



Full wwPDB EM Validation Report ⓘ

Jun 24, 2025 – 07:24 pm BST

PDB ID : 9FAJ / pdb_00009faj
EMDB ID : EMD-50273
Title : CryoEM structure of human full-length alpha1beta3gamma2 GABA(A) receptor in complex with GARLH4, the TMD of Neuroligin2, GABA and Megabody38, in a desensitised state (StateD1)
Authors : Kasaragod, V.B.; Aricescu, A.R.
Deposited on : 2024-05-10
Resolution : 2.60 Å (reported)
Based on initial model : 6HUO

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

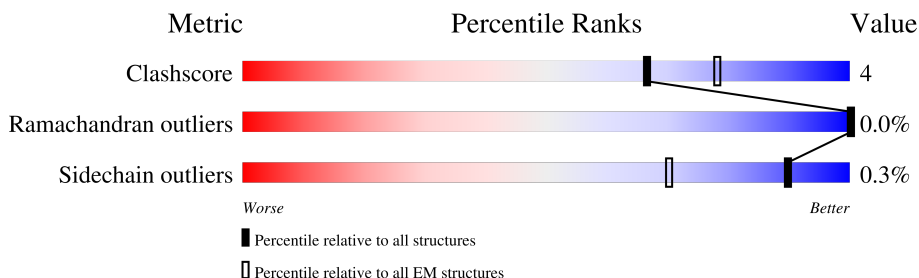
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
2	E	441	
3	C	405	
4	H	33	
5	L	193	
6	G	539	

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Mol	Chain	Length	Quality of chain
6	P	539	
7	F	10	
8	I	3	
8	O	3	
9	J	6	
9	N	6	
10	K	2	
11	M	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
17	CL	L	304	-	-	X	-

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 19645 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	3	0
			2904	1877	491	520	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
			2843	1861	466	500	16		
2	E	347	Total	C	N	O	S	5	0
			2887	1888	479	504	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	3	0
			2959	1943	480	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 Neuroligin-2.

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

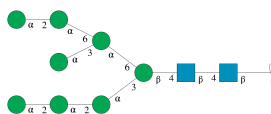
- Molecule 5 is a protein called LHFPL tetraspan subfamily member 4 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	193	Total	C	N	O	S	1	0
			1509	1001	238	254	16		

- Molecule 6 is a protein called Megabody38.

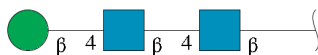
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	121	Total	C	N	O	S	1	0
			949	594	172	179	4		
6	P	121	Total	C	N	O	S	0	0
			941	589	169	179	4		

- 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.



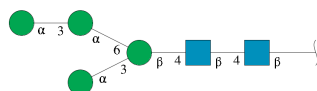
Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	10	Total	C	N	O		0	0
			116	64	2	50			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



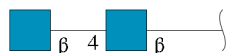
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	3	Total	C	N	O		0	0
			39	22	2	15			
8	O	3	Total	C	N	O		0	0
			39	22	2	15			

- Molecule 9 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.



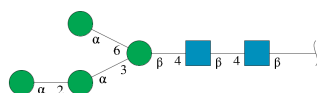
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	6	Total	C	N	O	0	0
			72	40	2	30		
9	N	6	Total	C	N	O	0	0
			72	40	2	30		

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



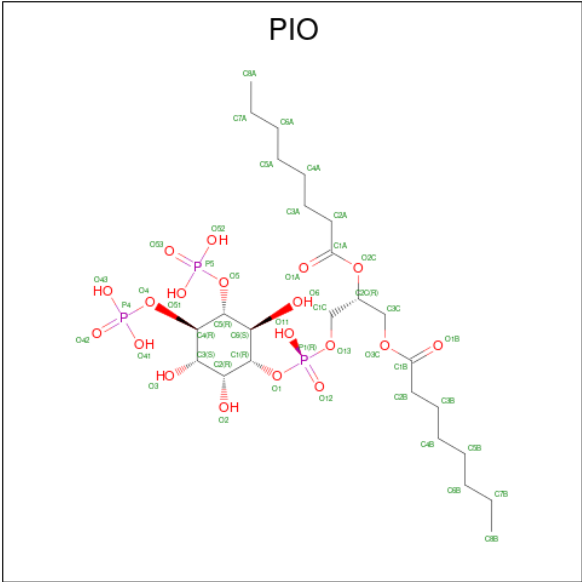
Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	2	Total	C	N	O	0	0
			28	16	2	10		

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



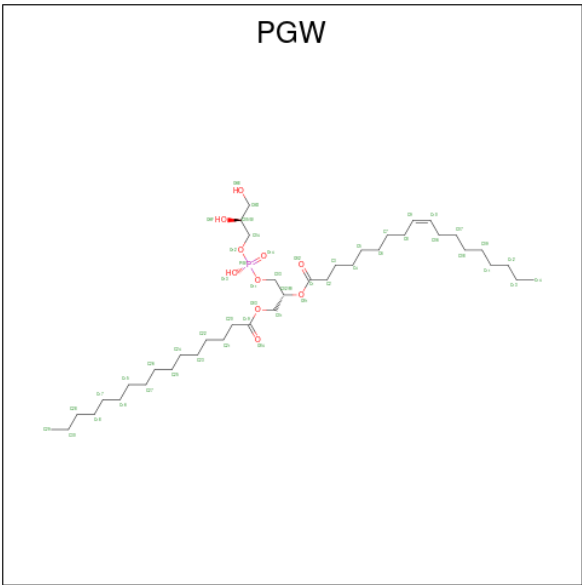
Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 12 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃).



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

- Molecule 13 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).



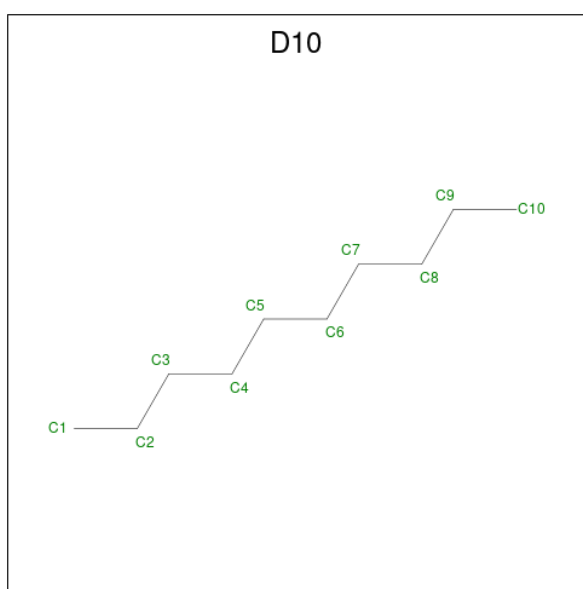
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	1
			102	80	20	2	

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Mol	Chain	Residues	Atoms				AltConf
13	D	1	Total	C	O	P	1
			102	80	20	2	
13	E	1	Total	C	O	P	0
			32	21	10	1	
13	L	1	Total	C	O	P	0
			51	40	10	1	
13	L	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 14 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



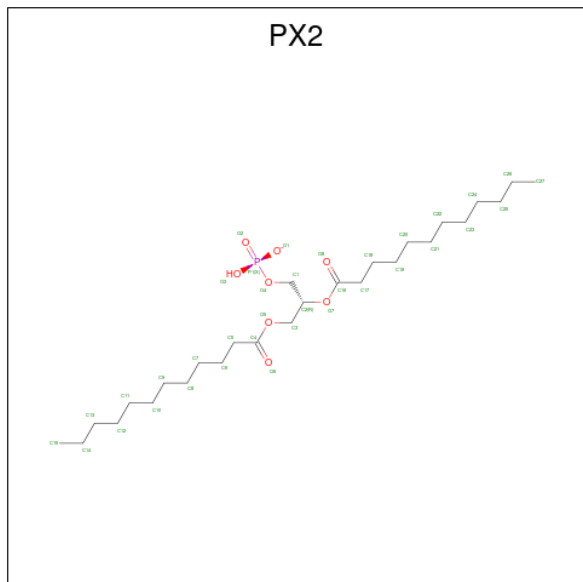
Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	C	0
			10	10	
14	A	1	Total	C	0
			10	10	
14	A	1	Total	C	0
			10	10	
14	A	1	Total	C	0
			10	10	
14	B	1	Total	C	0
			10	10	
14	B	1	Total	C	0
			10	10	
14	C	1	Total	C	0
			10	10	

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Mol	Chain	Residues	Atoms	AltConf
14	D	1	Total C 10 10	0
14	D	1	Total C 10 10	0
14	E	1	Total C 10 10	0
14	E	1	Total C 10 10	0
14	L	1	Total C 10 10	0

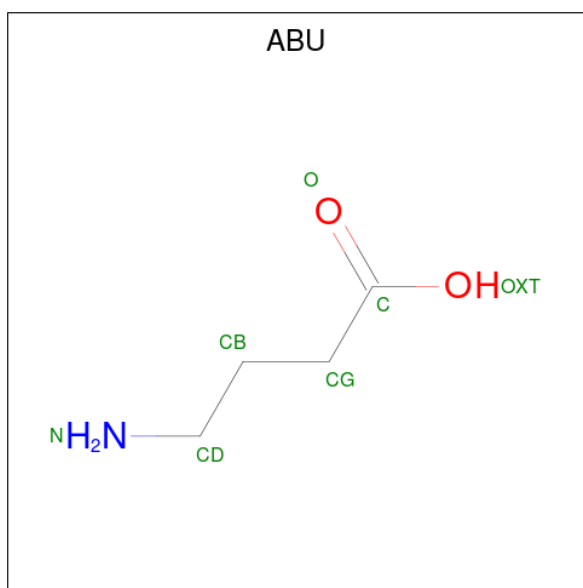
- Molecule 15 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C O P 36 27 8 1	0
15	B	1	Total C O P 36 27 8 1	0
15	C	1	Total C O P 36 27 8 1	0
15	D	1	Total C O P 36 27 8 1	0
15	E	1	Total C O P 36 27 8 1	0

- Molecule 16 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: $C_4H_9NO_2$)

(labeled as "Ligand of Interest" by depositor).

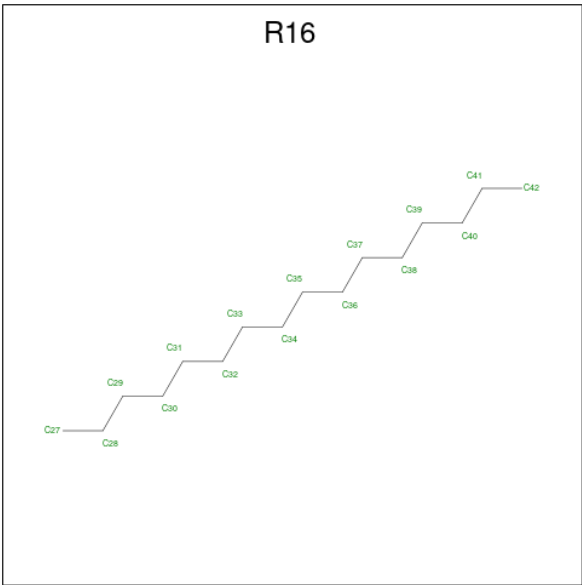


Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	N	O	0
			7	4	1	2	
16	E	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

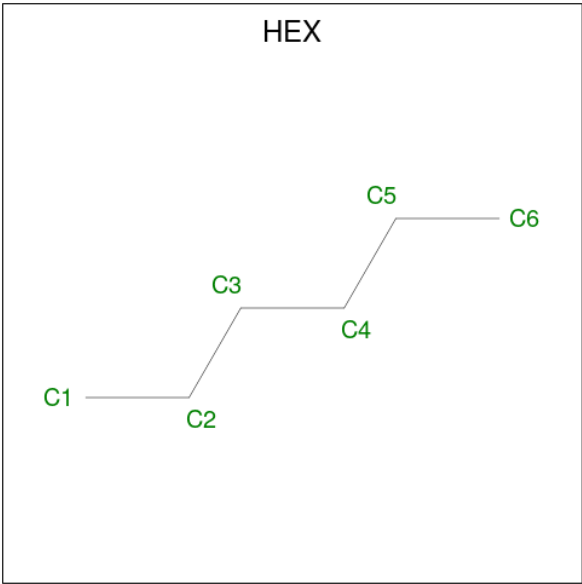
Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Cl	0
			1	1	
17	C	1	Total	Cl	0
			1	1	
17	D	1	Total	Cl	0
			1	1	
17	L	1	Total	Cl	0
			1	1	

- Molecule 18 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



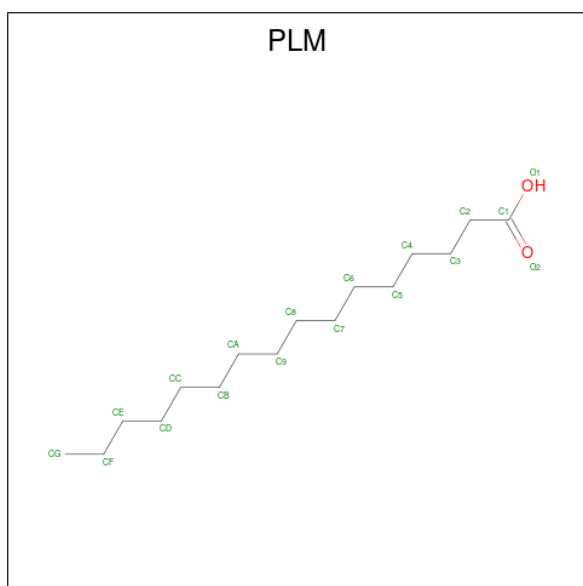
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	C	0
			16	16	
18	B	1	Total	C	0
			16	16	
18	E	1	Total	C	0
			16	16	
18	E	1	Total	C	0
			16	16	

- Molecule 19 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



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

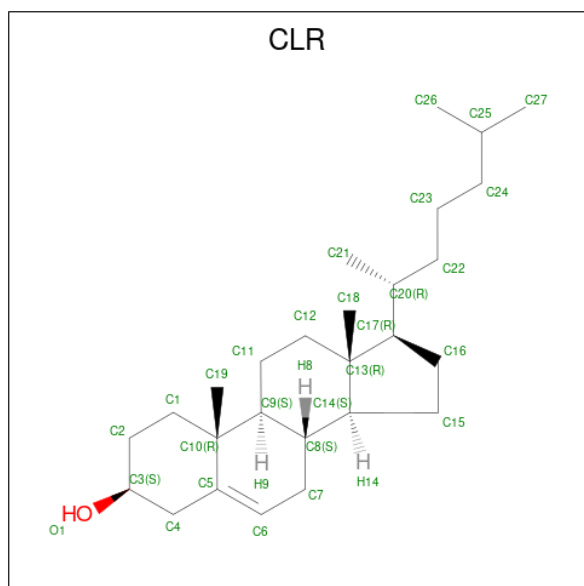
- Molecule 20 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
20	C	1	Total	C	O	0
			14	12	2	
20	C	1	Total	C	O	0
			18	16	2	
20	C	1	Total	C	O	0
			18	16	2	
20	C	1	Total	C	O	0
			18	16	2	
20	E	1	Total	C	O	0
			18	16	2	

- # OLC
-
- The chemical structure of OLC (Oleyl Linoleate) is shown. It consists of a long hydrocarbon chain with a double bond (C10=C11) and a terminal carboxylic acid group (C17=O18, O19). The chain is labeled with carbon atoms (C1 to C17) and oxygen atoms (O18, O19). The carboxylic acid group is shown in red, with the hydroxyl group (OH) and the carbonyl group (C=O) clearly visible.

- Molecule 22 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



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


- Molecule 23 is water.

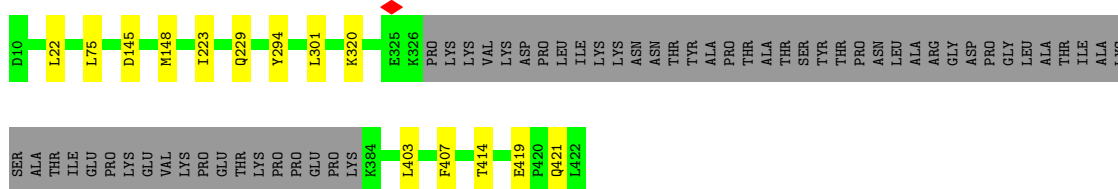
Mol	Chain	Residues	Atoms		AltConf
23	A	24	Total 24	O 24	0
23	B	21	Total 21	O 21	0
23	C	16	Total 16	O 16	0
23	D	13	Total 13	O 13	0
23	E	19	Total 19	O 19	0
23	L	1	Total 1	O 1	0
23	G	10	Total 10	O 10	0

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.

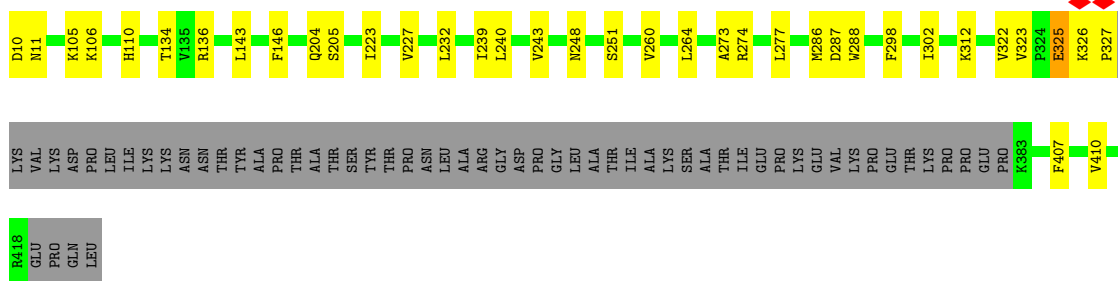
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain A: 



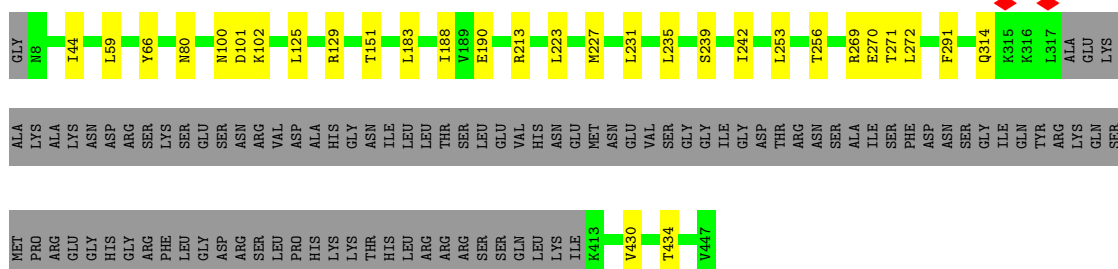
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

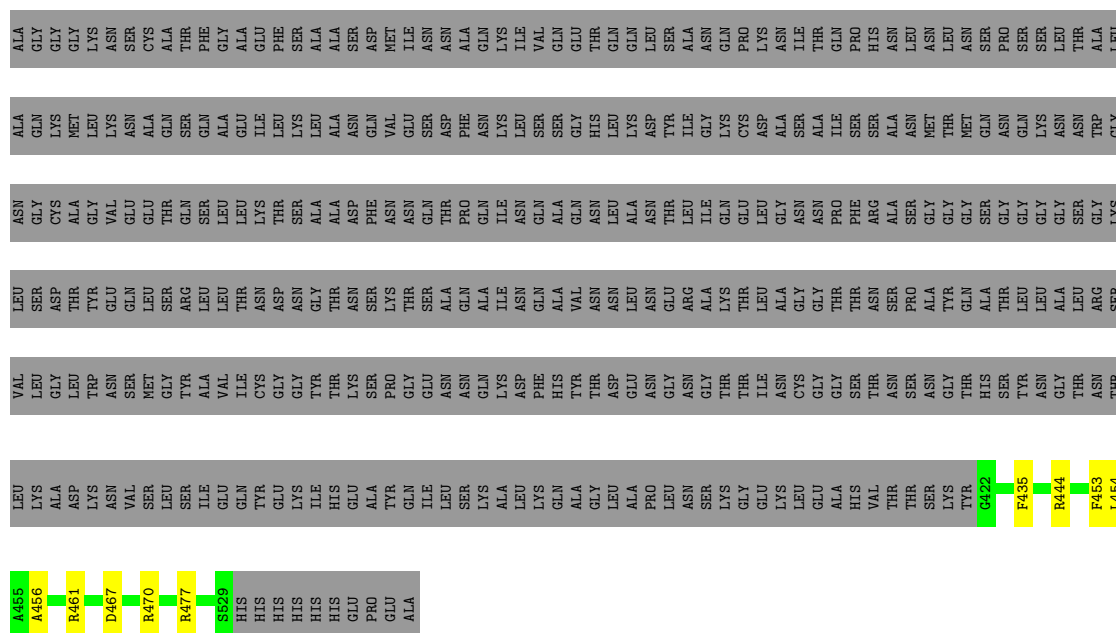
Chain D: 



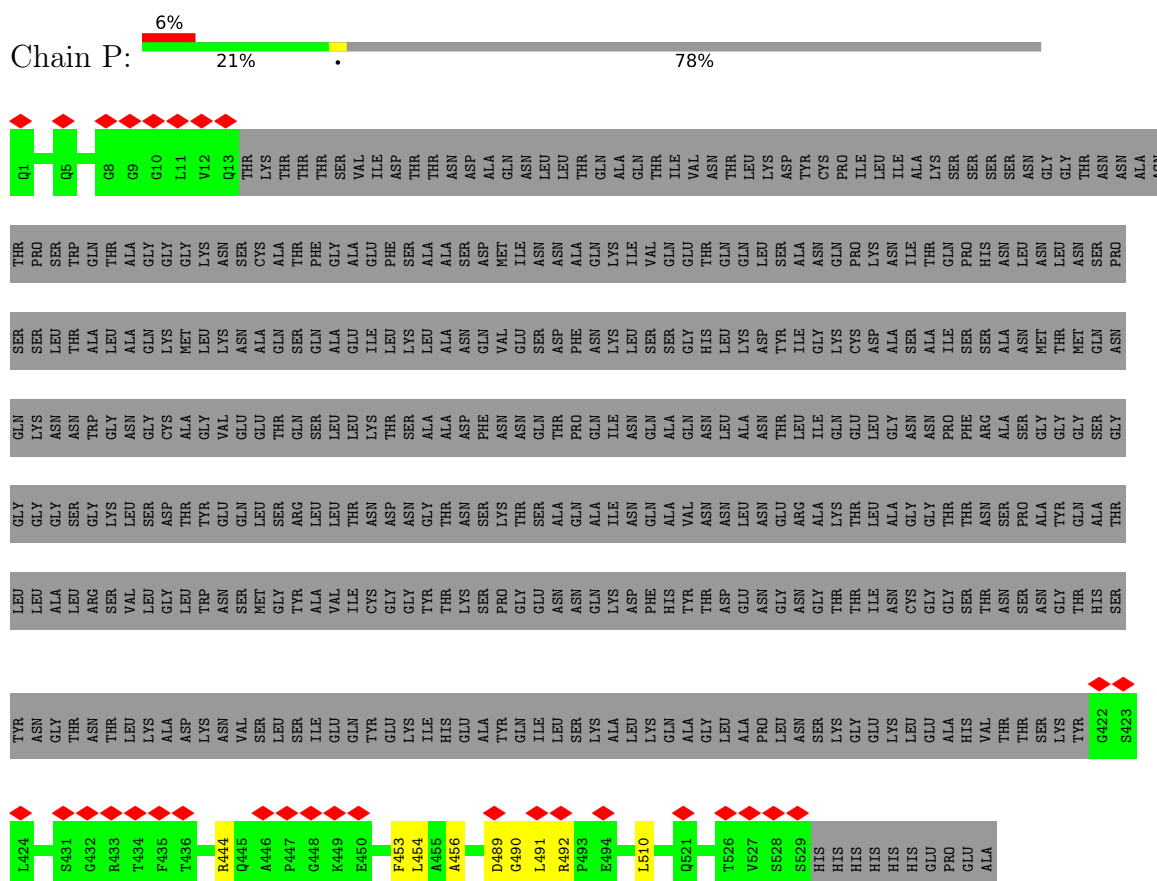
- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain B: 



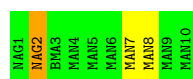


• Molecule 6: Megabody38



• 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:  70% 20% 10%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67% 33%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  33% 67% 33%



- Molecule 9: 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 J:  50% 50%



- Molecule 9: 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:  50% 50%




- 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)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

mido-2-deoxy-beta-D-glucopyranose

Chain M:  83% 17%

MAG1
MAG2
BNA3
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49871	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 ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	234.71912, 234.71912, 234.71912	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.79297, 0.79297, 0.79297	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.14	0/2986	0.33	0/4052
1	D	0.20	0/2937	0.37	0/3989
2	B	0.15	0/2921	0.35	0/3970
2	E	0.15	0/2974	0.34	0/4039
3	C	0.29	0/2976	0.51	3/4040 (0.1%)
4	H	0.17	0/260	0.35	0/352
5	L	0.16	0/1555	0.36	0/2112
6	G	0.15	0/972	0.35	0/1311
6	P	0.19	0/961	0.41	0/1297
All	All	0.19	0/18542	0.38	3/25162 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	372	GLY	N-CA-C	-6.47	106.75	115.36
3	C	304[A]	PHE	CA-C-O	5.92	126.83	120.55
3	C	304[B]	PHE	CA-C-O	5.92	126.83	120.55

There are no chirality outliers.

There are no planarity outliers.

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	2904	0	2909	15	0
1	D	2864	0	2858	28	0
2	B	2843	0	2850	27	0
2	E	2887	0	2907	19	0
3	C	2959	0	2977	39	0
4	H	256	0	256	2	0
5	L	1509	0	1504	13	0
6	G	949	0	907	6	0
6	P	941	0	894	5	0
7	F	116	0	97	3	0
8	I	39	0	34	4	0
8	O	39	0	34	1	0
9	J	72	0	61	0	0
9	N	72	0	61	0	0
10	K	28	0	25	6	0
11	M	72	0	61	0	0
12	A	47	0	44	0	0
12	D	47	0	44	2	0
13	A	102	0	152	0	0
13	D	102	0	152	1	0
13	E	32	0	34	0	0
13	L	102	0	152	9	0
14	A	40	0	88	0	0
14	B	20	0	44	0	0
14	C	10	0	22	0	0
14	D	20	0	44	0	0
14	E	20	0	44	0	0
14	L	10	0	22	0	0
15	A	36	0	52	5	0
15	B	36	0	52	0	0
15	C	36	0	52	0	0
15	D	36	0	52	5	0
15	E	36	0	52	1	0
16	A	7	0	0	0	0
16	E	7	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
17	L	1	0	0	4	0
18	B	32	0	68	0	0
18	E	32	0	68	0	0
19	B	18	0	42	0	0
19	D	12	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	E	12	0	28	0	0
20	C	68	0	113	0	0
20	E	18	0	31	0	0
21	C	21	0	29	0	0
22	C	28	0	46	4	0
23	A	24	0	0	0	0
23	B	21	0	0	0	0
23	C	16	0	0	1	0
23	D	13	0	0	0	0
23	E	19	0	0	1	0
23	G	10	0	0	2	0
23	L	1	0	0	0	0
All	All	19645	0	19990	146	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 4.

All (146) 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)
3:C:208:ASN:HD21	10:K:1:NAG:C1	0.92	1.54
3:C:208:ASN:ND2	10:K:1:NAG:C1	1.73	1.41
2:B:80:ASN:HD21	8:I:1:NAG:C1	1.43	1.31
2:B:80:ASN:ND2	8:I:1:NAG:C1	2.09	1.14
3:C:208:ASN:CG	10:K:1:NAG:C1	2.48	0.86
22:C:508:CLR:O1	17:L:304:CL:CL	2.36	0.80
2:B:80:ASN:CG	8:I:1:NAG:C1	2.54	0.80
1:A:301:LEU:HD23	2:E:235:LEU:HD11	1.65	0.79
15:D:3907:PX2:H13	15:D:3907:PX2:H21	1.69	0.75
5:L:140:VAL:HG12	5:L:144:MET:HE2	1.70	0.73
2:B:80:ASN:OD1	8:I:1:NAG:C1	2.41	0.69
5:L:80:SER:HA	17:L:304:CL:CL	2.31	0.68
2:B:235:LEU:HD11	3:C:273:VAL:HG11	1.75	0.66
1:A:229:GLN:NE2	2:B:270:GLU:OE2	2.30	0.65
2:E:48:ASP:OD2	23:E:601:HOH:O	2.15	0.65
1:D:204:GLN:NE2	1:D:205:SER:O	2.31	0.64
5:L:148:ASP:OD1	5:L:165:LYS:NZ	2.31	0.64
10:K:2:NAG:O7	10:K:2:NAG:O4	2.08	0.63
3:C:271:THR:CG2	1:D:264:LEU:HD11	2.28	0.63
1:A:229:GLN:OE1	2:B:269:ARG:NH1	2.32	0.63
1:A:407:PHE:HB2	15:A:3906:PX2:H26	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:81:PHE:N	17:L:304:CL:CL	2.69	0.62
5:L:83:ASP:HA	13:L:301:PGW:O04	2.00	0.62
3:C:304[A]:PHE:CD2	13:L:301:PGW:H12	2.35	0.62
3:C:208:ASN:ND2	10:K:1:NAG:C2	2.62	0.61
6:G:461[B]:ARG:NH2	23:G:602:HOH:O	2.33	0.61
13:L:303:PGW:O12	13:L:303:PGW:OAE	2.17	0.61
22:C:508:CLR:H162	13:L:301:PGW:H28	1.82	0.60
1:D:312:LYS:NZ	12:D:3901:PIO:O4	2.33	0.60
2:B:190:GLU:OE1	2:B:213:ARG:NH1	2.35	0.60
3:C:123:TRP:CD1	7:F:7:MAN:HO2	2.20	0.59
1:A:294:TYR:CE2	2:E:231:LEU:HD13	2.38	0.59
3:C:211:GLU:HG2	23:C:608:HOH:O	2.02	0.59
1:D:326:LYS:O	1:D:327:PRO:C	2.46	0.57
1:D:143:LEU:HD13	1:D:277:LEU:HD22	1.87	0.56
2:B:291:PHE:HE1	2:B:434:THR:HG23	1.71	0.56
5:L:80:SER:CA	17:L:304:CL:CL	2.91	0.56
1:D:325:GLU:HG3	1:D:327:PRO:HG2	1.88	0.55
2:E:44:ILE:HG21	2:E:181:ILE:HD11	1.88	0.55
3:C:63:GLY:N	3:C:73:THR:O	2.38	0.55
1:D:274:ARG:NH1	1:D:287:ASP:OD2	2.39	0.55
6:P:444:ARG:HB2	6:P:454:LEU:HD11	1.89	0.55
2:B:227:MET:O	2:B:231:LEU:HG	2.07	0.54
3:C:123:TRP:HB3	7:F:8:MAN:H62	1.89	0.54
3:C:236:PHE:HB3	3:C:296:MET:HE1	1.89	0.54
13:D:3903[A]:PGW:O12	13:D:3903[A]:PGW:OAE	2.19	0.54
22:C:508:CLR:C15	13:L:301:PGW:H17	2.37	0.54
3:C:380:P1L:SG	3:C:381:P1L:N	2.80	0.54
2:B:235:LEU:HD21	3:C:308:PHE:CD1	2.43	0.53
2:E:155:GLU:OE1	2:E:207:ARG:NE	2.40	0.53
1:D:248:ASN:OD1	1:D:251:SER:OG	2.21	0.53
1:D:298:PHE:CE2	1:D:302:ILE:HD11	2.44	0.53
2:B:223:LEU:HG	13:L:301:PGW:H3	1.91	0.52
2:E:47:ILE:HD12	2:E:181:ILE:HD13	1.92	0.52
3:C:161:ASP:OD2	3:C:163:HIS:NE2	2.43	0.52
2:B:430:VAL:O	2:B:434:THR:HG22	2.10	0.51
1:A:301:LEU:CD2	2:E:235:LEU:HD11	2.39	0.51
3:C:208:ASN:OD1	10:K:1:NAG:C1	2.59	0.51
2:E:44:ILE:CG2	2:E:181:ILE:HD11	2.41	0.50
2:E:66[A]:TYR:CZ	2:E:125:LEU:HD13	2.45	0.50
2:E:79:LEU:HA	8:O:1:NAG:H82	1.93	0.49
2:E:66[A]:TYR:CE1	2:E:125:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ASP:OD1	2:B:102:LYS:N	2.46	0.49
2:E:101:ASP:OD1	2:E:102:LYS:N	2.46	0.49
6:G:467:ASP:OD1	6:G:470:ARG:NH1	2.44	0.49
15:D:3907:PX2:H37	15:D:3907:PX2:H12	1.95	0.48
2:B:256:THR:HG23	3:C:274:LEU:HD11	1.94	0.48
6:G:435:PHE:O	6:G:477:ARG:NH2	2.47	0.48
2:B:66[A]:TYR:CZ	2:B:125:LEU:HD13	2.49	0.47
2:E:50:VAL:HG12	2:E:138:MET:HE1	1.95	0.47
5:L:29:PHE:HB2	5:L:190:LEU:HD21	1.96	0.47
12:D:3901:PIO:O41	12:D:3901:PIO:O3	2.31	0.47
1:A:414:THR:HG21	15:A:3906:PX2:H7	1.97	0.47
3:C:157:ASN:O	3:C:160:MET:N	2.47	0.47
1:D:239:ILE:O	1:D:243:VAL:HG23	2.13	0.47
1:D:240:LEU:HD11	2:E:296:LEU:HD23	1.97	0.47
3:C:383:GLU:O	3:C:385:P1L:N	2.48	0.46
6:P:491:LEU:O	6:P:492:ARG:NE	2.42	0.46
3:C:423:VAL:HG12	3:C:428:LEU:HD13	1.95	0.46
4:H:697:LEU:HD11	5:L:193:LEU:CD1	2.45	0.46
3:C:240:THR:HB	3:C:296:MET:HE2	1.96	0.46
1:D:326:LYS:N	1:D:327:PRO:HD2	2.30	0.46
1:D:105:LYS:N	1:D:136:ARG:O	2.48	0.46
1:A:403:LEU:HB3	15:A:3906:PX2:H28	1.97	0.46
2:B:235:LEU:CD1	3:C:273:VAL:HG11	2.42	0.46
3:C:380:P1L:H9C2	3:C:381:P1L:H102	1.98	0.46
1:D:110:HIS:NE2	1:D:134:THR:OG1	2.43	0.46
1:A:407:PHE:HD1	15:A:3906:PX2:H15	1.81	0.46
3:C:62:ILE:HD12	3:C:196:TRP:CZ3	2.50	0.46
1:A:148:MET:HG3	1:A:223:ILE:HD12	1.97	0.45
1:D:326:LYS:HB2	1:D:326:LYS:HE2	1.67	0.45
2:B:44:ILE:HD12	2:B:59:LEU:HD11	1.97	0.45
3:C:271:THR:HG23	1:D:264:LEU:HD11	1.97	0.45
1:D:223:ILE:HG12	1:D:227:VAL:HG23	1.99	0.45
1:D:227:VAL:O	1:D:232:LEU:HD23	2.17	0.45
1:D:243:VAL:HG22	15:E:501:PX2:H46	1.99	0.45
2:E:178:VAL:HA	2:E:181:ILE:HD12	1.98	0.45
3:C:370:LEU:HD12	3:C:371:ASP:N	2.32	0.44
3:C:373:LYS:HA	3:C:373:LYS:HD3	1.41	0.44
5:L:117:PHE:O	13:L:303:PGW:OAE	2.29	0.44
3:C:106:ILE:HD11	3:C:131:LEU:HD11	2.00	0.44
2:E:28:ARG:NH1	2:E:30:ASP:O	2.51	0.44
7:F:2:NAG:O3	7:F:7:MAN:H5	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ASN:ND2	2:B:151:THR:O	2.50	0.43
3:C:98:LEU:HD13	3:C:102:MET:SD	2.59	0.43
2:E:44:ILE:HD12	2:E:59:LEU:HD11	2.00	0.43
6:G:444:ARG:HB2	6:G:454:LEU:HD11	2.00	0.43
6:P:453:PHE:HE1	6:P:456:ALA:HB2	1.84	0.43
6:P:510:LEU:O	6:P:510:LEU:HD23	2.19	0.43
2:B:129:ARG:NH2	3:C:116:SER:O	2.51	0.43
1:D:146:PHE:CE1	1:D:277:LEU:HD21	2.54	0.42
1:D:273:ALA:HB1	1:D:286:MET:HE3	2.01	0.42
2:B:291:PHE:CE1	2:B:434:THR:HG23	2.52	0.42
6:G:1:GLN:NE2	6:G:2:VAL:O	2.52	0.42
3:C:271:THR:HG21	1:D:260:VAL:CG1	2.49	0.42
1:D:410:VAL:CG1	15:D:3907:PX2:H35	2.49	0.42
5:L:73:ARG:O	5:L:75:LEU:HD22	2.19	0.42
1:A:145:ASP:O	1:A:148:MET:N	2.53	0.42
2:B:256:THR:HG21	3:C:270:ILE:HG13	2.01	0.42
1:A:407:PHE:HA	15:A:3906:PX2:H21	2.01	0.42
1:D:322:VAL:O	1:D:323:VAL:C	2.62	0.42
1:D:407:PHE:HA	15:D:3907:PX2:H40	2.02	0.42
4:H:697:LEU:HD11	5:L:193:LEU:HD12	2.01	0.42
5:L:136:ALA:O	5:L:140:VAL:HG23	2.20	0.42
1:D:10:ASP:OD1	1:D:11:ASN:N	2.49	0.41
2:B:271:THR:HG23	2:B:272:LEU:HD22	2.01	0.41
1:A:419:GLU:O	1:A:421:GLN:NE2	2.52	0.41
1:A:22:LEU:HD22	1:A:75:LEU:HA	2.02	0.41
3:C:301:SER:OG	13:L:301:PGW:H13A	2.21	0.41
2:E:84:ASP:O	2:E:87:VAL:HG12	2.21	0.41
2:B:239:SER:HA	2:B:242:ILE:HD12	2.03	0.41
3:C:428:LEU:HB3	5:L:42:ILE:HG21	2.03	0.41
3:C:277:THR:HA	3:C:304[A]:PHE:HZ	1.86	0.41
1:A:320:LYS:O	2:B:314:GLN:NE2	2.54	0.40
22:C:508:CLR:H152	13:L:301:PGW:H17	2.02	0.40
6:G:453:PHE:HE1	6:G:456:ALA:HB2	1.86	0.40
6:P:489:ASP:OD1	6:P:490:GLY:N	2.55	0.40
2:B:183:LEU:HD12	2:B:188:ILE:HD11	2.03	0.40
2:B:239:SER:HB3	2:B:253:LEU:HD23	2.03	0.40
3:C:34:LEU:HD22	3:C:87:LEU:HA	2.03	0.40
3:C:34:LEU:HD21	3:C:89:PHE:HB3	2.03	0.40
3:C:247:ILE:HD11	3:C:275:THR:HG21	2.03	0.40
1:D:288:TRP:HB3	15:D:3907:PX2:C3	2.51	0.40
3:C:120:ASP:OD2	1:D:106:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:ASN:ND2	2:E:151:THR:O	2.49	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	355/413 (86%)	351 (99%)	4 (1%)	0	100	100
1	D	350/413 (85%)	342 (98%)	8 (2%)	0	100	100
2	B	342/441 (78%)	336 (98%)	6 (2%)	0	100	100
2	E	348/441 (79%)	341 (98%)	7 (2%)	0	100	100
3	C	347/405 (86%)	339 (98%)	7 (2%)	1 (0%)	37	59
4	H	31/33 (94%)	31 (100%)	0	0	100	100
5	L	192/193 (100%)	186 (97%)	6 (3%)	0	100	100
6	G	118/539 (22%)	113 (96%)	5 (4%)	0	100	100
6	P	117/539 (22%)	113 (97%)	4 (3%)	0	100	100
All	All	2200/3417 (64%)	2152 (98%)	47 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	384	ASP

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	321/367 (88%)	321 (100%)	0	100	100
1	D	316/367 (86%)	315 (100%)	1 (0%)	91	97
2	B	312/393 (79%)	312 (100%)	0	100	100
2	E	317/393 (81%)	317 (100%)	0	100	100
3	C	323/366 (88%)	317 (98%)	6 (2%)	52	75
4	H	27/27 (100%)	27 (100%)	0	100	100
5	L	160/159 (101%)	160 (100%)	0	100	100
6	G	95/435 (22%)	95 (100%)	0	100	100
6	P	94/435 (22%)	94 (100%)	0	100	100
All	All	1965/2942 (67%)	1958 (100%)	7 (0%)	90	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	304[A]	PHE
3	C	304[B]	PHE
3	C	369	CYS
3	C	370	LEU
3	C	373	LYS
3	C	377	SER
1	D	325	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	68	GLN
1	A	189	ASN
2	B	90	GLN
2	B	312	GLN
3	C	208	ASN
1	D	189	ASN
2	E	185	GLN
2	E	421	ASN
4	H	690	ASN
5	L	186	ASN

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Mol	Chain	Res	Type
6	G	3	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	1.08	1 (4%)	18,23,25	1.38	3 (16%)
3	P1L	C	381	3	21,22,23	0.64	0	18,23,25	1.55	3 (16%)
3	P1L	C	380	3	21,22,23	0.37	0	18,23,25	2.76	1 (5%)

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	-	9/20/22/24	-
3	P1L	C	381	3	-	5/20/22/24	-
3	P1L	C	380	3	-	9/20/22/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	385	P1L	O-C	4.13	1.36	1.19

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	380	P1L	CB-SG-C7	11.71	117.21	100.84
3	C	381	P1L	C8-C7-SG	-4.26	108.50	113.46
3	C	381	P1L	CB-SG-C7	3.84	106.21	100.84
3	C	385	P1L	C8-C7-SG	-3.74	109.11	113.46
3	C	385	P1L	CB-SG-C7	3.49	105.73	100.84
3	C	381	P1L	O7-C7-SG	2.44	125.78	122.61
3	C	385	P1L	O7-C7-SG	2.03	125.26	122.61

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	385	P1L	1	0
3	C	381	P1L	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	380	P1L	2	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	7,1	14,14,15	0.42	0	17,19,21	0.54	0
7	MAN	F	10	7	11,11,12	0.34	0	15,15,17	0.56	0
7	NAG	F	2	7	14,14,15	0.38	0	17,19,21	0.87	1 (5%)
7	BMA	F	3	7	11,11,12	0.57	0	15,15,17	0.73	0
7	MAN	F	4	7	11,11,12	0.30	0	15,15,17	0.53	0
7	MAN	F	5	7	11,11,12	0.46	0	15,15,17	0.47	0
7	MAN	F	6	7	11,11,12	0.37	0	15,15,17	0.58	0
7	MAN	F	7	7	11,11,12	0.70	0	15,15,17	0.85	0
7	MAN	F	8	7	11,11,12	0.36	0	15,15,17	0.56	0
7	MAN	F	9	7	11,11,12	0.38	0	15,15,17	0.49	0
8	NAG	I	1	8	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	I	2	8	14,14,15	0.21	0	17,19,21	0.61	0
8	BMA	I	3	8	11,11,12	0.57	0	15,15,17	0.75	0
9	NAG	J	1	2,9	14,14,15	0.31	0	17,19,21	0.37	0
9	NAG	J	2	9	14,14,15	0.21	0	17,19,21	0.42	0
9	BMA	J	3	9	11,11,12	0.59	0	15,15,17	0.78	0
9	MAN	J	4	9	11,11,12	0.68	0	15,15,17	1.22	2 (13%)
9	MAN	J	5	9	11,11,12	1.03	1 (9%)	15,15,17	1.30	2 (13%)
9	MAN	J	6	9	11,11,12	0.69	0	15,15,17	1.05	2 (13%)
10	NAG	K	1	10	14,14,15	0.17	0	17,19,21	0.81	1 (5%)
10	NAG	K	2	10	14,14,15	0.68	1 (7%)	17,19,21	0.53	0
11	NAG	M	1	11,1	14,14,15	0.38	0	17,19,21	0.60	0
11	NAG	M	2	11	14,14,15	0.41	0	17,19,21	0.56	0
11	BMA	M	3	11	11,11,12	0.33	0	15,15,17	0.68	0
11	MAN	M	4	11	11,11,12	0.37	0	15,15,17	0.58	0
11	MAN	M	5	11	11,11,12	0.26	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	M	6	11	11,11,12	0.30	0	15,15,17	0.94	1 (6%)
9	NAG	N	1	2,9	14,14,15	0.40	0	17,19,21	0.42	0
9	NAG	N	2	9	14,14,15	0.31	0	17,19,21	0.41	0
9	BMA	N	3	9	11,11,12	0.58	0	15,15,17	0.82	0
9	MAN	N	4	9	11,11,12	0.67	0	15,15,17	1.10	2 (13%)
9	MAN	N	5	9	11,11,12	0.72	0	15,15,17	1.36	3 (20%)
9	MAN	N	6	9	11,11,12	0.70	0	15,15,17	1.05	2 (13%)
8	NAG	O	1	2,8	14,14,15	0.39	0	17,19,21	0.68	0
8	NAG	O	2	8	14,14,15	0.39	0	17,19,21	0.67	0
8	BMA	O	3	8	11,11,12	0.30	0	15,15,17	0.65	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	7,1	-	0/6/23/26	0/1/1/1
7	MAN	F	10	7	-	0/2/19/22	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	-	0/2/19/22	0/1/1/1
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	-	0/2/19/22	0/1/1/1
7	MAN	F	9	7	-	0/2/19/22	0/1/1/1
8	NAG	I	1	8	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	2/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
9	NAG	J	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	J	2	9	-	1/6/23/26	0/1/1/1
9	BMA	J	3	9	-	0/2/19/22	0/1/1/1
9	MAN	J	4	9	-	0/2/19/22	1/1/1/1
9	MAN	J	5	9	-	0/2/19/22	0/1/1/1
9	MAN	J	6	9	-	0/2/19/22	0/1/1/1
10	NAG	K	1	10	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	3/6/23/26	0/1/1/1
11	NAG	M	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	M	2	11	-	2/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	5	MAN	O5-C1	-2.52	1.39	1.43
10	K	2	NAG	O5-C1	-2.41	1.39	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	4	MAN	C1-O5-C5	3.28	116.64	112.19
9	J	5	MAN	C1-O5-C5	3.27	116.63	112.19
9	N	5	MAN	C1-O5-C5	3.15	116.46	112.19
7	F	2	NAG	C2-N2-C7	2.70	126.74	122.90
11	M	6	MAN	C1-O5-C5	2.59	115.70	112.19
10	K	1	NAG	C2-N2-C7	2.52	126.48	122.90
9	N	5	MAN	O5-C1-C2	2.51	114.64	110.77
9	N	6	MAN	C1-O5-C5	2.37	115.40	112.19
9	N	5	MAN	O2-C2-C3	-2.36	105.40	110.14
9	N	4	MAN	C1-O5-C5	2.34	115.37	112.19
9	J	6	MAN	C1-O5-C5	2.29	115.29	112.19
9	J	5	MAN	O2-C2-C3	-2.27	105.60	110.14
9	J	6	MAN	O2-C2-C3	-2.24	105.66	110.14
9	N	6	MAN	O2-C2-C3	-2.22	105.69	110.14
9	J	4	MAN	O2-C2-C3	-2.20	105.74	110.14
9	N	4	MAN	O2-C2-C3	-2.18	105.77	110.14

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

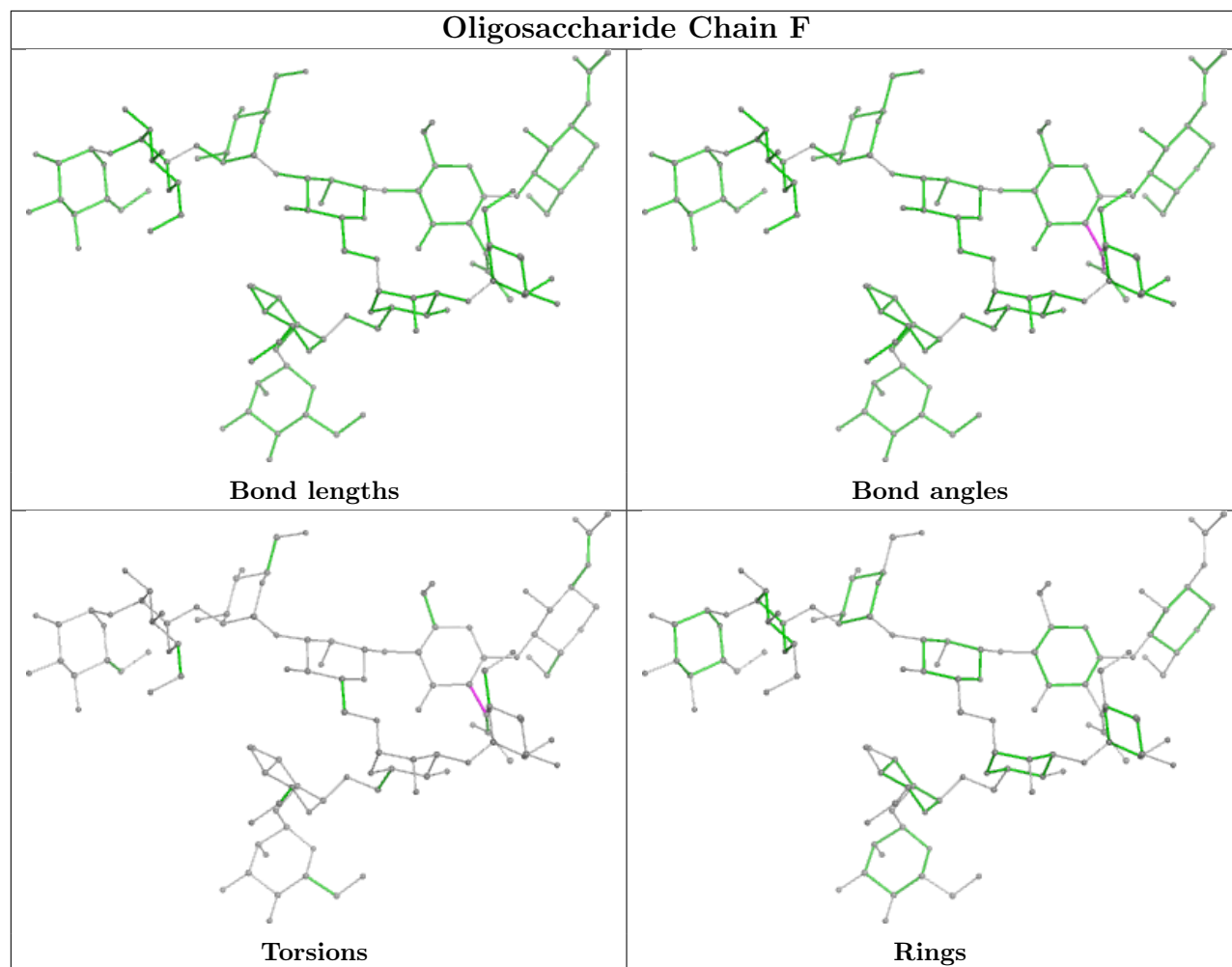
All (1) ring outliers are listed below:

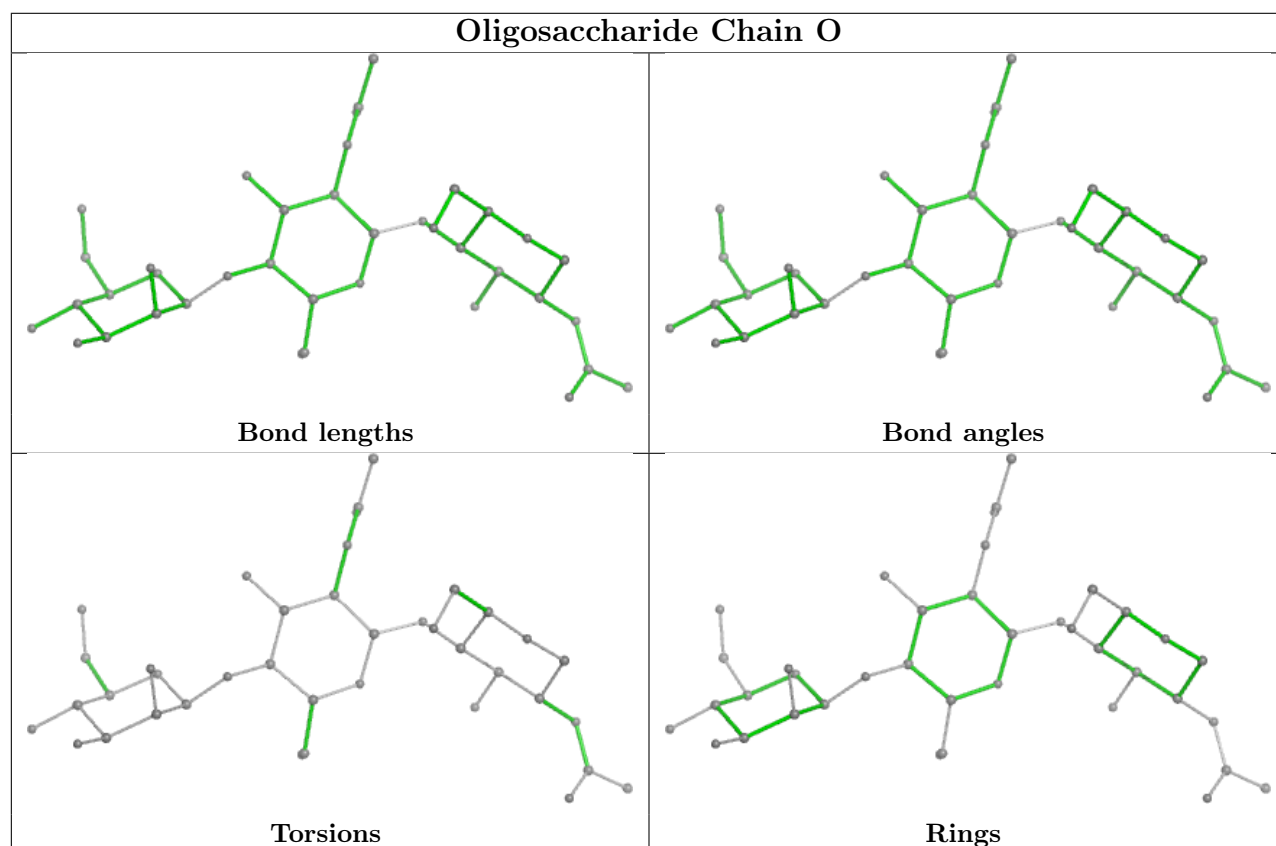
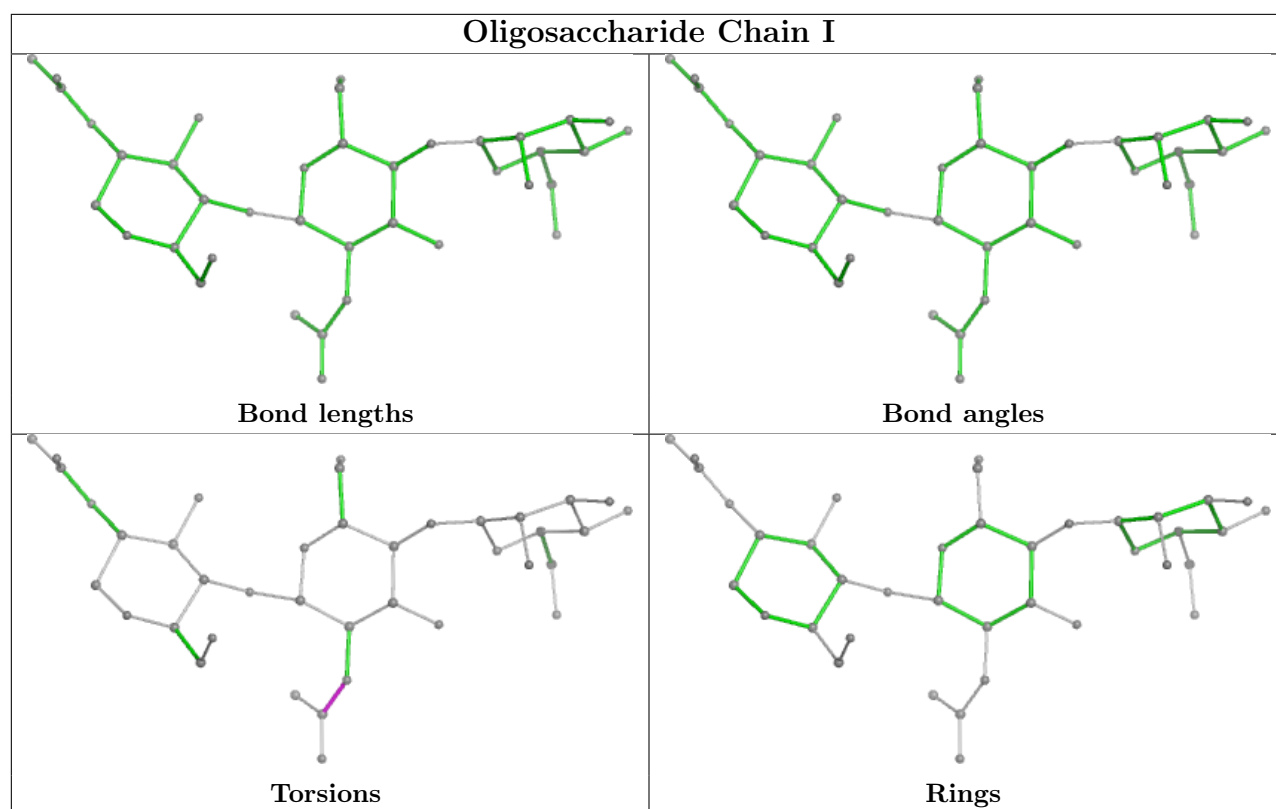
Mol	Chain	Res	Type	Atoms
9	J	4	MAN	C1-C2-C3-C4-C5-O5

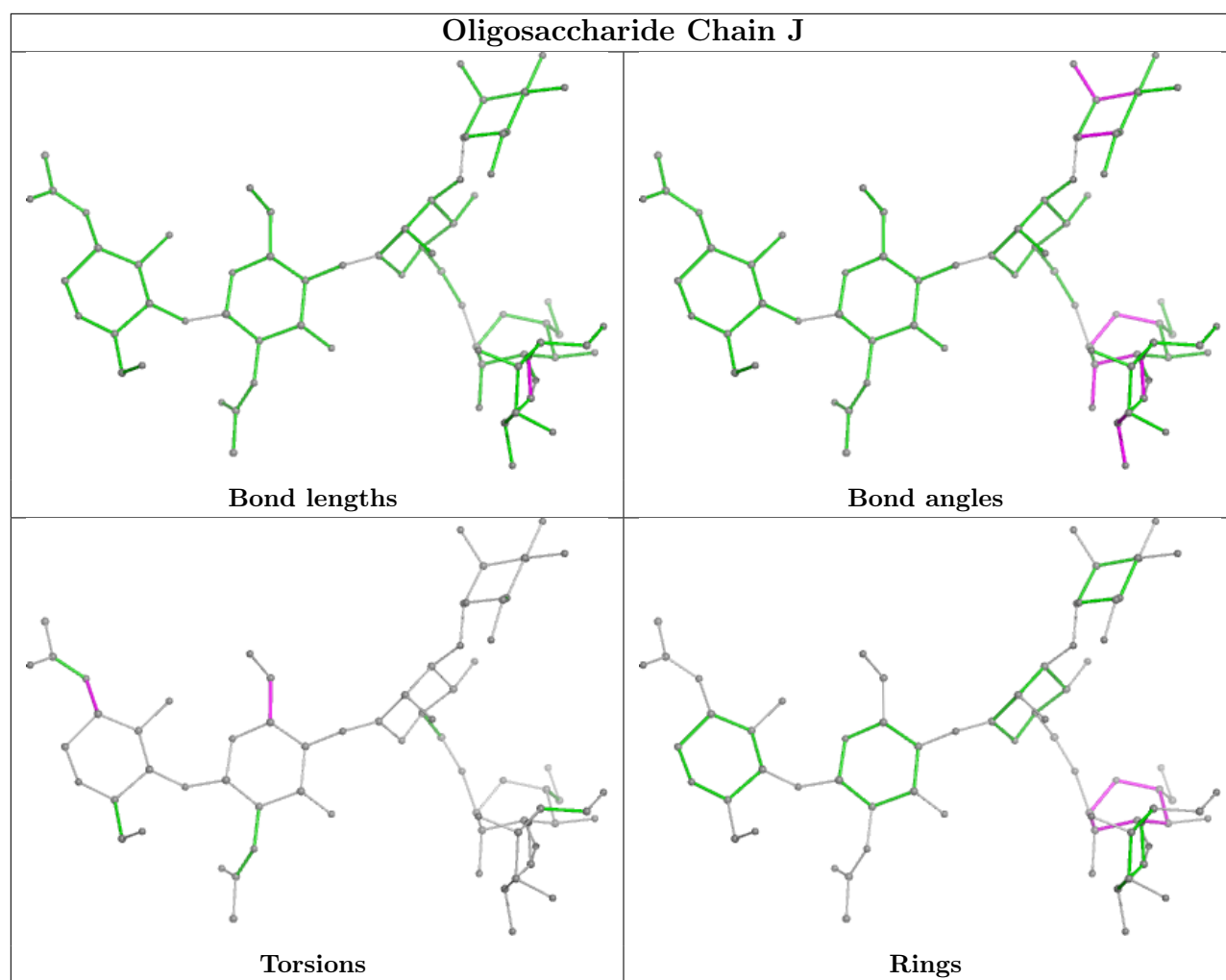
7 monomers are involved in 14 short contacts:

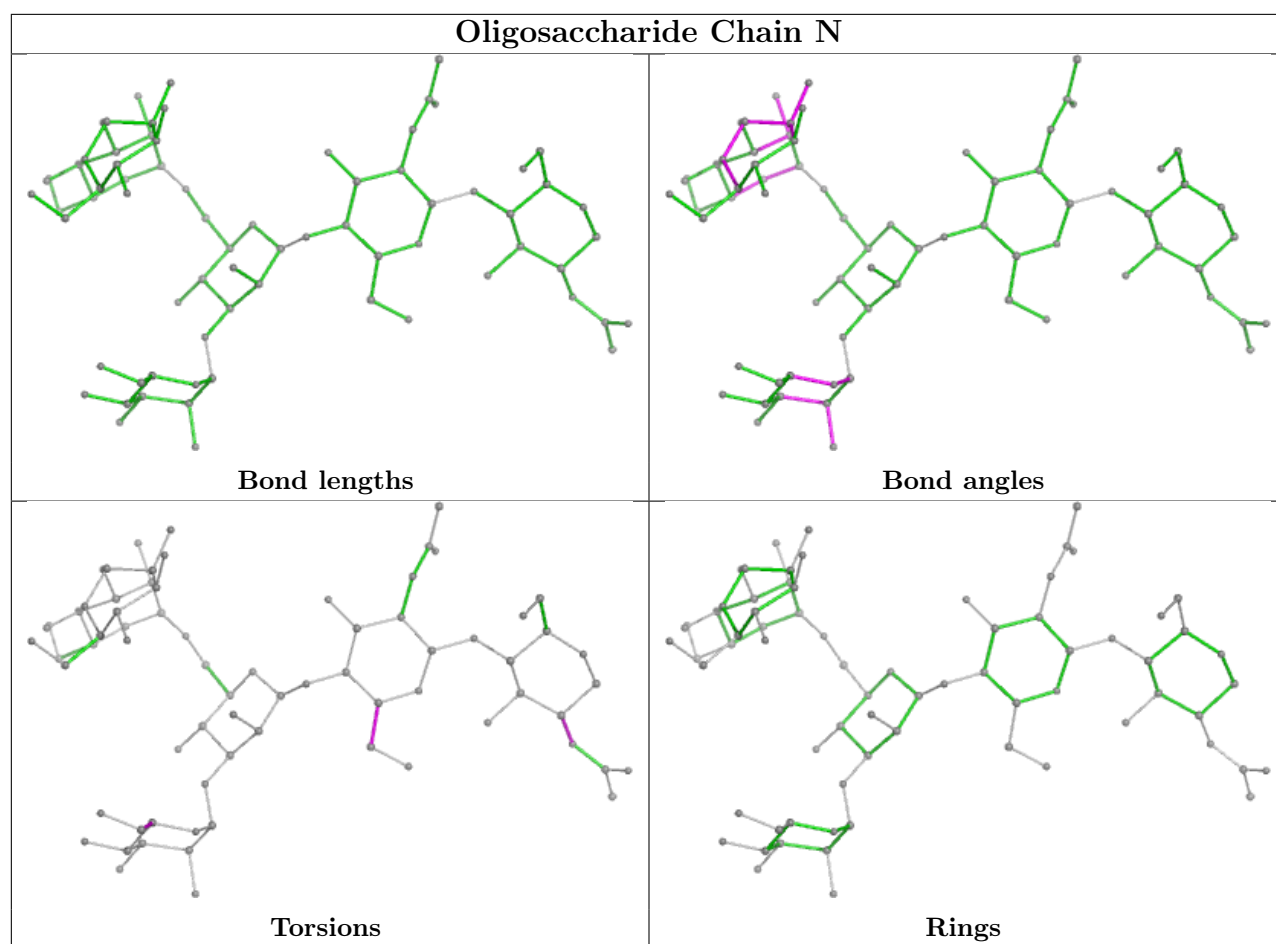
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	8	MAN	1	0
8	I	1	NAG	4	0
10	K	2	NAG	1	0
7	F	7	MAN	2	0
7	F	2	NAG	1	0
8	O	1	NAG	1	0
10	K	1	NAG	5	0

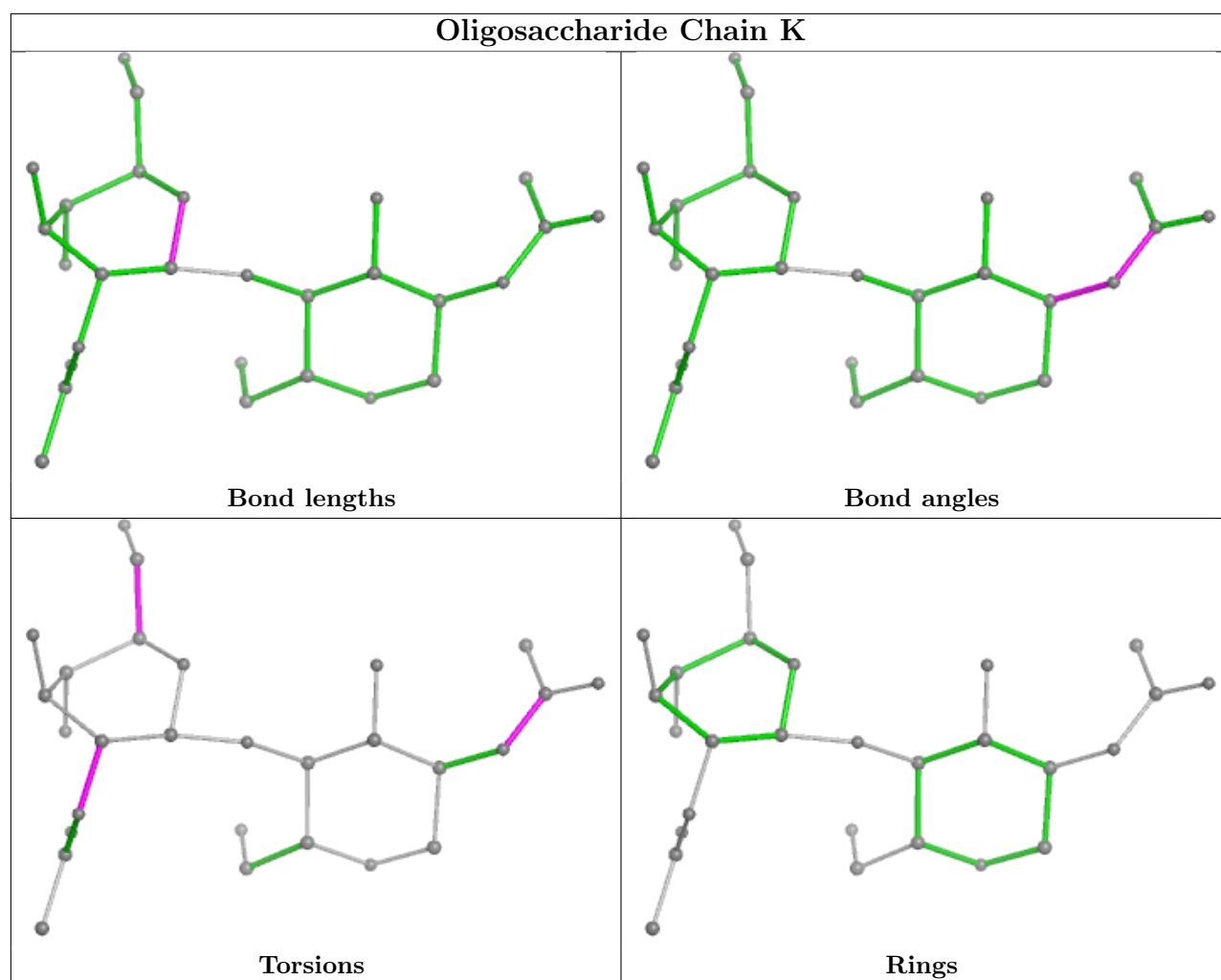
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

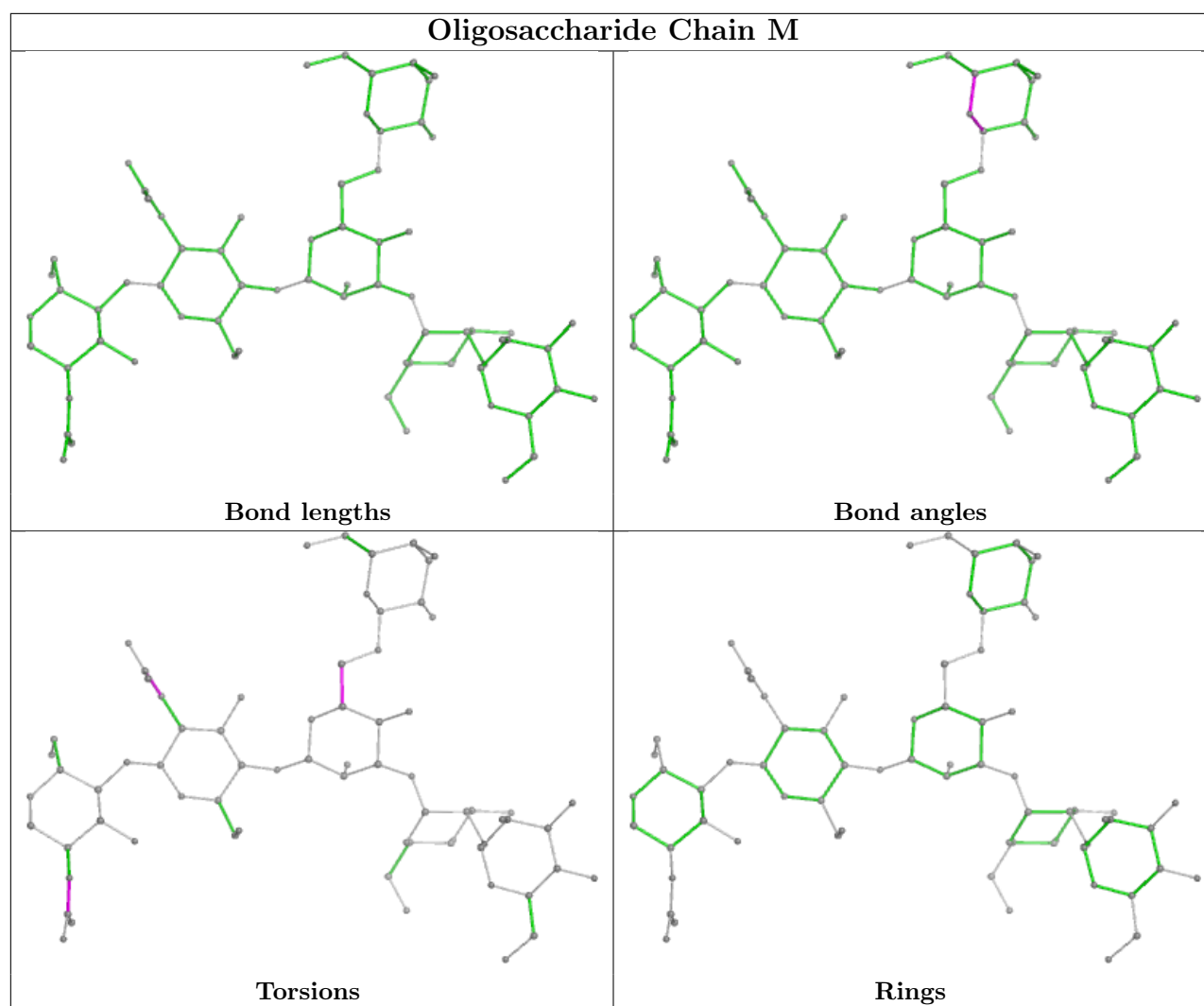












5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 4 are monoatomic - leaving 46 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	PLM	E	506	-	17,17,17	0.60	0	17,17,17	1.01	0
20	PLM	C	506	-	17,17,17	0.60	0	17,17,17	0.95	0
13	PGW	L	303	-	50,50,50	0.96	2 (4%)	53,56,56	1.04	2 (3%)
18	R16	B	506	-	15,15,15	0.35	0	14,14,14	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PX2	A	3906	-	35,35,35	0.31	0	39,40,40	0.34	0
20	PLM	C	507	-	17,17,17	0.57	0	17,17,17	1.10	0
20	PLM	C	505	-	17,17,17	0.60	0	17,17,17	1.07	0
14	D10	B	508	-	9,9,9	0.30	0	8,8,8	0.74	0
13	PGW	E	504	-	31,31,50	1.16	2 (6%)	34,37,56	1.08	2 (5%)
18	R16	E	507	-	15,15,15	0.32	0	14,14,14	0.69	0
12	PIO	D	3901	-	47,47,47	1.17	6 (12%)	61,65,65	1.09	4 (6%)
19	HEX	D	3902	-	5,5,5	0.31	0	4,4,4	0.54	0
19	HEX	B	505	-	5,5,5	0.31	0	4,4,4	0.55	0
14	D10	A	3908	-	9,9,9	0.30	0	8,8,8	0.71	0
12	PIO	A	3901	-	47,47,47	1.18	5 (10%)	61,65,65	1.08	3 (4%)
15	PX2	C	502	-	35,35,35	1.02	3 (8%)	39,40,40	1.21	2 (5%)
20	PLM	C	501	-	13,13,17	0.65	0	13,13,17	1.01	1 (7%)
13	PGW	L	301	-	50,50,50	0.31	0	53,56,56	0.31	0
14	D10	E	503	-	9,9,9	0.32	0	8,8,8	0.69	0
14	D10	L	302	-	9,9,9	0.31	0	8,8,8	0.71	0
18	R16	B	502	-	15,15,15	0.30	0	14,14,14	0.81	0
14	D10	A	3903	-	9,9,9	0.33	0	8,8,8	0.64	0
19	HEX	E	509	-	5,5,5	0.31	0	4,4,4	0.56	0
21	OLC	C	504	-	20,20,24	1.12	1 (5%)	21,21,25	1.13	2 (9%)
15	PX2	D	3907	-	35,35,35	0.32	0	39,40,40	0.32	0
16	ABU	A	3907	-	6,6,6	0.89	0	6,6,6	1.34	0
13	PGW	A	3902[B]	-	50,50,50	0.97	2 (4%)	53,56,56	1.01	2 (3%)
14	D10	A	3905	-	9,9,9	0.31	0	8,8,8	0.65	0
15	PX2	B	501	-	35,35,35	1.03	4 (11%)	39,40,40	1.13	2 (5%)
13	PGW	D	3903[B]	-	50,50,50	0.98	2 (4%)	53,56,56	0.96	2 (3%)
14	D10	D	3906	-	9,9,9	0.30	0	8,8,8	0.77	0
14	D10	C	503	-	9,9,9	0.29	0	8,8,8	0.76	0
13	PGW	A	3902[A]	-	50,50,50	0.96	2 (4%)	53,56,56	0.95	2 (3%)
19	HEX	D	3904	-	5,5,5	0.33	0	4,4,4	0.47	0
18	R16	E	502	-	15,15,15	0.30	0	14,14,14	0.82	0
16	ABU	E	510	-	6,6,6	0.87	0	6,6,6	1.40	1 (16%)
15	PX2	E	501	-	35,35,35	1.01	3 (8%)	39,40,40	1.09	2 (5%)
19	HEX	B	504	-	5,5,5	0.34	0	4,4,4	0.46	0
13	PGW	D	3903[A]	-	50,50,50	0.96	2 (4%)	53,56,56	0.95	2 (3%)
19	HEX	E	505	-	5,5,5	0.31	0	4,4,4	0.56	0
22	CLR	C	508	-	31,31,31	0.16	0	48,48,48	0.33	0
14	D10	D	3905	-	9,9,9	0.33	0	8,8,8	0.60	0
14	D10	E	508	-	9,9,9	0.29	0	8,8,8	0.78	0
14	D10	A	3904	-	9,9,9	0.31	0	8,8,8	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	HEX	B	507	-	5,5,5	0.31	0	4,4,4	0.57	0
14	D10	B	503	-	9,9,9	0.31	0	8,8,8	0.73	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	PLM	E	506	-	-	5/15/15/15	-
20	PLM	C	506	-	-	4/15/15/15	-
13	PGW	L	303	-	-	23/55/55/55	-
18	R16	B	506	-	-	4/13/13/13	-
15	PX2	A	3906	-	-	7/37/37/37	-
20	PLM	C	507	-	-	5/15/15/15	-
20	PLM	C	505	-	-	2/15/15/15	-
14	D10	B	508	-	-	1/7/7/7	-
13	PGW	E	504	-	-	16/36/36/55	-
18	R16	E	507	-	-	4/13/13/13	-
12	PIO	D	3901	-	-	17/44/68/68	0/1/1/1
19	HEX	D	3902	-	-	0/3/3/3	-
19	HEX	B	505	-	-	0/3/3/3	-
14	D10	A	3908	-	-	1/7/7/7	-
12	PIO	A	3901	-	-	13/44/68/68	0/1/1/1
15	PX2	C	502	-	-	15/37/37/37	-
20	PLM	C	501	-	-	5/11/11/15	-
13	PGW	L	301	-	-	15/55/55/55	-
14	D10	E	503	-	-	0/7/7/7	-
14	D10	L	302	-	-	1/7/7/7	-
18	R16	B	502	-	-	1/13/13/13	-
14	D10	A	3903	-	-	1/7/7/7	-
19	HEX	E	509	-	-	0/3/3/3	-
21	OLC	C	504	-	-	9/20/20/24	-
15	PX2	D	3907	-	-	7/37/37/37	-
16	ABU	A	3907	-	-	0/4/4/4	-
13	PGW	A	3902[B]	-	-	18/55/55/55	-
14	D10	A	3905	-	-	1/7/7/7	-
15	PX2	B	501	-	-	13/37/37/37	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PGW	D	3903[B]	-	-	36/55/55/55	-
14	D10	D	3906	-	-	0/7/7/7	-
14	D10	C	503	-	-	0/7/7/7	-
13	PGW	A	3902[A]	-	-	25/55/55/55	-
19	HEX	D	3904	-	-	1/3/3/3	-
18	R16	E	502	-	-	1/13/13/13	-
16	ABU	E	510	-	-	2/4/4/4	-
15	PX2	E	501	-	-	11/37/37/37	-
19	HEX	B	504	-	-	1/3/3/3	-
13	PGW	D	3903[A]	-	-	19/55/55/55	-
19	HEX	E	505	-	-	1/3/3/3	-
22	CLR	C	508	-	-	0/10/68/68	0/4/4/4
14	D10	D	3905	-	-	0/7/7/7	-
14	D10	E	508	-	-	1/7/7/7	-
14	D10	A	3904	-	-	1/7/7/7	-
19	HEX	B	507	-	-	0/3/3/3	-
14	D10	B	503	-	-	1/7/7/7	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	3901	PIO	P5-O5	3.27	1.65	1.59
12	D	3901	PIO	P5-O5	3.24	1.65	1.59
12	A	3901	PIO	P4-O4	3.11	1.65	1.59
12	D	3901	PIO	P4-O4	3.06	1.65	1.59
13	A	3902[B]	PGW	O03-C19	2.99	1.42	1.33
21	C	504	OLC	O20-C1	2.96	1.42	1.33
13	L	303	PGW	O03-C19	2.91	1.41	1.33
13	E	504	PGW	O03-C19	2.90	1.41	1.33
15	C	502	PX2	O5-C4	2.88	1.41	1.33
13	D	3903[B]	PGW	O03-C19	2.85	1.41	1.33
13	A	3902[A]	PGW	O01-C1	2.85	1.42	1.34
13	D	3903[A]	PGW	O03-C19	2.84	1.41	1.33
13	A	3902[B]	PGW	O01-C1	2.83	1.42	1.34
13	A	3902[A]	PGW	O03-C19	2.80	1.41	1.33
13	D	3903[A]	PGW	O01-C1	2.72	1.42	1.34
13	D	3903[B]	PGW	O01-C1	2.72	1.42	1.34
13	E	504	PGW	O01-C1	2.70	1.41	1.34
13	L	303	PGW	O01-C1	2.69	1.41	1.34
15	B	501	PX2	O5-C4	2.69	1.41	1.33
15	E	501	PX2	O5-C4	2.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	3901	PIO	O3C-C1B	2.60	1.40	1.33
15	E	501	PX2	O7-C16	2.52	1.41	1.34
15	B	501	PX2	O7-C2	-2.46	1.40	1.46
12	D	3901	PIO	O3C-C1B	2.42	1.40	1.33
12	A	3901	PIO	O2C-C1A	2.41	1.41	1.34
15	C	502	PX2	O7-C2	-2.37	1.40	1.46
15	B	501	PX2	O7-C16	2.31	1.40	1.34
12	D	3901	PIO	O2C-C1A	2.30	1.40	1.34
15	C	502	PX2	O7-C16	2.27	1.40	1.34
15	E	501	PX2	O7-C2	-2.19	1.41	1.46
12	A	3901	PIO	O2C-C2C	-2.12	1.41	1.46
12	D	3901	PIO	O3C-C3C	-2.09	1.40	1.45
12	D	3901	PIO	O2C-C2C	-2.06	1.41	1.46
15	B	501	PX2	O5-C3	-2.04	1.40	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	3901	PIO	O2C-C1A-C2A	5.23	122.78	111.50
12	D	3901	PIO	O2C-C1A-C2A	4.54	121.29	111.50
13	L	303	PGW	O01-C1-C2	4.32	120.82	111.50
15	B	501	PX2	O7-C16-C17	4.15	120.44	111.50
13	A	3902[B]	PGW	O01-C1-C2	4.01	120.14	111.50
15	C	502	PX2	O7-C16-C17	3.92	119.95	111.50
13	E	504	PGW	O01-C1-C2	3.89	119.88	111.50
15	E	501	PX2	O7-C16-C17	3.85	119.79	111.50
13	A	3902[A]	PGW	O01-C1-C2	3.78	119.66	111.50
13	D	3903[B]	PGW	O01-C1-C2	3.77	119.63	111.50
13	D	3903[A]	PGW	O01-C1-C2	3.74	119.56	111.50
21	C	504	OLC	C8-C9-C10	3.61	152.43	124.73
15	C	502	PX2	O5-C4-C5	3.27	122.17	111.91
12	D	3901	PIO	C5-C6-C1	2.73	114.62	108.96
15	B	501	PX2	O5-C4-C5	2.70	120.39	111.91
12	D	3901	PIO	O3C-C1B-C2B	2.69	120.35	111.91
13	D	3903[B]	PGW	O03-C19-C20	2.67	120.28	111.91
13	E	504	PGW	O03-C19-C20	2.55	119.92	111.91
15	E	501	PX2	O5-C4-C5	2.52	119.80	111.91
13	A	3902[B]	PGW	O03-C19-C20	2.50	119.74	111.91
12	A	3901	PIO	O3C-C1B-C2B	2.50	119.74	111.91
13	A	3902[A]	PGW	O03-C19-C20	2.47	119.66	111.91
13	L	303	PGW	O03-C19-C20	2.37	119.36	111.91
13	D	3903[A]	PGW	O03-C19-C20	2.31	119.15	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	504	OLC	O20-C1-C2	2.16	118.69	111.91
12	A	3901	PIO	O2C-C1A-O1A	-2.10	118.62	123.70
16	E	510	ABU	CB-CG-C	-2.08	109.24	114.47
12	D	3901	PIO	C6-C1-C2	2.01	113.75	110.85
20	C	501	PLM	C3-C2-C1	-2.01	109.41	114.47

There are no chirality outliers.

All (288) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	3901	PIO	O1A-C1A-O2C-C2C
12	A	3901	PIO	C2A-C1A-O2C-C2C
12	D	3901	PIO	C2-C1-O1-P1
12	D	3901	PIO	C6-C1-O1-P1
12	D	3901	PIO	C1C-O13-P1-O12
12	D	3901	PIO	C5-O5-P5-O53
12	D	3901	PIO	C2A-C1A-O2C-C2C
13	A	3902[A]	PGW	C03-O11-P-O13
13	A	3902[A]	PGW	O12-C04-C05-CAD
13	A	3902[B]	PGW	C2-C1-O01-C02
13	D	3903[A]	PGW	O12-C04-C05-CAD
13	D	3903[B]	PGW	C03-O11-P-O14
13	L	301	PGW	C03-O11-P-O14
13	L	303	PGW	C04-O12-P-O13
13	L	303	PGW	C2-C1-O01-C02
13	L	303	PGW	O02-C1-O01-C02
15	B	501	PX2	C1-O4-P1-O1
15	B	501	PX2	C1-O4-P1-O3
15	B	501	PX2	C17-C16-O7-C2
15	C	502	PX2	C1-O4-P1-O1
15	C	502	PX2	C1-O4-P1-O2
15	C	502	PX2	C1-O4-P1-O3
15	E	501	PX2	C1-O4-P1-O1
15	E	501	PX2	C1-O4-P1-O2
15	E	501	PX2	C1-O4-P1-O3
15	B	501	PX2	O6-C4-O5-C3
15	C	502	PX2	O6-C4-O5-C3
15	C	502	PX2	C5-C4-O5-C3
13	L	301	PGW	O04-C19-O03-C01
15	A	3906	PX2	O6-C4-O5-C3
12	D	3901	PIO	O1A-C1A-O2C-C2C
15	B	501	PX2	O8-C16-O7-C2

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Mol	Chain	Res	Type	Atoms
13	A	3902[A]	PGW	C20-C19-O03-C01
13	L	301	PGW	C20-C19-O03-C01
15	A	3906	PX2	C5-C4-O5-C3
15	B	501	PX2	C5-C4-O5-C3
21	C	504	OLC	C4-C5-C6-C7
13	A	3902[B]	PGW	O02-C1-O01-C02
13	A	3902[A]	PGW	O04-C19-O03-C01
13	A	3902[A]	PGW	O12-C04-C05-OAF
13	A	3902[A]	PGW	C2-C1-O01-C02
15	C	502	PX2	C17-C16-O7-C2
15	C	502	PX2	O8-C16-O7-C2
13	D	3903[B]	PGW	C20-C19-O03-C01
13	L	303	PGW	O12-C04-C05-CAD
13	A	3902[A]	PGW	O02-C1-O01-C02
13	D	3903[B]	PGW	O04-C19-O03-C01
12	D	3901	PIO	C1-O1-P1-O13
13	D	3903[A]	PGW	O12-C04-C05-OAF
13	L	303	PGW	O12-C04-C05-OAF
13	A	3902[A]	PGW	C1-C2-C3-C4
15	C	502	PX2	C19-C20-C21-C22
15	B	501	PX2	C16-C17-C18-C19
15	E	501	PX2	C2-C1-O4-P1
20	C	501	PLM	C2-C3-C4-C5
15	C	502	PX2	C2-C3-O5-C4
13	A	3902[A]	PGW	C03-O11-P-O12
13	D	3903[B]	PGW	C03-O11-P-O12
13	D	3903[B]	PGW	C04-O12-P-O11
13	L	301	PGW	C03-O11-P-O12
13	L	303	PGW	C04-O12-P-O11
21	C	504	OLC	C2-C1-O20-C21
15	A	3906	PX2	C18-C19-C20-C21
13	D	3903[A]	PGW	C2-C1-O01-C02
13	A	3902[B]	PGW	C5-C6-C7-C8
18	B	506	R16	C33-C34-C35-C36
20	C	507	PLM	C2-C3-C4-C5
13	D	3903[A]	PGW	O02-C1-O01-C02
20	C	507	PLM	C7-C8-C9-CA
13	A	3902[B]	PGW	C27-C15-C16-C17
14	A	3908	D10	C4-C5-C6-C7
13	D	3903[B]	PGW	C23-C24-C25-C26
18	B	506	R16	C28-C29-C30-C31
20	E	506	PLM	CC-CD-CE-CF

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Mol	Chain	Res	Type	Atoms
13	L	303	PGW	C24-C25-C26-C27
14	E	508	D10	C3-C4-C5-C6
13	L	303	PGW	C06-C07-C08-C09
13	D	3903[B]	PGW	C04-C05-CAD-OAE
13	E	504	PGW	C04-C05-CAD-OAE
21	C	504	OLC	O20-C21-C22-O23
13	D	3903[A]	PGW	C27-C15-C16-C17
13	D	3903[B]	PGW	C27-C15-C16-C17
13	L	303	PGW	C22-C23-C24-C25
20	C	506	PLM	C1-C2-C3-C4
13	A	3902[A]	PGW	C06-C07-C08-C09
13	A	3902[A]	PGW	C08-C09-C11-C12
13	D	3903[A]	PGW	C23-C24-C25-C26
13	L	303	PGW	C09-C11-C12-C13
14	A	3905	D10	C6-C7-C8-C9
13	A	3902[A]	PGW	C27-C15-C16-C17
13	L	303	PGW	C27-C15-C16-C17
14	B	508	D10	C5-C6-C7-C8
13	A	3902[B]	PGW	C2-C3-C4-C5
13	D	3903[A]	PGW	C5-C6-C7-C8
13	D	3903[A]	PGW	C06-C07-C08-C09
13	D	3903[A]	PGW	C08-C09-C11-C12
21	C	504	OLC	C2-C3-C4-C5
21	C	504	OLC	O19-C1-O20-C21
15	B	501	PX2	C5-C6-C7-C8
13	D	3903[B]	PGW	OAF-C05-CAD-OAE
15	B	501	PX2	C10-C11-C12-C13
21	C	504	OLC	C6-C7-C8-C9
13	A	3902[B]	PGW	C1-C2-C3-C4
15	C	502	PX2	C4-C5-C6-C7
15	E	501	PX2	C10-C11-C12-C13
13	E	504	PGW	C1-C2-C3-C4
13	A	3902[B]	PGW	C06-C07-C08-C09
13	L	303	PGW	C17-C18-C28-C30
18	E	502	R16	C34-C35-C36-C37
13	D	3903[B]	PGW	C08-C09-C11-C12
15	E	501	PX2	C6-C7-C8-C9
13	D	3903[B]	PGW	C10-C06-C07-C08
13	A	3902[B]	PGW	C09-C11-C12-C13
12	D	3901	PIO	C1C-O13-P1-O1
13	D	3903[A]	PGW	C09-C11-C12-C13
15	B	501	PX2	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	A	3902[B]	PGW	C6-C7-C8-C9
13	A	3902[B]	PGW	C23-C24-C25-C26
13	E	504	PGW	C23-C24-C25-C26
13	D	3903[B]	PGW	O03-C01-C02-C03
15	C	502	PX2	C6-C7-C8-C9
13	D	3903[B]	PGW	C16-C15-C27-C26
13	E	504	PGW	OAF-C05-CAD-OAE
15	A	3906	PX2	C17-C16-O7-C2
18	E	507	R16	C27-C28-C29-C30
19	E	505	HEX	C3-C4-C5-C6
21	C	504	OLC	O20-C21-C22-C24
12	D	3901	PIO	C1C-C2C-O2C-C1A
13	L	303	PGW	C03-C02-O01-C1
13	A	3902[A]	PGW	C05-C04-O12-P
15	B	501	PX2	C1-O4-P1-O2
13	D	3903[B]	PGW	C06-C07-C08-C09
18	E	507	R16	C34-C35-C36-C37
20	C	507	PLM	CC-CD-CE-CF
12	D	3901	PIO	C2B-C1B-O3C-C3C
15	B	501	PX2	C6-C7-C8-C9
15	D	3907	PX2	O5-C4-C5-C6
18	B	506	R16	C35-C36-C37-C38
12	A	3901	PIO	C1C-C2C-C3C-O3C
18	E	507	R16	C36-C37-C38-C39
12	A	3901	PIO	C1-O1-P1-O12
13	D	3903[B]	PGW	C07-C08-C09-C11
15	B	501	PX2	C11-C10-C9-C8
12	A	3901	PIO	C2B-C1B-O3C-C3C
12	D	3901	PIO	O1B-C1B-O3C-C3C
12	A	3901	PIO	O2C-C2C-C3C-O3C
13	E	504	PGW	O03-C01-C02-O01
15	A	3906	PX2	O8-C16-O7-C2
15	D	3907	PX2	O7-C16-C17-C18
13	A	3902[B]	PGW	C21-C22-C23-C24
13	D	3903[A]	PGW	C2-C3-C4-C5
13	A	3902[A]	PGW	C20-C21-C22-C23
14	B	503	D10	C7-C8-C9-C10
12	A	3901	PIO	O1B-C1B-O3C-C3C
12	A	3901	PIO	C5-O5-P5-O52
13	E	504	PGW	C3-C4-C5-C6
13	E	504	PGW	C4-C5-C6-C7
13	D	3903[A]	PGW	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
18	B	502	R16	C31-C32-C33-C34
12	D	3901	PIO	C1C-O13-P1-O11
13	A	3902[A]	PGW	C03-O11-P-O14
13	D	3903[B]	PGW	C03-O11-P-O13
13	D	3903[B]	PGW	C04-O12-P-O13
13	L	303	PGW	C04-O12-P-O14
13	D	3903[B]	PGW	C2-C1-O01-C02
12	D	3901	PIO	C1C-C2C-C3C-O3C
13	E	504	PGW	O03-C01-C02-C03
15	E	501	PX2	C21-C22-C23-C24
12	D	3901	PIO	O2C-C2C-C3C-O3C
13	D	3903[B]	PGW	O03-C01-C02-O01
13	A	3902[A]	PGW	C17-C18-C28-C30
13	D	3903[B]	PGW	C05-C04-O12-P
20	C	506	PLM	C6-C7-C8-C9
15	C	502	PX2	O7-C16-C17-C18
12	A	3901	PIO	C1-O1-P1-O13
13	D	3903[B]	PGW	C2-C3-C4-C5
20	E	506	PLM	C4-C5-C6-C7
13	D	3903[B]	PGW	O03-C19-C20-C21
13	L	301	PGW	C19-C20-C21-C22
13	A	3902[A]	PGW	C25-C26-C27-C15
13	A	3902[B]	PGW	C03-C02-O01-C1
13	D	3903[B]	PGW	O02-C1-O01-C02
18	B	506	R16	C27-C28-C29-C30
12	A	3901	PIO	C2B-C3B-C4B-C5B
12	D	3901	PIO	C2C-C1C-O13-P1
13	D	3903[A]	PGW	C02-C03-O11-P
15	C	502	PX2	C23-C24-C25-C26
13	A	3902[A]	PGW	C5-C6-C7-C8
15	D	3907	PX2	C17-C18-C19-C20
20	C	505	PLM	C9-CA-CB-CC
13	E	504	PGW	C04-O12-P-O11
13	L	301	PGW	C04-O12-P-O11
13	D	3903[B]	PGW	C17-C18-C28-C30
13	A	3902[B]	PGW	C7-C8-C9-C10
15	E	501	PX2	O7-C16-C17-C18
13	L	301	PGW	C7-C8-C9-C10
13	L	303	PGW	C07-C06-C10-C9
20	C	507	PLM	O1-C1-C2-C3
13	L	301	PGW	C07-C06-C10-C9
13	E	504	PGW	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
13	D	3903[B]	PGW	C15-C16-C17-C18
13	A	3902[B]	PGW	C20-C21-C22-C23
21	C	504	OLC	C9-C10-C11-C12
15	A	3906	PX2	C11-C10-C9-C8
12	A	3901	PIO	C1-O1-P1-O11
12	D	3901	PIO	C1-O1-P1-O11
19	D	3904	HEX	C1-C2-C3-C4
13	L	301	PGW	C01-C02-O01-C1
13	D	3903[A]	PGW	C7-C8-C9-C10
13	D	3903[A]	PGW	C21-C22-C23-C24
13	L	303	PGW	C19-C20-C21-C22
13	D	3903[A]	PGW	C20-C21-C22-C23
13	D	3903[B]	PGW	C1-C2-C3-C4
14	A	3903	D10	C4-C5-C6-C7
16	E	510	ABU	OXT-C-CG-CB
13	L	301	PGW	C10-C06-C07-C08
20	C	506	PLM	O1-C1-C2-C3
20	C	507	PLM	O2-C1-C2-C3
20	C	506	PLM	O2-C1-C2-C3
13	D	3903[B]	PGW	C18-C28-C30-C29
15	E	501	PX2	C7-C8-C9-C10
20	C	501	PLM	C4-C5-C6-C7
16	E	510	ABU	O-C-CG-CB
13	L	303	PGW	C4-C5-C6-C7
21	C	504	OLC	C7-C8-C9-C10
13	L	301	PGW	C2-C3-C4-C5
20	C	505	PLM	CB-CC-CD-CE
15	C	502	PX2	C9-C10-C11-C12
15	D	3907	PX2	C5-C6-C7-C8
15	D	3907	PX2	O6-C4-C5-C6
13	A	3902[A]	PGW	O03-C19-C20-C21
19	B	504	HEX	C1-C2-C3-C4
13	A	3902[A]	PGW	C03-C02-O01-C1
13	A	3902[B]	PGW	O03-C19-C20-C21
13	D	3903[B]	PGW	C24-C25-C26-C27
14	A	3904	D10	C3-C4-C5-C6
13	A	3902[B]	PGW	O01-C02-C03-O11
13	D	3903[B]	PGW	O01-C02-C03-O11
20	C	501	PLM	O1-C1-C2-C3
20	C	501	PLM	O2-C1-C2-C3
13	D	3903[B]	PGW	C07-C06-C10-C9
13	D	3903[B]	PGW	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
13	E	504	PGW	C01-C02-C03-O11
15	A	3906	PX2	C5-C6-C7-C8
13	L	303	PGW	O04-C19-O03-C01
20	C	501	PLM	C9-CA-CB-CC
20	E	506	PLM	O2-C1-C2-C3
13	E	504	PGW	O03-C19-C20-C21
14	L	302	D10	C3-C4-C5-C6
13	D	3903[B]	PGW	C7-C8-C9-C10
15	D	3907	PX2	C11-C10-C9-C8
20	E	506	PLM	C2-C3-C4-C5
13	L	301	PGW	C20-C21-C22-C23
13	L	303	PGW	C20-C19-O03-C01
13	A	3902[B]	PGW	O04-C19-C20-C21
13	D	3903[B]	PGW	C5-C6-C7-C8
15	E	501	PX2	C11-C10-C9-C8
13	E	504	PGW	O04-C19-C20-C21
13	A	3902[A]	PGW	C22-C23-C24-C25
13	L	303	PGW	C02-C03-O11-P
13	A	3902[A]	PGW	O04-C19-C20-C21
13	D	3903[A]	PGW	C03-O11-P-O14
13	D	3903[A]	PGW	C04-O12-P-O13
13	D	3903[B]	PGW	C04-O12-P-O14
13	L	301	PGW	C03-O11-P-O13
13	L	301	PGW	C04-O12-P-O14
13	A	3902[B]	PGW	C01-C02-C03-O11
13	D	3903[A]	PGW	C1-C2-C3-C4
15	D	3907	PX2	O8-C16-C17-C18
15	C	502	PX2	C5-C6-C7-C8
20	E	506	PLM	O1-C1-C2-C3
12	A	3901	PIO	C1C-C2C-O2C-C1A
12	A	3901	PIO	C3C-C2C-O2C-C1A
13	A	3902[A]	PGW	C01-C02-O01-C1
13	D	3903[B]	PGW	C01-C02-O01-C1
13	L	301	PGW	C03-C02-O01-C1
13	D	3903[B]	PGW	C21-C22-C23-C24
18	E	507	R16	C28-C29-C30-C31
13	L	303	PGW	O03-C19-C20-C21
13	E	504	PGW	O04-C19-O03-C01
13	E	504	PGW	O01-C02-C03-O11
15	E	501	PX2	C9-C10-C11-C12
13	A	3902[A]	PGW	O01-C1-C2-C3
13	L	303	PGW	C7-C8-C9-C10

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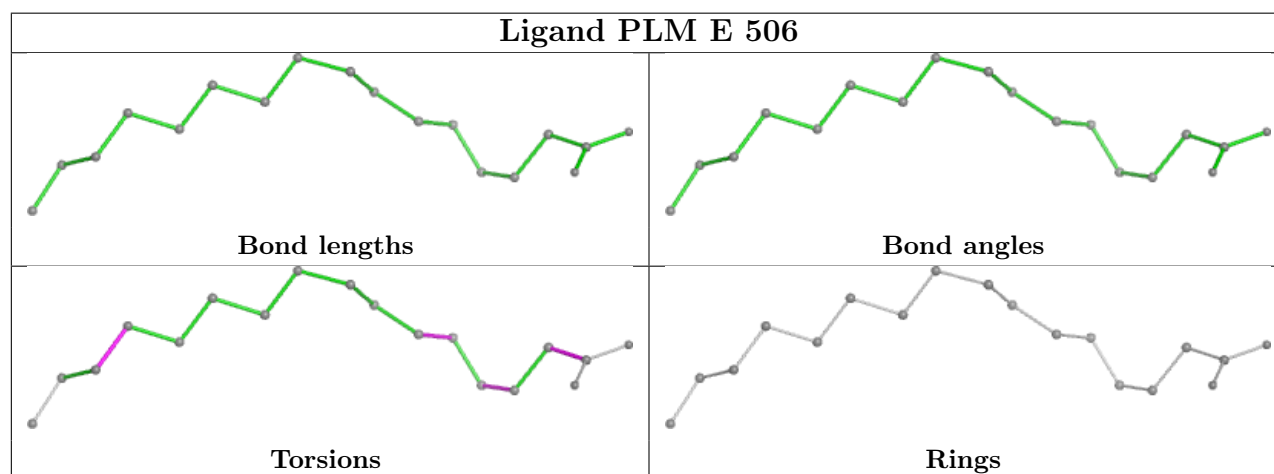
Mol	Chain	Res	Type	Atoms
12	D	3901	PIO	O2C-C1A-C2A-C3A
13	L	303	PGW	O04-C19-C20-C21
13	E	504	PGW	C20-C19-O03-C01
13	A	3902[A]	PGW	O02-C1-C2-C3

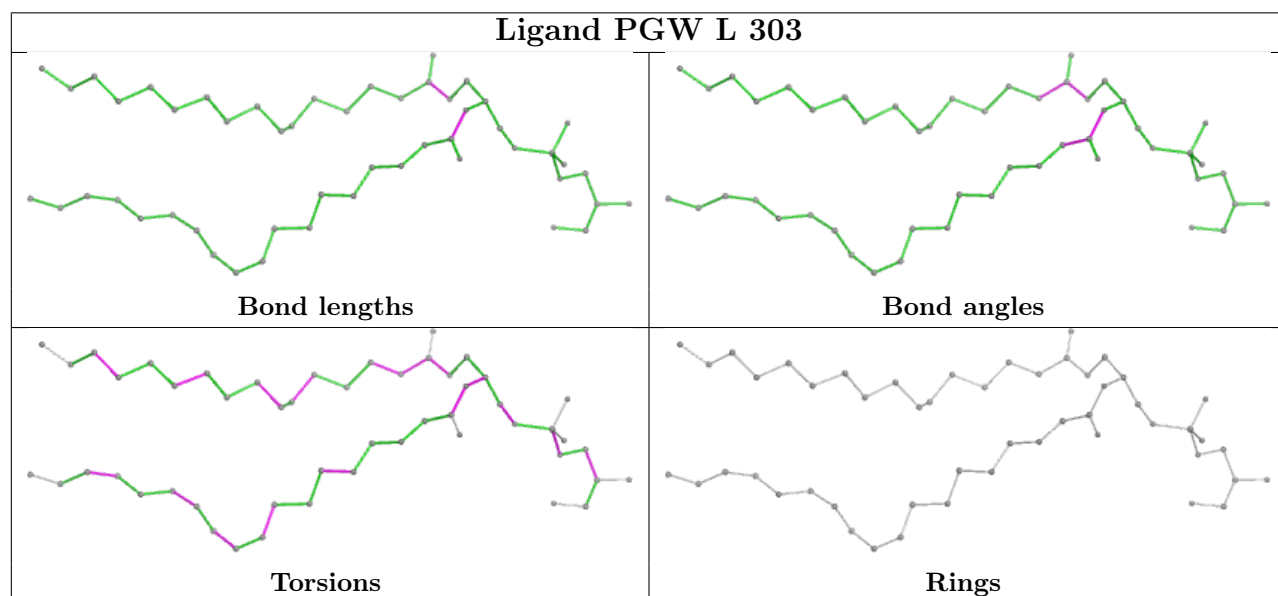
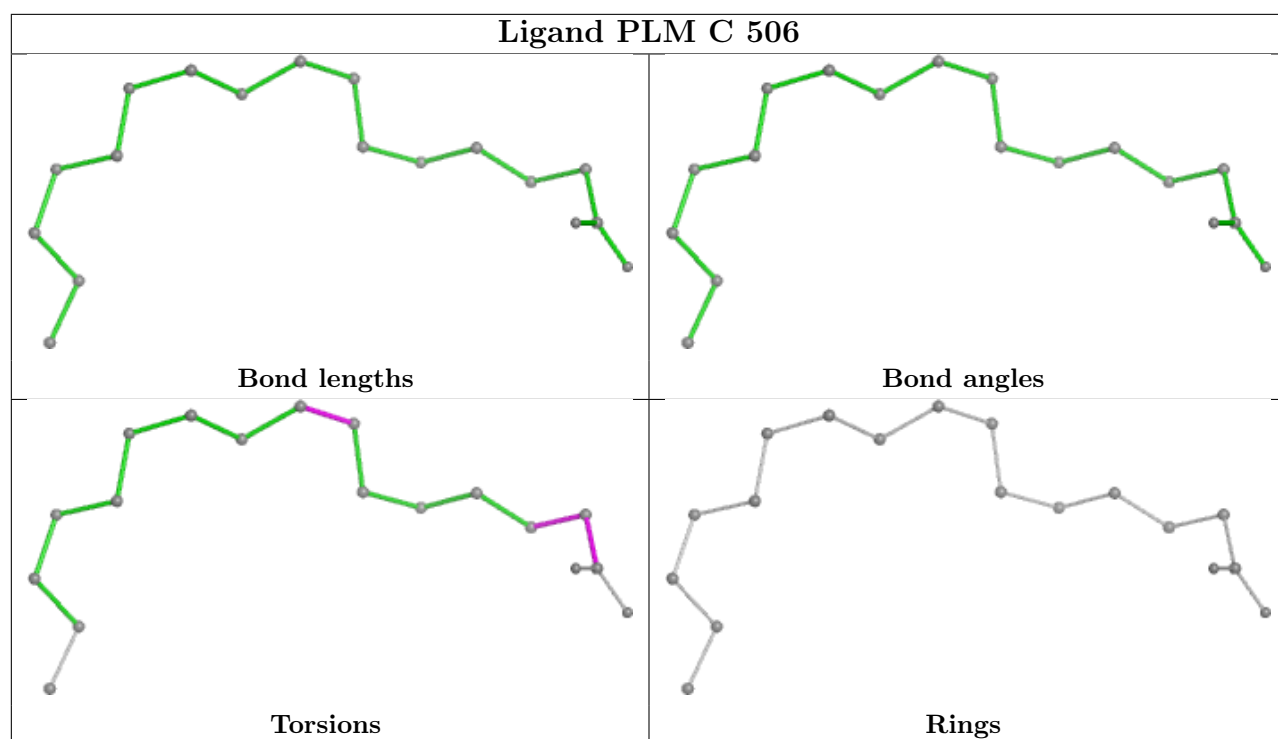
There are no ring outliers.

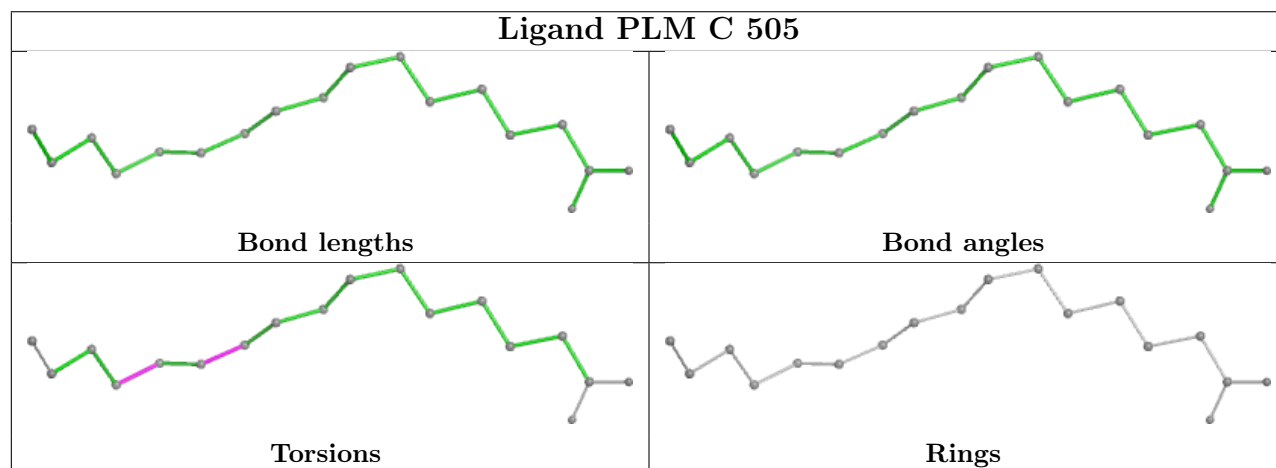
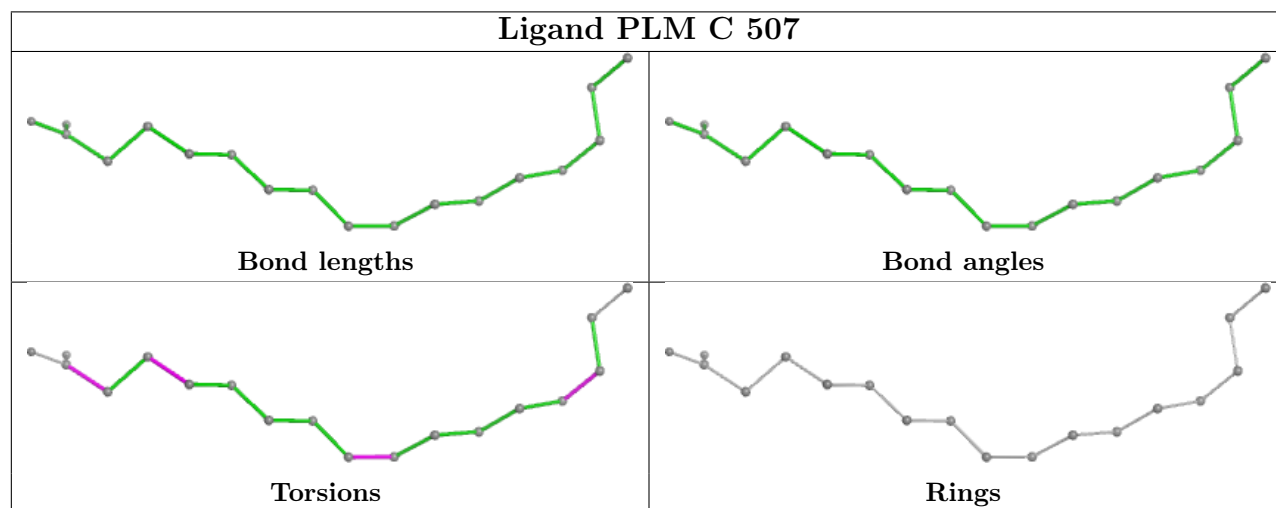
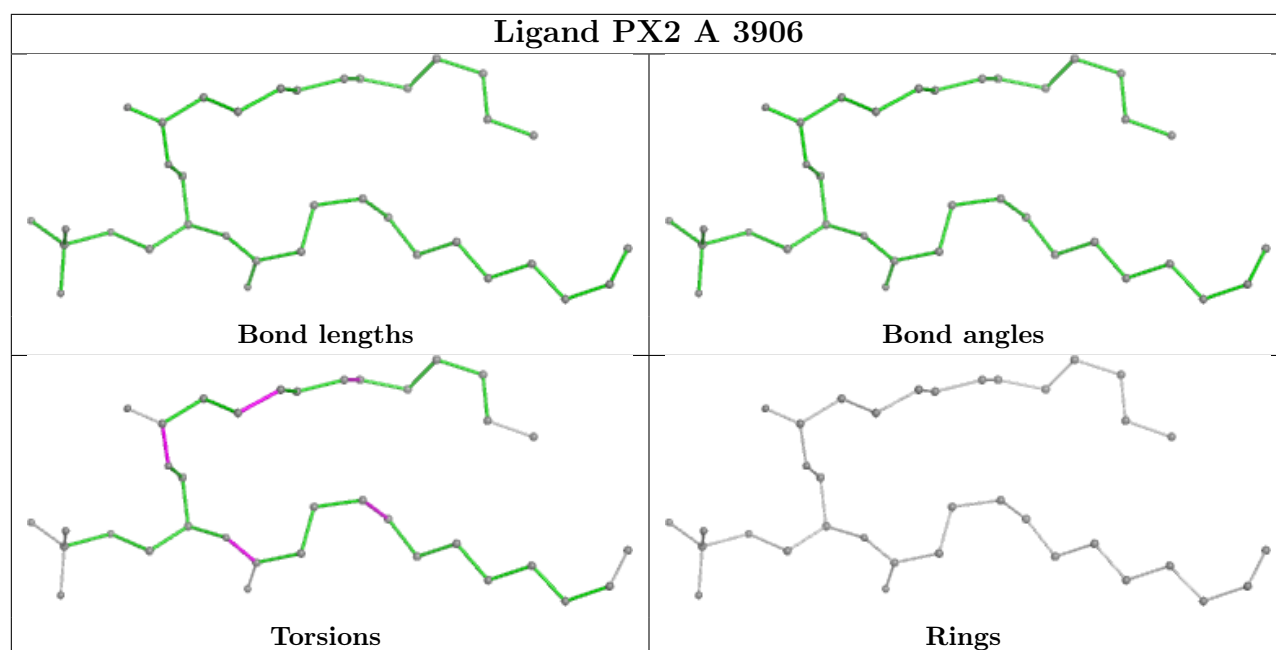
8 monomers are involved in 24 short contacts:

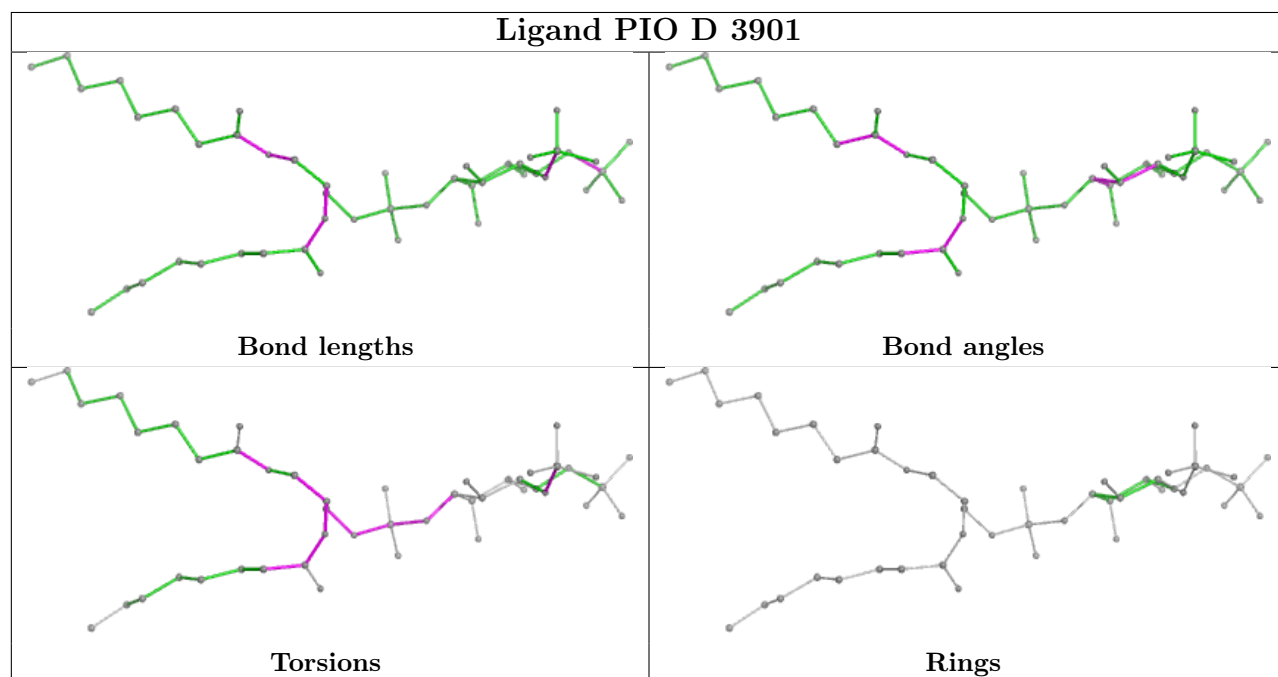
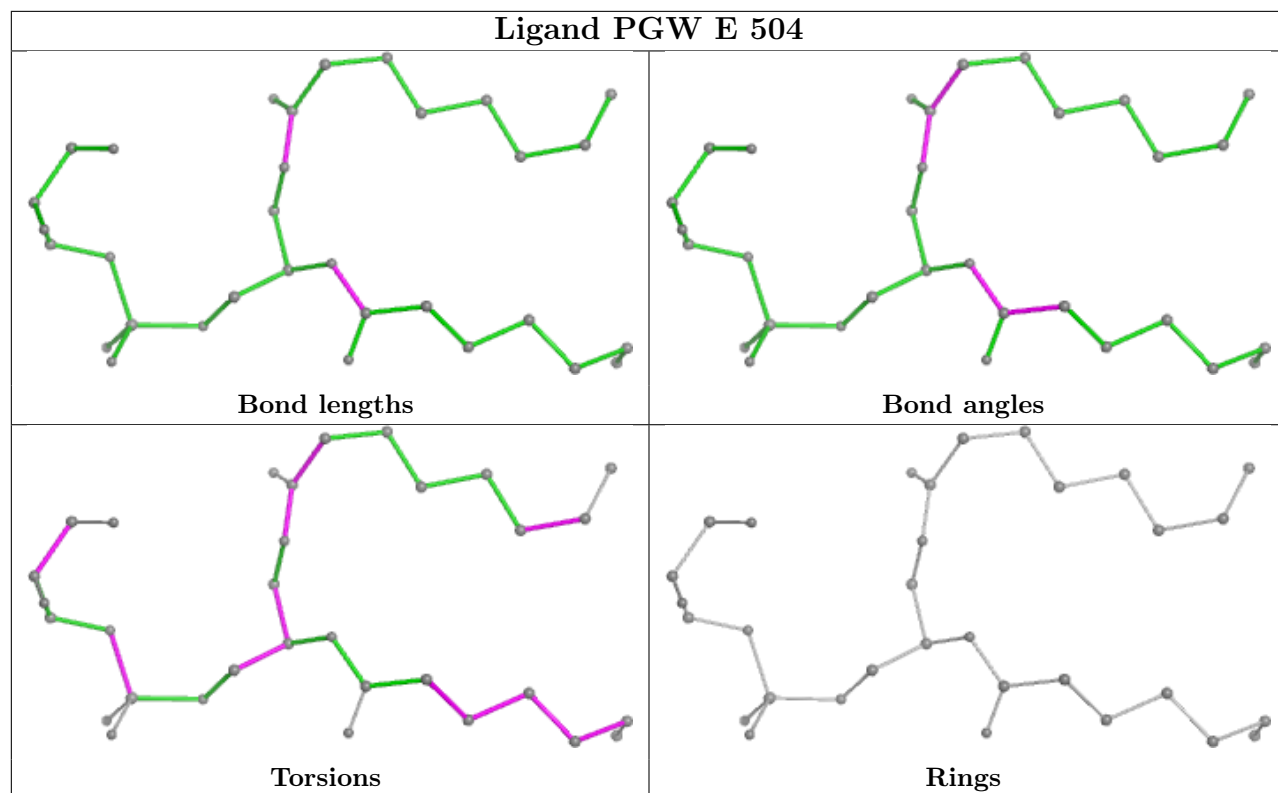
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	303	PGW	2	0
15	A	3906	PX2	5	0
12	D	3901	PIO	2	0
13	L	301	PGW	7	0
15	D	3907	PX2	5	0
15	E	501	PX2	1	0
13	D	3903[A]	PGW	1	0
22	C	508	CLR	4	0

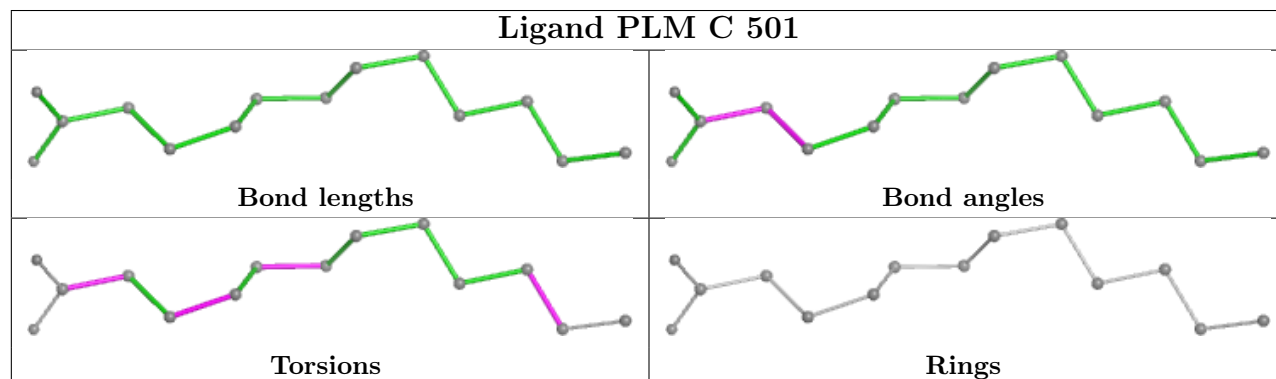
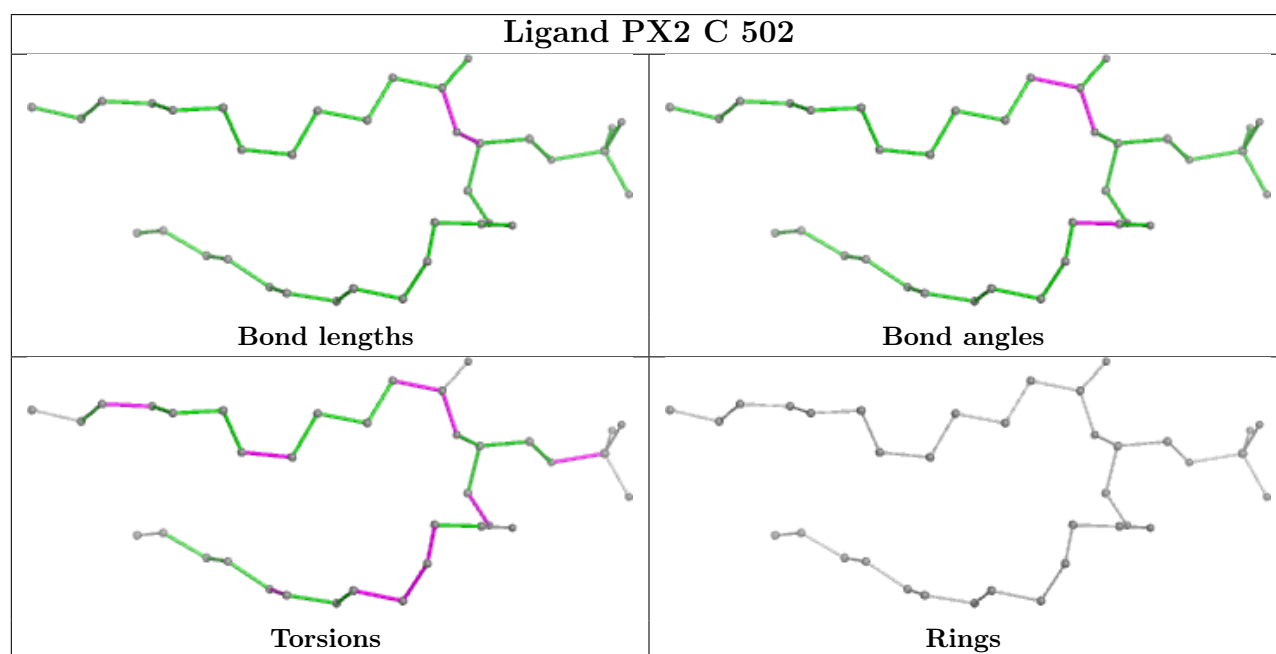
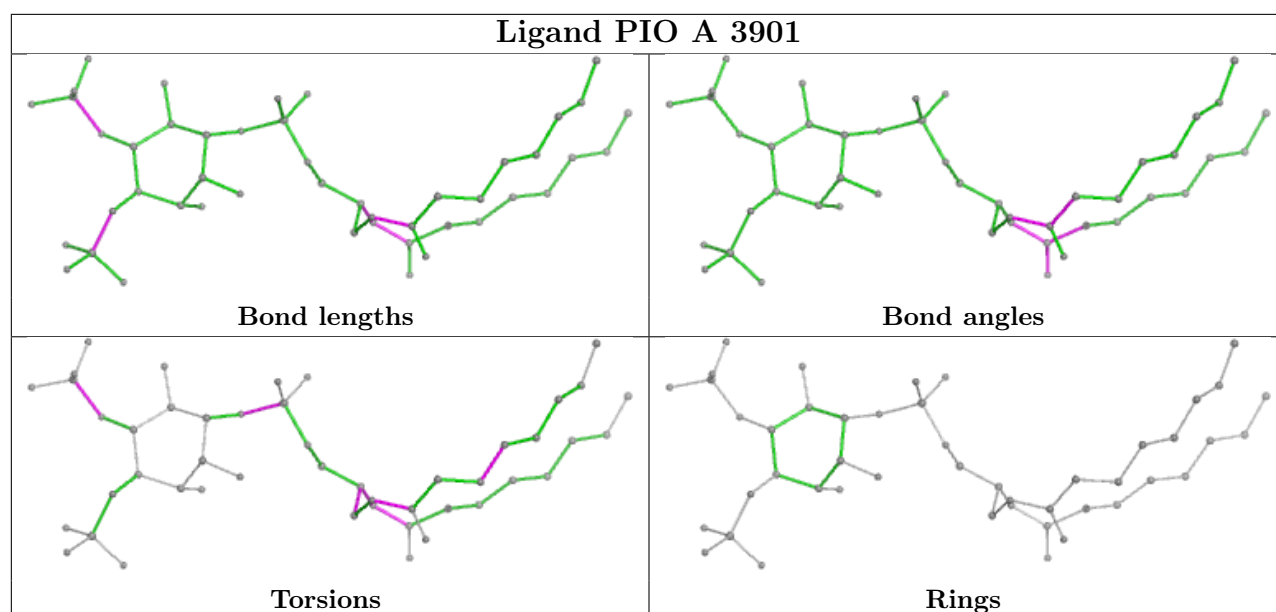
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

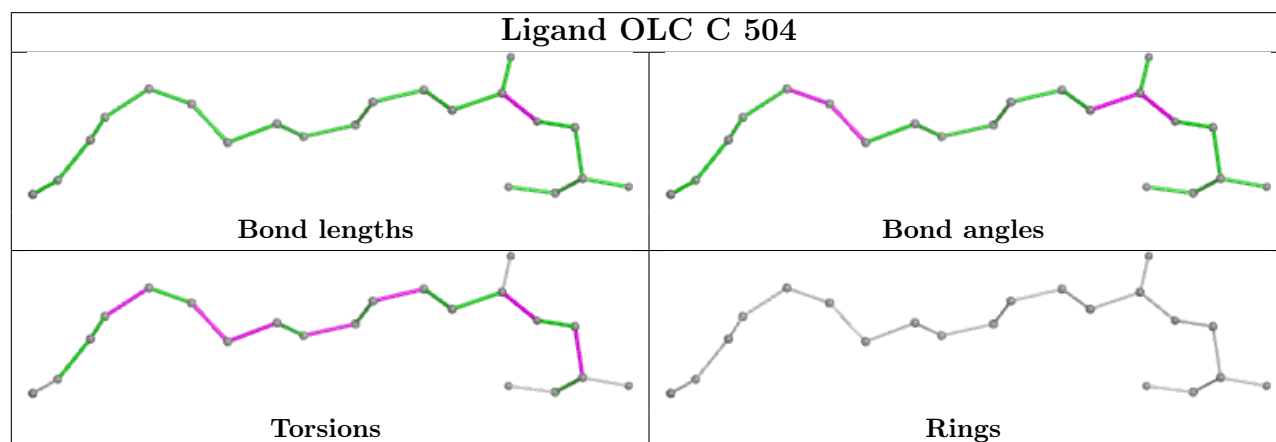
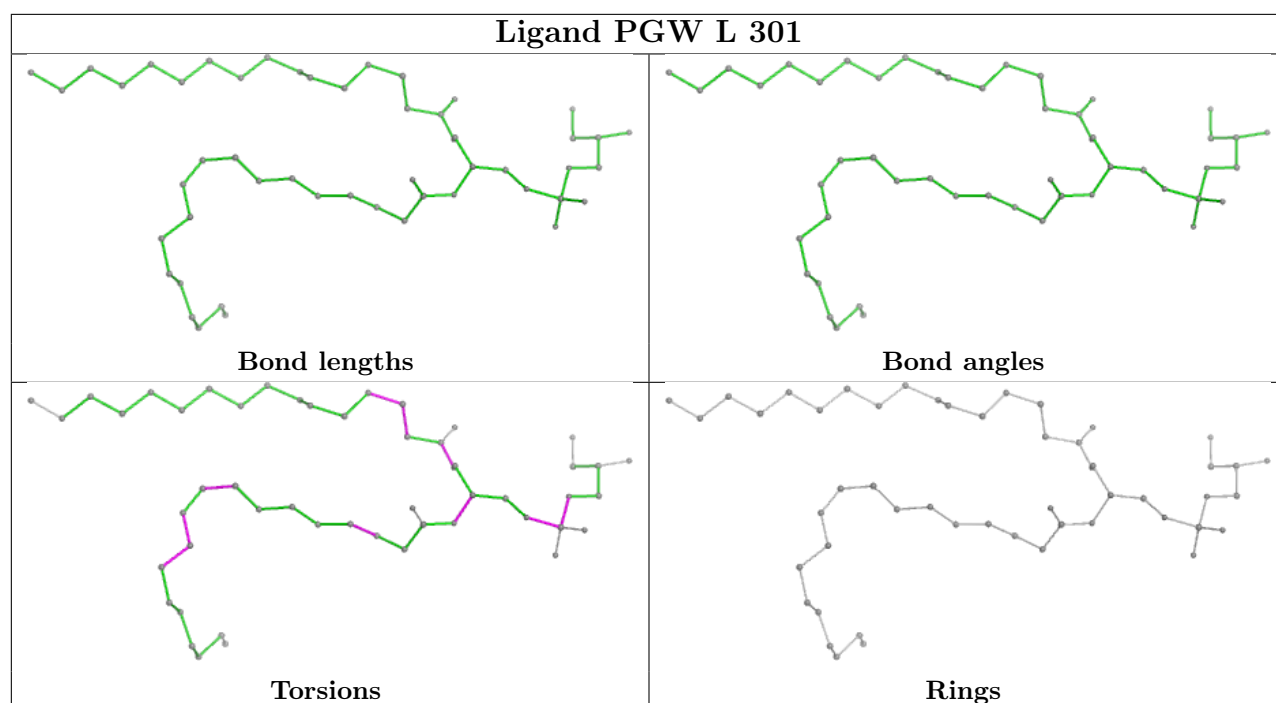


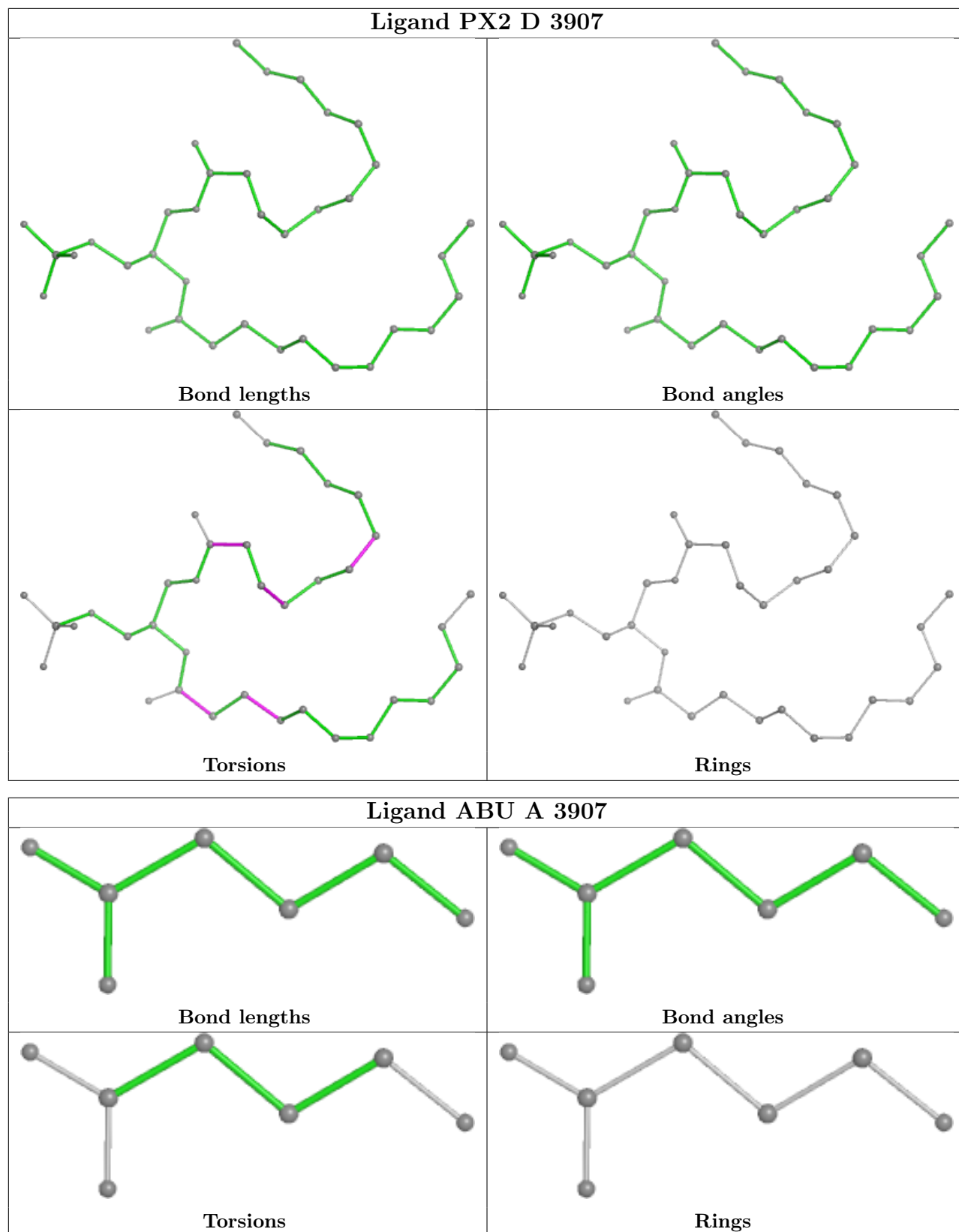


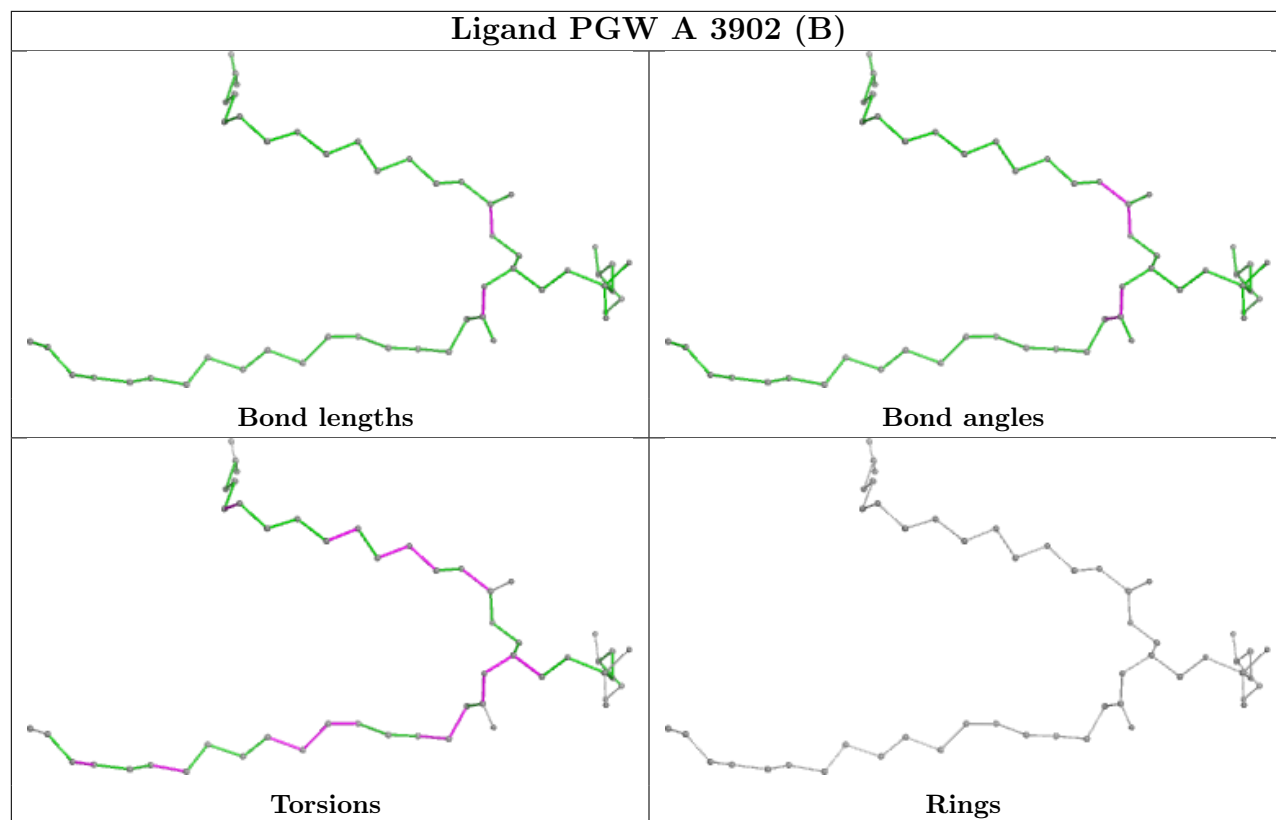


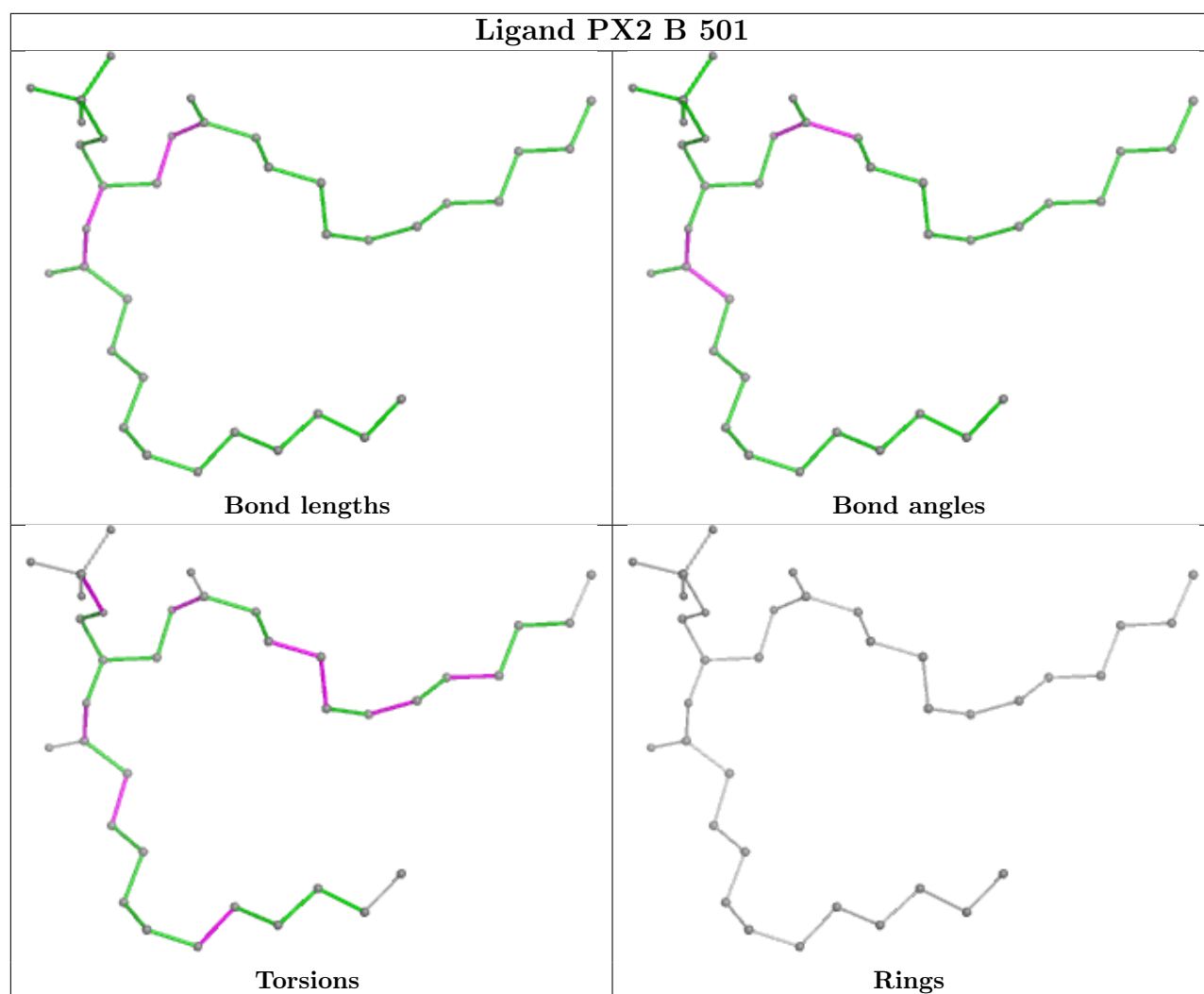


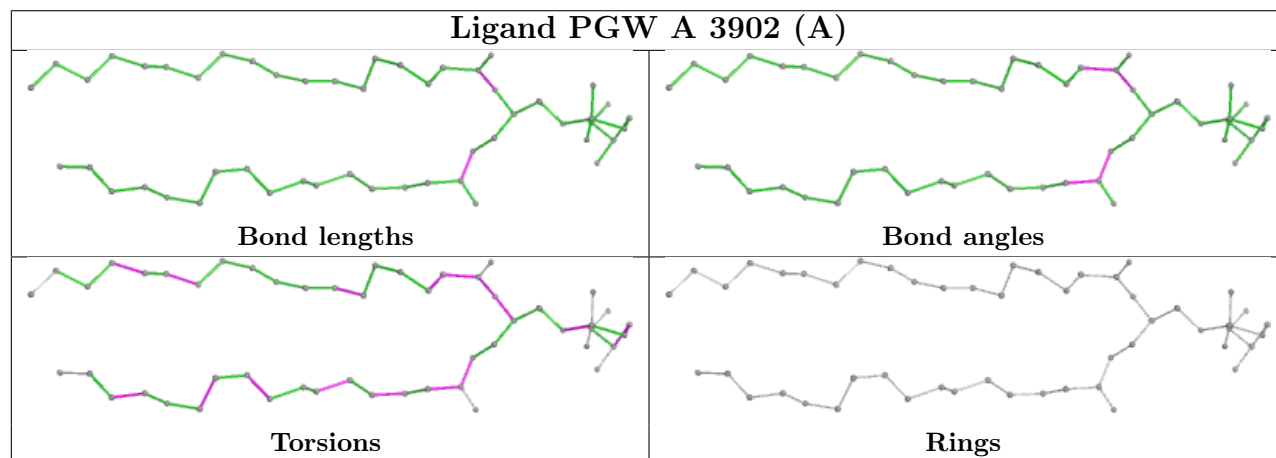
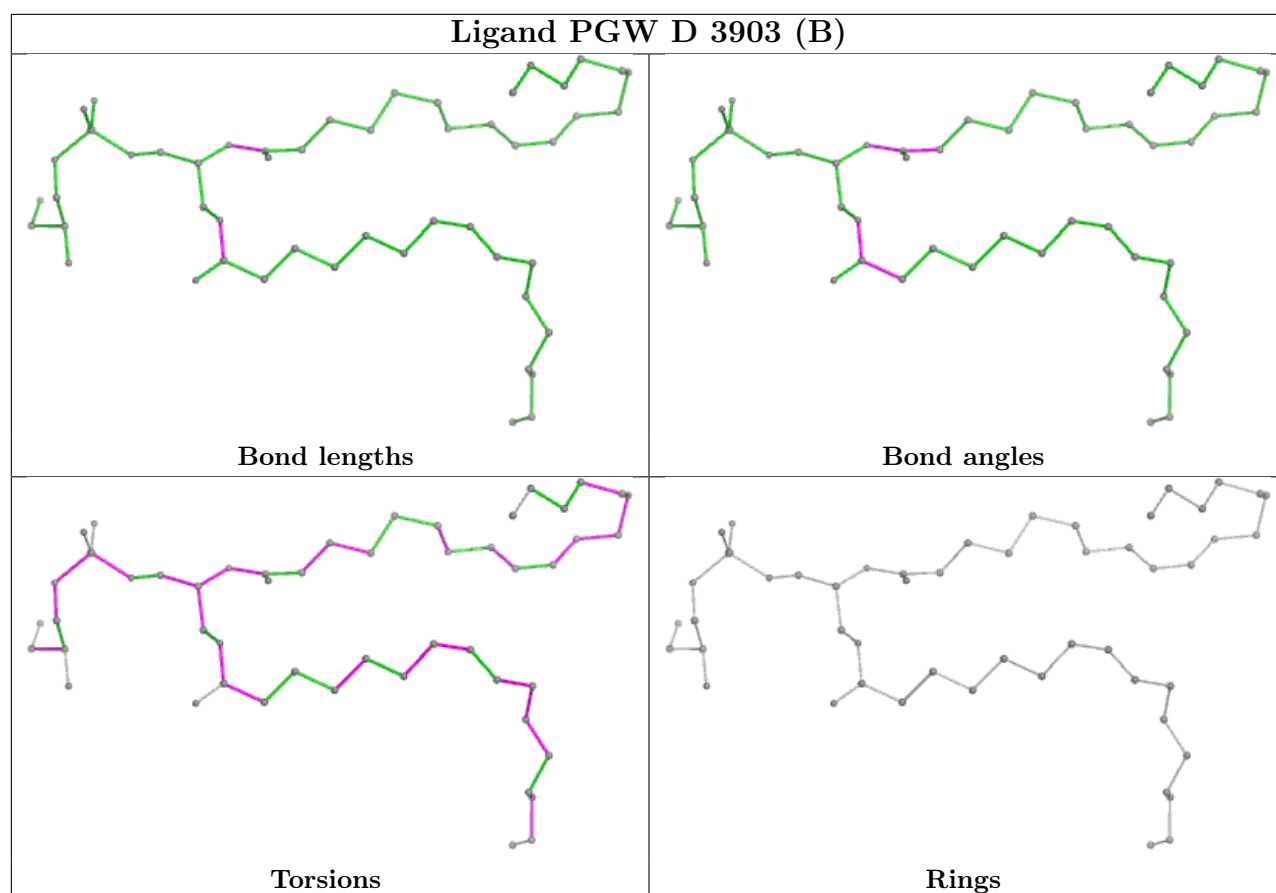


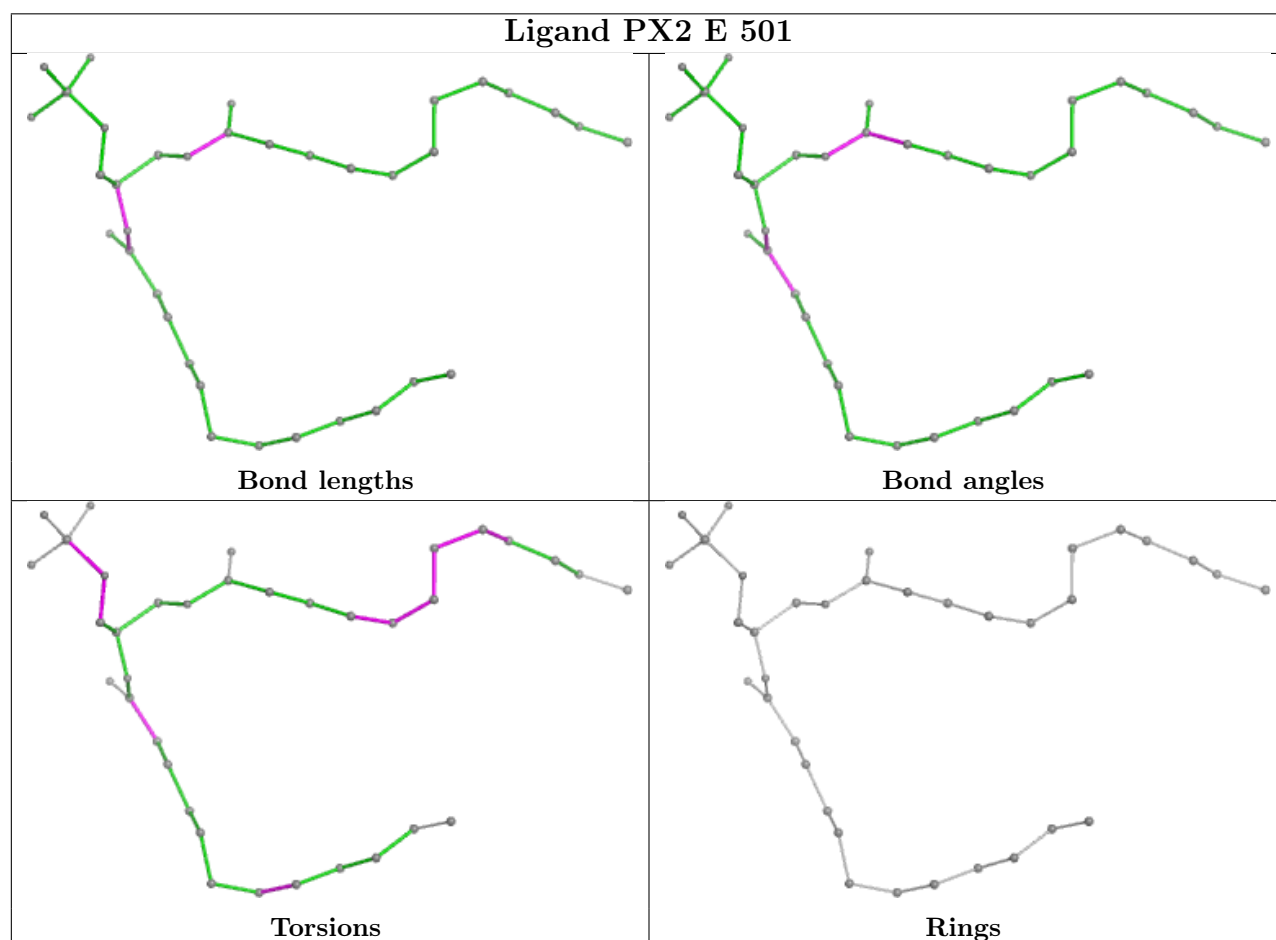
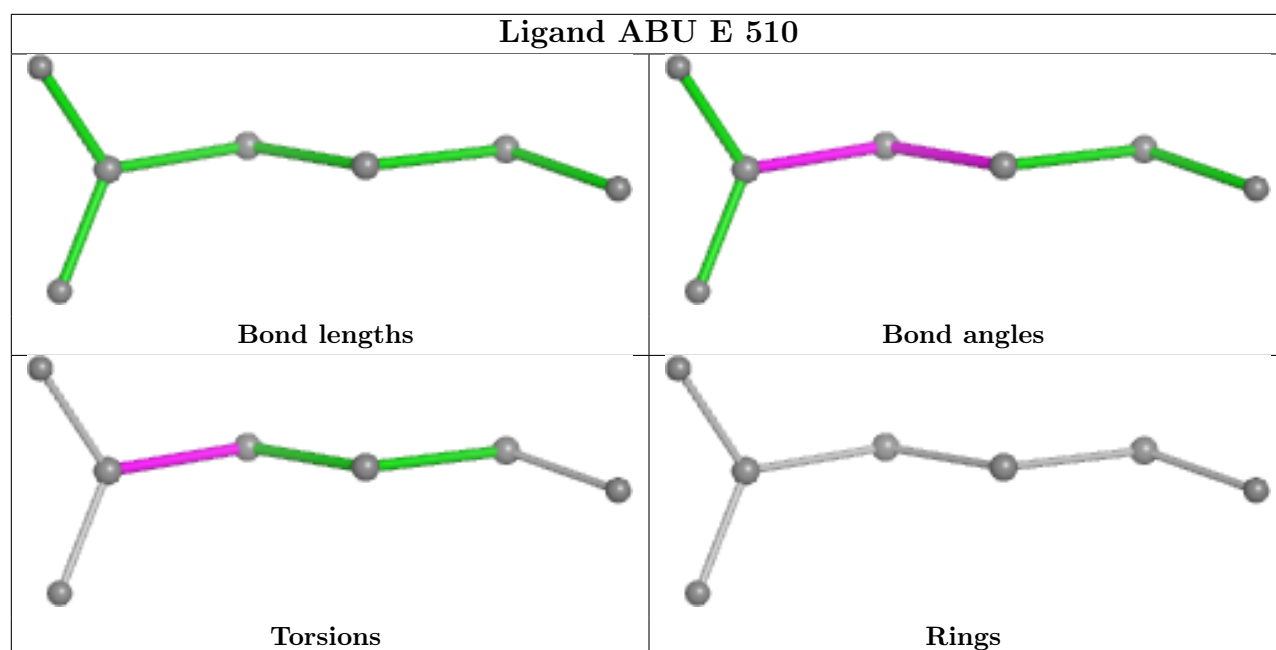


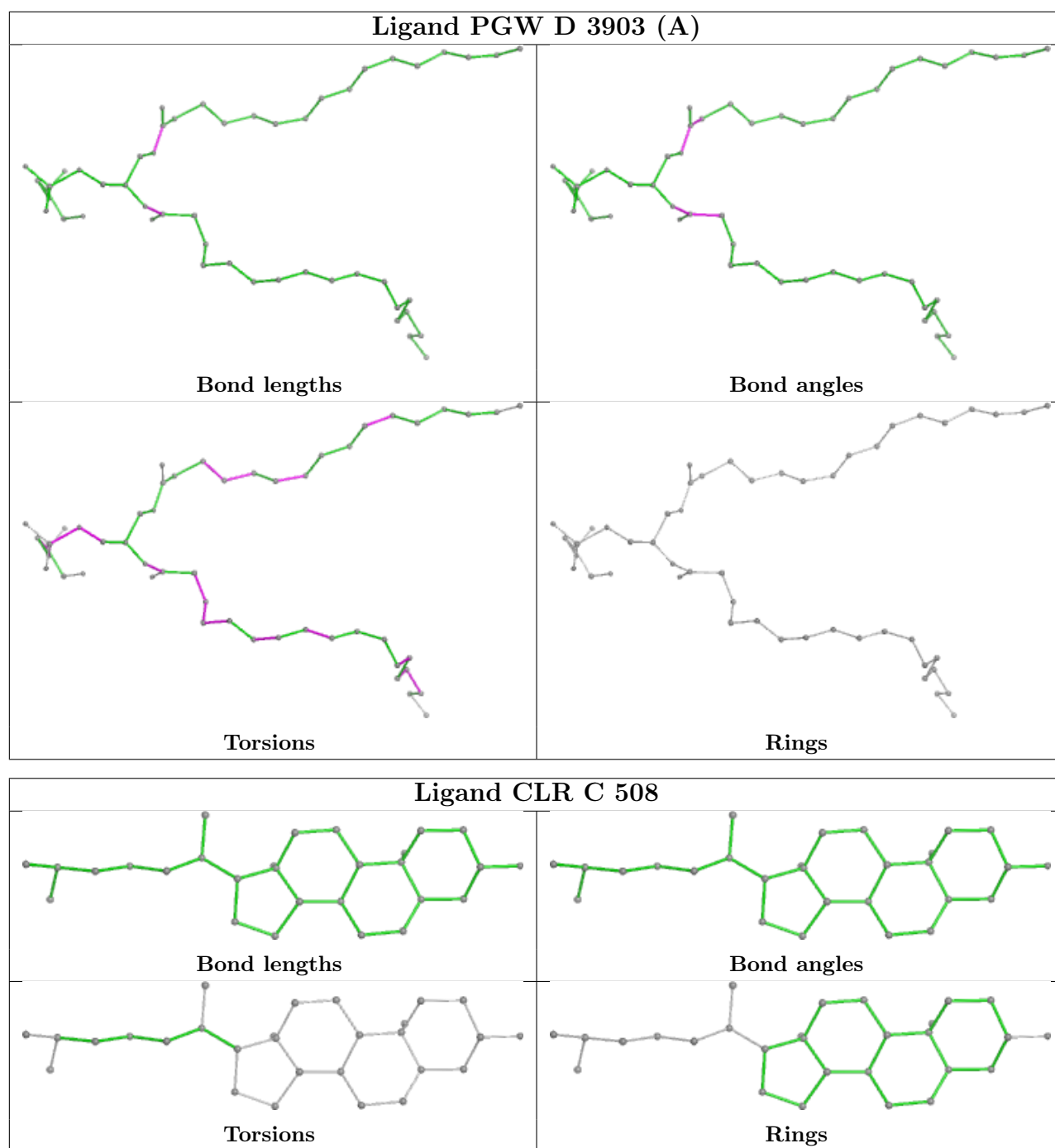












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

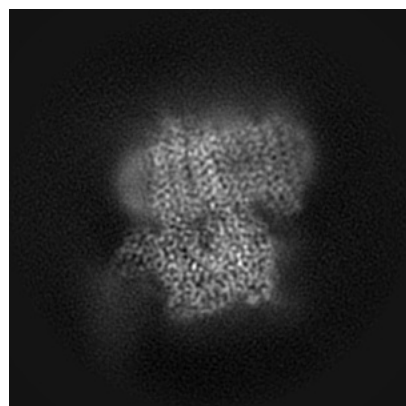
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50273. These allow visual inspection of the internal detail of the map and identification of artifacts.

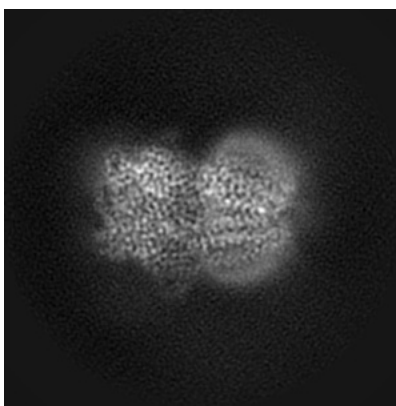
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

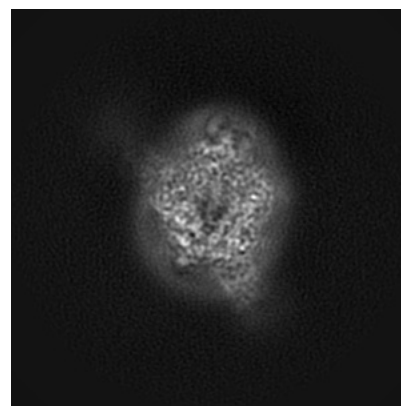
6.1.1 Primary map



X

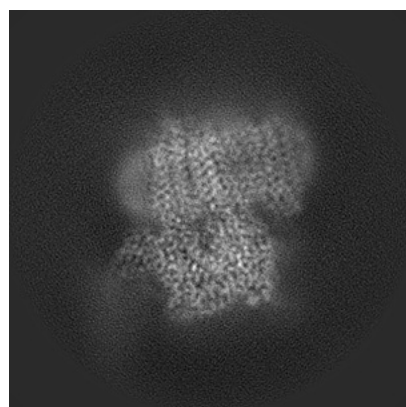


Y

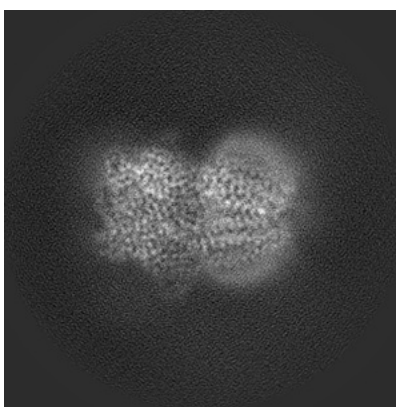


Z

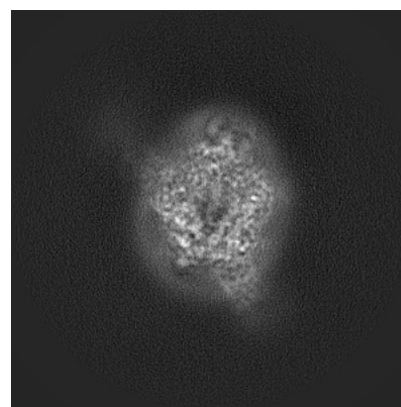
6.1.2 Raw map



X



Y

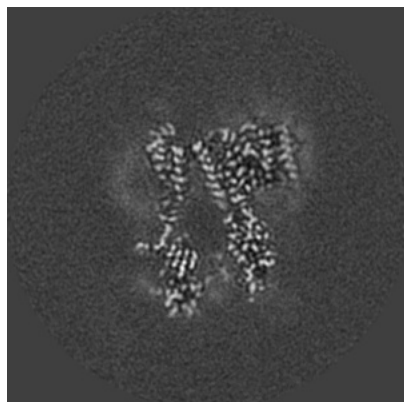


Z

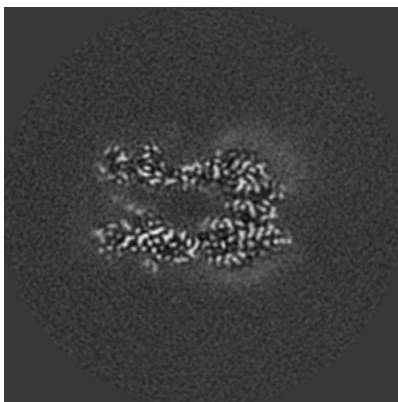
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

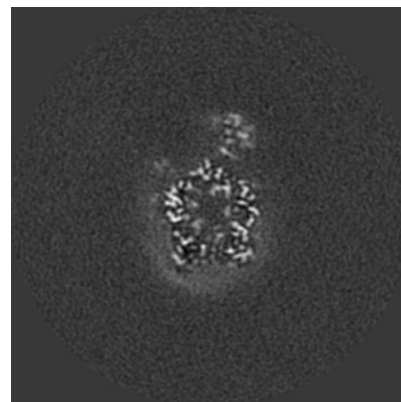
6.2.1 Primary map



X Index: 148

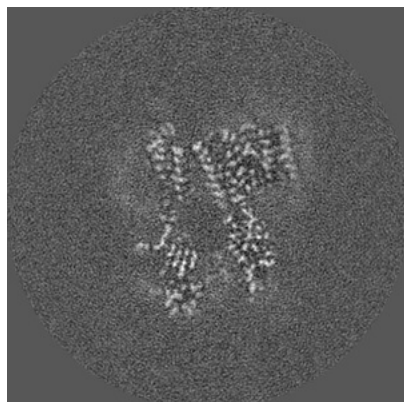


Y Index: 148

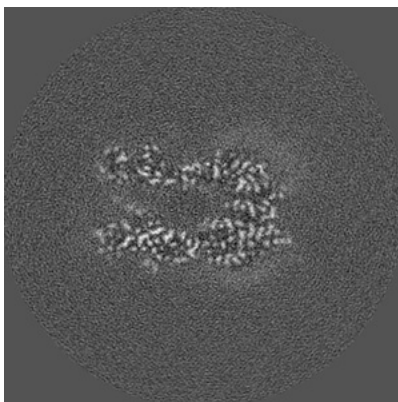


Z Index: 148

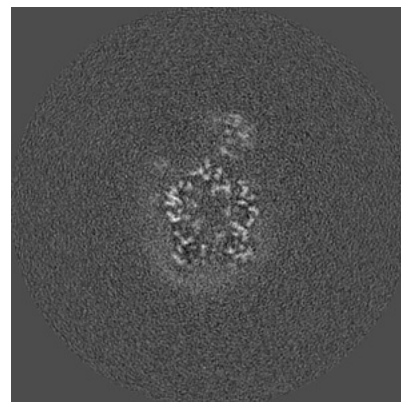
6.2.2 Raw map



X Index: 148



Y Index: 148

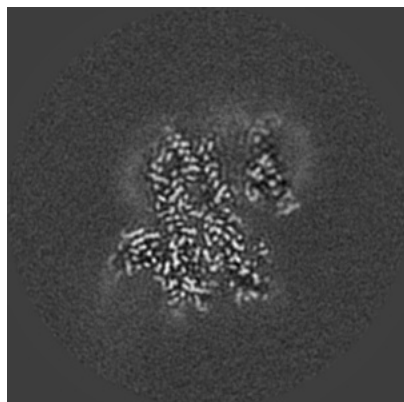


Z Index: 148

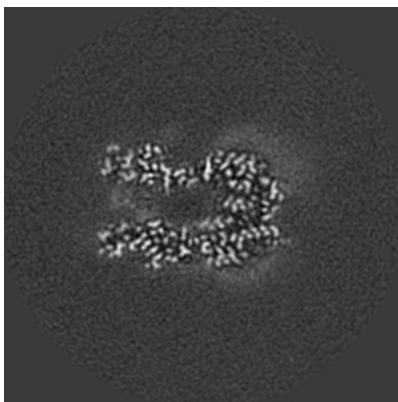
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

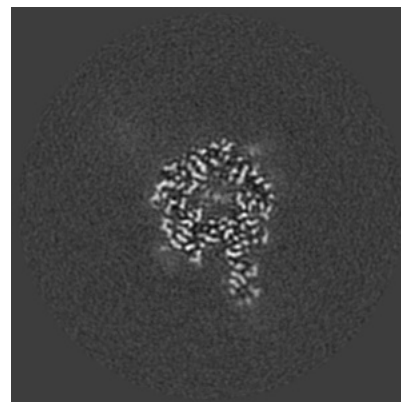
6.3.1 Primary map



X Index: 167

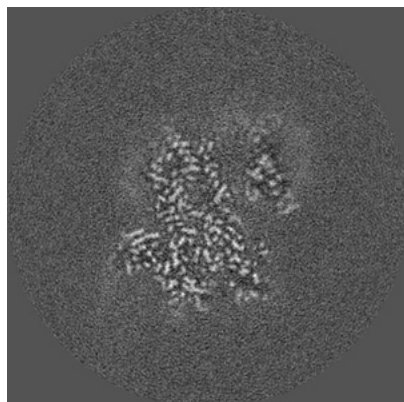


Y Index: 150

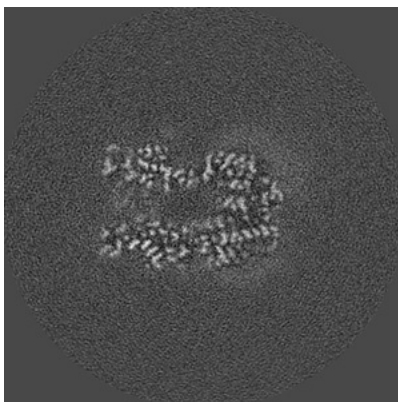


Z Index: 104

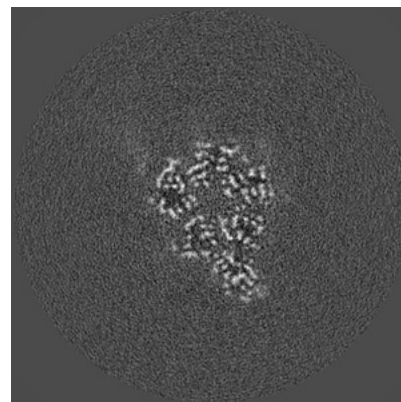
6.3.2 Raw map



X Index: 167



Y Index: 151

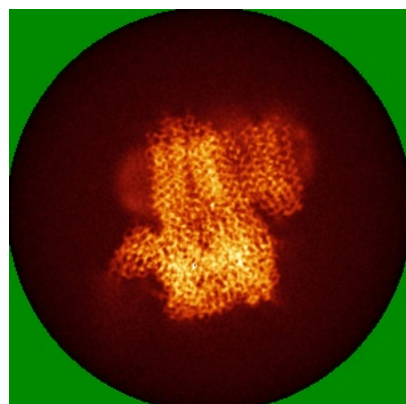


Z Index: 115

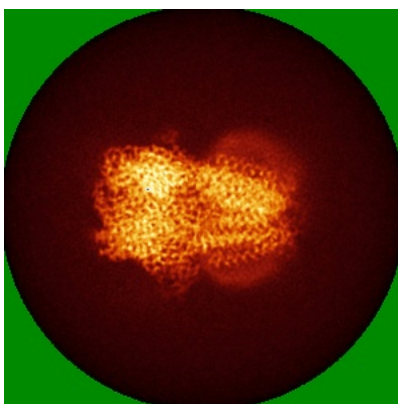
The images above show the largest variance slices of the map in three orthogonal directions.

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

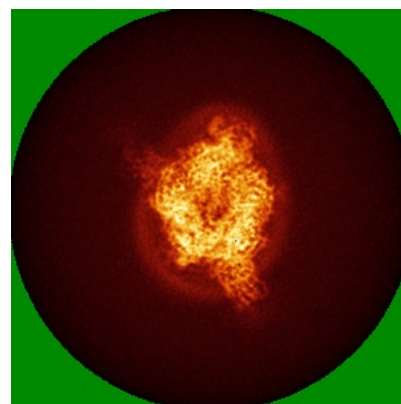
6.4.1 Primary map



X

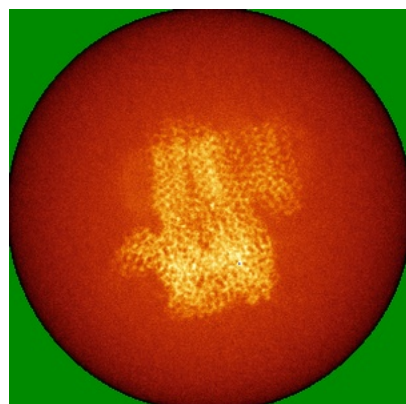


Y

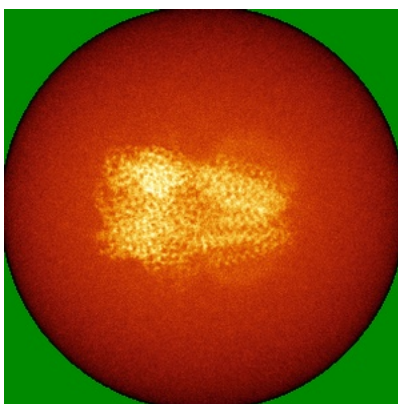


Z

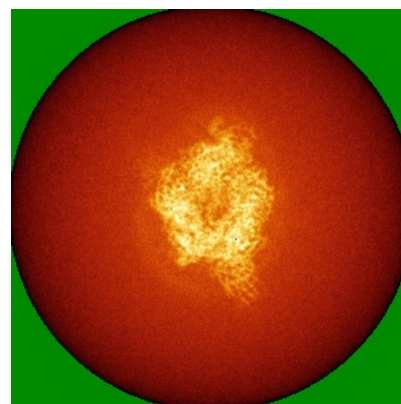
6.4.2 Raw map



X



Y

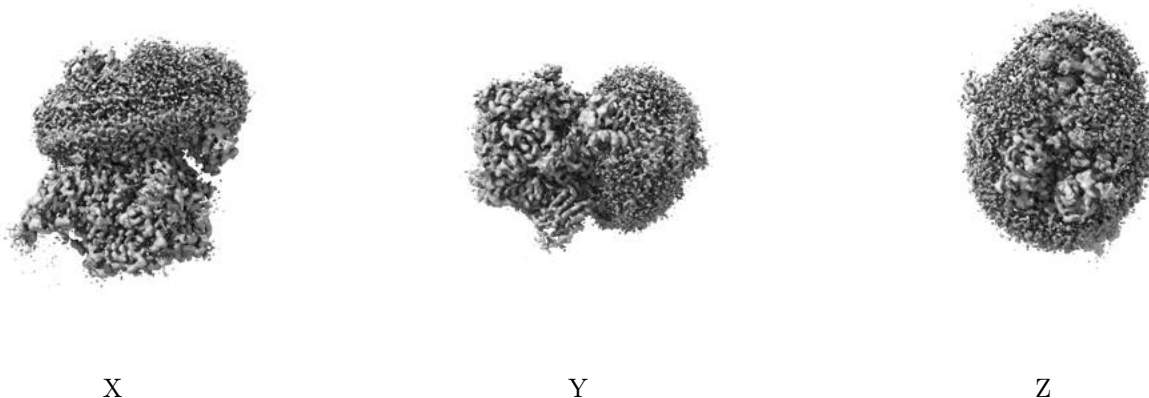


Z

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.

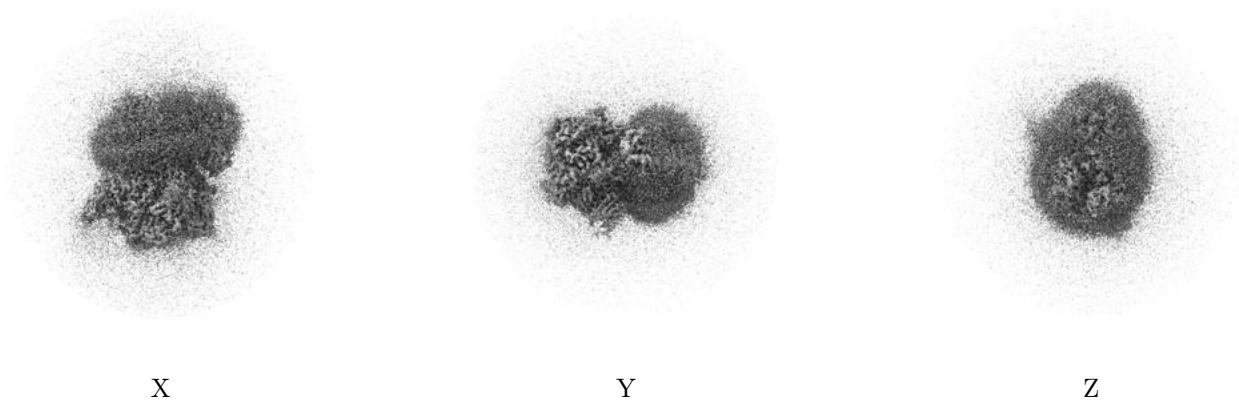
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

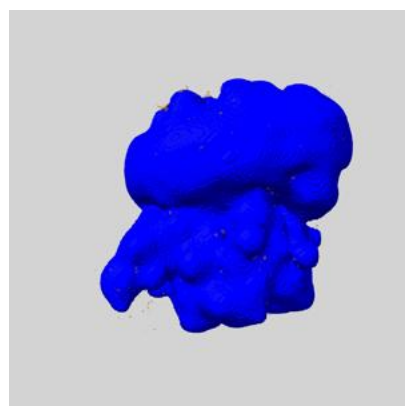
6.6 Mask visualisation [i](#)

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

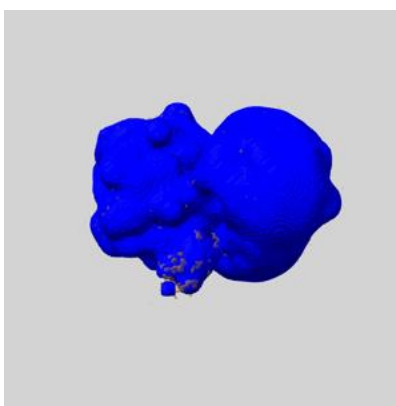
A mask typically either:

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

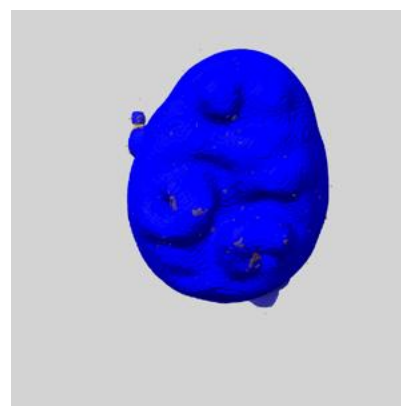
6.6.1 emd_50273_msk_1.map [i](#)



X



Y

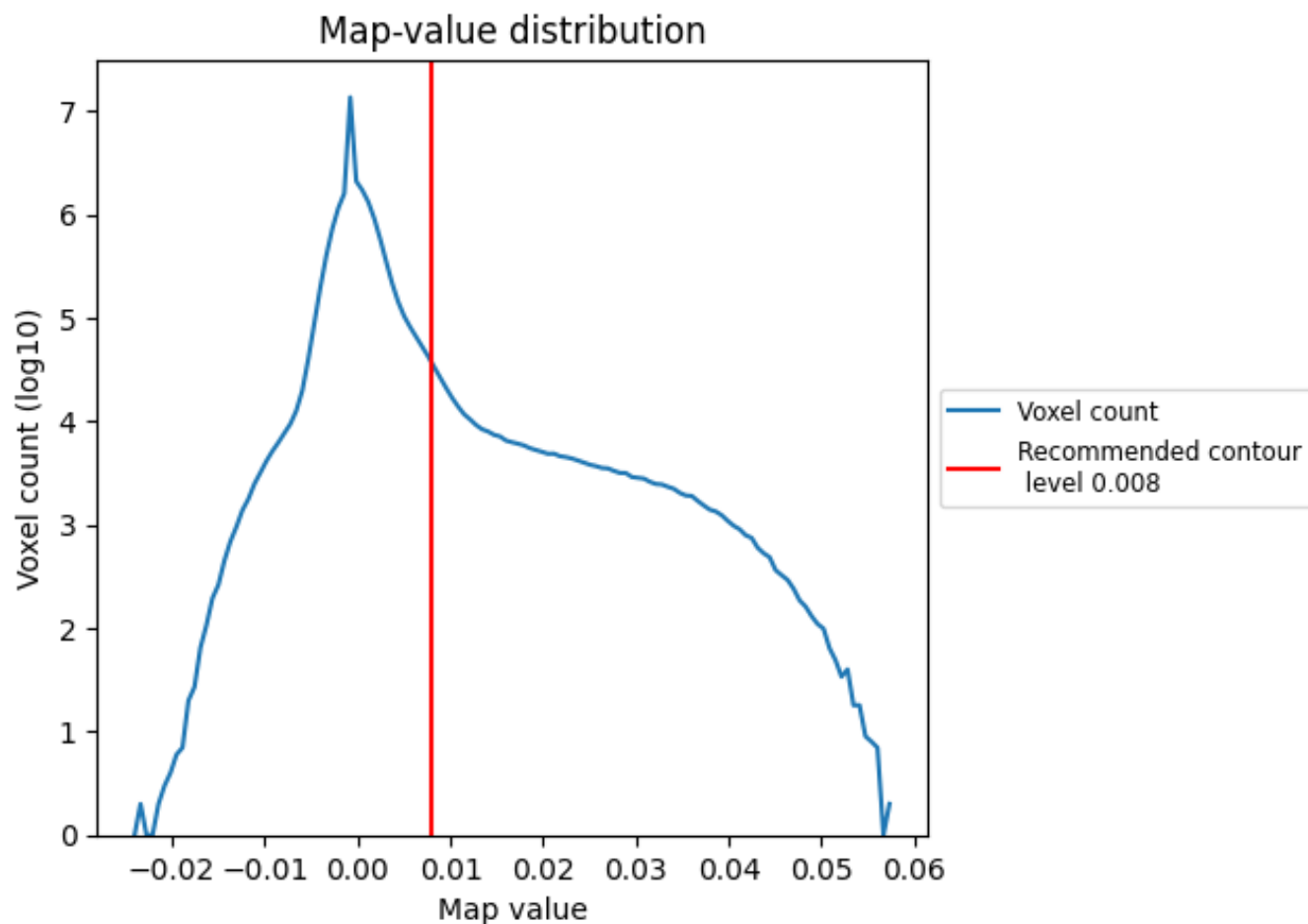


Z

7 Map analysis [i](#)

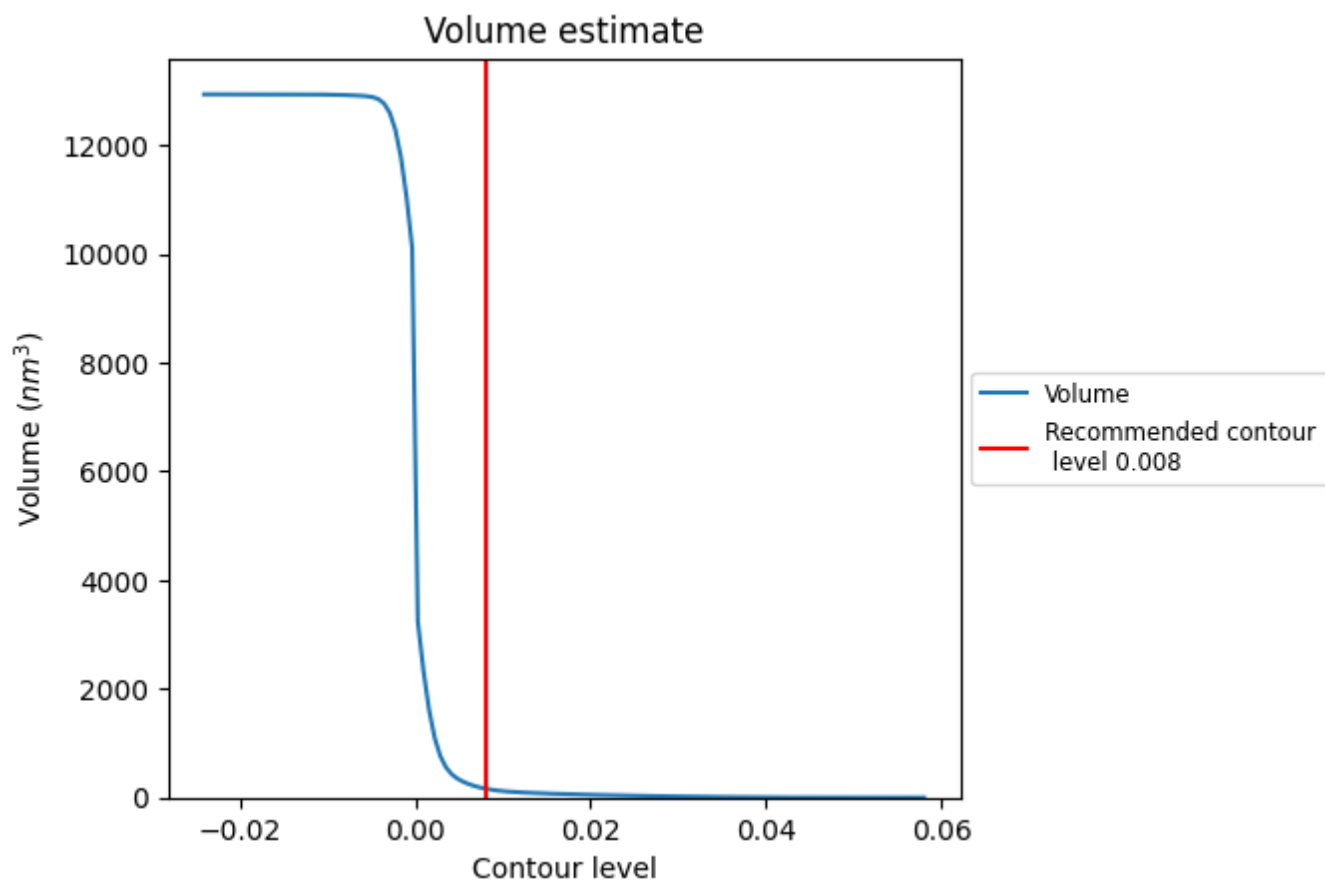
This section contains the results of statistical analysis of the map.

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.

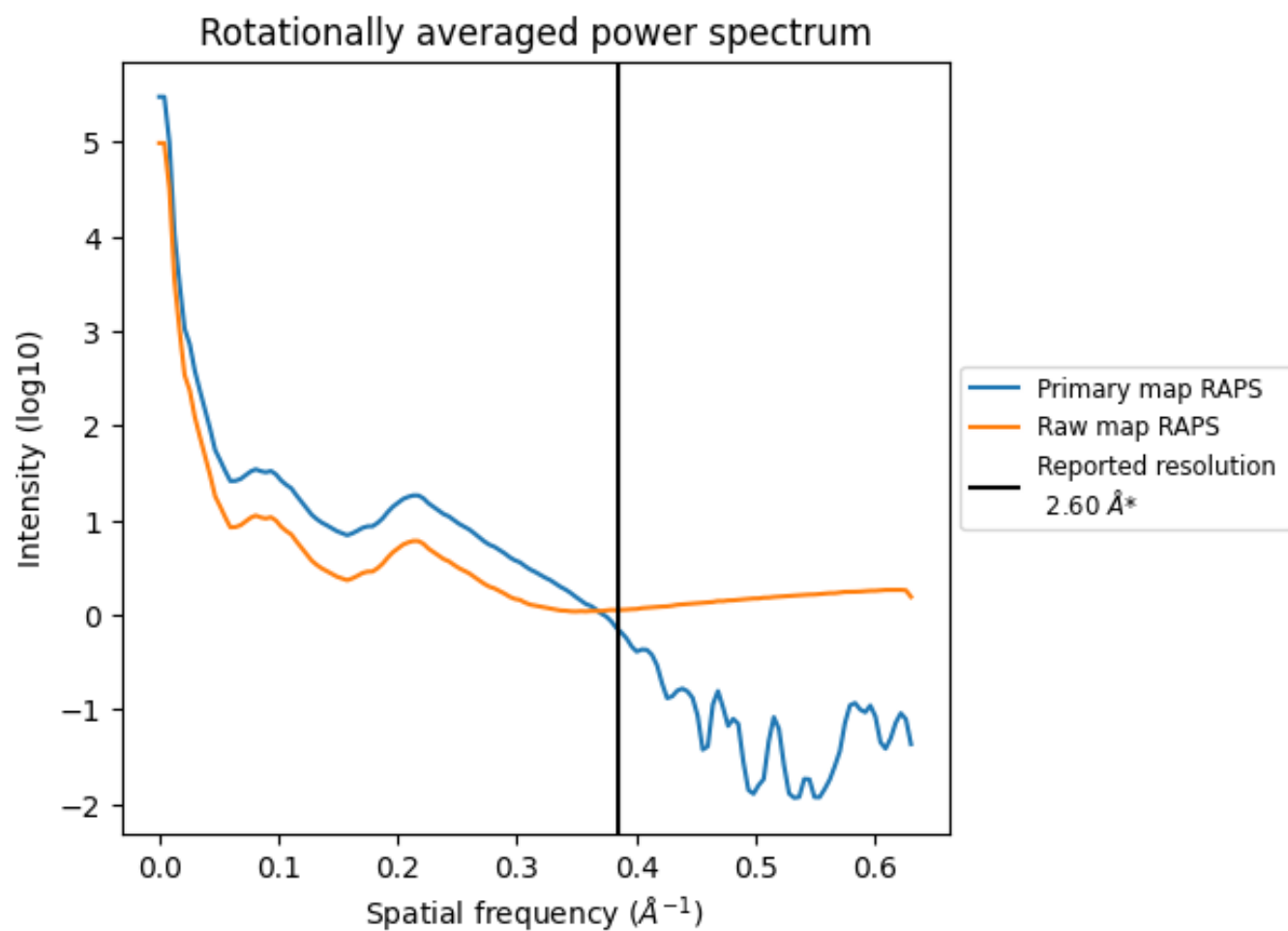
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm^3 ; this corresponds to an approximate mass of 148 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 ⓘ

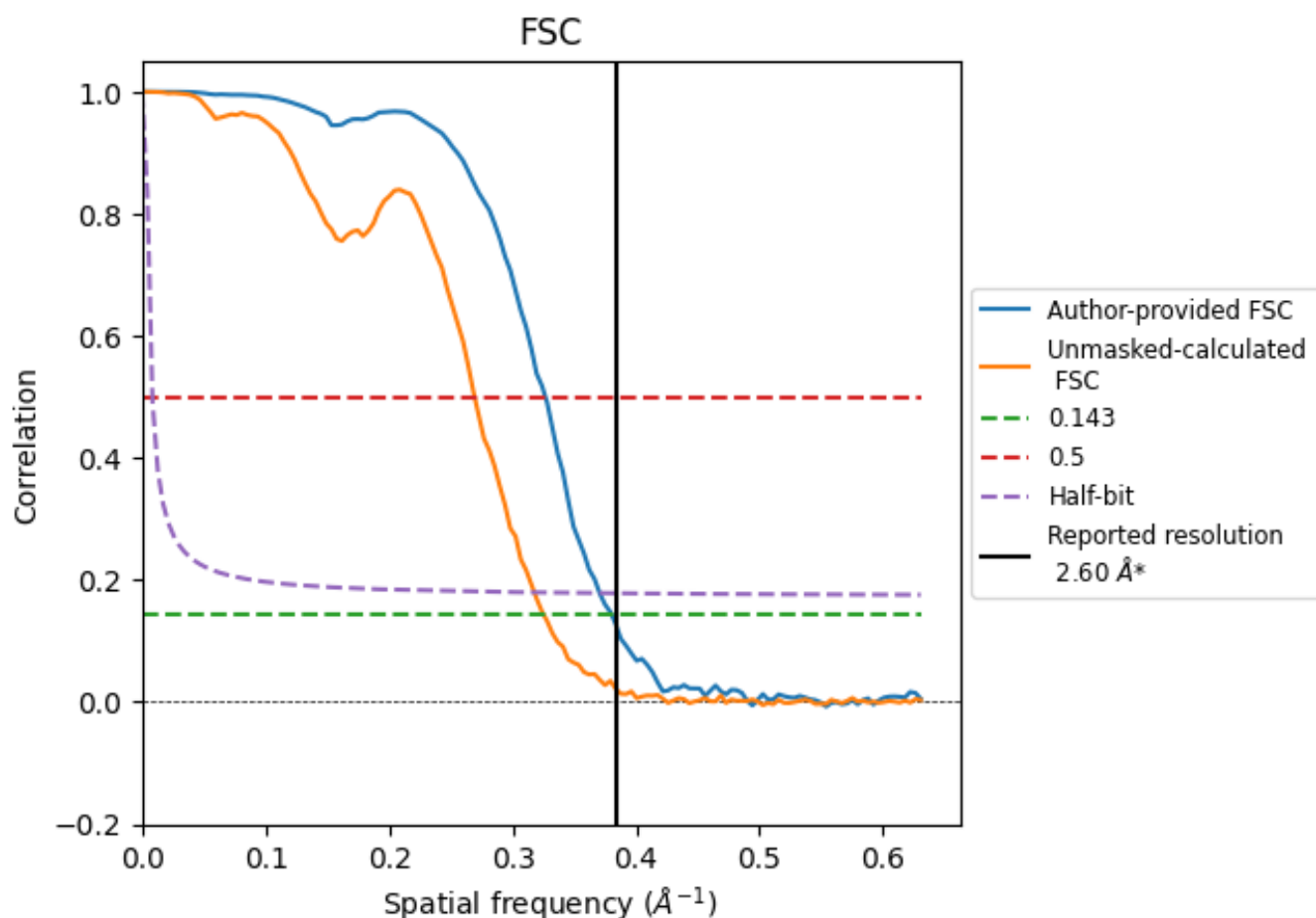


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

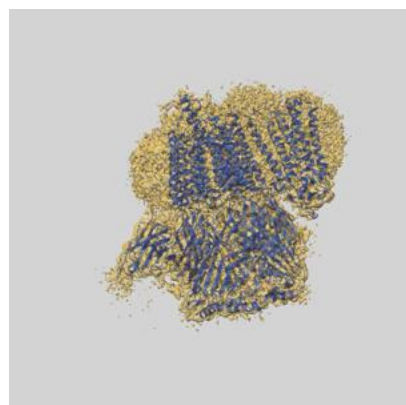
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.63	3.06	2.70
Unmasked-calculated*	3.08	3.71	3.15

*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 3.08 differs from the reported value 2.6 by more than 10 %

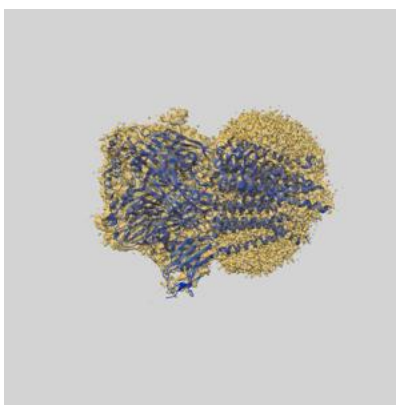
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50273 and PDB model 9FAJ. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

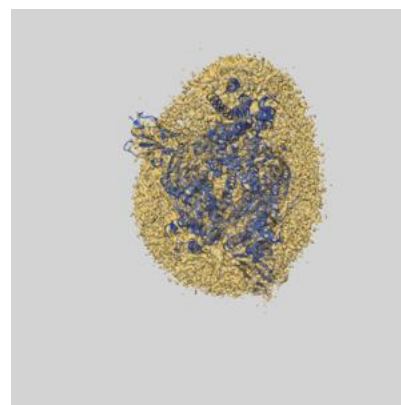
9.1 Map-model overlay [i](#)



X



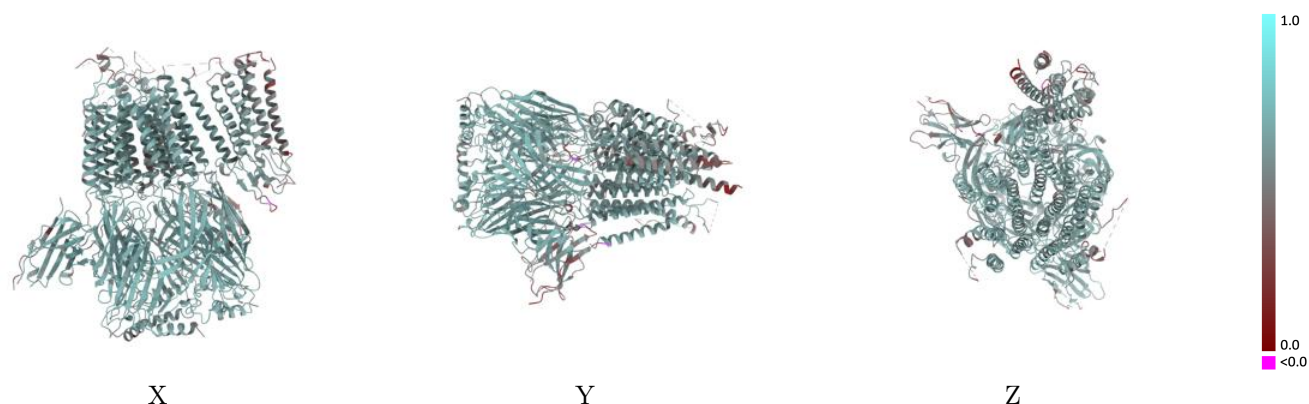
Y



Z

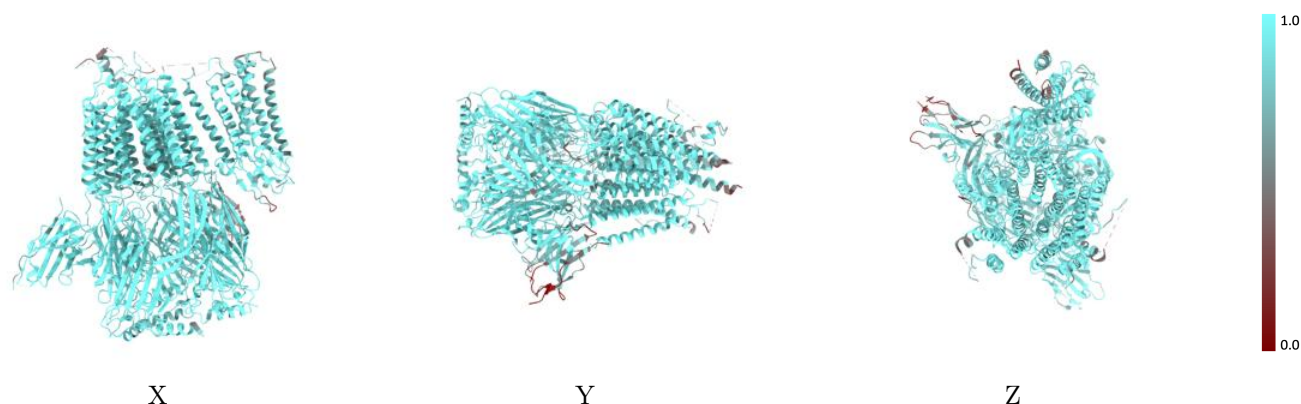
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



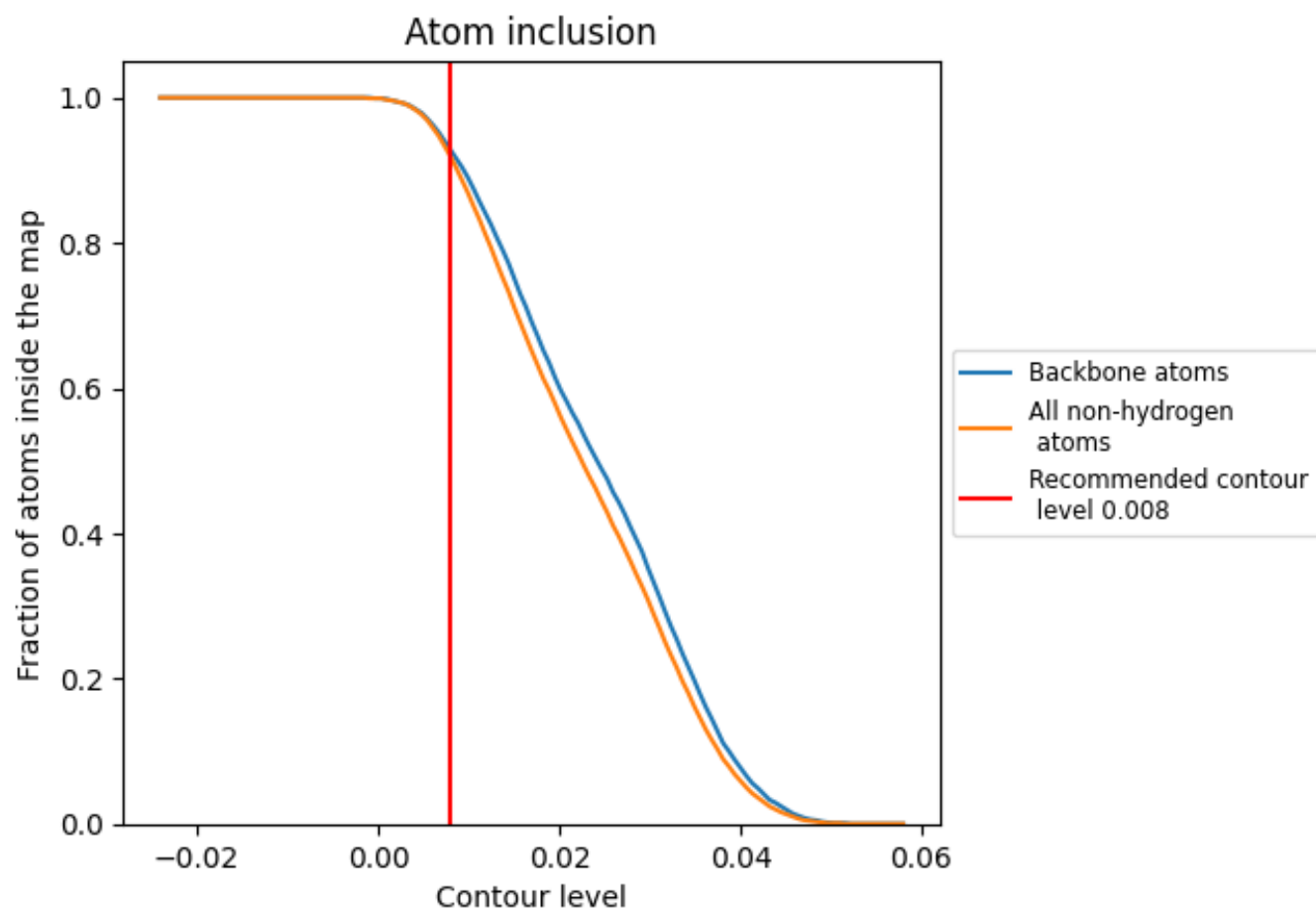
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9190	<div></div> 0.5960
A	<div></div> 0.9480	<div></div> 0.6200
B	<div></div> 0.9500	<div></div> 0.6130
C	<div></div> 0.9380	<div></div> 0.6030
D	<div></div> 0.9450	<div></div> 0.6170
E	<div></div> 0.9480	<div></div> 0.6150
F	<div></div> 0.9310	<div></div> 0.5580
G	<div></div> 0.9520	<div></div> 0.6030
H	<div></div> 0.7570	<div></div> 0.4360
I	<div></div> 0.7690	<div></div> 0.4550
J	<div></div> 0.9310	<div></div> 0.5800
K	<div></div> 0.8210	<div></div> 0.5190
L	<div></div> 0.8730	<div></div> 0.5310
M	<div></div> 0.8060	<div></div> 0.4890
N	<div></div> 0.9310	<div></div> 0.5720
O	<div></div> 0.7950	<div></div> 0.5430
P	<div></div> 0.6340	<div></div> 0.4790

1.0

0.0

<0.0