



Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 01:35 pm BST

PDB ID : 9RGD / pdb_00009rgd
EMDB ID : EMD-53948
Title : CryoEM structure of human alpha1beta3gamma2L GABA(A)R in CL47a
Authors : Kasaragod, V.B.; Aricescu, A.R.
Deposited on : 2025-06-06
Resolution : 2.00 Å(reported)
Based on initial model : 9EQG

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

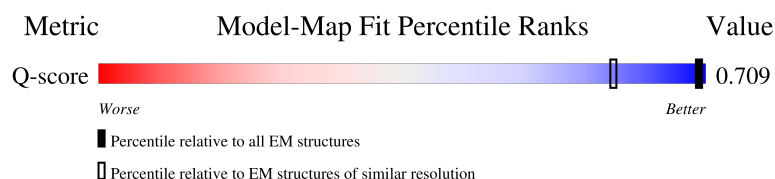
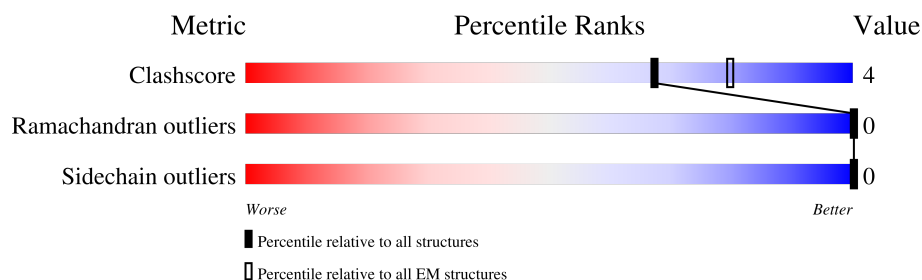
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.00 Å.

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



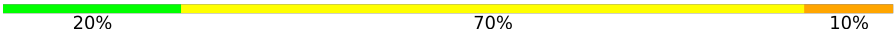


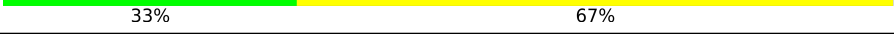
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1659 (1.50 - 2.50)

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	409	 78% 8% 14%
1	D	409	 81% 5% 14%
2	B	441	 72% 6% 22%
2	E	441	 72% 6% 22%

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Mol	Chain	Length	Quality of chain
3	C	415	 74%6%20%
4	F	10	 20%70%10%
5	G	6	 50%50%
5	J	6	 83%17%
5	K	6	 50%33%17%
6	H	3	 33%67%
6	L	3	 67%33%
7	I	2	 100%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 16242 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	353	Total	C	N	O	S	18	0
			2955	1925	492	521	17		
1	D	353	Total	C	N	O	S	5	0
			2894	1875	488	514	17		

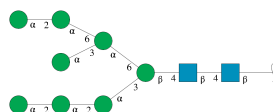
- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	344	Total	C	N	O	S	12	0
			2900	1911	473	500	16		
2	E	342	Total	C	N	O	S	12	0
			2897	1907	477	496	17		

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

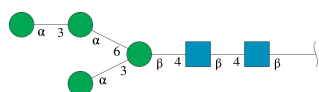
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	334	Total	C	N	O	S	9	0
			2800	1833	463	489	15		

- Molecule 4 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.



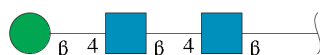
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 5 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
5	G	6	Total	C	N	O	0	0
			72	40	2	30		
5	J	6	Total	C	N	O	0	0
			72	40	2	30		
5	K	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 6 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.



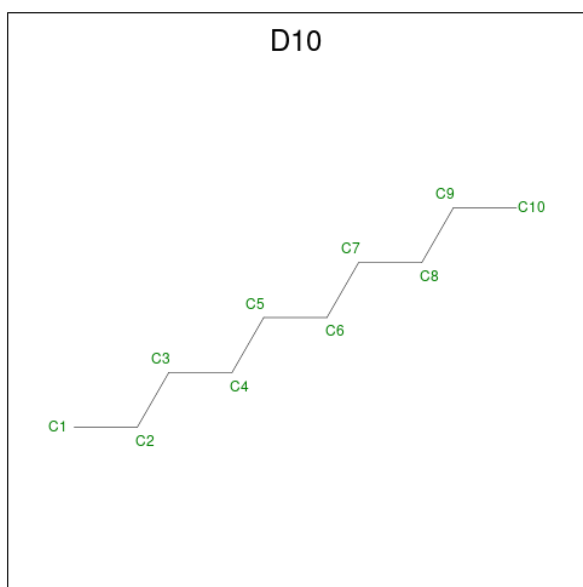
Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	3	Total	C	N	O	0	0
			39	22	2	15		
6	L	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



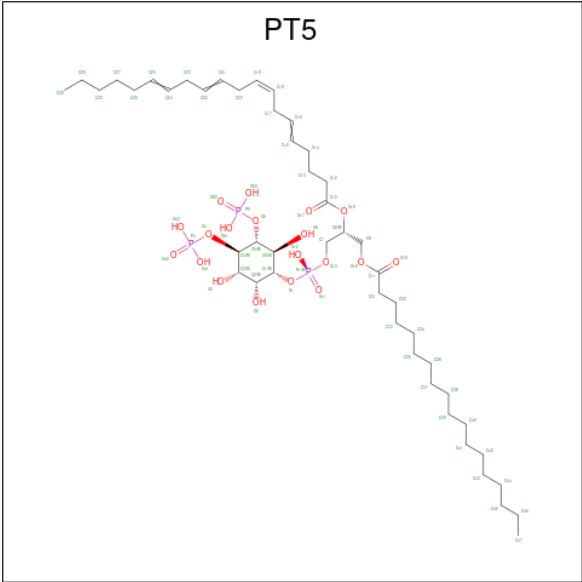
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



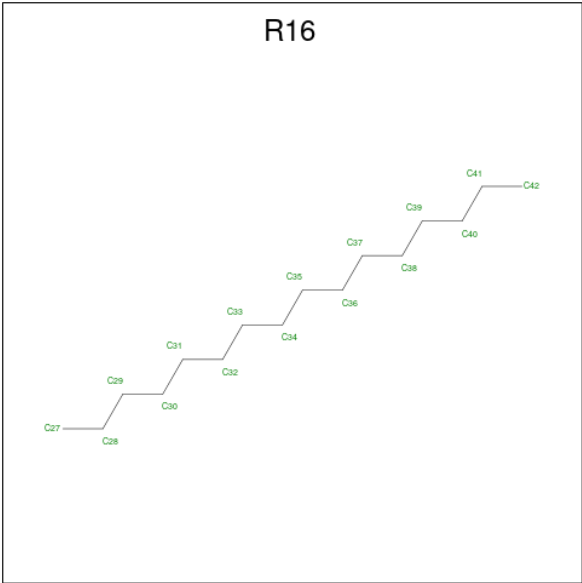
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C 10 10	0
8	A	1	Total C 10 10	0
8	B	1	Total C 10 10	0
8	B	1	Total C 10 10	0
8	B	1	Total C 10 10	0
8	D	1	Total C 10 10	0
8	D	1	Total C 10 10	0
8	E	1	Total C 10 10	0
8	E	1	Total C 10 10	0
8	E	1	Total C 10 10	0

- Molecule 9 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: C₄₇H₈₅O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			69	47	19	3	
9	D	1	Total	C	O	P	0
			69	47	19	3	

- Molecule 10 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



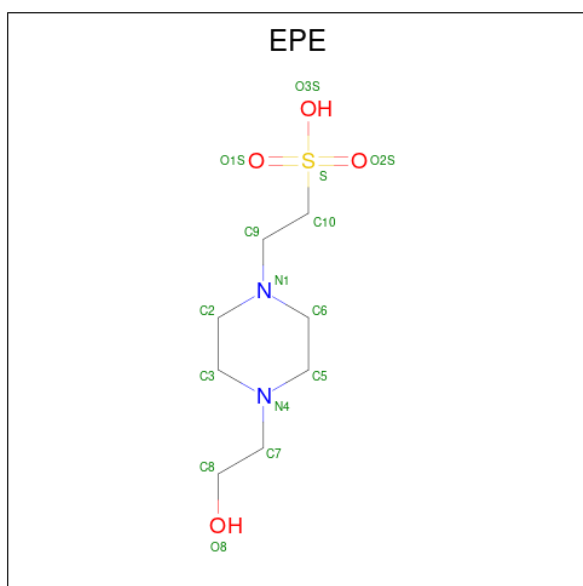
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	C	0
			16	16	
10	B	1	Total	C	0
			16	16	

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Mol	Chain	Residues	Atoms	AltConf
10	D	1	Total C 16 16	0
10	D	1	Total C 16 16	0
10	E	1	Total C 16 16	0

- Molecule 11 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C N O S 15 8 2 4 1	0

- Molecule 12 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).

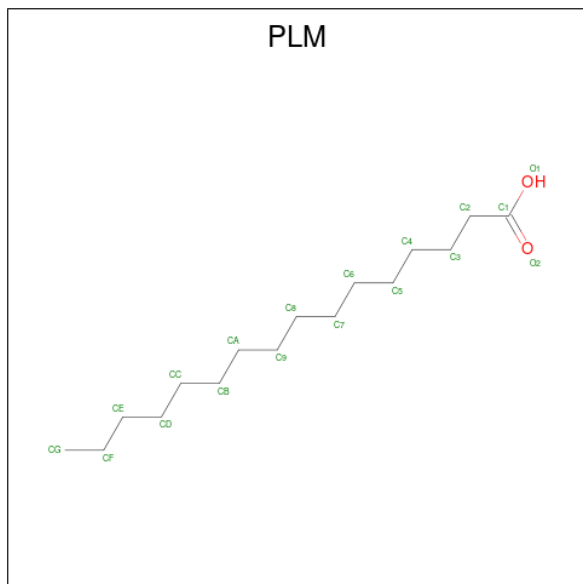


- Molecule 13 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



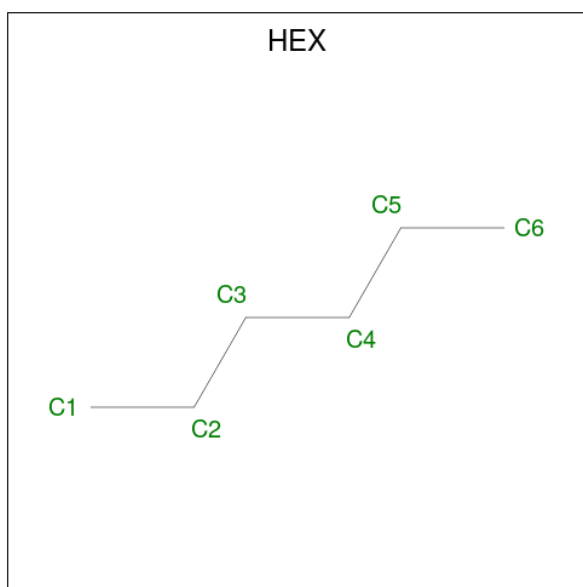
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			25	21	4	
13	B	1	Total	C	O	0
			25	21	4	
13	E	1	Total	C	O	0
			25	21	4	

- Molecule 14 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			18	16	2	
14	C	1	Total	C	O	0
			18	16	2	
14	C	1	Total	C	O	0
			18	16	2	

- Molecule 15 is HEXANE (CCD ID: HEX) (formula: C_6H_{14}).



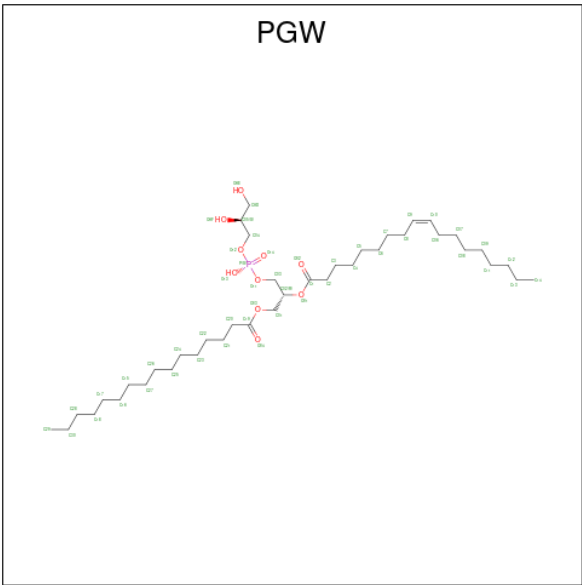
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 6 6	0
15	B	1	Total C 6 6	0
15	B	1	Total C 6 6	0
15	C	1	Total C 6 6	0
15	C	1	Total C 6 6	0
15	C	1	Total C 6 6	0
15	C	1	Total C 6 6	0
15	D	1	Total C 6 6	0
15	E	1	Total C 6 6	0
15	E	1	Total C 6 6	0
15	E	1	Total C 6 6	0

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 17 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
17	C	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 18 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
18	C	1	Total 1	Cl 1	0

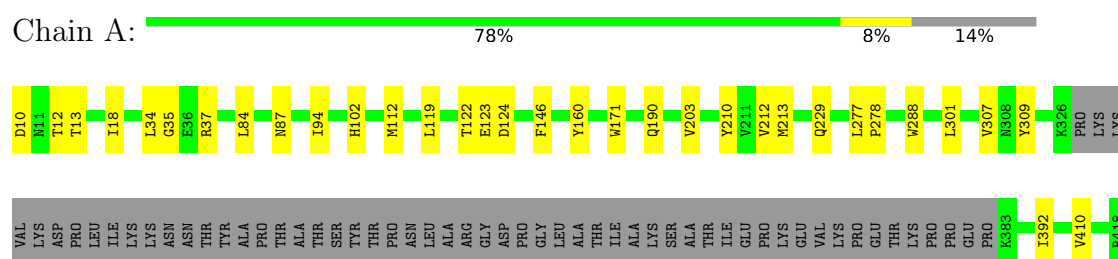
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	A	131	Total 131	O 131	0
19	B	132	Total 132	O 132	0
19	C	133	Total 133	O 133	0
19	D	132	Total 132	O 132	0
19	E	114	Total 114	O 114	0

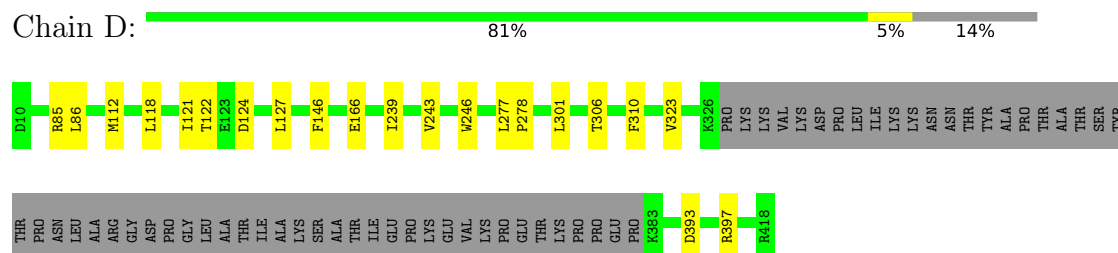
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

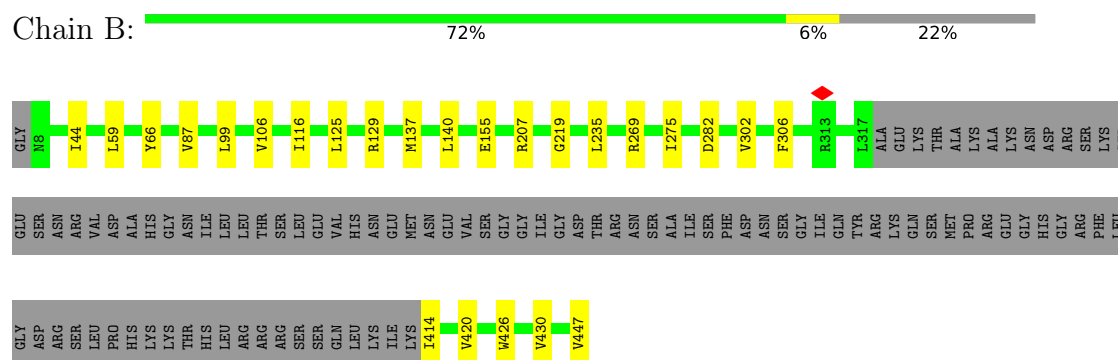
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1



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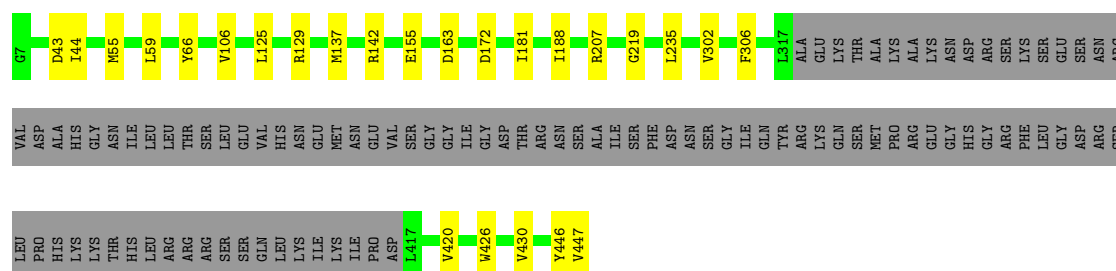


- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

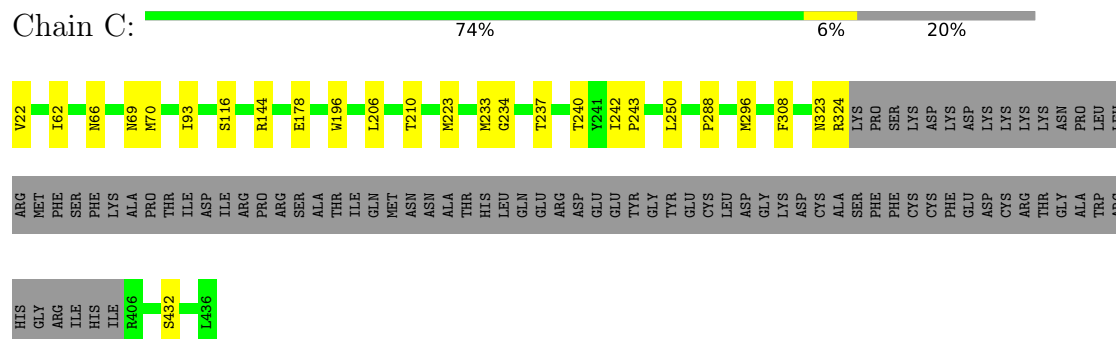


- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3





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



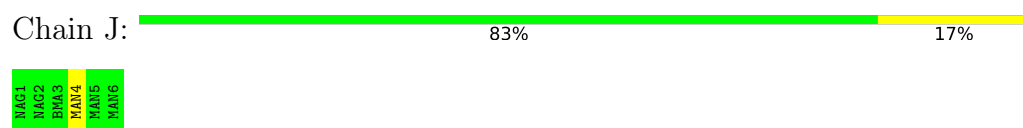
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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

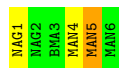


- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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 K:  50% 33% 17%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  67% 33%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	232597	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 ($e^-/\text{\AA}^2$)	53.2	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0025	Depositor
Map size (Å)	349.91998, 349.91998, 349.91998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NAG, BMA, HEX, EPE, PT5, D10, OLC, PGW, R16, PLM, MAN, PX2

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	0.19	0/3083	0.30	0/4187
1	D	0.25	0/2983	0.35	0/4048
2	B	0.19	0/3014	0.32	0/4101
2	E	0.19	0/3012	0.31	0/4091
3	C	0.20	0/2902	0.32	0/3947
All	All	0.21	0/14994	0.32	0/20374

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2955	0	3017	29	0
1	D	2894	0	2904	18	0
2	B	2900	0	2948	23	0
2	E	2897	0	2935	19	0
3	C	2800	0	2833	19	0
4	F	116	0	97	1	0
5	G	72	0	61	0	0
5	J	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	72	0	61	1	0
6	H	39	0	34	0	0
6	L	39	0	34	0	0
7	I	28	0	25	1	0
8	A	20	0	44	3	0
8	B	30	0	66	2	0
8	D	20	0	44	0	0
8	E	30	0	66	3	0
9	A	69	0	80	1	0
9	D	69	0	80	5	0
10	A	16	0	34	1	0
10	B	16	0	34	0	0
10	D	32	0	68	1	0
10	E	16	0	34	0	0
11	A	15	0	18	4	0
12	A	72	0	104	5	0
12	D	36	0	52	1	0
13	A	25	0	40	1	0
13	B	25	0	40	2	0
13	E	25	0	40	0	0
14	A	18	0	31	5	0
14	C	36	0	62	2	0
15	A	6	0	14	0	0
15	B	12	0	28	0	0
15	C	24	0	56	1	0
15	D	6	0	14	1	0
15	E	18	0	42	5	0
16	C	14	0	13	0	0
16	D	14	0	13	0	0
17	C	51	0	76	4	0
18	C	1	0	0	0	0
19	A	131	0	0	2	0
19	B	132	0	0	1	0
19	C	133	0	0	3	0
19	D	132	0	0	1	0
19	E	114	0	0	4	0
All	All	16242	0	16203	122	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 (122) 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)
7:I:1:NAG:H61	7:I:2:NAG:H2	1.61	0.82
1:A:229:GLN:OE1	2:B:269[B]:ARG:NH2	2.17	0.77
2:E:163:ASP:OD2	19:E:601:HOH:O	2.05	0.75
3:C:432:SER:HB3	14:C:504:PLM:H62	1.67	0.74
3:C:178:GLU:OE1	19:C:601:HOH:O	2.05	0.73
14:A:4208:PLM:H31	15:E:507:HEX:H12	1.72	0.71
2:B:44:ILE:HD12	2:B:59:LEU:HD11	1.73	0.69
14:A:4208:PLM:HF1	8:E:502:D10:H81	1.73	0.69
2:E:172:ASP:O	19:E:602:HOH:O	2.11	0.68
1:A:277:LEU:HD22	1:A:278:PRO:HD2	1.76	0.68
1:D:310:PHE:CE2	9:D:501:PT5:H18	2.29	0.68
1:D:277:LEU:HD12	1:D:278:PRO:HD2	1.77	0.67
1:A:160:TYR:O	11:A:4204:EPE:H72	1.95	0.66
2:B:87[A]:VAL:CG1	2:B:116[A]:ILE:HG21	2.25	0.66
1:D:166:GLU:OE2	19:D:601:HOH:O	2.13	0.65
3:C:66:ASN:ND2	3:C:69:ASN:OD1	2.30	0.65
2:E:306:PHE:HB2	2:E:420:VAL:HG11	1.80	0.64
1:A:112:MET:HE1	2:B:106:VAL:HG23	1.79	0.64
1:D:310:PHE:CZ	9:D:501:PT5:H18	2.33	0.64
1:A:37[B]:ARG:NH2	19:A:4304:HOH:O	2.26	0.63
3:C:234:GLY:HA2	17:C:505:PGW:H01	1.79	0.63
17:C:505:PGW:H18	12:D:508:PX2:H41	1.81	0.62
2:B:99[B]:LEU:HD11	2:B:155:GLU:HB2	1.82	0.61
8:E:502:D10:H71	15:E:507:HEX:C6	2.31	0.61
2:E:426[B]:TRP:CE2	2:E:430:VAL:HG21	2.36	0.61
12:A:4205:PX2:H14	12:A:4205:PX2:H21	1.83	0.60
3:C:144:ARG:NH1	19:C:605:HOH:O	2.35	0.60
2:E:44:ILE:HD12	2:E:59:LEU:HD11	1.84	0.59
1:A:122[B]:THR:OG1	1:A:124:ASP:OD1	2.17	0.59
2:B:426[A]:TRP:CE2	2:B:430:VAL:HG21	2.37	0.59
2:B:66:TYR:CE2	2:B:125:LEU:HD13	2.38	0.58
2:B:137:MET:O	19:B:601:HOH:O	2.17	0.58
3:C:240:THR:HG21	3:C:296:MET:SD	2.43	0.58
2:E:43:ASP:OD1	19:E:603:HOH:O	2.17	0.58
2:E:142[B]:ARG:NH2	2:E:446:TYR:O	2.36	0.57
12:A:4207:PX2:O6	12:A:4207:PX2:H3	2.04	0.57
1:A:210:TYR:CZ	11:A:4204:EPE:H71	2.41	0.56
2:B:235:LEU:HD13	3:C:308:PHE:CE2	2.41	0.56
1:A:94[A]:ILE:HD11	1:A:119:LEU:HD21	1.88	0.55
2:B:447:VAL:HG21	8:B:504:D10:H82	1.89	0.55
1:D:122:THR:OG1	1:D:124:ASP:OD1	2.25	0.55
2:B:87[A]:VAL:HG12	2:B:116[A]:ILE:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:501:PT5:H15	9:D:501:PT5:H20	1.91	0.53
1:D:86:LEU:HD11	1:D:121:ILE:HD11	1.90	0.52
2:E:129:ARG:NH1	19:E:611:HOH:O	2.41	0.52
19:C:731:HOH:O	4:F:3:BMA:O4	2.19	0.52
1:A:146:PHE:CD1	1:A:277:LEU:HD23	2.45	0.51
1:A:34:LEU:HD23	1:A:35:GLY:N	2.26	0.51
1:D:112:MET:HE1	2:E:106:VAL:HG23	1.92	0.51
2:B:129:ARG:NH2	3:C:116:SER:O	2.45	0.50
12:A:4207:PX2:H9	12:A:4207:PX2:H35	1.95	0.49
1:A:203[B]:VAL:HG21	11:A:4204:EPE:O3S	2.13	0.49
2:E:155:GLU:OE2	2:E:207:ARG:NE	2.40	0.49
2:B:306:PHE:HB2	2:B:420:VAL:HG11	1.94	0.48
1:D:306:THR:HG21	9:D:501:PT5:H53	1.96	0.48
2:E:188:ILE:HD12	2:E:188:ILE:N	2.28	0.48
14:C:504:PLM:H71	14:C:504:PLM:H22	1.96	0.48
2:B:302:VAL:HG13	2:B:420:VAL:HB	1.96	0.47
1:A:288:TRP:HH2	8:A:4210:D10:H52	1.78	0.47
2:B:140:LEU:HD13	2:B:275[A]:ILE:HD13	1.97	0.47
8:E:502:D10:H71	15:E:507:HEX:H63	1.97	0.47
1:A:146:PHE:CE1	1:A:277:LEU:HD23	2.50	0.47
1:A:102:HIS:CE1	1:A:212[B]:VAL:HG12	2.50	0.47
2:B:414:ILE:HG23	2:B:414:ILE:O	2.15	0.47
2:B:269[B]:ARG:NH1	2:B:282:ASP:OD1	2.49	0.46
2:E:66[A]:TYR:CZ	2:E:125:LEU:HD13	2.50	0.46
12:A:4207:PX2:H3	12:A:4207:PX2:C4	2.45	0.46
3:C:237:THR:HG21	17:C:505:PGW:H20A	1.98	0.46
3:C:323:ASN:O	3:C:324:ARG:NH1	2.41	0.46
1:D:239:ILE:O	1:D:243:VAL:HG23	2.16	0.46
1:D:306:THR:HG21	9:D:501:PT5:C32	2.46	0.45
2:E:302:VAL:HG13	2:E:420:VAL:HB	1.98	0.45
1:A:190:GLN:OE1	19:A:4301:HOH:O	2.21	0.45
15:D:503:HEX:H11	10:D:505:R16:H421	1.97	0.45
1:D:85:ARG:HG3	1:D:118:LEU:HD11	1.99	0.45
1:A:94[A]:ILE:CD1	1:A:119:LEU:HD21	2.46	0.45
1:D:86:LEU:HD11	1:D:121:ILE:CD1	2.46	0.45
2:E:44:ILE:HG21	2:E:181:ILE:HD11	1.99	0.45
1:A:10:ASP:CG	1:A:12:THR:HG22	2.41	0.45
1:D:146:PHE:CE1	1:D:277:LEU:HD13	2.52	0.45
2:E:66[B]:TYR:CZ	2:E:125:LEU:HD13	2.50	0.45
5:K:4:MAN:H3	5:K:5:MAN:H3	1.99	0.45
1:A:410:VAL:HG11	12:A:4207:PX2:H37	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:ASP:O	1:D:397:ARG:HD3	2.17	0.45
1:A:18:ILE:HG21	1:A:84:LEU:HD11	1.98	0.44
3:C:250:LEU:HD22	1:D:301:LEU:HD23	1.99	0.44
2:B:66:TYR:CZ	2:B:125:LEU:HD13	2.53	0.44
3:C:22:VAL:HG11	3:C:93:ILE:HD11	2.00	0.44
2:E:55[B]:MET:HE1	2:E:137:MET:SD	2.58	0.44
1:A:34:LEU:HD23	1:A:34:LEU:C	2.43	0.43
3:C:206:LEU:C	3:C:206:LEU:HD12	2.43	0.43
1:D:246[B]:TRP:CE2	1:D:397:ARG:HG2	2.54	0.43
8:A:4210:D10:H71	2:E:219:GLY:HA2	2.00	0.42
1:A:122[A]:THR:HG22	1:A:123:GLU:N	2.34	0.42
2:B:44:ILE:HG23	2:B:59:LEU:HD11	2.01	0.42
1:A:301:LEU:HD23	2:E:235:LEU:HD22	2.01	0.42
2:B:219:GLY:HA3	13:B:505:OLC:H7	2.00	0.42
14:A:4208:PLM:H42	15:E:507:HEX:H12	2.00	0.42
1:A:309:TYR:CD2	14:A:4208:PLM:H71	2.54	0.42
3:C:210:THR:HG23	3:C:223:MET:SD	2.59	0.42
2:B:447:VAL:HG22	2:B:447:VAL:O	2.19	0.42
1:A:10:ASP:O	1:A:13:THR:HG22	2.20	0.42
11:A:4204:EPE:O8	11:A:4204:EPE:H52	2.19	0.42
2:E:447:VAL:HG12	2:E:447:VAL:OXT	2.20	0.42
1:A:392:ILE:HD11	9:A:4202:PT5:H18	2.02	0.41
13:A:4206:OLC:C3	13:A:4206:OLC:H7A	2.47	0.41
8:B:503:D10:H61	8:B:503:D10:H91	1.89	0.41
13:B:505:OLC:H14	15:C:501:HEX:H11	2.02	0.41
3:C:233:MET:HB2	17:C:505:PGW:H03A	2.02	0.41
3:C:242:ILE:HB	3:C:243:PRO:HD3	2.02	0.41
1:D:127:LEU:HD12	1:D:127:LEU:N	2.35	0.41
1:A:277:LEU:HD13	1:A:278:PRO:N	2.36	0.41
2:B:155:GLU:OE2	2:B:207:ARG:NH2	2.44	0.41
14:A:4208:PLM:C3	15:E:507:HEX:H12	2.45	0.41
3:C:70:MET:HE2	3:C:288:PRO:HG3	2.02	0.41
1:D:323:VAL:O	1:D:323:VAL:HG23	2.20	0.41
1:A:171:TRP:CE2	1:A:213:MET:HE3	2.55	0.41
3:C:62:ILE:HD12	3:C:196:TRP:CZ3	2.56	0.41
1:A:307:VAL:HG22	1:A:392:ILE:HB	2.02	0.40
8:A:4201:D10:H21	10:A:4203:R16:H321	2.02	0.40
2:B:235:LEU:HD13	3:C:308:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	367/409 (90%)	360 (98%)	7 (2%)	0	100	100
1	D	354/409 (87%)	348 (98%)	6 (2%)	0	100	100
2	B	352/441 (80%)	347 (99%)	5 (1%)	0	100	100
2	E	350/441 (79%)	349 (100%)	1 (0%)	0	100	100
3	C	339/415 (82%)	331 (98%)	8 (2%)	0	100	100
All	All	1762/2115 (83%)	1735 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/363 (92%)	333 (100%)	0	100	100
1	D	320/363 (88%)	320 (100%)	0	100	100
2	B	322/393 (82%)	322 (100%)	0	100	100
2	E	319/393 (81%)	319 (100%)	0	100	100
3	C	317/380 (83%)	317 (100%)	0	100	100
All	All	1611/1892 (85%)	1611 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	242	GLN
2	B	421	ASN
3	C	66	ASN
3	C	69	ASN
1	D	88	ASN
1	D	102	HIS
1	D	242	GLN
2	E	90	GLN
2	E	119	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
4	NAG	F	1	4,1	14,14,15	0.82	0	17,19,21	0.85	0
4	MAN	F	10	4	11,11,12	0.86	1 (9%)	15,15,17	0.94	0
4	NAG	F	2	4	14,14,15	0.80	0	17,19,21	0.80	0
4	BMA	F	3	4	11,11,12	0.91	0	15,15,17	2.50	4 (26%)
4	MAN	F	4	4	11,11,12	0.86	1 (9%)	15,15,17	1.00	1 (6%)
4	MAN	F	5	4	11,11,12	0.90	1 (9%)	15,15,17	1.07	1 (6%)
4	MAN	F	6	4	11,11,12	0.85	1 (9%)	15,15,17	1.16	1 (6%)
4	MAN	F	7	4	11,11,12	0.91	1 (9%)	15,15,17	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	F	8	4	11,11,12	0.85	1 (9%)	15,15,17	1.04	1 (6%)
4	MAN	F	9	4	11,11,12	0.85	1 (9%)	15,15,17	1.04	1 (6%)
5	NAG	G	1	5,2	14,14,15	0.44	0	17,19,21	1.09	3 (17%)
5	NAG	G	2	5	14,14,15	0.43	0	17,19,21	0.54	0
5	BMA	G	3	5	11,11,12	0.38	0	15,15,17	0.73	0
5	MAN	G	4	5	11,11,12	0.35	0	15,15,17	0.76	1 (6%)
5	MAN	G	5	5	11,11,12	0.36	0	15,15,17	0.79	1 (6%)
5	MAN	G	6	5	11,11,12	0.43	0	15,15,17	0.51	0
6	NAG	H	1	6,2	14,14,15	0.80	0	17,19,21	0.83	0
6	NAG	H	2	6	14,14,15	0.74	0	17,19,21	0.95	1 (5%)
6	BMA	H	3	6	11,11,12	0.88	0	15,15,17	1.81	1 (6%)
7	NAG	I	1	7,3	14,14,15	0.41	0	17,19,21	0.97	1 (5%)
7	NAG	I	2	7	14,14,15	0.42	0	17,19,21	0.97	1 (5%)
5	NAG	J	1	5,1	14,14,15	0.41	0	17,19,21	0.76	0
5	NAG	J	2	5	14,14,15	0.40	0	17,19,21	0.62	0
5	BMA	J	3	5	11,11,12	0.42	0	15,15,17	0.60	0
5	MAN	J	4	5	11,11,12	0.34	0	15,15,17	1.02	2 (13%)
5	MAN	J	5	5	11,11,12	0.30	0	15,15,17	0.53	0
5	MAN	J	6	5	11,11,12	0.30	0	15,15,17	0.52	0
5	NAG	K	1	5,2	14,14,15	0.45	0	17,19,21	1.04	2 (11%)
5	NAG	K	2	5	14,14,15	0.43	0	17,19,21	0.60	0
5	BMA	K	3	5	11,11,12	0.52	0	15,15,17	0.51	0
5	MAN	K	4	5	11,11,12	0.33	0	15,15,17	0.58	0
5	MAN	K	5	5	11,11,12	0.29	0	15,15,17	0.85	1 (6%)
5	MAN	K	6	5	11,11,12	0.39	0	15,15,17	0.63	0
6	NAG	L	1	6,2	14,14,15	0.78	0	17,19,21	0.77	0
6	NAG	L	2	6	14,14,15	0.78	0	17,19,21	0.93	0
6	BMA	L	3	6	11,11,12	0.88	0	15,15,17	1.81	2 (13%)

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
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	MAN	F	10	4	-	2/2/19/22	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
4	MAN	F	8	4	-	2/2/19/22	0/1/1/1
4	MAN	F	9	4	-	1/2/19/22	0/1/1/1
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
5	MAN	G	6	5	-	1/2/19/22	0/1/1/1
6	NAG	H	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1
7	NAG	I	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	0/1/1/1
5	MAN	J	5	5	-	0/2/19/22	0/1/1/1
5	MAN	J	6	5	-	0/2/19/22	0/1/1/1
5	NAG	K	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	0/2/19/22	0/1/1/1
5	MAN	K	6	5	-	0/2/19/22	0/1/1/1
6	NAG	L	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	7	MAN	O5-C1	-2.44	1.39	1.43
4	F	5	MAN	O5-C1	-2.31	1.40	1.43
4	F	6	MAN	O5-C1	-2.28	1.40	1.43
4	F	8	MAN	O5-C1	-2.25	1.40	1.43
4	F	10	MAN	O5-C1	-2.24	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	4	MAN	O5-C1	-2.24	1.40	1.43
4	F	9	MAN	O5-C1	-2.17	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	C1-O5-C5	6.68	121.24	112.19
6	H	3	BMA	C1-O5-C5	5.02	119.00	112.19
6	L	3	BMA	C1-O5-C5	4.87	118.79	112.19
4	F	3	BMA	C3-C4-C5	4.37	118.03	110.24
4	F	6	MAN	C1-O5-C5	3.37	116.76	112.19
4	F	3	BMA	O4-C4-C3	-3.04	103.31	110.35
5	K	1	NAG	C2-N2-C7	2.78	126.86	122.90
5	G	1	NAG	C1-C2-N2	-2.67	105.93	110.49
4	F	3	BMA	C2-C3-C4	2.59	115.39	110.89
4	F	9	MAN	C1-O5-C5	2.53	115.62	112.19
4	F	8	MAN	C1-O5-C5	2.50	115.58	112.19
5	J	4	MAN	C1-O5-C5	2.44	115.50	112.19
5	G	1	NAG	C1-O5-C5	2.39	115.42	112.19
4	F	5	MAN	C1-O5-C5	2.35	115.38	112.19
5	K	5	MAN	C1-O5-C5	2.31	115.32	112.19
5	G	1	NAG	C2-N2-C7	2.29	126.16	122.90
4	F	7	MAN	C1-O5-C5	2.27	115.26	112.19
7	I	2	NAG	C1-C2-N2	-2.24	106.67	110.49
4	F	4	MAN	C1-O5-C5	2.19	115.16	112.19
6	L	3	BMA	C3-C4-C5	2.17	114.11	110.24
5	G	4	MAN	C1-O5-C5	2.16	115.12	112.19
7	I	1	NAG	C1-O5-C5	2.15	115.10	112.19
5	J	4	MAN	O3-C3-C2	-2.13	105.91	109.99
6	H	2	NAG	C4-C3-C2	-2.05	108.02	111.02
5	G	5	MAN	C1-O5-C5	2.04	114.96	112.19
5	K	1	NAG	C1-C2-N2	-2.03	107.02	110.49

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
4	F	10	MAN	O5-C5-C6-O6
4	F	10	MAN	C4-C5-C6-O6
4	F	8	MAN	O5-C5-C6-O6

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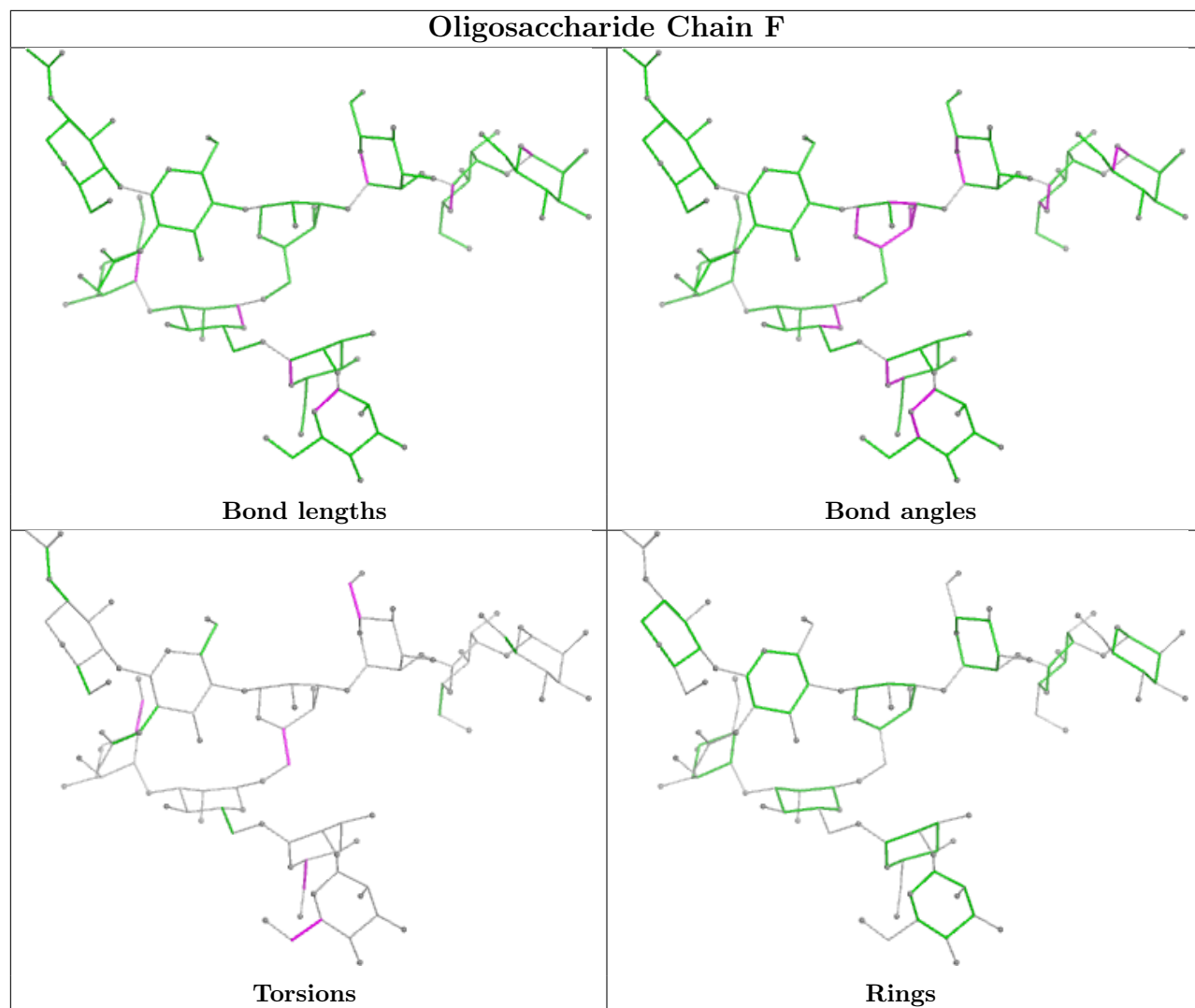
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
7	I	2	NAG	C8-C7-N2-C2
4	F	8	MAN	C4-C5-C6-O6
7	I	2	NAG	O7-C7-N2-C2
4	F	4	MAN	O5-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
5	G	6	MAN	O5-C5-C6-O6
6	L	2	NAG	C3-C2-N2-C7
4	F	9	MAN	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6

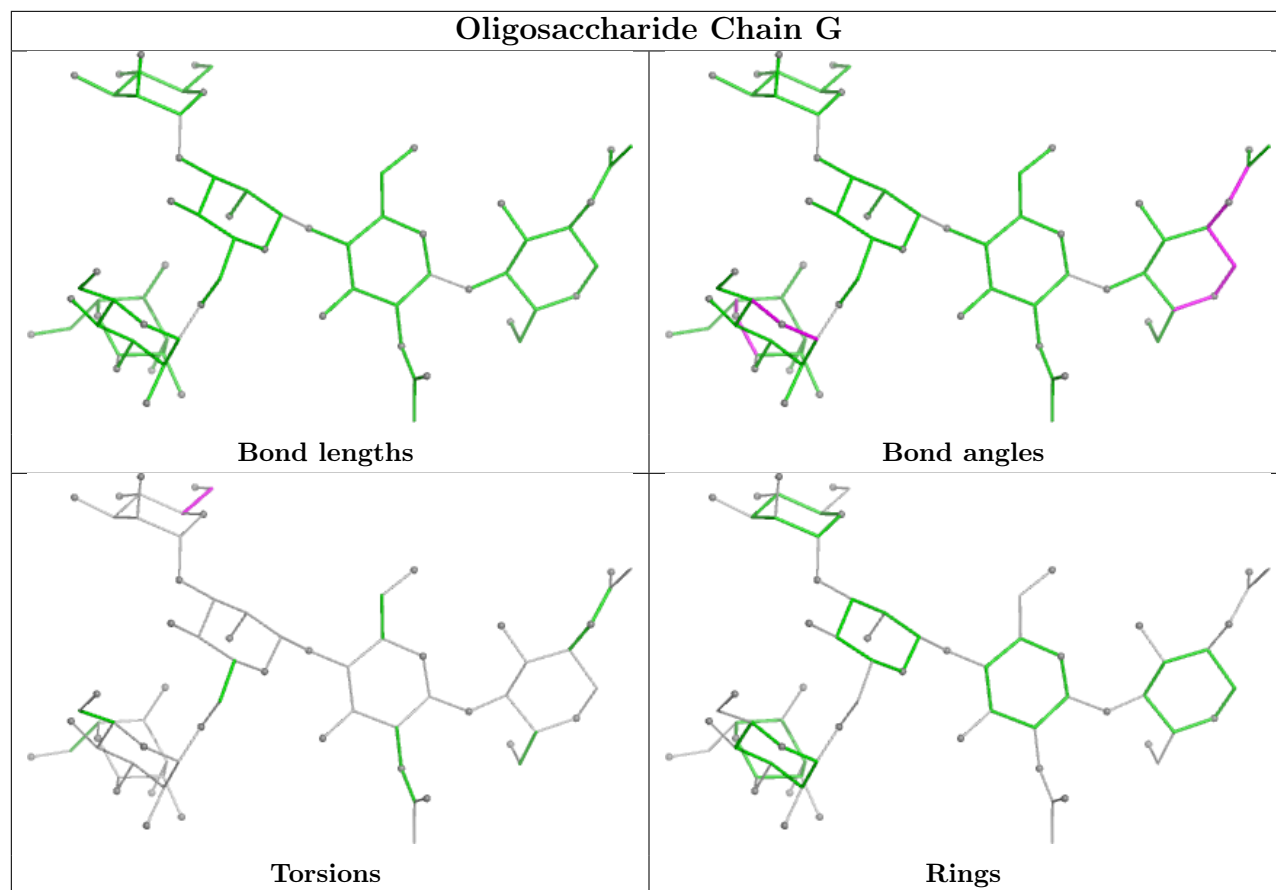
There are no ring outliers.

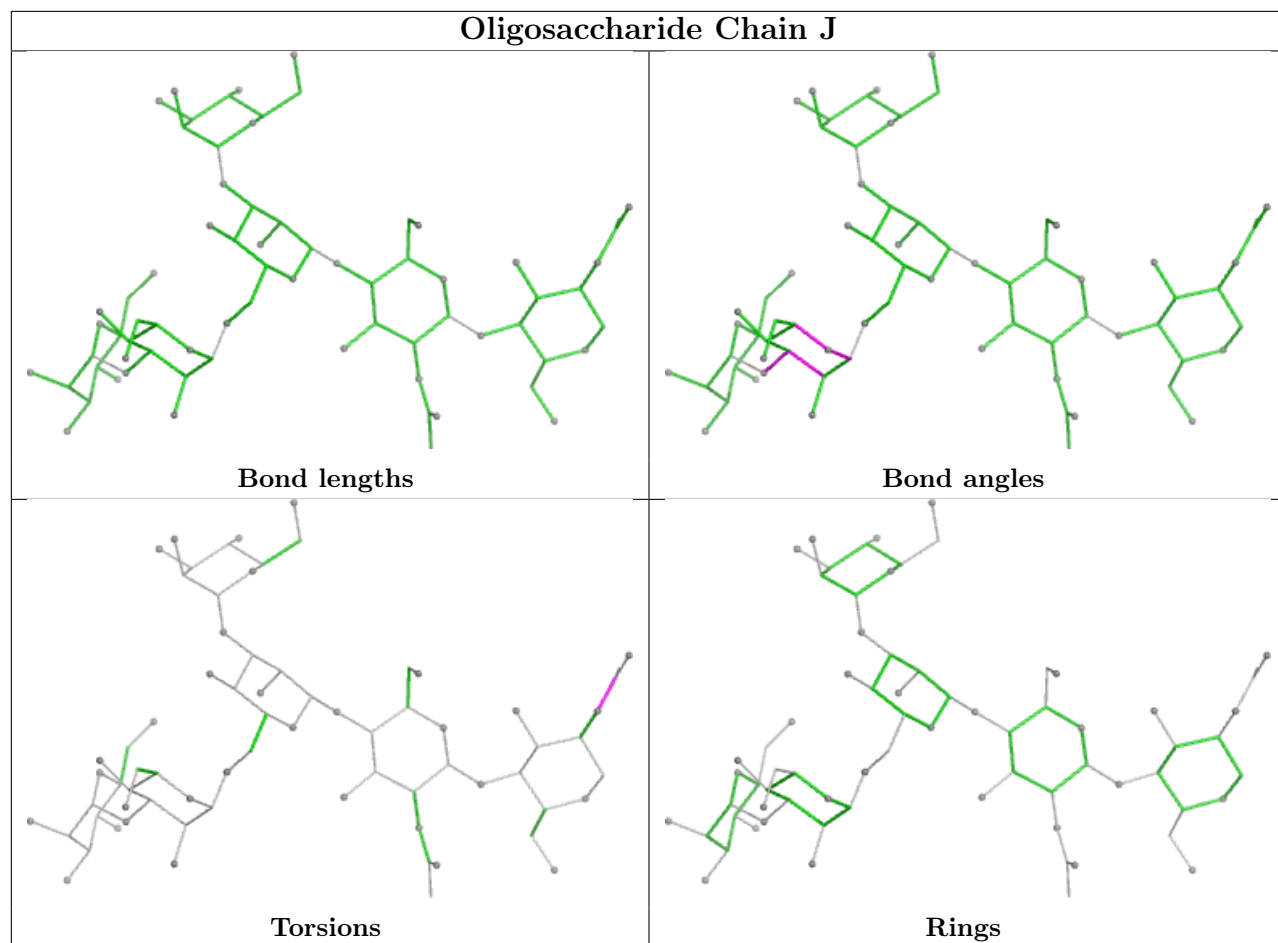
5 monomers are involved in 3 short contacts:

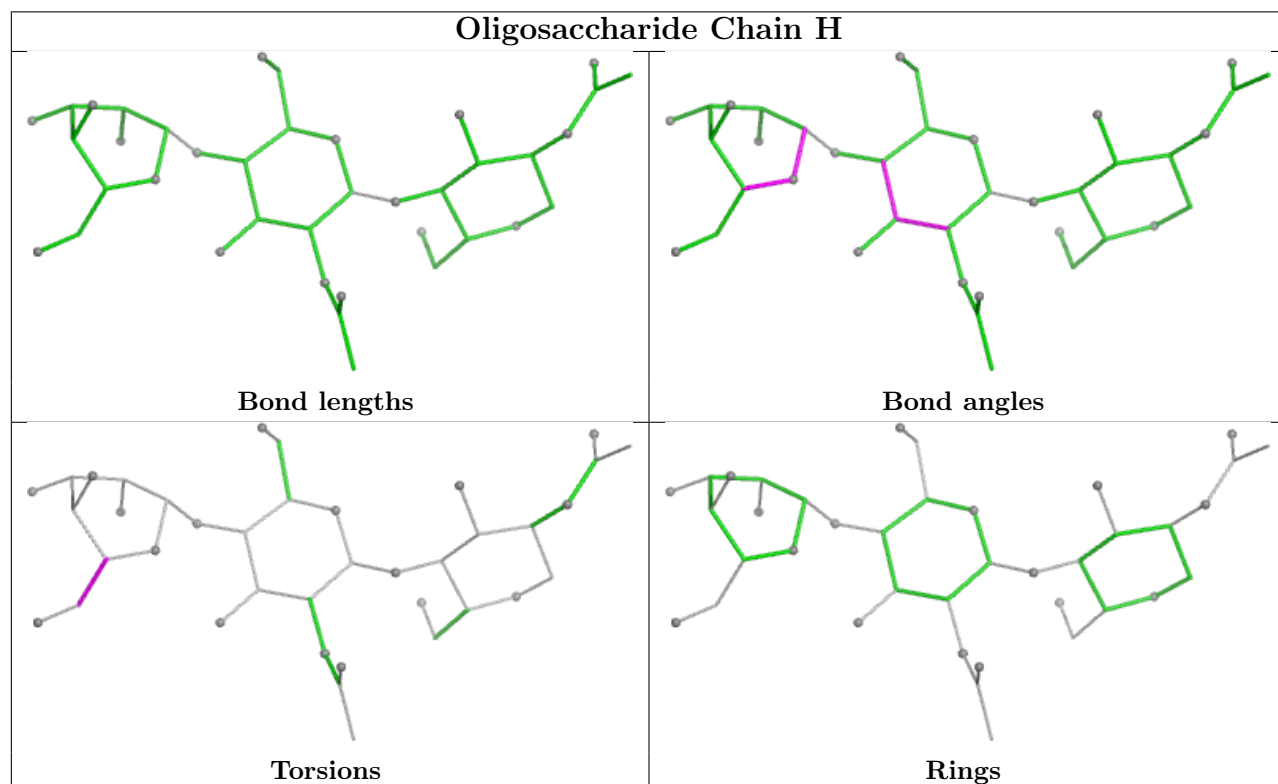
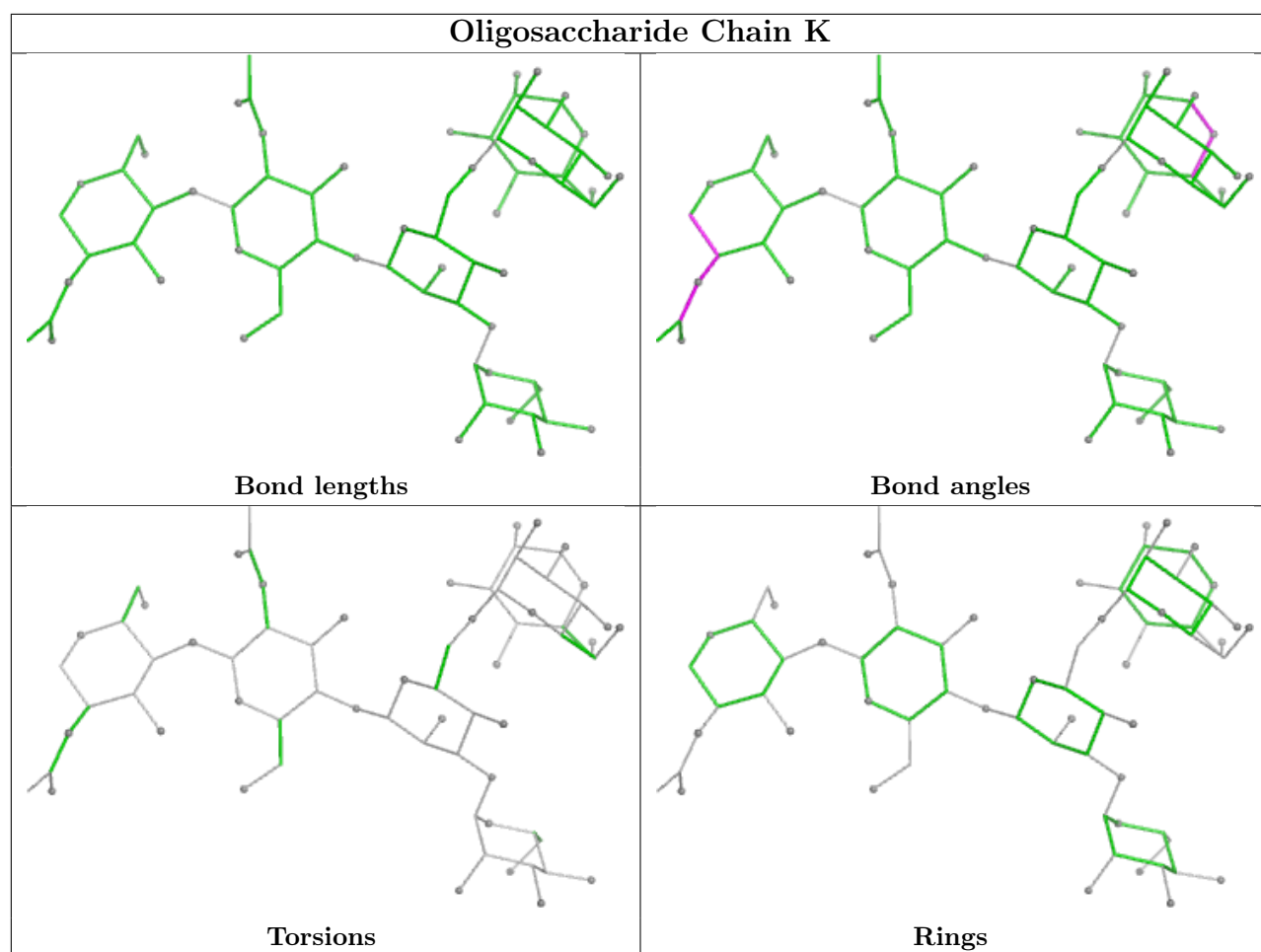
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3	BMA	1	0
5	K	5	MAN	1	0
7	I	2	NAG	1	0
7	I	1	NAG	1	0
5	K	4	MAN	1	0

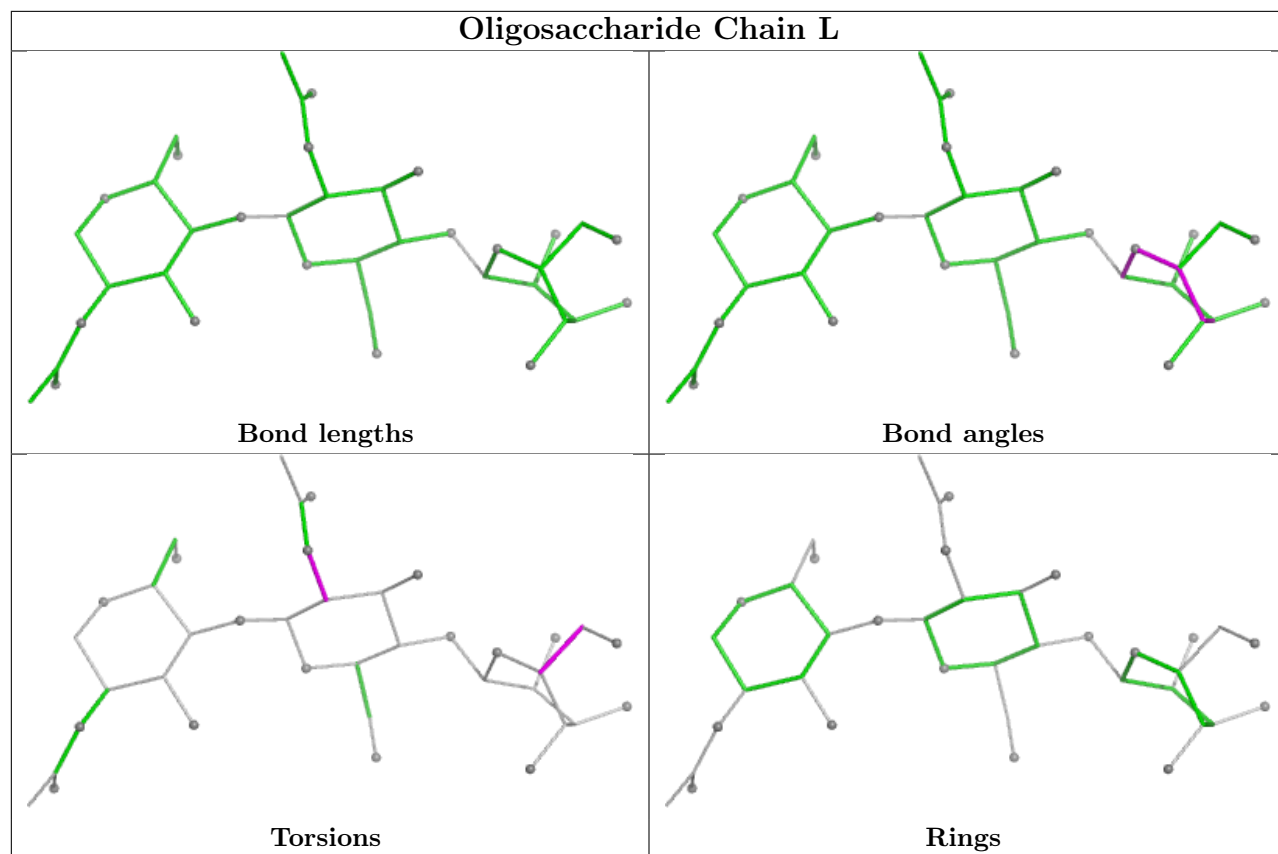
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

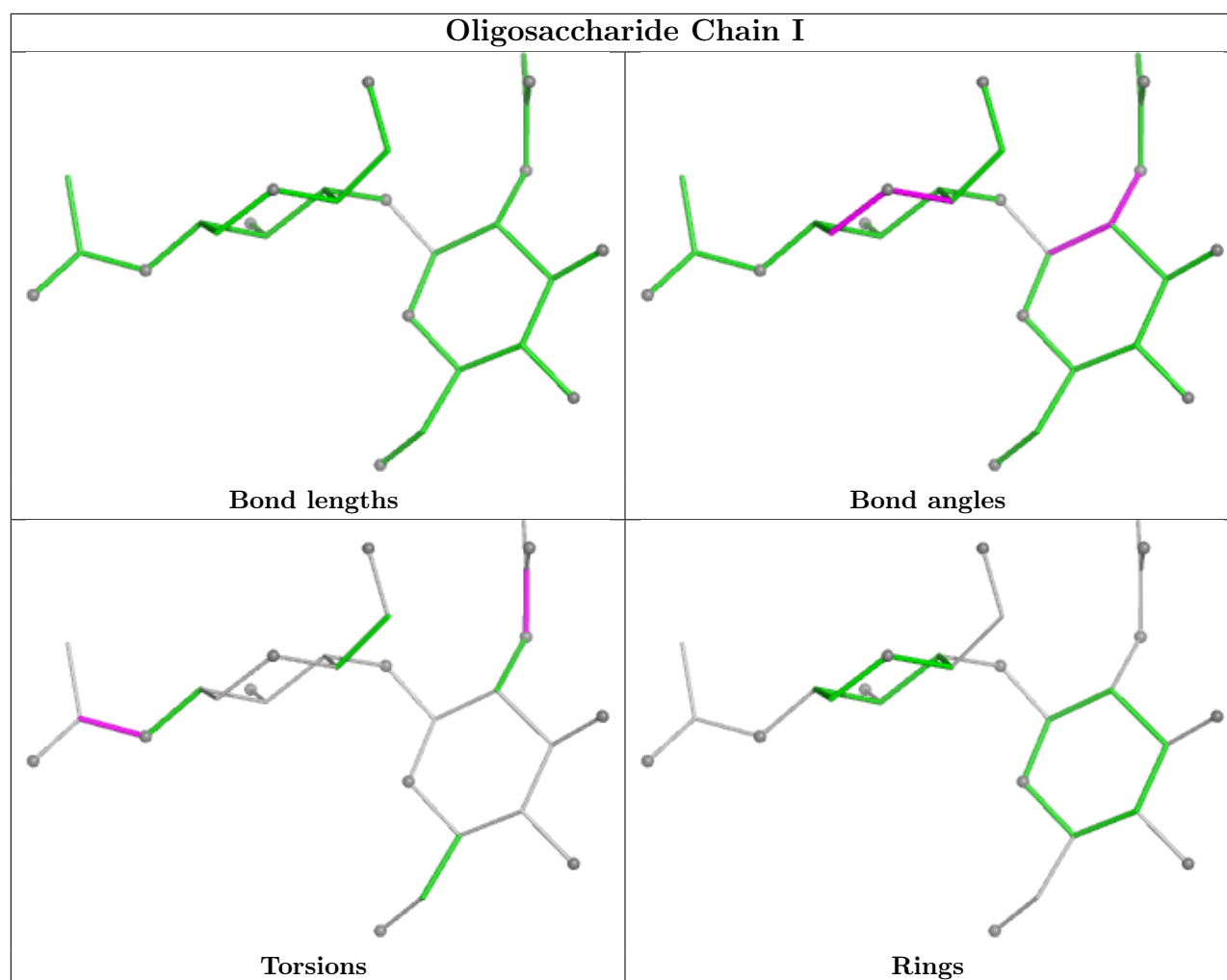












5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 1 is monoatomic - leaving 41 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	$\# Z > 2$
13	OLC	B	505	-	24,24,24	1.04	1 (4%)	25,25,25	1.16	2 (8%)
15	HEX	C	501	-	5,5,5	0.28	0	4,4,4	0.61	0
8	D10	D	507	-	9,9,9	0.29	0	8,8,8	0.81	0
15	HEX	E	508	-	5,5,5	0.30	0	4,4,4	0.58	0
14	PLM	C	504	-	17,17,17	0.55	0	17,17,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	NAG	D	502	1	14,14,15	0.69	0	17,19,21	1.11	1 (5%)
12	PX2	A	4205	-	35,35,35	1.37	4 (11%)	39,40,40	1.13	2 (5%)
8	D10	B	507	-	9,9,9	0.29	0	8,8,8	0.80	0
10	R16	A	4203	-	15,15,15	0.28	0	14,14,14	0.86	0
8	D10	A	4201	-	9,9,9	0.29	0	8,8,8	0.81	0
10	R16	D	506	-	15,15,15	0.29	0	14,14,14	0.84	0
8	D10	E	502	-	9,9,9	0.28	0	8,8,8	0.81	0
15	HEX	C	507	-	5,5,5	0.30	0	4,4,4	0.58	0
8	D10	B	503	-	9,9,9	0.30	0	8,8,8	0.77	0
15	HEX	A	4209	-	5,5,5	0.29	0	4,4,4	0.60	0
15	HEX	C	503	-	5,5,5	0.13	0	4,4,4	0.06	0
8	D10	B	504	-	9,9,9	0.29	0	8,8,8	0.81	0
15	HEX	E	503	-	5,5,5	0.29	0	4,4,4	0.56	0
9	PT5	A	4202	-	69,69,69	0.42	0	83,87,87	0.63	2 (2%)
15	HEX	D	503	-	5,5,5	0.30	0	4,4,4	0.59	0
16	NAG	C	502	3	14,14,15	0.39	0	17,19,21	1.72	2 (11%)
8	D10	E	505	-	9,9,9	0.28	0	8,8,8	0.82	0
11	EPE	A	4204	-	15,15,15	1.19	3 (20%)	18,20,20	1.83	5 (27%)
8	D10	E	504	-	9,9,9	0.28	0	8,8,8	0.81	0
14	PLM	A	4208	-	17,17,17	0.56	0	17,17,17	1.14	0
10	R16	D	505	-	15,15,15	0.31	0	14,14,14	0.70	0
15	HEX	B	502	-	5,5,5	0.30	0	4,4,4	0.58	0
15	HEX	E	507	-	5,5,5	0.30	0	4,4,4	0.59	0
12	PX2	D	508	-	35,35,35	1.37	4 (11%)	39,40,40	1.12	2 (5%)
12	PX2	A	4207	-	35,35,35	1.36	4 (11%)	39,40,40	1.15	2 (5%)
10	R16	B	506	-	15,15,15	0.29	0	14,14,14	0.81	0
15	HEX	C	506	-	5,5,5	0.30	0	4,4,4	0.58	0
17	PGW	C	505	-	50,50,50	0.32	0	53,56,56	0.34	0
13	OLC	E	501	-	24,24,24	1.02	1 (4%)	25,25,25	1.20	2 (8%)
10	R16	E	506	-	15,15,15	0.30	0	14,14,14	0.79	0
14	PLM	C	508	-	17,17,17	0.57	0	17,17,17	1.12	1 (5%)
9	PT5	D	501	-	69,69,69	0.45	0	83,87,87	0.57	1 (1%)
13	OLC	A	4206	-	24,24,24	1.04	1 (4%)	25,25,25	1.25	2 (8%)
15	HEX	B	501	-	5,5,5	0.30	0	4,4,4	0.56	0
8	D10	D	504	-	9,9,9	0.30	0	8,8,8	0.77	0
8	D10	A	4210	-	9,9,9	0.29	0	8,8,8	0.76	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
13	OLC	B	505	-	-	12/24/24/24	-
15	HEX	C	501	-	-	1/3/3/3	-
8	D10	D	507	-	-	2/7/7/7	-
15	HEX	E	508	-	-	0/3/3/3	-
14	PLM	C	504	-	-	6/15/15/15	-
16	NAG	D	502	1	-	2/6/23/26	0/1/1/1
12	PX2	A	4205	-	-	14/37/37/37	-
8	D10	B	507	-	-	1/7/7/7	-
10	R16	A	4203	-	-	2/13/13/13	-
8	D10	A	4201	-	-	1/7/7/7	-
10	R16	D	506	-	-	4/13/13/13	-
8	D10	E	502	-	-	1/7/7/7	-
15	HEX	C	507	-	-	0/3/3/3	-
8	D10	B	503	-	-	1/7/7/7	-
15	HEX	A	4209	-	-	0/3/3/3	-
15	HEX	C	503	-	-	0/3/3/3	-
8	D10	B	504	-	-	0/7/7/7	-
15	HEX	E	503	-	-	0/3/3/3	-
9	PT5	A	4202	-	-	18/66/90/90	0/1/1/1
15	HEX	D	503	-	-	0/3/3/3	-
16	NAG	C	502	3	-	1/6/23/26	0/1/1/1
8	D10	E	505	-	-	2/7/7/7	-
11	EPE	A	4204	-	-	2/9/19/19	0/1/1/1
8	D10	E	504	-	-	1/7/7/7	-
14	PLM	A	4208	-	-	8/15/15/15	-
10	R16	D	505	-	-	3/13/13/13	-
15	HEX	B	502	-	-	1/3/3/3	-
15	HEX	E	507	-	-	0/3/3/3	-
12	PX2	D	508	-	-	22/37/37/37	-
12	PX2	A	4207	-	-	21/37/37/37	-
10	R16	B	506	-	-	5/13/13/13	-
15	HEX	C	506	-	-	0/3/3/3	-
17	PGW	C	505	-	-	17/55/55/55	-
13	OLC	E	501	-	-	14/24/24/24	-
10	R16	E	506	-	-	2/13/13/13	-
14	PLM	C	508	-	-	3/15/15/15	-
9	PT5	D	501	-	-	22/66/90/90	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	OLC	A	4206	-	-	12/24/24/24	-
15	HEX	B	501	-	-	0/3/3/3	-
8	D10	D	504	-	-	0/7/7/7	-
8	D10	A	4210	-	-	3/7/7/7	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	4205	PX2	O7-C16	3.80	1.45	1.34
12	D	508	PX2	O7-C16	3.74	1.44	1.34
12	A	4207	PX2	O7-C16	3.74	1.44	1.34
12	A	4205	PX2	O5-C4	3.55	1.43	1.33
12	A	4207	PX2	O5-C4	3.48	1.43	1.33
12	D	508	PX2	O5-C4	3.44	1.43	1.33
13	B	505	OLC	O20-C1	2.96	1.42	1.33
13	E	501	OLC	O20-C1	2.90	1.41	1.33
11	A	4204	EPE	C10-S	2.88	1.81	1.77
13	A	4206	OLC	O20-C1	2.87	1.41	1.33
12	D	508	PX2	O7-C2	-2.35	1.40	1.46
12	D	508	PX2	C17-C16	2.33	1.57	1.50
12	A	4205	PX2	C17-C16	2.30	1.57	1.50
12	A	4207	PX2	O7-C2	-2.28	1.40	1.46
12	A	4205	PX2	O7-C2	-2.23	1.41	1.46
12	A	4207	PX2	C17-C16	2.20	1.57	1.50
11	A	4204	EPE	O2S-S	2.08	1.51	1.45
11	A	4204	EPE	O1S-S	2.08	1.51	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	502	NAG	C2-N2-C7	5.67	130.97	122.90
12	A	4205	PX2	O7-C16-C17	4.06	120.24	111.50
12	A	4207	PX2	O7-C16-C17	4.00	120.11	111.50
11	A	4204	EPE	O2S-S-C10	3.96	111.68	106.92
12	D	508	PX2	O7-C16-C17	3.89	119.88	111.50
16	C	502	NAG	C1-C2-N2	3.66	116.74	110.49
13	A	4206	OLC	C8-C9-C10	3.65	152.73	124.73
13	B	505	OLC	C8-C9-C10	3.64	152.64	124.73
11	A	4204	EPE	O1S-S-C10	3.60	111.25	106.92
11	A	4204	EPE	O2S-S-O1S	-3.59	101.54	113.95
13	E	501	OLC	C8-C9-C10	3.50	151.59	124.73
16	D	502	NAG	C2-N2-C7	3.37	127.71	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	4206	OLC	O20-C1-C2	2.91	121.03	111.91
13	B	505	OLC	O20-C1-C2	2.60	120.05	111.91
12	A	4207	PX2	O5-C4-C5	2.58	120.01	111.91
13	E	501	OLC	O20-C1-C2	2.58	120.00	111.91
9	A	4202	PT5	O16-C10-C12	2.57	117.05	111.50
12	A	4205	PX2	O5-C4-C5	2.51	119.79	111.91
12	D	508	PX2	O5-C4-C5	2.48	119.67	111.91
11	A	4204	EPE	C5-N4-C3	2.31	114.03	108.83
14	C	508	PLM	C3-C2-C1	-2.16	109.04	114.47
11	A	4204	EPE	O3S-S-C10	2.11	109.18	105.77
9	D	501	PT5	O16-C10-C12	2.09	116.00	111.50
9	A	4202	PT5	O12-P1-O11	2.05	122.36	112.24

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	4202	PT5	C12-C10-O16-C8
9	D	501	PT5	C7-O13-P1-O12
9	D	501	PT5	O17-C10-O16-C8
9	D	501	PT5	C12-C10-O16-C8
9	D	501	PT5	C17-C18-C19-C20
11	A	4204	EPE	C8-C7-N4-C5
12	A	4205	PX2	C1-O4-P1-O1
12	A	4205	PX2	C1-O4-P1-O3
12	A	4205	PX2	C1-C2-O7-C16
12	A	4205	PX2	C17-C16-O7-C2
12	A	4207	PX2	C1-O4-P1-O1
12	A	4207	PX2	C1-O4-P1-O3
12	D	508	PX2	C1-O4-P1-O1
12	D	508	PX2	C1-O4-P1-O3
12	D	508	PX2	O4-C1-C2-O7
12	D	508	PX2	C17-C16-O7-C2
13	E	501	OLC	O20-C21-C22-C24
16	C	502	NAG	C1-C2-N2-C7
17	C	505	PGW	C04-O12-P-O14
9	A	4202	PT5	O19-C11-O18-C9
12	D	508	PX2	O6-C4-O5-C3
12	A	4205	PX2	O8-C16-O7-C2
12	D	508	PX2	O8-C16-O7-C2
9	A	4202	PT5	C31-C11-O18-C9
12	D	508	PX2	C5-C4-O5-C3

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Mol	Chain	Res	Type	Atoms
9	A	4202	PT5	C17-C18-C19-C20
9	A	4202	PT5	C20-C21-C22-C23
9	A	4202	PT5	O17-C10-O16-C8
12	A	4207	PX2	C5-C6-C7-C8
13	A	4206	OLC	O20-C21-C22-C24
16	D	502	NAG	C8-C7-N2-C2
16	D	502	NAG	O7-C7-N2-C2
13	A	4206	OLC	O20-C21-C22-O23
13	E	501	OLC	O20-C21-C22-O23
12	A	4207	PX2	C16-C17-C18-C19
12	D	508	PX2	C17-C18-C19-C20
14	A	4208	PLM	C4-C5-C6-C7
12	A	4207	PX2	C5-C4-O5-C3
13	B	505	OLC	O20-C21-C22-O23
8	D	507	D10	C3-C4-C5-C6
10	D	505	R16	C33-C34-C35-C36
12	A	4207	PX2	C17-C16-O7-C2
12	A	4207	PX2	C19-C20-C21-C22
14	A	4208	PLM	C6-C7-C8-C9
17	C	505	PGW	C24-C25-C26-C27
13	B	505	OLC	O20-C21-C22-C24
9	D	501	PT5	C7-C8-O16-C10
12	A	4207	PX2	O8-C16-O7-C2
12	D	508	PX2	C21-C22-C23-C24
13	B	505	OLC	C13-C14-C15-C16
14	C	504	PLM	C2-C3-C4-C5
12	A	4207	PX2	C17-C18-C19-C20
13	E	501	OLC	C5-C6-C7-C8
8	A	4201	D10	C4-C5-C6-C7
12	D	508	PX2	C5-C6-C7-C8
13	A	4206	OLC	C4-C5-C6-C7
17	C	505	PGW	C25-C26-C27-C15
9	D	501	PT5	C39-C40-C41-C42
13	A	4206	OLC	C1-C2-C3-C4
13	E	501	OLC	C1-C2-C3-C4
12	A	4205	PX2	C7-C8-C9-C10
13	B	505	OLC	C4-C5-C6-C7
14	A	4208	PLM	C2-C3-C4-C5
14	C	504	PLM	C4-C5-C6-C7
12	A	4207	PX2	C21-C22-C23-C24
12	D	508	PX2	C10-C11-C12-C13
13	E	501	OLC	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
17	C	505	PGW	C5-C6-C7-C8
13	A	4206	OLC	C3-C4-C5-C6
12	A	4207	PX2	O6-C4-O5-C3
12	A	4205	PX2	C9-C10-C11-C12
14	C	504	PLM	C5-C6-C7-C8
17	C	505	PGW	C22-C23-C24-C25
17	C	505	PGW	C19-C20-C21-C22
12	D	508	PX2	C11-C10-C9-C8
12	A	4205	PX2	C21-C22-C23-C24
13	E	501	OLC	C2-C3-C4-C5
17	C	505	PGW	C21-C22-C23-C24
12	A	4207	PX2	C9-C10-C11-C12
14	A	4208	PLM	C1-C2-C3-C4
13	A	4206	OLC	C2-C3-C4-C5
10	B	506	R16	C30-C31-C32-C33
12	A	4205	PX2	C20-C21-C22-C23
12	A	4207	PX2	O4-C1-C2-C3
12	D	508	PX2	C19-C20-C21-C22
12	D	508	PX2	C16-C17-C18-C19
14	A	4208	PLM	CD-CE-CF-CG
9	A	4202	PT5	C41-C42-C43-C44
13	B	505	OLC	C2-C3-C4-C5
9	A	4202	PT5	C42-C43-C44-C45
12	D	508	PX2	C4-C5-C6-C7
10	D	505	R16	C39-C40-C41-C42
12	A	4207	PX2	C11-C10-C9-C8
15	B	502	HEX	C3-C4-C5-C6
9	D	501	PT5	C44-C45-C46-C47
10	E	506	R16	C33-C34-C35-C36
12	A	4205	PX2	C1-O4-P1-O2
12	D	508	PX2	C1-O4-P1-O2
9	A	4202	PT5	O13-C7-C8-O16
13	B	505	OLC	C6-C7-C8-C9
12	A	4207	PX2	C22-C23-C24-C25
8	E	502	D10	C2-C3-C4-C5
9	D	501	PT5	C14-C15-C16-C17
9	D	501	PT5	C20-C21-C22-C23
12	D	508	PX2	O4-C1-C2-C3
17	C	505	PGW	C01-C02-C03-O11
13	E	501	OLC	C2-C1-O20-C21
13	A	4206	OLC	C13-C14-C15-C16
13	E	501	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	A	4202	PT5	C19-C20-C21-C22
9	A	4202	PT5	C22-C23-C24-C25
9	D	501	PT5	C15-C16-C17-C18
9	D	501	PT5	C34-C35-C36-C37
13	E	501	OLC	O20-C1-C2-C3
9	D	501	PT5	C38-C39-C40-C41
13	B	505	OLC	C11-C12-C13-C14
17	C	505	PGW	C05-C04-O12-P
12	A	4205	PX2	C5-C6-C7-C8
13	A	4206	OLC	C5-C6-C7-C8
8	B	507	D10	C2-C3-C4-C5
9	D	501	PT5	C10-C12-C13-C14
10	A	4203	R16	C34-C35-C36-C37
9	D	501	PT5	C35-C36-C37-C38
9	A	4202	PT5	C9-C8-O16-C10
12	A	4207	PX2	C3-C2-O7-C16
12	D	508	PX2	C2-C3-O5-C4
13	E	501	OLC	O19-C1-O20-C21
13	A	4206	OLC	C14-C15-C16-C17
13	E	501	OLC	C12-C13-C14-C15
14	C	508	PLM	C6-C7-C8-C9
12	A	4205	PX2	C6-C7-C8-C9
17	C	505	PGW	C04-O12-P-O11
9	A	4202	PT5	O13-C7-C8-C9
17	C	505	PGW	O01-C02-C03-O11
14	C	508	PLM	C4-C5-C6-C7
9	D	501	PT5	C13-C14-C15-C16
10	A	4203	R16	C31-C32-C33-C34
10	D	506	R16	C38-C39-C40-C41
8	A	4210	D10	C1-C2-C3-C4
8	E	505	D10	C5-C6-C7-C8
9	A	4202	PT5	C35-C36-C37-C38
10	B	506	R16	C35-C36-C37-C38
10	B	506	R16	C39-C40-C41-C42
17	C	505	PGW	C16-C15-C27-C26
12	A	4207	PX2	O4-C1-C2-O7
14	C	504	PLM	C6-C7-C8-C9
12	D	508	PX2	C20-C21-C22-C23
10	D	506	R16	C36-C37-C38-C39
10	B	506	R16	C32-C33-C34-C35
13	E	501	OLC	C7-C8-C9-C10
13	A	4206	OLC	O20-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	D	508	PX2	C23-C24-C25-C26
8	E	505	D10	C6-C7-C8-C9
11	A	4204	EPE	C8-C7-N4-C3
12	D	508	PX2	C6-C7-C8-C9
10	D	506	R16	C39-C40-C41-C42
14	C	508	PLM	C8-C9-CA-CB
8	E	504	D10	C5-C6-C7-C8
12	A	4205	PX2	C2-C1-O4-P1
9	A	4202	PT5	C11-C31-C32-C33
13	B	505	OLC	C1-C2-C3-C4
13	B	505	OLC	C7-C8-C9-C10
10	D	505	R16	C29-C30-C31-C32
17	C	505	PGW	C4-C5-C6-C7
8	A	4210	D10	C5-C6-C7-C8
9	A	4202	PT5	C24-C25-C26-C27
12	A	4207	PX2	C23-C24-C25-C26
10	D	506	R16	C37-C38-C39-C40
8	D	507	D10	C5-C6-C7-C8
14	C	504	PLM	O1-C1-C2-C3
13	B	505	OLC	O20-C1-C2-C3
15	C	501	HEX	C1-C2-C3-C4
12	A	4205	PX2	C11-C10-C9-C8
14	C	504	PLM	O2-C1-C2-C3
13	E	501	OLC	C9-C10-C11-C12
8	A	4210	D10	C4-C5-C6-C7
9	D	501	PT5	C4-O4-P4-O42
14	A	4208	PLM	CB-CC-CD-CE
13	A	4206	OLC	C12-C13-C14-C15
13	A	4206	OLC	C9-C10-C11-C12
13	B	505	OLC	C15-C16-C17-C18
12	A	4207	PX2	C1-O4-P1-O2
13	E	501	OLC	O19-C1-C2-C3
9	D	501	PT5	C24-C25-C26-C27
12	A	4207	PX2	O7-C16-C17-C18
9	A	4202	PT5	C5-O5-P5-O53
9	D	501	PT5	C5-O5-P5-O53
17	C	505	PGW	C16-C17-C18-C28
8	B	503	D10	C6-C7-C8-C9
13	B	505	OLC	C9-C10-C11-C12
17	C	505	PGW	C20-C19-O03-C01
9	D	501	PT5	C7-O13-P1-O1
9	D	501	PT5	C7-O13-P1-O11

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Mol	Chain	Res	Type	Atoms
14	A	4208	PLM	O1-C1-C2-C3
9	A	4202	PT5	C12-C13-C14-C15
14	A	4208	PLM	O2-C1-C2-C3
17	C	505	PGW	C07-C08-C09-C11
17	C	505	PGW	O12-C04-C05-OAF
10	E	506	R16	C36-C37-C38-C39
10	B	506	R16	C31-C32-C33-C34
9	D	501	PT5	O18-C11-C31-C32
12	A	4207	PX2	O8-C16-C17-C18
12	D	508	PX2	C22-C23-C24-C25
9	D	501	PT5	O19-C11-C31-C32

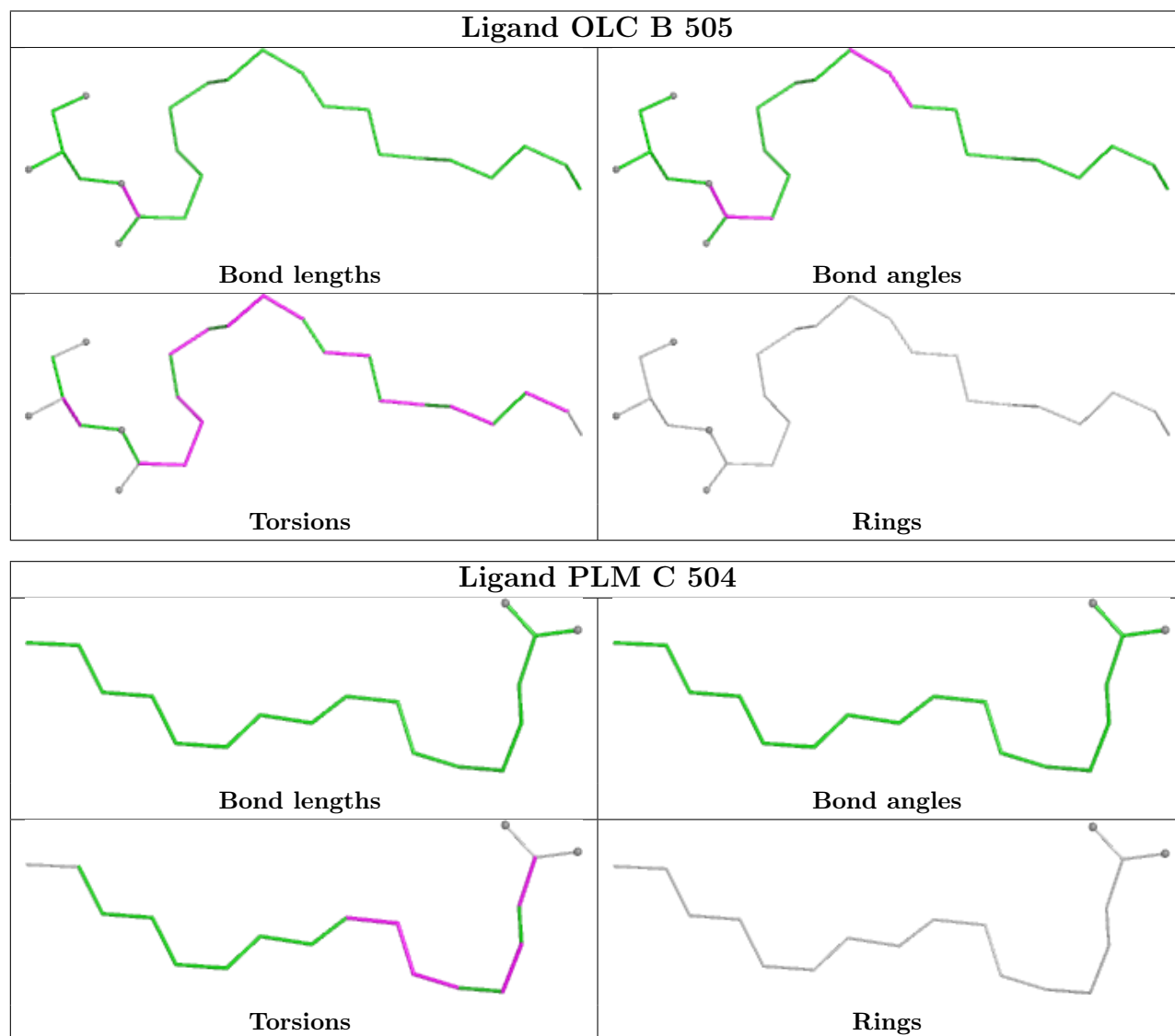
There are no ring outliers.

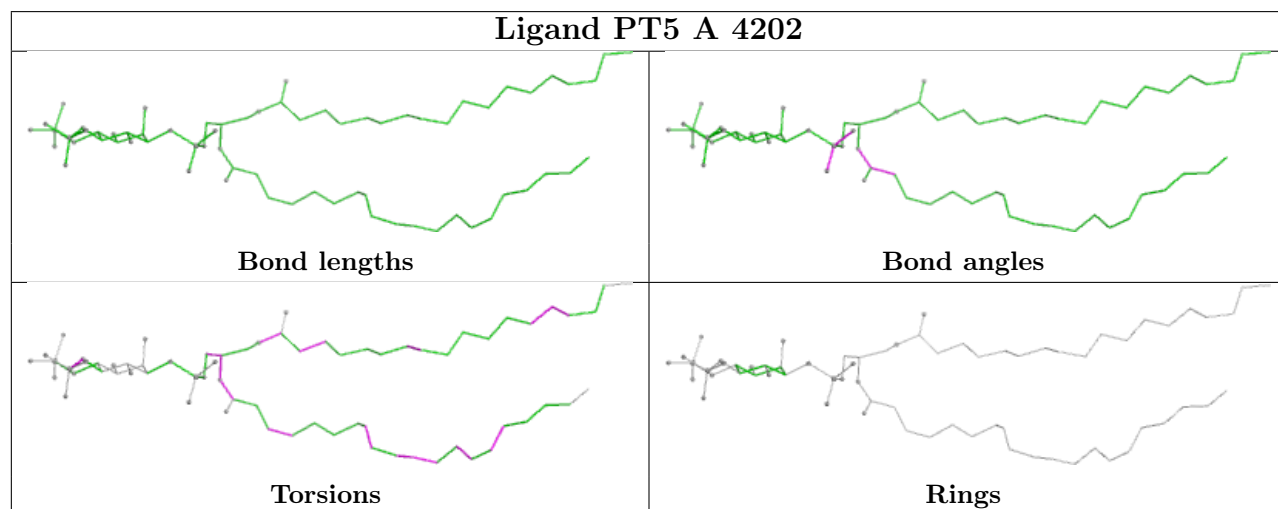
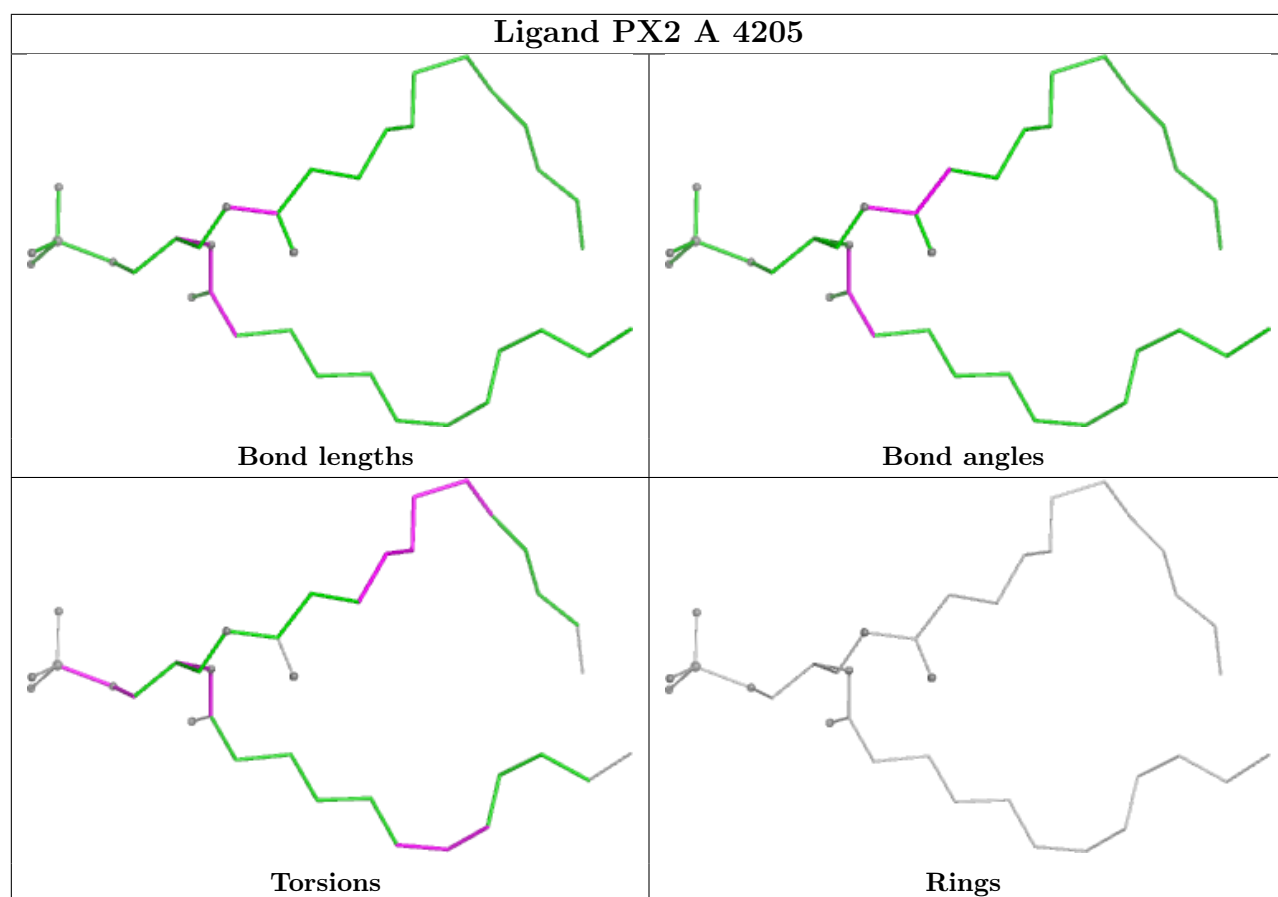
21 monomers are involved in 37 short contacts:

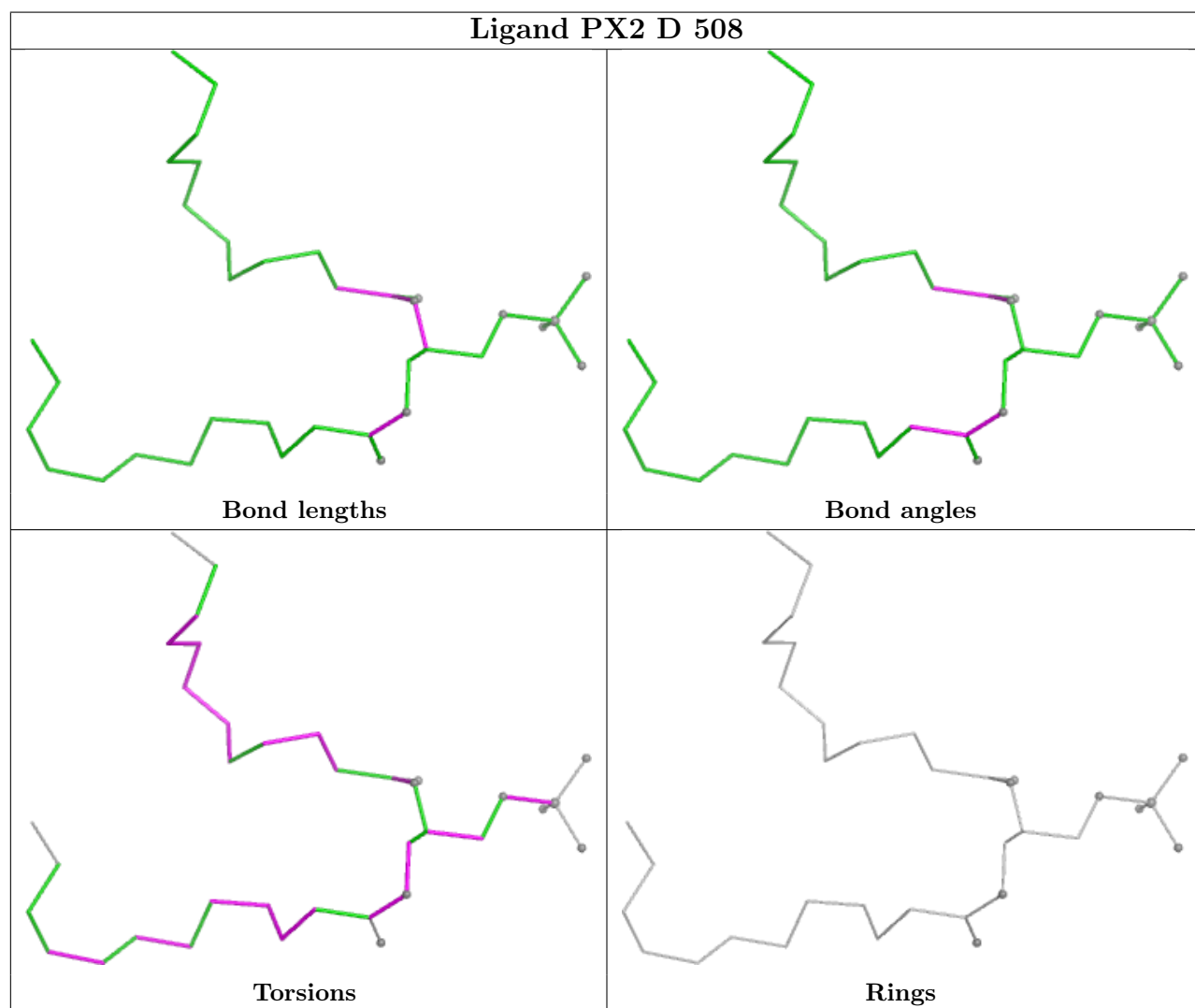
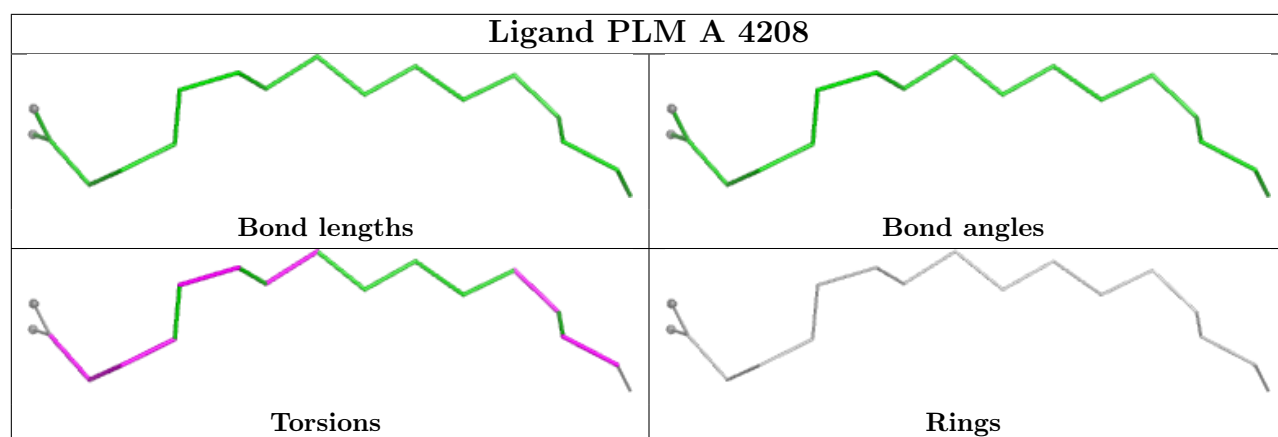
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	505	OLC	2	0
15	C	501	HEX	1	0
14	C	504	PLM	2	0
12	A	4205	PX2	1	0
10	A	4203	R16	1	0
8	A	4201	D10	1	0
8	E	502	D10	3	0
8	B	503	D10	1	0
8	B	504	D10	1	0
9	A	4202	PT5	1	0
15	D	503	HEX	1	0
11	A	4204	EPE	4	0
14	A	4208	PLM	5	0
10	D	505	R16	1	0
15	E	507	HEX	5	0
12	D	508	PX2	1	0
12	A	4207	PX2	4	0
17	C	505	PGW	4	0
9	D	501	PT5	5	0
13	A	4206	OLC	1	0
8	A	4210	D10	2	0

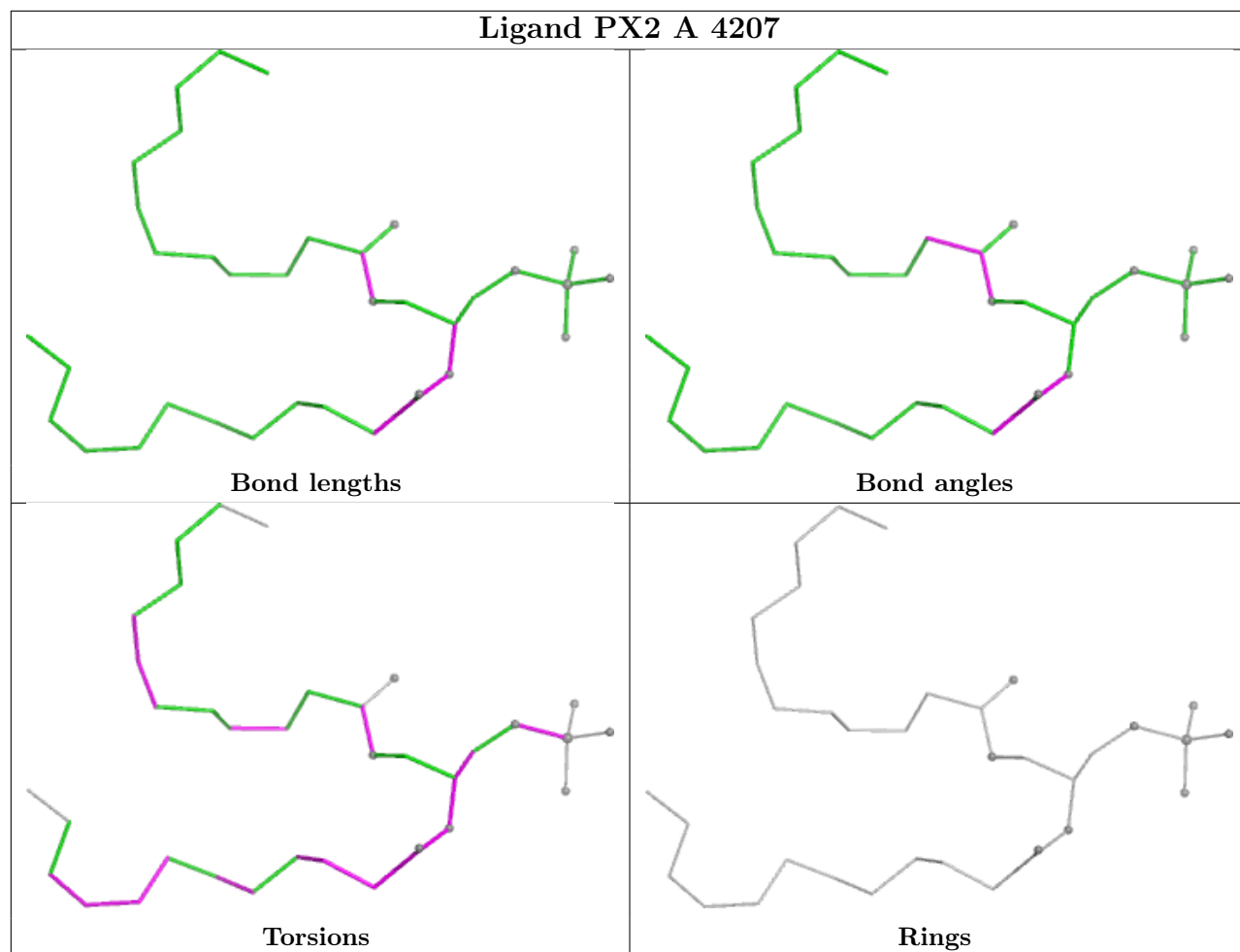
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

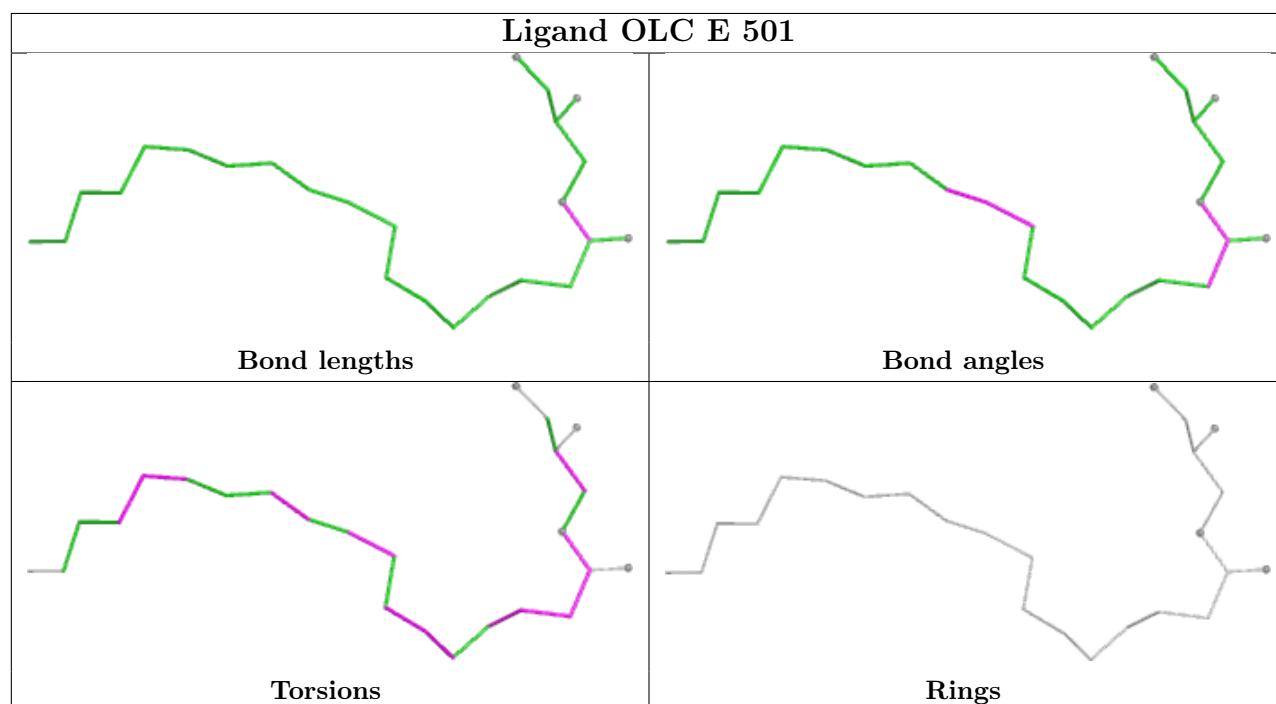
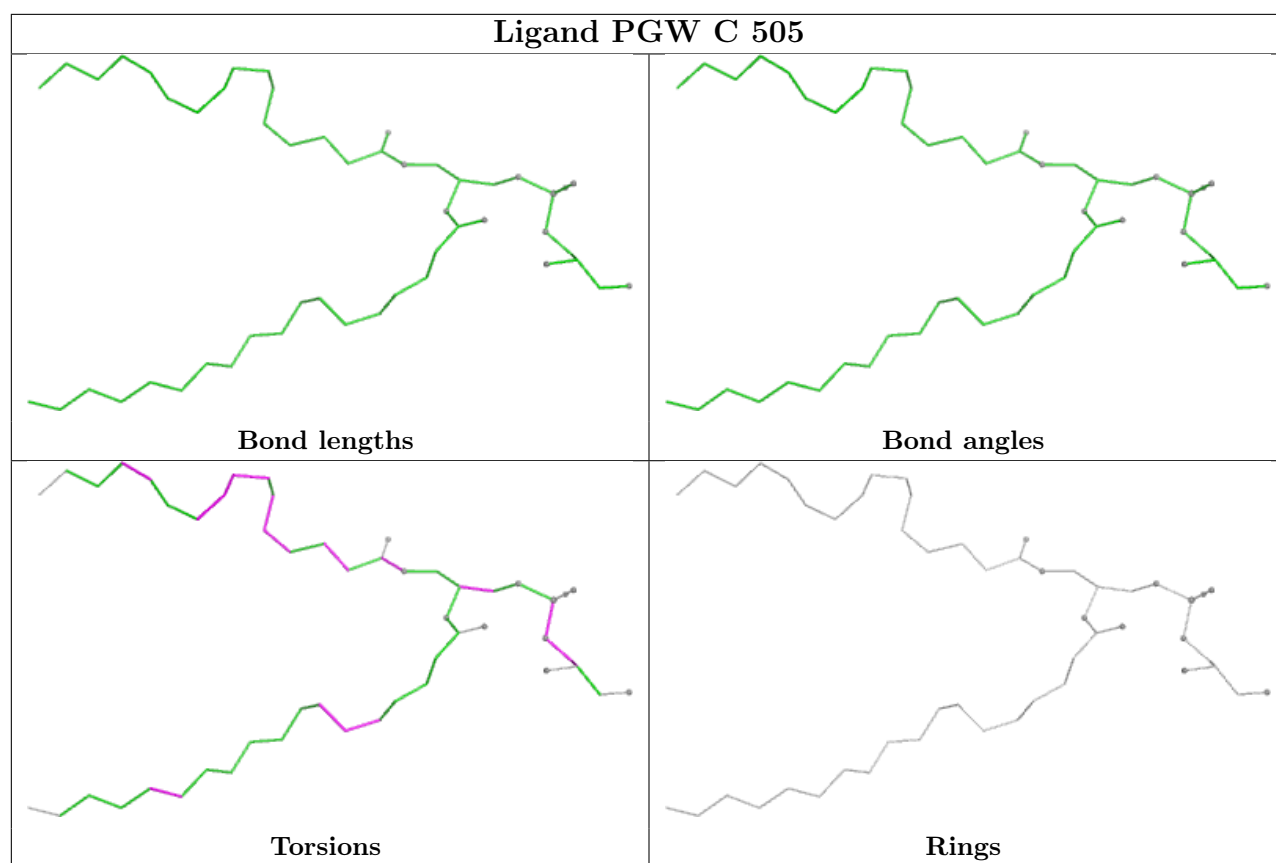
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

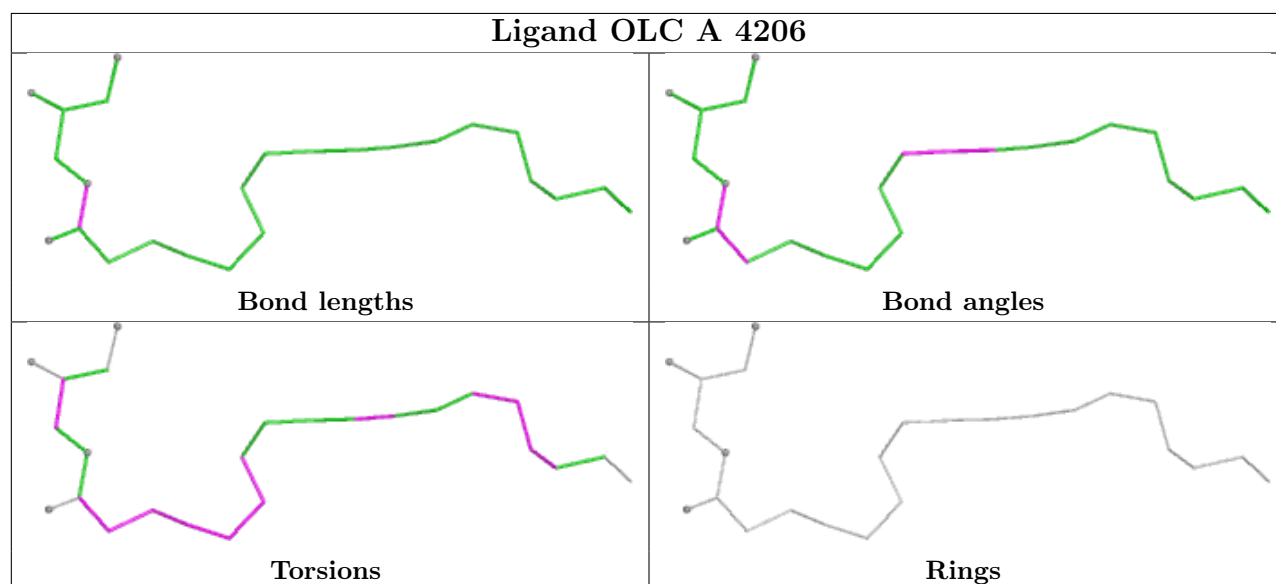
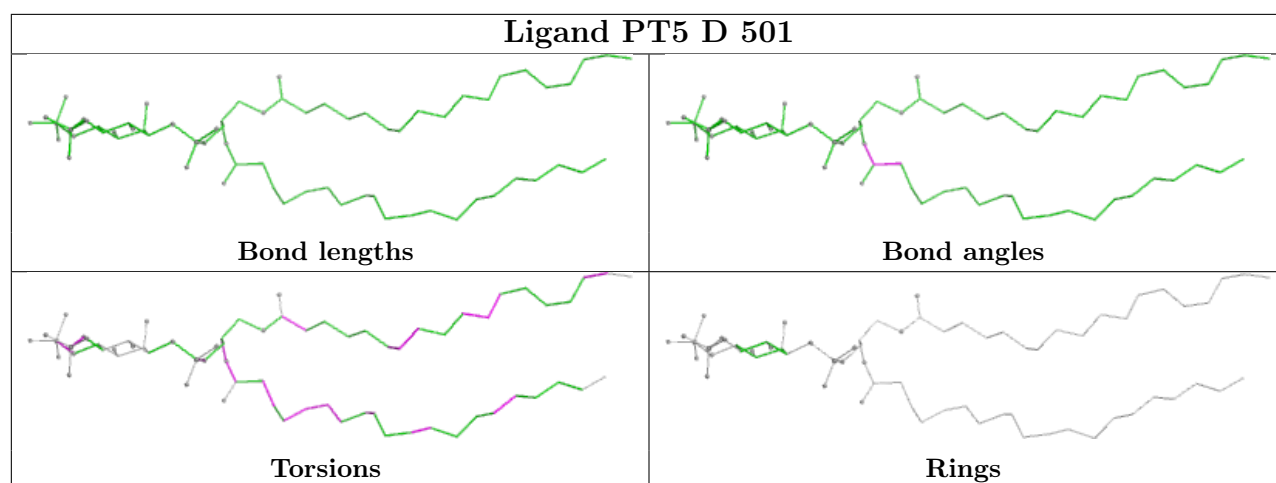
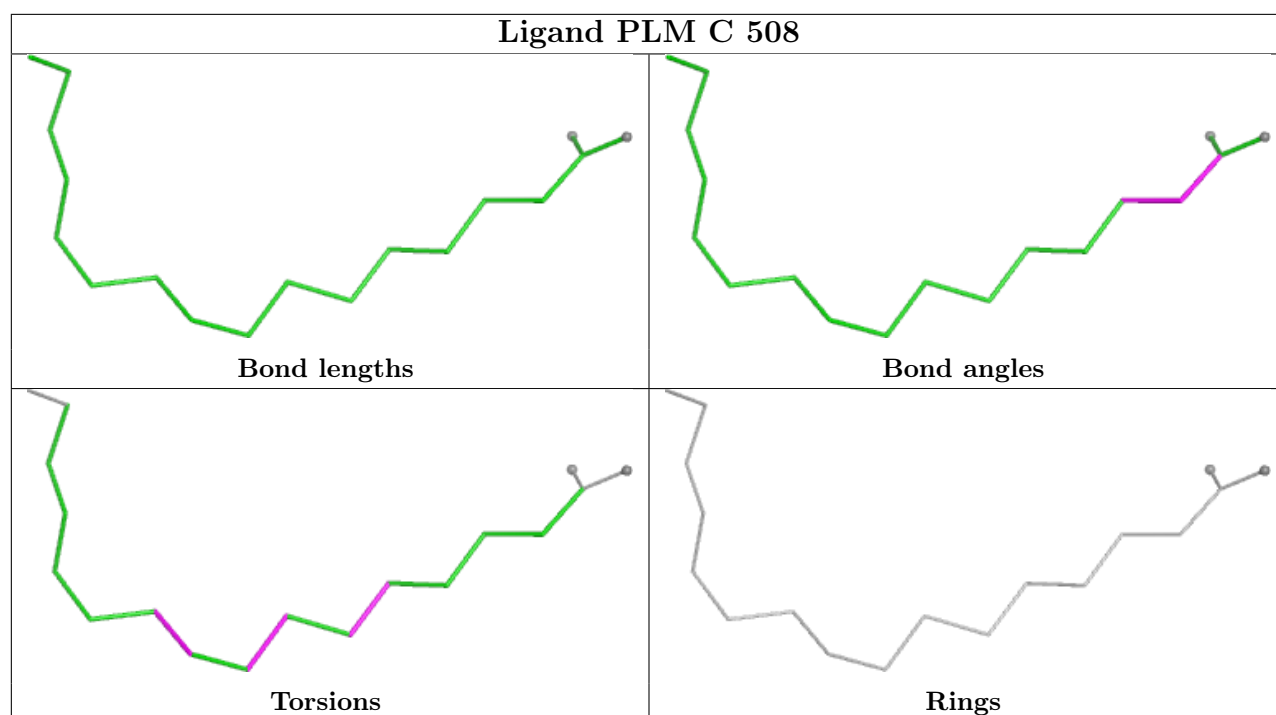












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

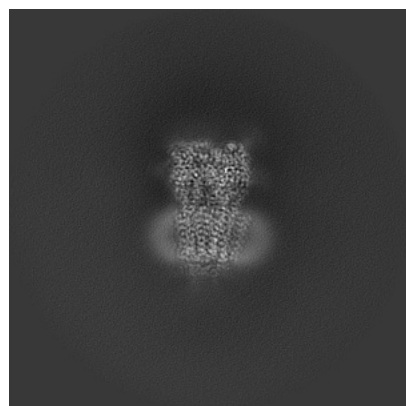
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53948. These allow visual inspection of the internal detail of the map and identification of artifacts.

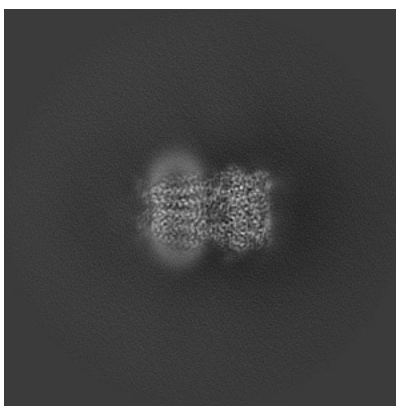
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

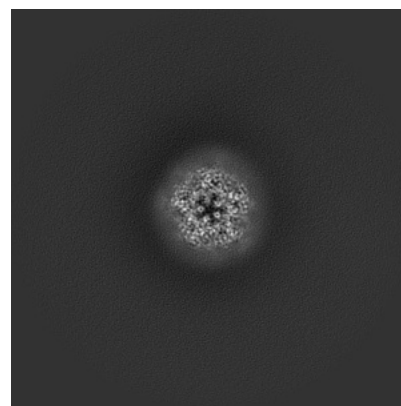
6.1.1 Primary map



X

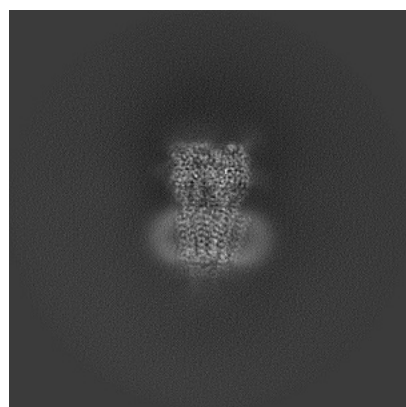


Y

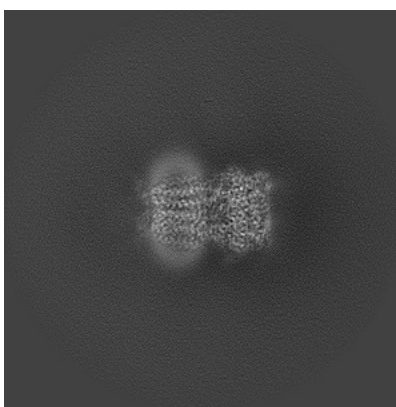


Z

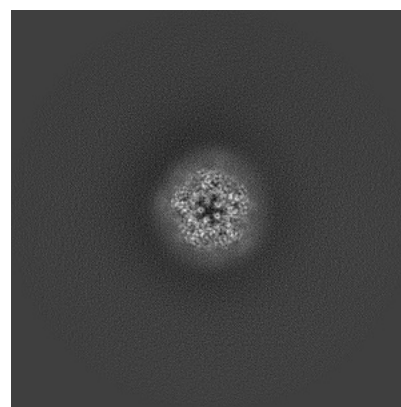
6.1.2 Raw map



X



Y

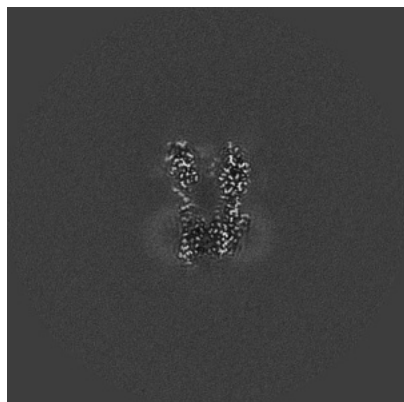


Z

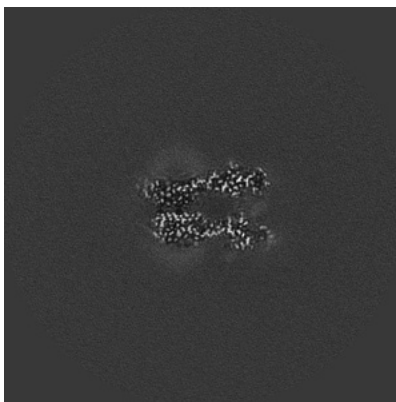
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

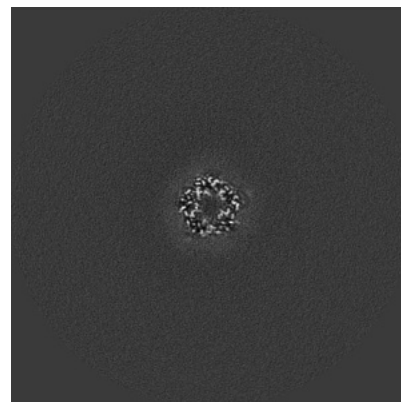
6.2.1 Primary map



X Index: 240

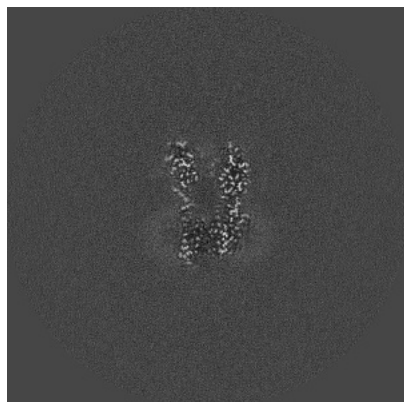


Y Index: 240

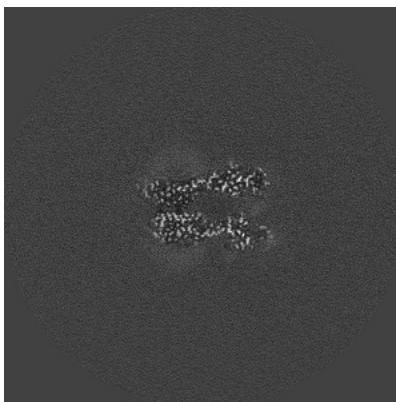


Z Index: 240

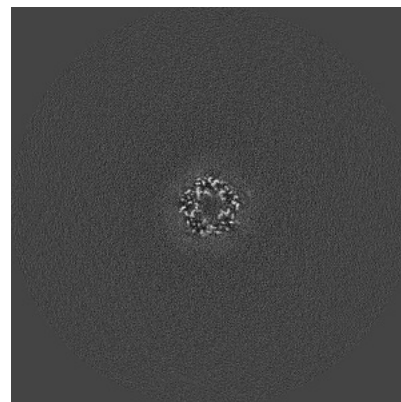
6.2.2 Raw map



X Index: 240



Y Index: 240

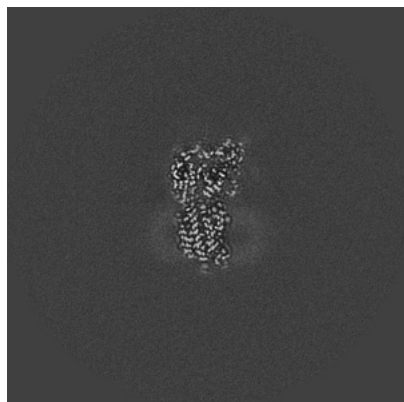


Z Index: 240

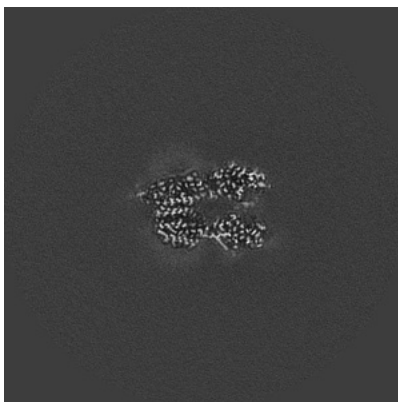
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

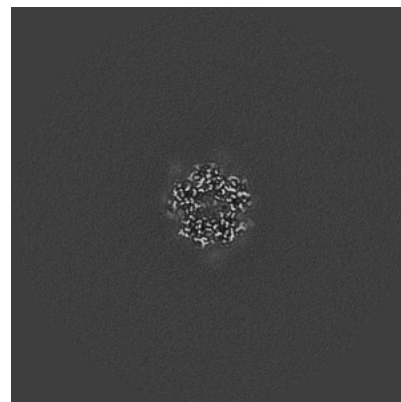
6.3.1 Primary map



X Index: 261

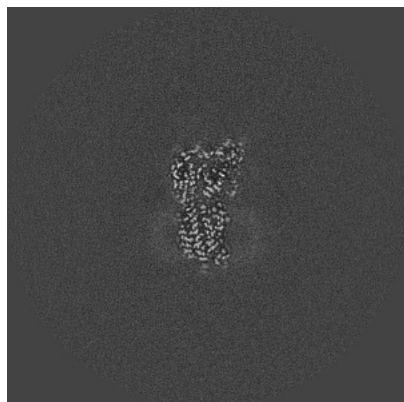


Y Index: 248

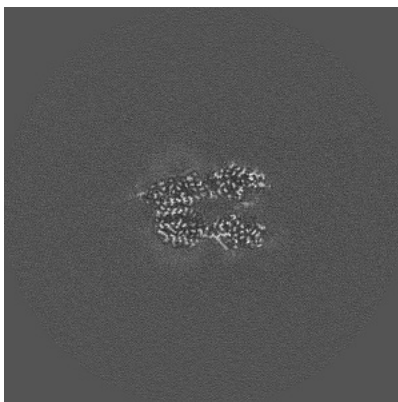


Z Index: 284

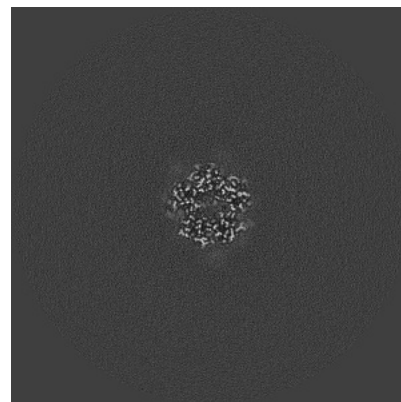
6.3.2 Raw map



X Index: 261



Y Index: 248

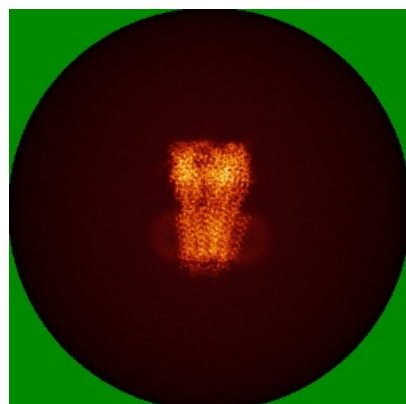


Z Index: 284

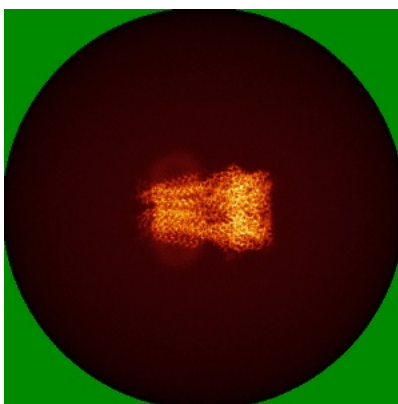
The images above show the largest variance slices of the map in three orthogonal directions.

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

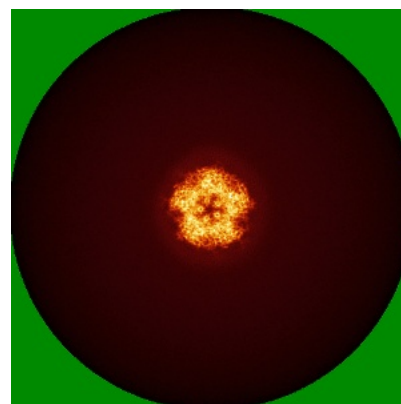
6.4.1 Primary map



X

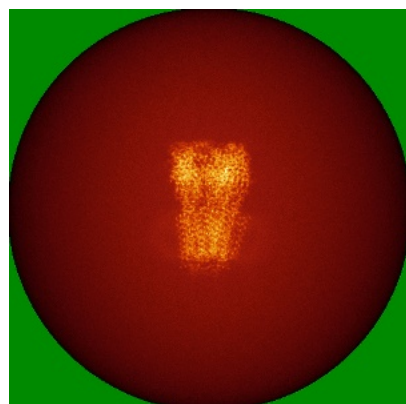


Y

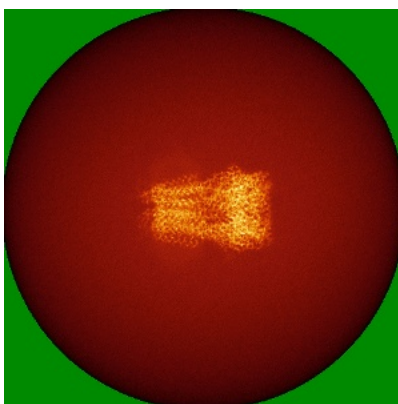


Z

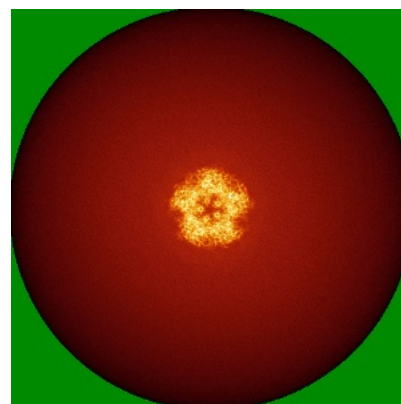
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

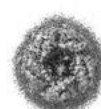
6.5.1 Primary map



X



Y



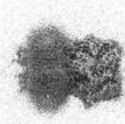
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

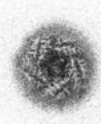
6.5.2 Raw map



X



Y



Z

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

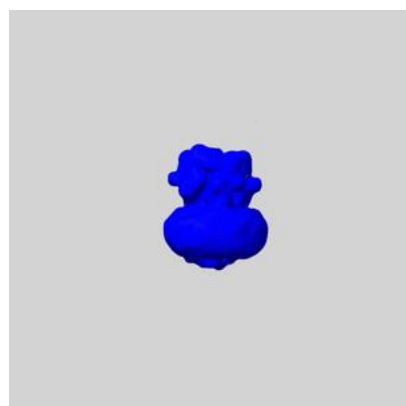
6.6 Mask visualisation [i](#)

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

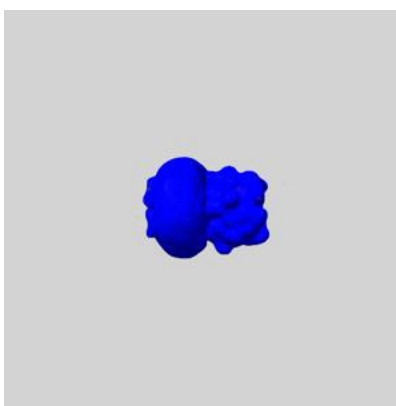
A mask typically either:

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

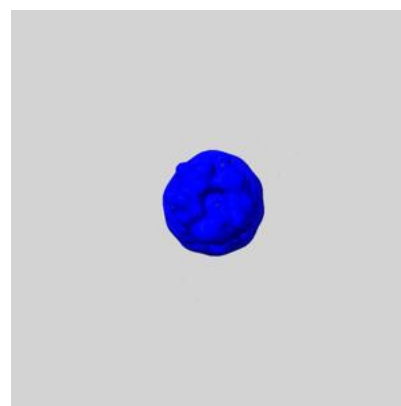
6.6.1 emd_53948_msk_1.map [i](#)



X



Y

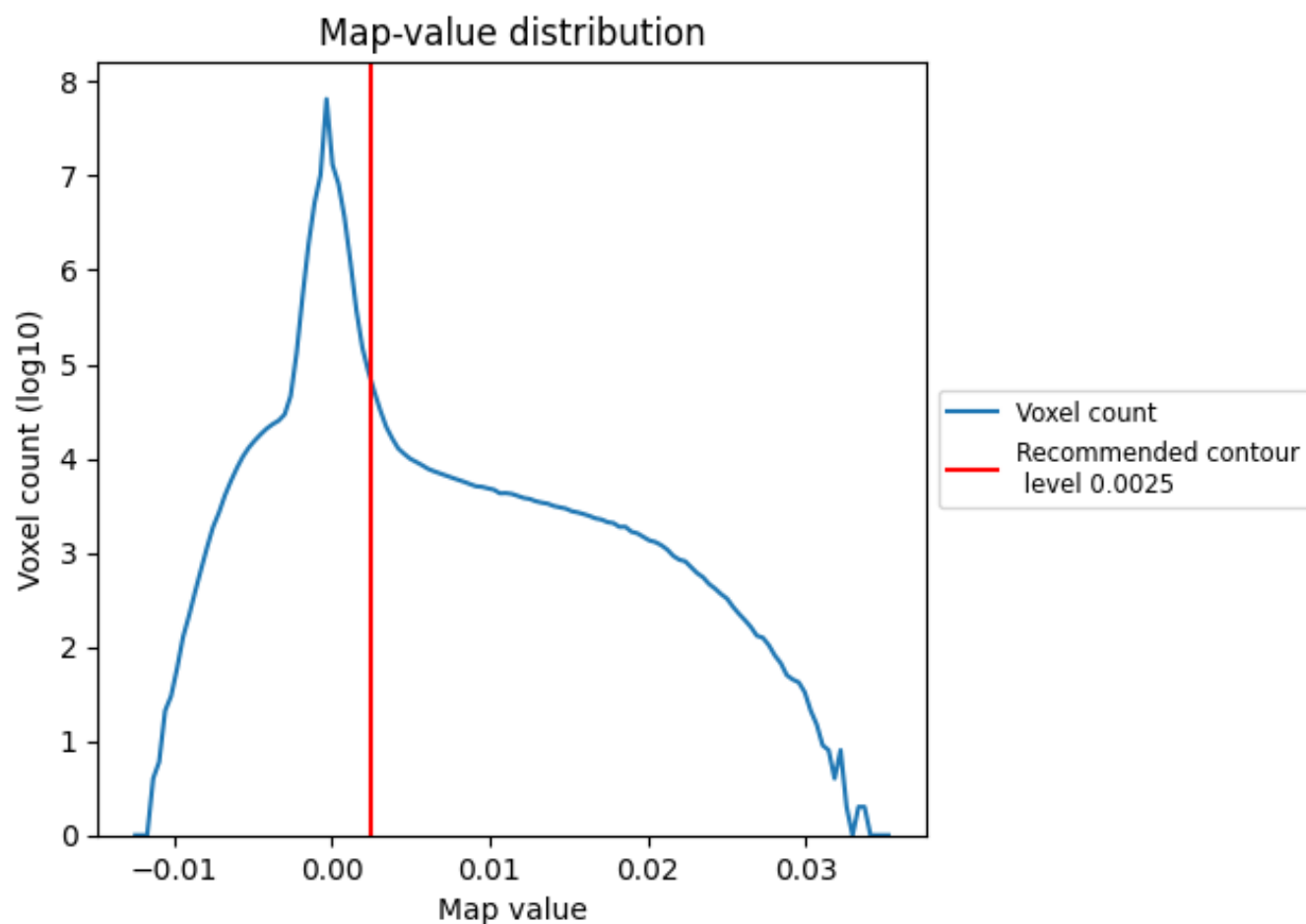


Z

7 Map analysis [i](#)

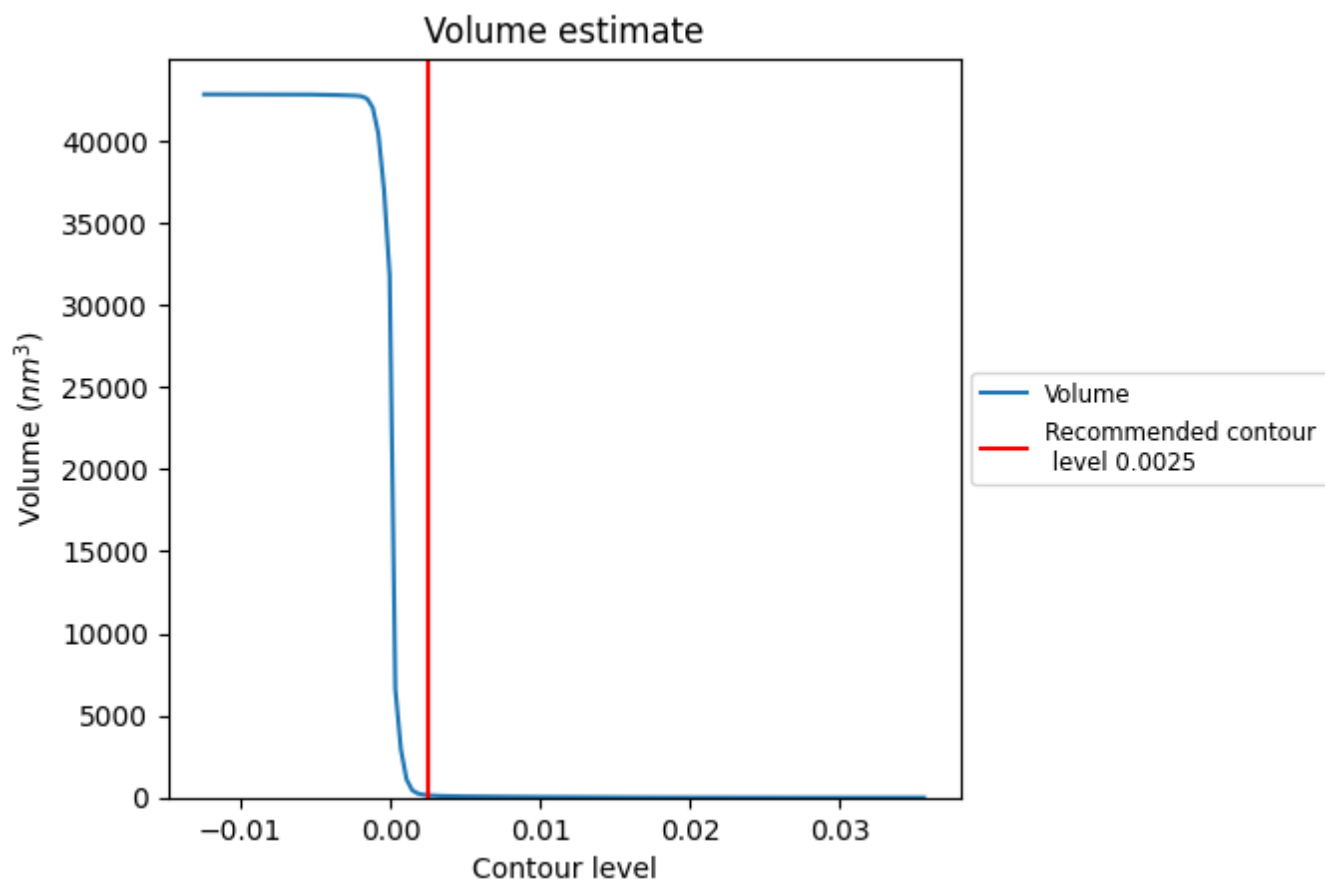
This section contains the results of statistical analysis of the map.

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.

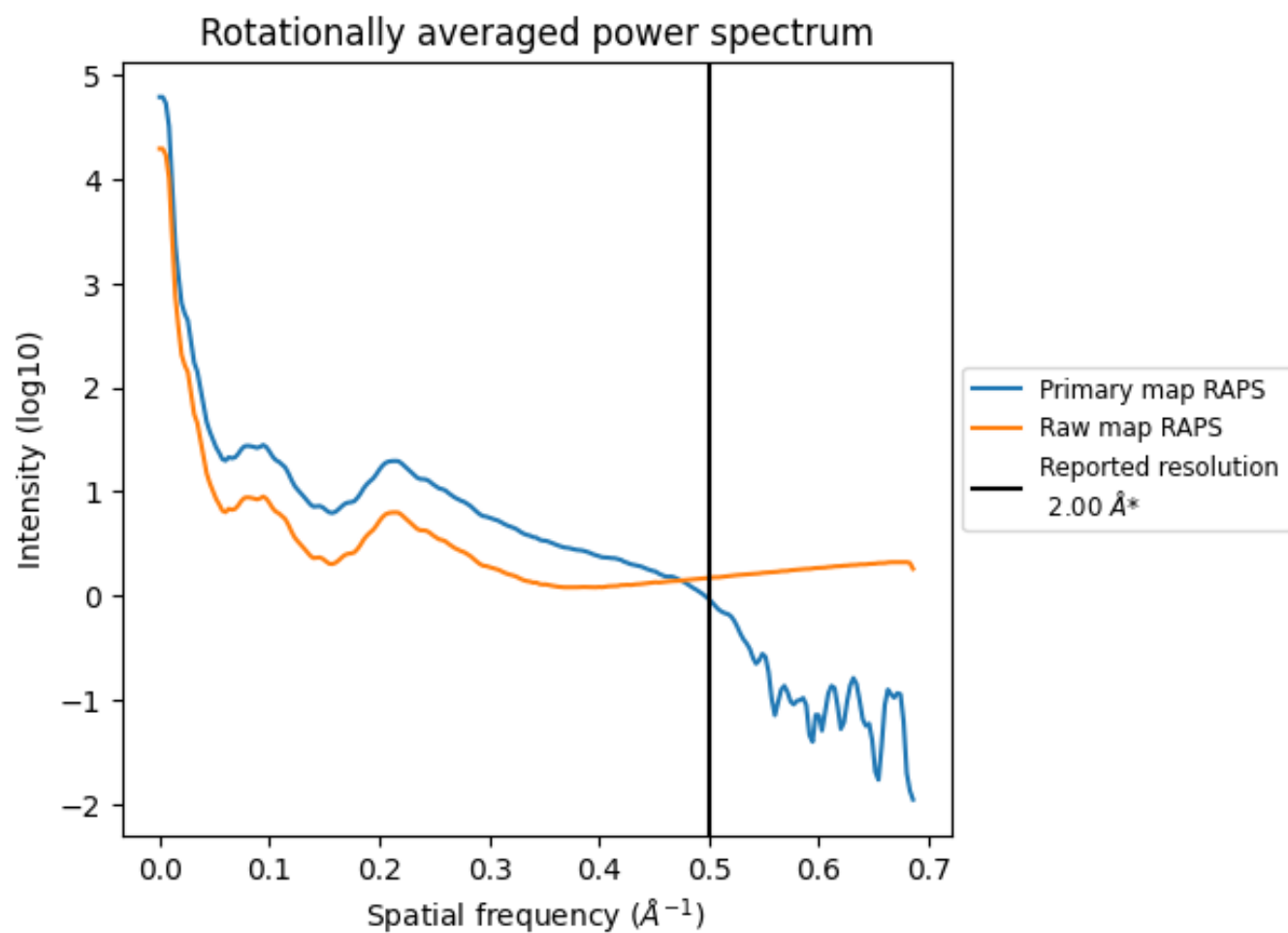
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 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 ⓘ

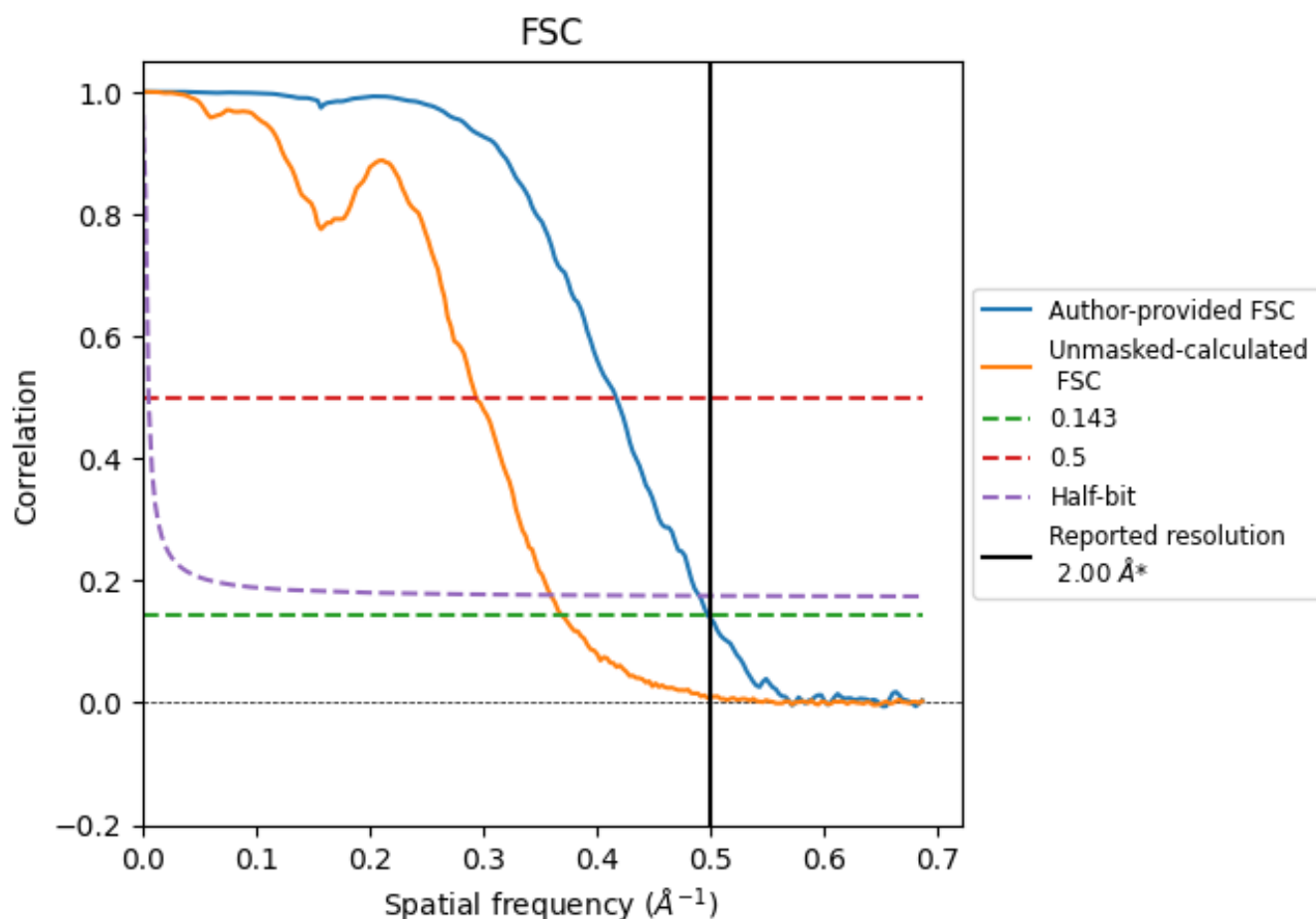


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

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 0.500 \AA^{-1}

8.2 Resolution estimates [i](#)

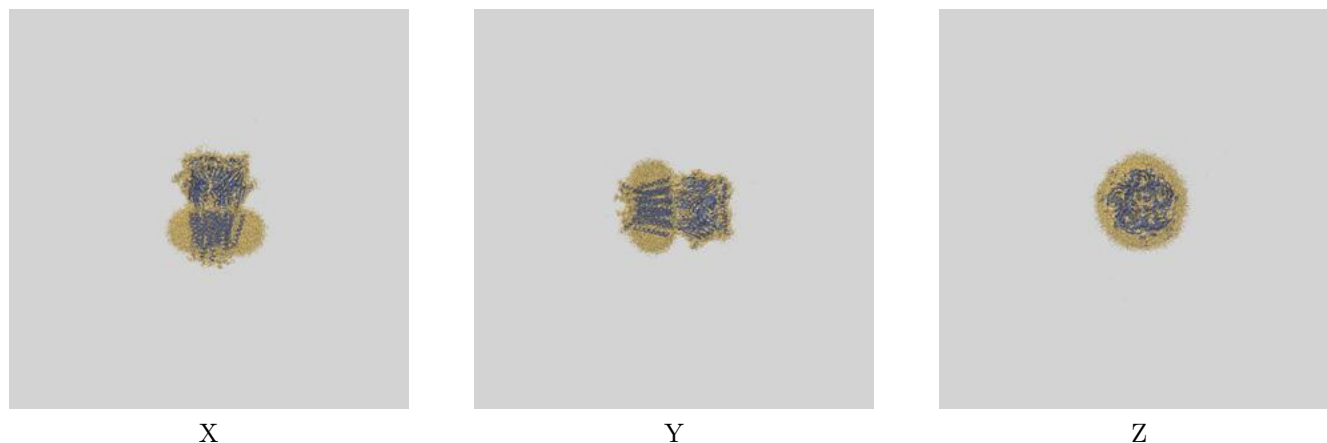
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	2.01	2.40	2.04
Unmasked-calculated*	2.71	3.41	2.78

*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 2.71 differs from the reported value 2.0 by more than 10 %

9 Map-model fit [i](#)

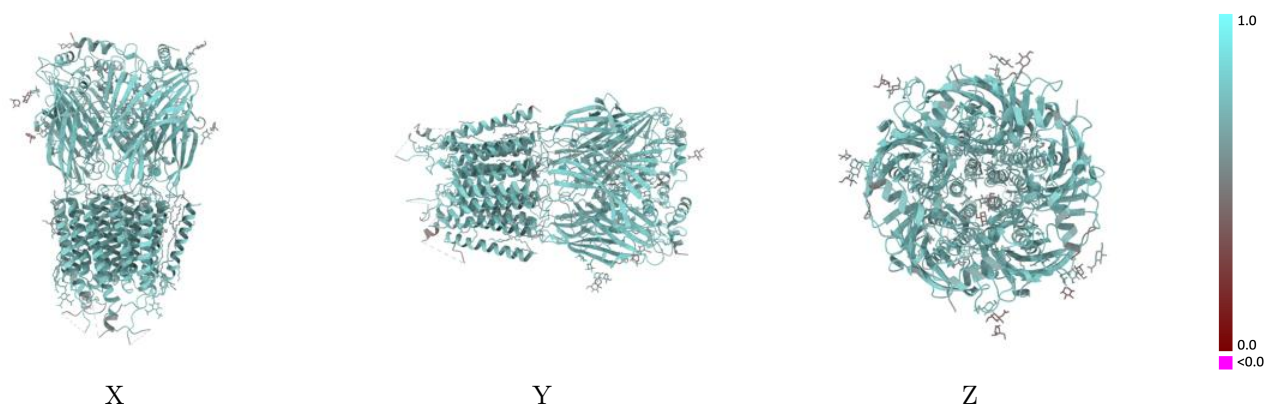
This section contains information regarding the fit between EMDB map EMD-53948 and PDB model 9RGD. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



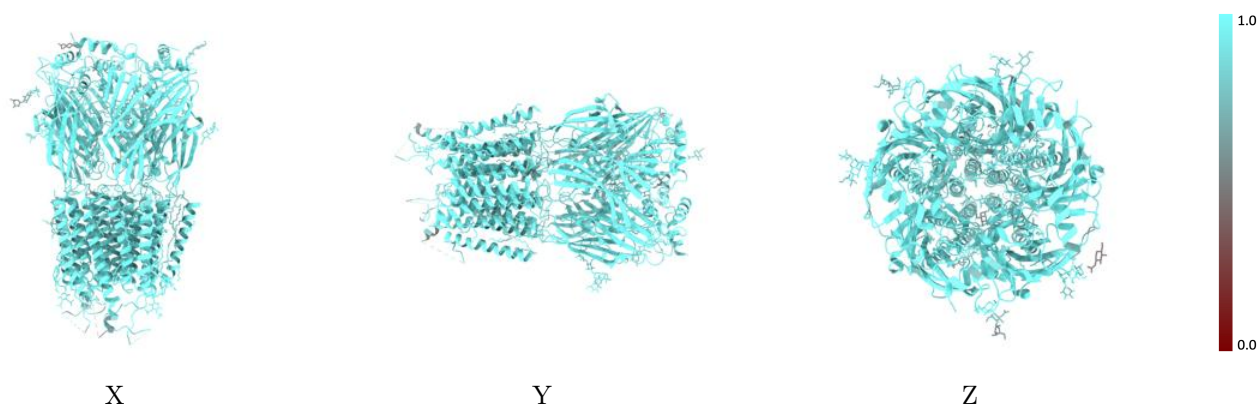
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



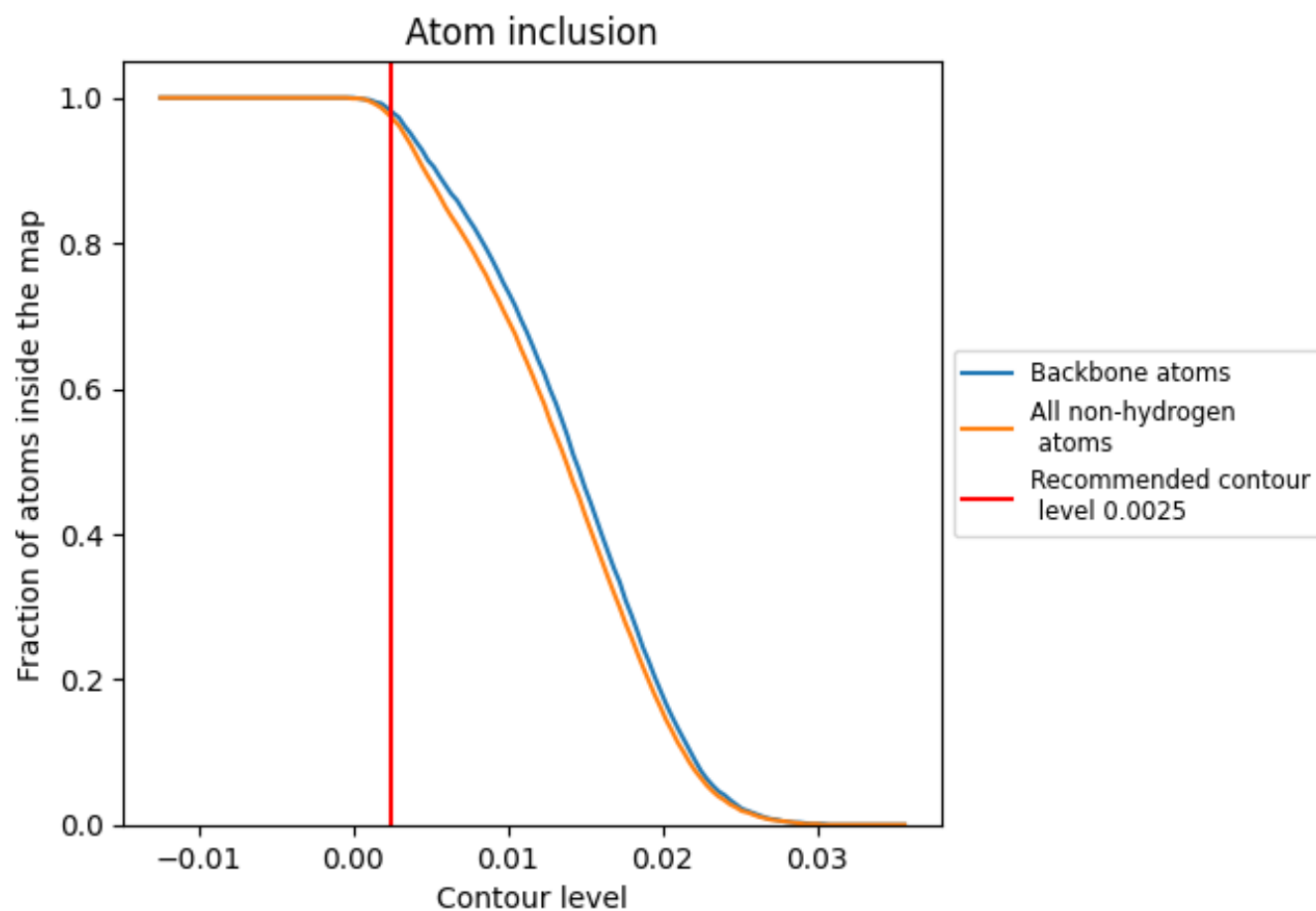
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9730</div>	<div><div></div>0.7090</div>
A	<div><div></div>0.9740</div>	<div><div></div>0.7070</div>
B	<div><div></div>0.9750</div>	<div><div></div>0.7150</div>
C	<div><div></div>0.9790</div>	<div><div></div>0.7190</div>
D	<div><div></div>0.9730</div>	<div><div></div>0.7140</div>
E	<div><div></div>0.9730</div>	<div><div></div>0.7090</div>
F	<div><div></div>0.9660</div>	<div><div></div>0.6360</div>
G	<div><div></div>0.9720</div>	<div><div></div>0.6180</div>
H	<div><div></div>0.8460</div>	<div><div></div>0.5300</div>
I	<div><div></div>0.9290</div>	<div><div></div>0.5380</div>
J	<div><div></div>0.8470</div>	<div><div></div>0.5500</div>
K	<div><div></div>0.9580</div>	<div><div></div>0.5720</div>
L	<div><div></div>0.7690</div>	<div><div></div>0.4880</div>

1.0

0.0

<0.0