



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2025 – 07:23 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 wwPDB EM Validation Summary 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

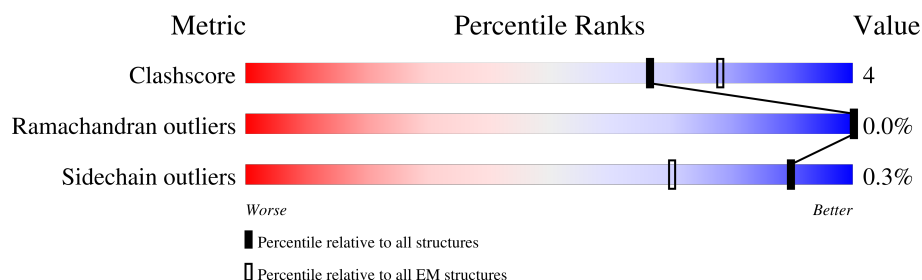
1 Overall quality at a glance

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

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		

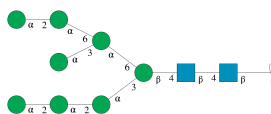
- Molecule 5 is a protein called LHFPL tetraspan subfamily member 4 protein.

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.

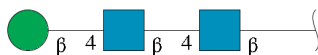
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	121	Total	C	N	O	S	1	0
			949	594	172	179	4		
6	P	121	Total	C	N	O	S	0	0
			941	589	169	179	4		

- 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.



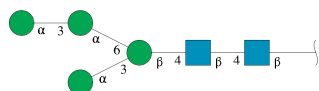
Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	10	Total	C	N	O		0	0
			116	64	2	50			

- 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.



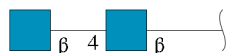
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	3	Total	C	N	O		0	0
			39	22	2	15			
8	O	3	Total	C	N	O		0	0
			39	22	2	15			

- 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.



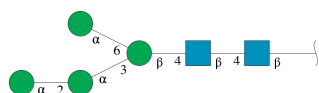
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	6	Total	C	N	O	0	0
			72	40	2	30		
9	N	6	Total	C	N	O	0	0
			72	40	2	30		

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



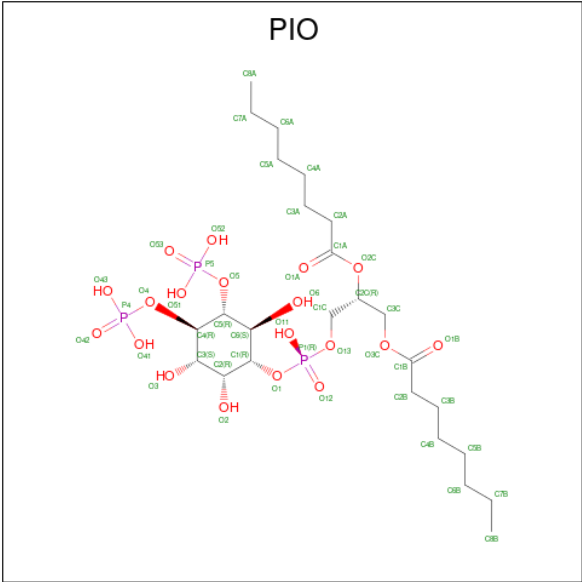
Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.



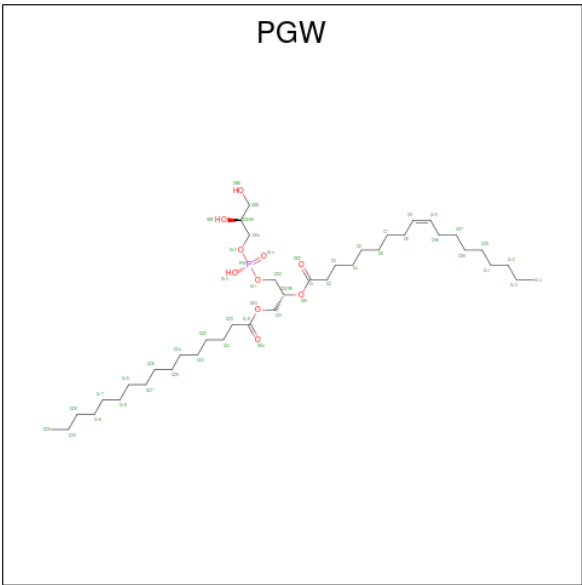
Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 12 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-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).



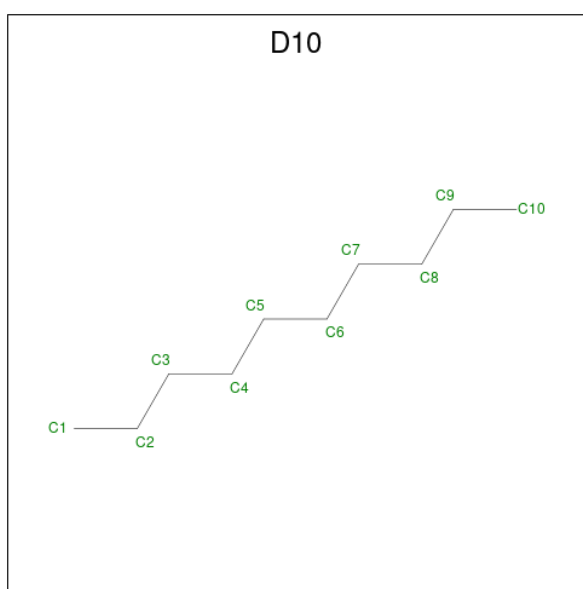
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	1
			102	80	20	2	

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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).



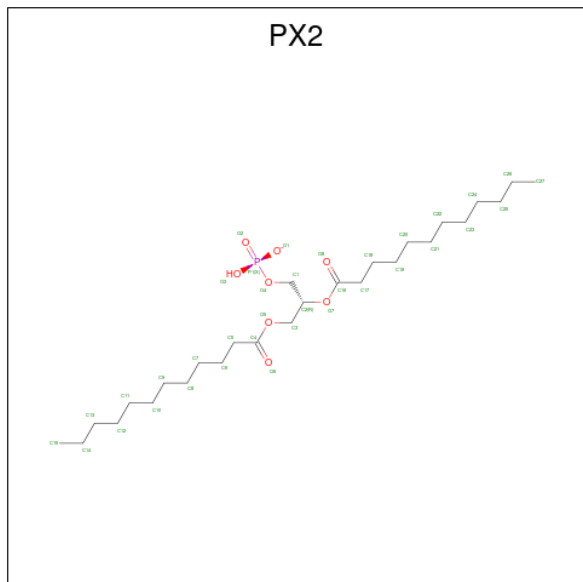
Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	C	0
			10	10	
14	A	1	Total	C	0
			10	10	
14	A	1	Total	C	0
			10	10	
14	A	1	Total	C	0
			10	10	
14	B	1	Total	C	0
			10	10	
14	B	1	Total	C	0
			10	10	
14	C	1	Total	C	0
			10	10	

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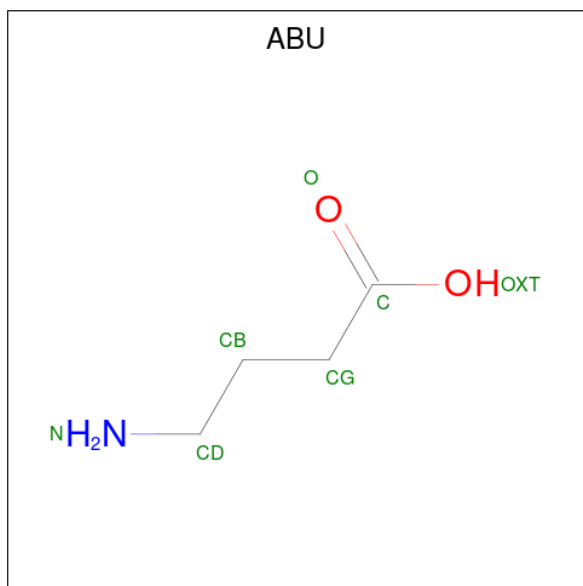
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Mol	Chain	Residues	Atoms	AltConf
14	D	1	Total C 10 10	0
14	D	1	Total C 10 10	0
14	E	1	Total C 10 10	0
14	E	1	Total C 10 10	0
14	L	1	Total C 10 10	0

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



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

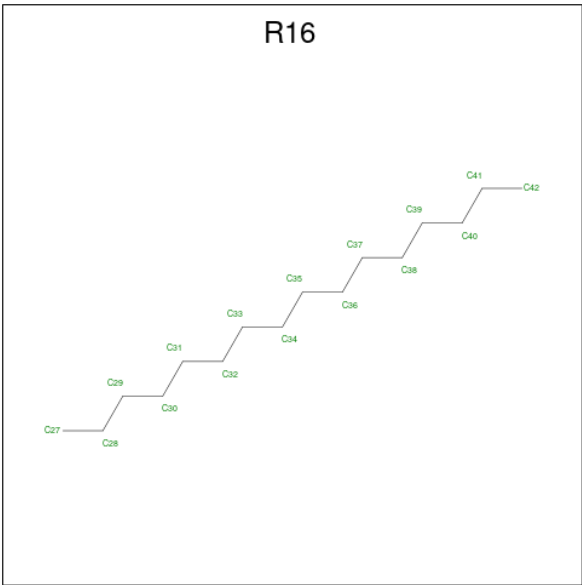


Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	N	O	0
			7	4	1	2	
16	E	1	Total	C	N	O	0
			7	4	1	2	

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

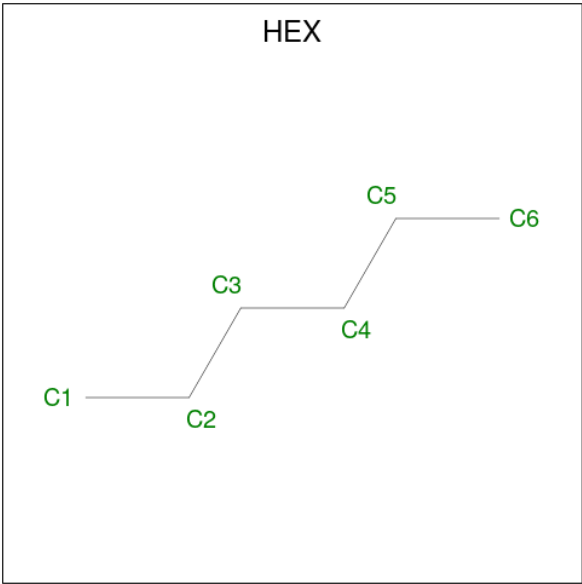
Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Cl	0
			1	1	
17	C	1	Total	Cl	0
			1	1	
17	D	1	Total	Cl	0
			1	1	
17	L	1	Total	Cl	0
			1	1	

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



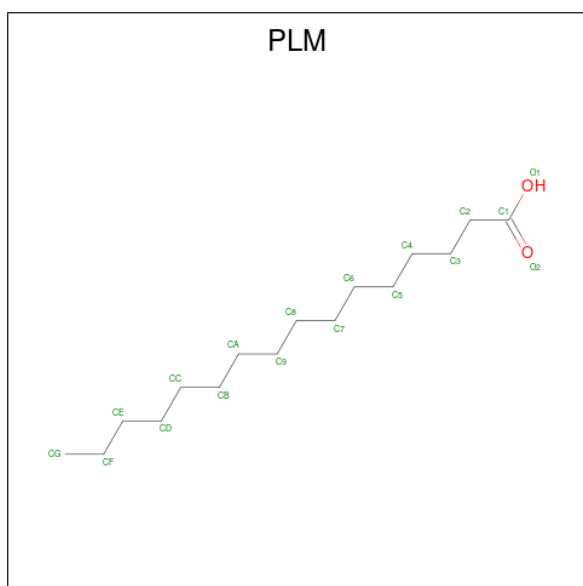
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	C	0
			16	16	
18	B	1	Total	C	0
			16	16	
18	E	1	Total	C	0
			16	16	
18	E	1	Total	C	0
			16	16	

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



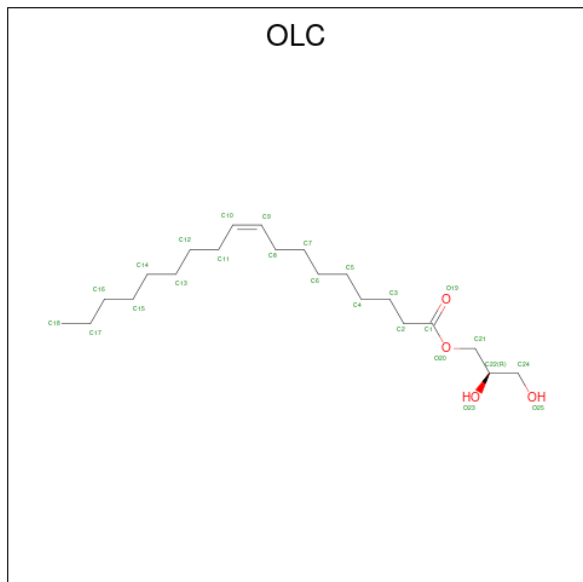
Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	C	0
			6	6	
19	B	1	Total	C	0
			6	6	
19	B	1	Total	C	0
			6	6	
19	D	1	Total	C	0
			6	6	
19	D	1	Total	C	0
			6	6	
19	E	1	Total	C	0
			6	6	
19	E	1	Total	C	0
			6	6	

- Molecule 20 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



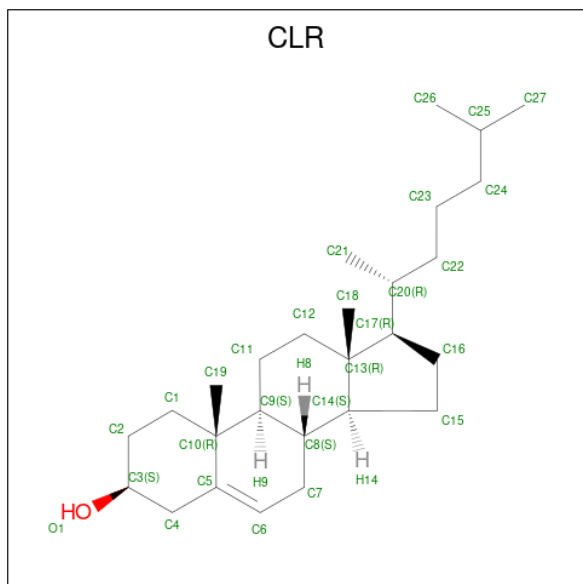
Mol	Chain	Residues	Atoms			AltConf
20	C	1	Total	C	O	0
			14	12	2	
20	C	1	Total	C	O	0
			18	16	2	
20	C	1	Total	C	O	0
			18	16	2	
20	C	1	Total	C	O	0
			18	16	2	
20	E	1	Total	C	O	0
			18	16	2	

- Molecule 21 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			AltConf
21	C	1	Total	C	O	0
			21	17	4	

- 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.

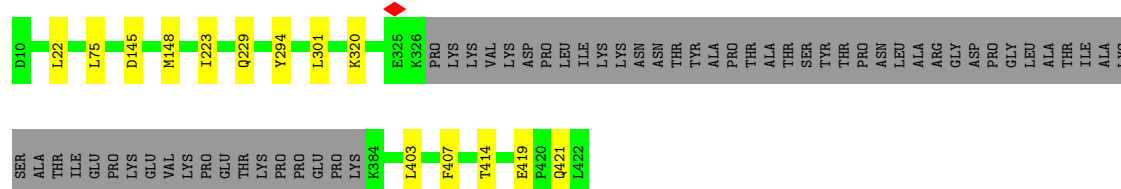
Mol	Chain	Residues	Atoms		AltConf
23	A	24	Total 24	O 24	0
23	B	21	Total 21	O 21	0
23	C	16	Total 16	O 16	0
23	D	13	Total 13	O 13	0
23	E	19	Total 19	O 19	0
23	L	1	Total 1	O 1	0
23	G	10	Total 10	O 10	0

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.

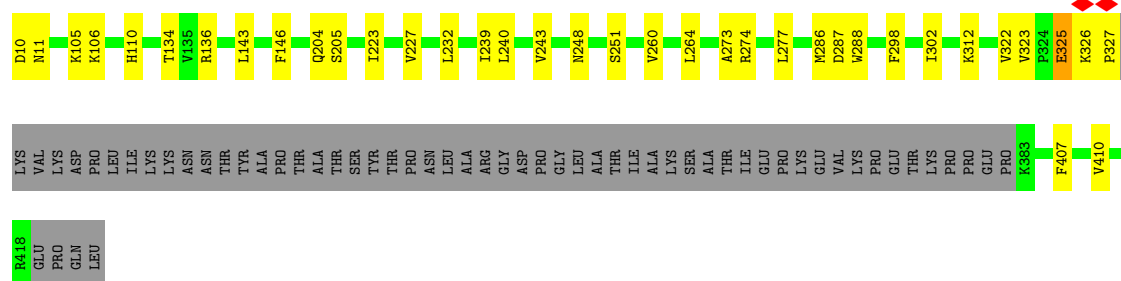
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain A: 



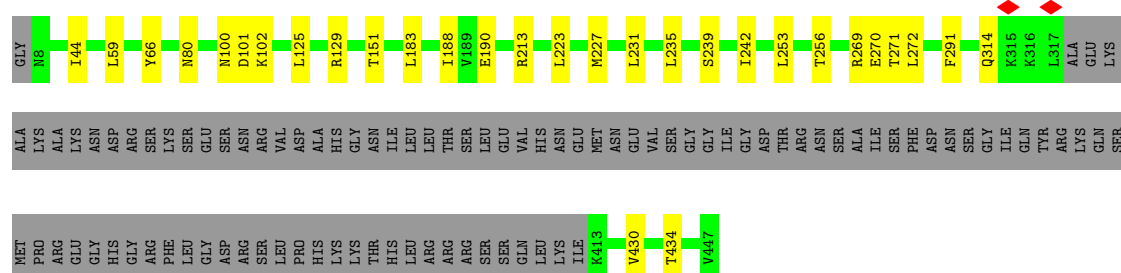
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

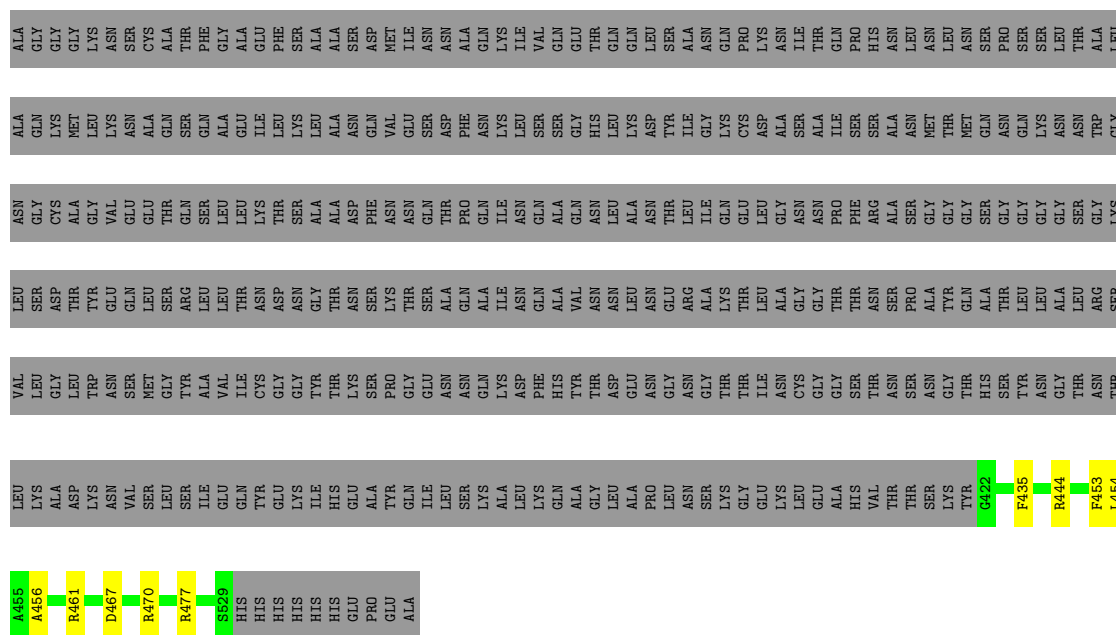
Chain D: 



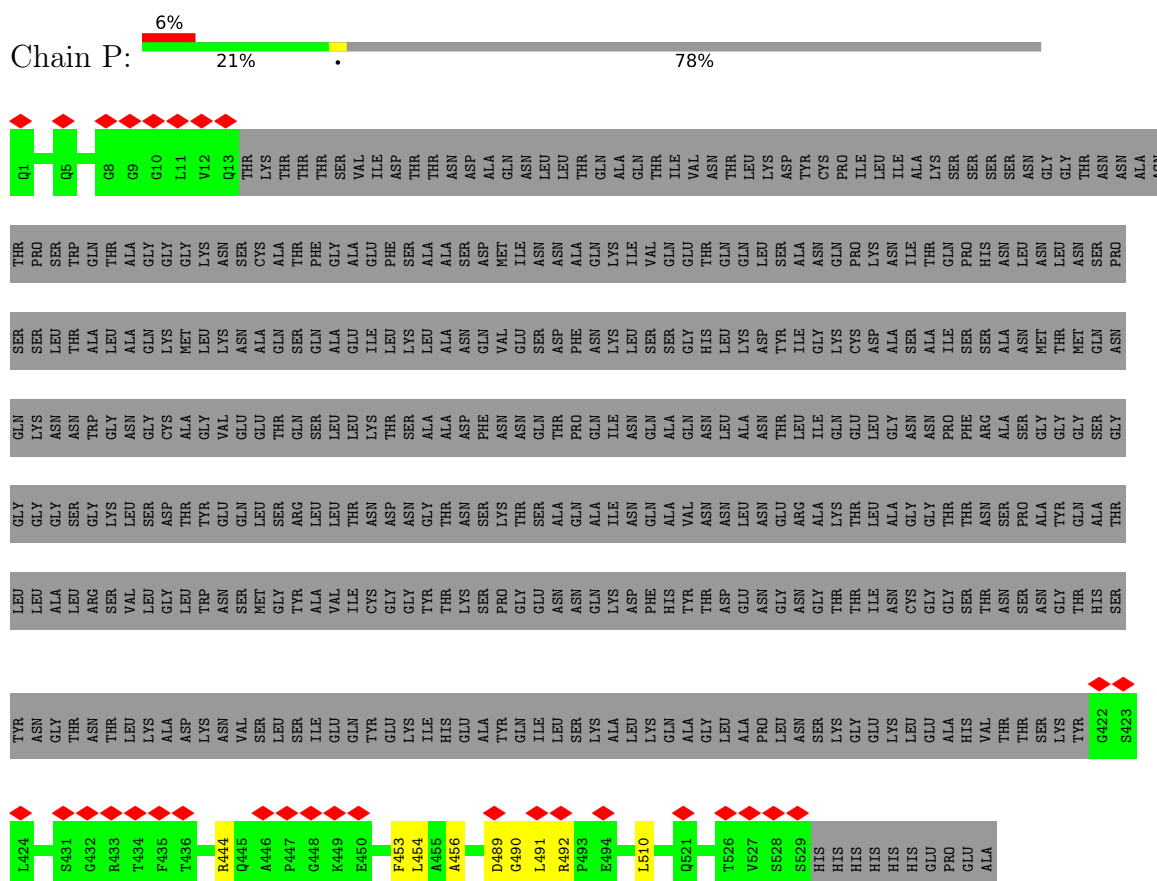
- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain B: 



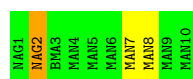


• Molecule 6: Megabody38



• 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(°)	Ideal(°)
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.

The worst 5 of 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

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 ⓘ

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

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	370	LEU
3	C	373	LYS
1	D	325	GLU
3	C	377	SER
3	C	369	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	185	GLN
2	E	421	ASN
6	G	3	GLN
4	H	690	ASN
2	B	90	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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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
3	C	380	P1L	2	0

5.5 Carbohydrates [i](#)

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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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:

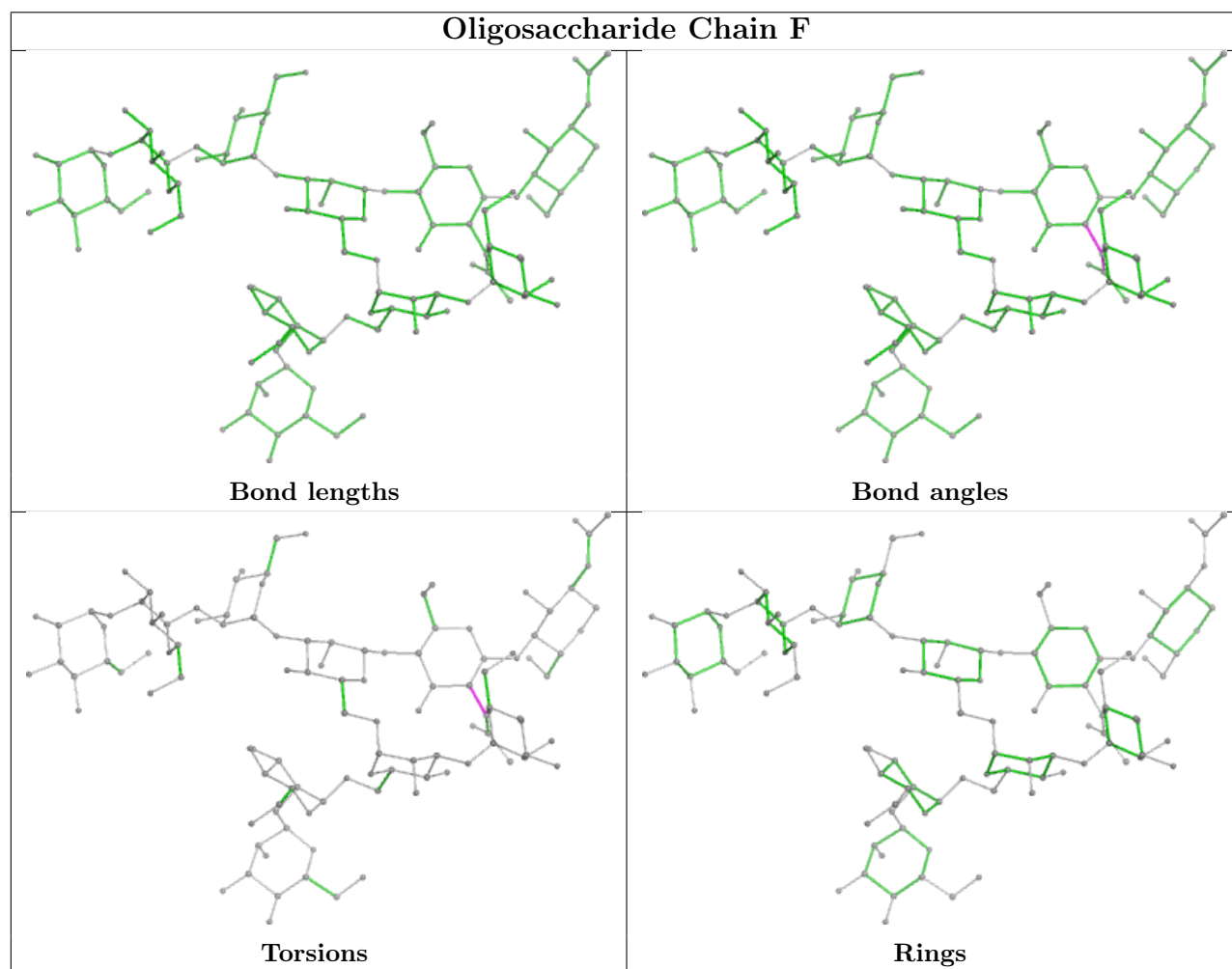
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	8	MAN	1	0
8	I	1	NAG	4	0

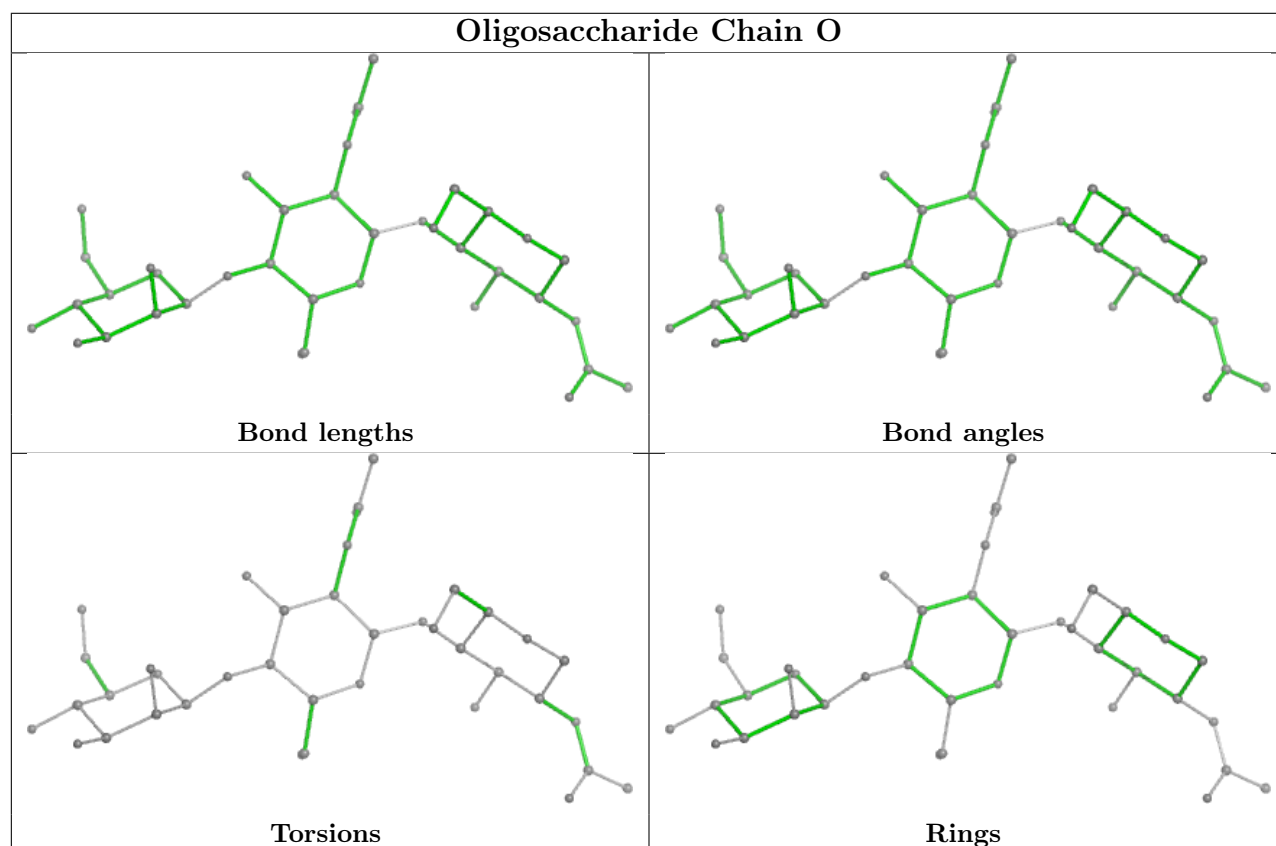
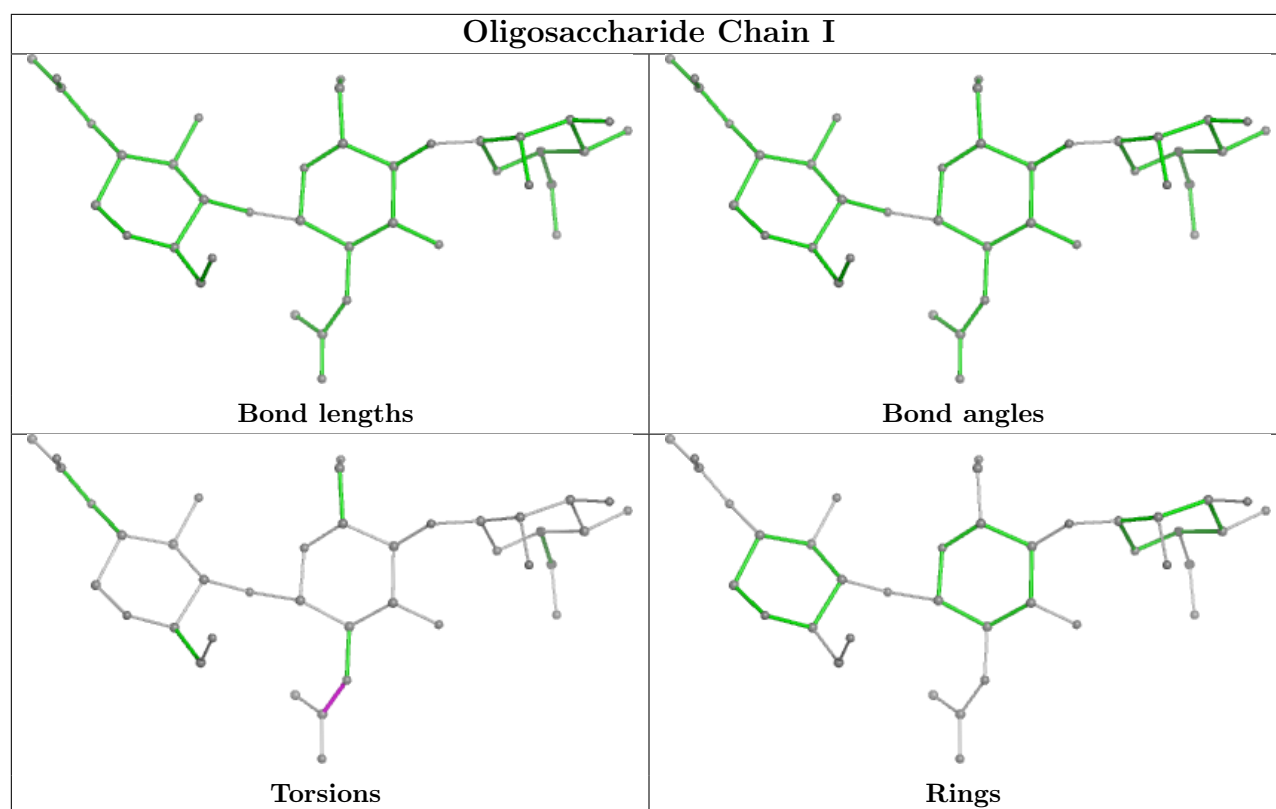
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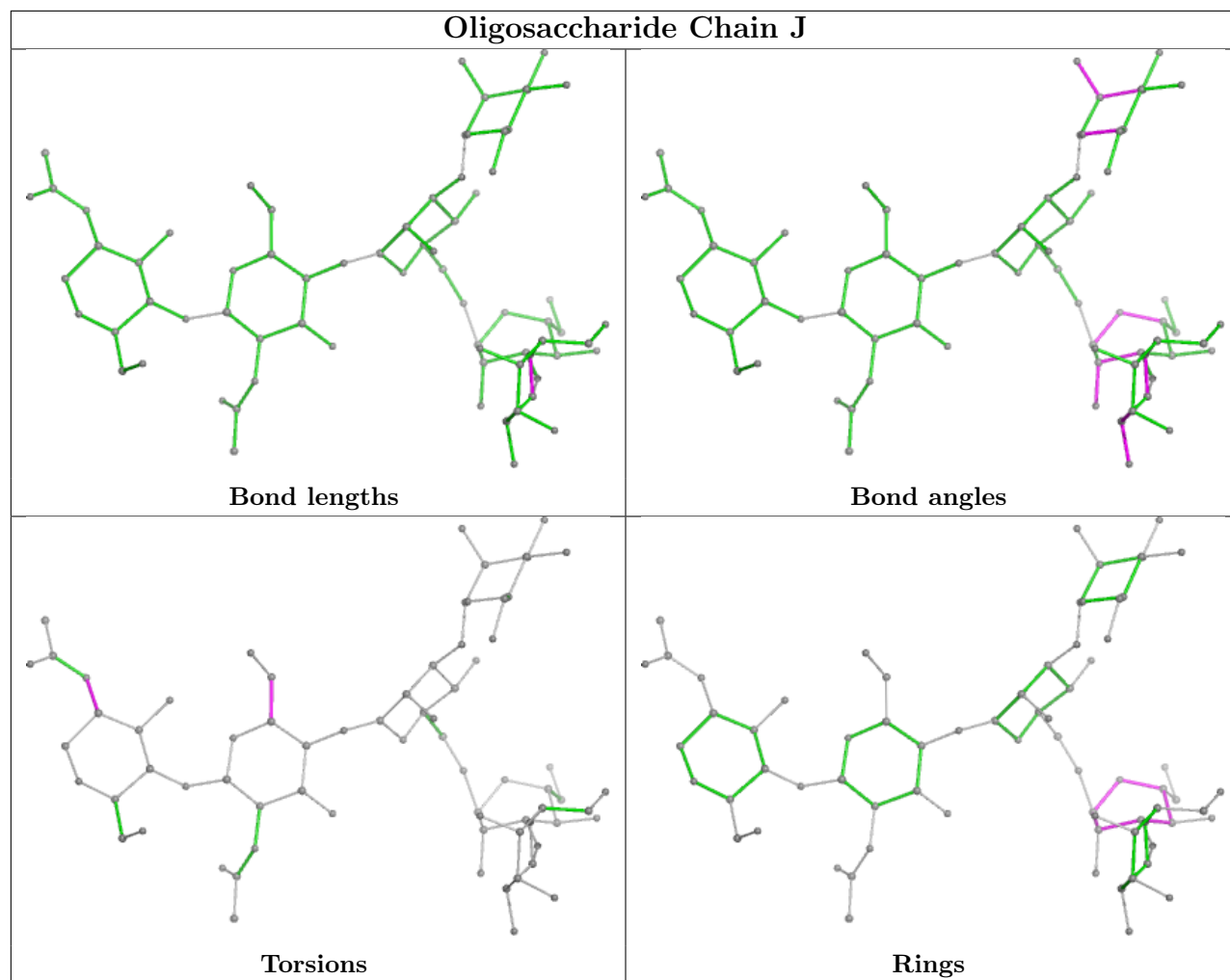
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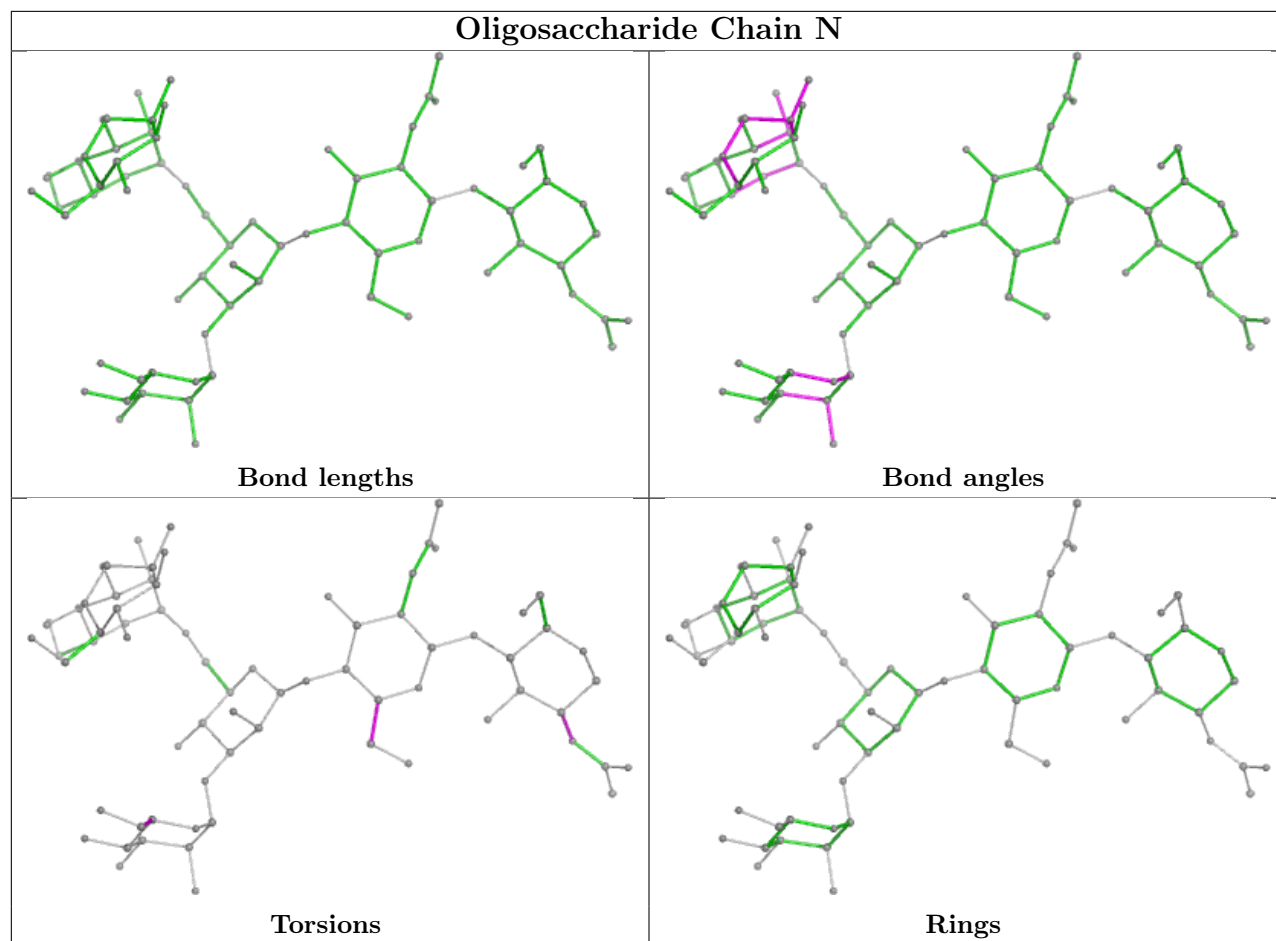
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	2	NAG	1	0
7	F	7	MAN	2	0
7	F	2	NAG	1	0
8	O	1	NAG	1	0
10	K	1	NAG	5	0

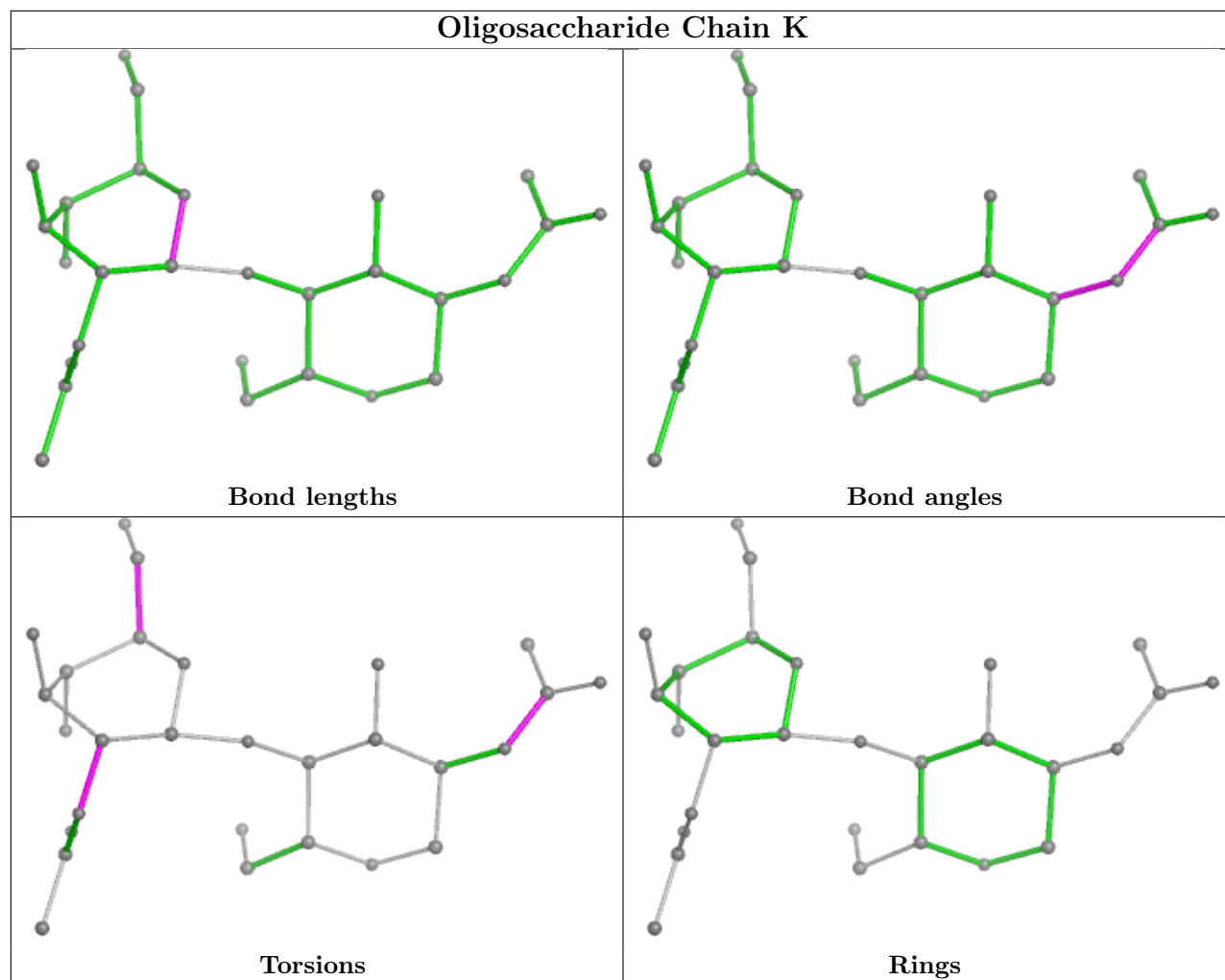
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

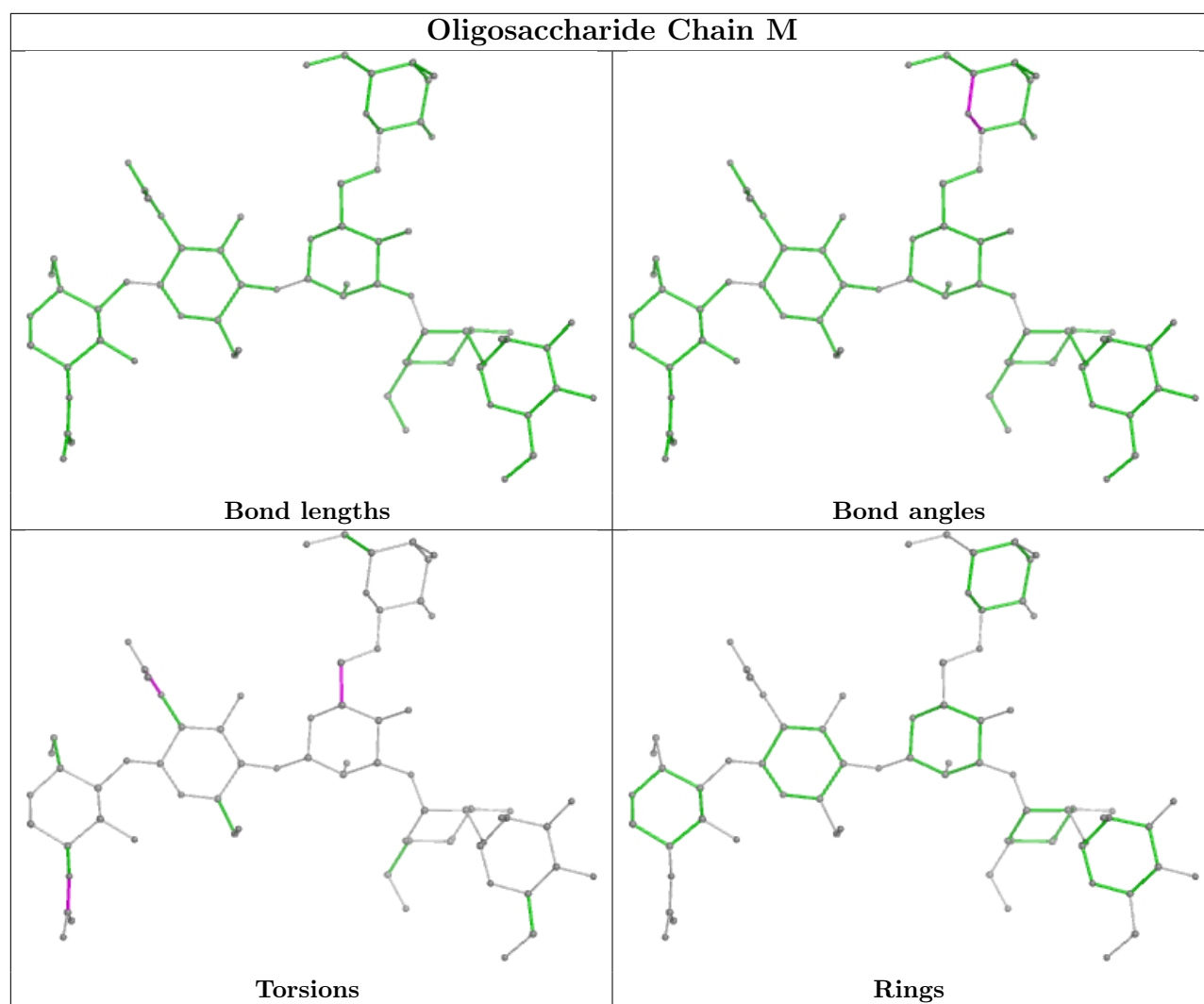












5.6 Ligand geometry [i](#)

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	-

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 288 torsion outliers are listed below:

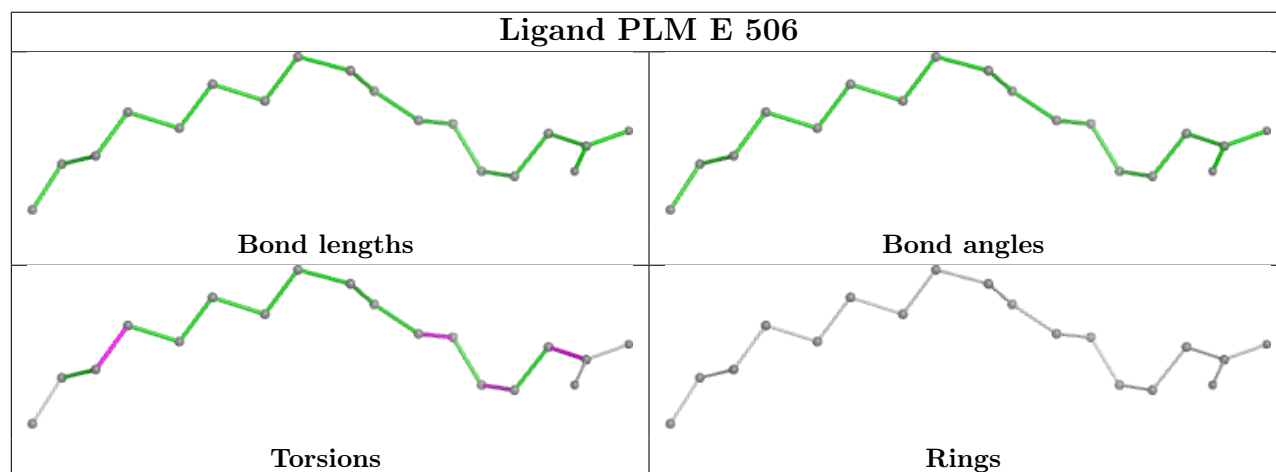
Mol	Chain	Res	Type	Atoms
12	A	3901	PIO	O1A-C1A-O2C-C2C
12	A	3901	PIO	C2A-C1A-O2C-C2C
12	D	3901	PIO	C2-C1-O1-P1
12	D	3901	PIO	C6-C1-O1-P1
12	D	3901	PIO	C1C-O13-P1-O12

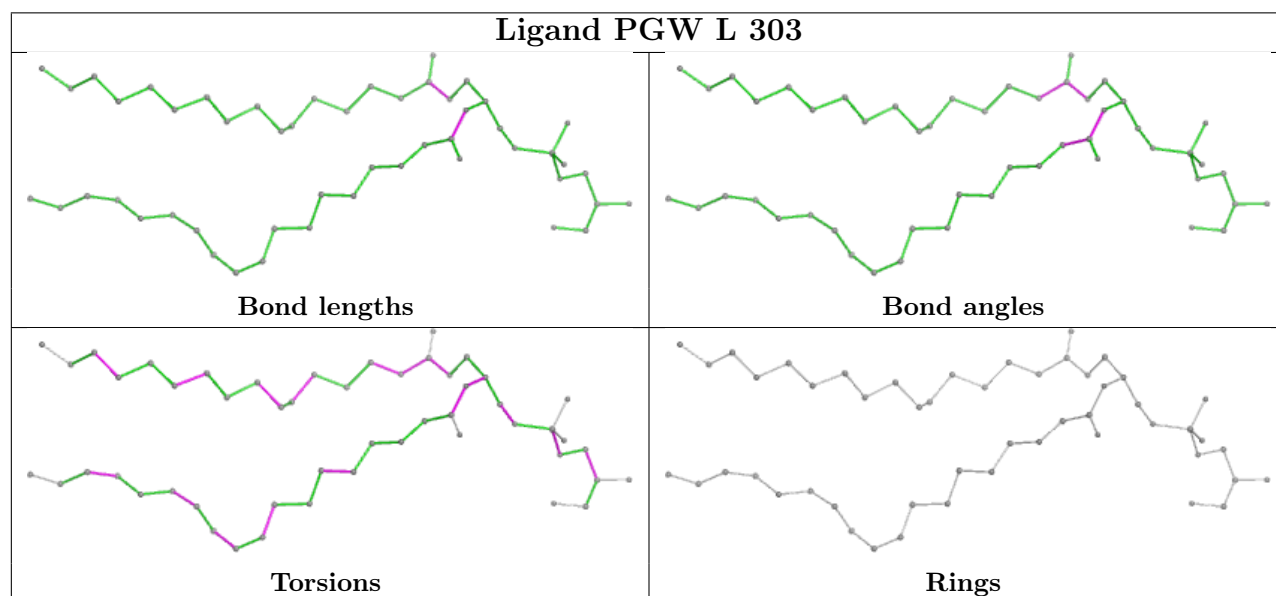
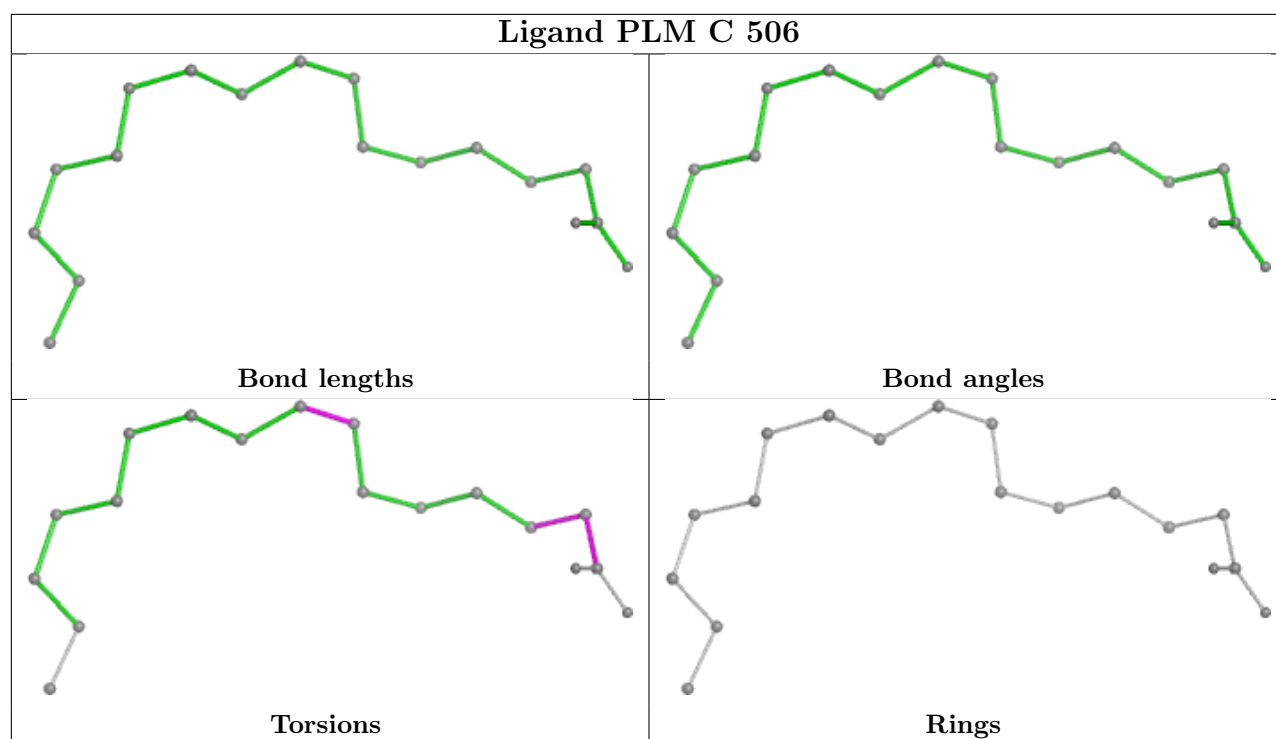
There are no ring outliers.

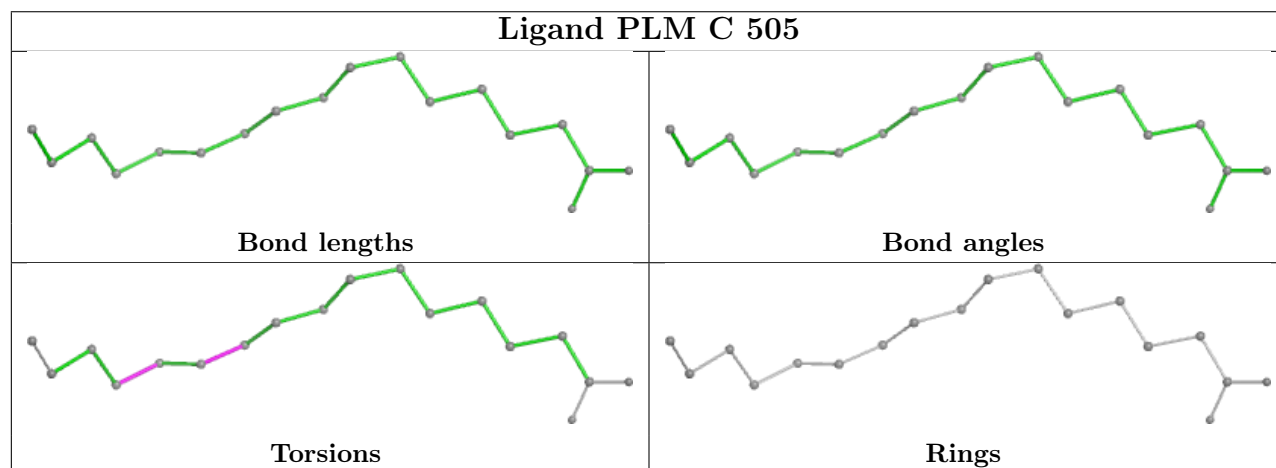
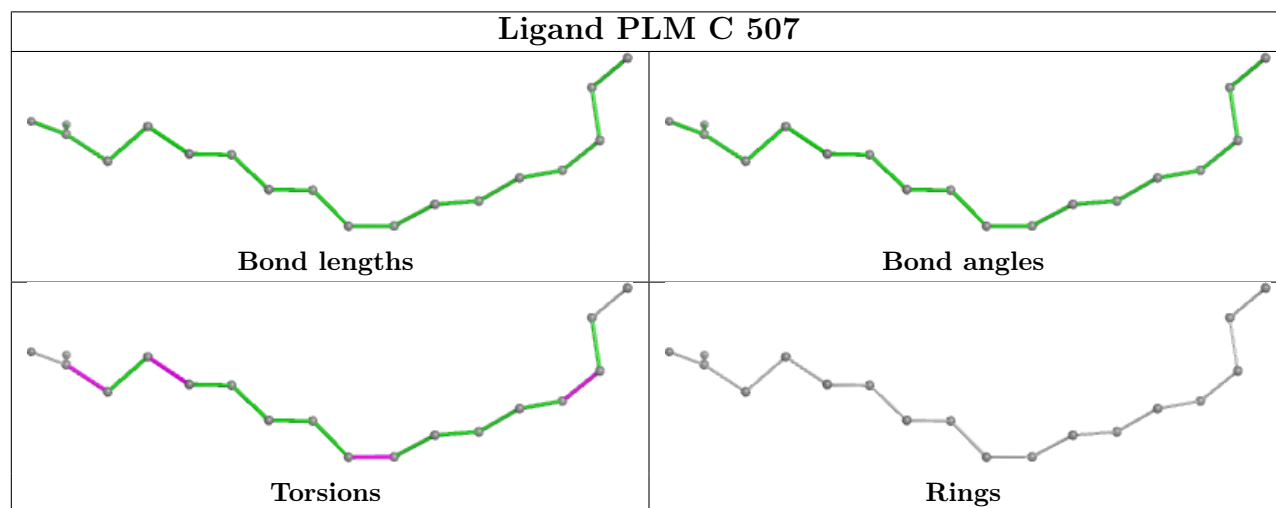
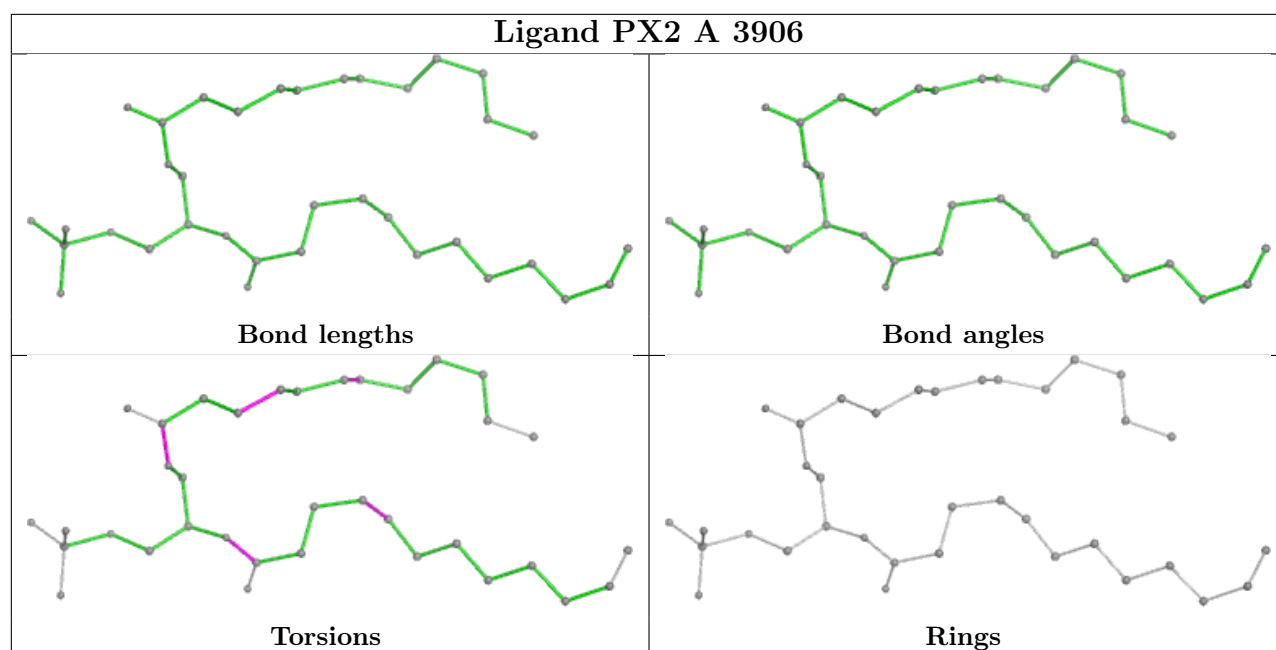
8 monomers are involved in 24 short contacts:

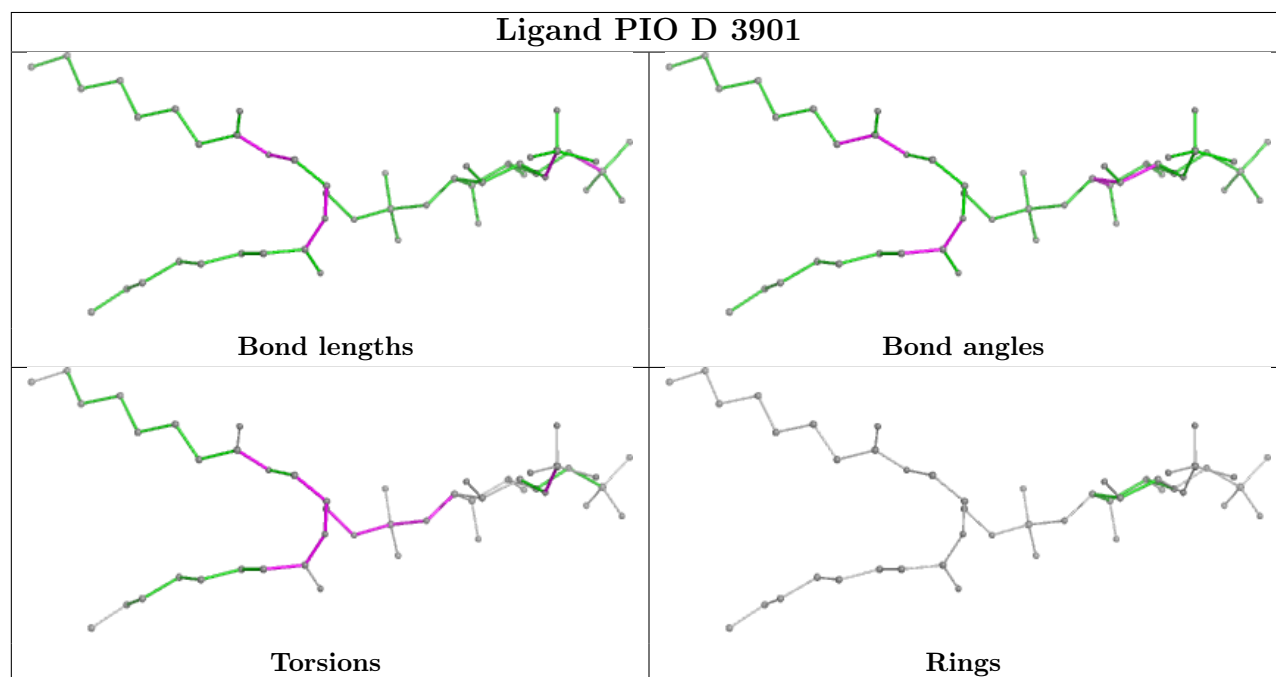
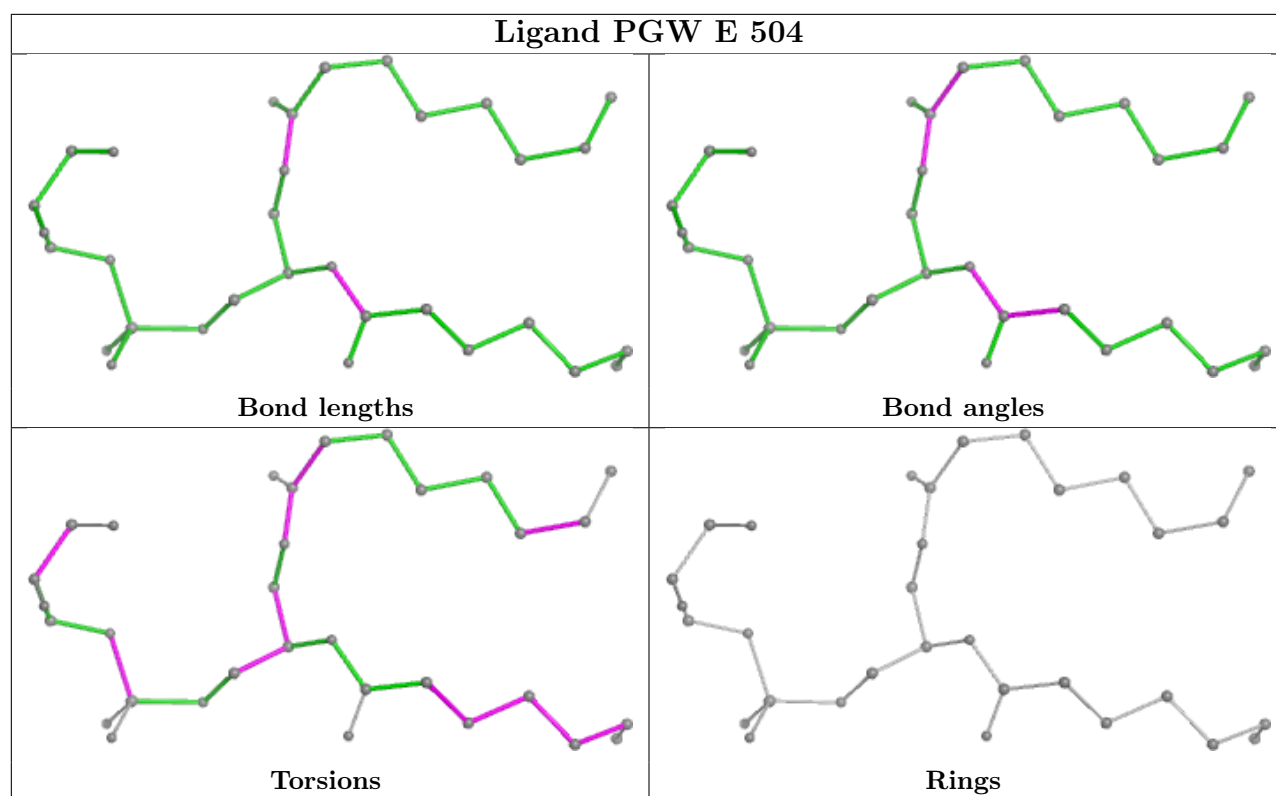
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	303	PGW	2	0
15	A	3906	PX2	5	0
12	D	3901	PIO	2	0
13	L	301	PGW	7	0
15	D	3907	PX2	5	0
15	E	501	PX2	1	0
13	D	3903[A]	PGW	1	0
22	C	508	CLR	4	0

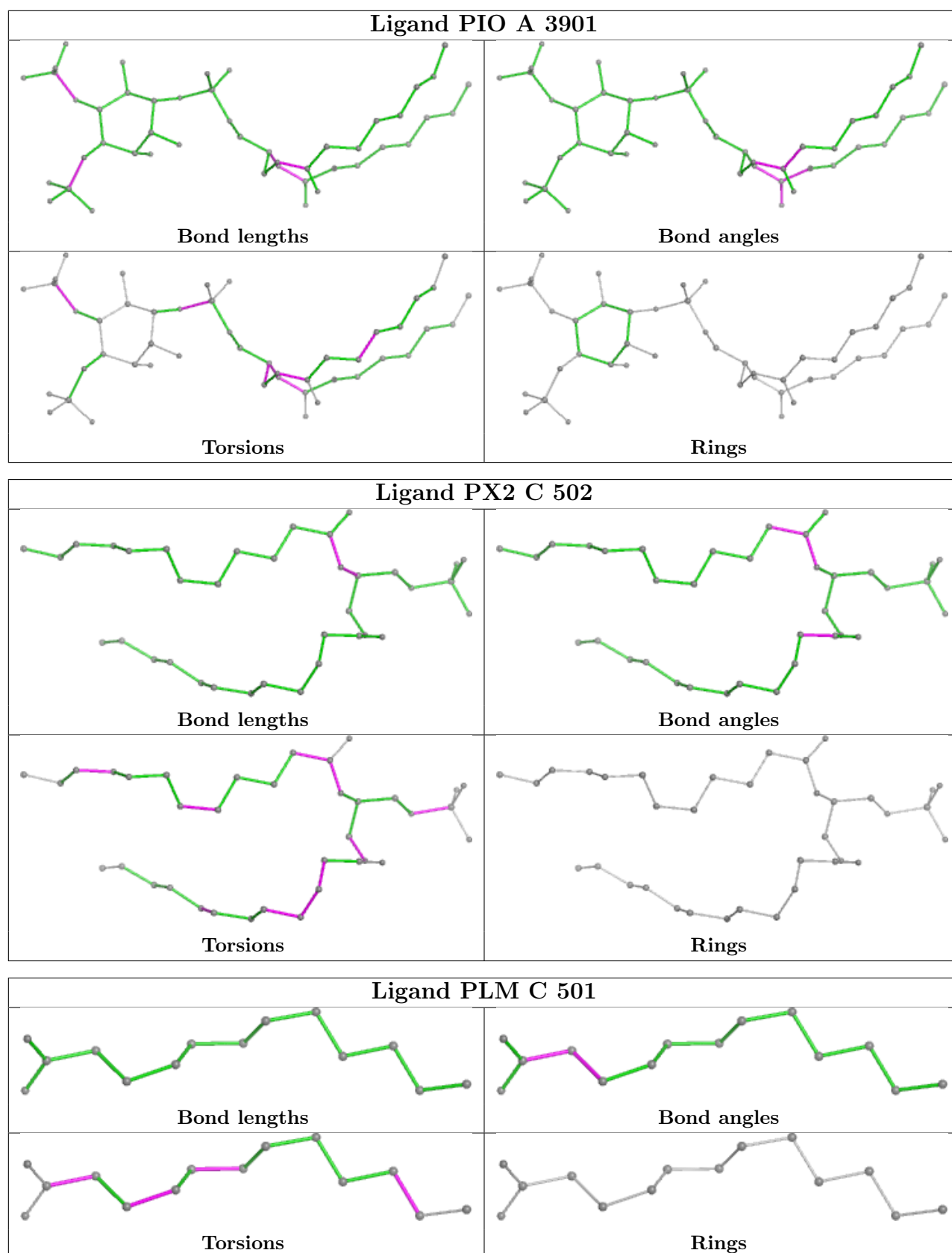
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

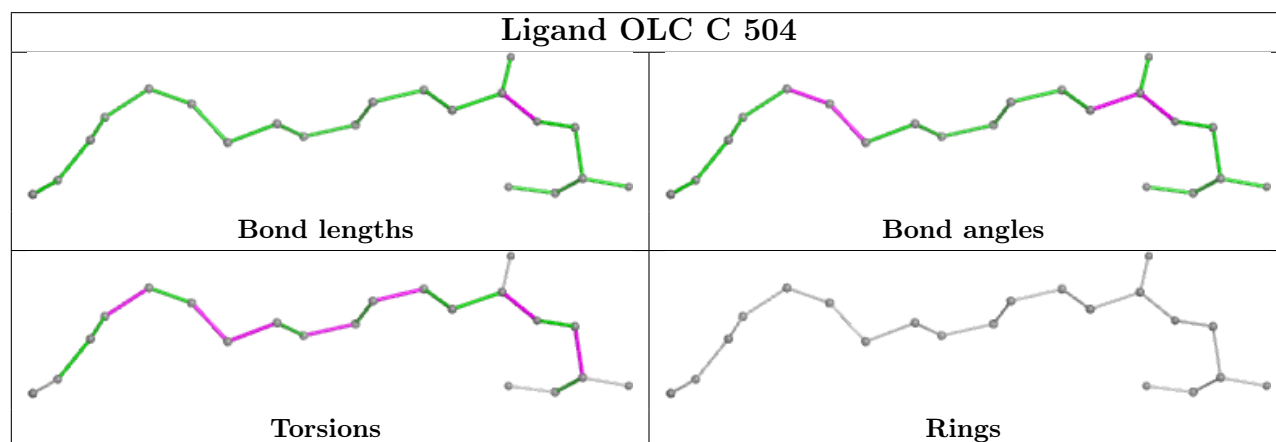
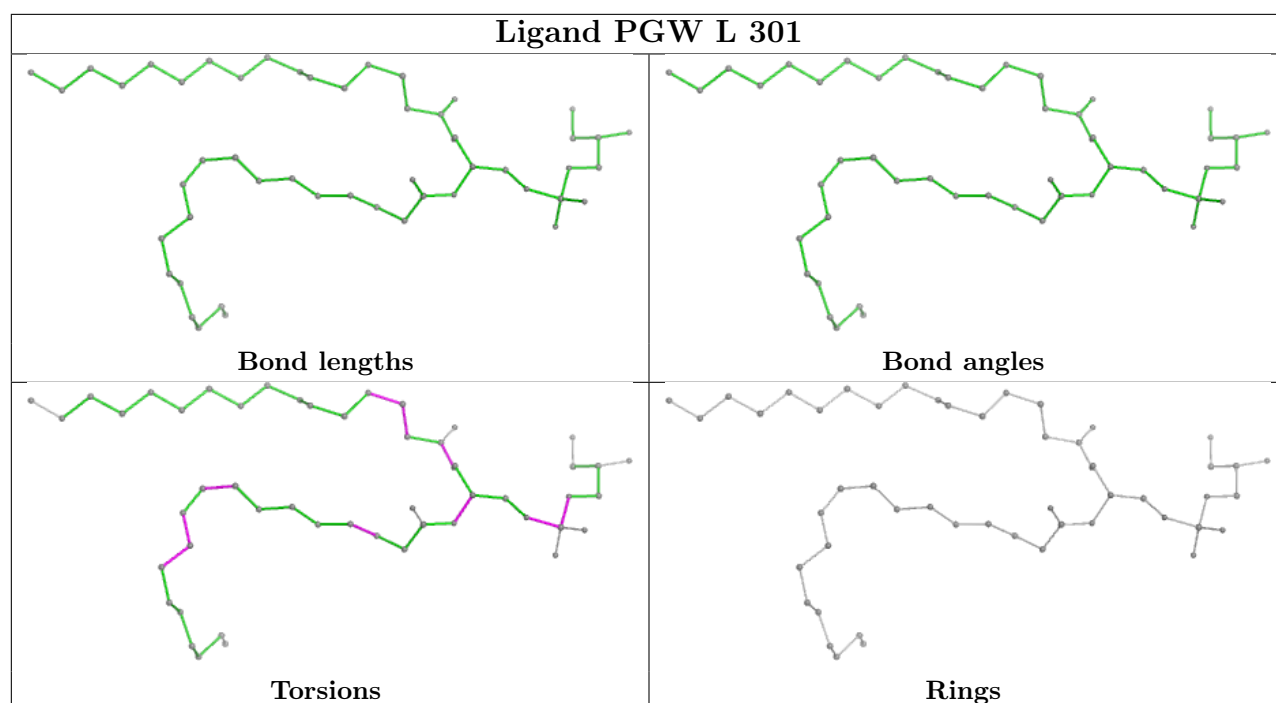


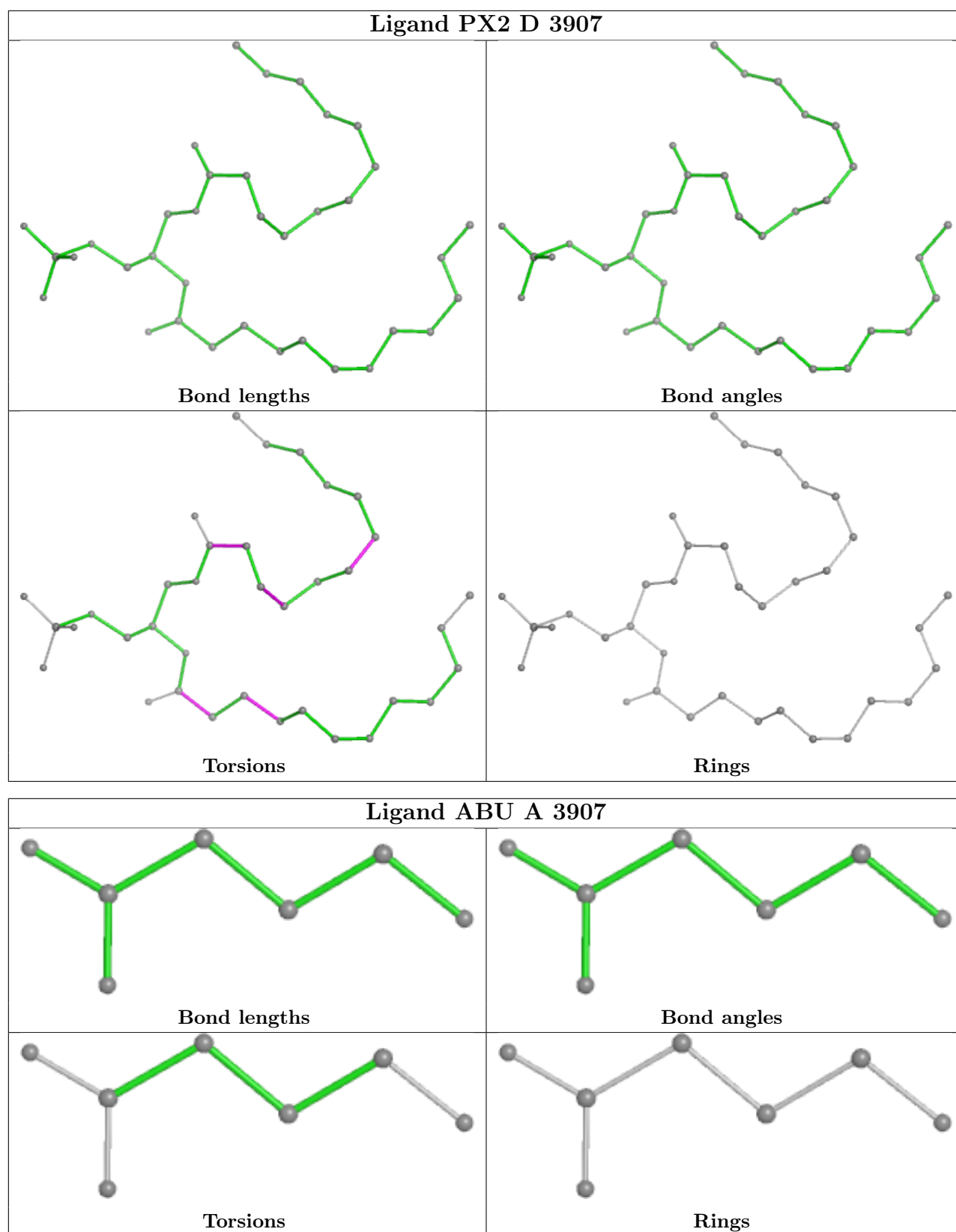


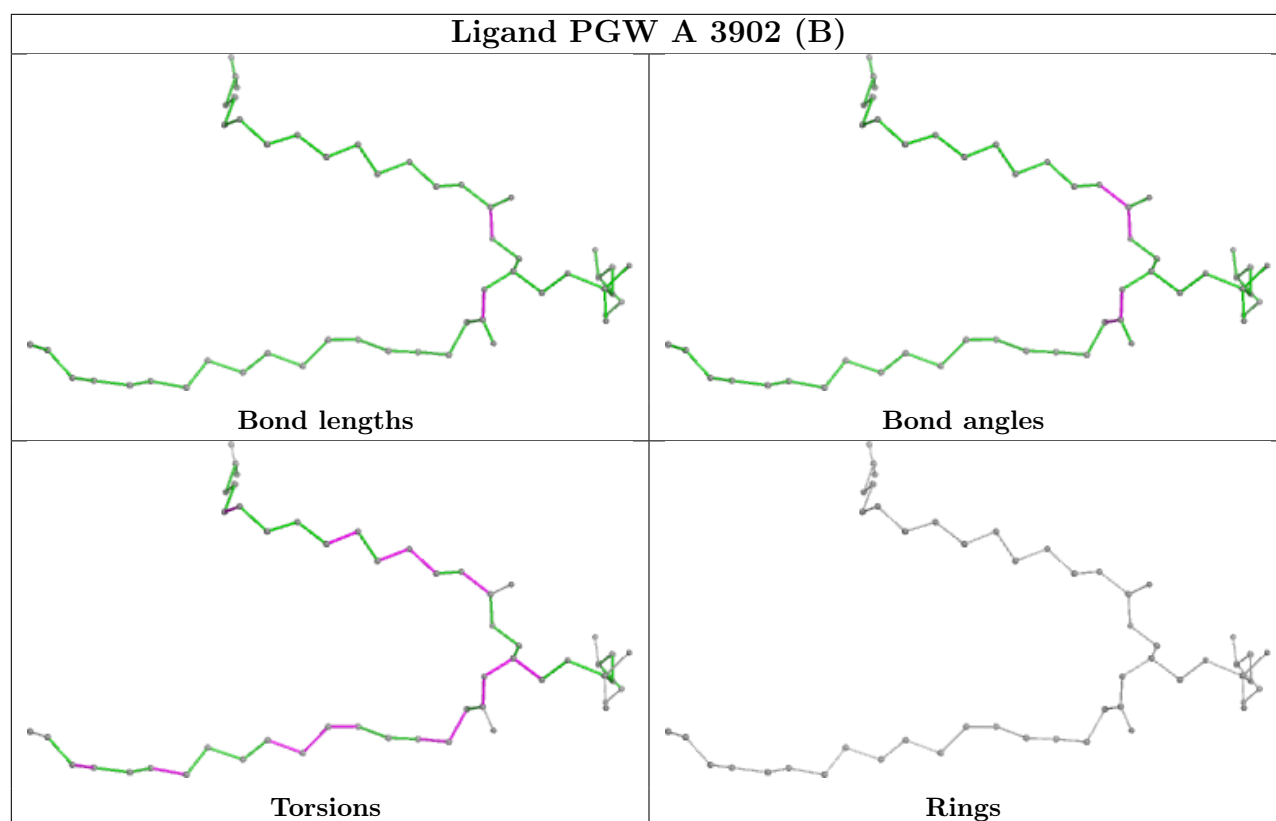


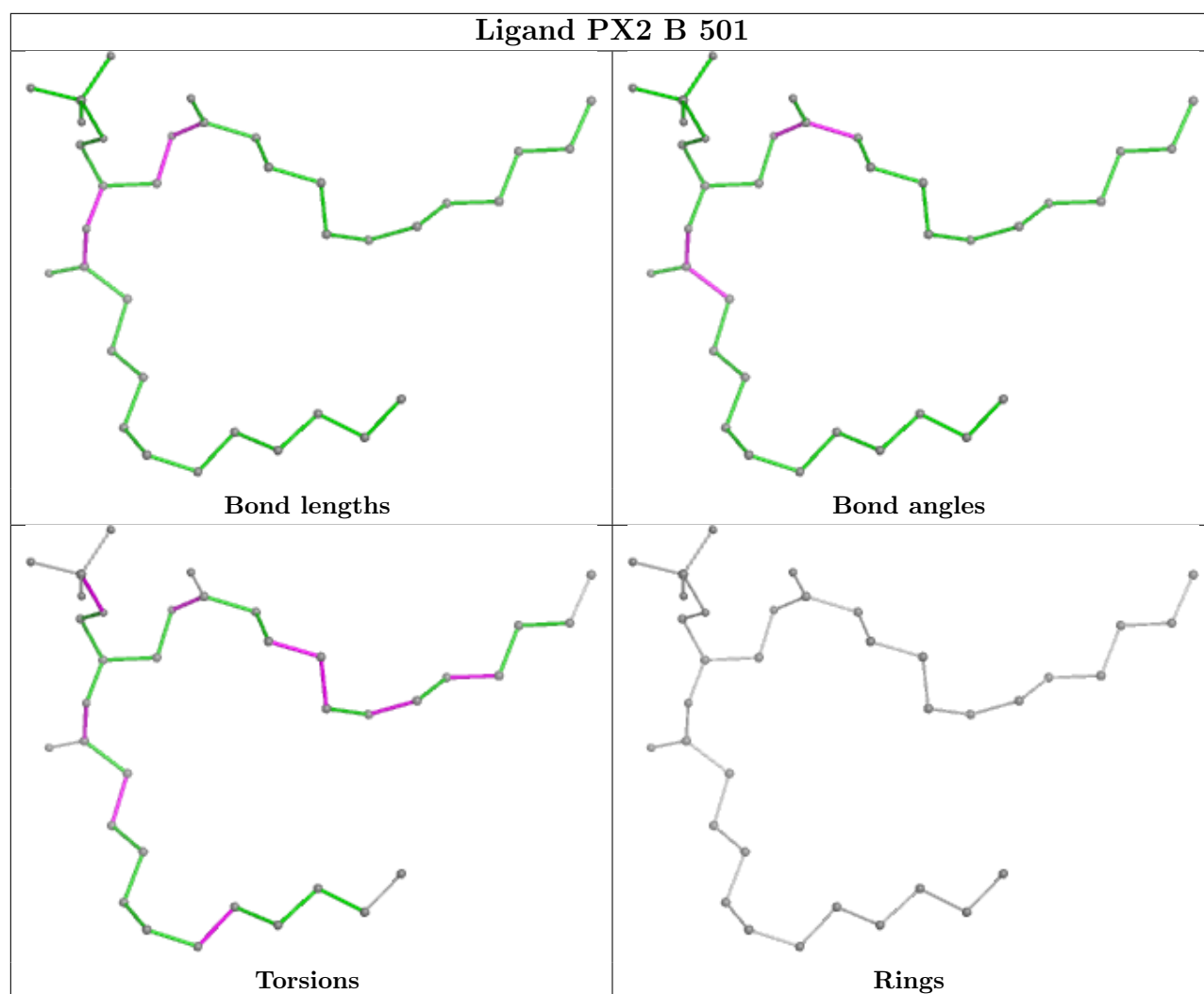


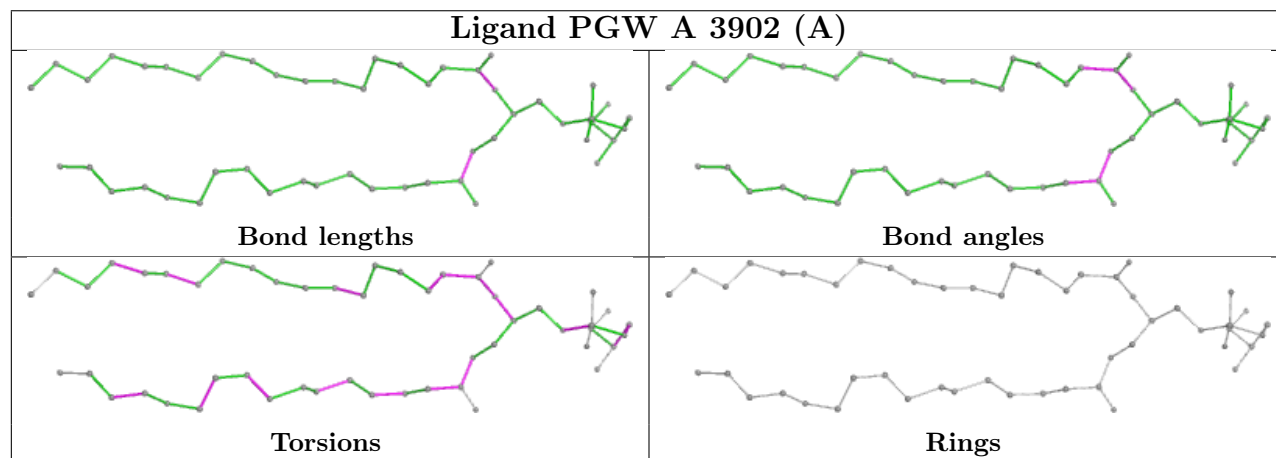
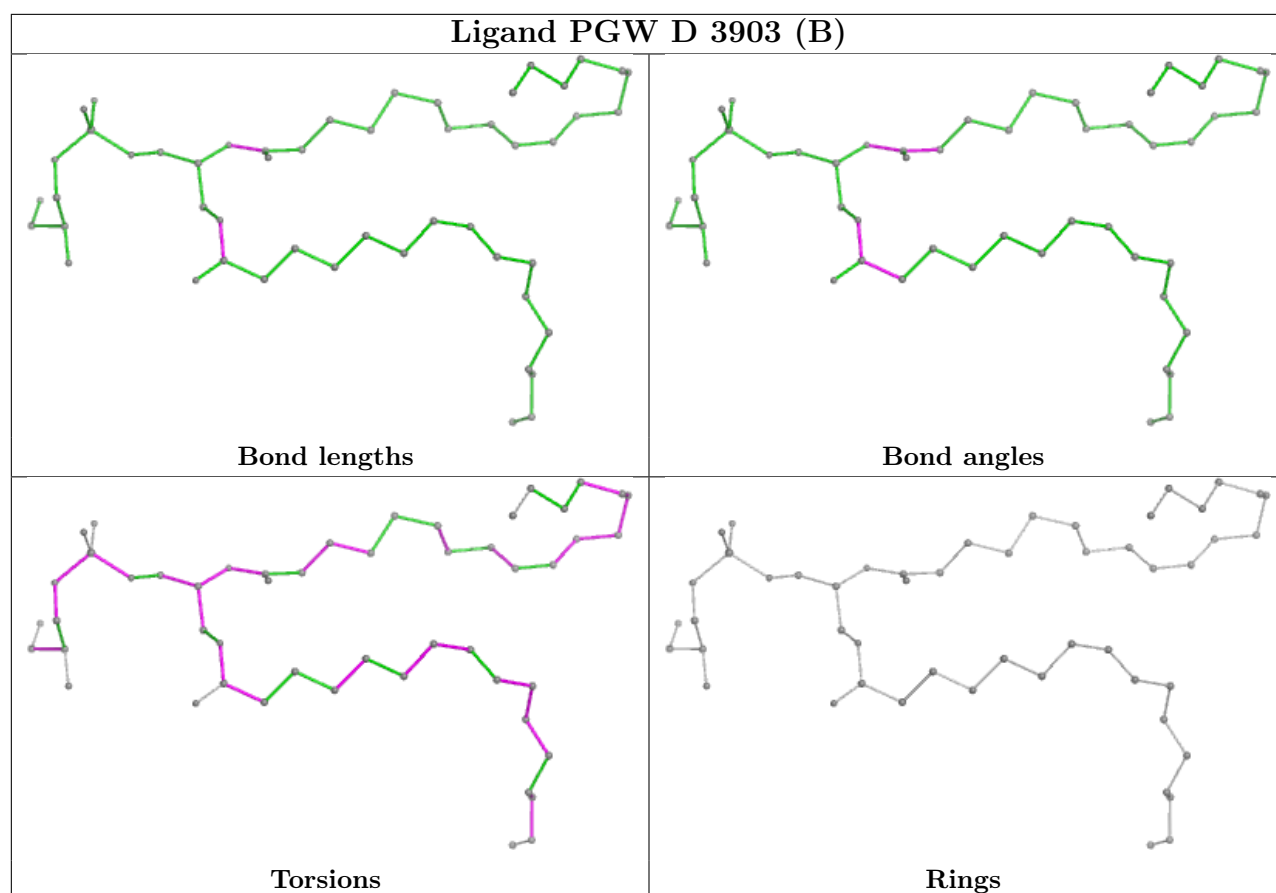


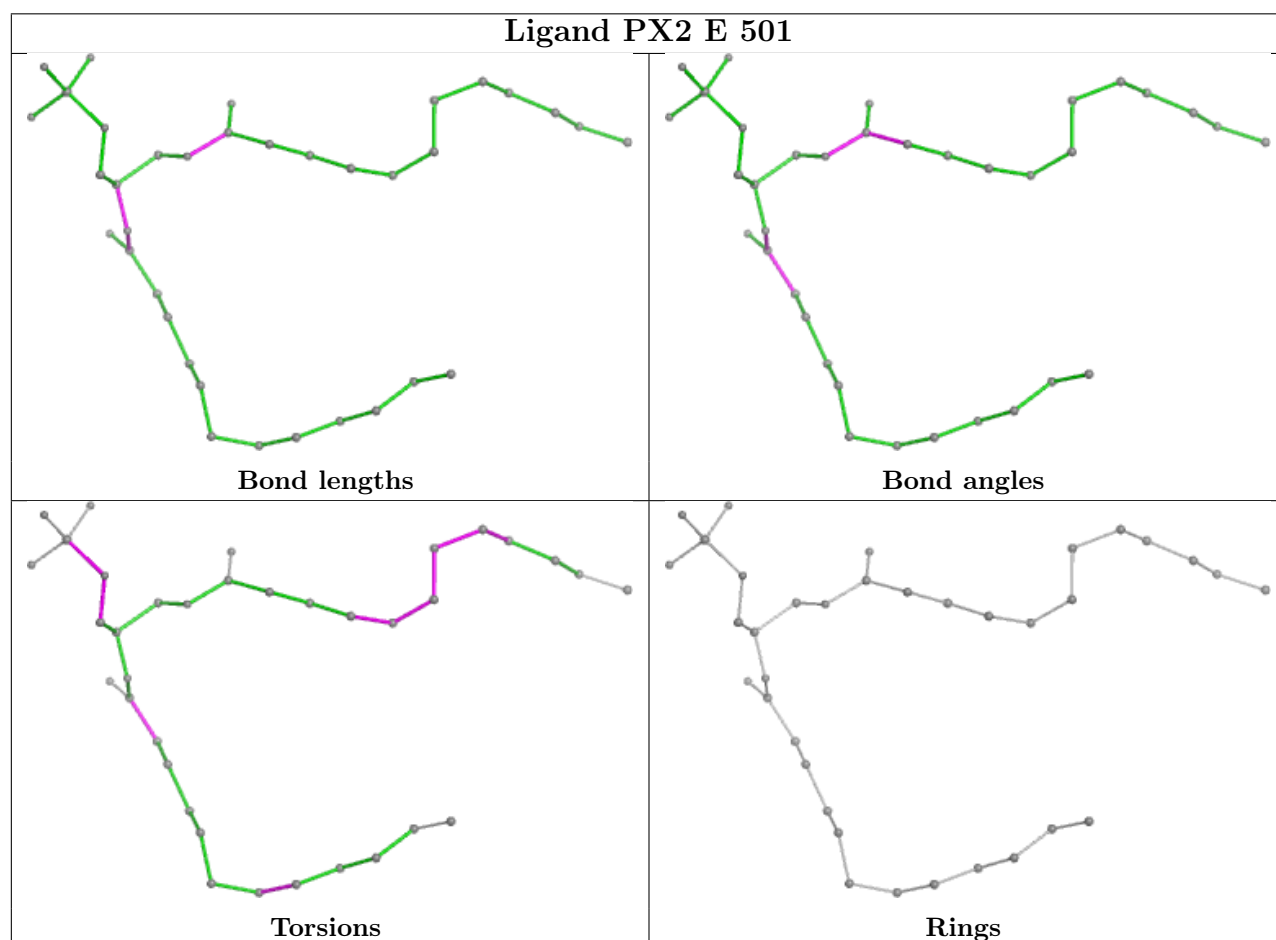
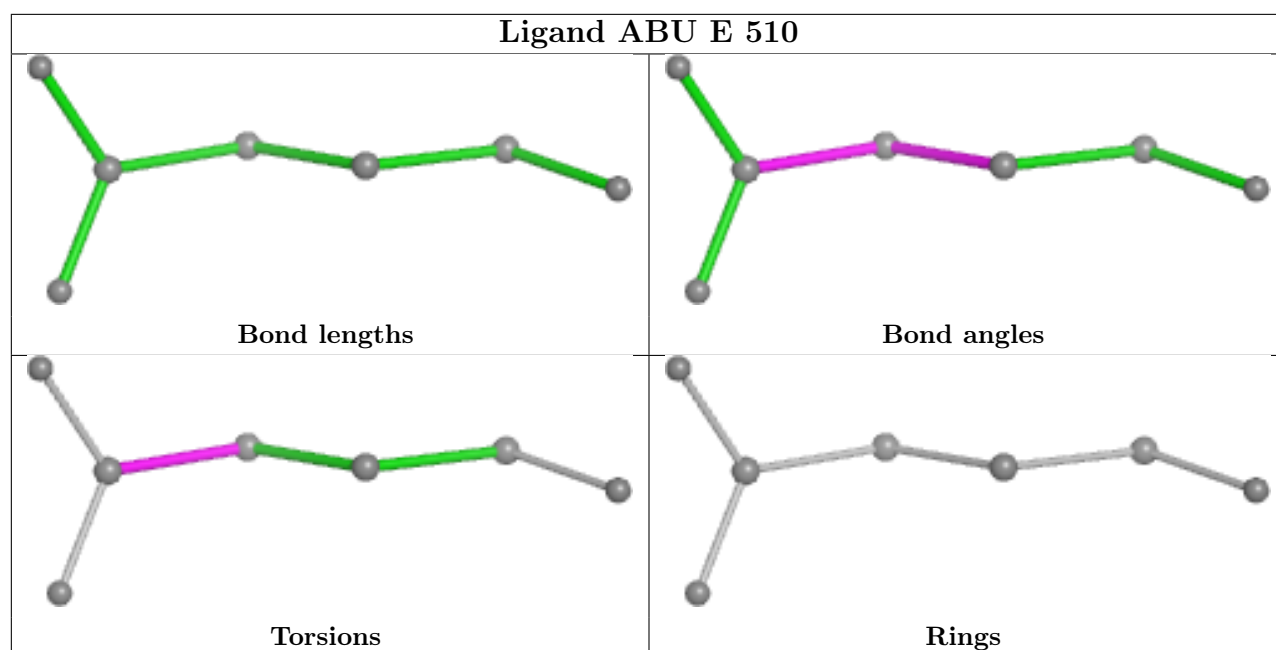


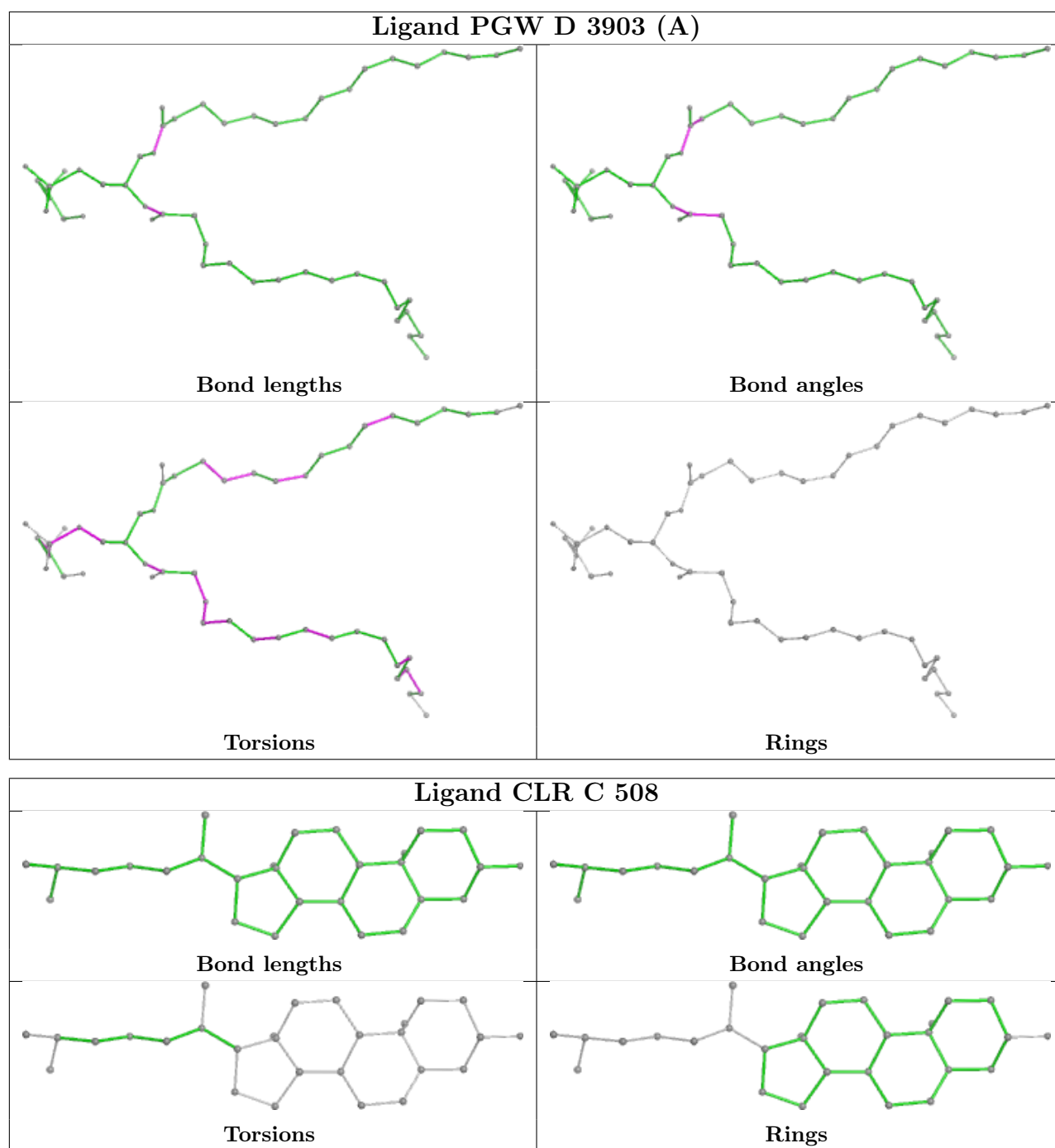












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

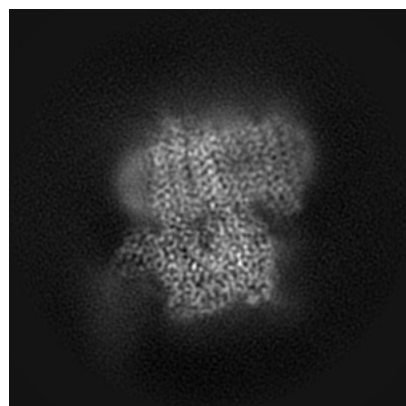
6 Map visualisation [i](#)

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.

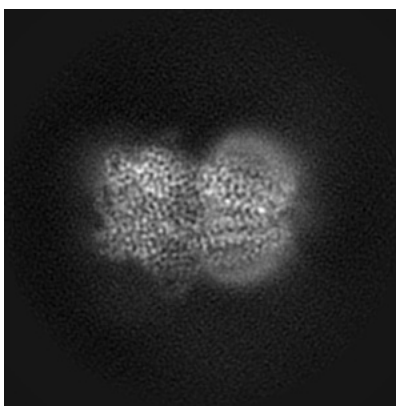
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

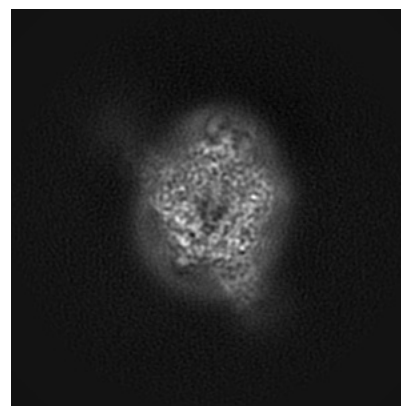
6.1.1 Primary map



X

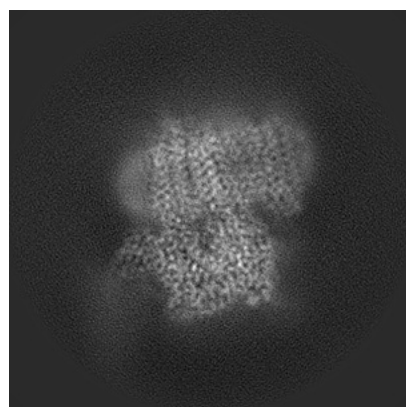


Y

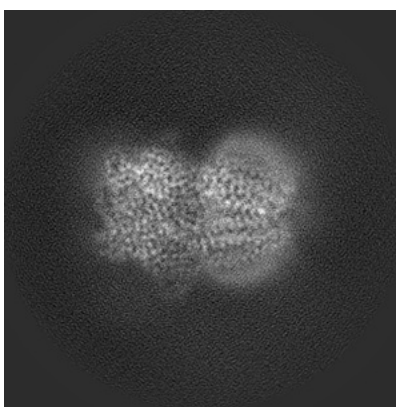


Z

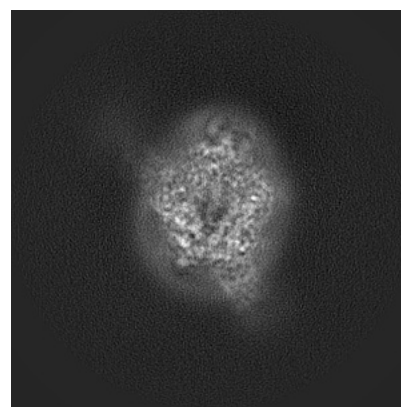
6.1.2 Raw map



X



Y

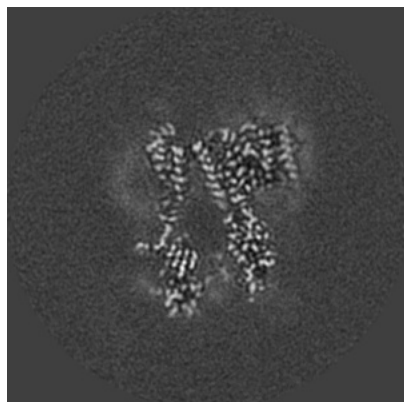


Z

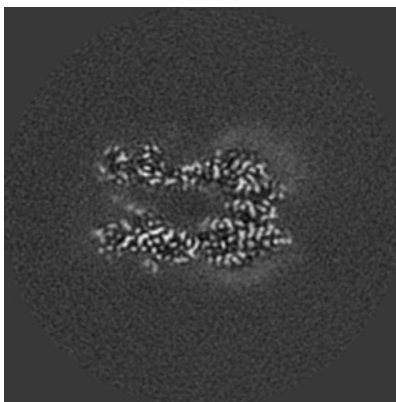
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

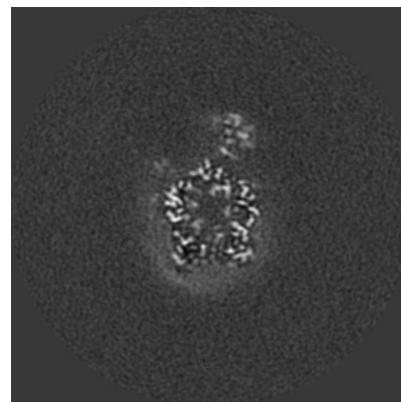
6.2.1 Primary map



X Index: 148

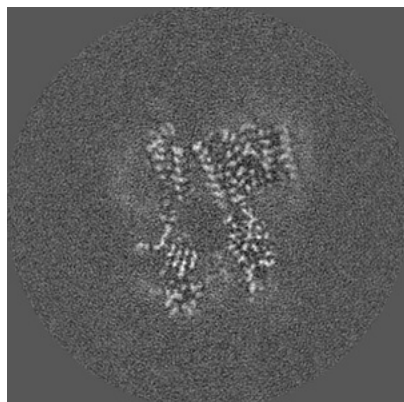


Y Index: 148

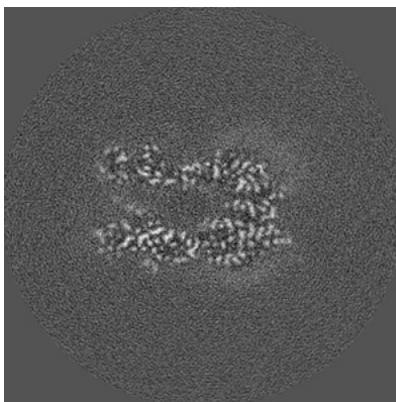


Z Index: 148

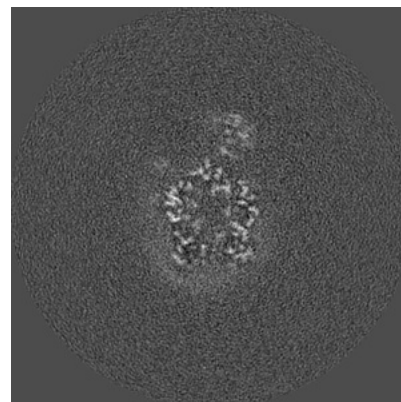
6.2.2 Raw map



X Index: 148



Y Index: 148

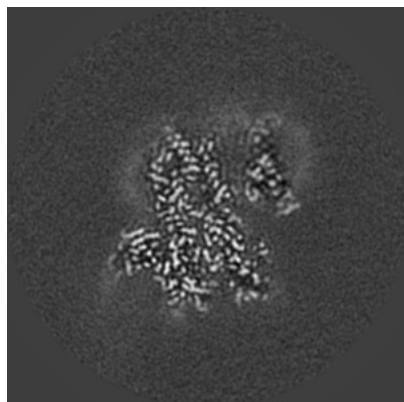


Z Index: 148

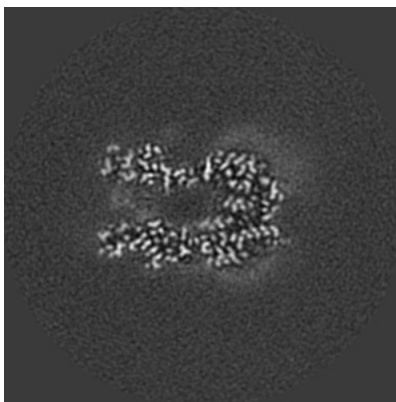
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

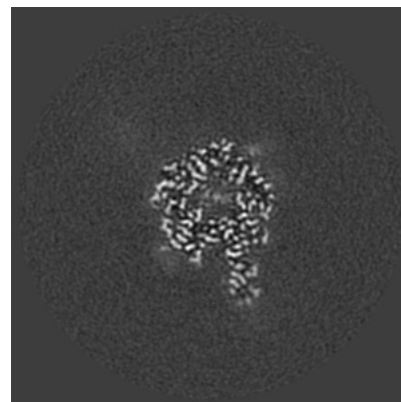
6.3.1 Primary map



X Index: 167

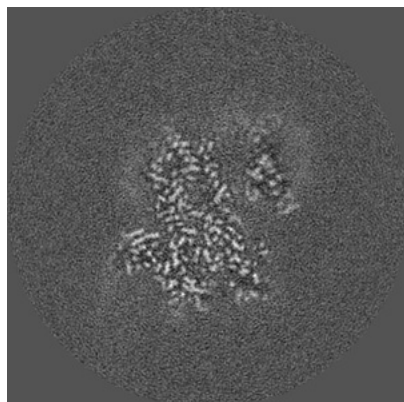


Y Index: 150

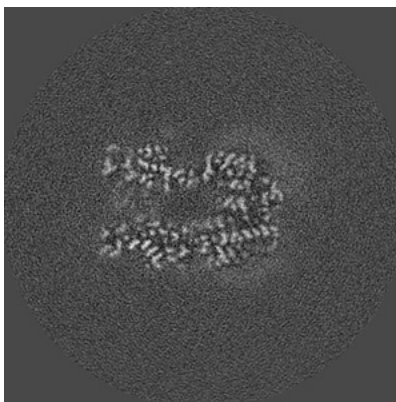


Z Index: 104

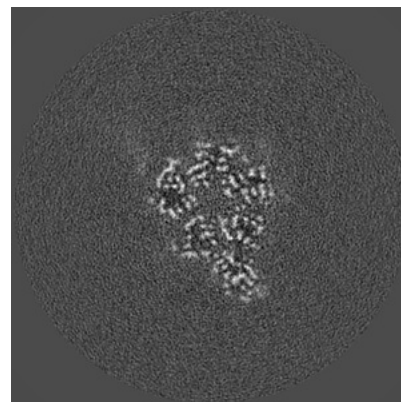
6.3.2 Raw map



X Index: 167



Y Index: 151

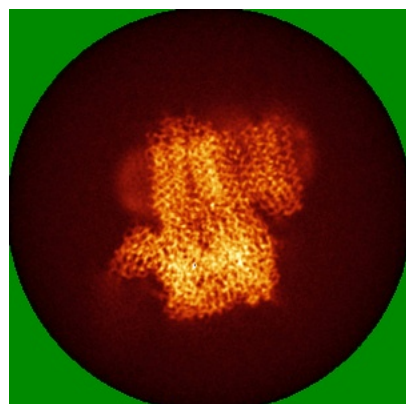


Z Index: 115

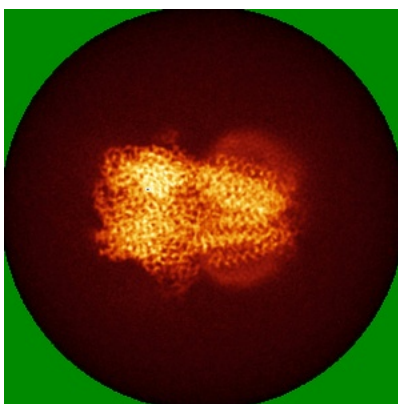
The images above show the largest variance slices of the map in three orthogonal directions.

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

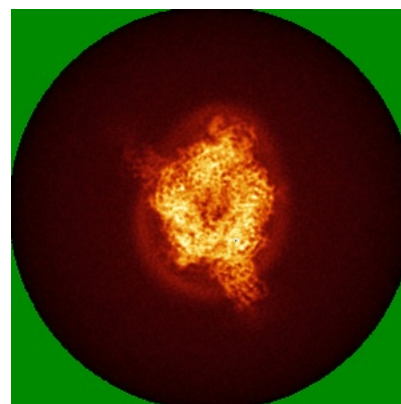
6.4.1 Primary map



X

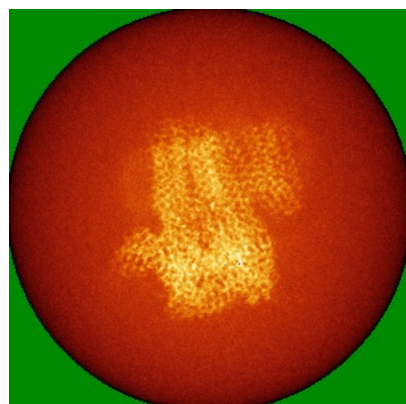


Y

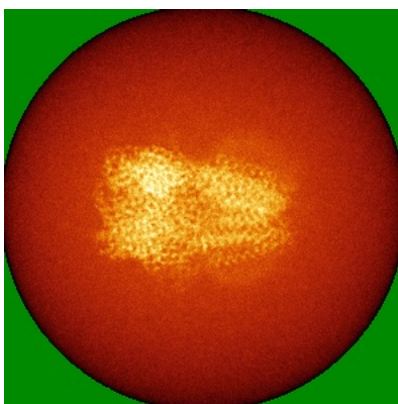


Z

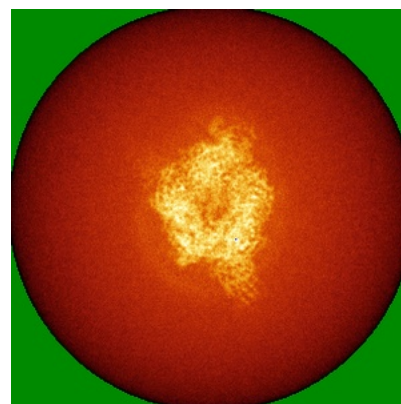
6.4.2 Raw map



X



Y

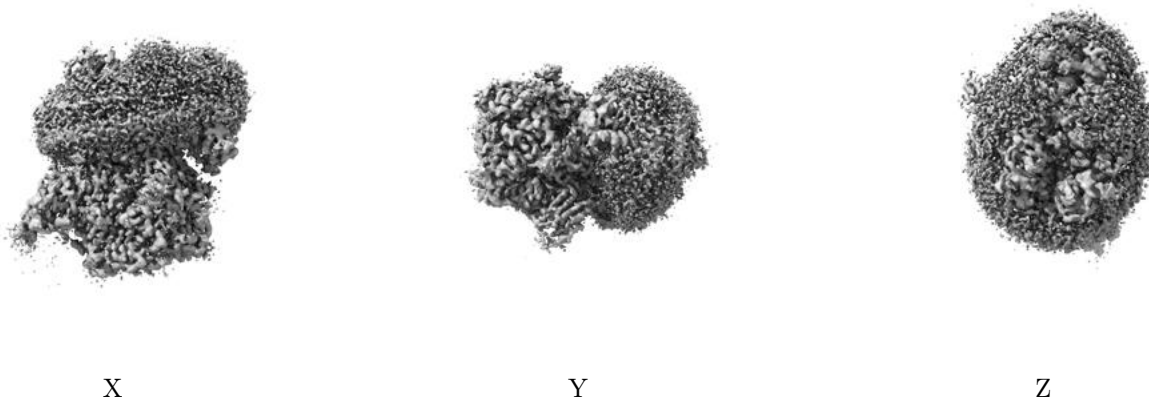


Z

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.

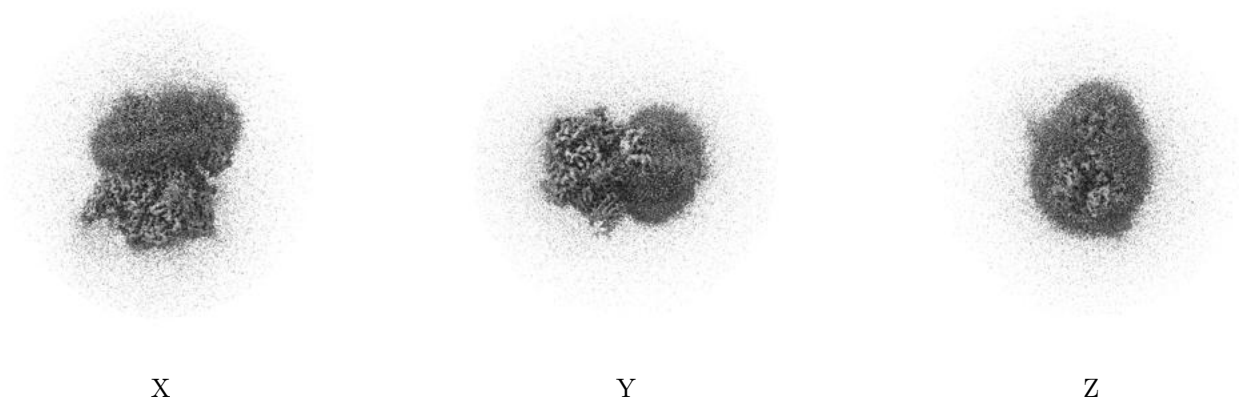
6.5 Orthogonal surface views [i](#)

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.

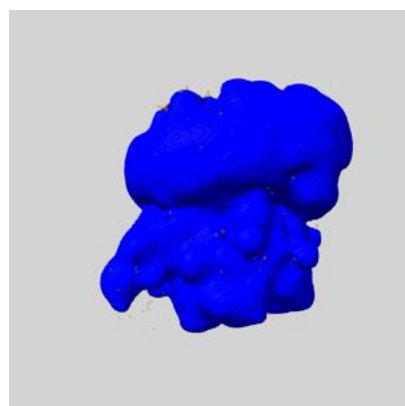
6.6 Mask visualisation [i](#)

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

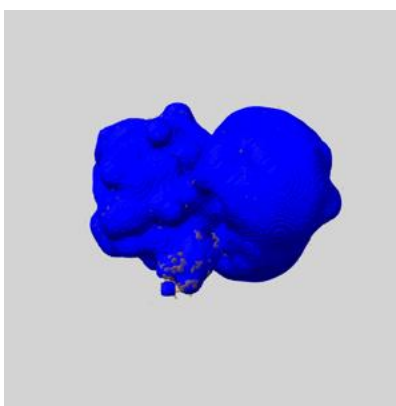
A mask typically either:

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

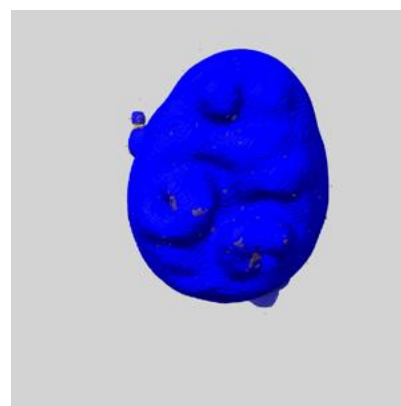
6.6.1 emd_50273_msk_1.map [i](#)



X



Y

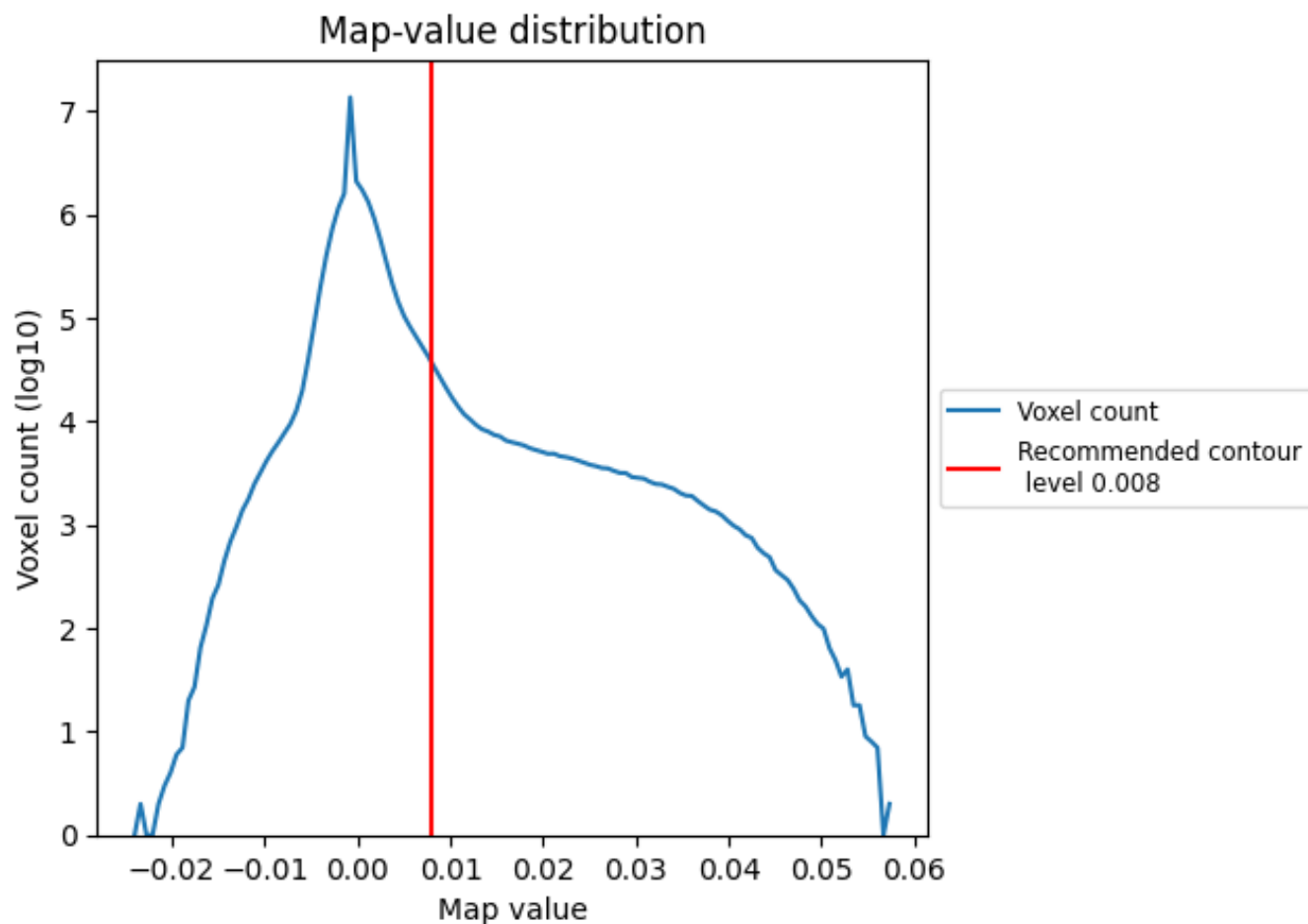


Z

7 Map analysis [i](#)

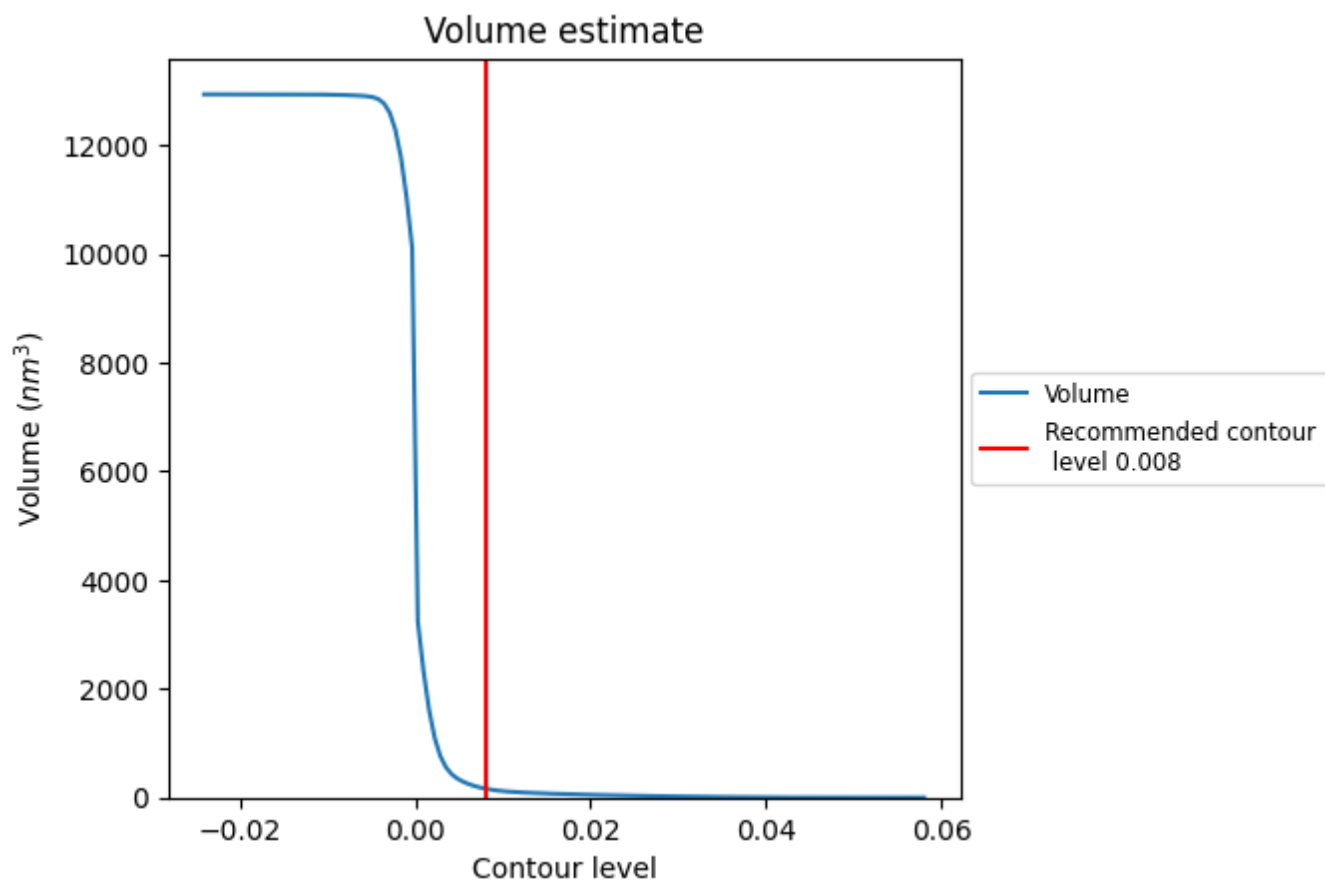
This section contains the results of statistical analysis of the map.

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.

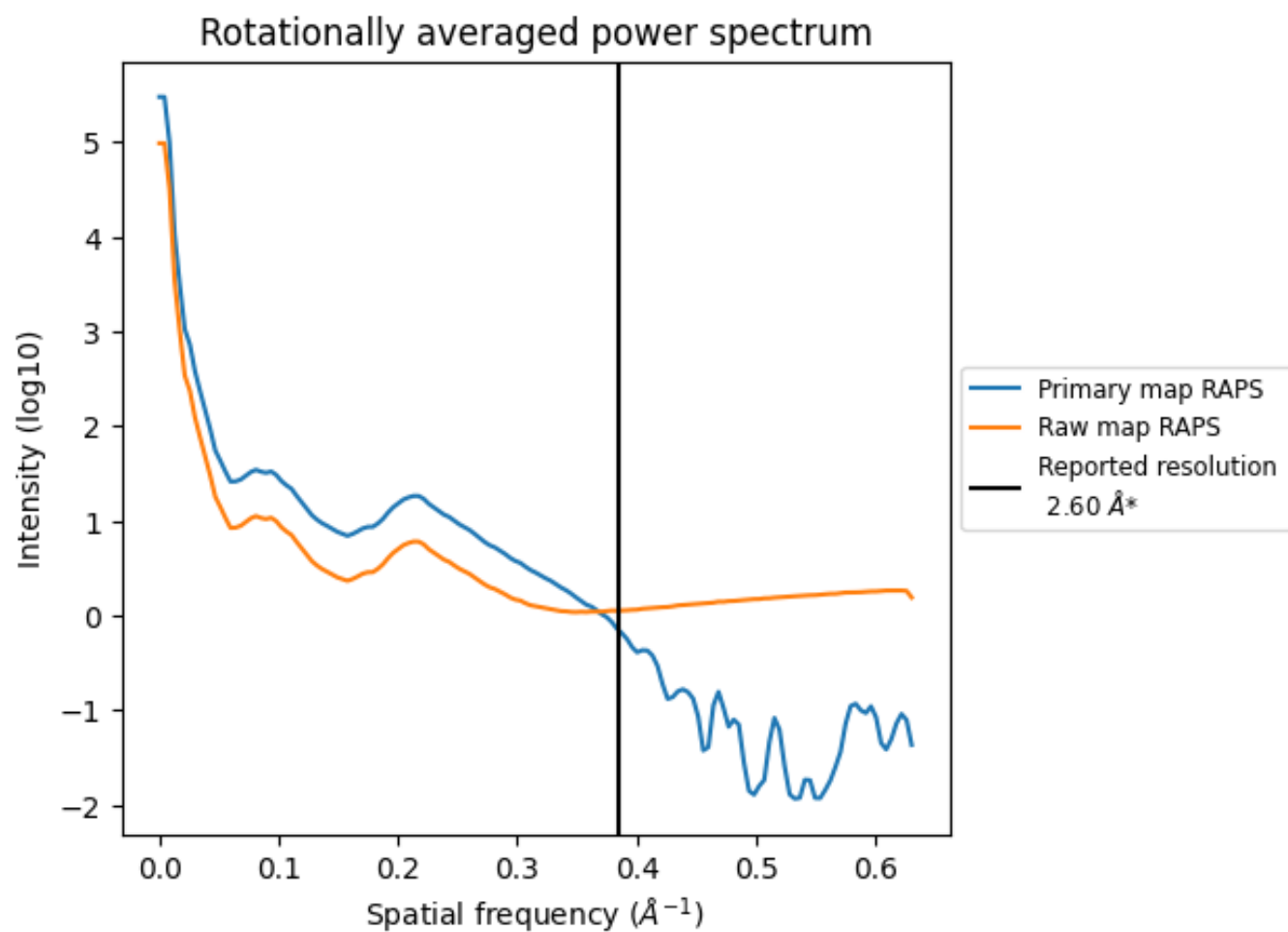
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm³; 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 ⓘ

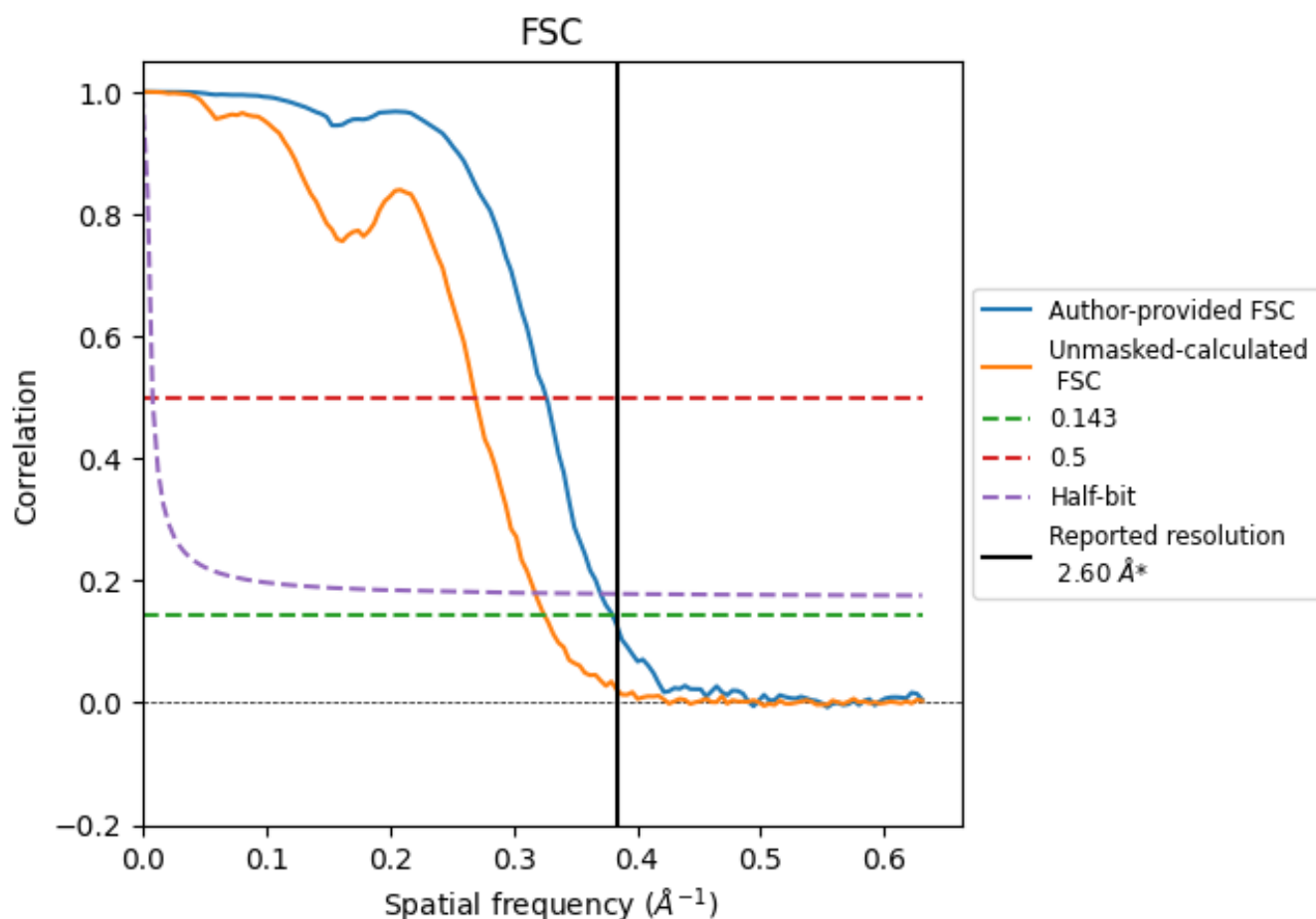


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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](#)

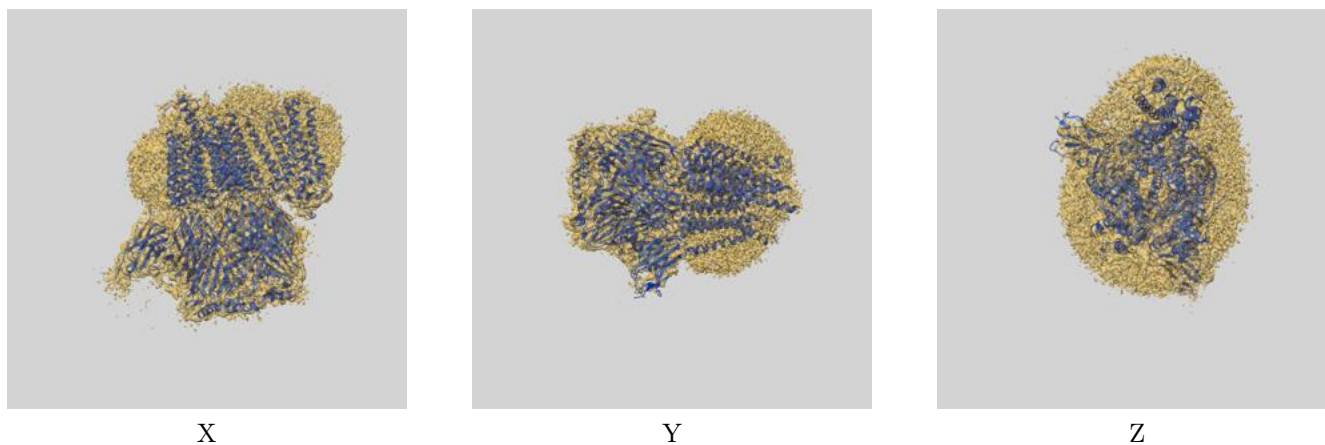
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.63	3.06	2.70
Unmasked-calculated*	3.08	3.71	3.15

*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](#)

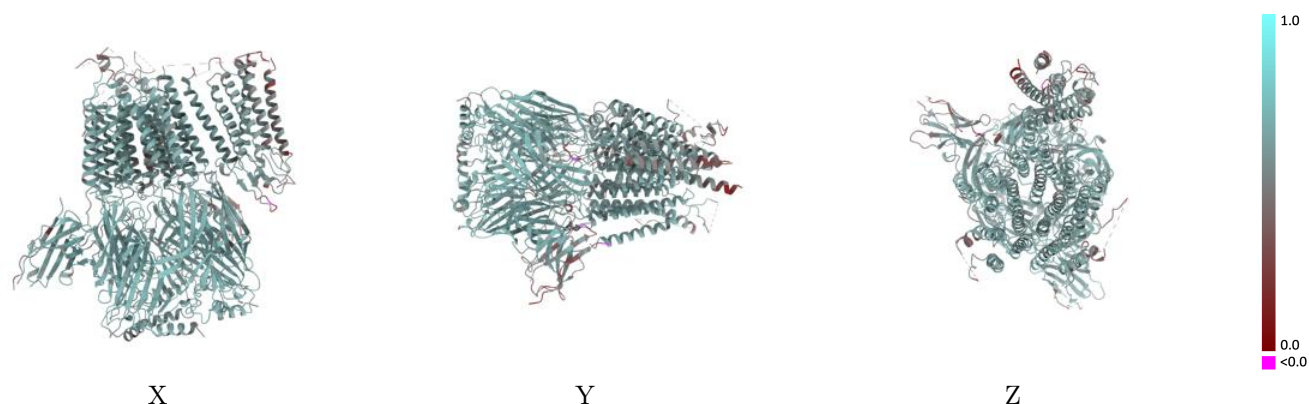
This section contains information regarding the fit between EMDB map EMD-50273 and PDB model 9FAJ. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



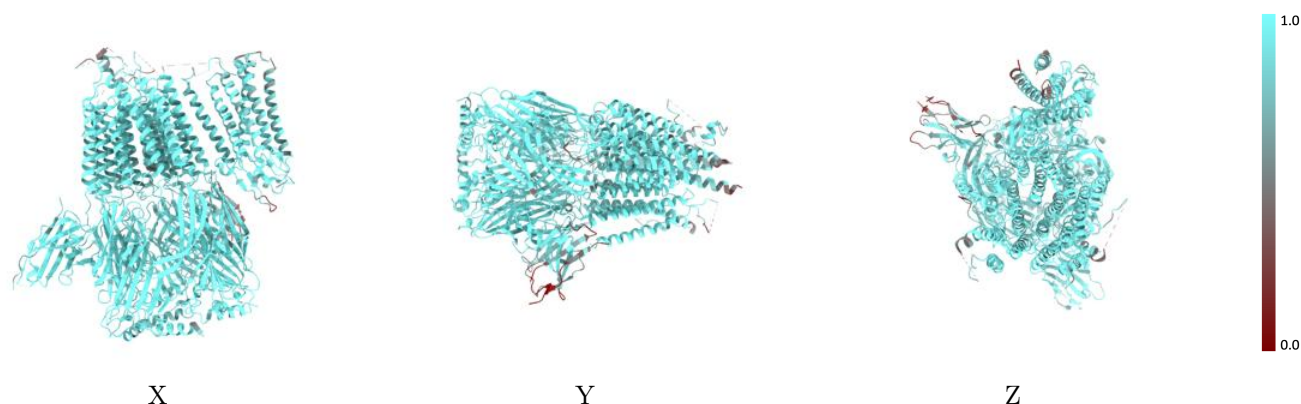
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



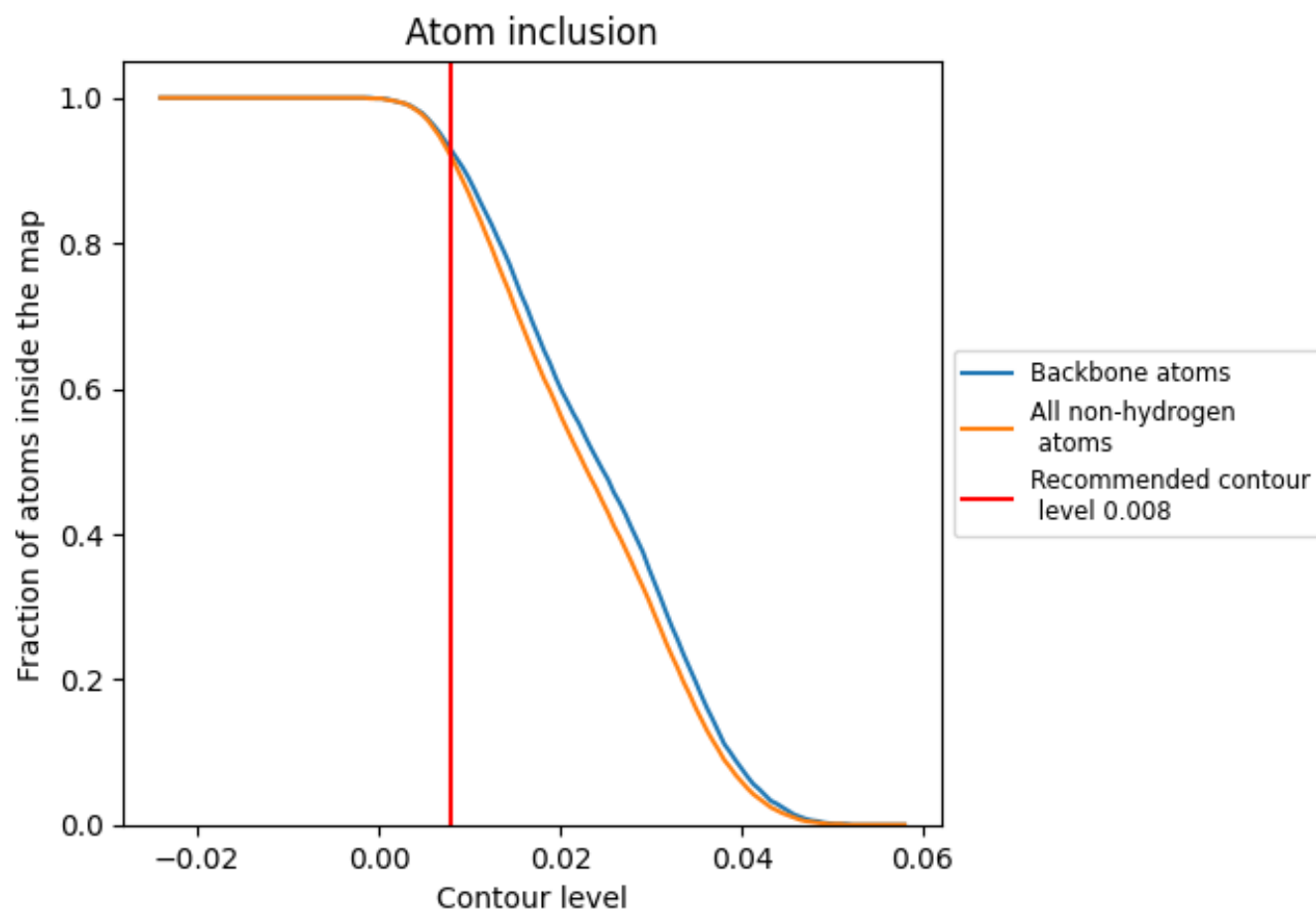
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9190	 0.5960
A	 0.9480	 0.6200
B	 0.9500	 0.6130
C	 0.9380	 0.6030
D	 0.9450	 0.6170
E	 0.9480	 0.6150
F	 0.9310	 0.5580
G	 0.9520	 0.6030
H	 0.7570	 0.4360
I	 0.7690	 0.4550
J	 0.9310	 0.5800
K	 0.8210	 0.5190
L	 0.8730	 0.5310
M	 0.8060	 0.4890
N	 0.9310	 0.5720
O	 0.7950	 0.5430
P	 0.6340	 0.4790

