



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 02:33 PM EDT

PDB ID : 6BE1
EMDB ID : EMD-7088
Title : Cryo-EM structure of serotonin receptor
Authors : Basak, S.; Chakrapani, S.
Deposited on : 2017-10-24
Resolution : 4.31 Å(reported)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
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)	:	2.39

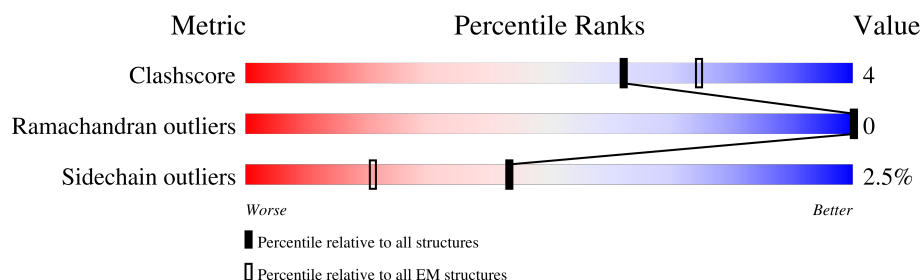
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.31 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	457	<div> <div>8%</div> <div>77%</div> <div>10%</div> <div>13%</div> </div>
1	B	457	<div> <div>7%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
1	C	457	<div> <div>7%</div> <div>75%</div> <div>11%</div> <div>13%</div> </div>
1	D	457	<div> <div>7%</div> <div>70%</div> <div>16%</div> <div>13%</div> </div>
1	E	457	<div> <div>8%</div> <div>76%</div> <div>11%</div> <div>13%</div> </div>
2	F	3	<div> <div>33%</div> <div>67%</div> <div>33%</div> </div>
2	K	3	<div> <div>33%</div> <div>67%</div> </div>
3	G	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	2	<div> <div>50%</div> <div>50%</div> </div>
3	J	2	<div> <div>50%</div> <div>100%</div> </div>
3	L	2	<div> <div>50%</div> <div>100%</div> </div>
3	N	2	<div> <div>100%</div> </div>
3	O	2	<div> <div>50%</div> <div>50%</div> </div>
3	P	2	<div> <div>50%</div> <div>50%</div> </div>
3	Q	2	<div> <div>50%</div> <div>50%</div> </div>
4	H	3	<div> <div>33%</div> <div>100%</div> </div>
5	M	3	<div> <div>33%</div> <div>67%</div> </div>

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
2	NAG	F	1	X	-	-	-
2	NAG	K	2	X	-	-	-
3	NAG	G	1	X	-	-	-
3	NAG	P	1	X	-	-	-
3	NAG	Q	1	X	-	-	-

2 Entry composition [i](#)

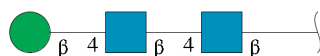
There are 11 unique types of molecules in this entry. The entry contains 16910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5-hydroxytryptamine receptor 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	399	Total	C	N	O	S	0	0
			3277	2155	536	576	10		
1	B	399	Total	C	N	O	S	0	0
			3265	2145	534	576	10		
1	C	399	Total	C	N	O	S	0	0
			3272	2150	534	578	10		
1	D	399	Total	C	N	O	S	0	0
			3266	2146	534	576	10		
1	E	399	Total	C	N	O	S	0	0
			3269	2147	534	578	10		

- Molecule 2 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.



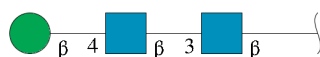
Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



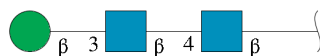
Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

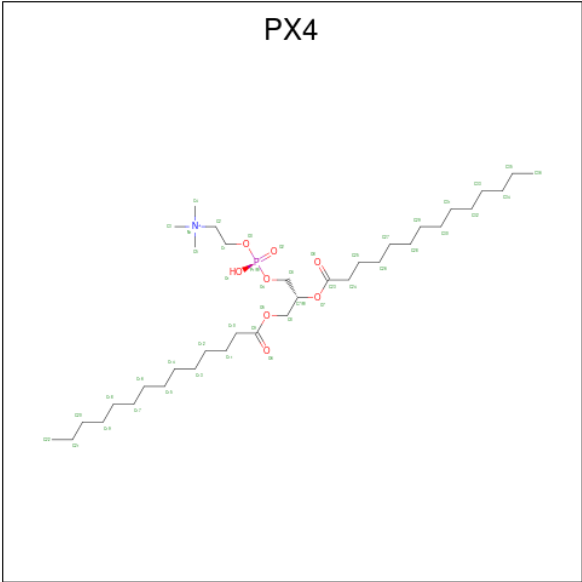


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			13	8	1	4	
6	A	1	Total	C	N	O	0
			15	8	1	6	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Na	0
			1	1	

- Molecule 8 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).

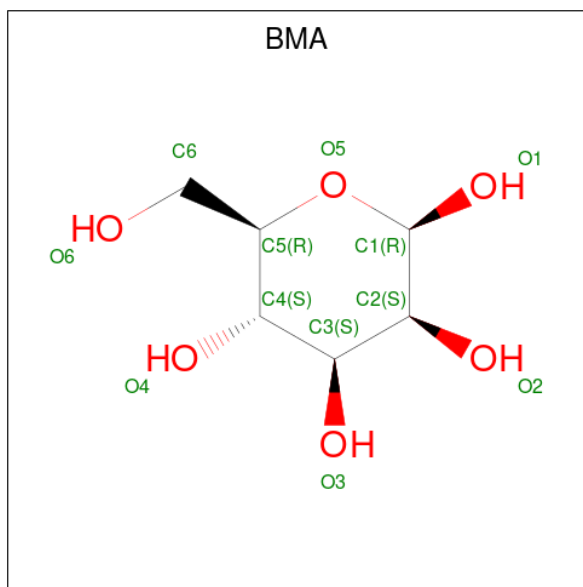


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	P	0
			18	10	7	1	
8	A	1	Total	C	O	P	0
			17	9	7	1	
8	C	1	Total	C	O	P	0
			18	10	7	1	
8	D	1	Total	C	O	P	0
			17	9	7	1	
8	E	1	Total	C	O	P	0
			17	9	7	1	

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
10	E	1	Total	C	O	0
			11	6	5	

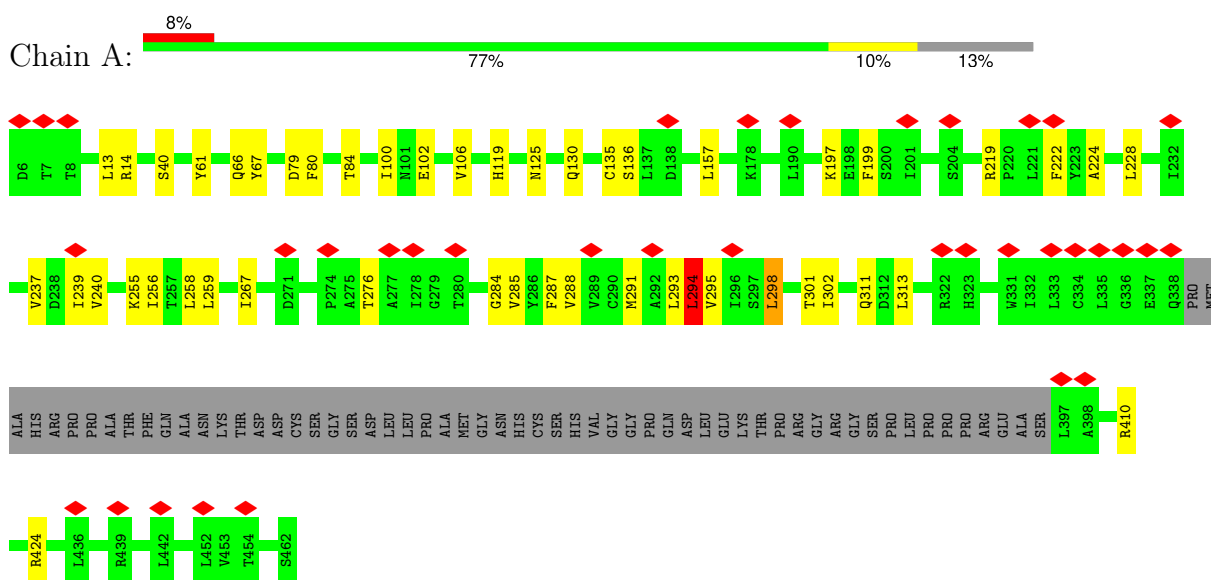
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	3	Total	O	0
			3	3	
11	B	1	Total	O	0
			1	1	
11	C	3	Total	O	0
			3	3	
11	D	2	Total	O	0
			2	2	
11	E	2	Total	O	0
			2	2	

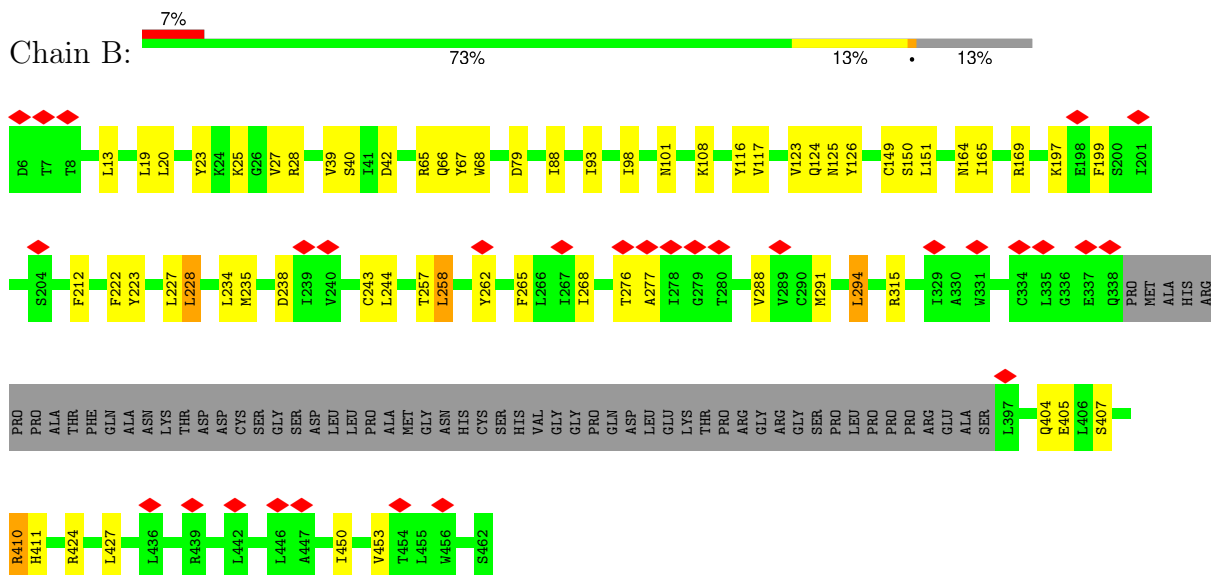
3 Residue-property plots

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

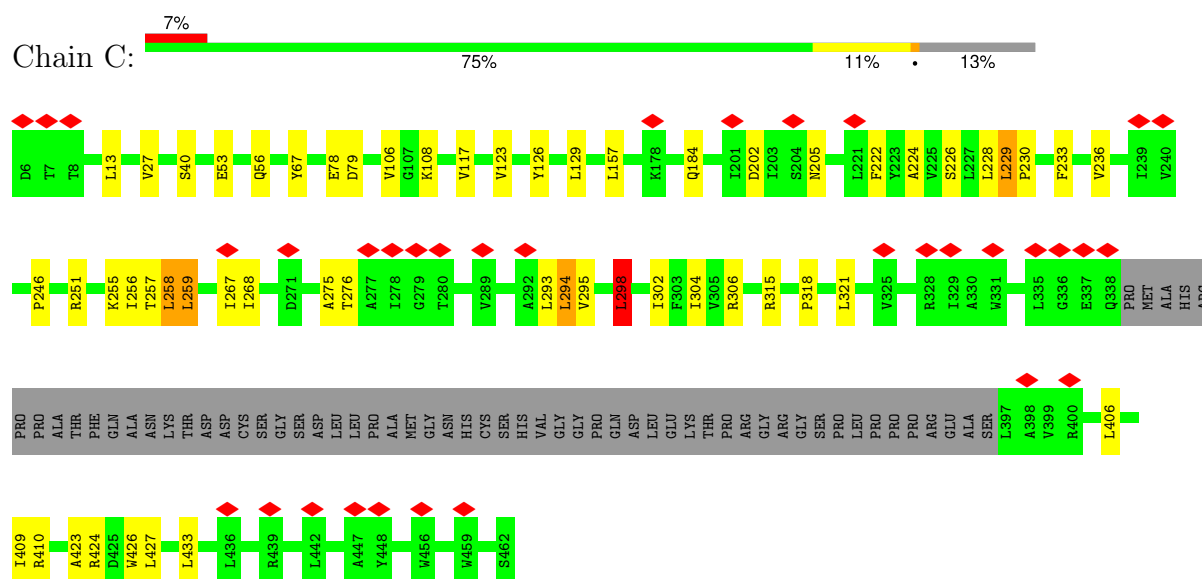
• Molecule 1: 5-hydroxytryptamine receptor 3A



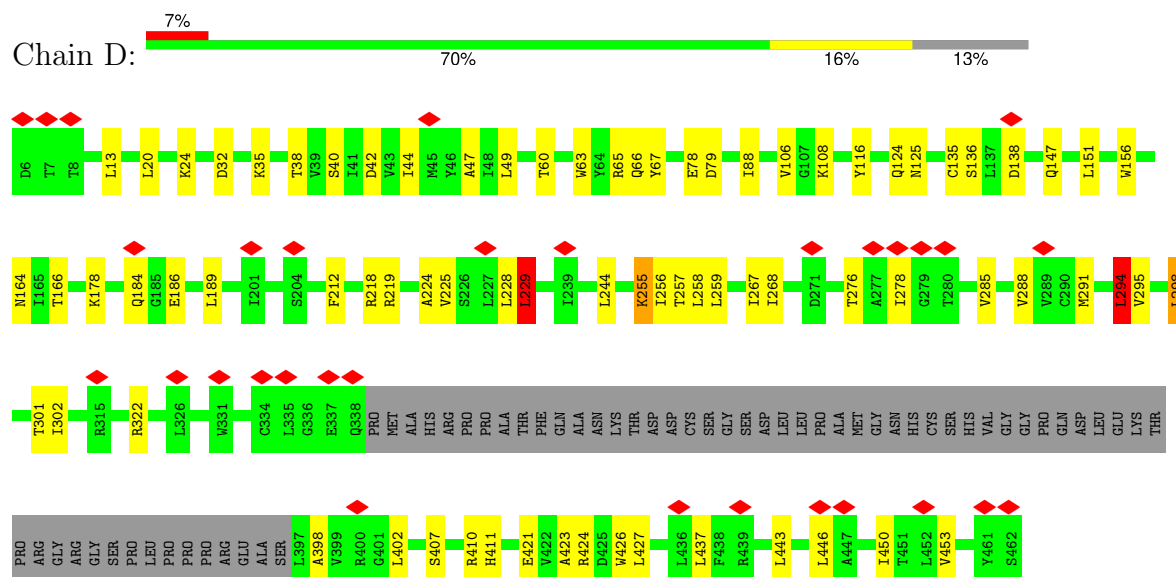
• Molecule 1: 5-hydroxytryptamine receptor 3A



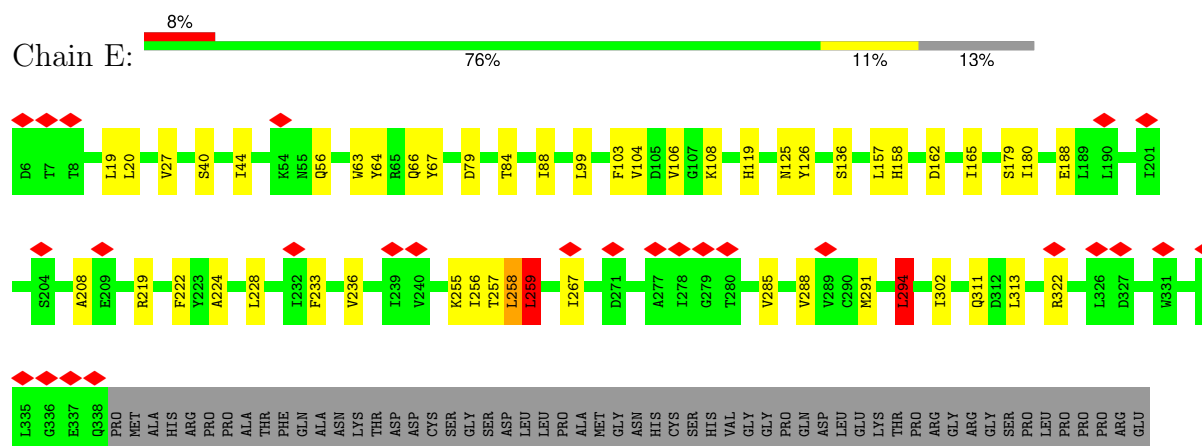
• Molecule 1: 5-hydroxytryptamine receptor 3A

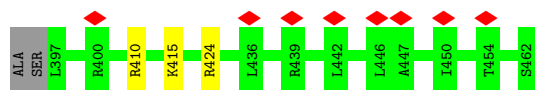


• Molecule 1: 5-hydroxytryptamine receptor 3A



• Molecule 1: 5-hydroxytryptamine receptor 3A





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



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



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	3D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, α =Not provided°, β =Not provided°, γ =Not provided°, space group=Not provided	Depositor
Number of particles used	108727	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	319.2, 319.2, 319.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, BMA, PX4, NA, 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	0.27	0/3367	0.62	4/4600 (0.1%)
1	B	0.27	0/3354	0.62	3/4583 (0.1%)
1	C	0.27	0/3361	0.65	8/4592 (0.2%)
1	D	0.27	0/3355	0.63	5/4584 (0.1%)
1	E	0.28	0/3358	0.61	3/4588 (0.1%)
All	All	0.27	0/16795	0.63	23/22947 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	ASP	CB-CG-OD1	7.90	125.41	118.30
1	C	229	LEU	CA-CB-CG	7.34	132.19	115.30
1	C	129	LEU	CA-CB-CG	7.28	132.03	115.30
1	D	79	ASP	CB-CG-OD1	7.16	124.74	118.30
1	B	294	LEU	CA-CB-CG	7.01	131.43	115.30
1	D	229	LEU	CA-CB-CG	6.51	130.27	115.30
1	C	298	LEU	CA-CB-CG	6.28	129.74	115.30
1	E	294	LEU	CA-CB-CG	6.27	129.72	115.30
1	C	294	LEU	CA-CB-CG	6.07	129.26	115.30
1	D	294	LEU	CA-CB-CG	5.86	128.78	115.30
1	C	293	LEU	CA-CB-CG	5.85	128.76	115.30
1	B	228	LEU	CA-CB-CG	5.76	128.54	115.30
1	E	259	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	79	ASP	CB-CG-OD1	5.63	123.36	118.30
1	E	79	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	78	GLU	C-N-CA	5.57	135.62	121.70
1	D	259	LEU	CA-CB-CG	5.51	127.96	115.30
1	C	259	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	79	ASP	CB-CG-OD1	5.44	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	259	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	78	GLU	C-N-CA	5.22	134.75	121.70
1	A	293	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3277	0	3278	24	0
1	B	3265	0	3254	35	0
1	C	3272	0	3266	34	0
1	D	3266	0	3255	43	0
1	E	3269	0	3257	32	0
2	F	39	0	33	0	0
2	K	39	0	33	0	0
3	G	28	0	24	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	24	0	0
3	P	28	0	24	0	0
3	Q	28	0	24	0	0
4	H	39	0	34	0	0
5	M	39	0	34	1	0
6	A	28	0	25	0	0
6	C	28	0	25	0	0
6	D	14	0	13	0	0
7	A	1	0	0	0	0
8	A	35	0	28	0	0
8	C	18	0	15	0	0
8	D	17	0	13	0	0
8	E	17	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	1	0	0	0	0
10	E	11	0	10	0	0
11	A	3	0	0	0	0
11	B	1	0	0	0	0
11	C	3	0	0	0	0
11	D	2	0	0	0	0
11	E	2	0	0	0	0
All	All	16910	0	16782	137	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 (137) 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)
1:D:66:GLN:HB2	1:D:125:ASN:HB3	1.76	0.66
1:D:224:ALA:O	1:D:228:LEU:HB2	1.99	0.62
1:A:157:LEU:HD12	1:E:126:TYR:HB2	1.82	0.61
1:B:238:ASP:HB3	1:B:258:LEU:HD11	1.82	0.61
1:B:40:SER:HB2	1:B:67:TYR:HB2	1.81	0.60
1:A:61:TYR:HD1	1:A:130:GLN:HB3	1.67	0.60
1:A:106:VAL:HB	1:E:108:LYS:HE2	1.85	0.59
1:C:40:SER:HB2	1:C:67:TYR:HB2	1.85	0.58
1:E:311:GLN:HB3	1:E:313:LEU:HD13	1.86	0.57
1:B:126:TYR:HB2	1:C:157:LEU:HD12	1.85	0.57
1:C:268:ILE:HG21	1:D:267:ILE:HD12	1.87	0.57
1:C:108:LYS:HE2	1:D:106:VAL:HB	1.87	0.56
1:C:257:THR:HG21	1:D:256:ILE:HB	1.87	0.56
1:D:255:LYS:NZ	1:D:301:THR:OG1	2.38	0.56
1:B:257:THR:HG21	1:C:256:ILE:HB	1.88	0.56
1:A:219:ARG:NH1	1:B:277:ALA:O	2.39	0.55
1:A:224:ALA:HA	1:A:228:LEU:HD23	1.87	0.55
1:C:202:ASP:HB2	1:C:205:ASN:HB2	1.87	0.55
1:A:311:GLN:HB3	1:A:313:LEU:HD13	1.87	0.55
1:D:40:SER:HB2	1:D:67:TYR:HB2	1.88	0.55
1:D:108:LYS:HE2	1:E:106:VAL:HB	1.88	0.54
1:A:255:LYS:NZ	1:A:301:THR:OG1	2.41	0.54
1:D:268:ILE:HG21	1:E:267:ILE:HD12	1.89	0.54
1:D:178:LYS:NZ	1:D:189:LEU:O	2.40	0.54
1:D:116:TYR:HB2	1:D:124:GLN:HB3	1.90	0.54
1:D:407:SER:O	1:D:411:HIS:ND1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:THR:HG22	1:D:164:ASN:HB3	1.90	0.53
1:D:166:THR:HG22	5:M:1:NAG:H61	1.90	0.53
1:B:42:ASP:OD1	1:B:169:ARG:NH1	2.41	0.53
1:B:66:GLN:HB2	1:B:125:ASN:HB3	1.90	0.53
1:E:158:HIS:HB3	1:E:162:ASP:HB3	1.90	0.52
1:D:257:THR:HG21	1:E:256:ILE:HB	1.91	0.52
1:B:42:ASP:HB3	1:B:65:ARG:HB2	1.91	0.51
1:B:108:LYS:HE2	1:C:106:VAL:HB	1.92	0.51
1:E:20:LEU:HD11	1:E:88:ILE:HD11	1.93	0.51
1:E:40:SER:HB2	1:E:67:TYR:HB2	1.93	0.51
1:B:13:LEU:HD12	1:C:27:VAL:HG11	1.93	0.51
1:E:165:ILE:HG12	1:E:208:ALA:HB1	1.93	0.51
1:D:244:LEU:HD22	1:E:302:ILE:HD11	1.92	0.50
1:C:304:ILE:HD13	1:C:433:LEU:HD12	1.92	0.50
1:B:222:PHE:HB2	1:C:276:THR:HB	1.93	0.50
1:C:233:PHE:HA	1:C:236:VAL:HG22	1.92	0.50
1:E:66:GLN:HB2	1:E:125:ASN:HB3	1.93	0.50
1:A:66:GLN:HB2	1:A:125:ASN:HB3	1.93	0.50
1:D:295:VAL:HA	1:D:298:LEU:HD23	1.94	0.49
1:B:149:CYS:SG	1:B:150:SER:N	2.86	0.49
1:E:255:LYS:HA	1:E:258:LEU:HD23	1.95	0.49
1:D:225:VAL:HG23	1:D:229:LEU:HD21	1.94	0.48
1:B:244:LEU:HD22	1:C:302:ILE:HD11	1.96	0.48
1:C:222:PHE:HB2	1:D:276:THR:HA	1.95	0.48
1:A:256:ILE:HB	1:E:257:THR:HG21	1.95	0.48
1:D:44:ILE:HB	1:D:63:TRP:HB2	1.95	0.48
1:C:224:ALA:O	1:C:228:LEU:HB2	2.13	0.48
1:B:291:MET:HA	1:B:294:LEU:HD23	1.95	0.48
1:E:256:ILE:HA	1:E:259:LEU:HD23	1.95	0.48
1:D:151:LEU:HB2	1:D:212:PHE:HB2	1.96	0.47
1:B:151:LEU:HB2	1:B:212:PHE:HB2	1.96	0.47
1:A:100:ILE:HD12	1:A:102:GLU:H	1.78	0.47
1:C:117:VAL:HA	1:C:123:VAL:HG12	1.96	0.47
1:C:229:LEU:HD23	1:C:230:PRO:HD3	1.97	0.47
1:D:47:ALA:O	1:D:60:THR:OG1	2.30	0.47
1:B:222:PHE:HD1	1:C:275:ALA:HB3	1.80	0.47
1:D:288:VAL:HA	1:D:291:MET:HG3	1.96	0.47
1:B:407:SER:O	1:B:411:HIS:ND1	2.36	0.46
1:E:84:THR:HG23	1:E:119:HIS:HD2	1.80	0.46
1:D:285:VAL:HA	1:D:288:VAL:HG12	1.95	0.46
1:D:42:ASP:HB3	1:D:65:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ARG:HE	1:B:411:HIS:CE1	2.34	0.46
1:D:20:LEU:HD21	1:D:88:ILE:HD11	1.98	0.46
1:D:116:TYR:OH	1:E:157:LEU:O	2.34	0.46
1:A:295:VAL:HA	1:A:298:LEU:HD23	1.97	0.46
1:D:291:MET:HA	1:D:294:LEU:HD23	1.97	0.46
1:D:398:ALA:HA	1:D:402:LEU:HD23	1.98	0.46
1:E:99:LEU:HB2	1:E:103:PHE:HE2	1.81	0.46
1:E:179:SER:OG	1:E:180:ILE:N	2.48	0.46
1:A:284:GLY:HA2	1:A:287:PHE:HD2	1.81	0.45
1:E:224:ALA:HA	1:E:228:LEU:HD23	1.98	0.45
1:A:222:PHE:HB3	1:B:276:THR:HG22	1.98	0.45
1:E:188:GLU:OE2	1:E:219:ARG:NE	2.49	0.45
1:A:13:LEU:HB3	1:B:27:VAL:HG11	1.98	0.45
1:A:197:LYS:HE2	1:A:199:PHE:HB2	1.98	0.45
1:B:288:VAL:HA	1:B:291:MET:HG3	1.99	0.45
1:B:116:TYR:HB2	1:B:124:GLN:HB2	1.97	0.44
1:C:184:GLN:HG2	1:D:278:ILE:HD13	2.00	0.44
1:C:267:ILE:HD12	1:C:267:ILE:HA	1.88	0.44
1:B:262:TYR:HE2	1:B:291:MET:HB3	1.82	0.44
1:A:40:SER:HB2	1:A:67:TYR:HB2	1.98	0.44
1:B:404:GLN:NE2	1:B:405:GLU:OE2	2.51	0.44
1:E:291:MET:HA	1:E:294:LEU:HD23	1.99	0.43
1:A:276:THR:HA	1:E:222:PHE:HB2	2.00	0.43
1:C:295:VAL:HA	1:C:298:LEU:HD23	2.01	0.43
1:D:184:GLN:H	1:D:219:ARG:HH22	1.67	0.43
1:D:423:ALA:HA	1:D:426:TRP:HD1	1.84	0.43
1:C:255:LYS:HA	1:C:258:LEU:HD23	2.00	0.43
1:D:32:ASP:HB3	1:D:35:LYS:HD3	2.00	0.43
1:A:84:THR:HG23	1:A:119:HIS:HD2	1.82	0.43
1:D:443:LEU:HD23	1:D:446:LEU:HD21	2.00	0.43
1:A:291:MET:HA	1:A:294:LEU:HD23	2.01	0.43
1:B:98:ILE:HG21	1:B:165:ILE:HD11	2.00	0.43
1:C:13:LEU:HD11	1:D:24:LYS:HD3	2.01	0.43
1:B:243:CYS:O	1:C:306:ARG:NH1	2.49	0.42
1:B:39:VAL:HG12	1:B:68:TRP:HB3	2.01	0.42
1:C:222:PHE:O	1:C:226:SER:OG	2.34	0.42
1:B:450:ILE:HA	1:B:453:VAL:HG22	2.02	0.42
1:E:233:PHE:HA	1:E:236:VAL:HG22	2.00	0.42
1:A:285:VAL:HA	1:A:288:VAL:HG12	2.00	0.42
1:C:126:TYR:O	1:D:156:TRP:NE1	2.36	0.42
1:C:246:PRO:HB3	1:C:251:ARG:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ALA:HA	1:C:426:TRP:HD1	1.85	0.42
1:E:44:ILE:HB	1:E:63:TRP:HB2	2.02	0.42
1:B:117:VAL:HA	1:B:123:VAL:HG12	2.02	0.41
1:A:237:VAL:HA	1:A:240:VAL:HG22	2.02	0.41
1:C:406:LEU:HA	1:C:409:ILE:HD12	2.02	0.41
1:A:14:ARG:HH22	1:A:80:PHE:HA	1.84	0.41
1:B:197:LYS:HE2	1:B:199:PHE:HB2	2.02	0.41
1:D:13:LEU:HD12	1:E:27:VAL:HG11	2.01	0.41
1:B:20:LEU:HD21	1:B:88:ILE:HD11	2.02	0.41
1:E:285:VAL:HA	1:E:288:VAL:HG12	2.03	0.41
1:B:223:TYR:O	1:B:227:LEU:HB2	2.21	0.41
1:B:23:TYR:HE2	1:B:93:ILE:HA	1.84	0.41
1:B:268:ILE:HG21	1:C:267:ILE:HG12	2.03	0.41
1:D:450:ILE:HA	1:D:453:VAL:HG22	2.02	0.41
1:E:64:TYR:HE2	1:E:66:GLN:HE21	1.69	0.41
1:C:53:GLU:O	1:C:56:GLN:NE2	2.54	0.41
1:E:56:GLN:HE21	1:E:136:SER:HA	1.85	0.41
1:A:239:ILE:HD13	1:A:239:ILE:HA	1.97	0.41
1:D:421:GLU:OE2	1:E:415:LYS:NZ	2.45	0.41
1:C:255:LYS:HA	1:C:255:LYS:HD3	1.91	0.40
1:E:255:LYS:HA	1:E:255:LYS:HD3	1.91	0.40
1:C:256:ILE:HA	1:C:259:LEU:HG	2.04	0.40
1:D:49:LEU:HD21	1:E:104:VAL:HB	2.04	0.40
1:D:186:GLU:OE2	1:D:218:ARG:NH1	2.54	0.40
1:A:135:CYS:SG	1:A:136:SER:N	2.94	0.40
1:B:265:PHE:HA	1:B:268:ILE:HG22	2.03	0.40
1:C:318:PRO:HA	1:C:321:LEU:HG	2.04	0.40
1:D:135:CYS:SG	1:D:136:SER:N	2.94	0.40
1:D:138:ASP:O	1:D:147:GLN:NE2	2.44	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	395/457 (86%)	367 (93%)	28 (7%)	0	100	100
1	B	395/457 (86%)	366 (93%)	29 (7%)	0	100	100
1	C	395/457 (86%)	366 (93%)	29 (7%)	0	100	100
1	D	395/457 (86%)	363 (92%)	32 (8%)	0	100	100
1	E	395/457 (86%)	373 (94%)	22 (6%)	0	100	100
All	All	1975/2285 (86%)	1835 (93%)	140 (7%)	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	364/419 (87%)	357 (98%)	7 (2%)	52	70
1	B	361/419 (86%)	348 (96%)	13 (4%)	30	52
1	C	363/419 (87%)	356 (98%)	7 (2%)	52	70
1	D	361/419 (86%)	350 (97%)	11 (3%)	36	57
1	E	362/419 (86%)	355 (98%)	7 (2%)	52	70
All	All	1811/2095 (86%)	1766 (98%)	45 (2%)	43	63

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	LEU
1	A	267	ILE
1	A	294	LEU
1	A	298	LEU
1	A	302	ILE
1	A	410	ARG
1	A	424	ARG
1	B	19	LEU
1	B	25	LYS
1	B	28	ARG

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Mol	Chain	Res	Type
1	B	101	ASN
1	B	164	ASN
1	B	228	LEU
1	B	234	LEU
1	B	235	MET
1	B	258	LEU
1	B	315	ARG
1	B	410	ARG
1	B	424	ARG
1	B	427	LEU
1	C	258	LEU
1	C	294	LEU
1	C	298	LEU
1	C	315	ARG
1	C	410	ARG
1	C	424	ARG
1	C	427	LEU
1	D	229	LEU
1	D	255	LYS
1	D	258	LEU
1	D	294	LEU
1	D	298	LEU
1	D	302	ILE
1	D	322	ARG
1	D	410	ARG
1	D	424	ARG
1	D	427	LEU
1	D	437	LEU
1	E	19	LEU
1	E	258	LEU
1	E	259	LEU
1	E	294	LEU
1	E	322	ARG
1	E	410	ARG
1	E	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	B	101	ASN
1	B	164	ASN

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Mol	Chain	Res	Type
1	D	119	HIS
1	D	124	GLN
1	E	9	GLN
1	E	56	GLN
1	E	119	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

28 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	F	1	1,2	14,14,15	0.66	1 (7%)	17,19,21	2.66	1 (5%)
2	NAG	F	2	2	14,14,15	0.26	0	17,19,21	0.58	0
2	BMA	F	3	2	11,11,12	0.78	0	15,15,17	0.81	0
3	NAG	G	1	3,1	14,14,15	0.66	1 (7%)	17,19,21	2.73	1 (5%)
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.49	0
4	NAG	H	1	4	14,14,15	0.75	0	17,19,21	1.63	5 (29%)
4	NAG	H	2	4	14,14,15	0.70	1 (7%)	17,19,21	1.99	2 (11%)
4	BMA	H	3	4	11,11,12	1.21	2 (18%)	15,15,17	1.07	1 (6%)
3	NAG	I	1	3,1	14,14,15	0.68	0	17,19,21	1.25	3 (17%)
3	NAG	I	2	3	14,14,15	0.37	0	17,19,21	0.55	0
3	NAG	J	1	3,1	14,14,15	0.23	0	17,19,21	0.56	0
3	NAG	J	2	3	14,14,15	0.47	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	K	1	1,2	14,14,15	0.59	0	17,19,21	0.76	1 (5%)
2	NAG	K	2	2	14,14,15	0.67	1 (7%)	17,19,21	2.75	1 (5%)
2	BMA	K	3	2	11,11,12	0.81	0	15,15,17	0.75	0
3	NAG	L	1	3,1	14,14,15	0.33	0	17,19,21	0.54	0
3	NAG	L	2	3	14,14,15	0.33	0	17,19,21	0.52	0
5	NAG	M	1	5,1	14,14,15	0.42	0	17,19,21	0.60	0
5	NAG	M	2	5	14,14,15	0.73	1 (7%)	17,19,21	2.33	2 (11%)
5	BMA	M	3	5	11,11,12	0.78	0	15,15,17	0.85	0
3	NAG	N	1	3,1	14,14,15	0.33	0	17,19,21	0.54	0
3	NAG	N	2	3	14,14,15	0.54	0	17,19,21	0.48	0
3	NAG	O	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	1.28	1 (5%)
3	NAG	O	2	3	14,14,15	0.31	0	17,19,21	0.50	0
3	NAG	P	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	2.96	1 (5%)
3	NAG	P	2	3	14,14,15	0.32	0	17,19,21	0.51	0
3	NAG	Q	1	3,1	14,14,15	1.33	2 (14%)	17,19,21	2.59	4 (23%)
3	NAG	Q	2	3	14,14,15	0.43	0	17,19,21	0.51	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	F	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	1/1/5/7	0/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	O5-C1	3.81	1.50	1.43
4	H	3	BMA	C2-C3	2.53	1.56	1.52
5	M	2	NAG	O3-C3	-2.10	1.37	1.43
4	H	3	BMA	C4-C3	2.10	1.57	1.52
3	G	1	NAG	O4-C4	-2.09	1.37	1.43
4	H	2	NAG	O4-C4	-2.08	1.37	1.43
2	F	1	NAG	O4-C4	-2.07	1.37	1.43
3	P	1	NAG	O4-C4	-2.06	1.37	1.43
3	O	1	NAG	O4-C4	-2.04	1.37	1.43
2	K	2	NAG	O4-C4	-2.04	1.37	1.43
3	Q	1	NAG	O4-C4	-2.00	1.38	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	NAG	O4-C4-C5	12.01	138.91	109.32
3	G	1	NAG	O4-C4-C3	11.00	136.30	110.38
2	K	2	NAG	O4-C4-C3	10.91	136.10	110.38
2	F	1	NAG	O4-C4-C3	10.73	135.66	110.38
5	M	2	NAG	O3-C3-C4	-8.99	89.19	110.38
3	Q	1	NAG	C1-O5-C5	8.52	123.61	112.19
4	H	2	NAG	O4-C4-C5	6.12	124.40	109.32
4	H	2	NAG	O4-C4-C3	-5.06	98.46	110.38
3	O	1	NAG	O4-C4-C3	4.76	121.60	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C2-N2-C7	3.66	127.81	122.90
3	Q	1	NAG	O4-C4-C3	3.51	118.64	110.38
3	Q	1	NAG	C3-C4-C5	3.41	116.41	110.23
3	I	1	NAG	C2-N2-C7	3.28	127.29	122.90
4	H	1	NAG	C4-C3-C2	2.87	115.22	111.02
4	H	1	NAG	C1-C2-N2	2.83	114.90	110.43
4	H	3	BMA	C2-C3-C4	2.75	115.70	110.86
4	H	1	NAG	C1-O5-C5	2.73	115.84	112.19
5	M	2	NAG	O3-C3-C2	-2.70	103.79	109.40
4	H	1	NAG	C3-C4-C5	2.44	114.65	110.23
3	Q	1	NAG	O4-C4-C5	2.29	114.97	109.32
3	I	1	NAG	C4-C3-C2	2.18	114.21	111.02
2	K	1	NAG	C1-O5-C5	2.09	114.99	112.19
3	I	1	NAG	C1-C2-N2	2.09	113.73	110.43

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C4
2	K	2	NAG	C4
3	G	1	NAG	C4
3	P	1	NAG	C4
3	Q	1	NAG	C4

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6

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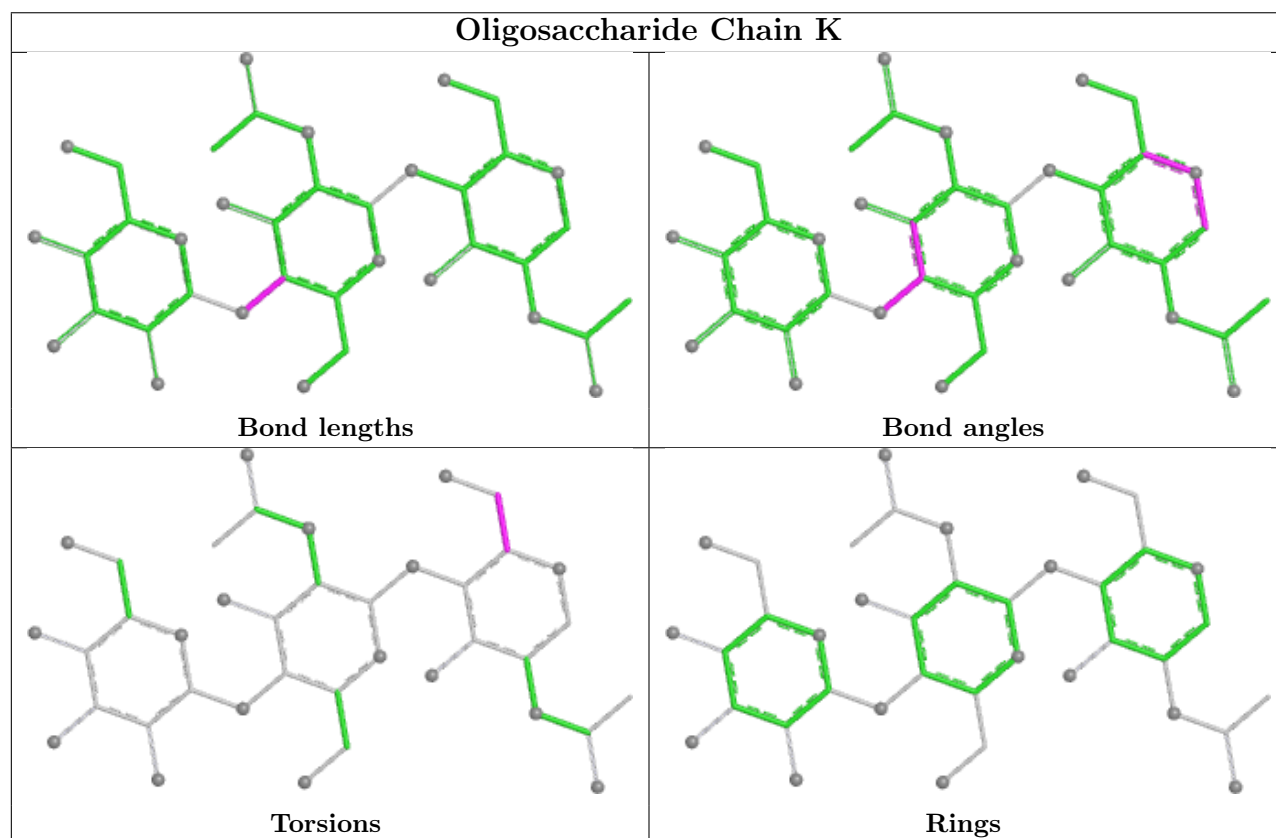
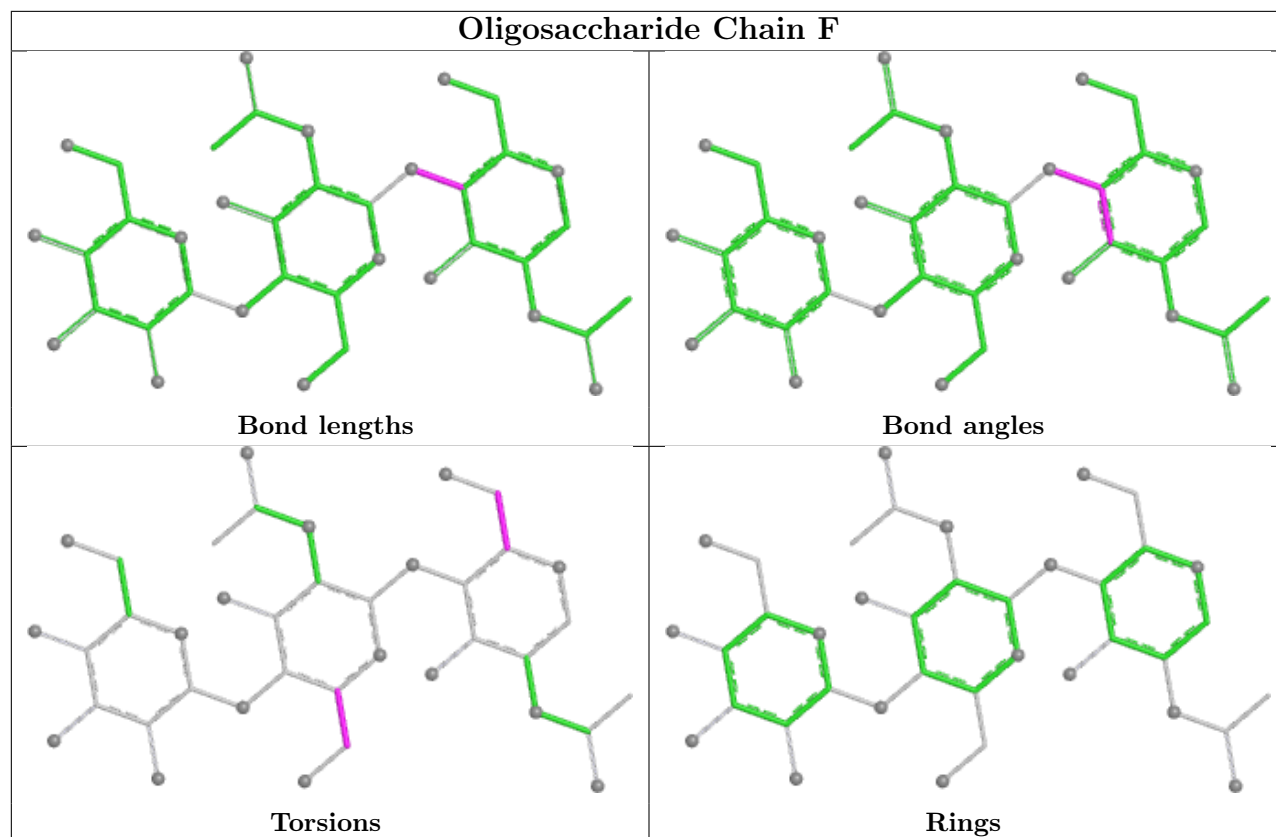
Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C1-C2-N2-C7
3	G	1	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
3	G	2	NAG	O5-C5-C6-O6
4	H	1	NAG	C1-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7

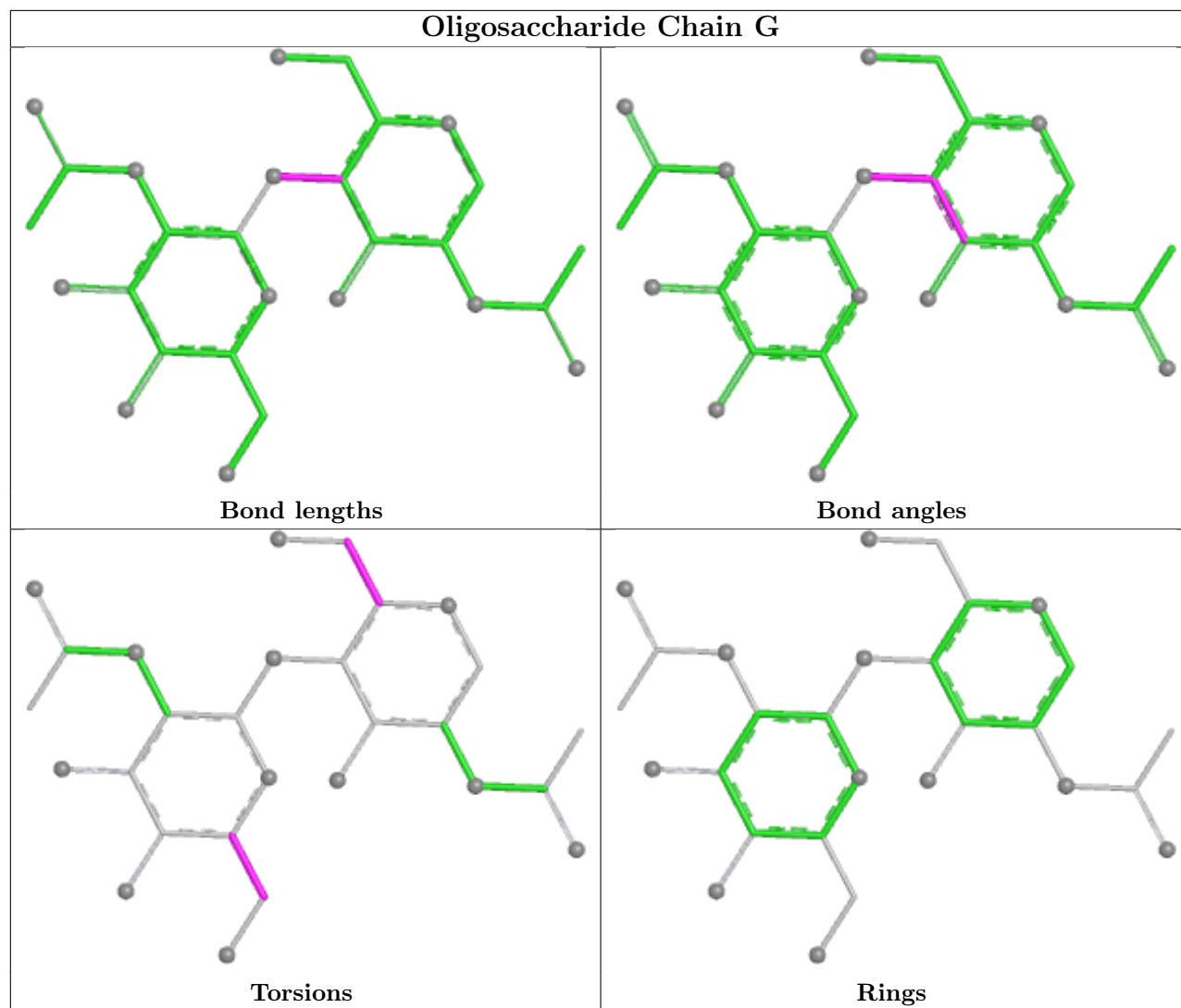
There are no ring outliers.

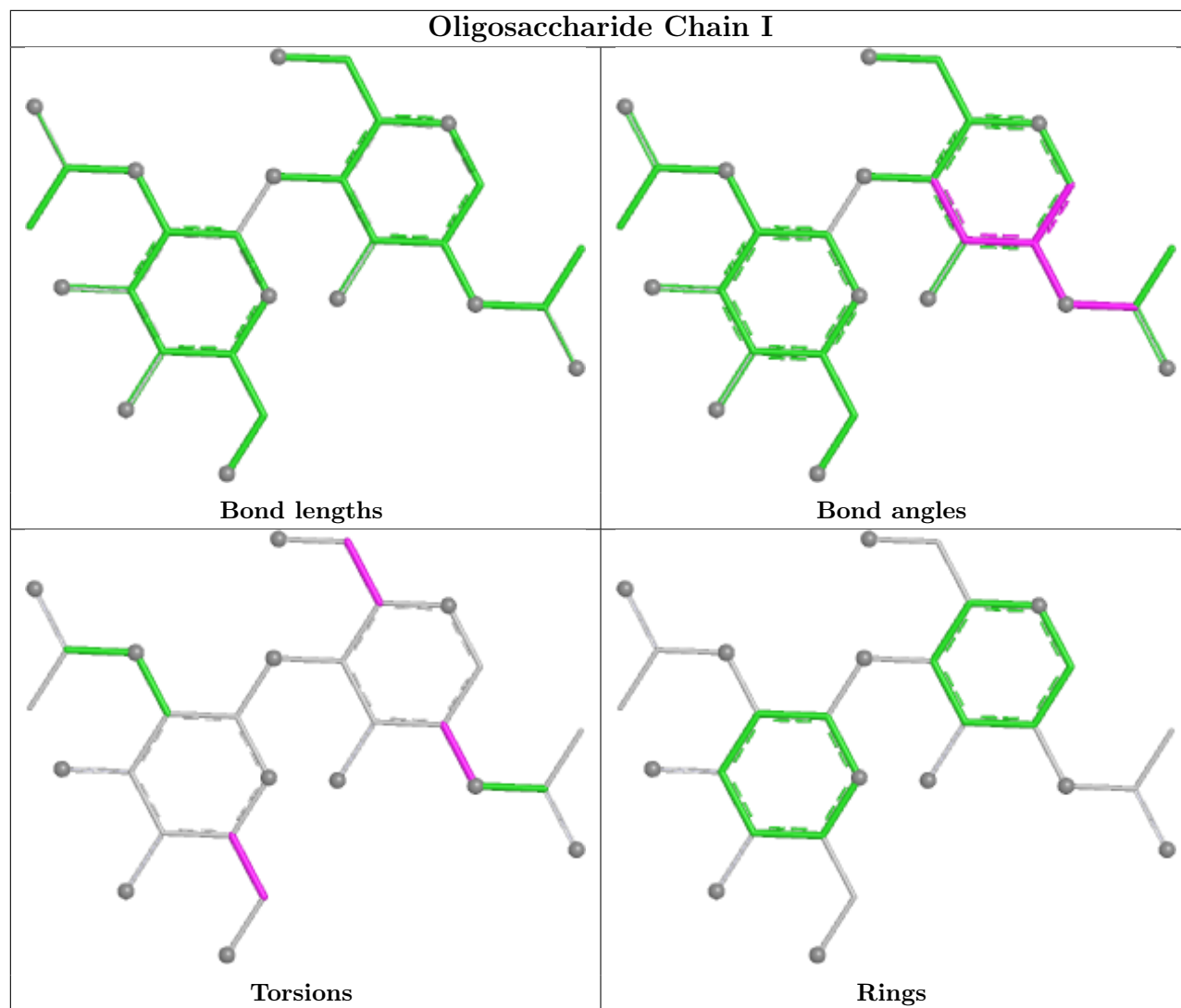
1 monomer is involved in 1 short contact:

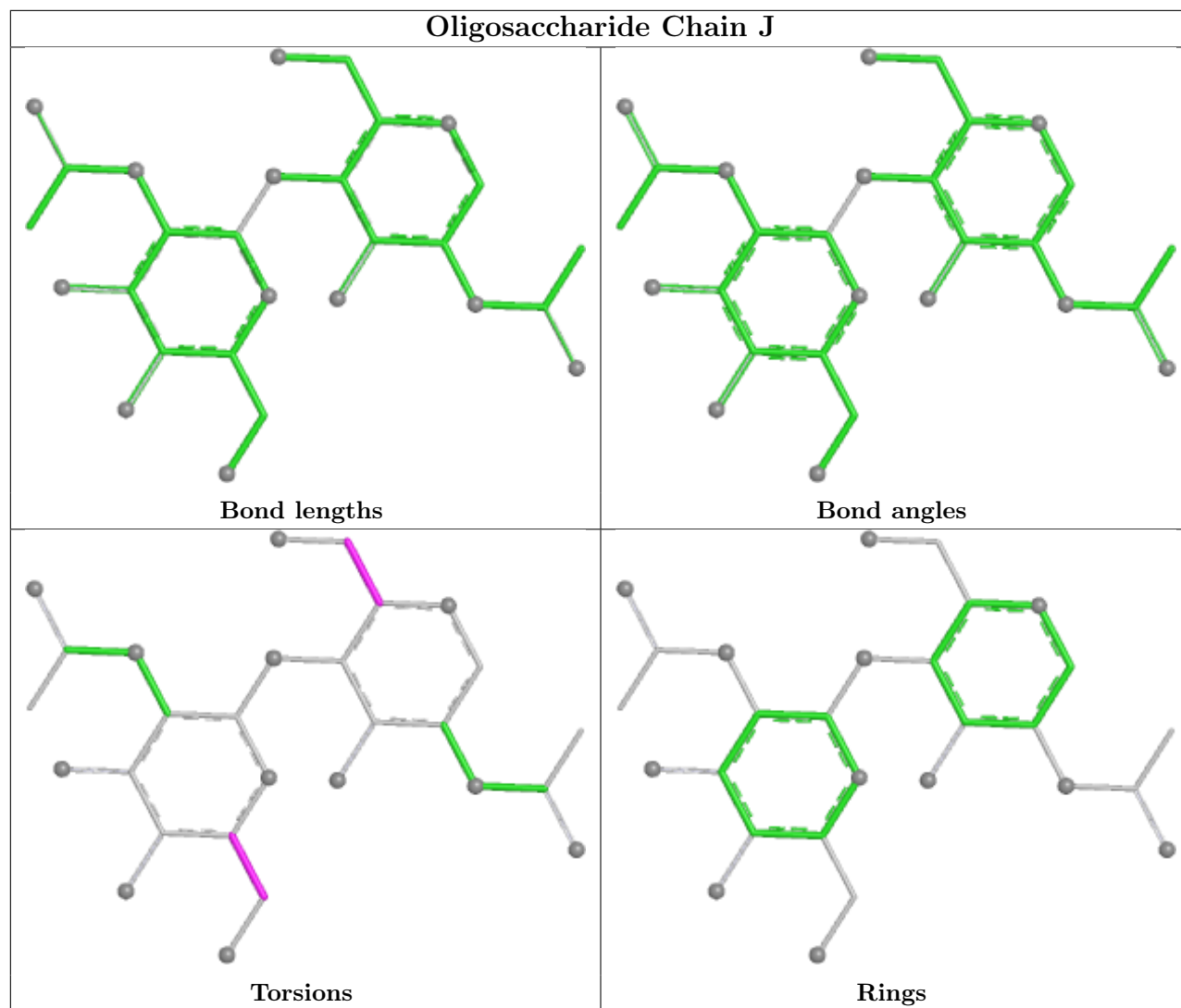
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1	NAG	1	0

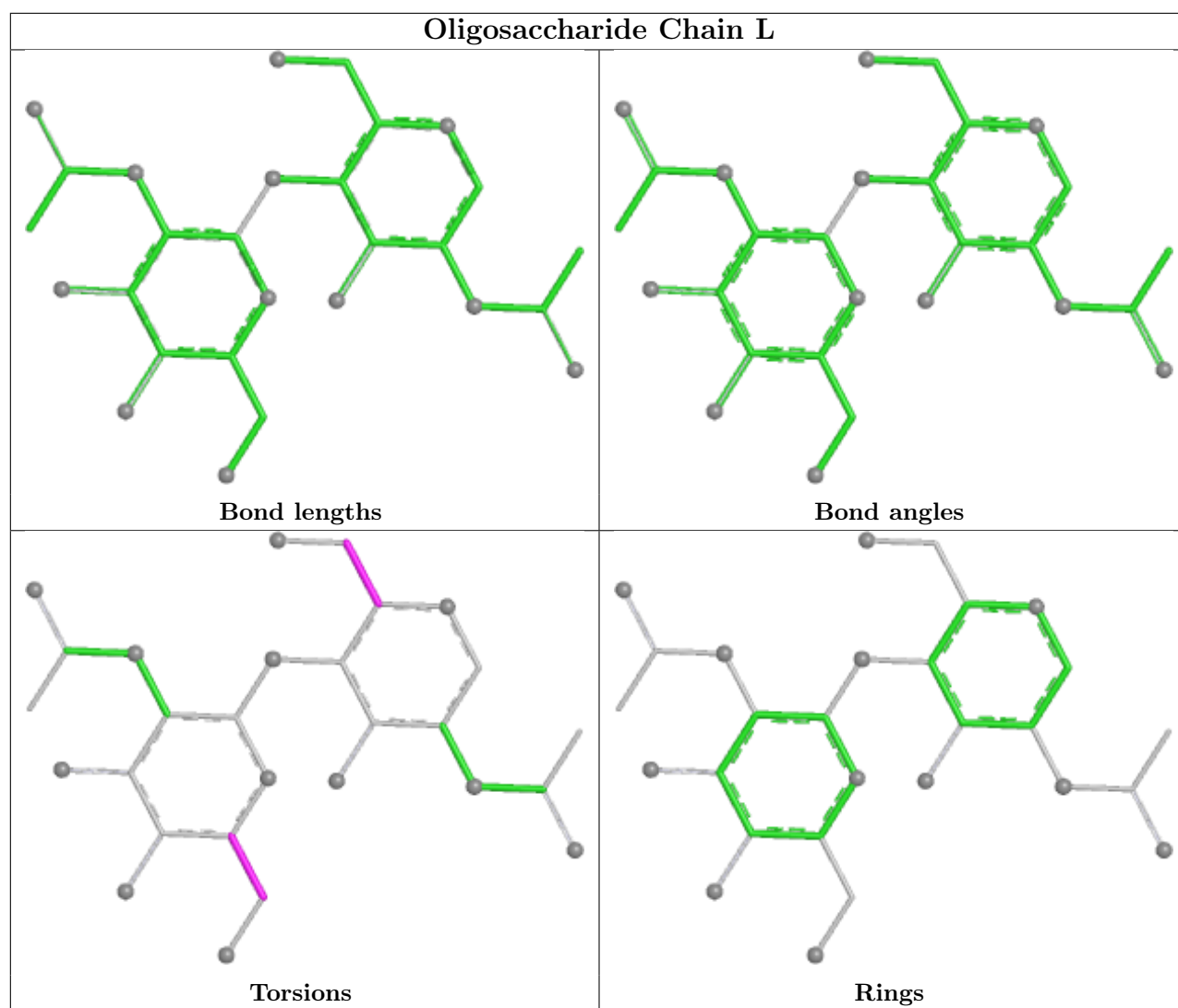
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

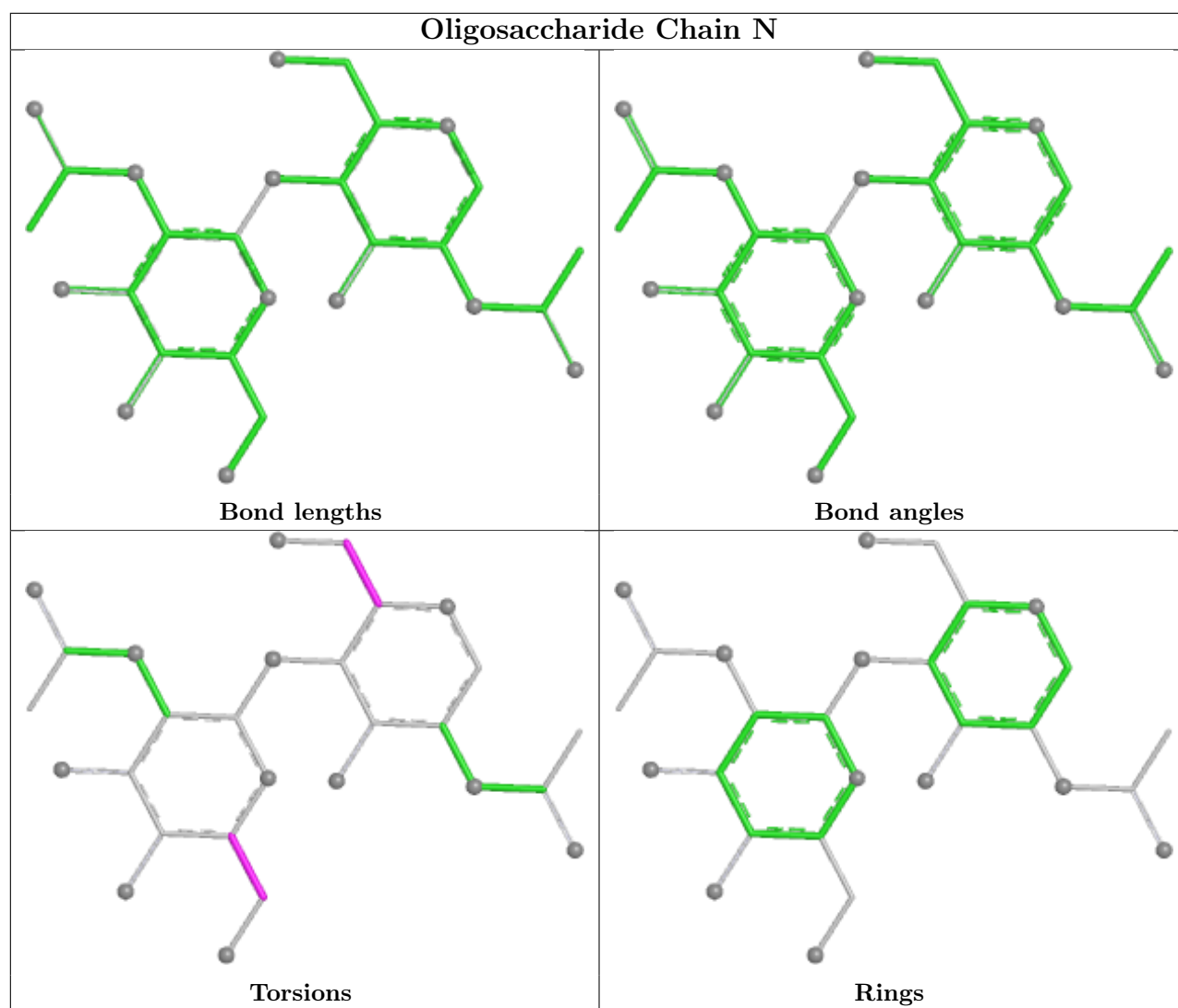


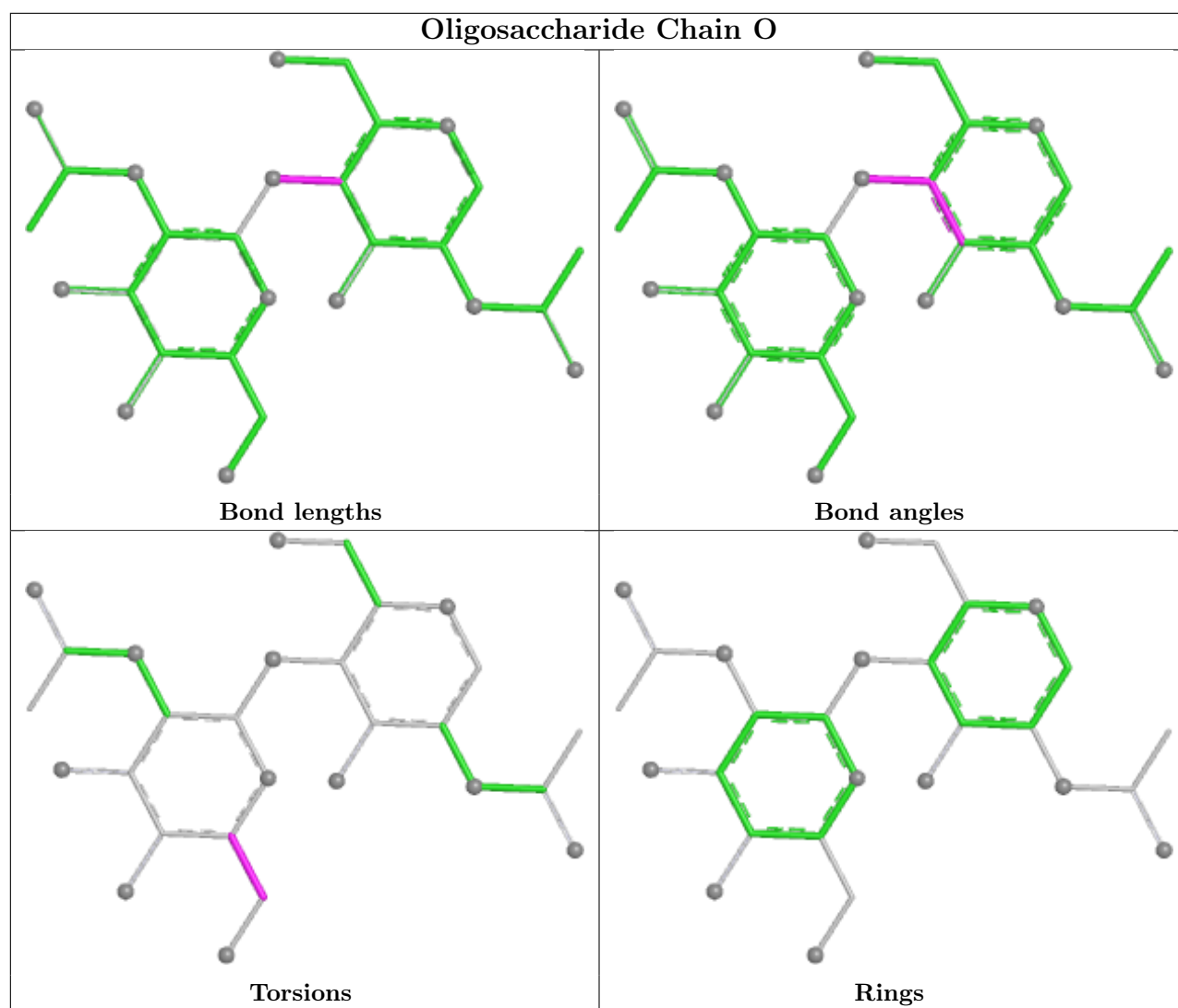


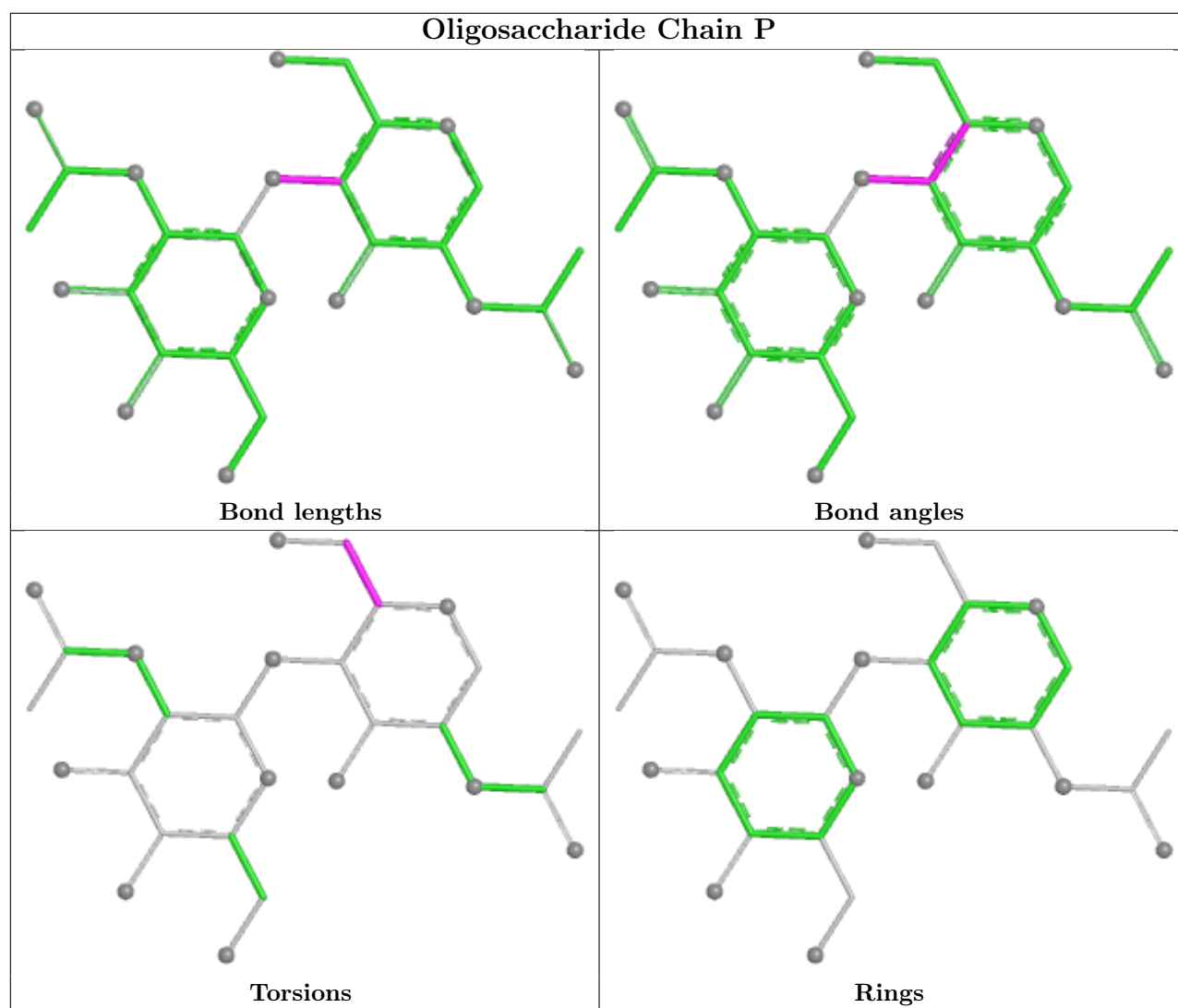


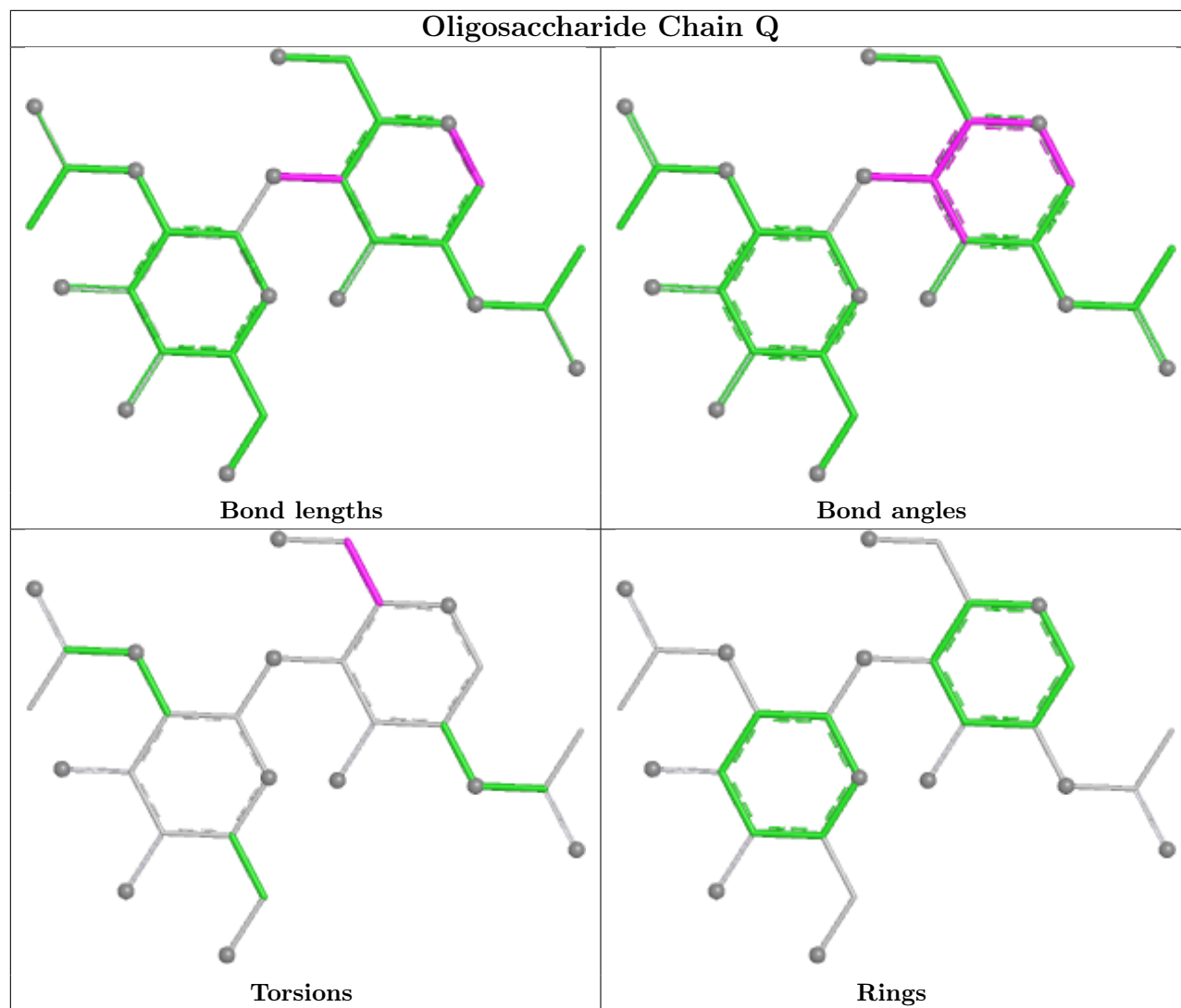


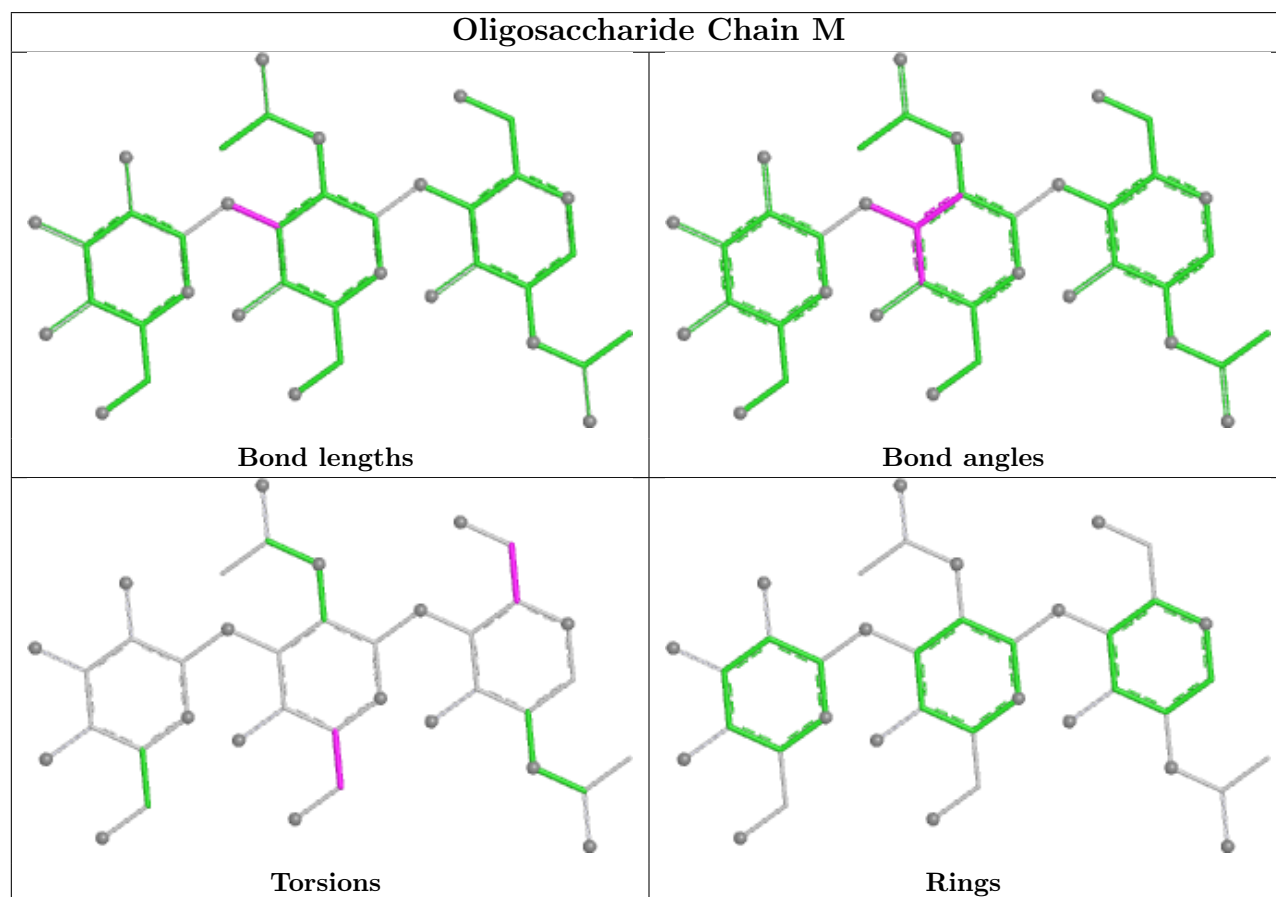
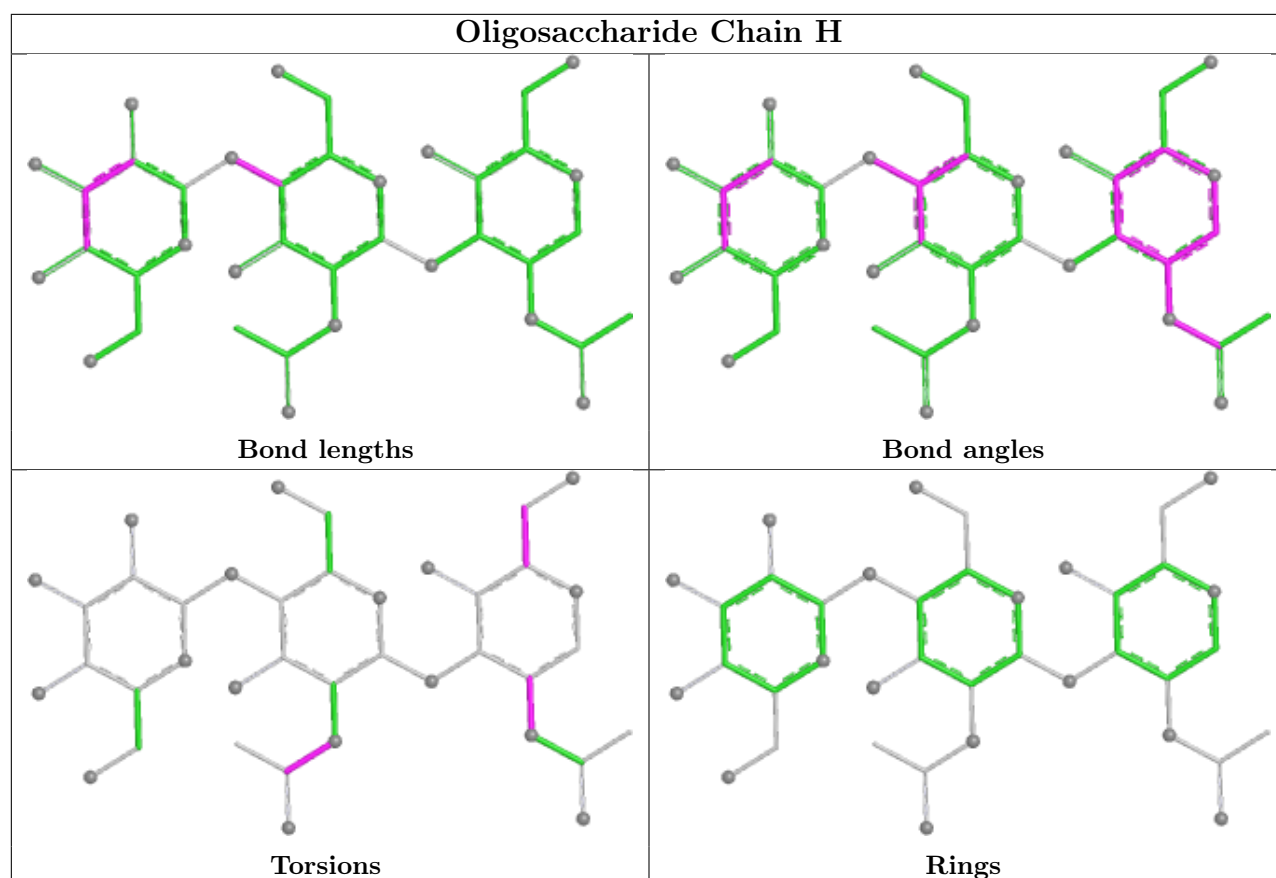












5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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
6	NAG	D	504	1	14,14,15	0.39	0	17,19,21	0.51	0
8	PX4	D	507	-	16,16,45	1.79	5 (31%)	18,20,53	1.29	2 (11%)
8	PX4	C	509	-	17,17,45	1.75	5 (29%)	19,21,53	1.28	2 (10%)
6	NAG	C	506	1	14,14,15	0.34	0	17,19,21	0.52	0
8	PX4	E	508	-	16,16,45	2.19	6 (37%)	18,20,53	1.21	1 (5%)
8	PX4	A	510	-	16,16,45	1.80	5 (31%)	18,20,53	1.29	2 (11%)
6	NAG	C	507	-	14,14,15	0.32	0	19,19,21	0.28	0
6	NAG	A	501	1	13,13,15	0.59	0	12,17,21	1.16	1 (8%)
6	NAG	A	502	-	15,15,15	0.33	0	21,21,21	0.19	0
8	PX4	A	509	-	17,17,45	2.13	6 (35%)	19,21,53	1.19	1 (5%)
10	BMA	E	503	-	11,11,12	0.81	0	15,15,17	0.95	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
6	NAG	D	504	1	-	0/6/23/26	0/1/1/1
8	PX4	D	507	-	-	5/16/16/49	-
8	PX4	C	509	-	-	6/17/17/49	-
6	NAG	C	506	1	-	1/6/23/26	0/1/1/1
8	PX4	E	508	-	-	5/16/16/49	-
8	PX4	A	510	-	-	3/16/16/49	-
6	NAG	C	507	-	-	0/6/22/26	0/1/1/1
6	NAG	A	501	1	-	2/6/19/26	0/1/1/1
6	NAG	A	502	-	-	2/6/26/26	0/1/1/1
8	PX4	A	509	-	-	7/17/17/49	-
10	BMA	E	503	-	-	0/2/18/22	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	508	PX4	P1-O2	6.14	1.69	1.50
8	A	509	PX4	P1-O2	6.12	1.69	1.50
8	A	510	PX4	P1-O3	4.01	1.69	1.54
8	D	507	PX4	P1-O3	4.00	1.69	1.54
8	C	509	PX4	P1-O3	3.99	1.69	1.54
8	A	509	PX4	O5-C9	3.50	1.43	1.33
8	C	509	PX4	O5-C9	3.49	1.43	1.33
8	A	510	PX4	O5-C9	3.48	1.43	1.33
8	D	507	PX4	O5-C9	3.47	1.43	1.33
8	E	508	PX4	O5-C9	3.46	1.43	1.33
8	E	508	PX4	P1-O1	-2.42	1.45	1.54
8	A	509	PX4	P1-O1	-2.42	1.45	1.54
8	A	510	PX4	C10-C9	2.32	1.57	1.50
8	A	509	PX4	C10-C9	2.31	1.57	1.50
8	D	507	PX4	C10-C9	2.31	1.57	1.50
8	E	508	PX4	C10-C9	2.30	1.57	1.50
8	C	509	PX4	C10-C9	2.29	1.57	1.50
8	E	508	PX4	P1-O4	2.22	1.67	1.60
8	A	510	PX4	P1-O4	2.21	1.67	1.60
8	A	509	PX4	P1-O4	2.20	1.67	1.60
8	D	507	PX4	P1-O4	2.19	1.67	1.60
8	C	509	PX4	P1-O4	2.19	1.67	1.60
8	D	507	PX4	P1-O1	-2.12	1.46	1.54
8	A	510	PX4	P1-O1	-2.11	1.47	1.54
8	E	508	PX4	P1-O3	-2.11	1.47	1.54
8	A	509	PX4	P1-O3	-2.11	1.47	1.54
8	C	509	PX4	P1-O1	-2.10	1.47	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	501	NAG	C2-N2-C7	3.25	127.25	122.90
8	E	508	PX4	O5-C9-C10	2.65	119.93	111.83
8	C	509	PX4	O5-C9-C10	2.63	119.85	111.83
8	A	510	PX4	O5-C9-C10	2.61	119.80	111.83
8	D	507	PX4	O5-C9-C10	2.61	119.78	111.83
8	A	509	PX4	O5-C9-C10	2.60	119.76	111.83
8	C	509	PX4	O1-P1-O2	-2.47	101.22	110.83
8	A	510	PX4	O1-P1-O2	-2.47	101.22	110.83
8	D	507	PX4	O1-P1-O2	-2.45	101.28	110.83

There are no chirality outliers.

All (31) torsion outliers are listed below:

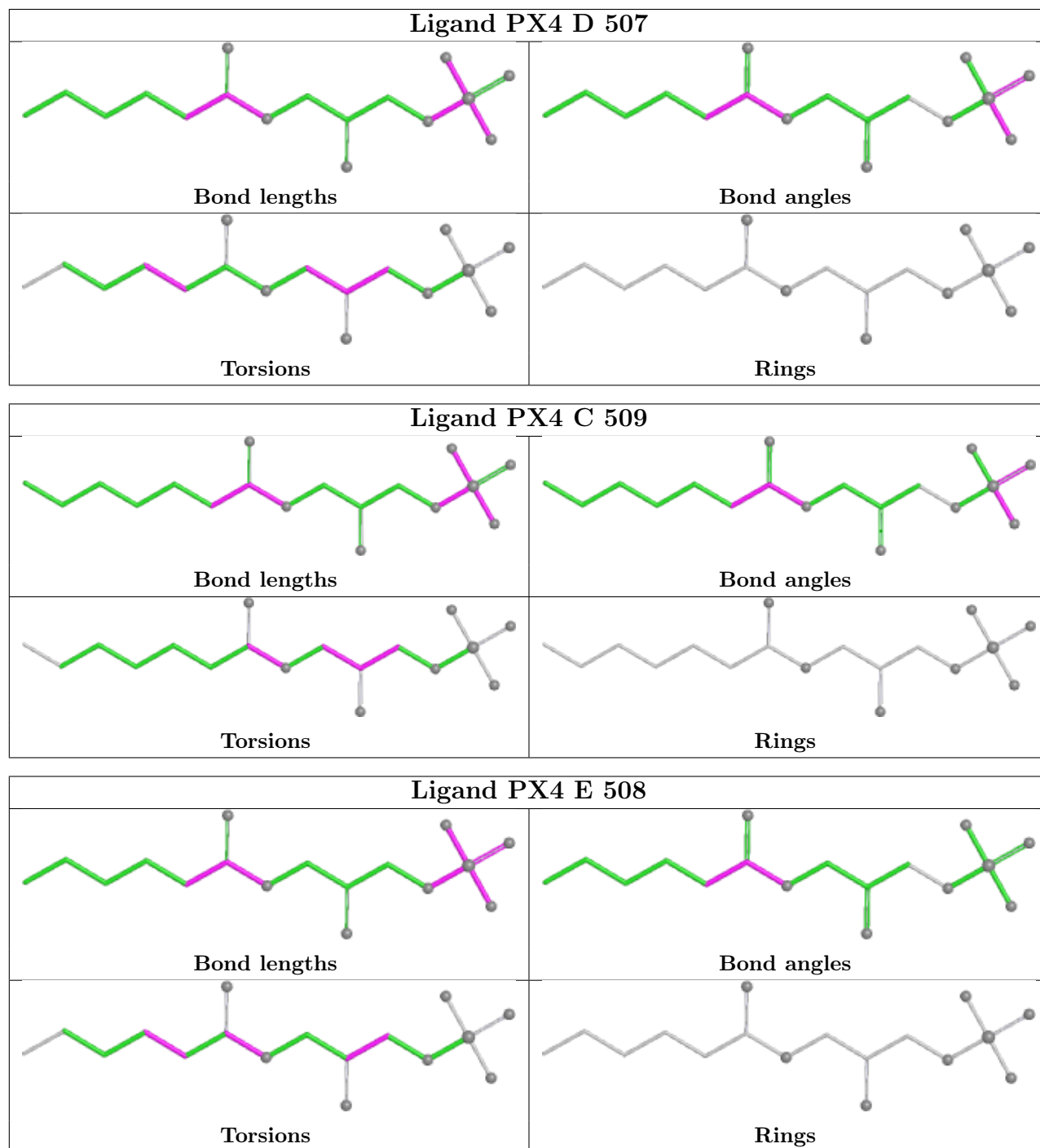
Mol	Chain	Res	Type	Atoms
8	E	508	PX4	O6-C9-O5-C8
8	E	508	PX4	C10-C9-O5-C8
8	E	508	PX4	O4-C6-C7-O7
6	A	502	NAG	O5-C5-C6-O6
8	E	508	PX4	O4-C6-C7-C8
8	A	509	PX4	C6-C7-C8-O5
8	A	509	PX4	O7-C7-C8-O5
8	A	510	PX4	O4-C6-C7-O7
8	C	509	PX4	O4-C6-C7-O7
8	D	507	PX4	O4-C6-C7-O7
8	C	509	PX4	O7-C7-C8-O5
8	A	510	PX4	O4-C6-C7-C8
8	C	509	PX4	O4-C6-C7-C8
8	D	507	PX4	O4-C6-C7-C8
6	A	502	NAG	C4-C5-C6-O6
8	C	509	PX4	C6-C7-C8-O5
8	A	509	PX4	C9-C10-C11-C12
6	C	506	NAG	O5-C5-C6-O6
8	D	507	PX4	C9-C10-C11-C12
8	A	510	PX4	C9-C10-C11-C12
8	E	508	PX4	C9-C10-C11-C12
8	D	507	PX4	C6-C7-C8-O5
8	A	509	PX4	C6-O4-P1-O2
8	D	507	PX4	O7-C7-C8-O5
6	A	501	NAG	C1-C2-N2-C7
6	A	501	NAG	C3-C2-N2-C7
8	A	509	PX4	C6-O4-P1-O1
8	C	509	PX4	O6-C9-O5-C8
8	C	509	PX4	C10-C9-O5-C8
8	A	509	PX4	C12-C13-C14-C15
8	A	509	PX4	O4-C6-C7-C8

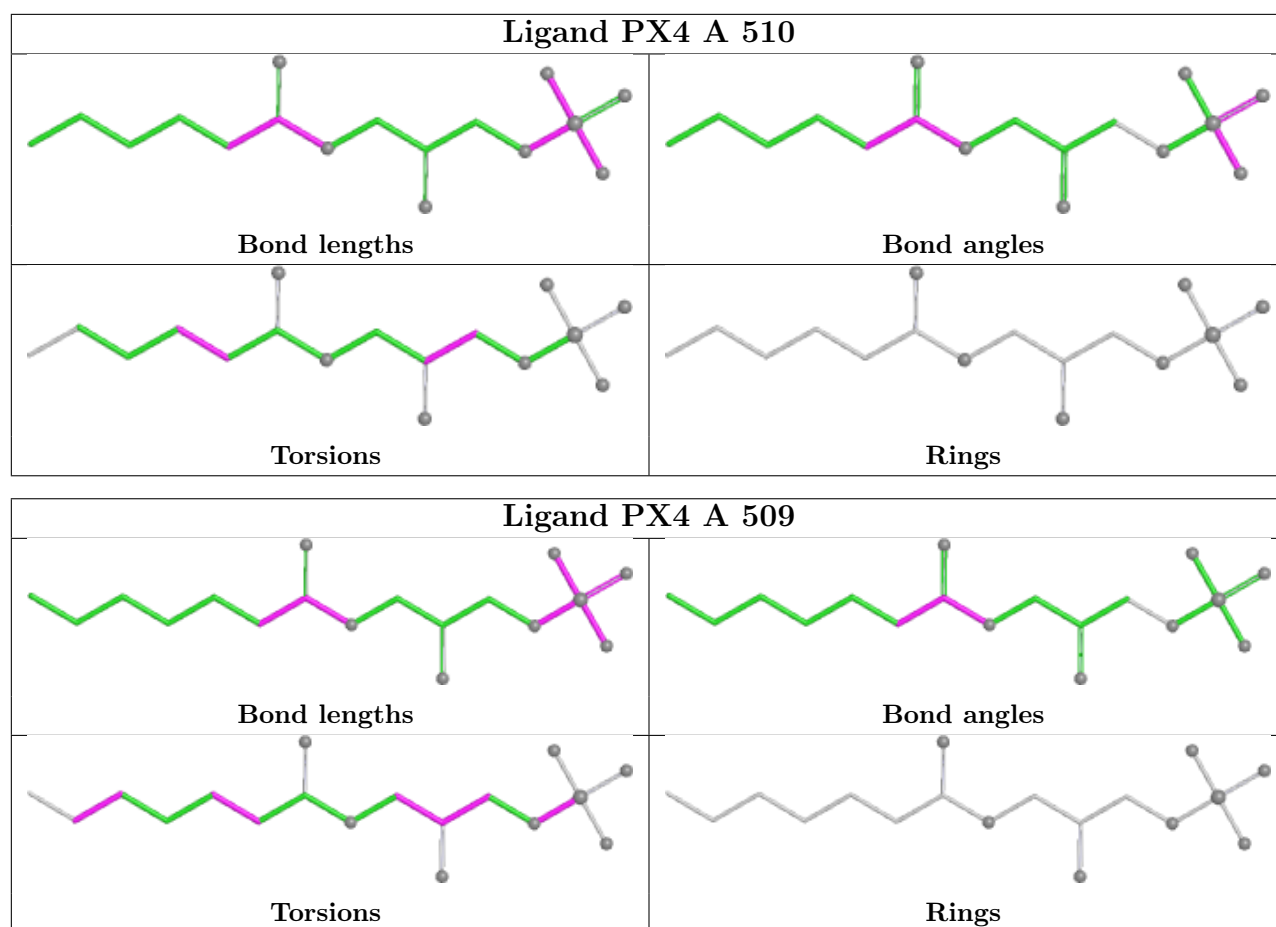
There are no ring outliers.

No monomer is involved in short contacts.

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.

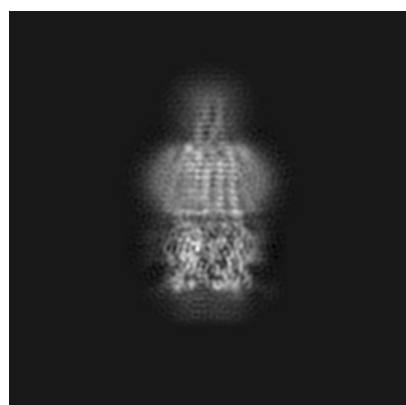
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7088. These allow visual inspection of the internal detail of the map and identification of artifacts.

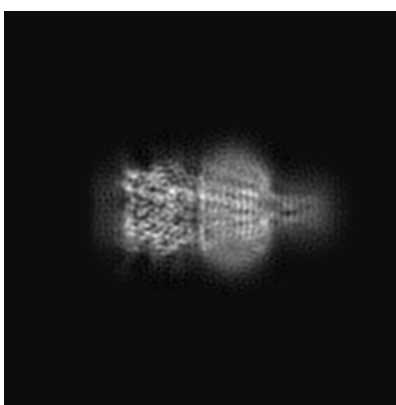
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

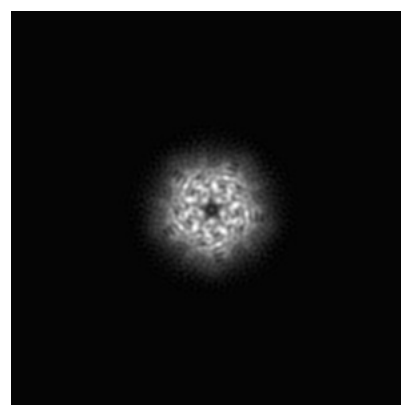
6.1.1 Primary map



X



Y

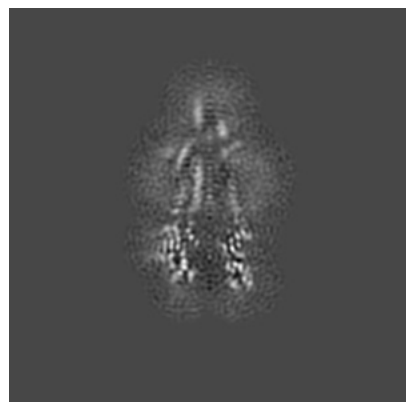


Z

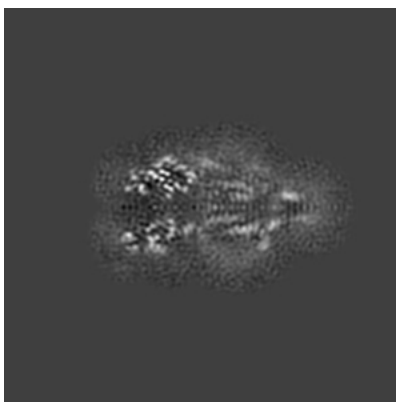
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

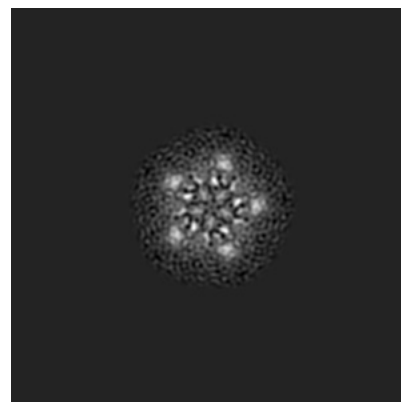
6.2.1 Primary map



X Index: 150



Y Index: 150

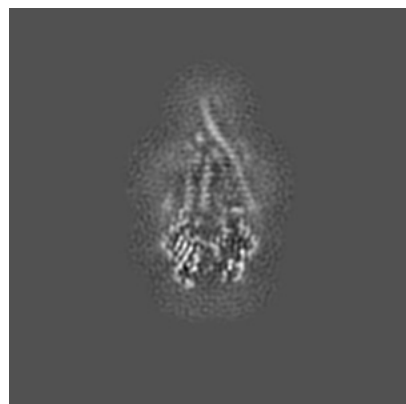


Z Index: 150

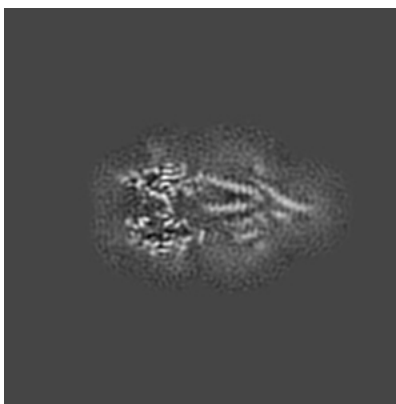
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

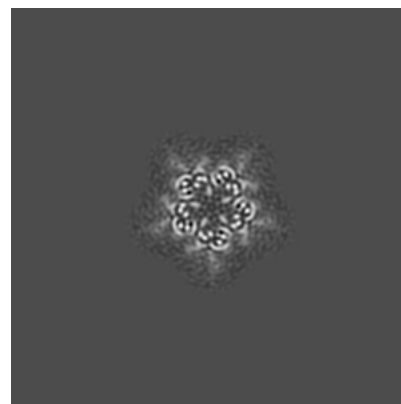
6.3.1 Primary map



X Index: 160



Y Index: 141

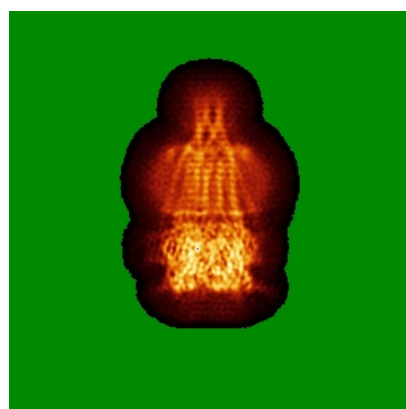


Z Index: 115

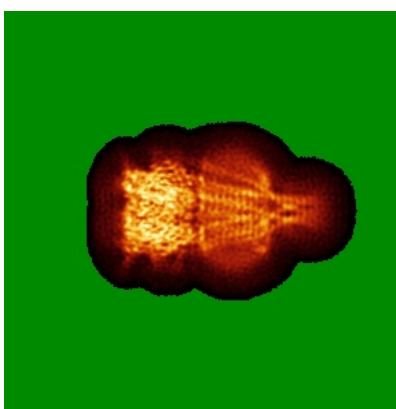
The images above show the largest variance slices of the map in three orthogonal directions.

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

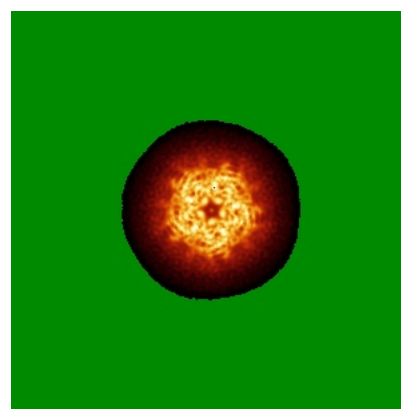
6.4.1 Primary map



X



Y



Z

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 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

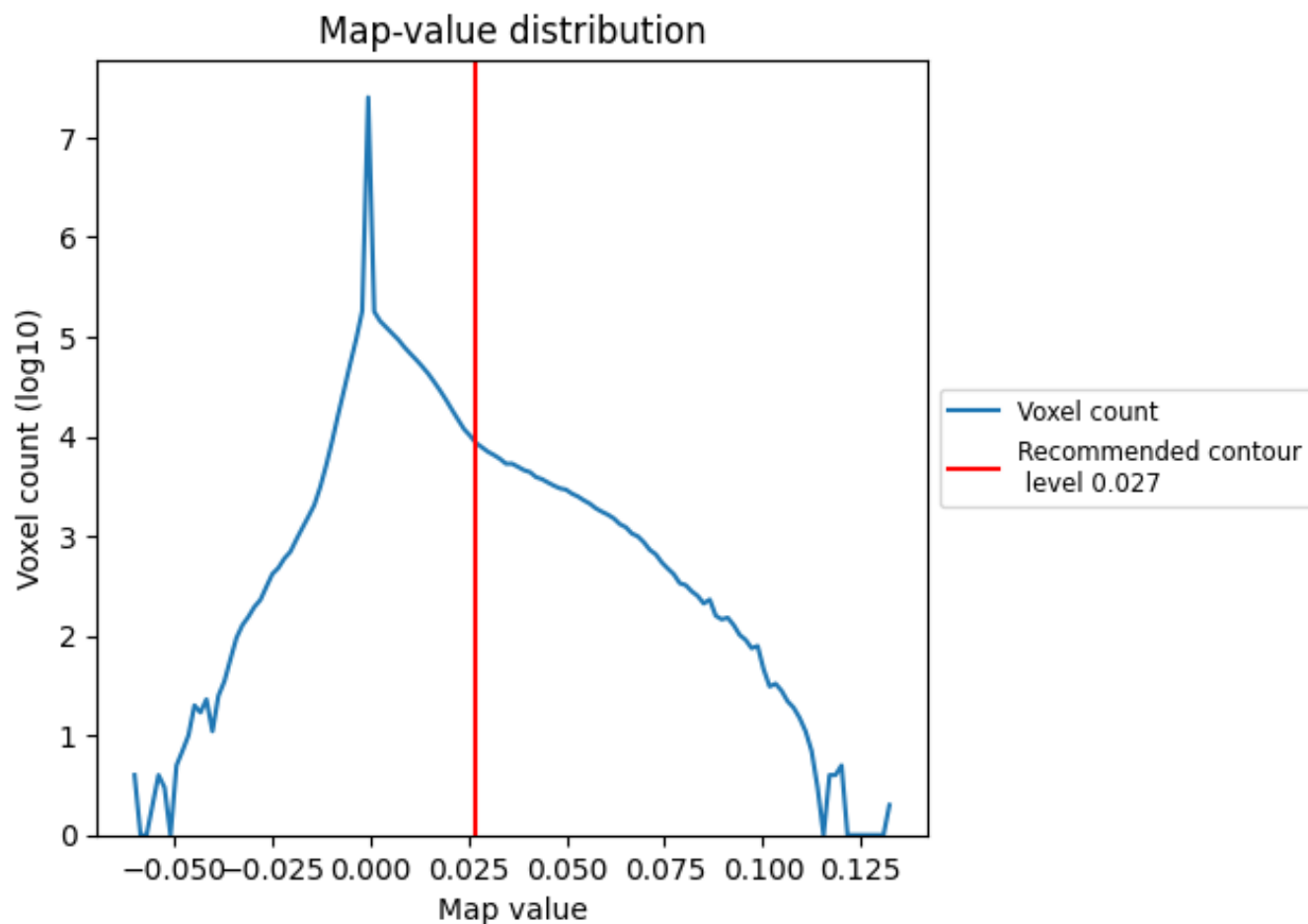
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

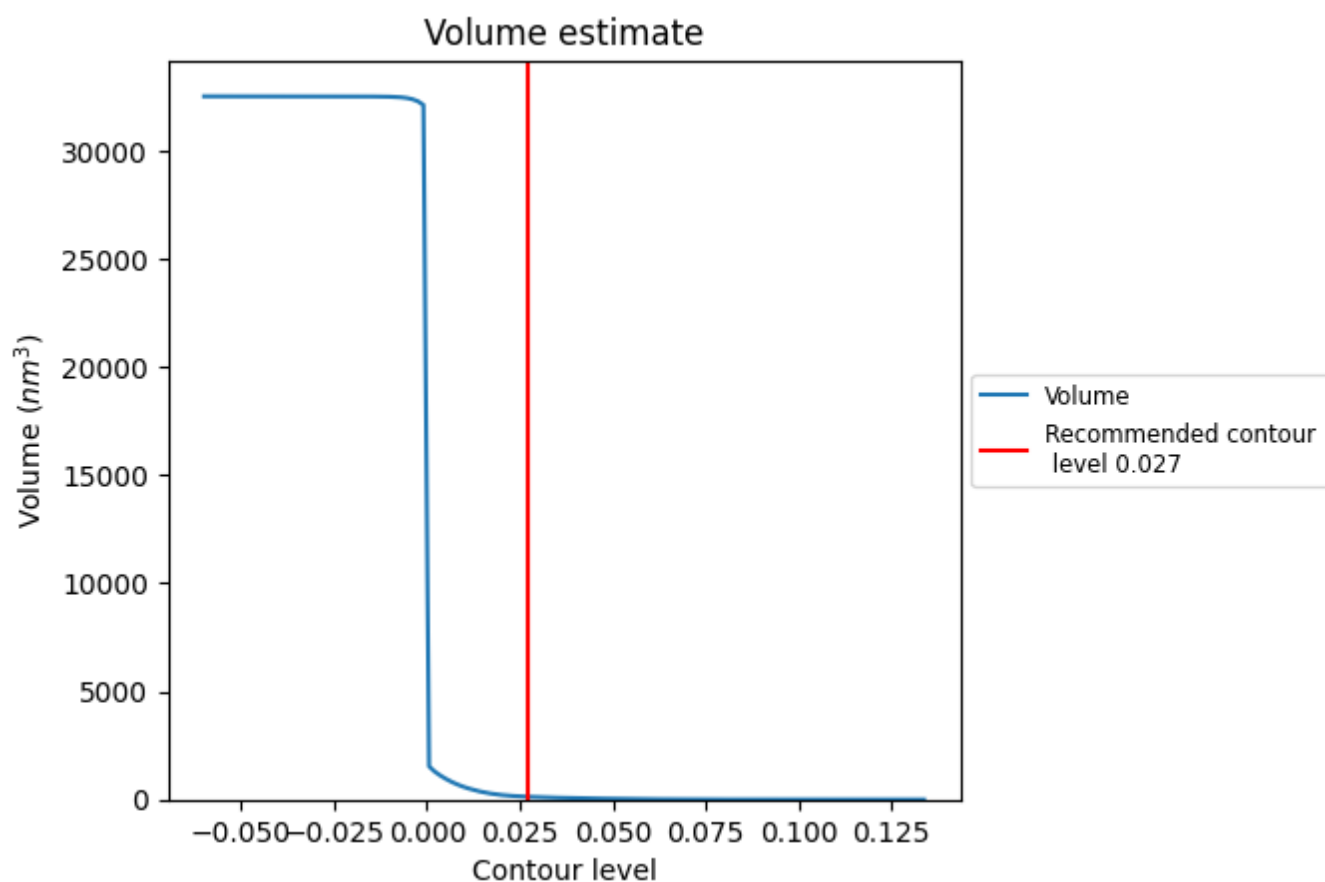
This section contains the results of statistical analysis of the map.

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.

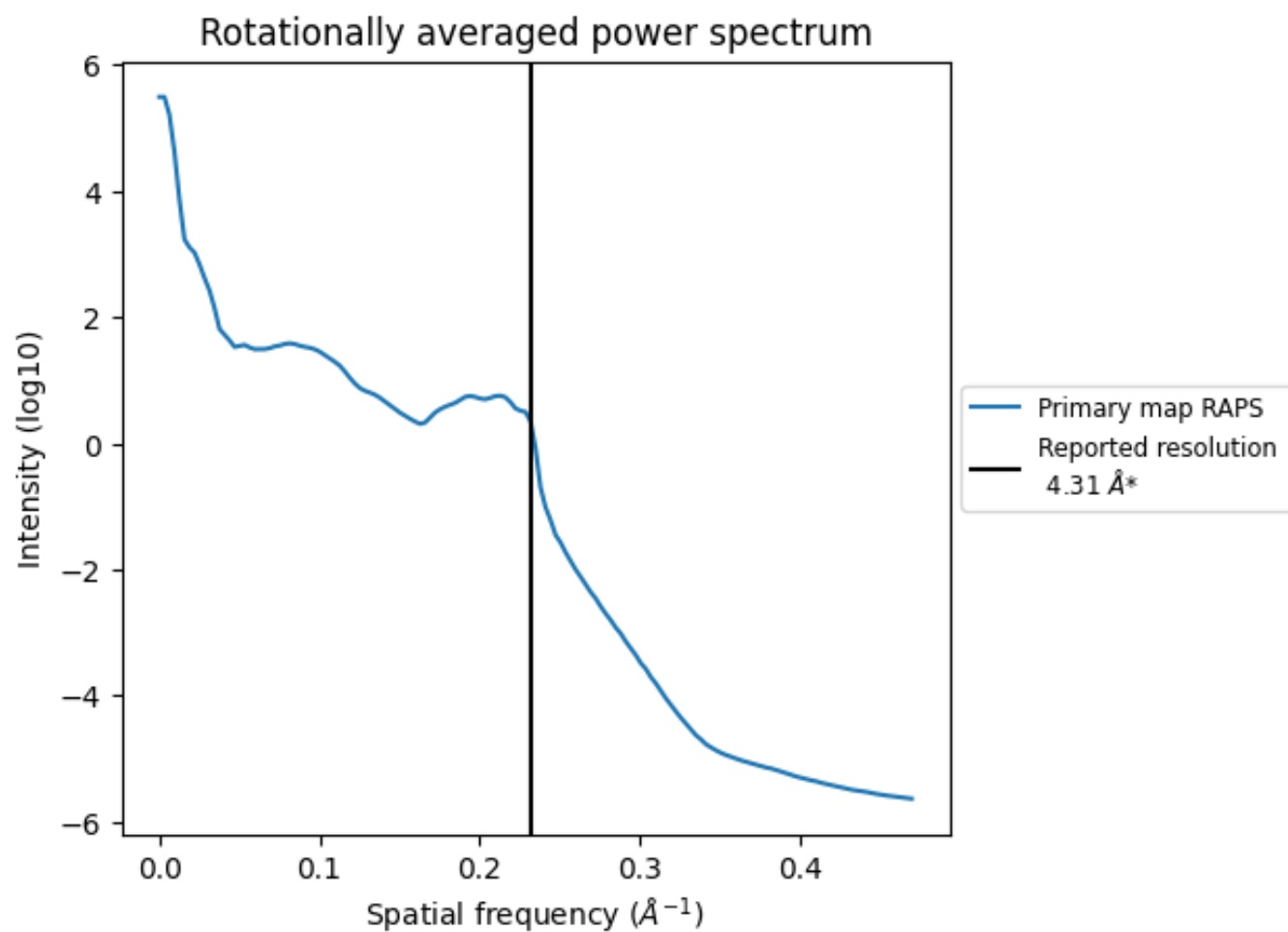
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm³; this corresponds to an approximate mass of 118 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 0.232 Å⁻¹

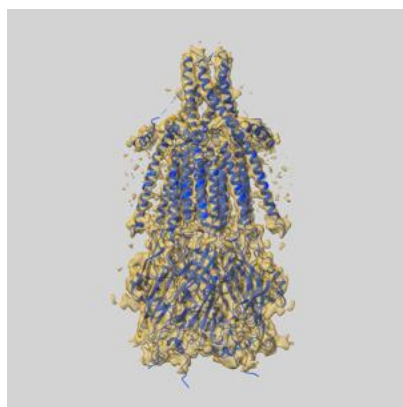
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

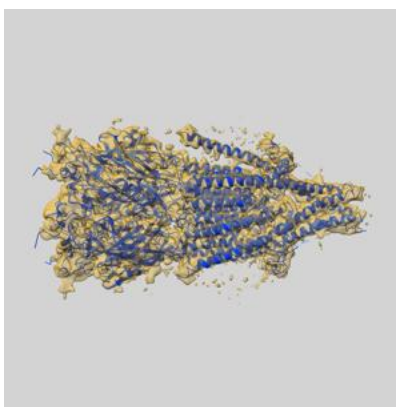
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7088 and PDB model 6BE1. Per-residue inclusion information can be found in section [3](#) on page [9](#).

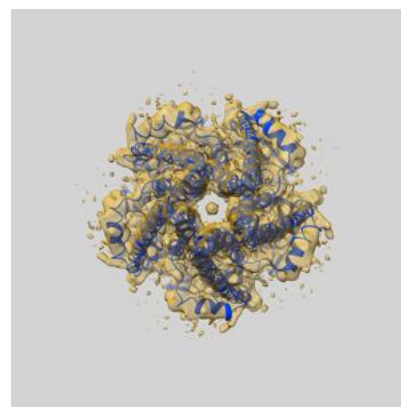
9.1 Map-model overlay [i](#)



X



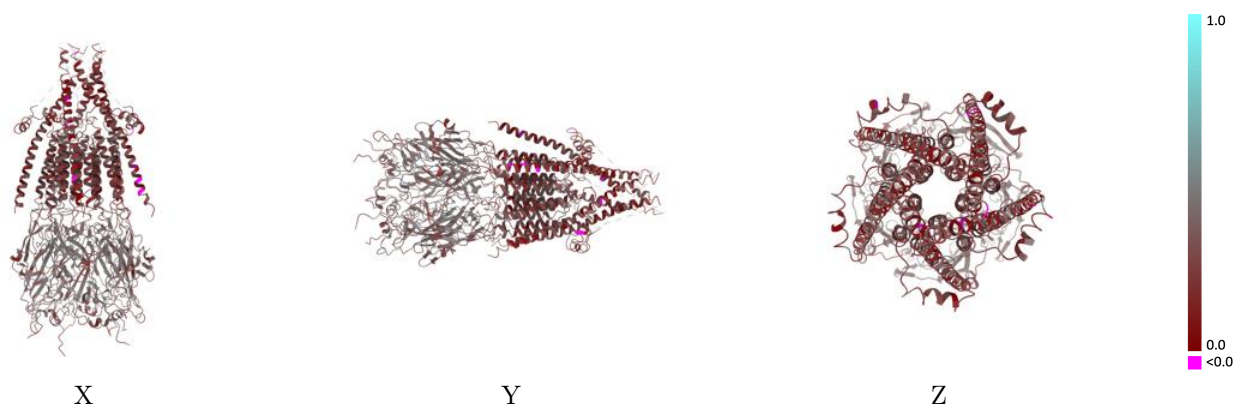
Y



Z

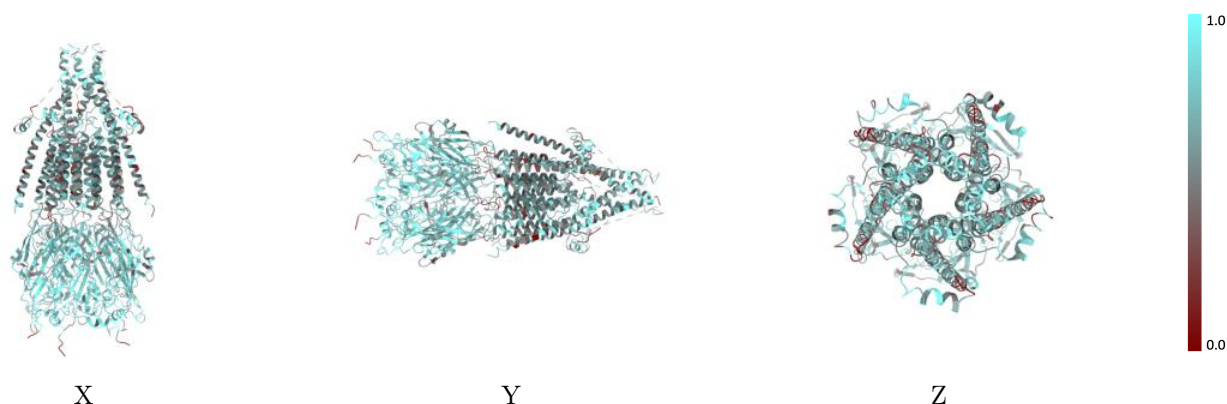
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



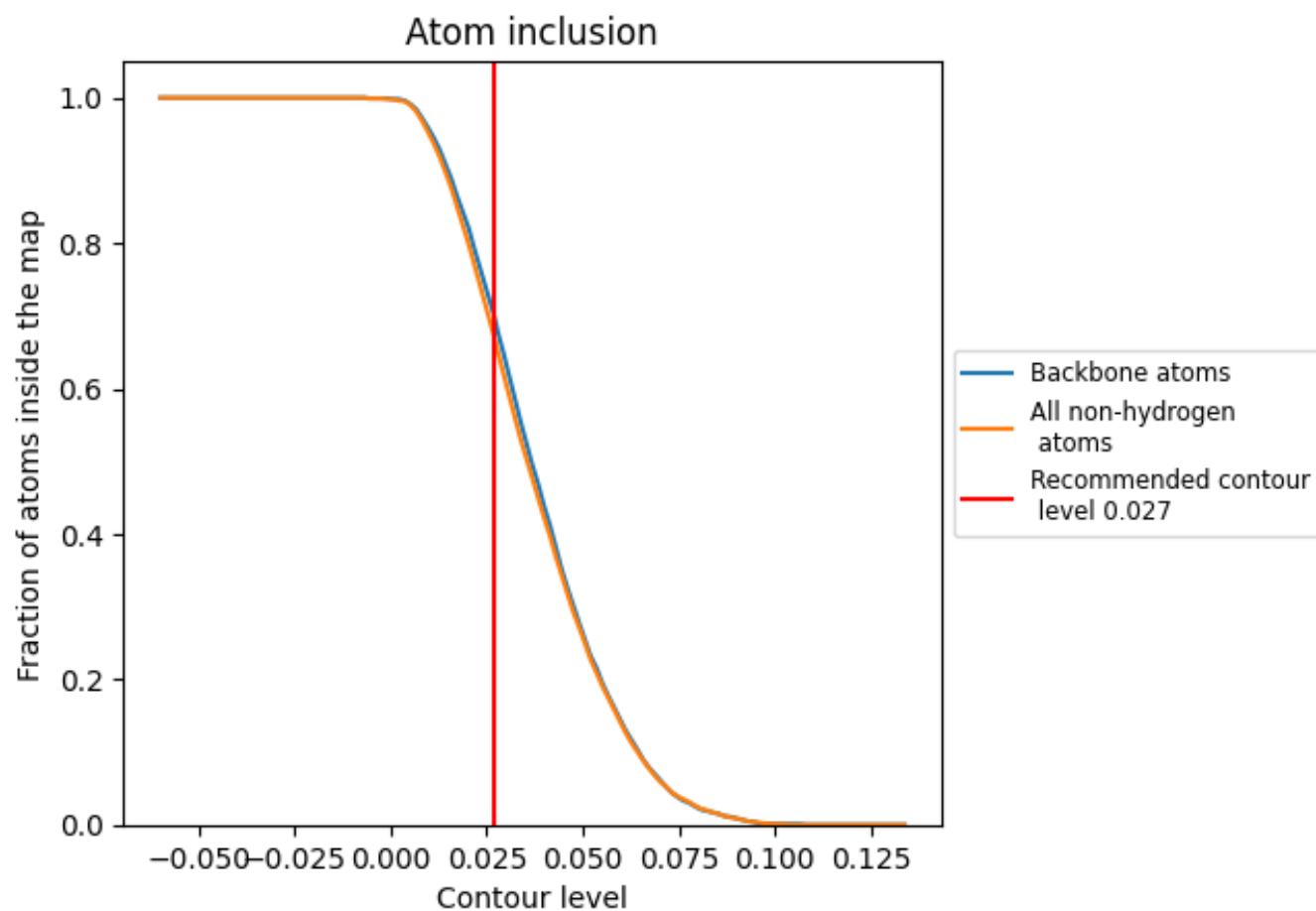
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 67% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6700	<div></div> 0.3210
A	<div></div> 0.6780	<div></div> 0.3200
B	<div></div> 0.6930	<div></div> 0.3250
C	<div></div> 0.6840	<div></div> 0.3160
D	<div></div> 0.6840	<div></div> 0.3150
E	<div></div> 0.6860	<div></div> 0.3210
F	<div></div> 0.5640	<div></div> 0.4470
G	<div></div> 0.6430	<div></div> 0.3890
H	<div></div> 0.5380	<div></div> 0.3610
I	<div></div> 0.4290	<div></div> 0.3100
J	<div></div> 0.6070	<div></div> 0.4110
K	<div></div> 0.5130	<div></div> 0.2980
L	<div></div> 0.4640	<div></div> 0.3820
M	<div></div> 0.6150	<div></div> 0.3750
N	<div></div> 0.6430	<div></div> 0.3230
O	<div></div> 0.7140	<div></div> 0.3900
P	<div></div> 0.3930	<div></div> 0.3400
Q	<div></div> 0.7140	<div></div> 0.4090

1.0

0.0

<0.0