



## Full wwPDB EM Validation Report ⓘ

Jun 24, 2025 – 07:26 pm BST

PDB ID : 9FAK / pdb\_00009fak  
EMDB ID : EMD-50274  
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 (StateD2)  
Authors : Kasaragod, V.B.; Aricescu, A.R.  
Deposited on : 2024-05-10  
Resolution : 2.60 Å (reported)  
Based on initial model : 6HUO

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

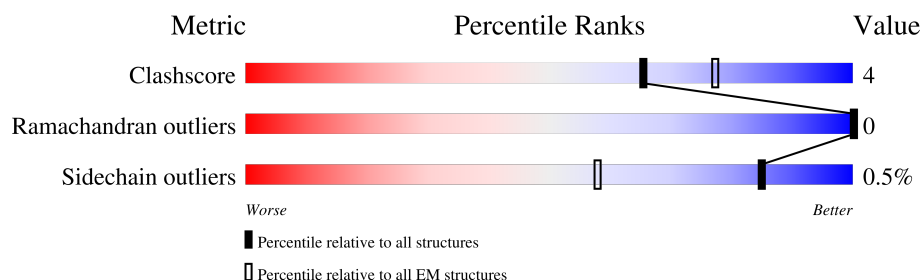
# 1 Overall quality at a glance

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.




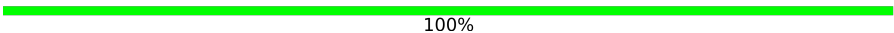
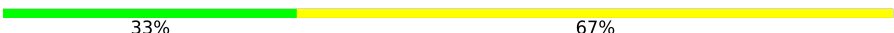




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	7	

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
18	CL	L	305	-	-	X	-

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 19569 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	4	0
			2912	1882	494	520	16		
1	D	354	Total	C	N	O	S	1	0
			2872	1857	485	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	4	0
			2879	1883	476	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	2	0
			2951	1938	477	516	20		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is a protein called Neuroligin-2.

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

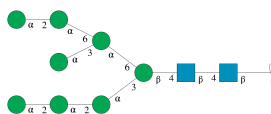
- Molecule 5 is a protein called LHFPL tetraspan subfamily member 4 protein.

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.

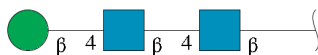
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	121	Total	C	N	O	S	1	0
			949	594	172	179	4		
6	P	121	Total	C	N	O	S	0	0
			941	589	169	179	4		

- 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.



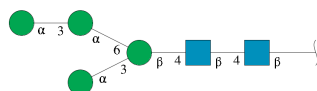
Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	10	Total	C	N	O		0	0
			116	64	2	50			

- 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.



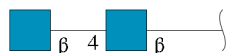
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	3	Total	C	N	O		0	0
			39	22	2	15			
8	O	3	Total	C	N	O		0	0
			39	22	2	15			

- 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.



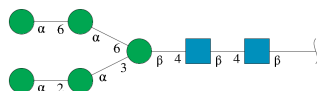
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	6	Total	C	N	O	0	0
			72	40	2	30		
9	N	6	Total	C	N	O	0	0
			72	40	2	30		

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



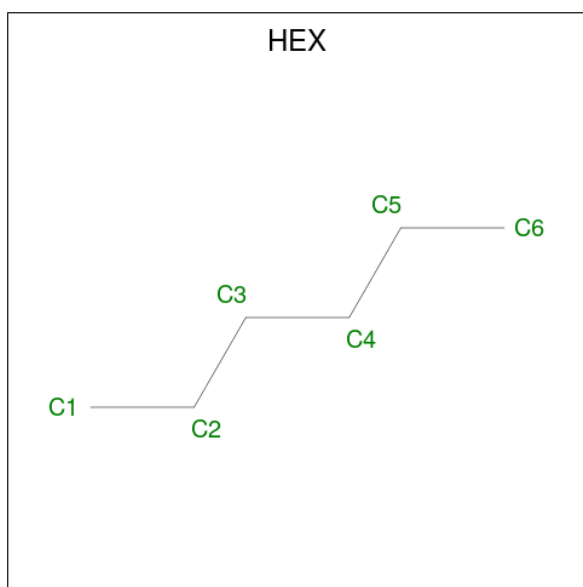
Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	2	Total	C	N	O	0	0
			28	16	2	10		

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



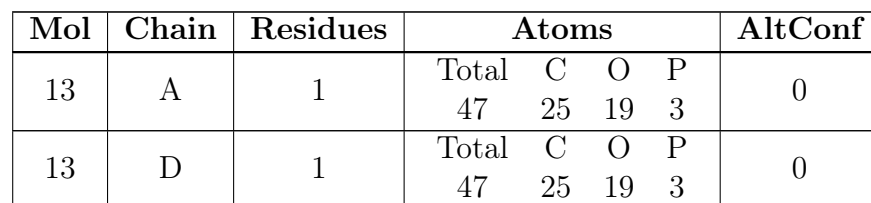
Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 12 is HEXANE (CCD ID: HEX) (formula: C<sub>6</sub>H<sub>14</sub>).



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

- Molecule 13 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C<sub>25</sub>H<sub>49</sub>O<sub>19</sub>P<sub>3</sub>).



- # PGW

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

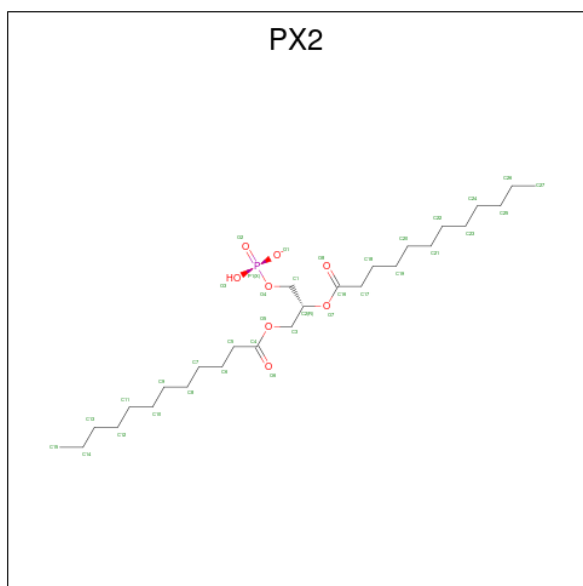
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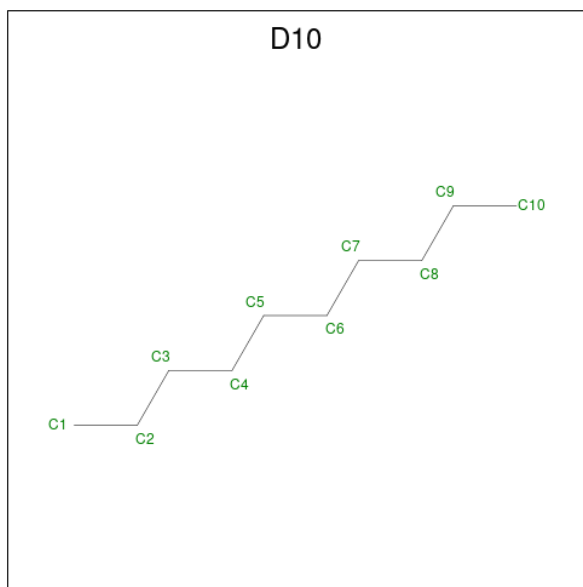


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Mol	Chain	Residues	Atoms				AltConf
14	D	1	Total	C	O	P	1
			102	80	20	2	
14	E	1	Total	C	O	P	0
			32	21	10	1	
14	L	1	Total	C	O	P	0
			51	40	10	1	
14	L	1	Total	C	O	P	0
			51	40	10	1	

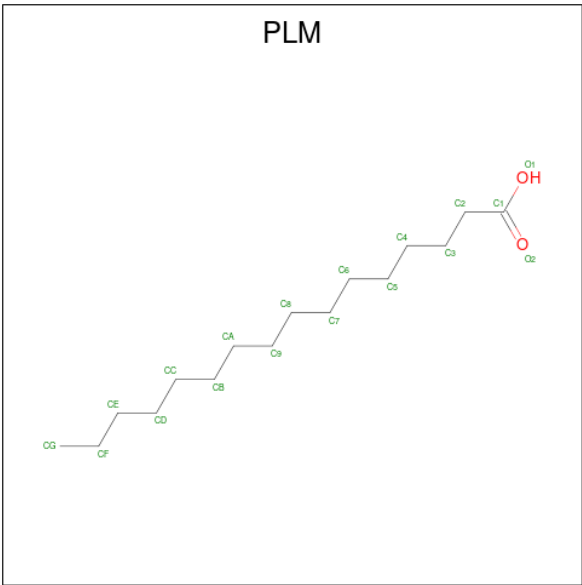
- Molecule 15 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula:  $C_{27}H_{52}O_8P$ ).





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

- Molecule 17 is PALMITIC ACID (CCD ID: PLM) (formula:  $C_{16}H_{32}O_2$ ).

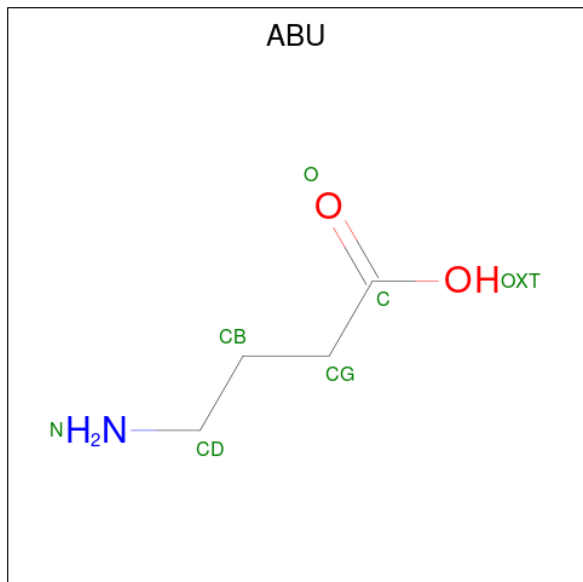


Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			18	16	2	
17	B	1	Total	C	O	0
			18	16	2	
17	C	1	Total	C	O	0
			14	12	2	
17	C	1	Total	C	O	0
			18	16	2	
17	C	1	Total	C	O	0
			18	16	2	
17	D	1	Total	C	O	0
			18	16	2	
17	E	1	Total	C	O	0
			18	16	2	
17	E	1	Total	C	O	0
			18	16	2	

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

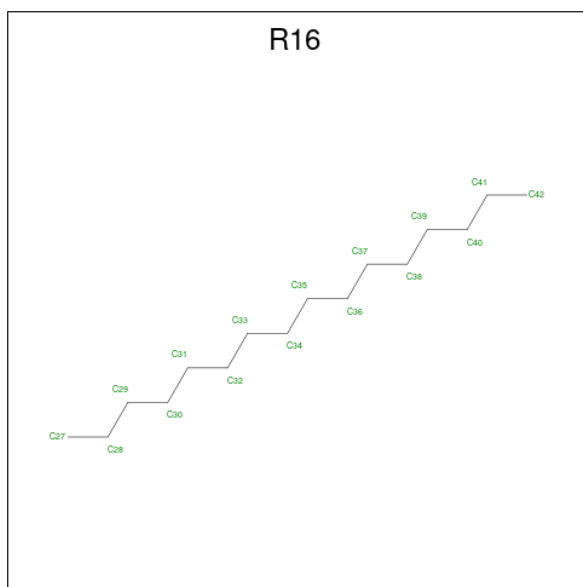
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Cl	0
			1	1	
18	C	1	Total	Cl	0
			1	1	
18	D	1	Total	Cl	0
			1	1	
18	L	1	Total	Cl	0
			1	1	

- Molecule 19 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula:  $C_4H_9NO_2$ ) (labeled as "Ligand of Interest" by depositor).



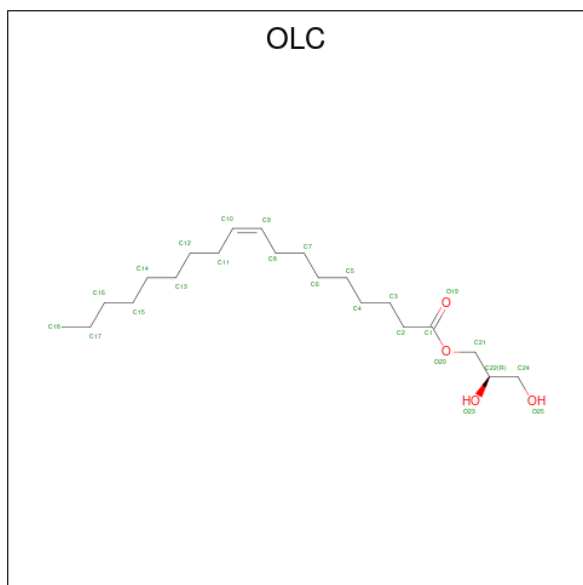
Mol	Chain	Residues	Atoms				AltConf
19	B	1	Total	C	N	O	0
			7	4	1	2	
19	E	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 20 is HEXADECANE (CCD ID: R16) (formula:  $C_{16}H_{34}$ ).



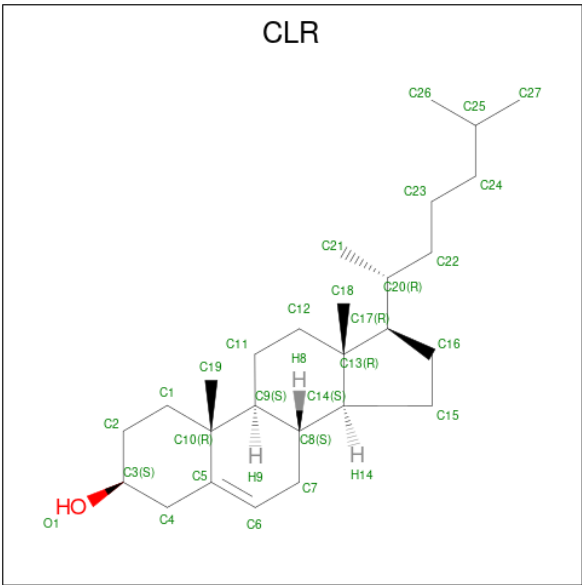
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 16 16	0
20	B	1	Total C 16 16	0
20	E	1	Total C 16 16	0

- 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 21 17 4	0

- 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	L	1	Total	C	O	0
			28	27	1	


- Molecule 23 is water.

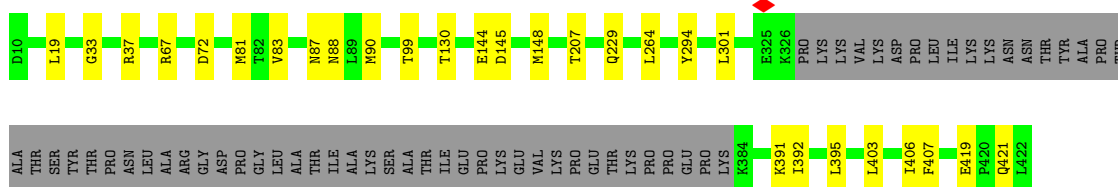
Mol	Chain	Residues	Atoms		AltConf
23	A	20	Total	O	0
			20	20	
23	B	19	Total	O	0
			19	19	
23	C	11	Total	O	0
			11	11	
23	D	17	Total	O	0
			17	17	
23	E	15	Total	O	0
			15	15	
23	G	4	Total	O	0
			4	4	

### 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.

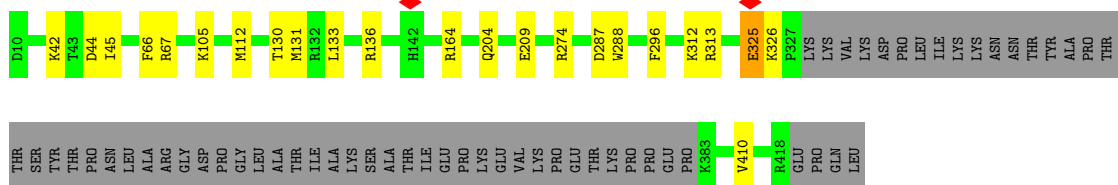
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain A: 



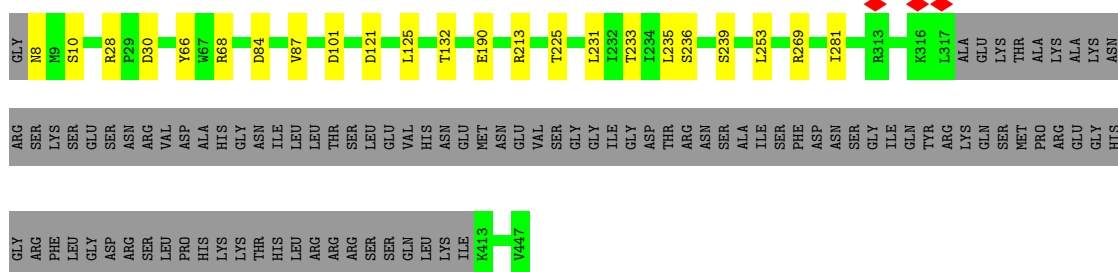
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain D: 



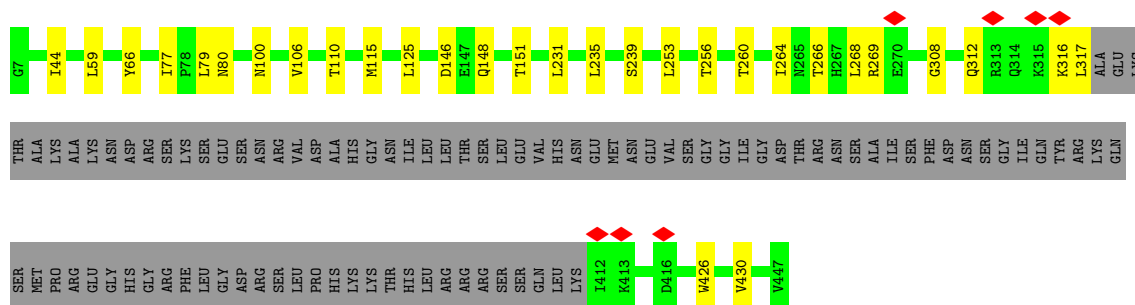
- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain B: 



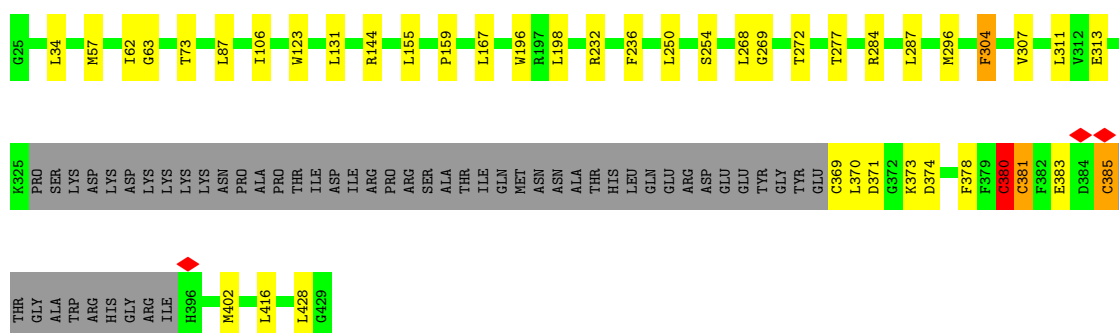
- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain E: 



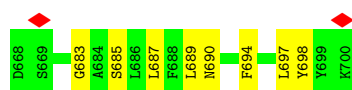
• Molecule 3: Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2

Chain C: 76% 10% 13%



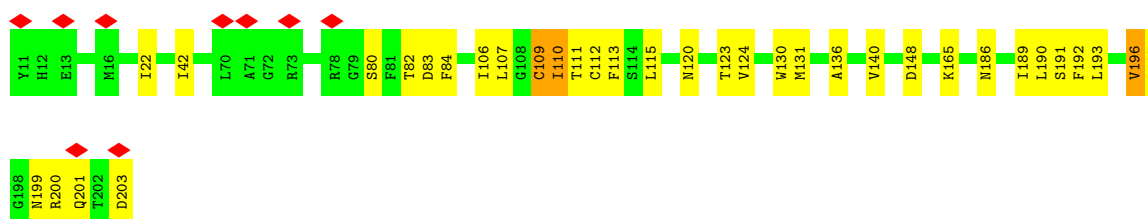
• Molecule 4: Neuroligin-2

Chain H: 6% 76% 24%



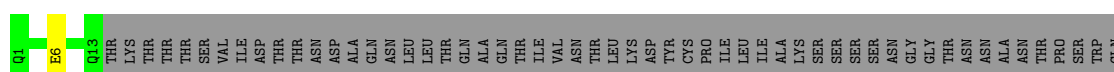
• Molecule 5: LHFPL tetraspan subfamily member 4 protein

Chain L: 5% 82% 17%

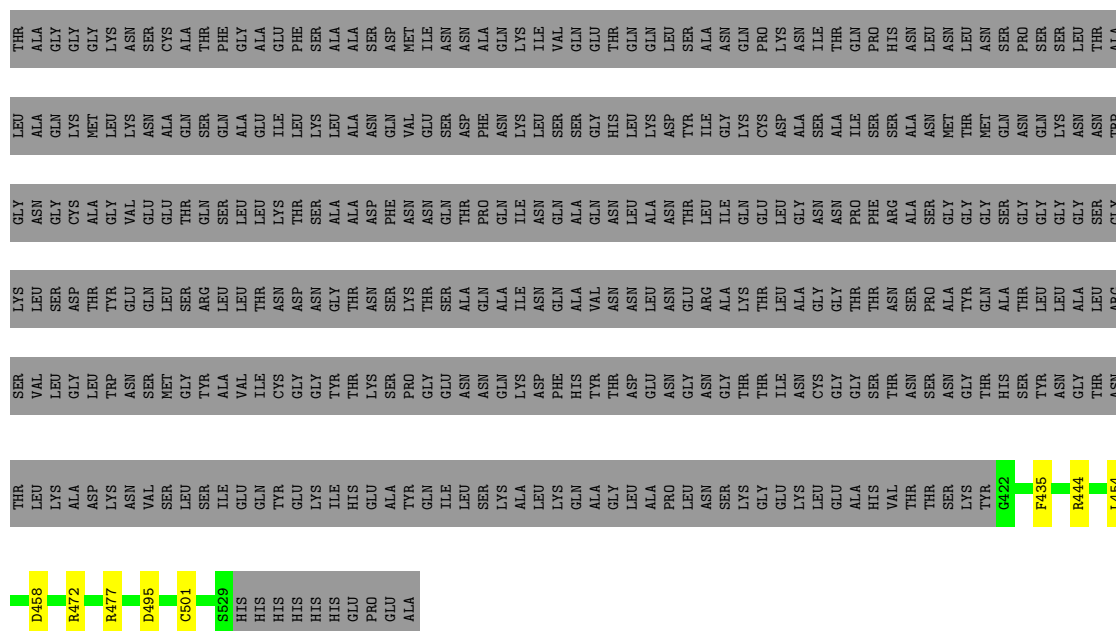


• Molecule 6: Megabody38

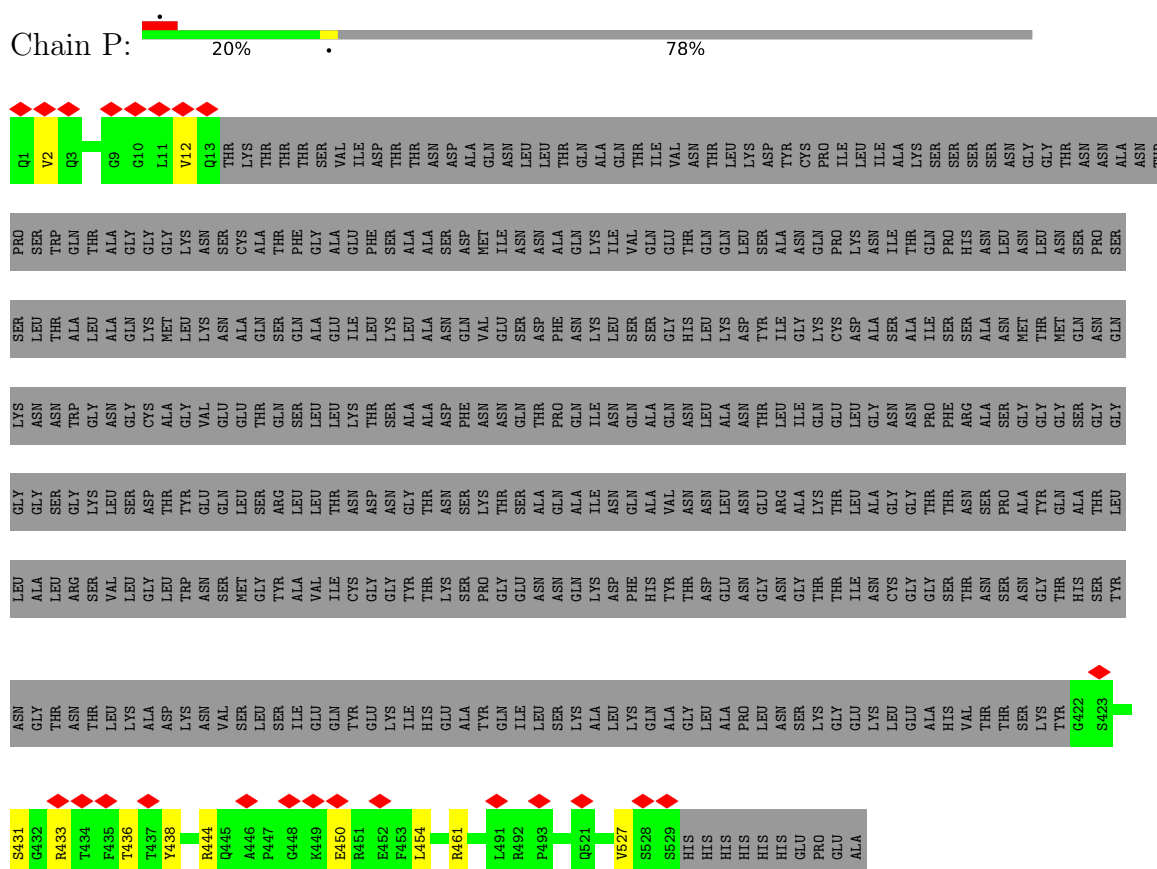
Chain G: 21% 78%





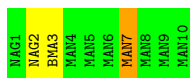


### • Molecule 6: Megabody38



### • 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

Chain I:  100%



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

Chain O:  33% 67%



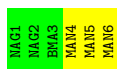
- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain N:  50% 50%

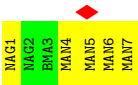


- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49663	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	0.057	Depositor
Minimum map value	-0.022	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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.19	0/2997	0.36	0/4066
1	D	0.22	0/2948	0.40	1/4003 (0.0%)
2	B	0.17	0/2921	0.37	0/3970
2	E	0.17	0/2963	0.38	0/4025
3	C	0.31	0/2965	0.53	2/4026 (0.0%)
4	H	0.28	0/260	0.40	0/352
5	L	0.52	2/1555 (0.1%)	0.79	2/2112 (0.1%)
6	G	0.20	0/972	0.39	0/1311
6	P	0.18	0/961	0.40	0/1297
All	All	0.26	2/18542 (0.0%)	0.46	5/25162 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	192[A]	PHE	C-O	6.89	1.31	1.24
5	L	192[B]	PHE	C-O	6.89	1.31	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	192[A]	PHE	CA-C-O	7.14	128.54	120.90
5	L	192[B]	PHE	CA-C-O	7.14	128.54	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	304[A]	PHE	CA-C-O	6.36	127.29	120.55
3	C	304[B]	PHE	CA-C-O	6.36	127.29	120.55
1	D	44	ASP	CA-CB-CG	5.30	117.90	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	380	P1L	Mainchain

## 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	2912	0	2922	24	0
1	D	2872	0	2871	17	0
2	B	2843	0	2849	13	0
2	E	2879	0	2894	20	0
3	C	2951	0	2963	32	0
4	H	256	0	256	6	0
5	L	1509	0	1504	29	0
6	G	949	0	907	6	0
6	P	941	0	894	7	0
7	F	116	0	97	3	0
8	I	39	0	34	0	0
8	O	39	0	34	0	0
9	J	72	0	61	1	0
9	N	72	0	61	0	0
10	K	28	0	25	0	0
11	M	83	0	70	2	0
12	A	6	0	14	0	0
12	B	12	0	28	0	0
12	D	6	0	14	0	0
12	E	12	0	28	0	0
13	A	47	0	44	3	0
13	D	47	0	44	4	0
14	A	51	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	D	102	0	152	0	0
14	E	32	0	34	0	0
14	L	102	0	152	9	0
15	A	72	0	104	7	0
15	C	36	0	52	0	0
15	D	72	0	104	3	0
16	A	10	0	22	0	0
16	B	10	0	22	0	0
16	D	20	0	44	0	0
16	E	20	0	44	0	0
16	L	10	0	22	0	0
17	A	18	0	31	0	0
17	B	18	0	31	0	0
17	C	50	0	82	1	0
17	D	18	0	31	0	0
17	E	36	0	62	0	0
18	A	1	0	0	0	0
18	C	1	0	0	0	0
18	D	1	0	0	0	0
18	L	1	0	0	5	0
19	B	7	0	0	0	0
19	E	7	0	0	1	0
20	B	32	0	68	0	0
20	E	16	0	34	0	0
21	C	21	0	28	0	0
22	L	28	0	46	2	0
23	A	20	0	0	1	0
23	B	19	0	0	0	0
23	C	11	0	0	1	0
23	D	17	0	0	0	0
23	E	15	0	0	0	0
23	G	4	0	0	2	0
All	All	19569	0	19855	150	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 (150) 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)
15:A:3706:PX2:H37	15:A:3706:PX2:H12	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD13	2:E:260:THR:HG22	1.58	0.85
1:A:301:LEU:HD23	2:E:235:LEU:HD11	1.59	0.82
22:L:302:CLR:O1	18:L:305:CL:CL	2.36	0.80
2:B:101:ASP:OD1	2:B:132:THR:OG1	2.04	0.75
5:L:80:SER:HA	18:L:305:CL:CL	2.25	0.73
1:A:229:GLN:OE1	2:B:269:ARG:NH2	2.21	0.73
2:E:308:GLY:O	2:E:312:GLN:NE2	2.26	0.68
3:C:381:P1L:H202	3:C:385:P1L:H222	1.76	0.68
1:D:288:TRP:HB3	15:D:3908:PX2:H4	1.74	0.68
3:C:416:LEU:HD12	5:L:111:THR:HG22	1.76	0.67
1:A:391:LYS:NZ	13:A:3702:PIO:O2	2.28	0.66
1:D:112:MET:HE1	2:E:106:VAL:HG23	1.76	0.66
3:C:277:THR:HA	3:C:304[B]:PHE:HZ	1.61	0.66
14:L:304:PGW:OAE	14:L:304:PGW:O12	2.12	0.65
2:E:146:ASP:OD2	2:E:148:GLN:NE2	2.30	0.65
5:L:80:SER:OG	18:L:305:CL:CL	2.53	0.64
5:L:200:ARG:O	5:L:203:ASP:N	2.30	0.64
6:G:6:GLU:OE2	6:G:501:CYS:N	2.30	0.64
2:E:256:THR:O	2:E:260:THR:HG23	1.99	0.63
13:D:3901:PIO:O41	13:D:3901:PIO:O3	2.16	0.63
1:A:406:ILE:HG22	15:A:3706:PX2:H17	1.81	0.61
3:C:381:P1L:H191	3:C:385:P1L:H182	1.82	0.61
1:D:312:LYS:NZ	13:D:3901:PIO:O51	2.25	0.61
3:C:144:ARG:NH1	23:C:601:HOH:O	2.34	0.61
5:L:80:SER:CA	18:L:305:CL:CL	2.86	0.61
1:A:294:TYR:CE1	2:E:231:LEU:HD13	2.36	0.61
5:L:112:CYS:O	5:L:113:PHE:C	2.42	0.60
2:B:225:THR:HG21	2:B:281:ILE:HD11	1.83	0.60
3:C:313:GLU:HG2	3:C:402:MET:HE2	1.83	0.60
3:C:123:TRP:CD1	7:F:7:MAN:HO2	2.20	0.60
6:P:450:GLU:N	6:P:450:GLU:OE1	2.35	0.59
1:D:410:VAL:HG11	15:D:3908:PX2:H38	1.86	0.58
2:B:233:THR:O	2:B:236:SER:OG	2.17	0.57
2:E:426:TRP:CE2	2:E:430:VAL:HG21	2.39	0.57
4:H:697:LEU:HD11	5:L:22:ILE:HG21	1.85	0.57
6:P:2:VAL:HG11	6:P:433:ARG:HH21	1.70	0.56
6:G:444:ARG:HB2	6:G:454:LEU:HD11	1.87	0.56
2:B:235:LEU:HD22	3:C:311:LEU:HD23	1.87	0.56
14:L:301:PGW:H3A	14:L:301:PGW:H20	1.88	0.55
2:B:84:ASP:O	2:B:87:VAL:HG12	2.06	0.55
5:L:80:SER:CB	18:L:305:CL:CL	2.92	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:107:LEU:O	5:L:111:THR:HG23	2.05	0.55
6:P:2:VAL:HG13	6:P:431:SER:O	2.07	0.55
7:F:7:MAN:H62	11:M:1:NAG:H82	1.88	0.55
2:E:66[A]:TYR:CZ	2:E:125:LEU:HD13	2.41	0.55
2:B:239:SER:HB3	2:B:253:LEU:HD23	1.89	0.55
13:D:3901:PIO:O11	13:D:3901:PIO:O2	2.19	0.55
3:C:381:P1L:C	3:C:383:GLU:H	2.19	0.54
5:L:148:ASP:OD1	5:L:165:LYS:NZ	2.39	0.54
2:B:28:ARG:NH1	2:B:30:ASP:O	2.42	0.53
3:C:381:P1L:H162	5:L:131:MET:HG2	1.91	0.52
1:A:81:MET:HE2	1:A:83:VAL:O	2.10	0.52
17:C:501:PLM:H22	5:L:123:THR:HG21	1.93	0.51
3:C:198:LEU:O	3:C:232:ARG:NH2	2.44	0.51
3:C:254:SER:HB2	3:C:268:LEU:HD22	1.93	0.51
5:L:109:CYS:O	5:L:110:ILE:C	2.54	0.51
1:A:19:LEU:HD22	1:A:90:MET:HE3	1.93	0.51
1:D:164:ARG:NH2	1:D:209:GLU:OE1	2.45	0.50
3:C:63:GLY:N	3:C:73:THR:O	2.43	0.50
1:A:72:ASP:OD2	23:A:3801:HOH:O	2.19	0.50
1:D:204:GLN:O	6:P:461:ARG:NH2	2.45	0.50
2:E:239:SER:HB3	2:E:253:LEU:HD23	1.94	0.50
2:B:66[A]:TYR:CZ	2:B:125:LEU:HD13	2.47	0.49
5:L:112:CYS:O	5:L:115:LEU:N	2.36	0.49
1:D:131:MET:HE2	1:D:133:LEU:HD21	1.95	0.49
3:C:381:P1L:H111	5:L:130:TRP:HB2	1.95	0.49
5:L:83:ASP:HA	14:L:301:PGW:O04	2.11	0.49
4:H:683:GLY:O	4:H:687:LEU:HD23	2.13	0.48
1:A:144:GLU:N	1:A:144:GLU:OE1	2.46	0.48
6:P:436:THR:O	6:P:438:TYR:N	2.44	0.48
1:A:67:ARG:HB3	1:A:130:THR:HG23	1.93	0.48
6:G:435:PHE:O	6:G:477:ARG:NH2	2.43	0.48
14:L:301:PGW:H4	14:L:301:PGW:H23A	1.96	0.48
1:A:407:PHE:HD1	15:A:3706:PX2:H9	1.79	0.48
1:A:419:GLU:O	1:A:421:GLN:NE2	2.47	0.48
1:A:301:LEU:CD2	2:E:235:LEU:HD11	2.38	0.47
1:A:403:LEU:HD13	15:A:3706:PX2:H28	1.95	0.47
3:C:428:LEU:HB3	5:L:42:ILE:HG21	1.97	0.47
2:E:44:ILE:HD12	2:E:59:LEU:HD11	1.97	0.47
2:B:231:LEU:CD1	14:L:301:PGW:H11	2.45	0.47
3:C:370:LEU:HD23	4:H:698:TYR:CE2	2.49	0.47
1:D:105:LYS:N	1:D:136:ARG:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:GLU:H	1:D:325:GLU:CD	2.22	0.47
5:L:200:ARG:O	5:L:201:GLN:C	2.58	0.47
4:H:690:ASN:OD1	5:L:186:ASN:ND2	2.48	0.47
1:A:33:GLY:HA3	1:A:37[B]:ARG:HG2	1.96	0.47
6:G:444:ARG:NH1	6:G:495:ASP:OD1	2.47	0.46
3:C:236:PHE:HB3	3:C:296:MET:HE1	1.97	0.46
6:G:458:ASP:OD1	23:G:602:HOH:O	2.21	0.46
4:H:685:SER:O	4:H:689:LEU:HD23	2.16	0.46
3:C:269:GLY:O	3:C:272:THR:OG1	2.31	0.45
3:C:250:LEU:O	3:C:268:LEU:HD21	2.15	0.45
1:A:207:THR:HG21	2:E:115:MET:HE1	1.98	0.45
1:D:326:LYS:HE2	1:D:326:LYS:HA	1.98	0.45
1:A:145:ASP:O	1:A:148:MET:N	2.49	0.45
5:L:106:ILE:O	5:L:110:ILE:HG12	2.17	0.45
1:A:99:THR:O	2:E:110:THR:OG1	2.32	0.44
3:C:159:PRO:HG3	3:C:296:MET:HE2	1.98	0.44
3:C:304[A]:PHE:HA	3:C:307:VAL:HG22	2.00	0.44
3:C:378:PHE:HA	5:L:199:ASN:OD1	2.18	0.44
3:C:284:ARG:HD2	3:C:287:LEU:HD12	1.99	0.44
2:E:316:LYS:C	2:E:317:LEU:HD12	2.42	0.44
3:C:277:THR:HA	3:C:304[B]:PHE:CZ	2.47	0.44
3:C:34:LEU:HD22	3:C:87:LEU:HA	2.00	0.43
3:C:57:MET:HE1	3:C:167:LEU:HD23	2.00	0.43
5:L:84:PHE:H	14:L:301:PGW:H21	1.83	0.43
5:L:120:ASN:O	5:L:124:VAL:HG23	2.17	0.43
1:D:45:ILE:HG12	1:D:66:PHE:HD1	1.83	0.43
3:C:155:LEU:HD13	3:C:287:LEU:HD22	2.00	0.43
2:E:77:ILE:HG22	2:E:79:LEU:HD23	2.01	0.43
6:G:472:ARG:NH2	6:G:495:ASP:OD2	2.51	0.43
1:D:67:ARG:HG3	1:D:130:THR:HG23	2.00	0.43
2:E:100:ASN:ND2	2:E:151:THR:O	2.50	0.43
5:L:82:THR:O	14:L:301:PGW:H20A	2.18	0.43
1:A:264:LEU:CD1	2:E:260:THR:HG22	2.38	0.43
1:D:274:ARG:NH1	1:D:287:ASP:OD2	2.47	0.42
1:A:407:PHE:CD1	15:A:3706:PX2:H9	2.53	0.42
15:A:3706:PX2:H42	15:A:3706:PX2:H34	2.00	0.42
14:L:301:PGW:H17	22:L:302:CLR:C15	2.50	0.42
3:C:381:P1L:C	3:C:383:GLU:N	2.82	0.42
1:D:67:ARG:NH2	19:E:4009:ABU:O	2.49	0.42
2:E:266:THR:HA	2:E:269:ARG:HG3	2.00	0.42
6:P:12:VAL:HG23	6:P:527:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:GLU:OE1	2:B:213:ARG:NH1	2.47	0.42
3:C:62:ILE:HD12	3:C:196:TRP:CZ3	2.54	0.42
3:C:106:ILE:HD11	3:C:131:LEU:HD11	2.00	0.42
1:A:87:ASN:OD1	1:A:88:ASN:N	2.53	0.42
1:D:112:MET:HA	1:D:112:MET:HE2	2.01	0.42
5:L:190:LEU:O	5:L:191:SER:C	2.62	0.42
1:A:392:ILE:HD11	13:A:3702:PIO:H2C	2.02	0.41
3:C:369:CYS:SG	3:C:373:LYS:O	2.75	0.41
5:L:136:ALA:O	5:L:140:VAL:HG23	2.20	0.41
9:J:4:MAN:H3	9:J:5:MAN:H2	1.74	0.41
3:C:380:P1L:H102	3:C:381:P1L:H122	2.03	0.41
1:D:313:ARG:NH2	13:D:3901:PIO:O43	2.53	0.41
15:A:3706:PX2:H44	15:A:3706:PX2:H24	2.02	0.41
1:D:296:PHE:CE1	15:D:3908:PX2:H28	2.56	0.41
2:E:264:ILE:O	2:E:268:LEU:HD23	2.21	0.41
4:H:694:PHE:CE2	5:L:189:ILE:HG23	2.55	0.41
2:B:8:ASN:OD1	2:B:10:SER:OG	2.30	0.41
1:A:395:LEU:HD23	13:A:3702:PIO:C6B	2.51	0.41
2:B:68:ARG:NH1	2:B:121:ASP:OD2	2.54	0.40
7:F:2:NAG:O3	7:F:7:MAN:H5	2.21	0.40
11:M:4:MAN:H2	11:M:5:MAN:H2	1.87	0.40
14:L:301:PGW:O02	14:L:301:PGW:H4A	2.21	0.40
6:P:444:ARG:HB2	6:P:454:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/413 (86%)	347 (98%)	9 (2%)	0	100	100
1	D	351/413 (85%)	346 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	342/441 (78%)	334 (98%)	8 (2%)	0	100	100
2	E	347/441 (79%)	342 (99%)	5 (1%)	0	100	100
3	C	346/405 (85%)	337 (97%)	9 (3%)	0	100	100
4	H	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
5	L	192/193 (100%)	184 (96%)	8 (4%)	0	100	100
6	G	118/539 (22%)	114 (97%)	4 (3%)	0	100	100
6	P	117/539 (22%)	110 (94%)	7 (6%)	0	100	100
All	All	2200/3417 (64%)	2143 (97%)	57 (3%)	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	322/367 (88%)	322 (100%)	0	100	100
1	D	317/367 (86%)	315 (99%)	2 (1%)	84	94
2	B	312/393 (79%)	312 (100%)	0	100	100
2	E	316/393 (80%)	315 (100%)	1 (0%)	91	97
3	C	322/366 (88%)	320 (99%)	2 (1%)	84	94
4	H	27/27 (100%)	27 (100%)	0	100	100
5	L	160/159 (101%)	156 (98%)	4 (2%)	42	68
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%)	1956 (100%)	9 (0%)	85	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	371	ASP

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Mol	Chain	Res	Type
3	C	374	ASP
1	D	42	LYS
1	D	325	GLU
2	E	80	ASN
5	L	109	CYS
5	L	110	ILE
5	L	196	VAL
5	L	197	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
2	B	185	GLN
3	C	54	HIS
3	C	80	GLN
3	C	200	GLN
1	D	110	HIS
1	D	142	HIS
1	D	204	GLN
2	E	90	GLN
2	E	267	HIS
2	E	421	ASN
4	H	690	ASN
5	L	120	ASN
5	L	186	ASN
6	G	517	HIS
6	P	524	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	P1L	C	380	3	21,22,23	0.41	0	18,23,25	3.55	1 (5%)
3	P1L	C	385	3	21,22,23	1.10	1 (4%)	18,23,25	1.35	3 (16%)
3	P1L	C	381	3	21,22,23	0.38	0	18,23,25	3.39	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	380	3	-	7/20/22/24	-
3	P1L	C	385	3	-	11/20/22/24	-
3	P1L	C	381	3	-	6/20/22/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	385	P1L	O-C	4.17	1.36	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	380	P1L	CB-SG-C7	14.95	121.75	100.84
3	C	381	P1L	CB-SG-C7	14.32	120.86	100.84
3	C	385	P1L	C8-C7-SG	-3.70	109.15	113.46
3	C	385	P1L	CB-SG-C7	3.25	105.38	100.84
3	C	385	P1L	O7-C7-SG	2.28	125.58	122.61

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	380	P1L	N-CA-CB-SG
3	C	380	P1L	C-CA-CB-SG
3	C	380	P1L	O7-C7-SG-CB
3	C	380	P1L	C8-C7-SG-CB

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

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	380	P1L	1	0
3	C	385	P1L	2	0
3	C	381	P1L	7	0

## 5.5 Carbohydrates

37 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	0.39	0	17,19,21	0.63	0
7	MAN	F	10	7	11,11,12	0.38	0	15,15,17	0.64	0
7	NAG	F	2	7	14,14,15	0.38	0	17,19,21	0.72	0
7	BMA	F	3	7	11,11,12	0.61	0	15,15,17	0.78	1 (6%)
7	MAN	F	4	7	11,11,12	0.44	0	15,15,17	0.60	0
7	MAN	F	5	7	11,11,12	0.35	0	15,15,17	0.56	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	0.72	1 (9%)	15,15,17	0.89	0
7	MAN	F	8	7	11,11,12	0.38	0	15,15,17	0.50	0
7	MAN	F	9	7	11,11,12	0.35	0	15,15,17	0.54	0
8	NAG	I	1	8	14,14,15	0.20	0	17,19,21	0.43	0
8	NAG	I	2	8	14,14,15	0.22	0	17,19,21	0.61	0
8	BMA	I	3	8	11,11,12	0.60	0	15,15,17	0.82	0
9	NAG	J	1	9,2	14,14,15	0.41	0	17,19,21	1.17	3 (17%)
9	NAG	J	2	9	14,14,15	0.42	0	17,19,21	0.63	0
9	BMA	J	3	9	11,11,12	0.50	0	15,15,17	0.50	0
9	MAN	J	4	9	11,11,12	0.33	0	15,15,17	0.64	0
9	MAN	J	5	9	11,11,12	0.30	0	15,15,17	0.54	0
9	MAN	J	6	9	11,11,12	0.28	0	15,15,17	0.50	0
10	NAG	K	1	10,3	14,14,15	0.40	0	17,19,21	0.40	0
10	NAG	K	2	10	14,14,15	0.39	0	17,19,21	0.79	1 (5%)
11	NAG	M	1	11,1	14,14,15	0.38	0	17,19,21	0.44	0
11	NAG	M	2	11	14,14,15	0.38	0	17,19,21	0.62	0
11	BMA	M	3	11	11,11,12	0.23	0	15,15,17	0.53	0
11	MAN	M	4	11	11,11,12	0.30	0	15,15,17	0.56	0
11	MAN	M	5	11	11,11,12	0.27	0	15,15,17	0.58	0
11	MAN	M	6	11	11,11,12	0.38	0	15,15,17	1.15	1 (6%)
11	MAN	M	7	11	11,11,12	0.33	0	15,15,17	0.95	1 (6%)
9	NAG	N	1	9,2	14,14,15	0.27	0	17,19,21	0.38	0
9	NAG	N	2	9	14,14,15	0.22	0	17,19,21	0.42	0
9	BMA	N	3	9	11,11,12	0.56	0	15,15,17	0.76	0
9	MAN	N	4	9	11,11,12	0.75	0	15,15,17	1.02	2 (13%)
9	MAN	N	5	9	11,11,12	0.67	0	15,15,17	1.13	3 (20%)
9	MAN	N	6	9	11,11,12	0.71	0	15,15,17	1.07	2 (13%)
8	NAG	O	1	8,2	14,14,15	0.41	0	17,19,21	0.94	2 (11%)
8	NAG	O	2	8	14,14,15	0.40	0	17,19,21	0.99	2 (11%)
8	BMA	O	3	8	11,11,12	0.33	0	15,15,17	0.41	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	-	1/2/19/22	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	-	4/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
9	NAG	J	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	J	2	9	-	0/6/23/26	0/1/1/1
9	BMA	J	3	9	-	0/2/19/22	0/1/1/1
9	MAN	J	4	9	-	0/2/19/22	0/1/1/1
9	MAN	J	5	9	-	1/2/19/22	0/1/1/1
9	MAN	J	6	9	-	0/2/19/22	0/1/1/1
10	NAG	K	1	10,3	-	3/6/23/26	0/1/1/1
10	NAG	K	2	10	-	1/6/23/26	0/1/1/1
11	NAG	M	1	11,1	-	4/6/23/26	0/1/1/1
11	NAG	M	2	11	-	0/6/23/26	0/1/1/1
11	BMA	M	3	11	-	1/2/19/22	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	-	2/2/19/22	0/1/1/1
11	MAN	M	7	11	-	0/2/19/22	0/1/1/1
9	NAG	N	1	9,2	-	0/6/23/26	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	-	2/2/19/22	0/1/1/1
9	MAN	N	5	9	-	0/2/19/22	0/1/1/1
9	MAN	N	6	9	-	0/2/19/22	0/1/1/1
8	NAG	O	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	O	2	8	-	2/6/23/26	0/1/1/1
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	7	MAN	C2-C3	-2.08	1.49	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	6	MAN	O5-C1-C2	3.50	116.17	110.77
8	O	2	NAG	C1-C2-N2	2.81	115.28	110.49
11	M	7	MAN	C1-O5-C5	2.78	115.96	112.19
9	J	1	NAG	C2-N2-C7	2.71	126.76	122.90
9	J	1	NAG	C1-O5-C5	2.41	115.45	112.19
8	O	1	NAG	C1-O5-C5	2.37	115.40	112.19
9	J	1	NAG	C1-C2-N2	2.32	114.45	110.49
8	O	1	NAG	C1-C2-N2	2.29	114.39	110.49
10	K	2	NAG	C2-N2-C7	2.23	126.08	122.90
8	O	2	NAG	C2-N2-C7	2.23	126.08	122.90
9	N	6	MAN	C1-O5-C5	2.22	115.20	112.19
9	N	6	MAN	O2-C2-C3	-2.22	105.69	110.14
9	N	5	MAN	O2-C2-C3	-2.20	105.74	110.14
9	N	5	MAN	C1-O5-C5	2.17	115.13	112.19
9	N	4	MAN	O2-C2-C3	-2.13	105.88	110.14
9	N	4	MAN	C1-O5-C5	2.05	114.98	112.19
9	N	5	MAN	O5-C1-C2	2.02	113.89	110.77
7	F	3	BMA	O3-C3-C2	-2.00	106.16	109.99

There are no chirality outliers.

All (28) torsion outliers are listed below:

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

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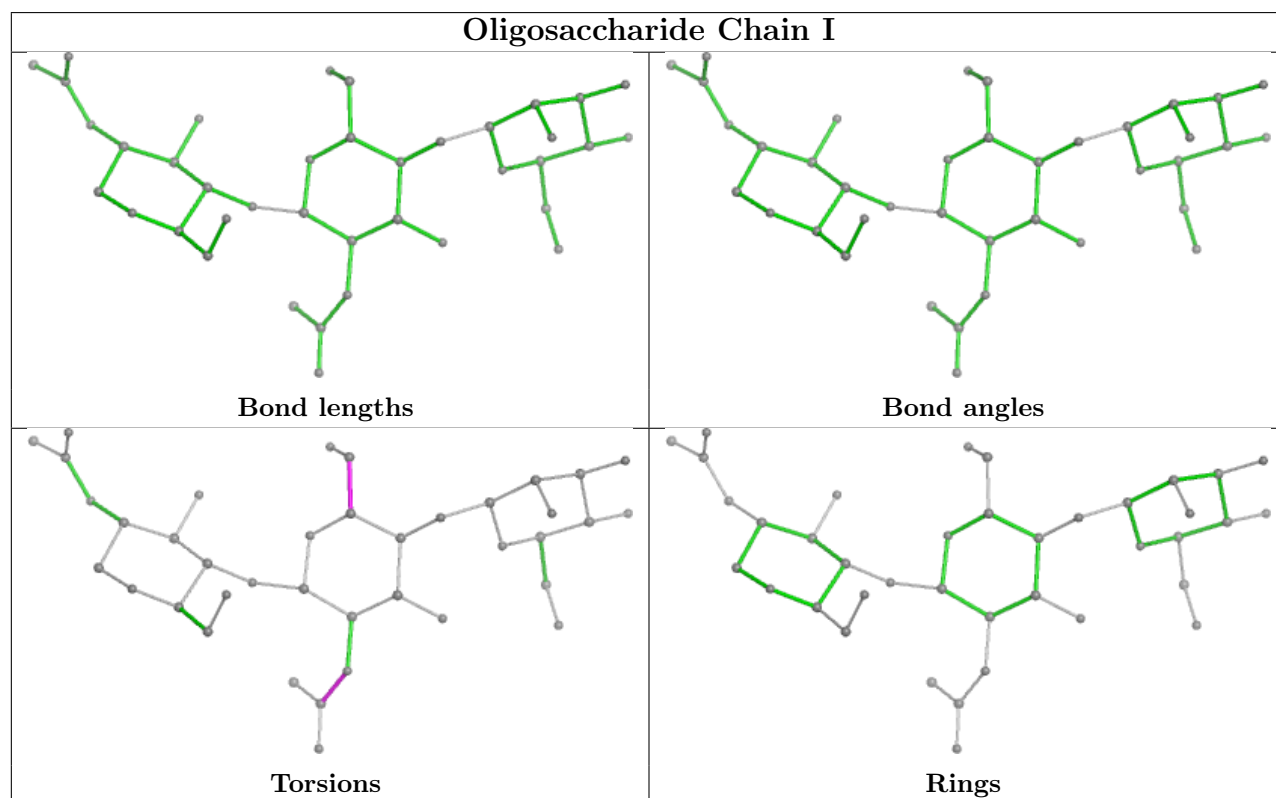
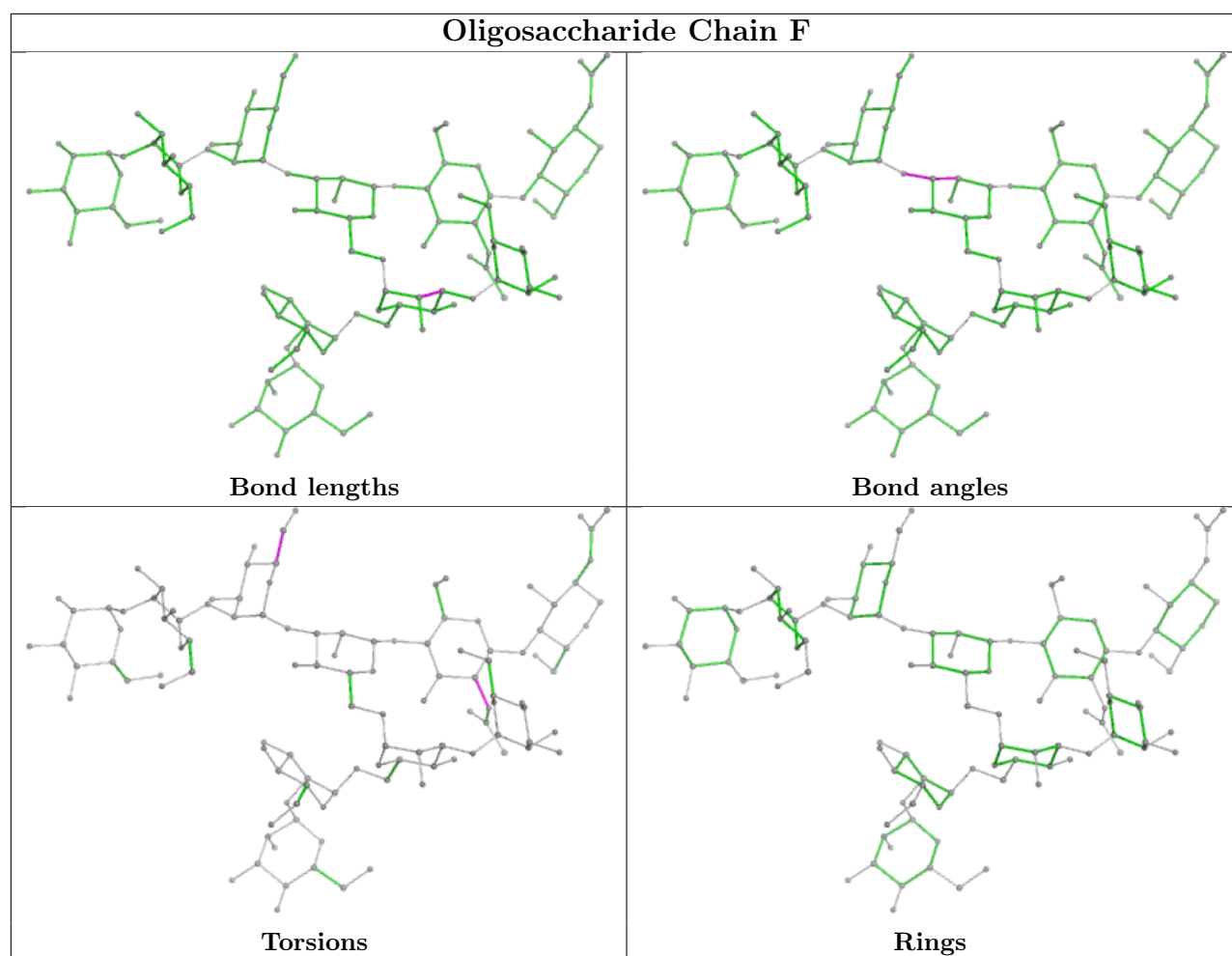
Mol	Chain	Res	Type	Atoms
11	M	1	NAG	C4-C5-C6-O6
8	O	1	NAG	O7-C7-N2-C2
11	M	1	NAG	O5-C5-C6-O6
11	M	3	BMA	O5-C5-C6-O6
7	F	4	MAN	O5-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
9	J	5	MAN	O5-C5-C6-O6
9	N	4	MAN	O5-C5-C6-O6
9	N	4	MAN	C4-C5-C6-O6
9	N	2	NAG	C4-C5-C6-O6
9	J	1	NAG	C1-C2-N2-C7
7	F	2	NAG	C3-C2-N2-C7
10	K	2	NAG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

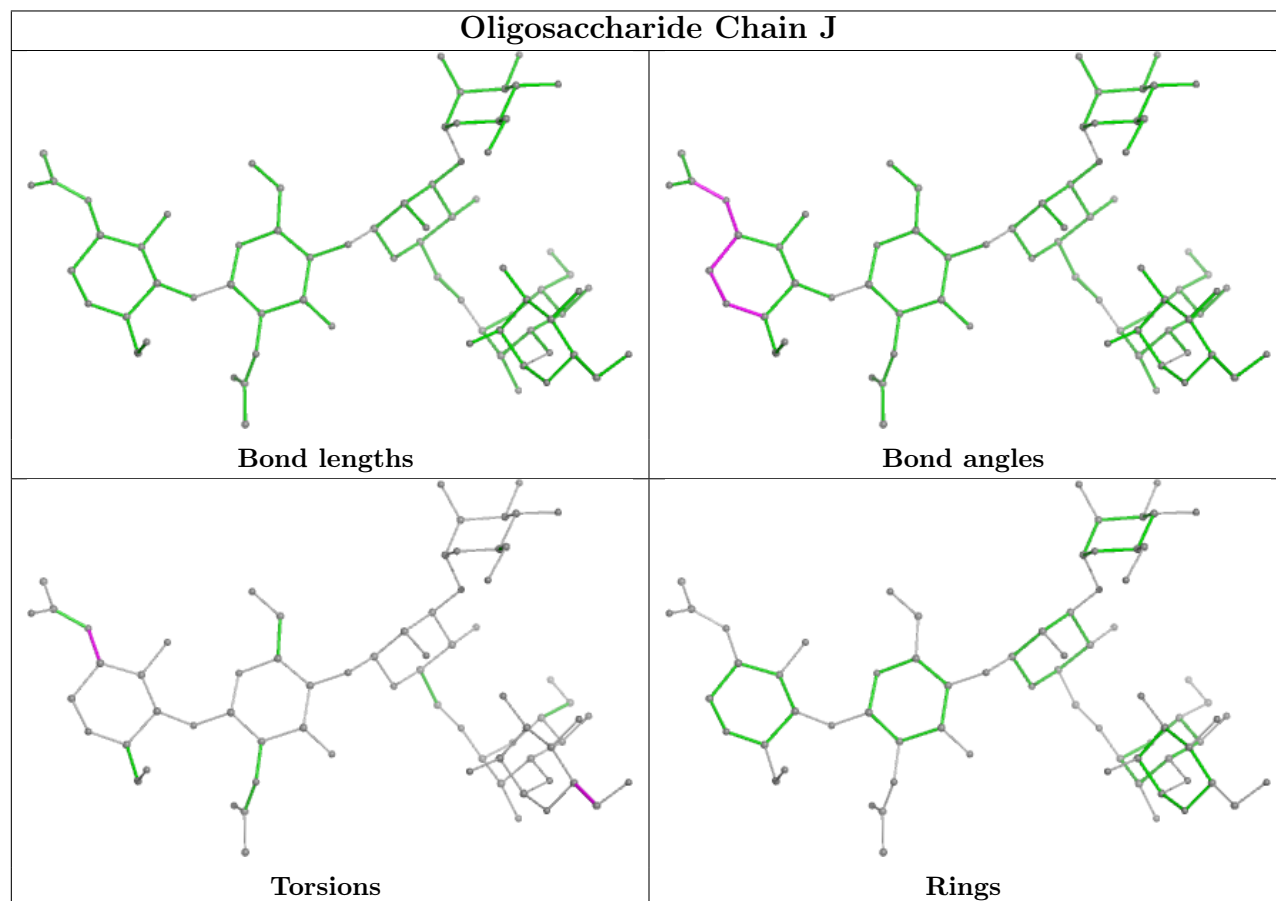
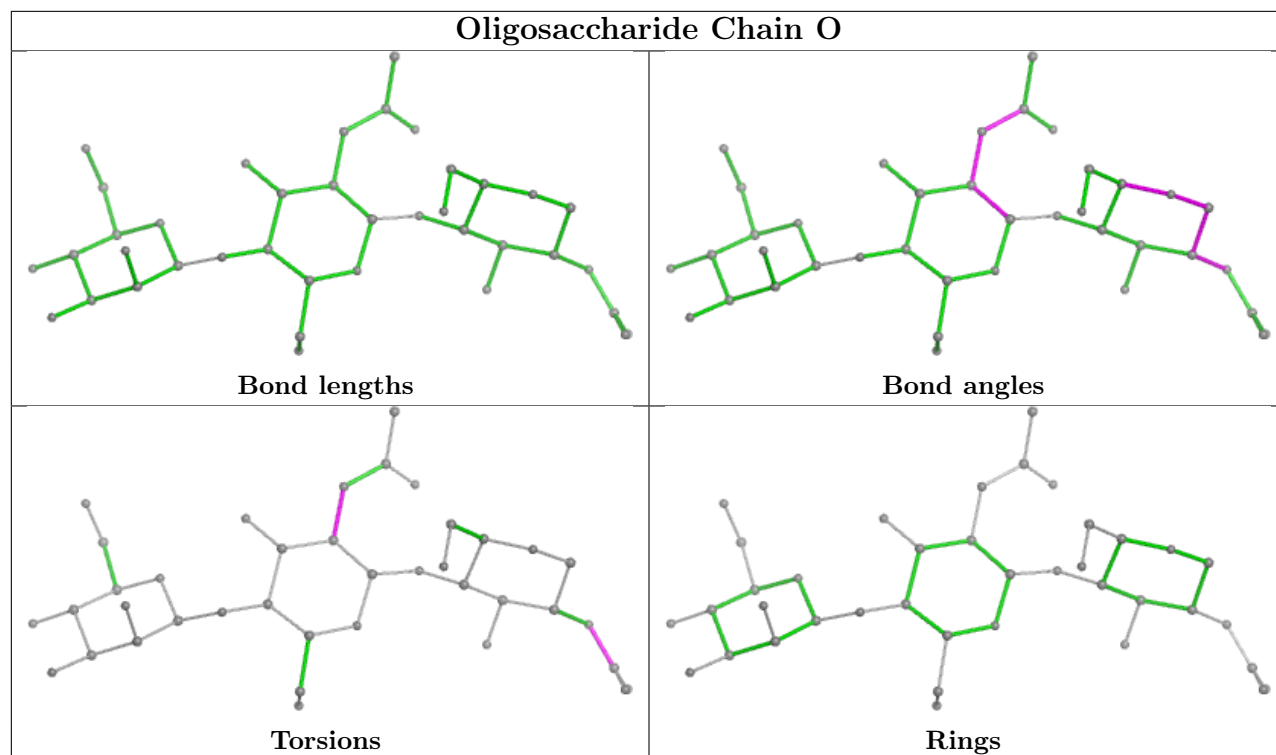
There are no ring outliers.

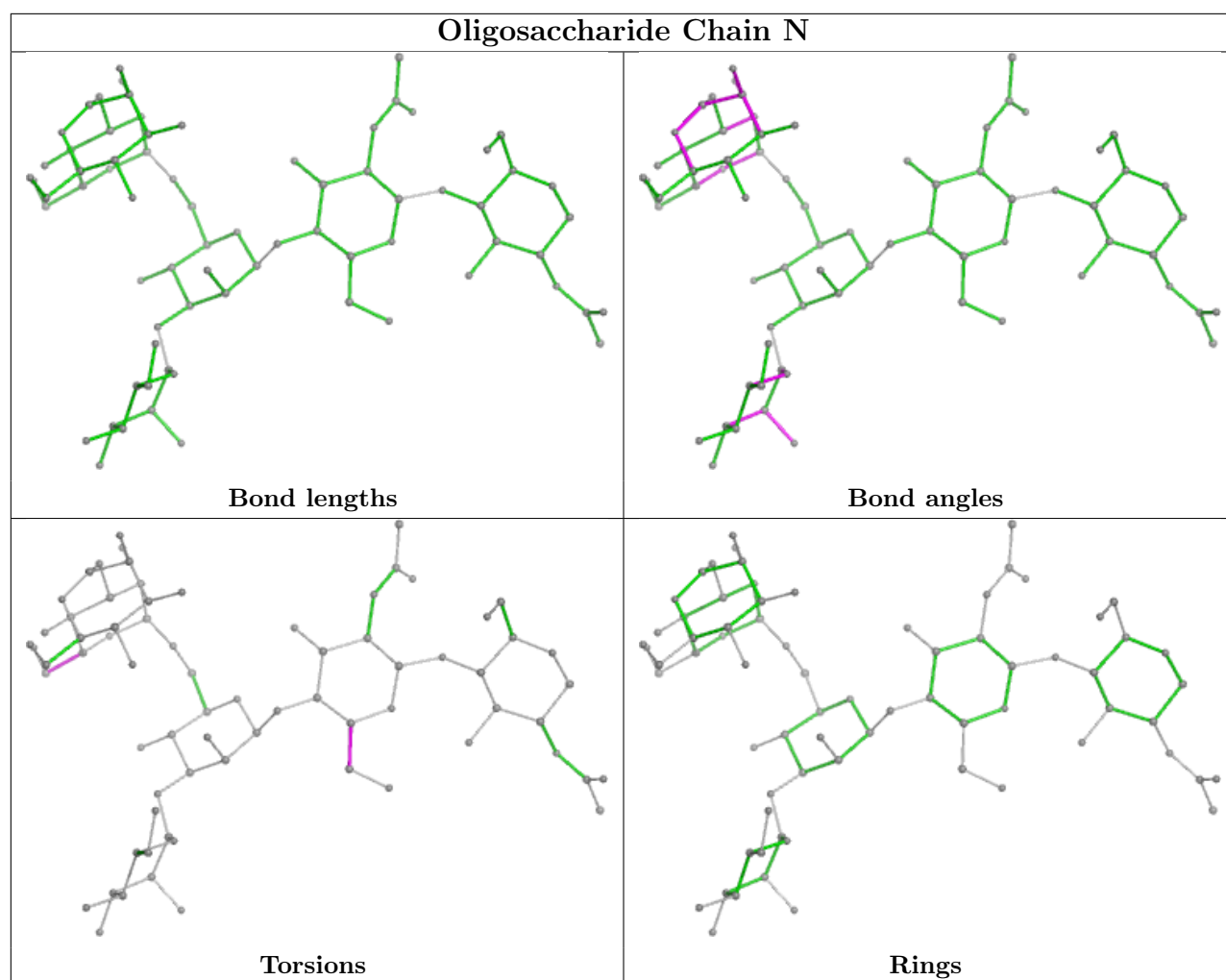
7 monomers are involved in 5 short contacts:

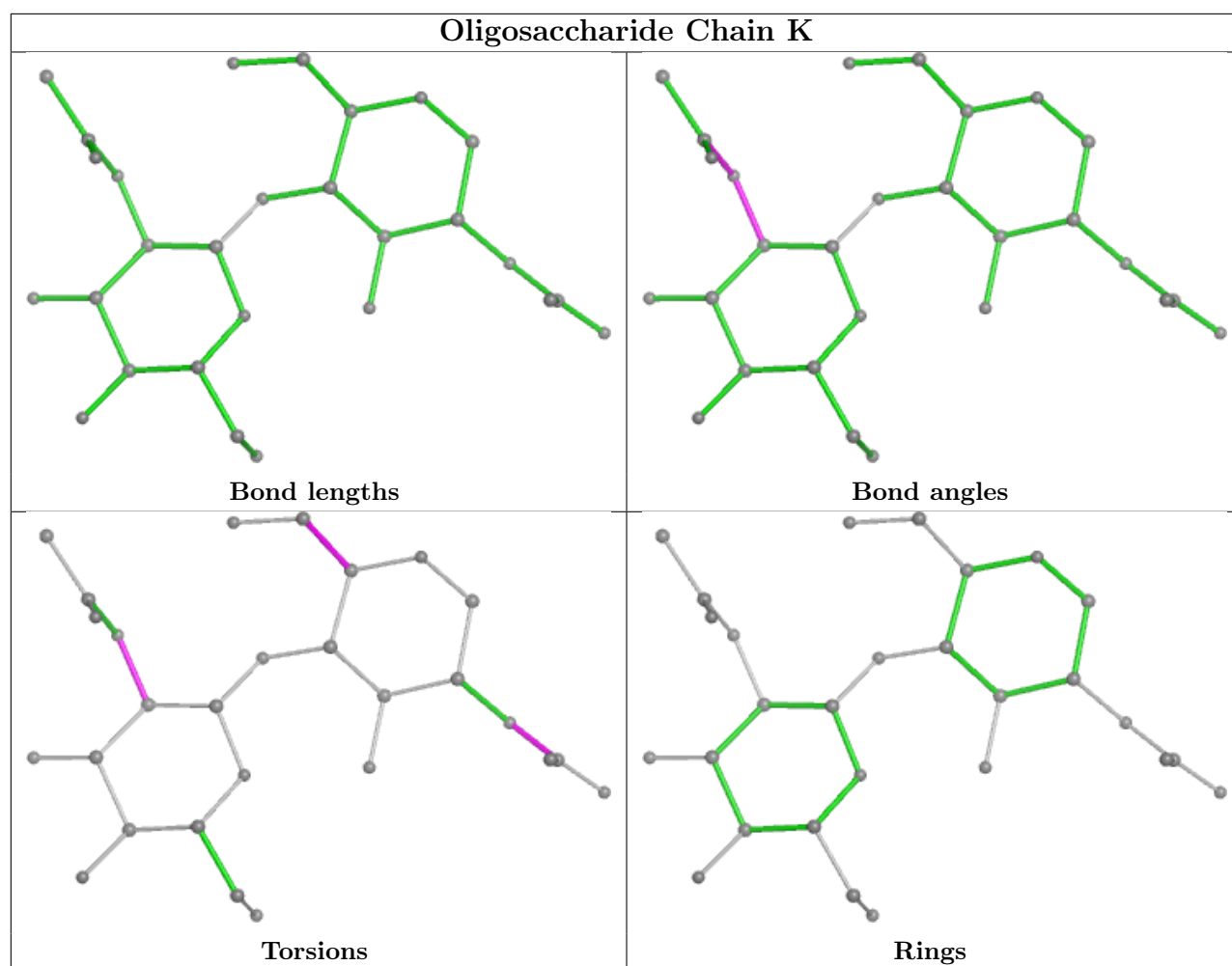
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	4	MAN	1	0
7	F	7	MAN	3	0
7	F	2	NAG	1	0
9	J	5	MAN	1	0
11	M	5	MAN	1	0
9	J	4	MAN	1	0
11	M	1	NAG	1	0

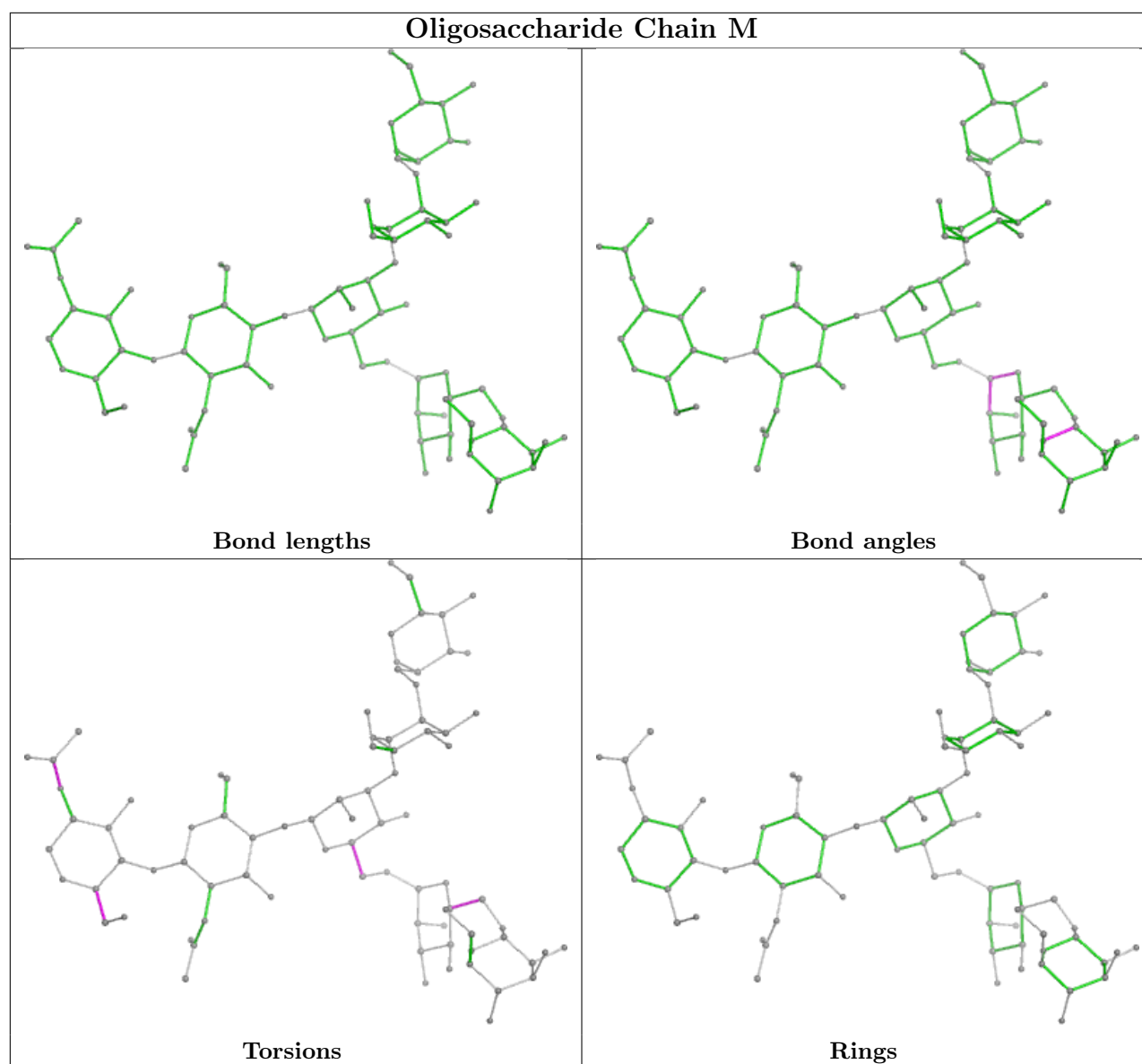
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 4 are 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	$\# Z  > 2$
12	HEX	D	3905	-	5,5,5	0.31	0	4,4,4	0.57	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	PGW	A	3703	-	50,50,50	0.97	2 (4%)	53,56,56	1.00	2 (3%)
19	ABU	B	1601	-	6,6,6	0.88	0	6,6,6	1.45	1 (16%)
15	PX2	A	3706	-	35,35,35	0.32	0	39,40,40	0.35	0
16	D10	L	303	-	9,9,9	0.33	0	8,8,8	0.67	0
17	PLM	B	1606	-	17,17,17	0.59	0	17,17,17	1.03	0
17	PLM	E	4007	-	17,17,17	0.59	0	17,17,17	1.00	0
20	R16	B	1602	-	15,15,15	0.29	0	14,14,14	0.81	0
17	PLM	C	504	-	17,17,17	0.57	0	17,17,17	1.05	0
12	HEX	A	3701	-	5,5,5	0.29	0	4,4,4	0.57	0
15	PX2	A	3704	-	35,35,35	1.03	4 (11%)	39,40,40	1.15	2 (5%)
16	D10	D	3906	-	9,9,9	0.32	0	8,8,8	0.59	0
12	HEX	E	4006	-	5,5,5	0.32	0	4,4,4	0.48	0
20	R16	B	1607	-	15,15,15	0.30	0	14,14,14	0.79	0
16	D10	E	4001	-	9,9,9	0.32	0	8,8,8	0.68	0
12	HEX	B	1604	-	5,5,5	0.33	0	4,4,4	0.47	0
16	D10	E	4003	-	9,9,9	0.31	0	8,8,8	0.72	0
17	PLM	C	501	-	13,13,17	0.65	0	13,13,17	1.05	0
17	PLM	C	505	-	17,17,17	0.60	0	17,17,17	0.96	0
17	PLM	E	4004	-	17,17,17	0.58	0	17,17,17	1.04	0
16	D10	B	1603	-	9,9,9	0.30	0	8,8,8	0.76	0
14	PGW	D	3902[A]	-	50,50,50	0.96	3 (6%)	53,56,56	1.00	2 (3%)
14	PGW	D	3902[B]	-	50,50,50	0.97	2 (4%)	53,56,56	0.93	2 (3%)
15	PX2	D	3908	-	35,35,35	0.31	0	39,40,40	0.42	0
16	D10	A	3705	-	9,9,9	0.32	0	8,8,8	0.71	0
15	PX2	D	3903	-	35,35,35	1.02	3 (8%)	39,40,40	1.16	2 (5%)
14	PGW	E	4005	-	31,31,50	1.16	3 (9%)	34,37,56	1.13	2 (5%)
12	HEX	B	1605	-	5,5,5	0.14	0	4,4,4	0.14	0
13	PIO	D	3901	-	47,47,47	1.17	6 (12%)	61,65,65	1.04	2 (3%)
17	PLM	A	3707	-	17,17,17	0.57	0	17,17,17	1.08	1 (5%)
12	HEX	E	4008	-	5,5,5	0.31	0	4,4,4	0.56	0
15	PX2	C	502	-	35,35,35	1.02	3 (8%)	39,40,40	1.17	2 (5%)
19	ABU	E	4009	-	6,6,6	0.87	0	6,6,6	1.44	1 (16%)
22	CLR	L	302	-	31,31,31	0.16	0	48,48,48	0.32	0
20	R16	E	4002	-	15,15,15	0.28	0	14,14,14	0.85	0
14	PGW	L	301	-	50,50,50	0.30	0	53,56,56	0.32	0
16	D10	D	3907	-	9,9,9	0.30	0	8,8,8	0.77	0
14	PGW	L	304	-	50,50,50	0.97	2 (4%)	53,56,56	1.00	2 (3%)
21	OLC	C	503	-	20,20,24	1.10	1 (5%)	21,21,25	1.26	2 (9%)
13	PIO	A	3702	-	47,47,47	1.17	6 (12%)	61,65,65	0.94	2 (3%)
17	PLM	D	3904	-	17,17,17	0.58	0	17,17,17	1.00	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
12	HEX	D	3905	-	-	1/3/3/3	-
14	PGW	A	3703	-	-	22/55/55/55	-
19	ABU	B	1601	-	-	0/4/4/4	-
15	PX2	A	3706	-	-	7/37/37/37	-
16	D10	L	303	-	-	0/7/7/7	-
17	PLM	B	1606	-	-	10/15/15/15	-
17	PLM	E	4007	-	-	7/15/15/15	-
20	R16	B	1602	-	-	0/13/13/13	-
17	PLM	C	504	-	-	6/15/15/15	-
12	HEX	A	3701	-	-	0/3/3/3	-
15	PX2	A	3704	-	-	18/37/37/37	-
16	D10	D	3906	-	-	0/7/7/7	-
12	HEX	E	4006	-	-	0/3/3/3	-
20	R16	B	1607	-	-	1/13/13/13	-
16	D10	E	4001	-	-	0/7/7/7	-
12	HEX	B	1604	-	-	1/3/3/3	-
16	D10	E	4003	-	-	1/7/7/7	-
17	PLM	C	501	-	-	3/11/11/15	-
17	PLM	C	505	-	-	5/15/15/15	-
17	PLM	E	4004	-	-	6/15/15/15	-
16	D10	B	1603	-	-	0/7/7/7	-
14	PGW	D	3902[A]	-	-	23/55/55/55	-
14	PGW	D	3902[B]	-	-	25/55/55/55	-
15	PX2	D	3908	-	-	8/37/37/37	-
16	D10	A	3705	-	-	1/7/7/7	-
15	PX2	D	3903	-	-	18/37/37/37	-
14	PGW	E	4005	-	-	18/36/36/55	-
12	HEX	B	1605	-	-	0/3/3/3	-
13	PIO	D	3901	-	-	12/44/68/68	0/1/1/1
17	PLM	A	3707	-	-	4/15/15/15	-
12	HEX	E	4008	-	-	0/3/3/3	-
15	PX2	C	502	-	-	20/37/37/37	-
19	ABU	E	4009	-	-	2/4/4/4	-
22	CLR	L	302	-	-	0/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	R16	E	4002	-	-	2/13/13/13	-
14	PGW	L	301	-	-	18/55/55/55	-
16	D10	D	3907	-	-	1/7/7/7	-
14	PGW	L	304	-	-	21/55/55/55	-
21	OLC	C	503	-	-	8/20/20/24	-
13	PIO	A	3702	-	-	11/44/68/68	0/1/1/1
17	PLM	D	3904	-	-	3/15/15/15	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	3901	PIO	P5-O5	3.37	1.65	1.59
13	A	3702	PIO	P5-O5	3.13	1.65	1.59
14	A	3703	PGW	O03-C19	3.04	1.42	1.33
21	C	503	OLC	O20-C1	3.02	1.42	1.33
13	D	3901	PIO	P4-O4	3.00	1.65	1.59
13	A	3702	PIO	P4-O4	2.99	1.65	1.59
14	L	304	PGW	O03-C19	2.91	1.41	1.33
14	E	4005	PGW	O03-C19	2.90	1.41	1.33
14	D	3902[B]	PGW	O03-C19	2.89	1.41	1.33
14	D	3902[A]	PGW	O03-C19	2.86	1.41	1.33
15	C	502	PX2	O5-C4	2.80	1.41	1.33
14	A	3703	PGW	O01-C1	2.78	1.42	1.34
14	L	304	PGW	O01-C1	2.73	1.42	1.34
14	D	3902[A]	PGW	O01-C1	2.71	1.42	1.34
14	D	3902[B]	PGW	O01-C1	2.69	1.41	1.34
14	E	4005	PGW	O01-C1	2.69	1.41	1.34
15	D	3903	PX2	O5-C4	2.64	1.41	1.33
15	A	3704	PX2	O5-C4	2.60	1.40	1.33
15	C	502	PX2	O7-C16	2.55	1.41	1.34
15	A	3704	PX2	O7-C2	-2.50	1.40	1.46
13	A	3702	PIO	O2C-C2C	-2.49	1.40	1.46
13	D	3901	PIO	O3C-C1B	2.43	1.40	1.33
15	D	3903	PX2	O7-C2	-2.42	1.40	1.46
13	A	3702	PIO	O3C-C1B	2.36	1.40	1.33
15	D	3903	PX2	O7-C16	2.35	1.40	1.34
15	A	3704	PX2	O7-C16	2.31	1.40	1.34
13	D	3901	PIO	O2C-C1A	2.21	1.40	1.34
13	A	3702	PIO	O2C-C1A	2.19	1.40	1.34
15	C	502	PX2	O7-C2	-2.17	1.41	1.46
13	A	3702	PIO	O3C-C3C	-2.17	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	3901	PIO	O3C-C3C	-2.08	1.40	1.45
13	D	3901	PIO	O2C-C2C	-2.07	1.41	1.46
14	E	4005	PGW	O01-C02	-2.07	1.41	1.46
15	A	3704	PX2	O5-C3	-2.06	1.40	1.45
14	D	3902[A]	PGW	O01-C02	-2.03	1.41	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	304	PGW	O01-C1-C2	4.30	120.77	111.50
13	D	3901	PIO	O2C-C1A-C2A	4.29	120.74	111.50
15	A	3704	PX2	O7-C16-C17	4.22	120.60	111.50
15	D	3903	PX2	O7-C16-C17	4.19	120.54	111.50
14	E	4005	PGW	O01-C1-C2	4.05	120.23	111.50
14	D	3902[B]	PGW	O01-C1-C2	3.99	120.10	111.50
14	D	3902[A]	PGW	O01-C1-C2	3.94	119.98	111.50
13	A	3702	PIO	O2C-C1A-C2A	3.93	119.97	111.50
14	A	3703	PGW	O01-C1-C2	3.80	119.69	111.50
21	C	503	OLC	C8-C9-C10	3.74	153.39	124.73
15	C	502	PX2	O7-C16-C17	3.71	119.50	111.50
15	C	502	PX2	O5-C4-C5	3.13	121.73	111.91
13	D	3901	PIO	O3C-C1B-C2B	2.88	120.95	111.91
14	A	3703	PGW	O03-C19-C20	2.81	120.72	111.91
13	A	3702	PIO	O3C-C1B-C2B	2.76	120.56	111.91
15	A	3704	PX2	O5-C4-C5	2.75	120.55	111.91
21	C	503	OLC	O20-C1-C2	2.67	120.29	111.91
14	E	4005	PGW	O03-C19-C20	2.57	119.98	111.91
14	D	3902[A]	PGW	O03-C19-C20	2.51	119.78	111.91
15	D	3903	PX2	O5-C4-C5	2.47	119.67	111.91
19	E	4009	ABU	CB-CG-C	-2.24	108.81	114.47
14	L	304	PGW	O03-C19-C20	2.21	118.86	111.91
19	B	1601	ABU	CB-CG-C	-2.17	109.01	114.47
14	D	3902[B]	PGW	O03-C19-C20	2.06	118.38	111.91
17	A	3707	PLM	O1-C1-C2	2.02	120.53	114.03

There are no chirality outliers.

All (283) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	3901	PIO	C2-C1-O1-P1
13	D	3901	PIO	C1-O1-P1-O11
13	D	3901	PIO	C5-O5-P5-O53

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Mol	Chain	Res	Type	Atoms
13	D	3901	PIO	O1A-C1A-O2C-C2C
14	A	3703	PGW	C03-O11-P-O12
14	A	3703	PGW	C03-O11-P-O13
14	A	3703	PGW	C03-O11-P-O14
14	A	3703	PGW	C04-O12-P-O11
14	A	3703	PGW	C04-O12-P-O13
14	A	3703	PGW	C04-O12-P-O14
14	A	3703	PGW	C2-C1-O01-C02
14	D	3902[A]	PGW	O12-C04-C05-CAD
14	D	3902[B]	PGW	C2-C1-O01-C02
14	E	4005	PGW	C04-C05-CAD-OAE
14	L	304	PGW	C2-C1-O01-C02
15	A	3704	PX2	C1-O4-P1-O1
15	A	3704	PX2	C1-O4-P1-O3
15	A	3704	PX2	C17-C16-O7-C2
15	C	502	PX2	C1-O4-P1-O1
15	C	502	PX2	C1-O4-P1-O2
15	C	502	PX2	C1-O4-P1-O3
15	D	3903	PX2	C1-O4-P1-O1
15	D	3903	PX2	C1-O4-P1-O2
15	D	3903	PX2	C1-O4-P1-O3
15	D	3903	PX2	C17-C16-O7-C2
15	A	3704	PX2	O6-C4-O5-C3
13	A	3702	PIO	O1B-C1B-O3C-C3C
14	L	301	PGW	O04-C19-O03-C01
15	C	502	PX2	O6-C4-O5-C3
14	A	3703	PGW	O02-C1-O01-C02
14	D	3902[B]	PGW	O02-C1-O01-C02
14	L	304	PGW	O02-C1-O01-C02
15	A	3704	PX2	O8-C16-O7-C2
15	D	3903	PX2	O8-C16-O7-C2
14	L	301	PGW	C20-C19-O03-C01
15	A	3704	PX2	C5-C4-O5-C3
15	C	502	PX2	C5-C4-O5-C3
13	D	3901	PIO	C2A-C1A-O2C-C2C
13	A	3702	PIO	C2B-C1B-O3C-C3C
14	E	4005	PGW	O02-C1-O01-C02
15	C	502	PX2	C2-C3-O5-C4
14	E	4005	PGW	C2-C1-O01-C02
14	L	304	PGW	O12-C04-C05-CAD
15	D	3903	PX2	C5-C4-O5-C3
15	A	3706	PX2	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	L	304	PGW	O12-C04-C05-OAF
15	D	3908	PX2	O7-C2-C3-O5
15	D	3903	PX2	O6-C4-O5-C3
15	A	3706	PX2	C17-C16-O7-C2
15	A	3704	PX2	C16-C17-C18-C19
14	E	4005	PGW	OAF-C05-CAD-OAE
14	L	304	PGW	C19-C20-C21-C22
14	D	3902[B]	PGW	C19-C20-C21-C22
15	D	3903	PX2	C16-C17-C18-C19
14	D	3902[A]	PGW	O12-C04-C05-OAF
14	L	301	PGW	C2-C1-O01-C02
14	L	304	PGW	C04-O12-P-O11
14	L	301	PGW	O02-C1-O01-C02
15	A	3706	PX2	O8-C16-O7-C2
14	D	3902[A]	PGW	C20-C19-O03-C01
13	D	3901	PIO	C1-O1-P1-O13
14	D	3902[A]	PGW	C27-C15-C16-C17
15	C	502	PX2	C21-C22-C23-C24
15	D	3903	PX2	C11-C10-C9-C8
14	A	3703	PGW	C2-C3-C4-C5
14	D	3902[B]	PGW	C2-C3-C4-C5
14	A	3703	PGW	C05-C04-O12-P
14	A	3703	PGW	C27-C15-C16-C17
14	D	3902[B]	PGW	C08-C09-C11-C12
17	C	505	PLM	C3-C4-C5-C6
15	A	3704	PX2	C5-C6-C7-C8
15	A	3704	PX2	C11-C10-C9-C8
16	E	4003	D10	C6-C7-C8-C9
14	D	3902[B]	PGW	C24-C25-C26-C27
15	C	502	PX2	C10-C11-C12-C13
15	C	502	PX2	C16-C17-C18-C19
14	D	3902[A]	PGW	C23-C24-C25-C26
14	L	304	PGW	C06-C07-C08-C09
15	C	502	PX2	C11-C10-C9-C8
14	A	3703	PGW	C08-C09-C11-C12
14	D	3902[B]	PGW	C04-C05-CAD-OAE
21	C	503	OLC	C21-C22-C24-O25
14	A	3703	PGW	C06-C07-C08-C09
14	L	304	PGW	C16-C15-C27-C26
17	A	3707	PLM	CC-CD-CE-CF
17	B	1606	PLM	CB-CC-CD-CE
15	A	3704	PX2	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	D	3902[B]	PGW	C16-C15-C27-C26
14	D	3902[A]	PGW	C17-C18-C28-C30
20	B	1607	R16	C36-C37-C38-C39
15	A	3704	PX2	C20-C21-C22-C23
13	A	3702	PIO	C2A-C1A-O2C-C2C
14	D	3902[A]	PGW	C08-C09-C11-C12
17	B	1606	PLM	C2-C3-C4-C5
14	D	3902[B]	PGW	C6-C7-C8-C9
14	A	3703	PGW	C5-C6-C7-C8
14	A	3703	PGW	C16-C15-C27-C26
14	D	3902[A]	PGW	O04-C19-O03-C01
15	C	502	PX2	C5-C6-C7-C8
15	C	502	PX2	O8-C16-O7-C2
15	D	3903	PX2	C2-C1-O4-P1
14	D	3902[A]	PGW	C2-C1-O01-C02
15	C	502	PX2	C17-C16-O7-C2
14	D	3902[A]	PGW	C6-C7-C8-C9
14	L	301	PGW	C6-C7-C8-C9
13	A	3702	PIO	O1A-C1A-O2C-C2C
21	C	503	OLC	C2-C1-O20-C21
14	D	3902[A]	PGW	C4-C5-C6-C7
14	D	3902[B]	PGW	C07-C08-C09-C11
17	D	3904	PLM	C7-C8-C9-CA
15	D	3908	PX2	C18-C19-C20-C21
17	E	4007	PLM	CB-CC-CD-CE
14	D	3902[A]	PGW	C1-C2-C3-C4
14	L	304	PGW	C17-C18-C28-C30
17	B	1606	PLM	C4-C5-C6-C7
14	E	4005	PGW	C03-O11-P-O12
14	L	304	PGW	C20-C21-C22-C23
14	L	304	PGW	C2-C3-C4-C5
14	D	3902[B]	PGW	C01-C02-C03-O11
14	D	3902[A]	PGW	O02-C1-O01-C02
17	C	504	PLM	C7-C8-C9-CA
17	D	3904	PLM	C4-C5-C6-C7
15	D	3908	PX2	C1-C2-C3-O5
17	C	504	PLM	CC-CD-CE-CF
15	D	3908	PX2	O5-C4-C5-C6
21	C	503	OLC	O19-C1-O20-C21
15	D	3903	PX2	C6-C7-C8-C9
21	C	503	OLC	O23-C22-C24-O25
17	E	4004	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
15	A	3704	PX2	C1-O4-P1-O2
14	E	4005	PGW	O03-C01-C02-O01
14	A	3703	PGW	C24-C25-C26-C27
13	D	3901	PIO	C6-C1-O1-P1
15	D	3903	PX2	C10-C11-C12-C13
15	A	3704	PX2	C21-C22-C23-C24
17	C	501	PLM	C3-C4-C5-C6
15	A	3706	PX2	C5-C4-O5-C3
15	A	3706	PX2	C20-C21-C22-C23
20	E	4002	R16	C33-C34-C35-C36
14	D	3902[B]	PGW	C27-C15-C16-C17
14	D	3902[B]	PGW	C17-C18-C28-C30
14	E	4005	PGW	C2-C3-C4-C5
14	D	3902[B]	PGW	C4-C5-C6-C7
13	A	3702	PIO	C1-O1-P1-O12
13	D	3901	PIO	C1-O1-P1-O12
15	A	3706	PX2	C11-C10-C9-C8
14	D	3902[B]	PGW	C04-O12-P-O11
14	L	304	PGW	C23-C24-C25-C26
14	D	3902[B]	PGW	O01-C02-C03-O11
14	D	3902[B]	PGW	C06-C07-C08-C09
16	A	3705	D10	C2-C3-C4-C5
14	L	301	PGW	C09-C11-C12-C13
14	E	4005	PGW	C23-C24-C25-C26
21	C	503	OLC	C6-C7-C8-C9
14	D	3902[A]	PGW	C2-C3-C4-C5
15	C	502	PX2	C24-C25-C26-C27
14	L	301	PGW	C7-C8-C9-C10
17	B	1606	PLM	C7-C8-C9-CA
17	C	504	PLM	C3-C4-C5-C6
13	D	3901	PIO	C1C-C2C-O2C-C1A
14	A	3703	PGW	C03-C02-O01-C1
14	L	304	PGW	C03-C02-O01-C1
15	D	3908	PX2	C5-C4-O5-C3
14	E	4005	PGW	O03-C01-C02-C03
15	D	3908	PX2	O7-C16-C17-C18
17	A	3707	PLM	C2-C3-C4-C5
16	D	3907	D10	C7-C8-C9-C10
15	A	3706	PX2	O6-C4-O5-C3
17	B	1606	PLM	C8-C9-CA-CB
17	D	3904	PLM	C6-C7-C8-C9
21	C	503	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
17	C	505	PLM	C9-CA-CB-CC
14	D	3902[B]	PGW	C15-C16-C17-C18
13	A	3702	PIO	C1-O1-P1-O13
15	D	3903	PX2	C21-C22-C23-C24
14	E	4005	PGW	C03-O11-P-O13
14	L	304	PGW	C04-O12-P-O14
17	B	1606	PLM	C6-C7-C8-C9
14	L	304	PGW	C20-C19-O03-C01
14	D	3902[A]	PGW	C07-C06-C10-C9
14	D	3902[A]	PGW	C3-C4-C5-C6
13	D	3901	PIO	C1C-C2C-C3C-O3C
13	D	3901	PIO	O2C-C2C-C3C-O3C
17	B	1606	PLM	CA-CB-CC-CD
14	L	304	PGW	O04-C19-O03-C01
15	D	3908	PX2	O6-C4-O5-C3
17	E	4004	PLM	C4-C5-C6-C7
17	E	4007	PLM	C6-C7-C8-C9
14	D	3902[A]	PGW	C7-C8-C9-C10
14	L	301	PGW	C01-C02-O01-C1
14	D	3902[A]	PGW	C21-C22-C23-C24
14	E	4005	PGW	C1-C2-C3-C4
14	E	4005	PGW	C04-O12-P-O11
14	L	301	PGW	C04-O12-P-O11
14	A	3703	PGW	O03-C01-C02-C03
14	L	301	PGW	C20-C21-C22-C23
15	D	3903	PX2	C20-C21-C22-C23
14	L	304	PGW	C09-C11-C12-C13
17	E	4007	PLM	C5-C6-C7-C8
14	D	3902[A]	PGW	O01-C02-C03-O11
12	B	1604	HEX	C1-C2-C3-C4
17	E	4007	PLM	C7-C8-C9-CA
14	A	3703	PGW	C17-C18-C28-C30
14	D	3902[B]	PGW	C07-C06-C10-C9
17	C	504	PLM	O1-C1-C2-C3
15	C	502	PX2	C4-C5-C6-C7
17	E	4004	PLM	C5-C6-C7-C8
14	A	3703	PGW	C3-C4-C5-C6
14	L	304	PGW	C07-C06-C10-C9
13	D	3901	PIO	C2A-C3A-C4A-C5A
20	E	4002	R16	C35-C36-C37-C38
13	A	3702	PIO	C1-O1-P1-O11
14	D	3902[A]	PGW	C20-C21-C22-C23

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
15	A	3704	PX2	C6-C7-C8-C9
14	D	3902[B]	PGW	C7-C8-C9-C10
17	C	504	PLM	O2-C1-C2-C3
13	A	3702	PIO	O2C-C2C-C3C-O3C
17	E	4007	PLM	CA-CB-CC-CD
15	D	3908	PX2	O6-C4-C5-C6
17	C	505	PLM	O1-C1-C2-C3
17	E	4007	PLM	O1-C1-C2-C3
14	A	3703	PGW	O03-C19-C20-C21
14	L	301	PGW	C05-C04-O12-P
15	A	3704	PX2	C23-C24-C25-C26
14	A	3703	PGW	C18-C28-C30-C29
17	C	505	PLM	O2-C1-C2-C3
17	E	4007	PLM	O2-C1-C2-C3
15	A	3704	PX2	C9-C10-C11-C12
17	C	501	PLM	O1-C1-C2-C3
17	C	501	PLM	O2-C1-C2-C3
14	E	4005	PGW	C3-C4-C5-C6
21	C	503	OLC	C9-C10-C11-C12
21	C	503	OLC	C7-C8-C9-C10
15	D	3903	PX2	C9-C10-C11-C12
19	E	4009	ABU	OXT-C-CG-CB
15	D	3903	PX2	O7-C16-C17-C18
17	E	4004	PLM	O2-C1-C2-C3
19	E	4009	ABU	O-C-CG-CB
17	B	1606	PLM	O2-C1-C2-C3
15	D	3903	PX2	C5-C6-C7-C8
17	A	3707	PLM	O2-C1-C2-C3
14	E	4005	PGW	O03-C19-C20-C21
15	A	3704	PX2	O5-C4-C5-C6
14	D	3902[A]	PGW	C01-C02-C03-O11
14	E	4005	PGW	C01-C02-C03-O11
15	C	502	PX2	O7-C16-C17-C18
17	E	4004	PLM	O1-C1-C2-C3
14	L	304	PGW	C7-C8-C9-C10
17	B	1606	PLM	O1-C1-C2-C3
13	A	3702	PIO	C5-O5-P5-O52
14	D	3902[B]	PGW	C20-C19-O03-C01
14	L	301	PGW	C07-C08-C09-C11
14	L	304	PGW	C22-C23-C24-C25
17	C	505	PLM	C4-C5-C6-C7
14	E	4005	PGW	O04-C19-C20-C21

*Continued on next page...*

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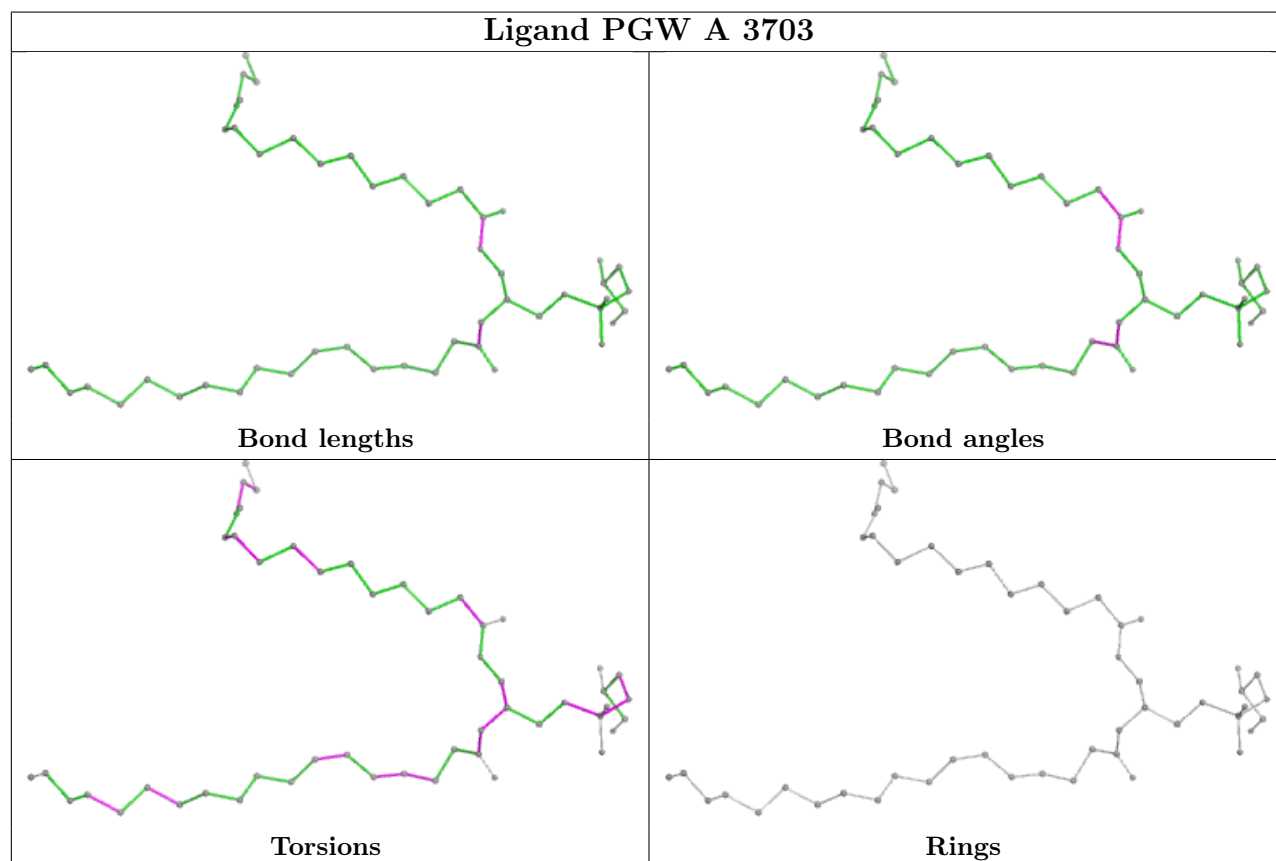
Mol	Chain	Res	Type	Atoms
15	C	502	PX2	O8-C16-C17-C18
15	C	502	PX2	O5-C4-C5-C6
17	E	4004	PLM	C6-C7-C8-C9
14	D	3902[B]	PGW	C04-O12-P-O13
14	E	4005	PGW	C04-O12-P-O14
14	L	301	PGW	C03-O11-P-O14
14	L	301	PGW	C04-O12-P-O14
14	L	304	PGW	C04-O12-P-O13
15	A	3704	PX2	O6-C4-C5-C6
15	D	3903	PX2	O8-C16-C17-C18
17	A	3707	PLM	O1-C1-C2-C3
14	D	3902[B]	PGW	O04-C19-O03-C01
15	C	502	PX2	C6-C7-C8-C9
12	D	3905	HEX	C1-C2-C3-C4
14	L	301	PGW	C11-C12-C13-C14
14	D	3902[A]	PGW	O01-C1-C2-C3
14	D	3902[B]	PGW	O03-C19-C20-C21
17	C	504	PLM	CA-CB-CC-CD
13	A	3702	PIO	O13-C1C-C2C-O2C
14	E	4005	PGW	O01-C02-C03-O11
13	A	3702	PIO	O3C-C1B-C2B-C3B
14	L	301	PGW	O01-C1-C2-C3
14	L	301	PGW	C2-C3-C4-C5
14	D	3902[A]	PGW	O02-C1-C2-C3
15	C	502	PX2	O6-C4-C5-C6
14	D	3902[B]	PGW	O01-C1-C2-C3
17	B	1606	PLM	C3-C4-C5-C6
14	L	301	PGW	O03-C19-C20-C21

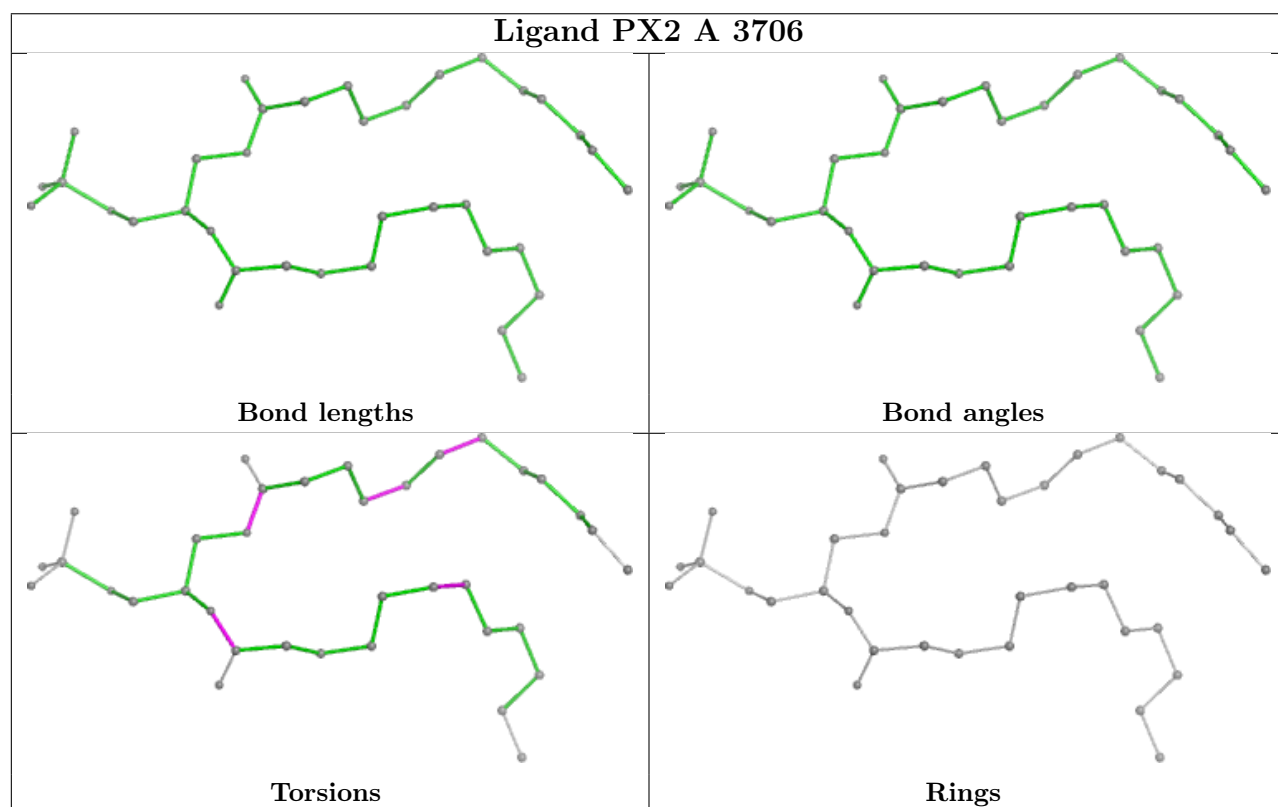
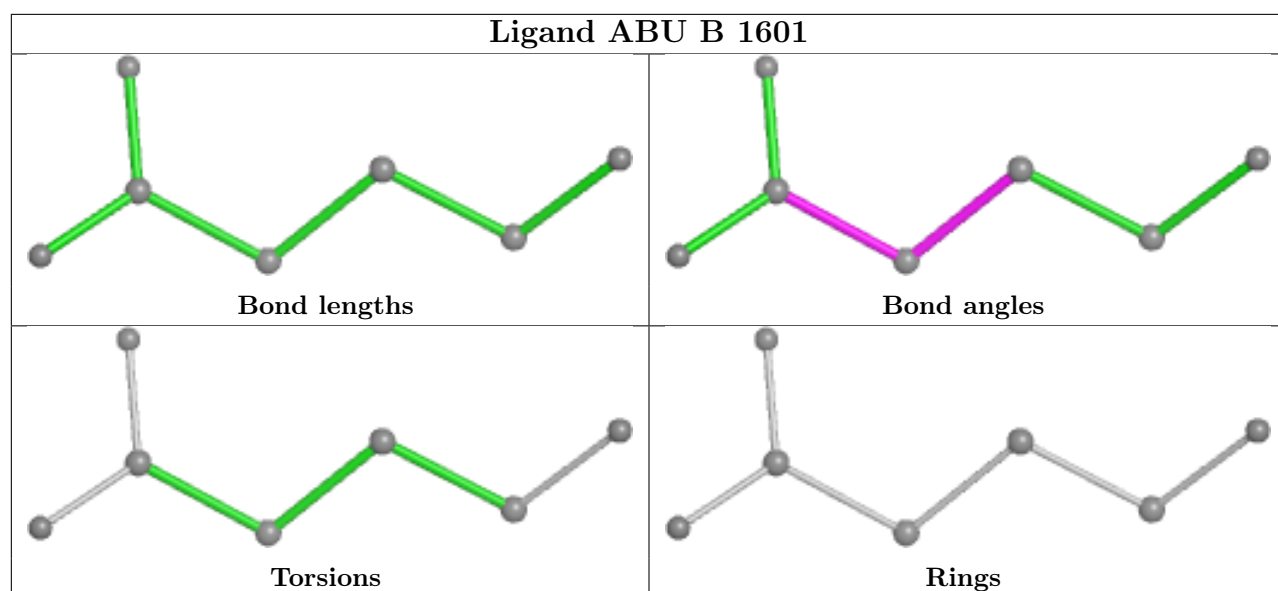
There are no ring outliers.

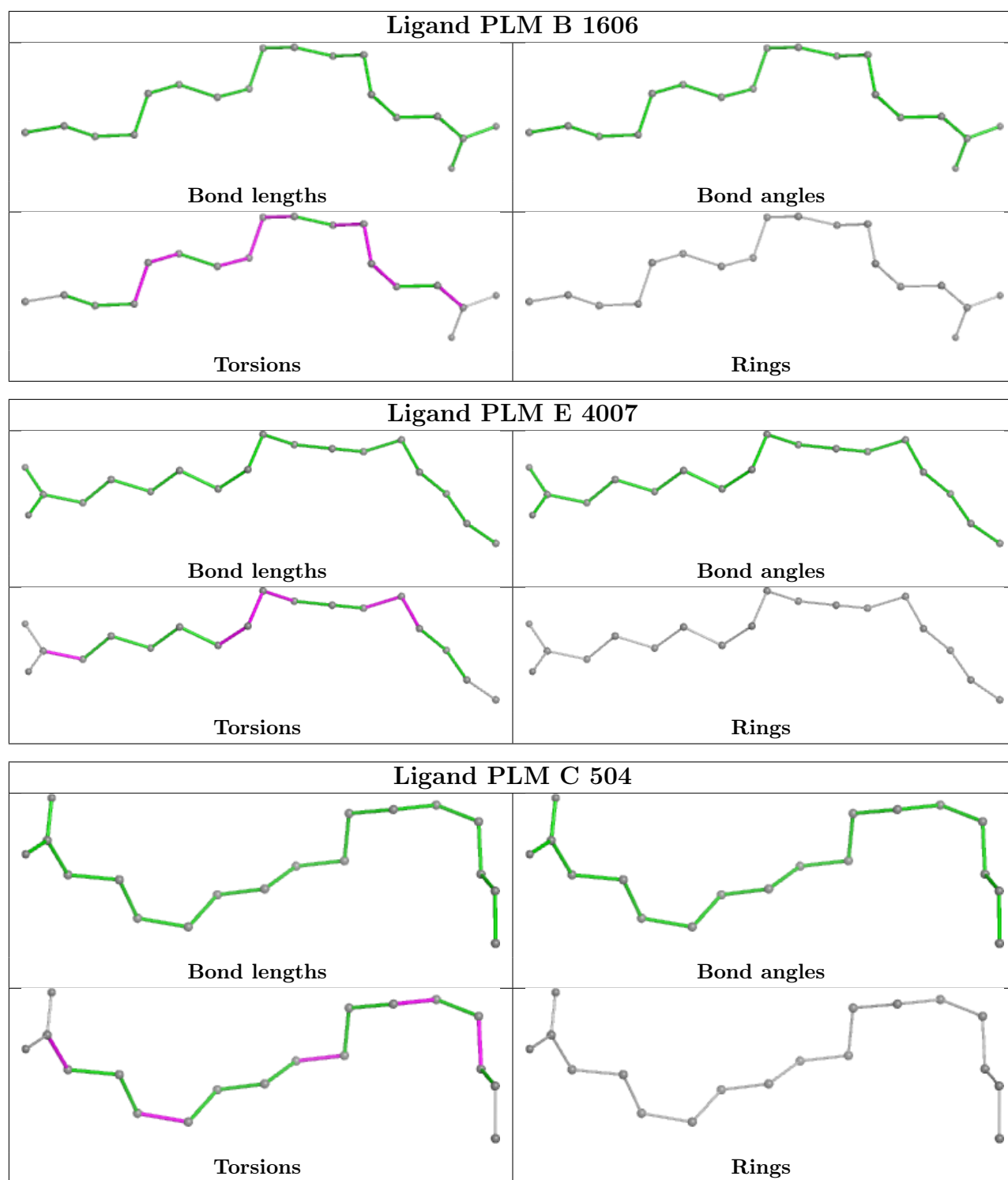
9 monomers are involved in 29 short contacts:

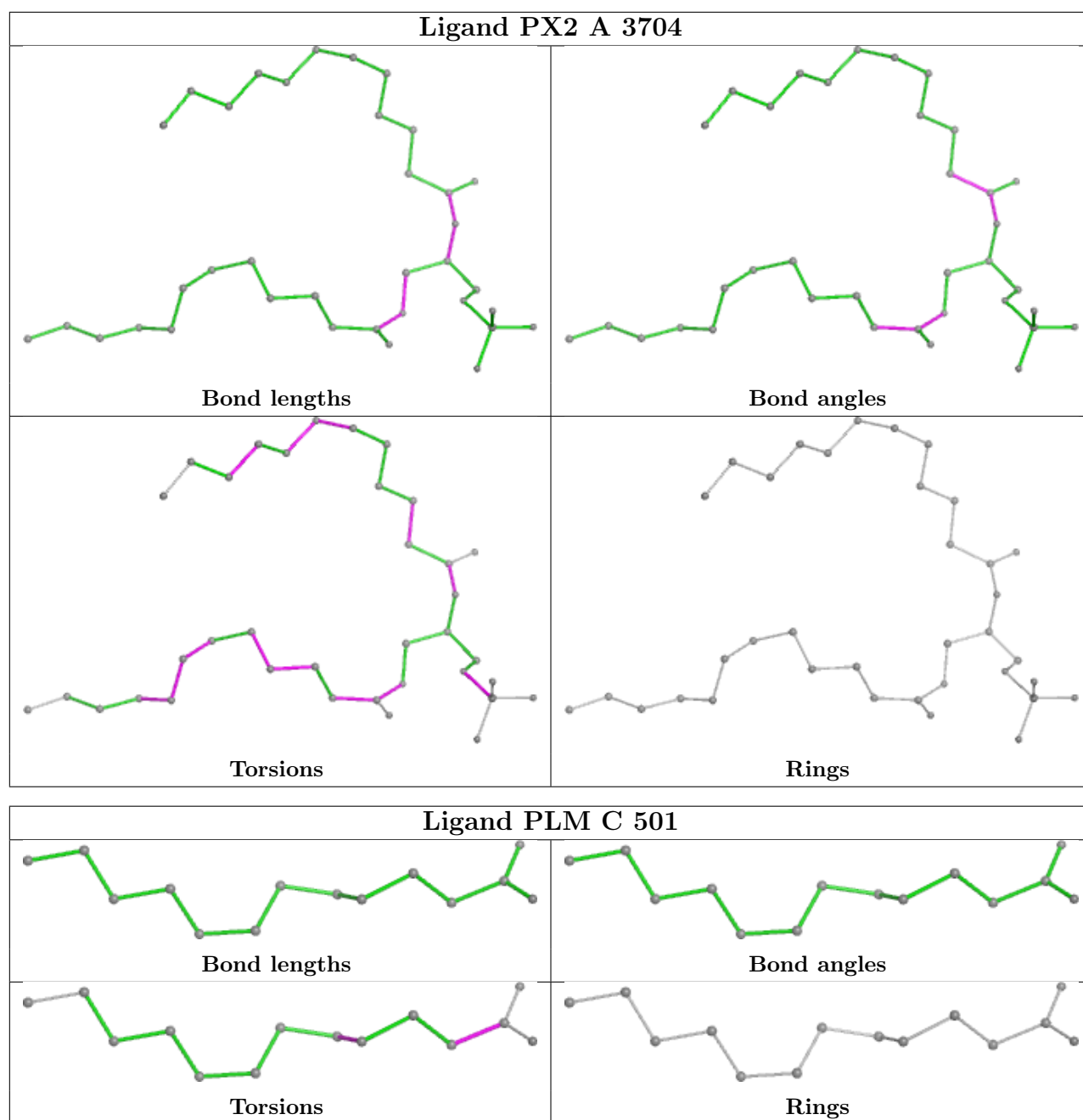
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	3706	PX2	7	0
17	C	501	PLM	1	0
15	D	3908	PX2	3	0
13	D	3901	PIO	4	0
19	E	4009	ABU	1	0
22	L	302	CLR	2	0
14	L	301	PGW	8	0
14	L	304	PGW	1	0
13	A	3702	PIO	3	0

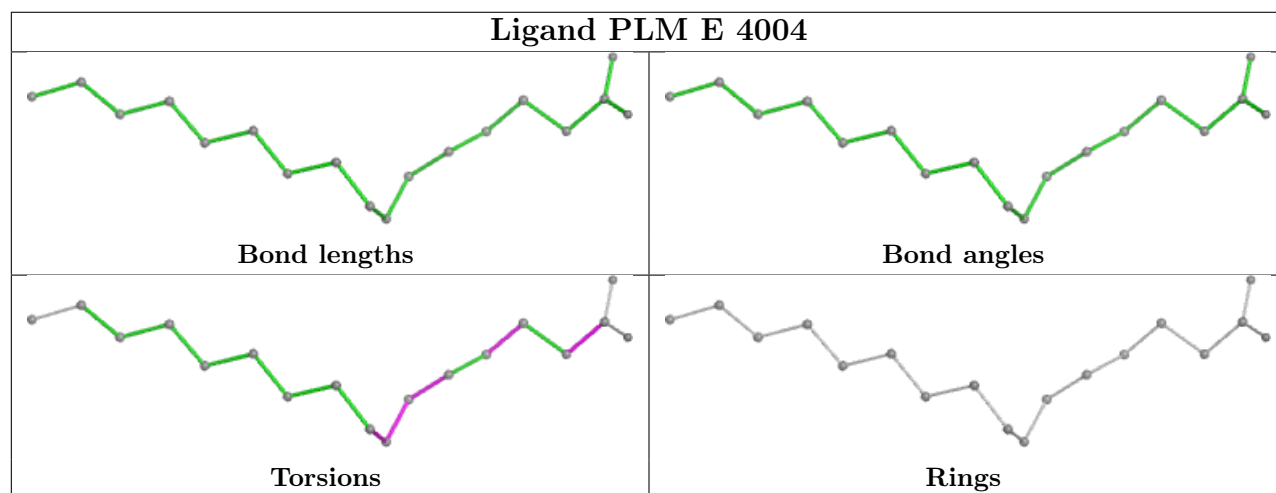
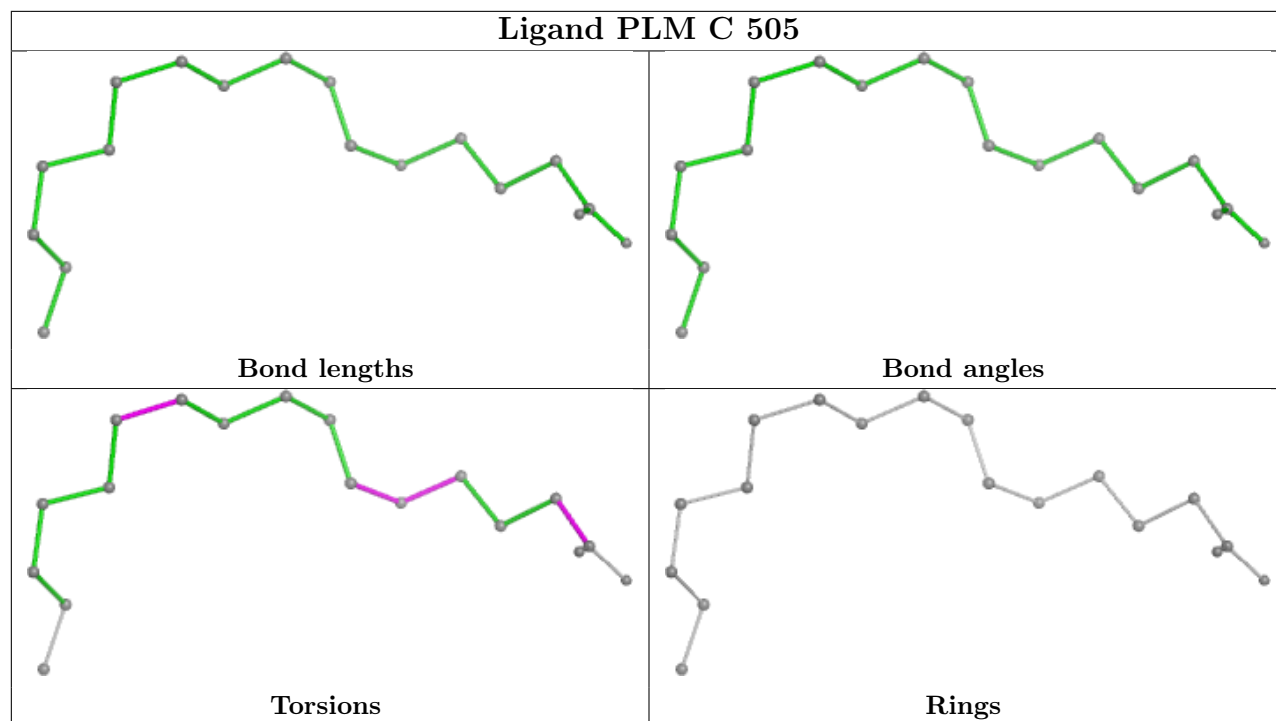
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





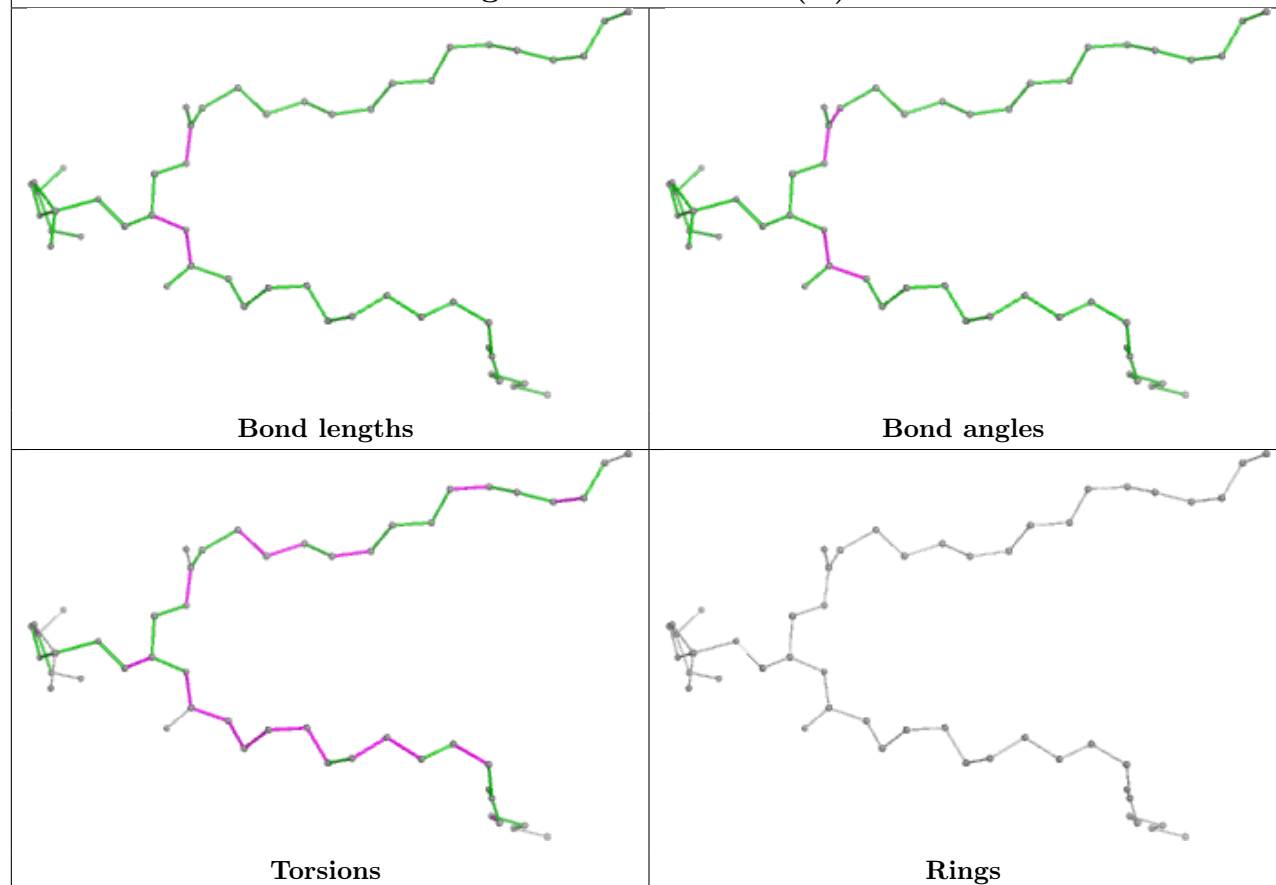




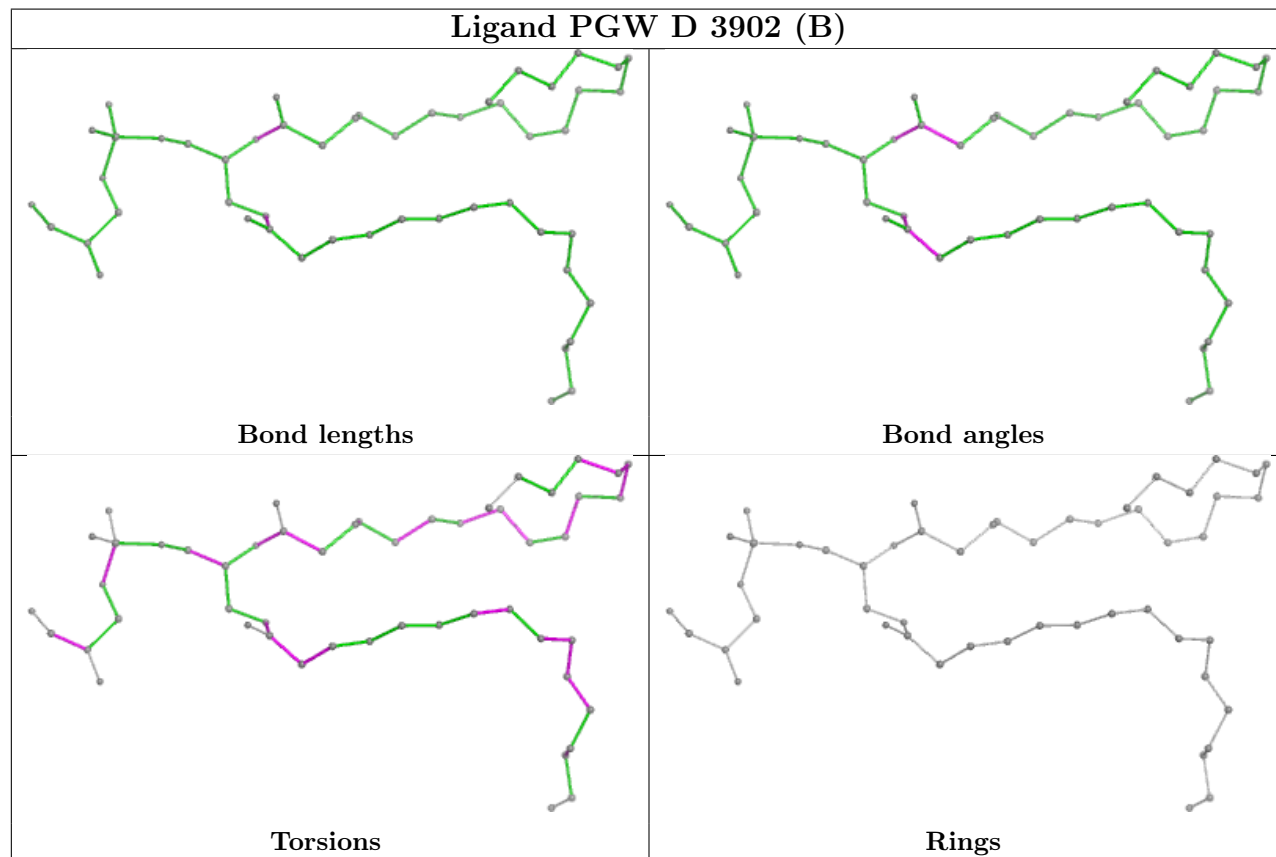


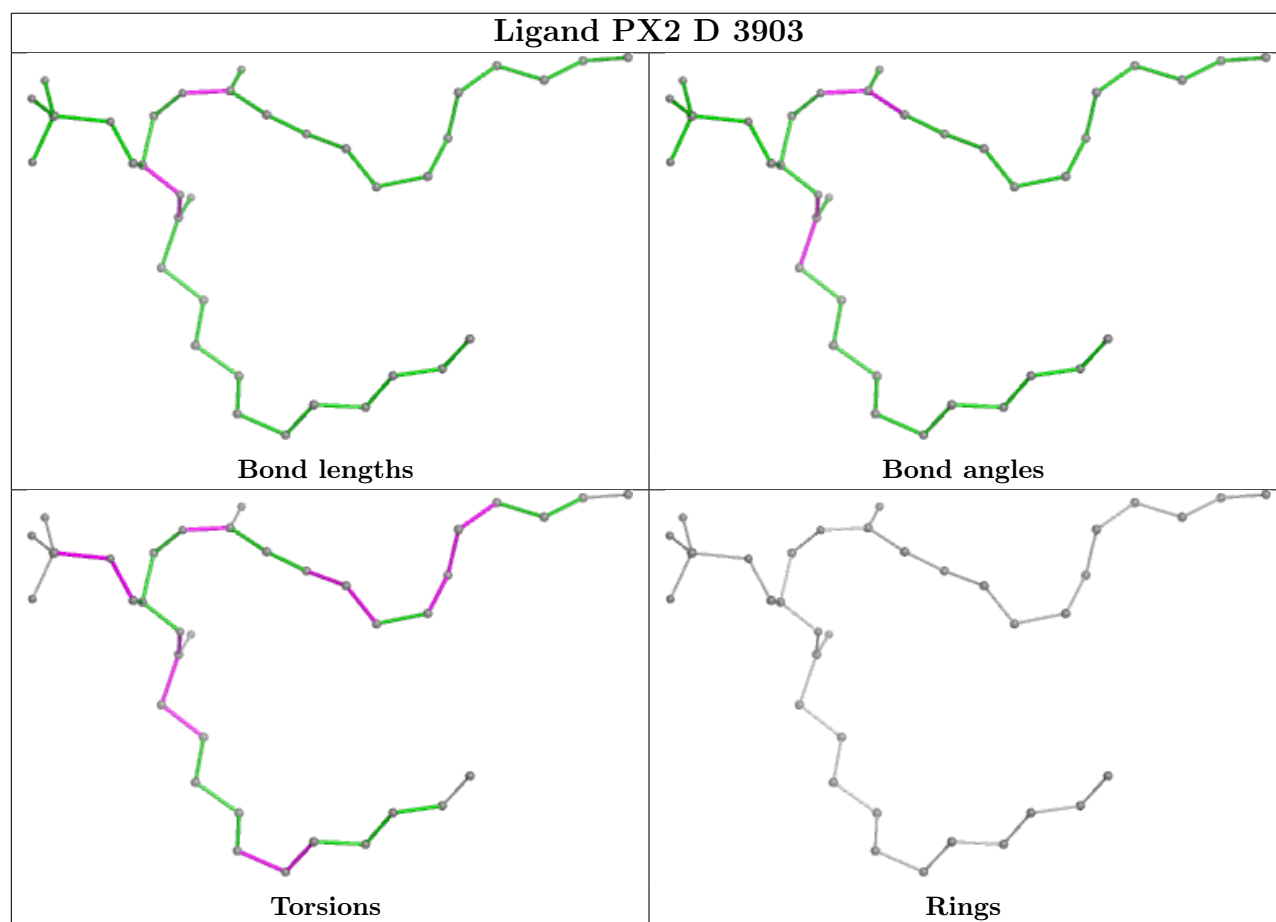
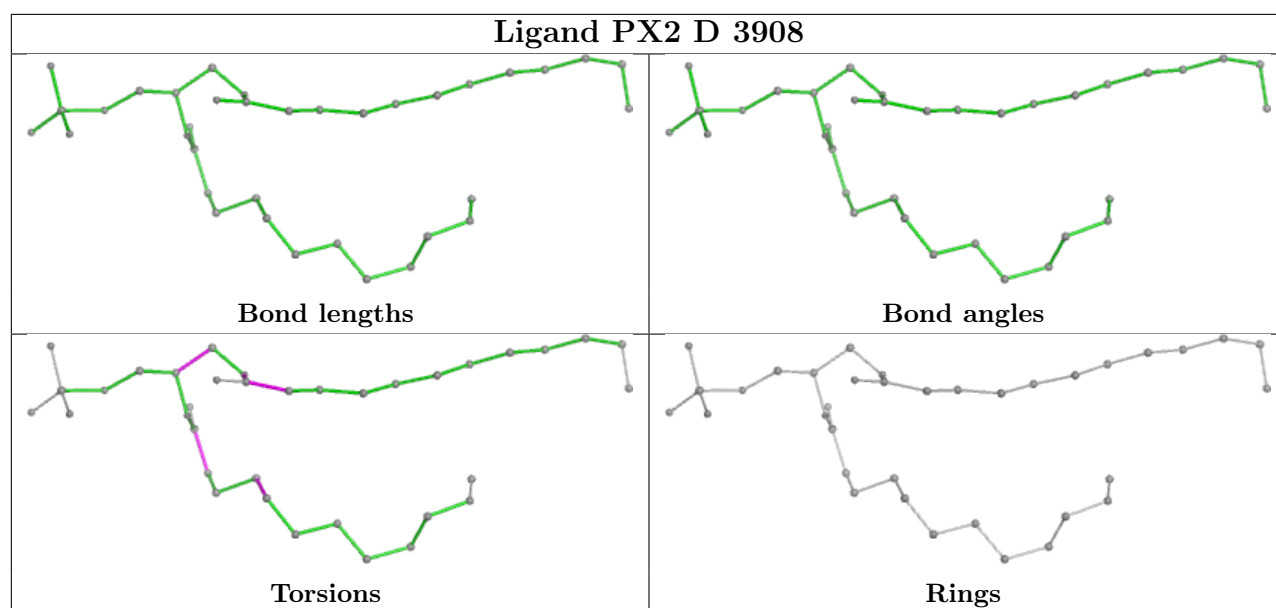


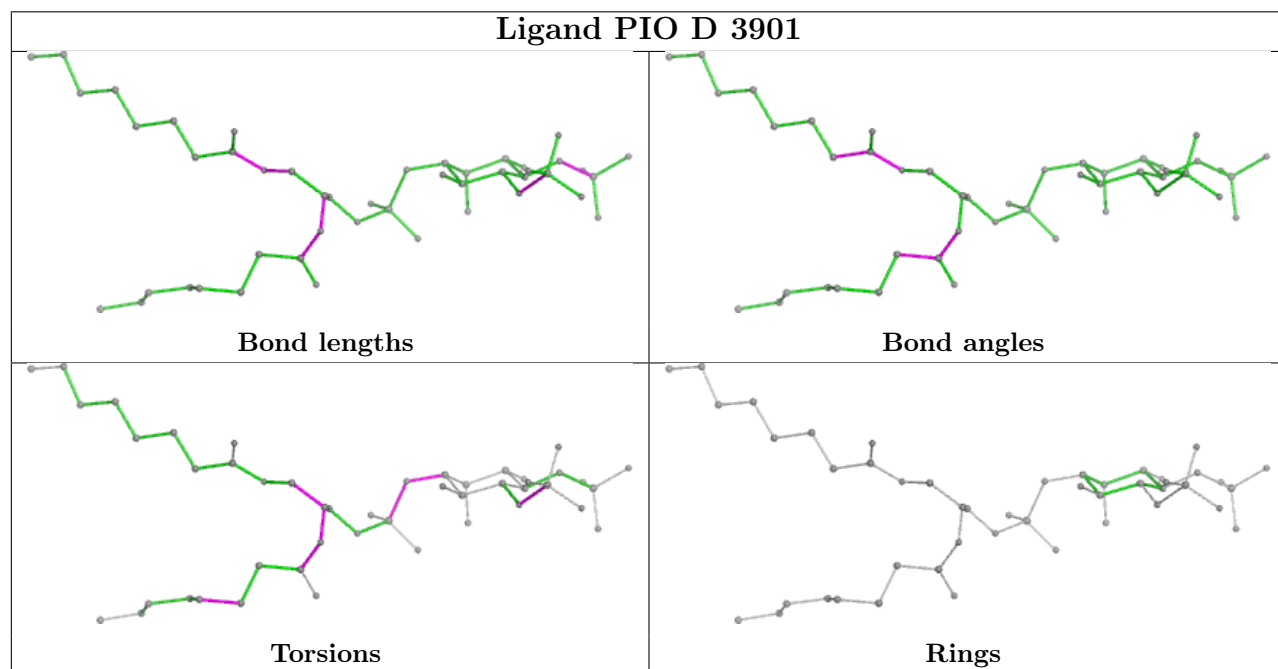
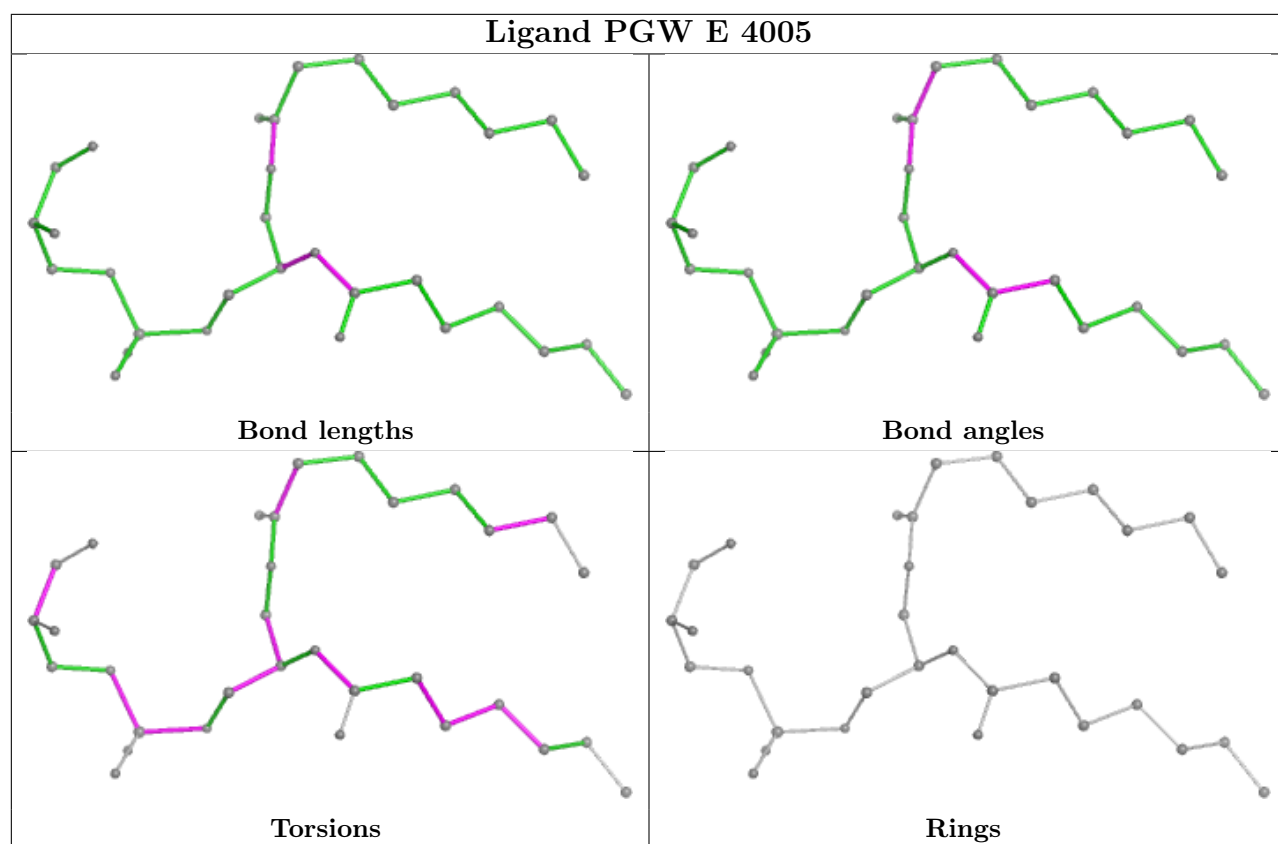
## Ligand PGW D 3902 (A)

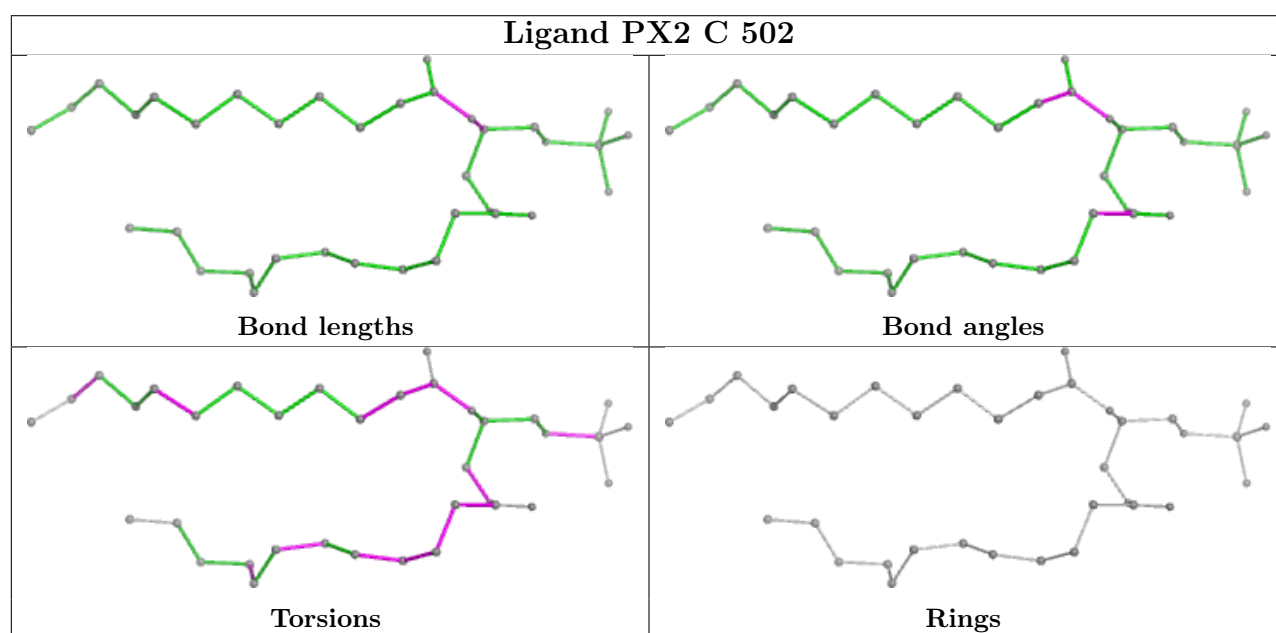
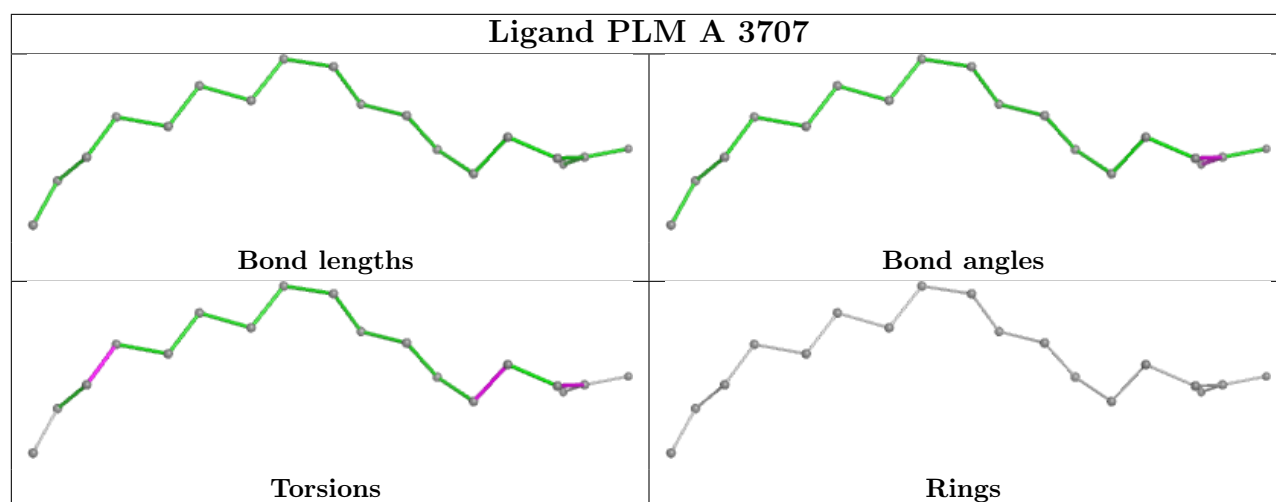


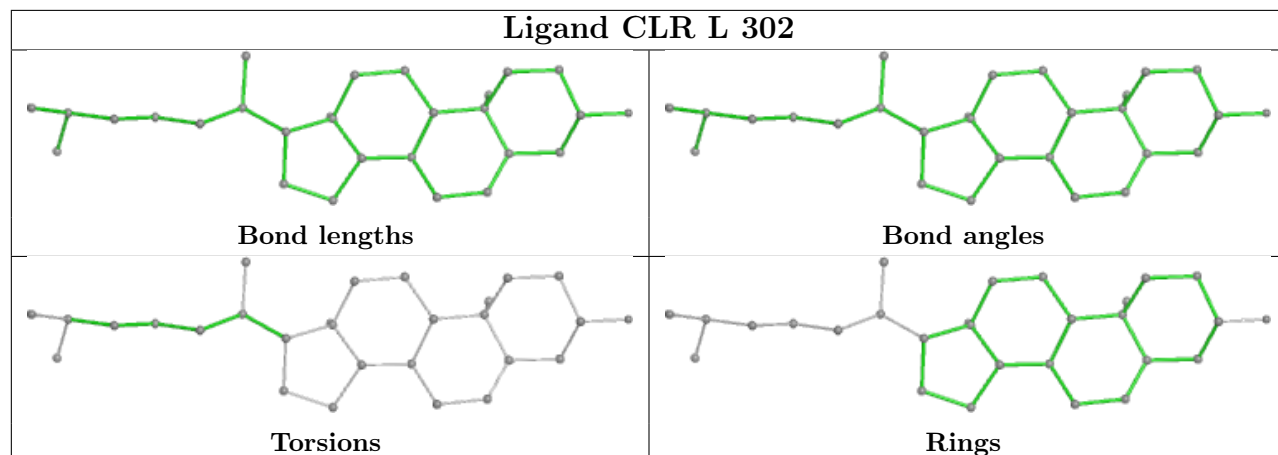
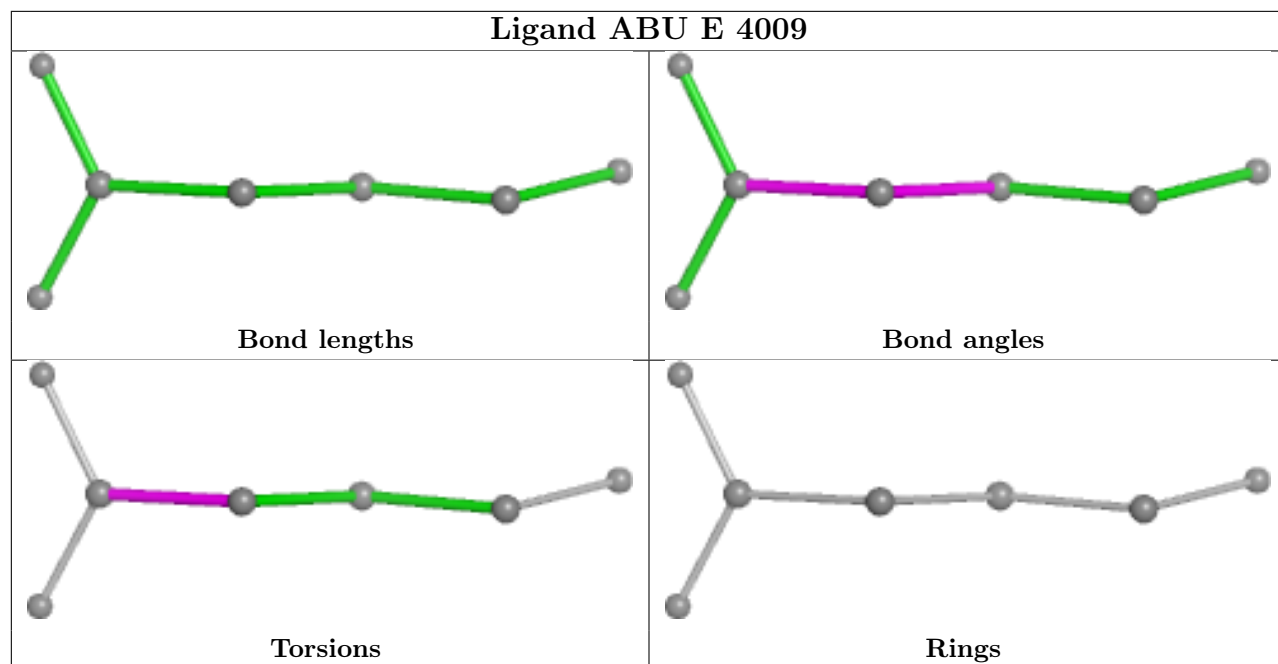
## Ligand PGW D 3902 (B)

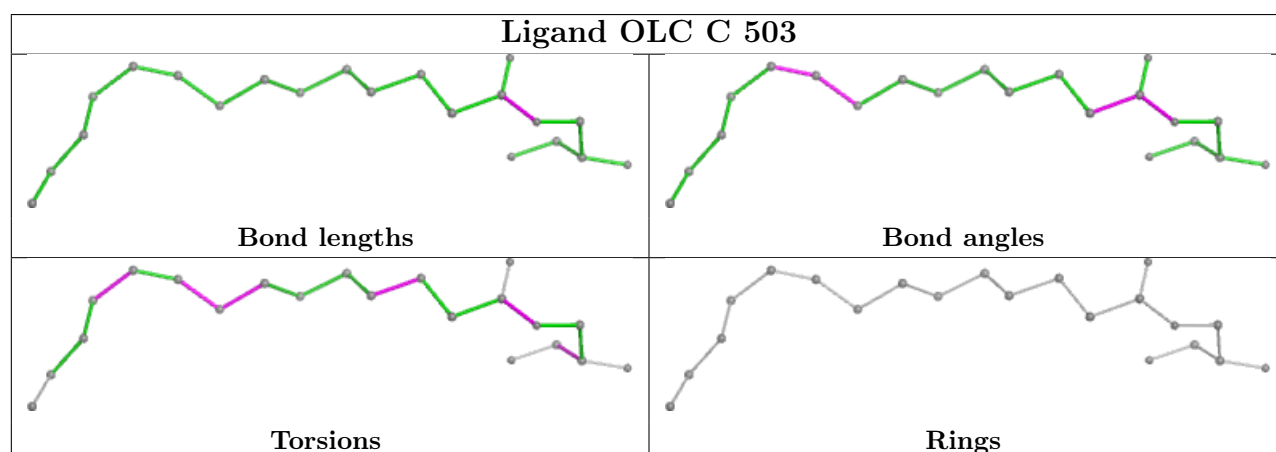
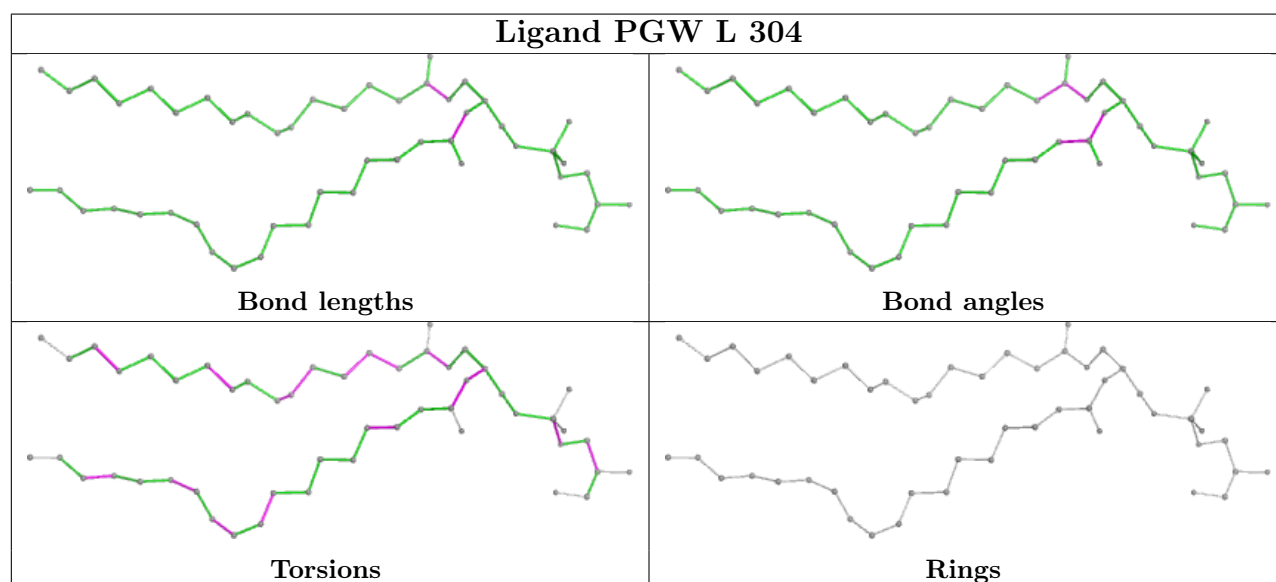
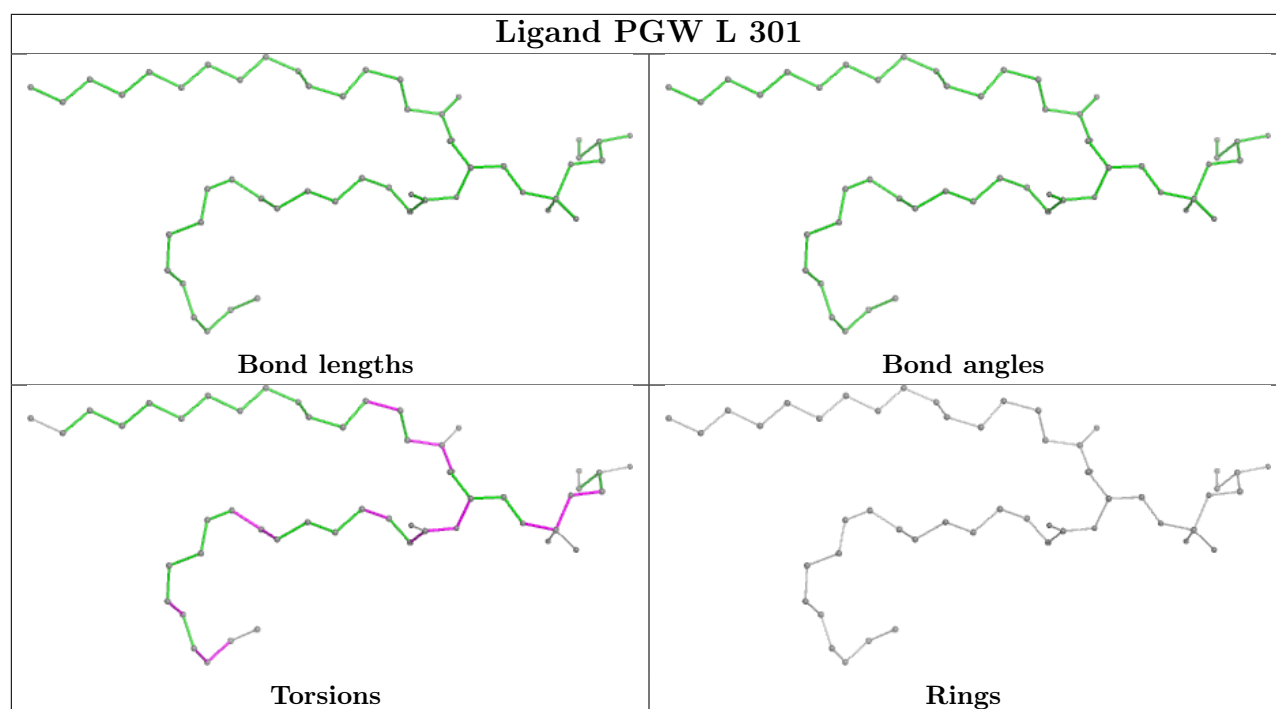


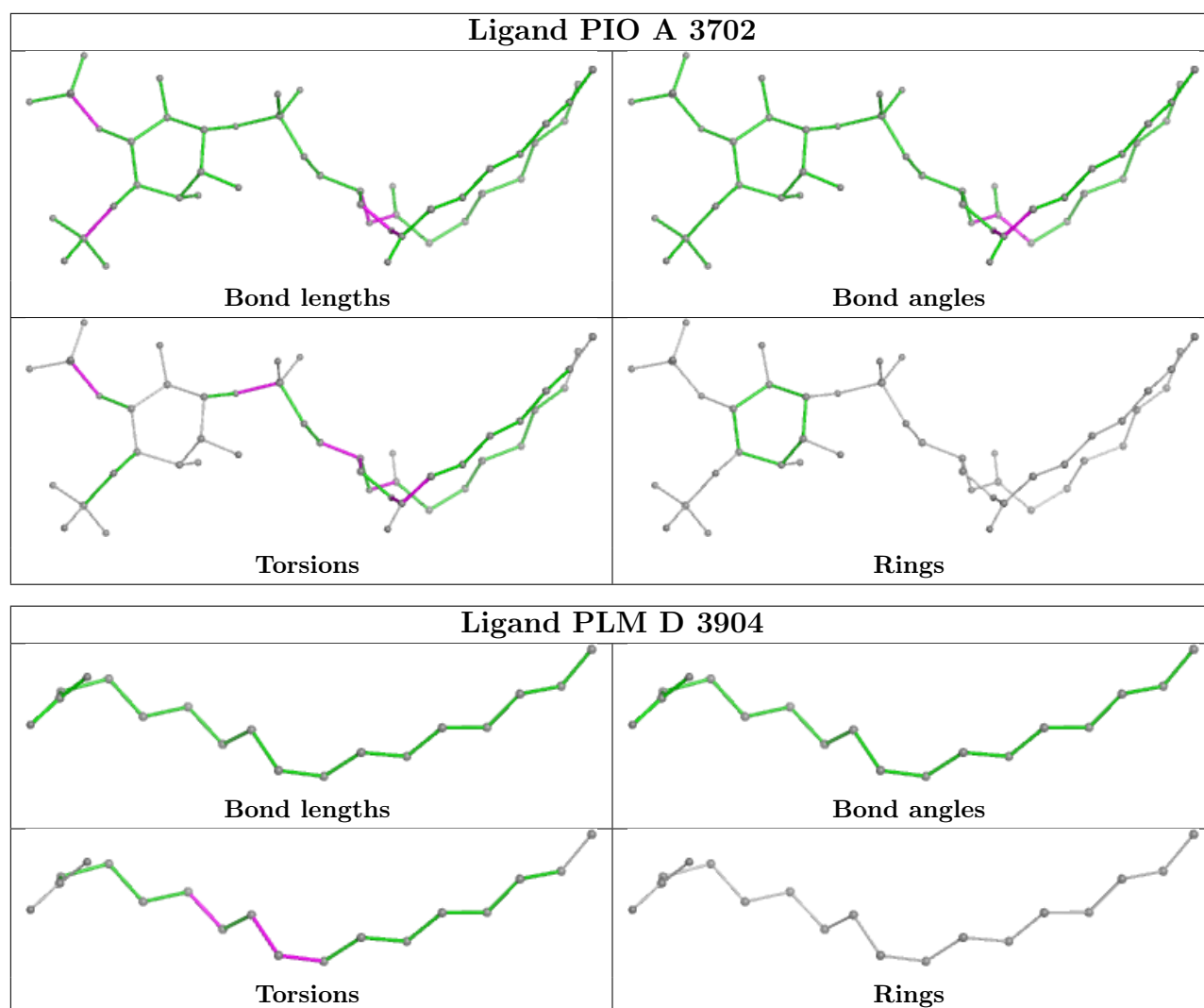












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

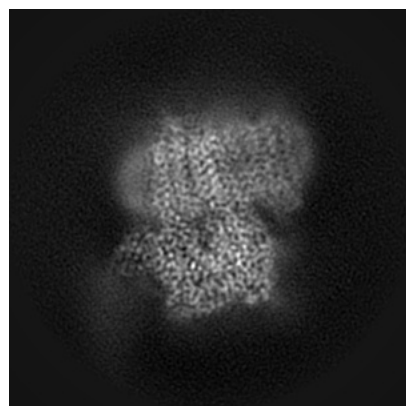
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50274. These allow visual inspection of the internal detail of the map and identification of artifacts.

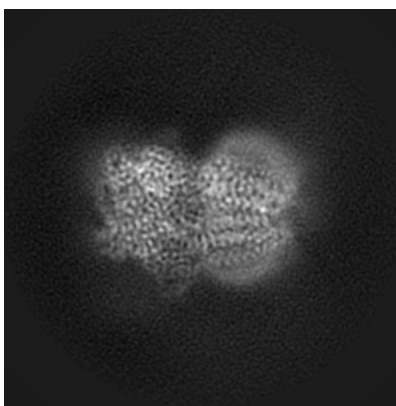
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

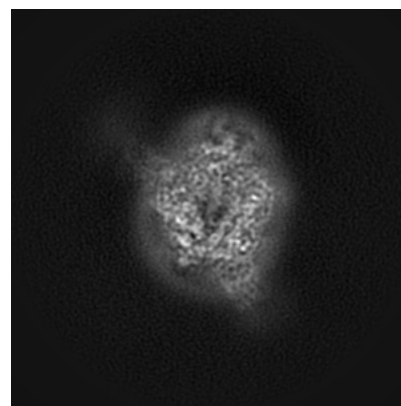
#### 6.1.1 Primary map



X

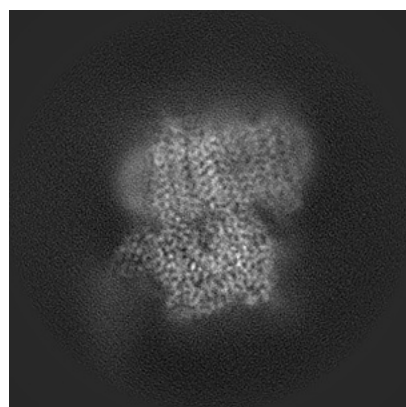


Y

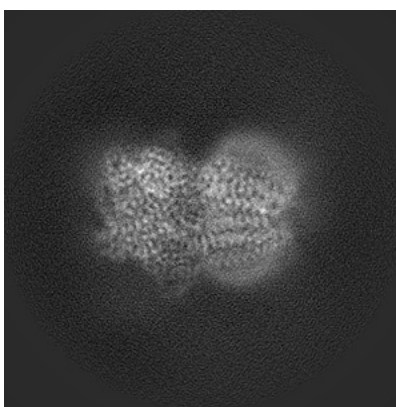


Z

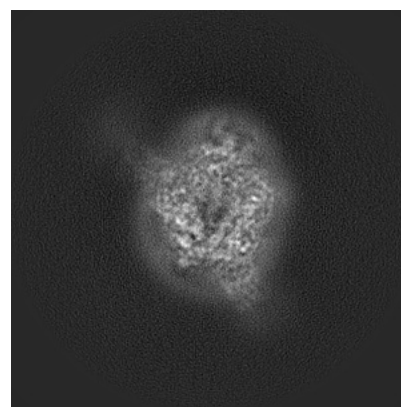
#### 6.1.2 Raw map



X



Y



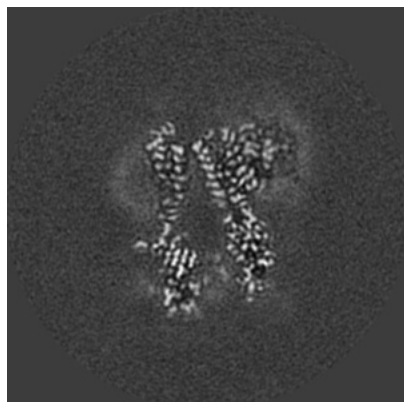
Z

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

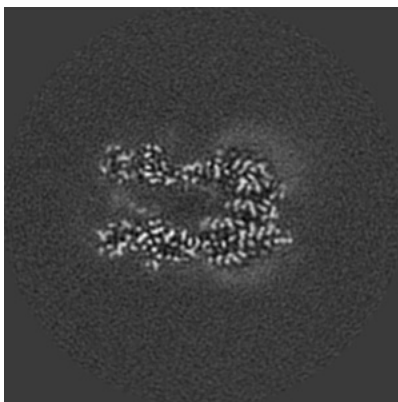


## 6.2 Central slices [i](#)

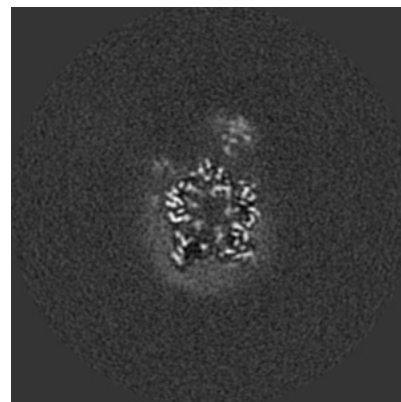
### 6.2.1 Primary map



X Index: 148

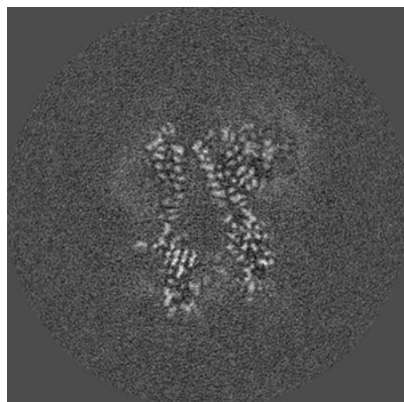


Y Index: 148

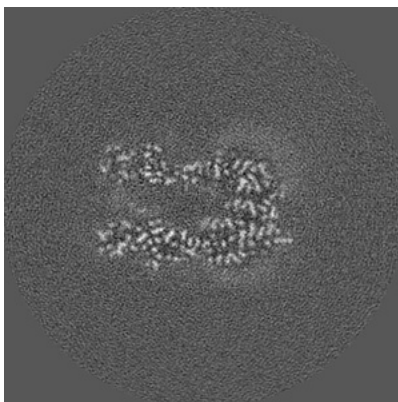


Z Index: 148

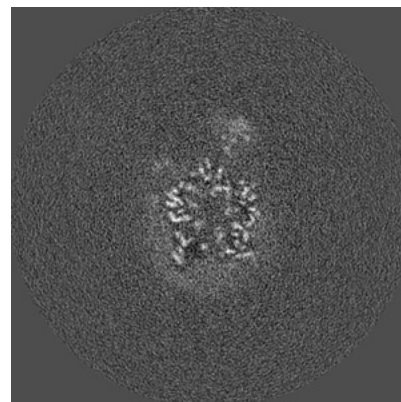
### 6.2.2 Raw map



X Index: 148



Y Index: 148

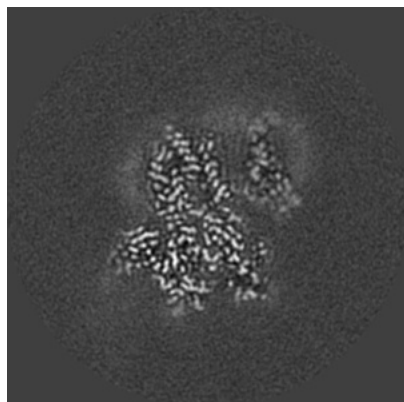


Z Index: 148

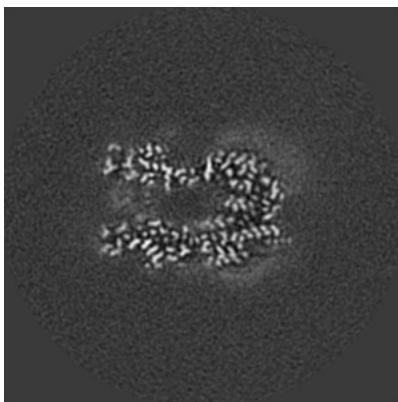
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

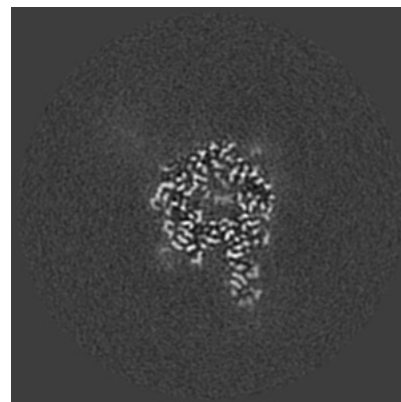
### 6.3.1 Primary map



X Index: 167

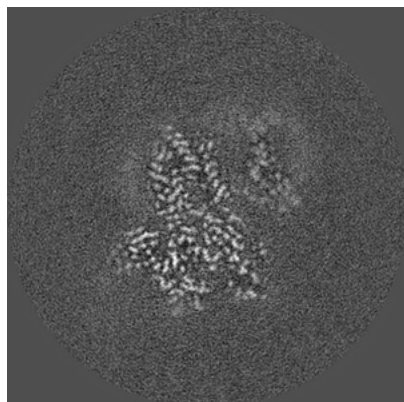


Y Index: 150

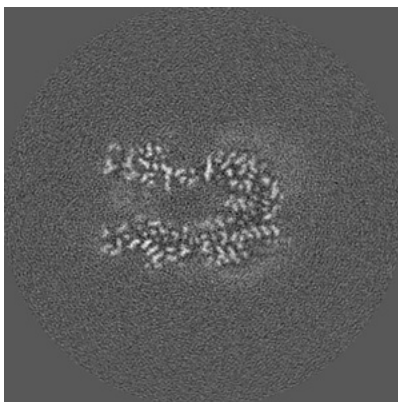


Z Index: 105

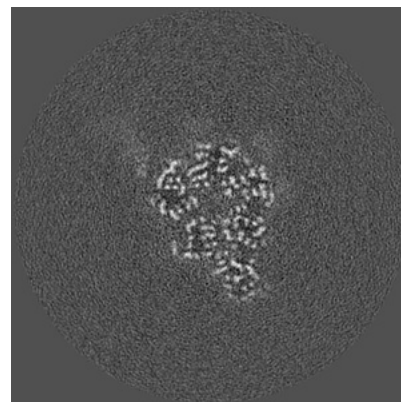
### 6.3.2 Raw map



X Index: 167



Y Index: 150

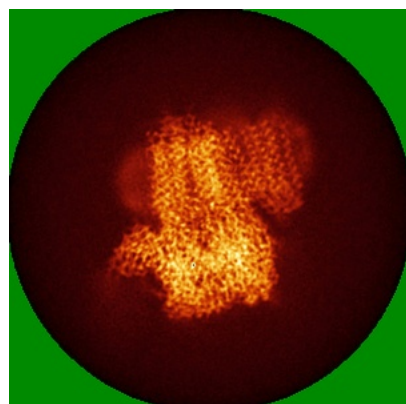


Z Index: 115

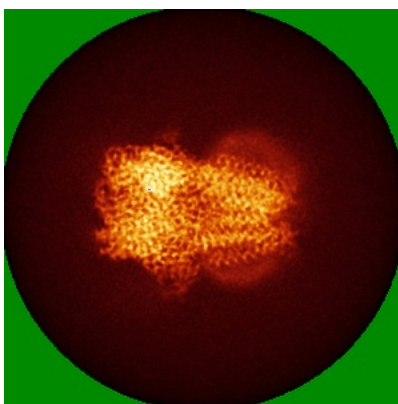
The images above show the largest variance slices of the map in three orthogonal directions.

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

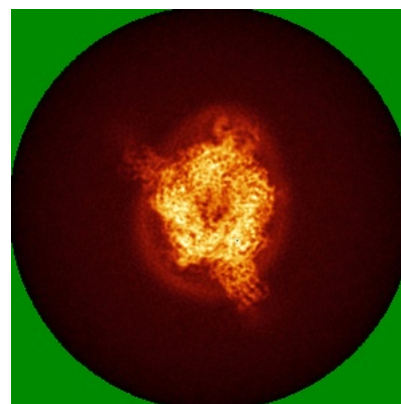
### 6.4.1 Primary map



X

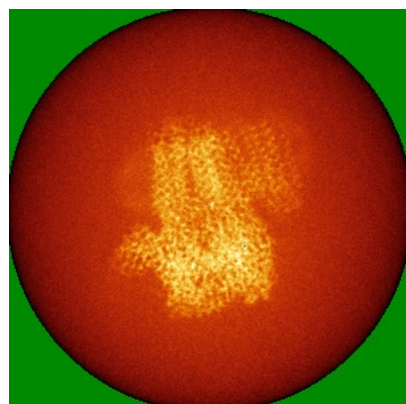


Y

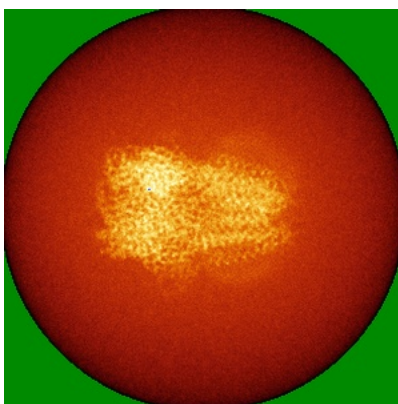


Z

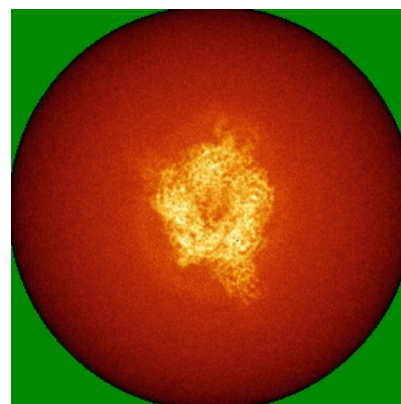
### 6.4.2 Raw map



X



Y

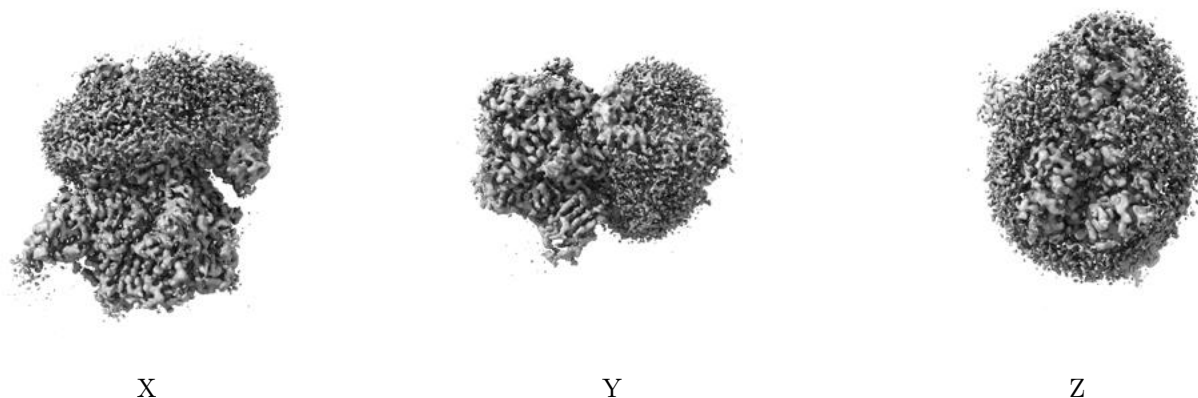


Z

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.

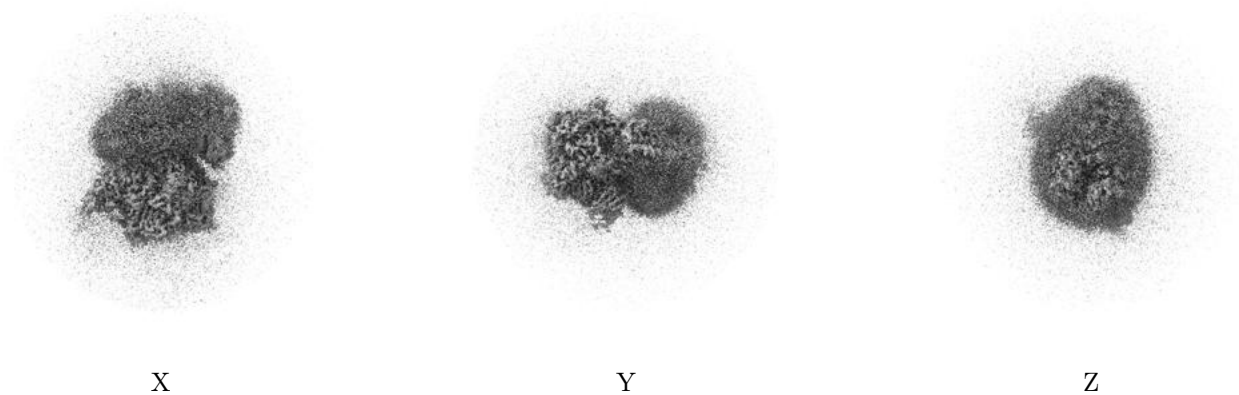
## 6.5 Orthogonal surface views [i](#)

### 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.



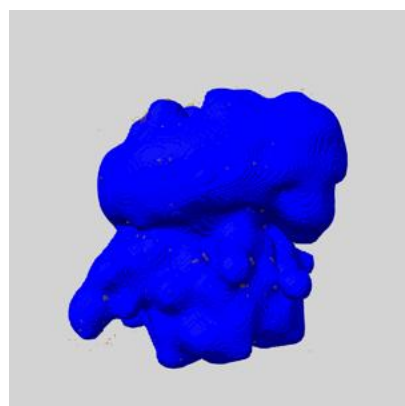
## 6.6 Mask visualisation [i](#)

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

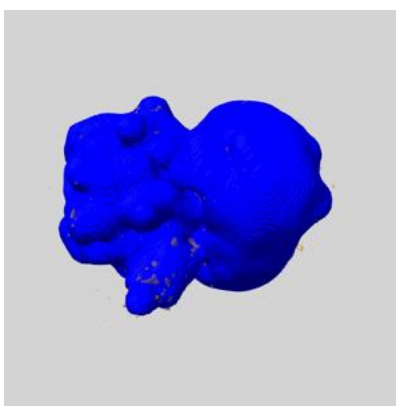
A mask typically either:

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

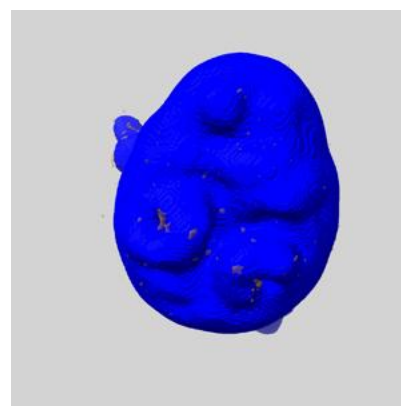
### 6.6.1 emd\_50274\_msk\_1.map [i](#)



X



Y

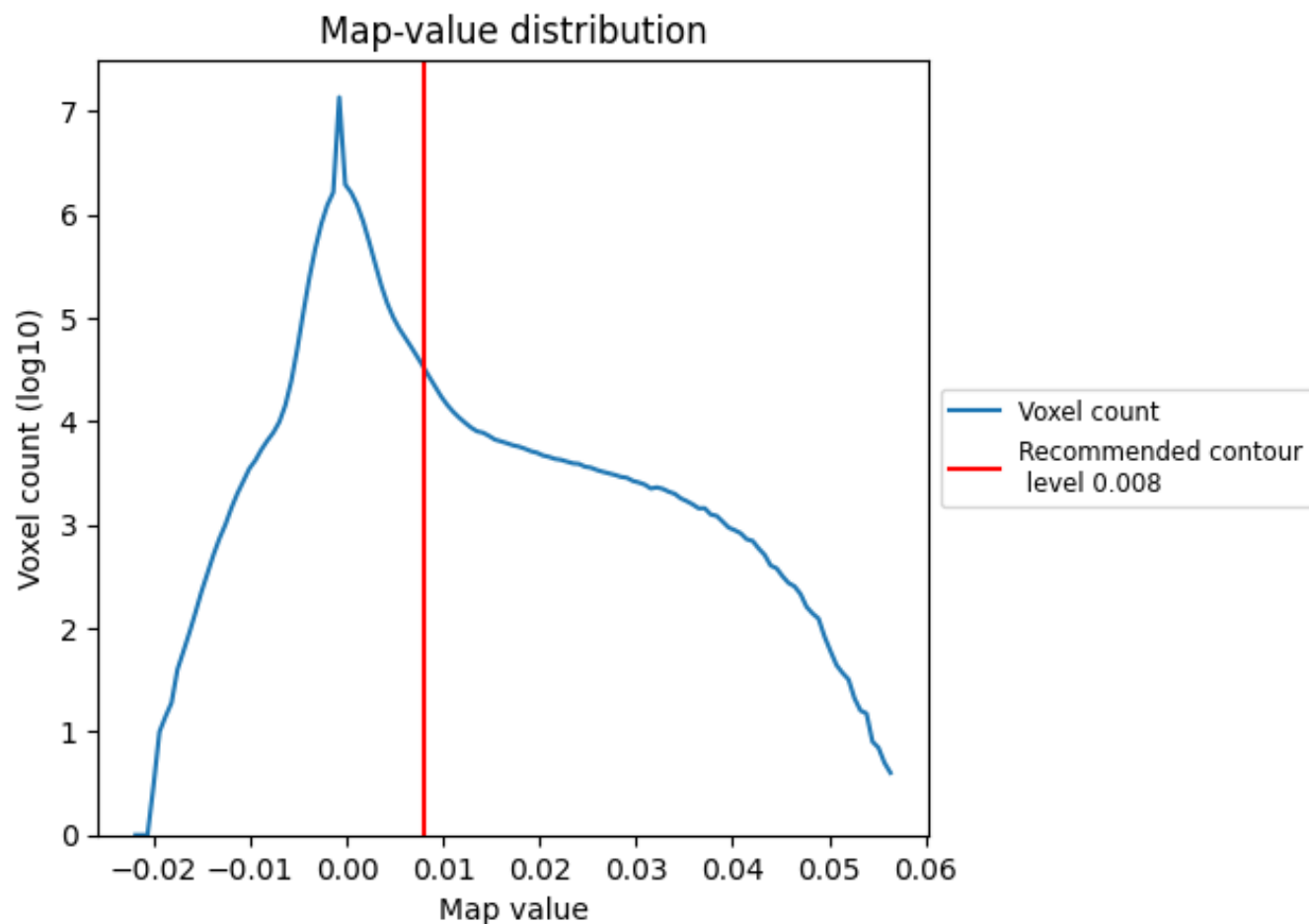


Z

## 7 Map analysis [i](#)

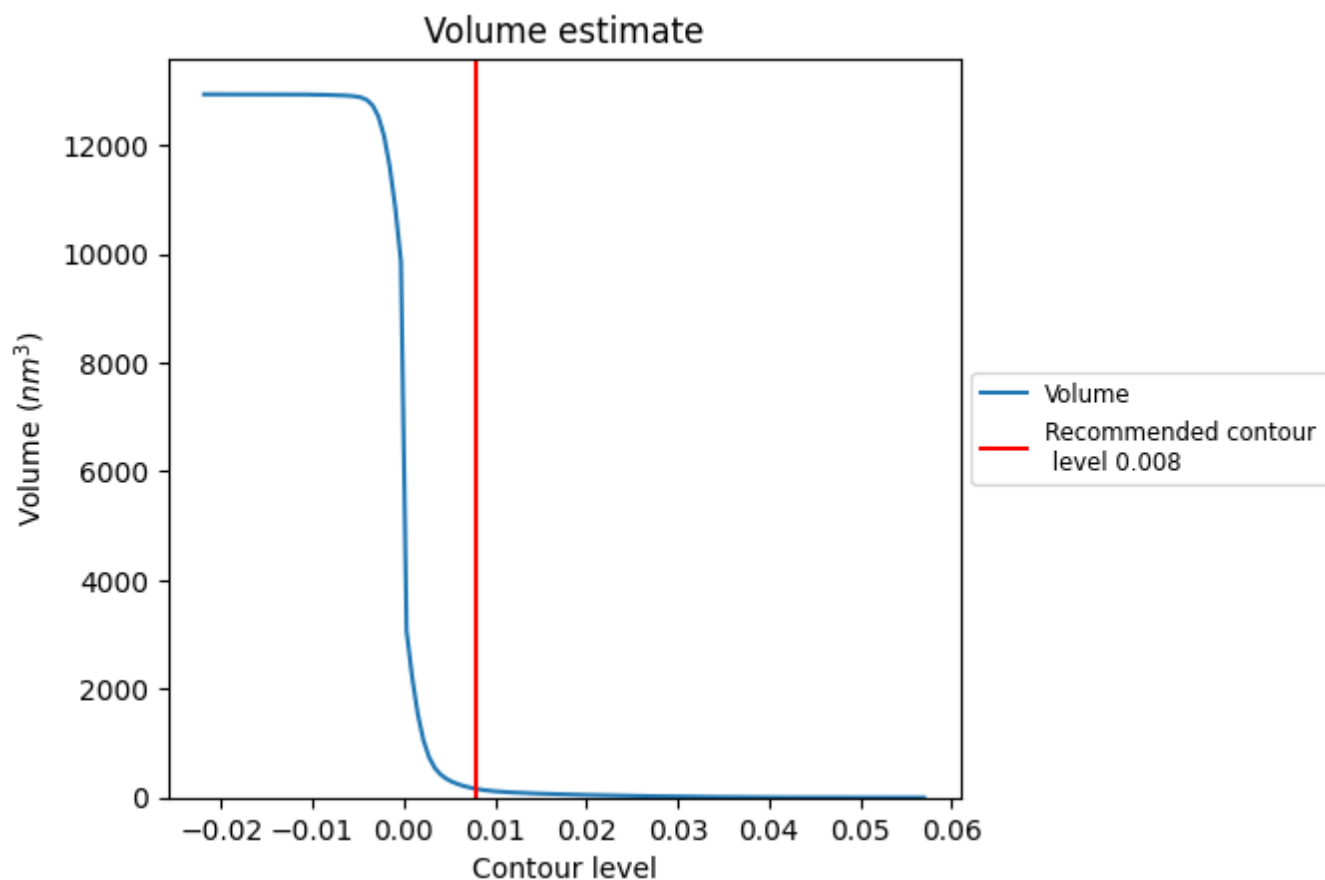
This section contains the results of statistical analysis of the map.

### 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.

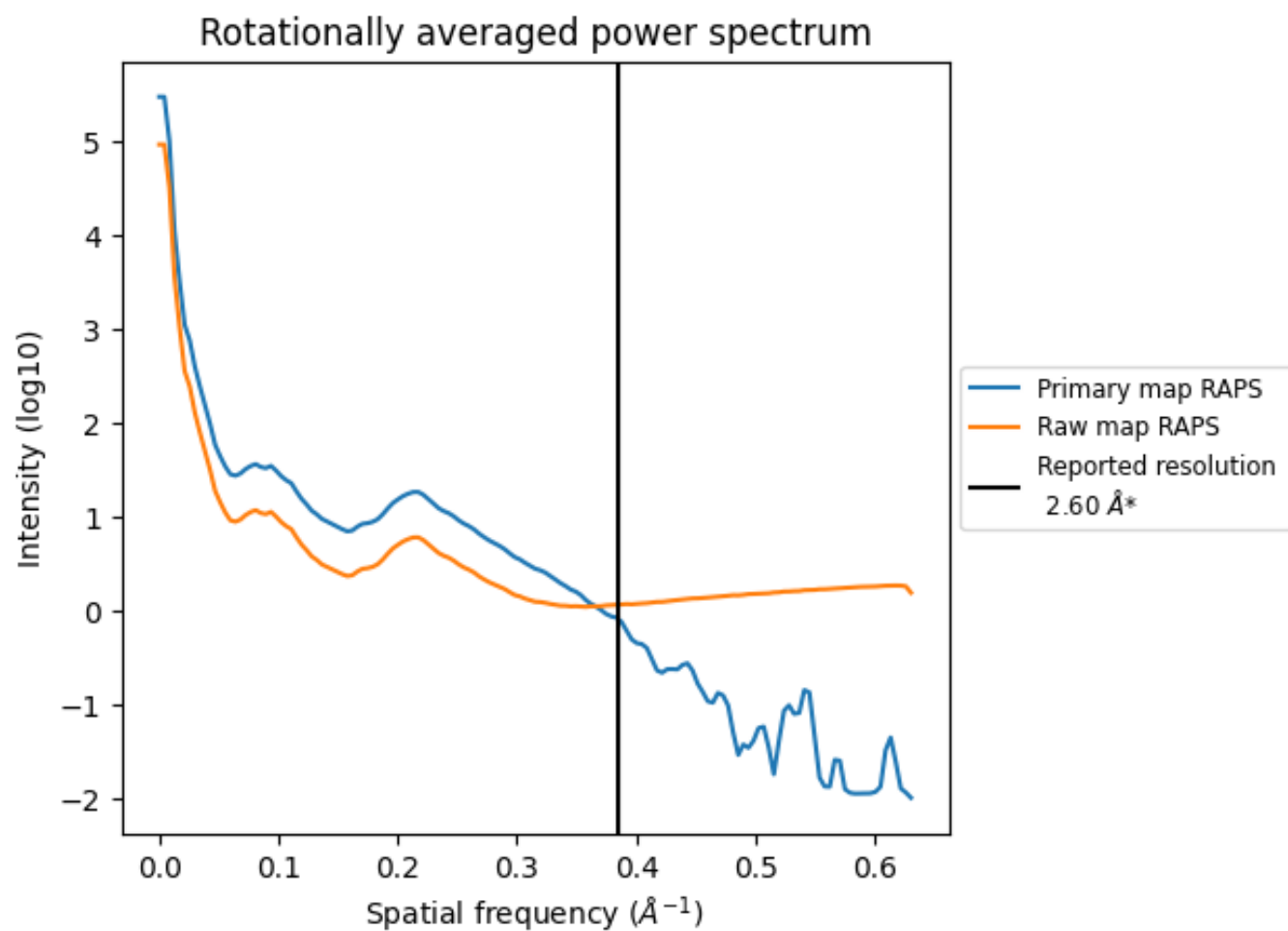
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158  $\text{nm}^3$ ; this corresponds to an approximate mass of 143 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 ⓘ



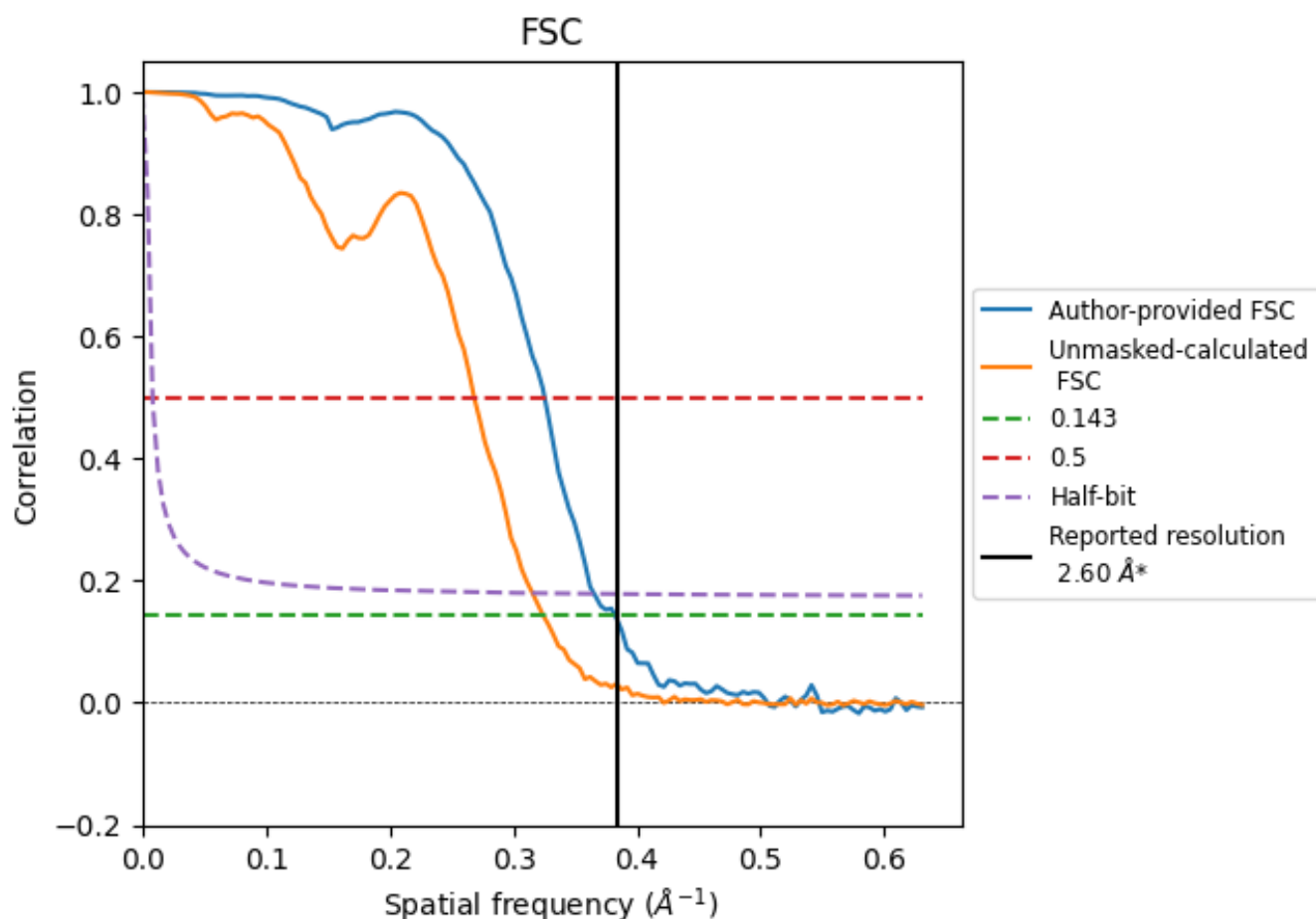
\*Reported resolution corresponds to spatial frequency of  $0.385 \text{ \AA}^{-1}$



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

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	3.07	2.74
Unmasked-calculated*	3.09	3.73	3.17

\*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 3.09 differs from the reported value 2.6 by more than 10 %

## 9 Map-model fit [i](#)

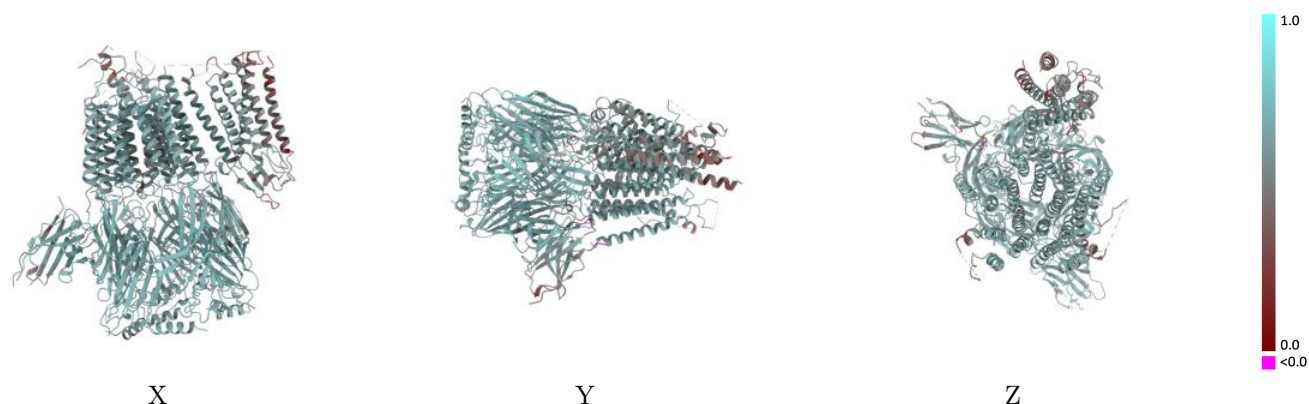
This section contains information regarding the fit between EMDB map EMD-50274 and PDB model 9FAK. Per-residue inclusion information can be found in section 3 on page 15.

### 9.1 Map-model overlay [i](#)



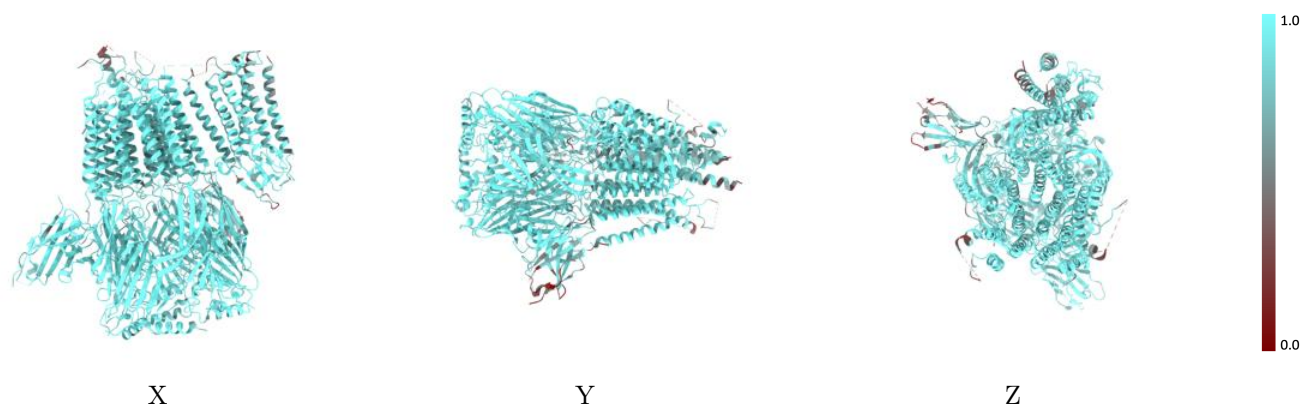
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



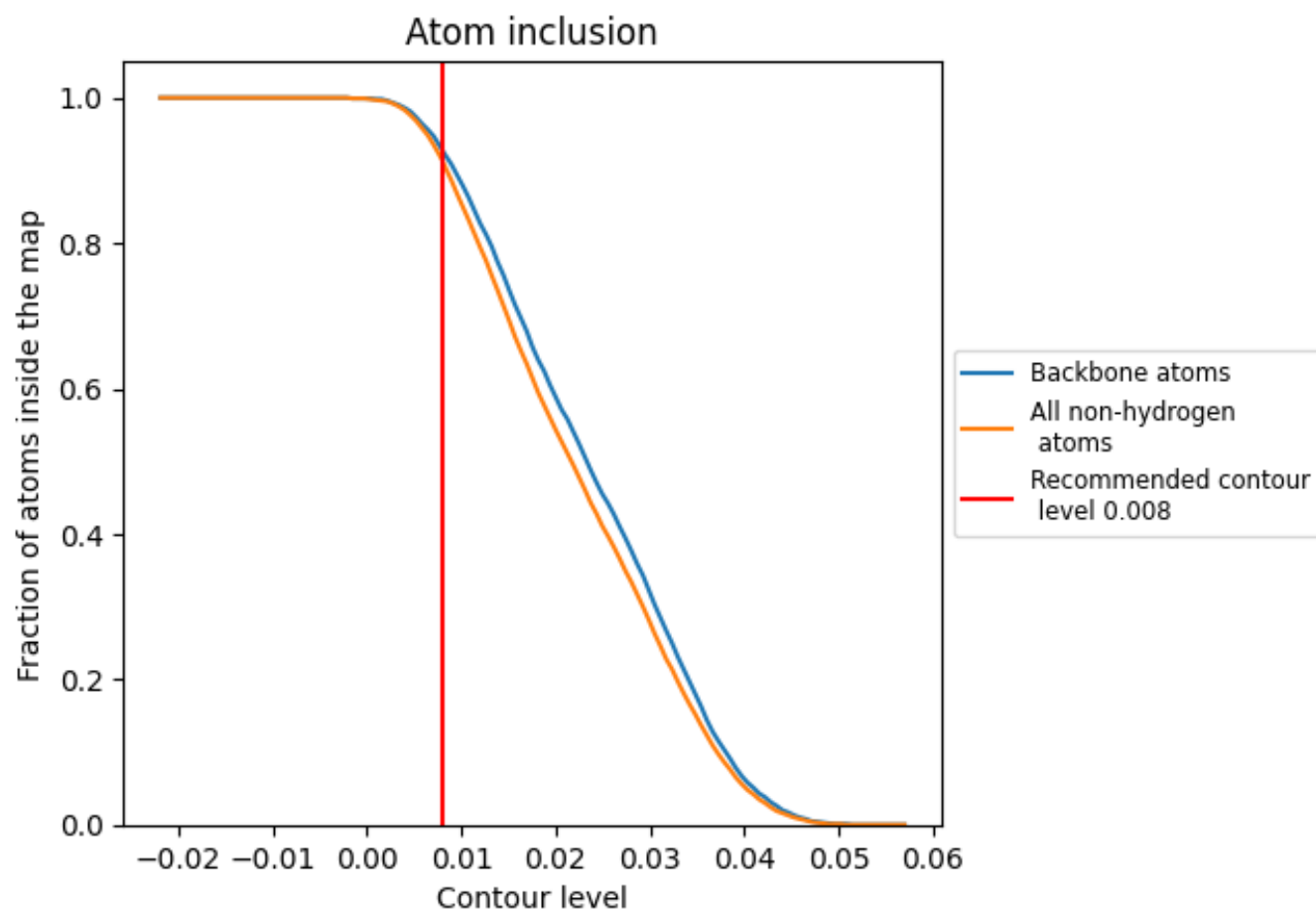
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9140	<div></div> 0.5920
A	<div></div> 0.9450	<div></div> 0.6170
B	<div></div> 0.9480	<div></div> 0.6150
C	<div></div> 0.9290	<div></div> 0.6060
D	<div></div> 0.9390	<div></div> 0.6130
E	<div></div> 0.9440	<div></div> 0.6120
F	<div></div> 0.9220	<div></div> 0.5590
G	<div></div> 0.9420	<div></div> 0.6040
H	<div></div> 0.7250	<div></div> 0.3840
I	<div></div> 0.7950	<div></div> 0.5130
J	<div></div> 0.9440	<div></div> 0.5650
K	<div></div> 0.5360	<div></div> 0.0860
L	<div></div> 0.8430	<div></div> 0.5090
M	<div></div> 0.6990	<div></div> 0.3810
N	<div></div> 0.9310	<div></div> 0.5790
O	<div></div> 0.7950	<div></div> 0.4620
P	<div></div> 0.7040	<div></div> 0.5010

1.0

0.0

<0.0