



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 11:24 PM UTC

PDB ID : 9DC4 / pdb\_00009dc4  
EMDB ID : EMD-46743  
Title : Transferrin Binding Protein A in complex with transferrin binding protein B, transferrin and globular domain of TonB  
Authors : Dubey, S.; Noinaj, N.  
Deposited on : 2024-08-25  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

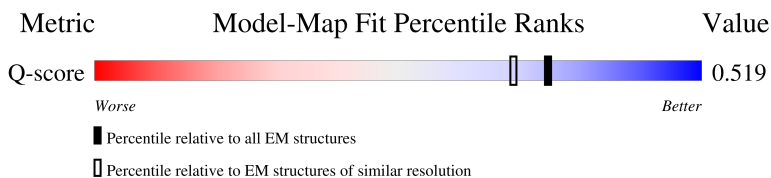
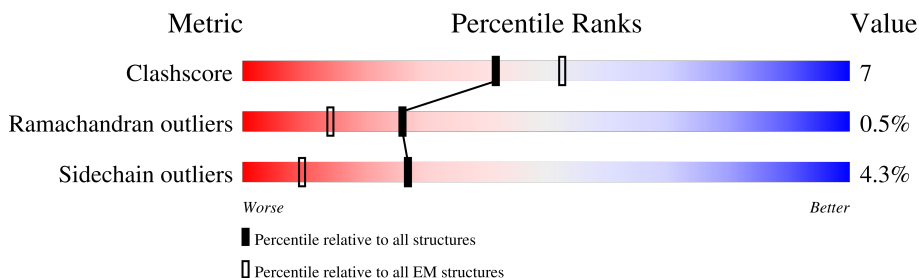
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 ( 2.60 - 3.60 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	915	
2	B	692	
3	F	698	
4	T	108	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCT	F	701	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17026 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 Transferrin-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	891	Total	C	N	O	S	0	0
			7000	4364	1281	1340	15		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9JPJ0
A	2	SER	-	expression tag	UNP Q9JPJ0
A	3	ASN	-	expression tag	UNP Q9JPJ0
A	4	HIS	-	expression tag	UNP Q9JPJ0
A	5	HIS	-	expression tag	UNP Q9JPJ0
A	6	HIS	-	expression tag	UNP Q9JPJ0
A	7	HIS	-	expression tag	UNP Q9JPJ0
A	8	HIS	-	expression tag	UNP Q9JPJ0
A	9	HIS	-	expression tag	UNP Q9JPJ0
A	10	HIS	-	expression tag	UNP Q9JPJ0
A	11	HIS	-	expression tag	UNP Q9JPJ0
A	12	HIS	-	expression tag	UNP Q9JPJ0
A	13	HIS	-	expression tag	UNP Q9JPJ0
A	14	GLU	-	expression tag	UNP Q9JPJ0
A	15	ASN	-	expression tag	UNP Q9JPJ0
A	16	LEU	-	expression tag	UNP Q9JPJ0
A	17	TYR	-	expression tag	UNP Q9JPJ0
A	18	PHE	-	expression tag	UNP Q9JPJ0
A	19	GLN	-	expression tag	UNP Q9JPJ0
A	20	GLY	-	expression tag	UNP Q9JPJ0
A	21	ALA	-	expression tag	UNP Q9JPJ0
A	22	MET	-	expression tag	UNP Q9JPJ0
A	23	ASP	-	expression tag	UNP Q9JPJ0
A	24	ILE	-	expression tag	UNP Q9JPJ0
A	490	ALA	THR	conflict	UNP Q9JPJ0
A	499	MET	VAL	conflict	UNP Q9JPJ0
A	510	MET	LEU	conflict	UNP Q9JPJ0
A	764	MET	VAL	conflict	UNP Q9JPJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	870	MET	LEU	conflict	UNP Q9JPJ0

- Molecule 2 is a protein called Transferrin-binding protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	532	Total	C	N	O	S	0	0
			4173	2619	710	838	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	MET	-	initiating methionine	UNP Q9JPI9

- Molecule 3 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	677	Total	C	N	O	S	1	0
			5196	3268	902	979	47		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	697	ALA	-	expression tag	UNP P02787
F	698	ALA	-	expression tag	UNP P02787

- Molecule 4 is a protein called Protein TonB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	86	Total	C	N	O	S	0	0
			652	409	119	123	1		

There are 22 discrepancies between the modelled and reference sequences:

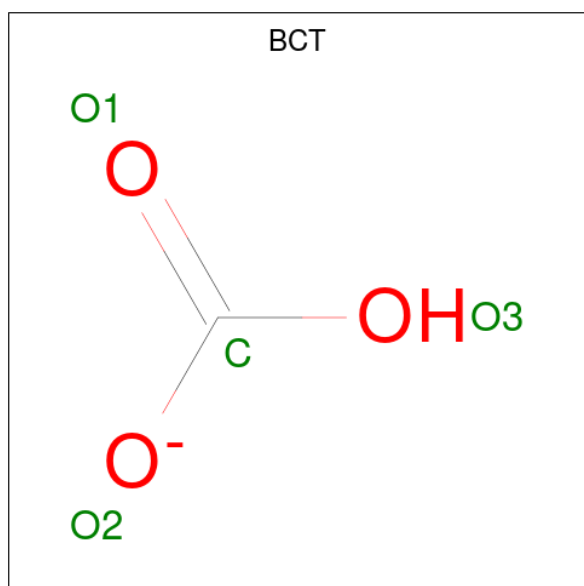
Chain	Residue	Modelled	Actual	Comment	Reference
T	173	HIS	-	expression tag	UNP P95374
T	174	HIS	-	expression tag	UNP P95374
T	175	HIS	-	expression tag	UNP P95374
T	176	HIS	-	expression tag	UNP P95374
T	177	HIS	-	expression tag	UNP P95374
T	178	HIS	-	expression tag	UNP P95374
T	179	ASP	-	expression tag	UNP P95374

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Chain	Residue	Modelled	Actual	Comment	Reference
T	180	TYR	-	expression tag	UNP P95374
T	181	ASP	-	expression tag	UNP P95374
T	182	ILE	-	expression tag	UNP P95374
T	183	PRO	-	expression tag	UNP P95374
T	184	THR	-	expression tag	UNP P95374
T	185	THR	-	expression tag	UNP P95374
T	186	GLU	-	expression tag	UNP P95374
T	187	ASN	-	expression tag	UNP P95374
T	188	LEU	-	expression tag	UNP P95374
T	189	TYR	-	expression tag	UNP P95374
T	190	PHE	-	expression tag	UNP P95374
T	191	GLN	-	expression tag	UNP P95374
T	192	GLY	-	expression tag	UNP P95374
T	193	ALA	-	expression tag	UNP P95374
T	194	MET	-	expression tag	UNP P95374

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	F	1	Total	C	O	0
			4	1	3	

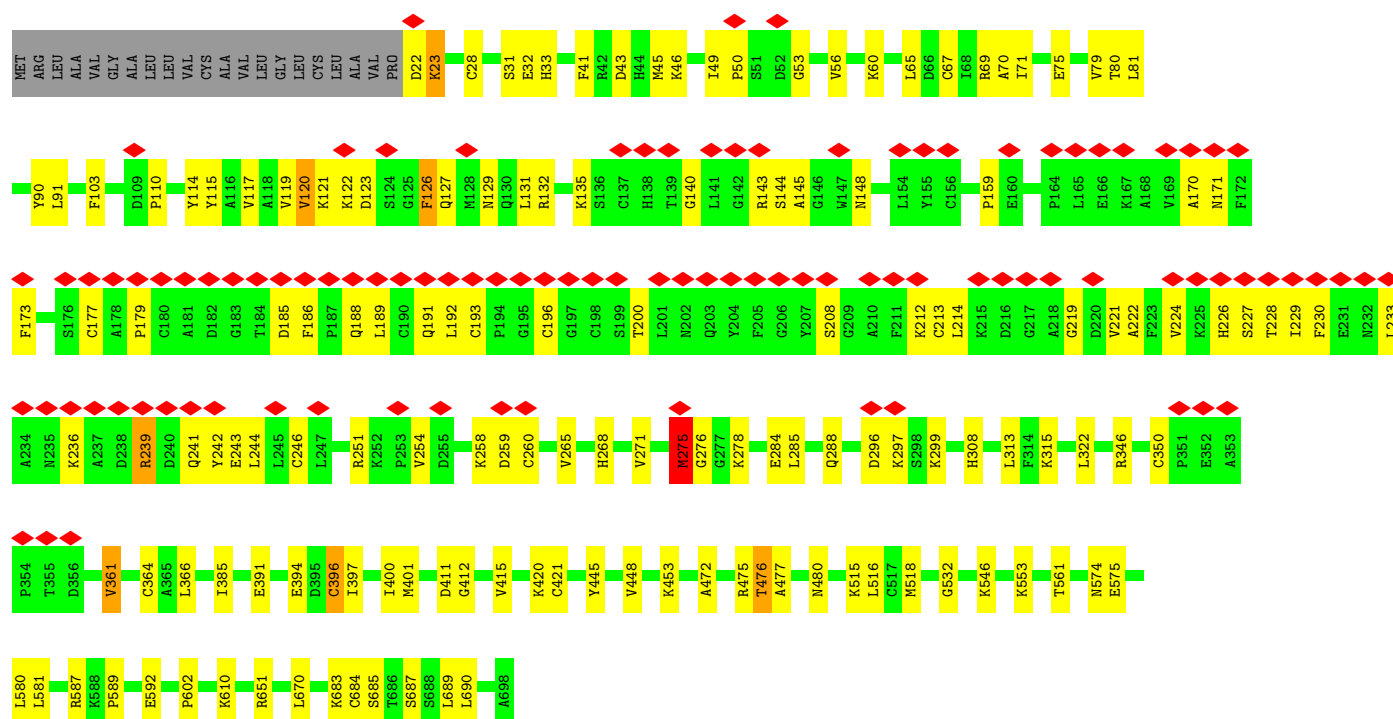
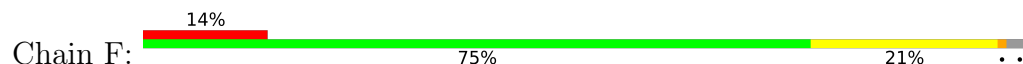
- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	F	1	Total 1	Fe 1	0

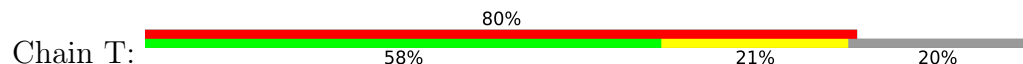




- Molecule 3: Serotransferrin



- Molecule 4: Protein TonB



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92329	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 ( $e^-/\text{\AA}^2$ )	65.81	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.624	Depositor
Minimum map value	-1.302	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.385	Depositor
Map size ( $\text{\AA}$ )	441.13998, 441.13998, 441.13998	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.959, 0.959, 0.959	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, FE

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	0/7152	0.37	1/9663 (0.0%)
2	B	0.15	0/4258	0.40	0/5729
3	F	0.15	0/5314	0.43	0/7189
4	T	0.12	0/666	0.33	0/902
All	All	0.15	0/17390	0.40	1/23483 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	ALA	CB-CA-C	-5.04	110.38	117.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	635	THR	Peptide
1	A	828	LEU	Peptide
2	B	506	CYS	Peptide

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Mol	Chain	Res	Type	Group
2	B	681	TYR	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	7000	0	6754	67	0
2	B	4173	0	3987	63	0
3	F	5196	0	4974	91	0
4	T	652	0	649	14	0
5	F	4	0	1	2	0
6	F	1	0	0	0	0
All	All	17026	0	16365	228	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 7.

All (228) 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)
3:F:71:ILE:HD11	3:F:79:VAL:HG23	1.58	0.85
4:T:202:ALA:HA	4:T:264:GLN:O	1.78	0.84
3:F:117:VAL:HG22	3:F:226:HIS:HA	1.61	0.82
1:A:521:ASN:O	1:A:554:GLY:HA2	1.79	0.81
3:F:49:ILE:HG12	3:F:53:GLY:HA3	1.64	0.80
1:A:639:ASP:HB2	1:A:683:VAL:HG13	1.66	0.77
3:F:236:LYS:HA	3:F:239:ARG:HD2	1.69	0.74
3:F:275:MET:HE2	3:F:276:GLY:H	1.51	0.74
3:F:119:VAL:HG11	3:F:214:LEU:HD22	1.70	0.73
1:A:631:VAL:HG23	1:A:641:THR:HG22	1.69	0.72
3:F:140:GLY:HA2	3:F:179:PRO:HG2	1.73	0.71
3:F:561:THR:HG21	3:F:575:GLU:HB3	1.73	0.70
3:F:43:ASP:HA	3:F:46:LYS:HE2	1.75	0.69
3:F:448:VAL:HG21	3:F:580:LEU:HD13	1.74	0.69
3:F:144:SER:HA	3:F:148:ASN:HB2	1.74	0.68
3:F:518:MET:HE2	3:F:532:GLY:HA3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:170:ALA:HA	3:F:173:PHE:HB2	1.75	0.67
1:A:728:ALA:HB2	1:A:775:ARG:HG3	1.74	0.67
1:A:455:CYS:O	1:A:456:ARG:NH1	2.24	0.67
2:B:280:ILE:HG22	2:B:295:GLN:HA	1.77	0.66
3:F:229:ILE:HG23	3:F:233:LEU:HB3	1.78	0.66
2:B:517:MET:HE2	2:B:547:MET:HE2	1.78	0.65
2:B:502:GLU:HG3	2:B:519:THR:HB	1.77	0.65
1:A:213:ILE:HG23	1:A:214:GLY:H	1.63	0.64
4:T:255:ARG:HH12	4:T:259:GLN:HG3	1.62	0.64
1:A:137:SER:OG	1:A:401:GLU:OE2	2.16	0.63
3:F:132:ARG:NH2	3:F:171:ASN:O	2.31	0.63
3:F:268:HIS:HB2	3:F:315:LYS:HE3	1.80	0.62
3:F:411:ASP:OD1	3:F:412:GLY:N	2.30	0.62
3:F:186:PHE:HB3	3:F:189:LEU:HB2	1.82	0.61
3:F:121:LYS:HA	3:F:242:TYR:HA	1.82	0.61
2:B:34:ASP:OD1	2:B:34:ASP:N	2.31	0.60
2:B:317:LYS:HA	2:B:330:VAL:HG13	1.85	0.59
2:B:223:ILE:HG22	2:B:224:ILE:HG12	1.83	0.59
3:F:476:THR:HA	3:F:480:ASN:HB2	1.86	0.58
3:F:135:LYS:HB3	3:F:219:GLY:HA2	1.85	0.58
2:B:45:GLN:NE2	2:B:709:GLN:OE1	2.36	0.58
1:A:540:ASN:OD1	1:A:540:ASN:N	2.36	0.57
4:T:228:VAL:HG22	4:T:239:VAL:HG13	1.85	0.57
2:B:237:PHE:HD1	2:B:237:PHE:H	1.52	0.57
2:B:57:ASP:O	2:B:59:GLY:N	2.38	0.57
1:A:748:TRP:HE1	1:A:750:LYS:HD3	1.70	0.56
3:F:394:GLU:OE2	3:F:687:SER:OG	2.23	0.56
1:A:489:ASP:OD1	1:A:490:ALA:N	2.38	0.56
1:A:521:ASN:O	1:A:554:GLY:CA	2.51	0.56
2:B:570:SER:OG	2:B:571:TRP:N	2.39	0.56
3:F:145:ALA:H	5:F:701:BCT:C	2.19	0.56
1:A:746:GLY:N	1:A:749:ASP:OD1	2.39	0.56
4:T:225:VAL:HG12	4:T:242:VAL:HB	1.87	0.55
1:A:177:THR:HG22	1:A:179:ASP:H	1.71	0.55
3:F:143:ARG:HB2	5:F:701:BCT:C	2.36	0.55
3:F:120:VAL:HG12	3:F:123:ASP:HA	1.87	0.55
1:A:221:ILE:HD12	1:A:313:LEU:HD22	1.88	0.55
2:B:510:LEU:HD22	2:B:674:GLU:HG2	1.88	0.55
3:F:122:LYS:HA	3:F:243:GLU:HB2	1.88	0.55
1:A:782:LEU:HD13	1:A:837:ALA:HB2	1.89	0.54
1:A:818:ILE:HB	1:A:841:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:119:VAL:HG21	3:F:224:VAL:HG22	1.88	0.54
2:B:554:THR:OG1	2:B:669:GLY:O	2.15	0.54
3:F:119:VAL:HG12	3:F:119:VAL:O	2.07	0.54
1:A:816:LYS:NZ	1:A:820:GLU:OE1	2.41	0.54
1:A:635:THR:O	1:A:637:TRP:N	2.41	0.53
3:F:41:PHE:HE1	3:F:45:MET:HE3	1.72	0.53
1:A:52:ASP:OD1	1:A:53:ASN:N	2.42	0.53
2:B:51:LYS:HG3	2:B:52:PRO:HD2	1.91	0.53
2:B:663:VAL:HA	2:B:679:PHE:HB3	1.91	0.53
2:B:353:LEU:HD13	2:B:360:ALA:HB2	1.91	0.53
3:F:41:PHE:HZ	3:F:285:LEU:HD21	1.74	0.53
1:A:799:GLN:HG2	1:A:802:GLY:H	1.74	0.52
1:A:650:LEU:HD23	1:A:672:PRO:HB3	1.91	0.52
2:B:224:ILE:HG21	2:B:230:GLN:HG3	1.91	0.52
2:B:438:LEU:HG	2:B:505:VAL:HG21	1.90	0.52
2:B:66:ARG:HG2	2:B:67:LEU:H	1.75	0.52
1:A:804:TRP:HB3	1:A:854:TYR:HD1	1.74	0.51
1:A:48:LYS:HG3	1:A:48:LYS:O	2.09	0.51
3:F:70:ALA:HB1	3:F:75:GLU:HB3	1.93	0.51
3:F:185:ASP:OD1	3:F:186:PHE:N	2.44	0.51
1:A:206:SER:HB2	1:A:223:THR:HG23	1.92	0.51
1:A:635:THR:O	1:A:635:THR:OG1	2.24	0.51
3:F:258:LYS:NZ	3:F:259:ASP:OD1	2.43	0.51
3:F:31:SER:HA	3:F:60:LYS:HD2	1.91	0.51
3:F:296:ASP:H	3:F:299:LYS:HD2	1.76	0.51
3:F:179:PRO:HA	3:F:196:CYS:HA	1.93	0.50
2:B:83:LEU:H	2:B:83:LEU:HD22	1.76	0.50
3:F:67:CYS:O	3:F:71:ILE:HG13	2.12	0.50
2:B:91:THR:HG21	2:B:188:HIS:HB3	1.93	0.50
1:A:568:THR:HG22	1:A:569:TYR:H	1.77	0.50
2:B:146:ALA:O	2:B:149:TYR:HB2	2.12	0.50
3:F:120:VAL:HA	3:F:221:VAL:HG11	1.93	0.50
4:T:225:VAL:HB	4:T:243:LYS:HB3	1.94	0.49
3:F:115:TYR:O	3:F:226:HIS:ND1	2.45	0.49
2:B:630:ASN:OD1	2:B:630:ASN:N	2.45	0.49
3:F:123:ASP:OD2	3:F:251:ARG:NH2	2.40	0.49
4:T:226:LEU:HD22	4:T:239:VAL:HG12	1.94	0.49
1:A:49:THR:N	1:A:52:ASP:OD2	2.30	0.49
1:A:247:VAL:HG22	1:A:248:PRO:HD2	1.93	0.49
2:B:333:SER:HB2	2:B:354:SER:HA	1.93	0.49
3:F:127:GLN:O	3:F:131:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:226:LEU:HD23	4:T:241:ILE:HA	1.94	0.49
3:F:81:LEU:HD21	3:F:271:VAL:HB	1.95	0.48
1:A:393:TYR:HB2	1:A:445:HIS:CD2	2.48	0.48
1:A:856:VAL:O	1:A:860:PHE:HB2	2.14	0.48
3:F:114:TYR:HB2	3:F:226:HIS:HE1	1.77	0.48
1:A:324:ARG:O	1:A:325:HIS:ND1	2.47	0.48
3:F:33:HIS:ND1	3:F:308:HIS:O	2.47	0.48
2:B:81:VAL:N	2:B:213:ASP:HB2	2.28	0.47
2:B:706:LYS:HG2	2:B:707:ARG:H	1.79	0.47
3:F:121:LYS:O	3:F:122:LYS:HG2	2.14	0.47
3:F:246:CYS:HB3	3:F:260:CYS:HB2	1.70	0.47
4:T:276:LYS:HG3	4:T:278:GLU:OE1	2.13	0.47
2:B:93:LEU:HD12	2:B:94:PRO:HD2	1.96	0.47
3:F:361:VAL:HG13	3:F:385:ILE:HD13	1.97	0.47
1:A:540:ASN:HB2	3:F:453:LYS:HD3	1.95	0.47
1:A:58:LEU:HD13	1:A:679:GLU:HG2	1.96	0.47
1:A:774:ASP:OD1	1:A:774:ASP:N	2.45	0.47
3:F:602:PRO:HG3	3:F:670:LEU:HD23	1.96	0.47
2:B:281:ARG:HE	2:B:296:TYR:HE2	1.62	0.47
1:A:269:TYR:OH	1:A:546:PRO:O	2.30	0.46
1:A:44:ALA:HB3	4:T:279:LEU:HD23	1.97	0.46
1:A:256:ALA:HB1	1:A:279:ASP:OD1	2.16	0.46
1:A:502:GLY:HA3	1:A:583:TYR:CE2	2.51	0.46
2:B:332:ASP:O	2:B:355:ASP:HB2	2.16	0.46
2:B:147:LYS:HD2	2:B:147:LYS:HA	1.60	0.46
3:F:80:THR:HG21	3:F:313:LEU:O	2.15	0.46
1:A:804:TRP:HB3	1:A:854:TYR:CD1	2.50	0.46
2:B:113:THR:O	2:B:113:THR:OG1	2.32	0.46
3:F:144:SER:OG	3:F:145:ALA:N	2.49	0.45
1:A:43:LYS:H	4:T:208:ARG:HH21	1.64	0.45
1:A:37:LEU:HD12	4:T:273:VAL:HG22	1.96	0.45
3:F:242:TYR:HB3	3:F:244:LEU:CD2	2.47	0.45
3:F:589:PRO:HG2	3:F:592:GLU:HG3	1.98	0.45
2:B:262:PHE:CE1	2:B:281:ARG:HD3	2.51	0.45
3:F:346:ARG:HA	3:F:346:ARG:HD3	1.75	0.45
3:F:581:LEU:HD23	3:F:587:ARG:HG2	1.98	0.45
2:B:147:LYS:HB3	2:B:149:TYR:HD2	1.82	0.45
2:B:206:GLY:HA3	2:B:365:ALA:HA	1.99	0.45
2:B:410:LEU:HG	2:B:417:VAL:HG12	1.98	0.45
3:F:135:LYS:HD3	3:F:135:LYS:HA	1.73	0.45
3:F:687:SER:C	3:F:689:LEU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:SER:OG	1:A:665:SER:O	2.32	0.45
2:B:283:ASN:OD1	2:B:294:THR:OG1	2.31	0.45
2:B:434:ILE:HD12	2:B:435:MET:H	1.82	0.45
1:A:151:VAL:HG13	1:A:173:PHE:CE1	2.52	0.44
1:A:147:ASN:HB3	1:A:313:LEU:HD13	1.98	0.44
2:B:66:ARG:HG2	2:B:67:LEU:N	2.31	0.44
3:F:103:PHE:HD2	3:F:322:LEU:HG	1.82	0.44
1:A:279:ASP:OD1	1:A:279:ASP:N	2.50	0.44
2:B:65:MET:HE2	2:B:87:ASP:HB2	2.00	0.44
2:B:265:ASN:OD1	2:B:266:LEU:N	2.51	0.44
2:B:279:LEU:HB2	2:B:297:TYR:HB2	1.98	0.44
1:A:376:TYR:C	1:A:378:GLY:H	2.26	0.44
2:B:577:ASN:ND2	2:B:655:LYS:O	2.46	0.44
3:F:472:ALA:HB3	3:F:475:ARG:HD3	1.99	0.44
1:A:49:THR:HG23	1:A:51:ARG:H	1.82	0.44
2:B:366:LYS:HG2	2:B:367:THR:N	2.31	0.44
3:F:132:ARG:HD2	3:F:132:ARG:HA	1.57	0.44
2:B:213:ASP:OD2	2:B:358:LYS:HA	2.18	0.44
3:F:126:PHE:HB2	3:F:131:LEU:HG	1.99	0.44
3:F:227:SER:O	3:F:229:ILE:N	2.51	0.44
3:F:230:PHE:HA	3:F:239:ARG:HH22	1.82	0.44
1:A:253:SER:OG	3:F:574:ASN:ND2	2.51	0.43
1:A:320:PHE:HD2	1:A:325:HIS:HB3	1.83	0.43
2:B:36:GLU:OE2	2:B:39:ARG:NH1	2.50	0.43
3:F:397:ILE:O	3:F:401:MET:HG3	2.17	0.43
3:F:420:LYS:HD2	3:F:690:LEU:HD11	2.01	0.43
3:F:515:LYS:HE3	3:F:515:LYS:HB2	1.73	0.43
1:A:728:ALA:HA	1:A:772:ARG:HD3	2.00	0.43
2:B:465:ASP:OD1	2:B:466:HIS:N	2.51	0.43
3:F:208:SER:O	3:F:212:LYS:HG3	2.17	0.43
2:B:36:GLU:OE1	2:B:37:ALA:N	2.31	0.43
3:F:396:CYS:O	3:F:400:ILE:HG13	2.19	0.43
3:F:401:MET:HE3	3:F:401:MET:HB3	1.87	0.43
1:A:236:ALA:HB2	2:B:28:PHE:CZ	2.54	0.43
3:F:188:GLN:O	3:F:191:GLN:HB2	2.19	0.43
1:A:322:ASN:OD1	1:A:322:ASN:N	2.51	0.43
3:F:275:MET:CE	3:F:276:GLY:H	2.27	0.43
2:B:53:GLN:OE1	2:B:53:GLN:N	2.44	0.42
2:B:578:ASP:OD2	2:B:696:ASN:ND2	2.44	0.42
1:A:160:VAL:HG21	1:A:627:ASN:HB3	2.01	0.42
1:A:617:SER:O	1:A:617:SER:OG	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:HIS:O	1:A:782:LEU:HD23	2.20	0.42
2:B:247:ASN:OD1	2:B:260:TYR:HA	2.19	0.42
3:F:121:LYS:H	3:F:121:LYS:HG3	1.54	0.42
2:B:208:TRP:NE1	2:B:262:PHE:HB3	2.34	0.42
2:B:225:GLN:O	2:B:227:SER:N	2.49	0.42
2:B:653:THR:O	2:B:653:THR:OG1	2.31	0.42
2:B:553:ARG:HG2	2:B:668:TYR:CE1	2.54	0.42
3:F:103:PHE:HB2	3:F:110:PRO:HB2	2.02	0.42
4:T:211:TYR:HB3	4:T:216:MET:SD	2.60	0.42
3:F:186:PHE:HE1	3:F:188:GLN:HB3	1.82	0.42
2:B:671:LYS:HD2	2:B:671:LYS:HA	1.89	0.42
3:F:65:LEU:HD23	3:F:65:LEU:HA	1.82	0.42
1:A:504:ASP:OD1	1:A:505:ARG:N	2.53	0.42
2:B:181:ASP:OD1	2:B:181:ASP:N	2.53	0.42
3:F:684:CYS:O	3:F:685:SER:OG	2.33	0.42
3:F:411:ASP:O	3:F:415:VAL:HG23	2.19	0.42
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.83	0.41
1:A:379:LEU:H	1:A:379:LEU:HG	1.54	0.41
1:A:425:TYR:HB3	1:A:485:LYS:HB3	2.02	0.41
2:B:577:ASN:OD1	2:B:578:ASP:N	2.53	0.41
2:B:113:THR:O	2:B:114:ASP:C	2.63	0.41
4:T:215:SER:HA	4:T:220:GLU:OE1	2.20	0.41
1:A:54:GLU:HG3	1:A:56:THR:H	1.86	0.41
1:A:324:ARG:O	1:A:325:HIS:CG	2.74	0.41
2:B:147:LYS:HB3	2:B:149:TYR:CD2	2.56	0.41
3:F:284:GLU:O	3:F:288:GLN:HG2	2.21	0.41
4:T:278:GLU:OE1	4:T:278:GLU:N	2.53	0.41
3:F:242:TYR:HB3	3:F:244:LEU:HD21	2.02	0.41
1:A:144:GLU:HG3	1:A:146:GLU:H	1.85	0.41
2:B:68:LYS:NZ	2:B:68:LYS:HB3	2.34	0.41
3:F:22:ASP:HB3	3:F:23:LYS:H	1.51	0.41
3:F:121:LYS:O	3:F:121:LYS:HD2	2.20	0.41
3:F:127:GLN:HG3	3:F:251:ARG:HH12	1.86	0.41
3:F:135:LYS:HD2	3:F:192:LEU:HD11	2.02	0.41
3:F:177:CYS:SG	3:F:193:CYS:N	2.94	0.41
3:F:516:LEU:HD22	3:F:546:LYS:HE2	2.02	0.41
1:A:192:SER:HB3	1:A:207:ILE:HD13	2.02	0.41
2:B:562:GLU:HB3	2:B:565:ILE:HD11	2.03	0.41
2:B:564:ASN:H	2:B:601:ASN:HD22	1.69	0.40
1:A:534:GLY:O	1:A:537:ILE:HG12	2.21	0.40
3:F:115:TYR:HB2	3:F:226:HIS:CG	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:214:LEU:HD23	3:F:222:ALA:HB3	2.02	0.40
1:A:811:THR:HG23	1:A:847:ILE:HG13	2.03	0.40
1:A:213:ILE:HG23	1:A:214:GLY:N	2.32	0.40
1:A:590:VAL:HB	1:A:598:VAL:HG22	2.04	0.40
2:B:647:GLN:NE2	3:F:391:GLU:O	2.55	0.40
3:F:401:MET:SD	3:F:421:CYS:HB3	2.61	0.40
3:F:445:TYR:CE1	3:F:553:LYS:HD2	2.57	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	889/915 (97%)	833 (94%)	55 (6%)	1 (0%)	48 78
2	B	510/692 (74%)	463 (91%)	43 (8%)	4 (1%)	16 47
3	F	676/698 (97%)	577 (85%)	93 (14%)	6 (1%)	14 44
4	T	84/108 (78%)	81 (96%)	3 (4%)	0	100 100
All	All	2159/2413 (90%)	1954 (90%)	194 (9%)	11 (0%)	26 57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	112	GLU
2	B	555	ASP
3	F	159	PRO
3	F	228	THR
2	B	58	GLN
3	F	477	ALA
3	F	275	MET
1	A	747	VAL

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Mol	Chain	Res	Type
2	B	148	ASP
3	F	50	PRO
3	F	350	CYS

### 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	722/749 (96%)	695 (96%)	27 (4%)	30	61
2	B	446/563 (79%)	427 (96%)	19 (4%)	26	57
3	F	549/583 (94%)	522 (95%)	27 (5%)	22	53
4	T	71/91 (78%)	68 (96%)	3 (4%)	26	58
All	All	1788/1986 (90%)	1712 (96%)	76 (4%)	27	57

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	VAL
1	A	144	GLU
1	A	194	THR
1	A	201	ARG
1	A	207	ILE
1	A	209	LEU
1	A	231	ARG
1	A	247	VAL
1	A	284	ASP
1	A	323	LYS
1	A	340	THR
1	A	359	LYS
1	A	376	TYR
1	A	379	LEU
1	A	395	THR
1	A	446	CYS
1	A	458	SER
1	A	497	LEU

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Mol	Chain	Res	Type
1	A	508	SER
1	A	540	ASN
1	A	609	THR
1	A	683	VAL
1	A	806	VAL
1	A	811	THR
1	A	859	HIS
1	A	870	MET
1	A	876	THR
2	B	34	ASP
2	B	36	GLU
2	B	68	LYS
2	B	99	GLU
2	B	147	LYS
2	B	182	ASP
2	B	203	THR
2	B	230	GLN
2	B	233	ARG
2	B	235	SER
2	B	237	PHE
2	B	238	SER
2	B	400	LYS
2	B	507	CYS
2	B	549	LEU
2	B	599	THR
2	B	601	ASN
2	B	607	ILE
2	B	663	VAL
3	F	23	LYS
3	F	28	CYS
3	F	32	GLU
3	F	56	VAL
3	F	69	ARG
3	F	90	TYR
3	F	91	LEU
3	F	120	VAL
3	F	126	PHE
3	F	129	ASN
3	F	200	THR
3	F	213	CYS
3	F	239	ARG
3	F	241	GLN

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Mol	Chain	Res	Type
3	F	254	VAL
3	F	265	VAL
3	F	275	MET
3	F	278	LYS
3	F	297	LYS
3	F	361	VAL
3	F	364	CYS
3	F	366	LEU
3	F	396	CYS
3	F	476	THR
3	F	610	LYS
3	F	651	ARG
3	F	683	LYS
4	T	200	LEU
4	T	223	THR
4	T	235	HIS

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

Mol	Chain	Res	Type
1	A	72	GLN
1	A	433	GLN
1	A	519	HIS
1	A	745	ASN
1	A	906	ASN
2	B	295	GLN
2	B	522	ASN
2	B	563	GLN
2	B	626	ASN
3	F	203	GLN
3	F	268	HIS
3	F	308	HIS
4	T	266	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
5	BCT	F	701	6	3,3,3	0.75	0	2,3,3	3.29	2 (100%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	701	BCT	O2-C-O1	3.94	129.76	119.68
5	F	701	BCT	O3-C-O1	-2.47	113.35	119.68

There are no chirality outliers.

There are no torsion outliers.

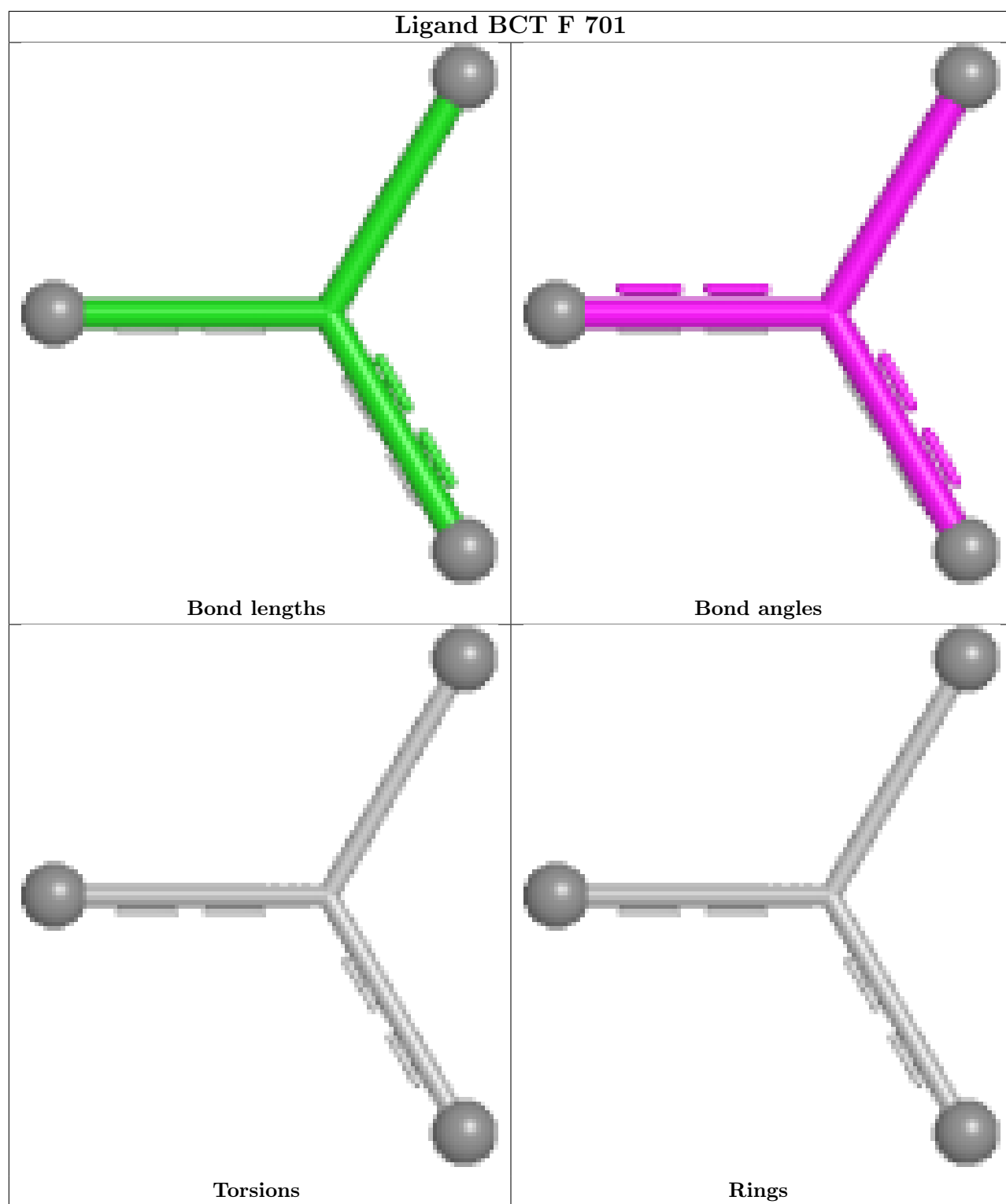
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	701	BCT	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 ⓘ

There are no chain breaks in this entry.

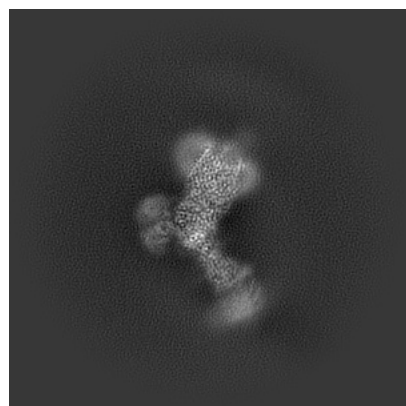
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46743. These allow visual inspection of the internal detail of the map and identification of artifacts.

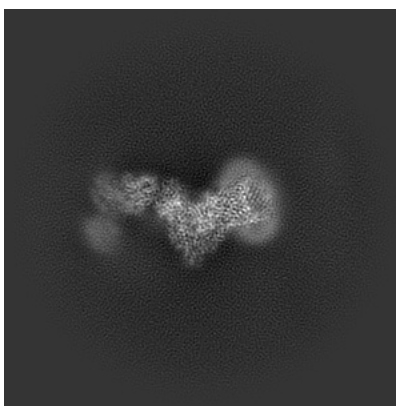
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

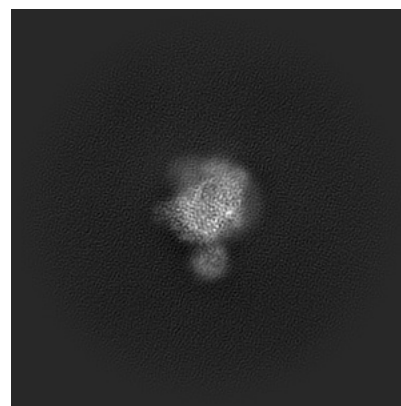
#### 6.1.1 Primary map



X

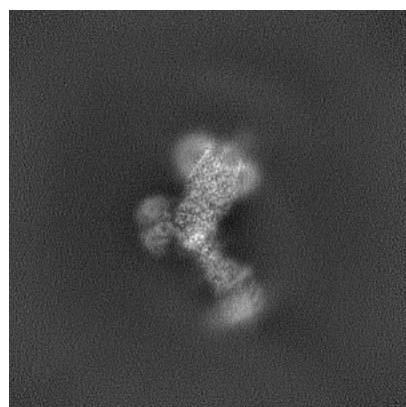


Y

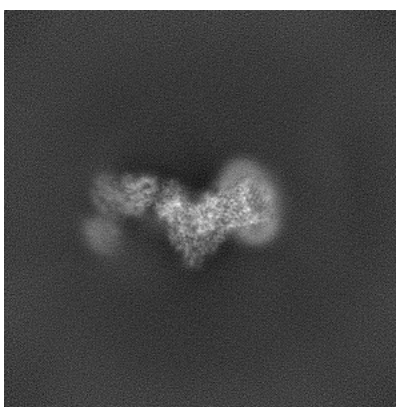


Z

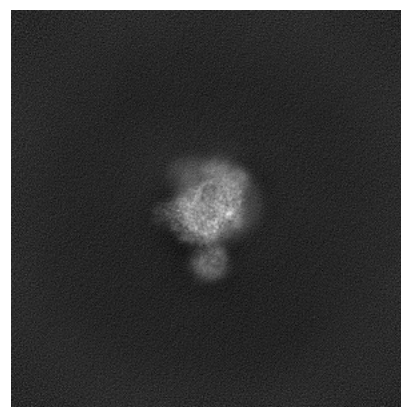
#### 6.1.2 Raw map



X



Y

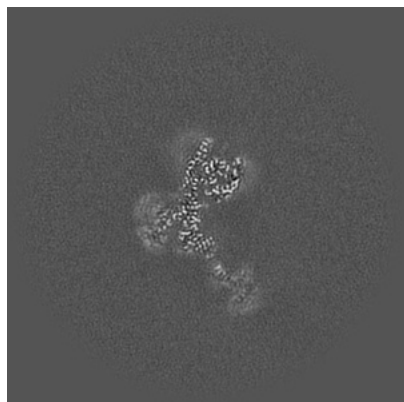


Z

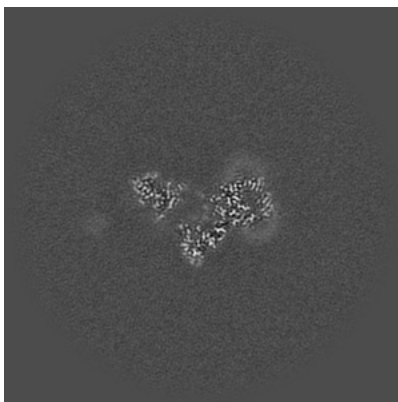
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

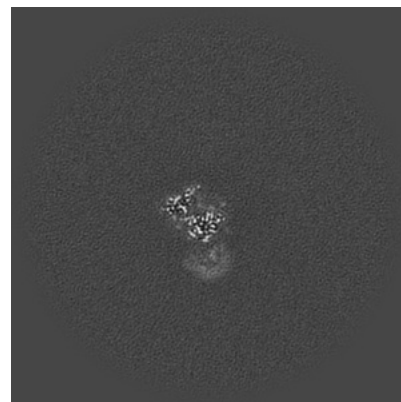
### 6.2.1 Primary map



X Index: 230

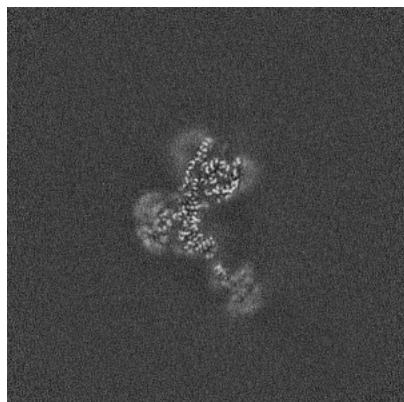


Y Index: 230

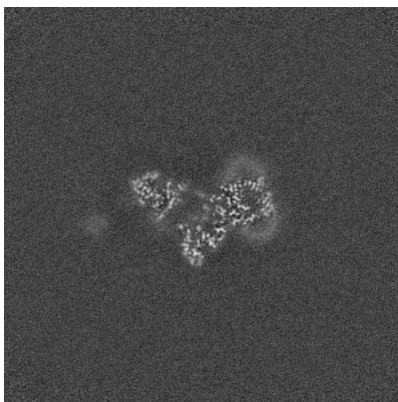


Z Index: 230

### 6.2.2 Raw map



X Index: 230



Y Index: 230

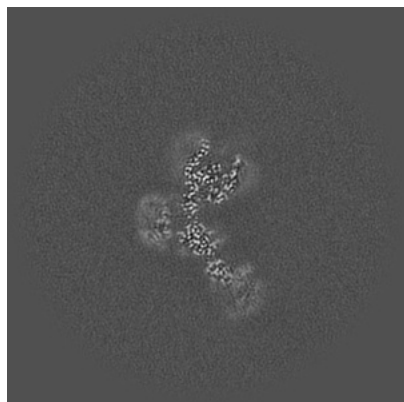


Z Index: 230

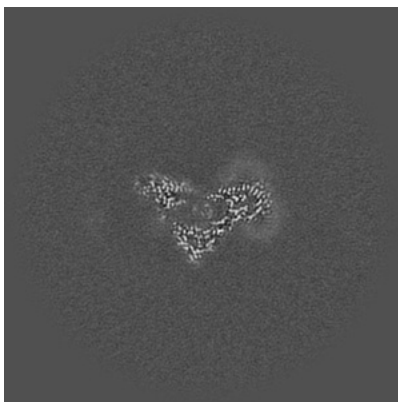
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

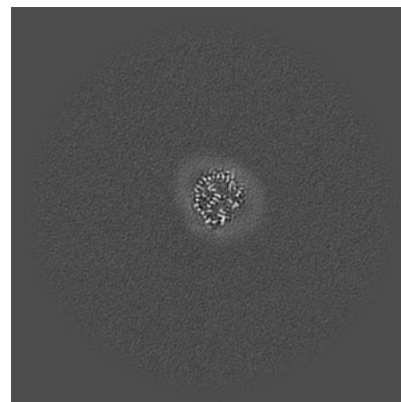
### 6.3.1 Primary map



X Index: 236

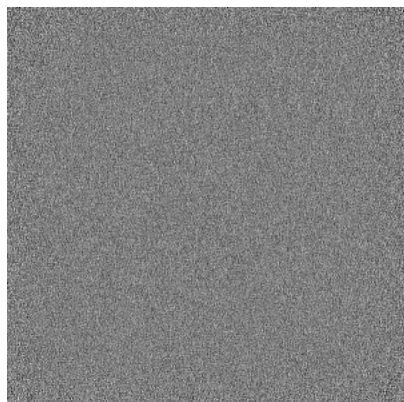


Y Index: 225

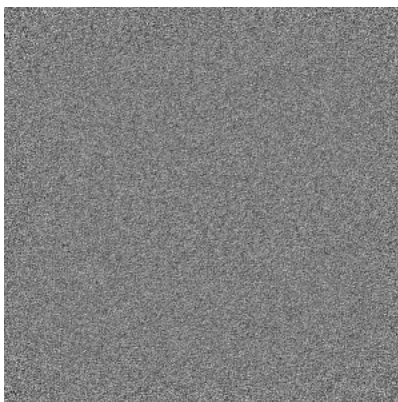


Z Index: 277

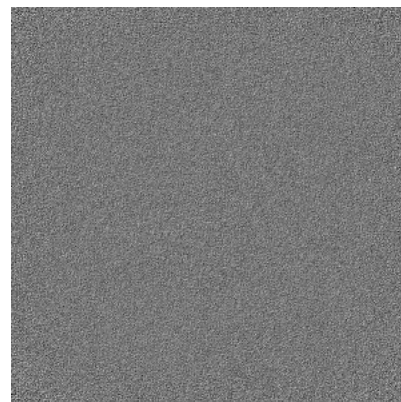
### 6.3.2 Raw map



X Index: 0



Y Index: 0



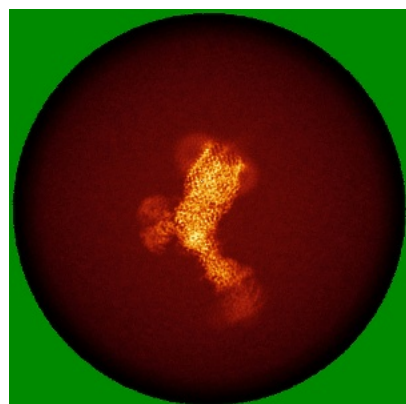
Z Index: 459

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

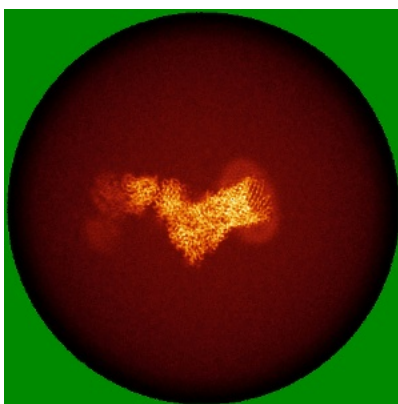


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

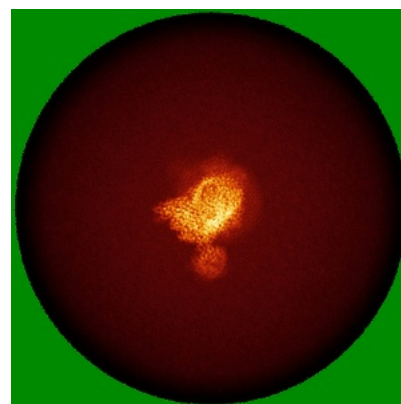
### 6.4.1 Primary map



X

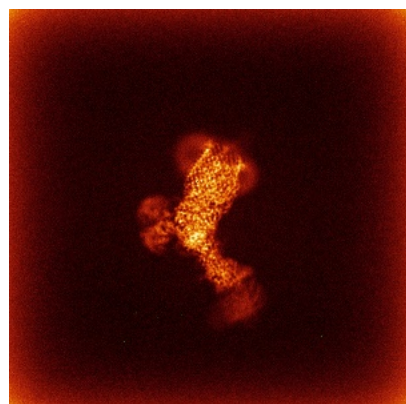


Y

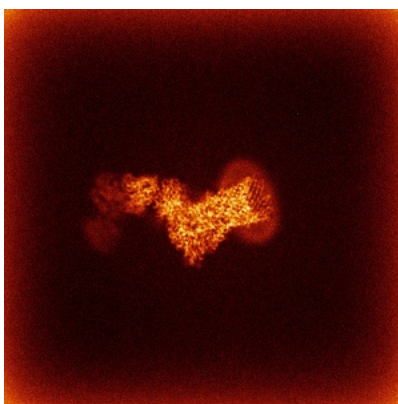


Z

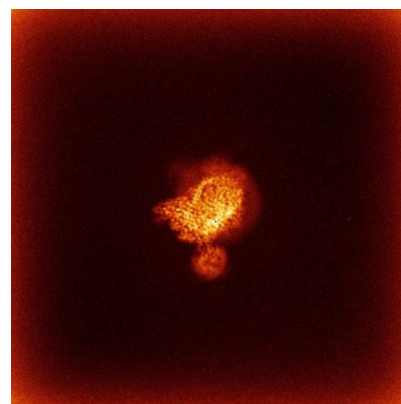
### 6.4.2 Raw map



X



Y

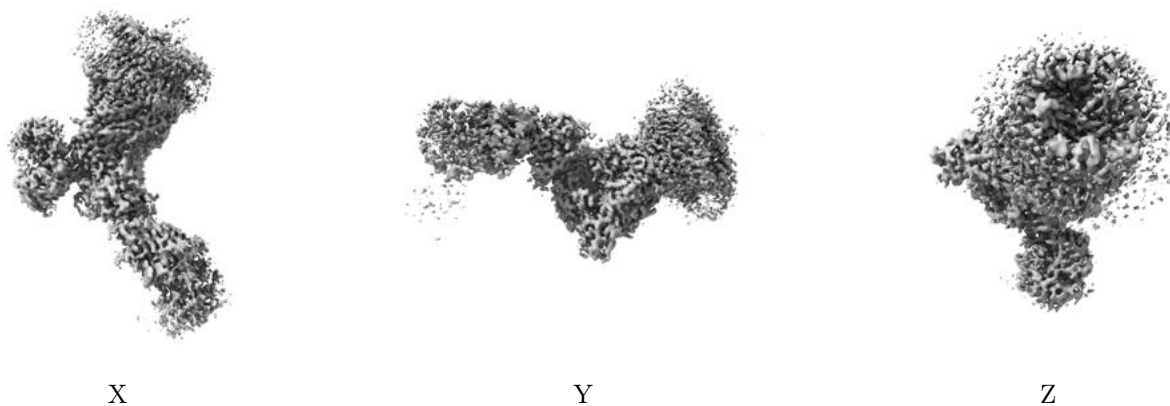


Z

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.

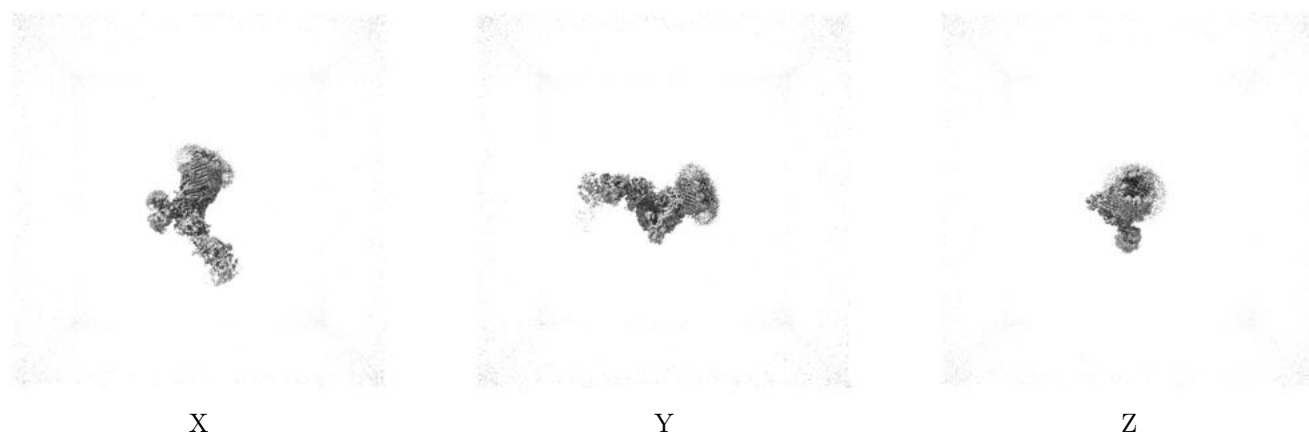
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.385. 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.

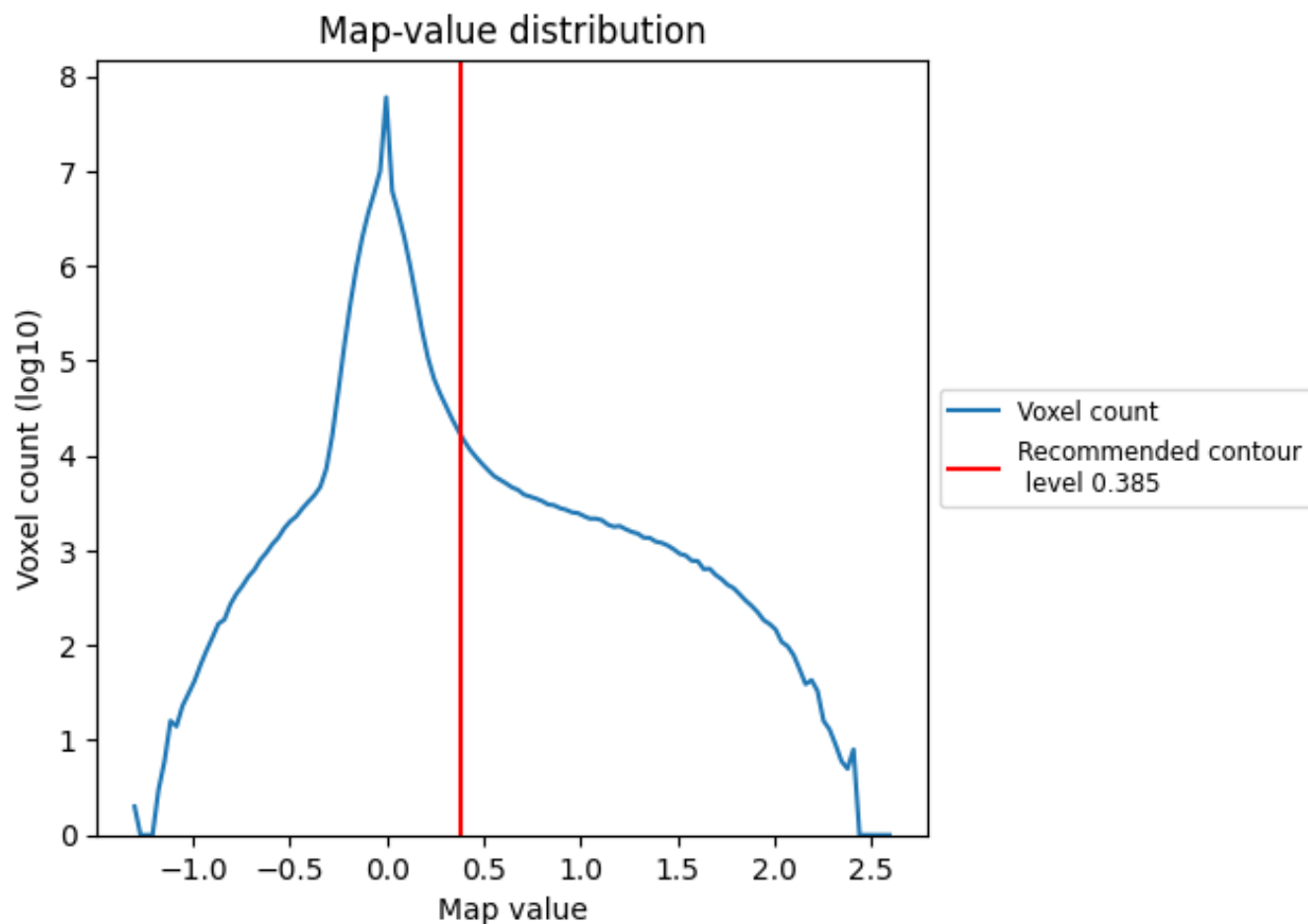
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

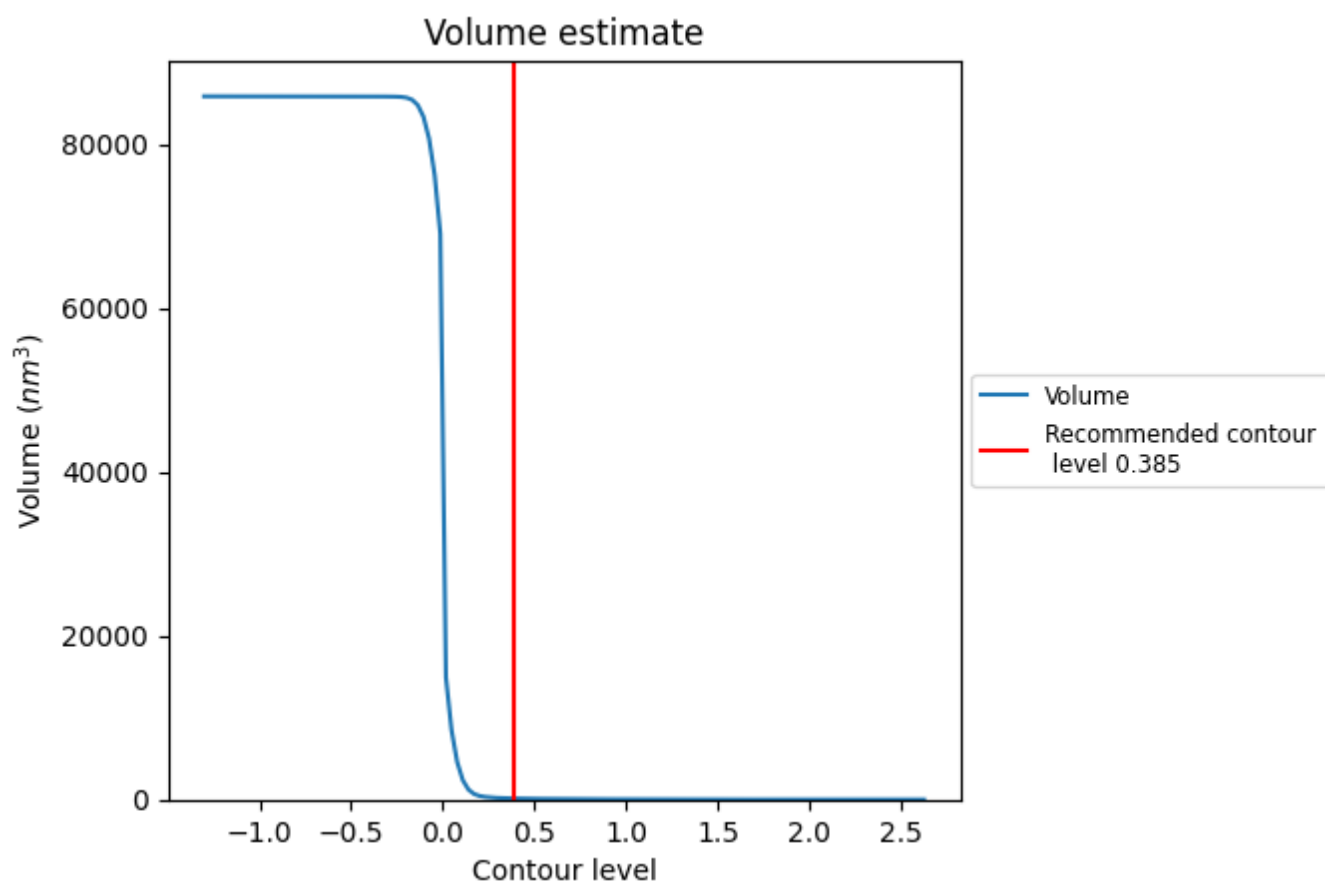
This section contains the results of statistical analysis of the map.

### 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](#)

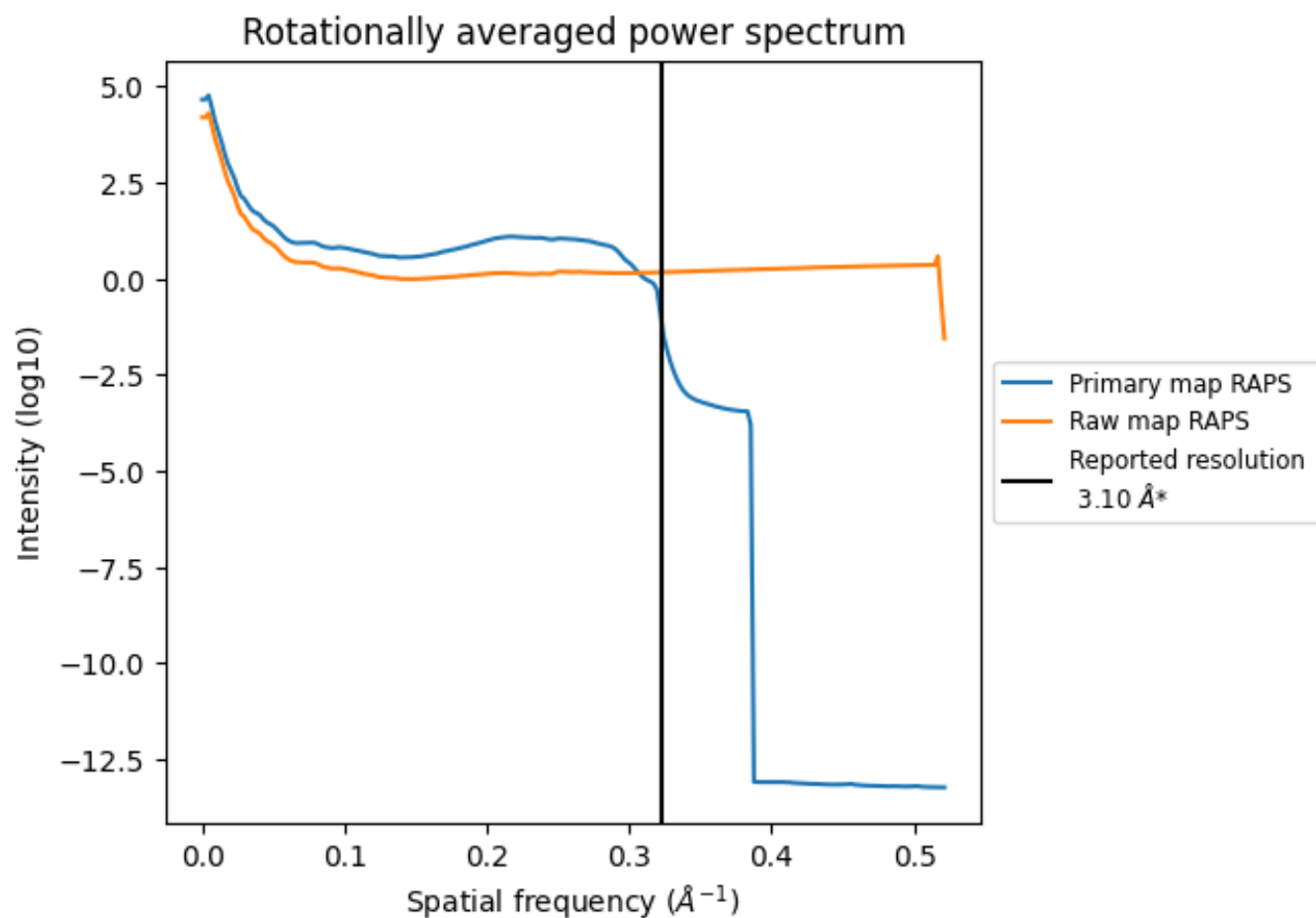


The volume at the recommended contour level is 132 nm<sup>3</sup>; this corresponds to an approximate mass of 119 kDa.

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 ⓘ

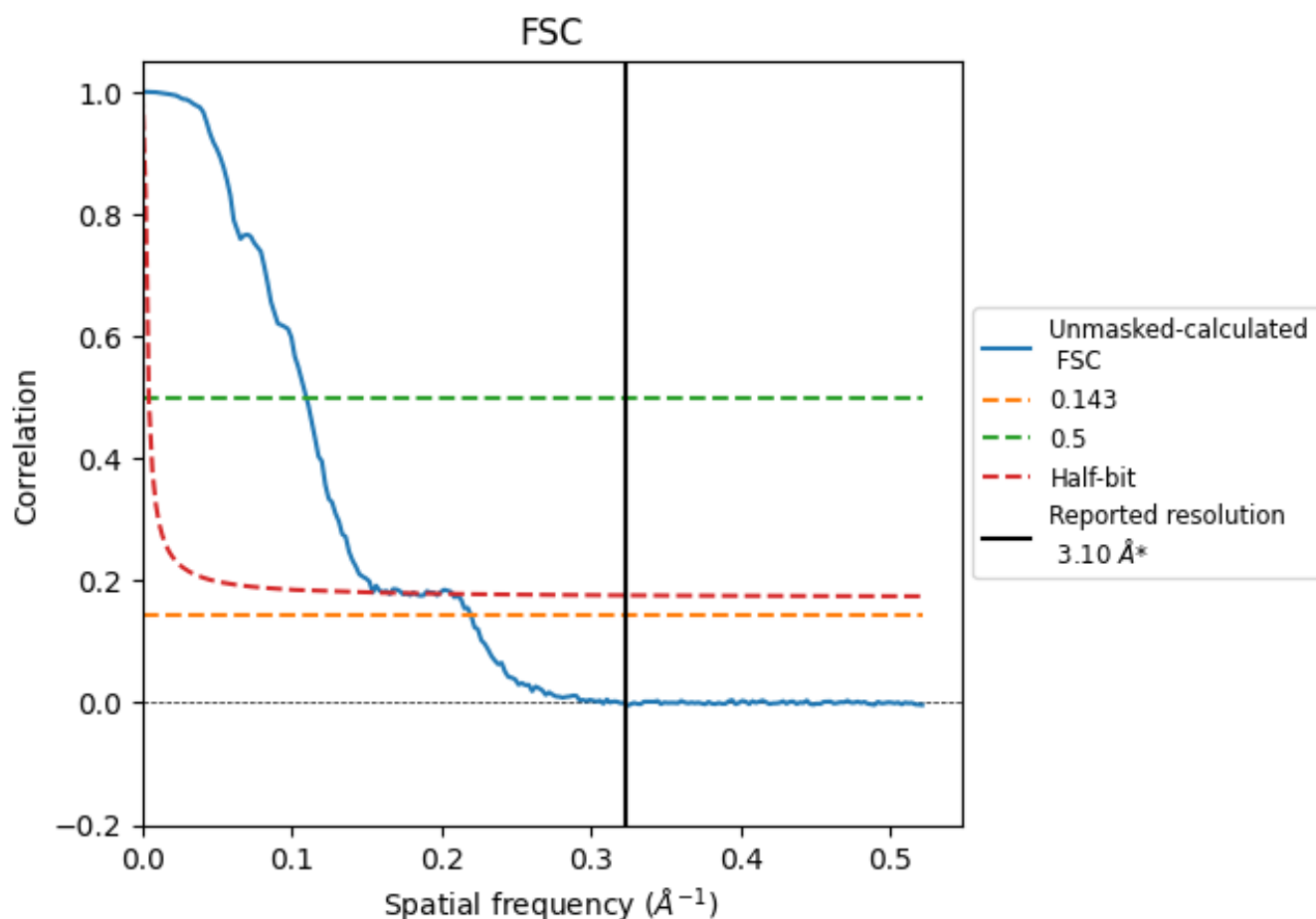


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

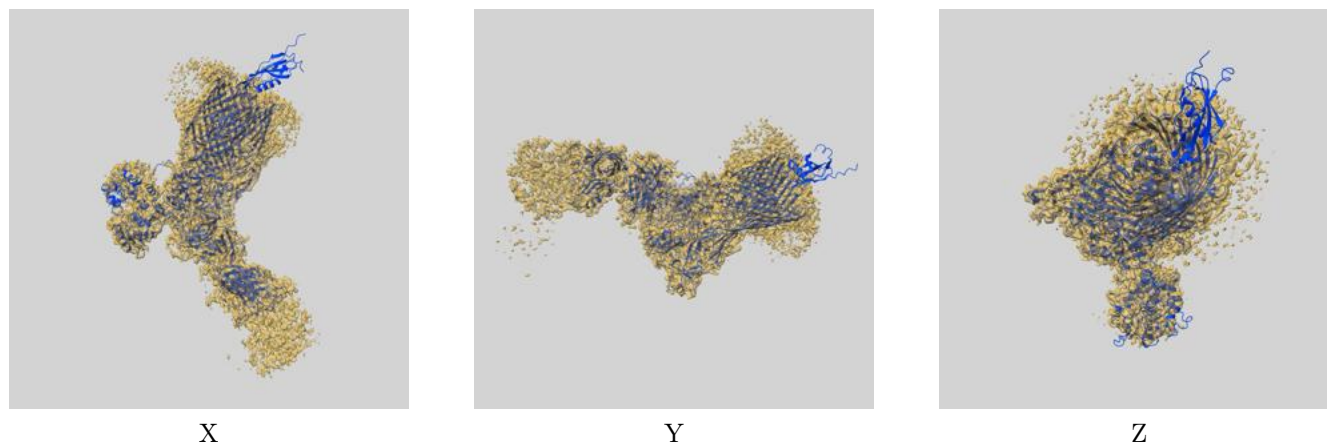
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.55	9.12	6.08

\*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 4.55 differs from the reported value 3.1 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46743 and PDB model 9DC4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



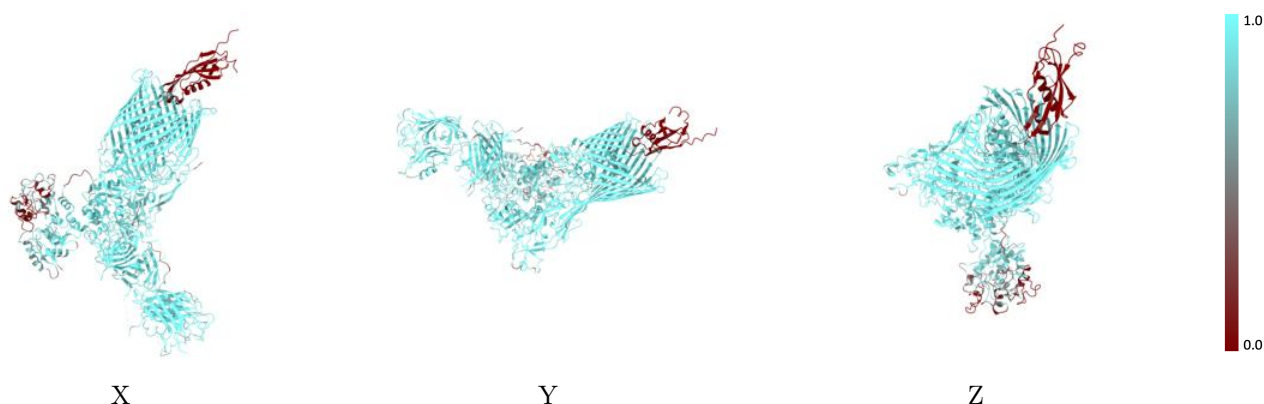
The images above show the 3D surface view of the map at the recommended contour level 0.385 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



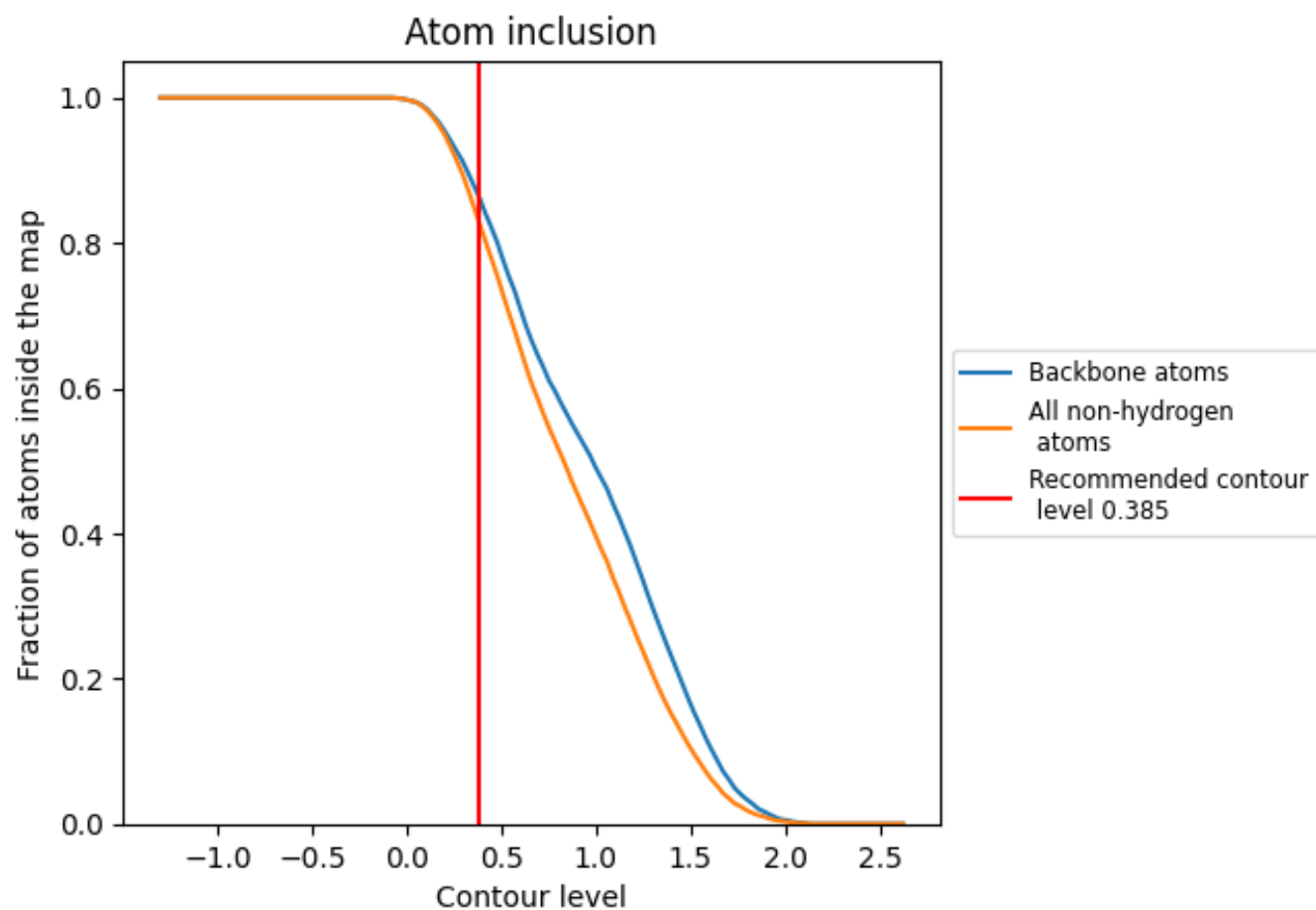
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.385).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.385) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8270	<div></div> 0.5190
A	<div></div> 0.9140	<div></div> 0.5600
B	<div></div> 0.8870	<div></div> 0.5510
F	<div></div> 0.7660	<div></div> 0.4850
T	<div></div> 0.0200	<div></div> 0.1400

