



Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 07:17 PM EST

PDB ID : 9NYD / pdb_00009nyd
EMDB ID : EMD-49931
Title : Cryo-EM structure of the glycosyltransferase GtrB in the pre-catalysis and product-bound state
Authors : Morgan, R.T.; Motta, S.; Gil-Iturbe, E.; di Muccio, G.; Bhattacharjee, B.; Romagnoli, A.; Anwar, M.T.; Mishra, B.; Ashraf, K.; Bang, I.; di Marino, D.; Lowary, T.L.; Quick, M.; Petrou, V.I.; Stowell, M.H.B.; Nygaard, R.; Mancia, F.
Deposited on : 2025-03-27
Resolution : 2.85 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.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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)

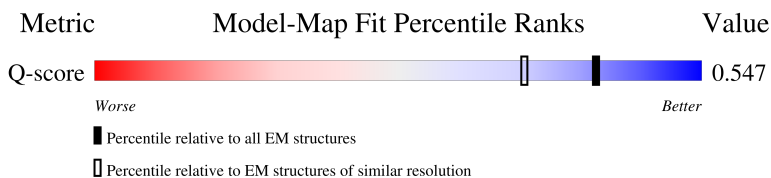
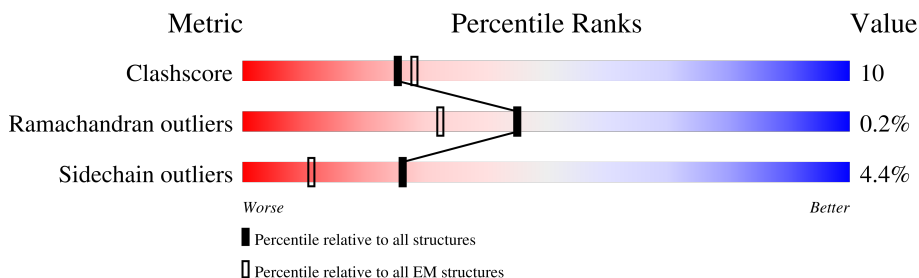
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	341	<div> <div>30%</div> <div>66%</div> <div>24%</div> <div>9%</div> </div>
1	B	341	<div> <div>28%</div> <div>65%</div> <div>23%</div> <div>11%</div> </div>
1	C	341	<div> <div>29%</div> <div>61%</div> <div>25%</div> <div>10%</div> </div>

Continued on next page...

Validation Pipeline (wwPDB-VP) : 2.47

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	D	341	<p>30% 69% 20% 11%</p>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10227 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 Uncharacterized glycosyltransferase sll0501.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	312	Total	C	N	O	S	0	0
			2541	1667	417	449	8		
1	B	305	Total	C	N	O	S	0	0
			2481	1630	404	439	8		
1	C	306	Total	C	N	O	S	0	0
			2492	1636	408	440	8		
1	D	305	Total	C	N	O	S	0	0
			2481	1630	404	439	8		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q55487
A	-21	HIS	-	expression tag	UNP Q55487
A	-20	HIS	-	expression tag	UNP Q55487
A	-19	HIS	-	expression tag	UNP Q55487
A	-18	HIS	-	expression tag	UNP Q55487
A	-17	HIS	-	expression tag	UNP Q55487
A	-16	HIS	-	expression tag	UNP Q55487
A	-15	SER	-	expression tag	UNP Q55487
A	-14	SER	-	expression tag	UNP Q55487
A	-13	GLY	-	expression tag	UNP Q55487
A	-12	VAL	-	expression tag	UNP Q55487
A	-11	ASP	-	expression tag	UNP Q55487
A	-10	LEU	-	expression tag	UNP Q55487
A	-9	GLY	-	expression tag	UNP Q55487
A	-8	THR	-	expression tag	UNP Q55487
A	-7	GLU	-	expression tag	UNP Q55487
A	-6	ASN	-	expression tag	UNP Q55487
A	-5	LEU	-	expression tag	UNP Q55487
A	-4	TYR	-	expression tag	UNP Q55487
A	-3	PHE	-	expression tag	UNP Q55487
A	-2	GLN	-	expression tag	UNP Q55487
A	-1	SER	-	expression tag	UNP Q55487

Continued on next page...

Continued from previous page...

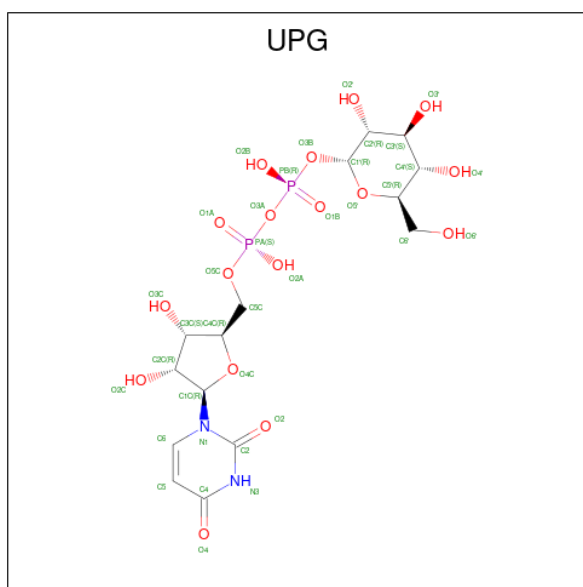
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASN	-	expression tag	UNP Q55487
A	1	ALA	-	expression tag	UNP Q55487
B	-22	MET	-	initiating methionine	UNP Q55487
B	-21	HIS	-	expression tag	UNP Q55487
B	-20	HIS	-	expression tag	UNP Q55487
B	-19	HIS	-	expression tag	UNP Q55487
B	-18	HIS	-	expression tag	UNP Q55487
B	-17	HIS	-	expression tag	UNP Q55487
B	-16	HIS	-	expression tag	UNP Q55487
B	-15	SER	-	expression tag	UNP Q55487
B	-14	SER	-	expression tag	UNP Q55487
B	-13	GLY	-	expression tag	UNP Q55487
B	-12	VAL	-	expression tag	UNP Q55487
B	-11	ASP	-	expression tag	UNP Q55487
B	-10	LEU	-	expression tag	UNP Q55487
B	-9	GLY	-	expression tag	UNP Q55487
B	-8	THR	-	expression tag	UNP Q55487
B	-7	GLU	-	expression tag	UNP Q55487
B	-6	ASN	-	expression tag	UNP Q55487
B	-5	LEU	-	expression tag	UNP Q55487
B	-4	TYR	-	expression tag	UNP Q55487
B	-3	PHE	-	expression tag	UNP Q55487
B	-2	GLN	-	expression tag	UNP Q55487
B	-1	SER	-	expression tag	UNP Q55487
B	0	ASN	-	expression tag	UNP Q55487
B	1	ALA	-	expression tag	UNP Q55487
C	-22	MET	-	initiating methionine	UNP Q55487
C	-21	HIS	-	expression tag	UNP Q55487
C	-20	HIS	-	expression tag	UNP Q55487
C	-19	HIS	-	expression tag	UNP Q55487
C	-18	HIS	-	expression tag	UNP Q55487
C	-17	HIS	-	expression tag	UNP Q55487
C	-16	HIS	-	expression tag	UNP Q55487
C	-15	SER	-	expression tag	UNP Q55487
C	-14	SER	-	expression tag	UNP Q55487
C	-13	GLY	-	expression tag	UNP Q55487
C	-12	VAL	-	expression tag	UNP Q55487
C	-11	ASP	-	expression tag	UNP Q55487
C	-10	LEU	-	expression tag	UNP Q55487
C	-9	GLY	-	expression tag	UNP Q55487
C	-8	THR	-	expression tag	UNP Q55487
C	-7	GLU	-	expression tag	UNP Q55487

Continued on next page...

Continued from previous page...

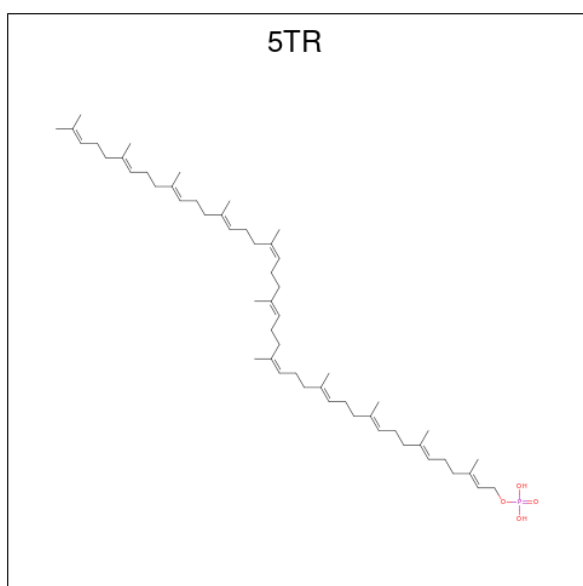
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASN	-	expression tag	UNP Q55487
C	-5	LEU	-	expression tag	UNP Q55487
C	-4	TYR	-	expression tag	UNP Q55487
C	-3	PHE	-	expression tag	UNP Q55487
C	-2	GLN	-	expression tag	UNP Q55487
C	-1	SER	-	expression tag	UNP Q55487
C	0	ASN	-	expression tag	UNP Q55487
C	1	ALA	-	expression tag	UNP Q55487
D	-22	MET	-	initiating methionine	UNP Q55487
D	-21	HIS	-	expression tag	UNP Q55487
D	-20	HIS	-	expression tag	UNP Q55487
D	-19	HIS	-	expression tag	UNP Q55487
D	-18	HIS	-	expression tag	UNP Q55487
D	-17	HIS	-	expression tag	UNP Q55487
D	-16	HIS	-	expression tag	UNP Q55487
D	-15	SER	-	expression tag	UNP Q55487
D	-14	SER	-	expression tag	UNP Q55487
D	-13	GLY	-	expression tag	UNP Q55487
D	-12	VAL	-	expression tag	UNP Q55487
D	-11	ASP	-	expression tag	UNP Q55487
D	-10	LEU	-	expression tag	UNP Q55487
D	-9	GLY	-	expression tag	UNP Q55487
D	-8	THR	-	expression tag	UNP Q55487
D	-7	GLU	-	expression tag	UNP Q55487
D	-6	ASN	-	expression tag	UNP Q55487
D	-5	LEU	-	expression tag	UNP Q55487
D	-4	TYR	-	expression tag	UNP Q55487
D	-3	PHE	-	expression tag	UNP Q55487
D	-2	GLN	-	expression tag	UNP Q55487
D	-1	SER	-	expression tag	UNP Q55487
D	0	ASN	-	expression tag	UNP Q55487
D	1	ALA	-	expression tag	UNP Q55487

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			36	15	2	17	2	
2	B	1	Total	C	N	O	P	0
			36	15	2	17	2	
2	D	1	Total	C	N	O	P	0
			36	15	2	17	2	

- Molecule 3 is [(2 {E},6 {E},10 {E},14 {E},18 {Z},22 {E},26 {Z},30 {E},34 {E},38 {E})-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaenyl] dihydrogen phosphate (CCD ID: 5TR) (formula: $C_{55}H_{91}O_4P$) (labeled as "Ligand of Interest" by depositor).

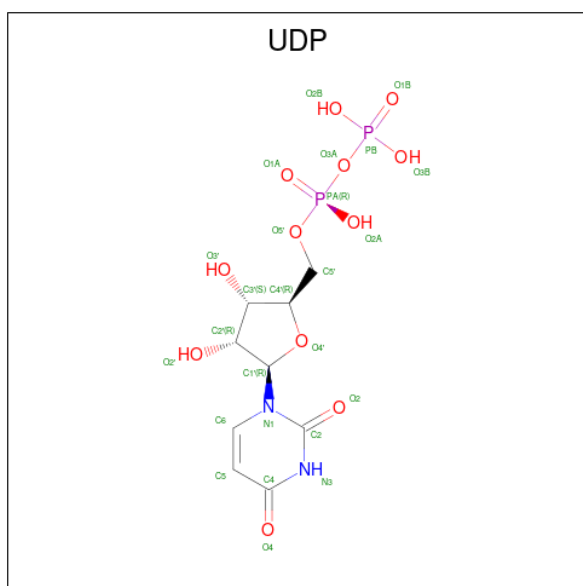


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			23	18	4	1	
3	B	1	Total	C	O	P	0
			23	18	4	1	
3	D	1	Total	C	O	P	0
			23	18	4	1	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

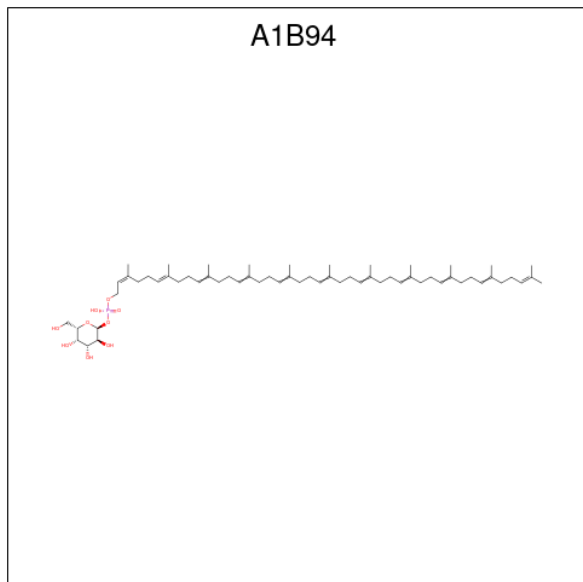
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).

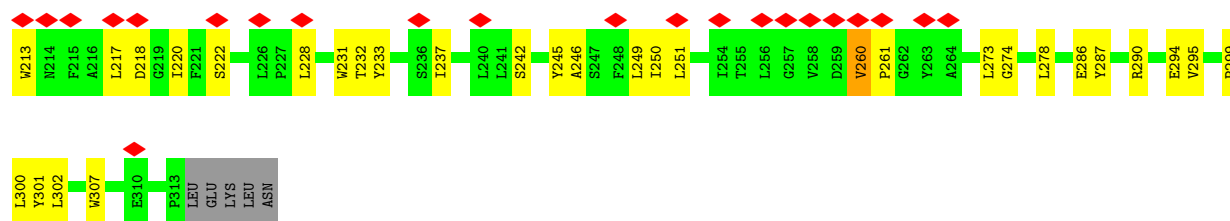


Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			25	9	2	12	2	

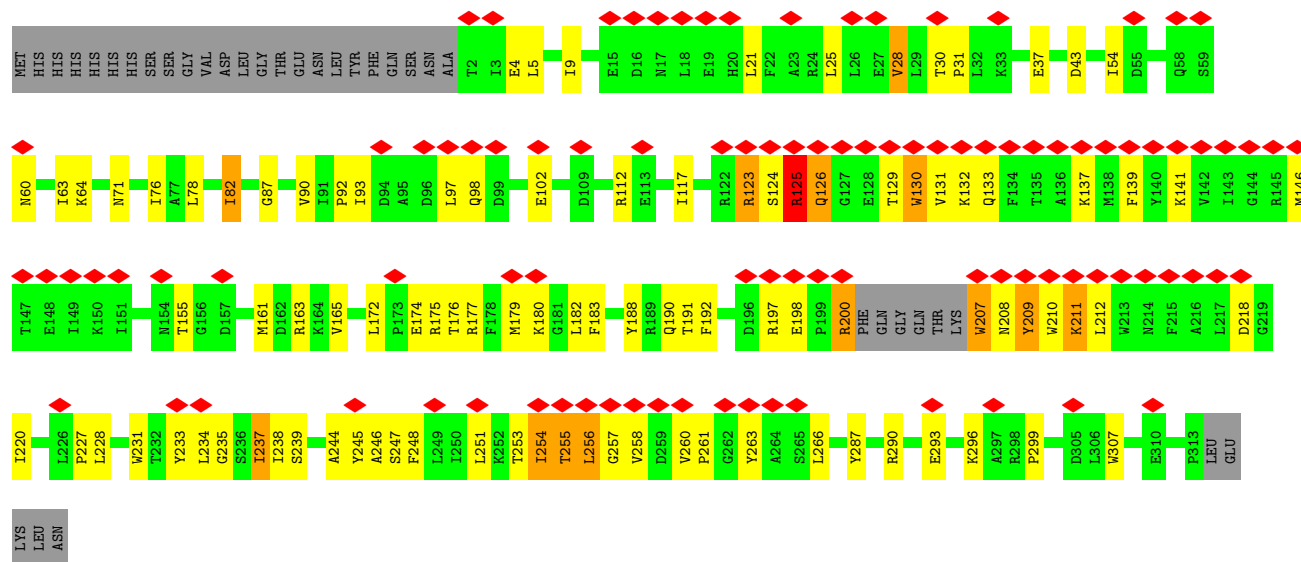
- Molecule 6 is undecaprenyl phosphate-glucose (CCD ID: A1B94) (formula: $C_{61}H_{101}O_9P$) (labeled as "Ligand of Interest" by depositor).



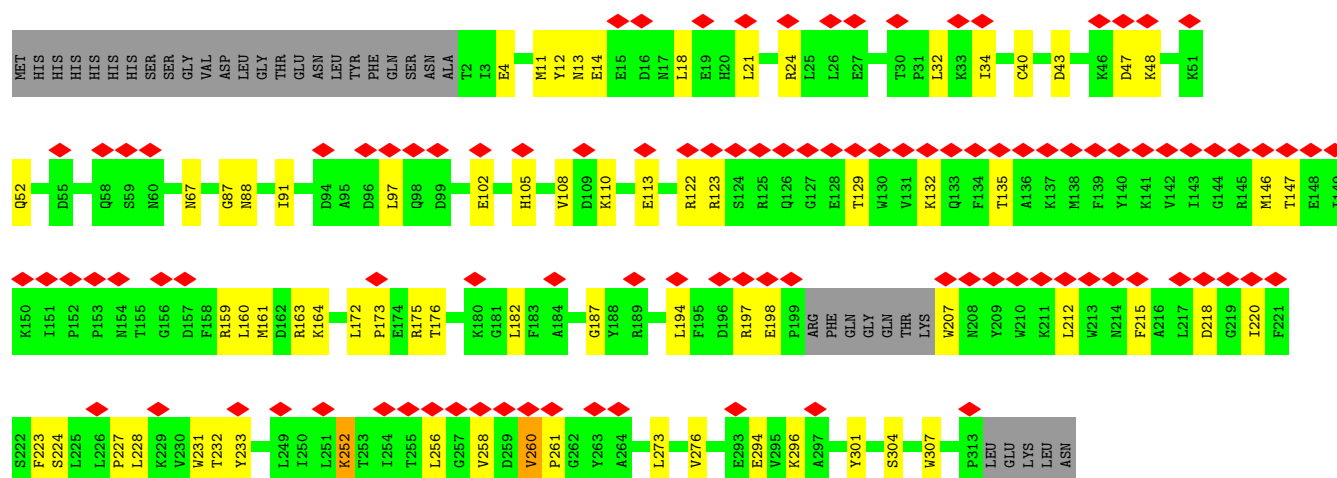
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
6	C	1	26	16	9	1	0



• Molecule 1: Uncharacterized glycosyltransferase sll0501



• Molecule 1: Uncharacterized glycosyltransferase sll0501



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46382	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 ($e^-/\text{\AA}^2$)	58.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.194	Depositor
Minimum map value	-0.827	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5TR, A1B94, UDP, UPG

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	0.26	1/2602 (0.0%)	0.42	0/3530
1	B	0.22	0/2540	0.39	0/3447
1	C	0.46	3/2551 (0.1%)	0.73	11/3461 (0.3%)
1	D	0.28	0/2540	0.44	0/3447
All	All	0.32	4/10233 (0.0%)	0.51	11/13885 (0.1%)

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
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	256	LEU	C-N	6.55	1.43	1.33
1	A	33	LYS	C-N	-6.48	1.25	1.33
1	C	234	LEU	C-N	5.63	1.40	1.33
1	C	255	THR	C-N	-5.05	1.26	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ILE	N-CA-C	-17.64	94.91	111.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	LEU	N-CA-C	-7.54	103.00	111.14
1	C	235	GLY	N-CA-C	-7.18	102.88	112.14
1	C	209	TYR	CB-CA-C	6.78	121.75	111.18
1	C	209	TYR	N-CA-C	-6.46	102.64	111.56
1	C	210	TRP	N-CA-C	-6.08	105.89	113.55
1	C	235	GLY	CA-C-O	-6.07	115.35	121.90
1	C	246	ALA	N-CA-C	-5.99	104.33	111.69
1	C	234	LEU	CA-C-N	-5.54	115.08	120.34
1	C	234	LEU	C-N-CA	-5.54	115.08	120.34
1	C	255	THR	N-CA-C	-5.20	101.81	109.86

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain
1	A	189	ARG	Sidechain
1	B	189	ARG	Sidechain
1	C	123	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	200	ARG	Sidechain
1	D	122	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2541	0	2598	62	0
1	B	2481	0	2536	58	0
1	C	2492	0	2549	62	0
1	D	2481	0	2536	45	0
2	A	36	0	21	3	0
2	B	36	0	21	6	0
2	D	36	0	21	2	0
3	A	23	0	29	3	0
3	B	23	0	29	2	0
3	D	23	0	29	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	25	0	10	0	0
6	C	26	0	0	2	0
All	All	10227	0	10379	207	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 10.

All (207) 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)
2:B:401:UPG:C4C	2:B:401:UPG:O4C	1.67	1.22
2:D:401:UPG:O4C	2:D:401:UPG:C4C	1.67	1.19
2:A:401:UPG:C4C	2:A:401:UPG:O4C	1.67	1.18
1:A:245:TYR:HA	1:A:248:PHE:HB3	1.62	0.79
1:D:32:LEU:HD11	1:D:108:VAL:HG21	1.65	0.77
1:A:187:GLY:O	1:B:69:SER:HB2	1.87	0.74
1:C:263:TYR:HB3	1:C:266:LEU:HD13	1.70	0.73
1:C:245:TYR:HA	1:C:248:PHE:HB3	1.71	0.73
1:C:124:SER:O	1:C:125:ARG:C	2.32	0.72
1:D:32:LEU:HB3	1:D:34:ILE:HG12	1.71	0.71
1:A:188:TYR:O	1:A:190:GLN:HG3	1.92	0.70
1:D:260:VAL:HB	1:D:261:PRO:HD3	1.77	0.67
1:B:96:ASP:OD2	2:B:401:UPG:H3C	1.95	0.67
1:C:198:GLU:HG2	1:C:200:ARG:H	1.60	0.66
1:B:260:VAL:HG12	1:B:261:PRO:HD2	1.78	0.65
1:A:274:GLY:HA3	1:D:273:LEU:HD13	1.78	0.65
1:B:161:MET:HE3	1:B:166:VAL:HG22	1.79	0.64
1:A:110:LYS:HD2	1:A:191:THR:HG21	1.80	0.64
1:A:212:LEU:HG	3:A:402:5TR:H81	1.80	0.63
1:C:4:GLU:OE2	1:C:112:ARG:NH2	2.32	0.63
1:A:122:ARG:HH22	1:A:125:ARG:HA	1.63	0.62
1:C:124:SER:O	1:C:126:GLN:N	2.32	0.62
1:C:28:VAL:HG21	1:C:102:GLU:HA	1.82	0.62
1:A:128:GLU:HG2	1:A:132:LYS:HG2	1.80	0.61
1:A:128:GLU:HB3	1:A:132:LYS:HB3	1.83	0.61
1:B:37:GLU:HG3	1:B:64:LYS:HE3	1.82	0.61
1:A:144:GLY:HA2	1:A:147:THR:HG22	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:PRO:O	1:D:175:ARG:NH1	2.33	0.61
1:D:18:LEU:HD12	1:D:52:GLN:HB2	1.83	0.60
1:C:263:TYR:CE1	1:D:261:PRO:HG2	2.37	0.60
1:B:74:LYS:NZ	1:B:94:ASP:OD1	2.35	0.60
1:B:233:TYR:O	1:B:237:ILE:HD12	2.01	0.60
1:A:60:ASN:HB3	1:A:63:ILE:HD12	1.83	0.59
1:B:286:GLU:OE1	1:B:290:ARG:NH1	2.33	0.59
1:A:101:PRO:O	1:A:104:ILE:HB	2.03	0.59
1:A:11:MET:SD	1:A:40:CYS:HB3	2.43	0.58
1:D:197:ARG:NH2	1:D:198:GLU:O	2.36	0.58
1:A:273:LEU:HD13	1:B:274:GLY:HA3	1.85	0.58
1:B:111:TRP:NE1	1:B:162:ASP:OD1	2.28	0.58
1:B:307:TRP:CE2	1:C:54:ILE:HD11	2.39	0.57
1:A:91:ILE:HD11	1:A:160:LEU:HD12	1.87	0.56
1:B:231:TRP:C	1:B:233:TYR:H	2.10	0.56
1:C:251:LEU:HA	1:C:254:ILE:HG12	1.87	0.56
1:A:233:TYR:OH	1:B:213:TRP:NE1	2.31	0.56
1:B:290:ARG:HH21	1:C:218:ASP:HA	1.70	0.56
1:C:82:ILE:HG13	1:C:90:VAL:HG11	1.87	0.56
1:A:11:MET:HE1	1:A:53:LEU:HD21	1.87	0.56
1:A:215:PHE:CD2	3:A:402:5TR:H80	2.41	0.56
1:D:231:TRP:C	1:D:233:TYR:H	2.12	0.55
1:A:307:TRP:HB2	1:B:65:ILE:HB	1.87	0.55
1:C:9:ILE:HD13	1:C:21:LEU:HD21	1.88	0.54
1:C:255:THR:O	1:C:256:LEU:C	2.48	0.54
1:B:43:ASP:OD2	2:B:401:UPG:H5	2.08	0.53
1:C:172:LEU:HD23	1:C:299:PRO:HD2	1.90	0.53
1:C:290:ARG:HH12	1:D:218:ASP:HA	1.73	0.53
1:A:82:ILE:HG13	1:A:90:VAL:HG11	1.90	0.53
1:B:245:TYR:O	1:B:249:LEU:HD22	2.08	0.53
1:A:232:THR:HG21	1:A:286:GLU:HG2	1.91	0.53
1:D:13:ASN:HA	1:D:47:ASP:HB3	1.91	0.53
1:D:24:ARG:NE	1:D:97:LEU:HD13	2.23	0.53
1:D:21:LEU:HA	1:D:97:LEU:HD11	1.90	0.53
1:D:110:LYS:HA	1:D:113:GLU:HG3	1.91	0.53
1:D:123:ARG:HA	1:D:194:LEU:HD22	1.90	0.52
1:C:129:THR:O	1:C:130:TRP:C	2.53	0.52
1:C:231:TRP:C	1:C:233:TYR:H	2.17	0.52
1:C:263:TYR:CZ	1:D:261:PRO:HG2	2.44	0.52
1:A:117:ILE:HB	1:A:190:GLN:HG2	1.92	0.51
1:B:301:TYR:HB3	1:C:76:ILE:HG22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:NH2	1:B:196:ASP:HB3	2.26	0.50
1:D:87:GLY:O	1:D:163:ARG:NH2	2.32	0.50
1:A:218:ASP:O	1:A:222:SER:HB3	2.10	0.50
1:A:296:LYS:NZ	1:D:294:GLU:OE2	2.44	0.50
1:B:128:GLU:HG2	1:B:132:LYS:HG2	1.93	0.50
1:D:91:ILE:HD11	1:D:160:LEU:HD12	1.94	0.49
1:B:132:LYS:HZ1	3:B:402:5TR:H69	1.75	0.49
1:D:47:ASP:OD1	1:D:48:LYS:N	2.44	0.49
1:A:231:TRP:C	1:A:233:TYR:H	2.21	0.49
1:A:295:VAL:HG23	1:B:295:VAL:HG21	1.94	0.49
1:A:135:THR:HB	3:A:402:5TR:H37	1.95	0.49
1:B:294:GLU:OE2	1:C:175:ARG:N	2.46	0.49
1:A:290:ARG:HH21	1:B:218:ASP:HA	1.78	0.48
1:A:307:TRP:CE2	1:B:54:ILE:HD11	2.48	0.48
1:C:117:ILE:HG12	1:C:165:VAL:HG21	1.95	0.48
1:A:65:ILE:HB	1:D:307:TRP:HB2	1.96	0.48
1:B:197:ARG:HH22	3:B:402:5TR:H83	1.77	0.48
1:D:159:ARG:HB2	1:D:159:ARG:HH11	1.79	0.48
1:C:43:ASP:OD2	1:C:71:ASN:ND2	2.46	0.48
1:D:102:GLU:O	1:D:105:HIS:HB2	2.14	0.48
1:A:287:TYR:CE2	1:B:228:LEU:HB2	2.49	0.48
1:C:139:PHE:HB2	6:C:403:A1B94:C04	2.43	0.48
1:C:258:VAL:HG23	1:C:260:VAL:HG22	1.96	0.48
1:C:176:THR:OG1	1:C:296:LYS:NZ	2.46	0.48
1:D:252:LYS:HE3	1:D:258:VAL:HG21	1.96	0.48
1:B:96:ASP:HB2	1:B:98:GLN:OE1	2.14	0.47
1:C:37:GLU:HB2	1:C:64:LYS:HE3	1.96	0.47
1:A:76:ILE:HG22	1:D:301:TYR:HB3	1.94	0.47
1:A:103:LEU:HD23	1:A:158:PHE:CE2	2.49	0.47
1:B:164:LYS:HE3	1:B:164:LYS:HB2	1.64	0.47
1:D:12:TYR:H	1:D:14:GLU:HG2	1.79	0.47
1:C:287:TYR:CE2	1:D:228:LEU:HB2	2.49	0.47
1:A:137:LYS:HD2	1:A:137:LYS:C	2.40	0.47
1:A:207:TRP:O	1:A:208:ASN:C	2.58	0.47
1:A:244:ALA:O	1:A:245:TYR:HB3	2.15	0.47
1:A:128:GLU:HG3	1:A:207:TRP:CZ2	2.50	0.47
1:B:172:LEU:HD13	1:B:182:LEU:HD23	1.96	0.47
6:C:403:A1B94:O22	6:C:403:A1B94:O20	2.32	0.47
1:D:4:GLU:OE1	1:D:88:ASN:ND2	2.45	0.47
1:D:215:PHE:HD2	3:D:402:5TR:H80	1.80	0.47
1:D:172:LEU:HD23	1:D:182:LEU:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TRP:HZ3	1:B:67:ASN:HB2	1.80	0.47
1:C:260:VAL:HB	1:C:261:PRO:HD2	1.96	0.47
1:B:218:ASP:O	1:B:222:SER:OG	2.28	0.46
1:D:147:THR:HG22	1:D:223:PHE:HE2	1.79	0.46
1:B:5:LEU:HD11	1:B:91:ILE:HG13	1.96	0.46
1:C:87:GLY:O	1:C:163:ARG:NH1	2.43	0.46
1:B:43:ASP:OD2	1:B:71:ASN:ND2	2.49	0.46
1:D:176:THR:OG1	1:D:296:LYS:NZ	2.48	0.46
1:A:149:ILE:HG13	1:A:184:ALA:O	2.16	0.46
1:B:78:LEU:HD22	1:B:92:PRO:HB3	1.97	0.46
1:A:276:VAL:HG12	1:B:278:LEU:HD21	1.97	0.46
1:C:191:THR:OG1	1:C:192:PHE:N	2.48	0.46
1:A:239:SER:O	1:A:243:LEU:HD23	2.15	0.46
1:B:96:ASP:OD2	2:B:401:UPG:H5C1	2.15	0.46
1:C:208:ASN:OD1	1:C:211:LYS:N	2.41	0.46
2:B:401:UPG:O4C	2:B:401:UPG:C5C	2.54	0.46
1:B:172:LEU:HD23	1:B:299:PRO:HD2	1.97	0.46
1:C:9:ILE:HG12	1:C:93:ILE:HG22	1.98	0.46
1:C:146:MET:HE1	1:C:227:PRO:HD3	1.98	0.46
2:A:401:UPG:O4C	2:A:401:UPG:C5C	2.54	0.45
1:B:117:ILE:HG12	1:B:165:VAL:HG11	1.97	0.45
1:B:10:PRO:O	2:B:401:UPG:O3C	2.24	0.45
1:B:196:ASP:N	1:B:196:ASP:OD1	2.48	0.45
1:B:9:ILE:HG12	1:B:93:ILE:HG22	1.97	0.45
1:A:146:MET:HG2	1:A:224:SER:OG	2.17	0.45
1:B:146:MET:HE1	1:B:220:ILE:HD13	1.98	0.45
1:D:164:LYS:NZ	1:D:304:SER:O	2.41	0.45
1:A:5:LEU:HD11	1:A:91:ILE:HG13	1.97	0.45
1:A:278:LEU:HD21	1:D:276:VAL:HG12	1.97	0.45
1:A:37:GLU:OE1	1:A:64:LYS:NZ	2.44	0.45
1:C:137:LYS:O	1:C:141:LYS:HG2	2.16	0.45
1:A:123:ARG:HG2	1:A:194:LEU:HB3	1.99	0.45
1:A:174:GLU:O	1:A:177:ARG:NH1	2.43	0.45
1:A:205:THR:O	1:A:206:LYS:C	2.59	0.45
1:B:117:ILE:HD12	1:B:190:GLN:HG2	1.99	0.45
1:B:287:TYR:CE2	1:C:228:LEU:HB2	2.52	0.44
1:C:82:ILE:HD11	1:C:92:PRO:HG3	1.98	0.44
1:B:125:ARG:O	1:B:127:GLY:N	2.50	0.44
1:C:125:ARG:HB3	1:C:133:GLN:HE21	1.83	0.44
1:B:115:TYR:CD1	1:B:191:THR:HB	2.53	0.44
1:A:48:LYS:HB3	1:A:48:LYS:HE3	1.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:THR:OG1	1:C:31:PRO:HD3	2.17	0.44
1:C:130:TRP:O	1:C:131:VAL:C	2.61	0.44
1:C:98:GLN:HB3	1:C:197:ARG:HH11	1.83	0.44
1:C:207:TRP:HA	1:C:207:TRP:CE3	2.52	0.44
1:B:125:ARG:NH1	1:B:154:ASN:OD1	2.51	0.44
1:D:132:LYS:HD3	1:D:207:TRP:CH2	2.53	0.43
1:A:70:ARG:HD3	1:D:187:GLY:HA3	2.00	0.43
1:A:208:ASN:OD1	1:A:208:ASN:N	2.51	0.43
1:C:180:LYS:H	1:C:180:LYS:HG2	1.61	0.43
1:B:24:ARG:NH1	1:B:102:GLU:OE2	2.51	0.43
1:B:186:VAL:HG12	1:B:302:LEU:HD11	2.01	0.43
1:A:182:LEU:O	1:A:186:VAL:HG22	2.18	0.43
1:C:125:ARG:HA	1:C:125:ARG:HD3	1.43	0.43
1:B:231:TRP:O	1:B:232:THR:HB	2.18	0.43
1:C:141:LYS:HZ3	1:C:141:LYS:HG3	1.70	0.43
1:A:206:LYS:H	1:A:206:LYS:HG3	1.59	0.43
1:A:43:ASP:OD2	2:A:401:UPG:H5	2.19	0.43
1:A:82:ILE:HG23	1:A:166:VAL:HG13	2.01	0.43
1:C:21:LEU:HA	1:C:97:LEU:HD11	2.00	0.42
1:B:24:ARG:NH1	1:B:101:PRO:HD2	2.34	0.42
1:C:179:MET:HG3	1:C:183:PHE:CE2	2.54	0.42
1:C:188:TYR:O	1:C:190:GLN:HG3	2.19	0.42
1:C:208:ASN:HB2	1:C:209:TYR:H	1.72	0.42
1:C:21:LEU:HD12	1:C:97:LEU:HG	2.00	0.42
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.88	0.42
1:D:43:ASP:OD2	2:D:401:UPG:H5	2.20	0.42
1:D:273:LEU:HD23	1:D:273:LEU:HA	1.86	0.42
1:D:231:TRP:O	1:D:232:THR:OG1	2.35	0.42
1:B:231:TRP:C	1:B:233:TYR:N	2.77	0.42
1:C:253:THR:HG23	1:C:258:VAL:HB	2.02	0.42
1:C:5:LEU:HD23	1:C:5:LEU:HA	1.91	0.42
1:A:215:PHE:CD2	1:A:215:PHE:C	2.98	0.42
1:B:101:PRO:O	1:B:104:ILE:HB	2.20	0.42
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.81	0.42
1:A:125:ARG:HB3	1:A:128:GLU:OE1	2.19	0.42
1:C:172:LEU:HD13	1:C:182:LEU:HD13	2.01	0.41
1:D:146:MET:SD	1:D:224:SER:OG	2.76	0.41
1:A:263:TYR:CG	1:A:264:ALA:N	2.88	0.41
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.93	0.41
3:D:402:5TR:H33	3:D:402:5TR:H21	1.91	0.41
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:HB2	1:A:188:TYR:HB3	2.03	0.41
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.80	0.41
1:C:251:LEU:HA	1:C:254:ILE:CG1	2.49	0.41
1:D:220:ILE:HG23	1:D:227:PRO:HG2	2.03	0.41
1:C:293:GLU:HG2	1:D:176:THR:HG22	2.03	0.41
1:C:174:GLU:O	1:C:177:ARG:NH1	2.42	0.40
1:C:244:ALA:O	1:C:245:TYR:HB3	2.21	0.40
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.84	0.40
1:D:212:LEU:HD23	1:D:212:LEU:HA	1.80	0.40
1:A:232:THR:O	1:A:236:SER:OG	2.25	0.40
1:C:307:TRP:HZ3	1:D:67:ASN:HB2	1.86	0.40
1:D:161:MET:HE3	1:D:161:MET:HB2	1.98	0.40
1:B:82:ILE:HG12	1:B:90:VAL:HG11	2.02	0.40
1:C:60:ASN:HB2	1:C:63:ILE:HD12	2.02	0.40
1:C:82:ILE:HG12	1:C:161:MET:HE1	2.03	0.40
1:B:246:ALA:O	1:B:250:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/341 (91%)	289 (93%)	20 (6%)	1 (0%)	37	55
1	B	301/341 (88%)	284 (94%)	17 (6%)	0	100	100
1	C	302/341 (89%)	279 (92%)	21 (7%)	2 (1%)	19	36
1	D	301/341 (88%)	285 (95%)	16 (5%)	0	100	100
All	All	1214/1364 (89%)	1137 (94%)	74 (6%)	3 (0%)	45	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	125	ARG
1	C	257	GLY
1	A	153	PRO

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	275/301 (91%)	266 (97%)	9 (3%)	33	59
1	B	269/301 (89%)	254 (94%)	15 (6%)	17	35
1	C	270/301 (90%)	253 (94%)	17 (6%)	15	30
1	D	269/301 (89%)	262 (97%)	7 (3%)	41	67
All	All	1083/1204 (90%)	1035 (96%)	48 (4%)	26	46

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	124	SER
1	A	145	ARG
1	A	146	MET
1	A	149	ILE
1	A	193	VAL
1	A	204	GLN
1	A	206	LYS
1	A	208	ASN
1	B	37	GLU
1	B	48	LYS
1	B	58	GLN
1	B	96	ASP
1	B	97	LEU
1	B	113	GLU
1	B	189	ARG
1	B	196	ASP
1	B	210	TRP
1	B	212	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	217	LEU
1	B	242	SER
1	B	251	LEU
1	B	260	VAL
1	B	300	LEU
1	C	28	VAL
1	C	82	ILE
1	C	123	ARG
1	C	125	ARG
1	C	126	GLN
1	C	130	TRP
1	C	132	LYS
1	C	155	THR
1	C	207	TRP
1	C	211	LYS
1	C	212	LEU
1	C	220	ILE
1	C	237	ILE
1	C	238	ILE
1	C	239	SER
1	C	247	SER
1	C	254	ILE
1	D	11	MET
1	D	40	CYS
1	D	129	THR
1	D	135	THR
1	D	252	LYS
1	D	256	LEU
1	D	260	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	190	GLN
1	B	133	GLN
1	C	71	ASN
1	C	86	GLN
1	C	126	GLN
1	C	133	GLN
1	C	171	GLN
1	D	42	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	133	GLN
1	D	277	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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
2	UPG	D	401	4	37,38,38	3.93	17 (45%)	55,58,58	1.26	5 (9%)
3	5TR	A	402	-	22,22,59	0.32	0	25,27,72	0.52	0
5	UDP	C	402	4	25,26,26	4.09	14 (56%)	38,40,40	1.60	7 (18%)
2	UPG	A	401	4	37,38,38	3.94	17 (45%)	55,58,58	1.25	5 (9%)
2	UPG	B	401	4	37,38,38	3.94	17 (45%)	55,58,58	1.21	4 (7%)
3	5TR	B	402	-	22,22,59	0.32	0	25,27,72	0.59	0
3	5TR	D	402	-	22,22,59	0.32	0	25,27,72	0.47	0
6	A1B94	C	403	-	25,26,71	1.53	5 (20%)	33,36,90	2.13	6 (18%)

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	UPG	D	401	4	-	9/23/59/59	0/3/3/3
3	5TR	A	402	-	-	3/23/23/67	-
5	UDP	C	402	4	-	6/16/32/32	0/2/2/2
2	UPG	A	401	4	-	8/23/59/59	0/3/3/3
2	UPG	B	401	4	-	7/23/59/59	0/3/3/3
3	5TR	B	402	-	-	5/23/23/67	-
3	5TR	D	402	-	-	5/23/23/67	-
6	A1B94	C	403	-	-	9/20/40/94	0/1/1/1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	UPG	O4C-C4C	9.99	1.67	1.45
2	A	401	UPG	O4C-C4C	9.95	1.67	1.45
2	D	401	UPG	O4C-C4C	9.92	1.67	1.45
5	C	402	UDP	C2-N3	9.31	1.54	1.38
2	B	401	UPG	C2-N1	9.25	1.52	1.38
2	A	401	UPG	C2-N1	9.14	1.52	1.38
2	D	401	UPG	C2-N1	8.98	1.52	1.38
5	C	402	UDP	C2-N1	8.89	1.52	1.38
2	D	401	UPG	C2-N3	8.74	1.53	1.38
2	B	401	UPG	C2-N3	8.74	1.53	1.38
2	A	401	UPG	C2-N3	8.64	1.53	1.38
5	C	402	UDP	C3'-C4'	-7.51	1.34	1.53
2	B	401	UPG	C3C-C4C	-7.31	1.34	1.53
2	A	401	UPG	C3C-C4C	-7.22	1.34	1.53
2	D	401	UPG	C3C-C4C	-7.17	1.34	1.53
2	A	401	UPG	PA-O3A	7.03	1.67	1.59
2	D	401	UPG	PB-O3A	6.91	1.67	1.59
2	A	401	UPG	PB-O3A	6.90	1.66	1.59
2	D	401	UPG	PA-O3A	6.89	1.66	1.59
2	B	401	UPG	PB-O3A	6.71	1.66	1.59
2	B	401	UPG	PA-O3A	6.67	1.66	1.59
5	C	402	UDP	C2'-C1'	-6.27	1.33	1.53
2	B	401	UPG	O4C-C1C	-5.68	1.28	1.42
2	D	401	UPG	O4C-C1C	-5.65	1.28	1.42
2	A	401	UPG	O4C-C1C	-5.65	1.28	1.42
5	C	402	UDP	C4-N3	5.55	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402	UDP	O4'-C1'	5.28	1.54	1.42
5	C	402	UDP	PA-O3A	5.05	1.64	1.59
2	B	401	UPG	C6-C5	4.34	1.45	1.35
2	D	401	UPG	C6-C5	4.29	1.45	1.35
2	B	401	UPG	O2C-C2C	-4.26	1.32	1.43
2	A	401	UPG	O2C-C2C	-4.24	1.32	1.43
5	C	402	UDP	O4'-C4'	4.23	1.54	1.45
2	A	401	UPG	C6-C5	4.22	1.44	1.35
2	D	401	UPG	O2C-C2C	-4.19	1.32	1.43
2	A	401	UPG	C4-N3	4.11	1.45	1.38
2	D	401	UPG	C4-N3	4.10	1.45	1.38
2	B	401	UPG	C4-N3	4.08	1.45	1.38
2	D	401	UPG	O5'-C1'	3.95	1.52	1.41
2	A	401	UPG	O5'-C1'	3.90	1.51	1.41
2	B	401	UPG	O5'-C1'	3.79	1.51	1.41
5	C	402	UDP	C6-C5	3.69	1.43	1.35
2	A	401	UPG	O2-C2	-3.64	1.16	1.23
2	D	401	UPG	O2-C2	-3.63	1.16	1.23
2	B	401	UPG	O2-C2	-3.60	1.16	1.23
2	D	401	UPG	O3C-C3C	3.22	1.50	1.43
2	B	401	UPG	O3C-C3C	3.17	1.50	1.43
2	A	401	UPG	O3C-C3C	3.09	1.50	1.43
2	D	401	UPG	C6-N1	2.96	1.45	1.38
2	B	401	UPG	C6-N1	2.92	1.45	1.38
2	A	401	UPG	C6-N1	2.89	1.45	1.38
2	D	401	UPG	PA-O5C	2.82	1.70	1.59
2	B	401	UPG	PA-O5C	2.76	1.70	1.59
2	B	401	UPG	O4-C4	-2.75	1.19	1.24
2	A	401	UPG	O4-C4	-2.75	1.19	1.24
2	D	401	UPG	O4-C4	-2.75	1.19	1.24
2	A	401	UPG	PA-O5C	2.74	1.70	1.59
5	C	402	UDP	C6-N1	2.71	1.44	1.38
6	C	403	A1B94	P12-O15	2.71	1.67	1.59
2	D	401	UPG	C2C-C1C	2.58	1.61	1.53
6	C	403	A1B94	C06-C07	2.55	1.56	1.51
2	A	401	UPG	C2C-C1C	2.49	1.61	1.53
6	C	403	A1B94	C10-C09	2.46	1.56	1.49
2	B	401	UPG	C2C-C1C	2.45	1.61	1.53
5	C	402	UDP	O2-C2	-2.37	1.18	1.23
5	C	402	UDP	PA-O5'	2.34	1.68	1.59
6	C	403	A1B94	O17-C16	2.33	1.47	1.41
5	C	402	UDP	C3'-C2'	2.27	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402	UDP	O2'-C2'	-2.14	1.37	1.43
6	C	403	A1B94	P12-O11	2.00	1.67	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	403	A1B94	C03-C02-C01	-7.97	96.25	114.59
6	C	403	A1B94	C05-C04-C02	-5.06	110.78	127.64
2	D	401	UPG	C5-C4-N3	4.06	120.49	114.80
5	C	402	UDP	C4-N3-C2	-4.06	121.58	126.61
2	A	401	UPG	C5-C4-N3	3.97	120.35	114.80
2	B	401	UPG	C5-C4-N3	3.93	120.31	114.80
5	C	402	UDP	C5-C4-N3	3.81	120.14	114.80
5	C	402	UDP	C2'-C1'-N1	3.76	123.72	113.25
6	C	403	A1B94	C10-C09-C07	-3.74	120.07	126.20
2	D	401	UPG	C4-N3-C2	-3.52	122.25	126.61
2	B	401	UPG	C4-N3-C2	-3.49	122.28	126.61
2	A	401	UPG	C4-N3-C2	-3.48	122.30	126.61
6	C	403	A1B94	C01-C02-C04	3.15	132.12	122.66
2	A	401	UPG	O4-C4-C5	-3.04	119.92	125.16
2	D	401	UPG	O4-C4-C5	-3.01	119.97	125.16
6	C	403	A1B94	C03-C02-C04	2.99	131.63	122.66
5	C	402	UDP	O4'-C1'-N1	-2.95	101.67	108.36
2	B	401	UPG	O4-C4-C5	-2.93	120.10	125.16
5	C	402	UDP	O4-C4-C5	-2.93	120.11	125.16
6	C	403	A1B94	C08-C07-C06	2.82	120.13	115.23
5	C	402	UDP	C2'-C3'-C4'	2.52	107.47	102.61
2	D	401	UPG	O5'-C1'-O3B	-2.27	108.40	111.36
2	D	401	UPG	C2C-C3C-C4C	2.12	106.71	102.61
5	C	402	UDP	C4'-O4'-C1'	-2.11	104.82	109.47
2	A	401	UPG	C1C-N1-C2	2.10	121.36	117.59
2	A	401	UPG	O5'-C1'-O3B	-2.04	108.70	111.36
2	B	401	UPG	O5'-C1'-O3B	-2.03	108.72	111.36

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	UPG	O4C-C4C-C5C-O5C
2	B	401	UPG	PA-O3A-PB-O3B
2	D	401	UPG	O5'-C1'-O3B-PB
6	C	403	A1B94	C16-O15-P12-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	403	A1B94	C16-O15-P12-O13
6	C	403	A1B94	C21-C18-C19-O20
6	C	403	A1B94	C05-C06-C07-C08
6	C	403	A1B94	C05-C06-C07-C09
6	C	403	A1B94	O17-C18-C19-O20
2	A	401	UPG	C3C-C4C-C5C-O5C
2	B	401	UPG	O4C-C4C-C5C-O5C
2	D	401	UPG	O4C-C4C-C5C-O5C
3	B	402	5TR	C45-C49-C52-C55
3	D	402	5TR	C45-C49-C52-C55
3	B	402	5TR	C45-C49-C52-C56
3	D	402	5TR	C45-C49-C52-C56
3	A	402	5TR	C34-C29-C31-C36
6	C	403	A1B94	C04-C05-C06-C07
2	A	401	UPG	O5'-C5'-C6'-O6'
2	A	401	UPG	C4'-C5'-C6'-O6'
2	D	401	UPG	O5'-C5'-C6'-O6'
2	B	401	UPG	C3C-C4C-C5C-O5C
6	C	403	A1B94	C09-C10-O11-P12
2	B	401	UPG	C2'-C1'-O3B-PB
2	D	401	UPG	C3C-C4C-C5C-O5C
2	D	401	UPG	O4C-C1C-N1-C2
2	D	401	UPG	O4C-C1C-N1-C6
3	B	402	5TR	C17-C19-C27-C20
3	D	402	5TR	C17-C19-C27-C20
3	B	402	5TR	C26-C17-C19-C27
2	D	401	UPG	PA-O3A-PB-O2B
2	B	401	UPG	O4C-C1C-N1-C6
6	C	403	A1B94	C10-O11-P12-O13
2	A	401	UPG	O4C-C1C-N1-C6
5	C	402	UDP	O4'-C1'-N1-C6
2	A	401	UPG	O5'-C1'-O3B-PB
3	A	402	5TR	C19-C17-C26-C43
3	A	402	5TR	C19-C17-C26-C34
2	B	401	UPG	O4C-C1C-N1-C2
3	D	402	5TR	C29-C31-C36-C50
3	B	402	5TR	C29-C31-C36-C50
2	A	401	UPG	O4C-C1C-N1-C2
5	C	402	UDP	PB-O3A-PA-O1A
5	C	402	UDP	C2'-C1'-N1-C6
2	D	401	UPG	PA-O3A-PB-O1B
2	D	401	UPG	C2'-C1'-O3B-PB

Continued on next page...

Continued from previous page...

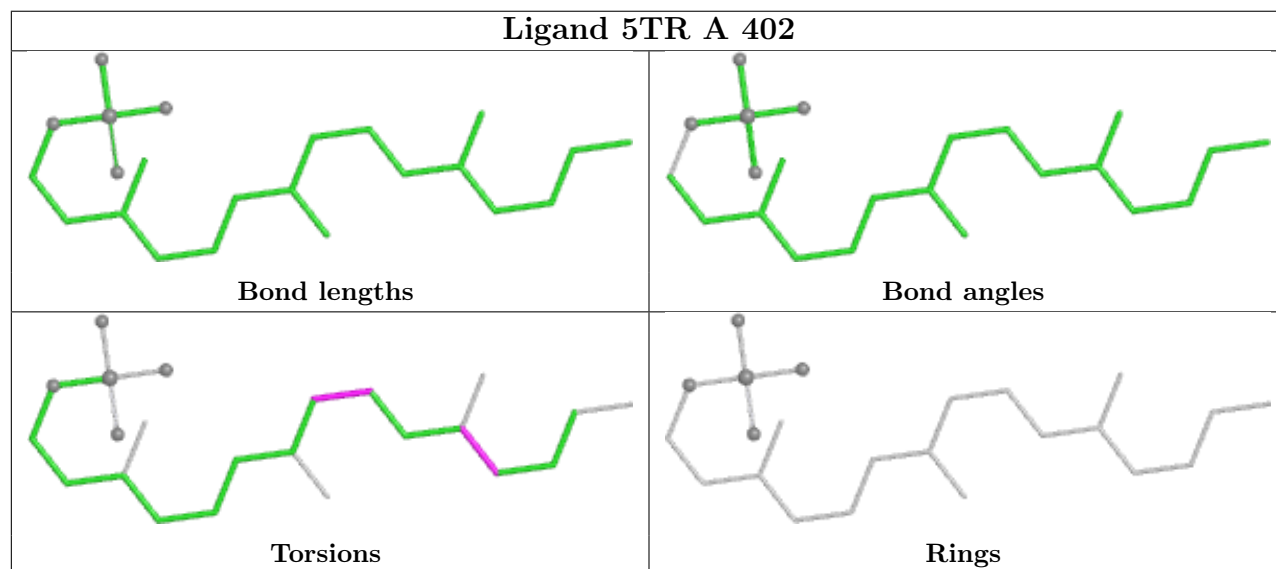
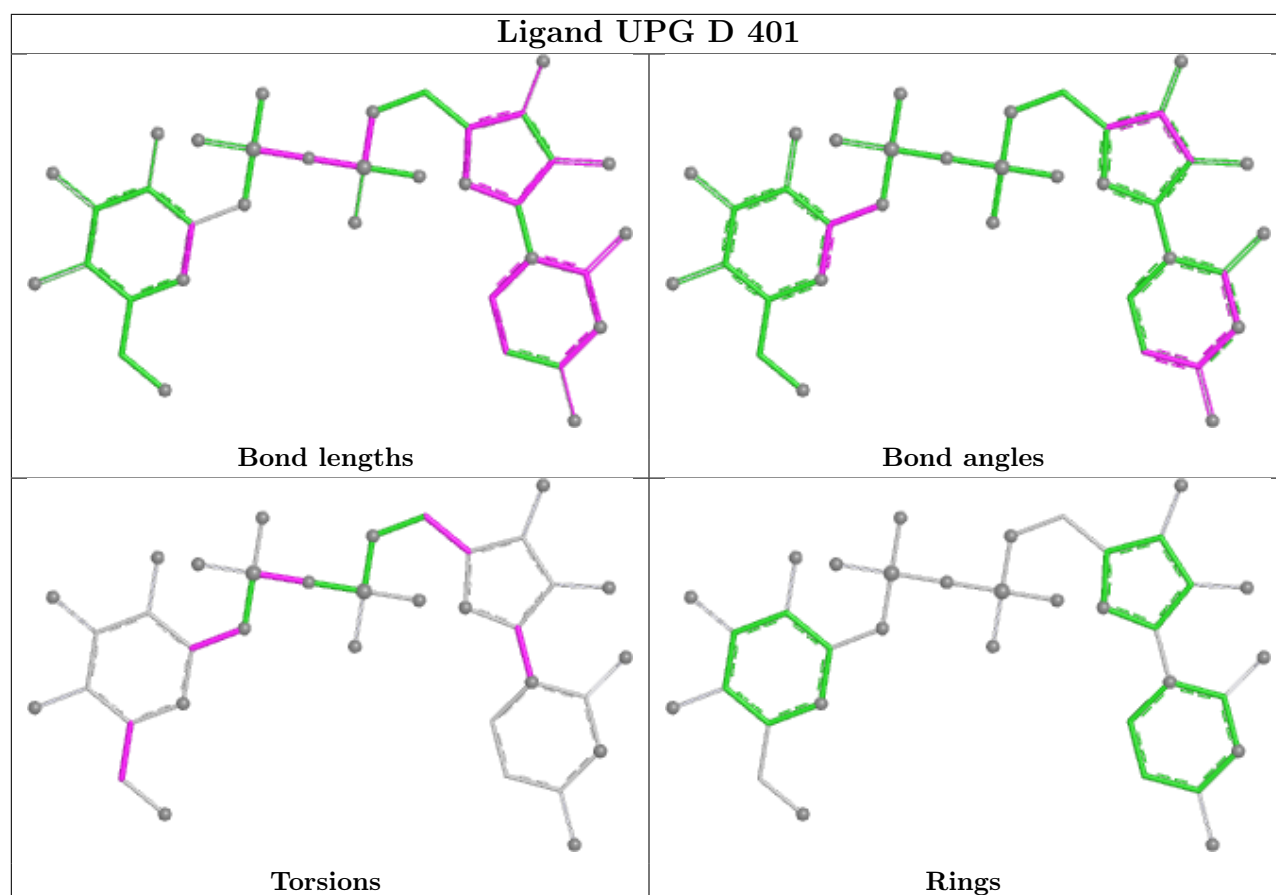
Mol	Chain	Res	Type	Atoms
3	D	402	5TR	C49-C45-C46-C36
5	C	402	UDP	O4'-C1'-N1-C2
2	B	401	UPG	C2C-C1C-N1-C2
2	A	401	UPG	C2C-C1C-N1-C2
5	C	402	UDP	C2'-C1'-N1-C2
5	C	402	UDP	PB-O3A-PA-O2A

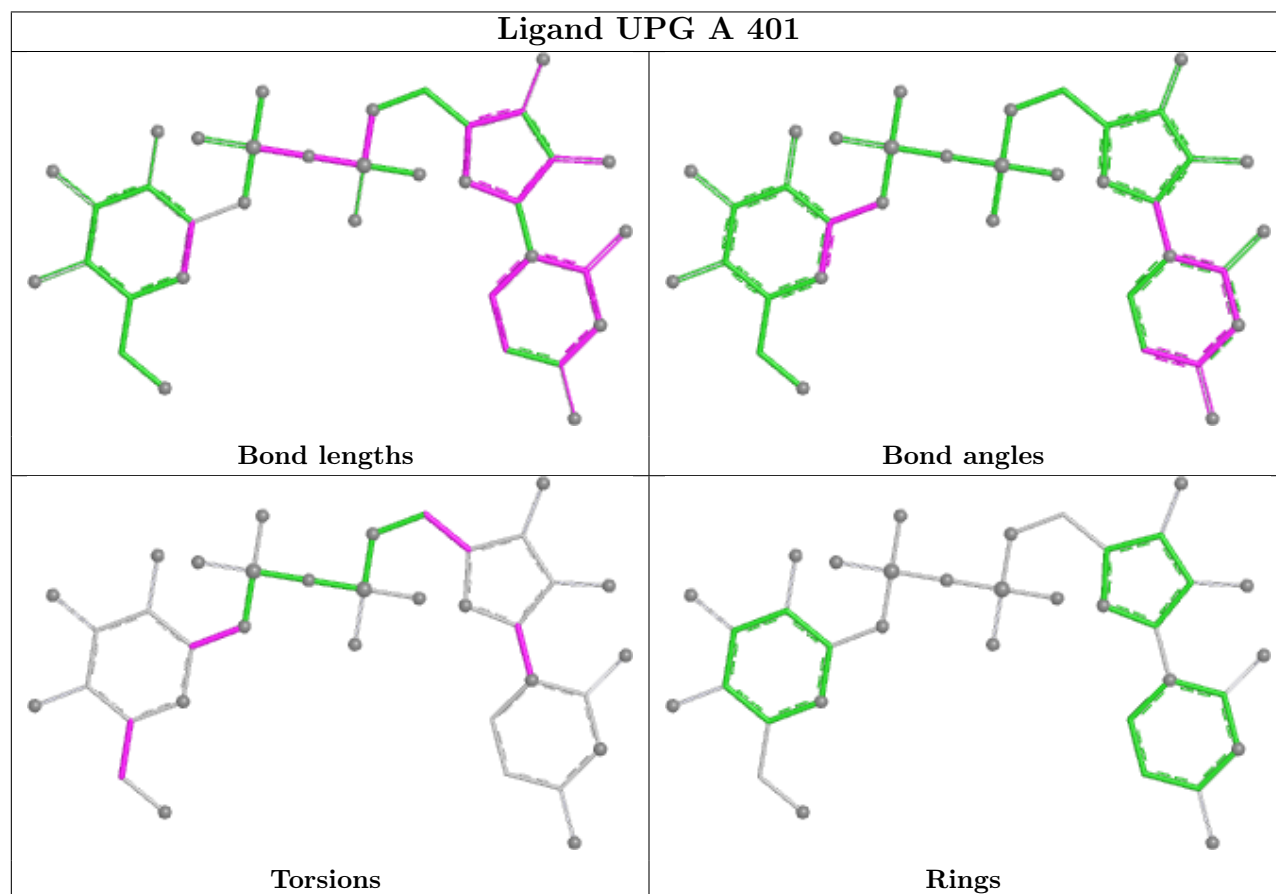
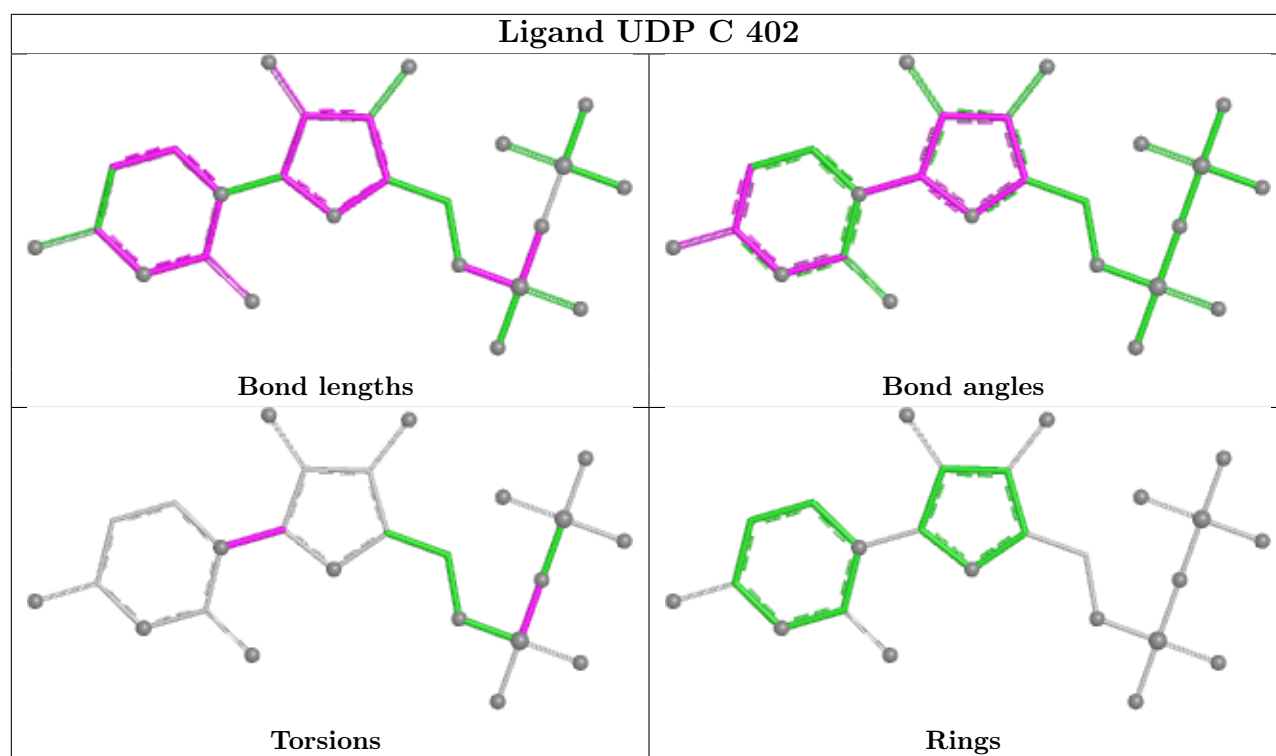
There are no ring outliers.

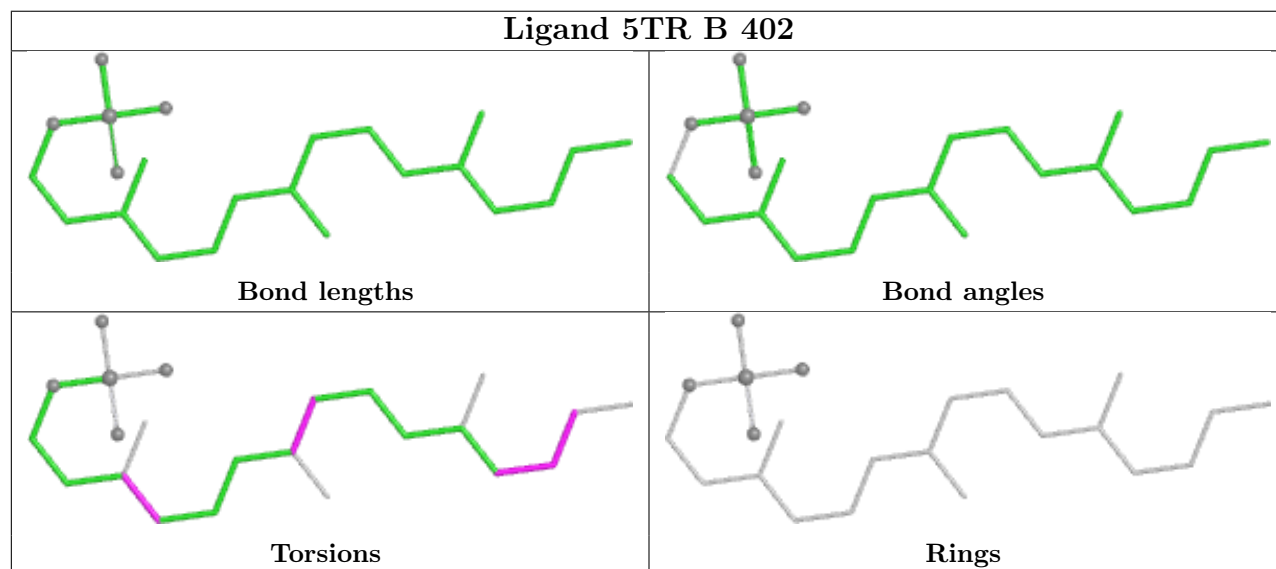
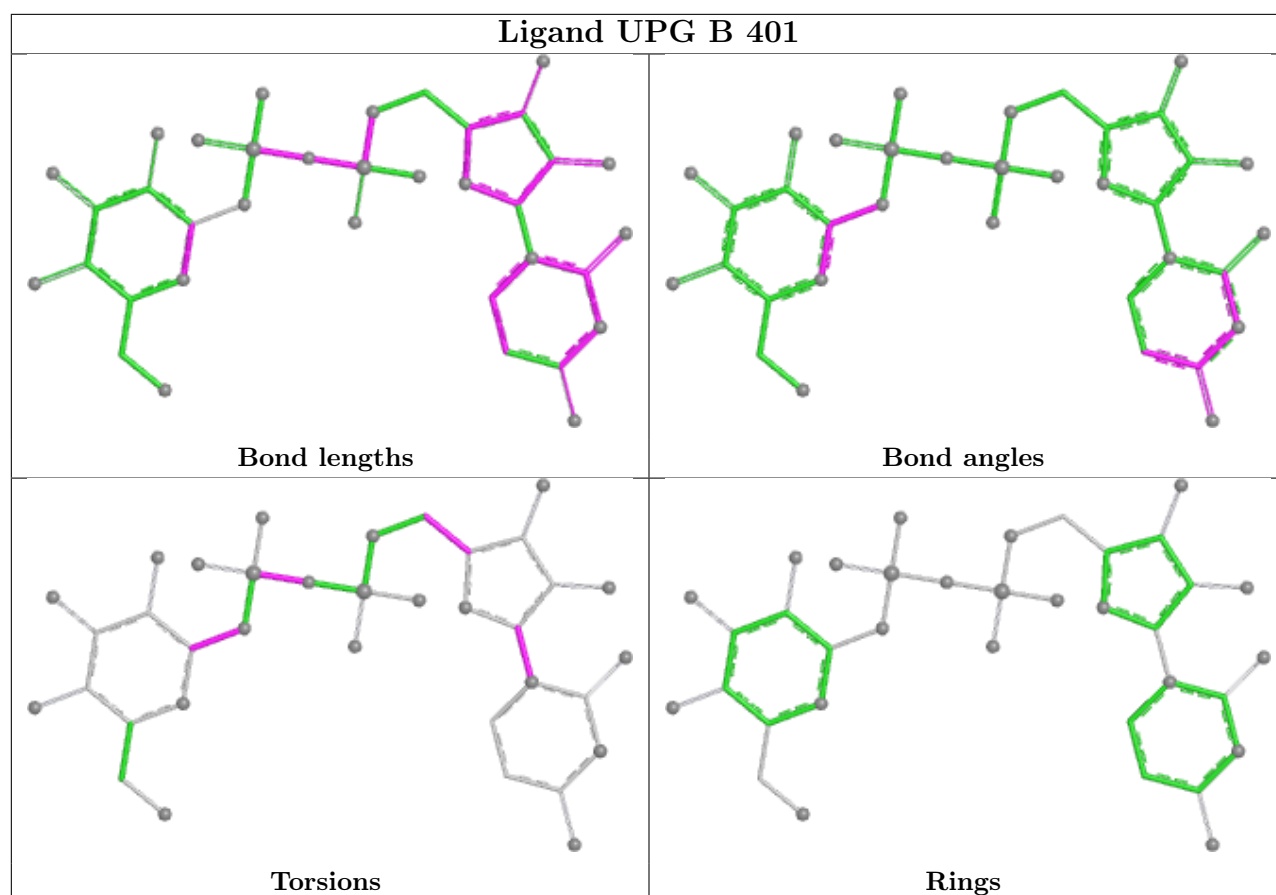
7 monomers are involved in 20 short contacts:

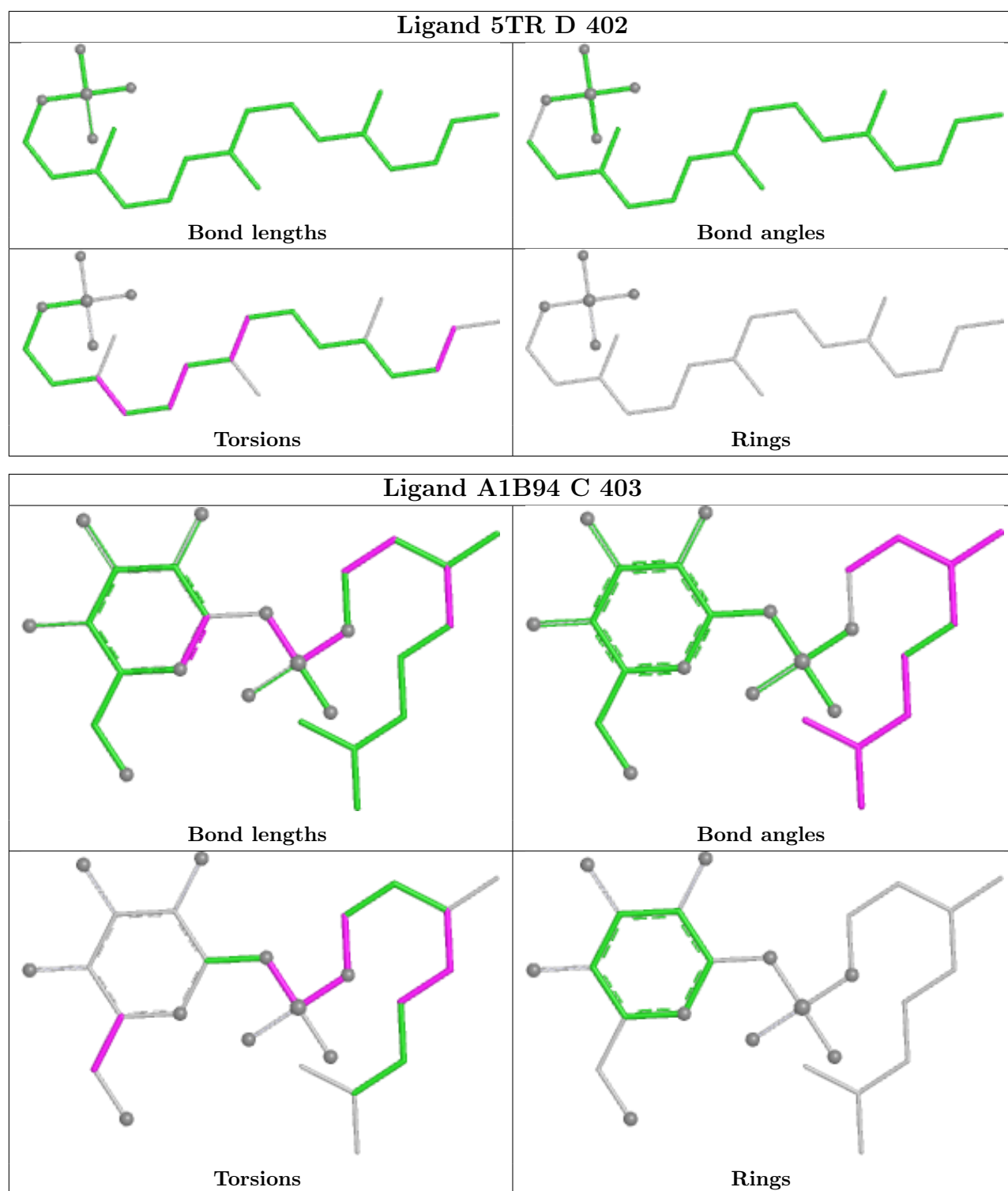
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	UPG	2	0
3	A	402	5TR	3	0
2	A	401	UPG	3	0
2	B	401	UPG	6	0
3	B	402	5TR	2	0
3	D	402	5TR	2	0
6	C	403	A1B94	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

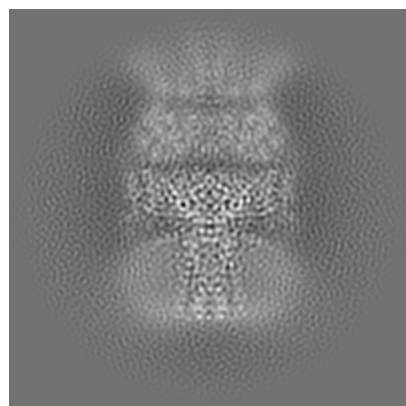
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49931. These allow visual inspection of the internal detail of the map and identification of artifacts.

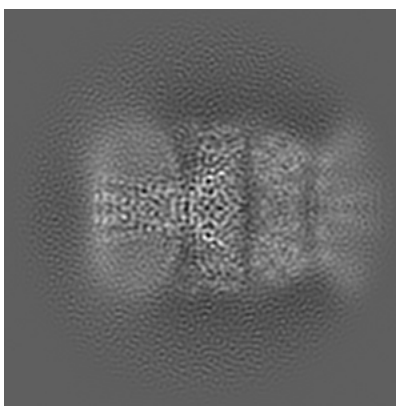
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

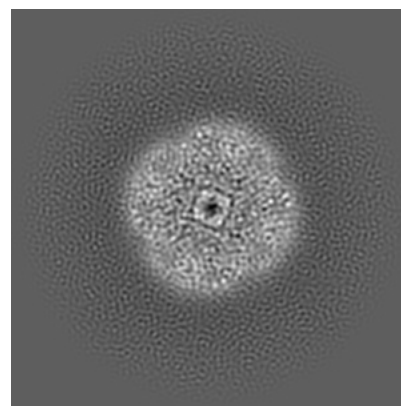
6.1.1 Primary map



X

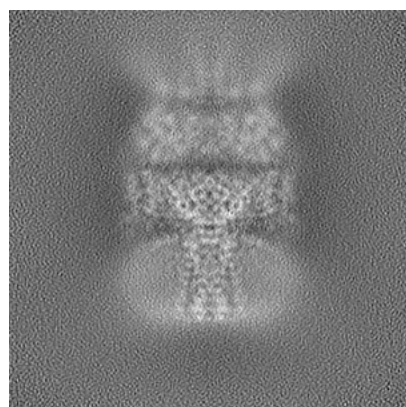


Y

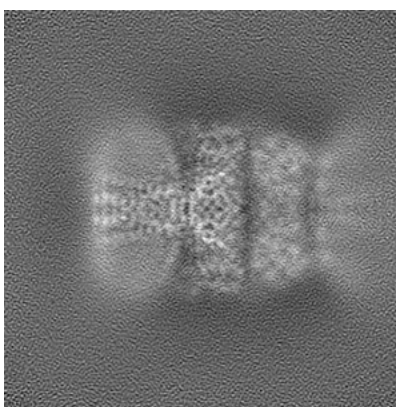


Z

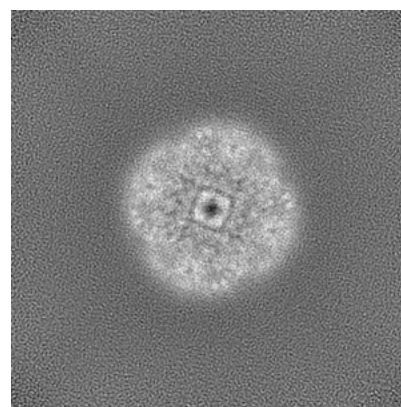
6.1.2 Raw map



X



Y

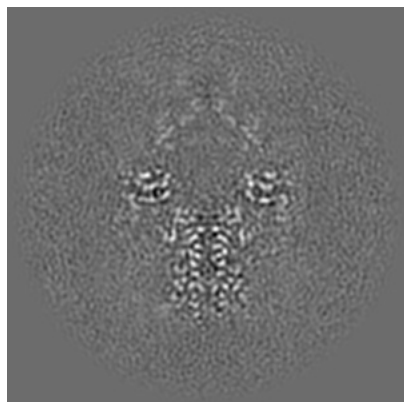


Z

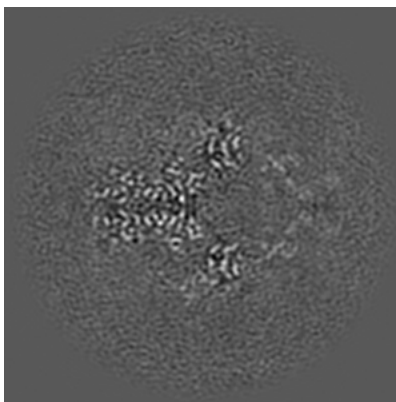
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

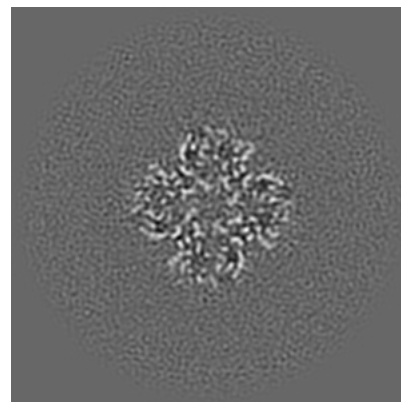
6.2.1 Primary map



X Index: 128

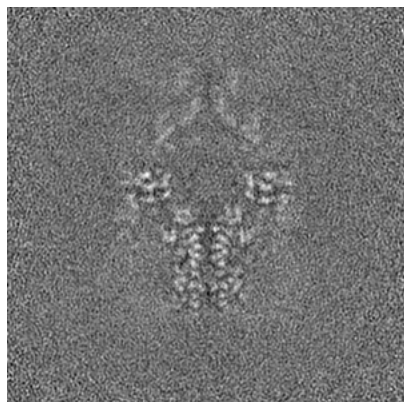


Y Index: 128

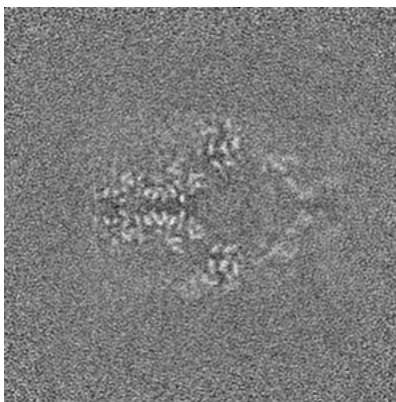


Z Index: 128

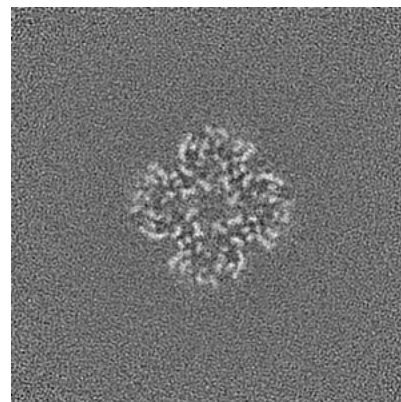
6.2.2 Raw map



X Index: 128



Y Index: 128

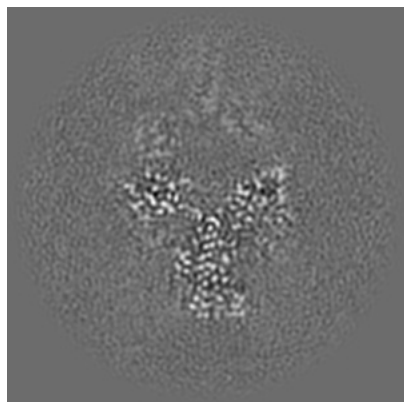


Z Index: 128

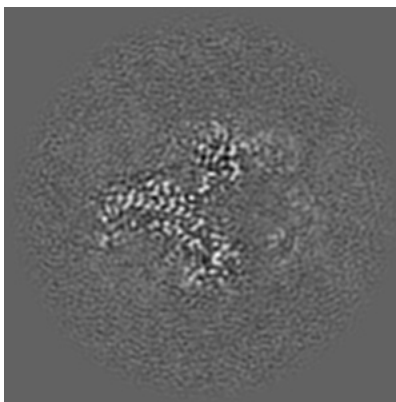
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

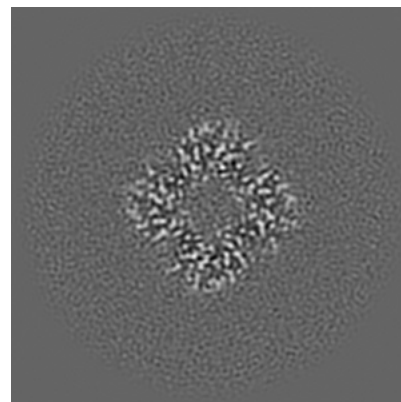
6.3.1 Primary map



X Index: 120

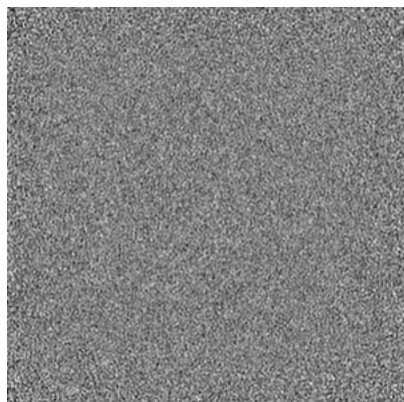


Y Index: 118

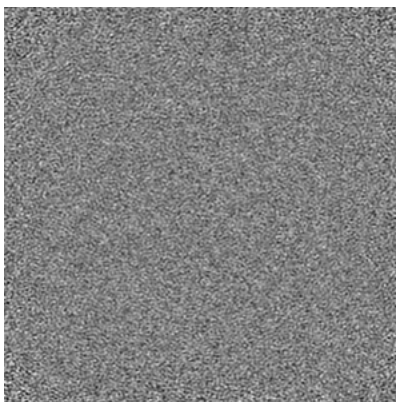


Z Index: 135

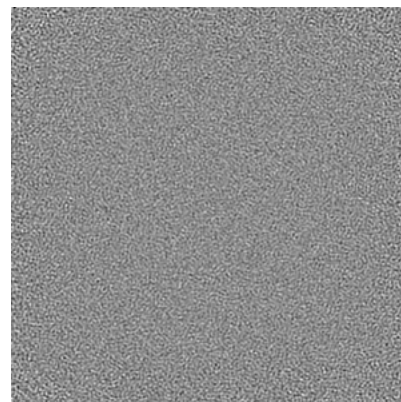
6.3.2 Raw map



X Index: 0



Y Index: 0

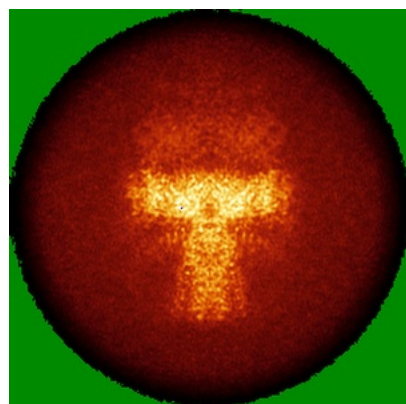


Z Index: 0

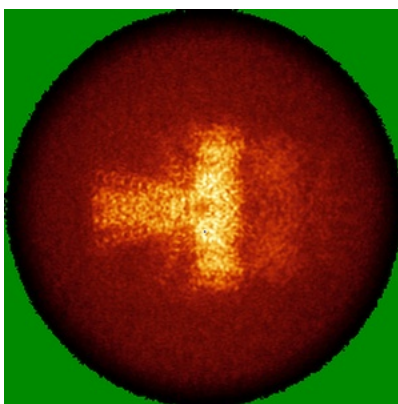
The images above show the largest variance slices of the map in three orthogonal directions.

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

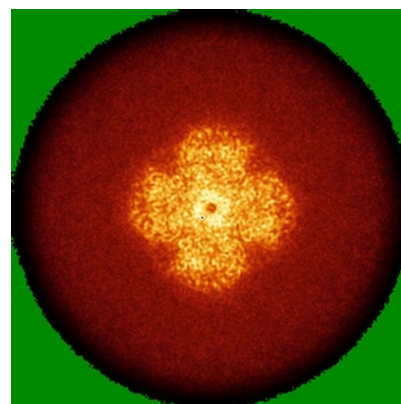
6.4.1 Primary map



X

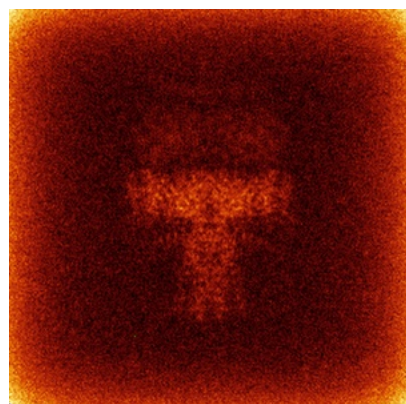


Y

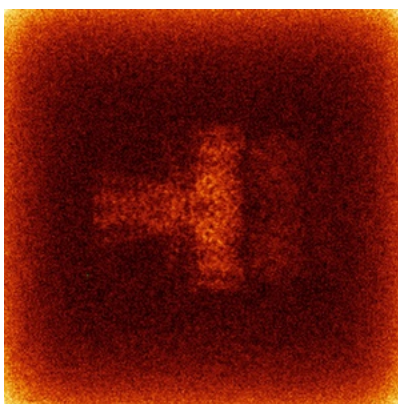


Z

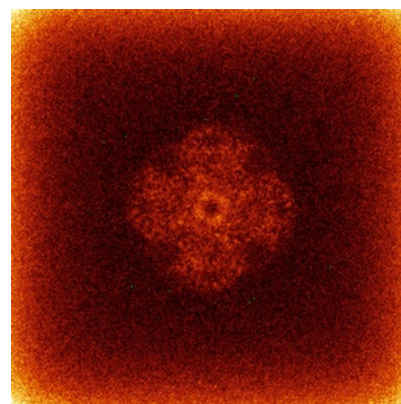
6.4.2 Raw map



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



X



Y



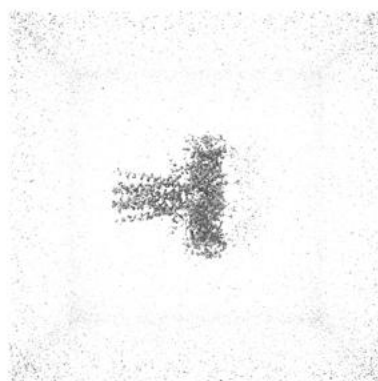
Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

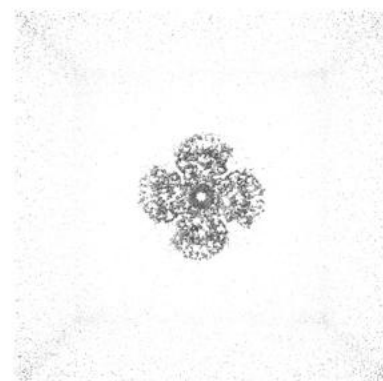
6.5.2 Raw map



X



Y



Z

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

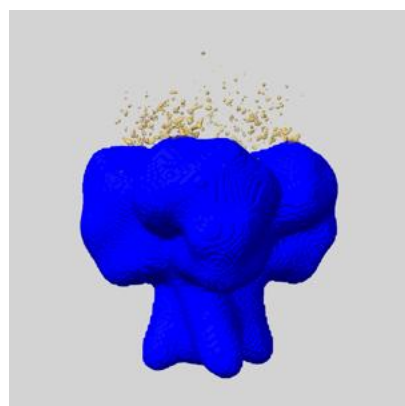
6.6 Mask visualisation [i](#)

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

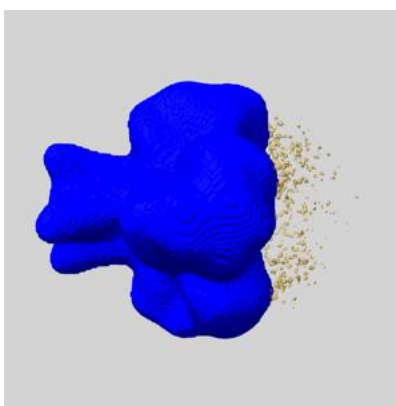
A mask typically either:

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

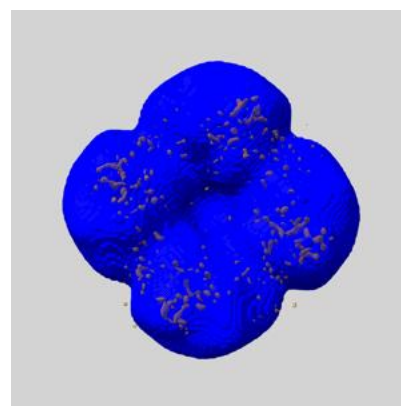
6.6.1 emd_49931_msk_1.map [i](#)



X



Y

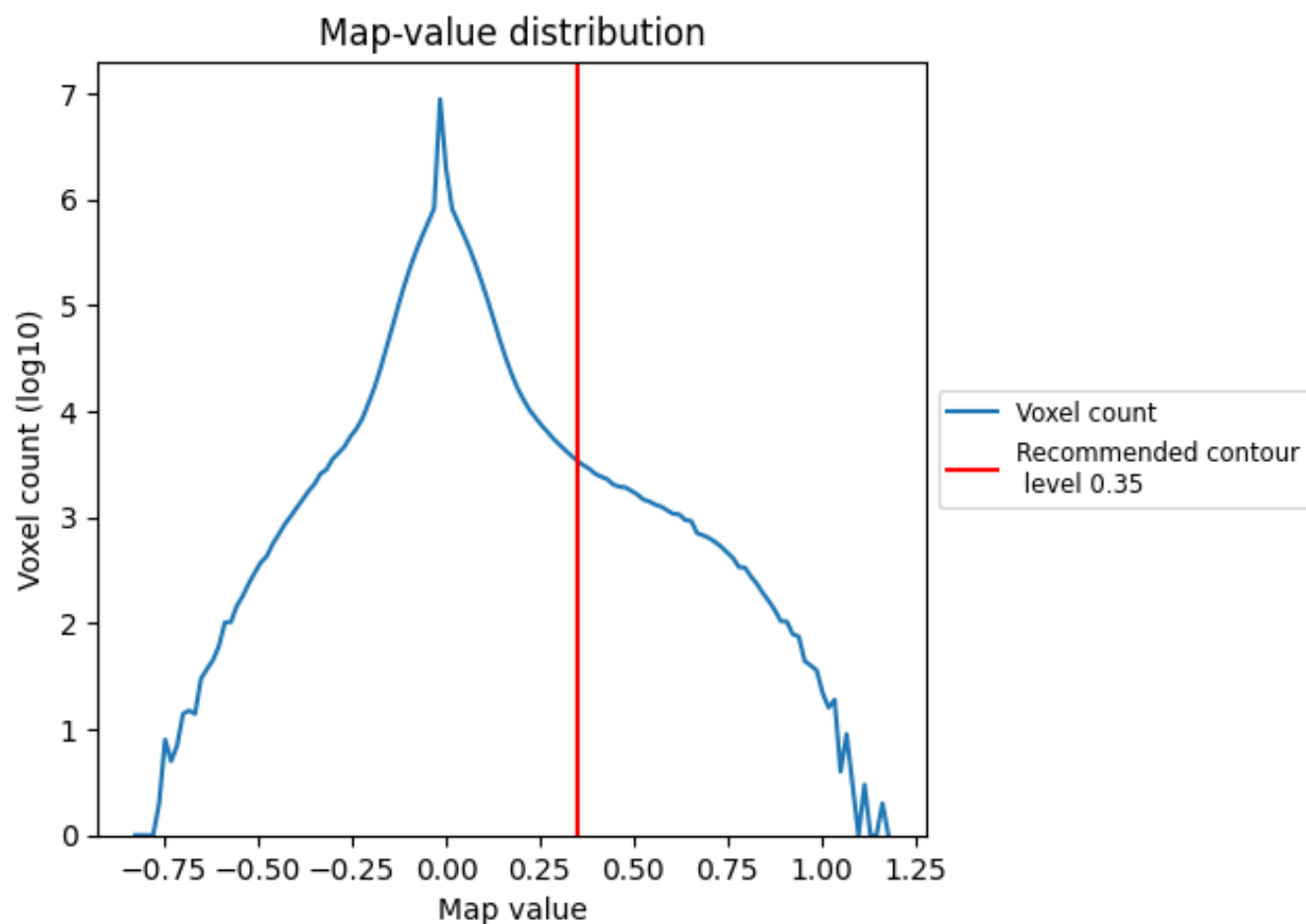


Z

7 Map analysis [i](#)

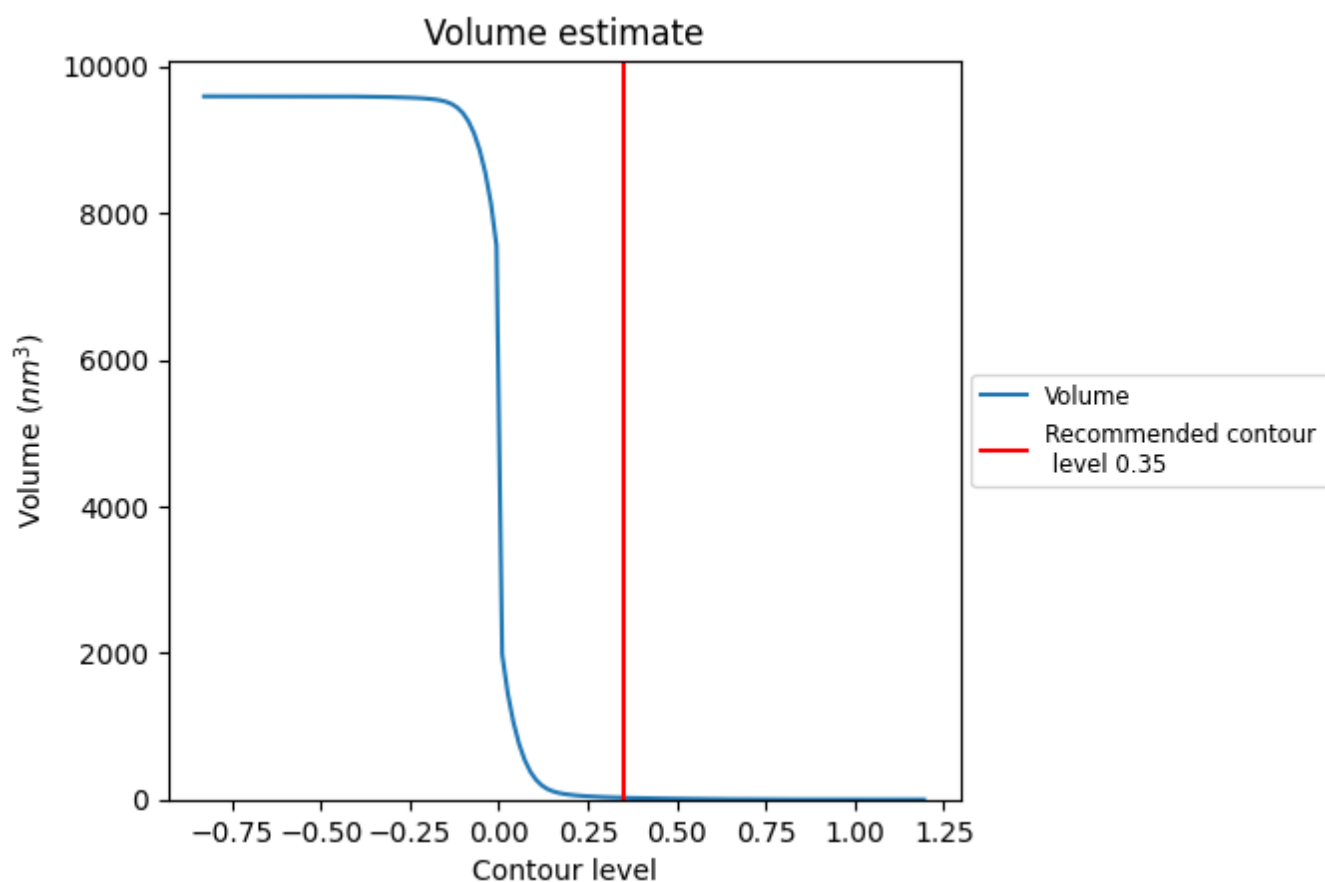
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

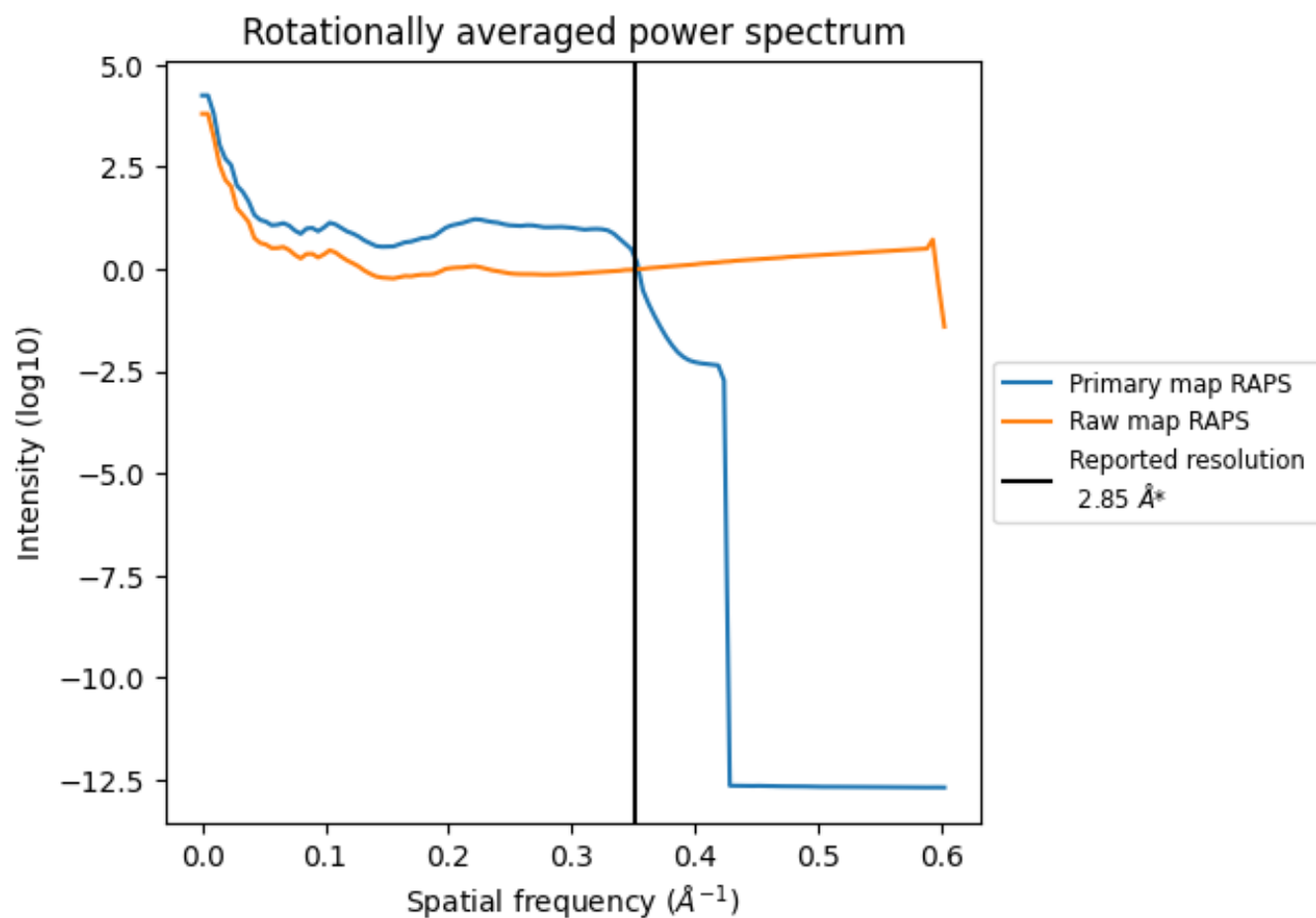
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25 nm³; this corresponds to an approximate mass of 22 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 ⓘ

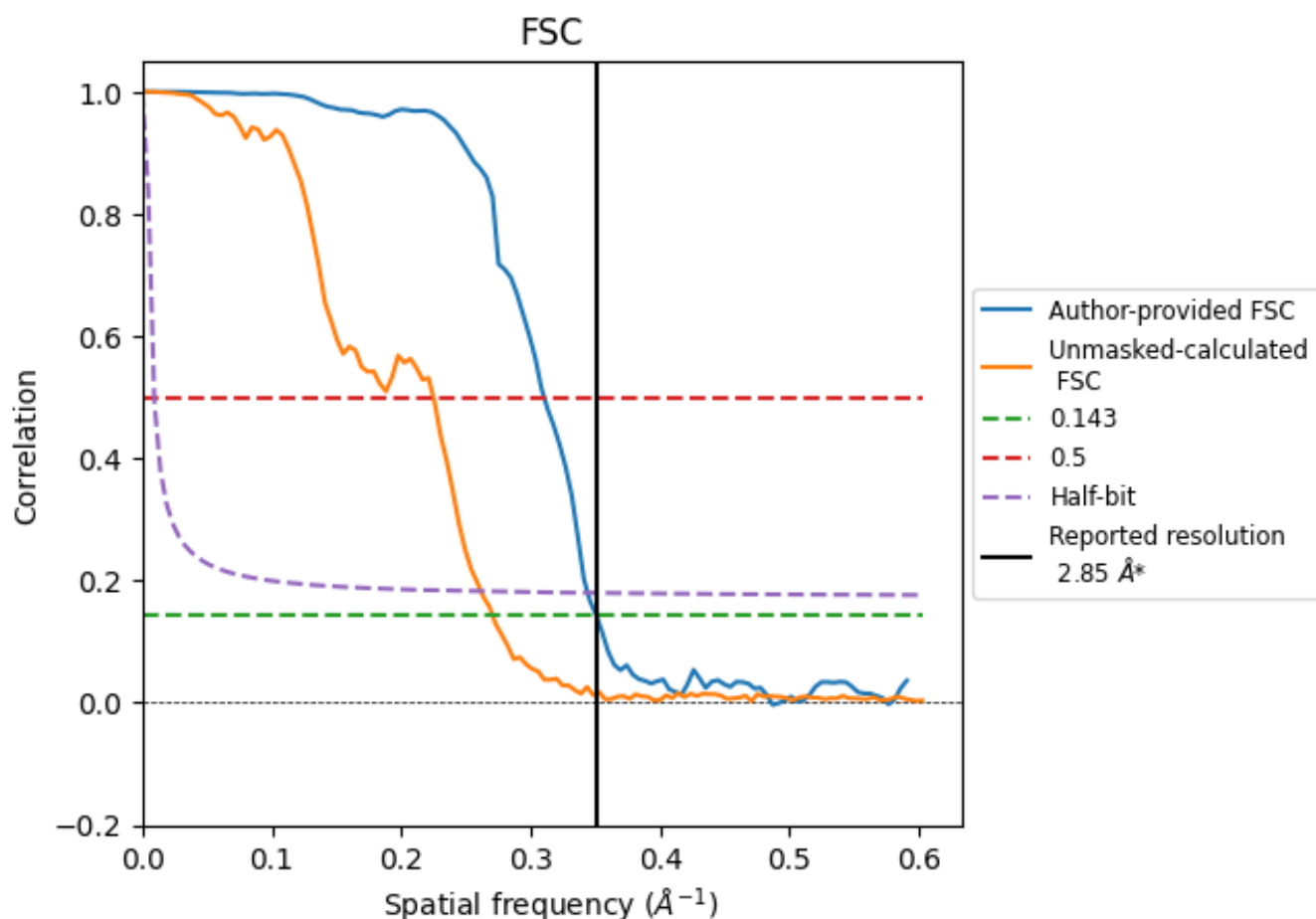


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 \AA^{-1}

8.2 Resolution estimates [i](#)

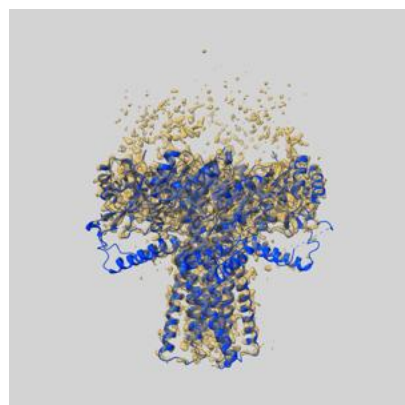
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.22	2.91
Unmasked-calculated*	3.70	4.45	3.82

*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 3.70 differs from the reported value 2.85 by more than 10 %

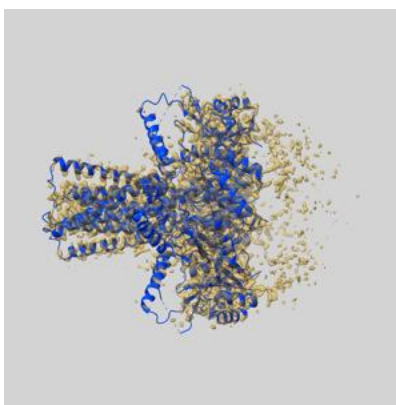
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49931 and PDB model 9NYD. Per-residue inclusion information can be found in section [3](#) on page [10](#).

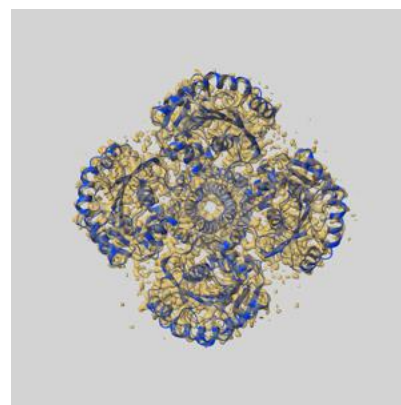
9.1 Map-model overlay [i](#)



X



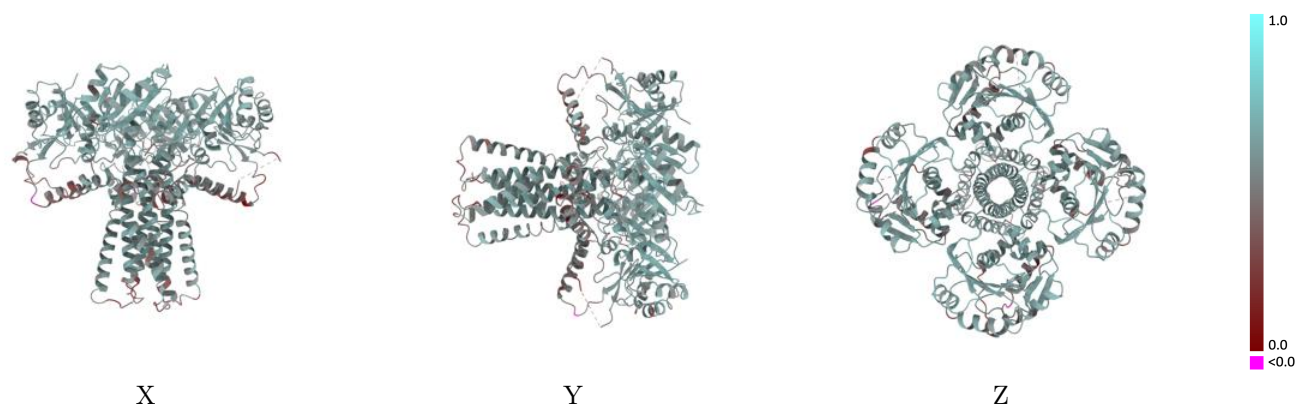
Y



Z

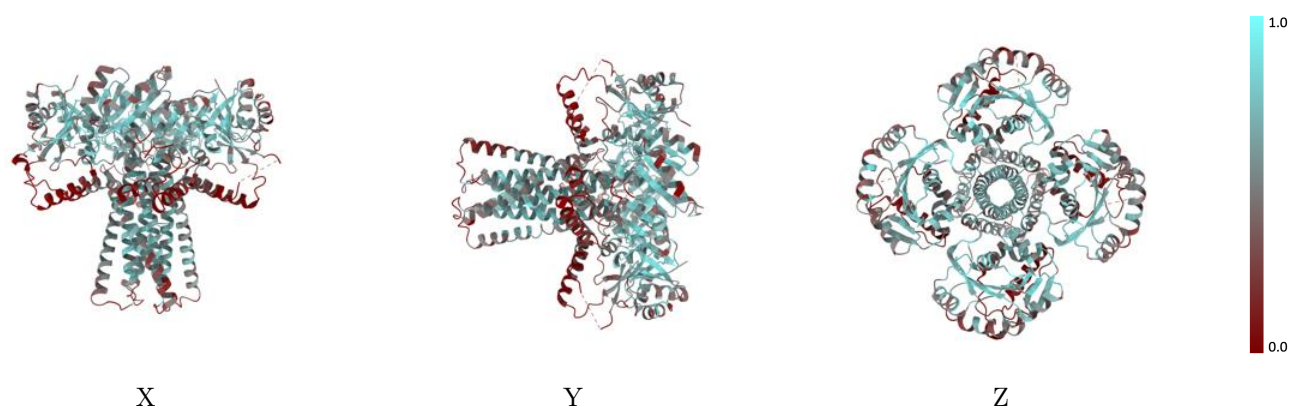
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



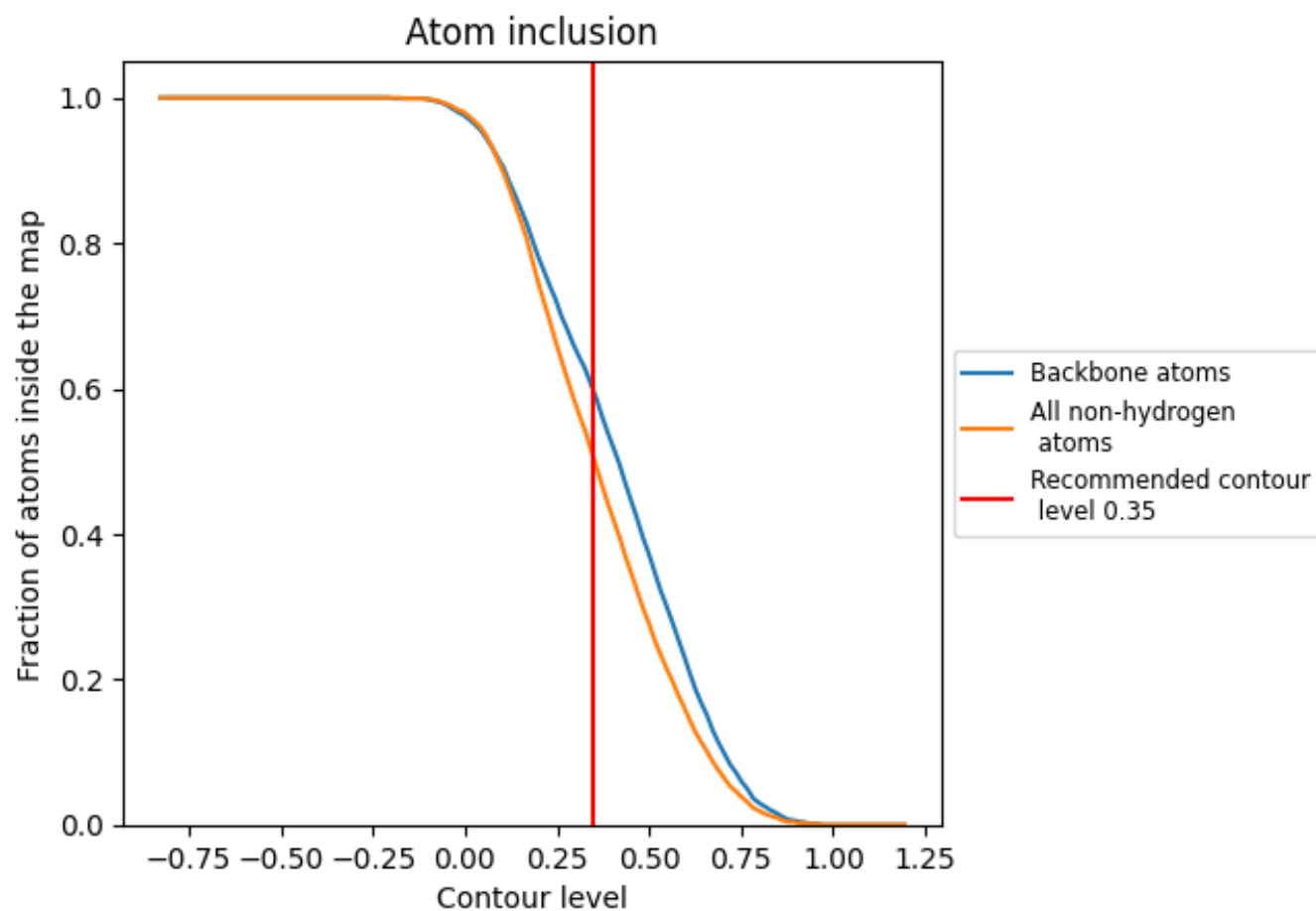
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 50% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5040	<div></div> 0.5470
A	<div></div> 0.4990	<div></div> 0.5470
B	<div></div> 0.5030	<div></div> 0.5490
C	<div></div> 0.5140	<div></div> 0.5430
D	<div></div> 0.5000	<div></div> 0.5490

