



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:54 PM BST

PDB ID : 2AYL
Title : 2.0 Angstrom Crystal Structure of Manganese Protoporphyrin IX-reconstituted Ovine Prostaglandin H2 Synthase-1 Complexed With Flurbiprofen
Authors : Gupta, K.; Selinsky, B.S.; Loll, P.J.
Deposited on : 2005-09-07
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

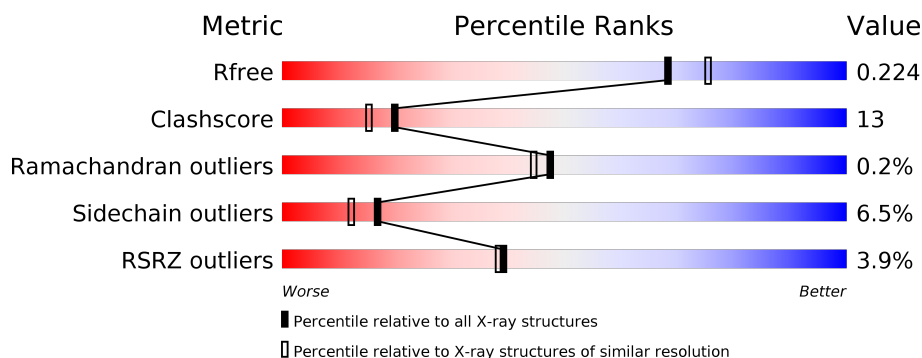
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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




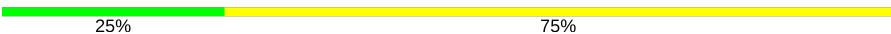
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div></div> </div> </div>
1	B	553	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div></div> </div> </div>
2	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>
3	D	5	<div> <div></div> <div> <div>20%</div> <div>80%</div> </div> </div>
3	G	5	<div> <div></div> <div> <div>20%</div> <div>20%</div> <div>60%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	4	 75%25%
4	H	4	 25%75%

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	C	2	X	-	-	X
2	NAG	F	2	X	-	-	X
3	NAG	D	2	X	-	X	-
3	MAN	D	3	X	-	X	X
3	MAN	D	4	-	-	-	X
3	MAN	D	5	X	-	-	X
3	NAG	G	2	X	-	-	-
3	MAN	G	3	X	-	-	X
3	MAN	G	4	X	-	-	X
3	MAN	G	5	X	-	-	X
4	MAN	E	3	X	-	-	X
4	MAN	E	4	X	-	-	X
4	MAN	H	4	X	-	-	X
5	BOG	A	752	-	-	-	X
5	BOG	A	754	-	-	-	X
5	BOG	B	1753	-	-	-	X
8	GOL	A	758	-	X	-	-
8	GOL	A	759	-	X	-	-
8	GOL	A	760	-	X	-	-
8	GOL	B	1759	-	X	-	-
8	GOL	B	1760	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10505 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Prostaglandin G/H synthase 1.

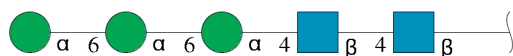
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	2	0
			4504	2918	762	795	29			
1	B	553	Total	C	N	O	S	0	2	0
			4504	2918	762	795	29			

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



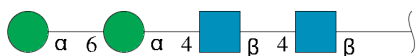
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



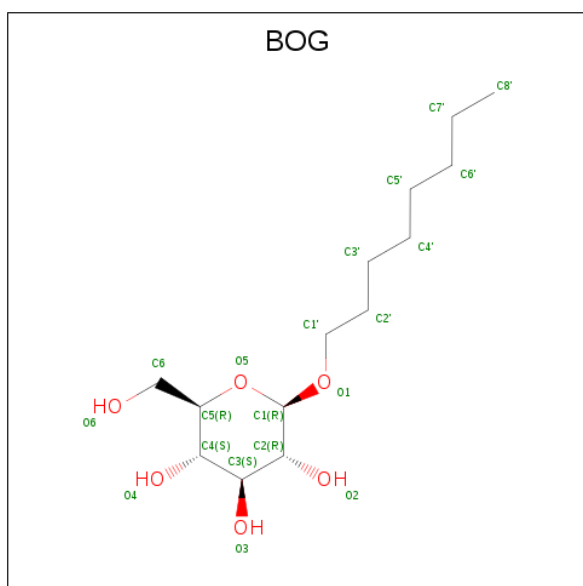
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



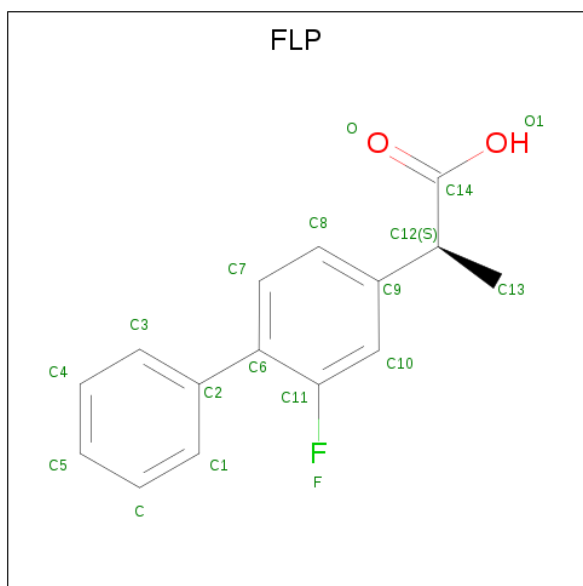
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		
5	B	1	Total	C	O	0	0
			20	14	6		
5	B	1	Total	C	O	0	0
			20	14	6		

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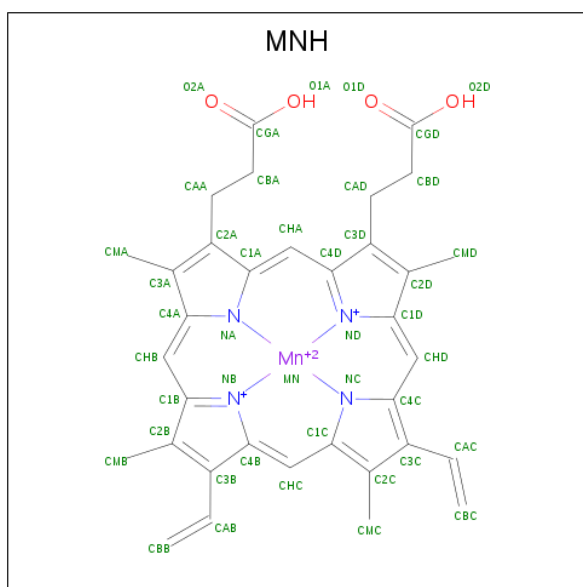
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 6 is FLURBIPROFEN (three-letter code: FLP) (formula: $C_{15}H_{13}FO_2$).



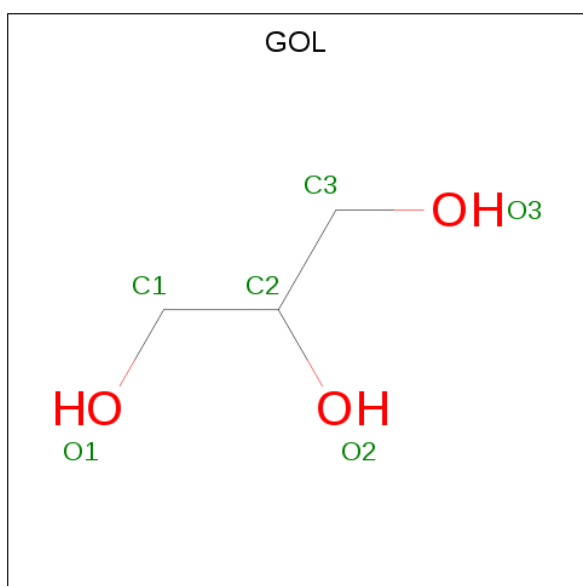
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	F	O	0	1
			36	30	2	4		
6	B	1	Total	C	F	O	0	1
			36	30	2	4		

- Molecule 7 is MANGANESE PROTOPORPHYRIN IX (three-letter code: MNH) (formula: $C_{34}H_{32}MnN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 43	C 34	Mn 1	N 4	O 4	0	0
7	B	1	Total 43	C 34	Mn 1	N 4	O 4	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

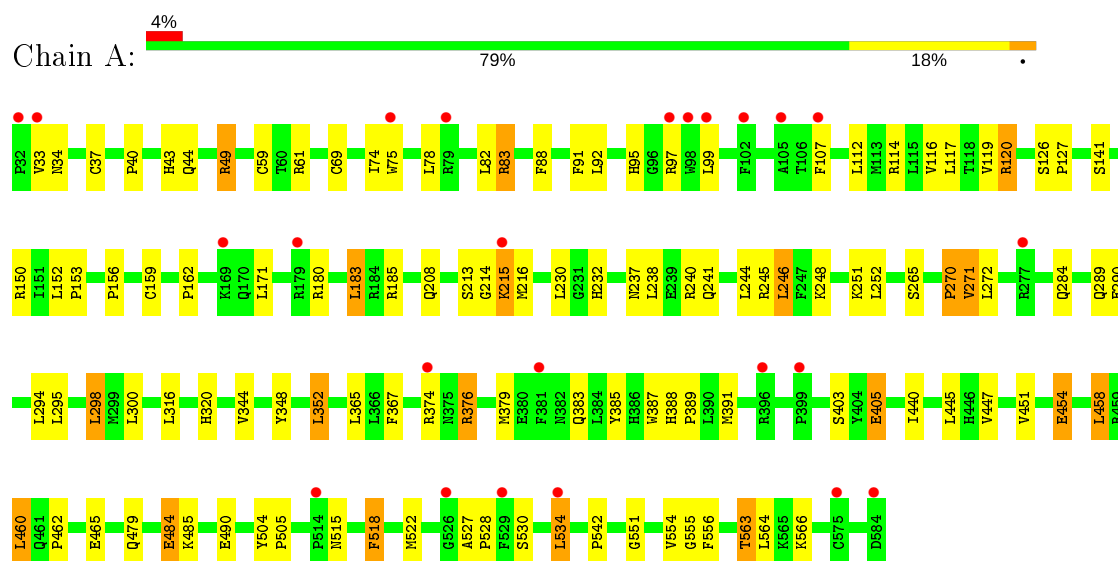
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	434	Total	O	0	0
			434	434		
9	B	457	Total	O	0	0
			457	457		

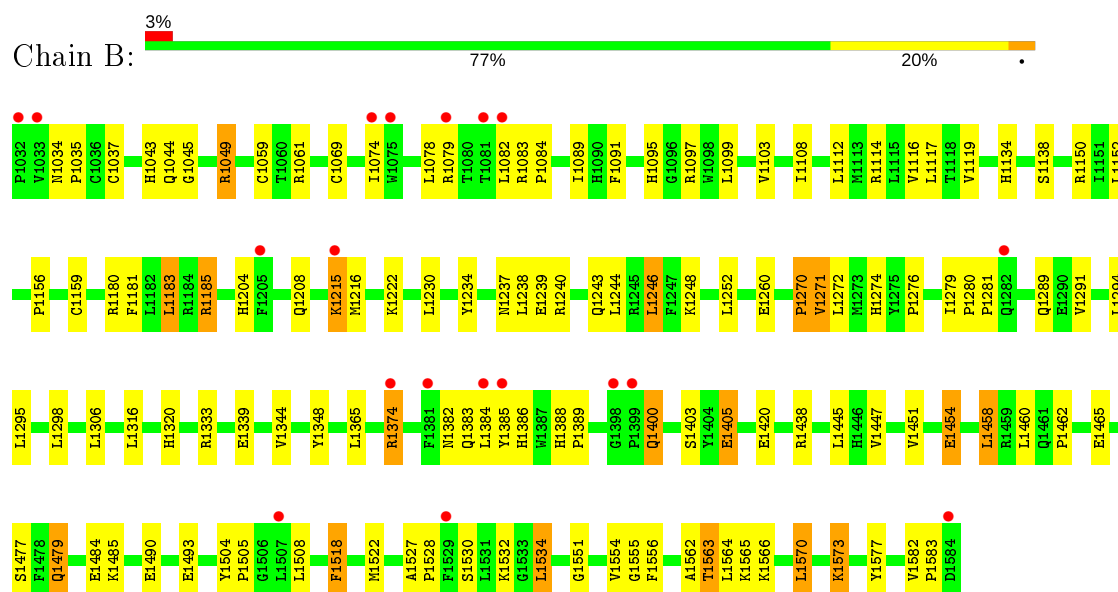
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Prostaglandin G/H synthase 1



• Molecule 1: Prostaglandin G/H synthase 1



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

Chain C:  50% 50%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain D:  20% 80%

MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain G:  20% 20% 60%

MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain E:  75% 25%

MAG1
MAG2
MAN3
MAN4

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

Chain H:  25% 75%

MAG1
MAG2
MAN3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.93Å 206.55Å 221.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.33 – 2.00 43.32 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.33-2.00) 99.4 (43.32-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.237 0.204 , 0.224	Depositor DCC
R_{free} test set	11371 reflections (6.44%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10505	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, FLP, MNH, BOG, MAN

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	0.34	0/4643	0.60	0/6302
1	B	0.35	0/4643	0.60	0/6302
All	All	0.34	0/9286	0.60	0/12604

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

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	4504	0	4407	103	0
1	B	4504	0	4405	114	0
2	C	28	0	25	1	0
2	F	28	0	25	1	0
3	D	61	0	52	13	0
3	G	61	0	52	8	0
4	E	50	0	43	3	0
4	H	50	0	43	2	0
5	A	80	0	112	7	0
5	B	60	0	84	5	0
6	A	36	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	36	0	24	0	0
7	A	43	0	30	3	0
7	B	43	0	30	0	0
8	A	18	0	12	2	0
8	B	12	0	8	0	0
9	A	434	0	0	8	0
9	B	457	0	0	13	0
All	All	10505	0	9376	236	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 13.

All (236) 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:B:1215:LYS:H	1:B:1215:LYS:HD3	1.28	0.98
1:B:1215:LYS:NZ	1:B:1222:LYS:HD2	1.84	0.93
1:A:83:ARG:HH12	5:A:751:BOG:H3	1.32	0.93
1:A:127:PRO:HD3	1:A:374:ARG:HH22	1.37	0.89
1:A:352:LEU:HD21	1:A:518:PHE:CZ	2.08	0.87
1:B:1276:PRO:HD2	1:B:1279:ILE:HD12	1.63	0.81
1:A:127:PRO:HD3	1:A:374:ARG:NH2	1.96	0.79
3:D:2:NAG:H4	3:D:3:MAN:O2	1.83	0.78
1:B:1374:ARG:NH1	1:B:1374:ARG:HB3	1.98	0.78
1:B:1454:GLU:OE1	1:B:1458:LEU:HD22	1.84	0.77
1:B:1294:LEU:HG	1:B:1295:LEU:HG	1.66	0.77
3:G:4:MAN:H62	3:G:4:MAN:O2	1.86	0.76
1:B:1083:ARG:NH1	5:B:1751:BOG:H3	2.02	0.75
1:B:1260:GLU:OE2	1:B:1573:LYS:HD2	1.87	0.74
1:A:49:ARG:O	1:B:1320:HIS:HD2	1.70	0.72
1:A:83:ARG:NH1	5:A:751:BOG:H3	2.04	0.72
1:B:1215:LYS:HZ3	1:B:1222:LYS:HD2	1.54	0.71
1:B:1374:ARG:HH11	1:B:1374:ARG:HB3	1.56	0.70
1:B:1374:ARG:HH11	1:B:1374:ARG:CB	2.05	0.70
1:A:150:ARG:HD3	1:A:152:LEU:O	1.92	0.69
1:B:1208:GLN:NE2	1:B:1230:LEU:H	1.90	0.69
1:B:1374:ARG:NH1	9:B:153:HOH:O	2.26	0.68
1:A:563:THR:HG22	1:A:566:LYS:H	1.58	0.67
1:A:270:PRO:HG2	3:G:5:MAN:H61	1.75	0.67
1:B:1420:GLU:OE2	1:B:1573:LYS:HE3	1.95	0.67
1:B:1462:PRO:HG2	1:B:1465:GLU:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1573:LYS:H	1:B:1573:LYS:HD3	1.61	0.66
1:A:563:THR:HG21	9:A:1950:HOH:O	1.95	0.65
1:B:1208:GLN:HE21	1:B:1230:LEU:H	1.42	0.65
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.79	0.64
1:A:320:HIS:HD2	1:B:1049:ARG:O	1.79	0.64
1:A:403:SER:OG	1:A:405:GLU:HG2	1.97	0.64
1:B:1215:LYS:HZ1	1:B:1222:LYS:HD2	1.59	0.64
1:B:1059:CYS:HG	1:B:1069[A]:CYS:HG	0.70	0.63
1:A:208:GLN:NE2	1:A:230:LEU:H	1.96	0.63
3:G:4:MAN:H62	3:G:5:MAN:O2	1.99	0.62
1:A:374:ARG:HB3	9:A:2116:HOH:O	1.97	0.62
1:A:88:PHE:O	1:A:92:LEU:HD13	2.00	0.62
1:B:1150:ARG:HD3	1:B:1152:LEU:O	2.00	0.62
1:A:216:MET:HG2	3:D:2:NAG:H83	1.80	0.61
1:B:1563:THR:HG21	9:B:434:HOH:O	2.00	0.61
1:A:49:ARG:HG3	9:A:1727:HOH:O	2.01	0.61
1:A:458:LEU:HB3	1:A:460:LEU:HD13	1.82	0.61
1:A:391:MET:HG3	7:A:601:MNH:HAB	1.82	0.60
1:B:1246:LEU:HD22	1:B:1248:LYS:HB3	1.82	0.60
1:A:114:ARG:HD3	1:A:365:LEU:O	2.02	0.60
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.37	0.60
1:A:59:CYS:HG	1:A:69[B]:CYS:HB2	1.65	0.59
4:E:2:NAG:H4	4:E:3:MAN:O2	2.02	0.59
1:B:1383:GLN:HE21	1:B:1454:GLU:CD	2.05	0.59
9:A:1879:HOH:O	1:B:1374:ARG:HG2	2.02	0.59
1:A:83:ARG:NH2	5:A:751:BOG:H5	2.18	0.59
3:G:4:MAN:H62	3:G:5:MAN:HO2	1.68	0.59
1:A:214:GLY:H	1:A:215:LYS:HZ2	1.49	0.59
1:B:1208:GLN:HE22	1:B:1230:LEU:HD12	1.68	0.59
1:B:1527:ALA:HB3	1:B:1528:PRO:HD3	1.85	0.58
1:A:61:ARG:NH2	9:A:1963:HOH:O	2.37	0.58
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.86	0.58
1:B:1215:LYS:N	1:B:1215:LYS:HD3	2.09	0.58
1:B:1276:PRO:HD2	1:B:1279:ILE:CD1	2.33	0.58
1:B:1518:PHE:CD1	1:B:1522:MET:HG2	2.38	0.57
1:A:127:PRO:HA	1:A:374:ARG:NH1	2.20	0.57
1:A:127:PRO:CD	1:A:374:ARG:HH22	2.13	0.57
1:A:530[B]:SER:O	1:A:534:LEU:HD22	2.05	0.56
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.86	0.56
1:A:99:LEU:HD23	5:A:754:BOG:H3'1	1.86	0.56
1:B:1240:ARG:NH1	1:B:1271:VAL:HG13	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1374:ARG:HH11	1:B:1374:ARG:CA	2.18	0.56
1:B:1239:GLU:HG2	9:B:113:HOH:O	2.05	0.55
3:D:2:NAG:O7	3:D:2:NAG:H3	2.05	0.55
1:A:352:LEU:CD2	1:A:518:PHE:CZ	2.86	0.55
1:B:1183:LEU:HG	1:B:1445:LEU:HD22	1.88	0.55
1:A:162:PRO:HB2	1:A:171:LEU:HD11	1.88	0.55
1:A:180:ARG:HD3	1:A:490:GLU:OE2	2.06	0.55
1:A:215:LYS:H	1:A:215:LYS:HD3	1.71	0.55
1:A:479:GLN:HG3	9:A:2120:HOH:O	2.07	0.55
1:A:208:GLN:HE21	1:A:230:LEU:H	1.52	0.55
1:B:1582:VAL:CG2	1:B:1583:PRO:HD2	2.37	0.55
1:A:215:LYS:H	1:A:215:LYS:CD	2.20	0.54
1:A:563:THR:HG23	9:A:1756:HOH:O	2.07	0.54
1:A:530[A]:SER:O	1:A:534:LEU:HD22	2.08	0.54
1:B:1112:LEU:O	1:B:1116:VAL:HG23	2.08	0.54
3:G:2:NAG:O7	3:G:2:NAG:H3	2.06	0.54
1:B:1216:MET:HG2	3:G:2:NAG:H83	1.90	0.54
1:B:1400:GLN:OE1	4:H:3:MAN:H3	2.08	0.53
1:A:83:ARG:HH22	5:A:751:BOG:H5	1.74	0.53
1:A:126:SER:OG	1:A:374:ARG:NH1	2.42	0.53
1:B:1451:VAL:O	1:B:1454:GLU:HG3	2.08	0.53
1:B:1454:GLU:HG2	9:B:719:HOH:O	2.08	0.53
3:D:2:NAG:O3	3:D:3:MAN:C1	2.57	0.53
1:A:208:GLN:HE22	1:A:230:LEU:HD12	1.74	0.52
1:A:150:ARG:CD	1:A:152:LEU:O	2.58	0.52
1:A:215:LYS:HD3	1:A:215:LYS:N	2.25	0.52
1:B:1504:TYR:HB3	1:B:1505:PRO:HD3	1.91	0.52
1:A:251:LYS:NZ	8:A:759:GOL:H12	2.25	0.52
2:F:1:NAG:H61	2:F:2:NAG:H82	1.91	0.52
1:A:290:GLU:H	1:A:290:GLU:CD	2.13	0.52
3:D:2:NAG:C4	3:D:3:MAN:O2	2.56	0.51
1:A:485:LYS:HD2	1:A:485:LYS:N	2.26	0.51
1:A:563:THR:HB	1:A:566:LYS:HD3	1.91	0.51
1:B:1049:ARG:HH11	1:B:1049:ARG:HG3	1.74	0.51
1:B:1563:THR:HG22	1:B:1565:LYS:N	2.25	0.51
1:B:1563:THR:HG23	9:B:147:HOH:O	2.11	0.51
1:A:240:ARG:NH1	1:A:271:VAL:HG13	2.26	0.51
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.50	0.51
1:A:40:PRO:HB3	2:C:1:NAG:H62	1.93	0.51
1:B:1119:VAL:HG12	5:B:1751:BOG:H62	1.92	0.51
3:D:4:MAN:H4	3:D:5:MAN:O2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:HIS:HE1	1:A:551:GLY:O	1.94	0.51
1:B:1074:ILE:HD12	1:B:1074:ILE:H	1.76	0.51
1:B:1260:GLU:CD	1:B:1573:LYS:HD2	2.31	0.51
1:A:447:VAL:O	1:A:451:VAL:HG23	2.11	0.50
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.47	0.50
3:D:2:NAG:O7	3:D:2:NAG:C3	2.60	0.50
1:B:1061:ARG:NH2	9:B:177:HOH:O	2.42	0.50
1:A:383:GLN:NE2	1:A:454:GLU:HG2	2.27	0.49
1:B:1530[B]:SER:O	1:B:1534:LEU:HD22	2.12	0.49
1:A:162:PRO:HB2	1:A:171:LEU:CD1	2.43	0.49
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.78	0.49
1:A:213:SER:OG	1:A:215:LYS:HG2	2.13	0.49
1:A:183:LEU:HG	1:A:445:LEU:HD22	1.94	0.49
1:A:484:GLU:C	1:A:485:LYS:HD2	2.34	0.48
3:D:4:MAN:H4	3:D:5:MAN:O3	2.13	0.48
1:A:388:HIS:N	1:A:389:PRO:CD	2.77	0.48
1:A:141:SER:O	1:A:376:ARG:NH2	2.46	0.48
1:A:554:VAL:HG13	1:A:555:GLY:N	2.27	0.48
1:B:1181:PHE:HZ	1:B:1490:GLU:HG2	1.78	0.48
1:B:1320:HIS:HE1	1:B:1551:GLY:O	1.95	0.48
1:A:107:PHE:C	1:A:107:PHE:CD1	2.87	0.48
1:B:1339:GLU:HG2	1:B:1562:ALA:HB2	1.96	0.48
1:B:1374:ARG:NH2	9:B:595:HOH:O	2.47	0.48
1:B:1405:GLU:CD	1:B:1405:GLU:H	2.18	0.48
4:E:2:NAG:C4	4:E:3:MAN:O2	2.61	0.48
1:B:1384:LEU:HG	1:B:1522:MET:SD	2.54	0.47
1:A:119:VAL:HG12	5:A:751:BOG:H62	1.96	0.47
1:A:127:PRO:N	1:A:374:ARG:HH12	2.12	0.47
1:B:1479:GLN:CD	1:B:1479:GLN:H	2.18	0.47
1:B:1563:THR:HG22	1:B:1566:LYS:H	1.79	0.47
1:B:1582:VAL:HG22	1:B:1583:PRO:HD2	1.96	0.47
1:A:251:LYS:HZ2	8:A:759:GOL:H12	1.80	0.47
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.79	0.47
1:B:1477:SER:OG	1:B:1479:GLN:HG2	2.15	0.47
1:B:1530[A]:SER:O	1:B:1534:LEU:HD22	2.15	0.47
1:B:1382:ASN:OD1	1:B:1386:HIS:HE1	1.99	0.46
1:B:1383:GLN:NE2	1:B:1454:GLU:CD	2.67	0.46
1:A:74:ILE:HG23	1:A:75:TRP:N	2.31	0.46
1:B:1270:PRO:HB2	3:D:5:MAN:H61	1.97	0.46
1:B:1185:ARG:CZ	1:B:1438:ARG:HH11	2.29	0.46
1:A:112:LEU:O	1:A:116:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1083:ARG:HH22	5:B:1751:BOG:H5	1.81	0.46
4:H:2:NAG:O3	4:H:3:MAN:C1	2.64	0.46
1:A:246:LEU:O	1:A:246:LEU:HD23	2.16	0.46
1:A:272:LEU:HD13	1:A:272:LEU:C	2.36	0.46
1:B:1099:LEU:HD23	5:B:1753:BOG:H3'1	1.98	0.46
1:A:454:GLU:HG3	1:A:458:LEU:HD22	1.98	0.46
1:B:1074:ILE:HD12	1:B:1074:ILE:N	2.31	0.46
1:A:120:ARG:NH1	5:A:751:BOG:H4	2.30	0.45
3:G:2:NAG:O7	3:G:2:NAG:C3	2.64	0.45
1:B:1272:LEU:HD13	1:B:1272:LEU:C	2.36	0.45
1:B:1384:LEU:HD23	1:B:1384:LEU:C	2.37	0.45
3:D:2:NAG:O3	3:D:3:MAN:H2	2.16	0.45
1:B:1215:LYS:H	1:B:1215:LYS:CD	2.04	0.45
1:B:1216:MET:HE1	9:B:84:HOH:O	2.17	0.45
1:A:240:ARG:HG3	1:A:271:VAL:HG22	1.98	0.45
1:B:1458:LEU:HB3	1:B:1460:LEU:HD13	1.99	0.45
1:B:1035:PRO:HD2	1:B:1049:ARG:NH1	2.32	0.45
1:A:83:ARG:NH1	9:A:2121:HOH:O	2.50	0.45
1:B:1240:ARG:CZ	1:B:1271:VAL:HG13	2.47	0.45
1:B:1573:LYS:N	1:B:1573:LYS:HD3	2.29	0.45
1:A:43:HIS:O	1:A:44:GLN:HB2	2.17	0.44
1:B:1114:ARG:HD3	1:B:1365:LEU:O	2.17	0.44
1:B:1239:GLU:HG3	9:B:592:HOH:O	2.18	0.44
1:A:387:TRP:HB2	7:A:601:MNH:HAC	1.99	0.44
1:B:1374:ARG:NH2	9:B:569:HOH:O	2.49	0.44
3:D:3:MAN:O4	3:D:4:MAN:H2	2.18	0.44
1:B:1504:TYR:CZ	1:B:1508:LEU:HD11	2.52	0.44
1:B:1083:ARG:NH1	1:B:1083:ARG:HG3	2.32	0.44
1:A:295:LEU:HD21	7:A:601:MNH:HBB1	1.98	0.44
1:A:352:LEU:HD21	1:A:518:PHE:CE1	2.52	0.44
1:B:1403:SER:OG	1:B:1405:GLU:HG2	2.17	0.44
1:A:246:LEU:HD22	1:A:248:LYS:HB3	2.00	0.44
1:A:320:HIS:CE1	1:A:551:GLY:O	2.71	0.44
1:A:389:PRO:HG3	1:A:440:ILE:HG12	2.00	0.43
1:B:1043:HIS:O	1:B:1044:GLN:HB2	2.17	0.43
1:B:1079:ARG:HH11	1:B:1079:ARG:HG2	1.83	0.43
3:D:2:NAG:O3	3:D:3:MAN:C2	2.66	0.43
1:B:1078:LEU:O	1:B:1082:LEU:HD13	2.18	0.43
1:B:1083:ARG:HH11	1:B:1083:ARG:HG3	1.84	0.43
1:B:1049:ARG:CG	1:B:1049:ARG:HH11	2.31	0.43
4:E:2:NAG:O3	4:E:3:MAN:C1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:CZ	1:A:271:VAL:HG13	2.48	0.43
1:A:295:LEU:HB2	1:A:298:LEU:HD22	2.01	0.43
1:A:265:SER:HA	1:A:284:GLN:O	2.19	0.43
1:B:1150:ARG:CD	1:B:1152:LEU:O	2.66	0.43
1:A:237:ASN:ND2	1:A:240:ARG:H	2.17	0.43
1:B:1280:PRO:HA	1:B:1281:PRO:HD3	1.88	0.43
1:A:127:PRO:CA	1:A:374:ARG:NH1	2.82	0.42
1:B:1274:HIS:HD2	1:B:1291:VAL:HG12	1.83	0.42
1:B:1344:VAL:O	1:B:1348:TYR:HB3	2.19	0.42
1:B:1045:GLY:HA3	1:B:1069[A]:CYS:SG	2.59	0.42
1:B:1566:LYS:O	1:B:1570:LEU:HB2	2.19	0.42
1:B:1374:ARG:O	1:B:1532:LYS:HE3	2.20	0.42
1:B:1554:VAL:HG13	1:B:1555:GLY:N	2.34	0.42
3:G:2:NAG:H4	3:G:3:MAN:H2	1.81	0.42
1:B:1083:ARG:NH2	5:B:1751:BOG:H5	2.34	0.42
1:A:241:GLN:HE21	1:A:245:ARG:HH11	1.67	0.42
1:B:1388:HIS:N	1:B:1389:PRO:CD	2.83	0.42
1:B:1049:ARG:NH1	9:B:3:HOH:O	2.52	0.42
1:B:1091:PHE:O	1:B:1095:HIS:HD2	2.03	0.42
1:B:1243:GLN:NE2	3:D:5:MAN:H62	2.35	0.42
1:A:344:VAL:HA	1:A:348:TYR:HB3	2.02	0.42
1:A:33:VAL:HG23	1:A:33:VAL:O	2.18	0.41
1:A:78:LEU:O	1:A:82:LEU:HD13	2.19	0.41
1:A:88:PHE:CE1	1:A:92:LEU:HD11	2.54	0.41
1:B:1306:LEU:C	1:B:1306:LEU:HD23	2.40	0.41
1:A:405:GLU:CD	1:A:405:GLU:H	2.23	0.41
1:A:367:PHE:CD2	1:A:542:PRO:HG3	2.55	0.41
1:A:126:SER:C	1:A:374:ARG:HH12	2.24	0.41
1:B:1577:TYR:CE2	1:B:1583:PRO:HD3	2.54	0.41
1:B:1134:HIS:HD2	1:B:1138:SER:OG	2.03	0.41
1:A:379:MET:SD	1:A:458:LEU:HG	2.60	0.41
1:B:1272:LEU:HD22	9:B:867:HOH:O	2.21	0.41
1:B:1237:ASN:ND2	1:B:1240:ARG:H	2.19	0.41
1:B:1204:HIS:HD2	9:B:87:HOH:O	2.03	0.41
1:A:150:ARG:HD2	1:A:153:PRO:HA	2.03	0.40
1:A:344:VAL:O	1:A:348:TYR:HB3	2.21	0.40
1:A:91:PHE:O	1:A:95:HIS:HD2	2.05	0.40
1:B:1103:VAL:HG13	1:B:1108:ILE:HB	2.03	0.40
1:B:1156:PRO:HB2	1:B:1159:CYS:SG	2.61	0.40
1:B:1388:HIS:CE1	1:B:1447:VAL:HG11	2.57	0.40
1:B:1034:ASN:HB3	1:B:1037:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1084:PRO:HG2	1:B:1089:ILE:HD11	2.03	0.40
1:B:1320:HIS:CE1	1:B:1551:GLY:O	2.74	0.40
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.62	0.40
1:B:1234:TYR:CE2	1:B:1333:ARG:HG3	2.56	0.40
1:B:1485:LYS:HA	1:B:1485:LYS:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	553/553 (100%)	538 (97%)	14 (2%)	1 (0%)	47	44
1	B	553/553 (100%)	538 (97%)	14 (2%)	1 (0%)	47	44
All	All	1106/1106 (100%)	1076 (97%)	28 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PRO
1	B	1270	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	490/488 (100%)	458 (94%)	32 (6%)	17	12
1	B	490/488 (100%)	459 (94%)	31 (6%)	18	13
All	All	980/976 (100%)	917 (94%)	63 (6%)	17	13

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	83	ARG
1	A	97	ARG
1	A	117	LEU
1	A	120	ARG
1	A	183	LEU
1	A	215	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	271	VAL
1	A	289	GLN
1	A	294	LEU
1	A	298	LEU
1	A	300	LEU
1	A	316	LEU
1	A	352	LEU
1	A	376	ARG
1	A	385	TYR
1	A	405	GLU
1	A	454	GLU
1	A	458	LEU
1	A	460	LEU
1	A	484	GLU
1	A	515	ASN
1	A	518	PHE
1	A	534	LEU
1	A	556	PHE
1	A	563	THR
1	A	564	LEU
1	B	1049	ARG
1	B	1097	ARG
1	B	1117	LEU

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Mol	Chain	Res	Type
1	B	1180	ARG
1	B	1183	LEU
1	B	1185	ARG
1	B	1215	LYS
1	B	1238	LEU
1	B	1244	LEU
1	B	1246	LEU
1	B	1252	LEU
1	B	1271	VAL
1	B	1289	GLN
1	B	1298	LEU
1	B	1316	LEU
1	B	1374	ARG
1	B	1385	TYR
1	B	1400	GLN
1	B	1405	GLU
1	B	1454	GLU
1	B	1458	LEU
1	B	1479	GLN
1	B	1484	GLU
1	B	1493	GLU
1	B	1518	PHE
1	B	1534	LEU
1	B	1556	PHE
1	B	1563	THR
1	B	1564	LEU
1	B	1570	LEU
1	B	1573	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	95	HIS
1	A	134	HIS
1	A	203	GLN
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	243	GLN
1	A	274	HIS
1	A	320	HIS

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Mol	Chain	Res	Type
1	A	375	ASN
1	A	386	HIS
1	A	443	HIS
1	A	479	GLN
1	B	1056	GLN
1	B	1095	HIS
1	B	1134	HIS
1	B	1203	GLN
1	B	1204	HIS
1	B	1208	GLN
1	B	1237	ASN
1	B	1241	GLN
1	B	1243	GLN
1	B	1274	HIS
1	B	1320	HIS
1	B	1375	ASN
1	B	1383	GLN
1	B	1386	HIS
1	B	1442	HIS
1	B	1443	HIS
1	B	1513	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 ⓘ

22 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	1,2	14,14,15	0.61	0	17,19,21	0.70	1 (5%)
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	0.83	0
3	NAG	D	1	1,3	14,14,15	0.68	0	17,19,21	0.85	0
3	NAG	D	2	3	14,14,15	0.77	0	17,19,21	1.79	3 (17%)
3	MAN	D	3	3	11,11,12	0.81	0	15,15,17	1.61	3 (20%)
3	MAN	D	4	3	11,11,12	0.63	0	15,15,17	1.15	1 (6%)
3	MAN	D	5	3	11,11,12	0.58	0	15,15,17	0.75	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.50	0	17,19,21	0.71	1 (5%)
4	NAG	E	2	4	14,14,15	0.65	0	17,19,21	0.70	0
4	MAN	E	3	4	11,11,12	0.72	0	15,15,17	0.97	1 (6%)
4	MAN	E	4	4	11,11,12	0.61	0	15,15,17	0.88	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.86	0	17,19,21	0.86	1 (5%)
2	NAG	F	2	2	14,14,15	0.65	0	17,19,21	0.82	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.66	0	17,19,21	0.80	0
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	1.51	2 (11%)
3	MAN	G	3	3	11,11,12	0.50	0	15,15,17	0.64	0
3	MAN	G	4	3	11,11,12	0.64	0	15,15,17	1.17	1 (6%)
3	MAN	G	5	3	11,11,12	0.66	0	15,15,17	0.86	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.46	0	17,19,21	0.63	0
4	NAG	H	2	4	14,14,15	0.52	0	17,19,21	0.82	0
4	MAN	H	3	4	11,11,12	0.50	0	15,15,17	0.74	0
4	MAN	H	4	4	11,11,12	0.54	0	15,15,17	0.87	1 (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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	1/1/5/7	1/6/23/26	0/1/1/1
3	MAN	D	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	1/1/1/1
3	MAN	D	5	3	1/1/4/5	1/2/19/22	1/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	E	3	4	1/1/4/5	1/2/19/22	1/1/1/1
4	MAN	E	4	4	1/1/4/5	2/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	1/1/5/7	1/6/23/26	0/1/1/1
3	MAN	G	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	G	4	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	G	5	3	1/1/4/5	1/2/19/22	1/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	MAN	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	1/1/4/5	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	MAN	C1-O5-C5	4.69	118.54	112.19
3	D	2	NAG	C1-O5-C5	4.42	118.18	112.19
3	D	2	NAG	C4-C3-C2	-4.24	104.80	111.02
3	G	2	NAG	C1-O5-C5	4.14	117.81	112.19
3	D	4	MAN	C1-O5-C5	3.51	116.95	112.19
3	G	2	NAG	C4-C3-C2	-3.45	105.96	111.02
3	G	4	MAN	C1-O5-C5	3.41	116.82	112.19
4	H	4	MAN	C1-O5-C5	2.95	116.19	112.19
4	E	3	MAN	C1-O5-C5	2.95	116.19	112.19
4	E	4	MAN	C1-O5-C5	2.92	116.15	112.19
3	G	5	MAN	C1-O5-C5	2.86	116.07	112.19
3	D	5	MAN	C1-O5-C5	2.66	115.80	112.19
3	D	2	NAG	C3-C4-C5	-2.59	105.61	110.24
3	D	3	MAN	C2-C3-C4	-2.50	106.57	110.89
2	F	1	NAG	C2-N2-C7	-2.16	119.83	122.90
3	D	3	MAN	O5-C1-C2	2.07	113.97	110.77
2	F	2	NAG	C2-N2-C7	-2.04	120.00	122.90
4	E	1	NAG	C2-N2-C7	-2.04	120.00	122.90
2	C	1	NAG	C2-N2-C7	-2.01	120.04	122.90

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	2	NAG	C1
2	C	2	NAG	C1
3	G	4	MAN	C1
4	H	4	MAN	C1
4	E	4	MAN	C1
3	G	5	MAN	C1
3	G	2	NAG	C1
3	D	2	NAG	C1
3	D	5	MAN	C1
4	E	3	MAN	C1
3	G	3	MAN	C1
3	D	3	MAN	C1

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C3-C2-N2-C7
3	D	4	MAN	C4-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	D	3	MAN	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	H	3	MAN	O5-C5-C6-O6
3	D	3	MAN	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
4	H	3	MAN	C4-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
4	E	3	MAN	O5-C5-C6-O6
3	G	5	MAN	O5-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
3	G	4	MAN	C4-C5-C6-O6

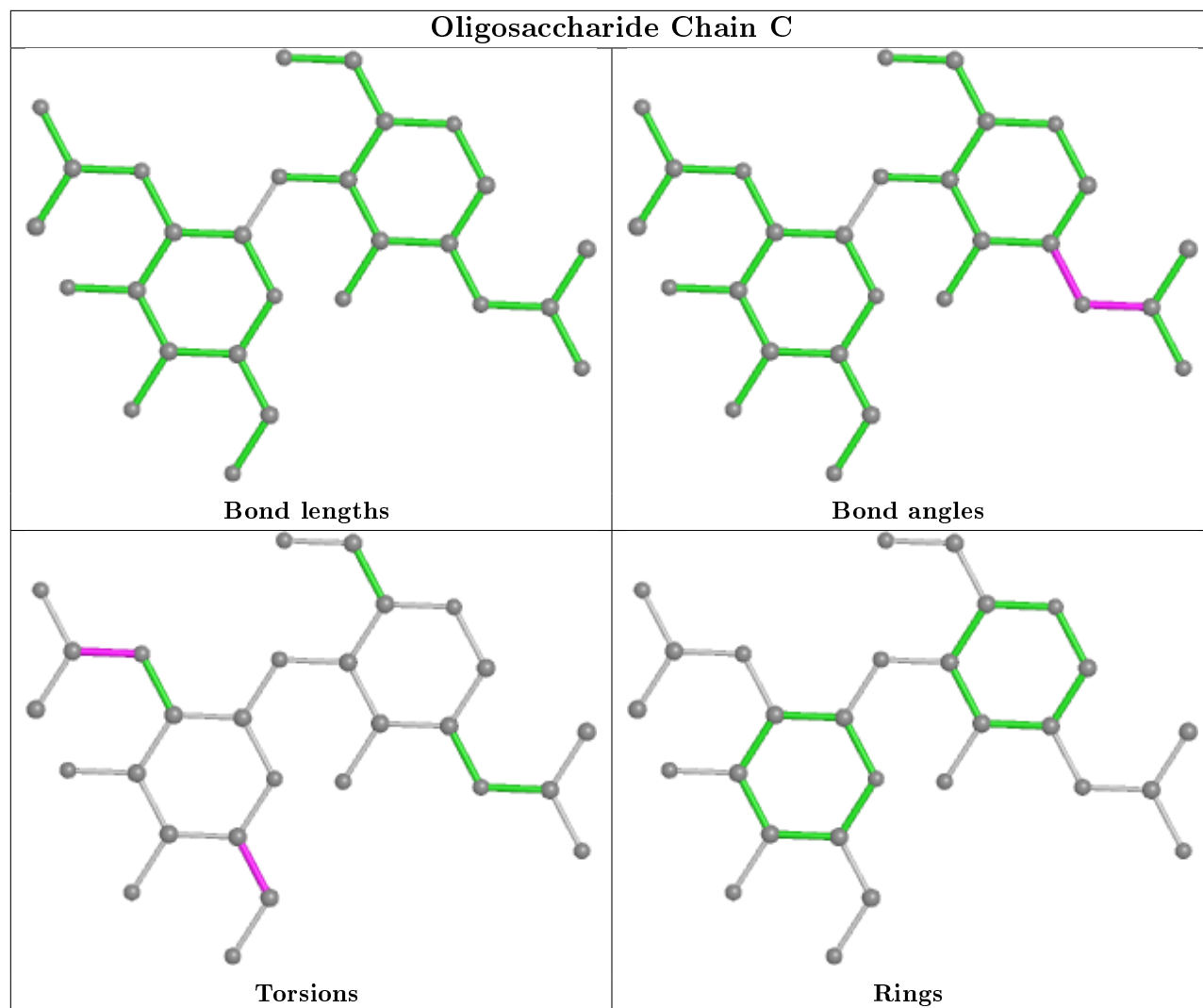
All (6) ring outliers are listed below:

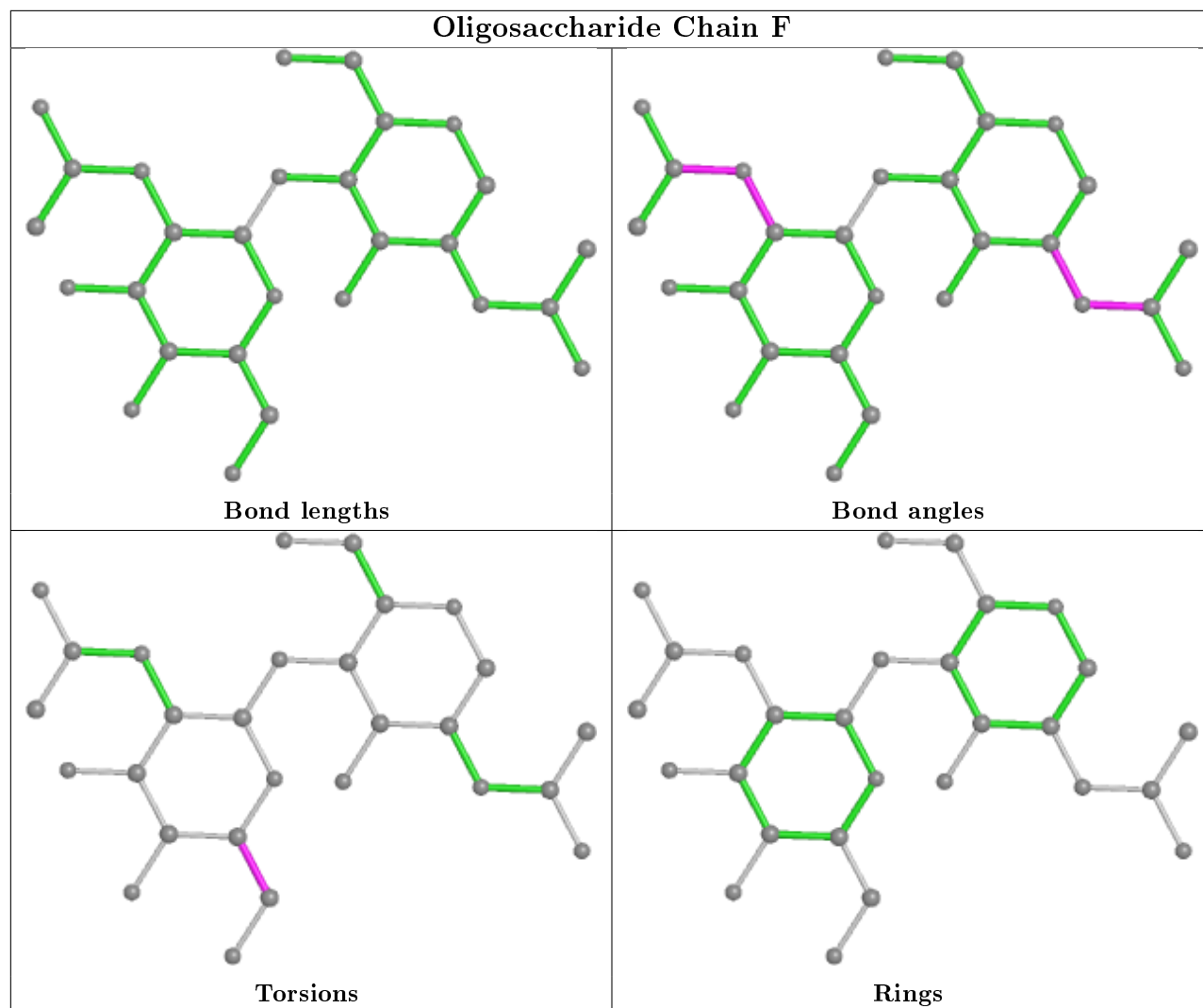
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	C1-C2-C3-C4-C5-O5
3	G	5	MAN	C1-C2-C3-C4-C5-O5
3	D	5	MAN	C1-C2-C3-C4-C5-O5
4	E	4	MAN	C1-C2-C3-C4-C5-O5
4	E	3	MAN	C1-C2-C3-C4-C5-O5
4	H	4	MAN	C1-C2-C3-C4-C5-O5

15 monomers are involved in 28 short contacts:

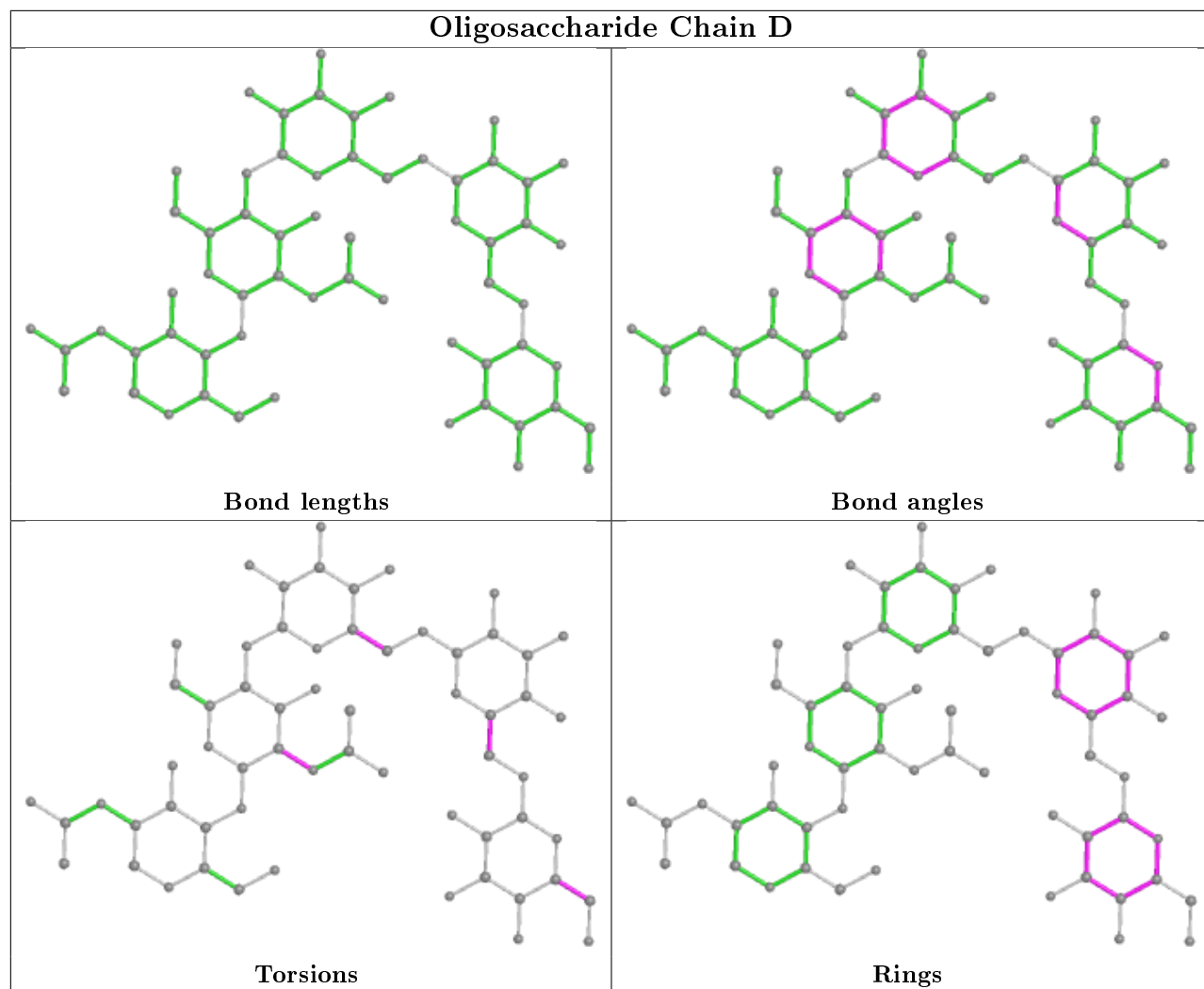
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	1	0
4	H	3	MAN	2	0
3	D	4	MAN	3	0
4	H	2	NAG	1	0
3	G	4	MAN	3	0
2	F	1	NAG	1	0
3	G	5	MAN	3	0
3	G	2	NAG	4	0
2	C	1	NAG	1	0
3	D	2	NAG	8	0
3	D	5	MAN	4	0
4	E	3	MAN	3	0
3	G	3	MAN	1	0
3	D	3	MAN	6	0
4	E	2	NAG	3	0

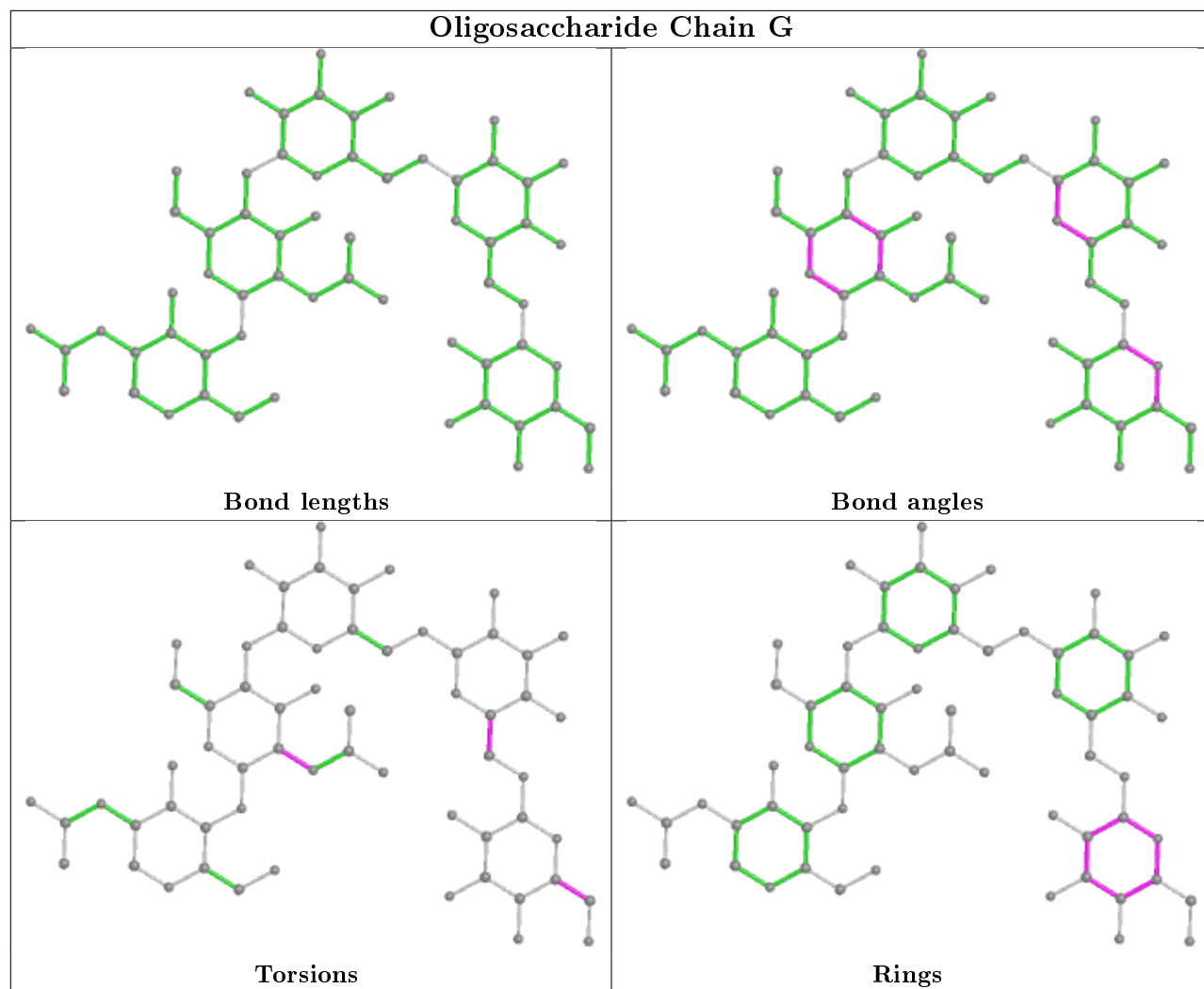
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

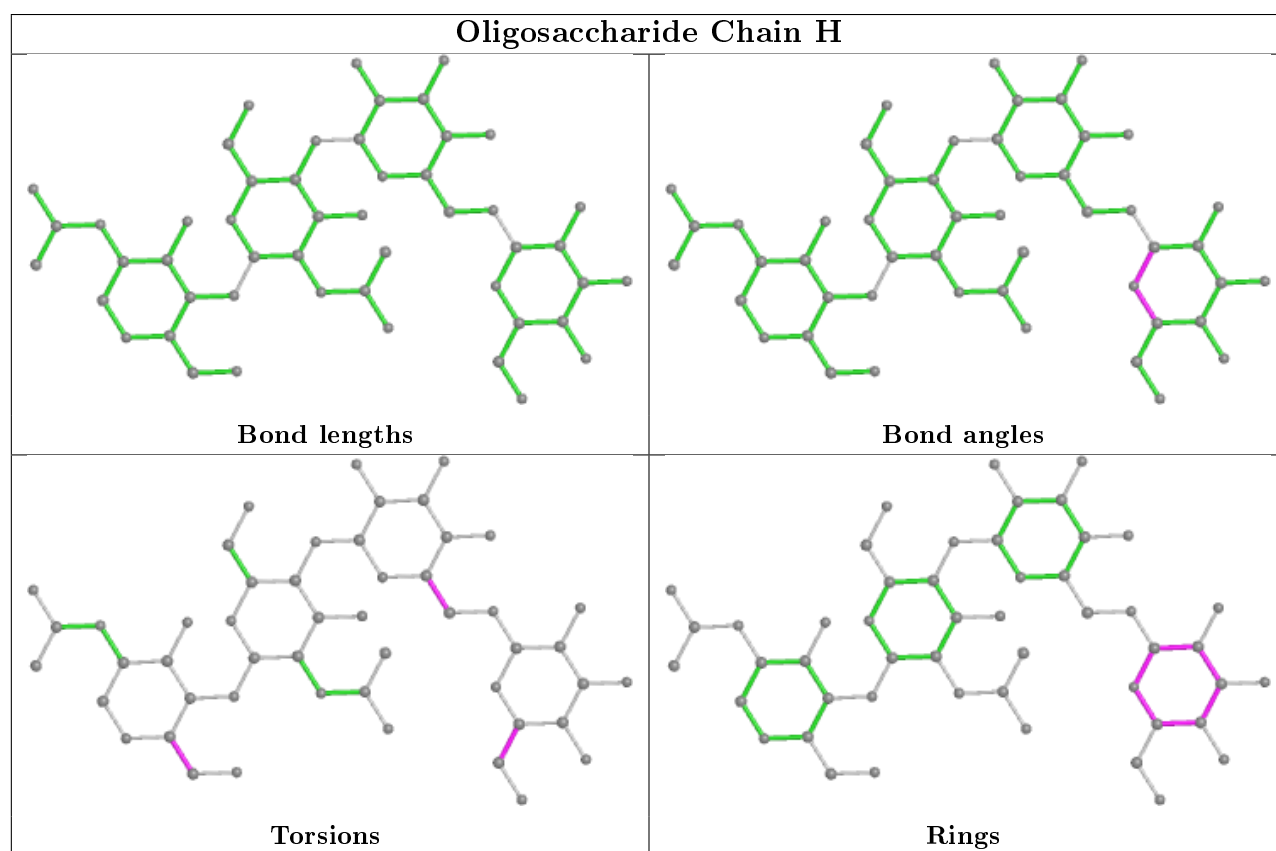
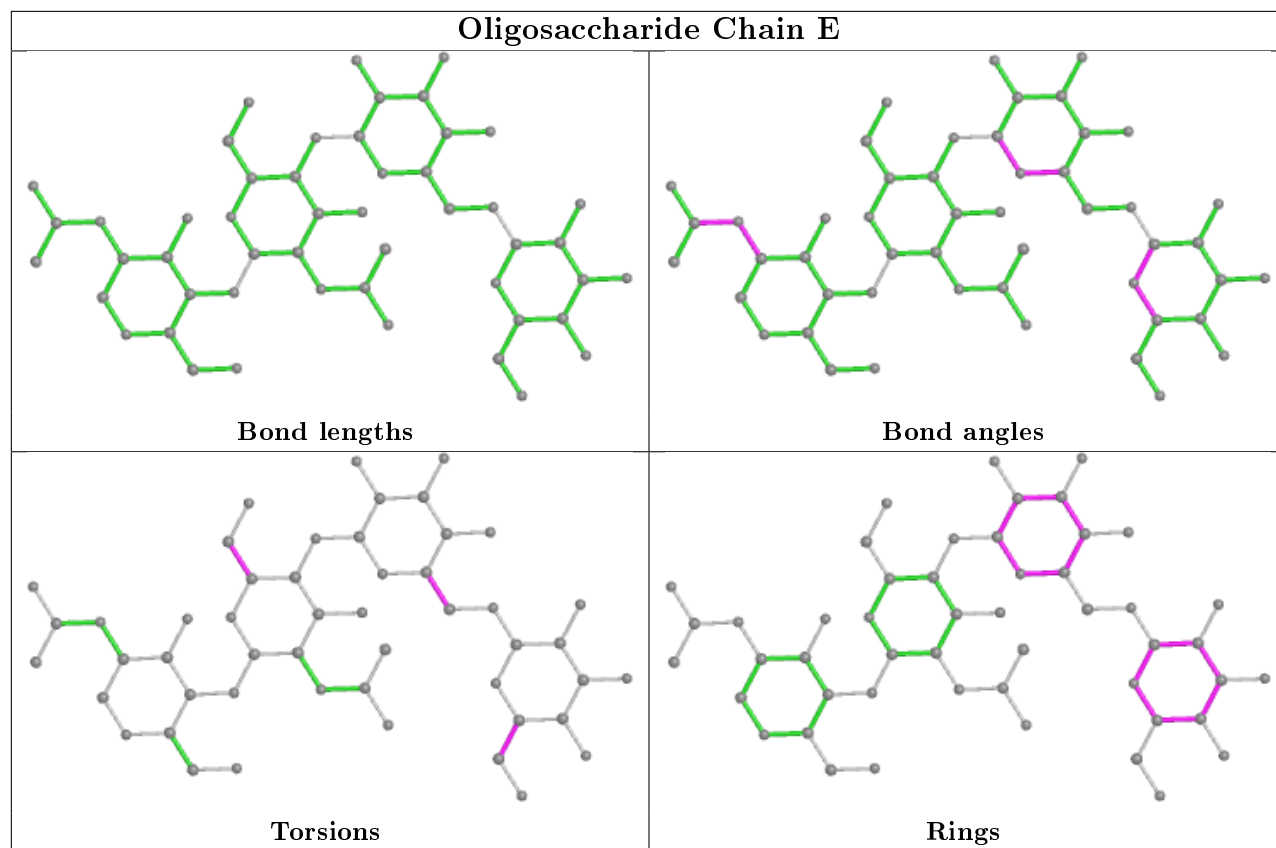




Oligosaccharide Chain D







5.6 Ligand geometry

18 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$
7	MNH	A	601	-	32,50,50	6.00	21 (65%)	19,82,82	7.11	15 (78%)
5	BOG	B	1750	-	20,20,20	1.71	5 (25%)	25,25,25	0.90	2 (8%)
6	FLP	A	1701[B]	-	16,19,19	2.27	7 (43%)	22,26,26	0.90	1 (4%)
5	BOG	A	754	-	20,20,20	1.71	5 (25%)	25,25,25	0.90	2 (8%)
8	GOL	A	760	-	5,5,5	4.54	5 (100%)	5,5,5	5.81	3 (60%)
8	GOL	A	758	-	5,5,5	4.46	5 (100%)	5,5,5	5.71	3 (60%)
7	MNH	B	1601	-	32,50,50	5.97	21 (65%)	19,82,82	7.38	12 (63%)
5	BOG	A	751	-	20,20,20	1.71	6 (30%)	25,25,25	0.81	1 (4%)
6	FLP	B	2701[A]	-	16,19,19	2.36	9 (56%)	22,26,26	0.88	0
8	GOL	B	1760	-	5,5,5	4.52	5 (100%)	5,5,5	5.70	3 (60%)
6	FLP	B	2701[B]	-	16,19,19	2.29	7 (43%)	22,26,26	0.91	1 (4%)
8	GOL	B	1759	-	5,5,5	4.52	5 (100%)	5,5,5	5.79	3 (60%)
8	GOL	A	759	-	5,5,5	4.52	5 (100%)	5,5,5	5.71	3 (60%)
5	BOG	A	752	-	20,20,20	1.79	5 (25%)	25,25,25	0.88	2 (8%)
6	FLP	A	1701[A]	-	16,19,19	2.34	9 (56%)	22,26,26	0.88	0
5	BOG	B	1751	-	20,20,20	1.72	6 (30%)	25,25,25	0.85	2 (8%)
5	BOG	B	1753	-	20,20,20	1.70	5 (25%)	25,25,25	0.88	2 (8%)
5	BOG	A	753	-	20,20,20	1.71	5 (25%)	25,25,25	0.88	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MNH	A	601	-	-	1/10/114/114	-
5	BOG	B	1750	-	-	4/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FLP	A	1701[B]	-	-	0/8/12/12	0/2/2/2
5	BOG	A	754	-	-	8/11/31/31	0/1/1/1
8	GOL	A	760	-	-	2/4/4/4	-
8	GOL	A	758	-	-	2/4/4/4	-
7	MNH	B	1601	-	-	1/10/114/114	-
5	BOG	A	751	-	-	6/11/31/31	0/1/1/1
6	FLP	B	2701[A]	-	-	0/8/12/12	0/2/2/2
8	GOL	B	1760	-	-	2/4/4/4	-
6	FLP	B	2701[B]	-	-	0/8/12/12	0/2/2/2
8	GOL	B	1759	-	-	3/4/4/4	-
8	GOL	A	759	-	-	2/4/4/4	-
5	BOG	A	752	-	-	7/11/31/31	0/1/1/1
6	FLP	A	1701[A]	-	-	0/8/12/12	0/2/2/2
5	BOG	B	1751	-	-	5/11/31/31	0/1/1/1
5	BOG	B	1753	-	-	8/11/31/31	0/1/1/1
5	BOG	A	753	-	-	4/11/31/31	0/1/1/1

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1601	MNH	C3C-C2C	-17.03	1.34	1.55
7	A	601	MNH	C3C-C2C	-17.02	1.34	1.55
7	A	601	MNH	CHD-C1D	-9.68	1.37	1.53
7	B	1601	MNH	CHD-C4C	-9.61	1.38	1.53
7	A	601	MNH	CHD-C4C	-9.57	1.38	1.53
7	B	1601	MNH	C4C-NC	-9.46	1.38	1.49
7	A	601	MNH	C4C-NC	-9.41	1.38	1.49
7	B	1601	MNH	CHD-C1D	-9.36	1.37	1.53
7	A	601	MNH	CHC-C1C	-9.17	1.39	1.53
7	A	601	MNH	C1C-NC	-9.08	1.38	1.49
7	B	1601	MNH	C1C-NC	-9.02	1.38	1.49
7	B	1601	MNH	CHC-C1C	-8.98	1.39	1.53
7	A	601	MNH	CHC-C4B	-8.65	1.38	1.53
7	B	1601	MNH	CHC-C4B	-8.43	1.39	1.53
7	B	1601	MNH	C3C-C4C	-7.98	1.45	1.54
7	A	601	MNH	C3C-C4C	-7.88	1.45	1.54
8	A	759	GOL	C3-C2	-7.46	1.21	1.51
8	B	1759	GOL	C3-C2	-7.40	1.21	1.51
8	B	1760	GOL	C3-C2	-7.38	1.21	1.51
8	A	760	GOL	C3-C2	-7.35	1.21	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	758	GOL	C3-C2	-7.13	1.22	1.51
7	A	601	MNH	C4A-C3A	6.18	1.46	1.38
7	B	1601	MNH	C4A-C3A	6.05	1.46	1.38
7	A	601	MNH	C1A-C2A	5.81	1.46	1.38
7	B	1601	MNH	C1A-C2A	5.53	1.45	1.38
7	A	601	MNH	CHB-C1B	-5.52	1.39	1.53
7	B	1601	MNH	CHB-C1B	-5.52	1.39	1.53
7	B	1601	MNH	CHB-C4A	-5.49	1.37	1.51
7	A	601	MNH	CHB-C4A	-5.46	1.37	1.51
7	A	601	MNH	CHA-C4D	-5.46	1.39	1.53
7	B	1601	MNH	CHA-C4D	-5.39	1.39	1.53
7	B	1601	MNH	CHA-C1A	-5.24	1.38	1.51
7	A	601	MNH	CHA-C1A	-5.11	1.38	1.51
7	B	1601	MNH	CBB-CAB	4.70	1.53	1.30
8	A	760	GOL	O1-C1	4.69	1.62	1.42
7	A	601	MNH	CBB-CAB	4.60	1.53	1.30
8	B	1760	GOL	O1-C1	4.59	1.61	1.42
7	B	1601	MNH	CBC-CAC	4.43	1.52	1.29
8	A	758	GOL	O1-C1	4.39	1.60	1.42
8	A	759	GOL	O1-C1	4.38	1.60	1.42
7	A	601	MNH	CBC-CAC	4.36	1.51	1.29
8	B	1759	GOL	O1-C1	4.20	1.60	1.42
6	B	2701[A]	FLP	C7-C6	4.17	1.46	1.40
6	B	2701[B]	FLP	C6-C11	4.03	1.44	1.39
7	A	601	MNH	C2C-C1C	-3.97	1.46	1.53
7	B	1601	MNH	C2C-C1C	-3.96	1.46	1.53
6	B	2701[A]	FLP	C6-C11	3.96	1.44	1.39
6	A	1701[A]	FLP	C7-C6	3.93	1.46	1.40
5	A	752	BOG	O5-C1	3.92	1.51	1.41
6	A	1701[A]	FLP	C6-C11	3.87	1.44	1.39
5	A	751	BOG	O5-C1	3.86	1.51	1.41
5	B	1751	BOG	O5-C1	3.81	1.51	1.41
6	B	2701[B]	FLP	C7-C6	3.80	1.45	1.40
6	A	1701[B]	FLP	C7-C6	3.77	1.45	1.40
5	A	753	BOG	O5-C1	3.76	1.51	1.41
5	B	1750	BOG	O5-C1	3.75	1.51	1.41
5	A	752	BOG	O5-C5	3.75	1.53	1.44
5	B	1753	BOG	O5-C1	3.74	1.51	1.41
6	A	1701[B]	FLP	C6-C11	3.74	1.44	1.39
5	A	754	BOG	O5-C1	3.72	1.51	1.41
8	A	758	GOL	O3-C3	3.68	1.57	1.42
5	A	754	BOG	O5-C5	3.55	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	753	BOG	O5-C5	3.53	1.52	1.44
5	B	1751	BOG	O5-C5	3.51	1.52	1.44
5	B	1750	BOG	O5-C5	3.49	1.52	1.44
5	B	1753	BOG	O5-C5	3.45	1.52	1.44
8	A	760	GOL	O3-C3	3.44	1.56	1.42
7	A	601	MNH	C2D-C3D	3.43	1.36	1.34
5	A	751	BOG	O5-C5	3.41	1.52	1.44
8	B	1760	GOL	O3-C3	3.41	1.56	1.42
6	A	1701[B]	FLP	C8-C9	3.35	1.44	1.39
8	B	1759	GOL	O3-C3	3.32	1.56	1.42
6	B	2701[B]	FLP	C8-C9	3.30	1.44	1.39
8	A	759	GOL	O3-C3	3.26	1.56	1.42
6	A	1701[B]	FLP	C1-C2	3.22	1.46	1.39
8	B	1759	GOL	C1-C2	-3.22	1.38	1.51
7	B	1601	MNH	C2D-C3D	3.20	1.36	1.34
6	B	2701[A]	FLP	C1-C2	3.18	1.46	1.39
6	B	2701[B]	FLP	C1-C2	3.18	1.46	1.39
6	A	1701[A]	FLP	C1-C2	3.14	1.46	1.39
8	A	759	GOL	C1-C2	-3.12	1.38	1.51
6	B	2701[A]	FLP	C8-C9	3.06	1.44	1.39
6	A	1701[A]	FLP	C8-C7	2.98	1.44	1.38
6	A	1701[A]	FLP	C8-C9	2.94	1.43	1.39
7	B	1601	MNH	CMB-C2B	2.93	1.55	1.50
6	B	2701[A]	FLP	C8-C7	2.92	1.44	1.38
8	B	1759	GOL	O2-C2	-2.88	1.34	1.43
8	A	758	GOL	O2-C2	-2.85	1.34	1.43
8	B	1760	GOL	O2-C2	-2.85	1.34	1.43
8	A	760	GOL	C1-C2	-2.83	1.40	1.51
8	A	758	GOL	C1-C2	-2.81	1.40	1.51
8	A	760	GOL	O2-C2	-2.68	1.35	1.43
8	B	1760	GOL	C1-C2	-2.66	1.40	1.51
7	A	601	MNH	CMB-C2B	2.64	1.54	1.50
5	A	752	BOG	C4-C3	2.63	1.59	1.52
8	A	759	GOL	O2-C2	-2.62	1.35	1.43
6	B	2701[B]	FLP	C8-C7	2.62	1.43	1.38
6	A	1701[B]	FLP	C8-C7	2.60	1.43	1.38
5	A	753	BOG	C4-C3	2.58	1.58	1.52
5	B	1750	BOG	C4-C3	2.57	1.58	1.52
5	B	1753	BOG	C3'-C2'	-2.52	1.37	1.51
5	A	752	BOG	C3'-C2'	-2.52	1.37	1.51
5	A	754	BOG	C3'-C2'	-2.51	1.37	1.51
5	A	753	BOG	C3'-C2'	-2.46	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	751	BOG	C4-C3	2.46	1.58	1.52
5	A	754	BOG	C4-C3	2.45	1.58	1.52
5	B	1750	BOG	C3'-C2'	-2.45	1.37	1.51
5	B	1751	BOG	C3'-C2'	-2.45	1.37	1.51
5	B	1753	BOG	C4-C3	2.44	1.58	1.52
5	A	751	BOG	C3'-C2'	-2.44	1.37	1.51
5	B	1751	BOG	C4-C3	2.41	1.58	1.52
5	A	752	BOG	C1-C2	2.32	1.59	1.52
5	B	1751	BOG	C1-C2	2.31	1.59	1.52
5	A	754	BOG	C1-C2	2.24	1.59	1.52
5	A	751	BOG	C1-C2	2.23	1.58	1.52
5	B	1750	BOG	C1-C2	2.22	1.58	1.52
5	A	753	BOG	C1-C2	2.19	1.58	1.52
6	A	1701[A]	FLP	C-C1	2.19	1.43	1.38
6	B	2701[B]	FLP	C-C1	2.18	1.43	1.38
6	B	2701[A]	FLP	C-C1	2.17	1.43	1.38
6	A	1701[A]	FLP	C4-C3	2.16	1.43	1.38
6	A	1701[A]	FLP	C9-C12	2.16	1.56	1.52
6	A	1701[B]	FLP	C4-C3	2.15	1.43	1.38
5	B	1753	BOG	C1-C2	2.15	1.58	1.52
7	A	601	MNH	C4D-C3D	-2.15	1.44	1.50
6	B	2701[B]	FLP	C4-C3	2.15	1.43	1.38
6	A	1701[B]	FLP	C-C1	2.14	1.43	1.38
6	B	2701[A]	FLP	C9-C12	2.11	1.56	1.52
6	A	1701[A]	FLP	C3-C2	2.07	1.43	1.39
7	A	601	MNH	C1B-C2B	-2.06	1.44	1.50
6	B	2701[A]	FLP	C3-C2	2.05	1.43	1.39
6	B	2701[A]	FLP	C4-C3	2.05	1.43	1.38
5	B	1751	BOG	C4-C5	-2.03	1.48	1.53
5	A	751	BOG	C4-C5	-2.03	1.48	1.53
7	B	1601	MNH	CMD-C2D	2.02	1.53	1.50
7	B	1601	MNH	C4D-C3D	-2.01	1.44	1.50

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	MNH	C4C-CHD-C1D	18.58	151.96	112.37
7	B	1601	MNH	C4C-CHD-C1D	17.80	150.31	112.37
7	B	1601	MNH	C1C-CHC-C4B	15.87	146.18	112.37
7	A	601	MNH	C1C-CHC-C4B	15.31	144.99	112.37
7	B	1601	MNH	CAA-C2A-C1A	-15.23	116.60	127.30
7	A	601	MNH	CAA-C2A-C1A	-12.02	118.85	127.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1759	GOL	O3-C3-C2	10.55	160.79	110.20
8	A	760	GOL	O3-C3-C2	10.52	160.63	110.20
8	B	1760	GOL	O3-C3-C2	10.41	160.12	110.20
8	A	758	GOL	O3-C3-C2	10.32	159.66	110.20
8	A	759	GOL	O3-C3-C2	10.17	158.97	110.20
7	B	1601	MNH	CMC-C2C-C3C	7.43	130.97	113.69
7	A	601	MNH	CMC-C2C-C3C	7.09	130.18	113.69
8	A	759	GOL	O2-C2-C3	7.01	140.00	109.12
8	A	760	GOL	O2-C2-C3	6.81	139.11	109.12
8	A	758	GOL	O2-C2-C3	6.79	139.04	109.12
8	B	1759	GOL	O2-C2-C3	6.67	138.51	109.12
7	A	601	MNH	CAA-CBA-CGA	6.63	123.79	112.67
8	B	1760	GOL	O2-C2-C3	6.59	138.17	109.12
7	B	1601	MNH	CAA-CBA-CGA	6.16	123.01	112.67
7	A	601	MNH	CBB-CAB-C3B	5.86	147.53	127.20
7	B	1601	MNH	CBB-CAB-C3B	5.85	147.53	127.20
7	A	601	MNH	CMB-C2B-C3B	5.21	138.59	129.73
7	B	1601	MNH	CMB-C2B-C3B	4.71	137.75	129.73
7	B	1601	MNH	CMA-C3A-C2A	4.58	133.57	124.94
7	B	1601	MNH	C4A-C3A-C2A	-4.51	101.00	105.81
7	A	601	MNH	CMA-C3A-C2A	4.24	132.93	124.94
7	B	1601	MNH	C1A-C2A-C3A	4.05	111.97	105.93
7	A	601	MNH	C4A-C3A-C2A	-3.54	102.04	105.81
8	A	760	GOL	O1-C1-C2	3.37	126.34	110.20
8	B	1759	GOL	O1-C1-C2	3.32	126.10	110.20
8	B	1760	GOL	O1-C1-C2	3.20	125.56	110.20
8	A	758	GOL	O1-C1-C2	3.18	125.43	110.20
8	A	759	GOL	O1-C1-C2	3.12	125.16	110.20
7	B	1601	MNH	CMD-C2D-C3D	2.97	132.34	128.33
5	A	753	BOG	C1'-O1-C1	2.84	118.55	113.84
7	A	601	MNH	C2C-C3C-CAC	2.83	127.52	113.83
7	A	601	MNH	CHB-C4A-C3A	2.82	134.34	129.45
7	A	601	MNH	C1A-C2A-C3A	2.82	110.13	105.93
5	A	754	BOG	C1'-O1-C1	2.79	118.47	113.84
7	A	601	MNH	CMD-C2D-C3D	2.75	132.05	128.33
5	B	1750	BOG	C1'-O1-C1	2.72	118.36	113.84
5	A	752	BOG	C1'-O1-C1	2.72	118.35	113.84
5	B	1753	BOG	C1'-O1-C1	2.61	118.17	113.84
7	A	601	MNH	CBA-CAA-C2A	-2.48	107.92	112.49
5	B	1751	BOG	O1-C1-C2	2.47	112.16	108.30
5	A	751	BOG	O1-C1-C2	2.45	112.13	108.30
5	B	1753	BOG	O1-C1-C2	2.40	112.05	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2701[B]	FLP	C10-C9-C12	-2.39	116.41	120.97
5	B	1750	BOG	O1-C1-C2	2.39	112.03	108.30
6	A	1701[B]	FLP	C10-C9-C12	-2.37	116.45	120.97
5	A	754	BOG	O1-C1-C2	2.36	111.99	108.30
5	B	1751	BOG	C1'-O1-C1	2.22	117.52	113.84
5	A	752	BOG	O1-C1-C2	2.18	111.71	108.30
7	B	1601	MNH	C2C-C3C-CAC	2.17	124.34	113.83
7	A	601	MNH	C3C-CAC-CBC	2.12	130.25	125.33
5	A	753	BOG	O1-C1-C2	2.10	111.59	108.30

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	MNH	C4C-C3C-CAC-CBC
8	A	759	GOL	O1-C1-C2-O2
8	A	759	GOL	C1-C2-C3-O3
8	A	758	GOL	C1-C2-C3-O3
8	B	1760	GOL	O1-C1-C2-O2
8	B	1760	GOL	C1-C2-C3-O3
8	B	1759	GOL	C1-C2-C3-O3
7	B	1601	MNH	C4C-C3C-CAC-CBC
8	A	760	GOL	O1-C1-C2-O2
8	A	760	GOL	C1-C2-C3-O3
5	B	1753	BOG	O5-C5-C6-O6
5	A	754	BOG	O5-C5-C6-O6
5	A	754	BOG	C4-C5-C6-O6
5	A	751	BOG	C2-C1-O1-C1'
5	B	1751	BOG	C2-C1-O1-C1'
5	B	1753	BOG	C2-C1-O1-C1'
5	B	1751	BOG	C3'-C4'-C5'-C6'
5	B	1750	BOG	C3'-C4'-C5'-C6'
5	A	751	BOG	C3'-C4'-C5'-C6'
5	A	752	BOG	C2'-C3'-C4'-C5'
5	A	753	BOG	C2'-C3'-C4'-C5'
8	A	758	GOL	O1-C1-C2-O2
5	B	1753	BOG	C4-C5-C6-O6
5	A	751	BOG	O5-C1-O1-C1'
5	B	1751	BOG	O5-C1-O1-C1'
5	B	1753	BOG	O5-C1-O1-C1'
5	B	1751	BOG	C1'-C2'-C3'-C4'
5	A	754	BOG	C2-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
5	B	1753	BOG	C3'-C4'-C5'-C6'
5	A	754	BOG	C1'-C2'-C3'-C4'
5	B	1753	BOG	O1-C1'-C2'-C3'
8	B	1759	GOL	O1-C1-C2-O2
5	A	751	BOG	C1'-C2'-C3'-C4'
5	A	754	BOG	C3'-C4'-C5'-C6'
5	A	752	BOG	C3'-C4'-C5'-C6'
5	A	751	BOG	O1-C1'-C2'-C3'
5	A	752	BOG	C2-C1-O1-C1'
5	A	753	BOG	O1-C1'-C2'-C3'
5	B	1751	BOG	O1-C1'-C2'-C3'
5	A	753	BOG	C4-C5-C6-O6
5	A	754	BOG	O5-C1-O1-C1'
5	B	1750	BOG	C1'-C2'-C3'-C4'
5	A	752	BOG	C4-C5-C6-O6
5	B	1753	BOG	C2'-C3'-C4'-C5'
5	A	752	BOG	O5-C5-C6-O6
5	A	754	BOG	C2'-C3'-C4'-C5'
5	A	754	BOG	O1-C1'-C2'-C3'
5	A	751	BOG	C2'-C3'-C4'-C5'
5	A	753	BOG	O5-C5-C6-O6
5	B	1750	BOG	C2-C1-O1-C1'
5	A	752	BOG	O1-C1'-C2'-C3'
5	B	1750	BOG	O5-C1-O1-C1'
5	A	752	BOG	O5-C1-O1-C1'
5	B	1753	BOG	C1'-C2'-C3'-C4'
8	B	1759	GOL	O1-C1-C2-C3

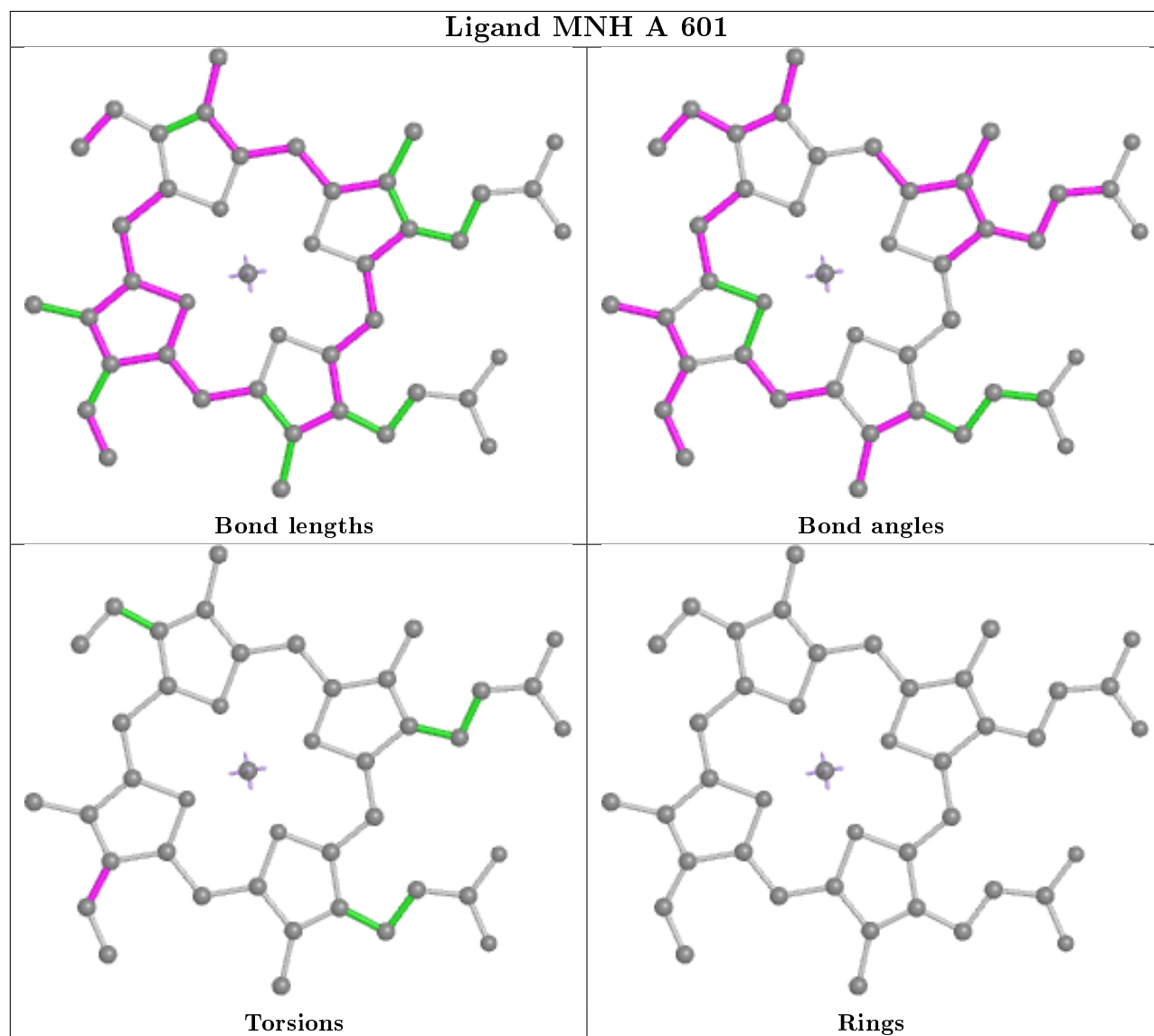
There are no ring outliers.

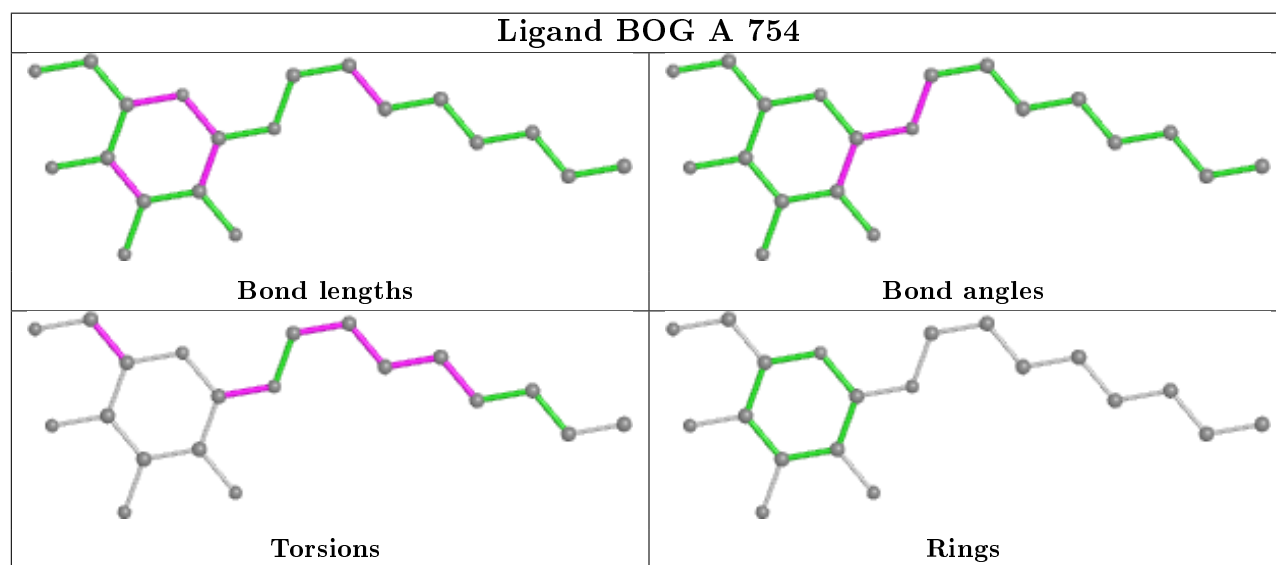
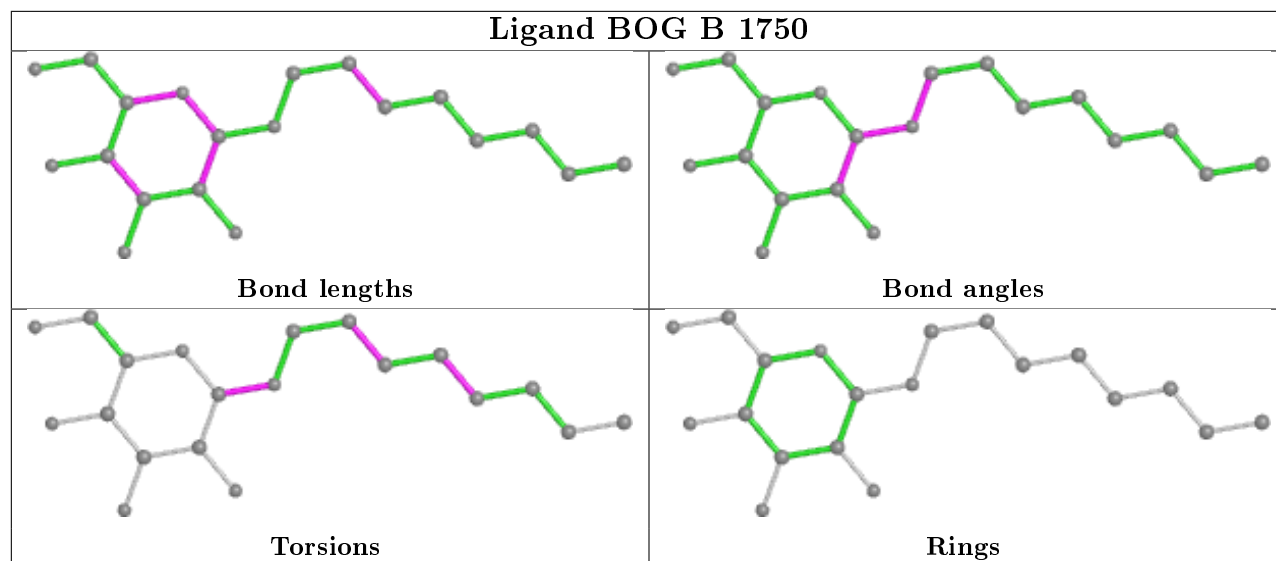
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	MNH	3	0
5	A	754	BOG	1	0
5	A	751	BOG	6	0
8	A	759	GOL	2	0
5	B	1751	BOG	4	0
5	B	1753	BOG	1	0

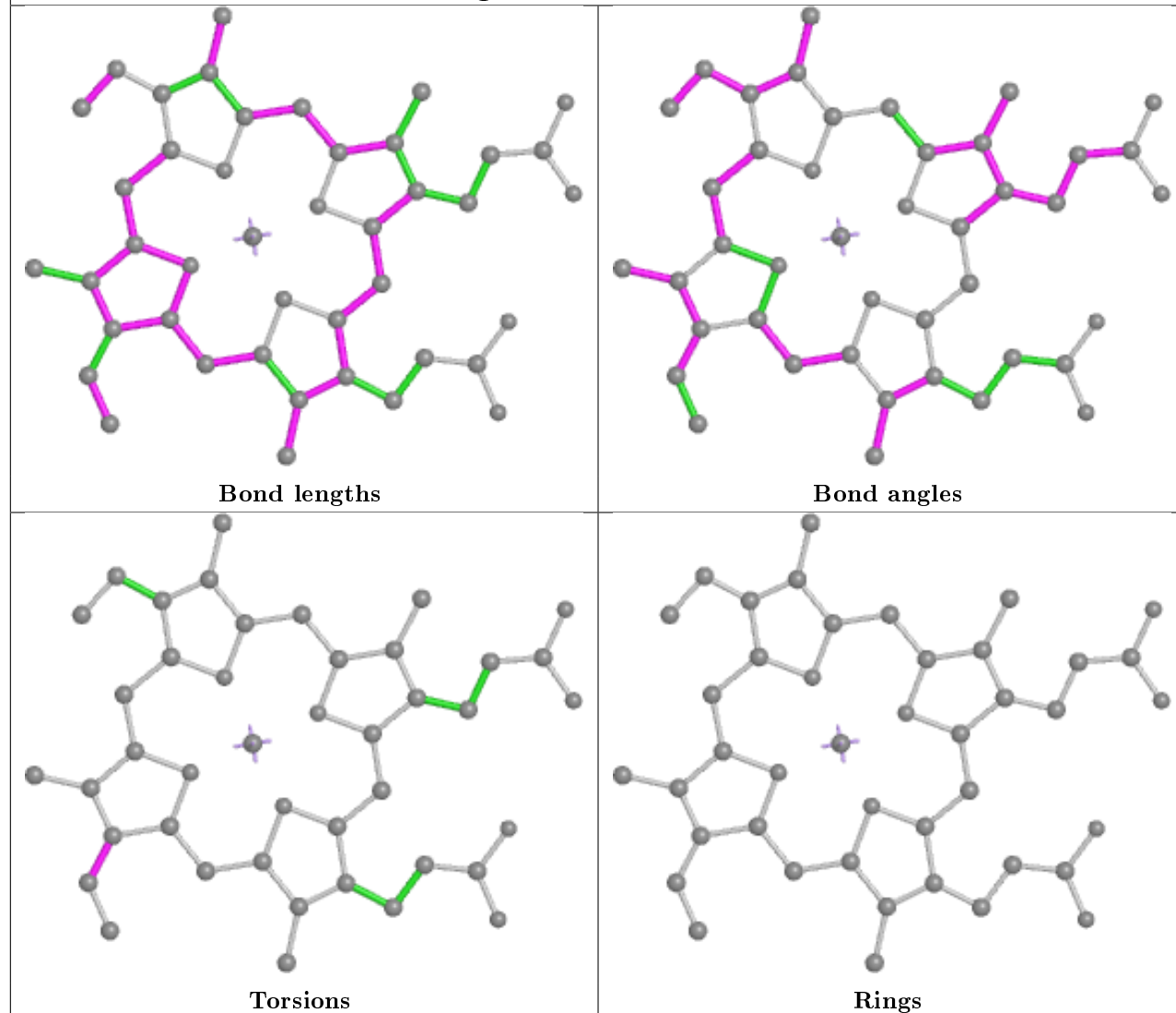
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

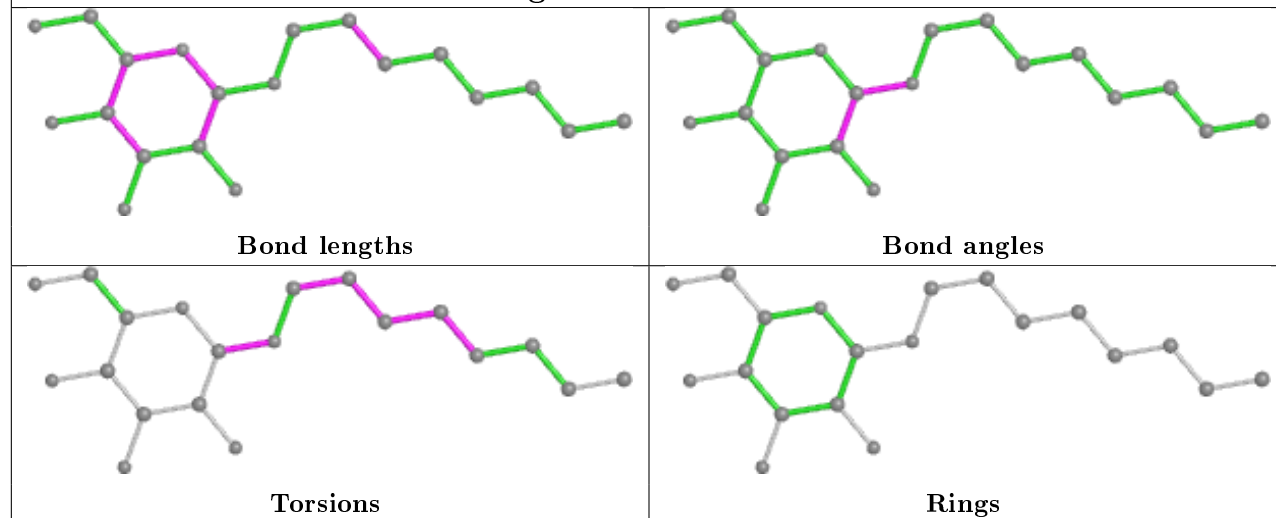


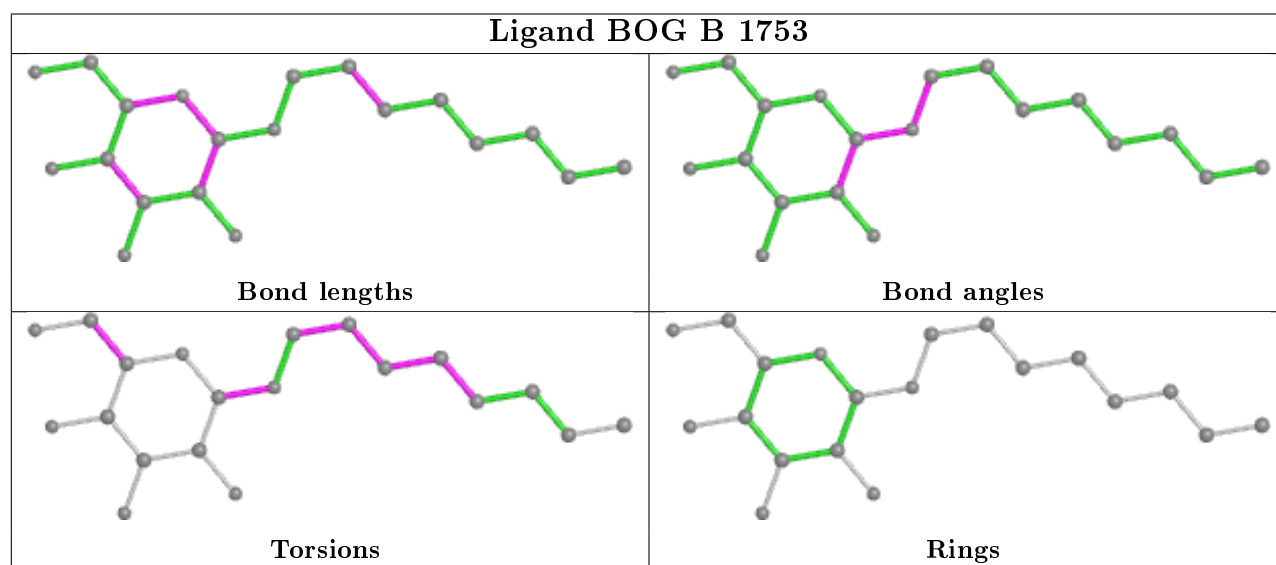
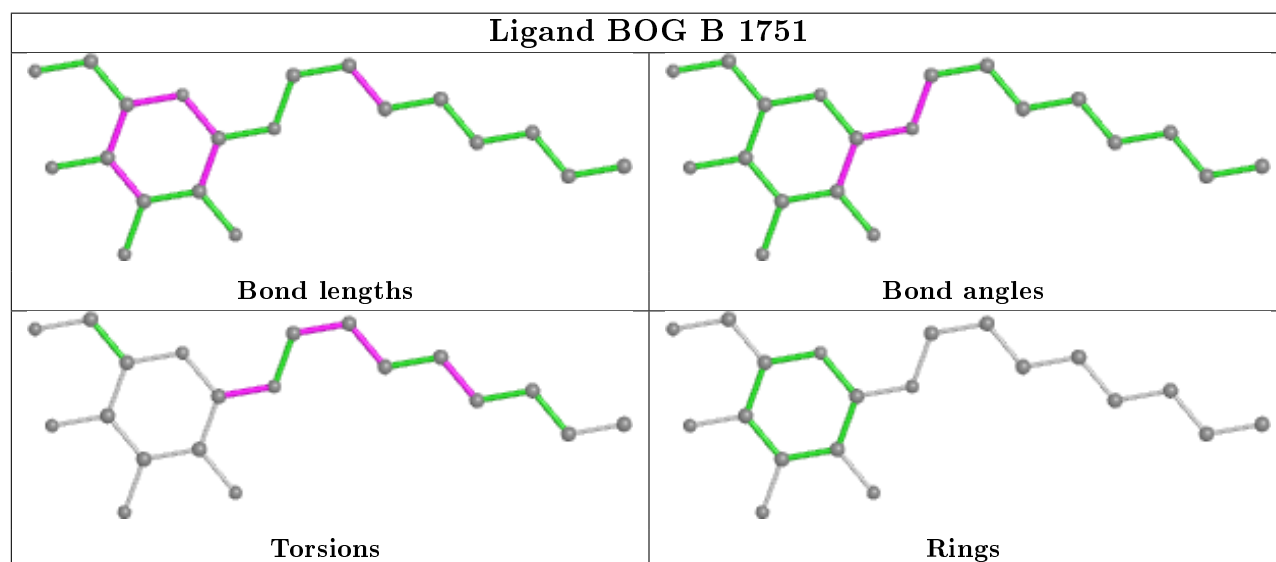
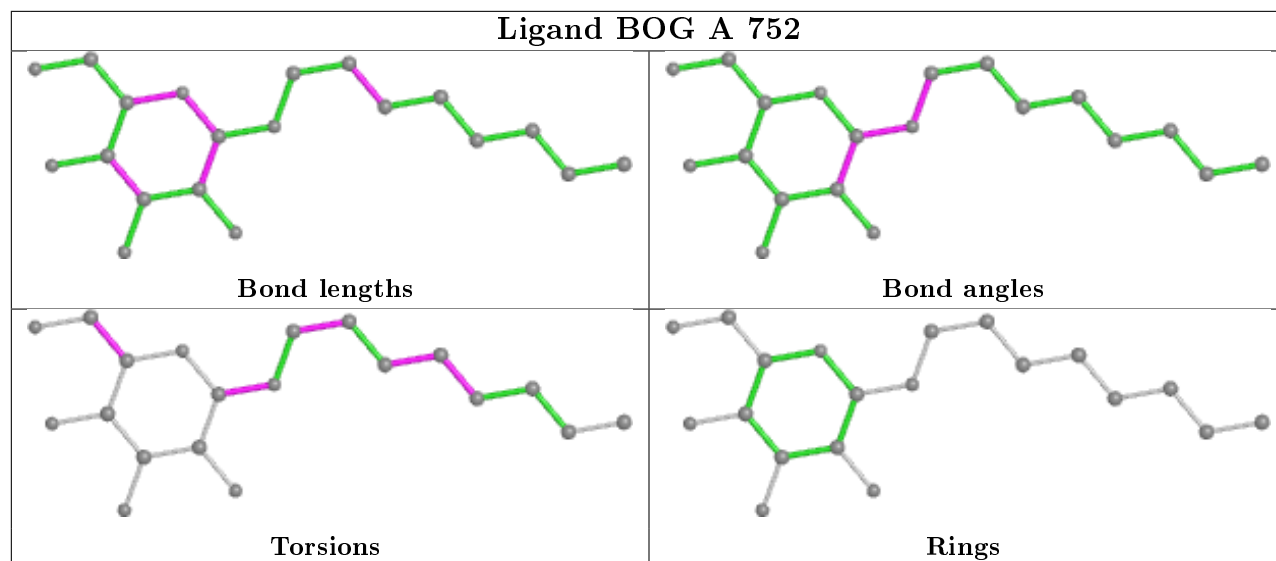


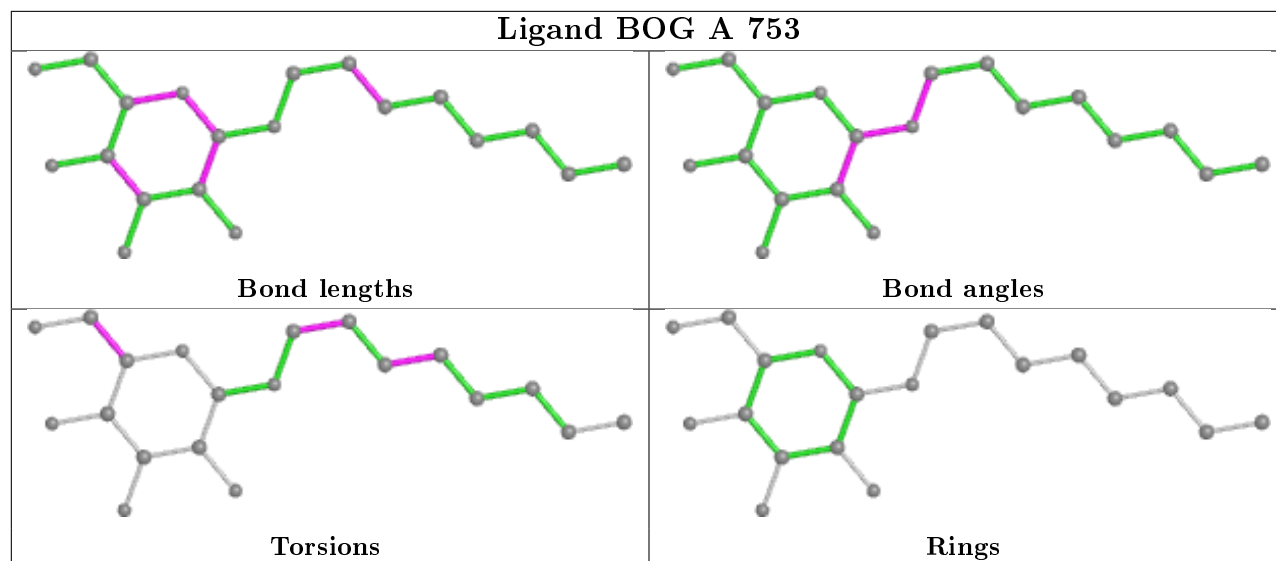
Ligand MNH B 1601



Ligand BOG A 751







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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	553/553 (100%)	0.09	24 (4%)	35	34	20, 30, 43, 53	0
1	B	553/553 (100%)	0.08	19 (3%)	45	44	20, 29, 42, 55	0
All	All	1106/1106 (100%)	0.09	43 (3%)	39	38	20, 29, 42, 55	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TRP	5.8
1	B	1584	ASP	5.5
1	A	107	PHE	5.4
1	A	584	ASP	5.4
1	B	1075	TRP	5.0
1	B	1032	PRO	3.6
1	A	32	PRO	3.5
1	A	75	TRP	3.4
1	B	1033	VAL	3.3
1	A	33	VAL	3.1
1	B	1079	ARG	3.1
1	B	1082	LEU	3.0
1	A	526	GLY	2.8
1	A	514	PRO	2.8
1	A	102	PHE	2.6
1	B	1399	PRO	2.6
1	B	1215	LYS	2.5
1	B	1282	GLN	2.5
1	B	1374	ARG	2.5
1	A	399	PRO	2.4
1	A	277	ARG	2.4
1	A	179	ARG	2.4
1	B	1081	THR	2.3
1	A	169	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	215	LYS	2.3
1	B	1529	PHE	2.3
1	A	374	ARG	2.3
1	A	105	ALA	2.2
1	A	97	ARG	2.2
1	B	1205	PHE	2.2
1	A	79	ARG	2.2
1	B	1507	LEU	2.2
1	A	529	PHE	2.1
1	B	1385	TYR	2.1
1	A	534	LEU	2.1
1	A	575	CYS	2.1
1	A	396	ARG	2.1
1	A	99	LEU	2.1
1	A	381	PHE	2.1
1	B	1074	ILE	2.0
1	B	1384	LEU	2.0
1	B	1381	PHE	2.0
1	B	1398	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

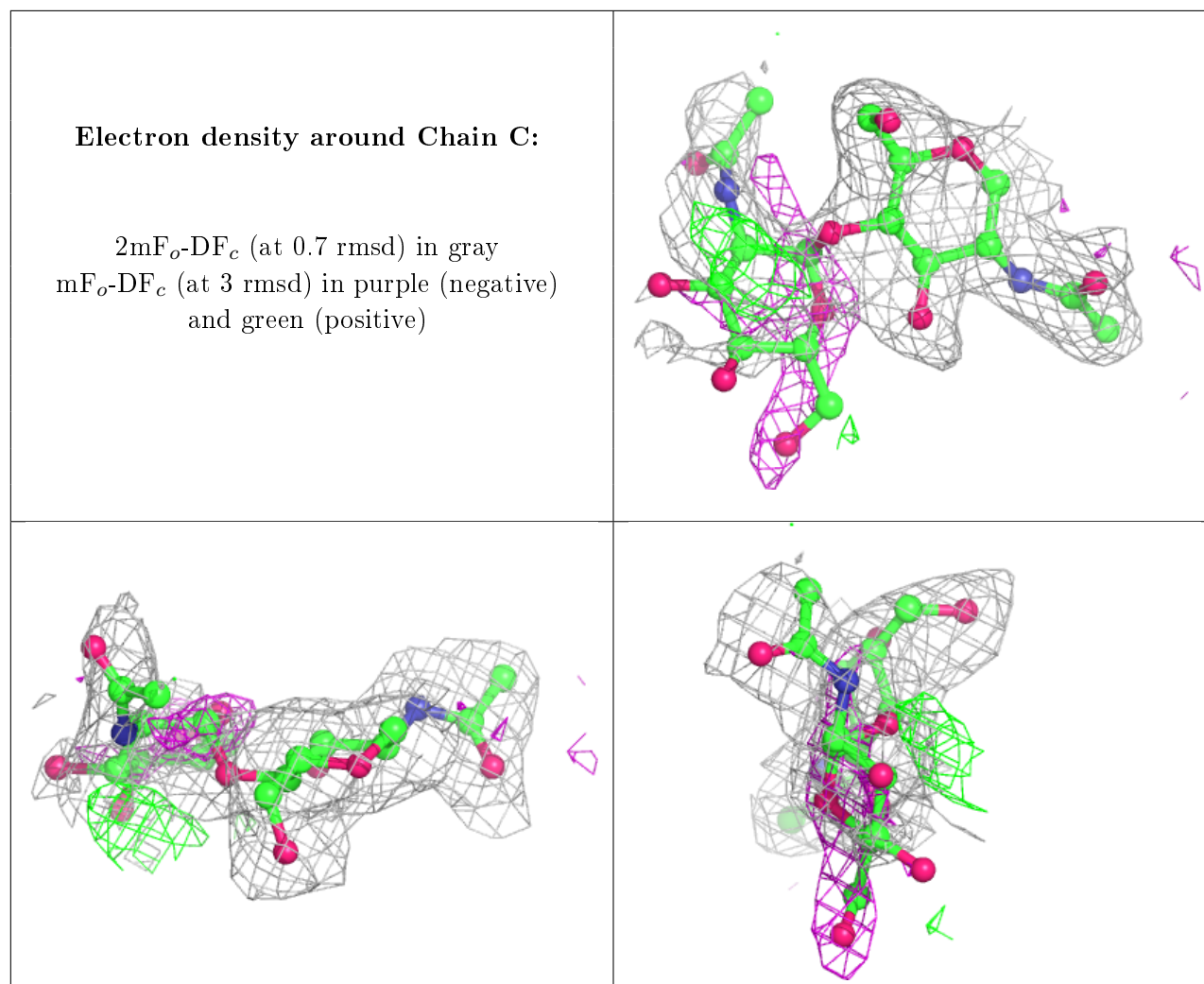
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	G	4	11/12	0.31	0.57	73,75,77,79	0
4	MAN	E	4	11/12	0.38	0.52	80,81,81,81	0
3	MAN	D	4	11/12	0.47	0.51	75,77,78,79	0
2	NAG	C	2	14/15	0.51	0.59	63,65,66,67	0
3	MAN	G	5	11/12	0.51	0.47	80,80,81,81	0
4	MAN	H	4	11/12	0.53	0.57	75,77,77,78	0
3	MAN	D	3	11/12	0.59	0.45	62,66,70,73	0
4	MAN	H	3	11/12	0.63	0.39	62,66,69,73	0
3	NAG	D	2	14/15	0.67	0.25	45,48,52,57	0

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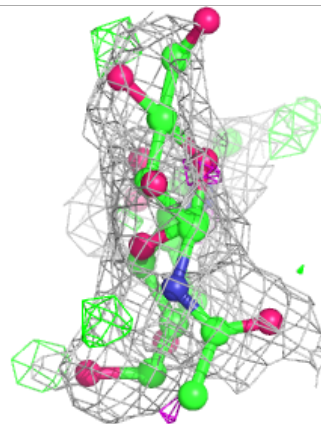
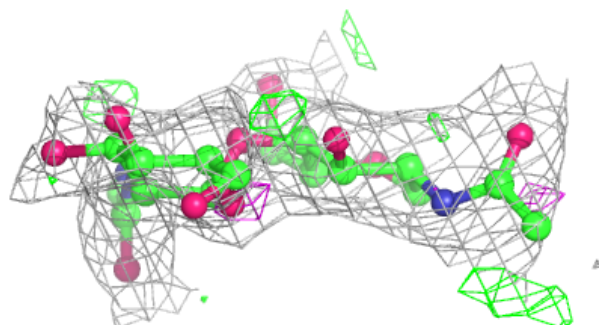
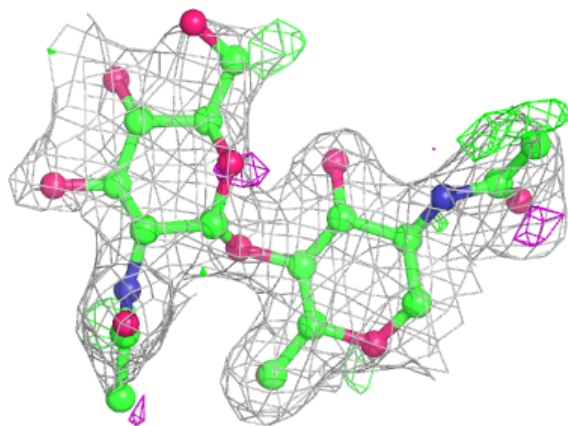
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	E	3	11/12	0.69	0.57	69,72,75,78	0
3	MAN	G	3	11/12	0.70	0.40	59,62,66,70	0
2	NAG	F	2	14/15	0.75	0.41	59,61,62,62	0
4	NAG	E	2	14/15	0.75	0.22	53,56,60,65	0
3	MAN	D	5	11/12	0.78	0.44	79,79,79,80	0
3	NAG	G	2	14/15	0.79	0.23	42,45,48,54	0
2	NAG	C	1	14/15	0.81	0.17	47,51,54,59	0
2	NAG	F	1	14/15	0.84	0.23	48,51,53,57	0
4	NAG	H	2	14/15	0.88	0.15	44,46,51,57	0
4	NAG	E	1	14/15	0.90	0.10	40,42,45,50	0
3	NAG	D	1	14/15	0.93	0.10	28,29,33,39	0
4	NAG	H	1	14/15	0.94	0.07	33,35,38,41	0
3	NAG	G	1	14/15	0.94	0.10	25,26,30,35	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



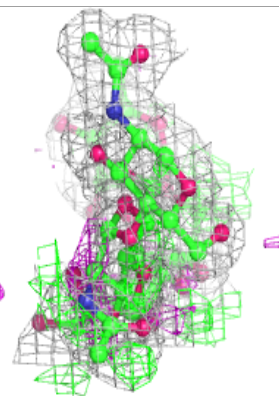
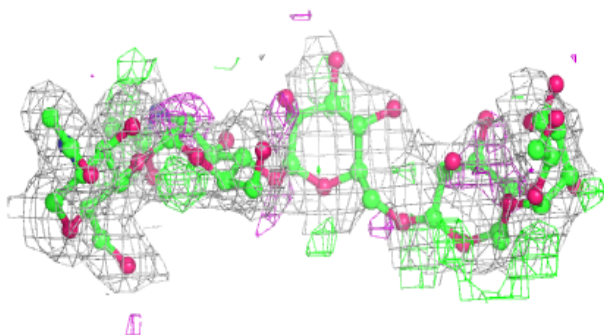
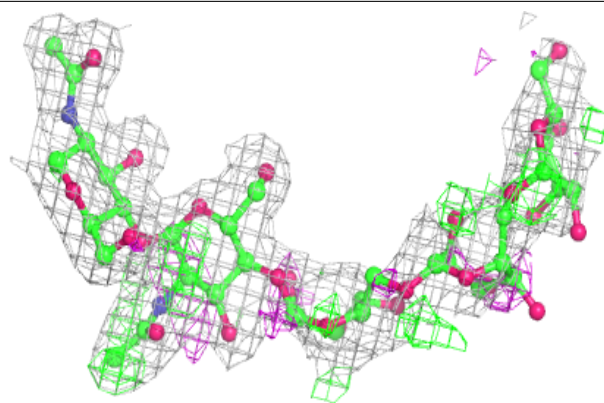
Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

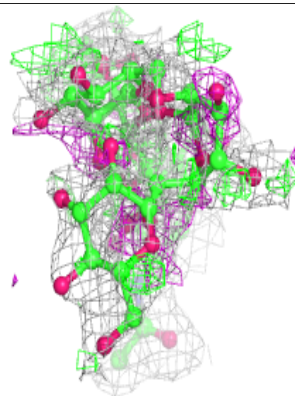
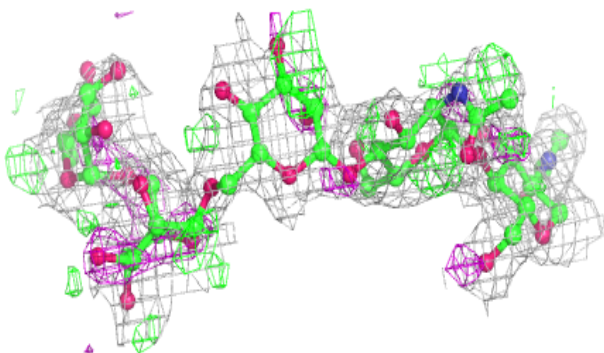
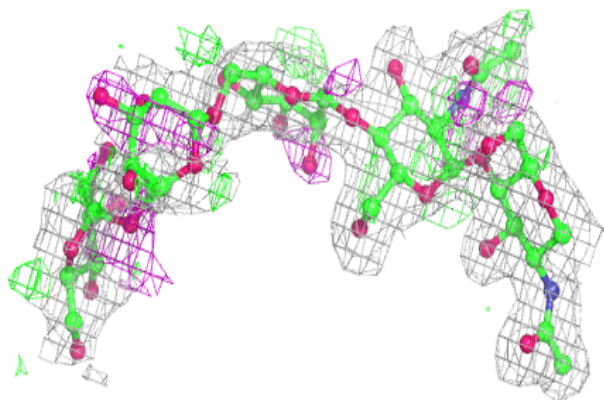


Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

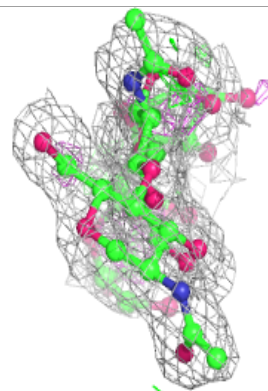
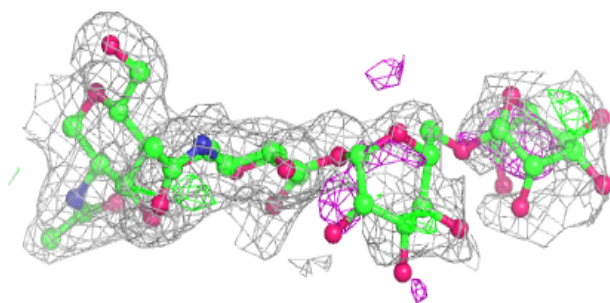
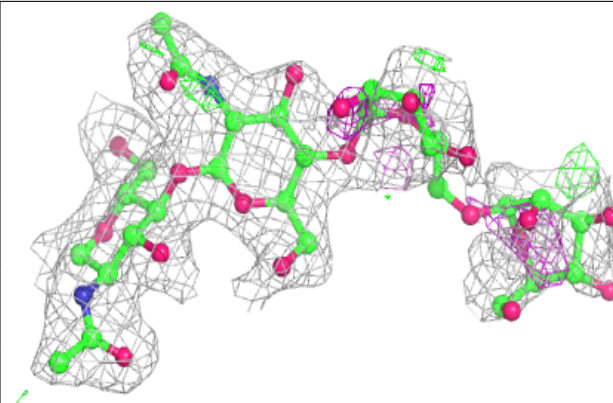
**Electron density around Chain G:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

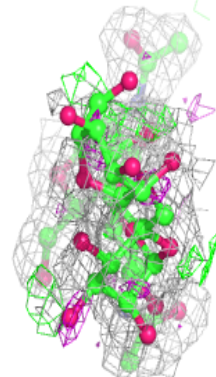
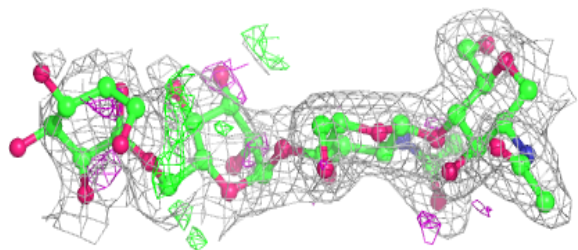
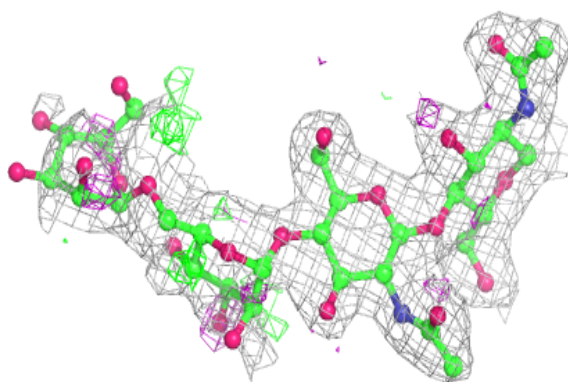


Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain H:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands ⓘ

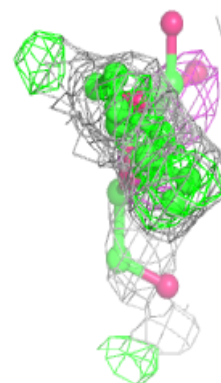
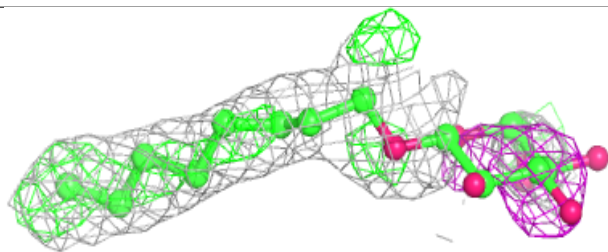
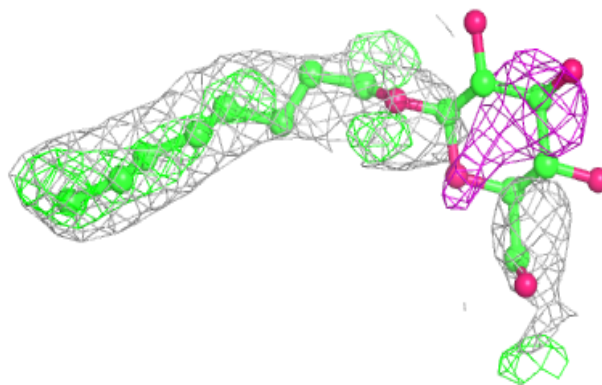
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BOG	A	752	20/20	0.04	0.52	94,101,102,102	0
5	BOG	A	754	20/20	0.32	0.54	96,99,99,100	0
5	BOG	B	1753	20/20	0.44	0.49	90,94,95,95	0
8	GOL	B	1760	6/6	0.55	0.36	66,67,67,68	0
5	BOG	B	1751	20/20	0.57	0.32	77,80,81,81	0
5	BOG	A	753	20/20	0.70	0.25	63,67,68,69	0
5	BOG	B	1750	20/20	0.72	0.40	84,84,89,89	0
5	BOG	A	751	20/20	0.73	0.26	69,70,71,71	0
8	GOL	A	760	6/6	0.76	0.20	61,62,62,63	0
8	GOL	A	758	6/6	0.78	0.28	38,44,45,45	0
8	GOL	B	1759	6/6	0.80	0.21	36,39,41,46	0
8	GOL	A	759	6/6	0.80	0.22	43,45,47,47	0
7	MNH	A	601	43/43	0.88	0.17	32,37,42,44	0
6	FLP	A	1701[B]	18/18	0.89	0.17	35,36,37,37	18
6	FLP	B	2701[B]	18/18	0.89	0.18	37,38,38,38	18
6	FLP	A	1701[A]	18/18	0.89	0.17	29,29,30,31	18
6	FLP	B	2701[A]	18/18	0.89	0.18	25,26,27,27	18
7	MNH	B	1601	43/43	0.90	0.16	32,36,42,44	0

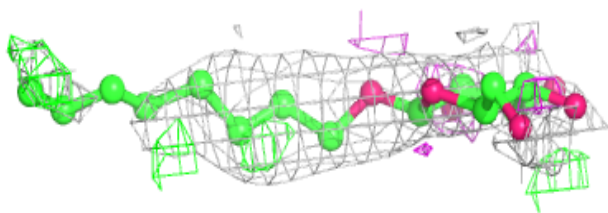
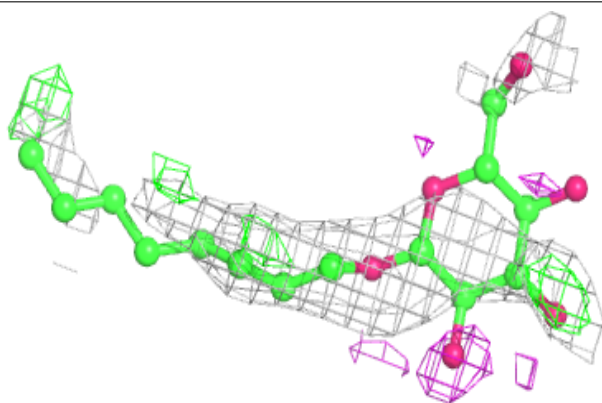
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BOG A 752:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

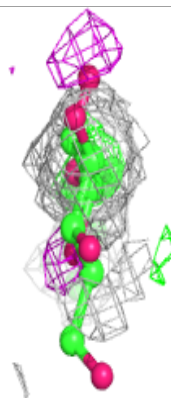
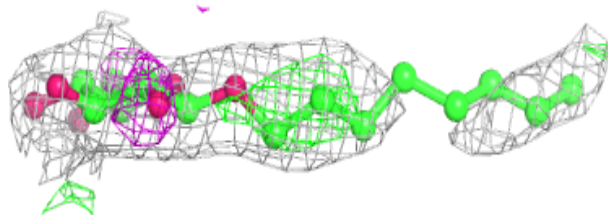
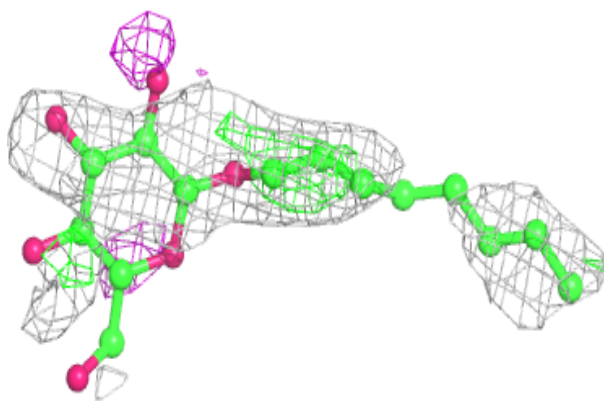
**Electron density around BOG A 754:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

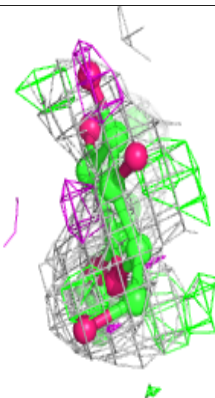
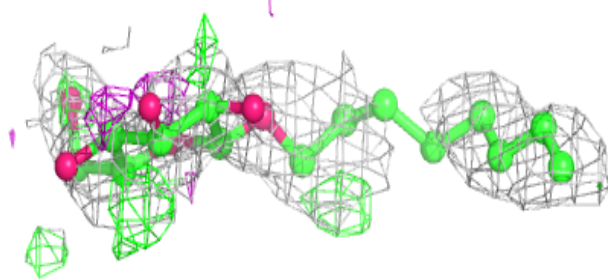
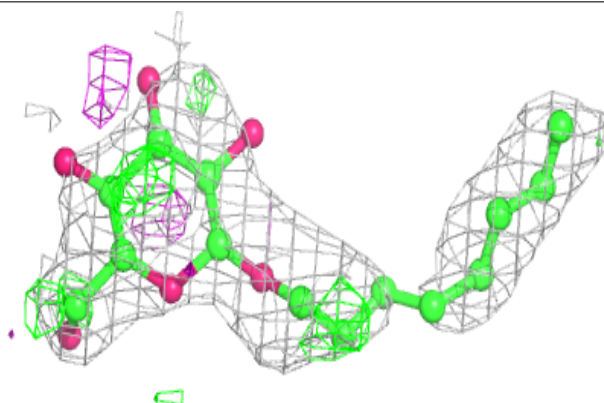


Electron density around BOG B 1753:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

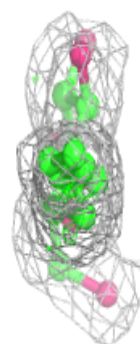
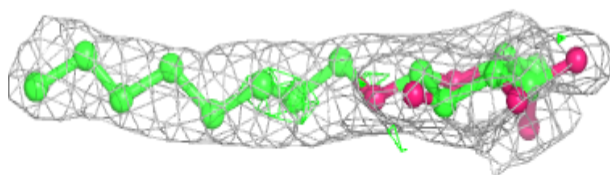
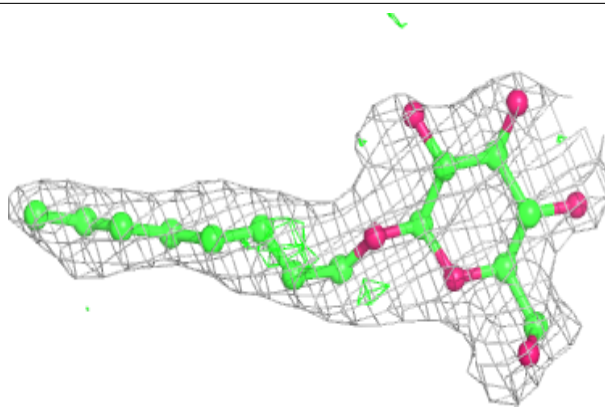
**Electron density around BOG B 1751:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

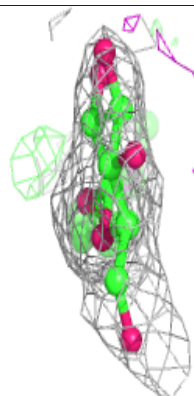
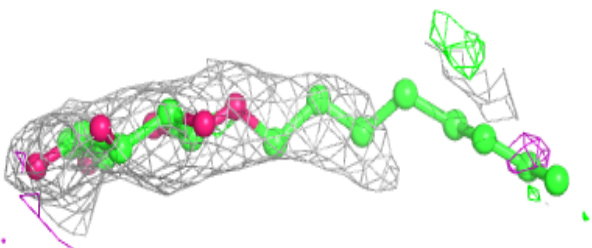
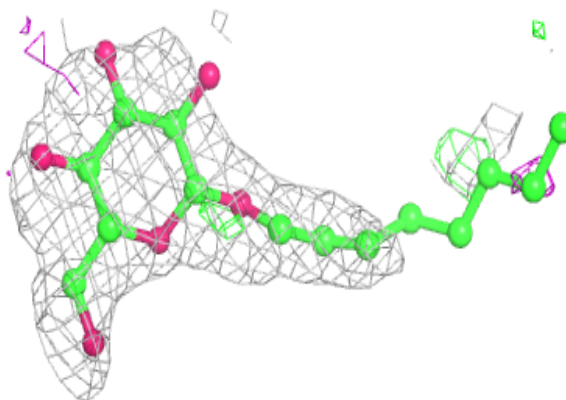


Electron density around BOG A 753:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

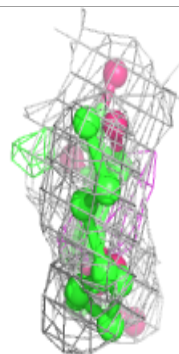
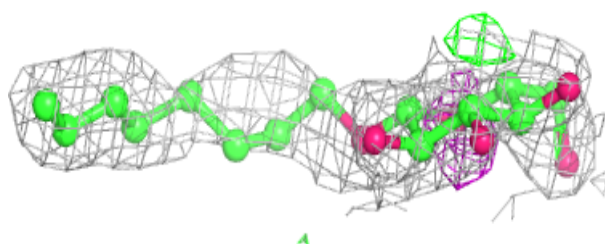
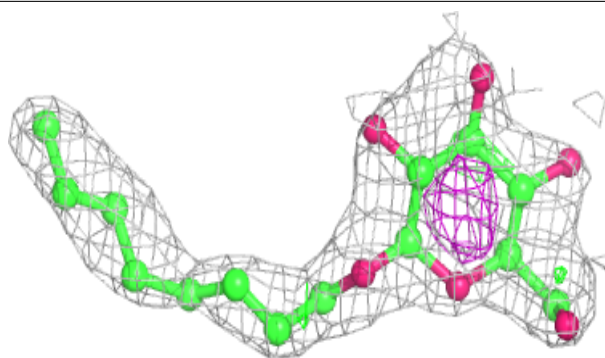
**Electron density around BOG B 1750:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



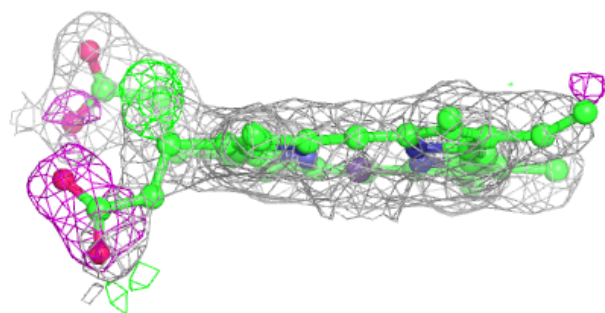
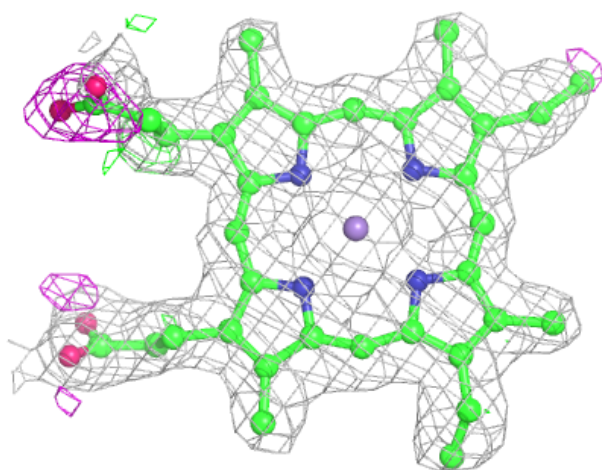
Electron density around BOG A 751:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



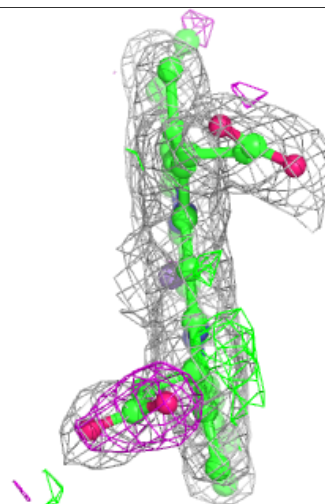
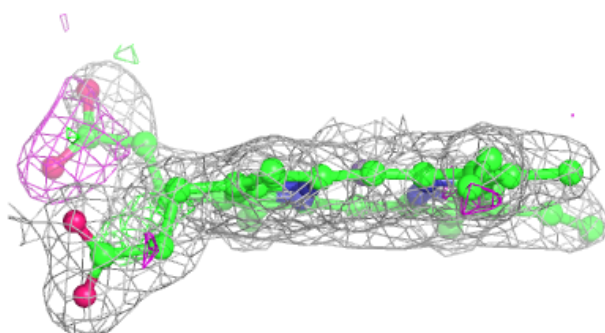
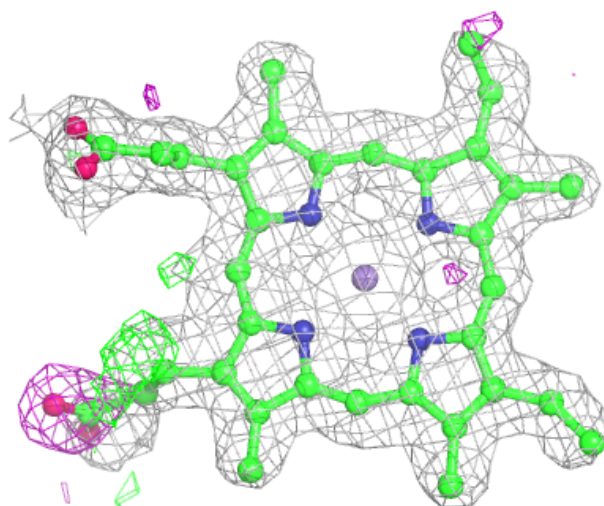
Electron density around MNH A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MNH B 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.