



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:34 AM UTC

PDB ID : 9FAT / pdb_00009fat
EMDB ID : EMD-50281
Title : CryoEM structure of human full-length alpha1beta3gamma2 GABA(A)R in complex with GARLH4, the TMD of Neuroligin2, Megabody38 and pregnenolone sulfate
Authors : Kasaragod, V.B.; Aricescu, A.R.
Deposited on : 2024-05-10
Resolution : 3.60 Å (reported)
Based on initial model : 6HUK

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

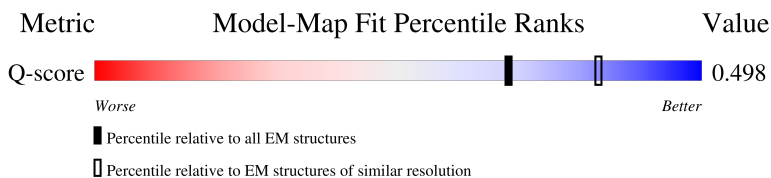
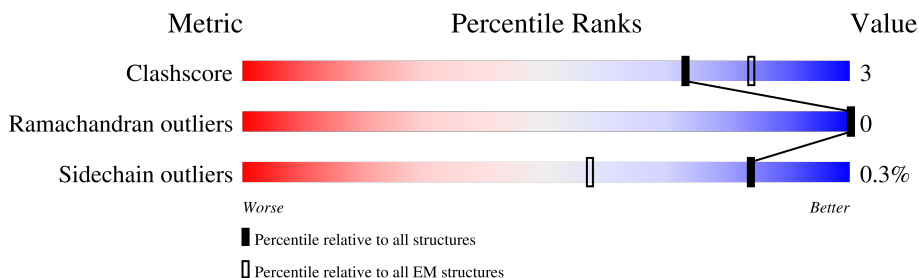
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



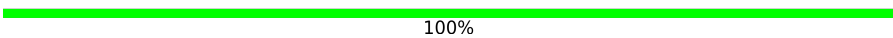
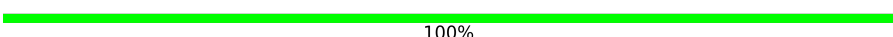
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	413	
1	D	413	
2	B	441	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	441	
3	C	405	
4	G	539	
5	H	33	
6	L	190	
7	F	10	
8	I	5	
9	J	3	
9	O	3	
10	K	2	
11	M	7	
12	N	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CL	L	302	-	-	X	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 17913 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 Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	356	Total	C	N	O	S	1	0
			2889	1867	487	519	16		
1	D	354	Total	C	N	O	S	0	0
			2864	1852	482	514	16		

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	345	Total	C	N	O	S	1	0
			2841	1858	469	498	16		
2	E	347	Total	C	N	O	S	0	0
			2845	1861	468	500	16		

- Molecule 3 is a protein called Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	352	Total	C	N	O	S	1	0
			2943	1930	477	516	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	429	GLY	-	expression tag	UNP P18507

- Molecule 4 is a protein called Megabody38.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	121	Total	C	N	O	S	0	0
			941	589	169	179	4		

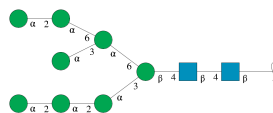
- Molecule 5 is a protein called Neuroligin-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	33	Total	C	N	O	0	0
			256	168	38	50		

- Molecule 6 is a protein called LHFPL tetraspan subfamily member 4 protein.

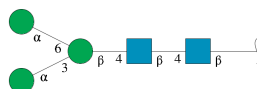
Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	190	Total	C	N	O	S	1	0
			1478	981	233	248	16		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



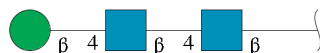
Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



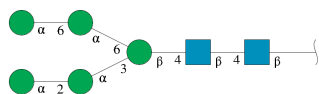
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	3	Total	C	N	O	0	0
			39	22	2	15		
9	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



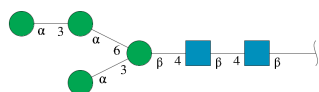
Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	7	Total	C	N	O	0	0
			83	46	2	35		

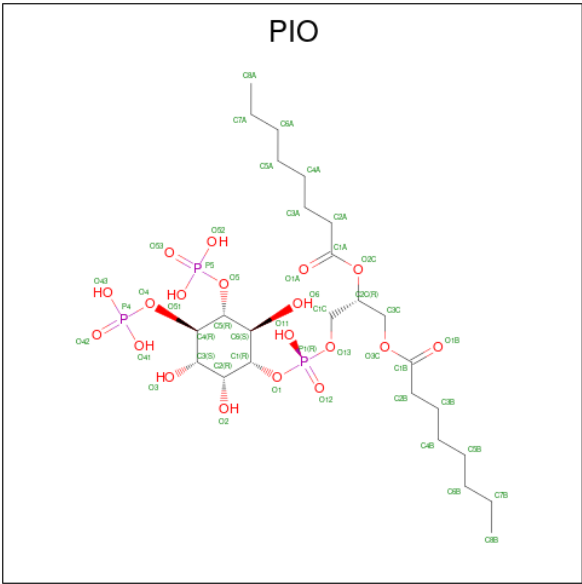
- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	N	6	Total	C	N	O	0	0
			72	40	2	30		

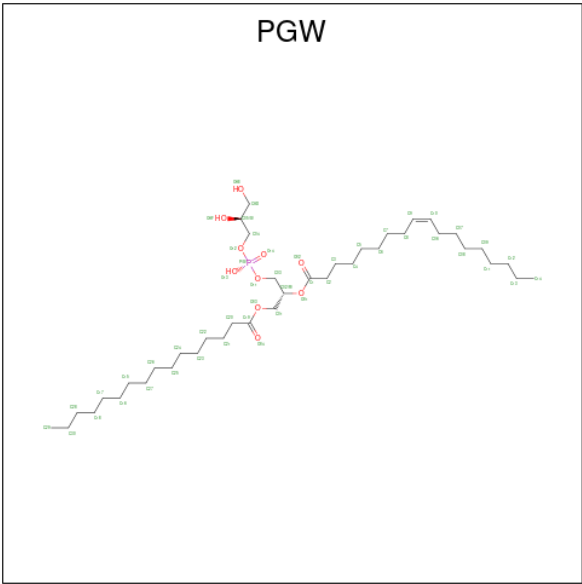
- Molecule 13 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidany

1)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO)
(formula: C₂₅H₄₉O₁₉P₃).



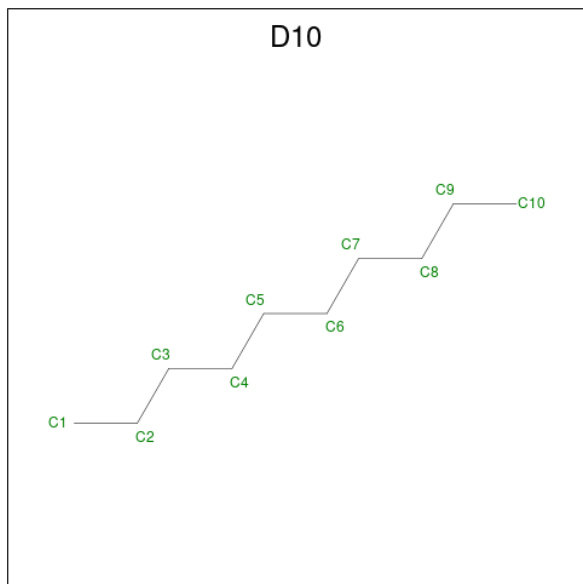
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			47	25	19	3	
13	D	1	Total	C	O	P	0
			47	25	19	3	

- Molecule 14 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			51	40	10	1	
14	B	1	Total	C	O	P	0
			51	40	10	1	
14	L	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 15 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).

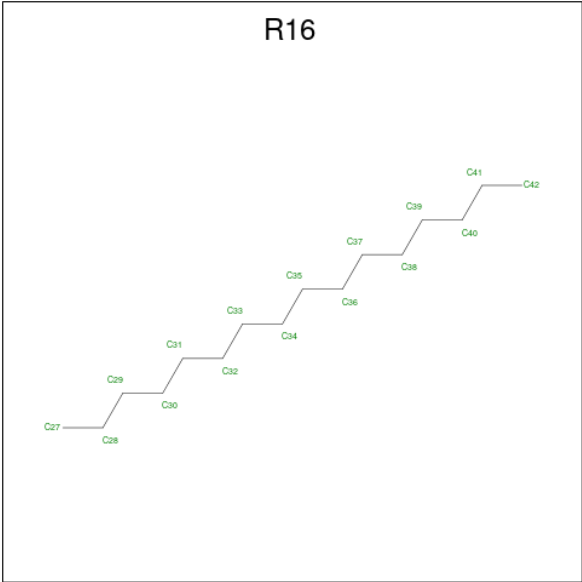


Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			10	10	
15	B	1	Total	C	0
			10	10	
15	C	1	Total	C	0
			10	10	

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

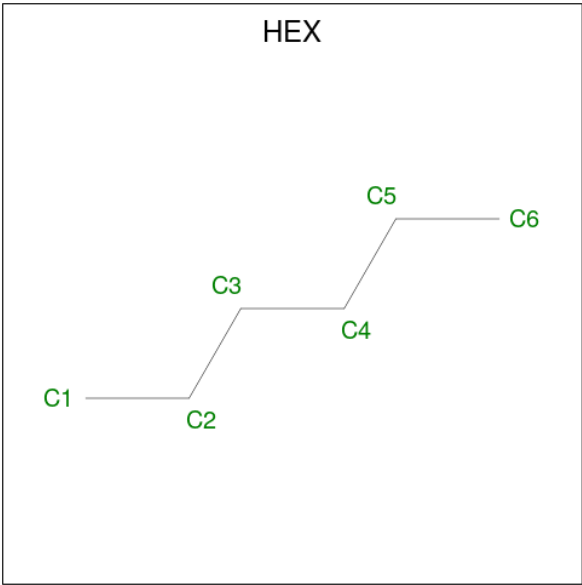
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Cl	0
			1	1	
16	L	1	Total	Cl	0
			1	1	

- Molecule 17 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



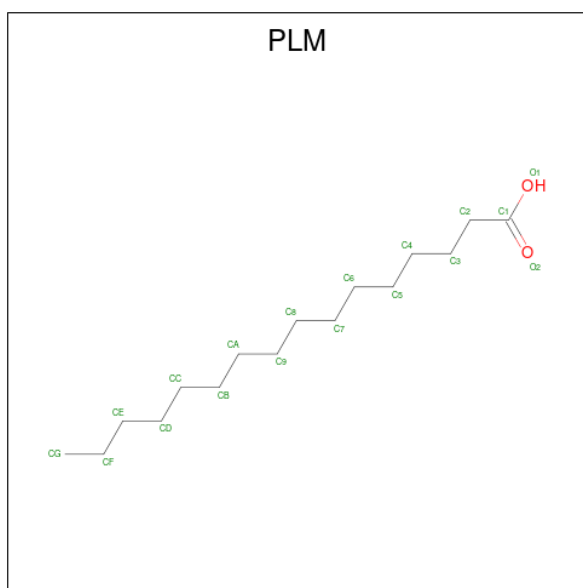
Mol	Chain	Residues	Atoms		AltConf
17	B	1	Total	C	0
			16	16	

- Molecule 18 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



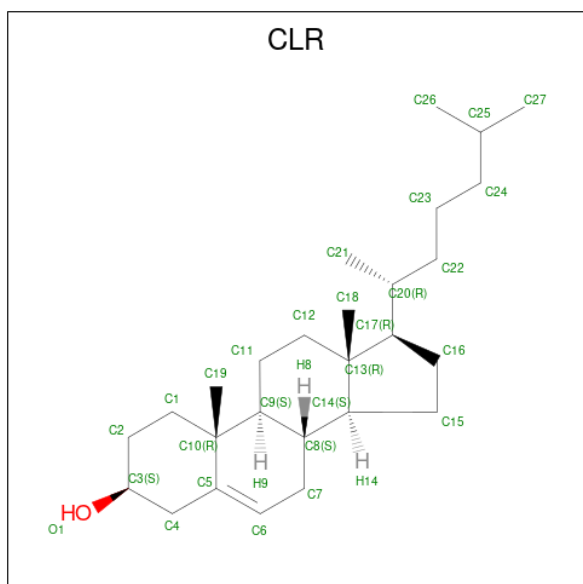
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	C	0
			6	6	
18	D	1	Total	C	0
			6	6	
18	E	1	Total	C	0
			6	6	

- Molecule 19 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



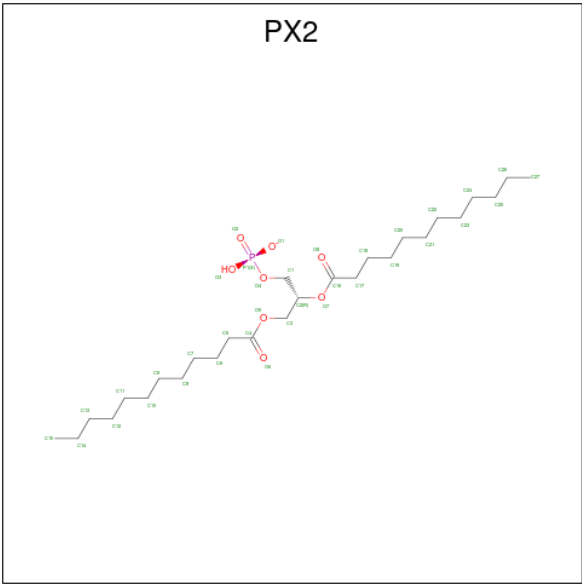
Mol	Chain	Residues	Atoms			AltConf
19	C	1	Total	C	O	0
			14	12	2	

- Molecule 20 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



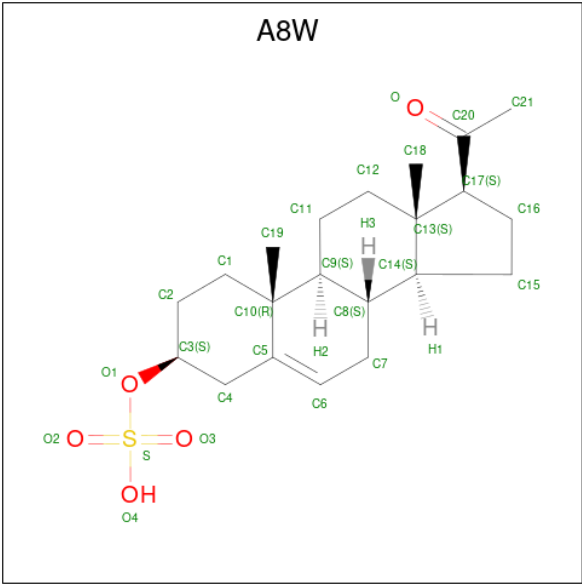
Mol	Chain	Residues	Atoms			AltConf
20	C	1	Total	C	O	0
			28	27	1	

- Molecule 21 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
21	D	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 22 is Pregnenolone sulfate (CCD ID: A8W) (formula: $C_{21}H_{32}O_5S$) (labeled as "Ligand of Interest" by depositor).

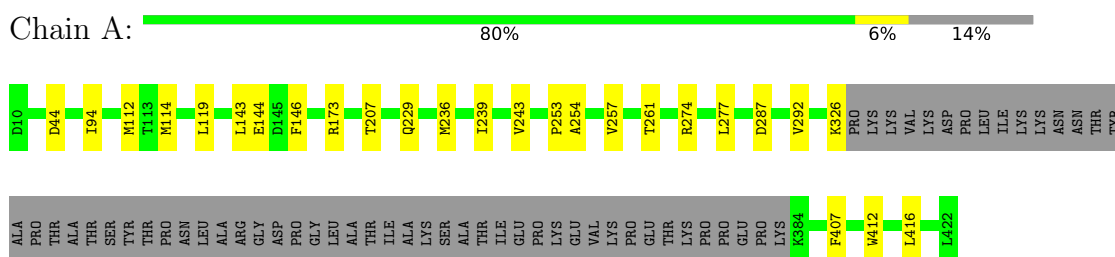


Mol	Chain	Residues	Atoms				AltConf
22	D	1	Total	C	O	S	0
			27	21	5	1	

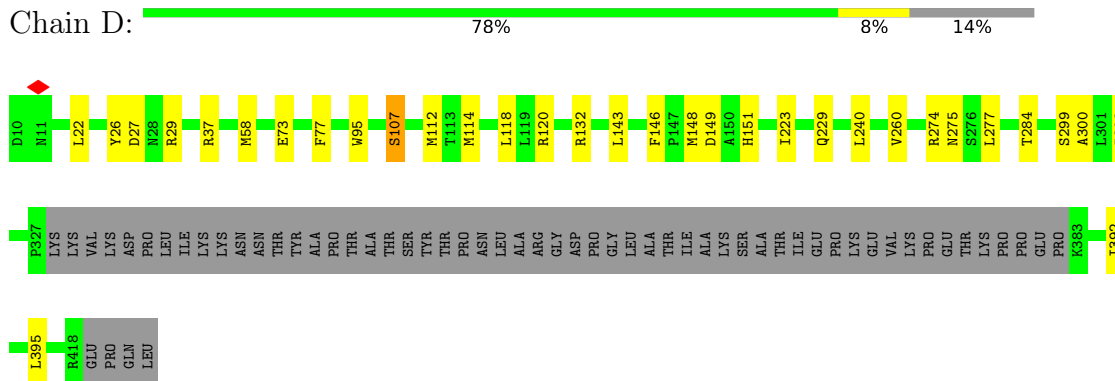
3 Residue-property plots [i](#)

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.

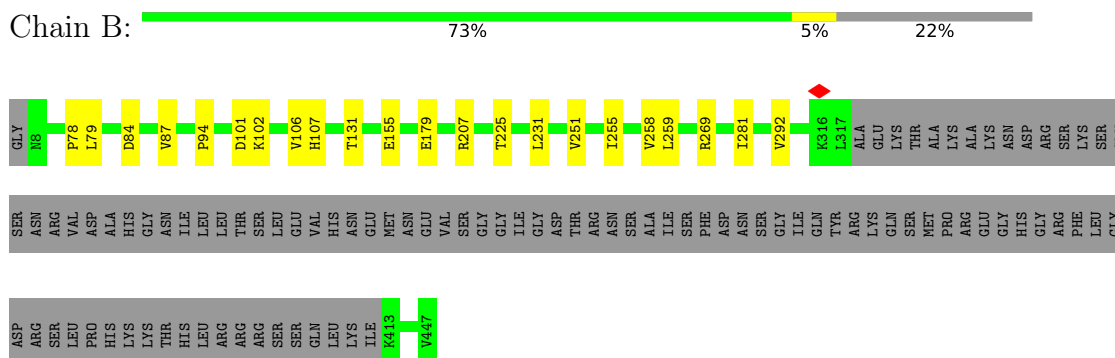
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1



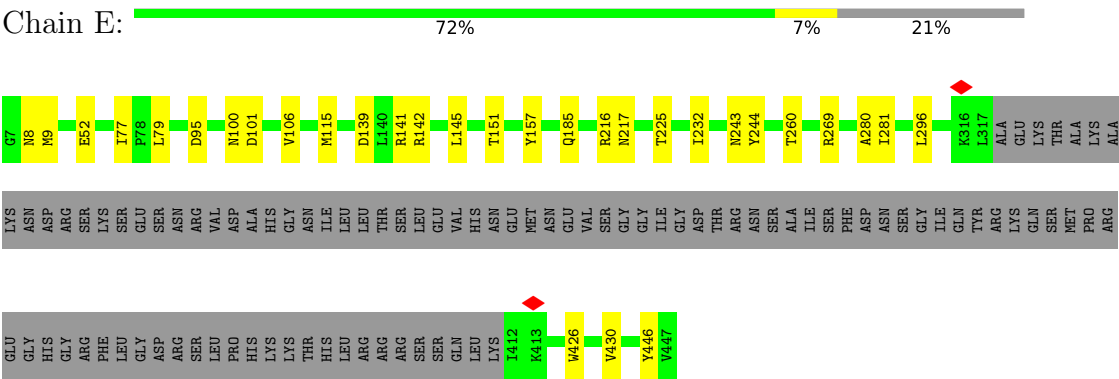
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1



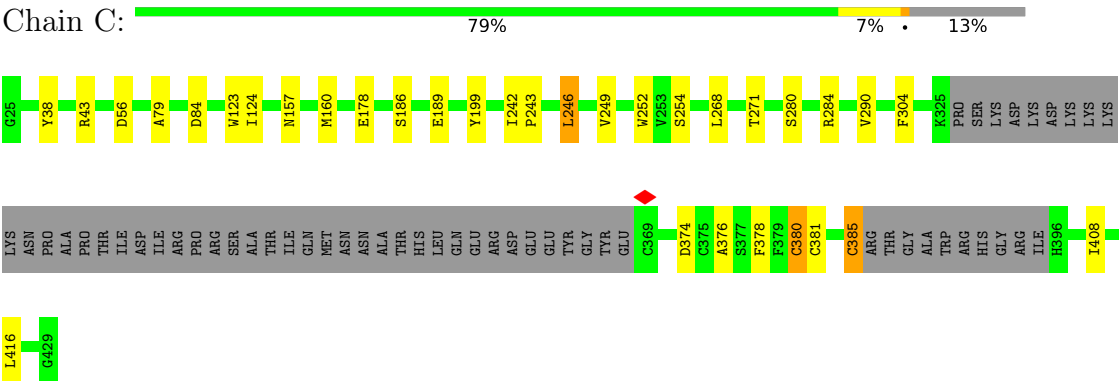
- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3



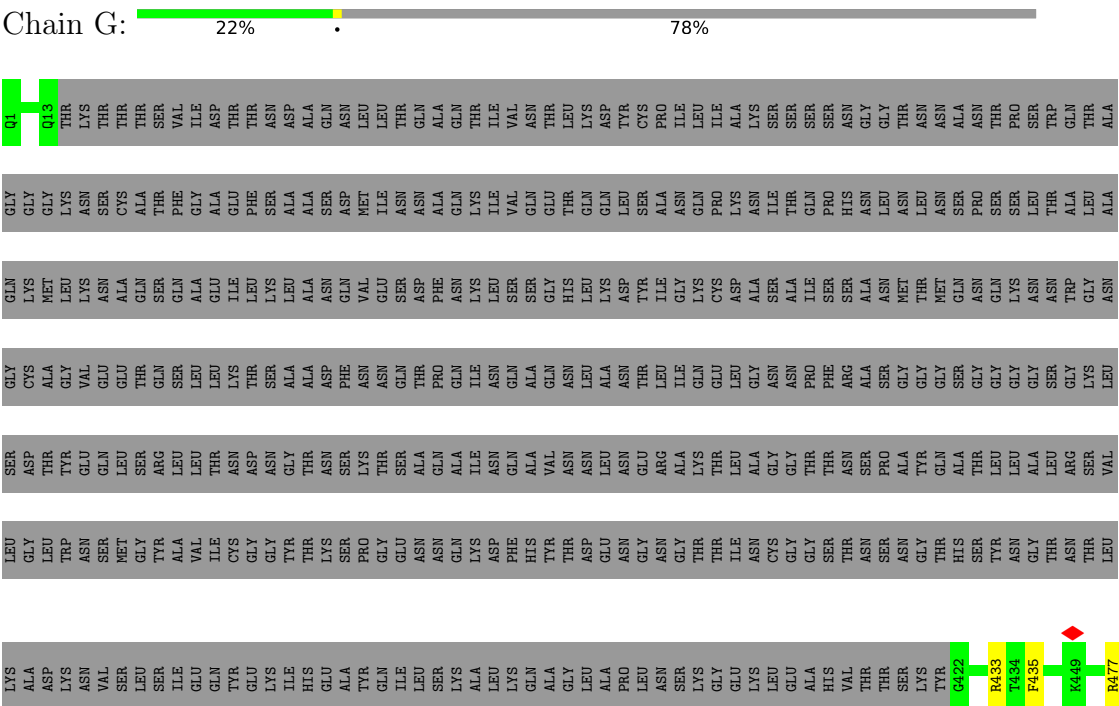
● Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

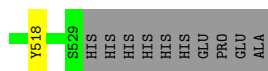


● Molecule 3: Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2



● Molecule 4: Megabody38





- Molecule 5: Neuroligin-2

Chain H: 88% 12%



- Molecule 6: LHFPL tetraspan subfamily member 4 protein

Chain L: 91% 9%



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 60% 20% 20%



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 60% 20% 20%



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 67% 33%



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 33% 33% 67%



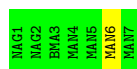
- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%



- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 86% 14%



- Molecule 12: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20534	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31.13	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	210.68031, 210.68031, 210.68031	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82297, 0.82297, 0.82297	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PGW, PLM, PX2, PIO, A8W, CL, CLR, MAN, HEX, BMA, D10, R16, P1L

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	0.18	0/2965	0.36	0/4027
1	D	0.42	0/2937	0.58	0/3989
2	B	0.18	0/2918	0.37	0/3966
2	E	0.18	0/2919	0.36	0/3968
3	C	0.23	0/2953	0.42	0/4010
4	G	0.17	0/961	0.33	0/1297
5	H	0.19	0/260	0.44	0/352
6	L	0.27	0/1522	0.49	0/2067
All	All	0.25	0/17435	0.43	0/23676

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2889	0	2883	22	0
1	D	2864	0	2858	25	0
2	B	2841	0	2853	18	0
2	E	2845	0	2854	22	0
3	C	2943	0	2954	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	941	0	894	2	0
5	H	256	0	256	4	0
6	L	1478	0	1482	15	0
7	F	116	0	97	4	0
8	I	61	0	52	1	0
9	J	39	0	34	0	0
9	O	39	0	34	1	0
10	K	28	0	25	0	0
11	M	83	0	70	0	0
12	N	72	0	61	0	0
13	A	47	0	44	1	0
13	D	47	0	44	3	0
14	A	51	0	76	1	0
14	B	51	0	76	1	0
14	L	51	0	76	1	0
15	A	10	0	22	0	0
15	B	10	0	22	0	0
15	C	10	0	22	1	0
16	A	1	0	0	0	0
16	L	1	0	0	3	0
17	B	16	0	34	0	0
18	B	6	0	14	0	0
18	D	6	0	14	0	0
18	E	6	0	14	0	0
19	C	14	0	20	0	0
20	C	28	0	46	1	0
21	D	36	0	52	2	0
22	D	27	0	0	0	0
All	All	17913	0	17983	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (117) 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)
20:C:502:CLR:O1	16:L:302:CL:CL	2.31	0.85
1:D:395:LEU:HD21	13:D:503:PIO:H4A	1.64	0.80
1:D:143:LEU:HD13	1:D:277:LEU:HD22	1.64	0.77
6:L:81:PHE:N	16:L:302:CL:CL	2.60	0.71
2:B:225:THR:HG21	2:B:281:ILE:HD11	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:TRP:HB3	7:F:8:MAN:H62	1.70	0.71
3:C:124:ILE:HD11	1:D:107:SER:HB2	1.74	0.69
3:C:376:ALA:O	3:C:380:P1L:O	2.11	0.69
3:C:385:P1L:SG	3:C:385:P1L:O	2.52	0.67
7:F:2:NAG:H2	7:F:10:MAN:H61	1.79	0.65
1:A:254:ALA:HB1	2:B:251:VAL:HG21	1.81	0.62
2:B:179:GLU:N	2:B:179:GLU:OE2	2.34	0.61
2:B:155:GLU:OE1	2:B:207:ARG:NE	2.34	0.60
1:A:229:GLN:OE1	2:B:269:ARG:NH1	2.35	0.60
1:D:112:MET:HE1	2:E:106:VAL:HG23	1.82	0.60
3:C:123:TRP:CD1	7:F:7:MAN:HO2	2.19	0.60
14:A:3902:PGW:O12	14:A:3902:PGW:OAE	2.17	0.59
1:A:326:LYS:NZ	13:A:3901:PIO:O4	2.35	0.59
6:L:29:PHE:HB3	6:L:190:LEU:HD21	1.85	0.58
3:C:38:TYR:OH	3:C:84:ASP:OD2	2.16	0.58
3:C:124:ILE:HD11	1:D:107:SER:CB	2.34	0.58
2:B:231:LEU:HD13	3:C:304:PHE:CE2	2.39	0.58
5:H:679:THR:HG21	6:L:175:TRP:HB2	1.86	0.57
2:B:107:HIS:NE2	2:B:131:THR:OG1	2.24	0.57
1:A:239:ILE:O	1:A:243:VAL:HG23	2.05	0.56
1:A:292:VAL:HG21	1:A:407:PHE:CZ	2.40	0.56
2:E:139:ASP:OD1	2:E:141:ARG:NH1	2.39	0.55
1:A:146:PHE:CE1	1:A:277:LEU:HD21	2.42	0.55
1:D:149:ASP:OD1	1:D:151:HIS:NE2	2.40	0.55
2:E:426:TRP:CE2	2:E:430:VAL:HG21	2.42	0.54
1:D:392:ILE:HG13	13:D:503:PIO:H1CA	1.89	0.54
5:H:675:GLU:O	5:H:679:THR:HG23	2.08	0.54
3:C:416:LEU:HD21	6:L:107:LEU:HD12	1.88	0.54
1:D:143:LEU:O	1:D:284:THR:HG22	2.08	0.54
2:E:225:THR:HG21	2:E:281:ILE:HD11	1.90	0.54
1:D:148:MET:HG2	1:D:223:ILE:HD12	1.91	0.53
6:L:29:PHE:CB	6:L:190:LEU:HD21	2.38	0.53
1:D:22:LEU:HD21	1:D:77:PHE:HB3	1.91	0.53
1:D:299:SER:O	1:D:302:ILE:N	2.42	0.53
3:C:408:ILE:HD11	21:D:501:PX2:H34	1.91	0.53
2:E:52:GLU:OE2	2:E:216:ARG:NH1	2.42	0.52
1:D:27:ASP:OD1	1:D:29:ARG:NE	2.39	0.52
1:A:146:PHE:CZ	1:A:277:LEU:HD21	2.44	0.52
2:B:101:ASP:OD1	2:B:102:LYS:N	2.43	0.51
2:B:225:THR:CG2	2:B:281:ILE:HD11	2.39	0.51
13:D:503:PIO:H5AA	13:D:503:PIO:H2BA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:LEU:HA	9:O:1:NAG:H82	1.93	0.51
1:A:114:MET:HE3	2:B:94:PRO:O	2.11	0.51
2:B:78:PRO:C	2:B:79:LEU:HD12	2.36	0.50
1:A:112:MET:HE1	2:B:106:VAL:HG23	1.93	0.50
1:D:118:LEU:HD21	1:D:120:ARG:HE	1.77	0.50
1:A:112:MET:HE1	2:B:106:VAL:CG2	2.42	0.50
4:G:435:PHE:O	4:G:477:ARG:NH2	2.45	0.49
14:L:301:PGW:O12	14:L:301:PGW:OAE	2.22	0.49
1:A:274[A]:ARG:NH1	1:A:287:ASP:OD1	2.46	0.49
1:D:274:ARG:O	1:D:275:ASN:C	2.55	0.49
3:C:199:TYR:CE1	1:D:58:MET:HE3	2.47	0.49
3:C:242:ILE:HB	3:C:243:PRO:HD3	1.95	0.49
5:H:697:LEU:HD13	6:L:22:ILE:HD12	1.95	0.48
1:D:229:GLN:OE1	2:E:269:ARG:NH2	2.46	0.48
1:A:236:MET:HA	1:A:236:MET:HE2	1.95	0.48
1:A:412:TRP:O	1:A:416:LEU:HD23	2.12	0.48
2:E:77:ILE:HG22	2:E:79:LEU:HD23	1.96	0.48
6:L:112:CYS:O	6:L:113:PHE:C	2.56	0.47
1:A:261:THR:HG22	2:B:259:LEU:HD11	1.95	0.47
2:E:232:ILE:CD1	2:E:260:THR:HG21	2.45	0.47
2:B:84:ASP:O	2:B:87:VAL:HG12	2.14	0.47
1:A:144:GLU:N	1:A:144:GLU:OE1	2.48	0.47
2:E:8:ASN:OD1	2:E:9:MET:N	2.48	0.46
3:C:408:ILE:HD11	21:D:501:PX2:C19	2.45	0.46
2:E:426:TRP:NE1	2:E:430:VAL:HG21	2.31	0.46
2:B:258:VAL:HG22	2:B:292:VAL:HG23	1.97	0.46
1:D:112:MET:HE2	1:D:112:MET:HB2	1.82	0.46
1:A:94:ILE:HD11	1:A:119:LEU:HD21	1.99	0.45
1:D:37:ARG:NH1	1:D:73:GLU:OE2	2.50	0.45
6:L:80:SER:OG	16:L:302:CL:CL	2.58	0.45
1:A:253:PRO:O	1:A:257:VAL:HG23	2.17	0.45
3:C:56:ASP:OD1	3:C:79:ALA:HB3	2.17	0.45
3:C:284:ARG:NH2	3:C:290:VAL:O	2.50	0.45
1:D:132:ARG:NH2	2:E:101:ASP:OD1	2.49	0.45
1:A:261:THR:HG22	2:B:259:LEU:CD1	2.47	0.45
1:D:146:PHE:CD1	1:D:277:LEU:HD21	2.51	0.45
1:D:299:SER:O	1:D:300:ALA:C	2.59	0.45
3:C:246:LEU:HD12	3:C:246:LEU:HA	1.77	0.44
3:C:374:ASP:O	3:C:378:PHE:N	2.47	0.44
6:L:50:SER:N	6:L:53:THR:OG1	2.50	0.44
1:A:207:THR:HG21	2:E:115:MET:HE1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:126:LYS:NZ	6:L:199:ASN:OD1	2.28	0.43
2:E:100:ASN:ND2	2:E:151:THR:O	2.49	0.43
3:C:254:SER:HB2	3:C:268:LEU:HD23	2.01	0.43
2:E:185:GLN:O	2:E:217:ASN:ND2	2.51	0.43
1:A:44:ASP:OD2	1:A:173:ARG:NH2	2.52	0.43
14:B:3504:PGW:H14	3:C:280:SER:OG	2.19	0.42
3:C:186:SER:OG	3:C:189:GLU:OE1	2.35	0.42
3:C:123:TRP:HB3	7:F:8:MAN:C6	2.44	0.42
3:C:271:THR:HG21	1:D:260:VAL:HG22	2.02	0.42
1:D:26:TYR:HE1	1:D:95:TRP:H	1.66	0.42
1:A:143:LEU:HD22	1:A:277:LEU:HD22	2.01	0.42
1:A:257:VAL:HG12	2:B:255:ILE:HD11	2.01	0.42
3:C:157:ASN:O	3:C:160:MET:N	2.52	0.42
1:D:240:LEU:HD11	2:E:296:LEU:HD23	2.02	0.42
3:C:43:ARG:NE	3:C:178:GLU:OE1	2.51	0.42
6:L:64:TYR:OH	6:L:78:ARG:NH2	2.49	0.42
2:E:95:ASP:OD2	2:E:157:TYR:N	2.53	0.41
5:H:670:ARG:NH2	6:L:50:SER:O	2.50	0.41
2:E:243:ASN:OD1	2:E:244:TYR:N	2.52	0.41
4:G:433:ARG:NH2	4:G:518:TYR:OH	2.54	0.41
3:C:416:LEU:CD2	6:L:107:LEU:HD12	2.50	0.41
15:C:503:D10:H101	6:L:107:LEU:HD11	2.03	0.41
1:D:22:LEU:HD23	1:D:22:LEU:HA	1.93	0.41
2:E:142:ARG:O	2:E:145:LEU:N	2.54	0.41
2:E:225:THR:CG2	2:E:281:ILE:HD11	2.50	0.41
8:I:3:BMA:H62	8:I:5:MAN:H2	1.85	0.40
2:E:232:ILE:HD11	2:E:260:THR:HG21	2.02	0.40
3:C:249:VAL:O	3:C:252:TRP:N	2.55	0.40
2:E:280:ALA:HB2	2:E:446:TYR:CE1	2.56	0.40
6:L:103:MET:HG3	6:L:107:LEU:HD23	2.03	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	353/413 (86%)	336 (95%)	17 (5%)	0	100	100
1	D	350/413 (85%)	333 (95%)	17 (5%)	0	100	100
2	B	342/441 (78%)	331 (97%)	11 (3%)	0	100	100
2	E	343/441 (78%)	336 (98%)	7 (2%)	0	100	100
3	C	345/405 (85%)	325 (94%)	20 (6%)	0	100	100
4	G	117/539 (22%)	112 (96%)	5 (4%)	0	100	100
5	H	31/33 (94%)	28 (90%)	3 (10%)	0	100	100
6	L	189/190 (100%)	182 (96%)	7 (4%)	0	100	100
All	All	2070/2875 (72%)	1983 (96%)	87 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	319/367 (87%)	319 (100%)	0	100	100
1	D	316/367 (86%)	314 (99%)	2 (1%)	78	79
2	B	312/393 (79%)	312 (100%)	0	100	100
2	E	312/393 (79%)	312 (100%)	0	100	100
3	C	321/366 (88%)	320 (100%)	1 (0%)	86	83
4	G	94/435 (22%)	94 (100%)	0	100	100
5	H	27/27 (100%)	27 (100%)	0	100	100
6	L	157/156 (101%)	155 (99%)	2 (1%)	61	72
All	All	1858/2504 (74%)	1853 (100%)	5 (0%)	84	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	246	LEU
1	D	107	SER
1	D	114	MET
6	L	109	CYS
6	L	128	CYS

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	102	HIS
2	B	64	GLN
2	B	197	ASN
2	B	267	HIS
3	C	54	HIS
3	C	418	ASN
1	D	190	GLN
1	D	417	ASN
4	G	445	GLN
4	G	517	HIS
4	G	524	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	P1L	C	385	3	21,22,23	1.13	1 (4%)	19,23,25	1.25	3 (15%)
3	P1L	C	381	3	21,22,23	0.68	0	19,23,25	1.35	3 (15%)
3	P1L	C	380	3	21,22,23	1.13	1 (4%)	19,23,25	1.43	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P1L	C	385	3	-	11/20/22/24	-
3	P1L	C	381	3	-	5/20/22/24	-
3	P1L	C	380	3	-	7/20/22/24	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	385	P1L	O-C	4.34	1.36	1.20
3	C	380	P1L	O-C	4.31	1.36	1.20

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	380	P1L	CB-SG-C7	4.07	106.35	100.76
3	C	381	P1L	C8-C7-SG	-3.60	109.11	113.40
3	C	380	P1L	C8-C7-SG	-3.53	109.20	113.40
3	C	381	P1L	CB-SG-C7	3.39	105.42	100.76
3	C	385	P1L	CB-SG-C7	3.27	105.26	100.76
3	C	385	P1L	C8-C7-SG	-3.14	109.66	113.40
3	C	380	P1L	O7-C7-SG	2.60	125.99	122.68
3	C	385	P1L	O7-C7-SG	2.48	125.84	122.68
3	C	381	P1L	O7-C7-SG	2.15	125.42	122.68

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	380	P1L	O7-C7-SG-CB
3	C	380	P1L	C8-C7-SG-CB
3	C	380	P1L	C7-C8-C9-C10
3	C	381	P1L	N-CA-CB-SG
3	C	381	P1L	O7-C7-SG-CB
3	C	381	P1L	C8-C7-SG-CB
3	C	385	P1L	N-CA-CB-SG
3	C	385	P1L	C-CA-CB-SG
3	C	385	P1L	C18-C19-C20-C21
3	C	385	P1L	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	385	P1L	C15-C16-C17-C18
3	C	385	P1L	C16-C17-C18-C19
3	C	380	P1L	C14-C15-C16-C17
3	C	385	P1L	C12-C13-C14-C15
3	C	380	P1L	N-CA-CB-SG
3	C	385	P1L	O7-C7-C8-C9
3	C	385	P1L	C8-C7-SG-CB
3	C	381	P1L	CA-CB-SG-C7
3	C	380	P1L	C11-C12-C13-C14
3	C	381	P1L	C19-C20-C21-C22
3	C	380	P1L	C10-C11-C12-C13
3	C	385	P1L	C14-C15-C16-C17
3	C	385	P1L	CA-CB-SG-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	385	P1L	1	0
3	C	380	P1L	1	0

5.5 Carbohydrates

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	F	1	1,7	14,14,15	0.37	0	17,19,21	0.58	0
7	MAN	F	10	7	11,11,12	0.30	0	15,15,17	0.60	0
7	NAG	F	2	7	14,14,15	0.38	0	17,19,21	0.82	1 (5%)
7	BMA	F	3	7	11,11,12	0.37	0	15,15,17	0.55	0
7	MAN	F	4	7	11,11,12	0.30	0	15,15,17	0.49	0
7	MAN	F	5	7	11,11,12	0.31	0	15,15,17	0.53	0
7	MAN	F	6	7	11,11,12	0.30	0	15,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	F	7	7	11,11,12	0.46	0	15,15,17	0.73	0
7	MAN	F	8	7	11,11,12	0.53	0	15,15,17	1.28	1 (6%)
7	MAN	F	9	7	11,11,12	0.32	0	15,15,17	0.55	0
8	NAG	I	1	2,8	14,14,15	0.38	0	17,19,21	0.64	0
8	NAG	I	2	8	14,14,15	0.37	0	17,19,21	0.59	0
8	BMA	I	3	8	11,11,12	0.33	0	15,15,17	0.62	0
8	MAN	I	4	8	11,11,12	0.28	0	15,15,17	0.51	0
8	MAN	I	5	8	11,11,12	0.49	0	15,15,17	1.31	2 (13%)
9	NAG	J	1	9,2	14,14,15	0.41	0	17,19,21	0.86	1 (5%)
9	NAG	J	2	9	14,14,15	0.20	0	17,19,21	0.46	0
9	BMA	J	3	9	11,11,12	0.56	0	15,15,17	0.73	0
10	NAG	K	1	3,10	14,14,15	0.38	0	17,19,21	0.46	0
10	NAG	K	2	10	14,14,15	0.37	0	17,19,21	0.40	0
11	NAG	M	1	1,11	14,14,15	0.38	0	17,19,21	0.53	0
11	NAG	M	2	11	14,14,15	0.38	0	17,19,21	0.60	0
11	BMA	M	3	11	11,11,12	0.27	0	15,15,17	0.54	0
11	MAN	M	4	11	11,11,12	0.30	0	15,15,17	0.54	0
11	MAN	M	5	11	11,11,12	0.27	0	15,15,17	0.55	0
11	MAN	M	6	11	11,11,12	0.30	0	15,15,17	0.90	1 (6%)
11	MAN	M	7	11	11,11,12	0.32	0	15,15,17	0.56	0
12	NAG	N	1	2,12	14,14,15	0.38	0	17,19,21	0.61	0
12	NAG	N	2	12	14,14,15	0.37	0	17,19,21	0.75	0
12	BMA	N	3	12	11,11,12	0.28	0	15,15,17	0.61	0
12	MAN	N	4	12	11,11,12	0.25	0	15,15,17	0.84	0
12	MAN	N	5	12	11,11,12	0.27	0	15,15,17	0.57	0
12	MAN	N	6	12	11,11,12	0.26	0	15,15,17	0.53	0
9	NAG	O	1	9,2	14,14,15	0.40	0	17,19,21	0.52	0
9	NAG	O	2	9	14,14,15	0.40	0	17,19,21	0.92	2 (11%)
9	BMA	O	3	9	11,11,12	0.27	0	15,15,17	0.54	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
7	NAG	F	1	1,7	-	0/6/23/26	0/1/1/1
7	MAN	F	10	7	-	1/2/19/22	0/1/1/1
7	NAG	F	2	7	-	1/6/23/26	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	0/1/1/1
7	MAN	F	4	7	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	F	5	7	-	0/2/19/22	0/1/1/1
7	MAN	F	6	7	-	0/2/19/22	0/1/1/1
7	MAN	F	7	7	-	0/2/19/22	0/1/1/1
7	MAN	F	8	7	-	1/2/19/22	0/1/1/1
7	MAN	F	9	7	-	0/2/19/22	0/1/1/1
8	NAG	I	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	3/6/23/26	0/1/1/1
8	BMA	I	3	8	-	1/2/19/22	0/1/1/1
8	MAN	I	4	8	-	0/2/19/22	0/1/1/1
8	MAN	I	5	8	-	0/2/19/22	0/1/1/1
9	NAG	J	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	J	2	9	-	0/6/23/26	0/1/1/1
9	BMA	J	3	9	-	0/2/19/22	0/1/1/1
10	NAG	K	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	0/6/23/26	0/1/1/1
11	NAG	M	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	M	2	11	-	2/6/23/26	0/1/1/1
11	BMA	M	3	11	-	2/2/19/22	0/1/1/1
11	MAN	M	4	11	-	0/2/19/22	0/1/1/1
11	MAN	M	5	11	-	1/2/19/22	0/1/1/1
11	MAN	M	6	11	-	2/2/19/22	0/1/1/1
11	MAN	M	7	11	-	0/2/19/22	0/1/1/1
12	NAG	N	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	N	2	12	-	2/6/23/26	0/1/1/1
12	BMA	N	3	12	-	0/2/19/22	0/1/1/1
12	MAN	N	4	12	-	0/2/19/22	0/1/1/1
12	MAN	N	5	12	-	0/2/19/22	0/1/1/1
12	MAN	N	6	12	-	0/2/19/22	0/1/1/1
9	NAG	O	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	O	2	9	-	4/6/23/26	0/1/1/1
9	BMA	O	3	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	8	MAN	O2-C2-C3	-3.75	102.39	110.15
8	I	5	MAN	C1-O5-C5	3.64	117.06	112.19
9	J	1	NAG	C2-N2-C7	2.83	126.69	122.90
11	M	6	MAN	C1-O5-C5	2.64	115.72	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	2	NAG	C2-N2-C7	2.54	126.31	122.90
8	I	5	MAN	C1-C2-C3	2.36	113.08	109.64
9	O	2	NAG	C1-C2-N2	2.30	114.06	110.43
9	O	2	NAG	C2-N2-C7	2.25	125.92	122.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

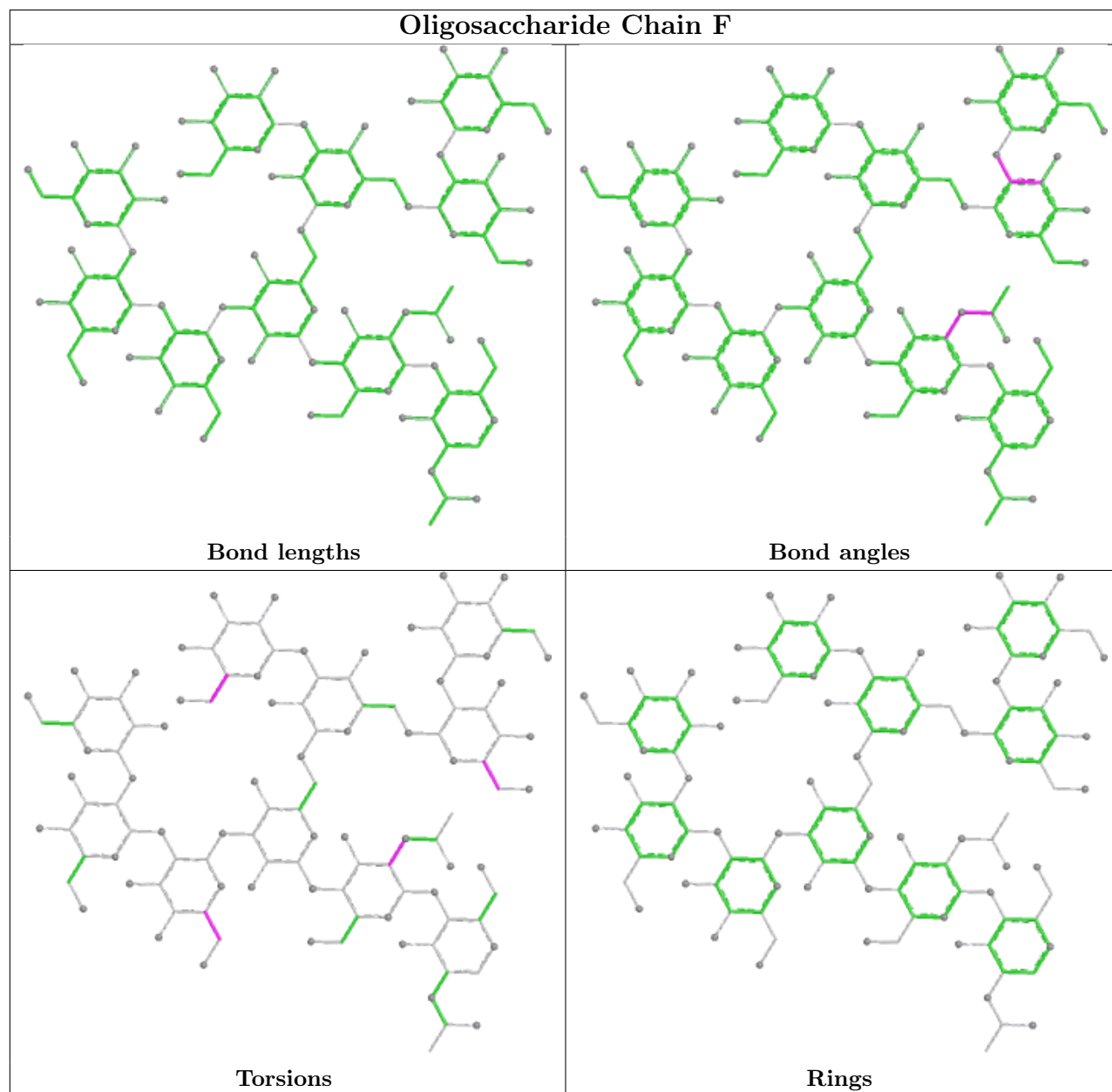
Mol	Chain	Res	Type	Atoms
9	O	2	NAG	C1-C2-N2-C7
11	M	6	MAN	O5-C5-C6-O6
11	M	3	BMA	O5-C5-C6-O6
8	I	1	NAG	C8-C7-N2-C2
8	I	1	NAG	O7-C7-N2-C2
8	I	2	NAG	C8-C7-N2-C2
8	I	2	NAG	O7-C7-N2-C2
9	J	1	NAG	C8-C7-N2-C2
9	J	1	NAG	O7-C7-N2-C2
10	K	1	NAG	C8-C7-N2-C2
10	K	1	NAG	O7-C7-N2-C2
11	M	1	NAG	C8-C7-N2-C2
11	M	1	NAG	O7-C7-N2-C2
11	M	2	NAG	C8-C7-N2-C2
11	M	2	NAG	O7-C7-N2-C2
11	M	6	MAN	C4-C5-C6-O6
12	N	2	NAG	C8-C7-N2-C2
12	N	2	NAG	O7-C7-N2-C2
8	I	2	NAG	O5-C5-C6-O6
7	F	10	MAN	O5-C5-C6-O6
8	I	3	BMA	O5-C5-C6-O6
11	M	5	MAN	O5-C5-C6-O6
7	F	4	MAN	O5-C5-C6-O6
9	O	2	NAG	C3-C2-N2-C7
11	M	3	BMA	C4-C5-C6-O6
9	O	2	NAG	C8-C7-N2-C2
7	F	2	NAG	C3-C2-N2-C7
9	O	2	NAG	O7-C7-N2-C2
7	F	8	MAN	O5-C5-C6-O6

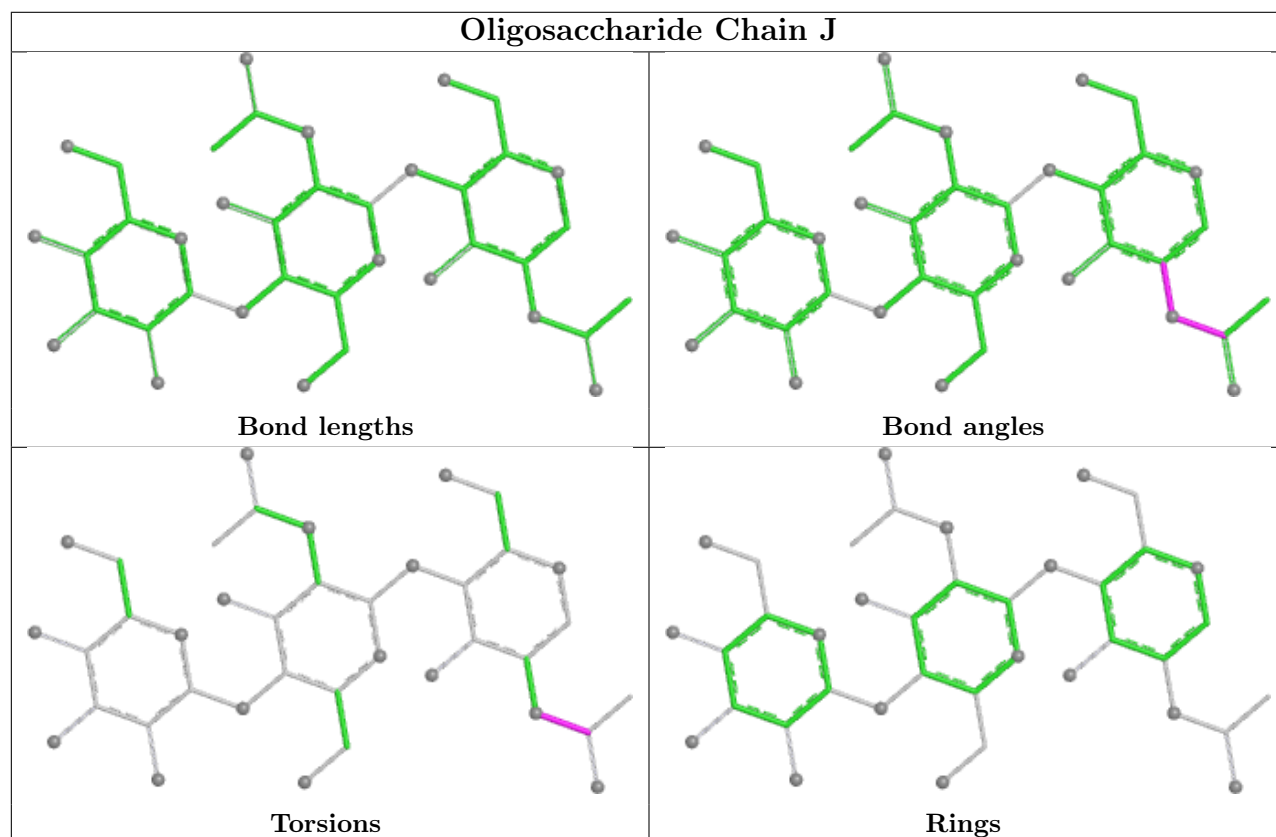
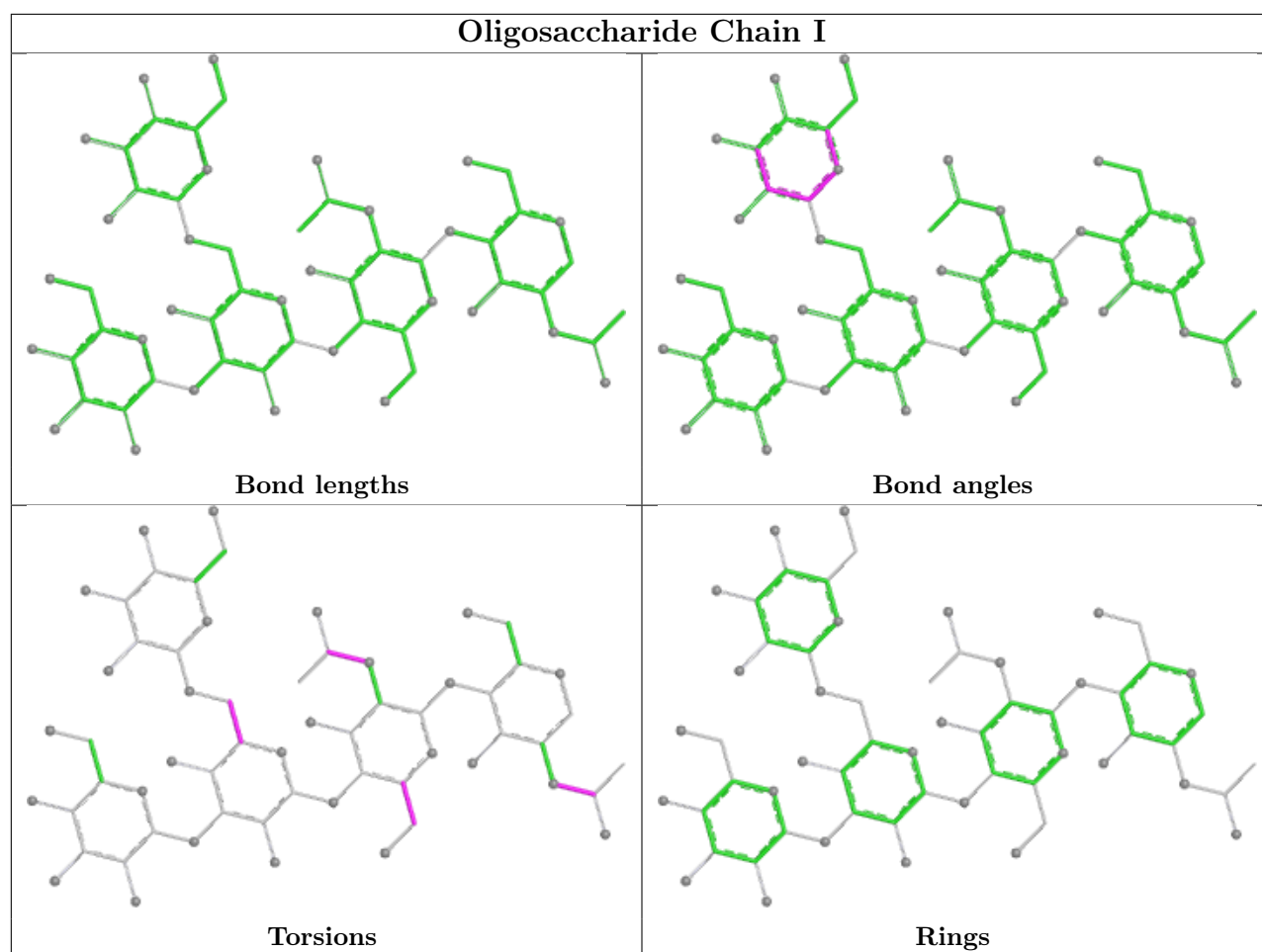
There are no ring outliers.

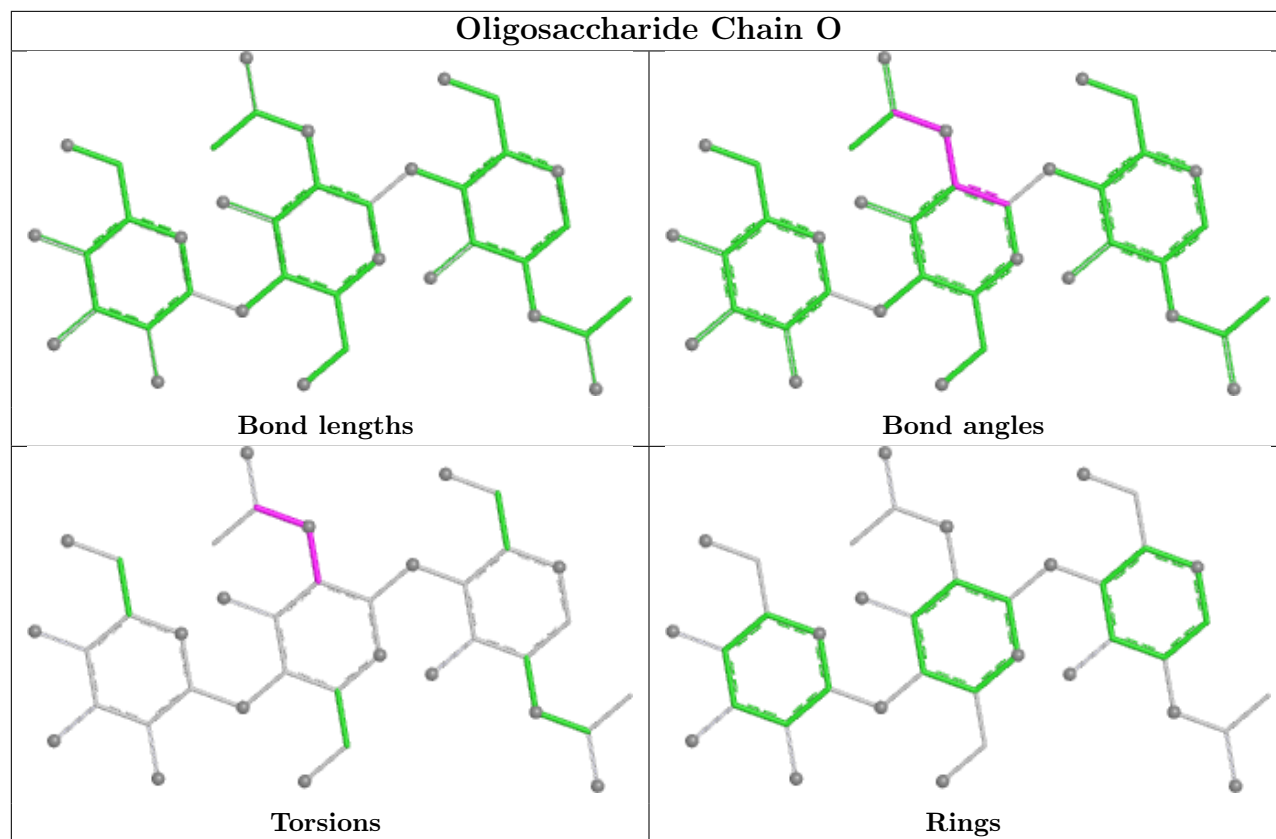
7 monomers are involved in 6 short contacts:

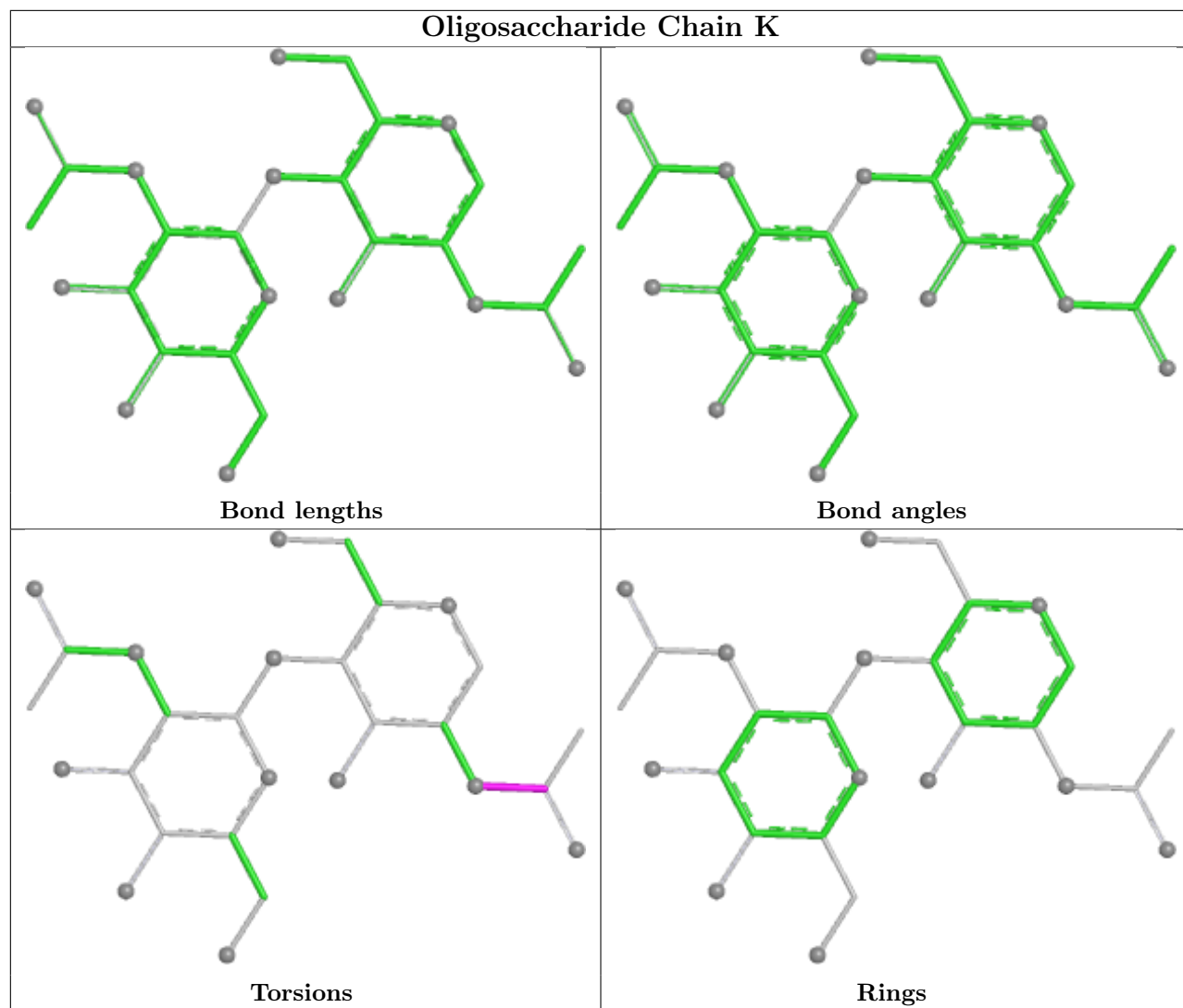
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	7	MAN	1	0
7	F	2	NAG	1	0
7	F	10	MAN	1	0
8	I	3	BMA	1	0
9	O	1	NAG	1	0
7	F	8	MAN	2	0
8	I	5	MAN	1	0

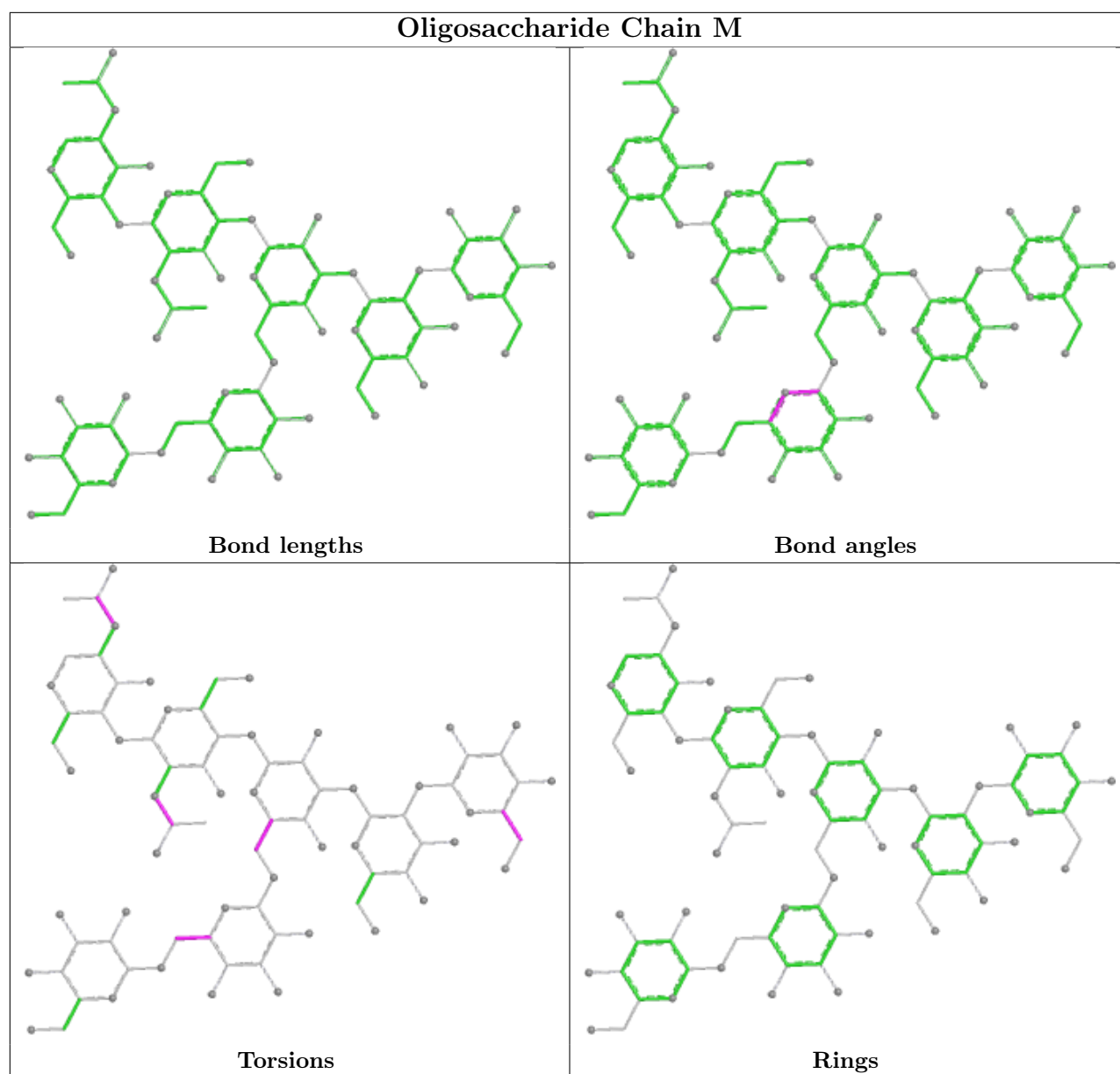
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

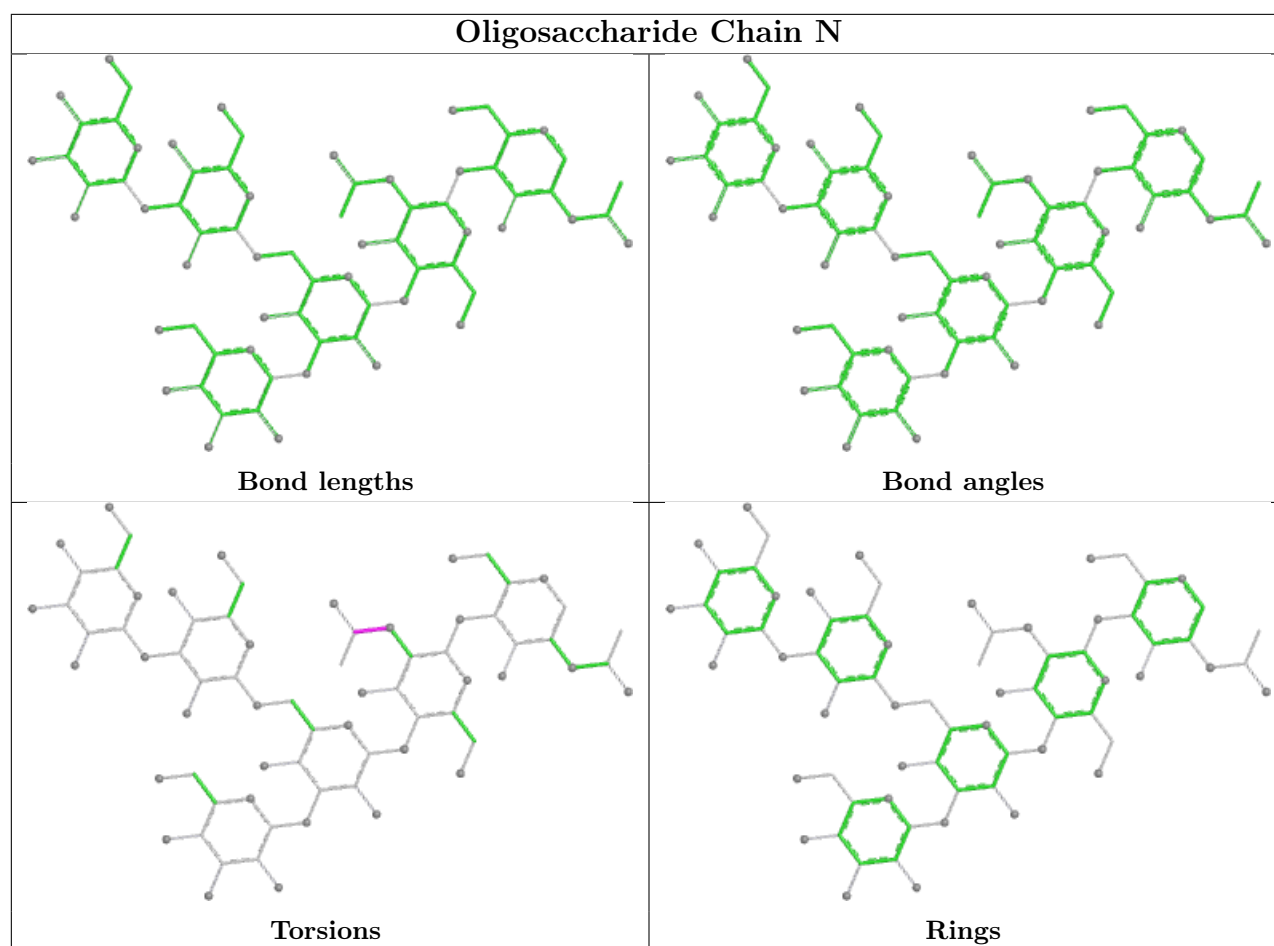












5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
20	CLR	C	502	-	31,31,31	0.16	0	48,48,48	0.32	0
15	D10	A	3903	-	9,9,9	0.32	0	8,8,8	0.75	0
14	PGW	L	301	-	50,50,50	0.97	2 (4%)	53,56,56	1.04	2 (3%)
14	PGW	B	3504	-	50,50,50	0.98	3 (6%)	53,56,56	1.01	2 (3%)
21	PX2	D	501	-	35,35,35	1.02	3 (8%)	38,40,40	1.10	2 (5%)
18	HEX	B	3503	-	5,5,5	0.33	0	4,4,4	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PIO	A	3901	-	47,47,47	1.21	7 (14%)	62,65,65	1.05	2 (3%)
22	A8W	D	502	-	30,30,30	0.35	0	45,49,49	0.91	2 (4%)
14	PGW	A	3902	-	50,50,50	0.98	3 (6%)	53,56,56	0.98	2 (3%)
15	D10	B	3502	-	9,9,9	0.30	0	8,8,8	0.78	0
18	HEX	D	504	-	5,5,5	0.33	0	4,4,4	0.52	0
19	PLM	C	501	-	13,13,17	0.70	0	13,13,17	1.07	1 (7%)
15	D10	C	503	-	9,9,9	0.32	0	8,8,8	0.67	0
13	PIO	D	503	-	47,47,47	0.47	0	62,65,65	0.43	0
17	R16	B	3501	-	15,15,15	0.30	0	14,14,14	0.81	0
18	HEX	E	4301	-	5,5,5	0.32	0	4,4,4	0.52	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
20	CLR	C	502	-	-	0/10/68/68	0/4/4/4
15	D10	A	3903	-	-	0/7/7/7	-
14	PGW	L	301	-	-	20/55/55/55	-
14	PGW	B	3504	-	-	24/55/55/55	-
21	PX2	D	501	-	-	14/37/37/37	-
18	HEX	B	3503	-	-	0/3/3/3	-
13	PIO	A	3901	-	-	15/44/68/68	0/1/1/1
22	A8W	D	502	-	-	1/9/67/67	0/4/4/4
14	PGW	A	3902	-	-	24/55/55/55	-
15	D10	B	3502	-	-	0/7/7/7	-
18	HEX	D	504	-	-	0/3/3/3	-
19	PLM	C	501	-	-	3/11/11/15	-
15	D10	C	503	-	-	0/7/7/7	-
13	PIO	D	503	-	-	6/44/68/68	0/1/1/1
17	R16	B	3501	-	-	1/13/13/13	-
18	HEX	E	4301	-	-	0/3/3/3	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	3901	PIO	P5-O5	3.26	1.65	1.59
13	A	3901	PIO	P4-O4	3.16	1.65	1.59
14	A	3902	PGW	O03-C19	3.00	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3504	PGW	O03-C19	2.83	1.41	1.33
14	L	301	PGW	O03-C19	2.81	1.41	1.33
14	A	3902	PGW	O01-C1	2.81	1.42	1.34
14	L	301	PGW	O01-C1	2.68	1.41	1.34
13	A	3901	PIO	O2C-C2C	-2.68	1.40	1.46
14	B	3504	PGW	O01-C1	2.67	1.41	1.34
21	D	501	PX2	O5-C4	2.60	1.40	1.33
21	D	501	PX2	O7-C2	-2.52	1.40	1.46
13	A	3901	PIO	O3C-C1B	2.50	1.40	1.33
21	D	501	PX2	O7-C16	2.44	1.41	1.34
13	A	3901	PIO	O3C-C3C	-2.15	1.40	1.45
13	A	3901	PIO	O2C-C1A	2.15	1.40	1.34
14	B	3504	PGW	O01-C02	-2.15	1.41	1.46
13	A	3901	PIO	P1-O1	2.08	1.65	1.59
14	A	3902	PGW	P-O12	2.03	1.67	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	3901	PIO	O2C-C1A-C2A	4.53	121.27	111.48
14	L	301	PGW	O01-C1-C2	4.14	120.44	111.48
14	B	3504	PGW	O01-C1-C2	3.95	120.03	111.48
14	A	3902	PGW	O01-C1-C2	3.76	119.62	111.48
21	D	501	PX2	O7-C16-C17	3.66	119.39	111.48
22	D	502	A8W	O4-S-O1	-3.45	98.43	106.37
22	D	502	A8W	O3-S-O2	3.37	125.22	112.24
13	A	3901	PIO	O3C-C1B-C2B	2.76	120.26	111.83
14	B	3504	PGW	O03-C19-C20	2.72	120.12	111.83
14	A	3902	PGW	O03-C19-C20	2.58	119.70	111.83
21	D	501	PX2	O5-C4-C5	2.56	119.65	111.83
19	C	501	PLM	O1-C1-C2	2.08	120.57	114.00
14	L	301	PGW	O03-C19-C20	2.06	118.10	111.83

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	3901	PIO	C1C-O13-P1-O1
13	A	3901	PIO	C1C-O13-P1-O11
13	A	3901	PIO	C1C-O13-P1-O12
13	A	3901	PIO	C2A-C1A-O2C-C2C
14	A	3902	PGW	C03-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	3902	PGW	C03-O11-P-O13
14	A	3902	PGW	C03-O11-P-O14
14	A	3902	PGW	C04-O12-P-O11
14	A	3902	PGW	C04-O12-P-O13
14	A	3902	PGW	C04-O12-P-O14
14	A	3902	PGW	C2-C1-O01-C02
14	B	3504	PGW	C04-O12-P-O11
14	B	3504	PGW	C04-O12-P-O14
14	B	3504	PGW	O03-C01-C02-O01
14	L	301	PGW	C03-O11-P-O12
14	L	301	PGW	C03-O11-P-O13
14	L	301	PGW	C03-O11-P-O14
14	L	301	PGW	C04-O12-P-O11
14	L	301	PGW	C2-C1-O01-C02
21	D	501	PX2	C1-O4-P1-O1
21	D	501	PX2	C1-O4-P1-O2
21	D	501	PX2	C1-O4-P1-O3
21	D	501	PX2	O6-C4-O5-C3
13	A	3901	PIO	O1A-C1A-O2C-C2C
14	A	3902	PGW	O02-C1-O01-C02
14	L	301	PGW	O02-C1-O01-C02
21	D	501	PX2	C5-C4-O5-C3
13	A	3901	PIO	C1B-C2B-C3B-C4B
14	A	3902	PGW	C04-C05-CAD-OAE
14	B	3504	PGW	C04-C05-CAD-OAE
14	L	301	PGW	C03-C02-O01-C1
21	D	501	PX2	C16-C17-C18-C19
14	B	3504	PGW	OAF-C05-CAD-OAE
14	A	3902	PGW	C2-C3-C4-C5
14	A	3902	PGW	C27-C15-C16-C17
13	D	503	PIO	C2A-C1A-O2C-C2C
14	B	3504	PGW	C2-C1-O01-C02
14	L	301	PGW	C06-C07-C08-C09
14	L	301	PGW	C27-C15-C16-C17
21	D	501	PX2	C11-C10-C9-C8
14	B	3504	PGW	C16-C15-C27-C26
14	B	3504	PGW	C22-C23-C24-C25
21	D	501	PX2	C17-C16-O7-C2
14	L	301	PGW	C20-C19-O03-C01
14	B	3504	PGW	O02-C1-O01-C02
21	D	501	PX2	C10-C11-C12-C13
14	L	301	PGW	O04-C19-O03-C01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	501	PX2	C6-C7-C8-C9
13	A	3901	PIO	O2C-C2C-C3C-O3C
13	D	503	PIO	O1A-C1A-O2C-C2C
14	B	3504	PGW	C20-C19-O03-C01
21	D	501	PX2	O8-C16-O7-C2
13	A	3901	PIO	C1C-C2C-C3C-O3C
22	D	502	A8W	C3-O1-S-O2
14	L	301	PGW	C17-C18-C28-C30
14	B	3504	PGW	O04-C19-O03-C01
14	L	301	PGW	C24-C25-C26-C27
14	L	301	PGW	C2-C3-C4-C5
14	A	3902	PGW	C23-C24-C25-C26
14	A	3902	PGW	C05-C04-O12-P
14	B	3504	PGW	C09-C11-C12-C13
14	A	3902	PGW	C06-C07-C08-C09
14	B	3504	PGW	O03-C01-C02-C03
17	B	3501	R16	C31-C32-C33-C34
14	A	3902	PGW	C1-C2-C3-C4
14	B	3504	PGW	C6-C7-C8-C9
14	A	3902	PGW	C08-C09-C11-C12
14	A	3902	PGW	O03-C19-C20-C21
14	B	3504	PGW	C24-C25-C26-C27
13	A	3901	PIO	C2B-C3B-C4B-C5B
14	L	301	PGW	C23-C24-C25-C26
14	B	3504	PGW	C11-C12-C13-C14
14	A	3902	PGW	C03-C02-O01-C1
14	A	3902	PGW	C17-C18-C28-C30
13	A	3901	PIO	C3B-C4B-C5B-C6B
14	A	3902	PGW	C5-C6-C7-C8
14	A	3902	PGW	C20-C21-C22-C23
14	B	3504	PGW	C17-C18-C28-C30
13	D	503	PIO	C1C-O13-P1-O12
14	L	301	PGW	C04-O12-P-O14
14	L	301	PGW	C02-C03-O11-P
14	B	3504	PGW	C1-C2-C3-C4
14	L	301	PGW	C22-C23-C24-C25
13	A	3901	PIO	C5-O5-P5-O51
13	D	503	PIO	C4-O4-P4-O43
13	D	503	PIO	C2B-C1B-O3C-C3C
21	D	501	PX2	C23-C24-C25-C26
14	A	3902	PGW	C09-C11-C12-C13
19	C	501	PLM	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	D	503	PIO	O1B-C1B-O3C-C3C
21	D	501	PX2	C5-C6-C7-C8
14	L	301	PGW	C7-C8-C9-C10
13	A	3901	PIO	O2C-C1A-C2A-C3A
14	B	3504	PGW	C07-C06-C10-C9
14	A	3902	PGW	O04-C19-C20-C21
14	B	3504	PGW	C06-C07-C08-C09
14	B	3504	PGW	C08-C09-C11-C12
19	C	501	PLM	O2-C1-C2-C3
13	A	3901	PIO	C2A-C3A-C4A-C5A
19	C	501	PLM	O1-C1-C2-C3
14	A	3902	PGW	C7-C8-C9-C10
13	A	3901	PIO	C1-O1-P1-O11
13	A	3901	PIO	C1-O1-P1-O12
14	L	301	PGW	C1-C2-C3-C4
21	D	501	PX2	C9-C10-C11-C12
14	B	3504	PGW	O03-C19-C20-C21
14	B	3504	PGW	O04-C19-C20-C21
14	B	3504	PGW	C7-C8-C9-C10

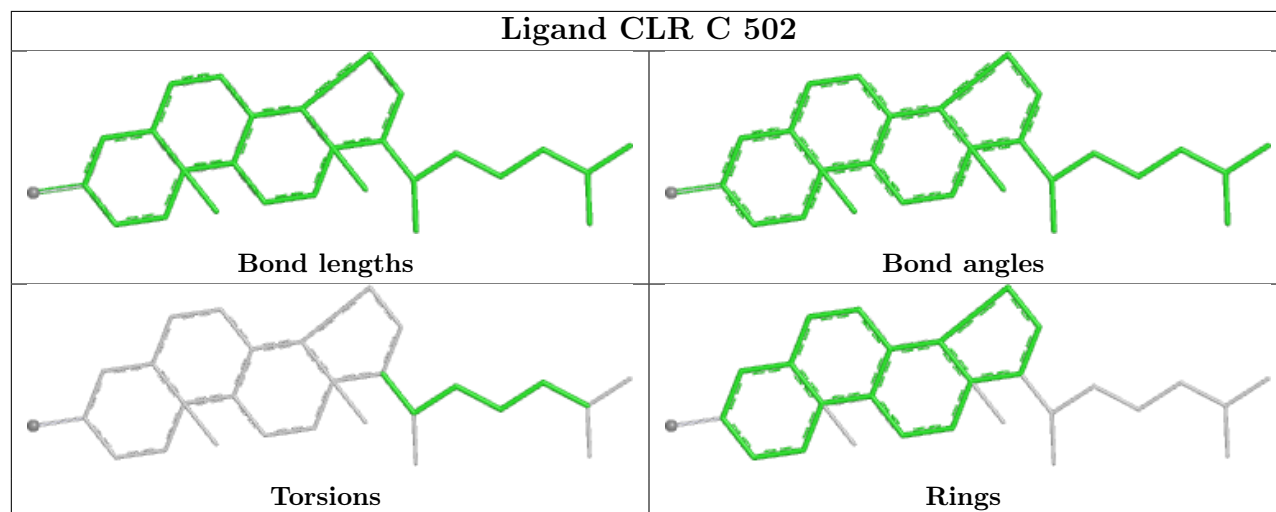
There are no ring outliers.

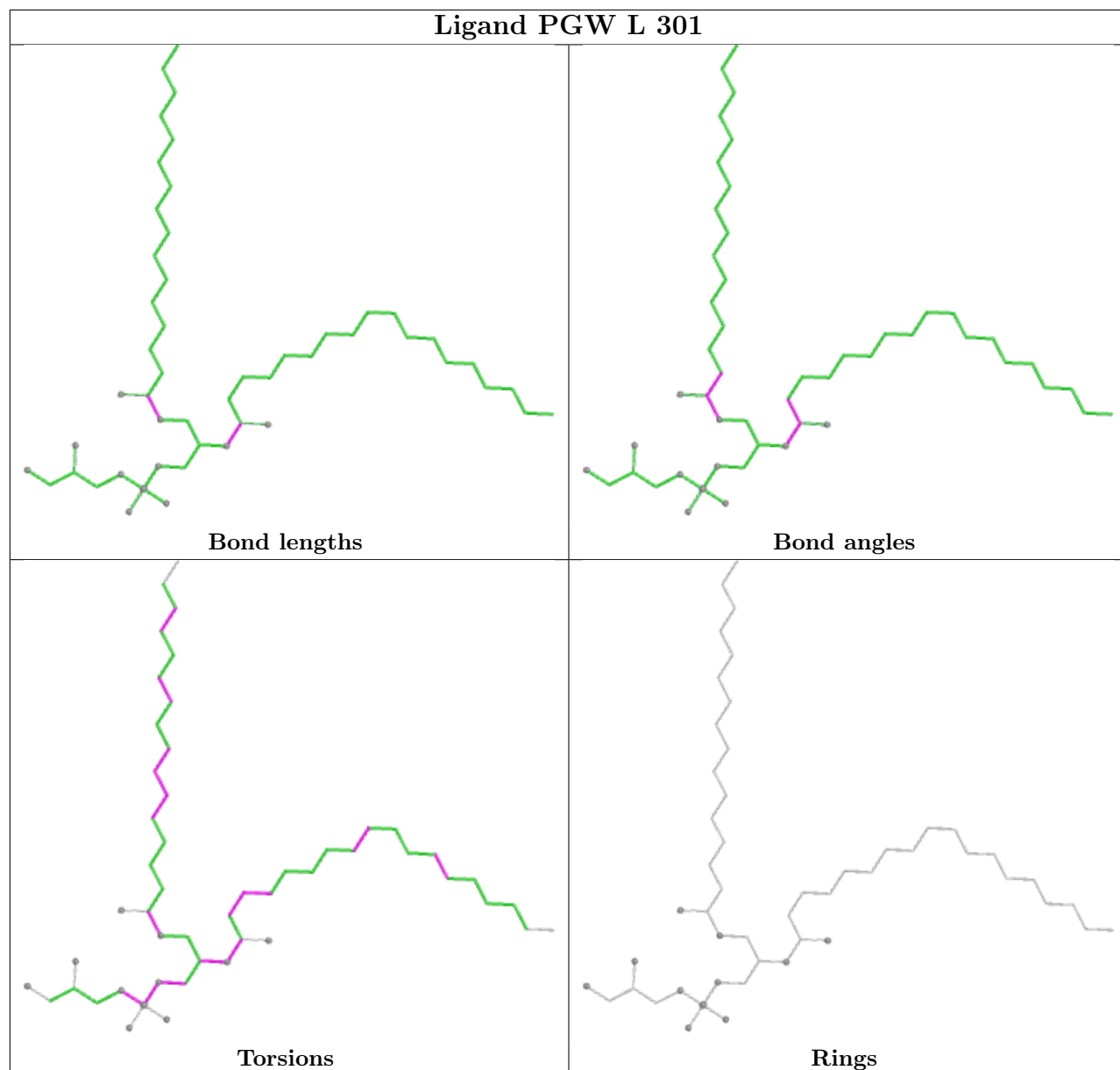
8 monomers are involved in 11 short contacts:

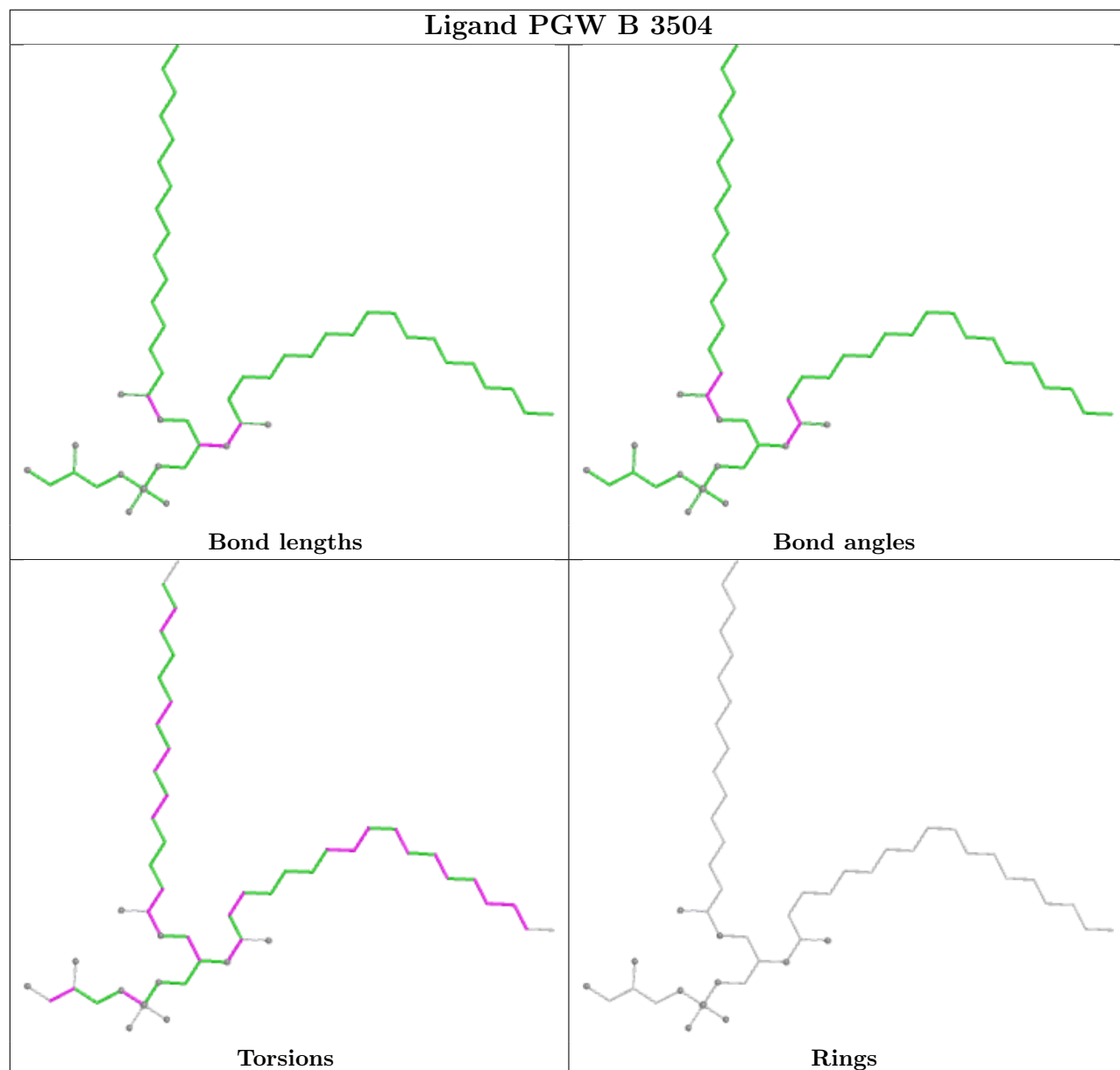
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	502	CLR	1	0
14	L	301	PGW	1	0
14	B	3504	PGW	1	0
21	D	501	PX2	2	0
13	A	3901	PIO	1	0
14	A	3902	PGW	1	0
15	C	503	D10	1	0
13	D	503	PIO	3	0

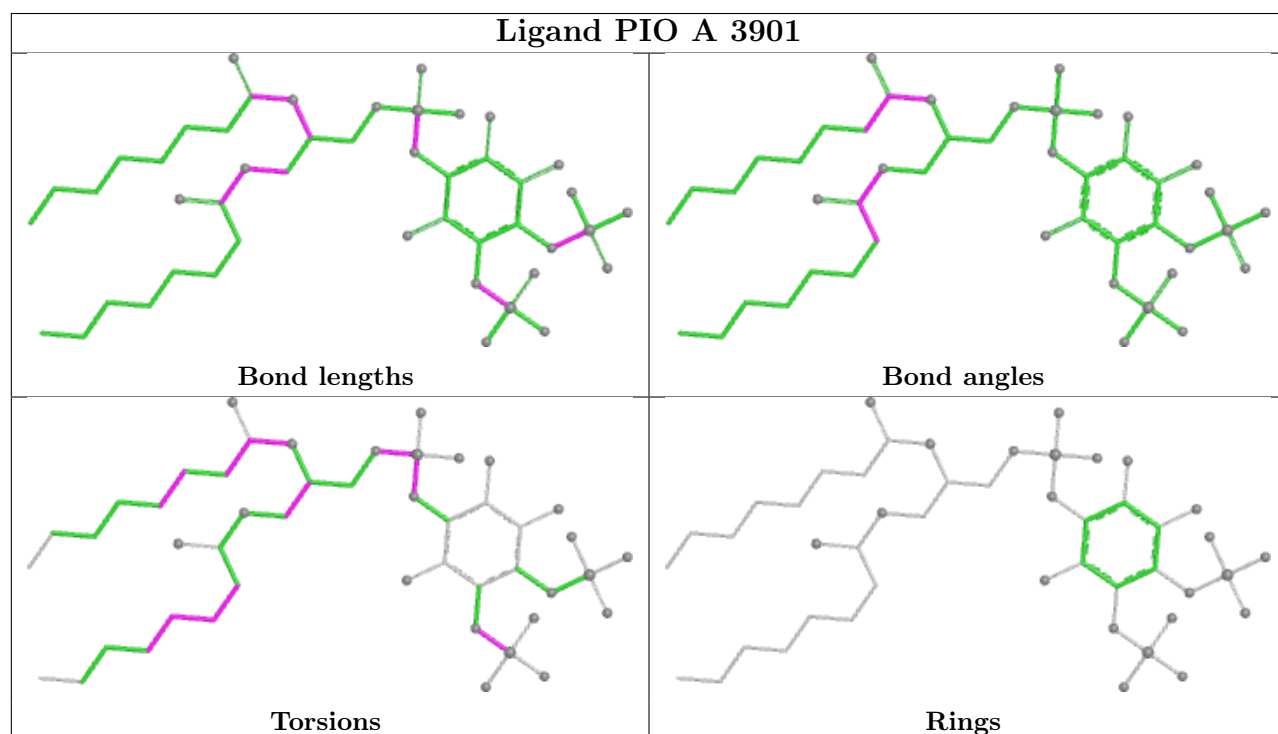
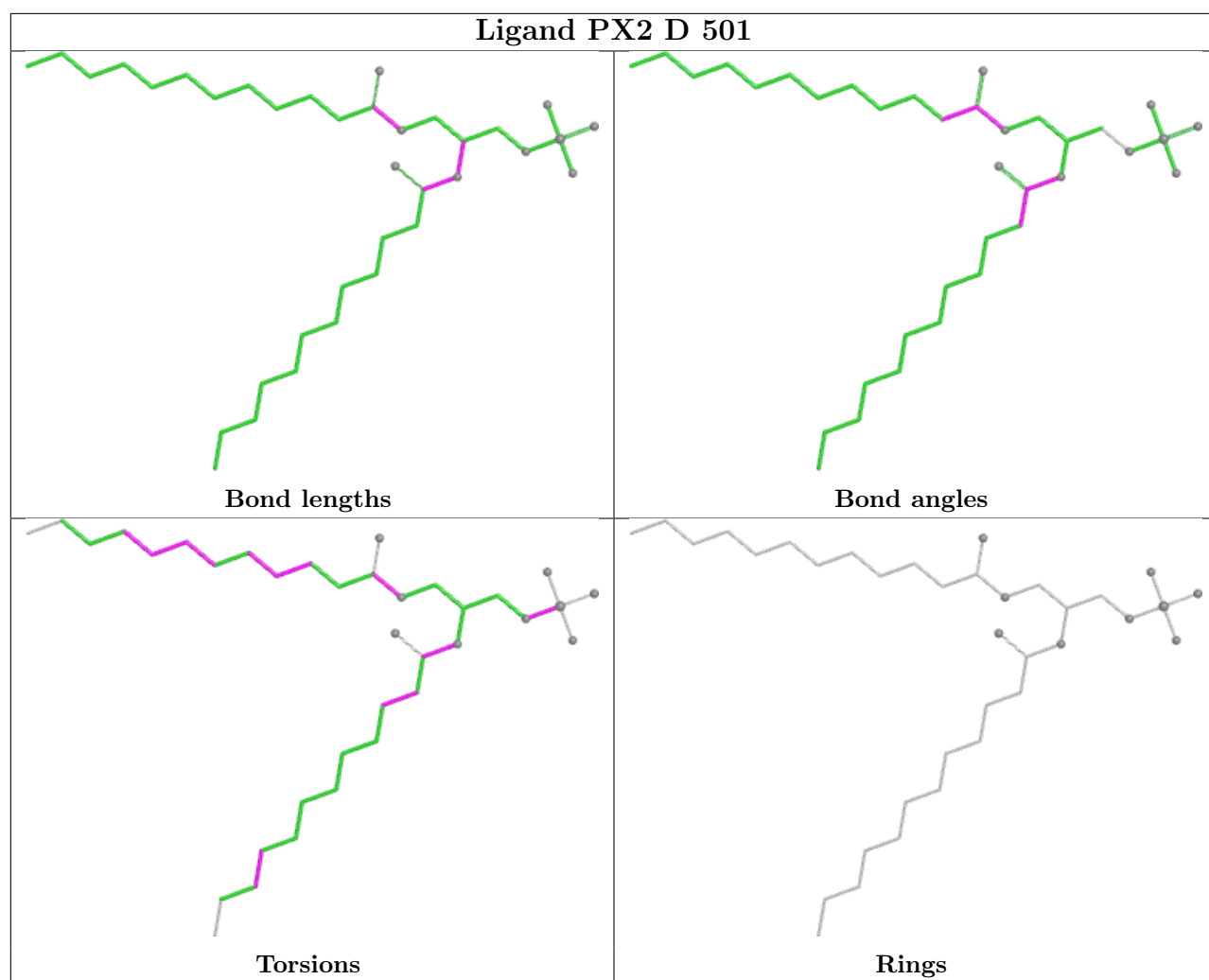
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

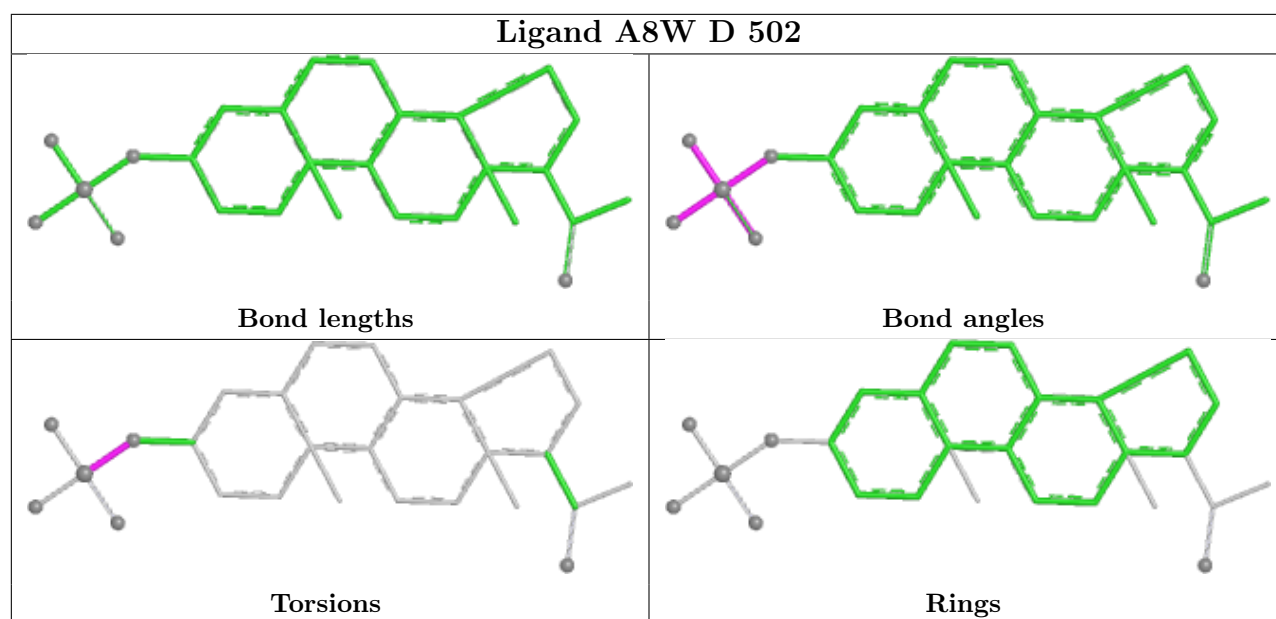
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

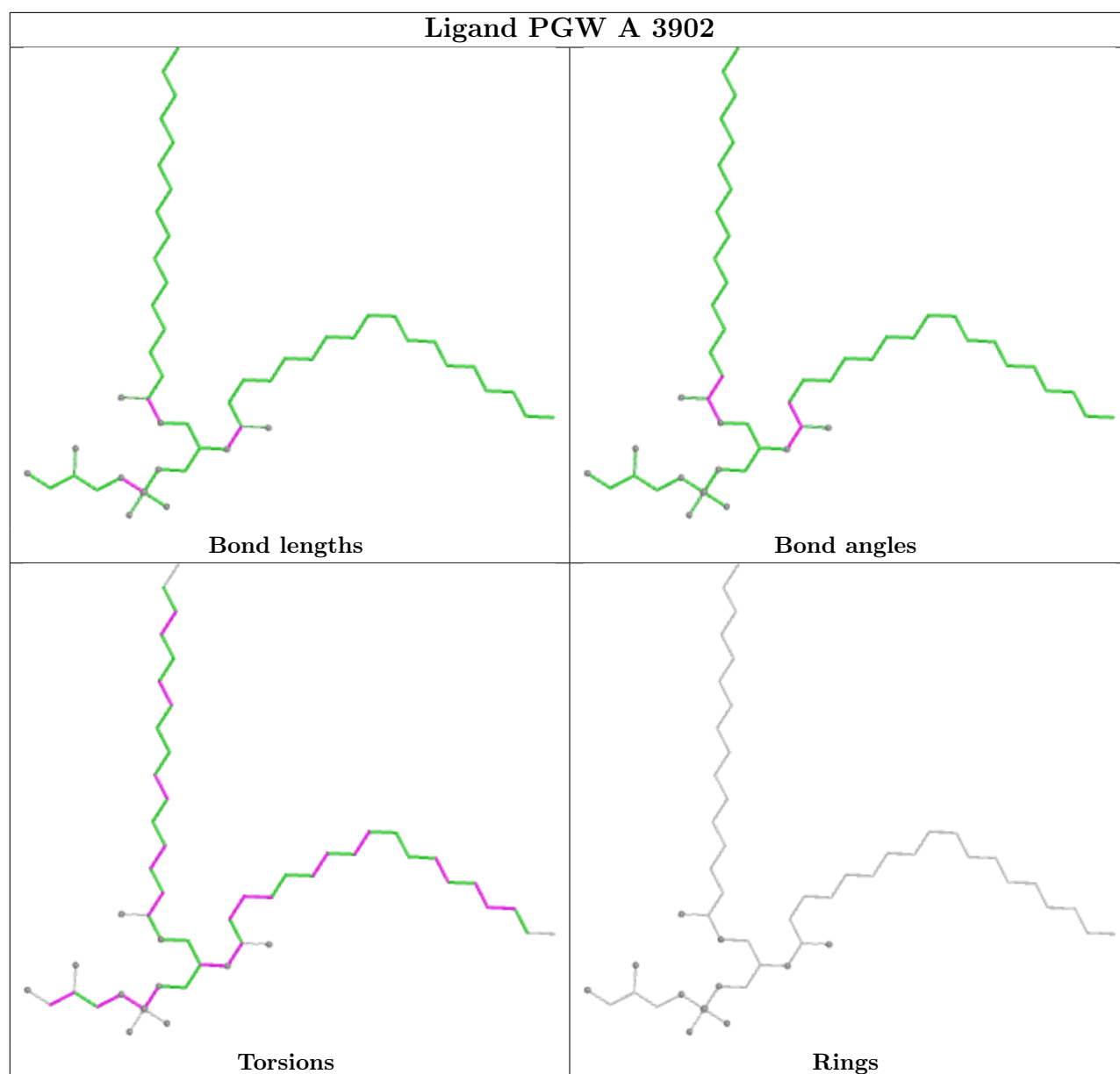


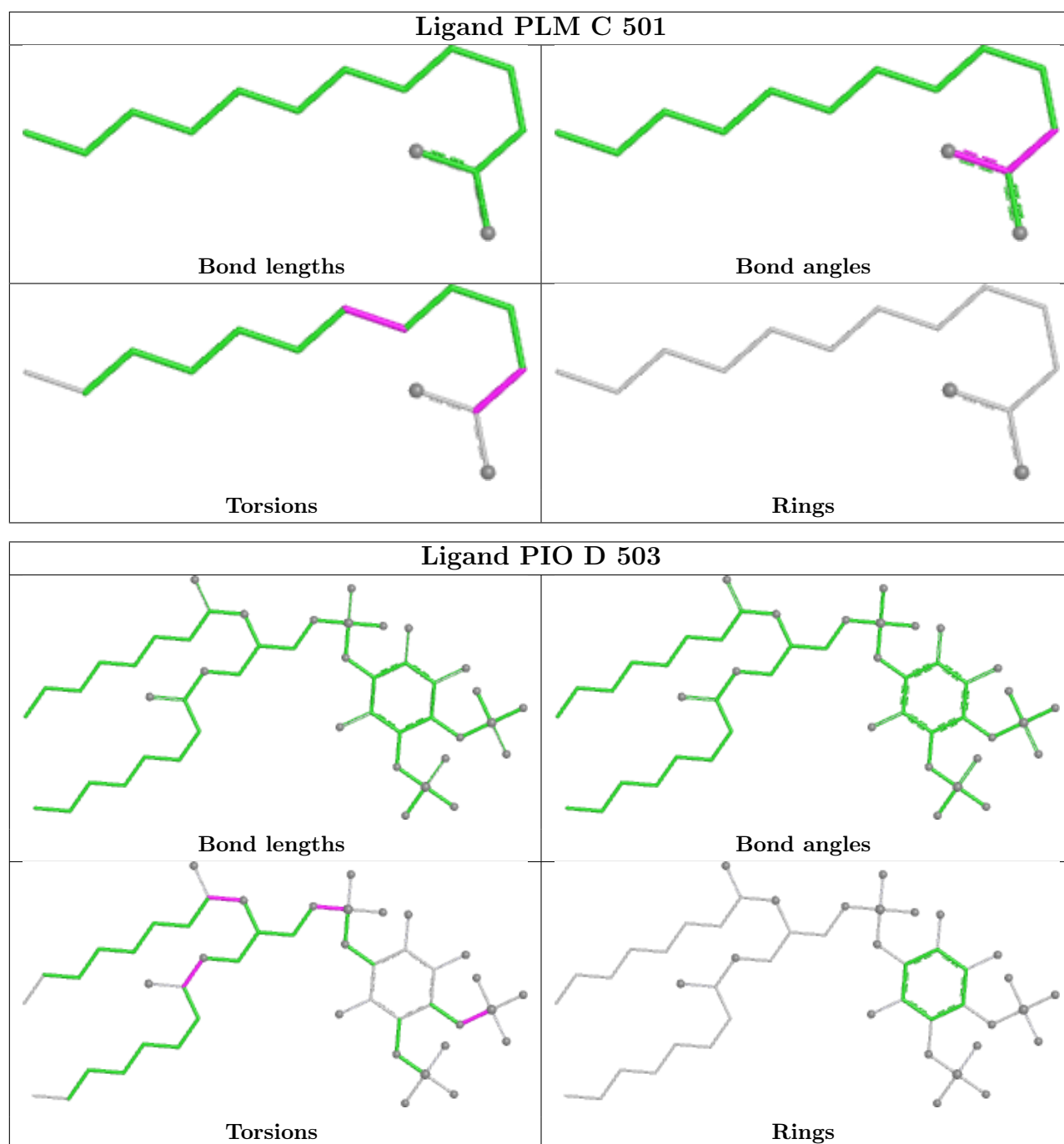












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

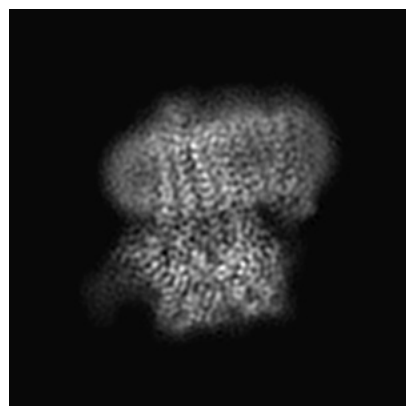
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50281. These allow visual inspection of the internal detail of the map and identification of artifacts.

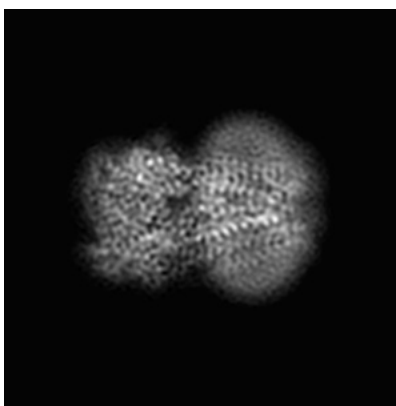
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

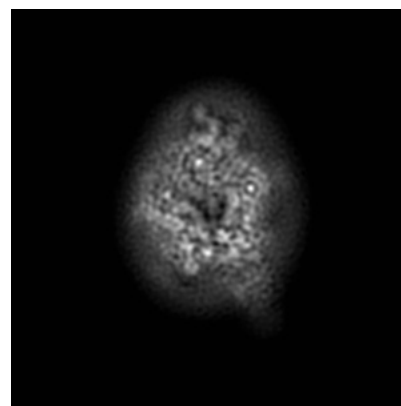
6.1.1 Primary map



X

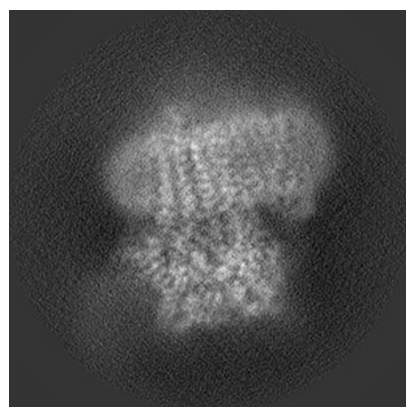


Y

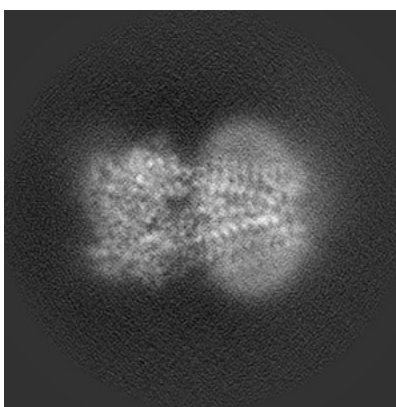


Z

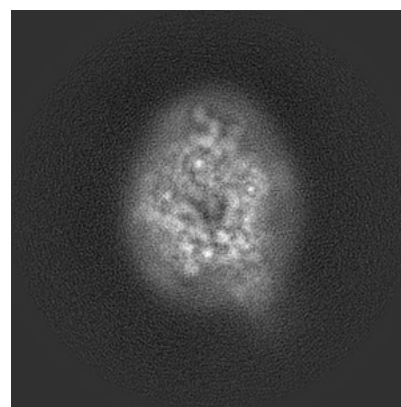
6.1.2 Raw map



X



Y

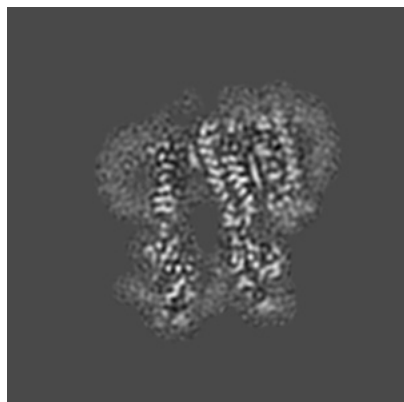


Z

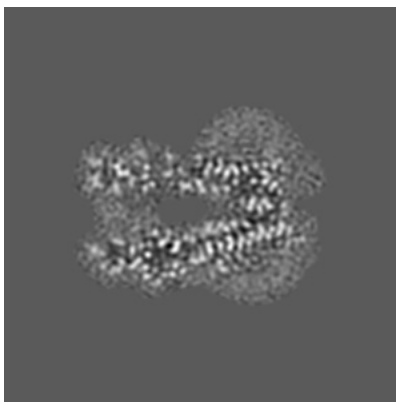
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

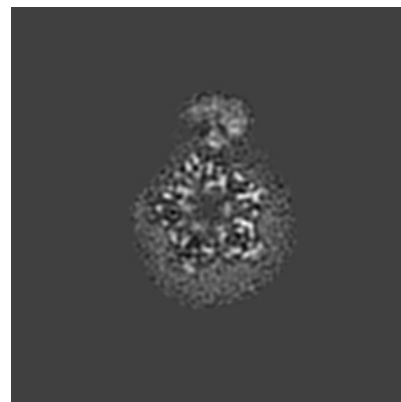
6.2.1 Primary map



X Index: 128

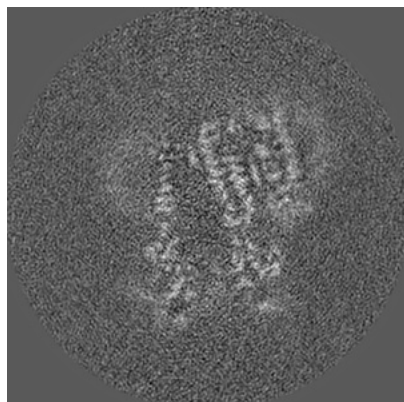


Y Index: 128

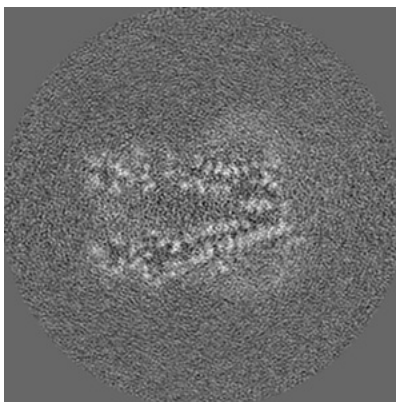


Z Index: 128

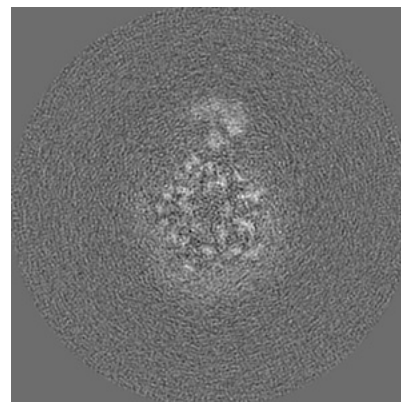
6.2.2 Raw map



X Index: 128



Y Index: 128

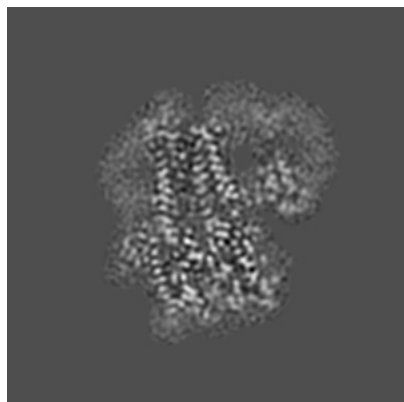


Z Index: 128

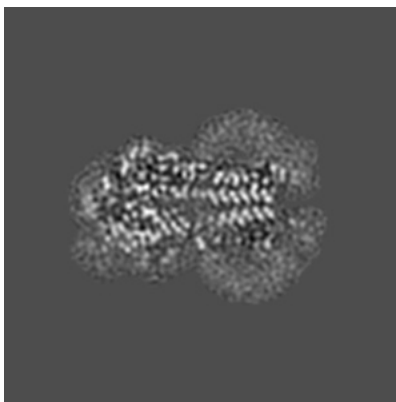
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

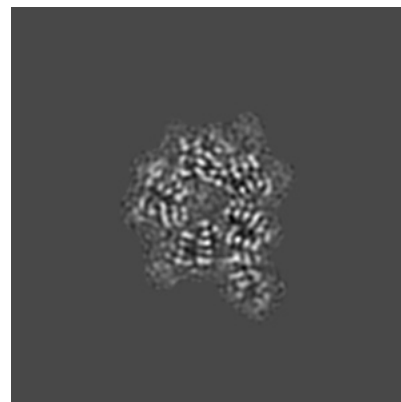
6.3.1 Primary map



X Index: 142

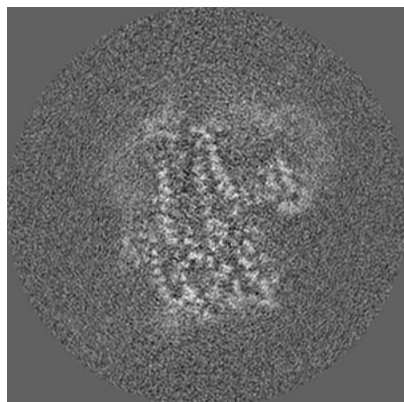


Y Index: 111

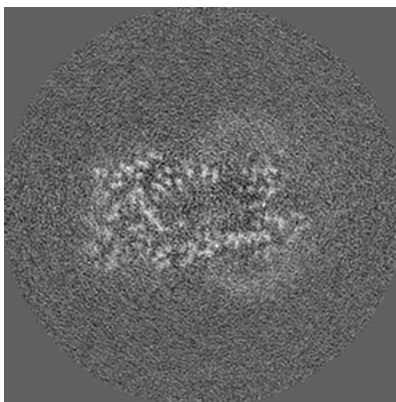


Z Index: 92

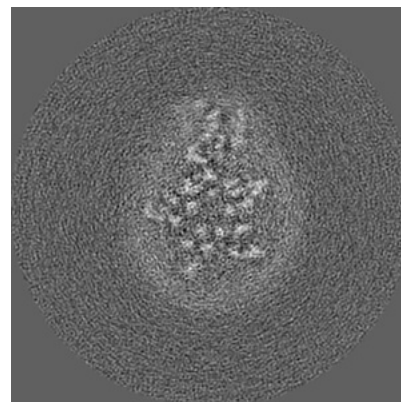
6.3.2 Raw map



X Index: 142



Y Index: 117

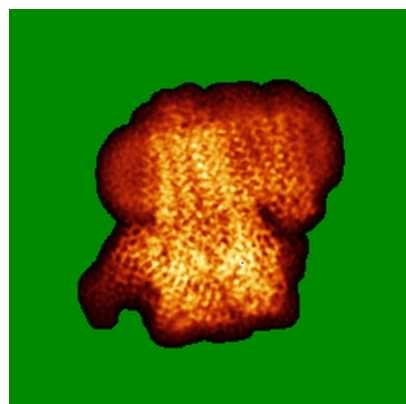


Z Index: 141

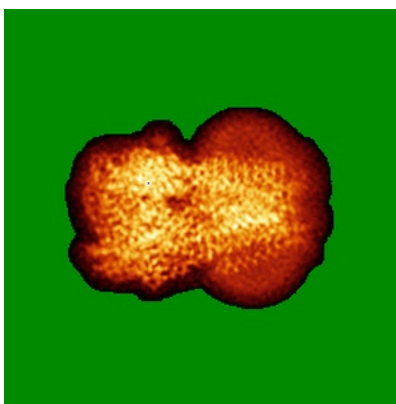
The images above show the largest variance slices of the map in three orthogonal directions.

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

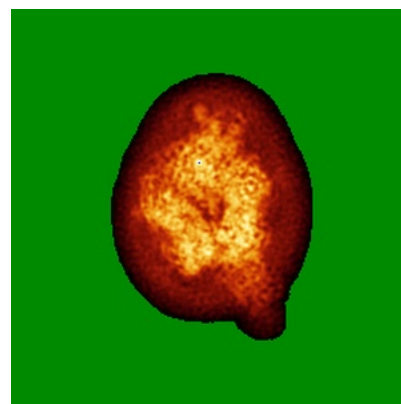
6.4.1 Primary map



X

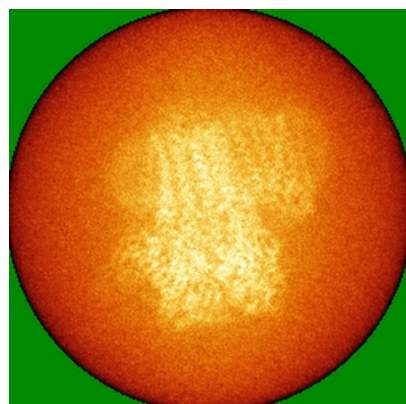


Y

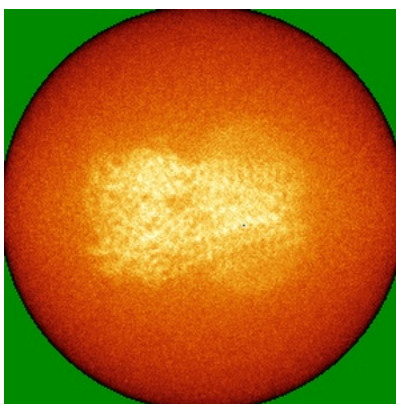


Z

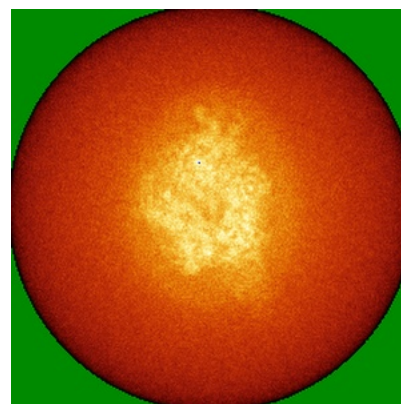
6.4.2 Raw map



X



Y

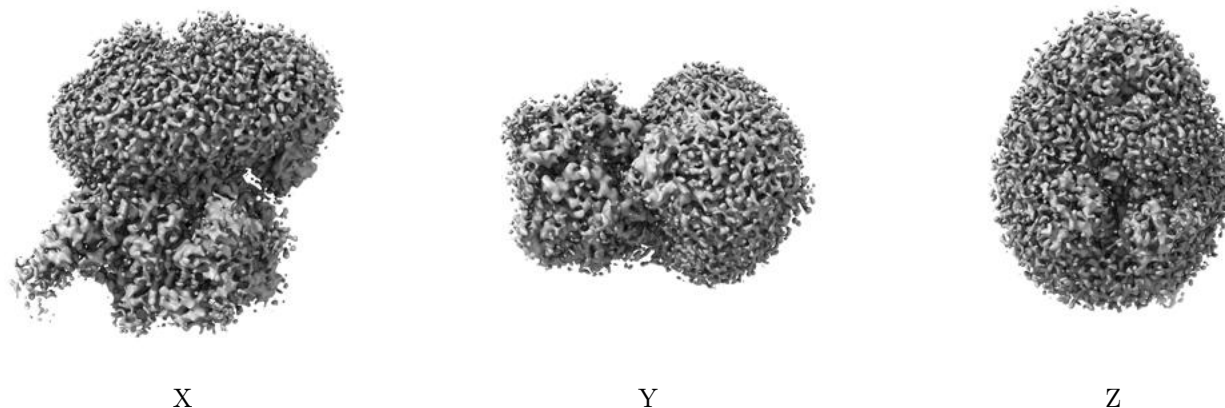


Z

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

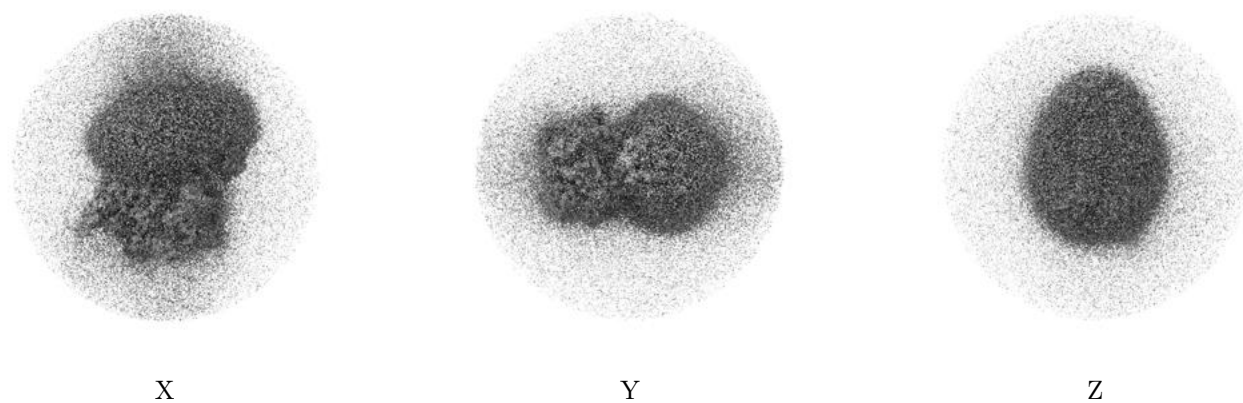
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

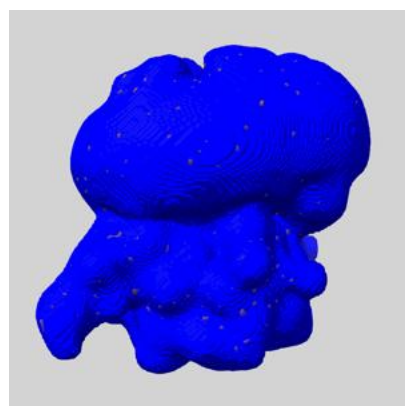
6.6 Mask visualisation [i](#)

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

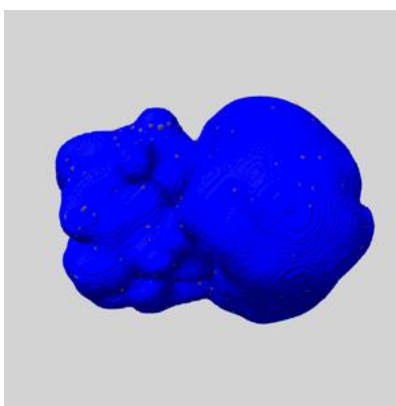
A mask typically either:

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

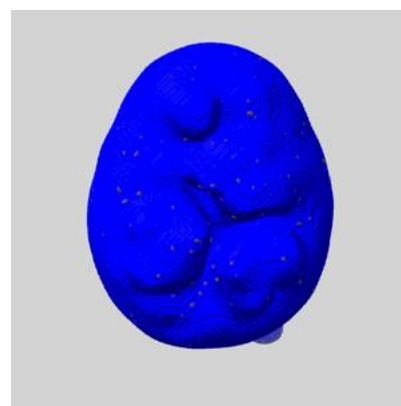
6.6.1 emd_50281_msk_1.map [i](#)



X



Y

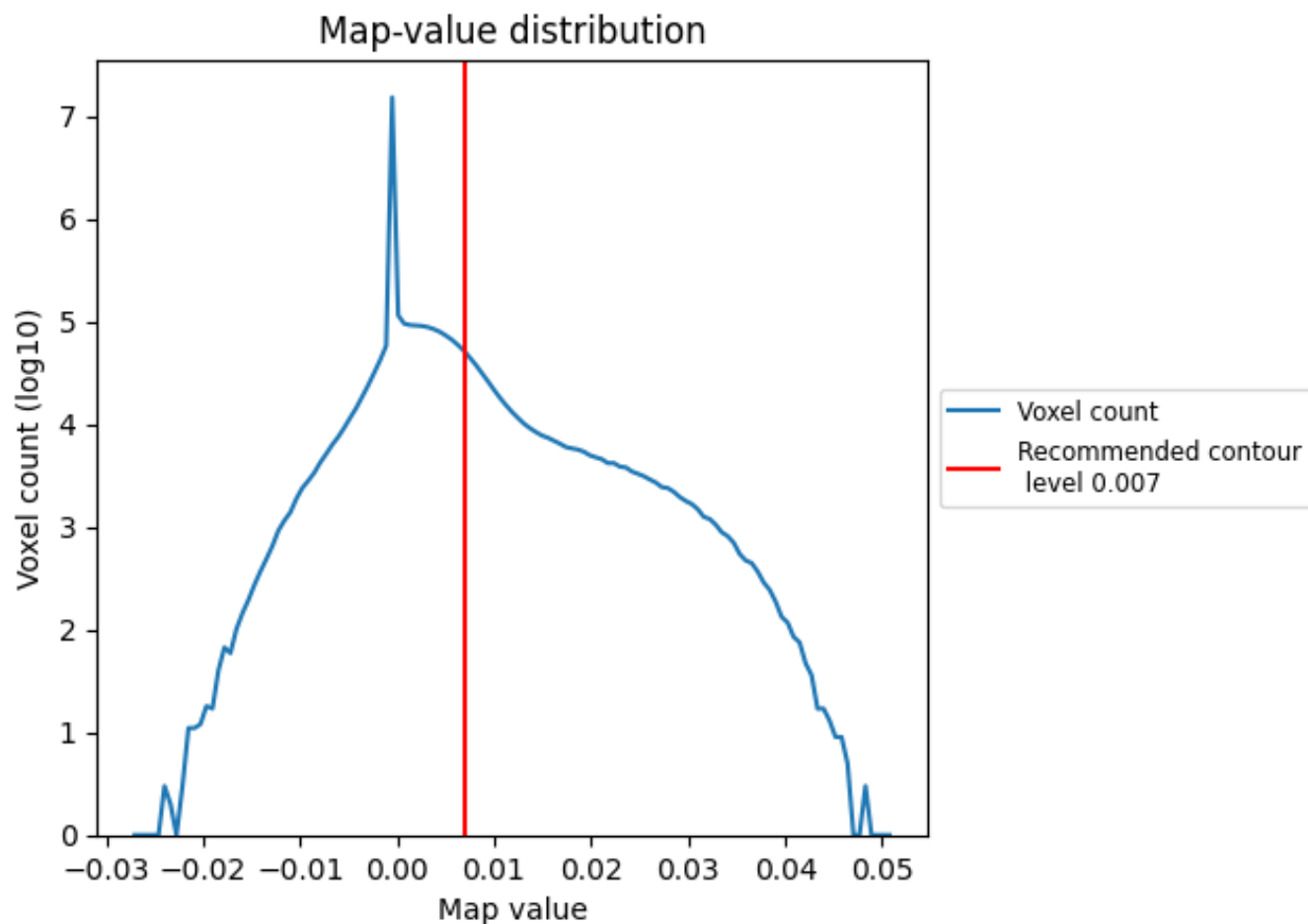


Z

7 Map analysis [i](#)

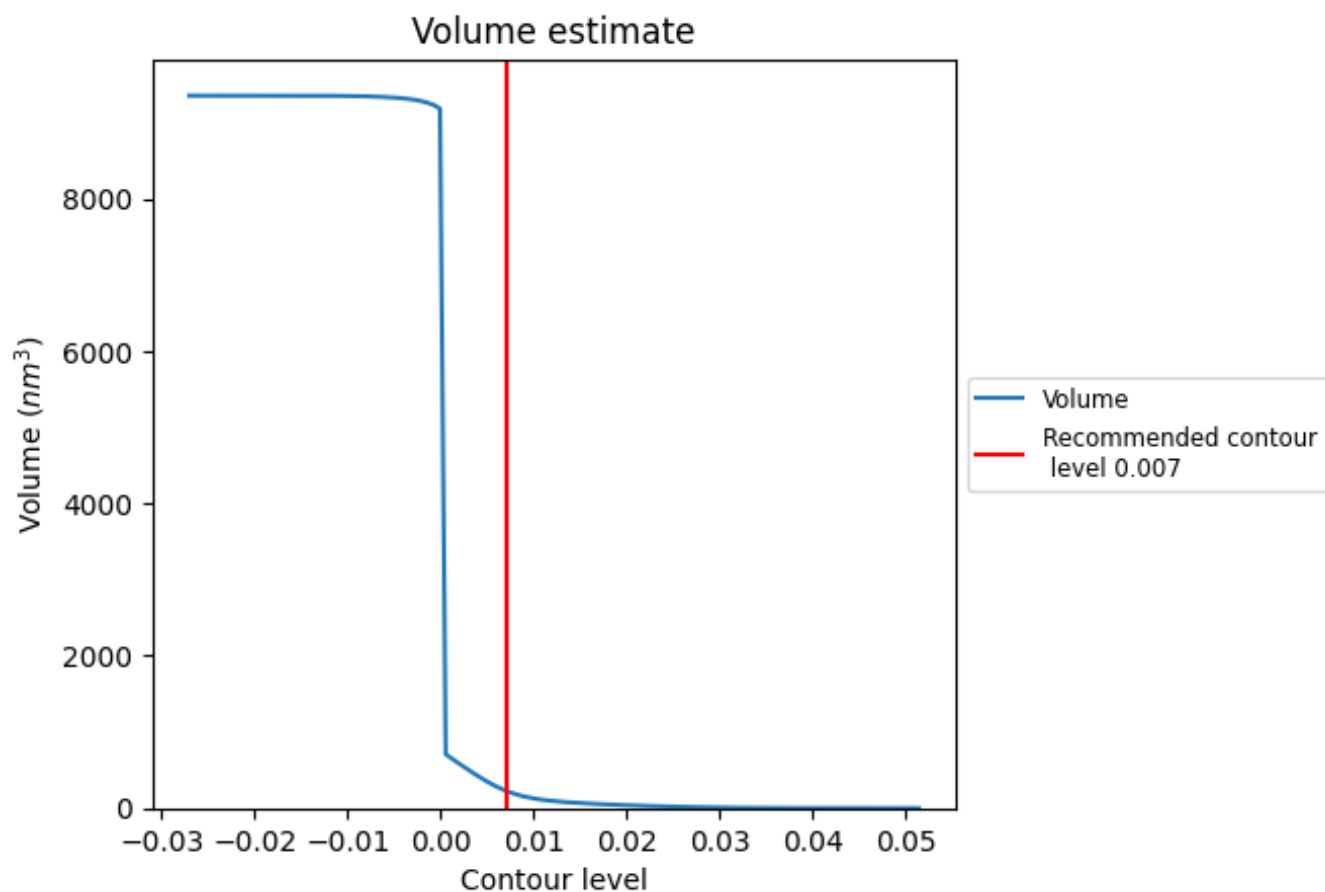
This section contains the results of statistical analysis of the map.

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.

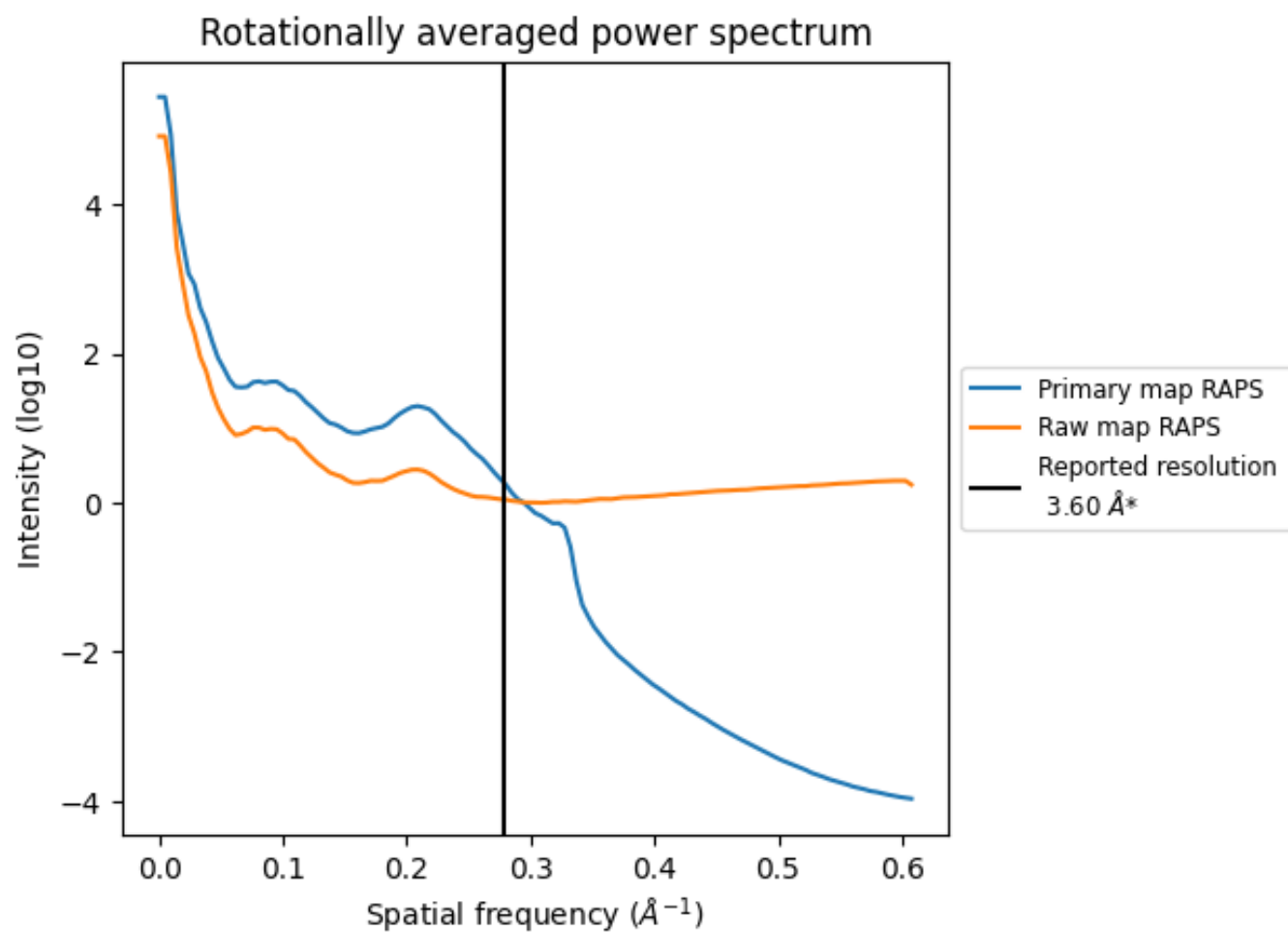
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm^3 ; this corresponds to an approximate mass of 206 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 ⓘ

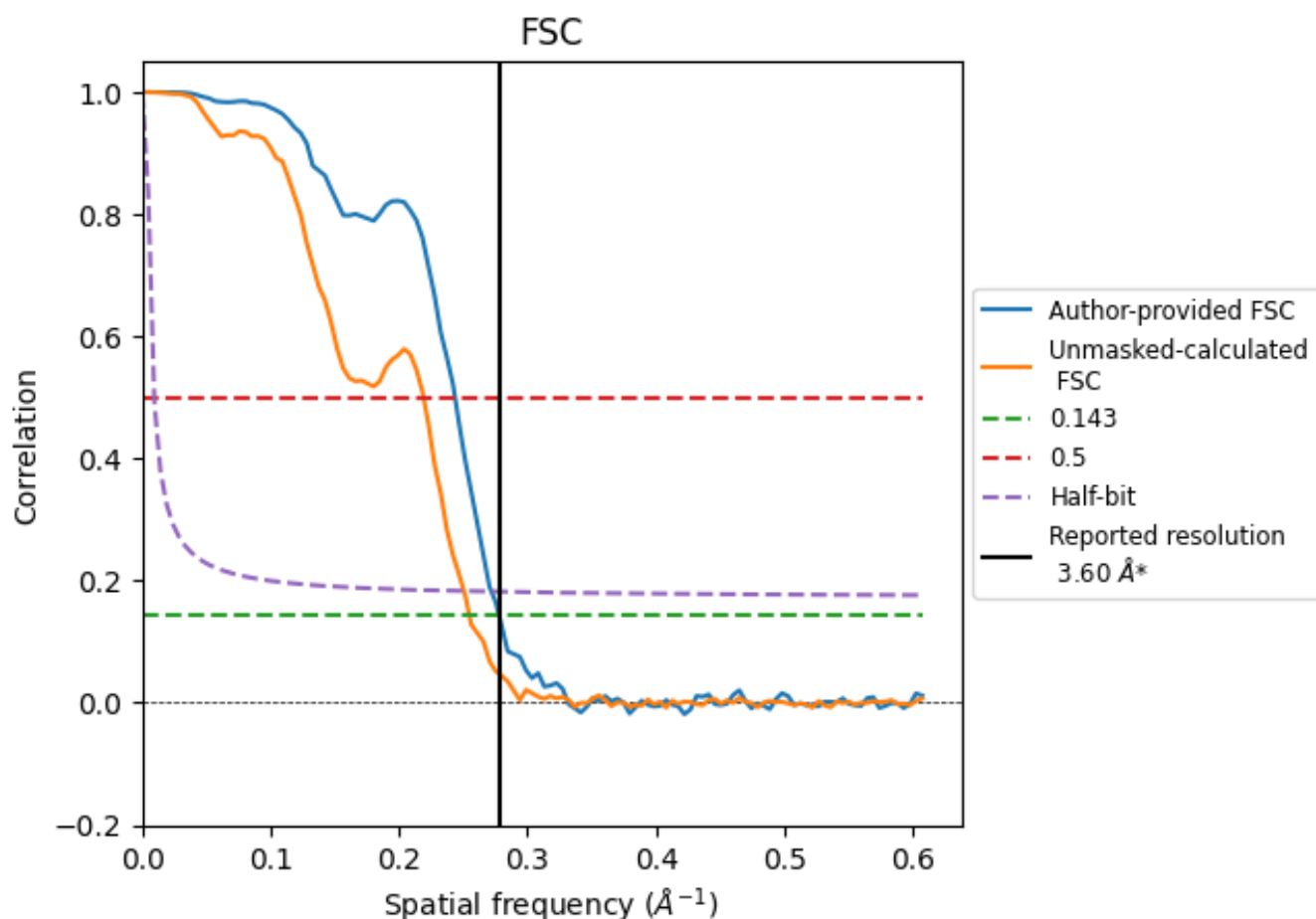


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

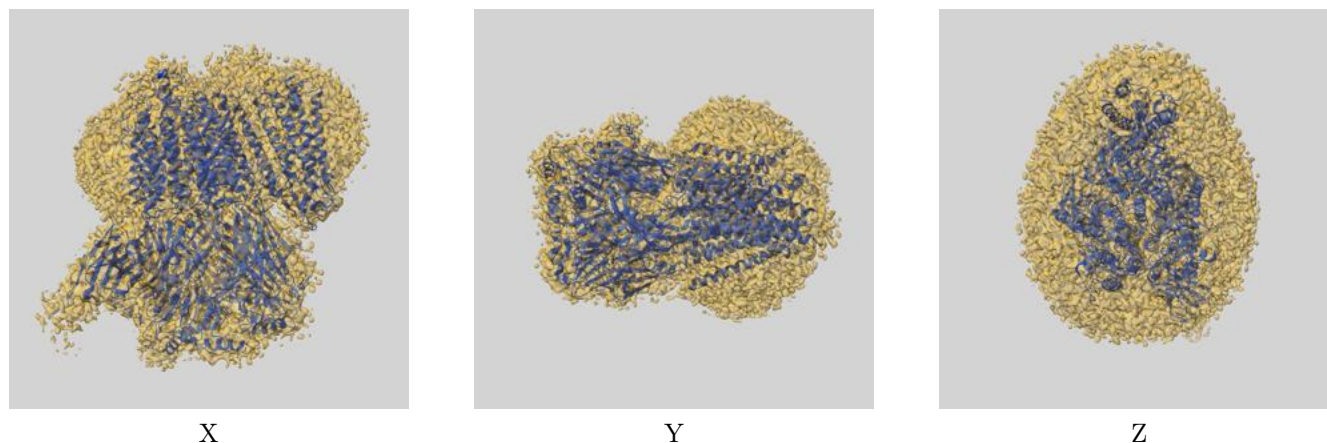
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.10	3.68
Unmasked-calculated*	3.92	4.56	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

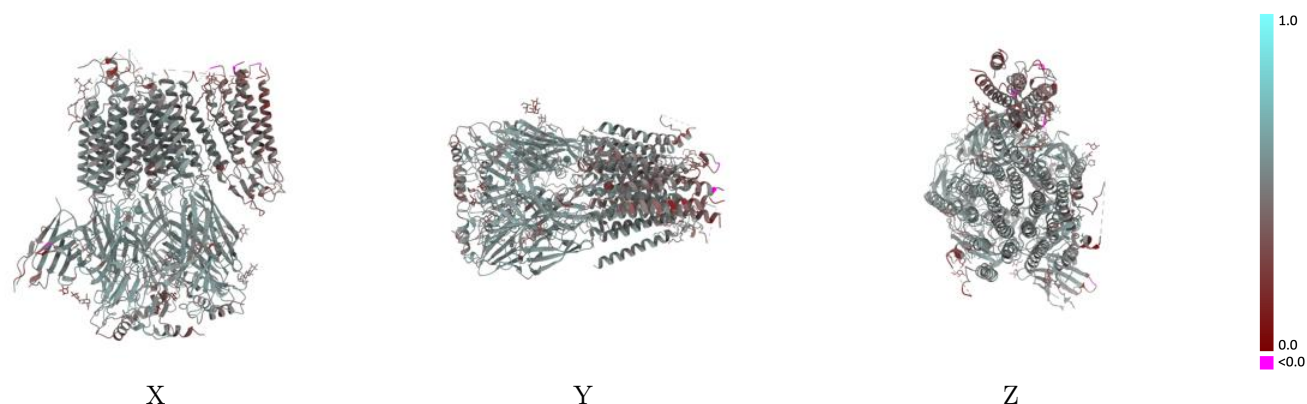
This section contains information regarding the fit between EMDB map EMD-50281 and PDB model 9FAT. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



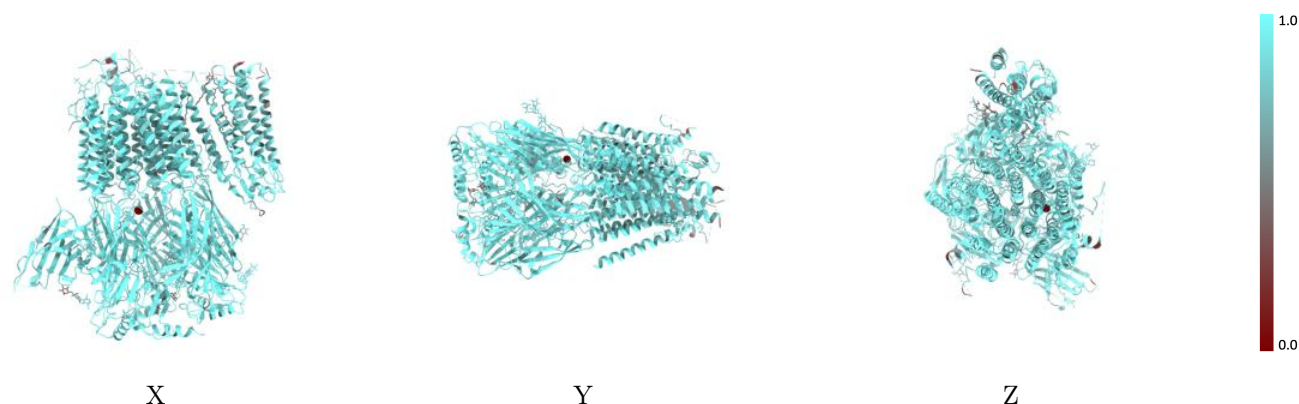
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



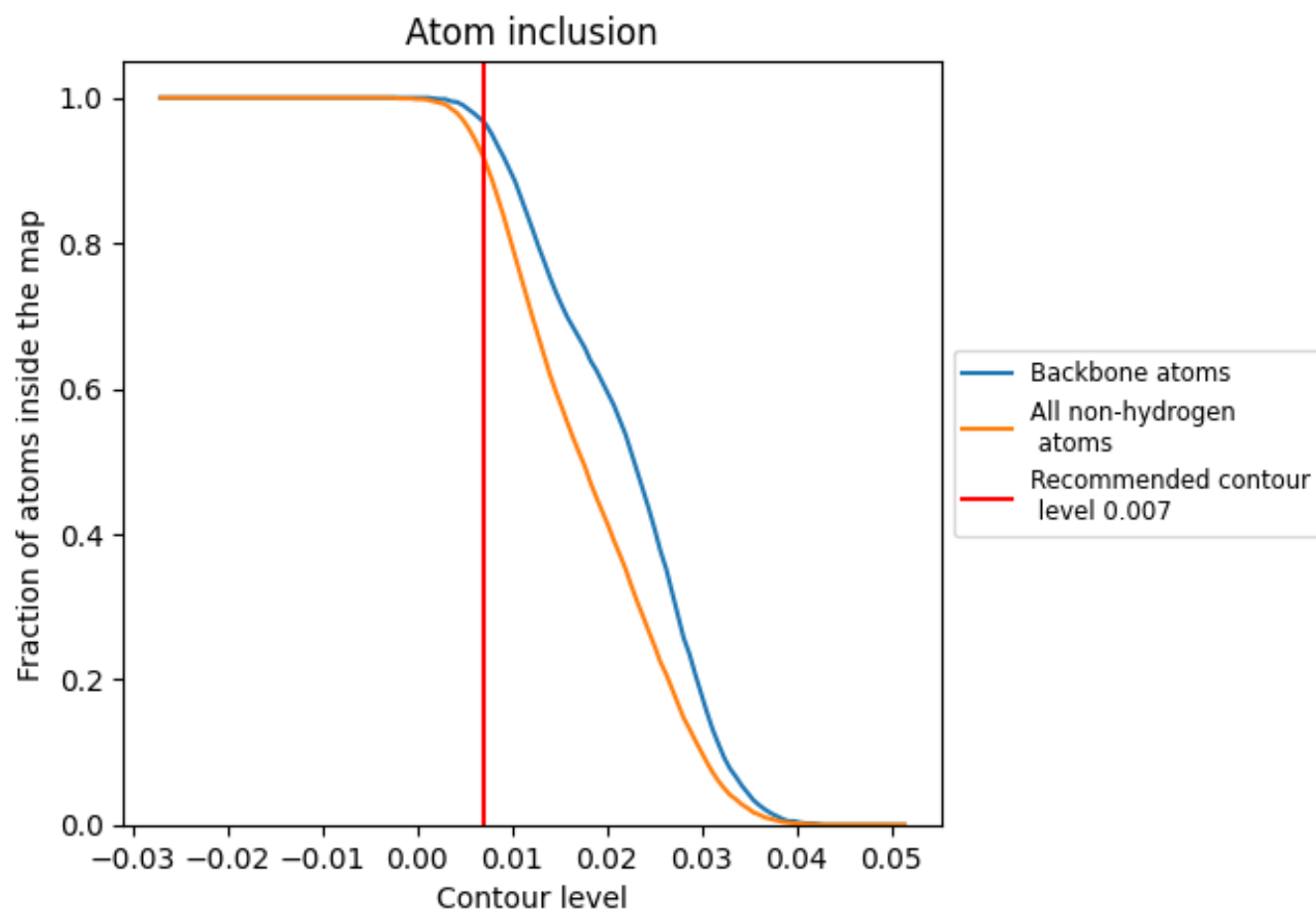
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.4980
A	0.9330	0.5140
B	0.9300	0.5110
C	0.9260	0.5070
D	0.9250	0.5170
E	0.9360	0.5080
F	0.8880	0.4430
G	0.9070	0.5020
H	0.7930	0.3380
I	0.8850	0.3850
J	0.8720	0.4330
K	0.7860	0.3200
L	0.8610	0.4280
M	0.6870	0.2990
N	0.8060	0.3430
O	0.6410	0.2820

