



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:03 PM UTC

PDB ID : 8WSA / pdb_00008wsa
EMDB ID : EMD-37803
Title : Cryo-EM Structure of Mouse TLR4/MD-2/DLAM5 Complex
Authors : Fu, Y.; Kim, H.; Zamyatina, A.; Kim, H.M.
Deposited on : 2023-10-17
Resolution : 3.10 Å(reported)
Based on initial model : 3VQ2

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

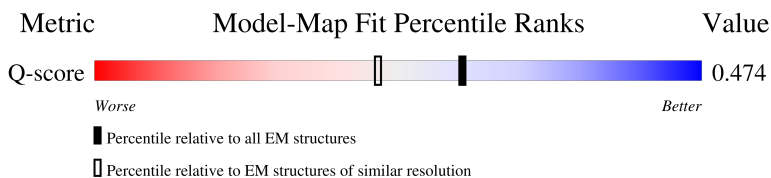
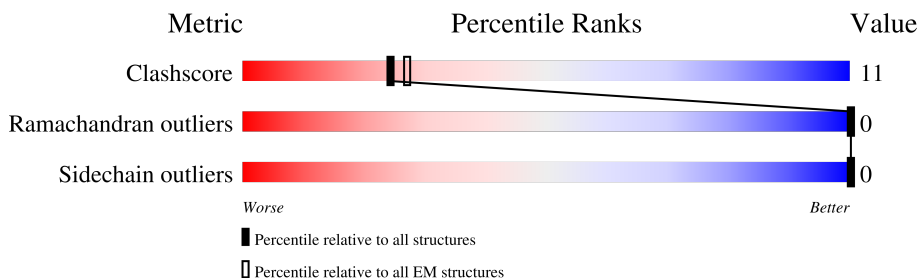
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	604	 76% 23% .
1	B	604	 76% 23% .
2	C	142	 65% 30% .
2	D	142	 65% 31% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12132 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.

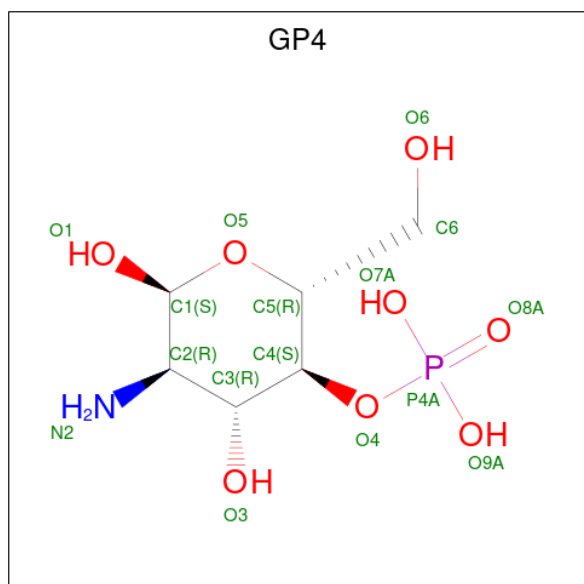
- Molecule 1 is a protein called Toll-like receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	595	Total	C	N	O	S	0	0
			4746	3041	780	898	27		
1	B	595	Total	C	N	O	S	0	0
			4746	3041	780	898	27		

- Molecule 2 is a protein called Lymphocyte antigen 96.

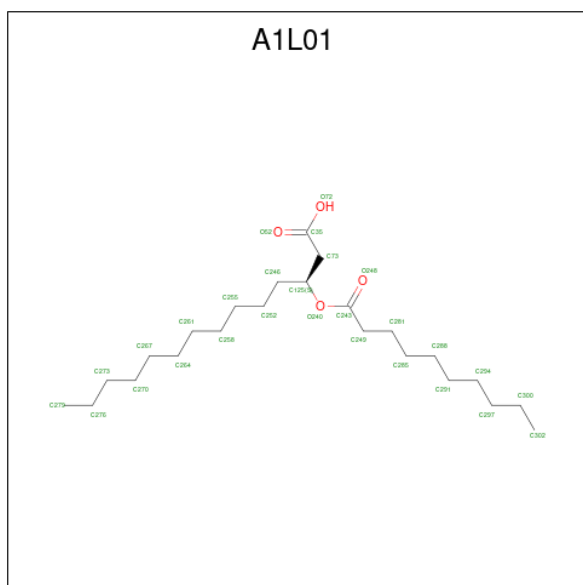
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	136	Total	C	N	O	S	0	0
			1103	712	186	198	7		
2	D	136	Total	C	N	O	S	0	0
			1103	712	186	198	7		

- Molecule 3 is 2-amino-2-deoxy-4-O-phosphono-alpha-D-glucopyranose (CCD ID: GP4) (formula: $C_6H_{14}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			14	6	1	6	1	
3	B	1	Total	C	N	O	P	0
			14	6	1	6	1	

- Molecule 4 is (3 {S})-3-decanoyloxytetradecanoic acid (CCD ID: A1L01) (formula: $C_{24}H_{46}O_4$) (labeled as "Ligand of Interest" by depositor).



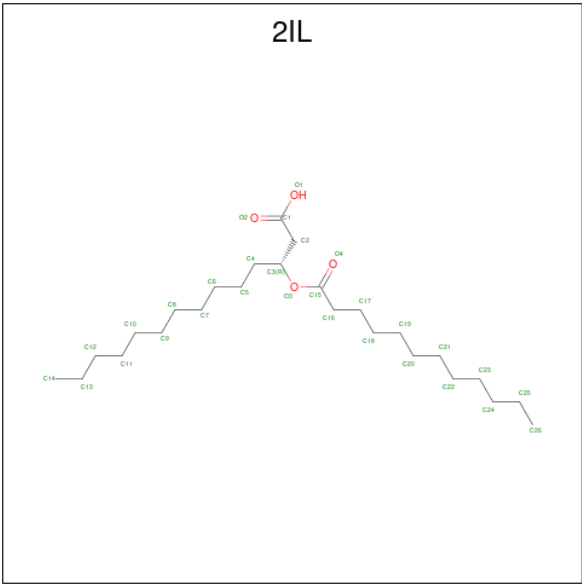
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	24	4	
4	C	1	Total	C	O	0
			28	24	4	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



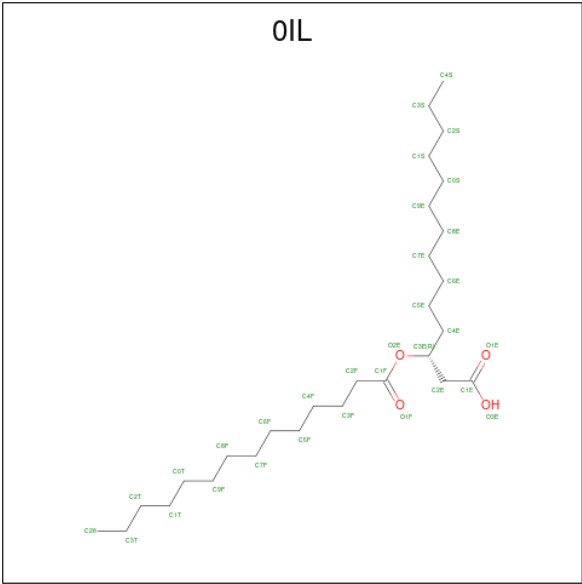
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is (3R)-3-(dodecanoyloxy)tetradecanoic acid (CCD ID: 2IL) (formula: $C_{26}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



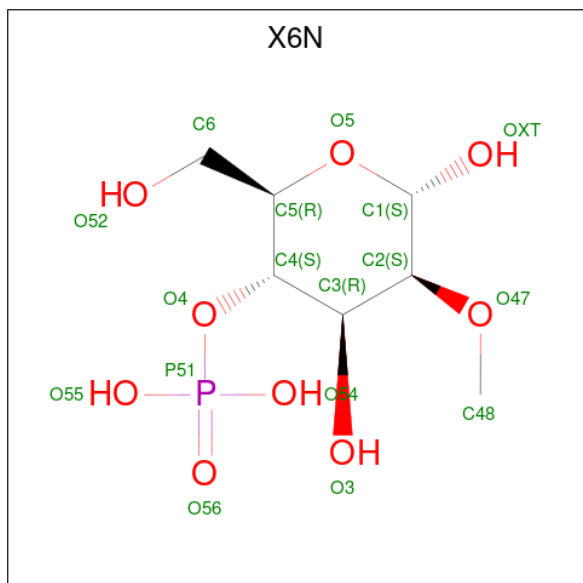
Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	C	O	0
			29	26	3	
6	D	1	Total	C	O	0
			29	26	3	

- Molecule 7 is (3R)-3-(tetradecanoyloxy)tetradecanoic acid (CCD ID: 0IL) (formula: $C_{28}H_{54}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	C	O	0
			32	28	4	
7	D	1	Total	C	O	0
			32	28	4	

- Molecule 8 is [(2 {R},3 {S},4 {R},5 {S})-2-(hydroxymethyl)-5-methoxy-4,6-bis(oxidanyl)oxan-3-yl] dihydrogen phosphate (CCD ID: X6N) (formula: C₇H₁₅O₉P) (labeled as "Ligand of Interest" by depositor).

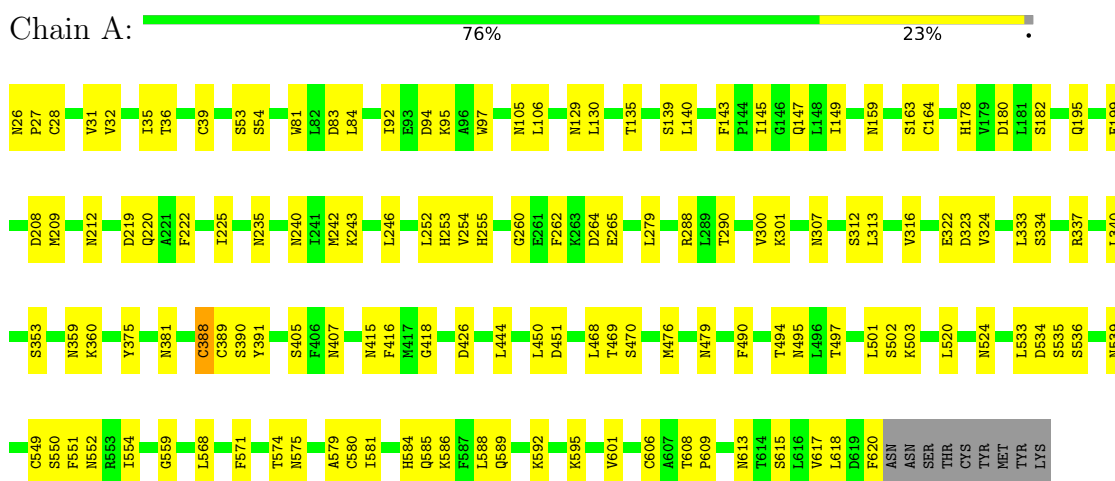


Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	O	P	0
			16	7	8	1	
8	D	1	Total	C	O	P	0
			16	7	8	1	

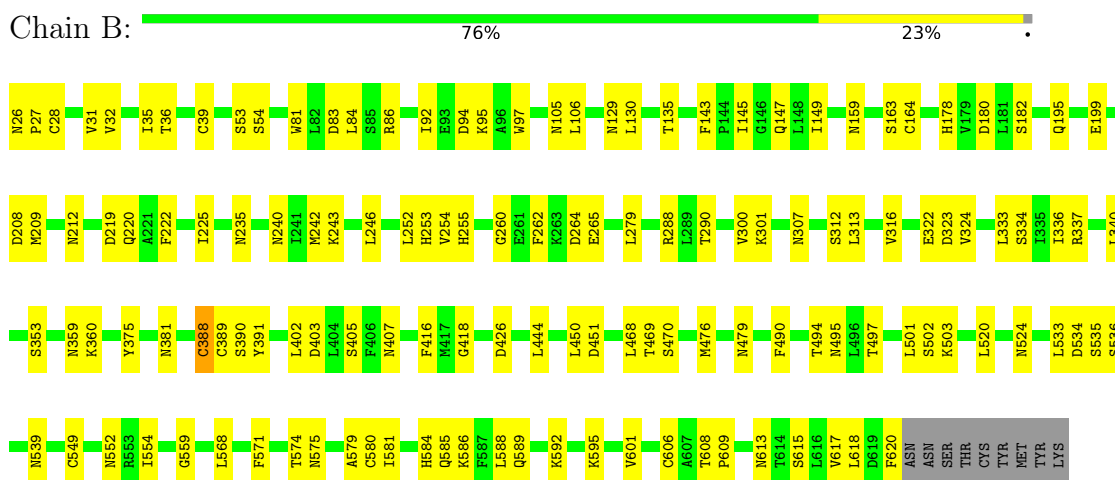
3 Residue-property plots

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: Toll-like receptor 4

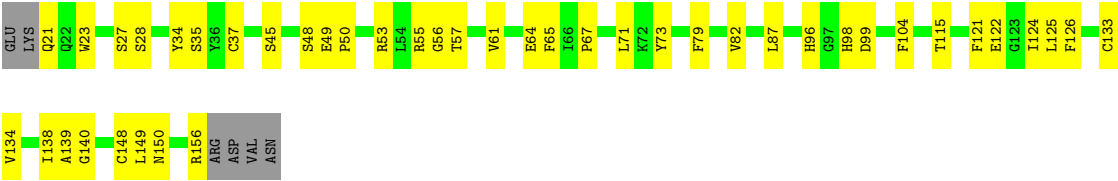


• Molecule 1: Toll-like receptor 4

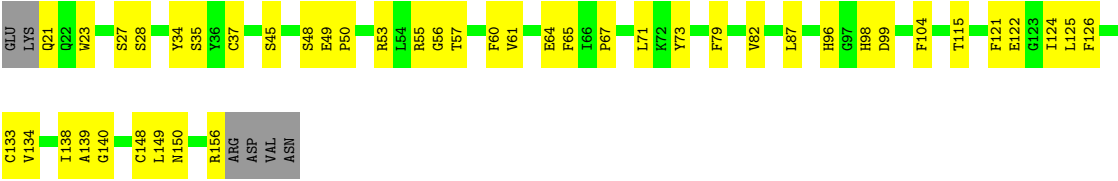


• Molecule 2: Lymphocyte antigen 96





● Molecule 2: Lymphocyte antigen 96



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	714161	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 ($e^-/\text{\AA}^2$)	40.1	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.484	Depositor
Minimum map value	-0.609	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	353.2, 353.2, 353.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.883, 0.883, 0.883	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, OIL, A1L01, GP4, 2IL, X6N

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	0.24	0/4846	0.50	0/6568
1	B	0.24	0/4846	0.50	0/6568
2	C	0.24	0/1134	0.48	0/1533
2	D	0.24	0/1134	0.48	0/1533
All	All	0.24	0/11960	0.50	0/16202

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	388	CYS	Peptide
1	B	388	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4746	0	4715	98	0
1	B	4746	0	4715	96	0
2	C	1103	0	1062	31	0
2	D	1103	0	1062	33	0
3	A	14	0	0	3	0
3	B	14	0	0	2	0
4	A	28	0	0	0	0
4	C	28	0	0	0	0
5	A	70	0	65	3	0
5	B	70	0	65	3	0
5	C	28	0	26	1	0
5	D	28	0	26	0	0
6	C	29	0	0	0	0
6	D	29	0	0	0	0
7	C	32	0	0	0	0
7	D	32	0	0	0	0
8	C	16	0	0	0	0
8	D	16	0	0	0	0
All	All	12132	0	11736	255	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 11.

All (255) 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:307:ASN:HD21	5:B:703:NAG:C1	1.03	1.65
1:A:307:ASN:HD21	5:A:704:NAG:C1	1.03	1.59
1:B:307:ASN:ND2	5:B:703:NAG:C1	1.86	1.34
1:A:307:ASN:ND2	5:A:704:NAG:C1	1.87	1.32
2:C:21:GLN:N	2:C:35:SER:HG	1.47	1.13
2:D:21:GLN:N	2:D:35:SER:HG	1.59	0.99
1:B:389:CYS:HB2	1:B:416:PHE:CE1	2.01	0.96
1:A:360:LYS:NZ	3:A:701:GP4:O8A	1.99	0.95
1:A:360:LYS:CE	3:A:701:GP4:O8A	2.14	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:CYS:HB2	1:A:416:PHE:CE1	2.01	0.94
1:A:360:LYS:HE2	3:A:701:GP4:O8A	1.73	0.88
1:B:35:ILE:HG22	1:B:36:THR:HG23	1.57	0.87
2:D:124:ILE:HD11	2:D:126:PHE:HE1	1.40	0.86
1:A:35:ILE:HG22	1:A:36:THR:HG23	1.57	0.85
2:D:124:ILE:HD11	2:D:126:PHE:CE1	2.11	0.85
1:B:360:LYS:HE2	3:B:701:GP4:O8A	1.78	0.82
1:A:313:LEU:HD12	1:A:316:VAL:HG21	1.65	0.78
1:B:313:LEU:HD12	1:B:316:VAL:HG21	1.66	0.77
1:B:580:CYS:HB3	1:B:608:THR:HG23	1.68	0.75
1:A:147:GLN:HE21	1:A:149:ILE:HG13	1.51	0.75
1:A:580:CYS:HB3	1:A:608:THR:HG23	1.68	0.75
1:B:336:ILE:HG22	1:B:337:ARG:HG3	1.69	0.74
1:B:147:GLN:HE21	1:B:149:ILE:HG13	1.51	0.73
1:B:288:ARG:HH22	2:D:99:ASP:CG	1.98	0.71
1:B:502:SER:OG	1:B:503:LYS:HG3	1.95	0.67
1:A:535:SER:HB3	1:A:559:GLY:HA3	1.77	0.67
1:A:31:VAL:HG12	1:A:32:VAL:HG23	1.77	0.67
1:B:535:SER:HB3	1:B:559:GLY:HA3	1.77	0.67
1:B:360:LYS:CE	3:B:701:GP4:O8A	2.42	0.67
2:D:79:PHE:HB2	2:D:134:VAL:HG12	1.76	0.67
1:A:502:SER:OG	1:A:503:LYS:HG3	1.95	0.66
2:C:23:TRP:HB3	2:C:34:TYR:HE1	1.61	0.66
2:D:53:ARG:H	2:D:57:THR:HG21	1.61	0.66
2:C:53:ARG:H	2:C:57:THR:HG21	1.61	0.66
2:C:79:PHE:HB2	2:C:134:VAL:HG12	1.76	0.66
1:A:135:THR:O	1:A:159:ASN:ND2	2.29	0.65
1:B:31:VAL:HG12	1:B:32:VAL:HG23	1.77	0.65
2:D:23:TRP:HB3	2:D:34:TYR:HE1	1.61	0.65
1:B:135:THR:O	1:B:159:ASN:ND2	2.29	0.65
1:B:595:LYS:HB3	1:B:601:VAL:HG21	1.79	0.65
1:B:592:LYS:NZ	1:B:617:VAL:O	2.30	0.65
1:A:595:LYS:HB3	1:A:601:VAL:HG21	1.79	0.64
1:A:592:LYS:NZ	1:A:617:VAL:O	2.30	0.64
2:C:67:PRO:HB3	2:C:71:LEU:HD13	1.80	0.64
2:D:21:GLN:N	2:D:35:SER:OG	2.29	0.64
1:A:301:LYS:NZ	1:A:323:ASP:O	2.23	0.64
2:D:67:PRO:HB3	2:D:71:LEU:HD13	1.80	0.63
1:B:240:ASN:HA	1:B:243:LYS:HD3	1.81	0.63
2:C:96:HIS:CE1	2:C:98:HIS:HB3	2.33	0.63
2:D:96:HIS:CE1	2:D:98:HIS:HB3	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:CYS:CB	1:A:416:PHE:CE1	2.81	0.63
1:B:389:CYS:CB	1:B:416:PHE:CE1	2.81	0.62
1:B:301:LYS:NZ	1:B:323:ASP:O	2.23	0.62
1:A:240:ASN:HA	1:A:243:LYS:HD3	1.81	0.62
1:B:533:LEU:HD23	1:B:554:ILE:HG13	1.82	0.61
2:C:124:ILE:HG12	2:C:125:LEU:H	1.65	0.61
1:A:337:ARG:O	1:A:337:ARG:HG2	2.01	0.61
1:A:533:LEU:HD23	1:A:554:ILE:HG13	1.82	0.60
2:C:28:SER:O	2:C:156:ARG:NH2	2.35	0.60
2:D:28:SER:O	2:D:156:ARG:NH2	2.35	0.59
1:A:534:ASP:OD1	1:A:535:SER:N	2.36	0.58
1:B:246:LEU:HD12	1:B:279:LEU:HD21	1.85	0.58
1:B:534:ASP:OD1	1:B:535:SER:N	2.36	0.58
1:B:209:MET:O	1:B:212:ASN:ND2	2.37	0.58
2:C:124:ILE:HG12	2:C:125:LEU:N	2.19	0.57
1:A:415:ASN:HD21	2:D:125:LEU:HB3	1.69	0.57
1:A:209:MET:O	1:A:212:ASN:ND2	2.37	0.57
1:A:246:LEU:HD12	1:A:279:LEU:HD21	1.85	0.57
1:A:105:ASN:OD1	1:A:106:LEU:N	2.38	0.57
1:B:105:ASN:OD1	1:B:106:LEU:N	2.38	0.56
1:B:301:LYS:HD3	1:B:324:VAL:HG22	1.89	0.55
1:A:264:ASP:OD1	1:A:264:ASP:N	2.39	0.55
1:B:163:SER:OG	1:B:164:CYS:N	2.39	0.55
1:A:163:SER:OG	1:A:164:CYS:N	2.39	0.55
2:D:45:SER:HB2	2:D:64:GLU:HG3	1.88	0.55
2:C:45:SER:HB2	2:C:64:GLU:HG3	1.88	0.54
2:D:124:ILE:CD1	2:D:126:PHE:CE1	2.87	0.54
1:B:288:ARG:NH2	2:D:99:ASP:OD2	2.29	0.54
1:A:389:CYS:HB2	1:A:416:PHE:CD1	2.42	0.54
1:A:301:LYS:HD3	1:A:324:VAL:HG22	1.89	0.54
1:B:182:SER:OG	1:B:208:ASP:OD2	2.26	0.54
1:B:264:ASP:OD1	1:B:264:ASP:N	2.39	0.54
1:B:381:ASN:O	1:B:407:ASN:ND2	2.33	0.54
1:A:212:ASN:H	1:A:235:ASN:HD22	1.56	0.53
1:A:182:SER:OG	1:A:208:ASP:OD2	2.26	0.53
1:B:389:CYS:HB2	1:B:416:PHE:CD1	2.42	0.53
2:C:104:PHE:CD2	2:C:115:THR:HG21	2.45	0.52
1:B:288:ARG:HG2	1:B:312:SER:HB3	1.92	0.52
1:B:618:LEU:HB3	1:B:620:PHE:HE1	1.74	0.52
1:A:288:ARG:HG2	1:A:312:SER:HB3	1.92	0.52
1:B:195:GLN:O	1:B:199:GLU:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ASN:H	1:B:235:ASN:HD22	1.56	0.52
1:A:618:LEU:HB3	1:A:620:PHE:HE1	1.74	0.52
2:D:104:PHE:CD2	2:D:115:THR:HG21	2.45	0.52
2:C:56:GLY:N	2:C:122:GLU:O	2.43	0.52
1:B:81:TRP:CZ3	1:B:83:ASP:HB2	2.45	0.52
1:A:81:TRP:CZ3	1:A:83:ASP:HB2	2.45	0.52
2:C:65:PHE:HZ	2:C:71:LEU:HD21	1.75	0.51
2:D:65:PHE:HZ	2:D:71:LEU:HD21	1.75	0.51
2:D:73:TYR:HB2	2:D:140:GLY:HA3	1.92	0.51
1:B:581:ILE:HD11	1:B:609:PRO:HD2	1.92	0.51
1:B:254:VAL:HG22	1:B:255:HIS:H	1.75	0.51
2:C:21:GLN:N	2:C:35:SER:OG	2.29	0.51
1:A:195:GLN:O	1:A:199:GLU:HG2	2.10	0.51
1:A:536:SER:O	1:A:539:ASN:ND2	2.44	0.51
1:A:254:VAL:HG22	1:A:255:HIS:H	1.75	0.51
1:B:242:MET:HG3	1:B:246:LEU:HD23	1.93	0.50
2:C:73:TYR:HB2	2:C:140:GLY:HA3	1.92	0.50
1:A:585:GLN:HA	1:A:588:LEU:HB2	1.92	0.50
1:B:524:ASN:HD22	5:B:702:NAG:H83	1.76	0.50
1:A:613:ASN:ND2	1:A:615:SER:OG	2.45	0.50
2:D:56:GLY:N	2:D:122:GLU:O	2.43	0.50
1:B:359:ASN:OD1	1:B:360:LYS:N	2.45	0.50
1:A:581:ILE:HD11	1:A:609:PRO:HD2	1.92	0.50
1:B:129:ASN:OD1	1:B:130:LEU:N	2.45	0.50
1:B:613:ASN:ND2	1:B:615:SER:OG	2.45	0.50
1:A:359:ASN:OD1	1:A:360:LYS:N	2.45	0.50
1:B:536:SER:O	1:B:539:ASN:ND2	2.44	0.50
1:A:586:LYS:O	1:A:589:GLN:HG3	2.12	0.50
1:B:586:LYS:O	1:B:589:GLN:HG3	2.12	0.50
1:B:300:VAL:O	1:B:301:LYS:HG2	2.12	0.49
1:A:129:ASN:OD1	1:A:130:LEU:N	2.45	0.49
1:B:581:ILE:HG12	1:B:608:THR:HG22	1.94	0.49
1:B:585:GLN:HA	1:B:588:LEU:HB2	1.92	0.49
1:A:300:VAL:O	1:A:301:LYS:HG2	2.12	0.49
1:A:524:ASN:HD22	5:A:703:NAG:H83	1.76	0.49
1:A:209:MET:SD	1:A:209:MET:N	2.86	0.49
2:C:124:ILE:CG1	2:C:125:LEU:H	2.24	0.49
2:C:82:VAL:HG12	2:C:87:LEU:HD11	1.94	0.49
1:B:92:ILE:HD13	1:B:97:TRP:HH2	1.78	0.48
1:B:209:MET:SD	1:B:209:MET:N	2.86	0.48
2:D:82:VAL:HG12	2:D:87:LEU:HD11	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:MET:HG3	1:A:246:LEU:HD23	1.93	0.48
1:A:92:ILE:HD13	1:A:97:TRP:HH2	1.78	0.48
1:A:581:ILE:HG12	1:A:608:THR:HG22	1.94	0.48
1:B:390:SER:OG	1:B:391:TYR:N	2.46	0.48
1:A:390:SER:OG	1:A:391:TYR:N	2.46	0.48
1:A:26:ASN:HB3	1:A:27:PRO:HD3	1.96	0.48
1:B:219:ASP:OD1	1:B:220:GLN:N	2.47	0.48
1:A:219:ASP:OD1	1:A:220:GLN:N	2.47	0.48
1:B:353:SER:HA	1:B:375:TYR:HB3	1.96	0.47
1:A:388:CYS:C	1:A:389:CYS:SG	2.97	0.47
1:A:585:GLN:OE1	1:A:585:GLN:N	2.43	0.47
1:B:580:CYS:HB2	1:B:606:CYS:HB2	1.59	0.47
1:A:209:MET:HB2	1:A:212:ASN:HD22	1.79	0.47
1:A:28:CYS:HB2	1:A:39:CYS:HA	1.96	0.47
1:A:353:SER:HA	1:A:375:TYR:HB3	1.96	0.47
1:B:26:ASN:HB3	1:B:27:PRO:HD3	1.96	0.47
1:B:209:MET:HB2	1:B:212:ASN:HD22	1.79	0.47
1:B:388:CYS:C	1:B:389:CYS:SG	2.98	0.47
1:B:450:LEU:HD12	1:B:451:ASP:H	1.80	0.47
2:C:34:TYR:HA	2:C:150:ASN:O	2.15	0.47
1:A:502:SER:OG	1:A:503:LYS:N	2.48	0.46
2:D:34:TYR:HA	2:D:150:ASN:O	2.15	0.46
1:A:618:LEU:HB3	1:A:620:PHE:CE1	2.50	0.46
1:A:381:ASN:O	1:A:407:ASN:ND2	2.33	0.46
1:B:468:LEU:HD12	1:B:468:LEU:O	2.16	0.46
1:B:502:SER:OG	1:B:503:LYS:N	2.48	0.46
2:C:56:GLY:HA2	2:C:121:PHE:O	2.15	0.46
2:C:124:ILE:CG1	2:C:125:LEU:N	2.78	0.46
2:D:124:ILE:CG1	2:D:126:PHE:CE1	2.99	0.46
1:A:260:GLY:HA3	1:A:290:THR:OG1	2.16	0.46
1:A:450:LEU:HD12	1:A:451:ASP:H	1.80	0.46
1:B:28:CYS:HB2	1:B:39:CYS:HA	1.96	0.46
1:B:262:PHE:HB2	1:B:265:GLU:OE1	2.16	0.46
1:A:262:PHE:HB2	1:A:265:GLU:OE1	2.16	0.46
2:C:27:SER:OG	2:C:28:SER:N	2.49	0.46
1:A:389:CYS:HB2	1:A:416:PHE:HE1	1.72	0.45
1:B:618:LEU:HB3	1:B:620:PHE:CE1	2.50	0.45
2:C:79:PHE:O	2:C:133:CYS:HA	2.16	0.45
2:D:79:PHE:O	2:D:133:CYS:HA	2.16	0.45
2:D:27:SER:OG	2:D:28:SER:N	2.49	0.45
2:D:56:GLY:HA2	2:D:121:PHE:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLY:HA3	1:B:290:THR:OG1	2.16	0.45
1:A:468:LEU:O	1:A:468:LEU:HD12	2.16	0.45
1:B:178:HIS:HE1	1:B:180:ASP:HB2	1.82	0.45
1:B:580:CYS:HB3	1:B:608:THR:CG2	2.44	0.45
1:A:494:THR:OG1	1:A:495:ASN:N	2.50	0.45
1:A:580:CYS:HB2	1:A:606:CYS:HB2	1.59	0.45
1:A:178:HIS:HE1	1:A:180:ASP:HB2	1.82	0.44
1:A:252:LEU:HD23	1:A:253:HIS:N	2.32	0.44
1:B:391:TYR:HB2	1:B:418:GLY:HA3	1.99	0.44
2:C:37:CYS:HB2	2:C:148:CYS:HB3	1.74	0.44
2:C:124:ILE:CG2	2:C:126:PHE:CE1	3.00	0.44
1:B:94:ASP:OD1	1:B:95:LYS:N	2.51	0.44
1:A:94:ASP:OD1	1:A:95:LYS:N	2.51	0.44
1:A:322:GLU:N	1:A:322:GLU:OE2	2.51	0.44
1:A:240:ASN:OD1	1:A:240:ASN:N	2.51	0.44
1:A:83:ASP:OD1	1:A:84:LEU:N	2.51	0.44
1:B:252:LEU:HD23	1:B:253:HIS:N	2.32	0.44
1:A:288:ARG:NH2	2:C:99:ASP:OD2	2.44	0.43
1:B:83:ASP:OD1	1:B:84:LEU:N	2.51	0.43
1:B:494:THR:OG1	1:B:495:ASN:N	2.50	0.43
1:B:585:GLN:OE1	1:B:585:GLN:N	2.43	0.43
2:C:96:HIS:HE1	2:C:98:HIS:HB3	1.82	0.43
1:A:143:PHE:HD2	1:A:145:ILE:HG13	1.83	0.43
2:D:37:CYS:HB2	2:D:148:CYS:HB3	1.74	0.43
1:B:322:GLU:OE2	1:B:322:GLU:N	2.51	0.43
2:D:48:SER:OG	2:D:60:PHE:O	2.31	0.43
1:A:391:TYR:HB2	1:A:418:GLY:HA3	1.99	0.43
1:A:53:SER:OG	1:A:54:SER:N	2.51	0.43
2:D:49:GLU:HA	2:D:50:PRO:HA	1.86	0.43
1:B:405:SER:OG	1:B:426:ASP:OD1	2.32	0.43
1:A:222:PHE:HA	1:A:225:ILE:HD12	2.01	0.42
1:B:568:LEU:HD21	1:B:571:PHE:CE1	2.54	0.42
1:A:574:THR:HG22	1:A:575:ASN:OD1	2.19	0.42
1:B:333:LEU:HD12	1:B:334:SER:H	1.84	0.42
1:A:579:ALA:HB3	1:A:584:HIS:NE2	2.35	0.42
2:D:138:ILE:HG22	2:D:139:ALA:O	2.19	0.42
1:B:497:THR:O	1:B:520:LEU:HD12	2.19	0.42
1:A:405:SER:OG	1:A:426:ASP:OD1	2.32	0.42
1:B:143:PHE:HD2	1:B:145:ILE:HG13	1.83	0.42
1:B:222:PHE:HA	1:B:225:ILE:HD12	2.01	0.42
1:B:574:THR:HG22	1:B:575:ASN:OD1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:ALA:HB3	1:B:584:HIS:NE2	2.35	0.42
1:A:333:LEU:HD12	1:A:334:SER:H	1.84	0.42
1:B:53:SER:OG	1:B:54:SER:N	2.51	0.42
2:C:48:SER:HA	2:C:61:VAL:HA	2.02	0.42
2:C:49:GLU:HA	2:C:50:PRO:HA	1.86	0.42
5:C:206:NAG:O6	5:C:206:NAG:O4	2.28	0.42
1:A:568:LEU:HD21	1:A:571:PHE:CE1	2.54	0.42
1:A:288:ARG:HE	1:A:288:ARG:HB3	1.46	0.42
1:A:497:THR:O	1:A:520:LEU:HD12	2.19	0.42
1:B:476:MET:HB3	1:B:479:ASN:HD22	1.85	0.41
2:C:138:ILE:HG22	2:C:139:ALA:O	2.19	0.41
2:D:96:HIS:HE1	2:D:98:HIS:HB3	1.82	0.41
1:A:490:PHE:CZ	1:A:501:LEU:HD21	2.56	0.41
1:B:254:VAL:HG22	1:B:255:HIS:N	2.35	0.41
1:B:469:THR:OG1	1:B:470:SER:N	2.54	0.41
1:A:585:GLN:HB3	1:A:620:PHE:CE2	2.55	0.41
1:B:212:ASN:H	1:B:235:ASN:ND2	2.18	0.41
1:B:240:ASN:OD1	1:B:240:ASN:N	2.51	0.41
1:B:490:PHE:CZ	1:B:501:LEU:HD21	2.56	0.41
2:C:55:ARG:O	2:C:57:THR:HG23	2.20	0.41
1:B:86:ARG:HD2	1:B:86:ARG:HA	1.93	0.41
2:D:55:ARG:O	2:D:57:THR:HG23	2.20	0.41
1:A:254:VAL:HG22	1:A:255:HIS:N	2.35	0.41
1:A:476:MET:HB3	1:A:479:ASN:HD22	1.85	0.41
1:A:469:THR:OG1	1:A:470:SER:N	2.54	0.41
1:B:340:LEU:HB3	1:B:359:ASN:HD21	1.85	0.41
2:C:34:TYR:HD2	2:C:149:LEU:HD22	1.86	0.41
2:D:48:SER:HA	2:D:61:VAL:HA	2.02	0.41
1:A:340:LEU:HB3	1:A:359:ASN:HD21	1.85	0.41
1:B:288:ARG:HE	1:B:288:ARG:HB3	1.46	0.41
1:B:416:PHE:HB2	1:B:444:LEU:HD21	2.03	0.41
1:A:549:CYS:C	1:A:552:ASN:HD21	2.29	0.40
1:A:416:PHE:HB2	1:A:444:LEU:HD21	2.03	0.40
1:A:31:VAL:HB	1:A:36:THR:OG1	2.22	0.40
1:B:402:LEU:HD12	1:B:403:ASP:H	1.87	0.40
1:B:549:CYS:C	1:B:552:ASN:HD21	2.30	0.40
1:B:585:GLN:HB3	1:B:620:PHE:CE2	2.55	0.40
1:A:212:ASN:H	1:A:235:ASN:ND2	2.18	0.40
2:D:34:TYR:HD2	2:D:149:LEU:HD22	1.86	0.40
1:A:139:SER:OG	1:A:140:LEU:N	2.54	0.40
1:A:550:SER:OG	1:A:551:PHE:HD1	2.05	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	593/604 (98%)	503 (85%)	90 (15%)	0	100	100
1	B	593/604 (98%)	502 (85%)	91 (15%)	0	100	100
2	C	134/142 (94%)	120 (90%)	14 (10%)	0	100	100
2	D	134/142 (94%)	120 (90%)	14 (10%)	0	100	100
All	All	1454/1492 (98%)	1245 (86%)	209 (14%)	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	554/563 (98%)	554 (100%)	0	100	100
1	B	554/563 (98%)	554 (100%)	0	100	100
2	C	123/129 (95%)	123 (100%)	0	100	100
2	D	123/129 (95%)	123 (100%)	0	100	100
All	All	1354/1384 (98%)	1354 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	147	GLN
1	A	212	ASN
1	A	235	ASN
1	A	255	HIS
1	A	307	ASN
1	A	401	HIS
1	A	415	ASN
1	A	429	HIS
1	A	495	ASN
1	A	540	GLN
1	A	552	ASN
1	A	613	ASN
1	B	111	ASN
1	B	147	GLN
1	B	212	ASN
1	B	235	ASN
1	B	255	HIS
1	B	307	ASN
1	B	401	HIS
1	B	428	GLN
1	B	429	HIS
1	B	495	ASN
1	B	540	GLN
1	B	552	ASN
1	B	613	ASN

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

24 ligands 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
5	NAG	B	704	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	A	707	1	14,14,15	0.40	0	17,19,21	0.76	0
7	OIL	D	202	3	31,31,31	1.96	4 (12%)	32,33,33	1.34	3 (9%)
5	NAG	D	205	2	14,14,15	0.40	0	17,19,21	0.75	0
6	2IL	C	201	3	28,28,29	1.70	3 (10%)	29,29,31	1.63	3 (10%)
5	NAG	C	205	2	14,14,15	0.33	0	17,19,21	0.50	0
5	NAG	D	204	2	14,14,15	0.33	0	17,19,21	0.50	0
5	NAG	B	705	1	14,14,15	0.40	0	17,19,21	0.76	0
5	NAG	C	206	2	14,14,15	0.40	0	17,19,21	0.75	0
5	NAG	A	706	1	14,14,15	0.41	0	17,19,21	0.75	0
8	X6N	C	203	3,4	16,16,17	2.30	5 (31%)	23,24,25	0.80	0
4	A1L01	C	204	8	27,27,27	2.15	4 (14%)	28,29,29	1.33	2 (7%)
5	NAG	B	703	-	14,14,15	0.35	0	17,19,21	0.42	0
5	NAG	B	706	1	14,14,15	0.41	0	17,19,21	0.76	0
7	OIL	C	202	3	31,31,31	1.96	4 (12%)	32,33,33	1.34	3 (9%)
3	GP4	A	701	8,6,7	14,14,16	2.64	4 (28%)	18,20,24	0.90	0
8	X6N	D	203	3,4	16,16,17	2.30	5 (31%)	23,24,25	0.80	0
4	A1L01	A	702	8	27,27,27	2.15	4 (14%)	28,29,29	1.32	2 (7%)
5	NAG	B	702	1	14,14,15	0.31	0	17,19,21	0.46	0
3	GP4	B	701	8,6,7	14,14,16	2.64	4 (28%)	18,20,24	0.90	0
5	NAG	A	705	1	14,14,15	0.24	0	17,19,21	0.46	0
6	2IL	D	201	3	28,28,29	1.70	3 (10%)	29,29,31	1.63	3 (10%)
5	NAG	A	703	1	14,14,15	0.31	0	17,19,21	0.46	0
5	NAG	A	704	-	14,14,15	0.34	0	17,19,21	0.42	0

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
5	NAG	B	704	1	-	2/6/23/26	0/1/1/1
5	NAG	A	707	1	-	2/6/23/26	0/1/1/1
7	0IL	D	202	3	-	15/32/32/32	-
5	NAG	D	205	2	-	2/6/23/26	0/1/1/1
6	2IL	C	201	3	-	14/29/29/30	-
5	NAG	C	205	2	-	0/6/23/26	0/1/1/1
5	NAG	D	204	2	-	0/6/23/26	0/1/1/1
5	NAG	B	705	1	-	1/6/23/26	0/1/1/1
5	NAG	C	206	2	-	2/6/23/26	0/1/1/1
5	NAG	A	706	1	-	1/6/23/26	0/1/1/1
8	X6N	C	203	3,4	-	0/7/27/29	0/1/1/1
4	A1L01	C	204	8	-	13/28/28/28	-
5	NAG	B	703	-	-	0/6/23/26	0/1/1/1
5	NAG	B	706	1	-	2/6/23/26	0/1/1/1
7	0IL	C	202	3	-	15/32/32/32	-
3	GP4	A	701	8,6,7	-	3/7/20/27	0/1/1/1
8	X6N	D	203	3,4	-	0/7/27/29	0/1/1/1
4	A1L01	A	702	8	-	13/28/28/28	-
5	NAG	B	702	1	-	4/6/23/26	0/1/1/1
3	GP4	B	701	8,6,7	-	3/7/20/27	0/1/1/1
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1
6	2IL	D	201	3	-	14/29/29/30	-
5	NAG	A	703	1	-	4/6/23/26	0/1/1/1
5	NAG	A	704	-	-	0/6/23/26	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	A1L01	O248-C243	7.22	1.44	1.22
4	C	204	A1L01	O248-C243	7.21	1.44	1.22
6	C	201	2IL	O4-C15	6.97	1.43	1.22
6	D	201	2IL	O4-C15	6.97	1.43	1.22
7	D	202	0IL	O1F-C1F	6.88	1.43	1.22
7	C	202	0IL	O1F-C1F	6.86	1.43	1.22
7	D	202	0IL	O1E-C1E	6.54	1.43	1.22
7	C	202	0IL	O1E-C1E	6.52	1.43	1.22
3	B	701	GP4	P4A-O4	6.36	1.70	1.59
3	A	701	GP4	P4A-O4	6.35	1.70	1.59
4	C	204	A1L01	O52-C35	6.29	1.42	1.22
4	A	702	A1L01	O52-C35	6.28	1.42	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	203	X6N	P51-O56	5.95	1.69	1.50
8	D	203	X6N	P51-O56	5.93	1.68	1.50
3	A	701	GP4	P4A-O8A	5.11	1.66	1.50
3	B	701	GP4	P4A-O8A	5.11	1.66	1.50
8	C	203	X6N	P51-O4	4.54	1.67	1.59
8	D	203	X6N	P51-O4	4.51	1.67	1.59
6	D	201	2IL	O2-C1	4.08	1.43	1.20
6	C	201	2IL	O2-C1	4.08	1.43	1.20
4	A	702	A1L01	O72-C35	3.87	1.43	1.30
4	C	204	A1L01	O72-C35	3.87	1.43	1.30
7	C	202	0IL	O3E-C1E	3.60	1.42	1.30
7	D	202	0IL	O3E-C1E	3.59	1.42	1.30
8	C	203	X6N	P51-O55	3.38	1.67	1.54
8	D	203	X6N	P51-O55	3.37	1.67	1.54
4	A	702	A1L01	O240-C243	3.33	1.43	1.34
4	C	204	A1L01	O240-C243	3.31	1.43	1.34
6	C	201	2IL	O3-C15	3.24	1.43	1.34
6	D	201	2IL	O3-C15	3.22	1.43	1.34
3	A	701	GP4	P4A-O9A	3.21	1.66	1.54
3	B	701	GP4	P4A-O9A	3.18	1.66	1.54
7	C	202	0IL	O2E-C1F	3.14	1.43	1.34
7	D	202	0IL	O2E-C1F	3.13	1.43	1.34
3	B	701	GP4	P4A-O7A	3.12	1.66	1.54
3	A	701	GP4	P4A-O7A	3.12	1.66	1.54
8	D	203	X6N	P51-O54	2.89	1.65	1.54
8	C	203	X6N	P51-O54	2.88	1.65	1.54
8	D	203	X6N	C1-C2	-2.49	1.50	1.52
8	C	203	X6N	C1-C2	-2.44	1.50	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	202	0IL	O2E-C1F-C2F	4.83	121.93	111.48
7	C	202	0IL	O2E-C1F-C2F	4.82	121.90	111.48
6	D	201	2IL	C4-C3-C2	-4.75	108.08	114.08
6	C	201	2IL	C4-C3-C2	-4.73	108.09	114.08
6	C	201	2IL	O3-C15-C16	4.43	121.08	111.48
6	D	201	2IL	O3-C15-C16	4.42	121.05	111.48
4	A	702	A1L01	O240-C243-C249	3.70	119.47	111.48
4	C	204	A1L01	O240-C243-C249	3.69	119.46	111.48
4	C	204	A1L01	O72-C35-C73	2.53	121.86	114.00
4	A	702	A1L01	O72-C35-C73	2.52	121.83	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	202	0IL	O2E-C3E-C2E	2.24	111.51	106.72
7	D	202	0IL	O2E-C3E-C2E	2.23	111.48	106.72
7	D	202	0IL	O2E-C1F-O1F	-2.10	118.79	123.70
7	C	202	0IL	O2E-C1F-O1F	-2.10	118.80	123.70
6	D	201	2IL	O2-C1-C2	-2.03	119.48	125.38
6	C	201	2IL	O2-C1-C2	-2.02	119.48	125.38

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	A1L01	O240-C125-C246-C252
4	A	702	A1L01	C73-C125-O240-C243
4	C	204	A1L01	O240-C125-C246-C252
4	C	204	A1L01	C73-C125-O240-C243
5	C	206	NAG	C3-C2-N2-C7
5	D	205	NAG	C3-C2-N2-C7
6	C	201	2IL	C2-C3-C4-C5
6	D	201	2IL	C2-C3-C4-C5
7	C	202	0IL	C1E-C2E-C3E-O2E
7	C	202	0IL	C1E-C2E-C3E-C4E
7	D	202	0IL	C1E-C2E-C3E-O2E
7	D	202	0IL	C1E-C2E-C3E-C4E
5	A	707	NAG	C4-C5-C6-O6
5	B	706	NAG	C4-C5-C6-O6
3	A	701	GP4	O5-C5-C6-O6
3	B	701	GP4	O5-C5-C6-O6
5	A	707	NAG	O5-C5-C6-O6
5	B	706	NAG	O5-C5-C6-O6
3	A	701	GP4	C4-C5-C6-O6
3	B	701	GP4	C4-C5-C6-O6
5	A	703	NAG	O5-C5-C6-O6
5	B	702	NAG	O5-C5-C6-O6
5	A	705	NAG	O5-C5-C6-O6
5	B	704	NAG	O5-C5-C6-O6
5	A	703	NAG	C8-C7-N2-C2
5	A	703	NAG	O7-C7-N2-C2
5	B	702	NAG	C8-C7-N2-C2
5	B	702	NAG	O7-C7-N2-C2
4	A	702	A1L01	C73-C125-C246-C252
4	C	204	A1L01	C73-C125-C246-C252
6	C	201	2IL	O3-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	201	2IL	O3-C3-C4-C5
4	A	702	A1L01	C243-C249-C281-C285
4	C	204	A1L01	C243-C249-C281-C285
7	C	202	0IL	C0S-C1S-C2S-C3S
7	D	202	0IL	C0S-C1S-C2S-C3S
6	C	201	2IL	C15-C16-C17-C18
6	D	201	2IL	C15-C16-C17-C18
6	C	201	2IL	C22-C23-C24-C25
6	D	201	2IL	C22-C23-C24-C25
7	C	202	0IL	C1F-C2F-C3F-C4F
7	D	202	0IL	C1F-C2F-C3F-C4F
4	A	702	A1L01	C252-C255-C258-C261
4	C	204	A1L01	C252-C255-C258-C261
6	C	201	2IL	C16-C17-C18-C19
6	D	201	2IL	C16-C17-C18-C19
4	A	702	A1L01	O248-C243-O240-C125
4	C	204	A1L01	O248-C243-O240-C125
7	C	202	0IL	C9F-C0T-C1T-C2T
7	D	202	0IL	C9F-C0T-C1T-C2T
4	A	702	A1L01	C246-C252-C255-C258
4	C	204	A1L01	C246-C252-C255-C258
4	A	702	A1L01	C285-C288-C291-C294
4	C	204	A1L01	C285-C288-C291-C294
5	C	206	NAG	O5-C5-C6-O6
5	D	205	NAG	O5-C5-C6-O6
6	C	201	2IL	C19-C20-C21-C22
6	D	201	2IL	C19-C20-C21-C22
7	D	202	0IL	C1S-C0S-C9E-C8E
7	C	202	0IL	C1S-C0S-C9E-C8E
7	C	202	0IL	C4F-C5F-C6F-C7F
7	D	202	0IL	C4F-C5F-C6F-C7F
7	C	202	0IL	C3F-C4F-C5F-C6F
7	D	202	0IL	C3F-C4F-C5F-C6F
7	C	202	0IL	C1S-C2S-C3S-C4S
7	D	202	0IL	C1S-C2S-C3S-C4S
4	C	204	A1L01	C249-C281-C285-C288
4	A	702	A1L01	C249-C281-C285-C288
7	C	202	0IL	C3E-C4E-C5E-C6E
7	D	202	0IL	C3E-C4E-C5E-C6E
4	A	702	A1L01	C255-C258-C261-C264
7	D	202	0IL	C7E-C8E-C9E-C0S
4	C	204	A1L01	C255-C258-C261-C264

Continued on next page...

Continued from previous page...

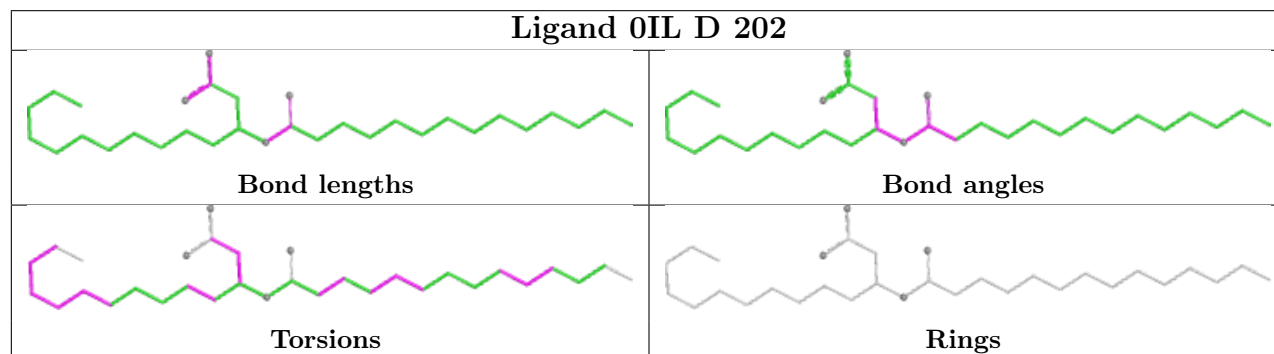
Mol	Chain	Res	Type	Atoms
7	C	202	0IL	C7E-C8E-C9E-C0S
4	C	204	A1L01	C291-C294-C297-C300
4	A	702	A1L01	C291-C294-C297-C300
5	A	703	NAG	C4-C5-C6-O6
5	B	702	NAG	C4-C5-C6-O6
6	C	201	2IL	O2-C1-C2-C3
6	D	201	2IL	O2-C1-C2-C3
7	C	202	0IL	O3E-C1E-C2E-C3E
7	D	202	0IL	O3E-C1E-C2E-C3E
7	C	202	0IL	O1E-C1E-C2E-C3E
7	D	202	0IL	O1E-C1E-C2E-C3E
6	C	201	2IL	O3-C15-C16-C17
6	D	201	2IL	O3-C15-C16-C17
4	A	702	A1L01	C294-C297-C300-C302
4	C	204	A1L01	C294-C297-C300-C302
5	A	706	NAG	C1-C2-N2-C7
5	B	705	NAG	C1-C2-N2-C7
5	A	705	NAG	C4-C5-C6-O6
5	B	704	NAG	C4-C5-C6-O6
7	C	202	0IL	C1T-C0T-C9F-C8F
7	D	202	0IL	C1T-C0T-C9F-C8F
6	D	201	2IL	C10-C11-C12-C13
6	C	201	2IL	C10-C11-C12-C13
6	C	201	2IL	C3-C4-C5-C6
6	D	201	2IL	C3-C4-C5-C6
6	C	201	2IL	C18-C19-C20-C21
6	D	201	2IL	C18-C19-C20-C21
6	C	201	2IL	C4-C5-C6-C7
6	D	201	2IL	C4-C5-C6-C7
6	C	201	2IL	C9-C10-C11-C12
6	D	201	2IL	C9-C10-C11-C12
6	C	201	2IL	C23-C24-C25-C26
6	D	201	2IL	C23-C24-C25-C26
3	A	701	GP4	C4-O4-P4A-O8A
3	B	701	GP4	C4-O4-P4A-O8A
4	A	702	A1L01	C125-C246-C252-C255
4	C	204	A1L01	C125-C246-C252-C255
7	D	202	0IL	C9E-C0S-C1S-C2S
7	C	202	0IL	C9E-C0S-C1S-C2S

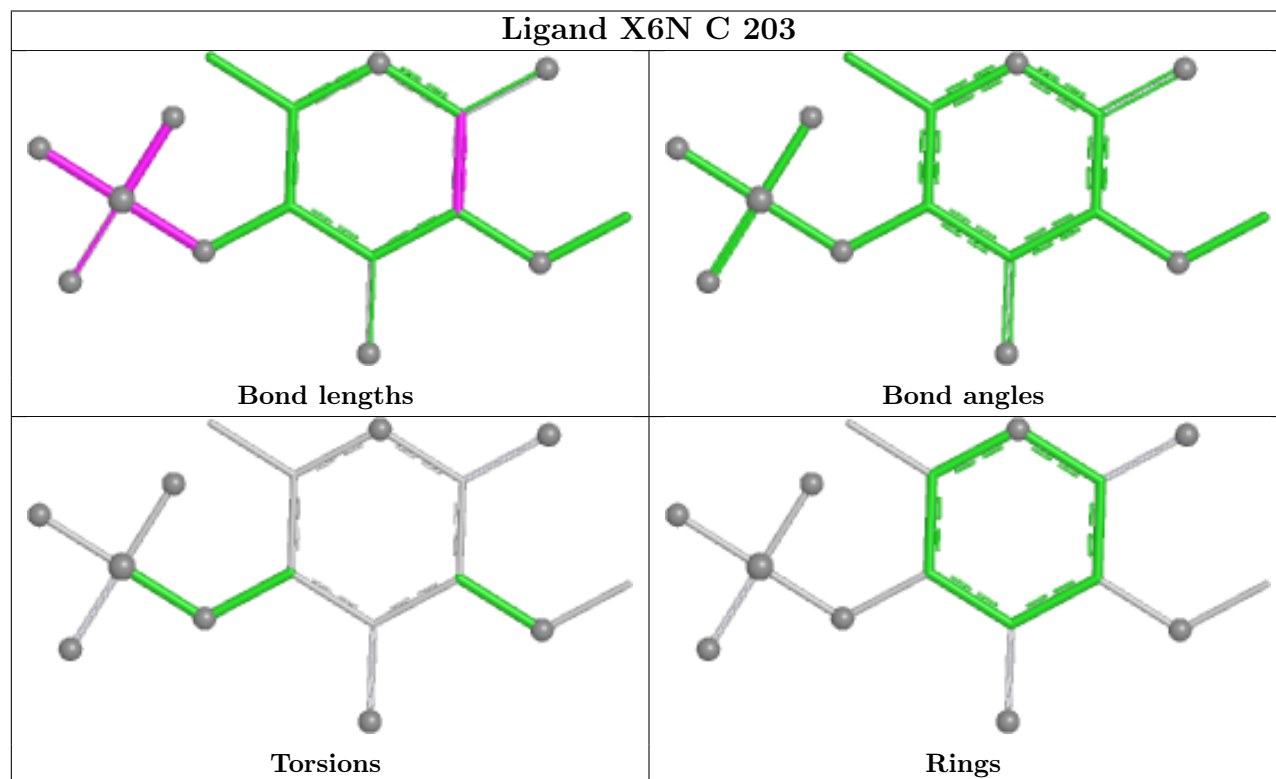
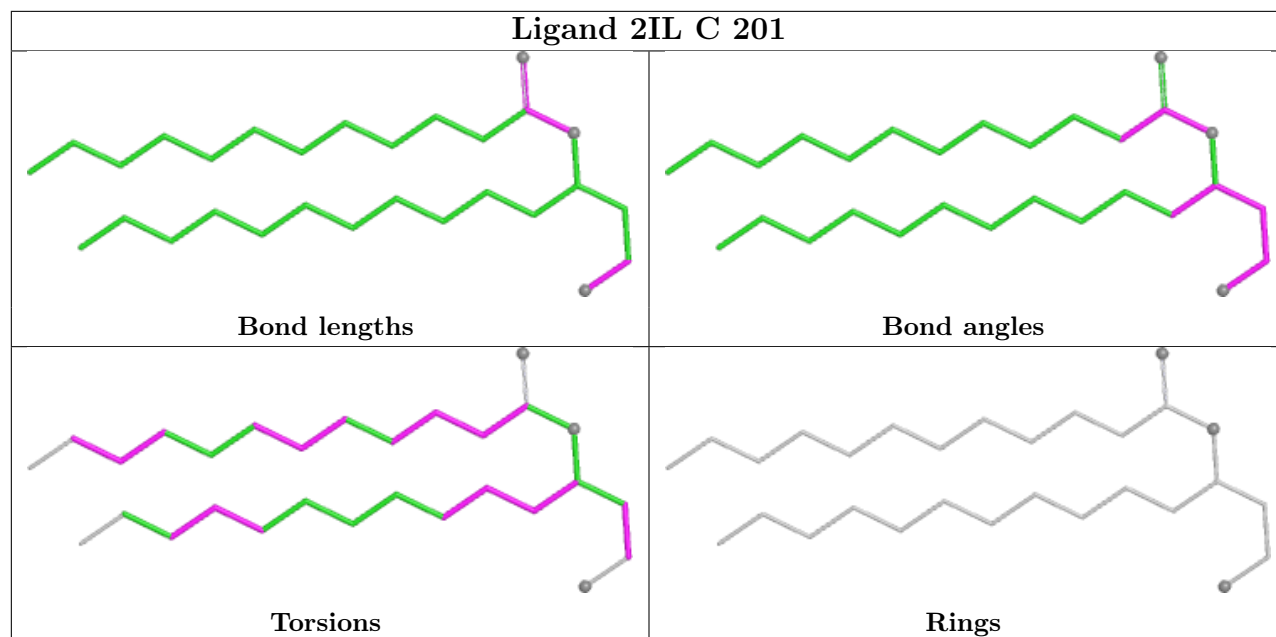
There are no ring outliers.

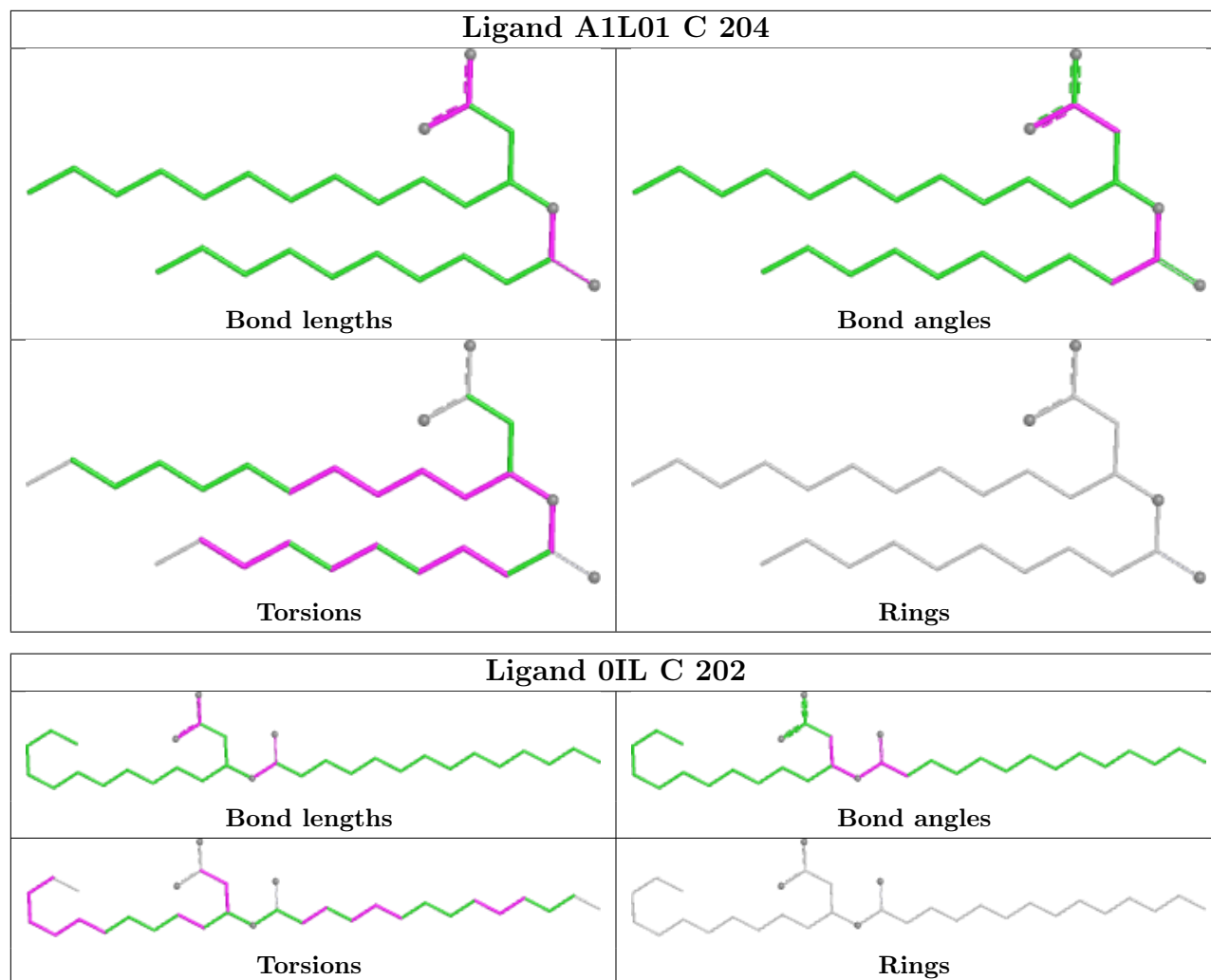
7 monomers are involved in 12 short contacts:

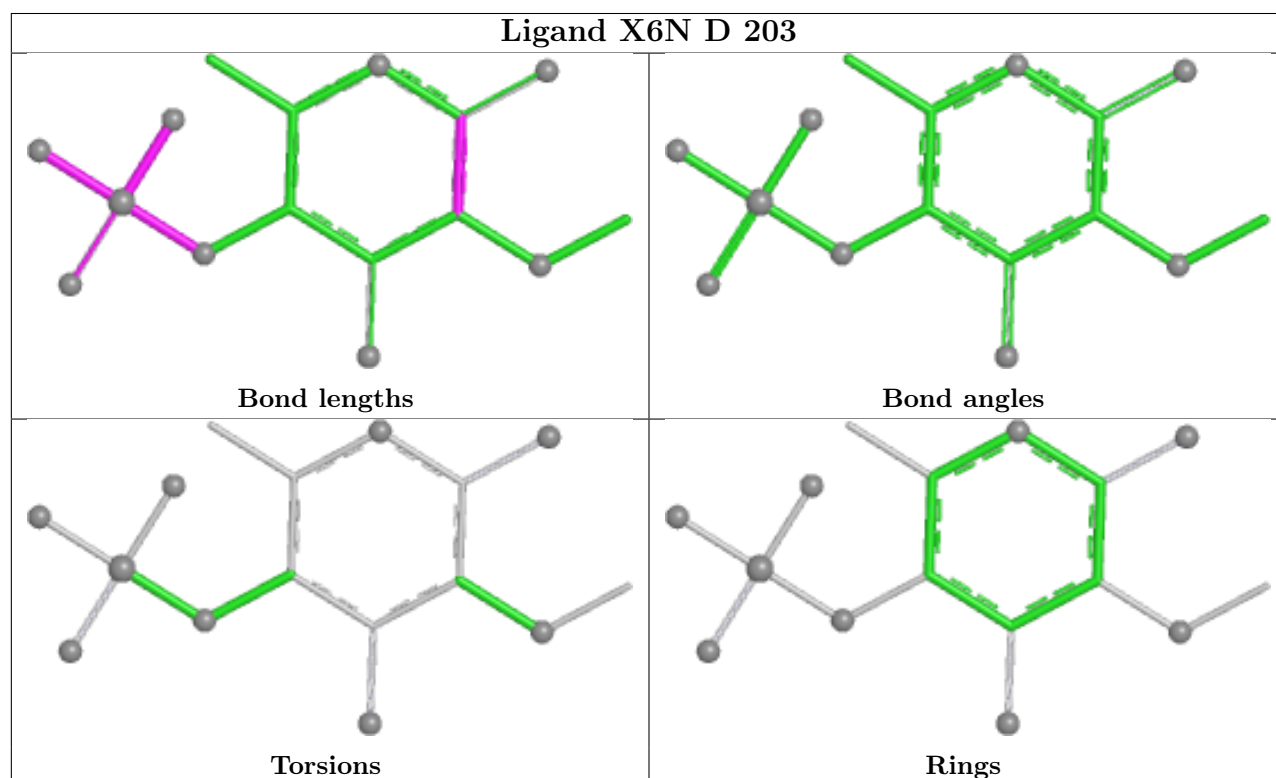
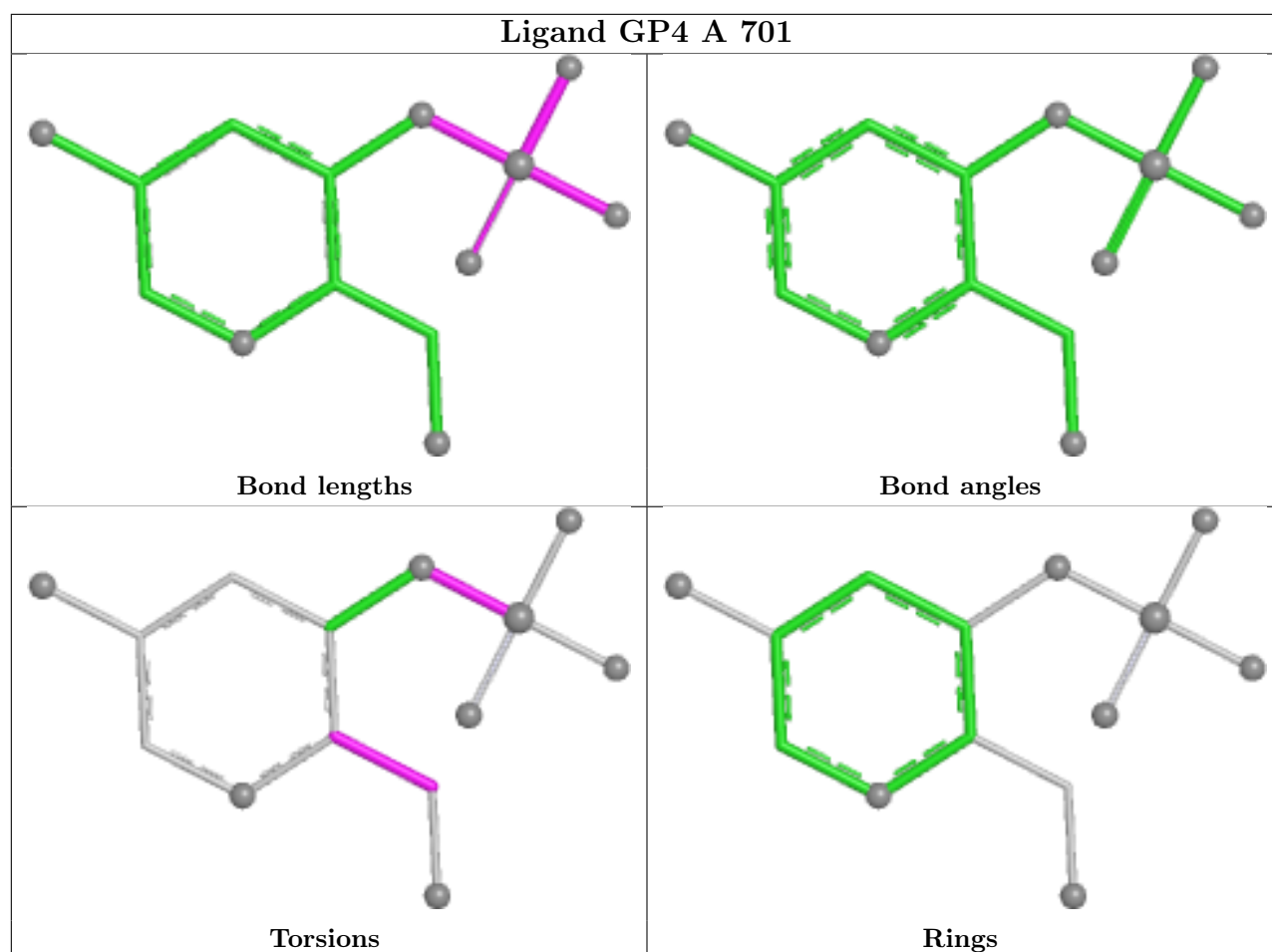
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	206	NAG	1	0
5	B	703	NAG	2	0
3	A	701	GP4	3	0
5	B	702	NAG	1	0
3	B	701	GP4	2	0
5	A	703	NAG	1	0
5	A	704	NAG	2	0

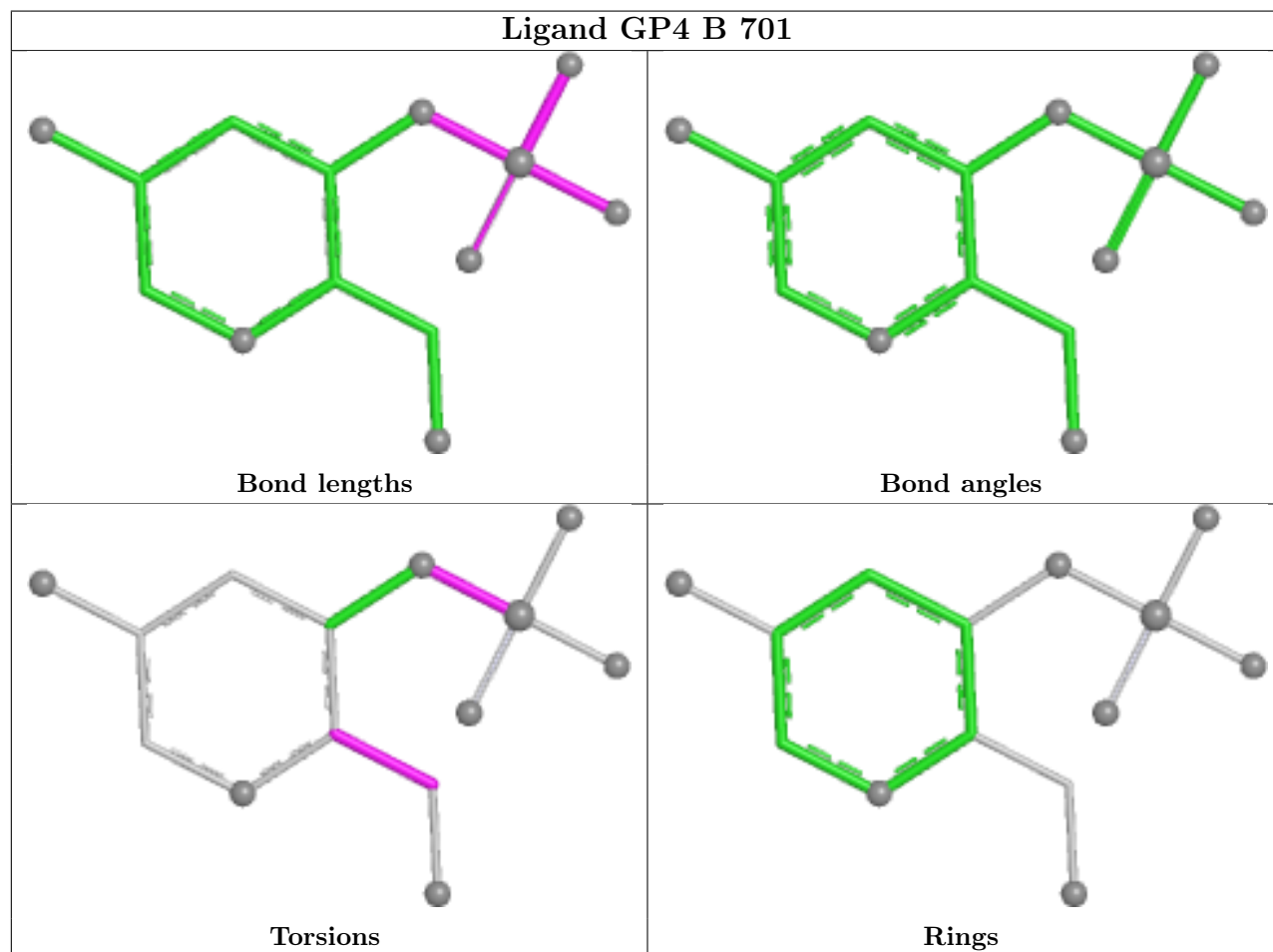
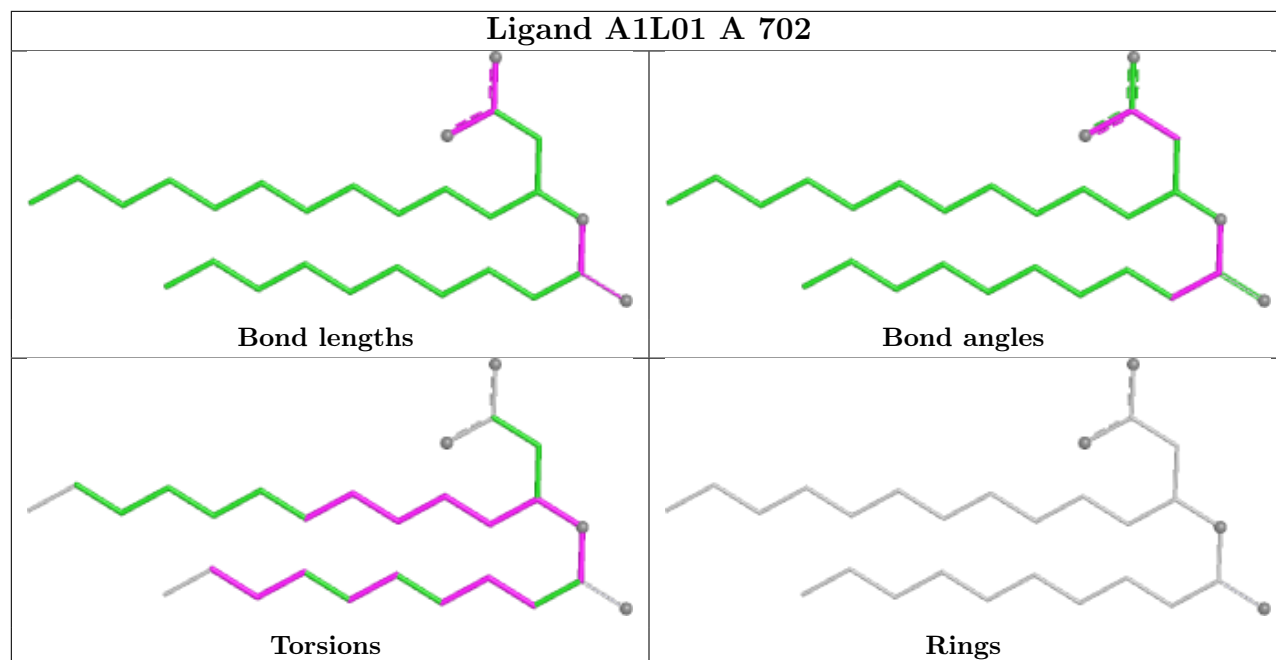
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

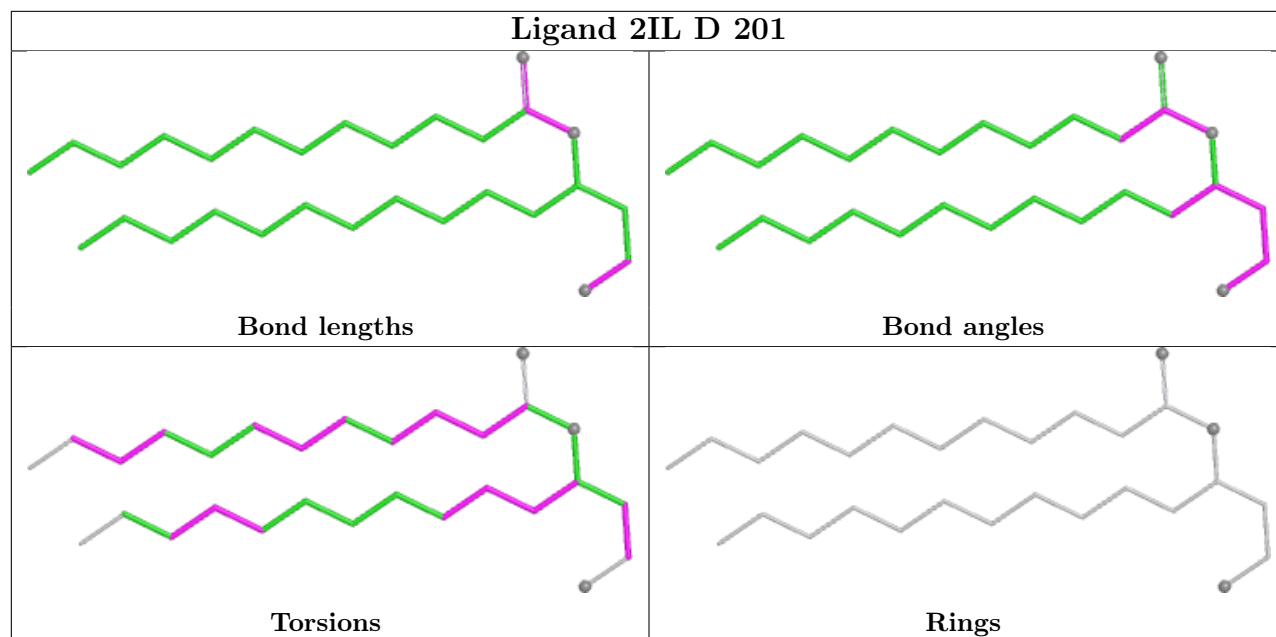












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

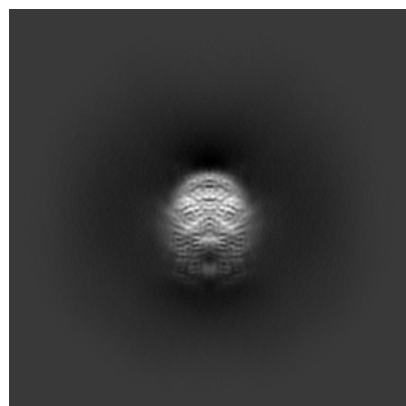
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37803. These allow visual inspection of the internal detail of the map and identification of artifacts.

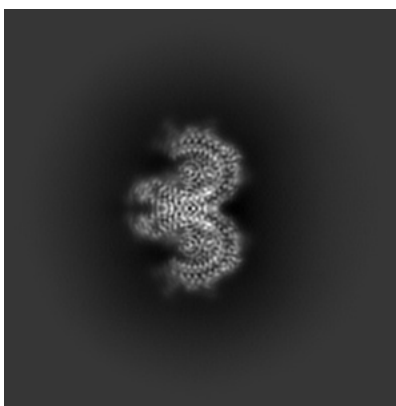
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

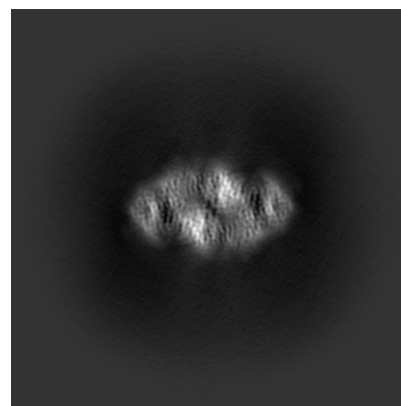
6.1.1 Primary map



X

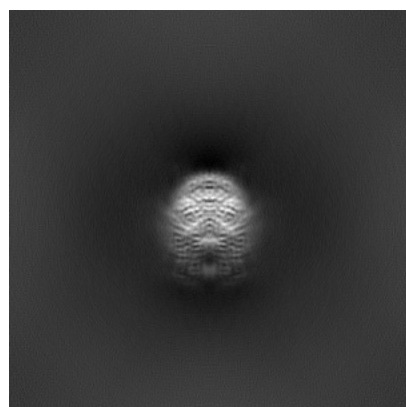


Y

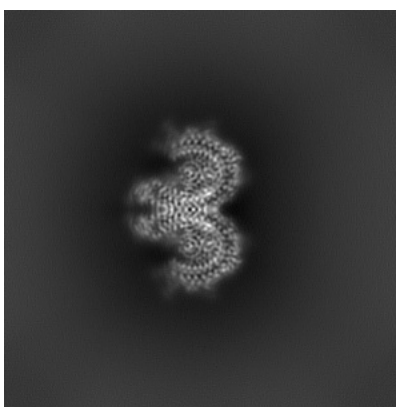


Z

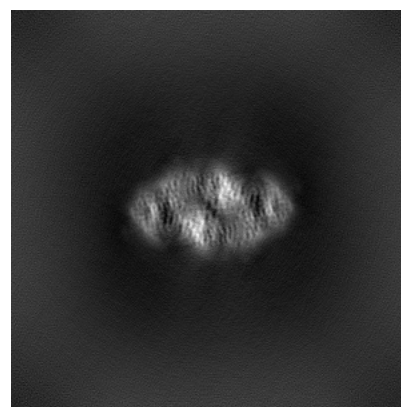
6.1.2 Raw map



X



Y

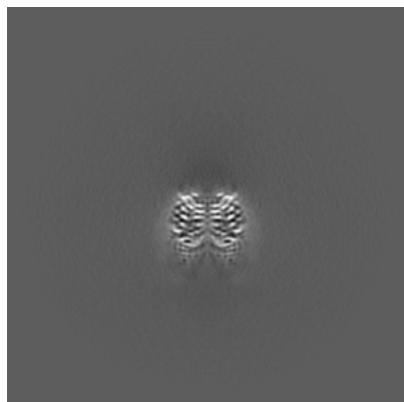


Z

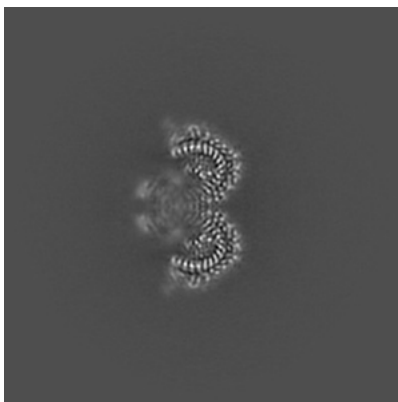
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

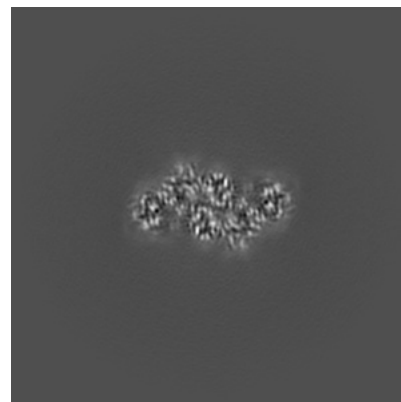
6.2.1 Primary map



X Index: 200

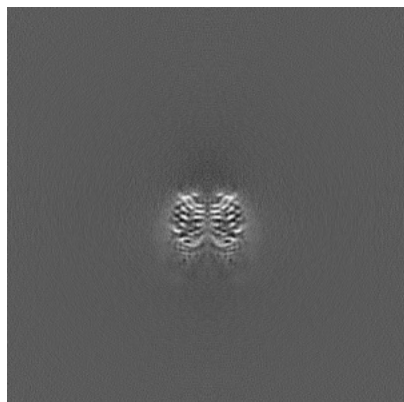


Y Index: 200

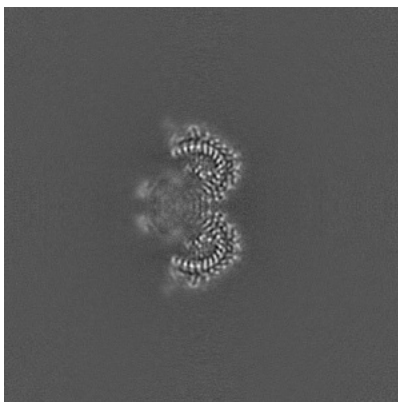


Z Index: 200

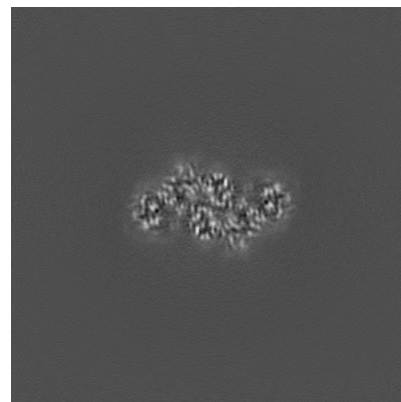
6.2.2 Raw map



X Index: 200



Y Index: 200

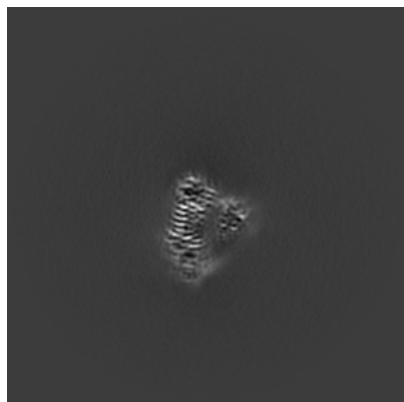


Z Index: 200

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

6.3 Largest variance slices [i](#)

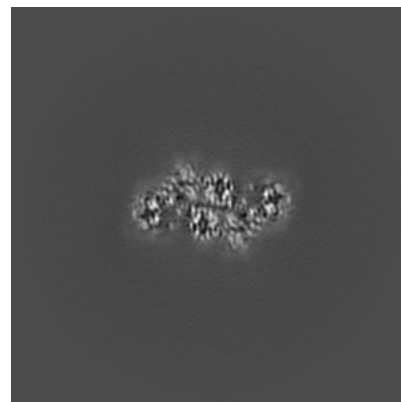
6.3.1 Primary map



X Index: 186

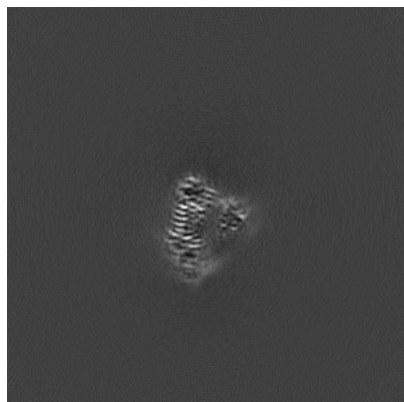


Y Index: 190

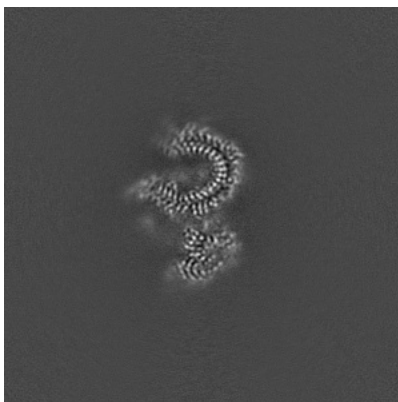


Z Index: 201

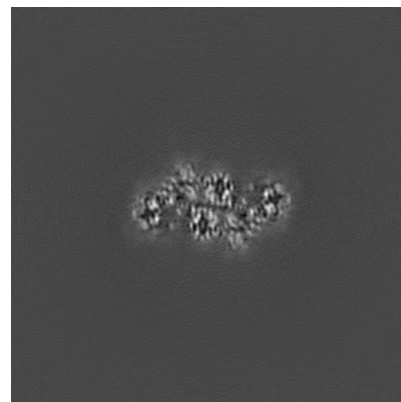
6.3.2 Raw map



X Index: 186



Y Index: 210

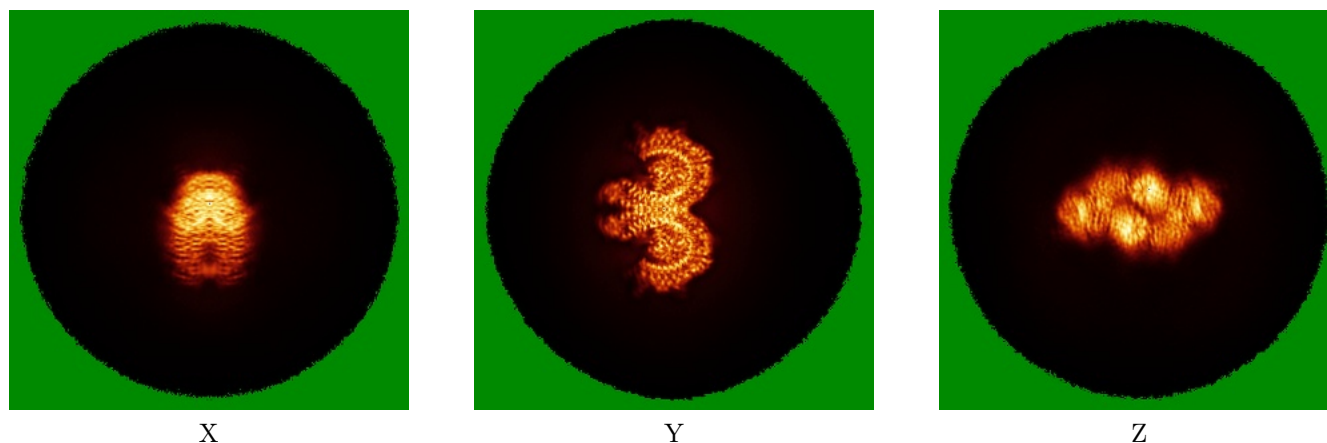


Z Index: 201

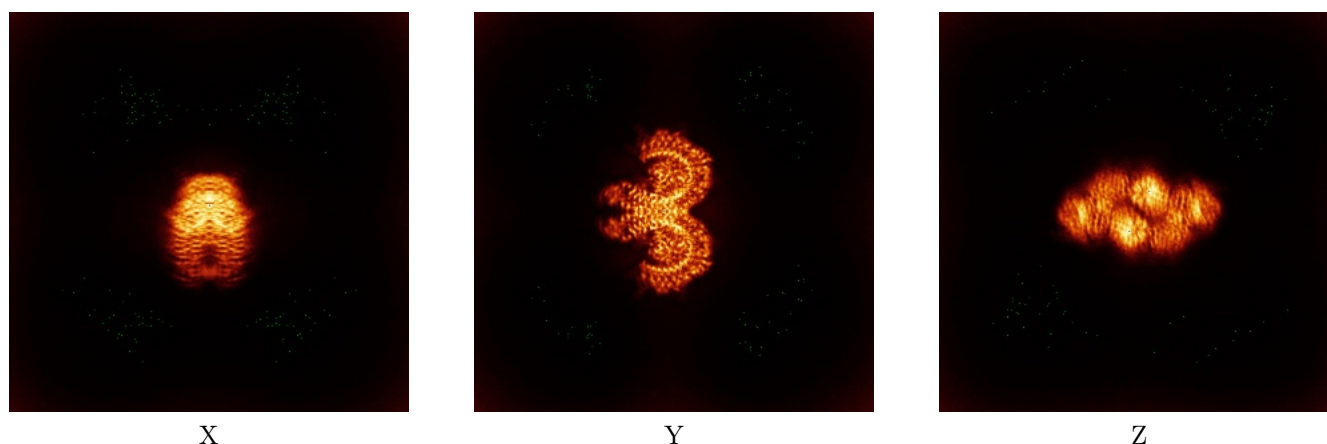
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

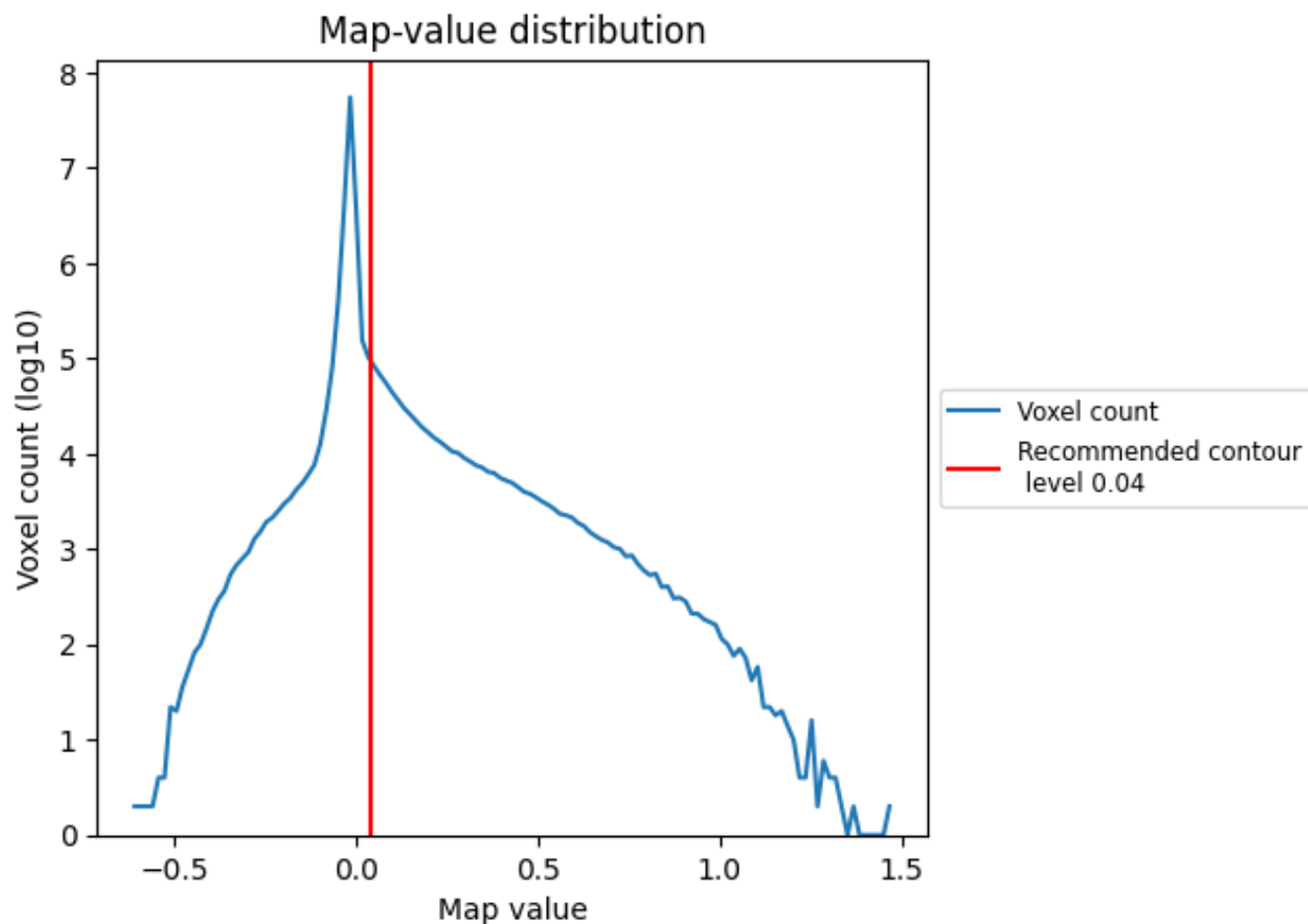
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

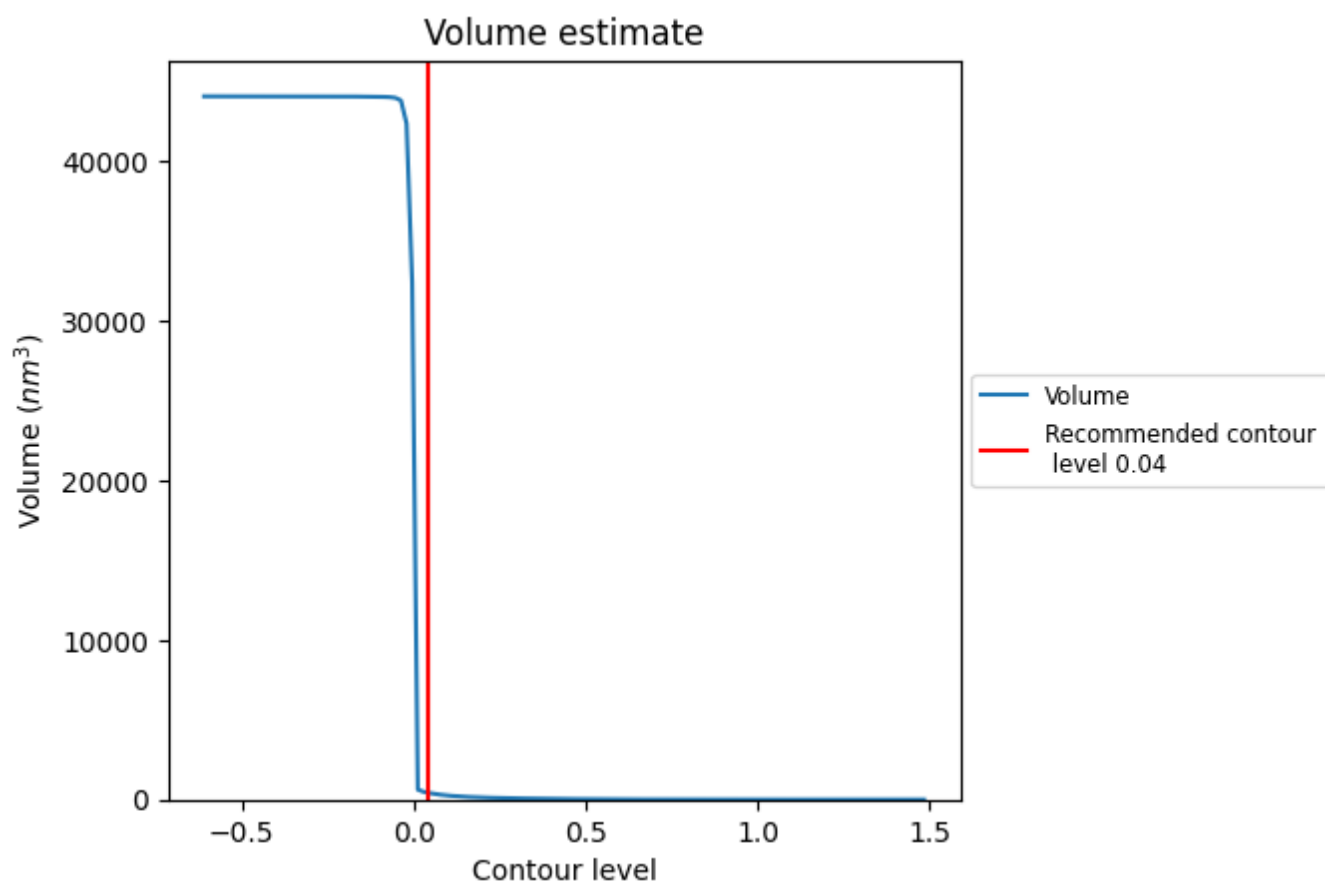
This section contains the results of statistical analysis of the map.

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.

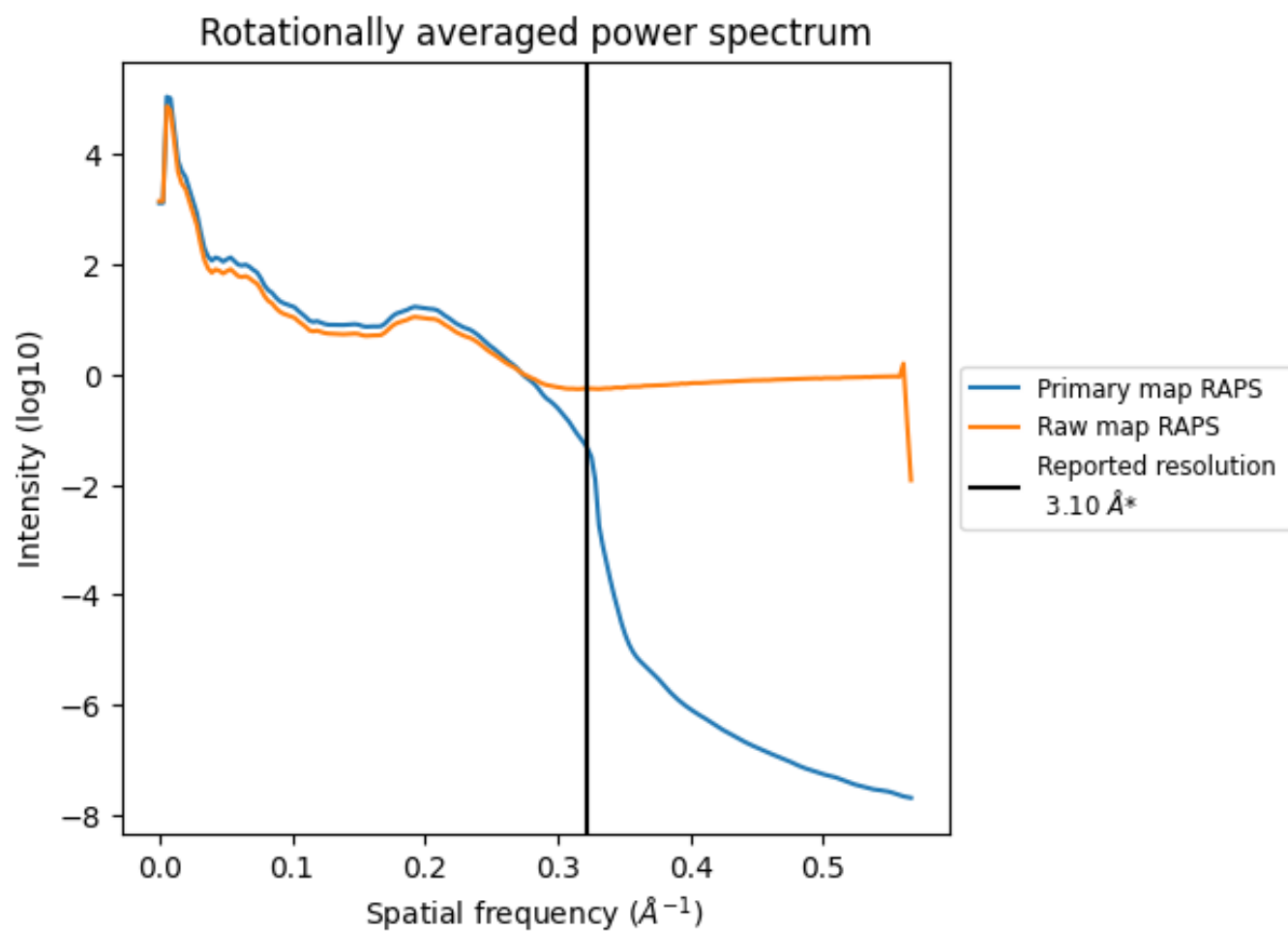
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 437 nm^3 ; this corresponds to an approximate mass of 394 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

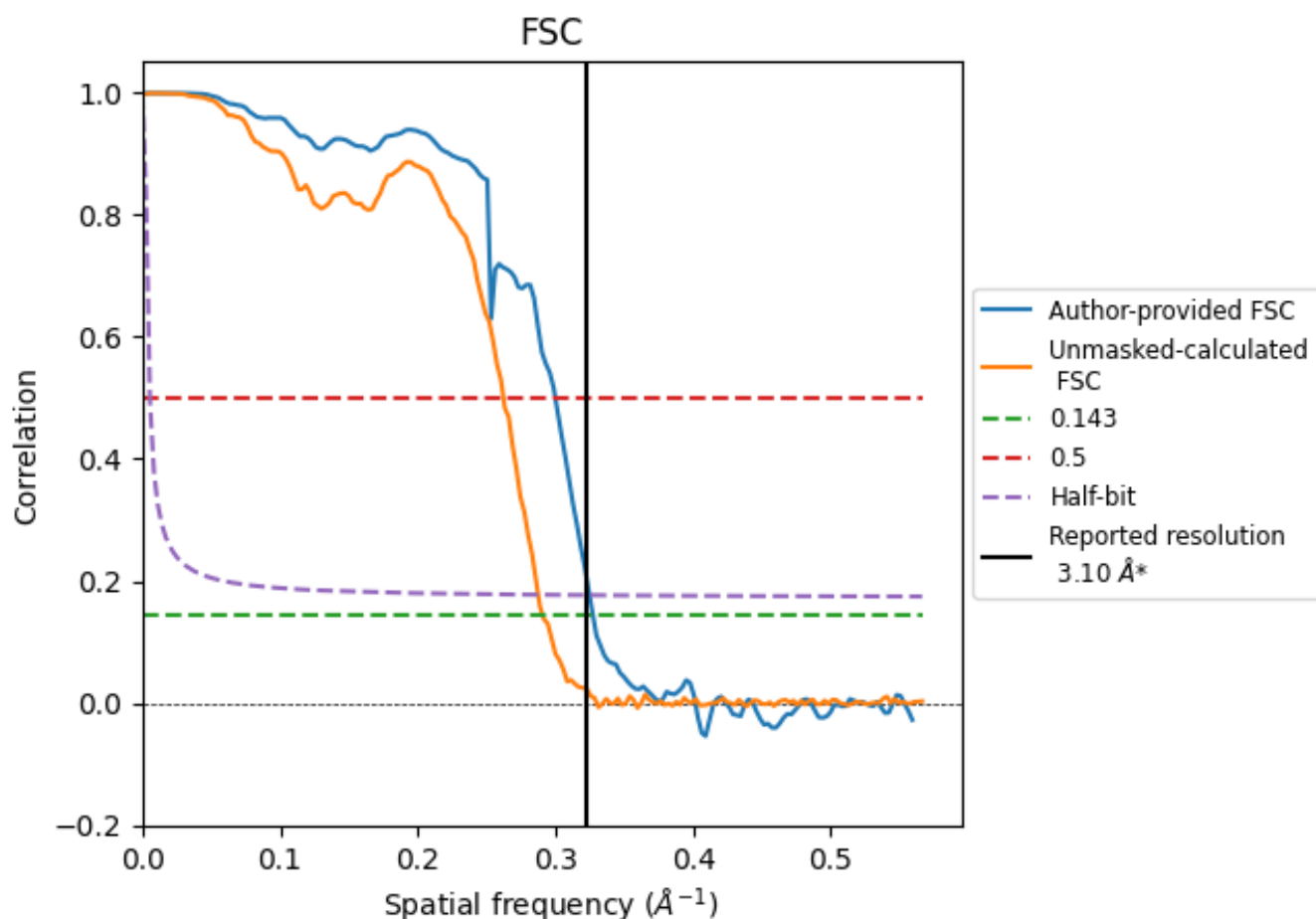


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.33	3.08
Unmasked-calculated*	3.44	3.81	3.48

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

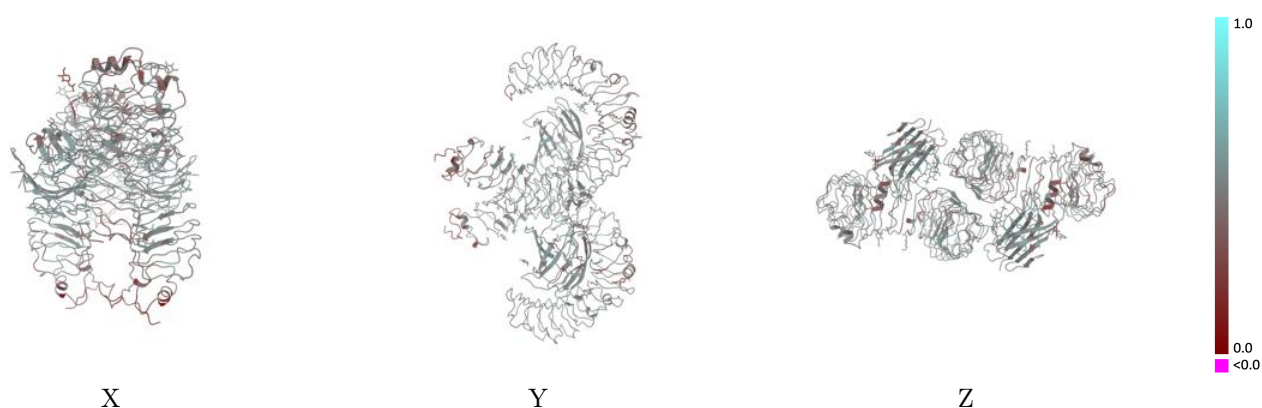
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37803 and PDB model 8WSA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)

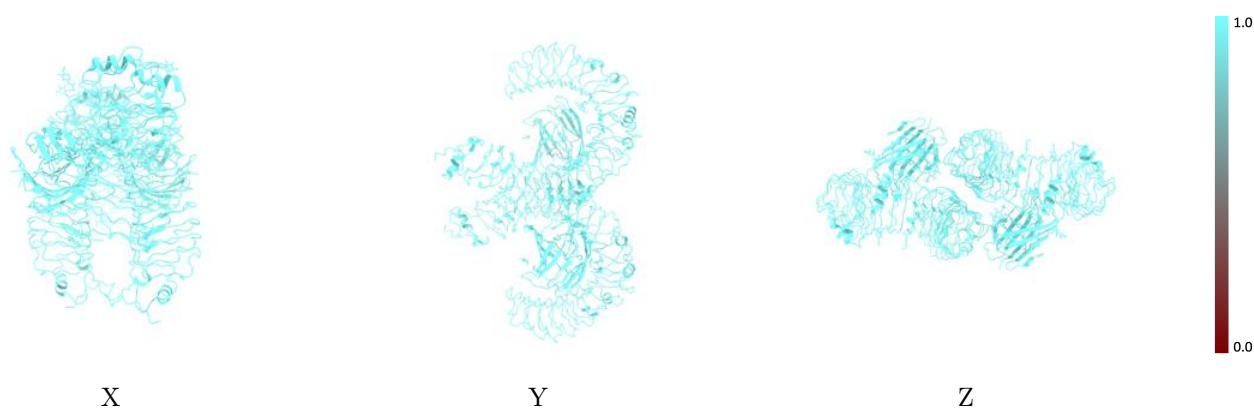
This section was not generated.

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



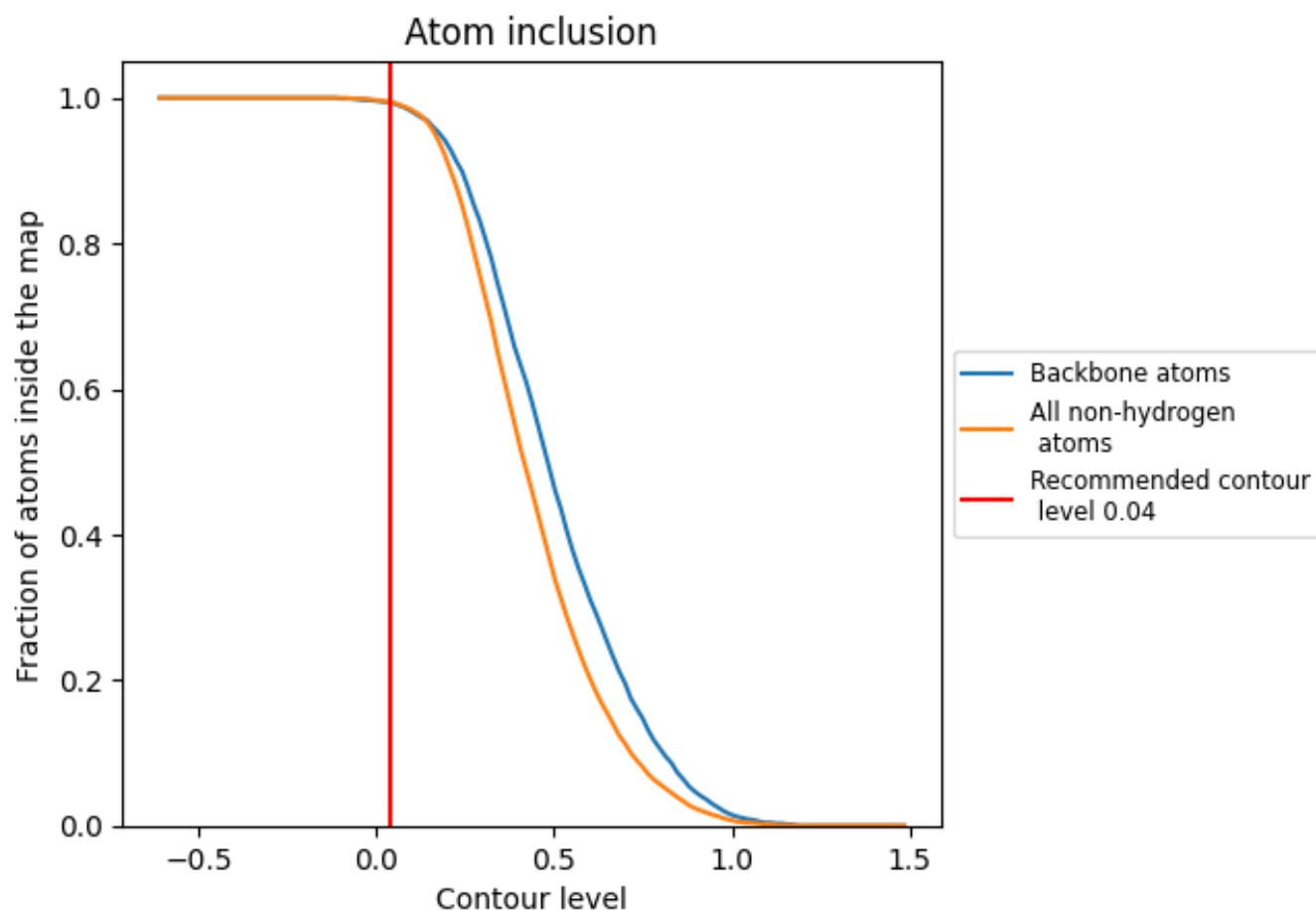
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9940	0.4740
A	0.9950	0.4760
B	0.9950	0.4600
C	0.9930	0.5000
D	0.9920	0.4990

