



## Full wwPDB EM Validation Report ⓘ

Jun 5, 2025 – 04:19 pm BST

PDB ID : 9G71 / pdb\_00009g71  
EMDB ID : EMD-51108  
Title : Cryo-EM structure of TTYH2 in complex with lipids in GDN  
Authors : Sukalskaia, A.; Weber, F.; Plochberger, B.; Dutzler, R.  
Deposited on : 2024-07-19  
Resolution : 2.74 Å(reported)

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) : 2.43.1

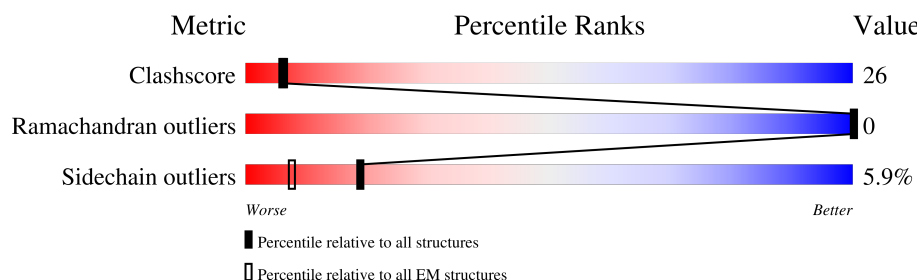
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

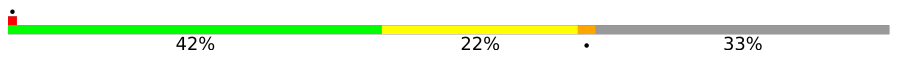
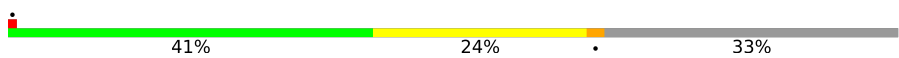
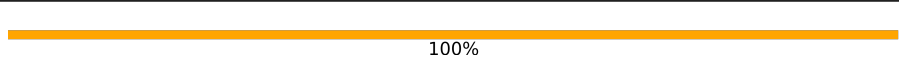


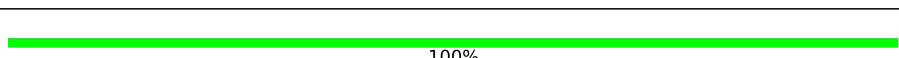
The reported resolution of this entry is 2.74 Å.

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	599	
1	B	599	
2	C	2	
2	D	2	
2	E	2	
2	F	2	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7510 atoms, of which 192 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 Protein tweety homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	399	Total	C	N	O	S	0	0
			3056	1976	492	563	25		
1	B	399	Total	C	N	O	S	0	0
			3056	1976	492	563	25		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q9BSA4
A	1	SER	-	expression tag	UNP Q9BSA4
A	535	ALA	-	expression tag	UNP Q9BSA4
A	536	LEU	-	expression tag	UNP Q9BSA4
A	537	GLU	-	expression tag	UNP Q9BSA4
A	538	VAL	-	expression tag	UNP Q9BSA4
A	539	LEU	-	expression tag	UNP Q9BSA4
A	540	PHE	-	expression tag	UNP Q9BSA4
A	541	GLN	-	expression tag	UNP Q9BSA4
A	542	GLY	-	expression tag	UNP Q9BSA4
A	543	PRO	-	expression tag	UNP Q9BSA4
A	544	GLN	-	expression tag	UNP Q9BSA4
A	545	GLY	-	expression tag	UNP Q9BSA4
A	546	THR	-	expression tag	UNP Q9BSA4
A	547	GLU	-	expression tag	UNP Q9BSA4
A	548	GLN	-	expression tag	UNP Q9BSA4
A	549	LYS	-	expression tag	UNP Q9BSA4
A	550	LEU	-	expression tag	UNP Q9BSA4
A	551	ILE	-	expression tag	UNP Q9BSA4
A	552	SER	-	expression tag	UNP Q9BSA4
A	553	GLU	-	expression tag	UNP Q9BSA4
A	554	GLU	-	expression tag	UNP Q9BSA4
A	555	ASP	-	expression tag	UNP Q9BSA4
A	556	LEU	-	expression tag	UNP Q9BSA4
A	557	ARG	-	expression tag	UNP Q9BSA4
A	558	GLY	-	expression tag	UNP Q9BSA4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	559	ALA	-	expression tag	UNP Q9BSA4
A	560	SER	-	expression tag	UNP Q9BSA4
A	561	MET	-	expression tag	UNP Q9BSA4
A	562	ASP	-	expression tag	UNP Q9BSA4
A	563	GLU	-	expression tag	UNP Q9BSA4
A	564	LYS	-	expression tag	UNP Q9BSA4
A	565	THR	-	expression tag	UNP Q9BSA4
A	566	THR	-	expression tag	UNP Q9BSA4
A	567	GLY	-	expression tag	UNP Q9BSA4
A	568	TRP	-	expression tag	UNP Q9BSA4
A	569	ARG	-	expression tag	UNP Q9BSA4
A	570	GLY	-	expression tag	UNP Q9BSA4
A	571	GLY	-	expression tag	UNP Q9BSA4
A	572	HIS	-	expression tag	UNP Q9BSA4
A	573	VAL	-	expression tag	UNP Q9BSA4
A	574	VAL	-	expression tag	UNP Q9BSA4
A	575	GLU	-	expression tag	UNP Q9BSA4
A	576	GLY	-	expression tag	UNP Q9BSA4
A	577	LEU	-	expression tag	UNP Q9BSA4
A	578	ALA	-	expression tag	UNP Q9BSA4
A	579	GLY	-	expression tag	UNP Q9BSA4
A	580	GLU	-	expression tag	UNP Q9BSA4
A	581	LEU	-	expression tag	UNP Q9BSA4
A	582	GLU	-	expression tag	UNP Q9BSA4
A	583	GLN	-	expression tag	UNP Q9BSA4
A	584	LEU	-	expression tag	UNP Q9BSA4
A	585	ARG	-	expression tag	UNP Q9BSA4
A	586	ALA	-	expression tag	UNP Q9BSA4
A	587	ARG	-	expression tag	UNP Q9BSA4
A	588	LEU	-	expression tag	UNP Q9BSA4
A	589	GLU	-	expression tag	UNP Q9BSA4
A	590	HIS	-	expression tag	UNP Q9BSA4
A	591	HIS	-	expression tag	UNP Q9BSA4
A	592	PRO	-	expression tag	UNP Q9BSA4
A	593	GLN	-	expression tag	UNP Q9BSA4
A	594	GLY	-	expression tag	UNP Q9BSA4
A	595	GLN	-	expression tag	UNP Q9BSA4
A	596	ARG	-	expression tag	UNP Q9BSA4
A	597	GLU	-	expression tag	UNP Q9BSA4
A	598	PRO	-	expression tag	UNP Q9BSA4
B	0	MET	-	initiating methionine	UNP Q9BSA4
B	1	SER	-	expression tag	UNP Q9BSA4

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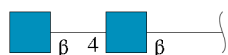
Chain	Residue	Modelled	Actual	Comment	Reference
B	535	ALA	-	expression tag	UNP Q9BSA4
B	536	LEU	-	expression tag	UNP Q9BSA4
B	537	GLU	-	expression tag	UNP Q9BSA4
B	538	VAL	-	expression tag	UNP Q9BSA4
B	539	LEU	-	expression tag	UNP Q9BSA4
B	540	PHE	-	expression tag	UNP Q9BSA4
B	541	GLN	-	expression tag	UNP Q9BSA4
B	542	GLY	-	expression tag	UNP Q9BSA4
B	543	PRO	-	expression tag	UNP Q9BSA4
B	544	GLN	-	expression tag	UNP Q9BSA4
B	545	GLY	-	expression tag	UNP Q9BSA4
B	546	THR	-	expression tag	UNP Q9BSA4
B	547	GLU	-	expression tag	UNP Q9BSA4
B	548	GLN	-	expression tag	UNP Q9BSA4
B	549	LYS	-	expression tag	UNP Q9BSA4
B	550	LEU	-	expression tag	UNP Q9BSA4
B	551	ILE	-	expression tag	UNP Q9BSA4
B	552	SER	-	expression tag	UNP Q9BSA4
B	553	GLU	-	expression tag	UNP Q9BSA4
B	554	GLU	-	expression tag	UNP Q9BSA4
B	555	ASP	-	expression tag	UNP Q9BSA4
B	556	LEU	-	expression tag	UNP Q9BSA4
B	557	ARG	-	expression tag	UNP Q9BSA4
B	558	GLY	-	expression tag	UNP Q9BSA4
B	559	ALA	-	expression tag	UNP Q9BSA4
B	560	SER	-	expression tag	UNP Q9BSA4
B	561	MET	-	expression tag	UNP Q9BSA4
B	562	ASP	-	expression tag	UNP Q9BSA4
B	563	GLU	-	expression tag	UNP Q9BSA4
B	564	LYS	-	expression tag	UNP Q9BSA4
B	565	THR	-	expression tag	UNP Q9BSA4
B	566	THR	-	expression tag	UNP Q9BSA4
B	567	GLY	-	expression tag	UNP Q9BSA4
B	568	TRP	-	expression tag	UNP Q9BSA4
B	569	ARG	-	expression tag	UNP Q9BSA4
B	570	GLY	-	expression tag	UNP Q9BSA4
B	571	GLY	-	expression tag	UNP Q9BSA4
B	572	HIS	-	expression tag	UNP Q9BSA4
B	573	VAL	-	expression tag	UNP Q9BSA4
B	574	VAL	-	expression tag	UNP Q9BSA4
B	575	GLU	-	expression tag	UNP Q9BSA4
B	576	GLY	-	expression tag	UNP Q9BSA4

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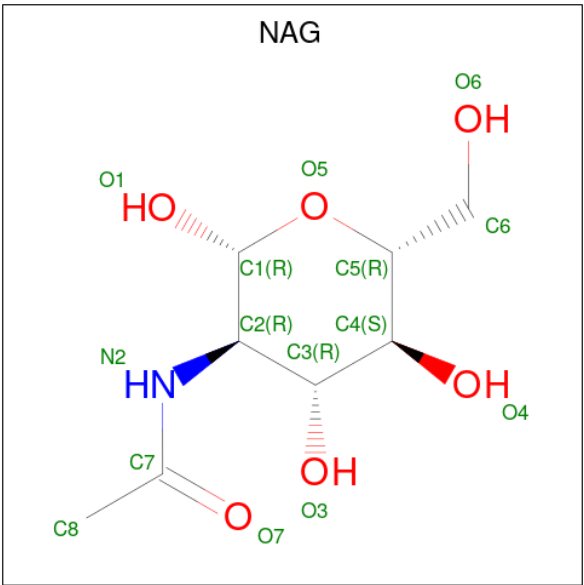
Chain	Residue	Modelled	Actual	Comment	Reference
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B	578	ALA	-	expression tag	UNP Q9BSA4
B	579	GLY	-	expression tag	UNP Q9BSA4
B	580	GLU	-	expression tag	UNP Q9BSA4
B	581	LEU	-	expression tag	UNP Q9BSA4
B	582	GLU	-	expression tag	UNP Q9BSA4
B	583	GLN	-	expression tag	UNP Q9BSA4
B	584	LEU	-	expression tag	UNP Q9BSA4
B	585	ARG	-	expression tag	UNP Q9BSA4
B	586	ALA	-	expression tag	UNP Q9BSA4
B	587	ARG	-	expression tag	UNP Q9BSA4
B	588	LEU	-	expression tag	UNP Q9BSA4
B	589	GLU	-	expression tag	UNP Q9BSA4
B	590	HIS	-	expression tag	UNP Q9BSA4
B	591	HIS	-	expression tag	UNP Q9BSA4
B	592	PRO	-	expression tag	UNP Q9BSA4
B	593	GLN	-	expression tag	UNP Q9BSA4
B	594	GLY	-	expression tag	UNP Q9BSA4
B	595	GLN	-	expression tag	UNP Q9BSA4
B	596	ARG	-	expression tag	UNP Q9BSA4
B	597	GLU	-	expression tag	UNP Q9BSA4
B	598	PRO	-	expression tag	UNP Q9BSA4

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



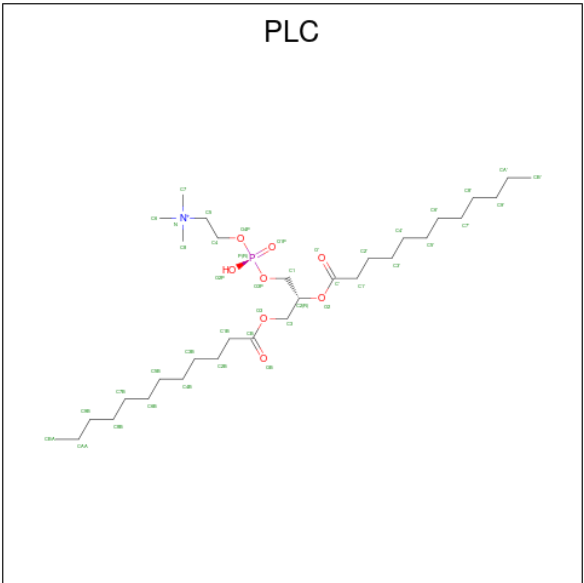
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



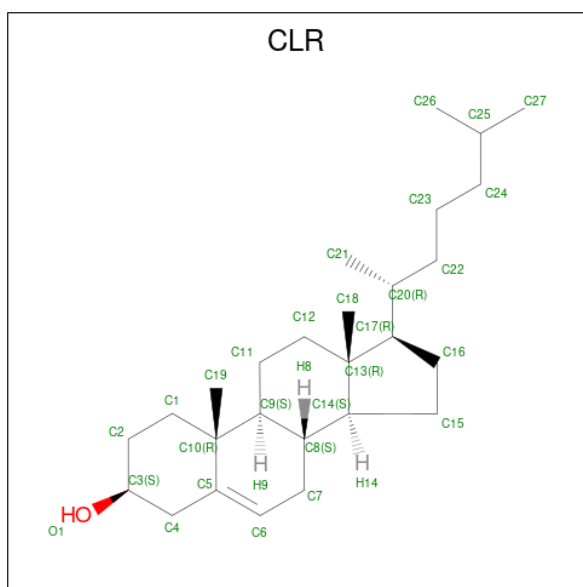
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0

- Molecule 4 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C<sub>32</sub>H<sub>65</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



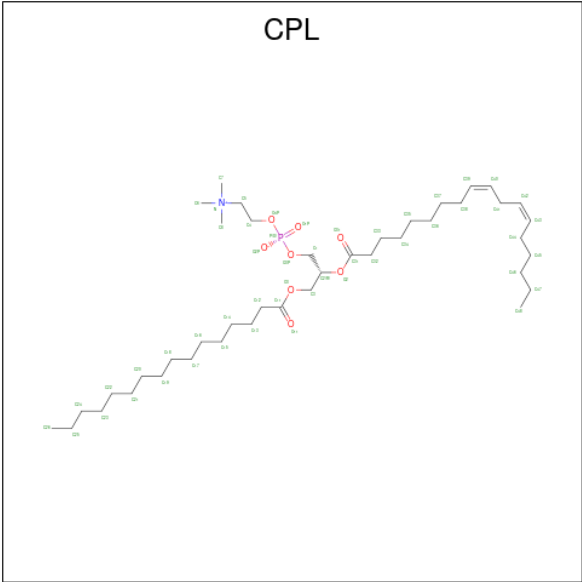
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total 42	C 32	N 1	O 8	P 1	0	
4	A	1	Total 42	C 32	N 1	O 8	P 1	0	
4	A	1	Total 42	C 32	N 1	O 8	P 1	0	
4	A	1	Total 42	C 32	N 1	O 8	P 1	0	
4	A	1	Total 42	C 32	N 1	O 8	P 1	0	
4	A	1	Total 42	C 32	N 1	O 8	P 1	0	
4	A	1	Total 42	C 32	N 1	O 8	P 1	0	
4	A	1	Total 106	C 32	H 64	N 1	O 8	P 1	0
4	B	1	Total 42	C 32	N 1	O 8	P 1	0	
4	B	1	Total 42	C 32	N 1	O 8	P 1	0	
4	B	1	Total 42	C 32	N 1	O 8	P 1	0	
4	B	1	Total 42	C 32	N 1	O 8	P 1	0	
4	B	1	Total 42	C 32	N 1	O 8	P 1	0	
4	B	1	Total 42	C 32	N 1	O 8	P 1	0	
4	B	1	Total 42	C 32	N 1	O 8	P 1	0	
4	B	1	Total 42	C 32	N 1	O 8	P 1	0	
4	B	1	Total 106	C 32	H 64	N 1	O 8	P 1	0
4	B	1	Total 106	C 32	H 64	N 1	O 8	P 1	0

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O) (labeled as "Ligand of Interest" by depositor).



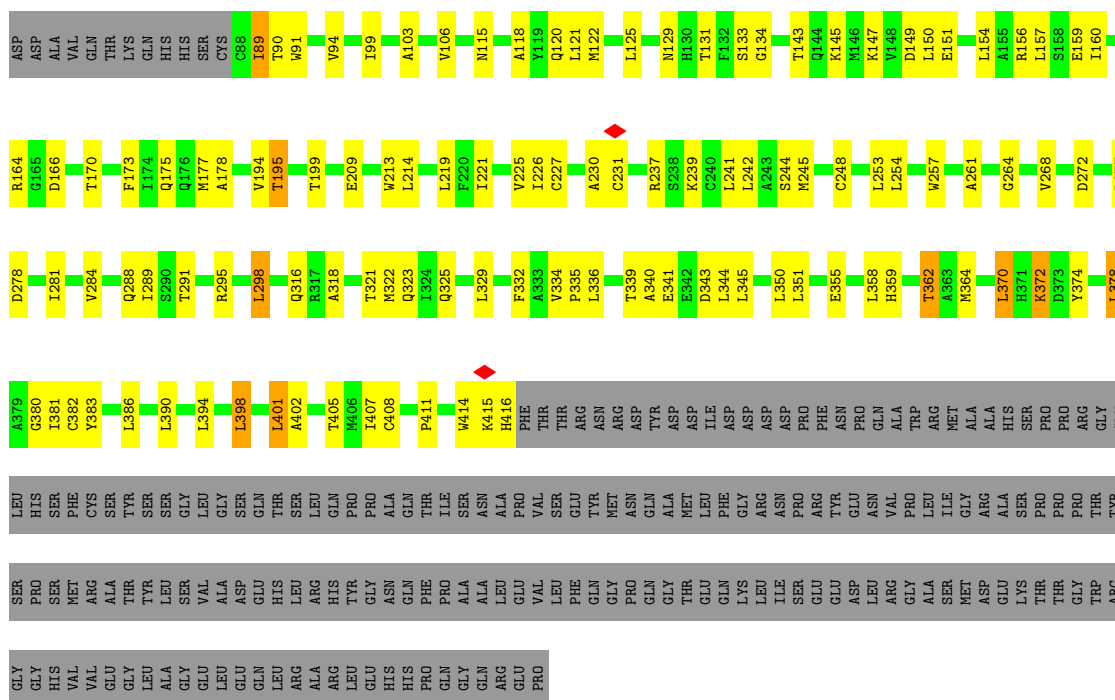
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	

- Molecule 6 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula:  $C_{42}H_{80}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
6	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
6	B	1	Total	C	N	O	P	0
			52	42	1	8	1	





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

Chain C:  100%



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

Chain D:  50% 50%



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

Chain E:  100%



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

Chain F:  100%

MAG  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2192921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	63	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	4.317	Depositor
Minimum map value	-3.069	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.271	Depositor
Map size ( $\text{\AA}$ )	286.44, 286.44, 286.44	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.302, 1.302, 1.302	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: PLC, CLR, CPL, NAG

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	0/3121	0.24	0/4253
1	B	0.18	0/3121	0.25	0/4253
All	All	0.18	0/6242	0.25	0/8506

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	3056	0	3052	147	0
1	B	3056	0	3052	141	0
2	C	28	0	25	3	0
2	D	28	0	25	0	0
2	E	28	0	25	3	0
2	F	28	0	25	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	336	64	512	50	0
4	B	378	128	574	32	0
5	A	112	0	184	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	56	0	92	9	0
6	A	104	0	160	22	0
6	B	52	0	80	14	0
All	All	7318	192	7858	392	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 26.

All (392) 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)
4:A:613:PLC:H1'1	4:A:613:PLC:H3A1	1.41	1.02
1:A:50:LEU:HB2	4:A:603:PLC:H5A1	1.46	0.96
1:A:121:LEU:HD13	1:A:381:ILE:HD11	1.54	0.89
1:A:99:ILE:HG22	1:A:402:ALA:HB2	1.53	0.88
1:A:89:ILE:HD11	1:A:412:ARG:HG2	1.54	0.88
1:B:103:ALA:HB2	1:B:398:LEU:HB3	1.55	0.87
6:B:603:CPL:H481	6:B:603:CPL:H262	1.57	0.85
6:A:610:CPL:H132	6:A:610:CPL:H332	1.58	0.85
1:B:25:LEU:HG	1:B:43:GLU:HG3	1.62	0.81
1:B:121:LEU:HD13	1:B:381:ILE:HD11	1.60	0.81
1:B:195:THR:O	1:B:199:THR:HG23	1.80	0.81
1:B:237:ARG:HE	1:B:237:ARG:HA	1.45	0.81
1:B:118:ALA:O	1:B:122:MET:HG3	1.82	0.80
4:B:606:PLC:H2A1	4:B:606:PLC:H2'1	1.63	0.80
6:B:603:CPL:H192	6:B:603:CPL:H242	1.65	0.79
1:A:43:GLU:HB2	6:A:610:CPL:H322	1.65	0.78
1:B:358:LEU:O	1:B:362:THR:HG22	1.83	0.78
1:B:291:THR:O	1:B:295:ARG:HG3	1.83	0.78
6:B:603:CPL:H221	6:B:603:CPL:H263	1.64	0.78
1:B:322:MET:HE2	1:B:351:LEU:HD21	1.66	0.78
4:A:615:PLC:H1A2	4:A:615:PLC:H1'2	1.67	0.77
1:B:143:THR:O	1:B:147:LYS:HG2	1.85	0.77
5:B:610:CLR:H21	5:B:611:CLR:H151	1.67	0.77
1:B:106:VAL:HG11	1:B:394:LEU:HD23	1.67	0.77
4:A:612:PLC:H62	4:A:613:PLC:H61	1.67	0.76
1:A:23:VAL:HG12	1:A:27:LEU:HA	1.68	0.74
1:A:160:ILE:HD13	1:A:340:ALA:HB2	1.69	0.74
5:A:608:CLR:H191	5:A:609:CLR:H71	1.70	0.73
1:A:154:LEU:HD13	1:A:175:GLN:HG3	1.70	0.73
1:B:156:ARG:HH11	1:B:156:ARG:HB2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG22	1:A:386:LEU:HD23	1.70	0.72
1:A:156:ARG:O	1:A:160:ILE:HG22	1.89	0.72
5:A:608:CLR:H221	5:A:608:CLR:H262	1.71	0.71
1:B:28:GLN:OE1	1:B:28:GLN:N	2.23	0.71
1:B:6:VAL:HG12	1:B:7:ASP:H	1.55	0.70
1:B:16:TRP:O	1:B:19:SER:OG	2.07	0.70
1:A:381:ILE:HD13	5:A:609:CLR:H261	1.72	0.70
1:A:225:VAL:HG12	4:A:614:PLC:HT'2	1.74	0.70
1:A:25:LEU:HD12	6:A:610:CPL:HC32	1.72	0.70
1:A:156:ARG:O	1:A:159:GLU:HG2	1.92	0.70
1:B:245:MET:HE2	1:B:245:MET:N	2.08	0.69
5:A:605:CLR:H151	5:A:606:CLR:C1	2.22	0.69
1:B:115:ASN:ND2	1:B:209:GLU:OE2	2.22	0.69
2:E:2:NAG:O7	2:E:2:NAG:O3	2.11	0.69
1:B:24:GLY:HA2	1:B:43:GLU:HG2	1.76	0.68
1:B:157:LEU:HD21	1:B:343:ASP:HB2	1.74	0.68
1:A:89:ILE:HD13	1:A:416:HIS:ND1	2.07	0.68
1:A:134:GLY:HA3	1:A:364:MET:HE1	1.75	0.68
1:B:38:ASP:O	1:B:42:GLN:HG3	1.93	0.68
2:C:2:NAG:O7	2:C:2:NAG:O3	2.10	0.68
1:A:123:TYR:OH	1:B:372:LYS:HE3	1.94	0.67
1:B:318:ALA:O	1:B:322:MET:HG3	1.95	0.67
1:B:154:LEU:HD13	1:B:175:GLN:HG3	1.75	0.67
1:B:170:THR:HG21	1:B:329:LEU:HG	1.77	0.67
1:B:226:ILE:CD1	1:B:248:CYS:HB3	2.25	0.67
6:B:603:CPL:H481	6:B:603:CPL:C26	2.25	0.67
1:A:129:ASN:OD1	1:A:195:THR:HG23	1.95	0.66
1:B:237:ARG:HA	1:B:237:ARG:NE	2.10	0.66
1:A:358:LEU:O	1:A:362:THR:HG22	1.96	0.66
5:A:609:CLR:H222	5:A:609:CLR:H272	1.77	0.66
4:A:612:PLC:H2'2	4:A:612:PLC:H6'1	1.78	0.65
1:A:25:LEU:HG	1:A:43:GLU:HG3	1.77	0.65
1:A:321:THR:O	1:A:325:GLN:HG2	1.96	0.65
1:B:147:LYS:O	1:B:151:GLU:HG2	1.98	0.64
1:B:408:CYS:O	1:B:411:PRO:HD2	1.98	0.64
1:A:150:LEU:HD23	1:A:178:ALA:HB2	1.80	0.64
1:B:323:GLN:NE2	1:B:355:GLU:OE2	2.28	0.64
1:A:221:ILE:O	1:A:225:VAL:HG13	1.97	0.64
1:A:237:ARG:NH1	1:A:416:HIS:O	2.26	0.64
6:A:610:CPL:H132	6:A:610:CPL:HC31	1.80	0.64
1:B:156:ARG:O	1:B:159:GLU:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LEU:O	1:B:405:THR:HG23	1.98	0.63
1:A:43:GLU:HB2	6:A:610:CPL:C32	2.29	0.63
1:A:109:TYR:OH	4:B:612:PLC:O1P	2.16	0.63
1:B:226:ILE:HD11	1:B:248:CYS:HB3	1.80	0.63
1:B:13:TRP:HB2	5:B:610:CLR:H261	1.79	0.63
1:B:160:ILE:HD13	1:B:340:ALA:HB2	1.80	0.63
1:B:230:ALA:CA	1:B:245:MET:HG3	2.29	0.62
4:B:606:PLC:HT'1	4:B:606:PLC:HEA2	1.79	0.62
1:B:27:LEU:HD23	5:B:611:CLR:C2	2.29	0.62
1:B:150:LEU:HD23	1:B:178:ALA:HB2	1.81	0.62
1:B:160:ILE:HD11	1:B:339:THR:OG1	1.98	0.62
5:A:609:CLR:H22	6:A:610:CPL:H381	1.81	0.61
4:A:612:PLC:H62	4:A:613:PLC:C6	2.30	0.61
1:A:27:LEU:HD12	5:A:605:CLR:C2	2.30	0.61
1:A:56:LEU:HD12	1:A:56:LEU:O	2.01	0.61
1:A:103:ALA:HB2	1:A:398:LEU:HB3	1.83	0.61
1:A:24:GLY:HA2	1:A:43:GLU:HG2	1.83	0.61
4:A:612:PLC:O1P	4:A:612:PLC:H63	2.01	0.61
1:A:89:ILE:CD1	1:A:412:ARG:HG2	2.27	0.60
1:A:90:THR:O	1:A:94:VAL:HG13	2.01	0.60
1:B:27:LEU:HD23	5:B:611:CLR:H22	1.83	0.60
1:B:244:SER:C	1:B:245:MET:HE2	2.26	0.60
1:B:213:TRP:CZ2	4:B:612:PLC:H51	2.37	0.60
1:A:157:LEU:HD21	1:A:343:ASP:HB2	1.84	0.60
4:A:603:PLC:O'	4:A:603:PLC:H12	2.01	0.59
1:B:145:LYS:HD2	1:B:350:LEU:HG	1.85	0.59
1:B:230:ALA:HA	1:B:245:MET:HG3	1.84	0.59
1:B:156:ARG:HB2	1:B:156:ARG:NH1	2.17	0.59
1:B:27:LEU:HD23	5:B:611:CLR:H11	1.83	0.58
1:A:48:LEU:CD1	1:A:268:VAL:HG21	2.33	0.58
1:A:229:ILE:HG21	1:A:245:MET:HE3	1.85	0.58
5:A:606:CLR:H222	5:A:606:CLR:H263	1.85	0.58
1:A:91:TRP:HE3	1:A:94:VAL:HG21	1.68	0.58
1:A:381:ILE:HG21	5:A:609:CLR:C26	2.34	0.58
1:B:120:GLN:HG2	1:B:380:GLY:HA3	1.85	0.58
5:A:609:CLR:H272	5:A:609:CLR:C22	2.34	0.58
4:A:615:PLC:H1'2	4:A:615:PLC:C1B	2.33	0.58
1:A:408:CYS:O	1:A:411:PRO:HD2	2.03	0.58
1:B:11:PRO:O	1:B:15:VAL:HG23	2.02	0.58
1:A:145:LYS:HG2	1:A:350:LEU:HD11	1.86	0.57
1:A:50:LEU:CD1	4:A:603:PLC:H1A2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:CB	4:A:603:PLC:H5A1	2.29	0.57
1:A:166:ASP:OD1	1:A:166:ASP:N	2.37	0.57
1:B:52:ALA:HB3	1:B:261:ALA:HB2	1.86	0.57
1:A:123:TYR:HE2	1:B:5:ARG:HA	1.69	0.57
4:A:604:PLC:HEA3	4:A:616:PLC:H8A2	1.85	0.57
1:B:131:THR:HG21	1:B:370:LEU:HD21	1.86	0.57
1:A:91:TRP:O	1:A:94:VAL:HG22	2.04	0.56
5:A:608:CLR:C19	5:A:609:CLR:H71	2.34	0.56
1:B:166:ASP:N	1:B:166:ASP:OD1	2.38	0.56
1:B:341:GLU:O	1:B:345:LEU:HD23	2.05	0.56
1:A:230:ALA:CA	1:A:245:MET:HG3	2.36	0.56
1:A:23:VAL:HG11	1:A:27:LEU:HD13	1.88	0.56
1:A:50:LEU:HD12	4:A:603:PLC:H1A2	1.88	0.56
1:A:193:GLU:O	1:A:197:GLU:HG2	2.06	0.56
1:B:284:VAL:HA	6:B:603:CPL:HC81	1.88	0.56
2:C:1:NAG:H61	2:C:2:NAG:O5	2.05	0.55
1:A:260:LEU:O	1:A:260:LEU:HD12	2.06	0.55
1:A:27:LEU:CD1	5:A:605:CLR:H11	2.36	0.55
1:B:214:LEU:HD23	4:B:613:PLC:H2'1	1.88	0.55
1:A:96:ALA:HB2	1:A:405:THR:CG2	2.37	0.55
1:B:129:ASN:OD1	1:B:195:THR:HG23	2.07	0.55
4:B:606:PLC:O2P	4:B:606:PLC:H51	2.07	0.55
1:B:145:LYS:HG3	1:B:350:LEU:HD11	1.88	0.55
1:A:27:LEU:HD12	5:A:605:CLR:H21	1.89	0.54
4:A:604:PLC:H3A1	4:A:616:PLC:H3A2	1.89	0.54
1:B:60:LEU:HD11	1:B:254:LEU:HD11	1.89	0.54
1:B:91:TRP:HA	1:B:94:VAL:HG22	1.88	0.54
4:B:609:PLC:H1A1	4:B:609:PLC:H2'2	1.88	0.54
1:A:237:ARG:HE	1:A:237:ARG:HA	1.73	0.54
1:B:157:LEU:HA	1:B:160:ILE:HG22	1.89	0.54
1:B:298:LEU:CD1	6:B:603:CPL:H241	2.38	0.54
4:A:603:PLC:H82	4:A:603:PLC:O2P	2.08	0.54
1:B:11:PRO:HG3	1:B:383:TYR:CZ	2.43	0.53
1:A:226:ILE:CD1	1:A:248:CYS:HB3	2.39	0.53
4:A:607:PLC:H31	4:A:607:PLC:H2'2	1.91	0.53
4:B:606:PLC:HT'1	4:B:606:PLC:CBA	2.38	0.53
1:B:27:LEU:HD23	5:B:611:CLR:C1	2.37	0.53
4:B:606:PLC:H2'1	4:B:606:PLC:C2B	2.38	0.53
1:A:25:LEU:N	1:A:43:GLU:OE2	2.39	0.53
1:A:27:LEU:HD12	5:A:605:CLR:H11	1.90	0.53
1:A:160:ILE:CD1	1:A:340:ALA:HB2	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:OD1	1:A:252:SER:OG	2.26	0.53
6:A:610:CPL:H332	6:A:610:CPL:C13	2.34	0.53
1:B:322:MET:CE	1:B:351:LEU:HD21	2.36	0.53
1:A:237:ARG:HA	1:A:237:ARG:NE	2.24	0.52
6:A:610:CPL:H43	4:A:613:PLC:CB'	2.39	0.52
4:B:612:PLC:HE'2	4:B:612:PLC:HEA2	1.90	0.52
4:B:609:PLC:H2'2	4:B:609:PLC:C1B	2.40	0.52
1:B:48:LEU:HD13	1:B:268:VAL:HG21	1.91	0.52
1:A:18:HIS:HE1	1:A:32:SER:O	1.92	0.52
1:B:31:ASN:OD1	1:B:33:THR:HG23	2.10	0.52
1:A:96:ALA:HB2	1:A:405:THR:HG23	1.91	0.52
1:A:194:VAL:HG21	1:A:289:ILE:HD11	1.92	0.52
5:A:608:CLR:H273	6:A:611:CPL:H232	1.91	0.52
5:A:608:CLR:H221	5:A:608:CLR:C26	2.40	0.51
4:B:612:PLC:HEA2	4:B:612:PLC:CB'	2.40	0.51
1:A:291:THR:O	1:A:295:ARG:HG3	2.10	0.51
6:A:610:CPL:H241	6:A:610:CPL:H40	1.92	0.51
4:A:604:PLC:H82	4:A:616:PLC:H12	1.93	0.51
4:A:612:PLC:H52	4:A:613:PLC:H81	1.93	0.51
4:A:603:PLC:H2'1	4:A:603:PLC:O1P	2.11	0.51
1:A:157:LEU:HA	1:A:160:ILE:CG2	2.41	0.51
1:A:203:ASP:HB3	6:A:611:CPL:HC61	1.92	0.51
1:A:25:LEU:HD12	6:A:610:CPL:C3	2.41	0.50
1:B:221:ILE:O	1:B:225:VAL:HG13	2.11	0.50
1:A:264:GLY:O	1:A:268:VAL:HG23	2.11	0.50
1:A:329:LEU:HD23	1:A:344:LEU:HD11	1.93	0.50
5:A:605:CLR:H72	5:A:606:CLR:H21	1.93	0.50
1:A:14:VAL:HG22	1:A:386:LEU:CD2	2.39	0.50
1:A:91:TRP:HA	1:A:94:VAL:HG22	1.92	0.50
5:A:608:CLR:H212	5:A:608:CLR:H183	1.93	0.50
1:B:150:LEU:HD21	1:B:322:MET:CE	2.42	0.50
1:B:322:MET:HE2	1:B:351:LEU:CD2	2.39	0.50
1:A:218:LEU:HD13	4:A:612:PLC:HTA1	1.93	0.50
1:A:381:ILE:HG21	5:A:609:CLR:H263	1.93	0.50
5:B:610:CLR:H222	5:B:610:CLR:H272	1.94	0.50
1:A:103:ALA:HB2	1:A:398:LEU:CB	2.41	0.50
1:B:321:THR:O	1:B:325:GLN:HG2	2.12	0.50
1:A:23:VAL:CG1	1:A:27:LEU:HA	2.40	0.50
1:A:118:ALA:HB3	1:A:209:GLU:HG2	1.93	0.50
1:B:245:MET:HE2	1:B:245:MET:CA	2.42	0.50
1:A:181:VAL:HG22	1:A:315:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:TRP:O	1:B:94:VAL:HG22	2.11	0.49
1:A:150:LEU:HD23	1:A:178:ALA:CB	2.42	0.49
1:A:12:TRP:HE3	1:A:16:TRP:HD1	1.59	0.49
1:A:27:LEU:HD21	4:A:603:PLC:H3'1	1.93	0.49
1:A:59:ASN:OD1	1:A:253:LEU:HD21	2.13	0.49
1:A:339:THR:O	1:A:340:ALA:HB3	2.13	0.49
1:B:173:PHE:HE1	1:B:177:MET:HE3	1.77	0.49
1:A:99:ILE:CG2	1:A:402:ALA:HB2	2.35	0.49
1:A:221:ILE:CD1	4:A:614:PLC:H4'2	2.43	0.49
1:B:48:LEU:CD1	1:B:268:VAL:HG21	2.41	0.49
1:B:277:PRO:O	1:B:281:ILE:HG12	2.13	0.49
1:B:264:GLY:O	1:B:268:VAL:HG23	2.13	0.48
6:B:603:CPL:H262	6:B:603:CPL:C48	2.36	0.48
1:A:381:ILE:HG21	5:A:609:CLR:H261	1.95	0.48
1:B:91:TRP:HA	1:B:91:TRP:CE3	2.48	0.48
1:A:56:LEU:HD21	1:A:254:LEU:HD23	1.95	0.48
2:C:1:NAG:H4	2:C:2:NAG:H2	1.55	0.48
1:A:91:TRP:CE3	1:A:94:VAL:HG21	2.47	0.48
1:A:226:ILE:HG12	1:A:248:CYS:HB3	1.95	0.48
1:A:48:LEU:HD13	1:A:268:VAL:HG21	1.95	0.48
4:A:613:PLC:H3A1	4:A:613:PLC:C1'	2.28	0.48
1:B:24:GLY:CA	1:B:43:GLU:HG2	2.44	0.48
1:B:213:TRP:CE2	4:B:612:PLC:H51	2.49	0.48
4:A:604:PLC:HE'1	5:A:605:CLR:H261	1.95	0.48
1:A:6:VAL:HG13	1:A:7:ASP:N	2.29	0.48
1:B:284:VAL:HG23	6:B:603:CPL:HC11	1.96	0.48
2:E:1:NAG:H61	2:E:2:NAG:O5	2.14	0.47
4:A:613:PLC:H1'1	4:A:613:PLC:C3B	2.27	0.47
1:A:14:VAL:CG2	1:A:386:LEU:HD23	2.41	0.47
1:A:288:GLN:HG3	1:A:289:ILE:HG13	1.96	0.47
1:B:89:ILE:C	1:B:89:ILE:HD13	2.39	0.47
1:B:339:THR:O	1:B:340:ALA:HB3	2.15	0.47
1:A:71:CYS:SG	1:A:72:HIS:N	2.86	0.47
1:B:103:ALA:CB	1:B:398:LEU:HB3	2.37	0.47
1:B:115:ASN:HA	1:B:209:GLU:OE2	2.15	0.47
1:A:145:LYS:CG	1:A:350:LEU:HD11	2.45	0.47
1:A:245:MET:N	1:A:245:MET:HE2	2.30	0.47
5:A:608:CLR:H112	6:A:611:CPL:H162	1.96	0.47
4:A:613:PLC:H31	4:A:613:PLC:O1P	2.14	0.47
1:B:26:ARG:O	1:B:27:LEU:HB2	2.15	0.47
4:B:612:PLC:H1A2	4:B:612:PLC:H2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ILE:HD11	4:A:614:PLC:H4'2	1.97	0.47
1:B:170:THR:HG21	1:B:329:LEU:CG	2.45	0.47
1:A:27:LEU:HD12	5:A:605:CLR:C1	2.45	0.47
1:A:272:ASP:O	1:A:275:VAL:HG12	2.14	0.47
4:A:604:PLC:H1A2	4:A:616:PLC:H1A1	1.96	0.47
1:B:17:LEU:HD11	1:B:390:LEU:HD21	1.96	0.47
1:B:52:ALA:CB	1:B:261:ALA:HB2	2.45	0.47
1:B:374:TYR:HB2	6:B:603:CPL:H252	1.97	0.47
4:B:612:PLC:H7'1	4:B:612:PLC:H4'1	1.71	0.46
1:A:50:LEU:HD12	4:A:603:PLC:H4A2	1.97	0.46
1:A:89:ILE:CG1	1:A:412:ARG:HG2	2.45	0.46
1:A:225:VAL:CG1	4:A:614:PLC:HT'2	2.42	0.46
1:B:55:CYS:SG	4:B:605:PLC:HT'2	2.55	0.46
1:B:60:LEU:HD21	1:B:253:LEU:HD23	1.96	0.46
1:B:56:LEU:HB2	1:B:257:TRP:CG	2.50	0.46
1:B:407:ILE:O	1:B:411:PRO:HD3	2.15	0.46
1:A:256:SER:OG	1:A:396:SER:O	2.33	0.46
1:A:154:LEU:CD1	1:A:175:GLN:HG3	2.43	0.46
1:A:381:ILE:HD13	5:A:609:CLR:C26	2.43	0.46
5:A:605:CLR:H151	5:A:606:CLR:H11	1.96	0.46
1:B:90:THR:O	1:B:94:VAL:HG13	2.16	0.46
4:B:612:PLC:H6'1	4:B:612:PLC:H7A1	1.98	0.46
1:A:97:GLY:HA2	1:A:227:CYS:SG	2.57	0.45
1:B:125:LEU:HD23	6:B:603:CPL:H462	1.97	0.45
1:A:242:LEU:HD13	1:A:242:LEU:O	2.16	0.45
1:A:149:ASP:OD1	1:A:149:ASP:N	2.48	0.45
1:B:134:GLY:HA3	1:B:364:MET:HE1	1.97	0.45
1:B:150:LEU:CD2	1:B:322:MET:HE1	2.46	0.45
1:A:18:HIS:ND1	1:A:272:ASP:OD1	2.45	0.45
6:B:603:CPL:H442	6:B:603:CPL:H472	1.78	0.45
4:B:608:PLC:H7A2	4:B:608:PLC:HTA1	1.72	0.45
2:E:1:NAG:H4	2:E:2:NAG:H2	1.57	0.45
1:A:415:LYS:NZ	1:A:415:LYS:HB2	2.32	0.45
1:A:164:ARG:HB2	1:A:167:TYR:HB2	1.98	0.45
1:B:221:ILE:HD12	4:B:613:PLC:HEA3	1.99	0.45
5:A:605:CLR:H151	5:A:606:CLR:H21	1.98	0.45
1:B:164:ARG:HB3	1:B:166:ASP:OD1	2.17	0.45
1:B:194:VAL:CG2	1:B:289:ILE:HD11	2.47	0.45
4:A:613:PLC:H4A1	4:A:613:PLC:H3'1	1.99	0.45
1:A:244:SER:C	1:A:245:MET:HE2	2.43	0.44
4:A:612:PLC:H63	4:A:612:PLC:H41	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:HB3	1:A:261:ALA:HB2	1.99	0.44
6:A:610:CPL:H43	4:A:613:PLC:HE'2	1.98	0.44
4:A:615:PLC:O2P	4:A:615:PLC:H32	2.17	0.44
1:B:151:GLU:OE2	1:B:175:GLN:HG2	2.17	0.44
1:A:28:GLN:NE2	1:A:43:GLU:OE2	2.50	0.44
1:A:222:LEU:O	1:A:225:VAL:HG22	2.18	0.44
1:A:382:CYS:O	1:A:386:LEU:HB2	2.17	0.44
4:A:613:PLC:H4'2	4:A:613:PLC:H7'2	1.75	0.44
1:B:63:LEU:HD23	1:B:63:LEU:HA	1.82	0.44
4:B:604:PLC:H82	4:B:604:PLC:H42	1.57	0.44
1:B:61:ILE:HD13	1:B:61:ILE:HA	1.91	0.44
1:B:150:LEU:HD23	1:B:178:ALA:CB	2.48	0.44
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.88	0.44
1:A:196:MET:HA	1:A:199:THR:HG22	2.00	0.44
6:A:611:CPL:O31	6:A:611:CPL:HC12	2.05	0.44
4:A:612:PLC:P	4:A:612:PLC:H82	2.57	0.44
1:A:109:TYR:HE2	1:A:391:TYR:CE2	2.36	0.44
4:A:603:PLC:H1A2	4:A:603:PLC:H4A2	1.58	0.44
1:B:150:LEU:HD21	1:B:322:MET:HE1	2.00	0.44
1:A:351:LEU:O	1:A:355:GLU:HG3	2.17	0.44
4:A:614:PLC:H9A1	4:A:614:PLC:H8'2	2.00	0.43
4:B:609:PLC:H73	4:B:609:PLC:H42	1.86	0.43
4:B:612:PLC:CB'	4:B:612:PLC:H9A1	2.48	0.43
1:B:134:GLY:HA3	1:B:364:MET:CE	2.49	0.43
1:B:382:CYS:O	1:B:386:LEU:HB2	2.18	0.43
4:A:604:PLC:HE'1	5:A:605:CLR:C26	2.49	0.43
1:B:6:VAL:HG12	1:B:7:ASP:N	2.29	0.43
1:A:16:TRP:HA	1:A:16:TRP:CE3	2.54	0.43
1:A:52:ALA:CB	1:A:261:ALA:HB2	2.48	0.43
4:A:603:PLC:H42	4:A:603:PLC:H83	1.43	0.43
1:B:39:GLU:OE1	1:B:39:GLU:HA	2.17	0.43
1:B:91:TRP:HA	1:B:91:TRP:HE3	1.84	0.43
4:B:612:PLC:H6'2	4:B:612:PLC:H9'2	1.57	0.43
6:B:603:CPL:H412	6:B:603:CPL:H441	1.85	0.43
4:B:608:PLC:H8'2	4:B:608:PLC:H5'2	1.76	0.43
1:A:23:VAL:HG12	1:A:23:VAL:O	2.18	0.43
1:A:118:ALA:CB	1:A:209:GLU:HG2	2.49	0.43
1:B:25:LEU:N	1:B:43:GLU:OE2	2.50	0.43
4:B:608:PLC:H72	4:B:608:PLC:H42	1.68	0.43
1:A:394:LEU:HD11	4:A:616:PLC:H8A1	2.00	0.43
1:B:194:VAL:HG21	1:B:289:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HD22	4:B:614:PLC:HEA1	2.00	0.43
1:B:5:ARG:H	1:B:5:ARG:HG2	1.61	0.43
4:A:612:PLC:HTA2	4:A:612:PLC:H7A1	1.76	0.42
1:B:149:ASP:N	1:B:149:ASP:OD1	2.51	0.42
1:A:238:SER:HB2	1:A:241:LEU:HB2	2.01	0.42
1:A:322:MET:O	1:A:326:VAL:HG23	2.19	0.42
1:B:332:PHE:O	1:B:336:LEU:HD13	2.19	0.42
6:A:610:CPL:H382	6:A:610:CPL:H411	1.74	0.42
1:B:278:ASP:OD1	1:B:278:ASP:N	2.52	0.42
6:A:610:CPL:H441	6:A:610:CPL:H472	1.61	0.42
5:A:608:CLR:C21	6:A:611:CPL:H221	2.49	0.42
1:B:9:ILE:HD12	1:B:9:ILE:HA	1.90	0.42
1:B:340:ALA:O	1:B:344:LEU:HD23	2.20	0.42
1:B:415:LYS:HE2	1:B:415:LYS:HB3	1.80	0.42
1:A:294:THR:O	1:A:298:LEU:HB2	2.19	0.42
1:A:331:GLN:O	1:A:331:GLN:HG2	2.17	0.42
4:A:604:PLC:HE'3	4:A:604:PLC:H8'2	1.82	0.42
1:B:288:GLN:HG3	1:B:289:ILE:HG13	2.01	0.42
1:B:370:LEU:HD13	1:B:370:LEU:HA	1.92	0.42
5:A:605:CLR:H151	5:A:606:CLR:C2	2.49	0.42
1:B:99:ILE:HG22	1:B:402:ALA:HB2	2.01	0.42
1:B:316:GLN:HB3	1:B:358:LEU:HD21	2.00	0.42
1:A:196:MET:O	1:A:199:THR:HG22	2.20	0.42
1:A:231:CYS:SG	1:A:232:LEU:N	2.92	0.42
1:A:344:LEU:HD13	1:A:344:LEU:HA	1.92	0.42
4:A:614:PLC:H1A2	4:B:607:PLC:OB	2.19	0.42
1:B:27:LEU:HD21	5:B:611:CLR:H193	2.01	0.42
5:A:608:CLR:H183	5:A:609:CLR:H17	2.02	0.42
1:B:12:TRP:HE3	1:B:16:TRP:HD1	1.68	0.42
1:B:239:LYS:CG	1:B:414:TRP:HE1	2.33	0.42
1:B:298:LEU:HD13	6:B:603:CPL:C23	2.49	0.42
1:B:157:LEU:HD21	1:B:343:ASP:CB	2.45	0.41
1:A:25:LEU:H	1:A:43:GLU:CG	2.33	0.41
4:B:612:PLC:H41	4:B:612:PLC:H62	1.84	0.41
1:A:50:LEU:HB2	4:A:603:PLC:C5B	2.31	0.41
1:B:41:TYR:OH	1:B:272:ASP:OD2	2.38	0.41
1:B:147:LYS:HB3	1:B:147:LYS:HE2	1.76	0.41
1:B:334:VAL:N	1:B:335:PRO:HD2	2.36	0.41
1:A:194:VAL:CG2	1:A:289:ILE:HD11	2.51	0.41
1:A:230:ALA:HA	1:A:245:MET:HG3	2.01	0.41
6:A:611:CPL:H341	6:A:611:CPL:H372	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:605:PLC:H72	4:B:605:PLC:O4P	2.20	0.41
4:B:606:PLC:H62	4:B:606:PLC:H41	1.74	0.41
1:A:391:TYR:CE1	4:A:604:PLC:H1'2	2.56	0.41
5:A:608:CLR:C27	6:A:611:CPL:H232	2.50	0.41
6:A:611:CPL:O1P	6:A:611:CPL:HC52	2.21	0.41
4:A:614:PLC:H82	4:A:614:PLC:H41	1.75	0.41
1:B:47:PHE:HE2	5:B:611:CLR:H212	1.85	0.41
1:A:35:SER:HB3	1:A:38:ASP:HB2	2.02	0.41
1:A:4:ALA:HB2	1:A:379:ALA:HB2	2.03	0.41
1:A:8:TYR:CD2	1:A:378:LEU:HD13	2.55	0.41
1:A:91:TRP:HA	1:A:91:TRP:CE3	2.55	0.41
1:A:177:MET:SD	1:A:318:ALA:HA	2.61	0.41
1:A:332:PHE:O	1:A:335:PRO:HD2	2.21	0.41
1:B:239:LYS:HG3	1:B:414:TRP:HE1	1.86	0.41
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.84	0.41
1:B:245:MET:HE2	1:B:245:MET:HA	2.02	0.41
4:B:606:PLC:H4A2	4:B:606:PLC:H1A1	1.61	0.41
1:B:131:THR:HG21	1:B:370:LEU:CD2	2.49	0.41
1:B:151:GLU:OE2	1:B:151:GLU:HA	2.20	0.41
4:B:604:PLC:H3'1	4:B:604:PLC:H6'2	1.93	0.41
1:A:26:ARG:O	1:A:26:ARG:HG3	2.19	0.40
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.95	0.40
1:A:299:TYR:O	1:A:300:CYS:C	2.63	0.40
1:A:170:THR:O	1:A:174:ILE:HG13	2.22	0.40
6:A:610:CPL:HC31	6:A:610:CPL:C13	2.46	0.40
1:B:129:ASN:O	1:B:133:SER:OG	2.29	0.40
1:B:145:LYS:HB3	1:B:145:LYS:HE2	1.93	0.40
1:A:230:ALA:N	1:A:245:MET:HG3	2.36	0.40
5:A:608:CLR:C18	5:A:609:CLR:H17	2.51	0.40
4:A:615:PLC:O4P	4:A:615:PLC:H82	2.21	0.40
1:B:359:HIS:HA	1:B:362:THR:CG2	2.51	0.40
6:B:603:CPL:HC41	6:B:603:CPL:HC73	1.85	0.40
1:A:6:VAL:HG13	1:A:7:ASP:H	1.86	0.40
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.92	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	395/599 (66%)	376 (95%)	19 (5%)	0	100	100
1	B	395/599 (66%)	380 (96%)	15 (4%)	0	100	100
All	All	790/1198 (66%)	756 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/500 (66%)	310 (94%)	21 (6%)	15	27
1	B	331/500 (66%)	313 (95%)	18 (5%)	18	33
All	All	662/1000 (66%)	623 (94%)	39 (6%)	19	29

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	64	VAL
1	A	68	VAL
1	A	149	ASP
1	A	193	GLU
1	A	195	THR
1	A	222	LEU
1	A	231	CYS

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Mol	Chain	Res	Type
1	A	242	LEU
1	A	254	LEU
1	A	298	LEU
1	A	323	GLN
1	A	341	GLU
1	A	344	LEU
1	A	350	LEU
1	A	370	LEU
1	A	386	LEU
1	A	405	THR
1	A	408	CYS
1	A	414	TRP
1	A	416	HIS
1	B	9	ILE
1	B	32	SER
1	B	64	VAL
1	B	67	LEU
1	B	68	VAL
1	B	89	ILE
1	B	195	THR
1	B	227	CYS
1	B	231	CYS
1	B	242	LEU
1	B	298	LEU
1	B	362	THR
1	B	370	LEU
1	B	372	LYS
1	B	378	LEU
1	B	398	LEU
1	B	401	LEU
1	B	416	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	GLN
1	B	184	GLN
1	B	371	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 ⓘ

8 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	$\# Z  > 2$
2	NAG	C	1	2,1	14,14,15	0.79	0	17,19,21	1.16	2 (11%)
2	NAG	C	2	2	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.81	0	17,19,21	0.99	1 (5%)
2	NAG	D	2	2	14,14,15	0.75	0	17,19,21	0.83	0
2	NAG	E	1	2,1	14,14,15	0.77	0	17,19,21	1.06	1 (5%)
2	NAG	E	2	2	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.80	0	17,19,21	0.94	0
2	NAG	F	2	2	14,14,15	0.76	0	17,19,21	0.82	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C2-N2-C7	2.56	126.56	122.90
2	E	2	NAG	C2-N2-C7	2.54	126.52	122.90
2	C	1	NAG	O5-C1-C2	-2.39	107.51	111.29
2	C	1	NAG	O4-C4-C3	-2.39	104.83	110.35
2	E	1	NAG	O4-C4-C3	-2.06	105.59	110.35
2	D	1	NAG	O4-C4-C3	-2.05	105.61	110.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

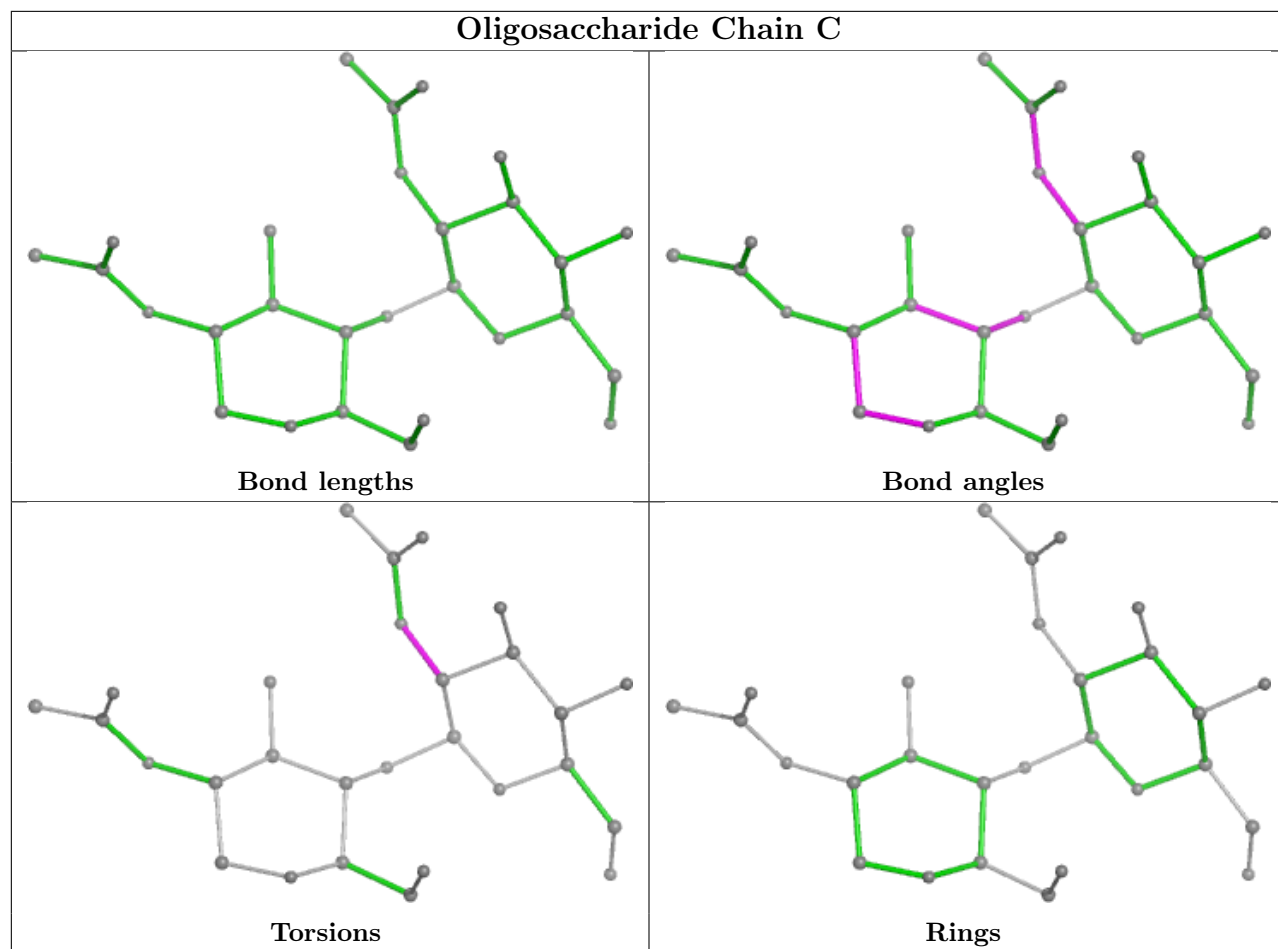
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C1-C2-N2-C7

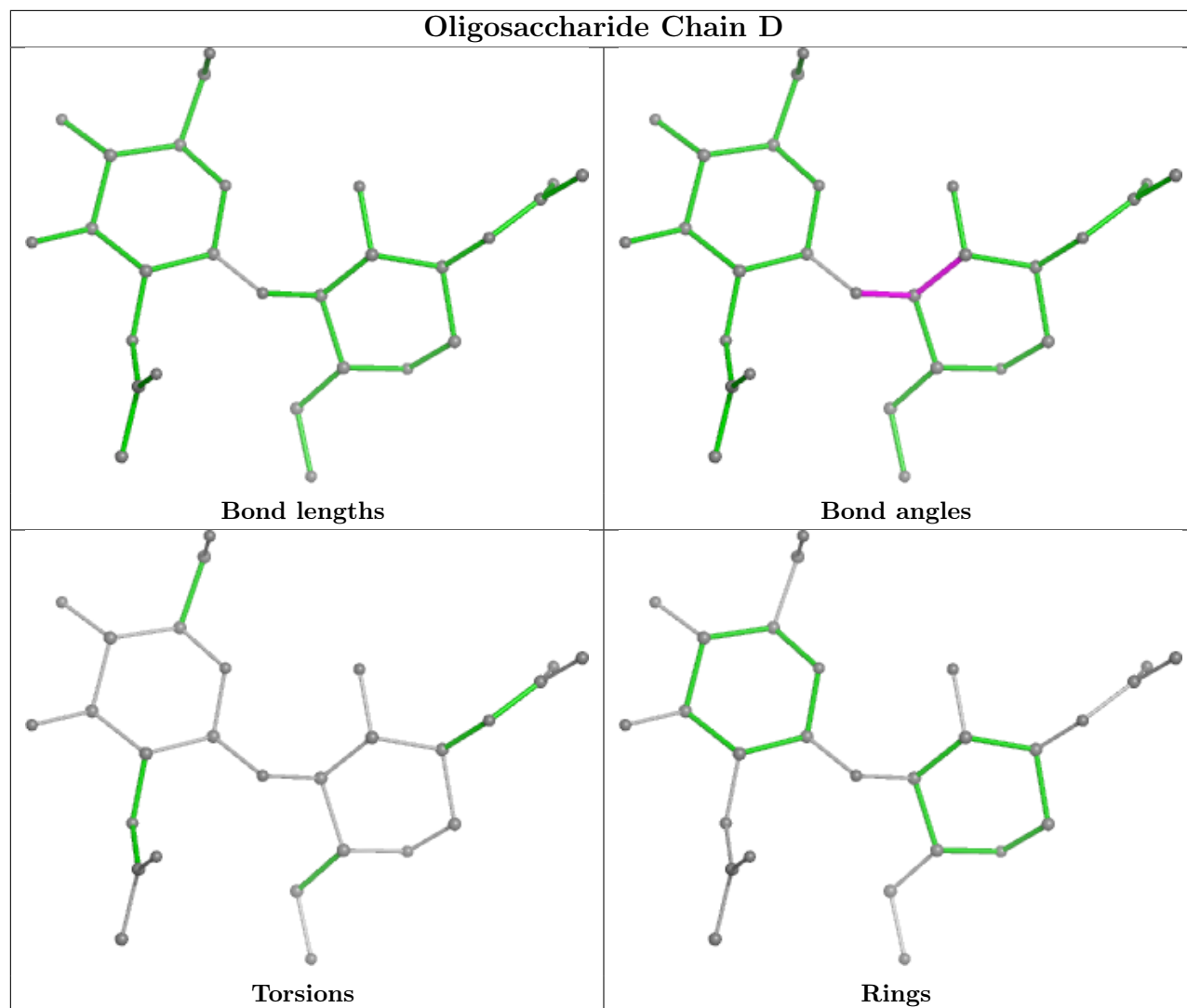
There are no ring outliers.

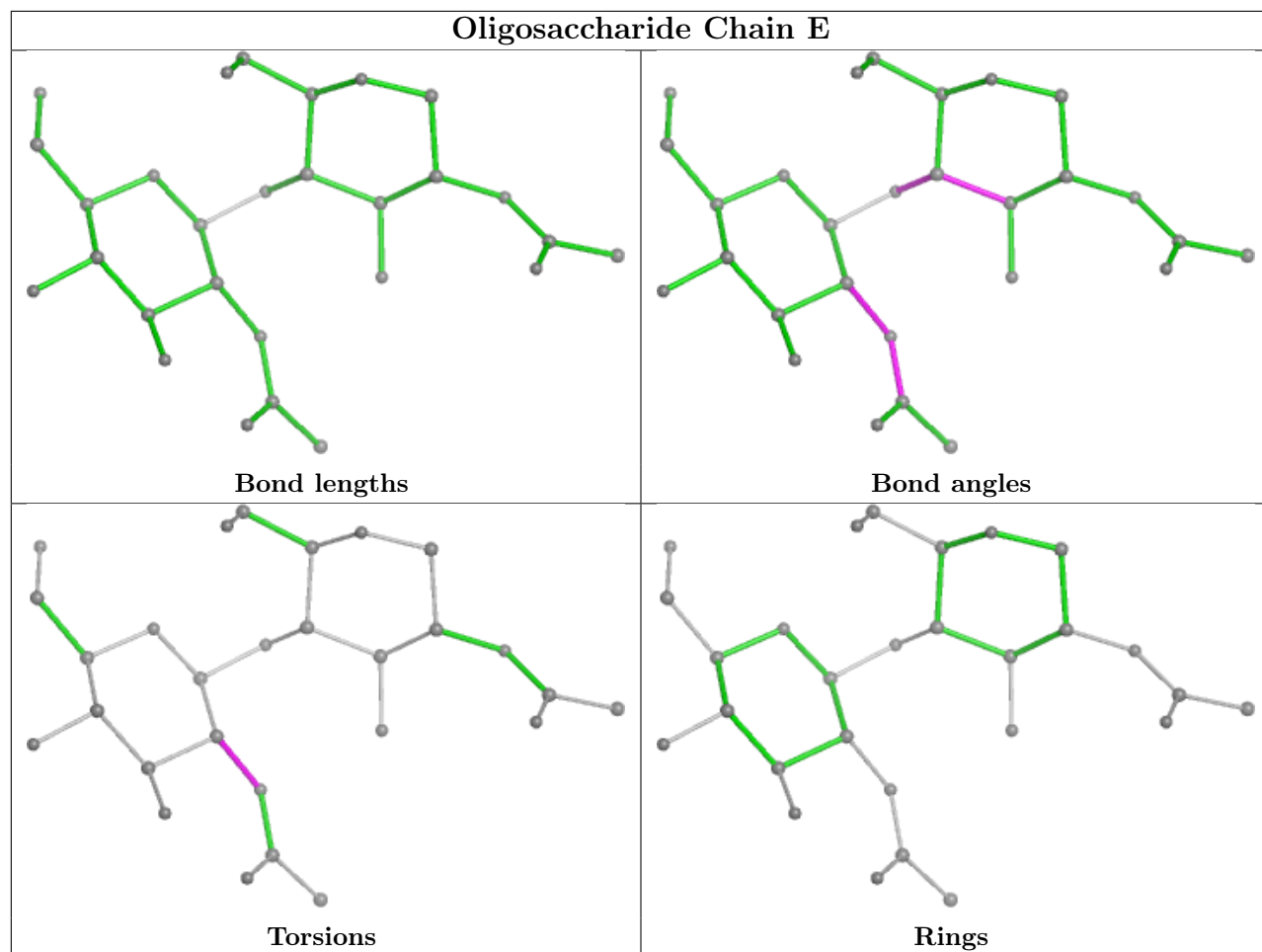
4 monomers are involved in 6 short contacts:

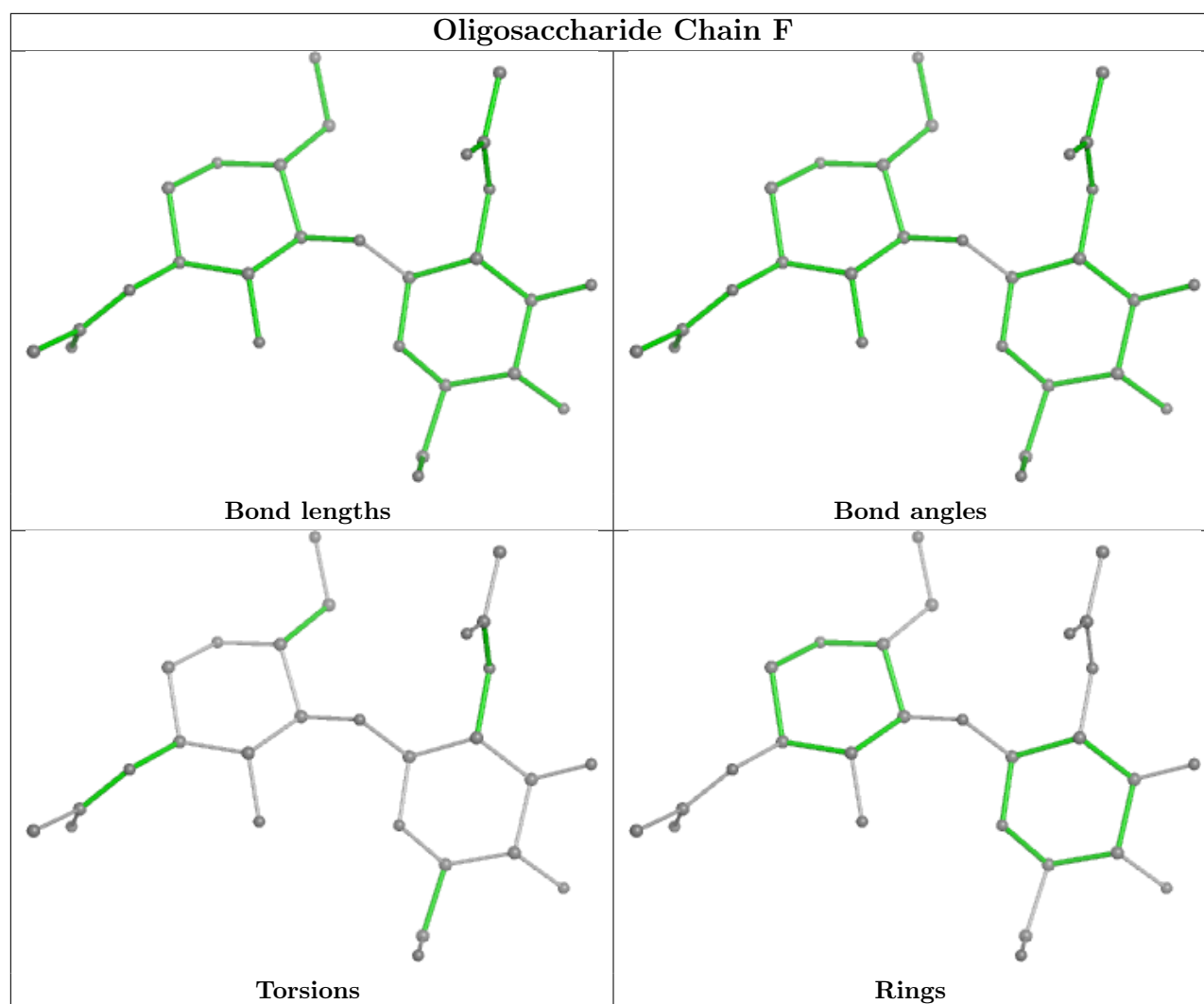
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	3	0
2	E	1	NAG	2	0
2	C	2	NAG	3	0
2	C	1	NAG	2	0

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









## 5.6 Ligand geometry [i](#)

30 ligands 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	PLC	A	607	-	41,41,41	1.10	3 (7%)	47,49,49	1.15	3 (6%)
4	PLC	B	613	-	41,41,41	1.10	4 (9%)	47,49,49	1.06	3 (6%)
4	PLC	B	614	-	41,41,41	1.10	4 (9%)	47,49,49	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CPL	A	611	-	51,51,51	1.50	7 (13%)	57,59,59	1.14	3 (5%)
5	CLR	A	606	-	31,31,31	0.37	0	48,48,48	0.51	0
3	NAG	A	602	1	14,14,15	0.76	0	17,19,21	0.81	0
4	PLC	A	614	-	41,41,41	1.11	4 (9%)	47,49,49	1.14	3 (6%)
5	CLR	A	605	-	31,31,31	0.39	0	48,48,48	0.59	0
4	PLC	B	604	-	41,41,41	1.11	4 (9%)	47,49,49	1.14	3 (6%)
3	NAG	B	601	1	14,14,15	0.75	0	17,19,21	0.78	0
3	NAG	A	601	1	14,14,15	0.79	0	17,19,21	0.78	0
4	PLC	B	608	-	41,41,41	1.11	4 (9%)	47,49,49	1.16	3 (6%)
5	CLR	B	611	-	31,31,31	0.37	0	48,48,48	0.49	0
3	NAG	B	602	1	14,14,15	0.75	0	17,19,21	0.81	0
6	CPL	B	603	-	51,51,51	1.49	7 (13%)	57,59,59	1.16	4 (7%)
4	PLC	A	604	-	41,41,41	1.10	4 (9%)	47,49,49	1.14	3 (6%)
4	PLC	B	607	-	41,41,41	1.11	4 (9%)	47,49,49	1.12	3 (6%)
4	PLC	B	612	-	41,41,41	1.12	4 (9%)	47,49,49	1.18	3 (6%)
4	PLC	B	609	-	41,41,41	1.12	3 (7%)	47,49,49	1.12	3 (6%)
4	PLC	A	616	-	41,41,41	1.11	4 (9%)	47,49,49	0.98	3 (6%)
5	CLR	B	610	-	31,31,31	0.39	0	48,48,48	0.45	0
4	PLC	A	615	-	41,41,41	1.11	4 (9%)	47,49,49	1.13	3 (6%)
4	PLC	B	606	-	41,41,41	1.11	4 (9%)	47,49,49	1.18	3 (6%)
4	PLC	A	612	-	41,41,41	1.11	4 (9%)	47,49,49	1.13	3 (6%)
5	CLR	A	608	-	31,31,31	0.49	0	48,48,48	0.82	0
6	CPL	A	610	-	51,51,51	1.51	7 (13%)	57,59,59	1.14	3 (5%)
5	CLR	A	609	-	31,31,31	0.43	0	48,48,48	0.60	0
4	PLC	B	605	-	41,41,41	1.12	4 (9%)	47,49,49	1.11	3 (6%)
4	PLC	A	613	-	41,41,41	1.11	4 (9%)	47,49,49	1.14	3 (6%)
4	PLC	A	603	-	41,41,41	1.12	4 (9%)	47,49,49	1.14	3 (6%)

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	PLC	A	607	-	-	18/45/45/45	-
4	PLC	B	613	-	-	18/45/45/45	-
4	PLC	B	614	-	-	20/45/45/45	-
6	CPL	A	611	-	-	30/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLR	A	606	-	-	5/10/68/68	0/4/4/4
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	PLC	A	614	-	-	11/45/45/45	-
5	CLR	A	605	-	-	0/10/68/68	0/4/4/4
4	PLC	B	604	-	-	12/45/45/45	-
3	NAG	B	601	1	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	PLC	B	608	-	-	14/45/45/45	-
5	CLR	B	611	-	-	2/10/68/68	0/4/4/4
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
6	CPL	B	603	-	-	24/55/55/55	-
4	PLC	A	604	-	-	17/45/45/45	-
4	PLC	B	607	-	-	16/45/45/45	-
4	PLC	B	612	-	-	17/45/45/45	-
4	PLC	B	609	-	-	21/45/45/45	-
4	PLC	A	616	-	-	26/45/45/45	-
5	CLR	B	610	-	-	1/10/68/68	0/4/4/4
4	PLC	A	615	-	-	13/45/45/45	-
4	PLC	B	606	-	-	19/45/45/45	-
4	PLC	A	612	-	-	12/45/45/45	-
5	CLR	A	608	-	-	1/10/68/68	0/4/4/4
6	CPL	A	610	-	-	30/55/55/55	-
5	CLR	A	609	-	-	7/10/68/68	0/4/4/4
4	PLC	B	605	-	-	14/45/45/45	-
4	PLC	A	613	-	-	15/45/45/45	-
4	PLC	A	603	-	-	21/45/45/45	-

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	610	CPL	C40-C39	4.21	1.56	1.31
6	A	611	CPL	C40-C39	4.17	1.55	1.31
6	B	603	CPL	C40-C39	4.13	1.55	1.31
6	A	611	CPL	C43-C42	3.95	1.54	1.31
6	A	610	CPL	C43-C42	3.93	1.54	1.31
6	B	603	CPL	C43-C42	3.91	1.54	1.31
6	B	603	CPL	O3-C11	3.64	1.44	1.33
6	A	610	CPL	O3-C11	3.62	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	611	CPL	O3-C11	3.60	1.43	1.33
6	A	611	CPL	O2-C31	3.28	1.43	1.34
6	A	610	CPL	O2-C31	3.25	1.43	1.34
6	B	603	CPL	O2-C31	3.16	1.43	1.34
6	B	603	CPL	O2-C2	-2.67	1.39	1.46
4	A	607	PLC	O2-C2	-2.65	1.40	1.46
4	B	609	PLC	O3-CB	2.63	1.41	1.33
4	A	612	PLC	O2-C2	-2.58	1.40	1.46
6	A	610	CPL	O2-C2	-2.57	1.40	1.46
6	A	611	CPL	O2-C2	-2.56	1.40	1.46
4	B	609	PLC	O2-C2	-2.55	1.40	1.46
4	A	615	PLC	O2-C2	-2.55	1.40	1.46
4	B	605	PLC	O2-C2	-2.54	1.40	1.46
4	A	614	PLC	O2-C2	-2.53	1.40	1.46
4	A	604	PLC	O2-C2	-2.52	1.40	1.46
4	A	613	PLC	O2-C2	-2.52	1.40	1.46
4	B	606	PLC	O2-C2	-2.52	1.40	1.46
4	B	604	PLC	O2-C2	-2.50	1.40	1.46
4	B	607	PLC	O2-C2	-2.50	1.40	1.46
4	B	612	PLC	O3-CB	2.49	1.40	1.33
4	B	612	PLC	O2-C2	-2.47	1.40	1.46
4	B	605	PLC	O3-CB	2.47	1.40	1.33
4	A	603	PLC	O3-CB	2.46	1.40	1.33
4	B	607	PLC	O3-CB	2.46	1.40	1.33
4	B	613	PLC	O2-C2	-2.45	1.40	1.46
4	A	616	PLC	O3-CB	2.44	1.40	1.33
4	A	614	PLC	O3-CB	2.44	1.40	1.33
4	A	616	PLC	O2-C2	-2.43	1.40	1.46
4	B	614	PLC	O2-C2	-2.42	1.40	1.46
4	A	603	PLC	O2-C2	-2.42	1.40	1.46
4	B	613	PLC	O3-CB	2.41	1.40	1.33
4	A	604	PLC	O3-CB	2.41	1.40	1.33
4	B	604	PLC	O3-CB	2.40	1.40	1.33
4	A	613	PLC	O3-CB	2.40	1.40	1.33
4	A	612	PLC	O3-CB	2.40	1.40	1.33
4	A	615	PLC	O3-CB	2.40	1.40	1.33
4	B	614	PLC	O3-CB	2.39	1.40	1.33
4	B	606	PLC	O3-CB	2.39	1.40	1.33
4	B	608	PLC	O3-CB	2.35	1.40	1.33
4	A	607	PLC	O3-CB	2.33	1.40	1.33
4	B	608	PLC	O2-C2	-2.32	1.40	1.46
4	B	608	PLC	O2-C'	2.28	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	616	PLC	O2-C'	2.22	1.40	1.34
6	A	610	CPL	P-O3P	2.21	1.68	1.59
4	A	603	PLC	O2-C'	2.20	1.40	1.34
4	B	606	PLC	O3-C3	-2.17	1.40	1.45
4	B	608	PLC	O3-C3	-2.16	1.40	1.45
6	B	603	CPL	P-O3P	2.15	1.68	1.59
4	A	614	PLC	O2-C'	2.15	1.40	1.34
6	A	611	CPL	P-O3P	2.14	1.68	1.59
4	B	612	PLC	O2-C'	2.14	1.40	1.34
4	B	607	PLC	O2-C'	2.14	1.40	1.34
4	B	605	PLC	O2-C'	2.14	1.40	1.34
4	B	604	PLC	O2-C'	2.12	1.40	1.34
4	B	606	PLC	O2-C'	2.12	1.40	1.34
4	B	614	PLC	O2-C'	2.12	1.40	1.34
4	B	604	PLC	O3-C3	-2.12	1.40	1.45
6	A	610	CPL	P-O4P	2.12	1.67	1.59
4	A	615	PLC	O3-C3	-2.11	1.40	1.45
4	A	613	PLC	O2-C'	2.11	1.40	1.34
6	B	603	CPL	P-O4P	2.11	1.67	1.59
6	A	611	CPL	P-O4P	2.11	1.67	1.59
4	A	612	PLC	O3-C3	-2.11	1.40	1.45
4	B	613	PLC	O2-C'	2.10	1.40	1.34
4	B	613	PLC	O3-C3	-2.10	1.40	1.45
4	A	615	PLC	O2-C'	2.10	1.40	1.34
4	B	609	PLC	O2-C'	2.09	1.40	1.34
4	A	607	PLC	O3-C3	-2.09	1.40	1.45
4	A	614	PLC	O3-C3	-2.08	1.40	1.45
4	A	603	PLC	O3-C3	-2.08	1.40	1.45
4	A	616	PLC	O3-C3	-2.07	1.40	1.45
4	A	613	PLC	O3-C3	-2.07	1.40	1.45
4	A	612	PLC	O2-C'	2.07	1.40	1.34
4	B	612	PLC	O3-C3	-2.06	1.40	1.45
4	A	604	PLC	O2-C'	2.05	1.40	1.34
4	B	607	PLC	O3-C3	-2.04	1.40	1.45
4	B	605	PLC	O3-C3	-2.02	1.40	1.45
4	B	614	PLC	O3-C3	-2.02	1.40	1.45
4	A	604	PLC	O3-C3	-2.02	1.40	1.45

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	606	PLC	O2-C'-C1'	4.26	120.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	612	PLC	O2-C'-C1'	4.09	120.32	111.50
4	A	603	PLC	O2-C'-C1'	4.06	120.25	111.50
6	A	610	CPL	O2-C31-C32	4.02	120.16	111.50
6	A	611	CPL	O2-C31-C32	4.02	120.16	111.50
4	B	604	PLC	O2-C'-C1'	4.01	120.14	111.50
4	B	608	PLC	O2-C'-C1'	3.98	120.08	111.50
4	B	609	PLC	O2-C'-C1'	3.95	120.02	111.50
4	A	613	PLC	O2-C'-C1'	3.94	119.98	111.50
4	A	607	PLC	O2-C'-C1'	3.93	119.97	111.50
4	A	612	PLC	O2-C'-C1'	3.92	119.95	111.50
4	A	614	PLC	O2-C'-C1'	3.90	119.90	111.50
4	A	604	PLC	O2-C'-C1'	3.88	119.87	111.50
4	A	615	PLC	O2-C'-C1'	3.85	119.80	111.50
4	B	613	PLC	O2-C'-C1'	3.85	119.79	111.50
4	B	614	PLC	O2-C'-C1'	3.84	119.78	111.50
4	B	607	PLC	O2-C'-C1'	3.84	119.78	111.50
4	B	605	PLC	O2-C'-C1'	3.80	119.69	111.50
6	B	603	CPL	O2-C31-C32	3.76	119.60	111.50
4	A	616	PLC	O2-C'-C1'	3.47	118.97	111.50
4	B	609	PLC	O3-CB-C1B	2.80	120.68	111.91
4	B	612	PLC	O3-CB-C1B	2.74	120.51	111.91
4	B	614	PLC	O3-CB-C1B	2.73	120.49	111.91
6	B	603	CPL	O3-C11-C12	2.71	120.41	111.91
4	B	607	PLC	O3-CB-C1B	2.71	120.40	111.91
4	A	603	PLC	O3-CB-C1B	2.69	120.36	111.91
4	B	605	PLC	O3-CB-C1B	2.68	120.33	111.91
4	B	604	PLC	O3-CB-C1B	2.68	120.31	111.91
4	A	614	PLC	O3-CB-C1B	2.66	120.24	111.91
4	A	604	PLC	O3-CB-C1B	2.61	120.10	111.91
4	A	613	PLC	O3-CB-C1B	2.60	120.06	111.91
4	A	607	PLC	O3-CB-C1B	2.60	120.05	111.91
4	A	615	PLC	O3-CB-C1B	2.57	119.98	111.91
4	B	613	PLC	O3-CB-C1B	2.56	119.95	111.91
4	B	606	PLC	O3-CB-C1B	2.56	119.95	111.91
6	A	610	CPL	O3-C11-C12	2.53	119.85	111.91
4	B	608	PLC	O3-CB-C1B	2.49	119.73	111.91
6	A	611	CPL	O3-C11-C12	2.46	119.63	111.91
4	A	612	PLC	O3-CB-C1B	2.43	119.54	111.91
4	A	616	PLC	O3-CB-C1B	2.43	119.52	111.91
4	B	613	PLC	O2P-P-O1P	-2.41	100.32	112.24
4	A	603	PLC	O2P-P-O1P	-2.38	100.50	112.24
4	B	609	PLC	O2P-P-O1P	-2.36	100.59	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	607	PLC	O2P-P-O1P	-2.32	100.77	112.24
4	A	616	PLC	O2P-P-O1P	-2.31	100.81	112.24
4	B	606	PLC	O2P-P-O1P	-2.30	100.85	112.24
4	B	612	PLC	O2P-P-O1P	-2.27	101.01	112.24
4	B	605	PLC	O2P-P-O1P	-2.27	101.02	112.24
6	A	611	CPL	O2P-P-O1P	-2.27	101.04	112.24
4	B	608	PLC	O2P-P-O1P	-2.26	101.06	112.24
4	B	607	PLC	O2P-P-O1P	-2.26	101.08	112.24
6	A	610	CPL	O2P-P-O1P	-2.25	101.11	112.24
4	B	604	PLC	O2P-P-O1P	-2.25	101.11	112.24
4	A	614	PLC	O2P-P-O1P	-2.25	101.12	112.24
4	B	614	PLC	O2P-P-O1P	-2.25	101.14	112.24
4	A	615	PLC	O2P-P-O1P	-2.25	101.14	112.24
4	A	612	PLC	O2P-P-O1P	-2.24	101.15	112.24
4	A	613	PLC	O2P-P-O1P	-2.24	101.17	112.24
6	B	603	CPL	O2P-P-O1P	-2.21	101.34	112.24
6	B	603	CPL	C4-C5-N	-2.20	108.44	115.78
4	A	604	PLC	O2P-P-O1P	-2.19	101.41	112.24

There are no chirality outliers.

All (386) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	PLC	O4P-C4-C5-N
4	A	603	PLC	C1'-C'-O2-C2
4	A	603	PLC	C4-O4P-P-O1P
4	A	604	PLC	C1-O3P-P-O1P
4	A	604	PLC	C4-O4P-P-O1P
4	A	604	PLC	C4-O4P-P-O2P
4	A	604	PLC	C4-O4P-P-O3P
4	A	607	PLC	C4-O4P-P-O1P
4	A	607	PLC	C4-O4P-P-O2P
4	A	607	PLC	C4-O4P-P-O3P
4	A	612	PLC	C1-O3P-P-O2P
4	A	613	PLC	C5-C4-O4P-P
4	A	613	PLC	C4-O4P-P-O1P
4	A	613	PLC	C4-O4P-P-O2P
4	A	613	PLC	C4-O4P-P-O3P
4	A	615	PLC	C4-O4P-P-O1P
4	A	615	PLC	C4-O4P-P-O3P
4	A	616	PLC	O3P-C1-C2-O2
4	A	616	PLC	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
4	A	616	PLC	C1-O3P-P-O2P
4	A	616	PLC	C1-O3P-P-O4P
4	B	604	PLC	C1'-C'-O2-C2
4	B	604	PLC	O'-C'-O2-C2
4	B	605	PLC	C1-O3P-P-O2P
4	B	605	PLC	C1-O3P-P-O4P
4	B	607	PLC	C1-O3P-P-O1P
4	B	607	PLC	C1-O3P-P-O2P
4	B	607	PLC	C1-O3P-P-O4P
4	B	609	PLC	O4P-C4-C5-N
4	B	609	PLC	C1'-C'-O2-C2
4	B	609	PLC	C1-O3P-P-O1P
4	B	609	PLC	C1-O3P-P-O2P
4	B	612	PLC	O4P-C4-C5-N
4	B	612	PLC	C1B-CB-O3-C3
4	B	612	PLC	OB-CB-O3-C3
4	B	612	PLC	C1-O3P-P-O2P
4	B	612	PLC	C4-O4P-P-O1P
4	B	613	PLC	O4P-C4-C5-N
4	B	613	PLC	C1'-C'-O2-C2
4	B	613	PLC	C4-O4P-P-O1P
4	B	614	PLC	C1-O3P-P-O1P
6	A	610	CPL	C12-C11-O3-C3
6	A	610	CPL	C40-C41-C42-C43
6	A	611	CPL	C2-C1-O3P-P
6	A	611	CPL	O4P-C4-C5-N
6	A	611	CPL	C5-C4-O4P-P
6	A	611	CPL	C32-C31-O2-C2
6	A	611	CPL	C1-O3P-P-O1P
6	A	611	CPL	C1-O3P-P-O2P
6	A	611	CPL	C4-O4P-P-O1P
6	A	611	CPL	C4-O4P-P-O2P
6	A	611	CPL	C4-O4P-P-O3P
6	B	603	CPL	O4P-C4-C5-N
6	B	603	CPL	C32-C31-O2-C2
6	B	603	CPL	O31-C31-O2-C2
6	B	603	CPL	C39-C40-C41-C42
4	A	607	PLC	OB-CB-O3-C3
6	A	610	CPL	O11-C11-O3-C3
4	B	609	PLC	C2-C3-O3-CB
4	B	607	PLC	C1B-CB-O3-C3
4	B	614	PLC	C1B-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
4	B	604	PLC	OB-CB-O3-C3
4	B	607	PLC	OB-CB-O3-C3
4	B	614	PLC	OB-CB-O3-C3
5	A	606	CLR	C13-C17-C20-C21
4	A	603	PLC	O'-C'-O2-C2
4	A	613	PLC	O'-C'-O2-C2
4	B	609	PLC	O'-C'-O2-C2
4	B	613	PLC	O'-C'-O2-C2
6	A	610	CPL	O31-C31-O2-C2
6	A	611	CPL	O31-C31-O2-C2
4	A	607	PLC	C1B-CB-O3-C3
4	B	604	PLC	C1B-CB-O3-C3
4	A	613	PLC	C1'-C'-O2-C2
6	A	610	CPL	C32-C31-O2-C2
4	A	603	PLC	OB-CB-O3-C3
5	A	606	CLR	C16-C17-C20-C21
5	A	606	CLR	C13-C17-C20-C22
4	A	613	PLC	OB-CB-O3-C3
4	A	613	PLC	C1B-CB-O3-C3
4	A	614	PLC	C1B-CB-O3-C3
4	B	606	PLC	C1B-CB-O3-C3
6	A	611	CPL	C12-C11-O3-C3
4	B	606	PLC	OB-CB-O3-C3
5	A	606	CLR	C16-C17-C20-C22
4	A	603	PLC	C1B-CB-O3-C3
4	B	613	PLC	C1B-CB-O3-C3
4	B	613	PLC	OB-CB-O3-C3
4	A	613	PLC	C2B-C3B-C4B-C5B
4	B	612	PLC	C6'-C7'-C8'-C9'
6	A	611	CPL	O11-C11-O3-C3
5	A	609	CLR	C21-C20-C22-C23
4	A	614	PLC	OB-CB-O3-C3
4	B	608	PLC	C1B-C2B-C3B-C4B
4	B	612	PLC	C4'-C5'-C6'-C7'
4	A	613	PLC	C4'-C5'-C6'-C7'
4	B	606	PLC	C4'-C5'-C6'-C7'
5	A	609	CLR	C17-C20-C22-C23
4	A	607	PLC	C1'-C'-O2-C2
6	A	611	CPL	C11-C12-C13-C14
4	A	603	PLC	O2-C2-C3-O3
4	A	604	PLC	C2B-C3B-C4B-C5B
6	A	611	CPL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
5	B	611	CLR	C22-C23-C24-C25
4	A	603	PLC	CB-C1B-C2B-C3B
4	B	607	PLC	C'-C1'-C2'-C3'
4	B	609	PLC	CB-C1B-C2B-C3B
4	B	612	PLC	CB-C1B-C2B-C3B
4	B	608	PLC	C3'-C4'-C5'-C6'
6	A	610	CPL	C44-C45-C46-C47
4	A	607	PLC	O'-C'-O2-C2
4	A	614	PLC	CB-C1B-C2B-C3B
4	B	613	PLC	C'-C1'-C2'-C3'
4	A	615	PLC	C1'-C'-O2-C2
4	B	614	PLC	C1'-C'-O2-C2
4	A	612	PLC	C3'-C4'-C5'-C6'
4	A	612	PLC	C1-O3P-P-O4P
4	A	613	PLC	C1-O3P-P-O4P
4	B	607	PLC	C4-O4P-P-O3P
4	B	609	PLC	C1-O3P-P-O4P
4	B	612	PLC	C1-O3P-P-O4P
4	B	612	PLC	C4-O4P-P-O3P
4	B	614	PLC	C1-O3P-P-O4P
6	A	610	CPL	C4-O4P-P-O3P
6	A	611	CPL	C1-O3P-P-O4P
6	B	603	CPL	C1-O3P-P-O4P
4	B	609	PLC	C1B-CB-O3-C3
4	A	615	PLC	O'-C'-O2-C2
4	B	614	PLC	O'-C'-O2-C2
4	A	615	PLC	C1B-CB-O3-C3
4	B	608	PLC	C5'-C6'-C7'-C8'
4	A	604	PLC	C1'-C'-O2-C2
4	A	616	PLC	C4B-C5B-C6B-C7B
4	B	606	PLC	C6B-C7B-C8B-C9B
4	B	609	PLC	C6B-C7B-C8B-C9B
4	B	614	PLC	C2'-C3'-C4'-C5'
6	B	603	CPL	C21-C22-C23-C24
6	A	611	CPL	C1-C2-O2-C31
4	A	604	PLC	O'-C'-O2-C2
4	B	613	PLC	C2'-C3'-C4'-C5'
6	B	603	CPL	C12-C11-O3-C3
4	B	613	PLC	C3B-C4B-C5B-C6B
6	A	610	CPL	C19-C20-C21-C22
4	A	604	PLC	C7'-C8'-C9'-CA'
6	A	611	CPL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
4	B	609	PLC	OB-CB-O3-C3
4	A	604	PLC	C4'-C5'-C6'-C7'
4	B	605	PLC	C4'-C5'-C6'-C7'
4	B	608	PLC	C1'-C2'-C3'-C4'
4	B	614	PLC	C2B-C3B-C4B-C5B
4	A	612	PLC	C2'-C3'-C4'-C5'
4	B	612	PLC	C3B-C4B-C5B-C6B
6	A	610	CPL	C18-C19-C20-C21
5	B	611	CLR	C20-C22-C23-C24
4	B	614	PLC	C1'-C2'-C3'-C4'
6	A	611	CPL	C22-C23-C24-C25
4	B	605	PLC	C1B-CB-O3-C3
4	A	612	PLC	C2B-C3B-C4B-C5B
4	A	614	PLC	C3B-C4B-C5B-C6B
4	B	604	PLC	C4'-C5'-C6'-C7'
4	B	608	PLC	C4'-C5'-C6'-C7'
6	A	610	CPL	C41-C42-C43-C44
4	A	607	PLC	C4'-C5'-C6'-C7'
4	A	615	PLC	OB-CB-O3-C3
4	A	616	PLC	C4'-C5'-C6'-C7'
4	B	608	PLC	C2'-C3'-C4'-C5'
4	B	604	PLC	C2B-C3B-C4B-C5B
4	B	613	PLC	C1B-C2B-C3B-C4B
6	B	603	CPL	O11-C11-O3-C3
4	B	609	PLC	C1B-C2B-C3B-C4B
4	B	605	PLC	OB-CB-O3-C3
6	A	611	CPL	C31-C32-C33-C34
6	B	603	CPL	C20-C21-C22-C23
4	A	616	PLC	C2B-C3B-C4B-C5B
4	A	616	PLC	C1'-C'-O2-C2
4	A	616	PLC	O'-C'-O2-C2
4	B	606	PLC	O2-C2-C3-O3
4	A	612	PLC	C4'-C5'-C6'-C7'
5	A	609	CLR	C13-C17-C20-C22
6	B	603	CPL	C11-C12-C13-C14
4	A	607	PLC	C2'-C3'-C4'-C5'
4	A	603	PLC	C4-O4P-P-O3P
6	A	611	CPL	C14-C15-C16-C17
4	A	616	PLC	C2-C1-O3P-P
4	A	616	PLC	O3P-C1-C2-C3
4	B	606	PLC	O3P-C1-C2-C3
6	A	611	CPL	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	610	CPL	C36-C37-C38-C39
4	A	607	PLC	C6'-C7'-C8'-C9'
4	B	606	PLC	C5B-C6B-C7B-C8B
4	B	607	PLC	C1B-C2B-C3B-C4B
4	A	603	PLC	C1-C2-C3-O3
4	A	616	PLC	C1-C2-C3-O3
6	A	610	CPL	C38-C39-C40-C41
4	B	614	PLC	C7B-C8B-C9B-CAA
4	A	604	PLC	C1'-C2'-C3'-C4'
4	B	608	PLC	C7'-C8'-C9'-CA'
4	A	603	PLC	C1B-C2B-C3B-C4B
6	B	603	CPL	C15-C16-C17-C18
4	A	616	PLC	C1'-C2'-C3'-C4'
6	A	610	CPL	C45-C46-C47-C48
4	B	614	PLC	C4'-C5'-C6'-C7'
4	B	608	PLC	C3B-C4B-C5B-C6B
4	B	605	PLC	O3P-C1-C2-O2
4	B	607	PLC	O3P-C1-C2-O2
4	B	613	PLC	O3P-C1-C2-O2
5	A	609	CLR	C16-C17-C20-C21
5	A	609	CLR	C13-C17-C20-C21
4	B	609	PLC	C4'-C5'-C6'-C7'
4	A	616	PLC	C5B-C6B-C7B-C8B
4	A	604	PLC	C4B-C5B-C6B-C7B
4	A	614	PLC	C1B-C2B-C3B-C4B
4	A	612	PLC	C1B-C2B-C3B-C4B
5	A	609	CLR	C16-C17-C20-C22
6	B	603	CPL	C23-C24-C25-C26
4	A	603	PLC	O3P-C1-C2-C3
4	A	607	PLC	O3P-C1-C2-C3
4	B	613	PLC	O3P-C1-C2-C3
6	A	610	CPL	O3P-C1-C2-C3
6	B	603	CPL	O3P-C1-C2-C3
4	B	614	PLC	CB-C1B-C2B-C3B
4	B	606	PLC	CB-C1B-C2B-C3B
4	A	616	PLC	C6'-C7'-C8'-C9'
6	A	610	CPL	C33-C34-C35-C36
4	B	606	PLC	C1-C2-C3-O3
4	A	604	PLC	C1-O3P-P-O4P
4	B	613	PLC	C4-O4P-P-O3P
6	A	610	CPL	C39-C40-C41-C42
6	A	611	CPL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
6	B	603	CPL	C40-C41-C42-C43
4	A	615	PLC	C2B-C3B-C4B-C5B
4	A	603	PLC	O3P-C1-C2-O2
4	A	607	PLC	O3P-C1-C2-O2
4	B	604	PLC	O3P-C1-C2-O2
6	A	611	CPL	C36-C37-C38-C39
4	B	605	PLC	C1B-C2B-C3B-C4B
4	A	616	PLC	C2'-C3'-C4'-C5'
4	B	613	PLC	C2-C1-O3P-P
4	B	614	PLC	C2-C1-O3P-P
4	B	605	PLC	O3P-C1-C2-C3
4	A	614	PLC	O2-C'-C1'-C2'
4	B	612	PLC	C1'-C2'-C3'-C4'
4	B	608	PLC	C2B-C3B-C4B-C5B
6	A	611	CPL	C42-C43-C44-C45
4	A	603	PLC	C1-C2-O2-C'
4	A	607	PLC	C3-C2-O2-C'
4	B	609	PLC	C1-C2-C3-O3
6	A	610	CPL	O3P-C1-C2-O2
6	B	603	CPL	C44-C45-C46-C47
4	B	614	PLC	C4B-C5B-C6B-C7B
4	B	609	PLC	C5B-C6B-C7B-C8B
6	A	611	CPL	C23-C24-C25-C26
4	A	616	PLC	O2-C2-C3-O3
4	B	606	PLC	C6'-C7'-C8'-C9'
4	B	614	PLC	C1B-C2B-C3B-C4B
4	A	615	PLC	C3B-C4B-C5B-C6B
4	A	603	PLC	C7B-C8B-C9B-CAA
4	A	612	PLC	C4-O4P-P-O3P
4	A	614	PLC	C4-O4P-P-O3P
4	A	615	PLC	C1-O3P-P-O4P
4	B	604	PLC	C4-O4P-P-O3P
4	B	608	PLC	C4-O4P-P-O3P
4	B	605	PLC	C3'-C4'-C5'-C6'
4	A	607	PLC	C2-C1-O3P-P
4	A	612	PLC	C1-O3P-P-O1P
4	A	612	PLC	C4-O4P-P-O2P
4	A	613	PLC	C1-O3P-P-O1P
4	A	615	PLC	C4-O4P-P-O2P
4	A	616	PLC	C1-O3P-P-O1P
4	B	605	PLC	C1-O3P-P-O1P
4	B	605	PLC	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
4	B	607	PLC	C4-O4P-P-O1P
4	B	612	PLC	C1-O3P-P-O1P
6	A	610	CPL	C4-O4P-P-O1P
6	A	610	CPL	C4-O4P-P-O2P
6	B	603	CPL	C1-O3P-P-O2P
6	B	603	CPL	C4-O4P-P-O2P
4	A	612	PLC	C5'-C6'-C7'-C8'
6	B	603	CPL	C32-C33-C34-C35
4	A	613	PLC	C7B-C8B-C9B-CAA
4	B	606	PLC	C1'-C2'-C3'-C4'
4	A	603	PLC	C5-C4-O4P-P
4	B	606	PLC	C5-C4-O4P-P
4	B	607	PLC	C5-C4-O4P-P
4	A	604	PLC	CB-C1B-C2B-C3B
4	B	608	PLC	O3P-C1-C2-O2
6	A	611	CPL	O3P-C1-C2-O2
6	B	603	CPL	O3P-C1-C2-O2
6	B	603	CPL	C37-C38-C39-C40
5	A	609	CLR	C22-C23-C24-C25
4	A	616	PLC	C7B-C8B-C9B-CAA
4	A	604	PLC	O4P-C4-C5-N
4	A	607	PLC	O4P-C4-C5-N
4	A	614	PLC	O4P-C4-C5-N
4	B	606	PLC	O4P-C4-C5-N
4	B	607	PLC	O4P-C4-C5-N
4	B	607	PLC	C7'-C8'-C9'-CA'
4	B	614	PLC	O4P-C4-C5-N
6	A	610	CPL	O4P-C4-C5-N
6	A	611	CPL	C1-C2-C3-O3
4	B	609	PLC	O2-C2-C3-O3
6	A	611	CPL	O2-C2-C3-O3
4	B	609	PLC	C2B-C3B-C4B-C5B
6	A	611	CPL	C33-C34-C35-C36
4	A	613	PLC	C2-C1-O3P-P
4	A	604	PLC	C1B-CB-O3-C3
4	A	616	PLC	C2-C3-O3-CB
4	A	603	PLC	C6B-C7B-C8B-C9B
6	A	610	CPL	C42-C43-C44-C45
4	A	607	PLC	C2B-C3B-C4B-C5B
4	A	616	PLC	OB-CB-O3-C3
4	B	613	PLC	C3-C2-O2-C'
4	B	607	PLC	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	608	PLC	O3P-C1-C2-C3
4	A	616	PLC	C1B-CB-O3-C3
4	A	604	PLC	OB-CB-O3-C3
4	B	606	PLC	O3P-C1-C2-O2
6	A	611	CPL	C37-C38-C39-C40
4	B	604	PLC	C1-O3P-P-O4P
4	B	606	PLC	C4-O4P-P-O3P
6	A	610	CPL	C1-O3P-P-O4P
6	B	603	CPL	C45-C46-C47-C48
4	B	609	PLC	C7B-C8B-C9B-CAA
4	B	614	PLC	O3P-C1-C2-C3
4	A	614	PLC	C1'-C2'-C3'-C4'
4	A	615	PLC	C2-C1-O3P-P
5	B	610	CLR	C22-C23-C24-C25
4	B	606	PLC	C2B-C3B-C4B-C5B
6	A	610	CPL	C3-C2-O2-C31
4	B	609	PLC	O3P-C1-C2-C3
4	B	614	PLC	C8B-C9B-CAA-CBA
4	B	613	PLC	C1'-C2'-C3'-C4'
5	A	606	CLR	C22-C23-C24-C25
4	A	603	PLC	C2B-C3B-C4B-C5B
4	B	605	PLC	C4-C5-N-C8
4	A	603	PLC	C1'-C2'-C3'-C4'
4	A	612	PLC	C7B-C8B-C9B-CAA
4	B	604	PLC	O3P-C1-C2-C3
5	A	608	CLR	C22-C23-C24-C25
6	A	610	CPL	C35-C36-C37-C38
6	A	610	CPL	O3-C11-C12-C13
4	A	616	PLC	C1B-C2B-C3B-C4B
4	B	604	PLC	O2-C'-C1'-C2'
4	B	608	PLC	C7B-C8B-C9B-CAA
4	A	615	PLC	C3'-C4'-C5'-C6'
6	A	610	CPL	C21-C22-C23-C24
4	A	607	PLC	O2-C'-C1'-C2'
4	B	613	PLC	C6'-C7'-C8'-C9'
6	A	610	CPL	C37-C38-C39-C40
4	B	605	PLC	C6'-C7'-C8'-C9'
4	B	614	PLC	C8'-C9'-CA'-CB'
3	A	601	NAG	C4-C5-C6-O6
4	B	613	PLC	C5B-C6B-C7B-C8B
6	B	603	CPL	O2-C31-C32-C33
4	A	603	PLC	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
4	A	615	PLC	C4-C5-N-C6
4	B	605	PLC	C8B-C9B-CAA-CBA
4	A	604	PLC	C8'-C9'-CA'-CB'
4	B	606	PLC	C1B-C2B-C3B-C4B
4	B	607	PLC	O2-C'-C1'-C2'
4	A	603	PLC	C4'-C5'-C6'-C7'
4	A	614	PLC	C4'-C5'-C6'-C7'
4	B	614	PLC	C6'-C7'-C8'-C9'
4	B	606	PLC	C4B-C5B-C6B-C7B
4	A	607	PLC	O'-C'-C1'-C2'
4	B	604	PLC	O'-C'-C1'-C2'
6	A	610	CPL	O11-C11-C12-C13
6	B	603	CPL	O31-C31-C32-C33
4	B	612	PLC	C1B-C2B-C3B-C4B
4	B	612	PLC	C2B-C1B-CB-O3
4	B	606	PLC	C2-C1-O3P-P
4	B	608	PLC	C4-O4P-P-O1P
4	B	609	PLC	C4-O4P-P-O1P
6	A	610	CPL	C22-C23-C24-C25
4	B	607	PLC	O'-C'-C1'-C2'
4	A	616	PLC	C5-C4-O4P-P
4	B	609	PLC	C5-C4-O4P-P
6	B	603	CPL	C5-C4-O4P-P
4	A	613	PLC	C2B-C1B-CB-O3
6	A	610	CPL	C15-C16-C17-C18
4	A	614	PLC	O'-C'-C1'-C2'
4	A	616	PLC	C7'-C8'-C9'-CA'
4	B	612	PLC	C2B-C1B-CB-OB
4	A	616	PLC	C6B-C7B-C8B-C9B
3	A	601	NAG	O5-C5-C6-O6
4	B	612	PLC	O2-C'-C1'-C2'

There are no ring outliers.

26 monomers are involved in 149 short contacts:

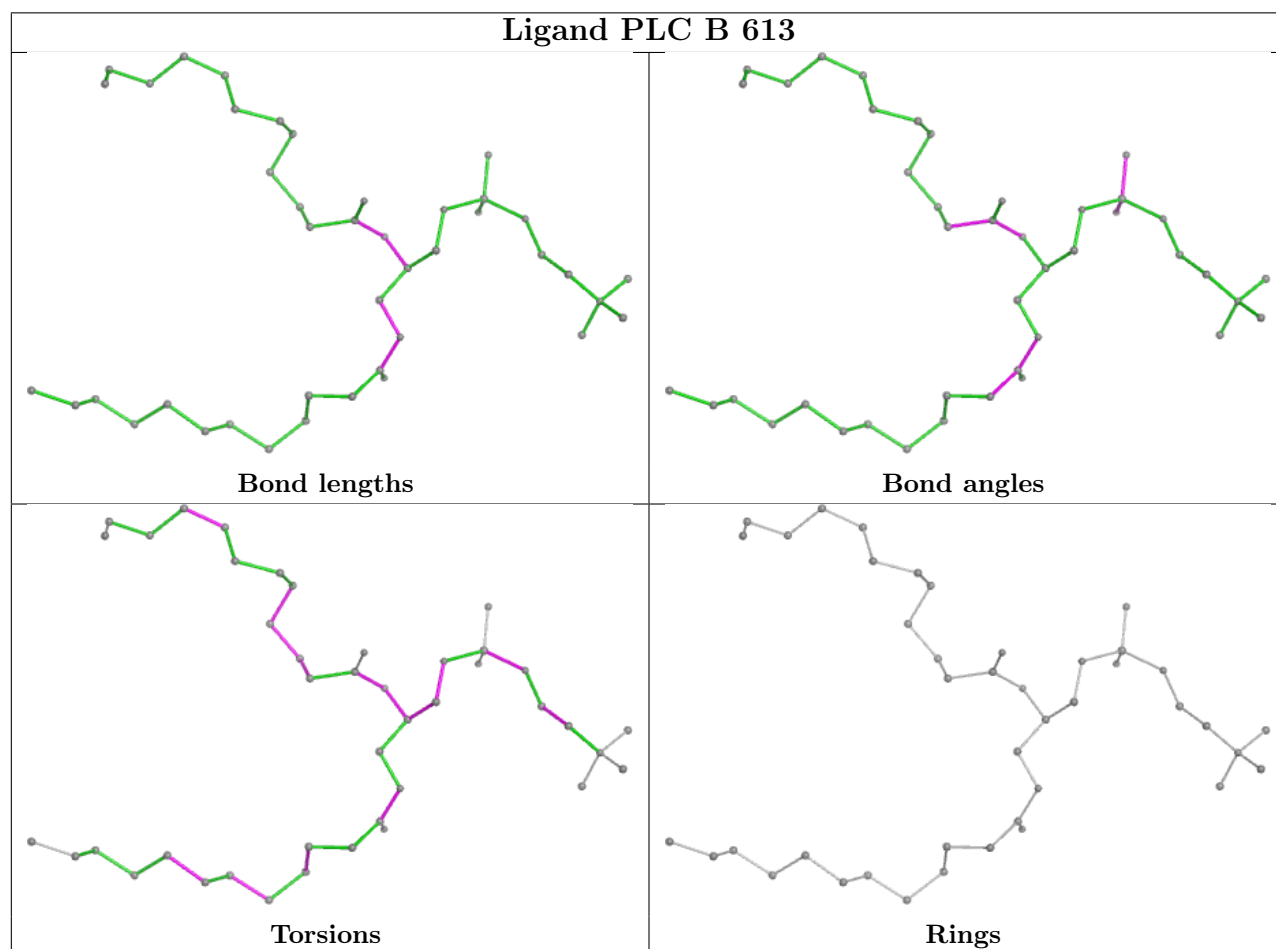
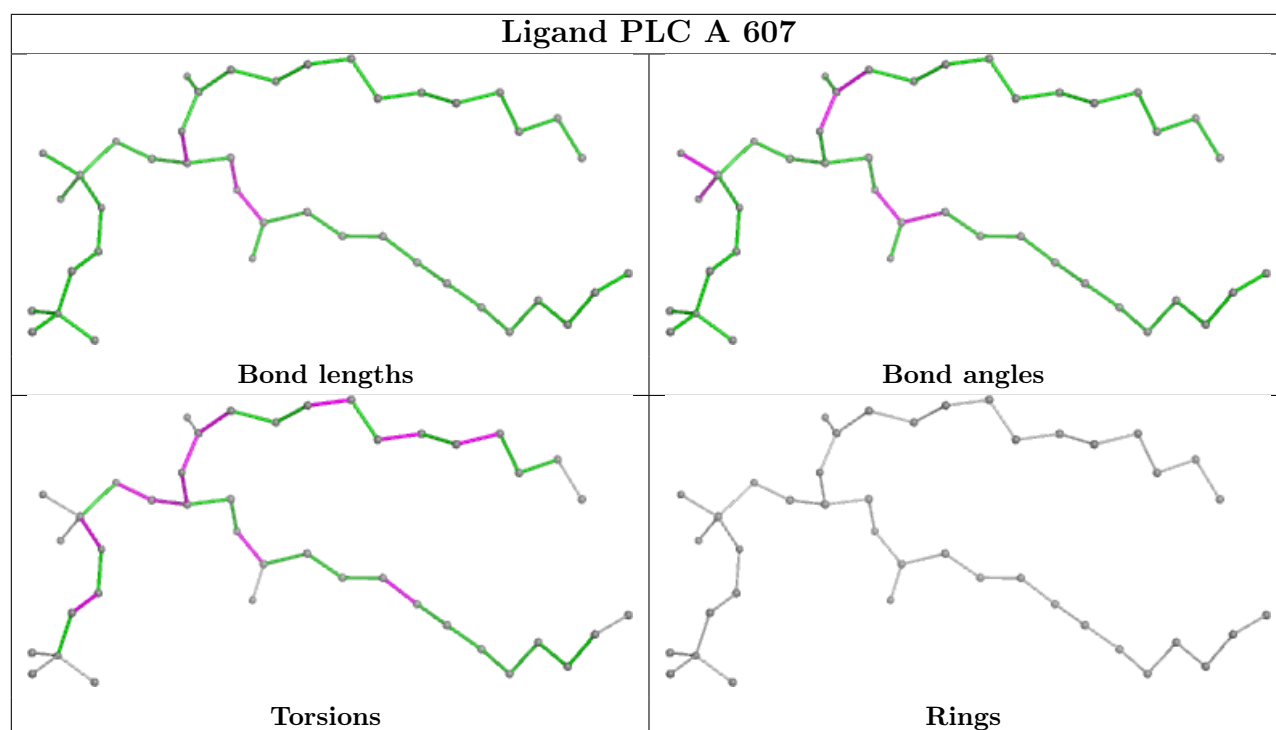
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	PLC	1	0
4	B	613	PLC	2	0
4	B	614	PLC	1	0
6	A	611	CPL	8	0
5	A	606	CLR	6	0
4	A	614	PLC	7	0

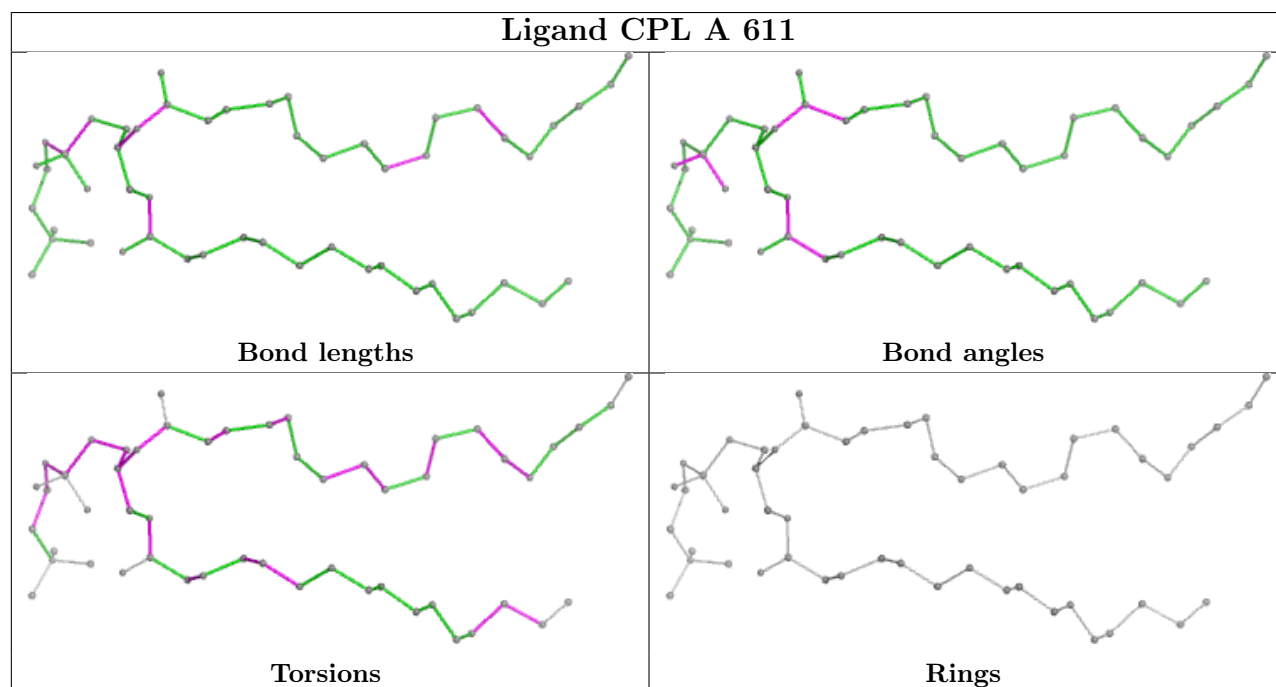
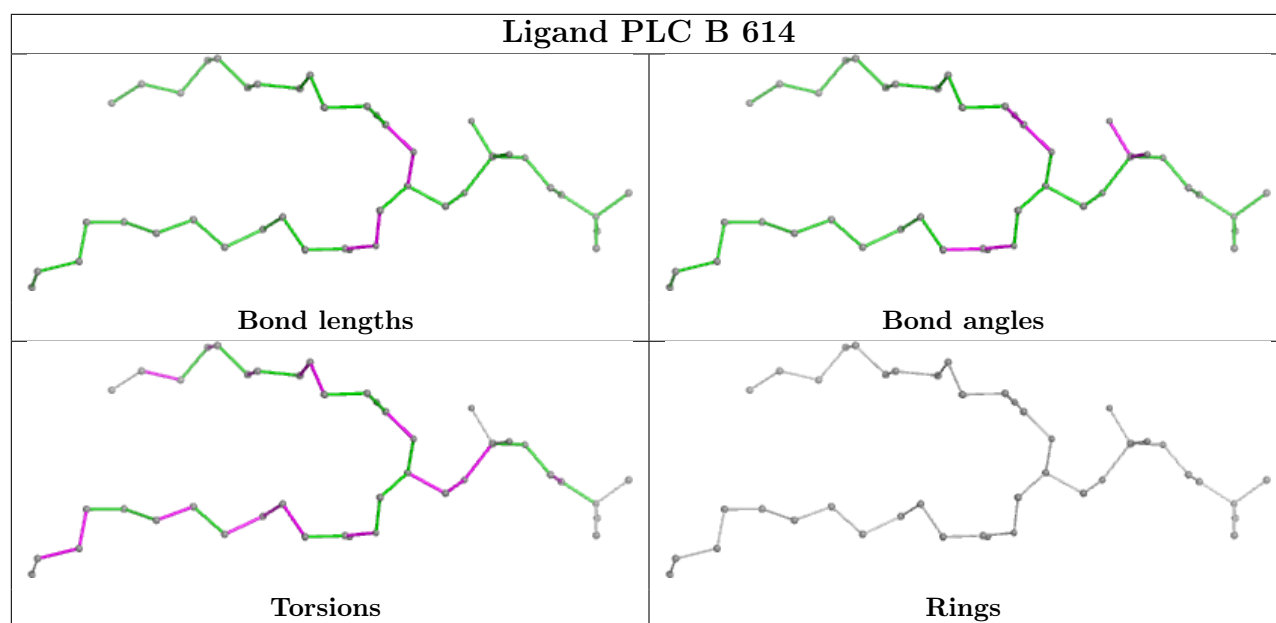
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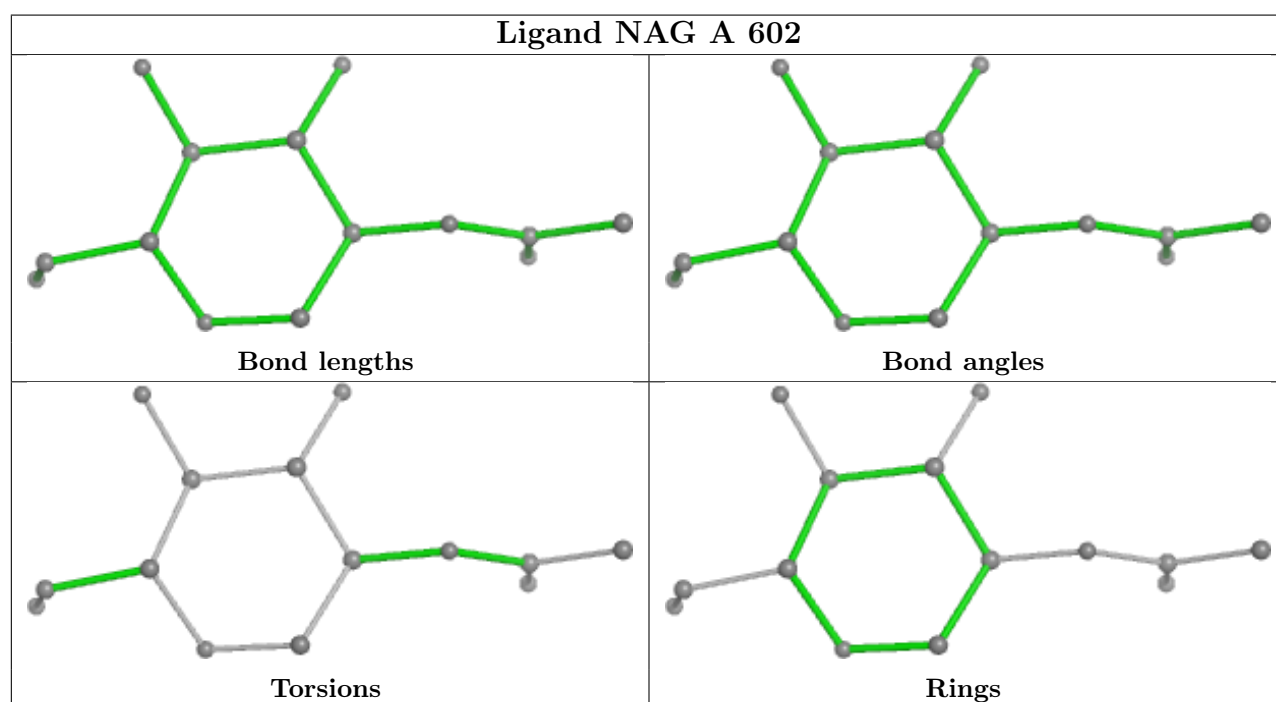
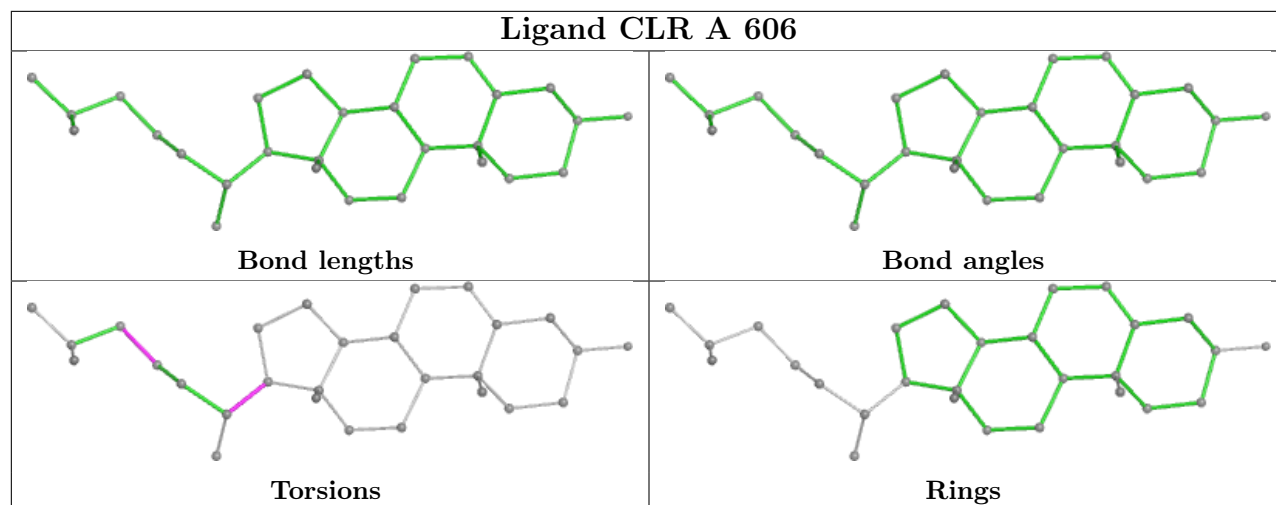
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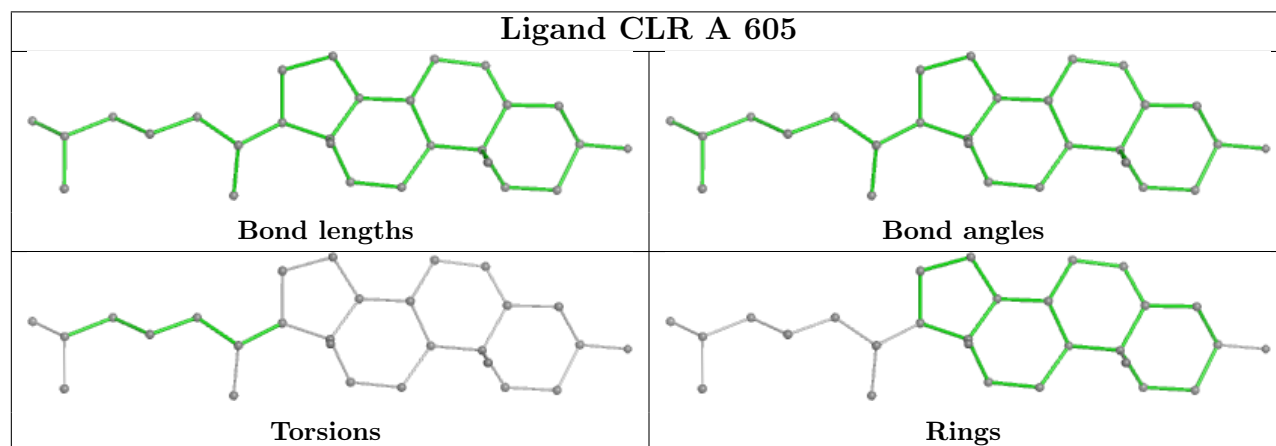
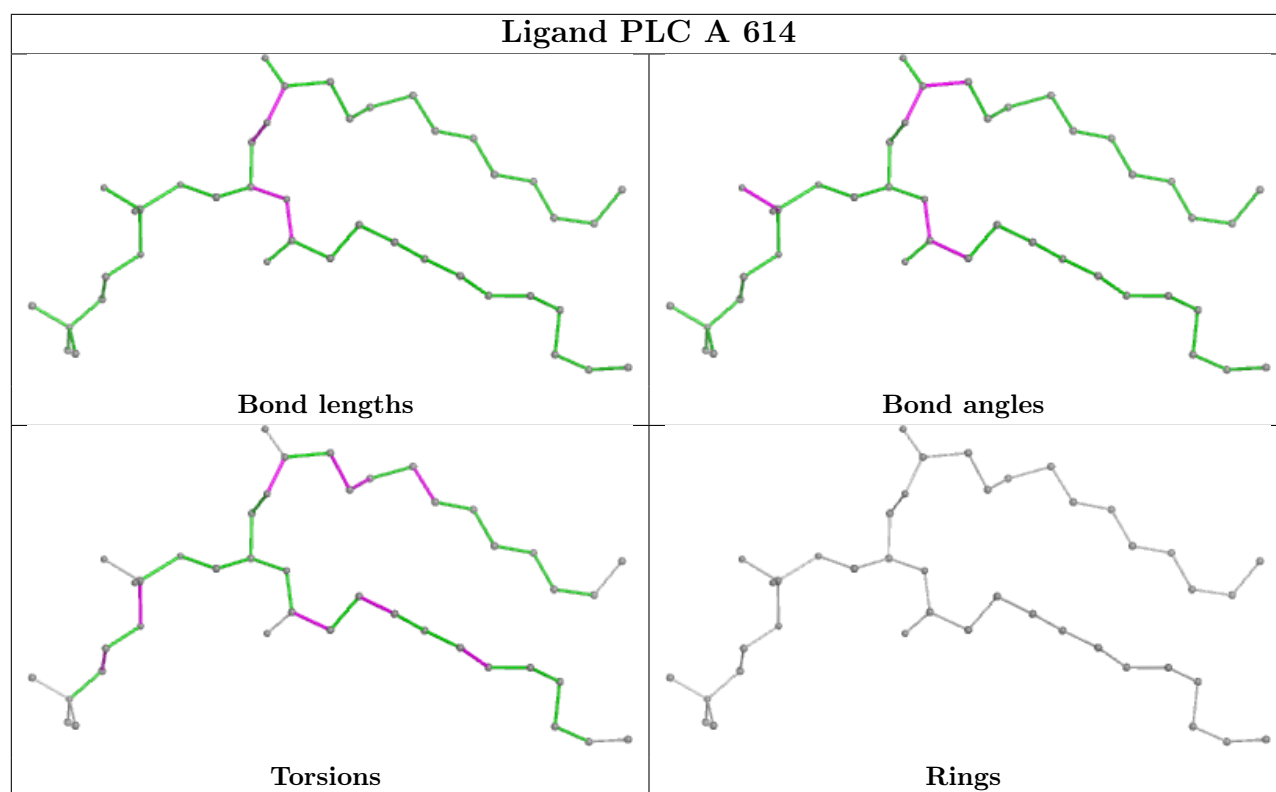
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	CLR	12	0
4	B	604	PLC	2	0
4	B	608	PLC	3	0
5	B	611	CLR	7	0
6	B	603	CPL	14	0
4	A	604	PLC	8	0
4	B	607	PLC	1	0
4	B	612	PLC	11	0
4	B	609	PLC	3	0
4	A	616	PLC	5	0
5	B	610	CLR	3	0
4	A	615	PLC	4	0
4	B	606	PLC	7	0
4	A	612	PLC	9	0
5	A	608	CLR	11	0
6	A	610	CPL	14	0
5	A	609	CLR	12	0
4	B	605	PLC	2	0
4	A	613	PLC	11	0
4	A	603	PLC	12	0

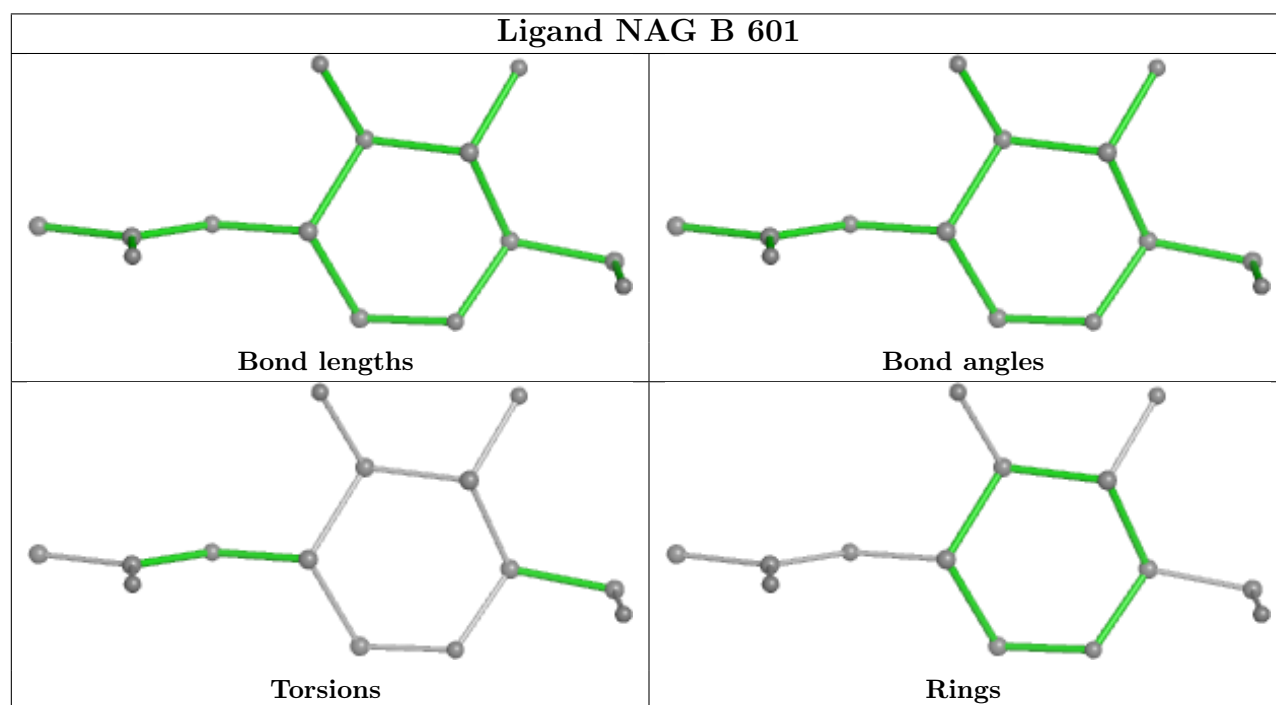
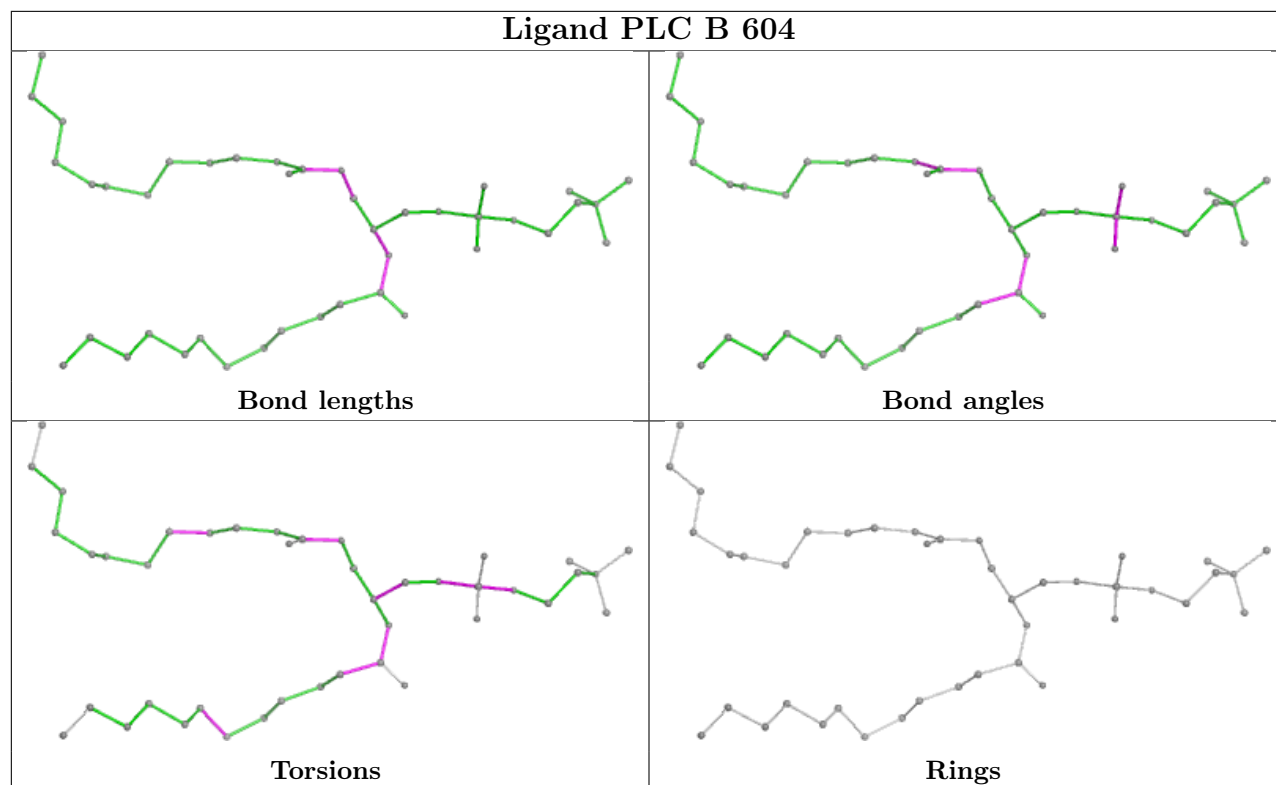
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

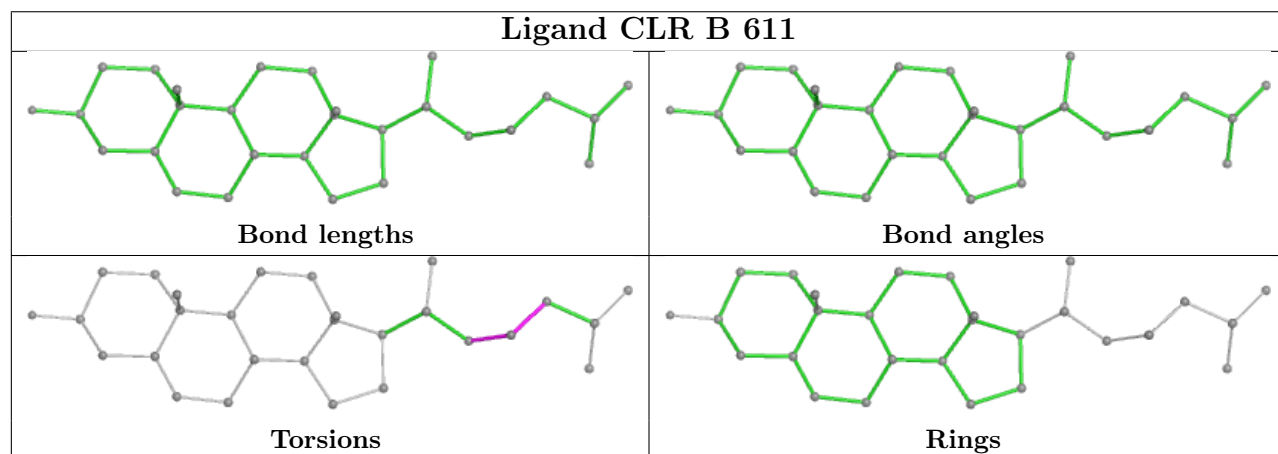
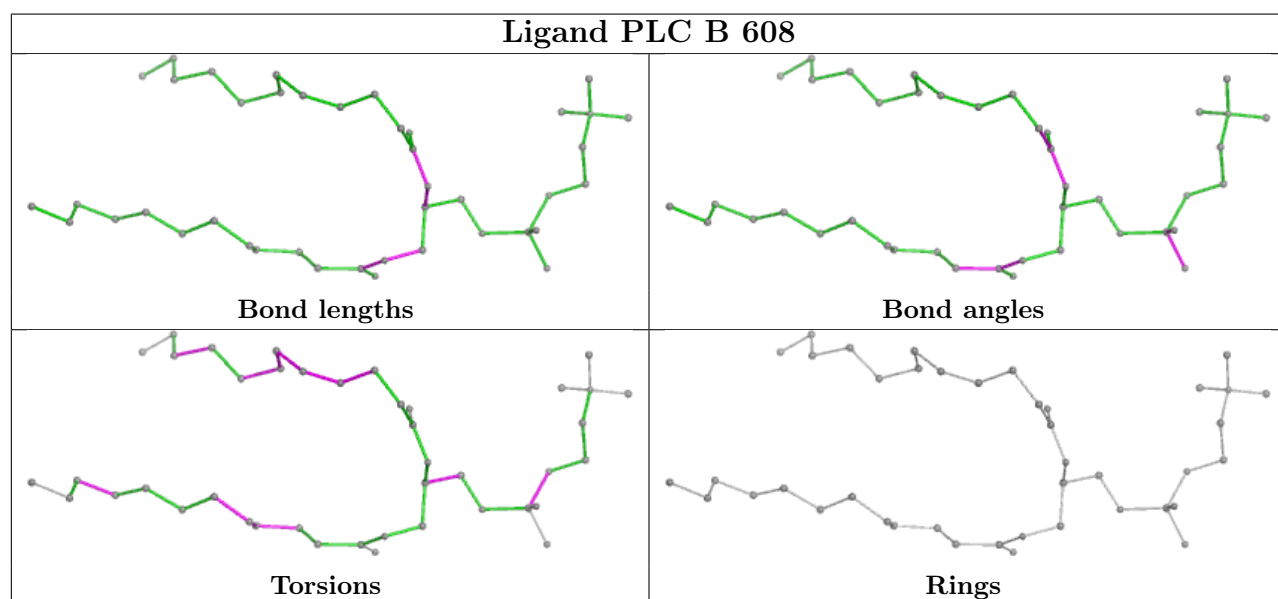
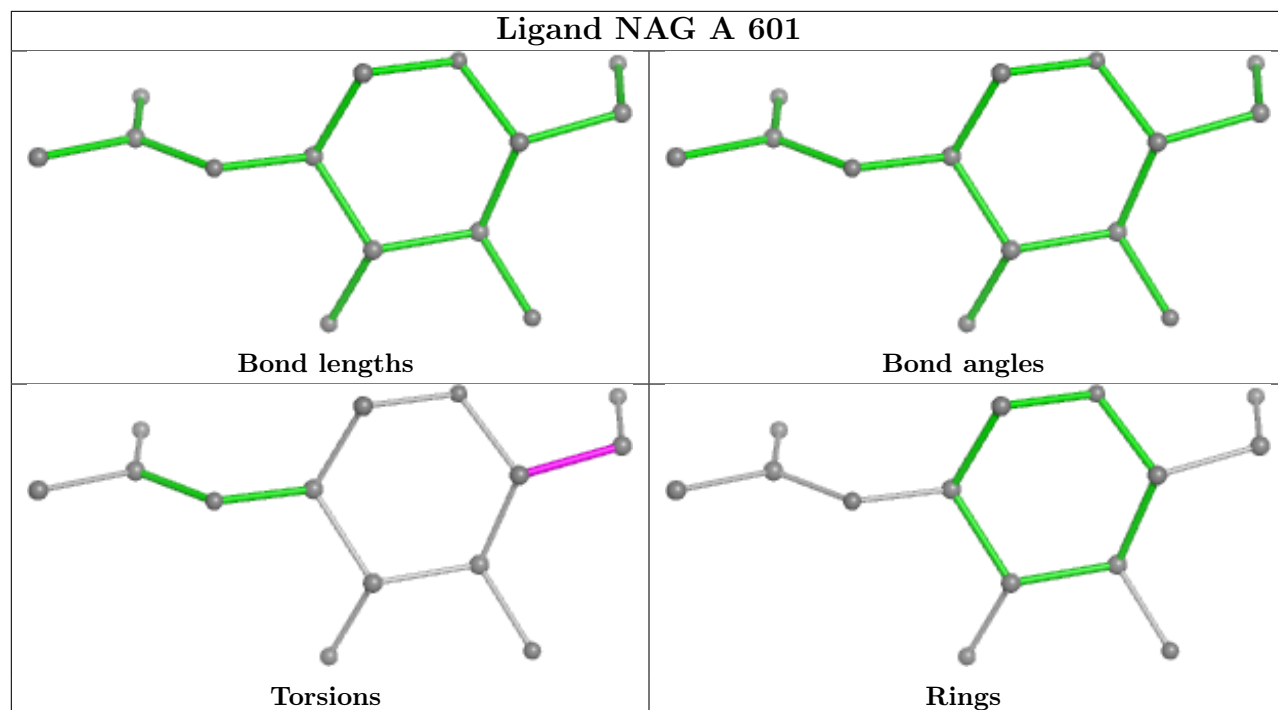


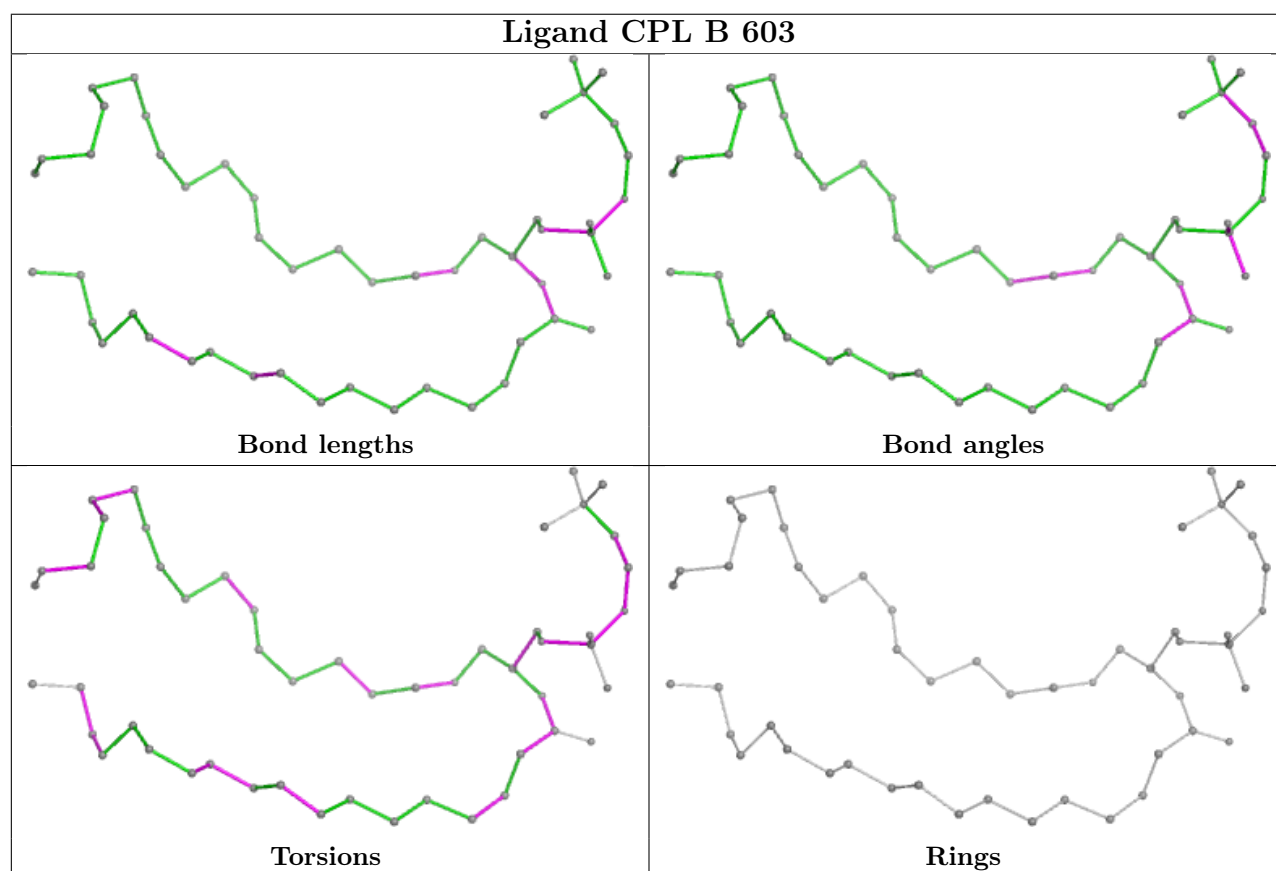
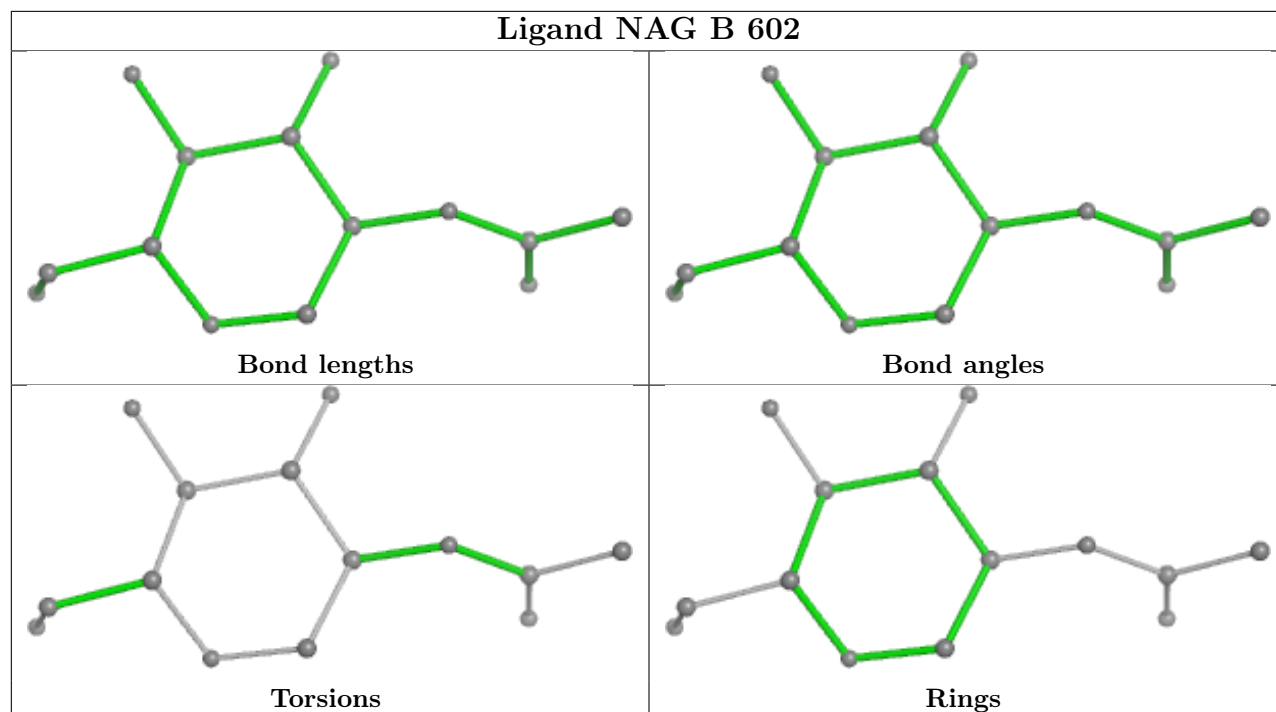


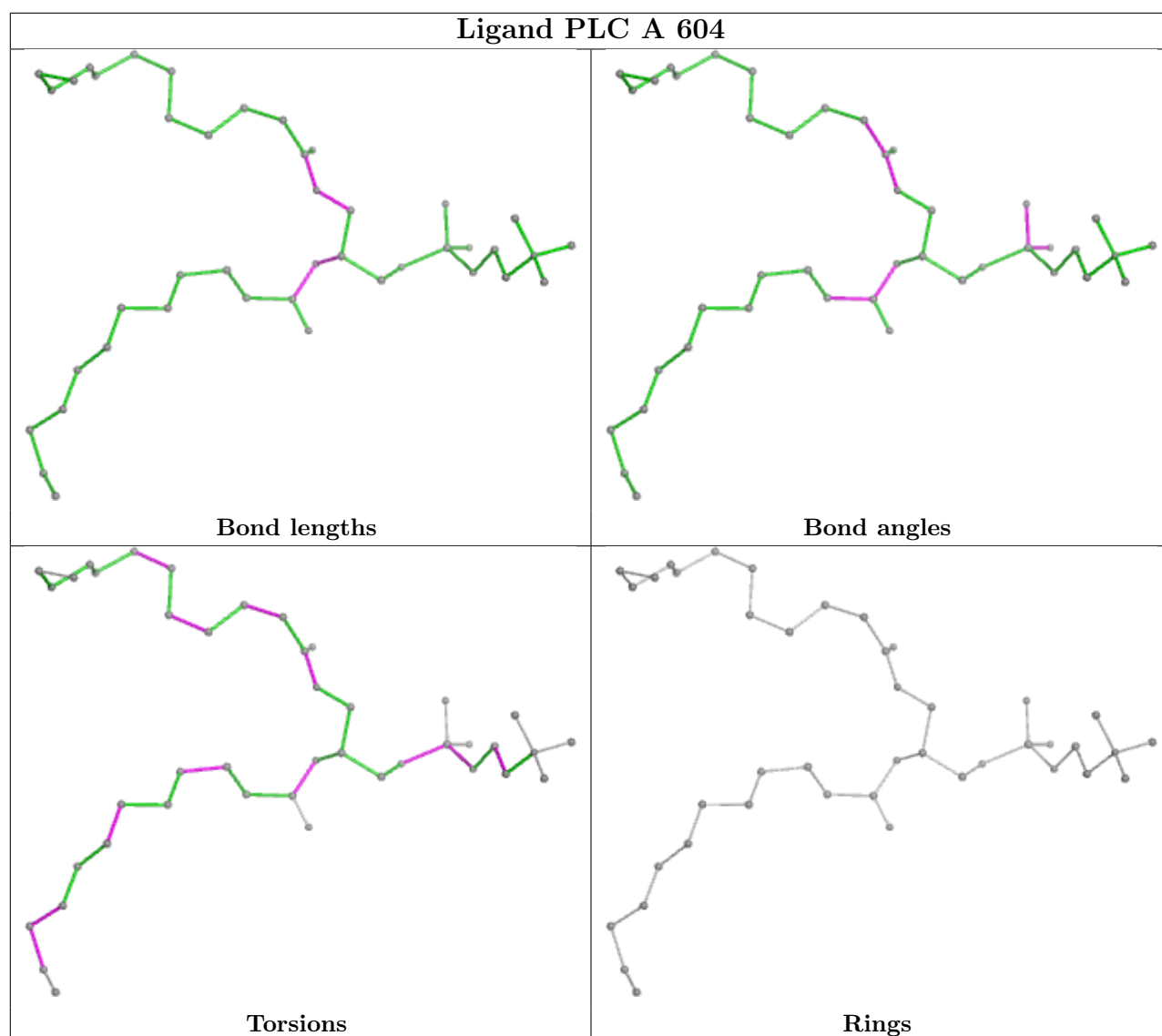


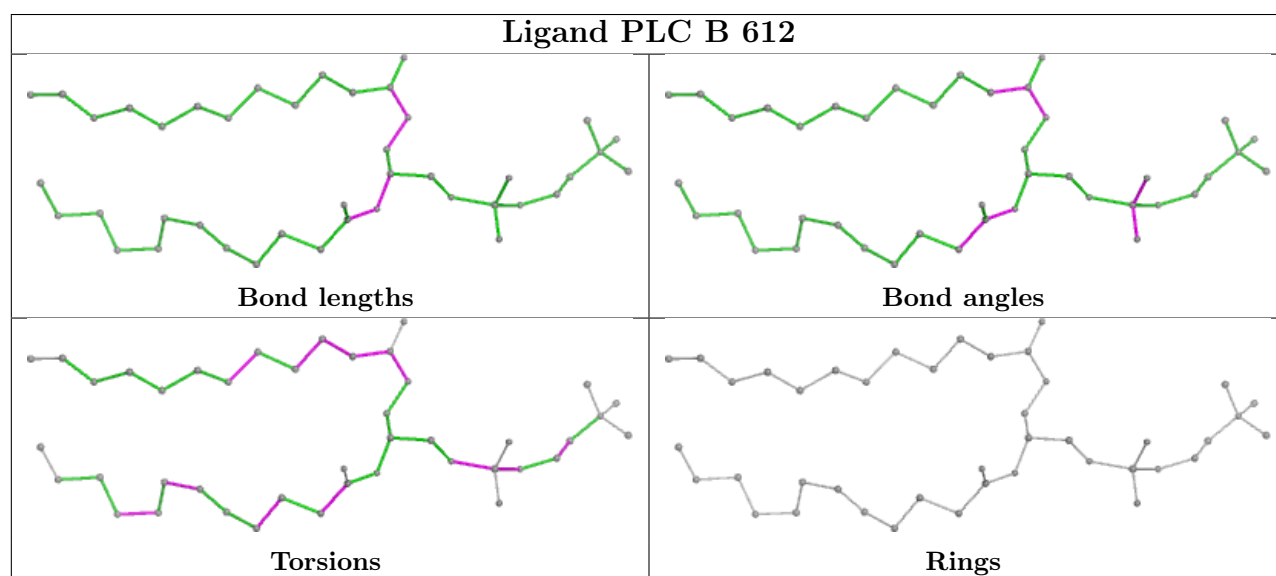
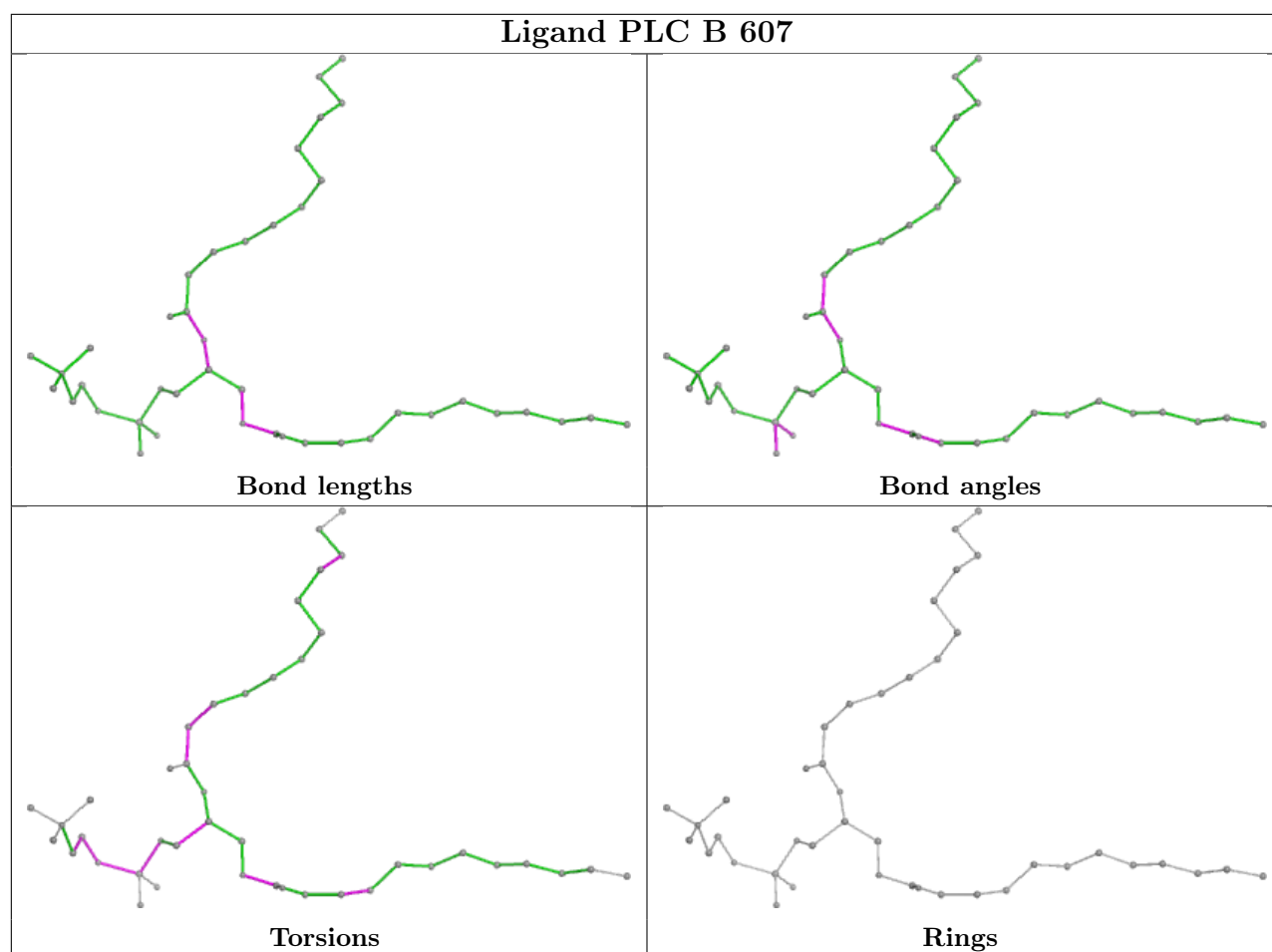


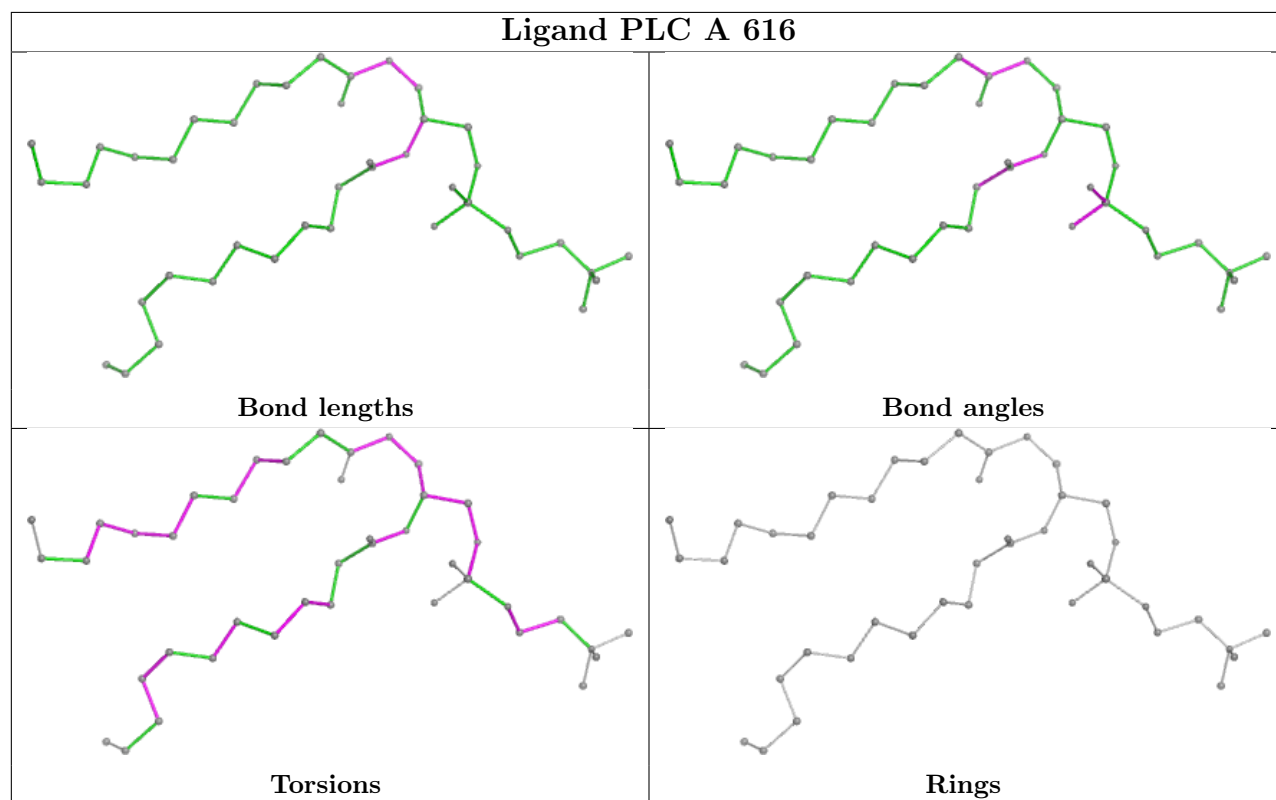
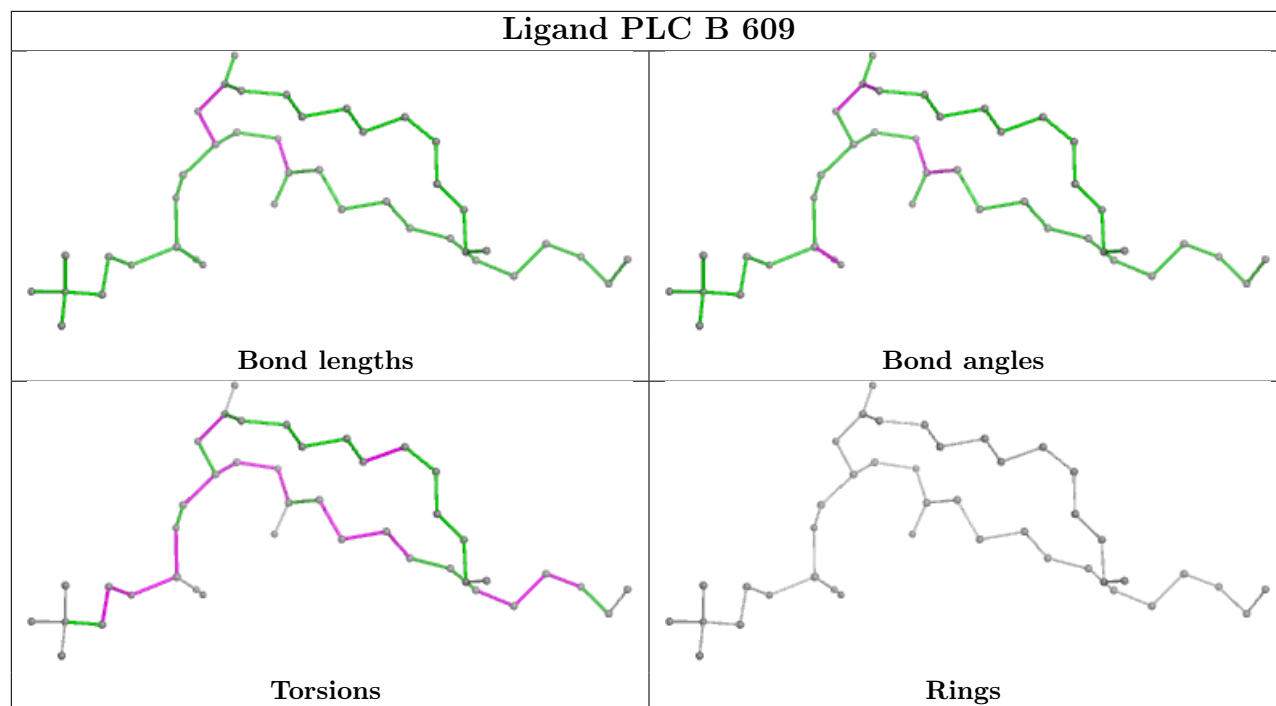


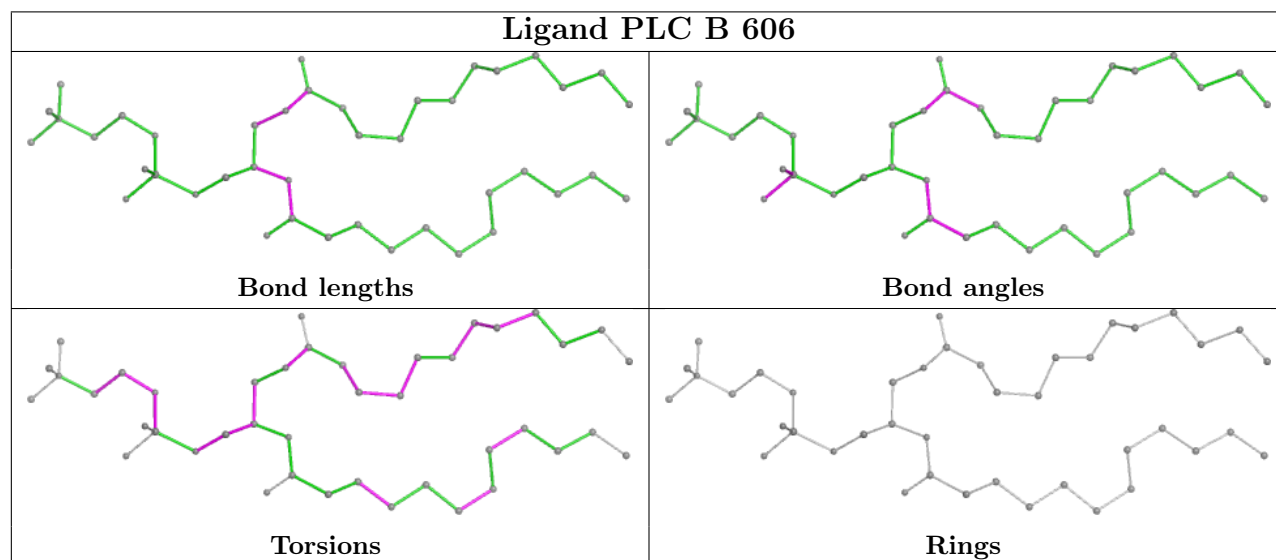
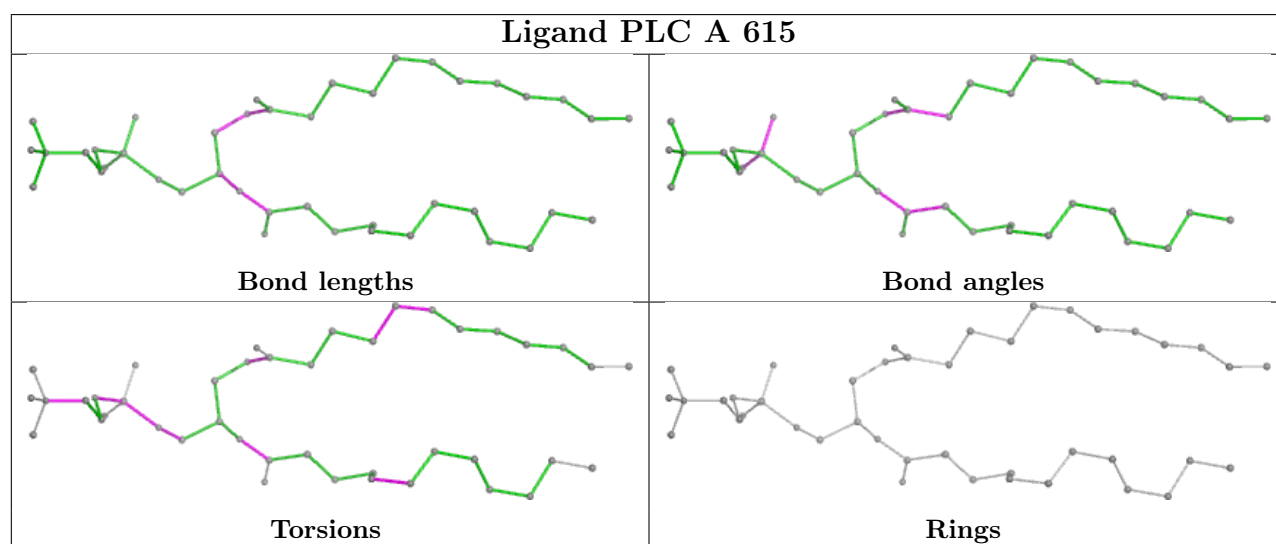
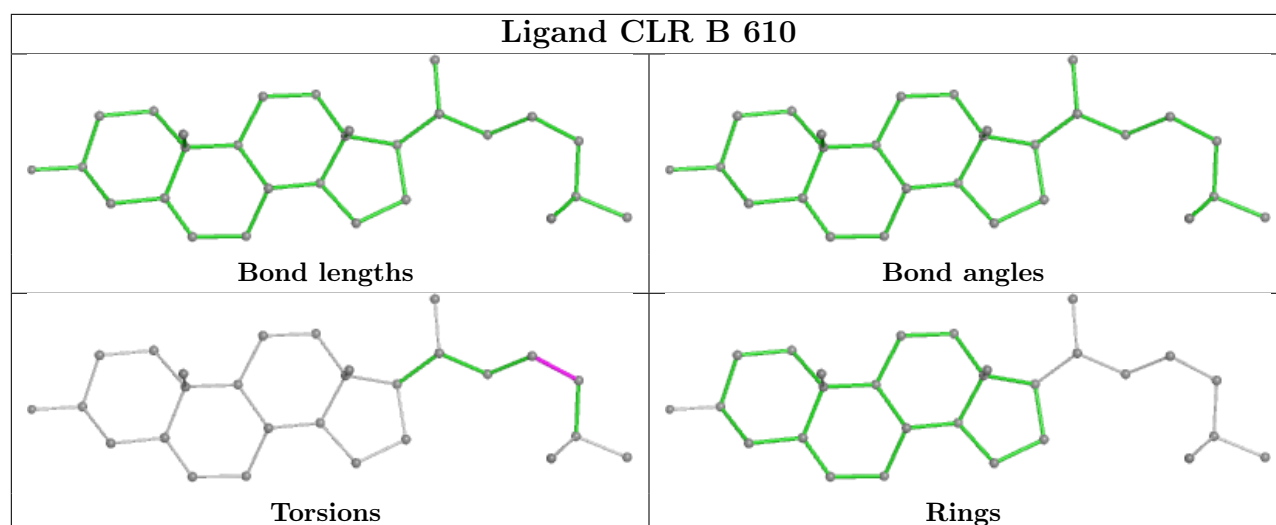


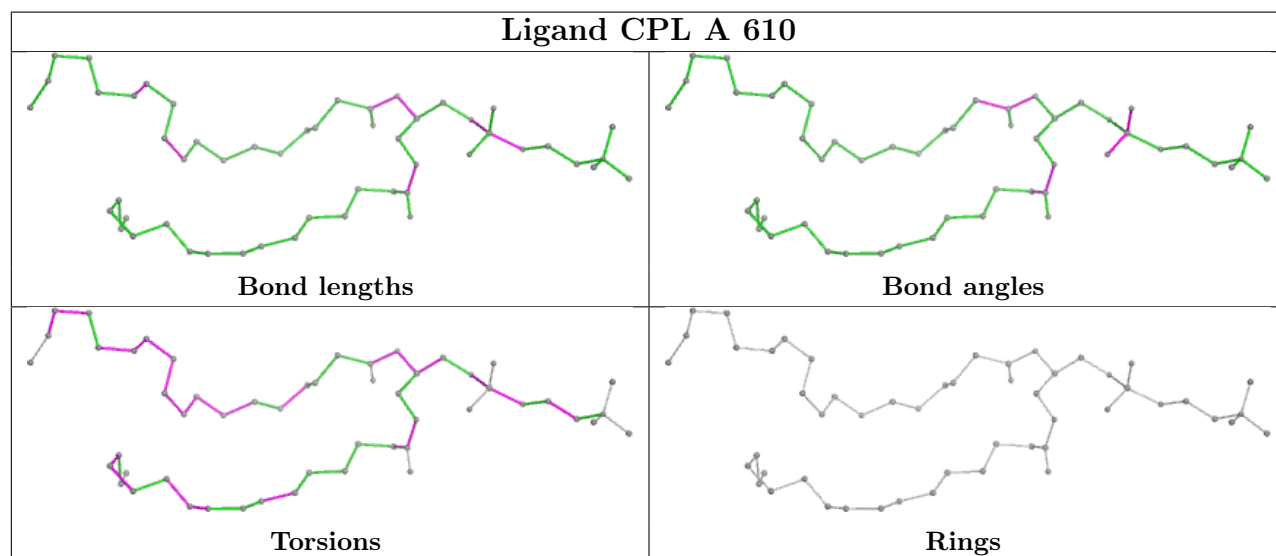
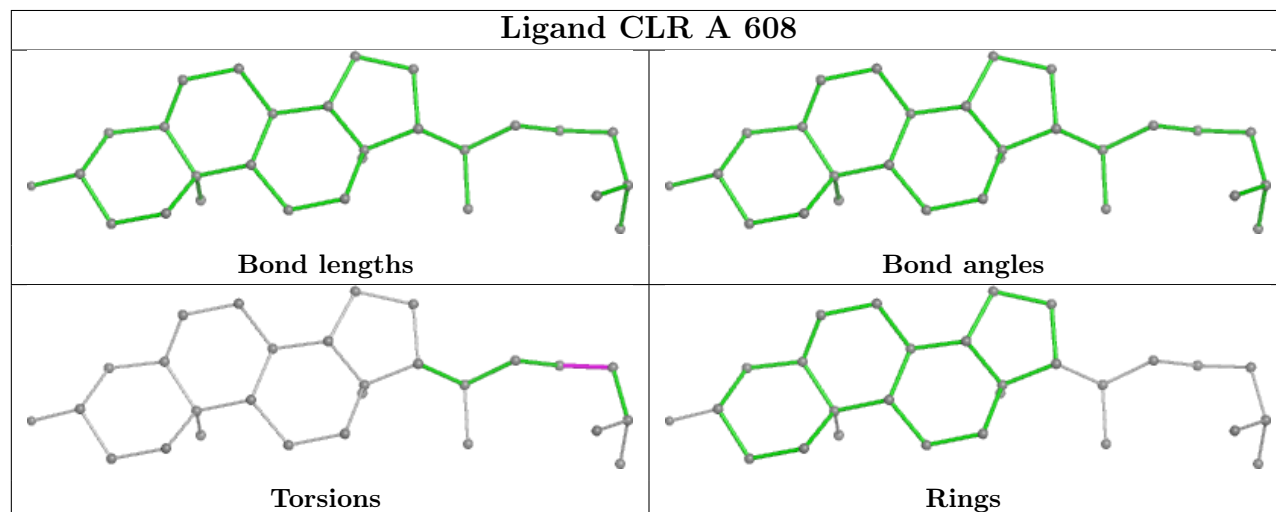
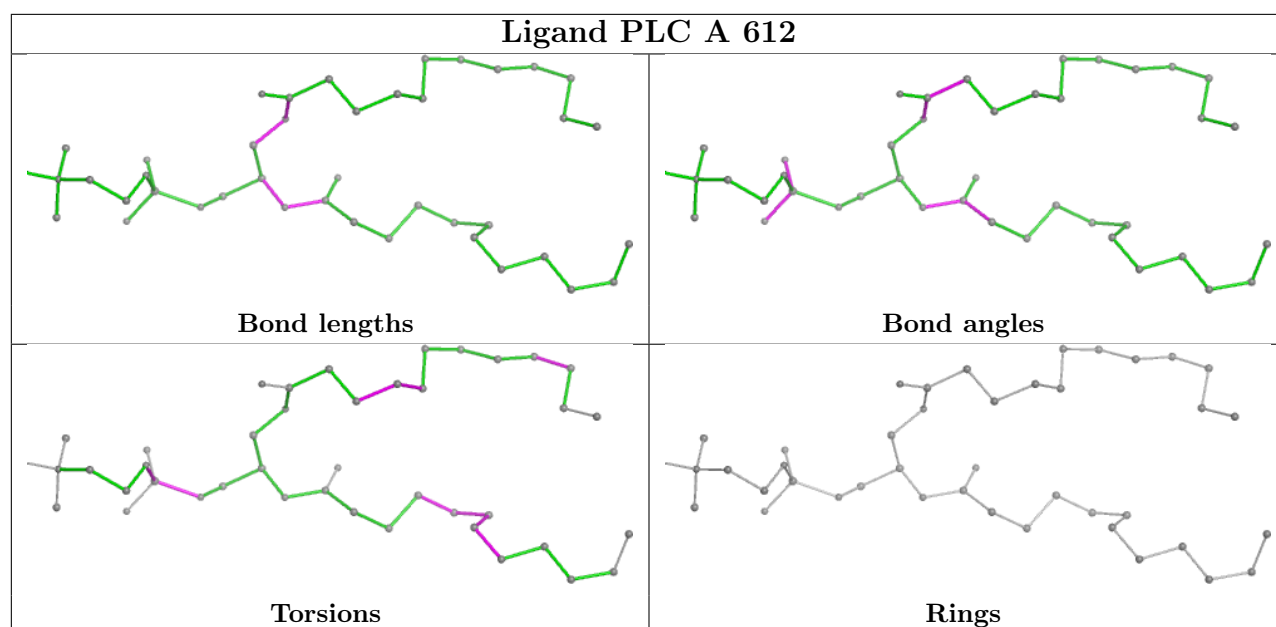


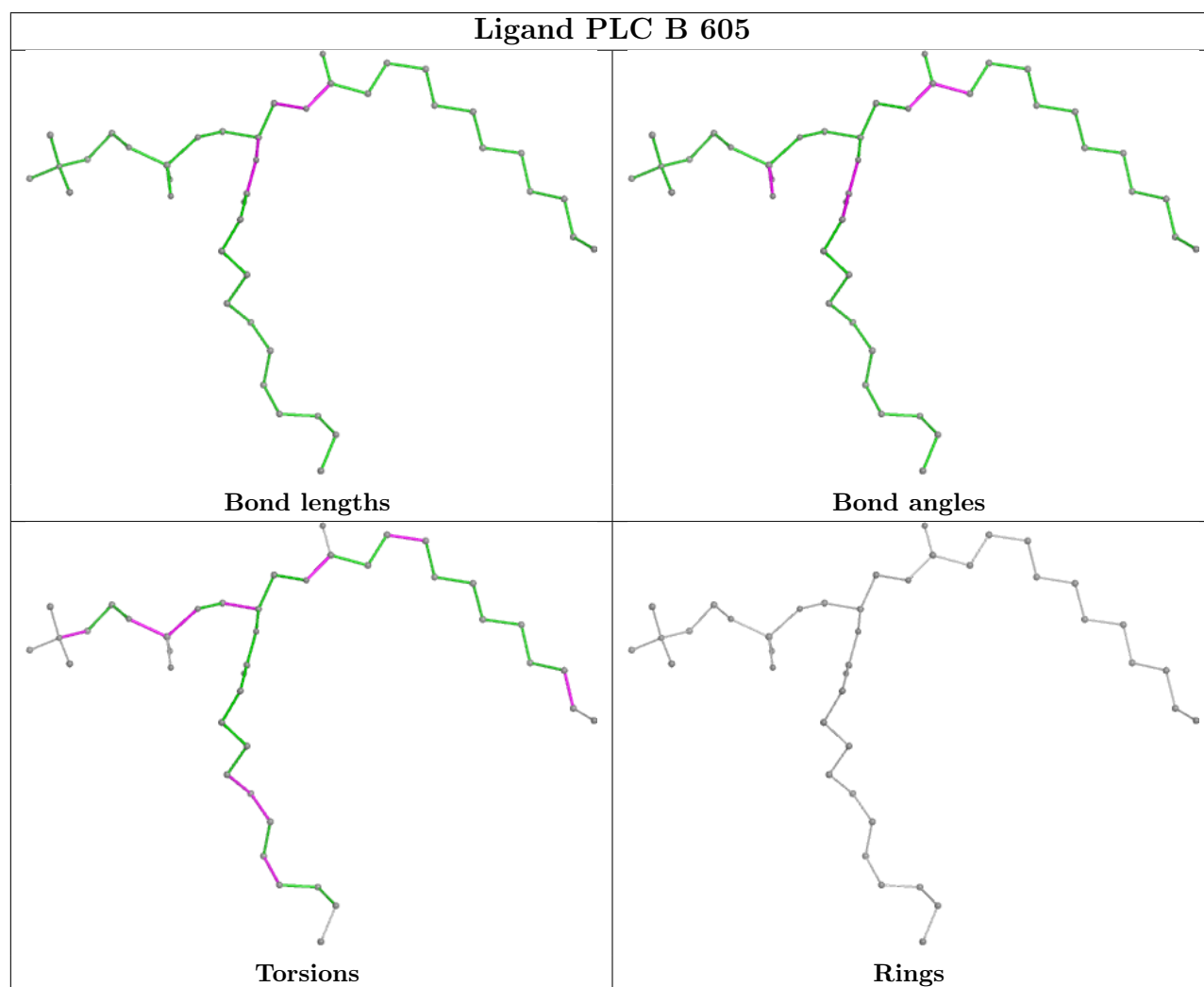
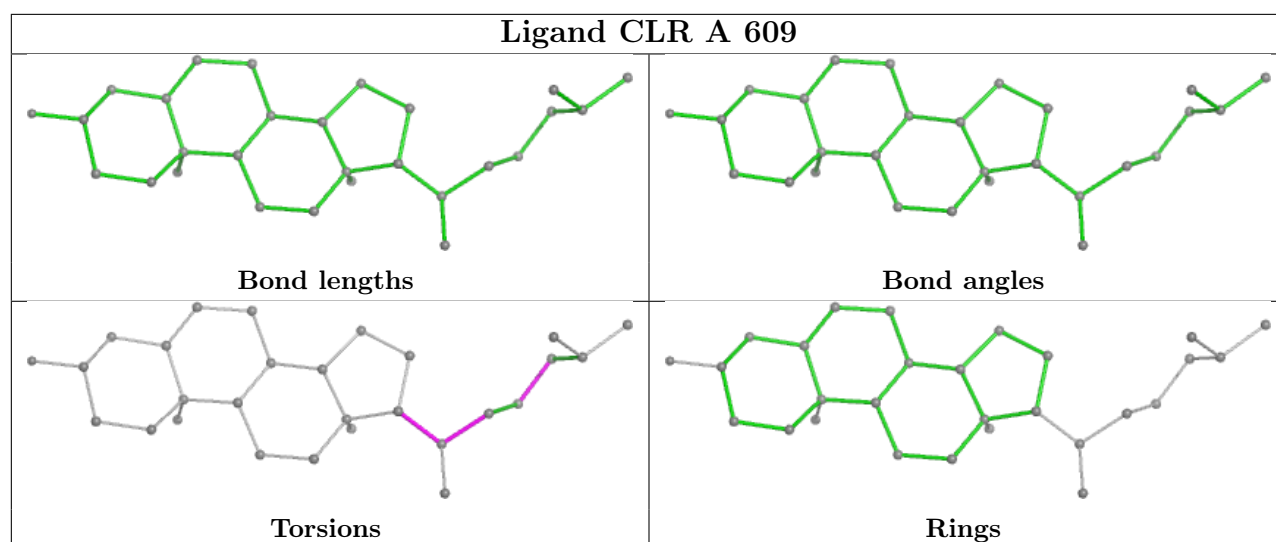


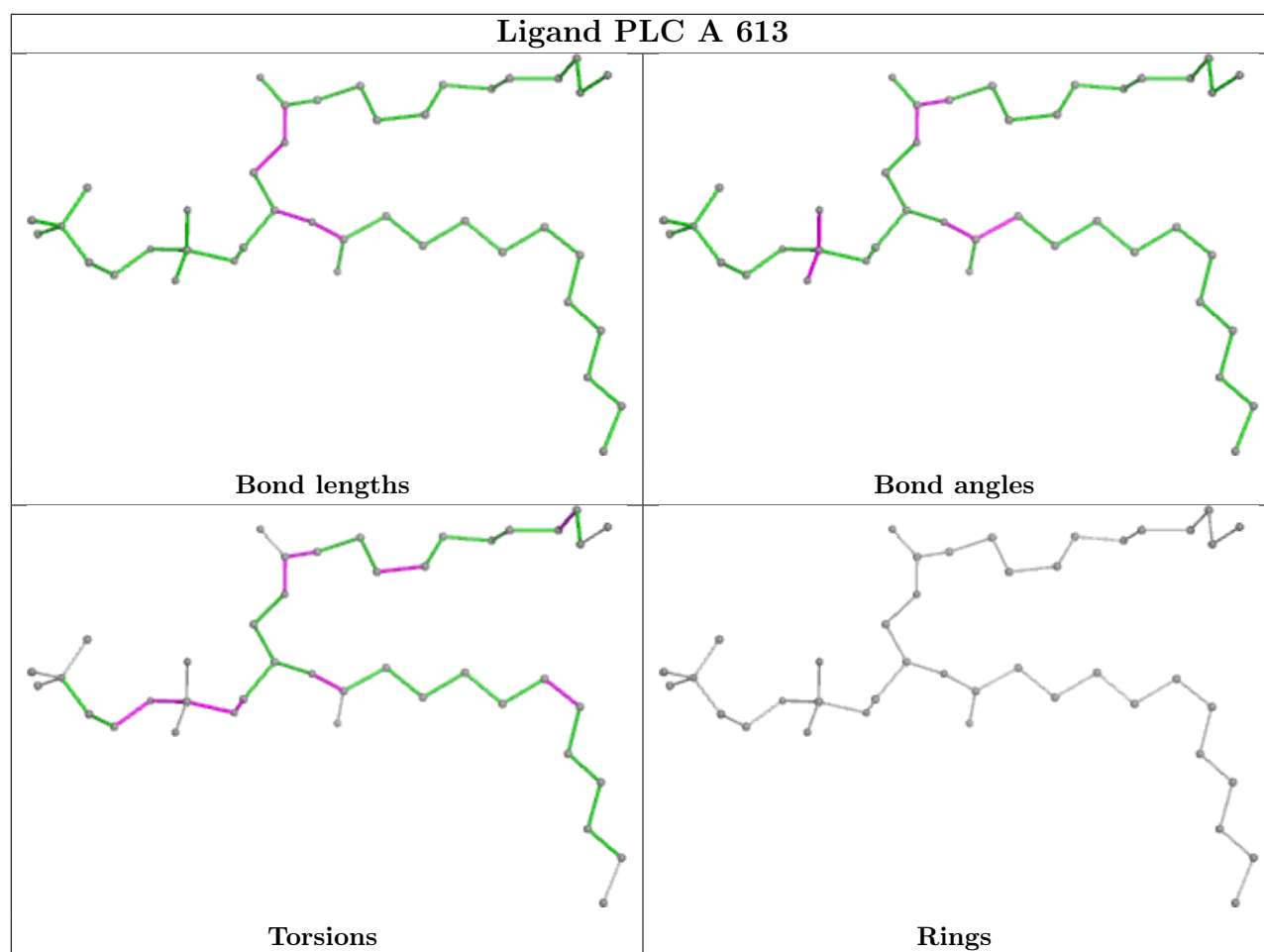


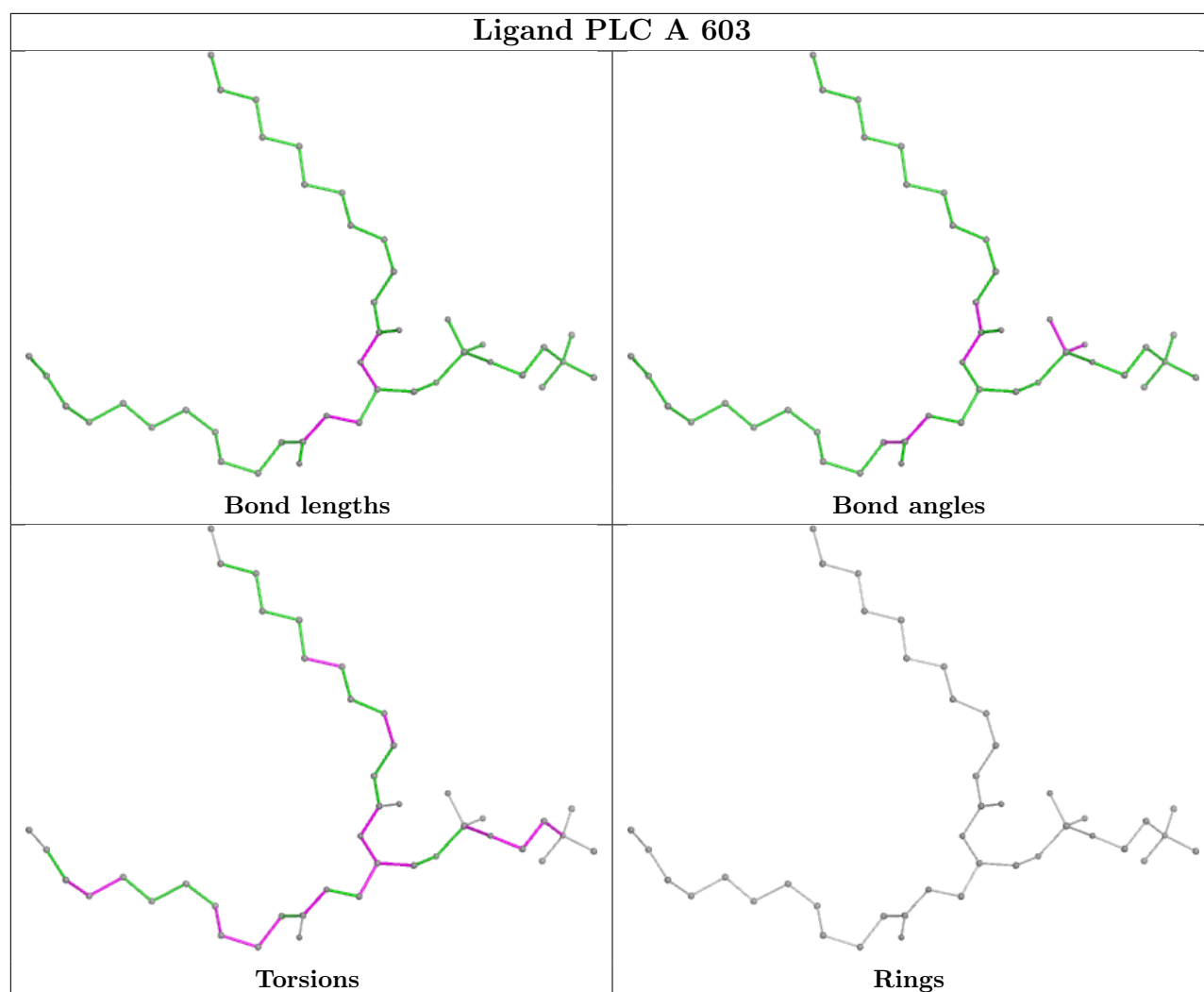












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

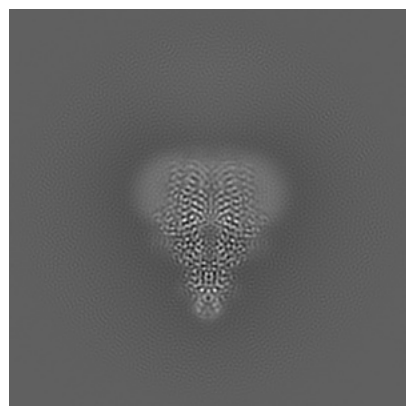
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51108. These allow visual inspection of the internal detail of the map and identification of artifacts.

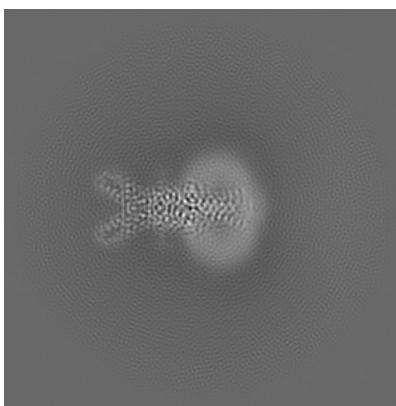
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

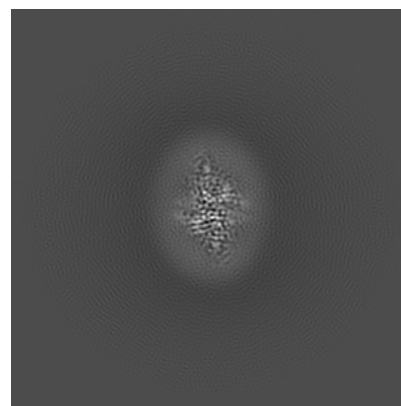
#### 6.1.1 Primary map



X

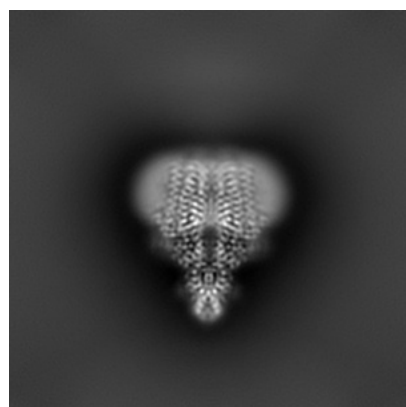


Y

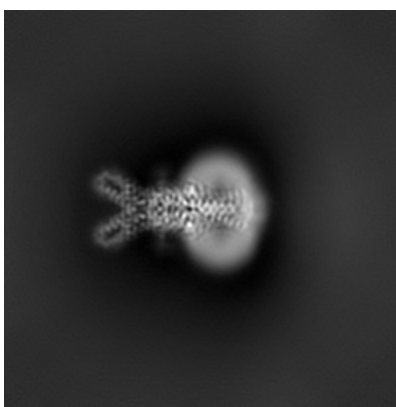


Z

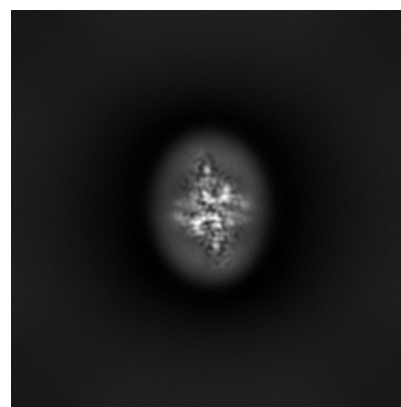
#### 6.1.2 Raw map



X



Y

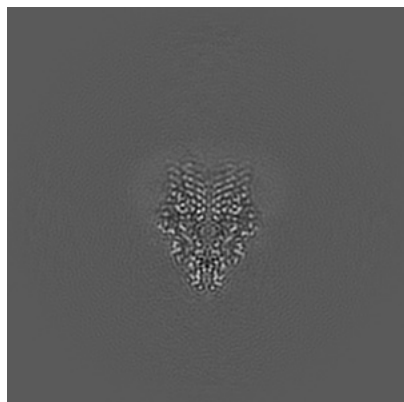


Z

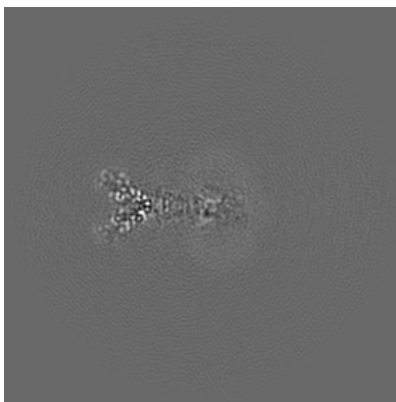
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

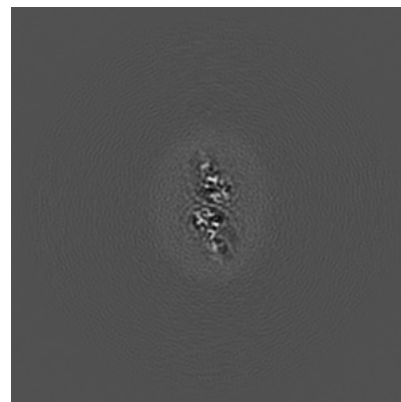
### 6.2.1 Primary map



X Index: 110

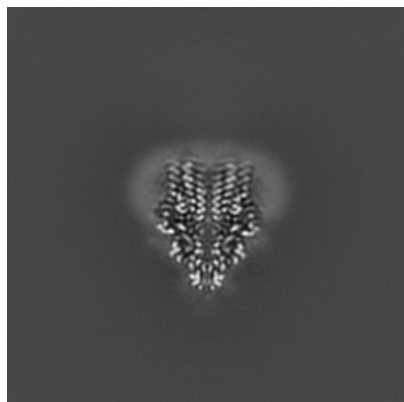


Y Index: 110

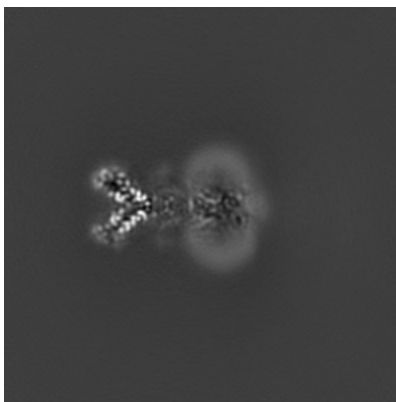


Z Index: 110

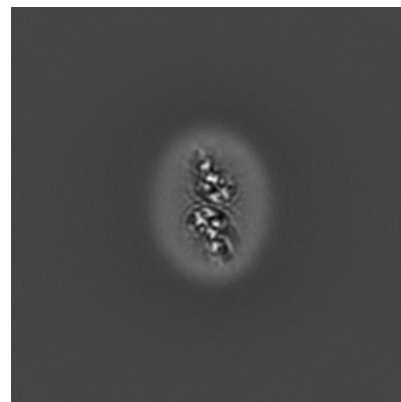
### 6.2.2 Raw map



X Index: 110



Y Index: 110

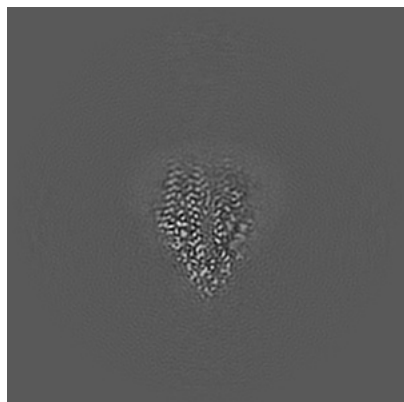


Z Index: 110

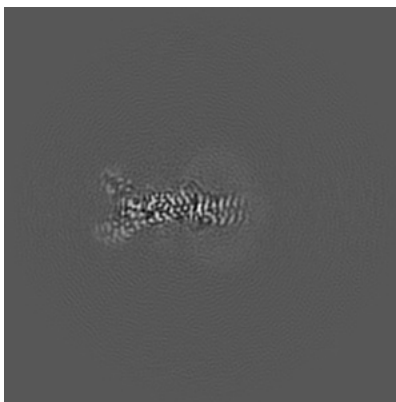
The images above show central slices of the map in three orthogonal directions.

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

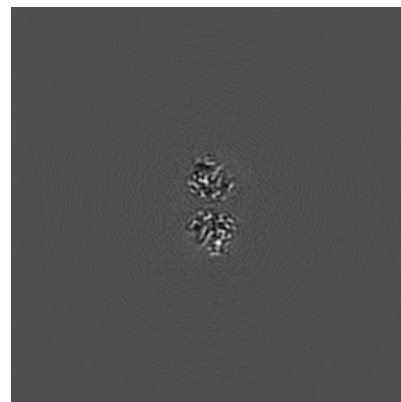
### 6.3.1 Primary map



X Index: 113

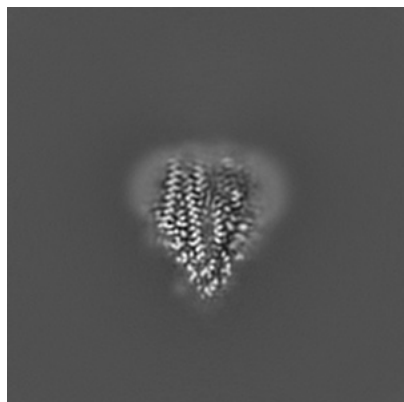


Y Index: 105

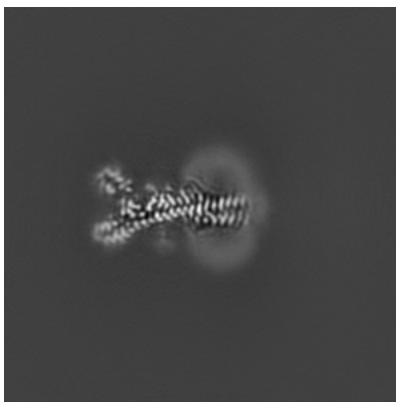


Z Index: 99

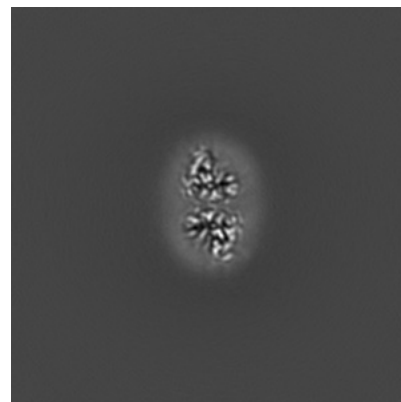
### 6.3.2 Raw map



X Index: 113



Y Index: 105

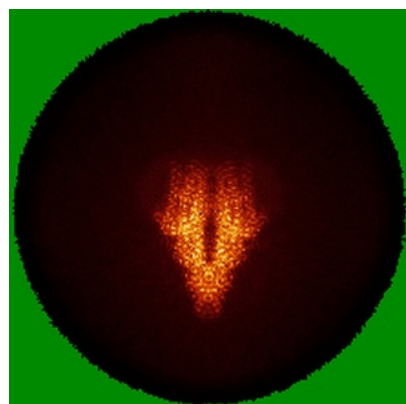


Z Index: 103

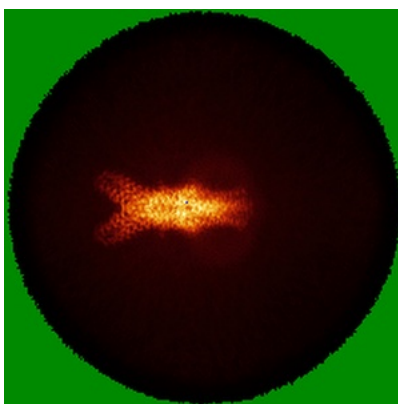
The images above show the largest variance slices of the map in three orthogonal directions.

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

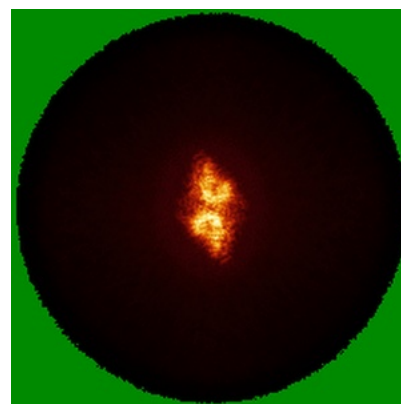
### 6.4.1 Primary map



X

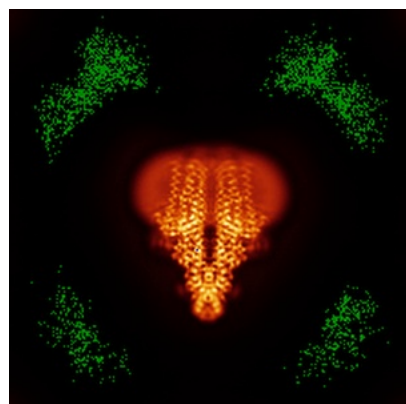


Y

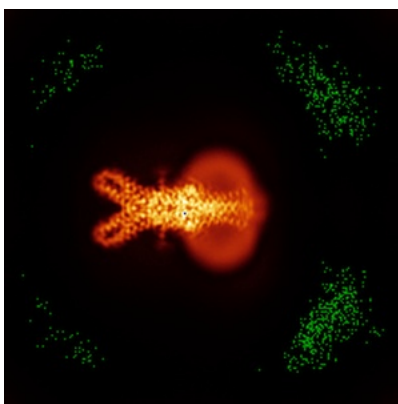


Z

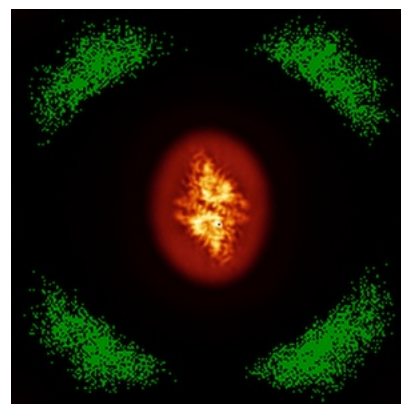
### 6.4.2 Raw map



X



Y

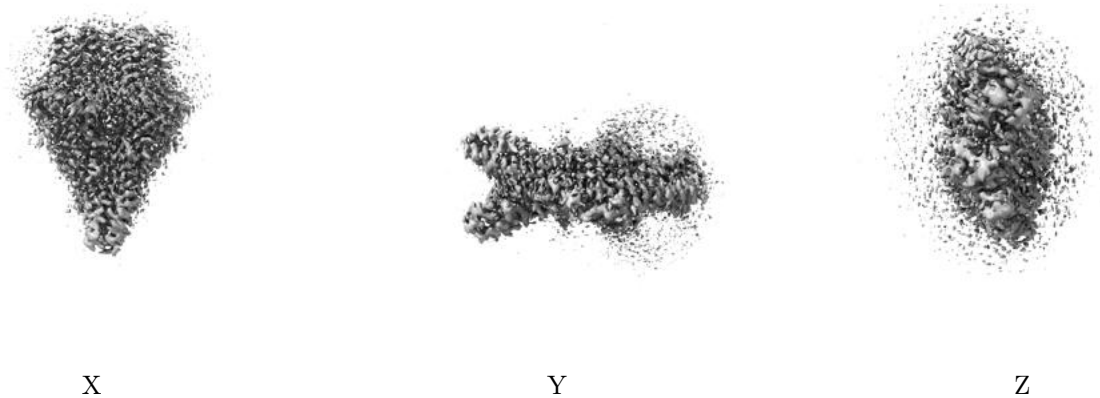


Z

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.

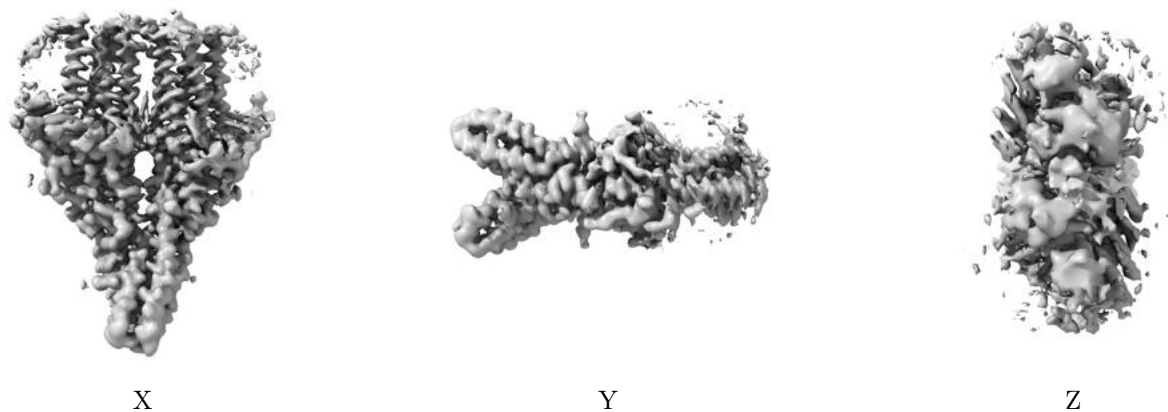
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.271. 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.

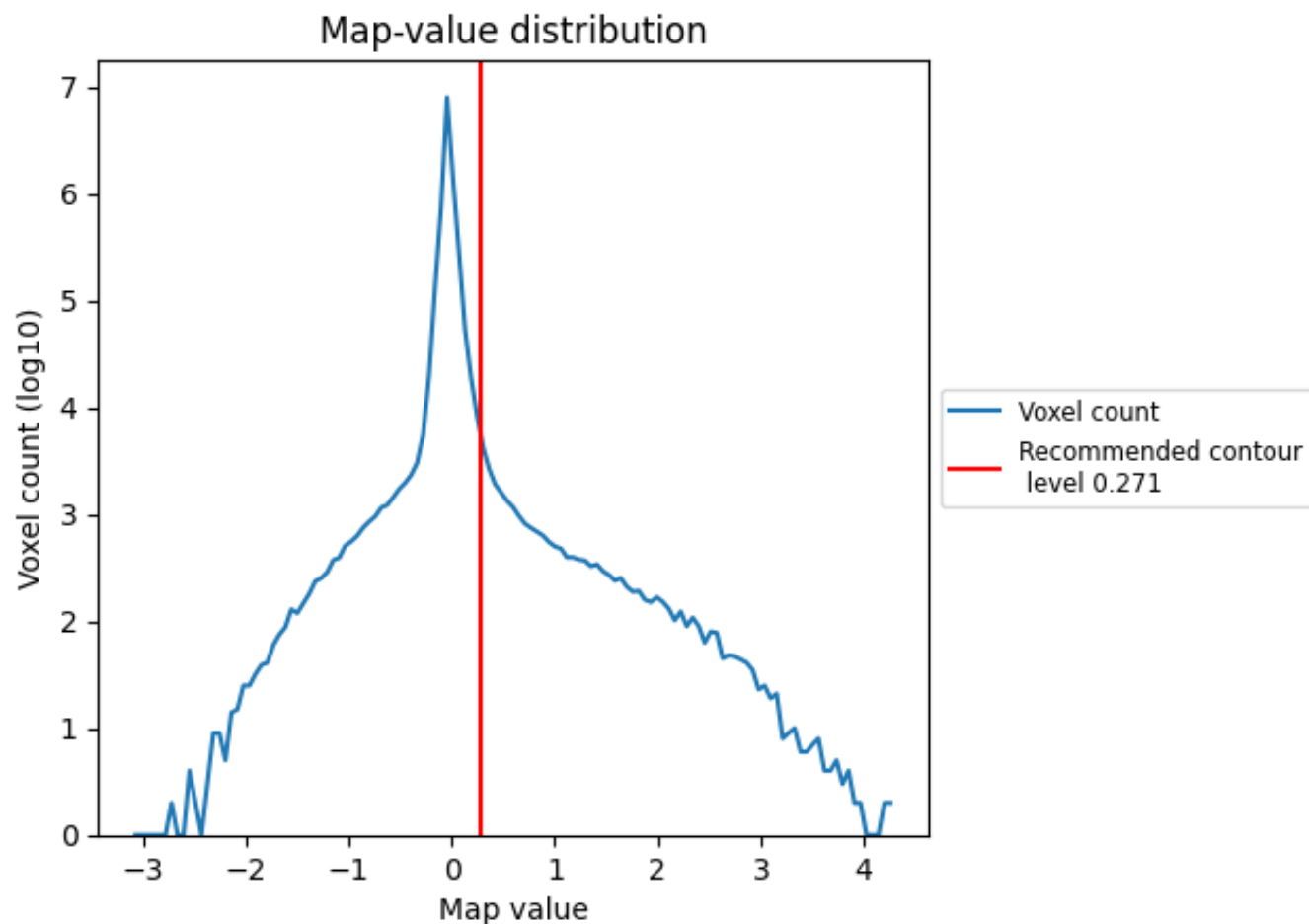
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

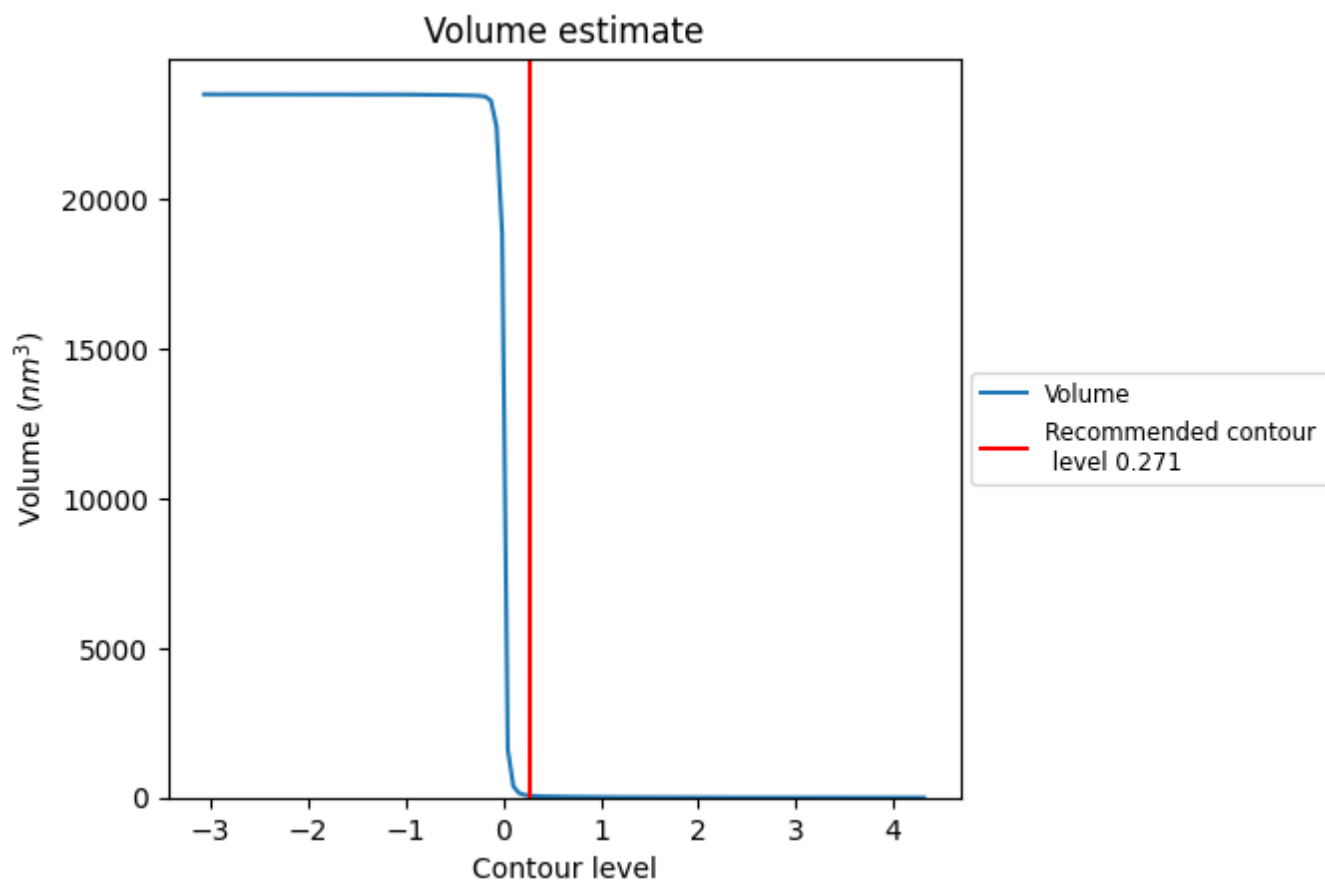
This section contains the results of statistical analysis of the map.

### 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.

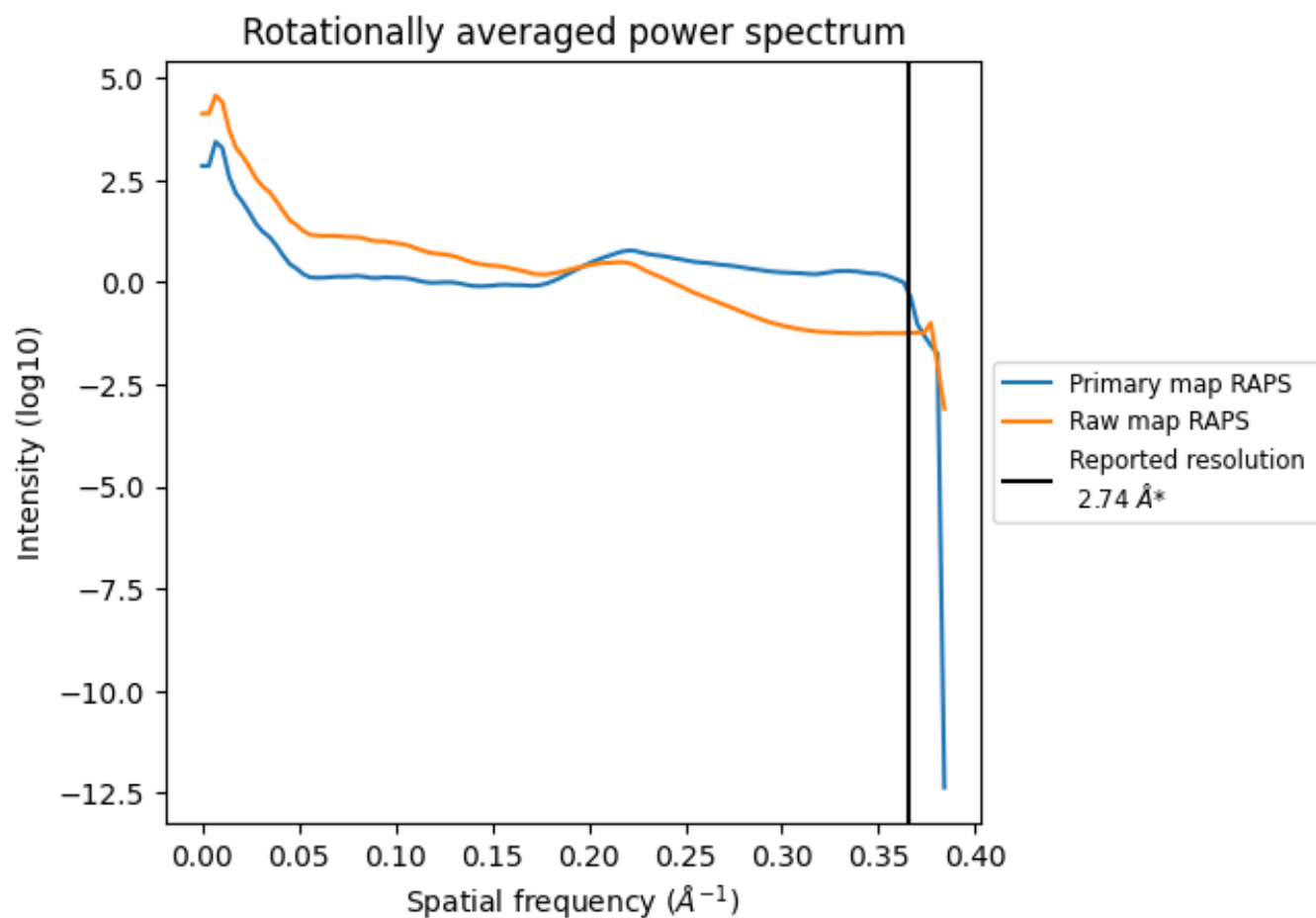
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm<sup>3</sup>; this corresponds to an approximate mass of 57 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 ⓘ

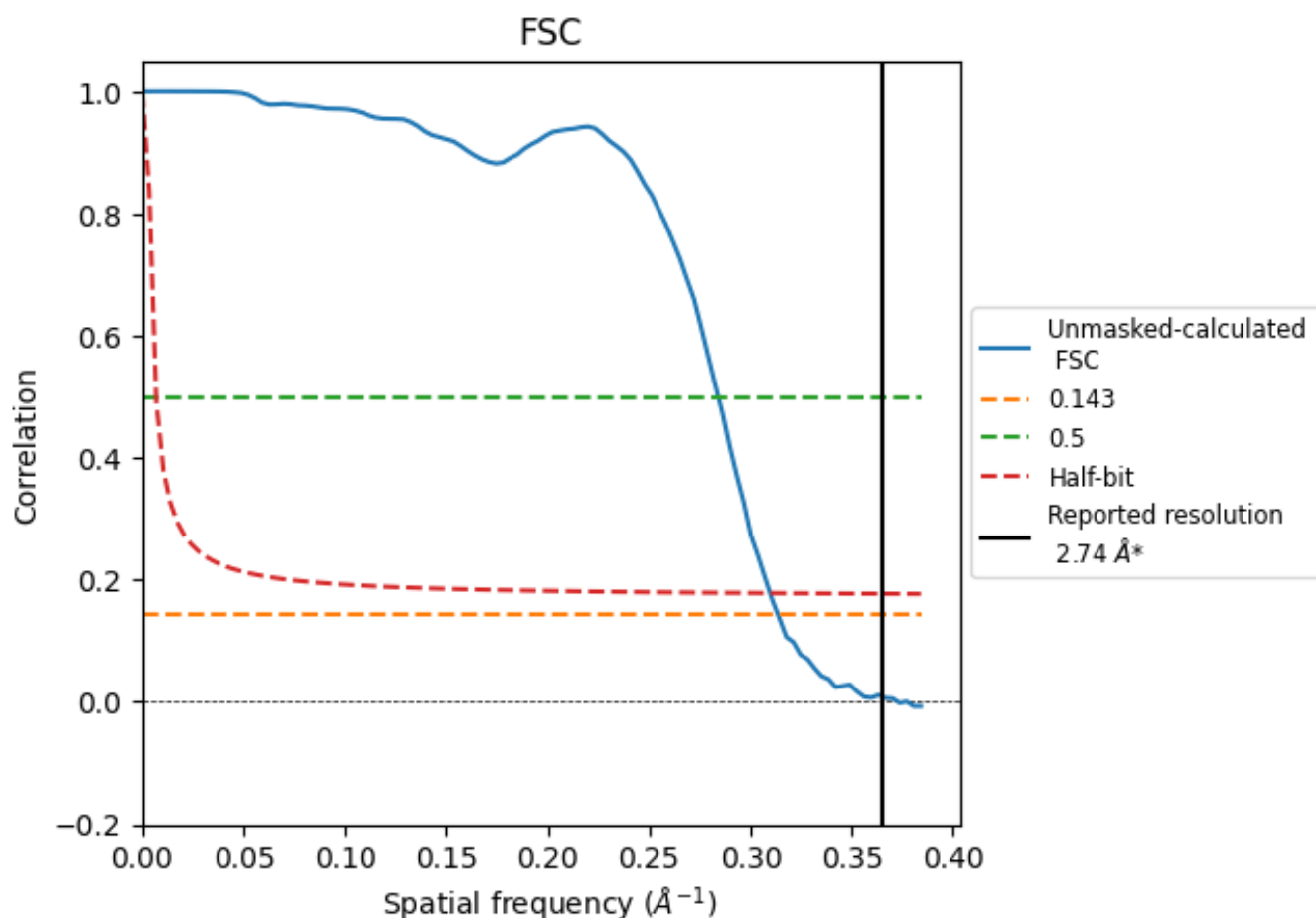


\*Reported resolution corresponds to spatial frequency of 0.365 Å<sup>-1</sup>

## 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  $0.365 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

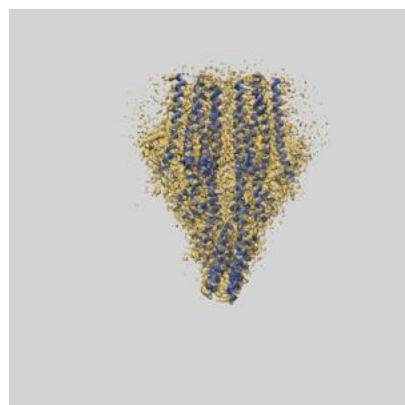
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.52	3.23

\*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 3.19 differs from the reported value 2.74 by more than 10 %

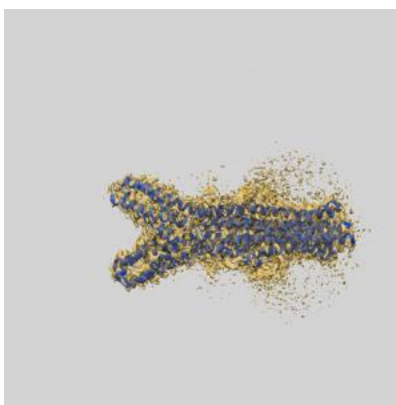
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51108 and PDB model 9G71. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

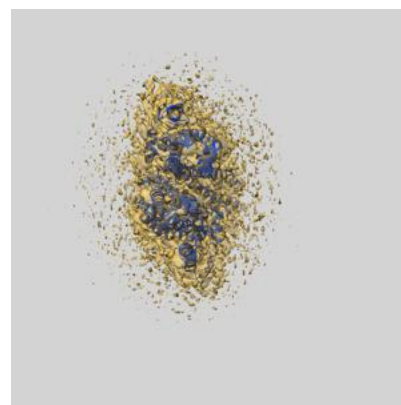
### 9.1 Map-model overlay [i](#)



X



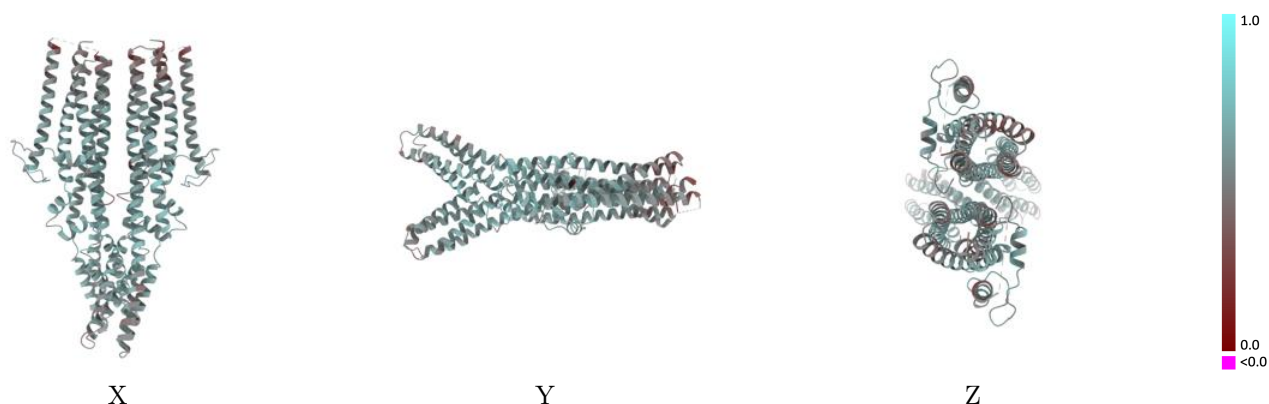
Y



Z

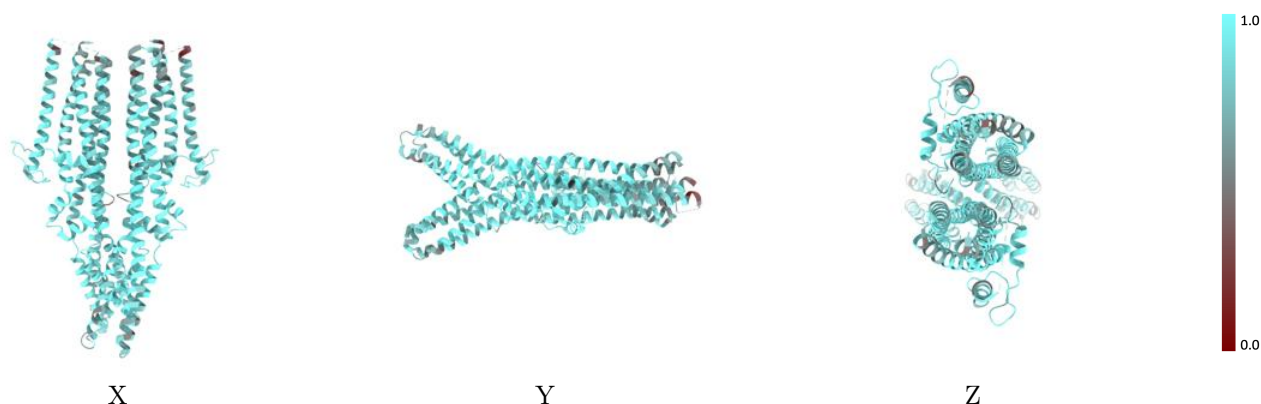
The images above show the 3D surface view of the map at the recommended contour level 0.271 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



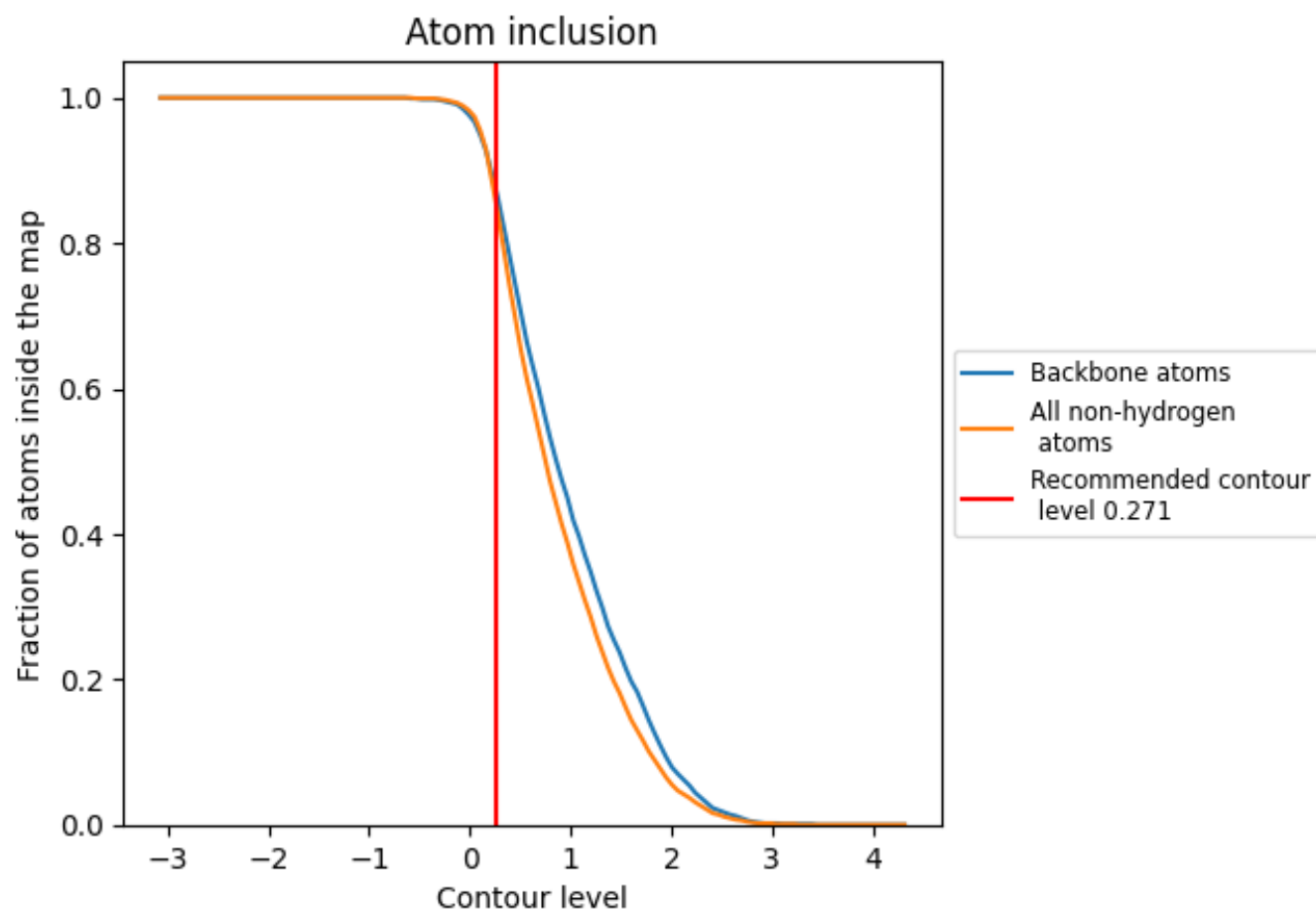
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.271).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8490	<div><div></div></div> 0.5520
A	<div><div></div></div> 0.8510	<div><div></div></div> 0.5580
B	<div><div></div></div> 0.8480	<div><div></div></div> 0.5470
C	<div><div></div></div> 0.6430	<div><div></div></div> 0.4890
D	<div><div></div></div> 0.9290	<div><div></div></div> 0.6130
E	<div><div></div></div> 0.6790	<div><div></div></div> 0.4490
F	<div><div></div></div> 0.8930	<div><div></div></div> 0.5170

1.0

0.0

<0.0