:180:VAL:HG22	1:A:184:LEU:HD12	1.86	0.58
1:A:558:SER:OG	3:D:857:VAL:CG1	2.47	0.57
1:A:559:PHE:CA	2:B:53:GLU:OE2	2.50	0.57
2:B:50:TYR:HD1	3:D:854:ARG:O	1.86	0.57
1:A:167:ASP:OD1	1:A:202:TYR:OH	2.21	0.57
1:A:612:GLN:NE2	3:D:871:PHE:HD1	2.02	0.57
2:B:74:ASP:OD1	2:B:75:LYS:N	2.37	0.57
1:A:559:PHE:CD2	2:B:54:GLU:HA	2.34	0.57
1:A:458:ARG:HD2	2:B:58:GLU:CD	2.30	0.57
1:A:247:ARG:O	1:A:343:ASN:ND2	2.36	0.57
1:A:603:VAL:HG21	2:B:57:TYR:CG	2.40	0.56
1:A:483:CYS:SG	1:A:556:ALA:HB1	2.45	0.56
1:A:561:HIS:NE2	3:D:859:TYR:CA	2.50	0.56
1:A:594:TRP:O	1:A:601:ILE:HD11	2.06	0.56
1:A:612:GLN:HE21	3:D:871:PHE:HD1	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:GLN:CD	2:B:54:GLU:HB2	2.31	0.55
1:A:603:VAL:HG22	2:B:57:TYR:CZ	2.42	0.55
1:A:564:SER:HB2	3:D:862:LEU:CD1	2.35	0.54
1:A:611:THR:O	1:A:611:THR:HG22	2.08	0.54
1:A:165:ARG:NH2	1:A:274:PRO:O	2.35	0.54
1:A:231:CYS:SG	1:A:235:GLN:NE2	2.73	0.54
2:B:73:LEU:HD21	3:D:859:TYR:HB2	1.89	0.54
1:A:623:ILE:HG23	1:A:637:VAL:CG1	2.38	0.54
2:B:73:LEU:HD22	3:D:859:TYR:HB2	1.88	0.54
1:A:484:ILE:HG23	1:A:484:ILE:O	2.08	0.54
1:A:560:SER:O	3:D:862:LEU:HD11	2.07	0.54
1:A:558:SER:OG	3:D:857:VAL:CG2	2.52	0.54
1:A:641:LEU:O	1:A:645:ILE:HG13	2.08	0.54
1:A:371:MET:HB2	2:B:100:TYR:CZ	2.42	0.53
2:B:108:ASP:OD1	2:B:108:ASP:O	2.26	0.53
2:B:109:ARG:NH2	2:B:143:ASP:OD2	2.40	0.53
1:A:180:VAL:O	1:A:184:LEU:HD12	2.08	0.53
1:A:650:LYS:HZ2	2:B:65:ASP:HB2	1.73	0.53
1:A:458:ARG:HD3	2:B:58:GLU:CB	2.33	0.53
1:A:174:LEU:O	1:A:178:PRO:HD3	2.09	0.52
1:A:370:VAL:HA	1:A:373:THR:HG22	1.90	0.52
2:B:50:TYR:CD1	3:D:854:ARG:O	2.62	0.52
2:B:82:GLY:O	2:B:146:ARG:NH2	2.43	0.52
1:A:368:ILE:HG21	2:B:100:TYR:CD2	2.39	0.52
1:A:558:SER:HB2	1:A:561:HIS:HD1	1.75	0.52
1:A:650:LYS:NZ	2:B:65:ASP:HB2	2.25	0.52
2:B:73:LEU:HD21	3:D:859:TYR:CB	2.40	0.52
1:A:279:ASP:OD1	1:A:279:ASP:N	2.40	0.51
1:A:559:PHE:C	2:B:53:GLU:CD	2.78	0.51
2:B:33:GLU:OE2	2:B:33:GLU:HA	2.11	0.51
1:A:421:LEU:HG	1:A:426:PHE:HA	1.93	0.50
1:A:580:ASP:OD1	1:A:580:ASP:N	2.43	0.50
1:A:458:ARG:CD	2:B:58:GLU:HB2	2.35	0.50
1:A:606:ASP:OD1	1:A:606:ASP:C	2.55	0.50
1:A:180:VAL:HG13	1:A:184:LEU:CD1	2.42	0.50
1:A:561:HIS:CE1	3:D:859:TYR:HA	2.38	0.50
1:A:738:PRO:O	1:A:742:ASN:ND2	2.44	0.50
1:A:640:ILE:O	1:A:644:THR:HG23	2.13	0.49
2:B:95:GLU:O	2:B:99:ARG:HG3	2.12	0.49
3:D:851:GLY:O	3:D:853:PRO:HD3	2.13	0.49
1:A:489:ASP:OD1	1:A:490:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ASP:OD1	2:B:142:TYR:N	2.45	0.49
1:A:557:LYS:CE	3:D:858:GLU:O	2.58	0.48
1:A:317:ASN:ND2	1:A:339:TYR:OH	2.40	0.48
1:A:733:THR:HG22	1:A:734:SER:H	1.78	0.48
2:B:152:LEU:HD12	2:B:153:ALA:N	2.28	0.48
1:A:368:ILE:HG22	2:B:100:TYR:CE2	2.39	0.48
1:A:165:ARG:O	1:A:166:ARG:C	2.56	0.48
1:A:354:VAL:O	1:A:358:GLU:HG3	2.14	0.47
2:B:114:ASP:OD1	2:B:115:TRP:O	2.32	0.47
3:D:868:VAL:HG12	3:D:869:ASP:N	2.29	0.47
1:A:153:VAL:HG21	1:A:195:ILE:HG23	1.97	0.47
1:A:368:ILE:CG2	2:B:100:TYR:CD2	2.95	0.47
1:A:559:PHE:N	2:B:53:GLU:CD	2.71	0.47
3:D:863:ASP:OD1	3:D:863:ASP:C	2.58	0.47
1:A:505:ALA:HB1	1:A:509:LYS:NZ	2.30	0.47
1:A:624:PHE:CD2	1:A:716:ARG:HB3	2.50	0.47
1:A:423:ASN:O	2:B:105:ARG:CD	2.62	0.47
2:B:25:PHE:CD1	2:B:26:ARG:N	2.83	0.46
2:B:136:ASP:OD2	2:B:146:ARG:NH1	2.48	0.46
1:A:411:ASP:OD1	1:A:635:LEU:CD2	2.63	0.46
1:A:265:GLN:OE1	1:A:265:GLN:HA	2.15	0.46
1:A:369:ASP:HA	1:A:372:TYR:HD2	1.81	0.46
1:A:598:PRO:HB3	1:A:636:PHE:CG	2.50	0.46
2:B:78:LYS:CG	3:D:860:ARG:HA	2.45	0.46
1:A:329:ARG:HG3	1:A:378:GLU:HG3	1.97	0.46
2:B:114:ASP:OD1	2:B:114:ASP:C	2.58	0.46
1:A:458:ARG:CG	2:B:58:GLU:HG2	2.45	0.46
1:A:83:LEU:HD12	1:A:130:PHE:HD1	1.81	0.46
1:A:105:VAL:O	1:A:109:ILE:HG12	2.15	0.46
1:A:440:ASP:O	1:A:446:PRO:HG3	2.15	0.46
1:A:370:VAL:CG1	2:B:100:TYR:HB2	2.46	0.45
1:A:559:PHE:C	2:B:53:GLU:OE2	2.58	0.45
1:A:599:GLN:OE1	2:B:54:GLU:HG3	2.15	0.45
1:A:75:VAL:HG11	1:A:86:TYR:CD1	2.51	0.45
1:A:582:GLY:O	1:A:586:VAL:HG23	2.17	0.45
1:A:293:ASP:OD1	1:A:294:TYR:N	2.50	0.45
1:A:505:ALA:HB1	1:A:509:LYS:HZ1	1.80	0.45
1:A:458:ARG:CD	2:B:58:GLU:CB	2.94	0.45
2:B:61:SER:HA	2:B:64:GLY:O	2.17	0.45
2:B:129:ARG:NH1	2:B:137:GLU:OE2	2.49	0.45
1:A:123:GLU:O	1:A:127:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLN:O	1:A:426:PHE:C	2.59	0.44
1:A:175:SER:O	1:A:178:PRO:HD2	2.18	0.44
1:A:612:GLN:NE2	3:D:871:PHE:CD1	2.83	0.44
1:A:108:MET:CE	1:A:130:PHE:CD2	3.01	0.44
1:A:542:LEU:O	1:A:546:VAL:HG12	2.18	0.44
1:A:173:PHE:CD1	1:A:173:PHE:C	2.95	0.43
1:A:688:LEU:O	1:A:692:ILE:HG12	2.18	0.43
1:A:457:MET:HB2	1:A:465:ILE:HG13	2.00	0.43
1:A:223:HIS:NE2	1:A:292:PHE:O	2.51	0.43
1:A:305:GLY:O	1:A:308:SER:OG	2.34	0.43
1:A:754:HIS:O	1:A:758:ILE:HG13	2.18	0.43
2:B:55:GLN:NE2	2:B:107:ASP:OD2	2.49	0.43
1:A:249:ILE:HD12	1:A:249:ILE:H	1.84	0.43
1:A:74:THR:HG22	2:B:6:LEU:HD21	2.00	0.43
2:B:7:LYS:HA	2:B:10:ARG:HG2	2.00	0.43
1:A:132:SER:HB3	1:A:180:VAL:HG11	1.99	0.43
1:A:423:ASN:HA	2:B:105:ARG:HB2	2.01	0.43
1:A:455:LYS:NZ	1:A:639:GLU:OE2	2.49	0.43
1:A:45:SER:O	1:A:49:ASN:OD1	2.37	0.42
1:A:696:GLN:O	1:A:699:VAL:HG22	2.19	0.42
1:A:742:ASN:O	1:A:746:ARG:HG2	2.19	0.42
1:A:761:TYR:O	1:A:762:MET:C	2.62	0.42
1:A:609:ILE:CD1	1:A:644:THR:HG22	2.49	0.42
1:A:152:PHE:O	1:A:155:VAL:HB	2.19	0.42
1:A:379:LEU:HB3	1:A:387:LEU:CD2	2.49	0.42
1:A:603:VAL:HG22	2:B:57:TYR:CG	2.48	0.42
1:A:174:LEU:HB2	1:A:232:LEU:HD21	2.02	0.42
1:A:467:ASP:C	1:A:467:ASP:OD1	2.63	0.42
1:A:304:PRO:O	1:A:311:ARG:NH1	2.52	0.42
1:A:53:LEU:O	1:A:57:LEU:HG	2.19	0.42
1:A:458:ARG:O	2:B:55:GLN:CB	2.64	0.42
2:B:84:CYS:SG	2:B:85:PHE:N	2.92	0.42
1:A:451:GLU:OE1	1:A:635:LEU:HG	2.20	0.41
1:A:733:THR:HG22	1:A:734:SER:N	2.35	0.41
1:A:132:SER:HB3	1:A:180:VAL:CG1	2.50	0.41
1:A:458:ARG:HG2	2:B:58:GLU:HG2	2.01	0.41
1:A:136:ASN:OD1	1:A:180:VAL:HG23	2.19	0.41
1:A:232:LEU:HA	1:A:235:GLN:OE1	2.21	0.41
1:A:442:GLU:HG3	1:A:442:GLU:O	2.20	0.41
1:A:121:TYR:HB3	1:A:168:TRP:NE1	2.36	0.41
1:A:421:LEU:O	1:A:424:PHE:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:TYR:HB2	1:A:260:LEU:CD1	2.50	0.41
1:A:370:VAL:CG2	2:B:100:TYR:CB	2.97	0.41
1:A:370:VAL:CG1	2:B:100:TYR:HD2	2.32	0.41
1:A:655:ILE:HD11	1:A:698:LYS:HB3	2.03	0.41
1:A:164:VAL:CG2	1:A:283:PRO:O	2.69	0.40
1:A:311:ARG:O	1:A:315:GLU:HG2	2.20	0.40
1:A:368:ILE:HG12	1:A:370:VAL:HG12	2.02	0.40
1:A:590:MET:HE1	1:A:601:ILE:HD13	2.03	0.40
1:A:624:PHE:CD2	1:A:716:ARG:CB	3.04	0.40
2:B:116:ASP:OD2	2:B:118:GLY:O	2.39	0.40
1:A:488:GLY:O	1:A:491:SER:HB3	2.20	0.40
1:A:604:LEU:O	1:A:608:MET:HG3	2.21	0.40
2:B:44:VAL:HG13	2:B:111:ILE:HG23	2.02	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	741/772 (96%)	720 (97%)	20 (3%)	1 (0%)	48	78
2	B	150/156 (96%)	149 (99%)	1 (1%)	0	100	100
3	D	19/729 (3%)	12 (63%)	5 (26%)	2 (10%)	0	4
All	All	910/1657 (55%)	881 (97%)	26 (3%)	3 (0%)	37	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	865	PRO
1	A	426	PHE
3	D	863	ASP

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	685/708 (97%)	684 (100%)	1 (0%)	88	88
2	B	127/130 (98%)	127 (100%)	0	100	100
3	D	18/634 (3%)	18 (100%)	0	100	100
All	All	830/1472 (56%)	829 (100%)	1 (0%)	87	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	325	HIS
1	A	348	ASN
1	A	493	ASN
1	A	540	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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$
4	MGT	B	201	-	34,35,35	1.33	4 (11%)	45,56,56	2.20	8 (17%)

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
4	MGT	B	201	-	-	2/22/50/50	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	201	MGT	C5-C4	3.38	1.48	1.37
4	B	201	MGT	C4-N9	-2.73	1.34	1.37
4	B	201	MGT	PA-O3A	2.49	1.62	1.59
4	B	201	MGT	C5-N7	-2.23	1.32	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	201	MGT	N9-C4-N3	9.10	138.79	125.46
4	B	201	MGT	C5-C4-N3	-5.56	117.70	128.13
4	B	201	MGT	C2-N3-C4	4.76	120.49	112.30
4	B	201	MGT	N9-C8-N7	-4.51	96.99	103.37
4	B	201	MGT	O4'-C1'-N9	3.88	114.58	109.30
4	B	201	MGT	C5-C6-N1	3.05	116.30	110.94
4	B	201	MGT	O6-C6-C5	-2.57	121.31	127.62
4	B	201	MGT	C5-C4-N9	-2.21	103.51	106.33

There are no chirality outliers.

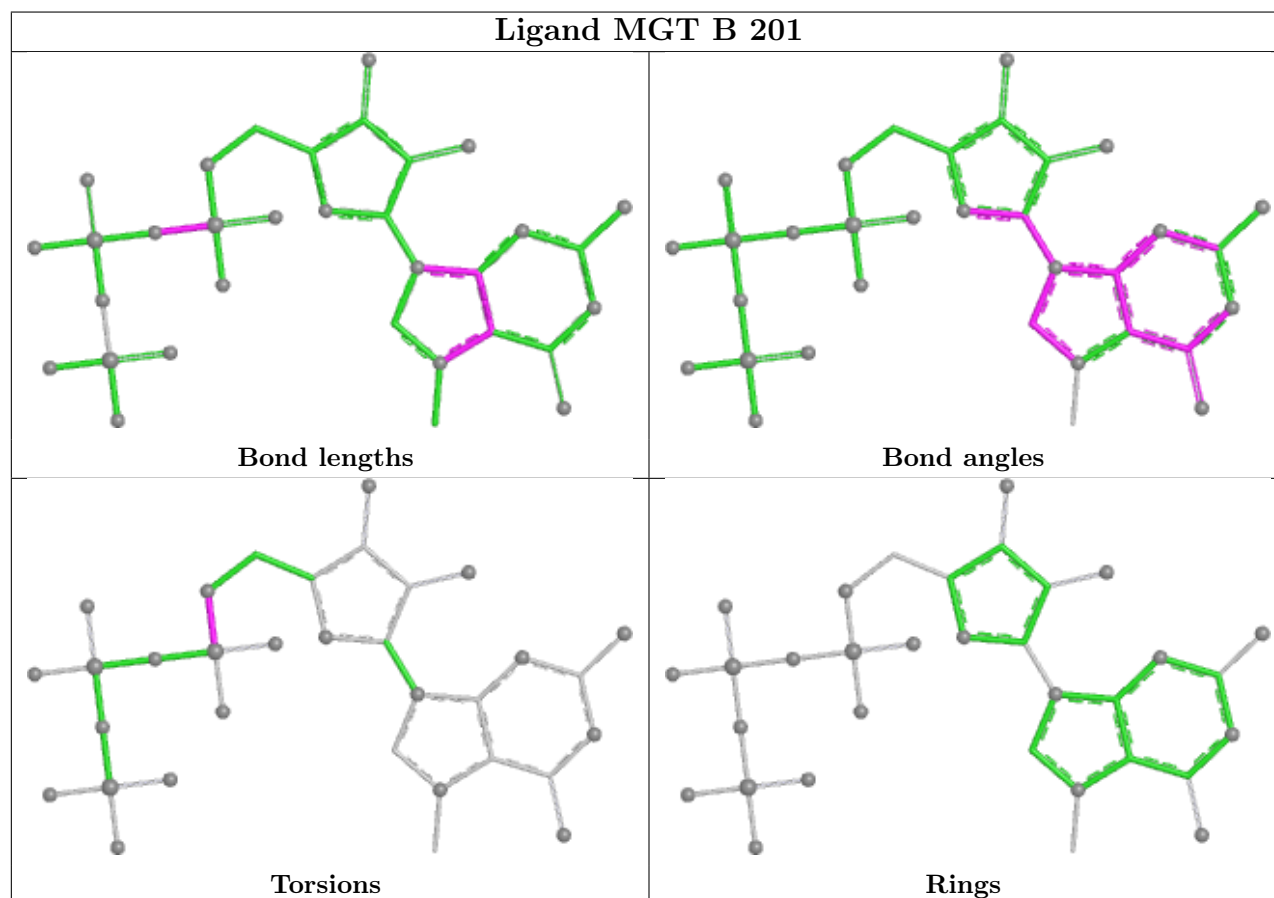
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	201	MGT	C5'-O5'-PA-O3A
4	B	201	MGT	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

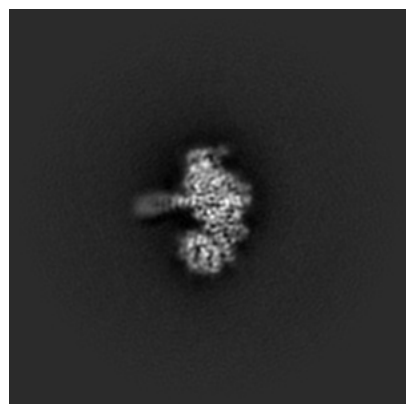
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17763. These allow visual inspection of the internal detail of the map and identification of artifacts.

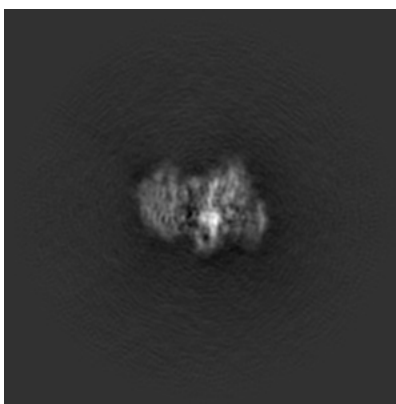
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

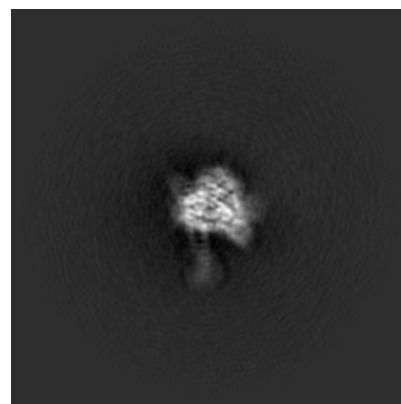
6.1.1 Primary map



X

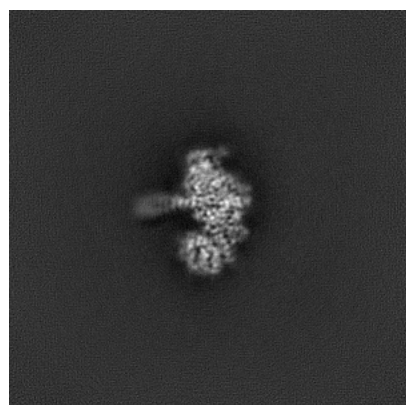


Y

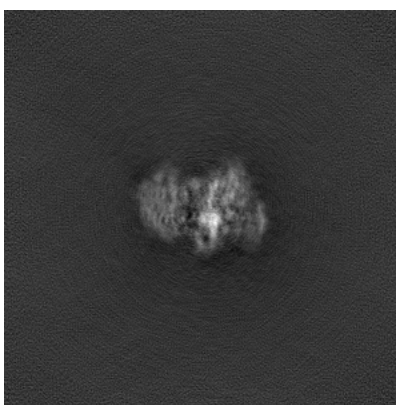


Z

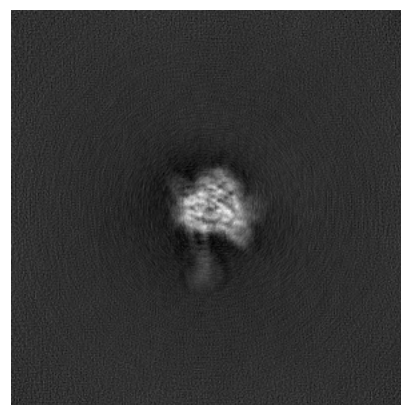
6.1.2 Raw map



X



Y

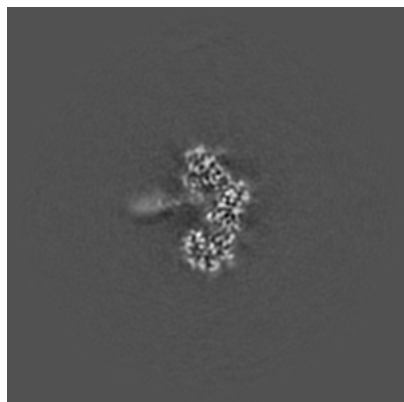


Z

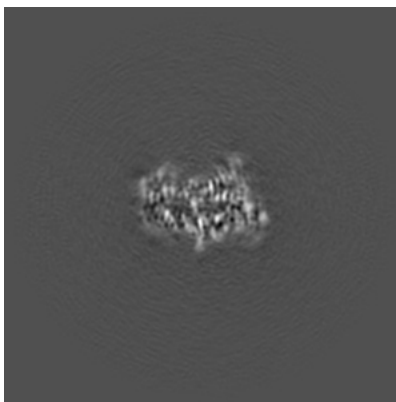
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

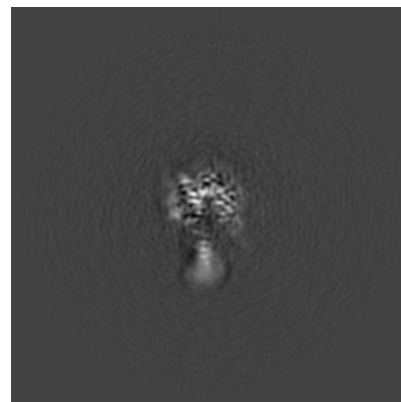
6.2.1 Primary map



X Index: 180

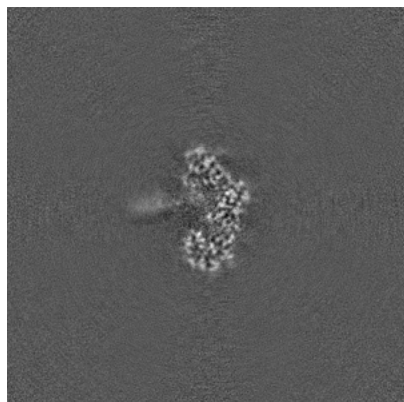


Y Index: 180

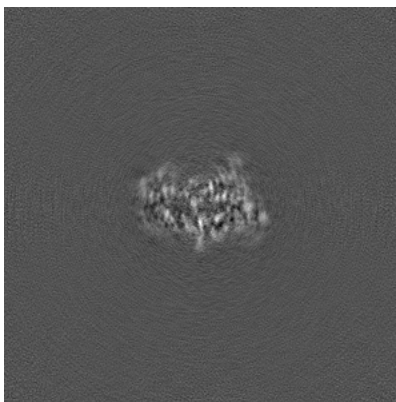


Z Index: 180

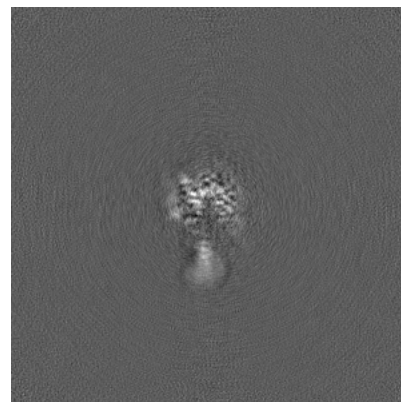
6.2.2 Raw map



X Index: 180



Y Index: 180

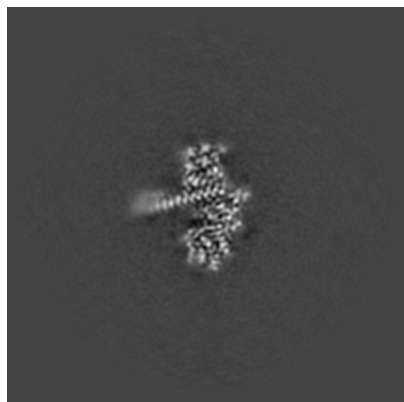


Z Index: 180

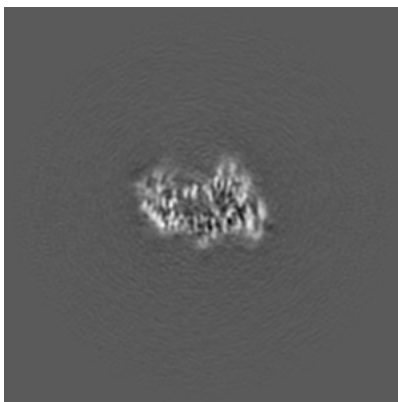
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

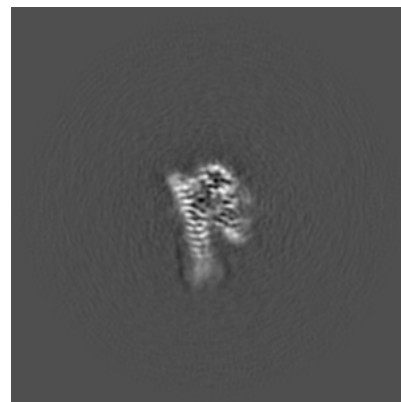
6.3.1 Primary map



X Index: 172

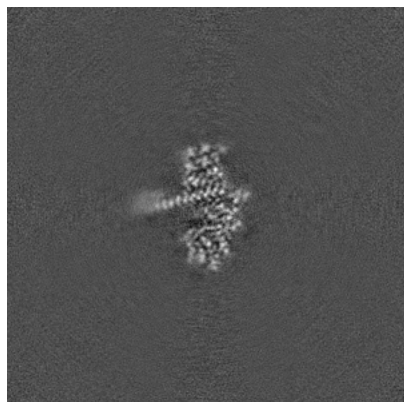


Y Index: 176

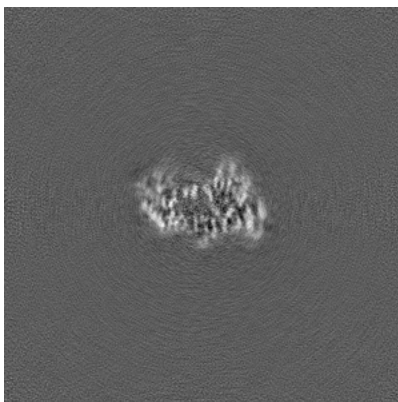


Z Index: 187

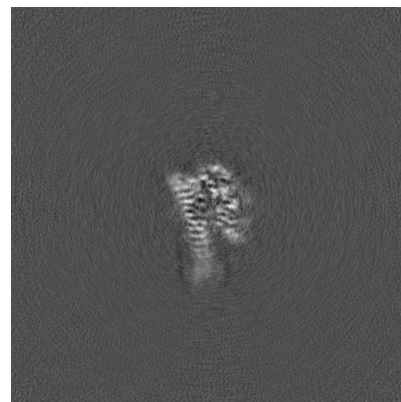
6.3.2 Raw map



X Index: 172



Y Index: 176

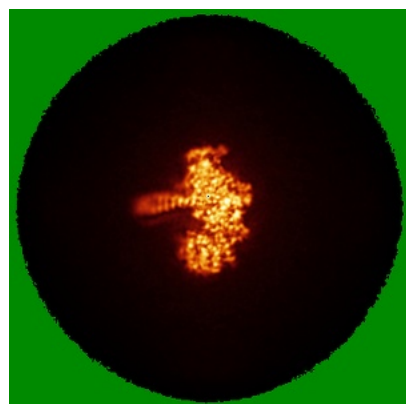


Z Index: 186

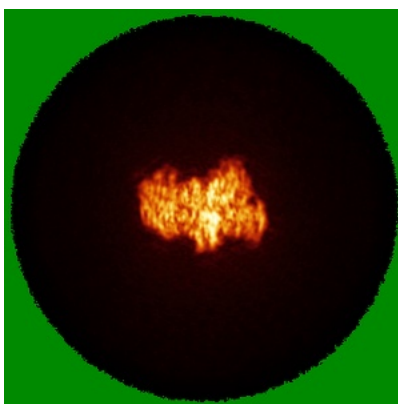
The images above show the largest variance slices of the map in three orthogonal directions.

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

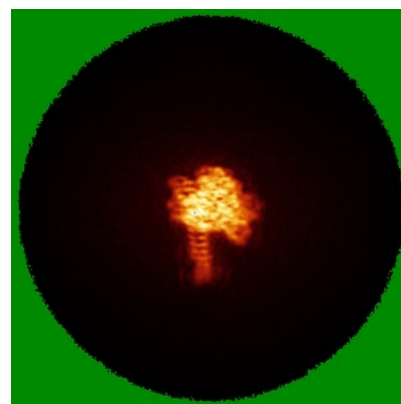
6.4.1 Primary map



X

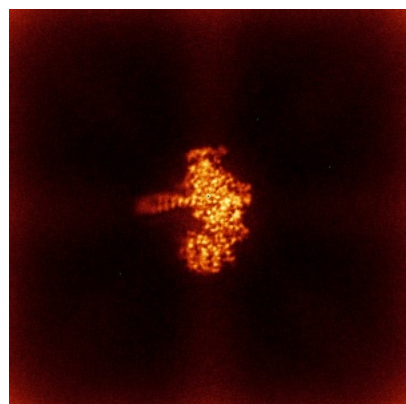


Y

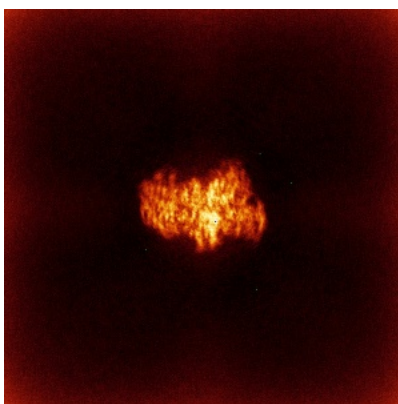


Z

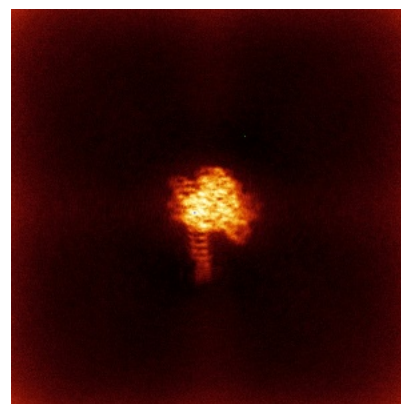
6.4.2 Raw map



X



Y

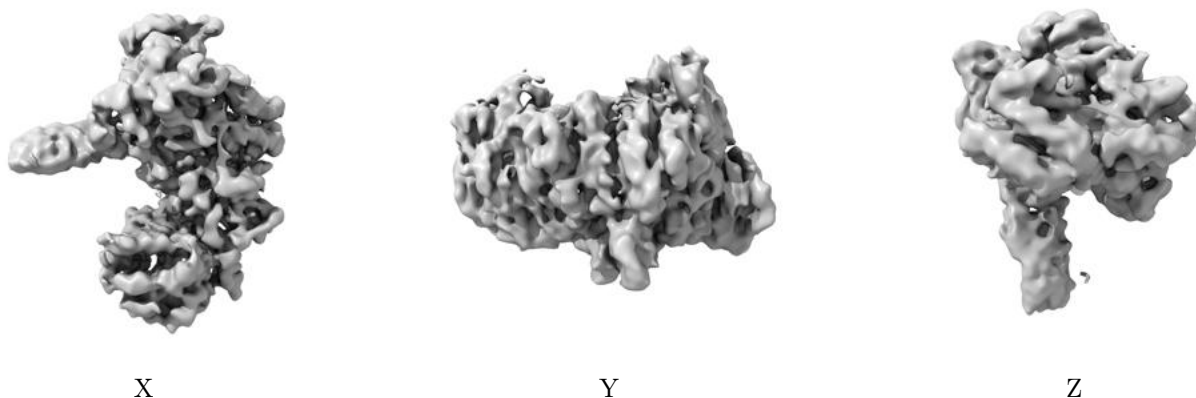


Z

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.

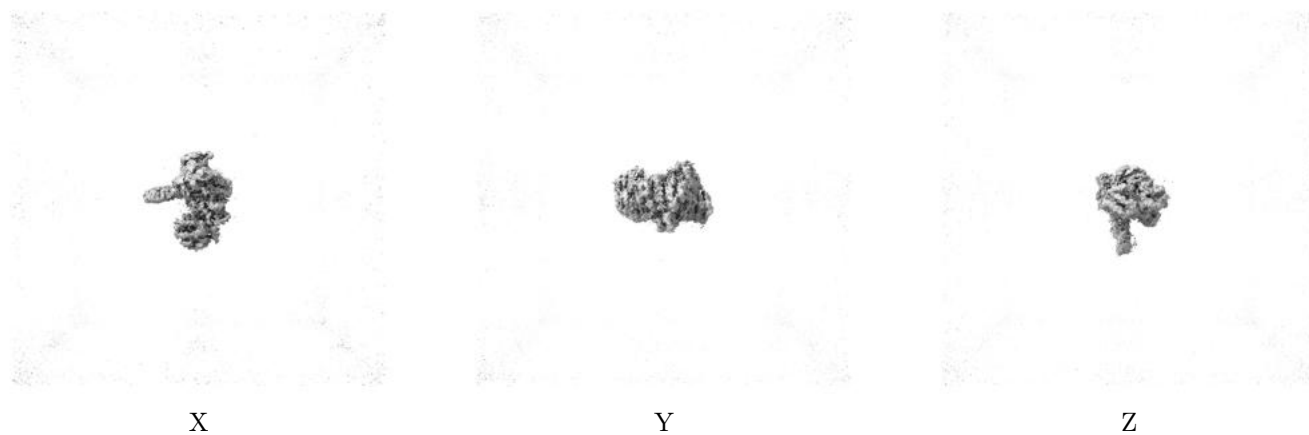
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

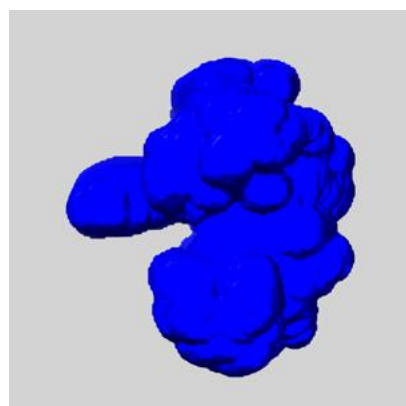
6.6 Mask visualisation [i](#)

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

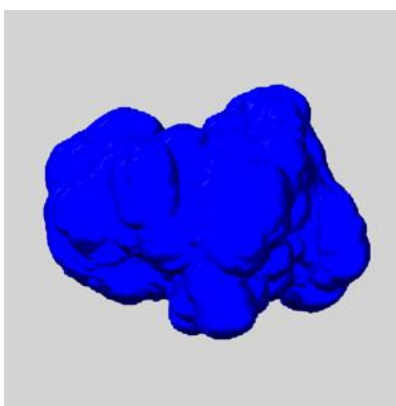
A mask typically either:

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

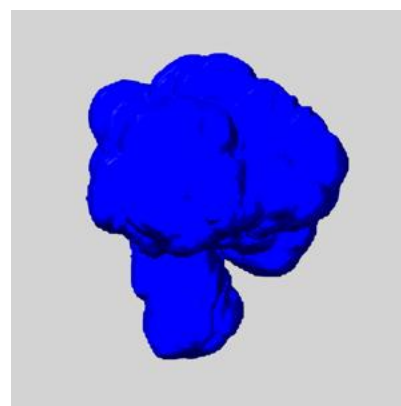
6.6.1 emd_17763_msk_1.map [i](#)



X



Y

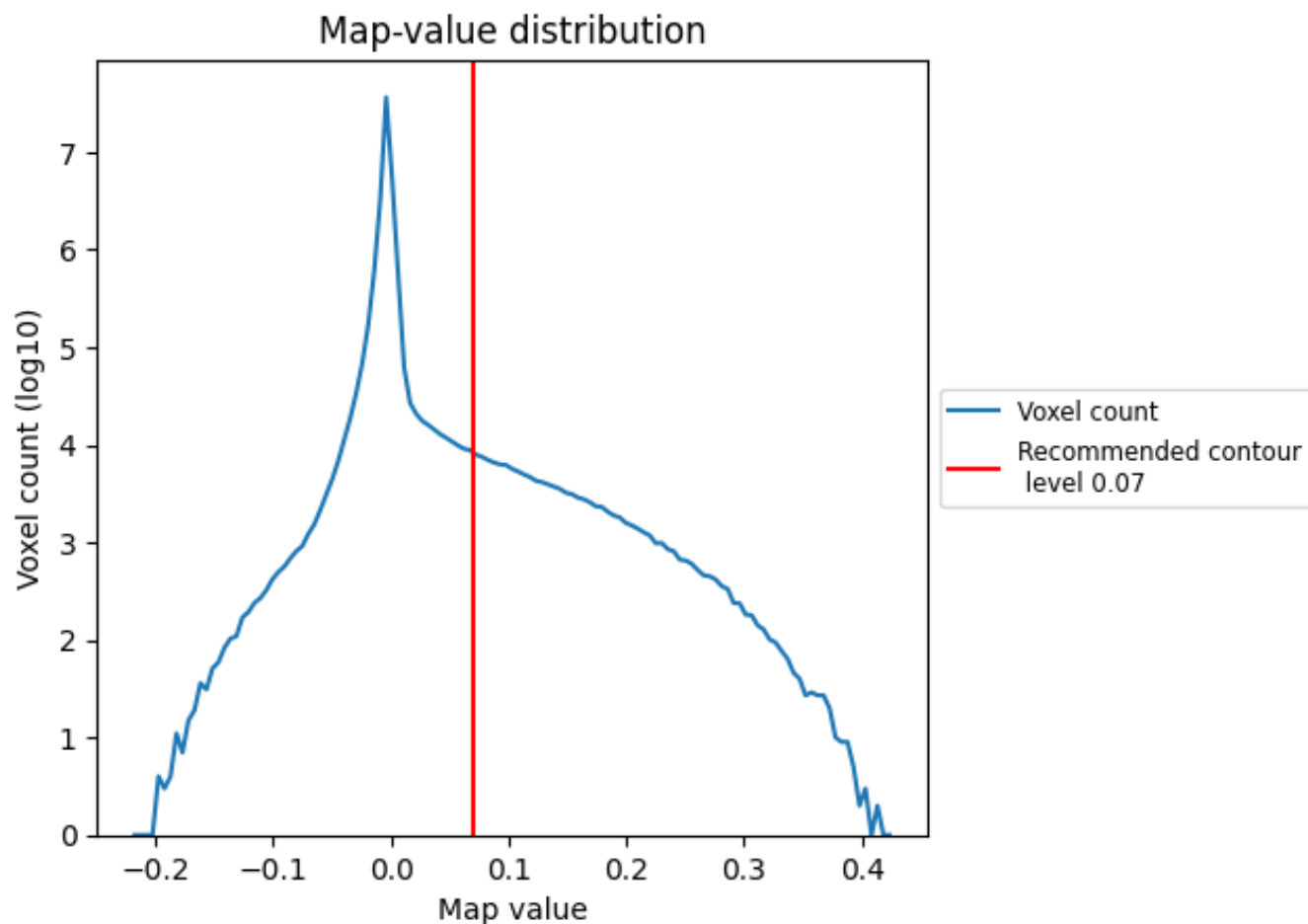


Z

7 Map analysis [i](#)

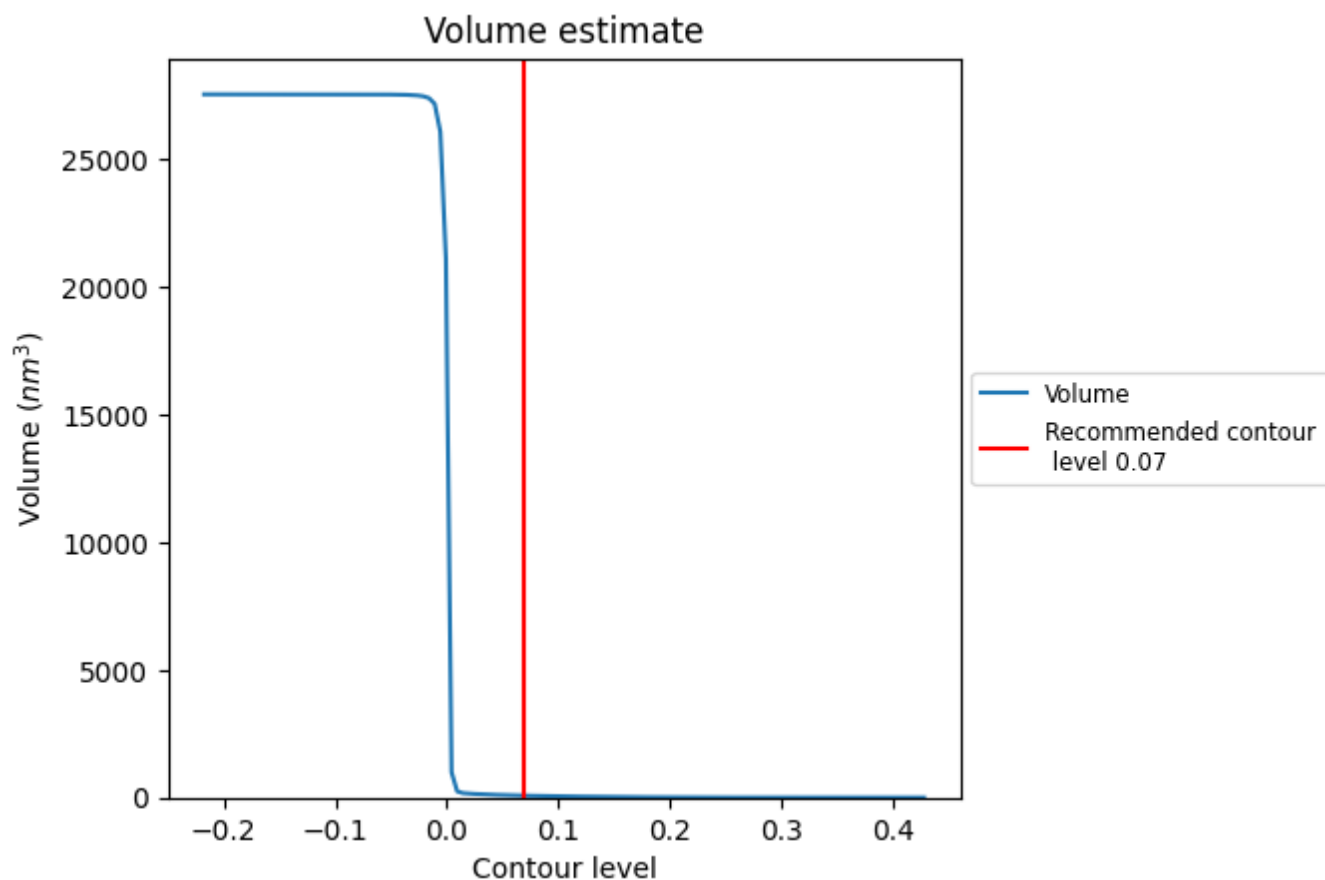
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

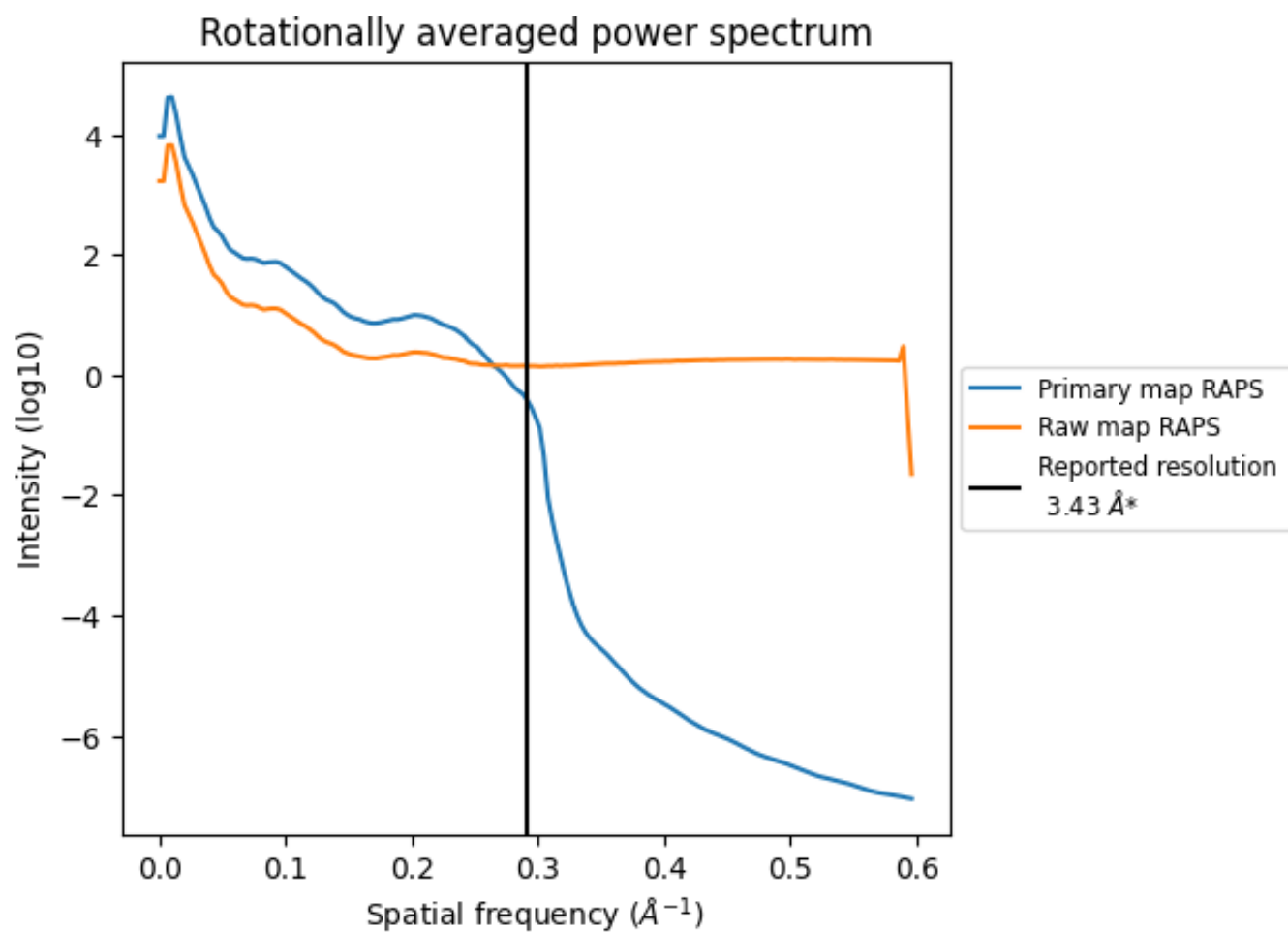
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm^3 ; this corresponds to an approximate mass of 68 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 ⓘ

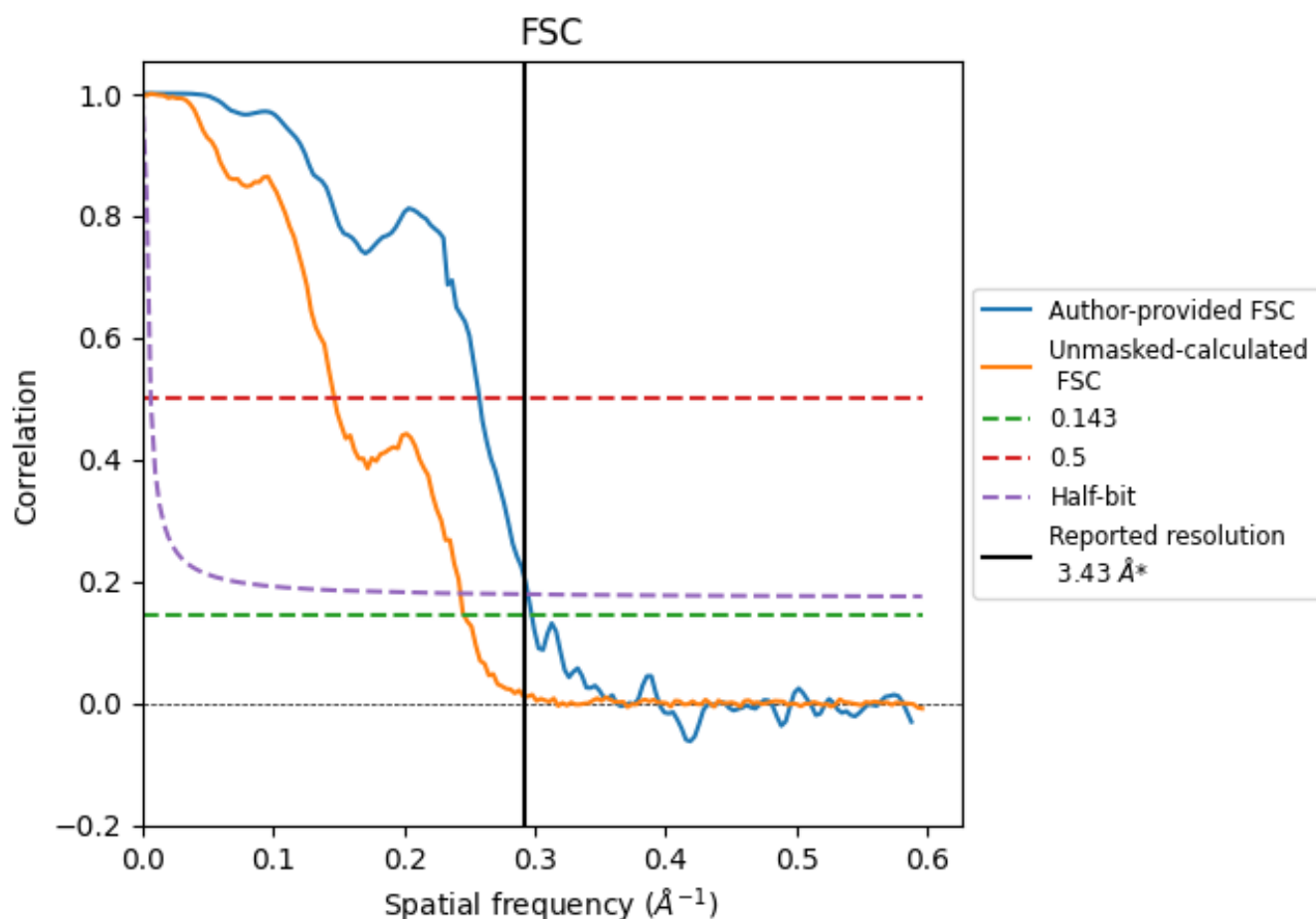


*Reported resolution corresponds to spatial frequency of 0.292 $\text{\AA}^{-1}$

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 0.292 Å⁻¹

8.2 Resolution estimates [i](#)

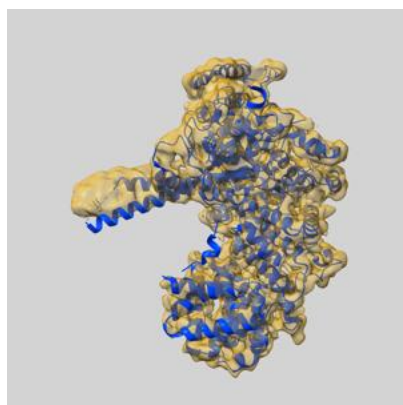
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	3.36	3.88	3.39
Unmasked-calculated*	4.06	6.81	4.11

*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 4.06 differs from the reported value 3.43 by more than 10 %

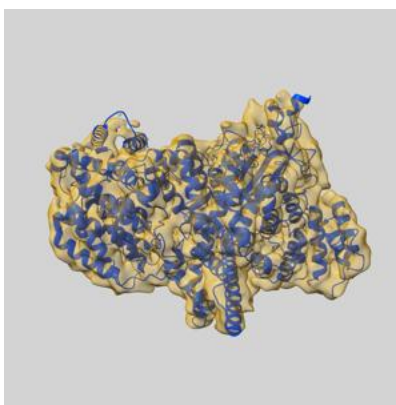
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17763 and PDB model 8PMP. Per-residue inclusion information can be found in section [3](#) on page [5](#).

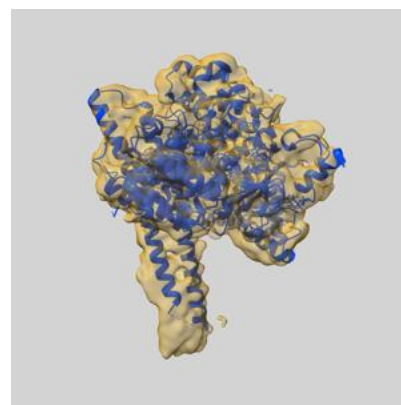
9.1 Map-model overlay [i](#)



X



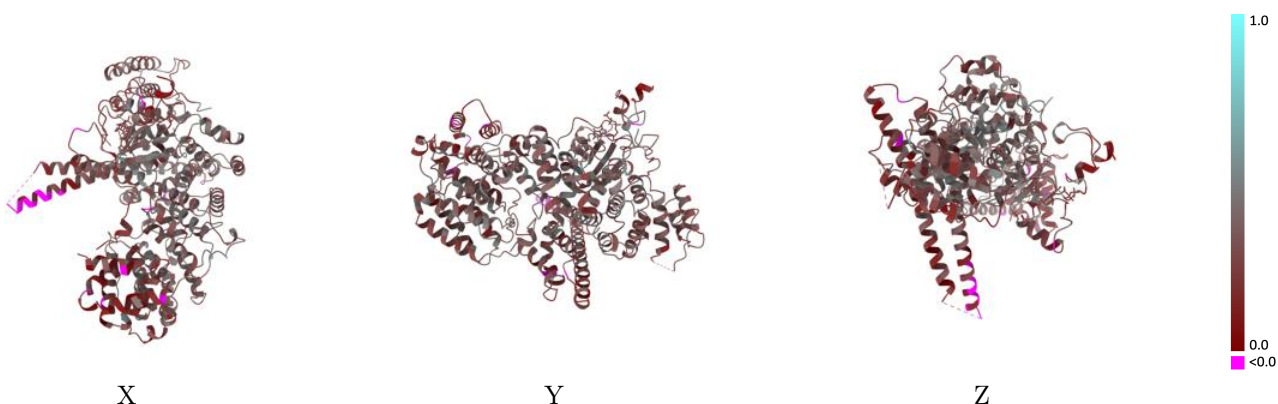
Y



Z

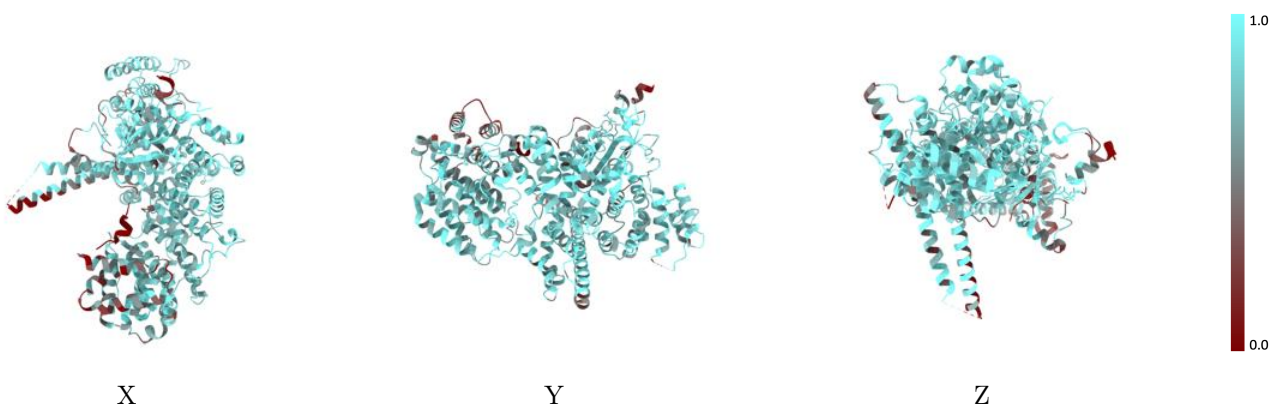
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



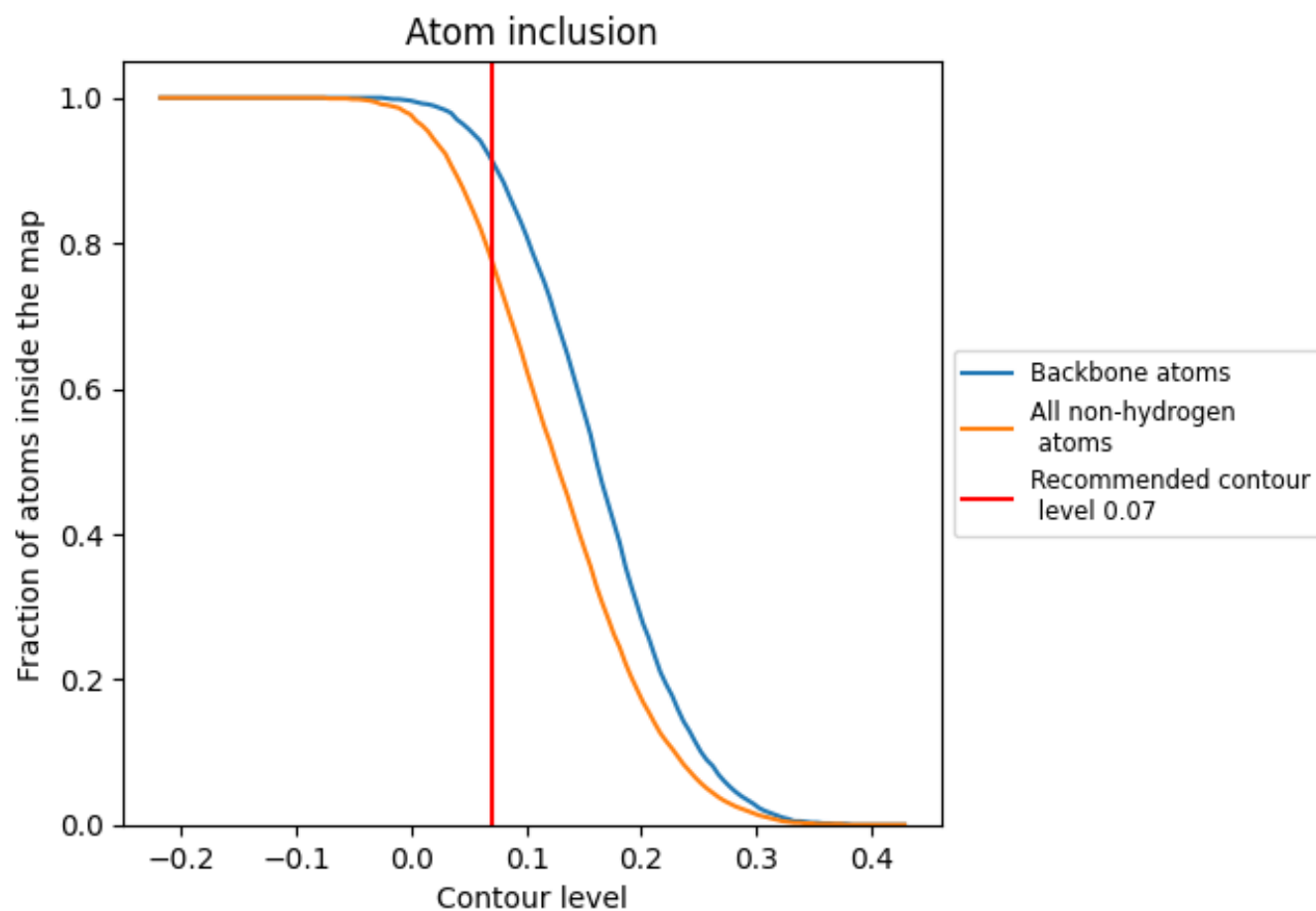
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 78% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.3180
A	0.7870	0.3180
B	0.7320	0.3210
D	0.7070	0.3000

