



Full wwPDB EM Validation Report ⓘ

Sep 13, 2026 – 02:14 am BST

PDB ID : 9T8H / pdb_00009t8h
EMDB ID : EMD-55686
Title : Murine RNF213 bound to maltoheptaose
Authors : Yip, M.C.J.; Naydenova, K.; Randow, F.
Deposited on : 2025-11-12
Resolution : 3.00 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

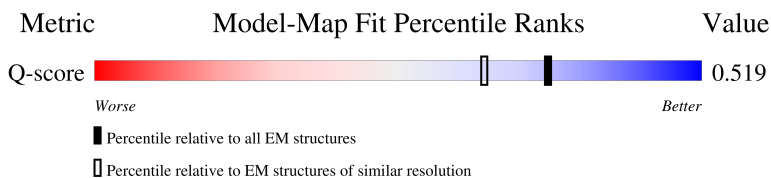
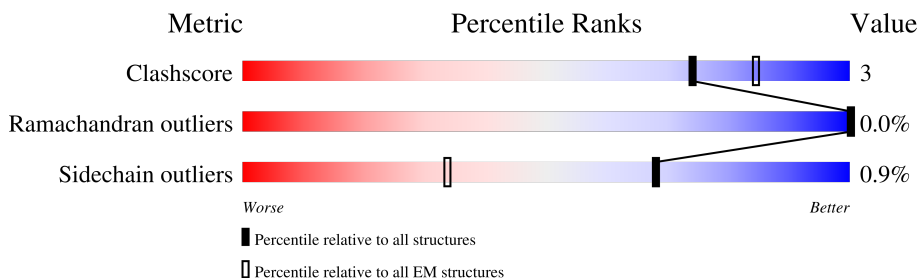
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	B	5188	
2	F	4	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36555 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 E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	4534	Total	C	N	O	S	0	0
			36478	23264	6271	6718	225		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-39	MET	-	initiating methionine	UNP E9Q555
B	-38	ALA	-	expression tag	UNP E9Q555
B	-37	SER	-	expression tag	UNP E9Q555
B	-36	TRP	-	expression tag	UNP E9Q555
B	-35	SER	-	expression tag	UNP E9Q555
B	-34	HIS	-	expression tag	UNP E9Q555
B	-33	PRO	-	expression tag	UNP E9Q555
B	-32	GLN	-	expression tag	UNP E9Q555
B	-31	PHE	-	expression tag	UNP E9Q555
B	-30	GLU	-	expression tag	UNP E9Q555
B	-29	LYS	-	expression tag	UNP E9Q555
B	-28	GLY	-	expression tag	UNP E9Q555
B	-27	SER	-	expression tag	UNP E9Q555
B	-26	ALA	-	expression tag	UNP E9Q555
B	-25	GLY	-	expression tag	UNP E9Q555
B	-24	SER	-	expression tag	UNP E9Q555
B	-23	ALA	-	expression tag	UNP E9Q555
B	-22	ALA	-	expression tag	UNP E9Q555
B	-21	GLY	-	expression tag	UNP E9Q555
B	-20	SER	-	expression tag	UNP E9Q555
B	-19	GLY	-	expression tag	UNP E9Q555
B	-18	ALA	-	expression tag	UNP E9Q555
B	-17	GLY	-	expression tag	UNP E9Q555
B	-16	TRP	-	expression tag	UNP E9Q555
B	-15	SER	-	expression tag	UNP E9Q555
B	-14	HIS	-	expression tag	UNP E9Q555
B	-13	PRO	-	expression tag	UNP E9Q555
B	-12	GLN	-	expression tag	UNP E9Q555

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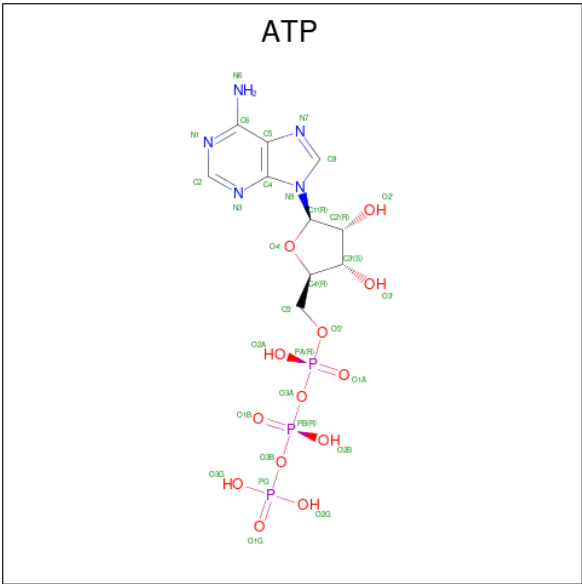
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	PHE	-	expression tag	UNP E9Q555
B	-10	GLU	-	expression tag	UNP E9Q555
B	-9	LYS	-	expression tag	UNP E9Q555
B	-8	GLU	-	expression tag	UNP E9Q555
B	-7	ASN	-	expression tag	UNP E9Q555
B	-6	LEU	-	expression tag	UNP E9Q555
B	-5	TYR	-	expression tag	UNP E9Q555
B	-4	PHE	-	expression tag	UNP E9Q555
B	-3	GLN	-	expression tag	UNP E9Q555
B	-2	ALA	-	expression tag	UNP E9Q555
B	-1	MET	-	expression tag	UNP E9Q555
B	0	SER	-	expression tag	UNP E9Q555

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
2	F	4	Total	C	O	0	0
			44	24	20		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

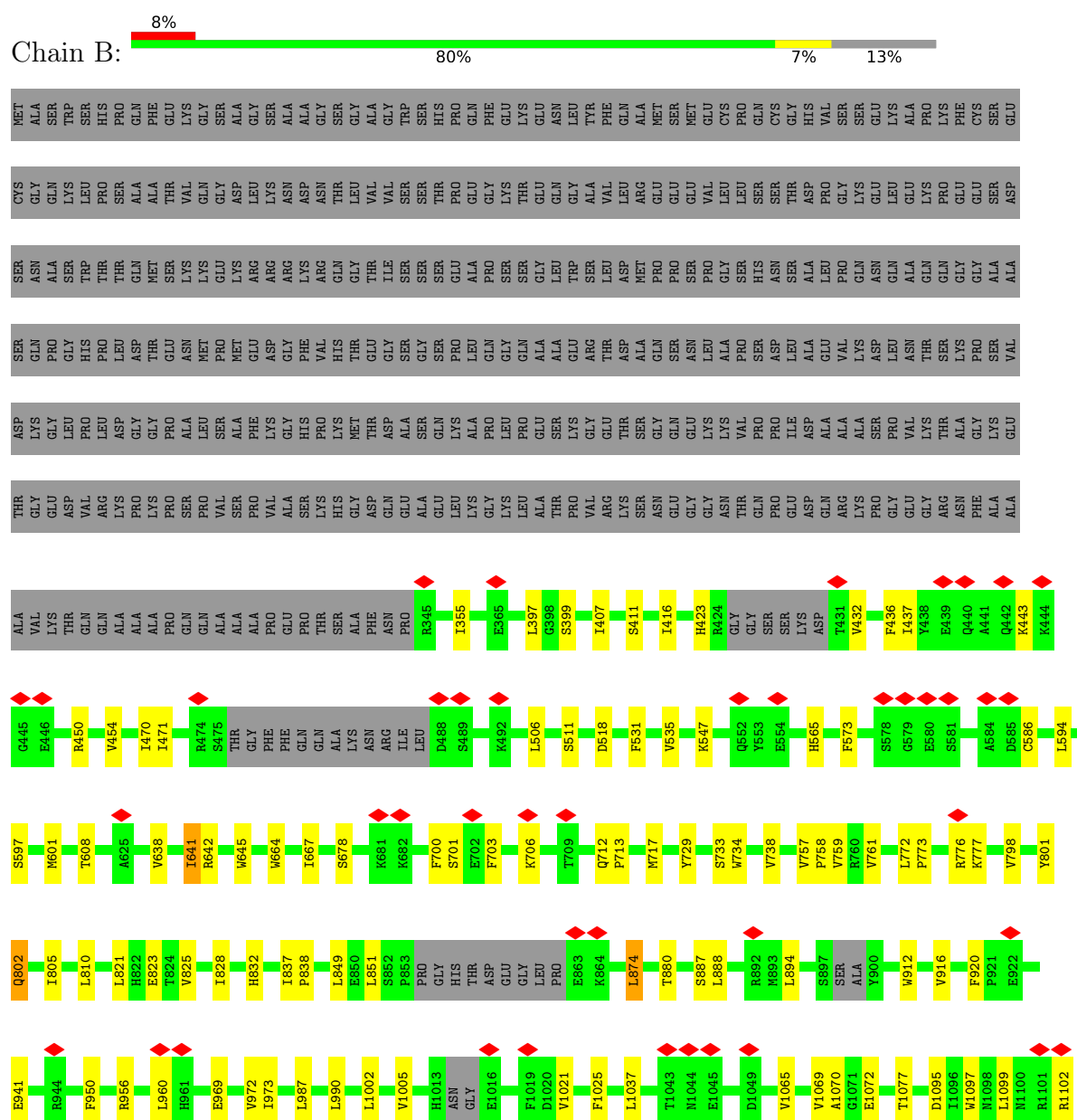
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total	Zn	0
			2	2	

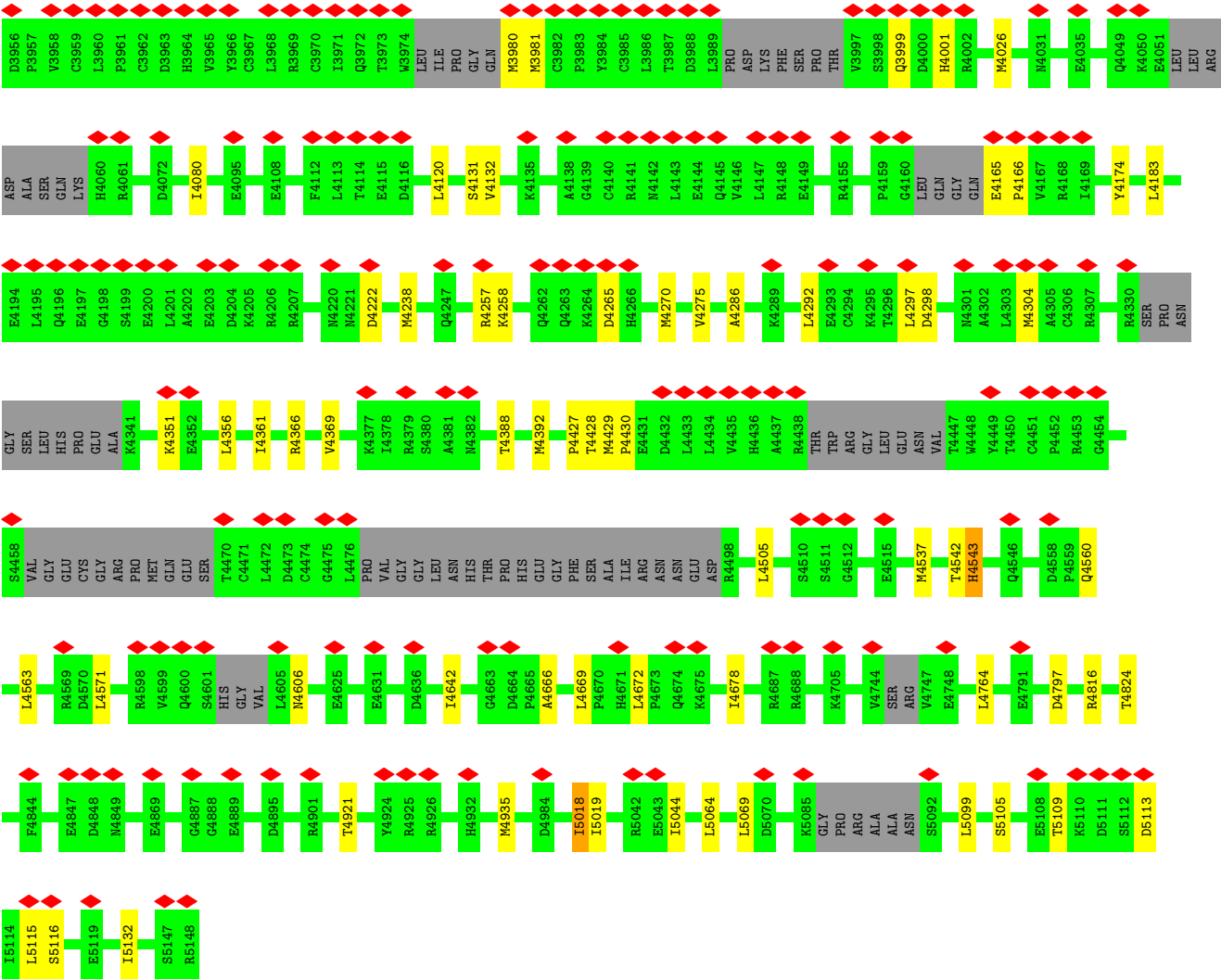
3 Residue-property plots

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: E3 ubiquitin-protein ligase RNF213







● Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	557952	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	373.19998, 373.19998, 373.19998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.244, 1.244, 1.244	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: GLC, ATP, ZN

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	B	0.21	0/37222	0.29	0/50317

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	B	36478	0	36644	232	0
2	F	44	0	37	0	0
3	B	31	0	12	1	0
4	B	2	0	0	0	0
All	All	36555	0	36693	232	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 3.

All (232) 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:B:4429:MET:HE3	1:B:4429:MET:HA	1.59	0.85
1:B:3503:MET:HE2	1:B:3503:MET:H	1.49	0.77
1:B:3014:ILE:HG21	1:B:3138:VAL:HG21	1.69	0.74
1:B:2608:VAL:HG22	1:B:2722:LEU:HD12	1.70	0.73
1:B:3529:MET:HE3	1:B:3530:ARG:N	2.05	0.72
1:B:987:LEU:HD21	1:B:1005:VAL:HG21	1.72	0.71
1:B:4304:MET:HE3	1:B:4304:MET:O	1.90	0.71
1:B:2450:ALA:HB1	1:B:2459:ILE:HD13	1.73	0.70
1:B:437:ILE:HD11	1:B:450:ARG:HG2	1.74	0.70
1:B:2924:VAL:HG13	1:B:2935:LEU:HD11	1.74	0.70
1:B:3529:MET:HE3	1:B:3529:MET:C	2.18	0.69
1:B:3852:LEU:HD22	1:B:3863:ILE:HD13	1.76	0.68
1:B:2608:VAL:HG22	1:B:2722:LEU:CD1	2.26	0.66
1:B:3833:LEU:HD11	1:B:3881:GLU:HB2	1.78	0.65
1:B:1785:LYS:N	1:B:1785:LYS:HE2	2.12	0.65
1:B:4392:MET:HE1	1:B:4571:LEU:HD11	1.76	0.65
1:B:2648:MET:SD	1:B:2689:VAL:HG21	2.37	0.65
1:B:3649:LYS:HE2	1:B:3649:LYS:HA	1.79	0.64
1:B:437:ILE:HD11	1:B:450:ARG:CG	2.26	0.64
1:B:874:LEU:HD11	1:B:920:PHE:CD1	2.32	0.64
1:B:5105:SER:O	1:B:5109:THR:HG23	1.97	0.64
1:B:3846:VAL:O	1:B:3852:LEU:HD21	1.99	0.62
1:B:3005:LEU:CD2	1:B:3116:VAL:HG21	2.30	0.62
1:B:3176:VAL:HG13	1:B:3225:ALA:CB	2.31	0.60
1:B:3852:LEU:CD2	1:B:3863:ILE:HD13	2.31	0.60
1:B:4257:ARG:NE	1:B:4257:ARG:H	2.00	0.60
1:B:4388:THR:HG22	1:B:4392:MET:HE2	1.84	0.59
1:B:1981:PRO:HG2	1:B:2014:VAL:HG22	1.85	0.58
1:B:443:LYS:HD2	1:B:443:LYS:C	2.28	0.58
1:B:990:LEU:O	1:B:990:LEU:HD12	2.04	0.57
1:B:3852:LEU:HD11	1:B:3863:ILE:HG21	1.85	0.57
1:B:2116:ASP:H	3:B:5301:ATP:HN61	1.53	0.55
1:B:717:MET:HE2	1:B:734:TRP:HB3	1.89	0.55
1:B:397:LEU:HD13	1:B:397:LEU:O	2.06	0.55
1:B:3858:MET:HE3	1:B:3858:MET:C	2.32	0.54
1:B:3480:LEU:HD21	1:B:3574:VAL:HG12	1.90	0.54
1:B:1070:ALA:HB1	1:B:1097:TRP:CZ3	2.43	0.54
1:B:1737:MET:HE2	1:B:1737:MET:HA	1.89	0.54
1:B:3859:THR:HG22	1:B:3863:ILE:HD12	1.90	0.53
1:B:547:LYS:HE2	1:B:547:LYS:HA	1.90	0.53
1:B:874:LEU:HD11	1:B:920:PHE:CE1	2.43	0.53
1:B:2579:VAL:HG11	1:B:2650:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:VAL:HG13	1:B:645:TRP:CD1	2.44	0.52
1:B:573:PHE:CE2	1:B:594:LEU:HD22	2.44	0.52
1:B:1934:ARG:NH1	1:B:1934:ARG:HB2	2.24	0.52
1:B:1710:CYS:SG	1:B:1767:CYS:HA	2.50	0.52
1:B:3981:MET:HE3	1:B:3981:MET:N	2.25	0.52
1:B:4292:LEU:HD13	1:B:4292:LEU:O	2.10	0.52
1:B:506:LEU:HD23	1:B:565:HIS:HD2	1.75	0.51
1:B:4543:HIS:ND1	1:B:4543:HIS:C	2.68	0.51
1:B:4935:MET:N	1:B:4935:MET:HE2	2.25	0.51
1:B:3788:VAL:HG21	1:B:3816:CYS:SG	2.50	0.51
1:B:2378:ILE:HG12	1:B:2540:VAL:HG22	1.93	0.50
1:B:2468:VAL:CG2	1:B:2473:LEU:HD21	2.41	0.50
1:B:4429:MET:HE3	1:B:4430:PRO:HD3	1.93	0.50
1:B:518:ASP:OD1	1:B:518:ASP:C	2.53	0.50
1:B:3345:ARG:HA	1:B:3345:ARG:NE	2.27	0.50
1:B:1196:MET:HE2	1:B:1238:LEU:HB2	1.94	0.50
1:B:4257:ARG:H	1:B:4257:ARG:HE	1.58	0.50
1:B:950:PHE:HB2	1:B:972:VAL:HG21	1.93	0.49
1:B:4429:MET:HA	1:B:4429:MET:CE	2.39	0.49
1:B:987:LEU:CD2	1:B:1005:VAL:HG21	2.42	0.49
1:B:641:ILE:O	1:B:642:ARG:C	2.55	0.49
1:B:1751:MET:HE3	1:B:1755:LEU:HD12	1.95	0.49
1:B:1361:PRO:HA	1:B:1364:ILE:HB	1.95	0.49
1:B:5113:ASP:OD2	1:B:5113:ASP:C	2.56	0.49
1:B:2579:VAL:CG1	1:B:2650:ILE:HD11	2.43	0.48
1:B:3399:VAL:HG12	1:B:3400:HIS:N	2.28	0.48
1:B:3820:LEU:HD21	1:B:3835:LEU:HG	1.95	0.48
1:B:2866:PRO:HG2	1:B:2871:LEU:HD21	1.95	0.48
1:B:3570:LEU:O	1:B:3574:VAL:HG23	2.13	0.48
1:B:597:SER:O	1:B:601:MET:HG3	2.14	0.48
1:B:4265:ASP:OD2	1:B:4265:ASP:C	2.57	0.48
1:B:531:PHE:CE1	1:B:535:VAL:HG21	2.49	0.48
1:B:3256:VAL:HG22	1:B:3292:LEU:CD1	2.44	0.48
1:B:1597:LEU:HB2	1:B:1751:MET:HE1	1.96	0.47
1:B:2371:PHE:CE1	1:B:2377:VAL:HG21	2.49	0.47
1:B:506:LEU:HD23	1:B:565:HIS:CD2	2.49	0.47
1:B:1037:LEU:HD13	1:B:1037:LEU:C	2.40	0.47
1:B:1727:PRO:O	1:B:1731:LEU:HD23	2.14	0.47
1:B:1935:LEU:HD23	1:B:1936:LEU:N	2.29	0.47
1:B:1981:PRO:CG	1:B:2014:VAL:HG22	2.44	0.47
1:B:3255:PHE:CE1	1:B:3259:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3833:LEU:HD11	1:B:3881:GLU:CB	2.41	0.47
1:B:4764:LEU:O	1:B:4764:LEU:HD12	2.14	0.47
1:B:1095:ASP:O	1:B:1099:LEU:HD13	2.15	0.47
1:B:5018:ILE:HG23	1:B:5019:ILE:N	2.29	0.47
1:B:355:ILE:HG21	1:B:397:LEU:CD1	2.44	0.47
1:B:3999:GLN:OE1	1:B:3999:GLN:N	2.48	0.47
1:B:3006:THR:HB	1:B:3011:ALA:HB2	1.97	0.47
1:B:3919:ARG:NH1	1:B:3919:ARG:HB2	2.30	0.46
1:B:960:LEU:C	1:B:960:LEU:HD13	2.40	0.46
1:B:1811:MET:CE	1:B:1921:ILE:HA	2.45	0.46
1:B:4666:ALA:HB1	1:B:4669:LEU:HD12	1.98	0.46
1:B:2611:TRP:CG	1:B:2722:LEU:HD21	2.51	0.46
1:B:3830:LYS:O	1:B:3830:LYS:HD3	2.16	0.46
1:B:3849:GLU:OE2	1:B:3849:GLU:O	2.34	0.46
1:B:411:SER:HB3	1:B:416:ILE:HD11	1.98	0.45
1:B:2082:PHE:CD1	1:B:2082:PHE:C	2.93	0.45
1:B:2562:LEU:HB2	1:B:2606:VAL:HG11	1.98	0.45
1:B:2924:VAL:CG1	1:B:2935:LEU:HD11	2.43	0.45
1:B:4275:VAL:HG12	1:B:4642:ILE:HG21	1.97	0.45
1:B:912:TRP:O	1:B:916:VAL:HG23	2.16	0.45
1:B:832:HIS:HA	1:B:888:LEU:HD21	1.99	0.45
1:B:1285:LYS:O	1:B:1289:THR:HG23	2.16	0.45
1:B:1127:LEU:HD21	1:B:1163:LEU:HD11	1.98	0.45
1:B:2274:MET:HE2	1:B:2274:MET:H	1.82	0.45
1:B:2894:ALA:HB3	1:B:2895:PRO:HD3	1.99	0.45
1:B:4174:TYR:CE2	1:B:4678:ILE:HD13	2.51	0.45
1:B:1099:LEU:HD12	1:B:1102:ARG:HH12	1.81	0.45
1:B:2618:MET:HE2	1:B:2759:CYS:CB	2.47	0.45
1:B:987:LEU:HD11	1:B:1002:LEU:HD23	1.99	0.45
1:B:3919:ARG:NH1	1:B:3919:ARG:CB	2.80	0.45
1:B:2284:GLU:HB2	1:B:2294:ILE:HD12	1.97	0.44
1:B:3814:MET:HE3	1:B:3818:GLU:HG3	1.99	0.44
1:B:3046:ILE:HG13	1:B:3092:LEU:HD21	1.98	0.44
1:B:758:PRO:O	1:B:761:VAL:HG23	2.17	0.44
1:B:837:ILE:HB	1:B:838:PRO:HD3	1.99	0.44
1:B:4429:MET:HE1	1:B:4505:LEU:HG	1.98	0.44
1:B:4132:VAL:HG11	1:B:4183:LEU:HD13	1.98	0.44
1:B:3610:LEU:HD23	1:B:3656:PRO:HD2	1.98	0.44
1:B:1390:LEU:HD12	1:B:1479:LEU:HD13	2.00	0.44
1:B:3283:LEU:HD22	1:B:3337:GLN:HB3	1.98	0.44
1:B:3862:VAL:O	1:B:3866:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3874:PHE:HD2	1:B:4026:MET:HE3	1.82	0.44
1:B:407:ILE:HD11	1:B:454:VAL:HG21	1.99	0.44
1:B:4222:ASP:HB2	1:B:4672:LEU:HD23	2.00	0.44
1:B:4238:MET:CE	1:B:4270:MET:HE3	2.48	0.44
1:B:355:ILE:HG21	1:B:397:LEU:HD13	1.99	0.44
1:B:717:MET:HE1	1:B:738:VAL:HG23	2.00	0.43
1:B:1025:PHE:CZ	1:B:1069:VAL:HG11	2.54	0.43
1:B:5064:LEU:HD22	1:B:5069:LEU:HD21	1.99	0.43
1:B:5044:ILE:HG21	1:B:5132:ILE:HD11	2.00	0.43
1:B:423:HIS:CE1	1:B:432:VAL:HG13	2.54	0.43
1:B:4351:LYS:NZ	1:B:4366:ARG:HE	2.17	0.43
1:B:4542:THR:HG22	1:B:4560:GLN:CD	2.42	0.43
1:B:706:LYS:O	1:B:706:LYS:CG	2.66	0.43
1:B:713:PRO:O	1:B:717:MET:HG3	2.18	0.43
1:B:4165:GLU:N	1:B:4166:PRO:CD	2.81	0.43
1:B:4606:ASN:O	1:B:4606:ASN:CG	2.62	0.43
1:B:3825:LEU:HD21	1:B:3902:VAL:HG11	2.00	0.43
1:B:4537:MET:HE2	1:B:4563:LEU:HD21	1.99	0.43
1:B:4824:THR:HG22	1:B:4824:THR:O	2.18	0.43
1:B:849:LEU:CD1	1:B:874:LEU:HD13	2.49	0.43
1:B:1072:GLU:OE1	1:B:1077:THR:HG23	2.19	0.43
1:B:776:ARG:NH1	1:B:776:ARG:HA	2.34	0.43
1:B:798:VAL:HA	1:B:805:ILE:HD11	2.01	0.43
1:B:3980:MET:HB3	1:B:3981:MET:HE3	2.01	0.43
1:B:801:TYR:O	1:B:802:GLN:C	2.61	0.43
1:B:823:GLU:HA	1:B:880:THR:HG21	2.01	0.43
1:B:969:GLU:O	1:B:973:ILE:HD13	2.19	0.43
1:B:2421:ILE:O	1:B:2425:VAL:HG23	2.18	0.43
1:B:3188:VAL:HG13	1:B:3216:ILE:CG2	2.48	0.43
1:B:3645:MET:HE3	1:B:3653:ASN:HB3	2.01	0.43
1:B:4356:LEU:HD22	1:B:4361:ILE:HG22	2.01	0.43
1:B:4797:ASP:OD2	1:B:4797:ASP:C	2.61	0.42
1:B:777:LYS:HA	1:B:828:ILE:O	2.19	0.42
1:B:821:LEU:O	1:B:825:VAL:HG23	2.19	0.42
1:B:1503:ILE:HG23	1:B:1528:LEU:HD21	2.02	0.42
1:B:3350:VAL:HG13	1:B:3375:PHE:CE1	2.54	0.42
1:B:700:PHE:CD1	1:B:701:SER:N	2.87	0.42
1:B:1323:LEU:HD22	1:B:1342:LEU:HD11	2.00	0.42
1:B:2983:ILE:CD1	1:B:3108:ILE:HD11	2.49	0.42
1:B:4080:ILE:HD13	1:B:4120:LEU:HD13	2.01	0.42
1:B:437:ILE:HD11	1:B:450:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3619:LYS:HD3	1:B:3619:LYS:N	2.35	0.42
1:B:4366:ARG:HA	1:B:4369:VAL:HG22	2.01	0.42
1:B:832:HIS:CB	1:B:888:LEU:HD21	2.50	0.42
1:B:956:ARG:NH1	1:B:956:ARG:HG2	2.35	0.42
1:B:1803:LEU:HB2	1:B:1804:PRO:HD3	2.01	0.42
1:B:3852:LEU:HD22	1:B:3863:ILE:CD1	2.46	0.42
1:B:759:VAL:HG13	1:B:810:LEU:CD1	2.50	0.42
1:B:664:TRP:HA	1:B:667:ILE:HD12	2.01	0.42
1:B:1339:ASN:N	1:B:1340:PRO:HD2	2.34	0.42
1:B:1404:LEU:O	1:B:1405:LYS:C	2.62	0.42
1:B:436:PHE:C	1:B:436:PHE:CD2	2.98	0.42
1:B:798:VAL:CG1	1:B:851:LEU:HD11	2.50	0.42
1:B:3361:ILE:O	1:B:3365:GLN:HB2	2.20	0.42
1:B:3508:ILE:HG22	1:B:3512:LEU:HD12	2.02	0.42
1:B:678:SER:HA	1:B:729:TYR:CZ	2.55	0.41
1:B:1141:LEU:HD22	1:B:1150:VAL:HG21	2.01	0.41
1:B:1763:ALA:O	1:B:1767:CYS:SG	2.79	0.41
1:B:2933:ARG:HB2	1:B:2933:ARG:NH1	2.35	0.41
1:B:3665:LEU:HD21	1:B:3689:PHE:CE1	2.54	0.41
1:B:4816:ARG:HH21	1:B:4921:THR:HG21	1.84	0.41
1:B:2825:LEU:HD21	1:B:2842:PHE:CG	2.55	0.41
1:B:3731:MET:SD	1:B:3731:MET:O	2.78	0.41
1:B:5099:LEU:HD13	1:B:5099:LEU:C	2.46	0.41
1:B:608:THR:O	1:B:608:THR:HG23	2.19	0.41
1:B:5115:LEU:O	1:B:5116:SER:C	2.63	0.41
1:B:1596:MET:SD	1:B:1672:VAL:HG13	2.61	0.41
1:B:2933:ARG:NH1	1:B:2933:ARG:CB	2.84	0.41
1:B:4427:PRO:C	1:B:4428:THR:HG23	2.46	0.41
1:B:3884:LEU:O	1:B:3888:GLU:HG2	2.20	0.41
1:B:4286:ALA:O	1:B:4298:ASP:OD2	2.38	0.41
1:B:1021:VAL:HG13	1:B:1065:VAL:HG22	2.02	0.41
1:B:3852:LEU:CD1	1:B:3863:ILE:HG21	2.51	0.41
1:B:4258:LYS:HD2	1:B:4258:LYS:C	2.45	0.41
1:B:712:GLN:N	1:B:713:PRO:CD	2.84	0.41
1:B:1447:ASN:OD1	1:B:1448:PHE:N	2.54	0.41
1:B:2186:GLN:HB3	1:B:2216:MET:HE3	2.03	0.41
1:B:2537:ILE:N	1:B:2538:PRO:HD2	2.36	0.41
1:B:2624:ASP:O	1:B:2628:HIS:ND1	2.54	0.41
1:B:2638:GLU:C	1:B:2638:GLU:OE2	2.64	0.41
1:B:2720:ILE:HG21	1:B:2747:MET:HE1	2.02	0.41
1:B:3192:ALA:HB1	1:B:3212:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:VAL:HG13	1:B:837:ILE:HG22	2.02	0.40
1:B:2124:ALA:HB1	1:B:2181:TRP:CD1	2.56	0.40
1:B:3134:ASP:OD1	1:B:3137:THR:HG23	2.21	0.40
1:B:3714:LEU:HD12	1:B:3764:VAL:HG13	2.03	0.40
1:B:712:GLN:O	1:B:713:PRO:C	2.65	0.40
1:B:2079:ALA:HB3	1:B:2080:PRO:HD3	2.03	0.40
1:B:2563:VAL:CG1	1:B:2568:VAL:HG21	2.51	0.40
1:B:2618:MET:HE2	1:B:2759:CYS:HB2	2.02	0.40
1:B:3761:LEU:N	1:B:3762:PRO:CD	2.85	0.40
1:B:3919:ARG:HB2	1:B:3919:ARG:CZ	2.52	0.40
1:B:950:PHE:CG	1:B:972:VAL:HG21	2.55	0.40
1:B:2402:VAL:HG12	1:B:2403:GLU:N	2.36	0.40
1:B:3005:LEU:HD23	1:B:3116:VAL:HG21	2.03	0.40
1:B:3833:LEU:HD11	1:B:3881:GLU:CA	2.51	0.40
1:B:470:ILE:HG22	1:B:471:ILE:O	2.22	0.40
1:B:849:LEU:HD13	1:B:874:LEU:HD13	2.03	0.40
1:B:894:LEU:HD12	1:B:941:GLU:HG3	2.03	0.40
1:B:3549:TRP:CD1	1:B:3549:TRP:H	2.39	0.40
1:B:4292:LEU:HD13	1:B:4292:LEU:C	2.47	0.40
1:B:4429:MET:HE1	1:B:4505:LEU:CD2	2.52	0.40
1:B:772:LEU:N	1:B:773:PRO:HD2	2.36	0.40
1:B:776:ARG:O	1:B:777:LYS:C	2.63	0.40
1:B:1645:PHE:HB2	1:B:1744:MET:HE3	2.02	0.40
1:B:3142:TRP:CD1	1:B:3201:LEU:HD22	2.56	0.40
1:B:3690:GLN:HG3	1:B:3757:PHE:CD1	2.56	0.40
1:B:4258:LYS:HE2	1:B:4669:LEU:HD23	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	B	4466/5188 (86%)	4309 (96%)	156 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	802	GLN

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	B	4086/4623 (88%)	4050 (99%)	36 (1%)	70	85

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	399	SER
1	B	511	SER
1	B	586	CYS
1	B	641	ILE
1	B	703	PHE
1	B	733	SER
1	B	757	VAL
1	B	874	LEU
1	B	887	SER
1	B	1183	ARG
1	B	1420	ILE
1	B	1495	SER
1	B	1692	SER
1	B	1745	MET
1	B	1855	SER
1	B	1950	ILE
1	B	2040	TYR
1	B	2123	GLU
1	B	2260	GLU
1	B	2340	LEU

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Mol	Chain	Res	Type
1	B	2380	MET
1	B	2407	MET
1	B	2468	VAL
1	B	2485	CYS
1	B	2569	ASN
1	B	3053	MET
1	B	3094	THR
1	B	3278	THR
1	B	3588	HIS
1	B	3683	LYS
1	B	3891	ILE
1	B	4001	HIS
1	B	4131	SER
1	B	4297	LEU
1	B	4543	HIS
1	B	5018	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	449	ASN
1	B	561	ASN
1	B	718	GLN
1	B	749	ASN
1	B	1089	HIS
1	B	1310	HIS
1	B	1313	HIS
1	B	1314	GLN
1	B	1418	ASN
1	B	1624	GLN
1	B	1664	ASN
1	B	1849	GLN
1	B	2010	GLN
1	B	2017	HIS
1	B	2439	HIS
1	B	2480	HIS
1	B	2613	HIS
1	B	2769	GLN
1	B	3013	GLN
1	B	3024	GLN
1	B	3148	GLN
1	B	3169	HIS

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Mol	Chain	Res	Type
1	B	3191	GLN
1	B	3690	GLN
1	B	4101	GLN
1	B	4347	ASN
1	B	4420	ASN
1	B	4503	HIS
1	B	4521	GLN
1	B	4619	ASN
1	B	4697	HIS
1	B	4836	ASN
1	B	4886	GLN
1	B	5077	HIS

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](#)

4 monosaccharides are 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	$\# Z > 2$
2	GLC	F	1	2	11,11,12	0.71	0	15,15,17	0.75	0
2	GLC	F	2	2	11,11,12	0.76	0	15,15,17	1.14	2 (13%)
2	GLC	F	3	2	11,11,12	0.71	0	15,15,17	0.92	1 (6%)
2	GLC	F	4	2	11,11,12	0.64	0	15,15,17	1.47	1 (6%)

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
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	0/2/19/22	0/1/1/1
2	GLC	F	4	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	GLC	C1-O5-C5	4.55	118.36	112.19
2	F	3	GLC	O5-C1-C2	-2.31	107.21	110.77
2	F	2	GLC	C1-C2-C3	2.26	112.45	109.67
2	F	2	GLC	O5-C1-C2	-2.06	107.60	110.77

There are no chirality outliers.

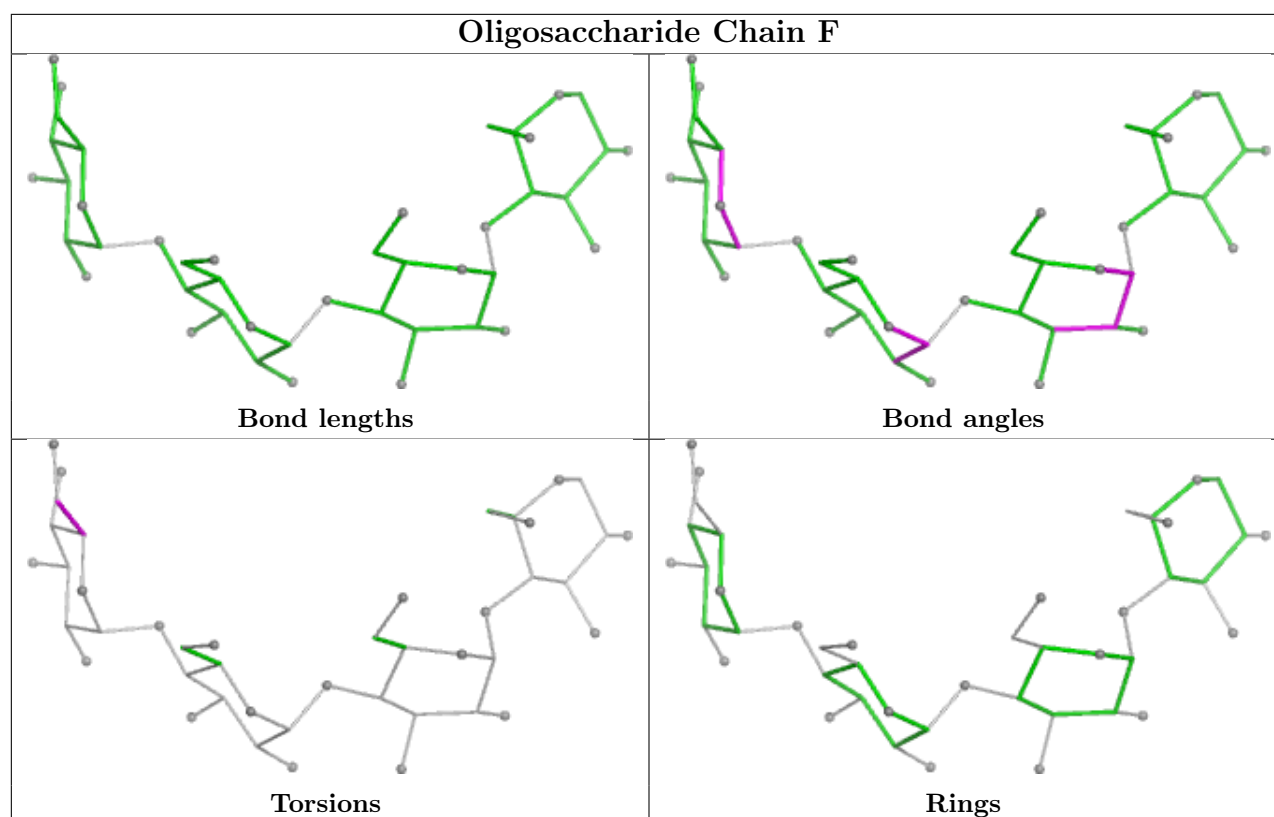
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	4	GLC	O5-C5-C6-O6

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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are 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	$\# Z > 2$
3	ATP	B	5301	-	29,33,33	0.45	0	44,52,52	0.86	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5301	-	-	10/22/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5301	ATP	O3'-C3'-C4'	-2.13	104.89	111.05
3	B	5301	ATP	PB-O3B-PG	2.06	139.90	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

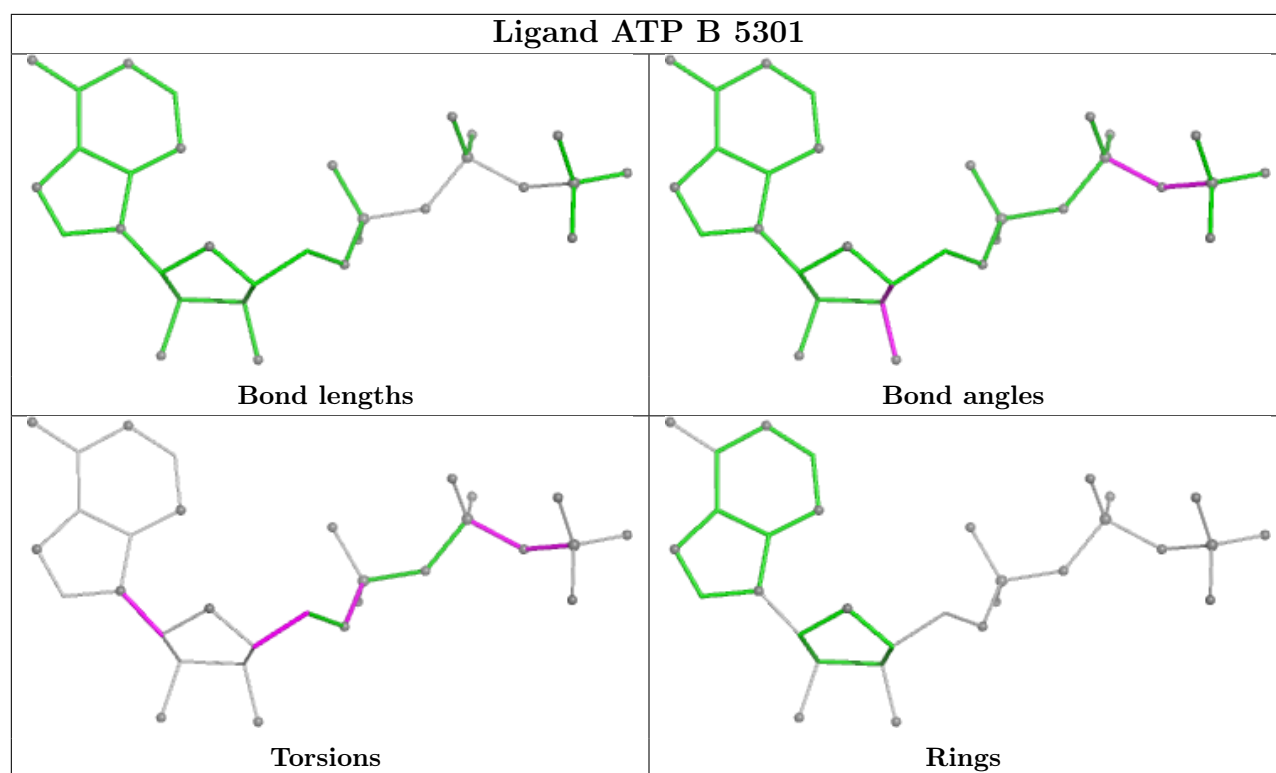
Mol	Chain	Res	Type	Atoms
3	B	5301	ATP	PB-O3B-PG-O3G
3	B	5301	ATP	C5'-O5'-PA-O1A
3	B	5301	ATP	C5'-O5'-PA-O2A
3	B	5301	ATP	O4'-C4'-C5'-O5'
3	B	5301	ATP	O4'-C1'-N9-C4
3	B	5301	ATP	O4'-C1'-N9-C8
3	B	5301	ATP	C3'-C4'-C5'-O5'
3	B	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	PB-O3B-PG-O2G
3	B	5301	ATP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

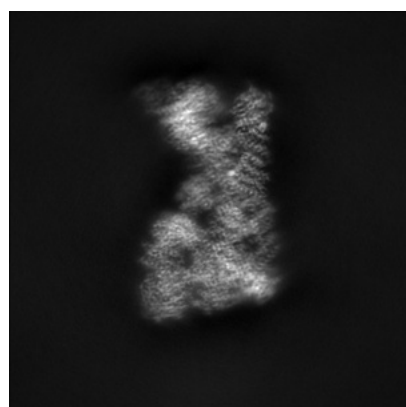
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55686. These allow visual inspection of the internal detail of the map and identification of artifacts.

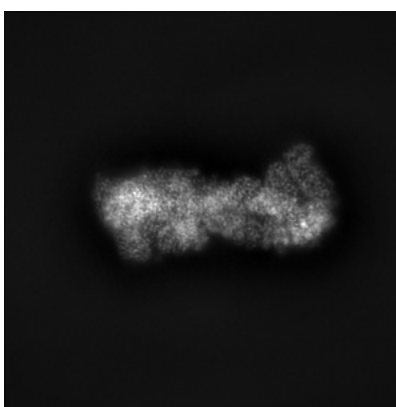
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

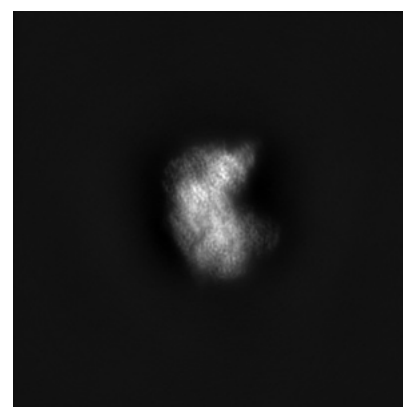
6.1.1 Primary map



X



Y

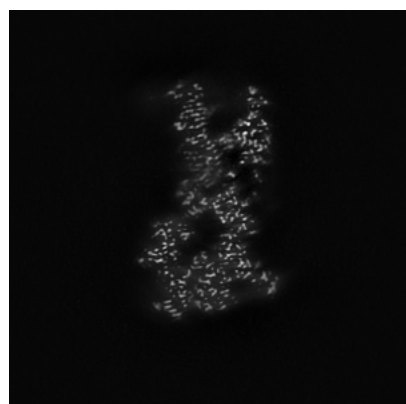


Z

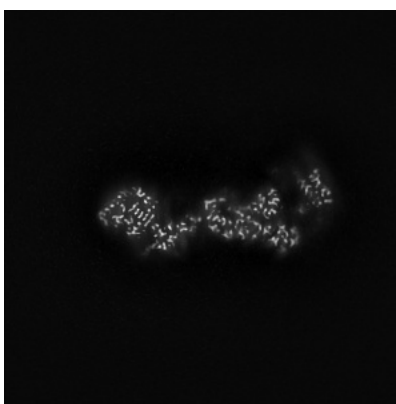
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

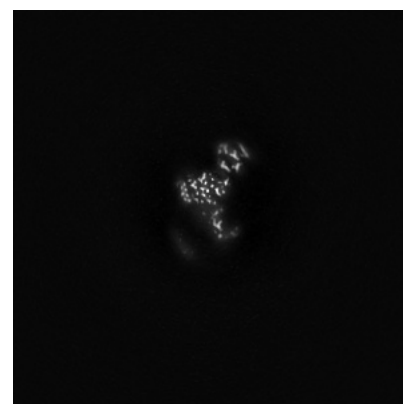
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

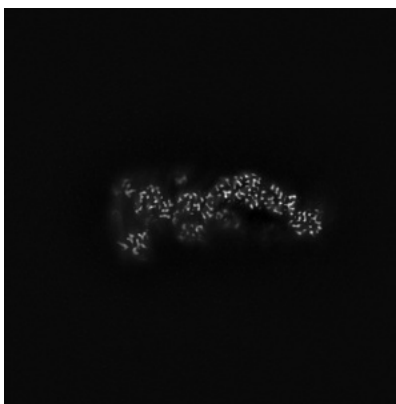
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

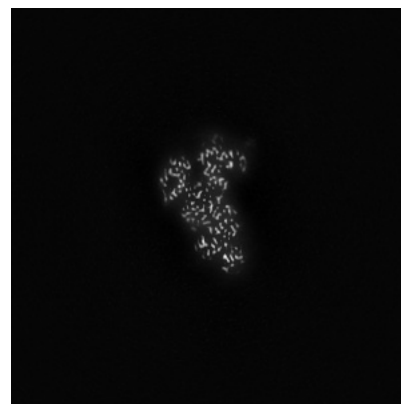
6.3.1 Primary map



X Index: 156



Y Index: 174

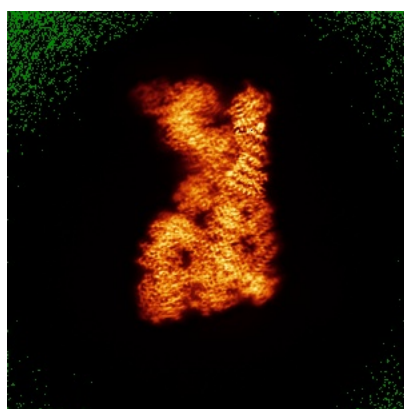


Z Index: 100

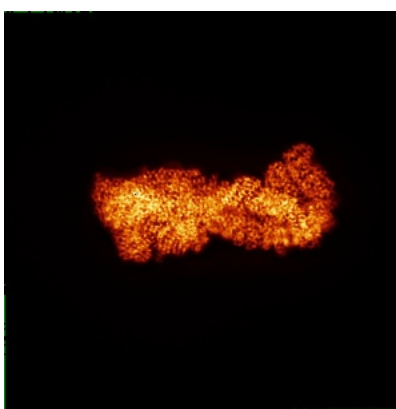
The images above show the largest variance slices of the map in three orthogonal directions.

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

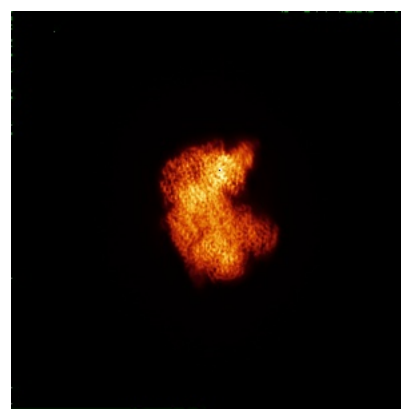
6.4.1 Primary map



X



Y



Z

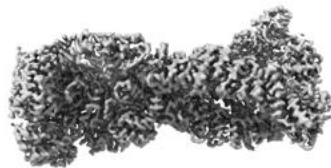
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

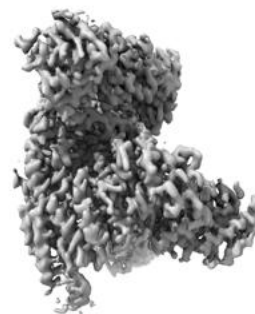
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

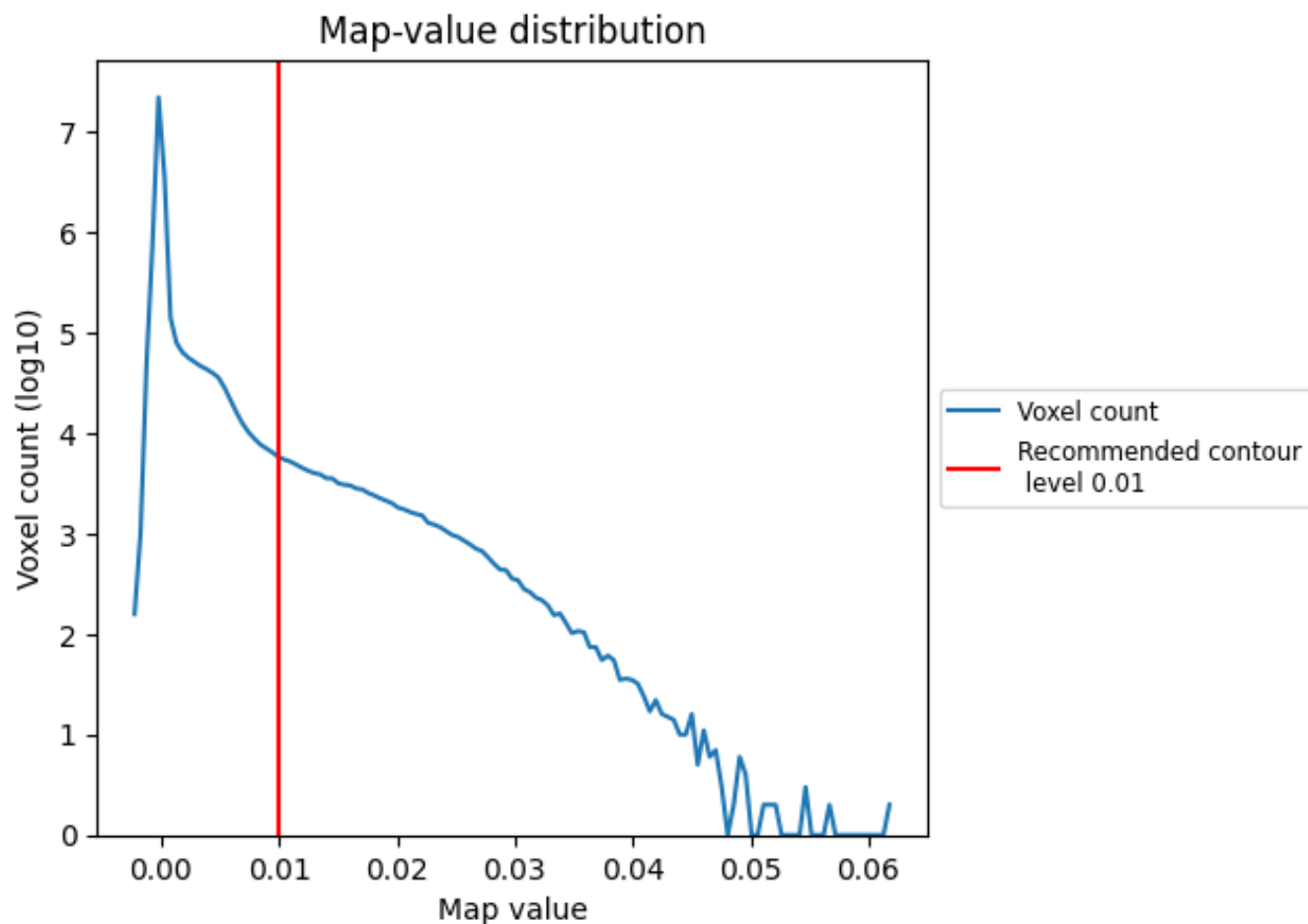
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

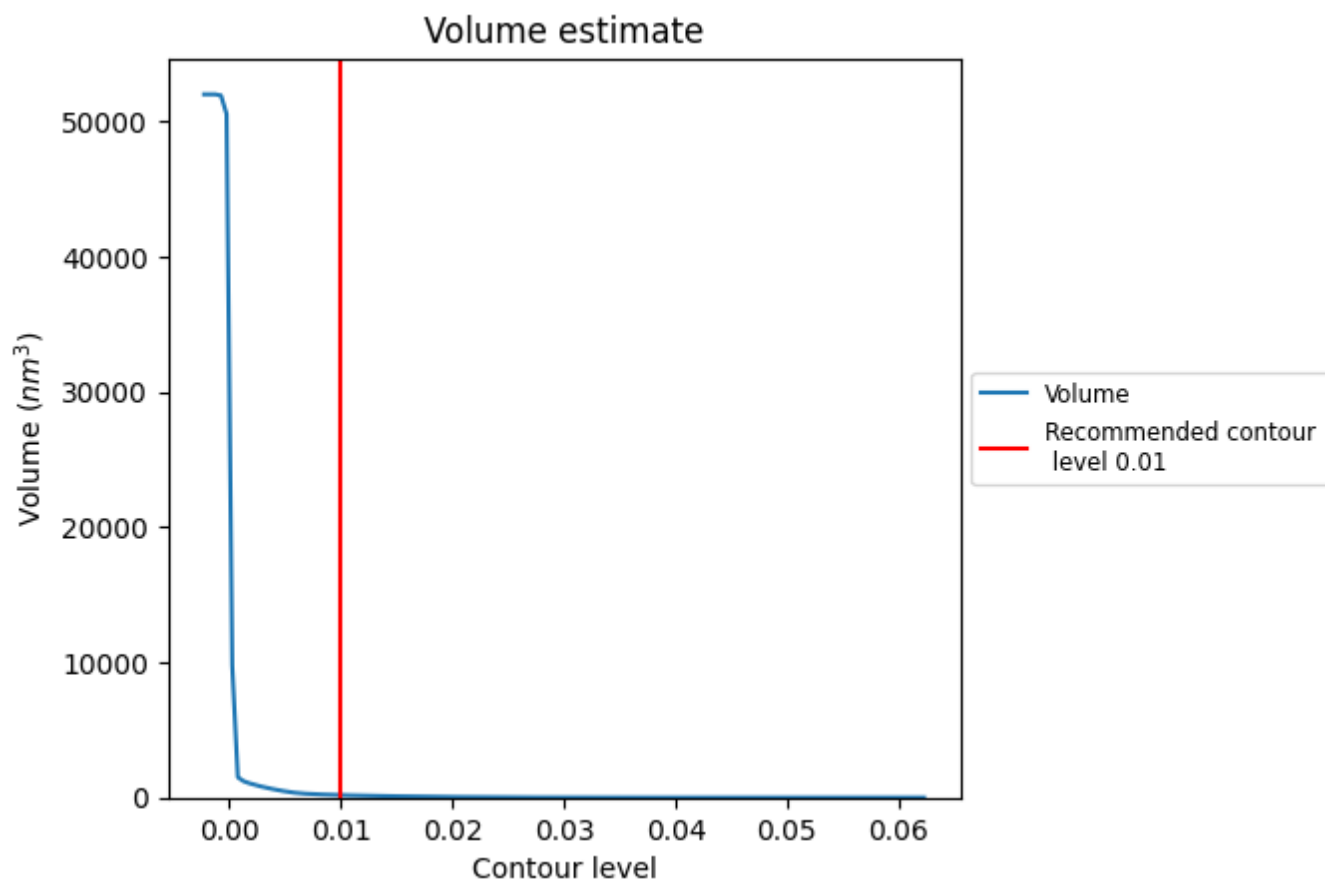
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

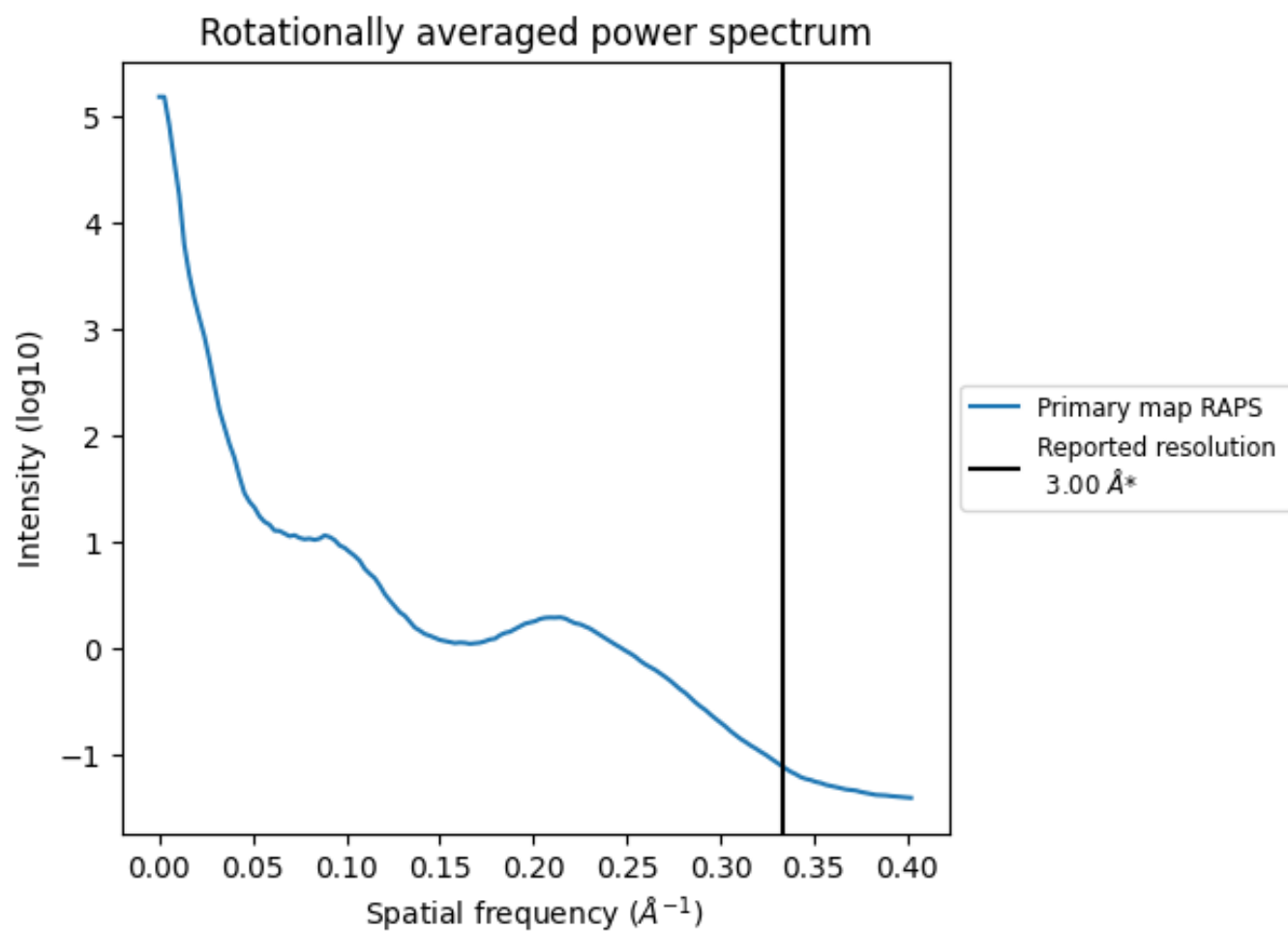
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 163 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 0.333 $\text{\AA}^{-1}$

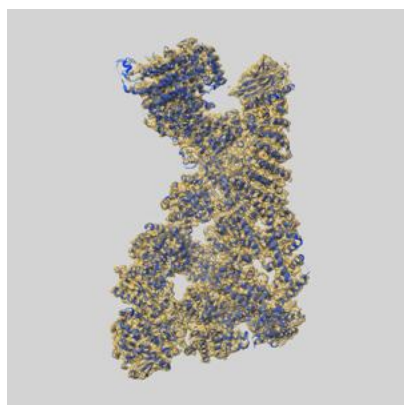
8 Fourier-Shell correlation ⓘ

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

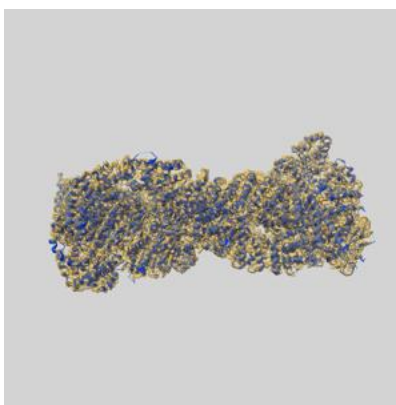
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55686 and PDB model 9T8H. Per-residue inclusion information can be found in section [3](#) on page [6](#).

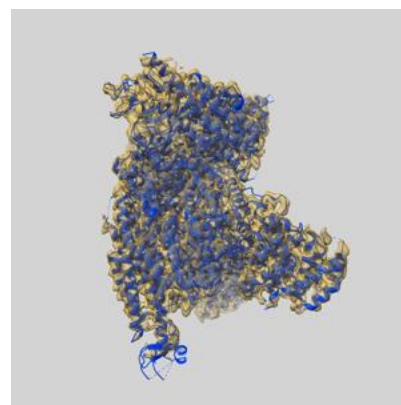
9.1 Map-model overlay [i](#)



X



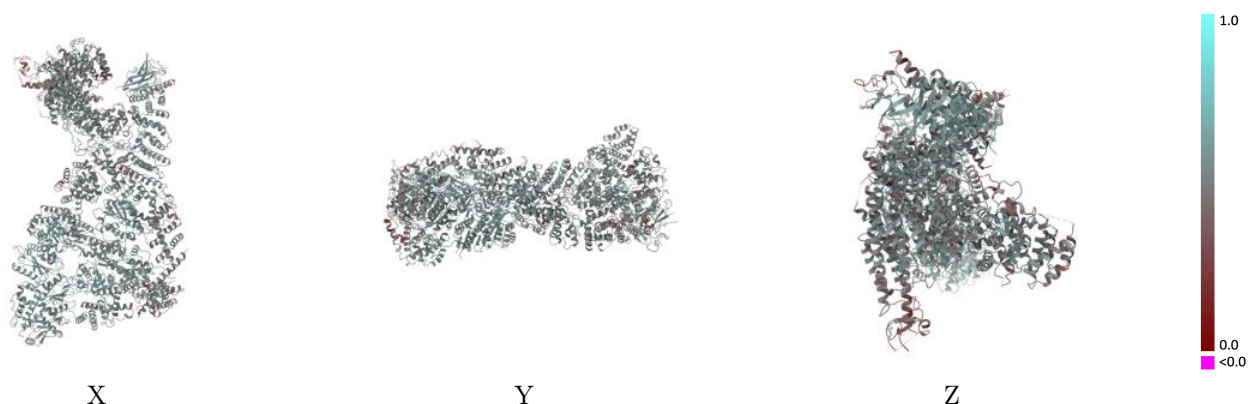
Y



Z

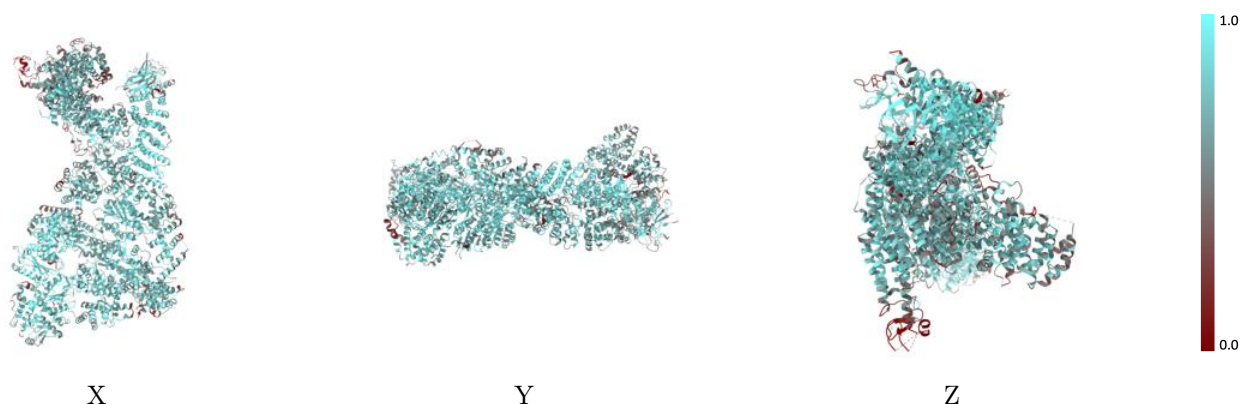
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



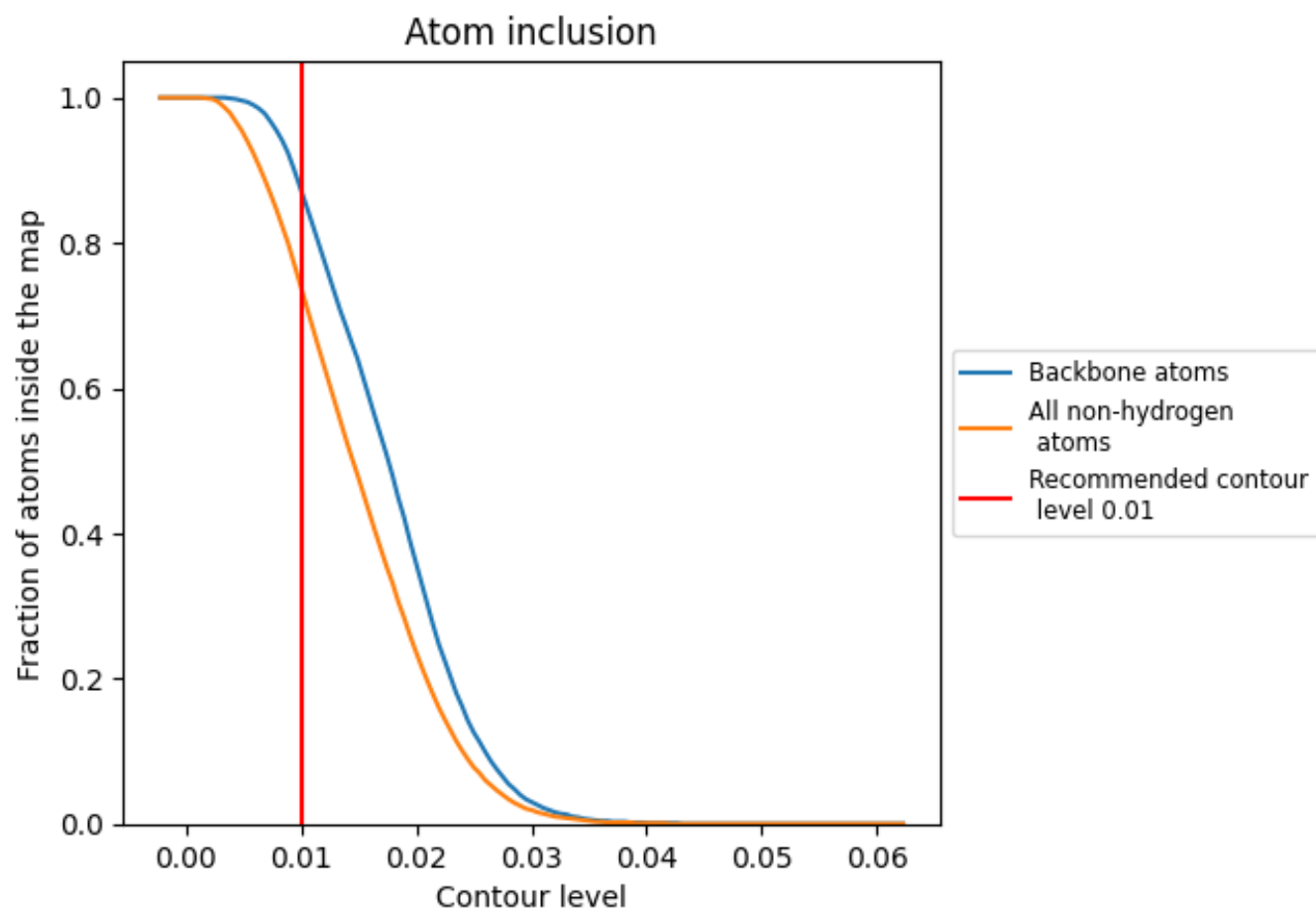
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.5190
B	0.7380	0.5190
F	0.6140	0.4600

