



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 02:24 AM UTC

PDB ID : 9CMG / pdb_00009cmg
EMDB ID : EMD-45747
Title : Transferrin Binding Protein A in complex with transferrin binding protein B and transferrin (iron bound in both lobes of Tf)
Authors : Dubey, S.; Noinaj, N.
Deposited on : 2024-07-15
Resolution : 3.71 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

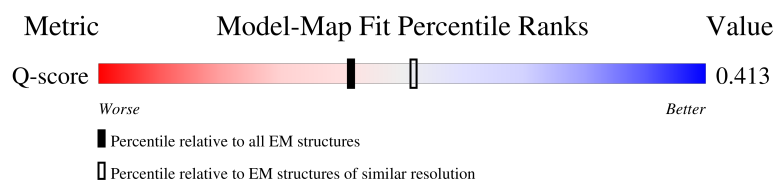
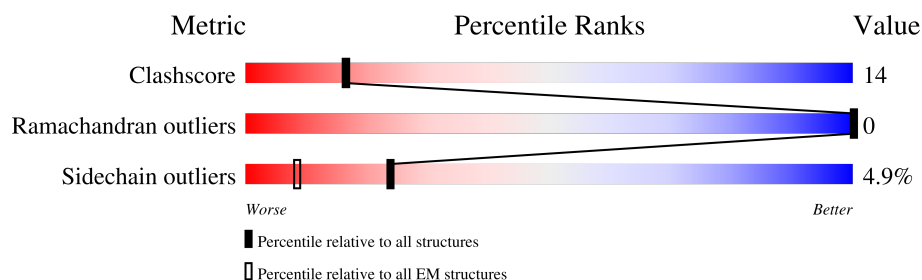
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.71 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	10534 (3.21 - 4.21)

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	915	 15% 63% 29% • 6%
2	F	698	 15% 66% 29% • •
3	B	696	 29% 56% 25% • 17%

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
4	BCT	F	702	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16460 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	859	Total	C	N	O	S	2	0
			6735	4197	1231	1291	16		

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	499	MET	VAL	conflict	UNP Q9JPJ0
A	510	MET	LEU	conflict	UNP Q9JPJ0
A	590	MET	VAL	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.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	677	Total	C	N	O	S	0	0
			5198	3268	899	984	47		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	448	VAL	ILE	conflict	UNP P02787

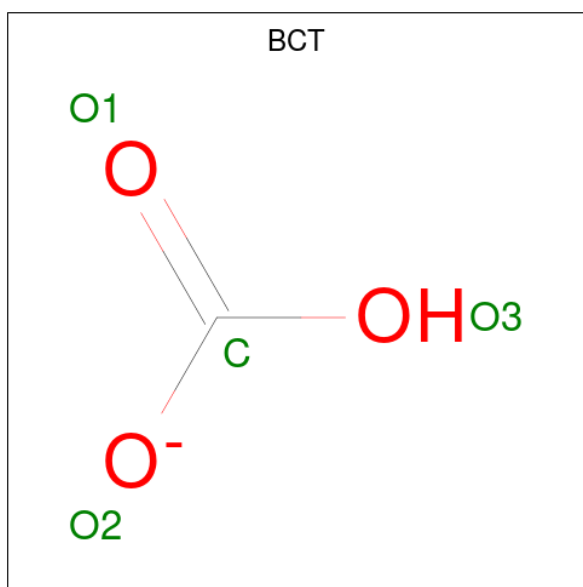
- Molecule 3 is a protein called Transferrin-binding protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	576	Total	C	N	O	S	0	0
			4517	2815	780	916	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	GLY	-	expression tag	UNP Q9JPI9
B	17	ALA	-	expression tag	UNP Q9JPI9
B	18	MET	-	expression tag	UNP Q9JPI9

- Molecule 4 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).

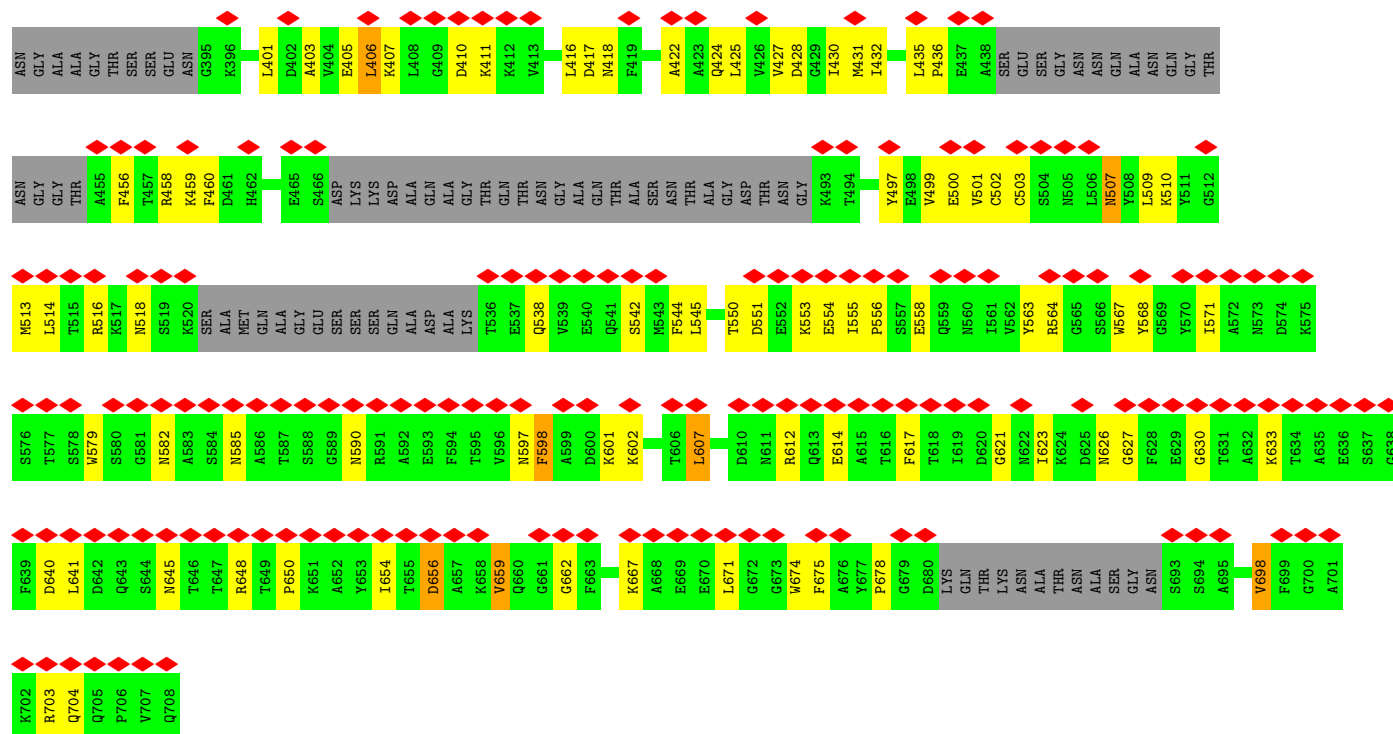


Mol	Chain	Residues	Atoms			AltConf
4	F	1	Total	C	O	0
			4	1	3	
4	F	1	Total	C	O	0
			4	1	3	

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	F	2	Total	Fe	0
			2	2	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84242	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	1.410	Depositor
Minimum map value	-0.841	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.24	Depositor
Map size (\AA)	264.0, 264.0, 264.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	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: FE, BCT

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	0.16	0/6882	0.37	0/9301
2	F	0.14	0/5317	0.34	0/7193
3	B	0.12	0/4608	0.30	0/6204
All	All	0.15	0/16807	0.35	0/22698

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6735	0	6437	192	0
2	F	5198	0	4982	146	0
3	B	4517	0	4302	135	0
4	F	8	0	2	2	0
5	F	2	0	0	0	0
All	All	16460	0	15723	453	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 14.

All (453) 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:794:GLY:HA3	1:A:809:MET:HG2	1.60	0.83
1:A:299:ARG:HB3	1:A:899:ARG:HD2	1.63	0.81
1:A:294:TYR:O	1:A:299:ARG:NH1	2.18	0.77
1:A:631:VAL:HG22	1:A:641:THR:HG22	1.67	0.76
1:A:779:GLN:HE22	1:A:835:THR:HG21	1.50	0.76
1:A:521:ASN:O	1:A:554:GLY:HA3	1.87	0.73
1:A:729:GLN:NE2	1:A:780:SER:O	2.21	0.71
1:A:832:SER:O	3:B:71:GLN:NE2	2.23	0.71
1:A:332:GLU:HG2	1:A:407:ARG:HG2	1.73	0.70
1:A:741:LYS:HE3	1:A:756:TYR:HB2	1.73	0.69
1:A:221:ILE:HB	1:A:313:LEU:HB3	1.74	0.69
3:B:459:LYS:HD3	3:B:500:GLU:HB2	1.74	0.69
1:A:91:GLN:HE22	1:A:93:ARG:HE	1.41	0.69
1:A:649:ARG:NE	1:A:673:GLU:OE2	2.26	0.68
1:A:93:ARG:HD3	1:A:399:TYR:HD2	1.59	0.67
2:F:235:ASN:HD21	2:F:237:ALA:HB3	1.59	0.67
2:F:167:LYS:HE2	2:F:167:LYS:HA	1.77	0.67
3:B:267:HIS:O	3:B:553:LYS:NZ	2.27	0.67
3:B:422:ALA:HB1	3:B:510:LYS:HG2	1.77	0.66
1:A:745:ASN:HA	1:A:747:VAL:H	1.60	0.66
2:F:627:PHE:HB3	2:F:638:PHE:HZ	1.61	0.66
2:F:282:ILE:HA	2:F:285:LEU:HD12	1.76	0.66
1:A:531:GLN:NE2	1:A:534:GLY:O	2.28	0.66
2:F:580:LEU:HG	2:F:590:VAL:HA	1.79	0.65
1:A:54:GLU:OE1	1:A:587:ARG:NH2	2.29	0.65
1:A:256:ALA:HB2	2:F:576:LYS:HG2	1.78	0.65
1:A:91:GLN:HG3	1:A:139:ALA:HB2	1.78	0.65
1:A:257:TYR:HE1	1:A:278:LYS:HE2	1.61	0.65
1:A:134:ALA:HB2	1:A:441:PHE:HB3	1.78	0.65
1:A:135:GLY:O	1:A:439:ASN:ND2	2.29	0.65
1:A:357:ASN:ND2	1:A:382:ASN:O	2.30	0.65
1:A:162:GLN:HG3	1:A:170:SER:HB2	1.79	0.65
3:B:159:HIS:ND1	3:B:177:ASP:OD1	2.30	0.65
3:B:550:THR:O	3:B:626:ASN:ND2	2.30	0.65
1:A:279:ASP:OD1	1:A:280:VAL:N	2.29	0.64
3:B:120:TYR:OH	3:B:153:SER:O	2.13	0.64
1:A:102:ARG:HD2	1:A:698:ASN:HD21	1.62	0.64
3:B:219:ILE:HG22	3:B:220:ILE:HG12	1.78	0.64
1:A:521:ASN:O	1:A:554:GLY:CA	2.45	0.64
2:F:70:ALA:HB1	2:F:75:GLU:HB2	1.79	0.64
2:F:367:SER:OG	2:F:368:HIS:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:141:LEU:HA	2:F:147:TRP:HZ3	1.62	0.63
1:A:204:THR:OG1	1:A:225:ARG:NH1	2.32	0.63
3:B:90:PRO:HG2	3:B:186:LYS:HG3	1.80	0.63
3:B:230:TYR:OH	3:B:236:ASP:OD2	2.17	0.63
3:B:503:CYS:O	3:B:510:LYS:NZ	2.32	0.63
3:B:607:LEU:HB2	3:B:617:PHE:HB2	1.80	0.63
2:F:653:ASP:OD1	2:F:653:ASP:N	2.20	0.62
2:F:128:MET:HE1	2:F:247:LEU:HA	1.80	0.62
1:A:305:LEU:HD13	1:A:340:THR:HG22	1.81	0.62
3:B:57:TYR:OH	3:B:417:ASP:OD2	2.15	0.62
3:B:564:ARG:HH21	3:B:704:GLN:HB2	1.65	0.62
1:A:705:VAL:HG21	1:A:778:ILE:HG23	1.82	0.61
1:A:105:ASP:OD2	1:A:881:ARG:NH2	2.33	0.61
1:A:577:ILE:HG22	1:A:611:SER:HB2	1.82	0.61
2:F:150:PRO:HG2	2:F:151:ILE:HD12	1.82	0.61
3:B:612:ARG:HE	3:B:614:GLU:H	1.48	0.61
2:F:99:VAL:HG23	2:F:100:VAL:HG23	1.82	0.61
3:B:57:TYR:HD2	3:B:89:LEU:HA	1.64	0.61
3:B:286:GLN:N	3:B:286:GLN:OE1	2.34	0.61
1:A:227:ALA:HB3	1:A:307:TYR:HD2	1.65	0.60
2:F:651:ARG:NH2	2:F:653:ASP:OD2	2.34	0.60
3:B:656:ASP:N	3:B:656:ASP:OD1	2.34	0.60
1:A:105:ASP:OD1	1:A:105:ASP:N	2.33	0.60
2:F:287:ASN:OD1	2:F:288:GLN:N	2.34	0.60
3:B:417:ASP:OD1	3:B:417:ASP:N	2.34	0.60
3:B:405:GLU:HB2	3:B:416:LEU:HD11	1.83	0.60
2:F:604:HIS:NE2	4:F:702:BCT:O2	2.32	0.59
1:A:199:LYS:HB3	1:A:906:ASN:HD22	1.67	0.59
1:A:821:LEU:HD21	1:A:877:TRP:HZ2	1.66	0.59
2:F:483:MET:HA	2:F:483:MET:HE3	1.84	0.59
1:A:411:GLU:OE1	1:A:427:ARG:NH1	2.31	0.59
1:A:141:ASN:HD21	1:A:405:LYS:HB2	1.68	0.59
2:F:325:PRO:HD2	2:F:328:MET:HG3	1.83	0.59
1:A:768:ASP:N	1:A:768:ASP:OD1	2.36	0.59
1:A:223:THR:HB	1:A:311:SER:HB3	1.85	0.59
2:F:295:LYS:NZ	2:F:318:ALA:O	2.36	0.59
3:B:71:GLN:OE1	3:B:71:GLN:N	2.31	0.59
3:B:297:ALA:HA	3:B:306:GLY:HA3	1.85	0.59
1:A:315:ARG:HD3	1:A:330:ILE:HD13	1.82	0.58
2:F:67:CYS:HB3	2:F:79:VAL:HG21	1.85	0.58
1:A:414:TYR:HB3	1:A:426:ALA:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:566:PRO:HG2	3:B:217:ARG:NH1	2.17	0.58
1:A:567:ASN:ND2	1:A:663:VAL:O	2.36	0.58
2:F:82:ASP:OD1	2:F:268:HIS:NE2	2.37	0.58
3:B:190:ARG:NH2	3:B:416:LEU:O	2.32	0.58
3:B:458:ARG:HE	3:B:460:PHE:HB3	1.68	0.58
1:A:829:ASN:HB2	3:B:167:LYS:HZ1	1.67	0.58
2:F:401:MET:HE1	2:F:421:CYS:HB3	1.85	0.58
1:A:93:ARG:HD3	1:A:399:TYR:CD2	2.39	0.57
1:A:442:GLN:OE1	1:A:466:TYR:OH	2.22	0.57
2:F:306:SER:HB3	2:F:312:LEU:HD11	1.87	0.57
2:F:132:ARG:O	2:F:134:LYS:NZ	2.37	0.57
3:B:516:ARG:NH2	3:B:542:SER:OG	2.37	0.57
1:A:484:PHE:HB2	1:A:499:MET:HE2	1.85	0.57
3:B:65:ARG:NH1	3:B:178:ASP:OD2	2.38	0.57
3:B:507:ASN:OD1	3:B:507:ASN:N	2.38	0.57
1:A:80:THR:HG22	1:A:80:THR:O	2.04	0.57
1:A:55:VAL:HG21	1:A:599:GLY:HA3	1.87	0.57
1:A:164:SER:HB3	1:A:650:LEU:HD12	1.86	0.57
2:F:165:LEU:HD12	2:F:168:ALA:HB3	1.87	0.57
2:F:470:HIS:HD2	2:F:504:ALA:HB2	1.69	0.57
2:F:160:GLU:HG2	2:F:161:PRO:HA	1.87	0.57
2:F:337:GLU:N	2:F:337:GLU:OE2	2.37	0.57
1:A:85:GLY:H	1:A:787:GLN:HE21	1.51	0.57
1:A:416:ASN:ND2	1:A:420:ASP:OD1	2.38	0.57
2:F:148:ASN:OD1	2:F:148:ASN:N	2.38	0.57
2:F:372:LEU:HD12	3:B:224:LYS:HB2	1.88	0.56
3:B:275:LEU:HB2	3:B:293:TYR:HB2	1.86	0.56
1:A:257:TYR:HD2	1:A:543:GLU:HA	1.69	0.56
1:A:863:ARG:NH1	1:A:912:GLU:OE2	2.38	0.56
1:A:732:ARG:HG3	1:A:767:ARG:HB3	1.88	0.56
1:A:299:ARG:HE	1:A:301:LEU:H	1.53	0.56
1:A:93:ARG:NH2	1:A:889:ASN:OD1	2.39	0.56
1:A:841:ARG:HG3	3:B:30:ASP:HB2	1.87	0.56
2:F:290:GLN:NE2	2:F:321:PHE:HB2	2.21	0.56
3:B:659:VAL:HA	3:B:675:PHE:HB3	1.88	0.55
1:A:524:TYR:HE1	1:A:549:VAL:HG22	1.71	0.55
1:A:616:VAL:HG23	1:A:657:TYR:HA	1.87	0.55
3:B:122:LYS:HD3	3:B:123:PRO:HD2	1.87	0.55
2:F:255:ASP:OD1	2:F:255:ASP:N	2.38	0.55
2:F:481:ILE:HD12	2:F:599:ALA:HB3	1.88	0.55
3:B:201:LYS:NZ	3:B:254:GLU:OE1	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:MET:HE1	2:F:333:TYR:HA	1.88	0.55
1:A:411:GLU:OE2	1:A:412:TYR:N	2.39	0.55
2:F:156:CYS:SG	2:F:351:PRO:HD2	2.47	0.55
2:F:178:ALA:HB3	2:F:189:LEU:HB3	1.88	0.55
3:B:195:SER:HA	3:B:266:PHE:HB2	1.89	0.55
3:B:627:GLY:HA2	3:B:662:GLY:HA2	1.89	0.55
3:B:431:MET:HE3	3:B:431:MET:HA	1.87	0.55
1:A:833:ARG:HD2	3:B:71:GLN:HE22	1.71	0.55
2:F:417:ILE:HG12	2:F:690:LEU:HG	1.89	0.55
1:A:671:ASP:HB3	1:A:727:ASN:ND2	2.22	0.55
3:B:54:GLN:N	3:B:54:GLN:OE1	2.40	0.55
3:B:202:GLY:O	3:B:260:SER:N	2.40	0.54
1:A:787:GLN:OE1	1:A:790:ARG:NH2	2.40	0.54
1:A:190:ILE:HG22	1:A:209:LEU:HD23	1.90	0.54
1:A:457:PRO:HG2	1:A:518:GLN:HG3	1.90	0.54
2:F:325:PRO:HG2	2:F:692:ALA:HA	1.89	0.54
2:F:147:TRP:O	2:F:152:GLY:N	2.40	0.54
2:F:456:SER:O	2:F:587:ARG:NH1	2.41	0.54
1:A:141:ASN:OD1	1:A:142:GLU:N	2.40	0.53
2:F:389:SER:O	2:F:399:LYS:NZ	2.38	0.53
3:B:202:GLY:HA3	3:B:361:ALA:HA	1.90	0.53
2:F:39:GLN:OE1	2:F:42:ARG:NH1	2.42	0.53
2:F:166:GLU:HB2	2:F:189:LEU:HD11	1.90	0.53
3:B:163:GLU:N	3:B:163:GLU:OE1	2.41	0.53
3:B:64:LYS:O	3:B:231:SER:OG	2.23	0.53
1:A:104:MET:HB3	1:A:108:ARG:HD2	1.90	0.53
2:F:23:LYS:HE3	2:F:24:THR:H	1.74	0.53
2:F:26:ARG:HB2	2:F:76:ALA:HA	1.91	0.53
2:F:394:GLU:OE2	2:F:687:SER:OG	2.27	0.53
2:F:566:PRO:HG2	3:B:217:ARG:HH12	1.74	0.53
1:A:515:TYR:CD1	1:A:561:ILE:HB	2.44	0.53
3:B:127:GLN:HB2	3:B:131:THR:HB	1.90	0.53
2:F:356:ASP:HB2	2:F:357:GLU:HG3	1.91	0.52
2:F:64:TYR:CD1	2:F:85:LEU:HD21	2.43	0.52
2:F:553:LYS:HD2	2:F:651:ARG:HH12	1.74	0.52
3:B:342:GLU:OE1	3:B:342:GLU:N	2.40	0.52
3:B:516:ARG:HH22	3:B:542:SER:H	1.57	0.52
1:A:146:GLU:OE2	1:A:225:ARG:NH2	2.42	0.52
1:A:704:ILE:HA	1:A:727:ASN:HA	1.91	0.52
3:B:102:SER:OG	3:B:106:LYS:NZ	2.42	0.52
1:A:867:TYR:HB2	1:A:906:ASN:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:TRP:CD1	2:F:151:ILE:HD13	2.45	0.52
1:A:407:ARG:NH2	1:A:431:ASP:OD2	2.35	0.52
3:B:255:GLY:O	3:B:278:ASN:ND2	2.42	0.52
3:B:597:ASN:N	3:B:602:LYS:O	2.43	0.52
3:B:645:ASN:ND2	3:B:648:ARG:O	2.43	0.52
1:A:299:ARG:NE	1:A:300:PHE:H	2.06	0.52
3:B:366:LYS:NZ	3:B:367:PRO:O	2.39	0.52
3:B:436:PRO:HB3	3:B:458:ARG:HH12	1.73	0.52
1:A:782:LEU:HD22	1:A:837:ALA:HB2	1.93	0.51
2:F:42:ARG:HG2	2:F:56:VAL:HG13	1.92	0.51
1:A:257:TYR:CD2	1:A:543:GLU:HA	2.45	0.51
1:A:263:GLU:OE1	1:A:277:LYS:NZ	2.29	0.51
3:B:500:GLU:HB3	3:B:513:MET:SD	2.50	0.51
1:A:178:ALA:HA	1:A:219:LEU:HD21	1.92	0.51
1:A:279:ASP:OD2	2:F:576:LYS:NZ	2.42	0.51
3:B:291:GLN:HE21	3:B:311:THR:HG21	1.76	0.51
1:A:489:ASP:O	1:A:492:LYS:N	2.43	0.51
1:A:702:ASP:HB3	1:A:727:ASN:HD22	1.76	0.51
1:A:807:ASN:OD1	1:A:808:GLY:N	2.44	0.51
1:A:128:LEU:HD12	2:F:625:HIS:HA	1.92	0.51
2:F:374:CYS:HB3	2:F:649:LEU:HD11	1.92	0.51
2:F:503:CYS:HB2	2:F:516:LEU:HB2	1.91	0.51
3:B:332:LEU:HA	3:B:348:PHE:HB3	1.92	0.51
1:A:68:LEU:HG	1:A:73:VAL:HG11	1.92	0.51
2:F:112:THR:OG1	2:F:696:ARG:O	2.21	0.51
2:F:291:GLU:O	2:F:297:LYS:NZ	2.43	0.51
3:B:266:PHE:HA	3:B:269:LYS:HD2	1.93	0.51
1:A:341:ARG:HD3	1:A:398:PHE:HE1	1.76	0.50
2:F:230:PHE:HA	2:F:239:ARG:HH22	1.76	0.50
2:F:662:ASP:OD1	2:F:662:ASP:N	2.43	0.50
3:B:403:ALA:HB1	3:B:416:LEU:HB2	1.94	0.50
3:B:551:ASP:HB3	3:B:554:GLU:HG2	1.93	0.50
1:A:266:ASN:N	1:A:266:ASN:OD1	2.45	0.50
1:A:515:TYR:HD1	1:A:561:ILE:HB	1.75	0.50
1:A:728:ALA:HB2	1:A:775:ARG:HD2	1.93	0.50
2:F:406:ASP:N	2:F:406:ASP:OD1	2.40	0.50
3:B:79:LEU:HD23	3:B:209:ASP:HB3	1.93	0.50
1:A:455:CYS:SG	1:A:456:ARG:N	2.84	0.50
1:A:299:ARG:HE	1:A:300:PHE:H	1.60	0.49
2:F:138:HIS:NE2	2:F:140:GLY:O	2.46	0.49
1:A:469:ASP:OD1	1:A:470:ARG:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:453:LYS:NZ	2:F:579:GLU:HB2	2.28	0.49
1:A:187:GLN:N	1:A:187:GLN:OE1	2.45	0.49
1:A:393:TYR:O	1:A:445:HIS:NE2	2.44	0.49
1:A:84:PRO:HB2	1:A:762:ASN:HB2	1.93	0.49
1:A:615:SER:OG	1:A:660:ARG:NH2	2.46	0.49
1:A:194:THR:HG22	1:A:205:GLN:OE1	2.12	0.49
1:A:359:LYS:HD2	2:F:559:GLN:HE22	1.77	0.49
1:A:663:VAL:HG12	2:F:621:ARG:HH21	1.78	0.49
3:B:407:LYS:HB3	3:B:410:ASP:HB2	1.95	0.49
3:B:401:LEU:HD11	3:B:418:ASN:HD21	1.78	0.49
2:F:36:THR:HB	2:F:37:LYS:HZ2	1.77	0.48
3:B:295:LEU:HD23	3:B:332:LEU:HD21	1.94	0.48
2:F:202:ASN:HB3	2:F:205:PHE:HB2	1.95	0.48
2:F:229:ILE:HG12	2:F:239:ARG:NH2	2.28	0.48
3:B:436:PRO:HB3	3:B:458:ARG:NH1	2.28	0.48
2:F:469:CYS:SG	2:F:547:GLY:HA3	2.53	0.48
3:B:115:ILE:HD13	3:B:158:LYS:HG3	1.96	0.48
2:F:34:GLU:HG3	2:F:313:LEU:HG	1.94	0.48
1:A:257:TYR:CE1	1:A:278:LYS:HE2	2.47	0.48
1:A:427:ARG:NH1	1:A:429:SER:OG	2.47	0.48
3:B:308:ALA:HB2	3:B:332:LEU:HD22	1.96	0.48
1:A:299:ARG:NH1	1:A:343:MET:SD	2.87	0.48
2:F:517:CYS:HB3	2:F:531:GLU:OE2	2.13	0.48
1:A:682:ILE:HG23	1:A:693:ALA:HB3	1.96	0.48
1:A:878:GLU:N	1:A:878:GLU:OE1	2.47	0.48
1:A:449:ASP:HA	1:A:450:GLY:HA3	1.50	0.48
3:B:518:ASN:H	3:B:538:GLN:NE2	2.12	0.47
1:A:85:GLY:H	1:A:787:GLN:NE2	2.13	0.47
1:A:102:ARG:HA	1:A:764:MET:HE1	1.95	0.47
1:A:143:ILE:HD13	1:A:173:PHE:CD2	2.49	0.47
2:F:323:LYS:HB3	2:F:323:LYS:HE3	1.66	0.47
2:F:439:ASP:OD1	2:F:661:HIS:NE2	2.47	0.47
2:F:568:PRO:HG2	3:B:241:TYR:CE2	2.49	0.47
1:A:421:THR:HG23	1:A:423:ALA:H	1.80	0.47
3:B:226:GLN:N	3:B:226:GLN:OE1	2.46	0.47
1:A:756:TYR:OH	1:A:807:ASN:ND2	2.48	0.47
2:F:283:TRP:CD1	2:F:323:LYS:HD3	2.50	0.47
2:F:369:HIS:ND1	2:F:529:ASN:HB3	2.29	0.47
2:F:371:ARG:O	2:F:375:ASP:HB2	2.15	0.47
3:B:54:GLN:O	3:B:424:GLN:NE2	2.47	0.47
3:B:204:TRP:NE1	3:B:258:PHE:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:435:LEU:HD12	3:B:436:PRO:HD2	1.97	0.47
1:A:833:ARG:HD2	3:B:71:GLN:NE2	2.30	0.47
2:F:376:GLU:OE2	2:F:638:PHE:HB2	2.15	0.47
3:B:113:ASN:OD1	3:B:113:ASN:N	2.48	0.47
2:F:45:MET:HE3	2:F:45:MET:HB2	1.84	0.47
1:A:755:TRP:HE3	1:A:797:TYR:HB2	1.79	0.46
1:A:384:GLU:OE2	1:A:465:TYR:OH	2.31	0.46
1:A:637:TRP:HB3	1:A:685:LYS:O	2.15	0.46
1:A:728:ALA:HA	1:A:772:ARG:HD3	1.97	0.46
2:F:418:ALA:HB1	2:F:423:LEU:HB2	1.98	0.46
1:A:638:LEU:HD22	1:A:684:PHE:HE2	1.80	0.46
2:F:278:LYS:HB3	2:F:281:LEU:HD13	1.97	0.46
3:B:558:GLU:OE2	3:B:703:ARG:NH2	2.42	0.46
1:A:196:TYR:HD1	1:A:203:LEU:HD13	1.80	0.46
3:B:571:ILE:HD12	3:B:579:TRP:CD1	2.51	0.46
1:A:76:ILE:HG22	1:A:88:VAL:HG11	1.98	0.46
1:A:218:ALA:HA	1:A:315:ARG:O	2.16	0.46
2:F:627:PHE:HB3	2:F:638:PHE:CZ	2.47	0.46
1:A:86:ILE:HG23	1:A:101:ILE:HG12	1.97	0.46
1:A:207:ILE:HD13	1:A:207:ILE:HA	1.85	0.46
1:A:141:ASN:ND2	1:A:405:LYS:HB2	2.31	0.46
1:A:575:ARG:HD3	1:A:657:TYR:CE1	2.51	0.46
1:A:833:ARG:HA	3:B:71:GLN:HE21	1.81	0.46
2:F:44:HIS:ND1	2:F:300:GLU:OE2	2.49	0.46
2:F:141:LEU:HA	2:F:147:TRP:CZ3	2.46	0.46
2:F:553:LYS:HE2	2:F:555:GLN:HG3	1.97	0.46
3:B:65:ARG:NH2	3:B:163:GLU:OE2	2.49	0.45
1:A:532:ASN:HA	1:A:533:ASN:HA	1.65	0.45
1:A:659:TRP:CH2	2:F:626:LEU:HB2	2.50	0.45
1:A:697:ASN:OD1	1:A:732:ARG:NH2	2.48	0.45
1:A:831:ASN:OD1	1:A:832:SER:N	2.50	0.45
1:A:870:MET:N	1:A:870:MET:SD	2.90	0.45
2:F:23:LYS:HE3	2:F:23:LYS:HB3	1.73	0.45
2:F:33:HIS:O	2:F:37:LYS:NZ	2.48	0.45
2:F:86:VAL:O	2:F:90:TYR:N	2.48	0.45
3:B:425:LEU:O	3:B:432:ILE:HG12	2.17	0.45
1:A:779:GLN:NE2	1:A:835:THR:HG21	2.26	0.45
1:A:250:GLU:OE2	1:A:278:LYS:HG3	2.17	0.45
3:B:502:CYS:HA	3:B:503:CYS:HA	1.65	0.45
2:F:312:LEU:HD23	2:F:312:LEU:H	1.81	0.45
2:F:356:ASP:HA	2:F:357:GLU:HA	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:505:PRO:HB2	2:F:527:PRO:HA	1.98	0.45
3:B:237:ASP:OD1	3:B:237:ASP:N	2.49	0.45
1:A:125:GLN:NE2	1:A:660:ARG:O	2.38	0.45
1:A:868:ASN:ND2	1:A:870:MET:O	2.50	0.45
3:B:633:LYS:HA	3:B:654:ILE:HG22	1.99	0.45
2:F:555:GLN:C	2:F:558:PRO:HD2	2.41	0.44
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.74	0.44
1:A:892:LYS:HA	1:A:893:ASN:HA	1.61	0.44
2:F:413:GLY:N	2:F:476:THR:OG1	2.41	0.44
2:F:477:ALA:N	4:F:702:BCT:O3	2.39	0.44
3:B:563:TYR:C	3:B:564:ARG:HD3	2.42	0.44
1:A:588:ASP:OD2	1:A:588:ASP:C	2.61	0.44
1:A:726:LEU:HD12	1:A:775:ARG:HD3	1.99	0.44
3:B:111:SER:OG	3:B:112:ASP:OD1	2.35	0.44
1:A:547:TYR:CZ	2:F:589:PRO:HB3	2.53	0.44
2:F:585:GLY:N	2:F:586:THR:HA	2.31	0.44
3:B:269:LYS:HE2	3:B:299:VAL:HB	2.00	0.44
1:A:214:GLY:HA3	1:A:215:GLY:HA3	1.56	0.44
3:B:177:ASP:HB2	3:B:230:TYR:CE2	2.52	0.44
3:B:621:GLY:HA2	3:B:630:GLY:HA3	1.98	0.44
1:A:303:ASP:OD1	1:A:303:ASP:N	2.48	0.44
1:A:398:PHE:HZ	1:A:451:SER:HB2	1.82	0.44
2:F:104:TYR:OH	2:F:315:LYS:HE3	2.18	0.44
2:F:104:TYR:HD2	2:F:318:ALA:HA	1.82	0.44
3:B:65:ARG:HA	3:B:230:TYR:HA	1.98	0.44
3:B:514:LEU:O	3:B:516:ARG:NH1	2.50	0.44
3:B:601:LYS:HB3	3:B:623:ILE:HB	2.00	0.44
1:A:449:ASP:OD2	1:A:451:SER:OG	2.21	0.44
1:A:755:TRP:HB2	1:A:796:GLY:O	2.18	0.44
3:B:406:LEU:HD21	3:B:674:TRP:CD1	2.53	0.44
2:F:37:LYS:O	2:F:41:PHE:N	2.43	0.43
2:F:104:TYR:CD1	2:F:114:TYR:HB3	2.53	0.43
2:F:138:HIS:CG	2:F:139:THR:N	2.86	0.43
2:F:178:ALA:N	2:F:189:LEU:O	2.47	0.43
3:B:640:ASP:OD1	3:B:640:ASP:N	2.51	0.43
1:A:828:LEU:HA	1:A:829:ASN:HA	1.69	0.43
2:F:470:HIS:CD2	2:F:504:ALA:HB2	2.51	0.43
3:B:148:PHE:CE1	3:B:362:LYS:HB3	2.53	0.43
3:B:516:ARG:HH22	3:B:542:SER:N	2.16	0.43
3:B:497:TYR:CE1	3:B:516:ARG:HG2	2.53	0.43
1:A:833:ARG:HA	3:B:71:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:459:LYS:NZ	3:B:460:PHE:O	2.46	0.43
3:B:641:LEU:HB2	3:B:650:PRO:HB2	2.01	0.43
1:A:381:THR:OG1	1:A:382:ASN:N	2.51	0.43
1:A:439:ASN:OD1	1:A:440:HIS:N	2.51	0.43
1:A:624:LEU:HD12	1:A:625:SER:N	2.34	0.43
2:F:127:GLN:HG2	2:F:249:ASN:C	2.43	0.43
1:A:713:LYS:HD2	1:A:713:LYS:HA	1.71	0.43
2:F:388:VAL:HG21	2:F:405:ALA:HB2	2.00	0.43
2:F:436:ASN:O	2:F:440:THR:OG1	2.37	0.43
1:A:315:ARG:NH1	1:A:330:ILE:HD11	2.34	0.42
1:A:815:ALA:HB2	1:A:844:PRO:HD3	2.01	0.42
2:F:286:LEU:O	2:F:290:GLN:HG3	2.19	0.42
2:F:325:PRO:O	2:F:328:MET:HB2	2.19	0.42
2:F:459:THR:OG1	2:F:462:ASN:OD1	2.36	0.42
3:B:216:PHE:CZ	3:B:324:PRO:HB3	2.54	0.42
1:A:82:TYR:CD2	1:A:809:MET:HE1	2.54	0.42
1:A:727:ASN:OD1	1:A:727:ASN:N	2.49	0.42
3:B:61:MET:HE3	3:B:61:MET:HB2	1.91	0.42
2:F:100:VAL:HB	2:F:270:VAL:HG22	2.02	0.42
2:F:273:ARG:NH2	2:F:276:GLY:O	2.52	0.42
2:F:626:LEU:HD23	2:F:627:PHE:CD2	2.53	0.42
1:A:78:ASP:OD1	1:A:199:LYS:NZ	2.50	0.42
1:A:269:TYR:HB2	1:A:548:TRP:CZ3	2.54	0.42
1:A:634:PRO:O	1:A:635:THR:HG22	2.20	0.42
1:A:778:ILE:HD12	1:A:778:ILE:N	2.34	0.42
2:F:138:HIS:HB3	2:F:178:ALA:HA	2.02	0.42
2:F:177:CYS:HB2	2:F:192:LEU:HB2	2.00	0.42
3:B:264:VAL:HG13	3:B:271:LEU:HD12	2.01	0.42
1:A:478:ARG:O	1:A:504:ASP:HA	2.19	0.42
2:F:103:PHE:HD2	2:F:322:LEU:HG	1.84	0.42
2:F:148:ASN:ND2	2:F:342:ILE:HD11	2.34	0.42
3:B:119:PRO:HB3	3:B:138:PRO:HG2	2.00	0.42
1:A:102:ARG:HD2	1:A:698:ASN:ND2	2.33	0.42
1:A:695:TRP:HE1	1:A:736:ILE:HD12	1.84	0.42
2:F:368:HIS:NE2	2:F:372:LEU:HD21	2.34	0.42
1:A:268:SER:O	1:A:271:THR:HG22	2.20	0.42
1:A:688:PHE:O	1:A:743:ASP:N	2.53	0.42
2:F:399:LYS:HG2	2:F:404:GLU:HB3	2.01	0.42
3:B:74:GLU:OE1	3:B:74:GLU:N	2.53	0.42
3:B:344:LEU:HD21	3:B:361:ALA:HB3	2.00	0.42
1:A:122:TYR:HE1	1:A:510:MET:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:MET:SD	1:A:786:ILE:HD11	2.59	0.42
2:F:28:CYS:HB2	2:F:79:VAL:HG22	2.00	0.42
2:F:306:SER:HB3	2:F:312:LEU:HD21	2.01	0.42
3:B:354:LYS:HG3	3:B:355:VAL:HG23	2.02	0.42
3:B:427:VAL:HG12	3:B:428:ASP:OD1	2.19	0.42
1:A:836:LYS:HD3	1:A:836:LYS:HA	1.83	0.42
2:F:131:LEU:HB2	2:F:172:PHE:CE2	2.54	0.42
2:F:401:MET:CE	2:F:421:CYS:HB3	2.47	0.42
3:B:568:TYR:HD1	3:B:582:ASN:HA	1.85	0.42
3:B:568:TYR:HB2	3:B:698:VAL:HG13	2.01	0.42
1:A:425:TYR:HB3	1:A:485:LYS:HG3	2.02	0.42
1:A:729:GLN:HE22	1:A:780:SER:C	2.23	0.42
2:F:481:ILE:HB	2:F:482:PRO:HD3	2.01	0.42
3:B:411:LYS:HD3	3:B:678:PRO:HD2	2.02	0.42
1:A:539:PRO:HB2	1:A:547:TYR:HD1	1.85	0.41
1:A:648:PHE:HB3	1:A:674:LYS:HD3	2.01	0.41
1:A:776:THR:C	1:A:778:ILE:HD12	2.45	0.41
2:F:375:ASP:O	2:F:378:SER:OG	2.33	0.41
3:B:204:TRP:CD1	3:B:275:LEU:HD22	2.55	0.41
1:A:397:VAL:HG13	1:A:441:PHE:CE1	2.54	0.41
2:F:81:LEU:HD12	2:F:85:LEU:HB3	2.01	0.41
1:A:808:GLY:HA2	1:A:849:ASP:O	2.20	0.41
2:F:65:LEU:O	2:F:69:ARG:HG2	2.20	0.41
2:F:138:HIS:CG	2:F:139:THR:H	2.38	0.41
2:F:397:ILE:O	2:F:401:MET:HG2	2.21	0.41
2:F:400:ILE:CD1	2:F:408:MET:HG2	2.50	0.41
2:F:663:ARG:HG2	2:F:668:LYS:HB3	2.03	0.41
3:B:206:PHE:HB3	3:B:357:VAL:HG22	2.03	0.41
3:B:208:THR:HG22	3:B:355:VAL:HG22	2.01	0.41
1:A:785:ALA:HA	1:A:881:ARG:NH1	2.35	0.41
2:F:144:SER:HB3	2:F:265:VAL:HG11	2.02	0.41
2:F:163:LYS:HA	2:F:164:PRO:HA	1.90	0.41
2:F:299:LYS:HD2	2:F:299:LYS:HA	1.84	0.41
3:B:209:ASP:OD1	3:B:354:LYS:HD3	2.21	0.41
3:B:556:PRO:HD2	3:B:598:PHE:CE2	2.56	0.41
1:A:89:VAL:HG13	1:A:97:SER:HB2	2.02	0.41
1:A:527:ASN:OD1	1:A:527:ASN:N	2.53	0.41
1:A:562:CYS:HB2	1:A:572:CYS:HB3	1.44	0.41
1:A:894:VAL:HA	1:A:895:GLY:HA3	1.67	0.41
3:B:497:TYR:HE1	3:B:516:ARG:HG2	1.84	0.41
3:B:555:ILE:HG23	3:B:598:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.89	0.41
1:A:225:ARG:HB2	1:A:309:SER:HB3	2.03	0.41
1:A:705:VAL:HG21	1:A:778:ILE:CG2	2.47	0.41
1:A:812:TYR:HD1	1:A:846:TYR:HB3	1.85	0.41
2:F:224:VAL:HG22	2:F:228:THR:HG21	2.03	0.41
2:F:36:THR:HB	2:F:37:LYS:NZ	2.36	0.41
3:B:221:GLN:O	3:B:226:GLN:NE2	2.54	0.41
3:B:354:LYS:HB2	3:B:354:LYS:HE2	1.83	0.41
1:A:710:ALA:HA	1:A:719:ALA:HA	2.02	0.41
1:A:330:ILE:HD13	1:A:330:ILE:HA	1.83	0.41
1:A:420:ASP:OD1	1:A:420:ASP:N	2.54	0.41
1:A:575:ARG:HD3	1:A:657:TYR:CZ	2.56	0.41
1:A:732:ARG:HE	1:A:767:ARG:HD2	1.85	0.41
3:B:57:TYR:CD2	3:B:89:LEU:HA	2.49	0.41
3:B:509:LEU:O	3:B:510:LYS:HD2	2.21	0.41
1:A:440:HIS:HE2	1:A:442:GLN:CD	2.30	0.41
1:A:896:VAL:O	1:A:899:ARG:HG2	2.21	0.41
2:F:268:HIS:ND1	2:F:315:LYS:HD3	2.35	0.41
3:B:456:PHE:CE1	3:B:585:ASN:HB3	2.57	0.41
1:A:389:VAL:HB	1:A:445:HIS:CE1	2.56	0.40
1:A:651:PRO:HG2	1:A:670:ILE:CG2	2.51	0.40
3:B:401:LEU:HD11	3:B:418:ASN:ND2	2.36	0.40
3:B:407:LYS:NZ	3:B:542:SER:OG	2.42	0.40
3:B:226:GLN:HG3	3:B:230:TYR:CE1	2.56	0.40
1:A:267:GLY:HA3	1:A:271:THR:HG21	2.03	0.40
1:A:829:ASN:HB2	3:B:167:LYS:NZ	2.36	0.40
1:A:860:PHE:N	1:A:860:PHE:CD1	2.88	0.40
2:F:200:THR:HA	2:F:205:PHE:CD2	2.56	0.40
2:F:690:LEU:HD23	2:F:690:LEU:HA	1.77	0.40
2:F:315:LYS:HB2	2:F:315:LYS:HE2	1.83	0.40
2:F:415:VAL:O	2:F:419:GLY:N	2.41	0.40
2:F:646:LYS:C	2:F:647:ASP:OD1	2.65	0.40
3:B:73:LYS:H	3:B:73:LYS:HG2	1.55	0.40
3:B:405:GLU:HB3	3:B:416:LEU:HD21	2.03	0.40
3:B:501:VAL:HG12	3:B:544:PHE:HZ	1.87	0.40
3:B:563:TYR:CE2	3:B:703:ARG:HB2	2.56	0.40
3:B:563:TYR:CZ	3:B:703:ARG:HB2	2.57	0.40
2:F:155:TYR:HA	2:F:165:LEU:HD21	2.04	0.40
2:F:520:SER:OG	3:B:245:ASN:ND2	2.44	0.40
2:F:576:LYS:HD3	2:F:576:LYS:HA	1.92	0.40
3:B:362:LYS:NZ	3:B:363:THR:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:567:TRP:NE1	3:B:590:ASN:HB3	2.36	0.40
3:B:667:LYS:HA	3:B:667:LYS:HD2	1.75	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	855/915 (93%)	806 (94%)	49 (6%)	0	100	100
2	F	675/698 (97%)	624 (92%)	51 (8%)	0	100	100
3	B	562/696 (81%)	531 (94%)	31 (6%)	0	100	100
All	All	2092/2309 (91%)	1961 (94%)	131 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	690/750 (92%)	656 (95%)	34 (5%)	22	48
2	F	555/585 (95%)	524 (94%)	31 (6%)	19	45
3	B	483/564 (86%)	463 (96%)	20 (4%)	27	52
All	All	1728/1899 (91%)	1643 (95%)	85 (5%)	24	48

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	54	GLU
1	A	56	THR
1	A	73	VAL
1	A	107	ASN
1	A	151	VAL
1	A	207	ILE
1	A	280	VAL
1	A	295	THR
1	A	299	ARG
1	A	320	PHE
1	A	420	ASP
1	A	449	ASP
1	A	537	ILE
1	A	549	VAL
1	A	551	ILE
1	A	607[A]	ARG
1	A	607[B]	ARG
1	A	608	SER
1	A	656	MET
1	A	675	SER
1	A	682	ILE
1	A	718	GLU
1	A	755	TRP
1	A	792	VAL
1	A	798	ASP
1	A	811	THR
1	A	838	THR
1	A	847	ILE
1	A	866	VAL
1	A	875	VAL
1	A	876	THR
1	A	888	VAL
1	A	912	GLU
2	F	23	LYS
2	F	45	MET
2	F	59	VAL
2	F	60	LYS
2	F	94	ASN
2	F	119	VAL
2	F	148	ASN
2	F	223	PHE

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Mol	Chain	Res	Type
2	F	345	LEU
2	F	349	THR
2	F	355	THR
2	F	396	CYS
2	F	406	ASP
2	F	448	VAL
2	F	450	VAL
2	F	462	ASN
2	F	513	LEU
2	F	553	LYS
2	F	556	THR
2	F	592	GLU
2	F	623	GLN
2	F	625	HIS
2	F	626	LEU
2	F	629	SER
2	F	638	PHE
2	F	648	LEU
2	F	653	ASP
2	F	656	CYS
2	F	662	ASP
2	F	684	CYS
2	F	690	LEU
3	B	69	TYR
3	B	76	GLU
3	B	109	THR
3	B	113	ASN
3	B	181	ILE
3	B	183	TYR
3	B	250	THR
3	B	300	THR
3	B	349	LEU
3	B	406	LEU
3	B	430	ILE
3	B	499	VAL
3	B	507	ASN
3	B	545	LEU
3	B	598	PHE
3	B	607	LEU
3	B	656	ASP
3	B	659	VAL
3	B	671	LEU

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Mol	Chain	Res	Type
3	B	698	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	416	ASN
1	A	433	GLN
1	A	442	GLN
1	A	518	GLN
1	A	532	ASN
1	A	621	HIS
1	A	690	ASN
1	A	779	GLN
2	F	235	ASN
2	F	241	GLN
2	F	288	GLN
2	F	290	GLN
2	F	302	GLN
2	F	344	ASN
2	F	529	ASN
2	F	560	ASN
2	F	565	ASN
2	F	617	HIS
3	B	191	GLN
3	B	414	GLN
3	B	421	ASN
3	B	424	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BCT	F	701	5	3,3,3	0.81	0	2,3,3	3.30	2 (100%)
4	BCT	F	702	5	3,3,3	0.81	0	2,3,3	3.03	2 (100%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	701	BCT	O2-C-O1	3.98	129.86	119.68
4	F	702	BCT	O2-C-O1	3.68	129.08	119.68
4	F	701	BCT	O3-C-O1	-2.43	113.47	119.68
4	F	702	BCT	O3-C-O1	-2.21	114.01	119.68

There are no chirality outliers.

There are no torsion outliers.

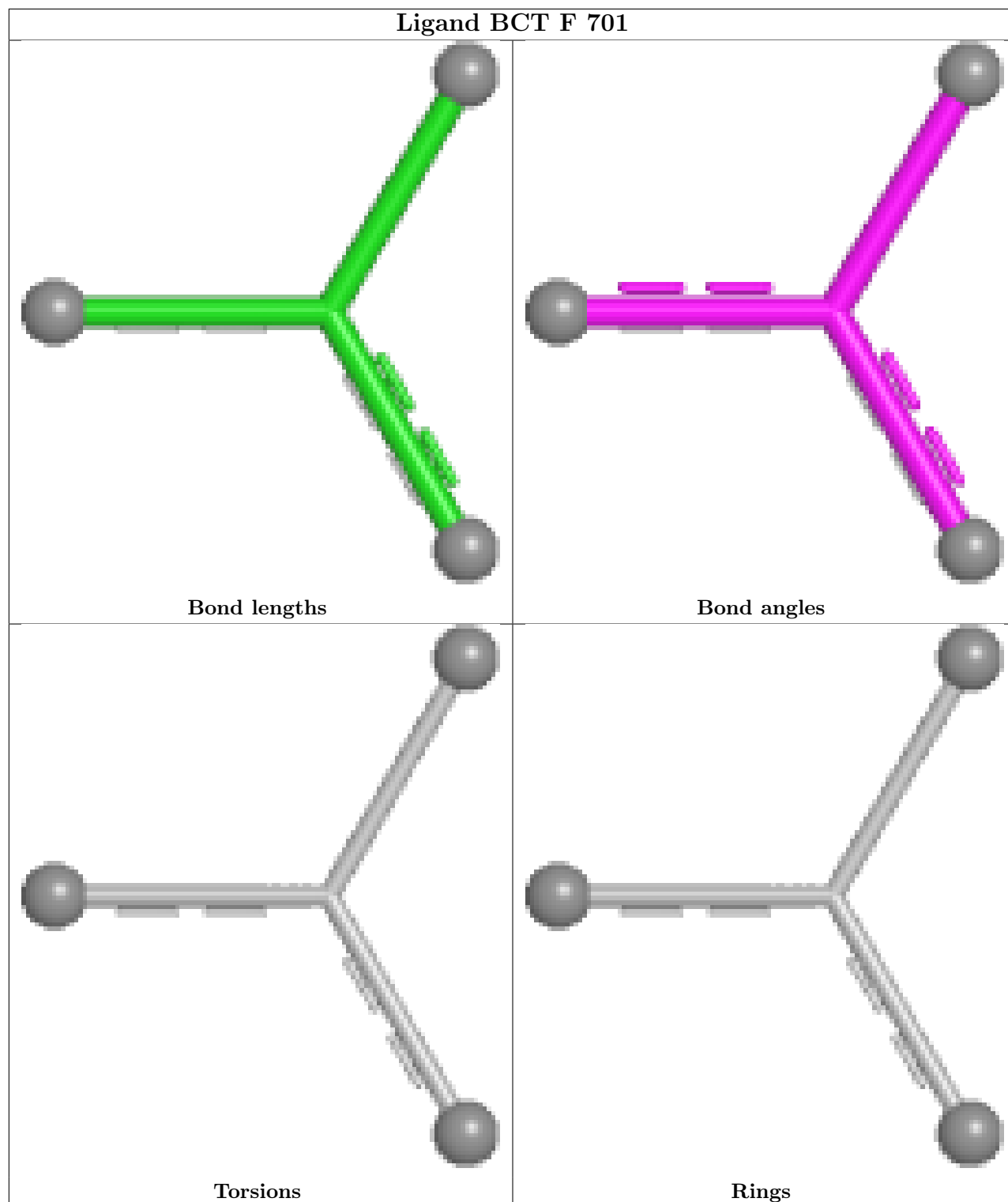
There are no ring outliers.

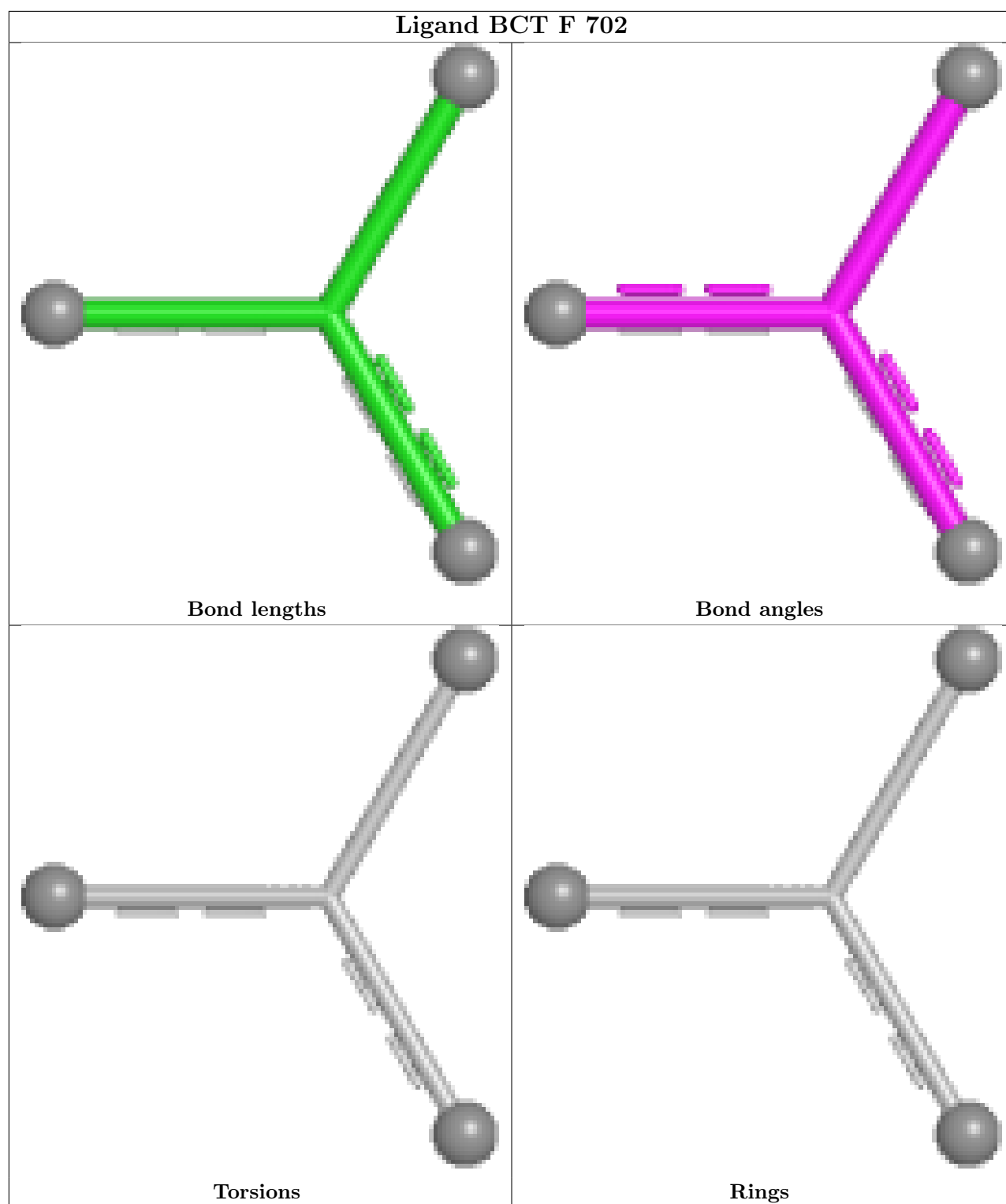
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	702	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.

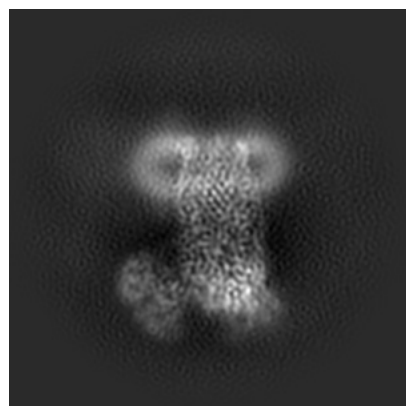
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45747. These allow visual inspection of the internal detail of the map and identification of artifacts.

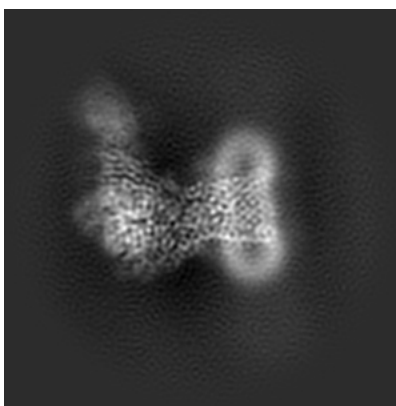
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

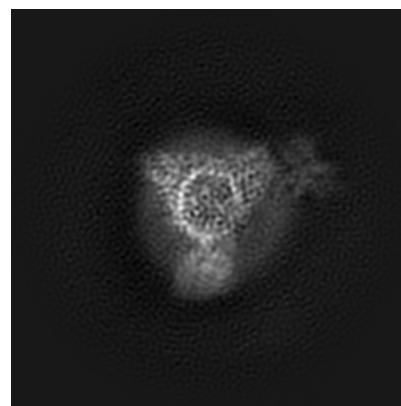
6.1.1 Primary map



X

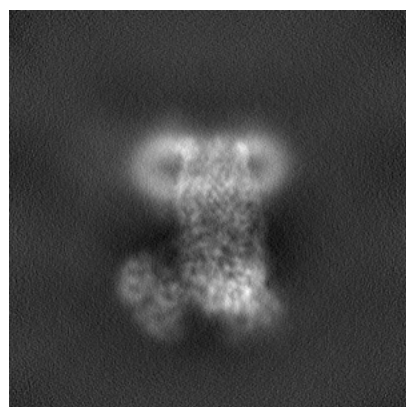


Y

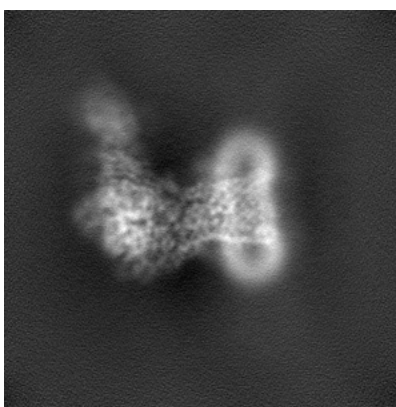


Z

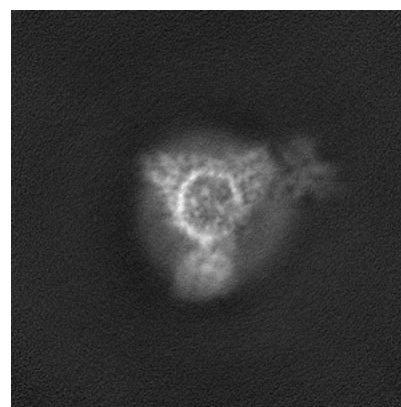
6.1.2 Raw map



X



Y

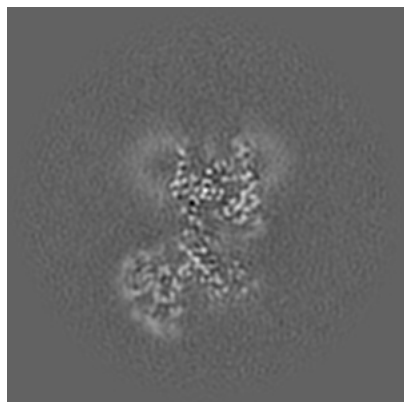


Z

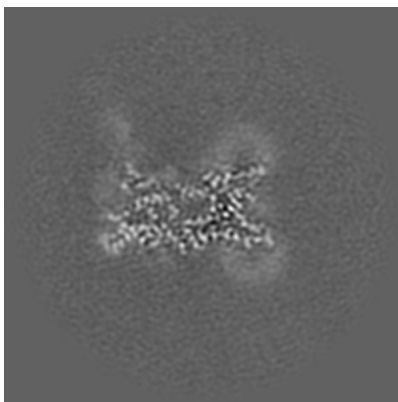
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

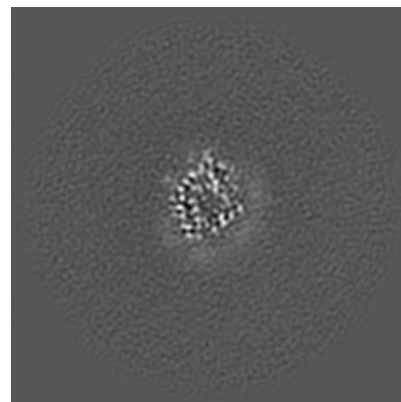
6.2.1 Primary map



X Index: 160

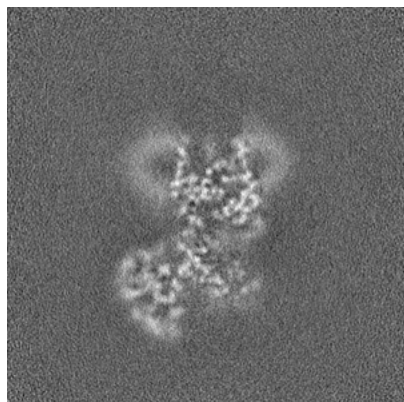


Y Index: 160

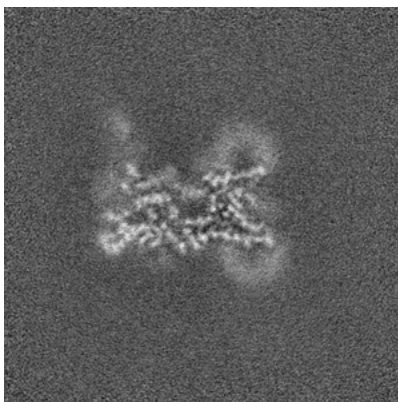


Z Index: 160

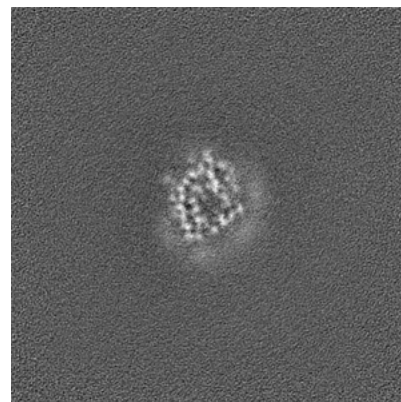
6.2.2 Raw map



X Index: 160



Y Index: 160

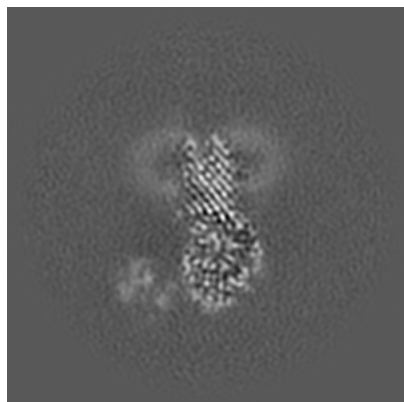


Z Index: 160

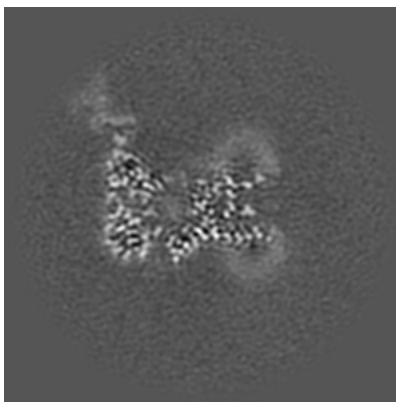
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

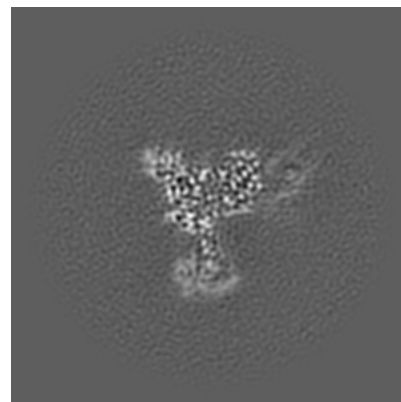
6.3.1 Primary map



X Index: 136

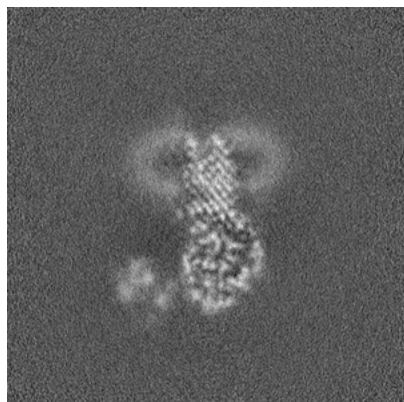


Y Index: 174

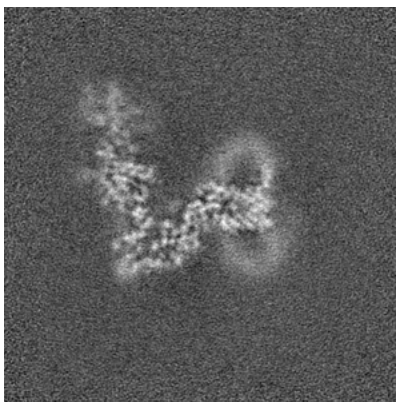


Z Index: 105

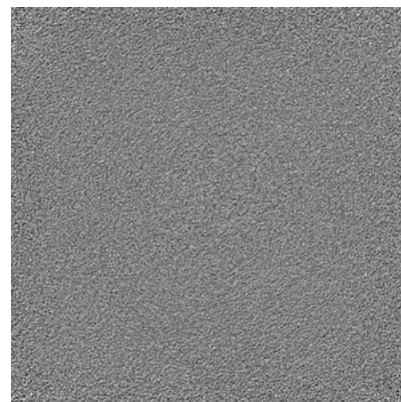
6.3.2 Raw map



X Index: 136



Y Index: 188

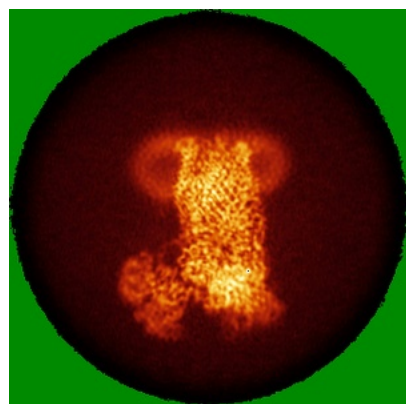


Z Index: 0

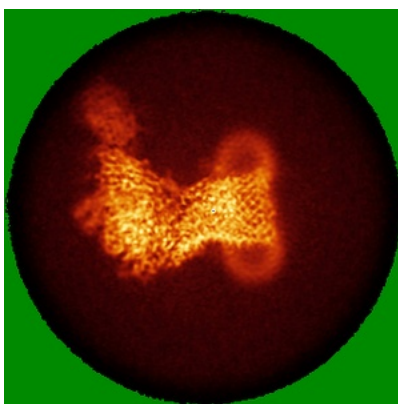
The images above show the largest variance slices of the map in three orthogonal directions.

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

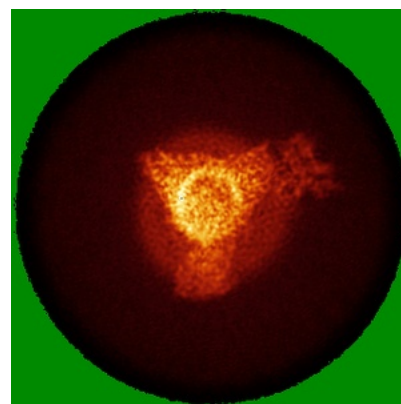
6.4.1 Primary map



X

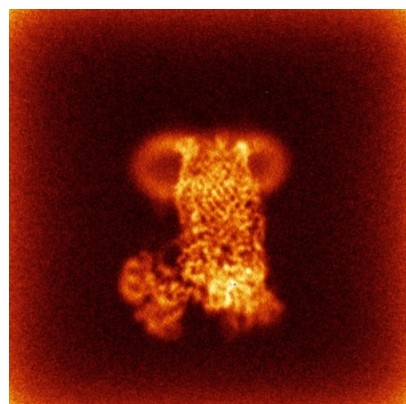


Y

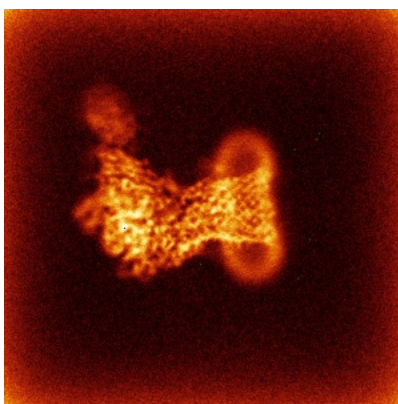


Z

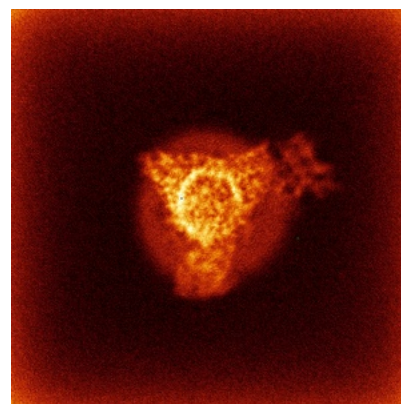
6.4.2 Raw map



X



Y

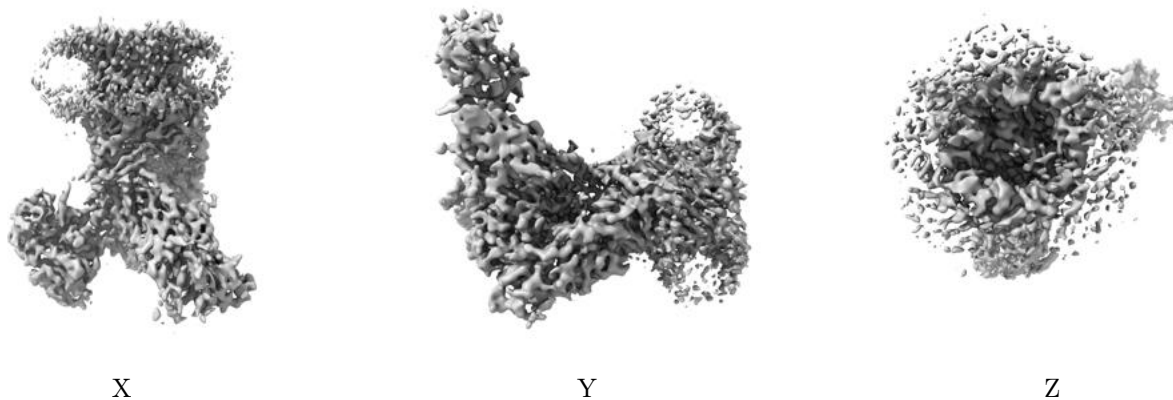


Z

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

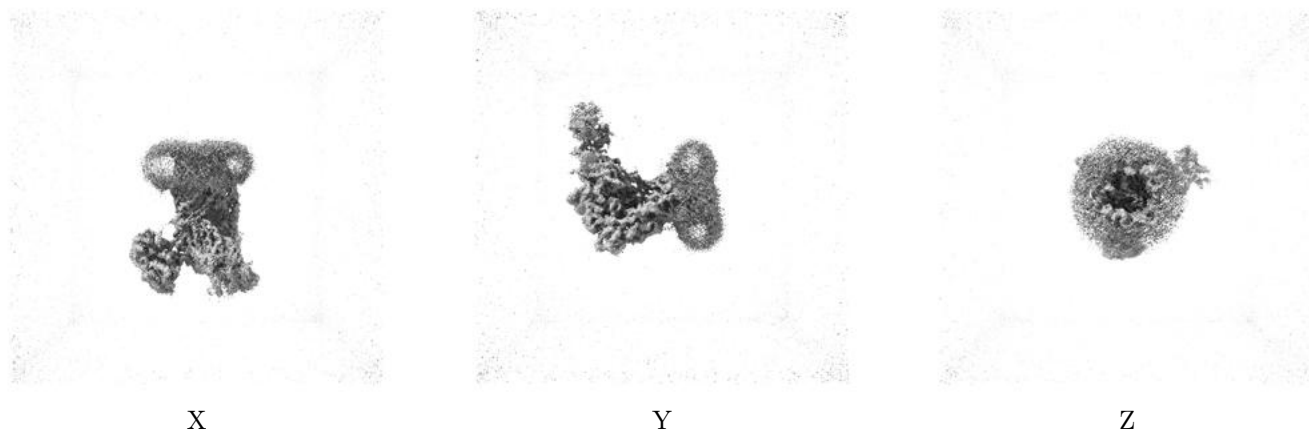
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. 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.

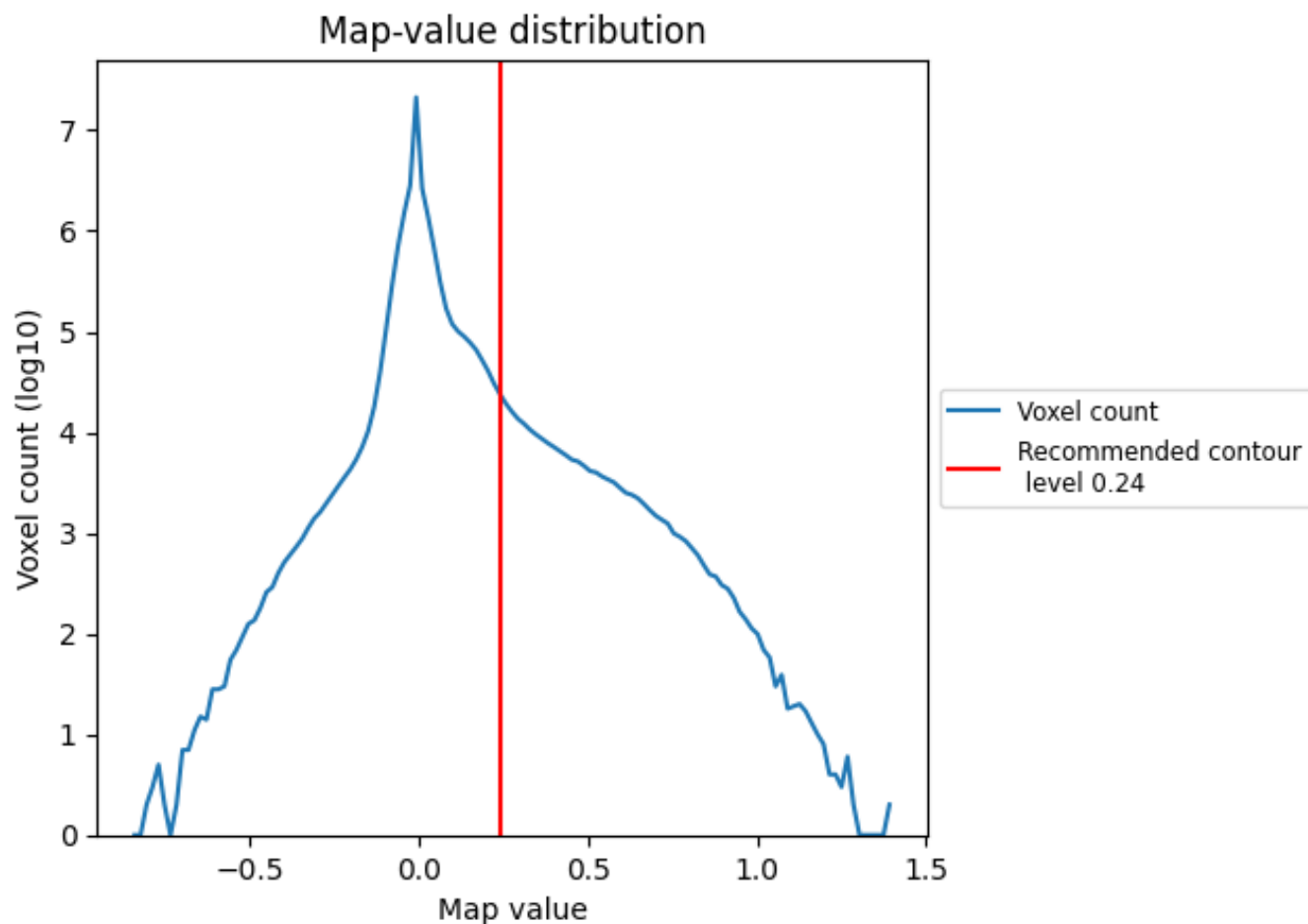
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

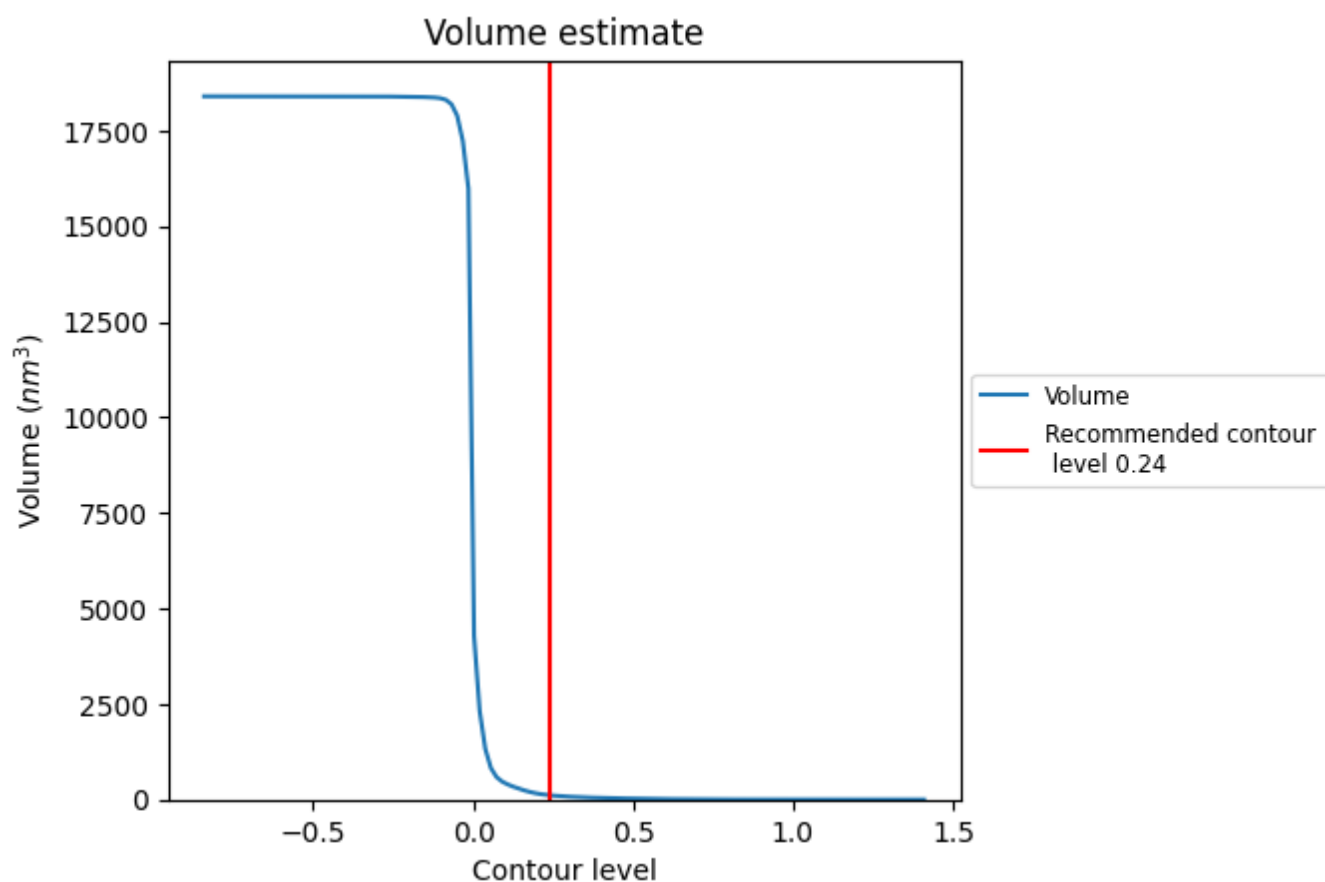
This section contains the results of statistical analysis of the map.

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.

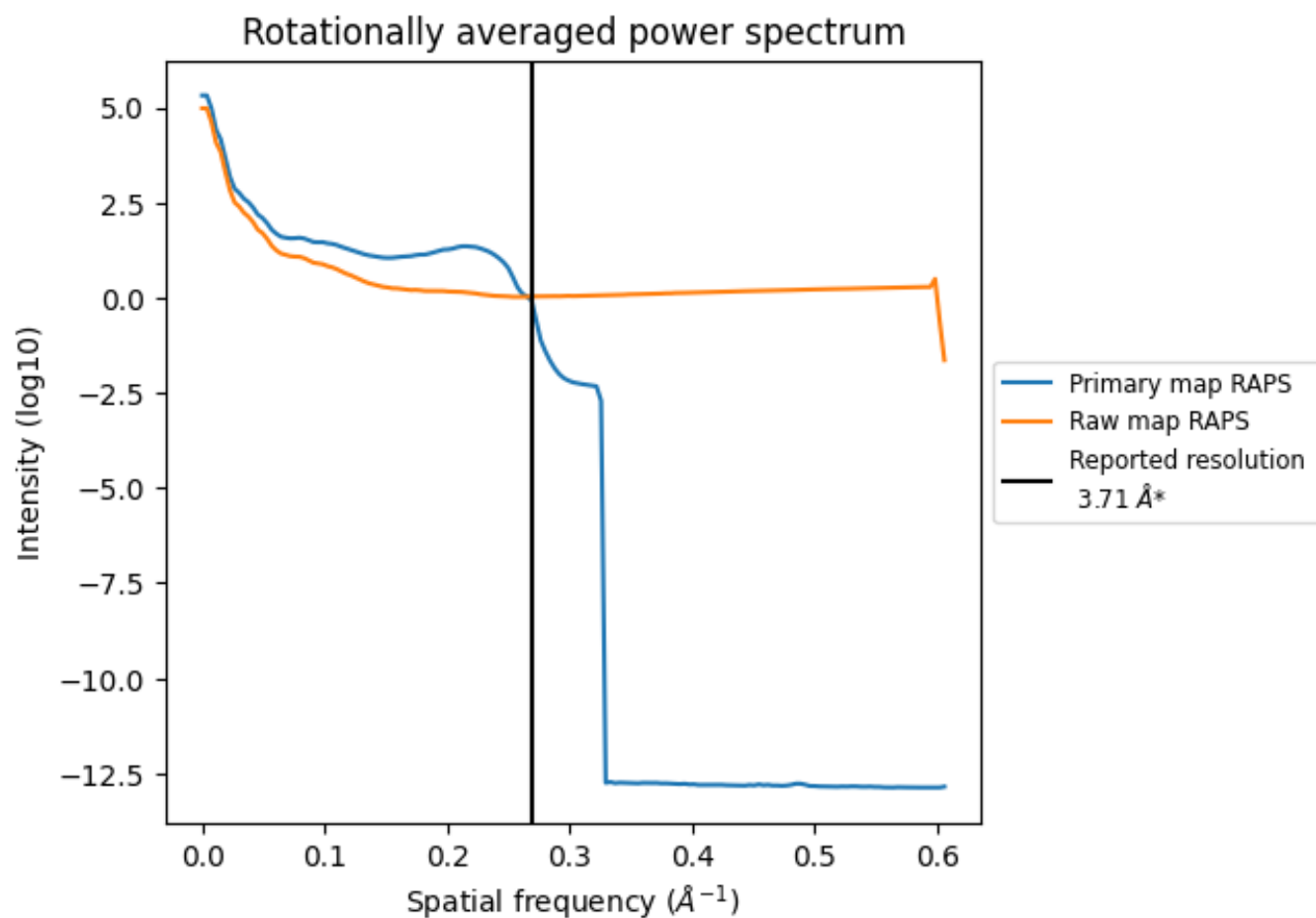
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm³; this corresponds to an approximate mass of 101 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 ⓘ

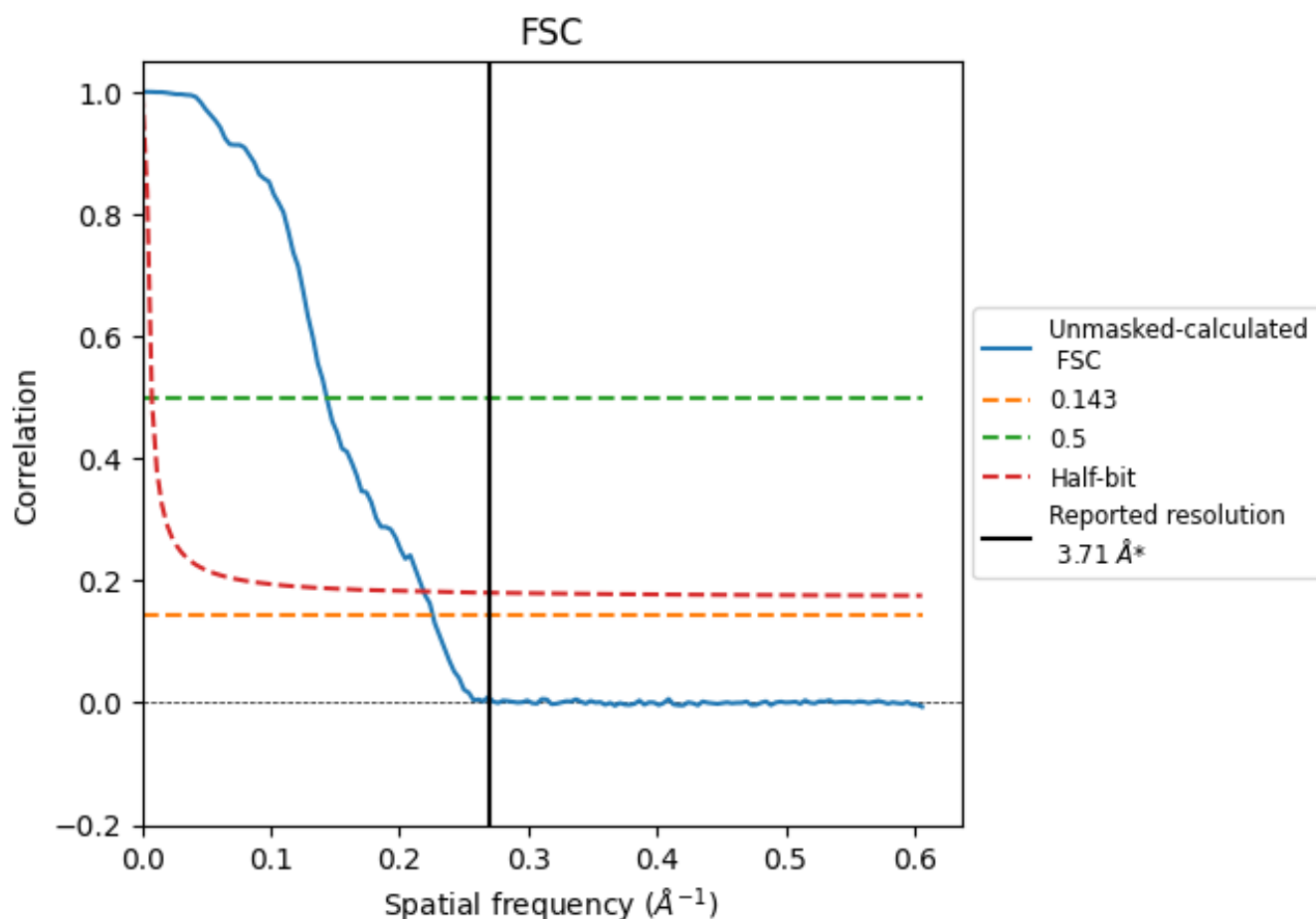


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

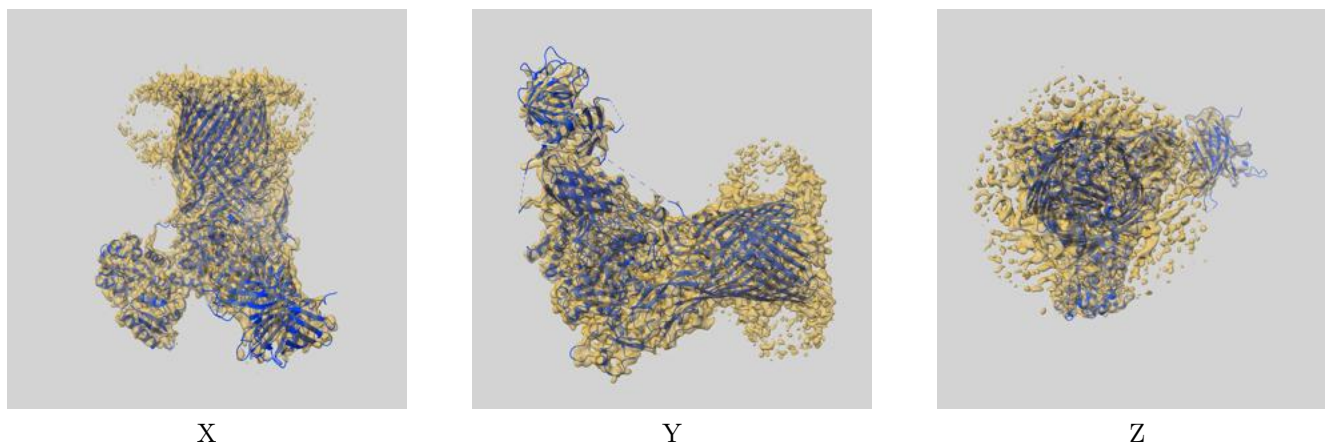
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.43	6.98	4.57

*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 4.43 differs from the reported value 3.71 by more than 10 %

9 Map-model fit [i](#)

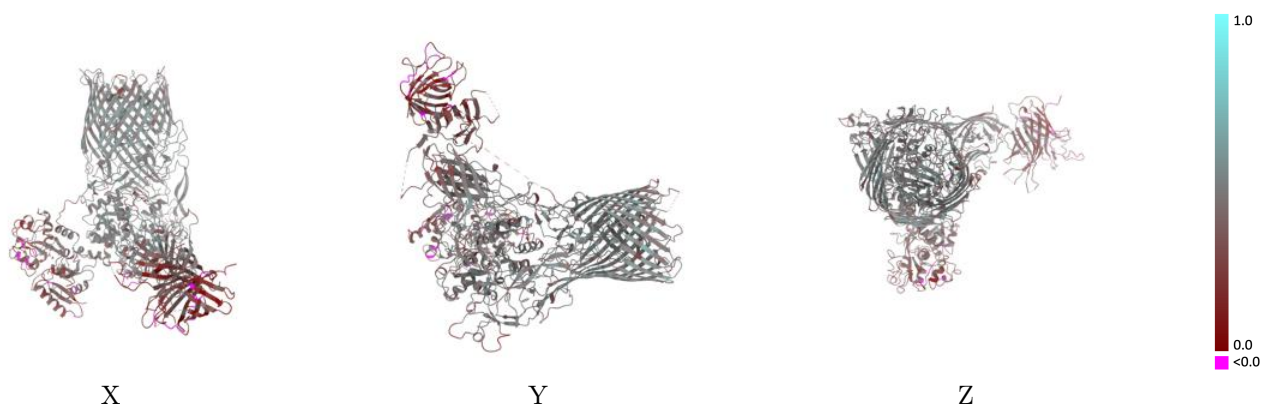
This section contains information regarding the fit between EMDB map EMD-45747 and PDB model 9CMG. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



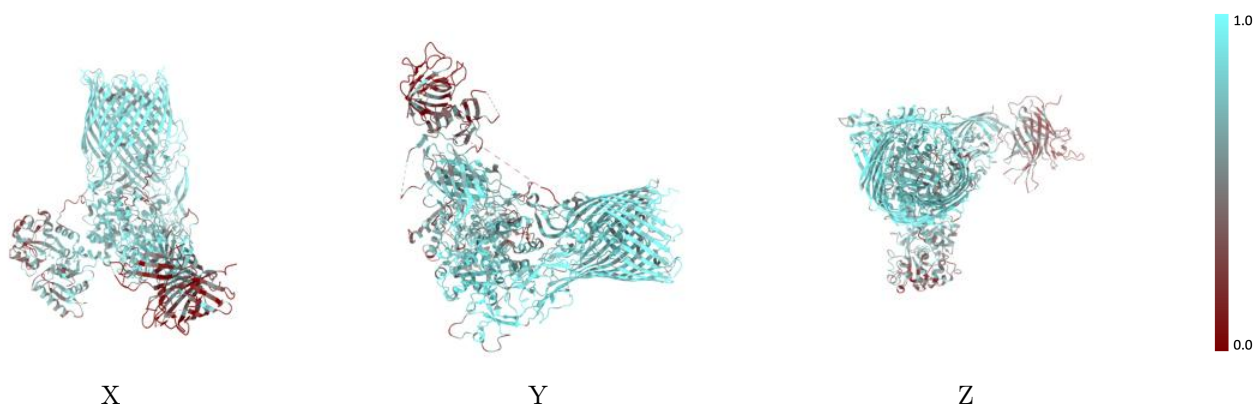
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



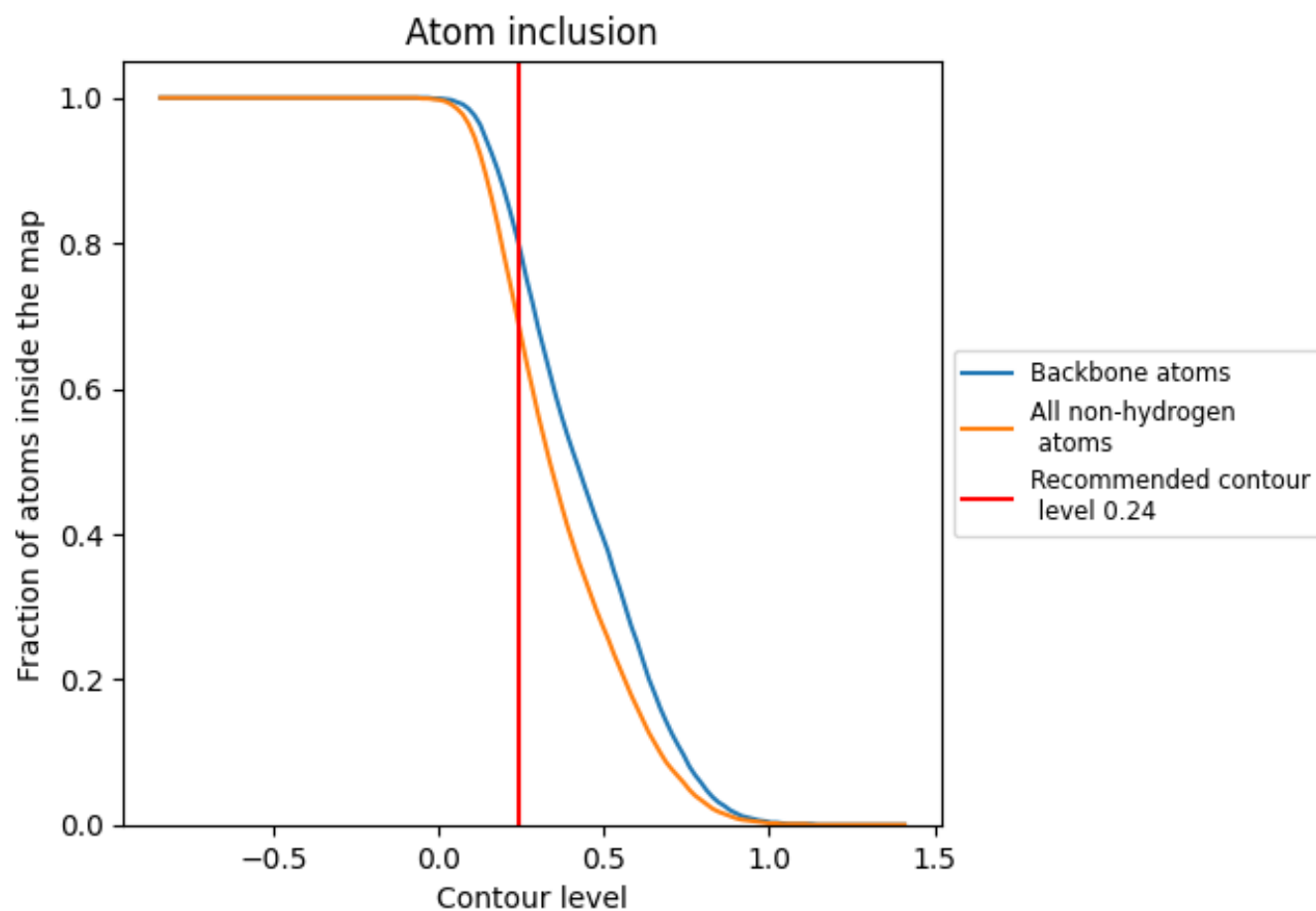
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6930	<div></div> 0.4130
A	<div></div> 0.8170	<div></div> 0.4720
B	<div></div> 0.5140	<div></div> 0.3570
F	<div></div> 0.6900	<div></div> 0.3860

