



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:08 PM UTC

PDB ID : 8YUI / pdb_00008yui
Title : X-ray Crystal structure of glycoside hydrolase family 18 chitinase from *Serratia marcescens* hexahistidine-tagged SmChiB with triacetyl chitotriose
Authors : Ebi, S.; Sunagawa, N.; Yamaguchi, S.; Igarashi, K.
Deposited on : 2024-03-27
Resolution : 1.43 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 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

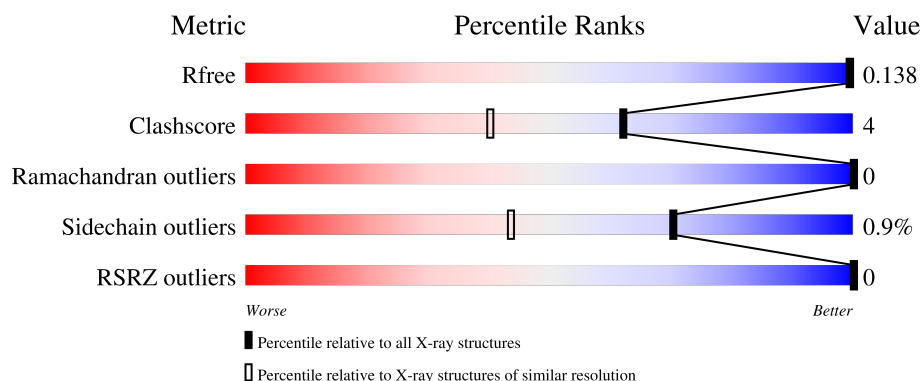
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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}	180053	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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 of 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	511	 90% 7%
1	B	511	 91% 6%
2	C	2	 50% 50%
2	D	2	 50% 50%

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
3	GOL	A	634	-	-	X	-
3	GOL	B	613	-	-	X	-
3	GOL	B	646	-	-	X	-
4	NGO	A	610	-	-	X	-
5	ACT	A	630	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10766 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 Chitinase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	45	0
			4287	2731	724	807	25			
1	B	498	Total	C	N	O	S	0	49	0
			4308	2744	729	811	24			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P11797
A	1	ASP	-	expression tag	UNP P11797
A	500	ALA	-	expression tag	UNP P11797
A	501	ALA	-	expression tag	UNP P11797
A	502	ALA	-	expression tag	UNP P11797
A	503	LEU	-	expression tag	UNP P11797
A	504	GLU	-	expression tag	UNP P11797
A	505	HIS	-	expression tag	UNP P11797
A	506	HIS	-	expression tag	UNP P11797
A	507	HIS	-	expression tag	UNP P11797
A	508	HIS	-	expression tag	UNP P11797
A	509	HIS	-	expression tag	UNP P11797
A	510	HIS	-	expression tag	UNP P11797
B	0	MET	-	initiating methionine	UNP P11797
B	1	ASP	-	expression tag	UNP P11797
B	500	ALA	-	expression tag	UNP P11797
B	501	ALA	-	expression tag	UNP P11797
B	502	ALA	-	expression tag	UNP P11797
B	503	LEU	-	expression tag	UNP P11797
B	504	GLU	-	expression tag	UNP P11797
B	505	HIS	-	expression tag	UNP P11797
B	506	HIS	-	expression tag	UNP P11797
B	507	HIS	-	expression tag	UNP P11797
B	508	HIS	-	expression tag	UNP P11797
B	509	HIS	-	expression tag	UNP P11797

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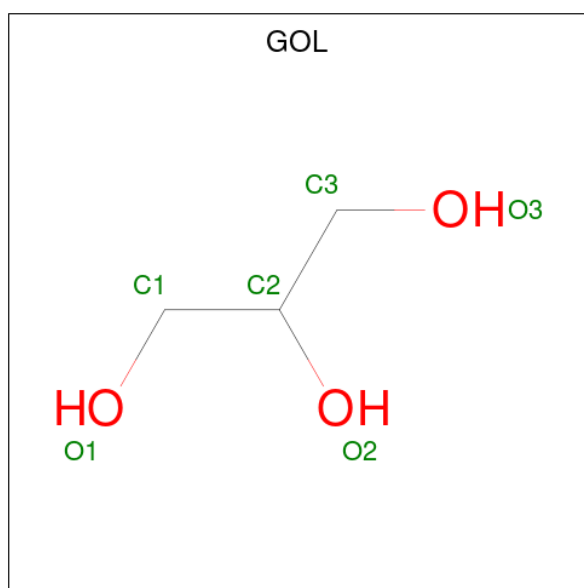
Chain	Residue	Modelled	Actual	Comment	Reference
B	510	HIS	-	expression tag	UNP P11797

- 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
			29	16	2	11			
2	D	2	Total	C	N	O	0	0	0
			29	16	2	11			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

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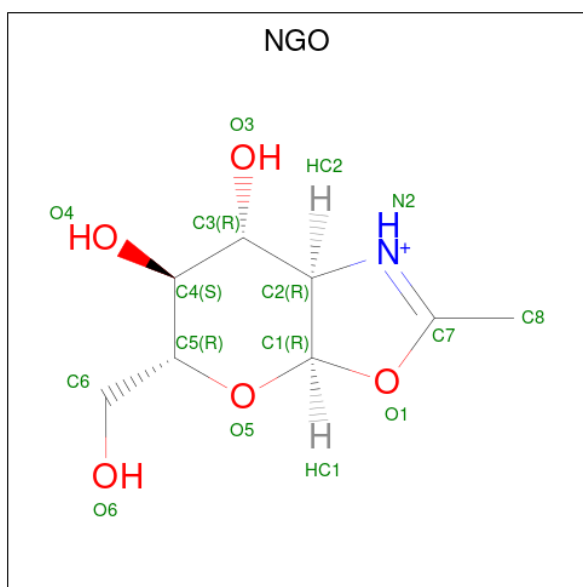
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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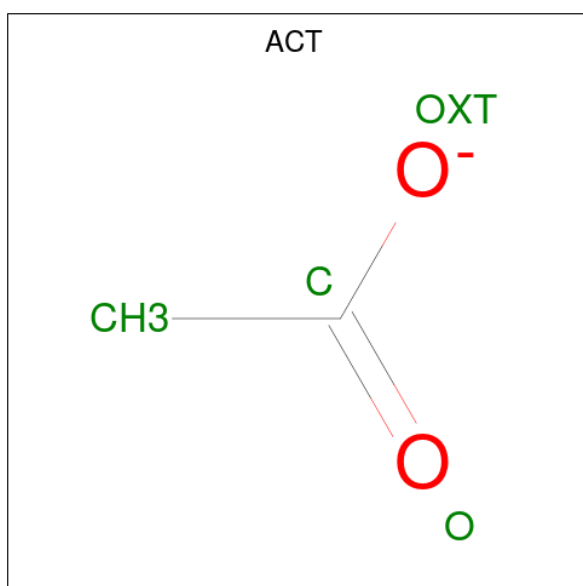
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

- Molecule 4 is 2-METHYL-4,5-DIHYDRO-(1,2-DIDEOXY-ALPHA-D-GLUCOPYRANO SO)[2,1-D]-1,3-OXAZOLE (CCD ID: NGO) (formula: C₈H₁₄NO₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



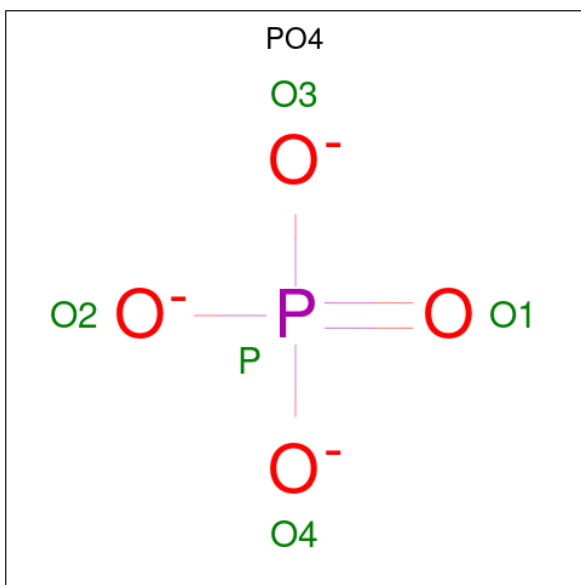
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	800	Total	O	0	0
			800	800		
7	B	781	Total	O	0	0
			781	781		

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.

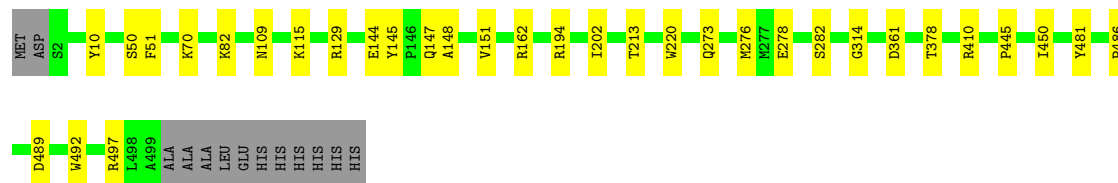
- Molecule 1: Chitinase B

Chain A: 



- Molecule 1: Chitinase B

Chain B: 



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

Chain C: 



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.38Å 97.38Å 197.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.69 – 1.43 48.69 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.69-1.43) 99.9 (48.69-1.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.43Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.124 , 0.138 0.125 , 0.138	Depositor DCC
R_{free} test set	2008 reflections (0.58%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.488 for k,h,-l	Xtriage
F_o, F_c correlation	0.99	EDS
Total number of atoms	10766	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ACT, NAG, GOL, NGO

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	0.25	0/4399	0.48	0/5981
1	B	0.25	0/4429	0.47	0/6022
All	All	0.25	0/8828	0.48	0/12003

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4287	0	4098	32	0
1	B	4308	0	4126	32	0
2	C	29	0	27	1	0
2	D	29	0	27	2	0
3	A	204	0	270	17	0
3	B	192	0	253	17	0
4	A	14	0	14	6	0
4	B	14	0	14	3	0
5	A	44	0	33	2	0
5	B	44	0	33	1	0
6	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	0	0	0
7	A	800	0	0	6	0
7	B	781	0	0	6	0
All	All	10766	0	8895	74	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 (74) 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:A:282:SER:H	3:A:628:GOL:H31	1.24	1.02
1:B:282:SER:H	3:B:646:GOL:H31	1.38	0.88
1:B:162:ARG:HG3	3:B:621:GOL:H12	1.65	0.77
1:A:162:ARG:HG3	3:A:617:GOL:H12	1.67	0.77
1:B:145:TYR:OH	2:D:1:NAG:H81	1.86	0.75
1:B:194:ARG:HG2	3:B:613:GOL:H32	1.70	0.72
1:A:145:TYR:OH	2:C:1:NAG:H81	1.90	0.72
1:A:194:ARG:HG2	3:A:634:GOL:H11	1.71	0.71
1:A:470:TYR:HA	3:A:608:GOL:H2	1.77	0.66
1:B:314:GLY:H	3:B:603:GOL:H2	1.61	0.65
1:A:450[A]:ILE:HD13	1:A:497:ARG:HG3	1.82	0.62
1:B:109:ASN:HD21	3:B:642:GOL:H32	1.64	0.62
1:B:450:ILE:HD13	1:B:497[A]:ARG:HG3	1.81	0.62
4:A:610:NGO:HC61	3:A:629:GOL:H2	1.82	0.59
3:B:646:GOL:H32	7:B:1007:HOH:O	2.04	0.58
1:B:82[B]:LYS:NZ	7:B:709:HOH:O	2.36	0.58
1:A:489:ASP:HB2	3:B:613:GOL:H2	1.85	0.58
1:A:148[B]:ALA:HB2	3:A:634:GOL:H12	1.84	0.57
3:A:634:GOL:H2	1:B:489:ASP:HB2	1.86	0.57
1:B:314:GLY:N	3:B:603:GOL:H2	2.19	0.57
1:B:147[A]:GLN:O	1:B:151:VAL:HG23	2.05	0.57
1:A:147[B]:GLN:O	1:A:151:VAL:HG23	2.05	0.56
1:A:278[A]:GLU:HG3	1:A:445:PRO:HB2	1.88	0.55
1:A:10:TYR:OH	4:A:610:NGO:HC82	2.06	0.55
1:A:10:TYR:CZ	4:A:610:NGO:HC82	2.43	0.54
1:A:347:GLN:OE1	3:A:619:GOL:H32	2.07	0.54
1:B:10:TYR:CZ	4:B:611:NGO:HC82	2.44	0.53
3:A:628:GOL:H32	7:A:1017:HOH:O	2.08	0.53
1:B:278[B]:GLU:HG3	1:B:445:PRO:HB2	1.91	0.53
1:B:282:SER:H	3:B:646:GOL:C3	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115[B]:LYS:NZ	7:B:715:HOH:O	2.44	0.51
1:B:109:ASN:HD21	3:B:642:GOL:C3	2.24	0.50
1:B:220:TRP:CD1	3:B:623:GOL:H2	2.47	0.50
1:A:162:ARG:HG3	3:A:617:GOL:C1	2.40	0.49
1:A:349[B]:LEU:HD21	1:A:368:LEU:HD22	1.93	0.49
3:A:622:GOL:O1	3:A:622:GOL:O3	2.19	0.49
1:B:148[A]:ALA:HB2	3:B:613:GOL:H31	1.93	0.49
1:B:129[A]:ARG:NH2	5:B:638:ACT:O	2.35	0.49
1:A:212[A]:MET:SD	4:A:610:NGO:HC1	2.53	0.48
1:A:273:GLN:HA	1:A:276[A]:MET:HE2	1.95	0.48
1:B:194:ARG:HA	3:B:613:GOL:H12	1.96	0.48
1:A:212[B]:MET:SD	4:A:610:NGO:HC1	2.54	0.48
5:A:630:ACT:H3	7:A:1120:HOH:O	2.13	0.47
1:B:162:ARG:HG3	3:B:621:GOL:C1	2.39	0.47
1:A:82[B]:LYS:NZ	7:A:718:HOH:O	2.48	0.46
4:B:611:NGO:HC2	7:B:821:HOH:O	2.15	0.46
1:B:273:GLN:HA	1:B:276[A]:MET:HE2	1.97	0.46
1:A:194:ARG:HA	3:A:634:GOL:H31	1.97	0.46
1:B:361[B]:ASP:OD1	3:B:615:GOL:O2	2.27	0.46
1:B:282:SER:N	3:B:646:GOL:H31	2.19	0.46
1:A:94[B]:ILE:HD12	1:A:141[B]:ILE:HD13	1.98	0.46
1:A:91[B]:MET:HE3	1:A:91[B]:MET:HB3	1.72	0.46
1:B:144:GLU:HA	1:B:145:TYR:CG	2.52	0.45
1:A:353:TYR:CZ	3:A:609:GOL:H11	2.51	0.45
1:A:454:PRO:HG2	7:A:1109:HOH:O	2.16	0.44
1:A:144:GLU:HA	1:A:145:TYR:CG	2.52	0.44
1:A:60[B]:CYS:SG	1:A:94[B]:ILE:HD13	2.57	0.44
1:A:282:SER:N	3:A:628:GOL:H31	2.09	0.44
1:A:450[B]:ILE:HD13	1:A:497:ARG:HG3	1.99	0.44
1:B:10:TYR:OH	4:B:611:NGO:HC82	2.18	0.43
1:B:410:ARG:NH2	3:B:610:GOL:H11	2.34	0.43
2:D:1:NAG:O1	2:D:1:NAG:H83	2.19	0.42
1:B:273:GLN:HA	1:B:276[B]:MET:HE2	2.02	0.42
1:B:486:PRO:HA	1:B:492:TRP:CD1	2.54	0.42
1:A:129[A]:ARG:HD3	7:A:761:HOH:O	2.18	0.41
1:A:212[B]:MET:SD	4:A:610:NGO:HC83	2.60	0.41
1:B:50:SER:HA	1:B:51:PHE:HA	1.81	0.41
3:A:645:GOL:H12	7:B:1222:HOH:O	2.21	0.41
5:A:630:ACT:H2	1:B:481:TYR:HD2	1.86	0.41
3:A:637:GOL:H11	7:A:767:HOH:O	2.20	0.41
1:B:70[A]:LYS:HA	1:B:70[A]:LYS:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PRO:HA	1:A:492:TRP:CD1	2.55	0.41
1:A:196:TYR:O	1:A:277[A]:MET:HE2	2.21	0.41
3:A:645:GOL:H32	7:B:1070:HOH:O	2.21	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	542/511 (106%)	532 (98%)	10 (2%)	0	100	100
1	B	545/511 (107%)	533 (98%)	12 (2%)	0	100	100
All	All	1087/1022 (106%)	1065 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	445/412 (108%)	439 (99%)	6 (1%)	61	29
1	B	449/412 (109%)	445 (99%)	4 (1%)	70	44
All	All	894/824 (108%)	884 (99%)	10 (1%)	70	35

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70[A]	LYS
1	A	70[B]	LYS
1	A	213	THR
1	A	223[A]	ILE
1	A	223[B]	ILE
1	A	378	THR
1	B	202[A]	ILE
1	B	202[B]	ILE
1	B	213	THR
1	B	378	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	201	GLN
1	B	16	ASN
1	B	201	GLN
1	B	350	GLN
1	B	423	ASN

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 ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2	15,15,15	0.24	0	21,21,21	0.70	0
2	NAG	C	2	2	14,14,15	0.29	0	17,19,21	0.37	0
2	NAG	D	1	2	15,15,15	0.28	0	21,21,21	0.72	0
2	NAG	D	2	2	14,14,15	0.34	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	3/6/26/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2	-	2/6/26/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

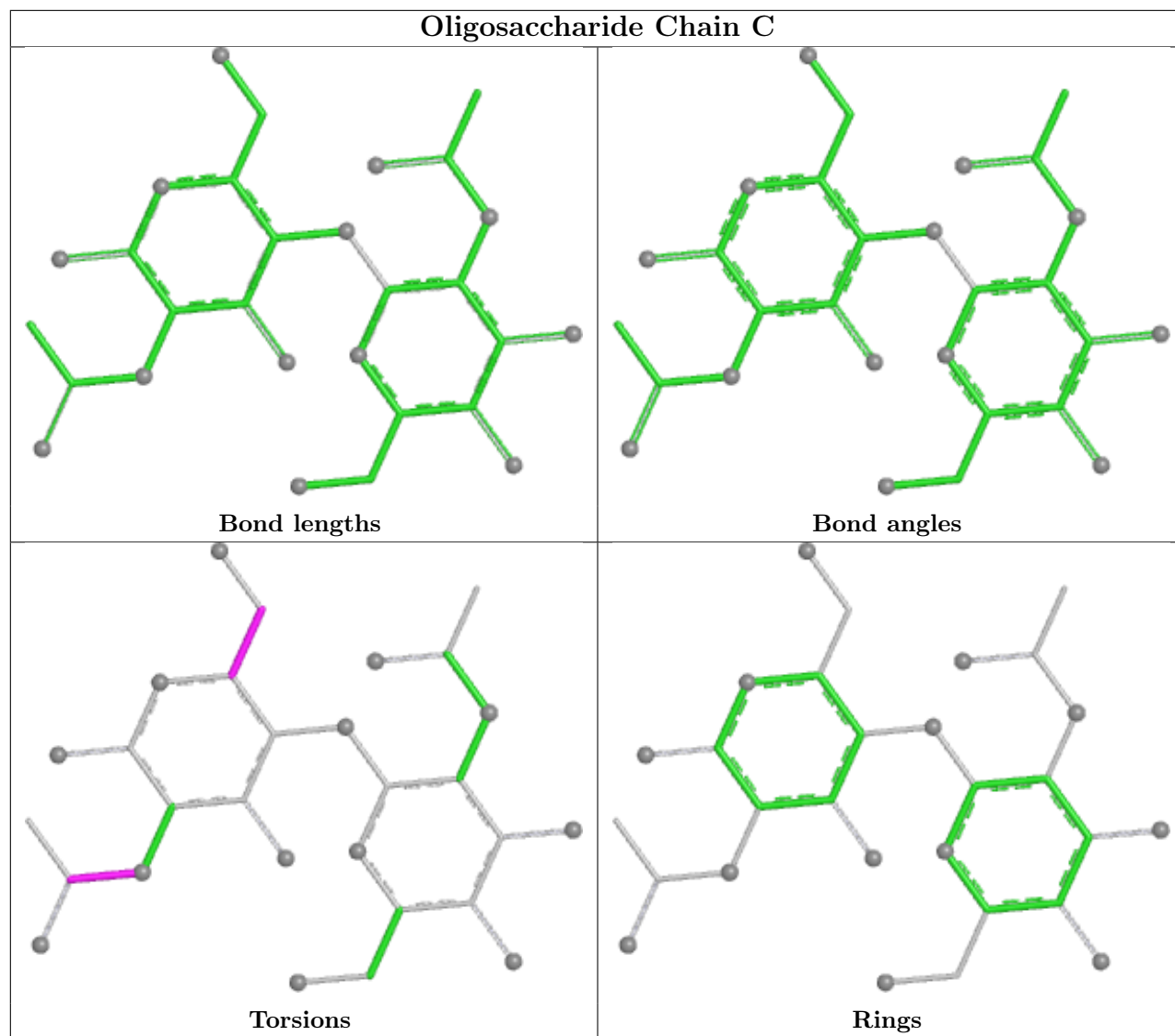
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6

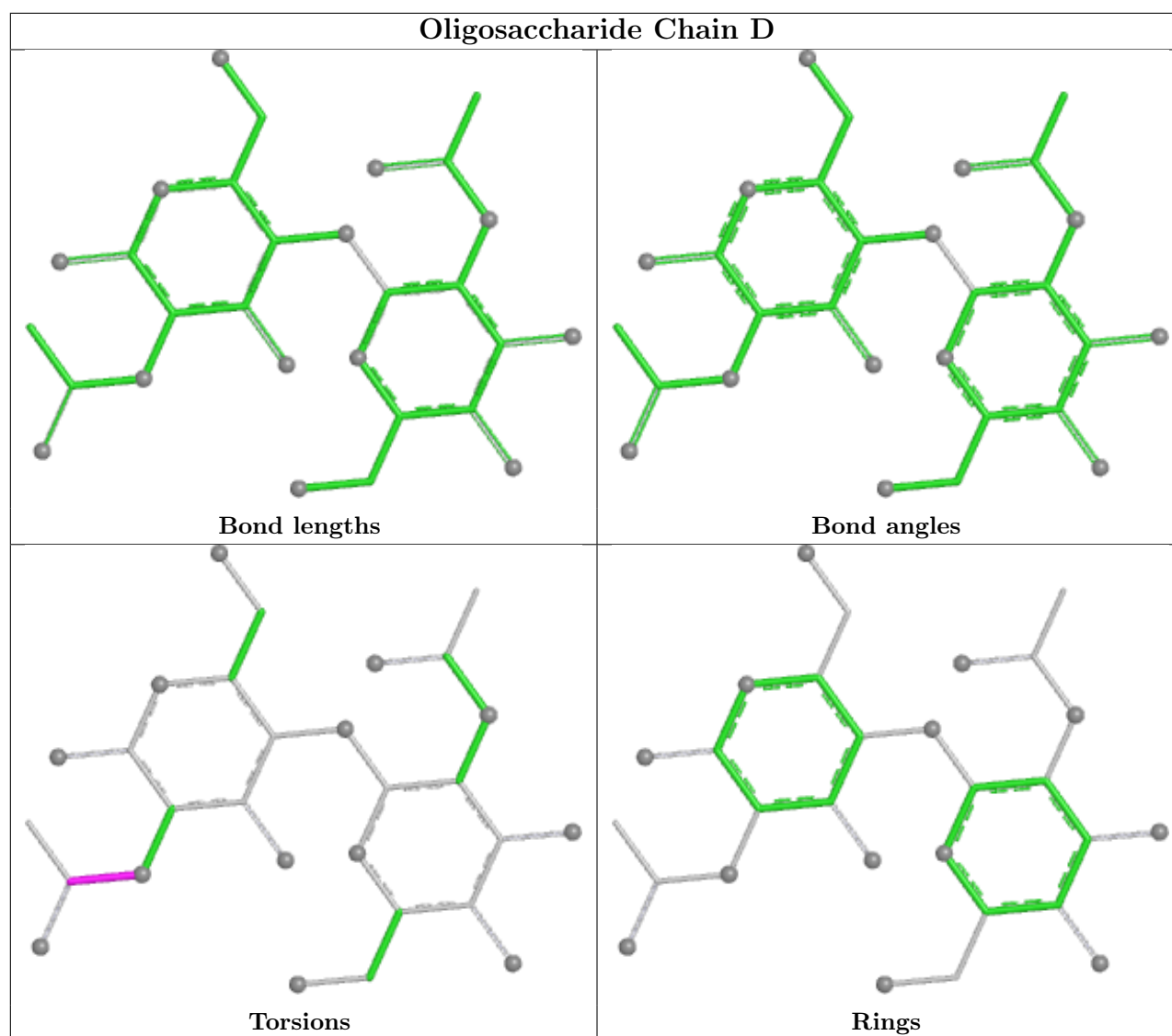
There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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





5.6 Ligand geometry [i](#)

94 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	$\# Z > 2$
3	GOL	B	601	-	5,5,5	0.71	0	5,5,5	1.00	0
3	GOL	B	615	-	5,5,5	0.86	0	5,5,5	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	618	-	5,5,5	0.72	0	5,5,5	1.09	0
4	NGO	B	611	-	14,15,15	0.75	0	15,22,22	1.51	2 (13%)
3	GOL	B	622	-	5,5,5	1.07	0	5,5,5	1.07	0
6	PO4	A	646	-	4,4,4	0.94	0	6,6,6	0.50	0
3	GOL	B	612	-	5,5,5	0.85	0	5,5,5	1.13	1 (20%)
3	GOL	A	615	-	5,5,5	0.93	0	5,5,5	1.15	1 (20%)
3	GOL	A	636	-	5,5,5	1.00	0	5,5,5	1.13	0
3	GOL	B	634	-	5,5,5	0.84	0	5,5,5	1.11	0
3	GOL	A	612	-	5,5,5	0.87	0	5,5,5	1.13	0
3	GOL	A	604	-	5,5,5	1.29	1 (20%)	5,5,5	0.72	0
3	GOL	B	637	-	5,5,5	1.00	0	5,5,5	1.16	0
3	GOL	B	607	-	5,5,5	0.84	0	5,5,5	1.08	0
3	GOL	A	619	-	5,5,5	0.97	0	5,5,5	0.95	0
3	GOL	B	640	-	5,5,5	0.90	0	5,5,5	1.06	0
3	GOL	A	621	-	5,5,5	0.93	0	5,5,5	0.97	0
5	ACT	A	632	-	3,3,3	1.37	0	3,3,3	1.37	0
3	GOL	B	610	-	5,5,5	1.08	0	5,5,5	1.17	1 (20%)
5	ACT	B	636	-	3,3,3	1.43	1 (33%)	3,3,3	1.37	0
3	GOL	B	642	-	5,5,5	1.09	0	5,5,5	1.07	0
3	GOL	A	607	-	5,5,5	0.83	0	5,5,5	1.02	0
5	ACT	B	628	-	3,3,3	1.41	1 (33%)	3,3,3	1.38	0
5	ACT	A	643	-	3,3,3	1.40	1 (33%)	3,3,3	1.36	0
3	GOL	B	625	-	5,5,5	0.91	0	5,5,5	1.13	1 (20%)
3	GOL	A	645	-	5,5,5	0.83	0	5,5,5	1.10	1 (20%)
5	ACT	B	639	-	3,3,3	1.29	0	3,3,3	1.38	0
3	GOL	A	644	-	5,5,5	0.96	0	5,5,5	1.09	0
3	GOL	B	626	-	5,5,5	0.90	0	5,5,5	1.08	0
3	GOL	B	618	-	5,5,5	0.90	0	5,5,5	1.17	1 (20%)
3	GOL	A	616	-	5,5,5	0.99	0	5,5,5	1.06	1 (20%)
3	GOL	B	609	-	5,5,5	1.03	0	5,5,5	1.19	1 (20%)
3	GOL	B	619	-	5,5,5	1.34	1 (20%)	5,5,5	0.70	0
3	GOL	B	621	-	5,5,5	1.45	1 (20%)	5,5,5	1.21	0
3	GOL	B	646	-	5,5,5	0.96	0	5,5,5	0.87	0
5	ACT	B	641	-	3,3,3	1.46	1 (33%)	3,3,3	1.40	0
3	GOL	A	603	-	5,5,5	1.01	0	5,5,5	0.87	0
3	GOL	A	601	-	5,5,5	0.94	0	5,5,5	0.90	0
4	NGO	A	610	-	14,15,15	0.80	0	15,22,22	1.75	3 (20%)
3	GOL	A	617	-	5,5,5	1.45	1 (20%)	5,5,5	1.21	0
5	ACT	B	630	-	3,3,3	1.36	0	3,3,3	1.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	608	-	5,5,5	1.11	0	5,5,5	1.02	0
3	GOL	A	637	-	5,5,5	0.95	0	5,5,5	1.02	0
3	GOL	B	633	-	5,5,5	0.98	0	5,5,5	1.00	0
3	GOL	A	613	-	5,5,5	0.87	0	5,5,5	1.12	0
3	GOL	B	613	-	5,5,5	0.91	0	5,5,5	1.16	1 (20%)
5	ACT	A	641	-	3,3,3	1.37	0	3,3,3	1.36	0
5	ACT	A	630	-	3,3,3	1.31	0	3,3,3	1.40	0
3	GOL	A	606	-	5,5,5	0.85	0	5,5,5	1.11	1 (20%)
5	ACT	A	627	-	3,3,3	1.40	1 (33%)	3,3,3	1.38	0
3	GOL	B	624	-	5,5,5	0.88	0	5,5,5	1.13	0
5	ACT	B	631	-	3,3,3	1.36	1 (33%)	3,3,3	1.40	0
3	GOL	A	628	-	5,5,5	0.94	0	5,5,5	0.89	0
3	GOL	A	622	-	5,5,5	1.09	0	5,5,5	1.01	0
5	ACT	B	638	-	3,3,3	1.41	1 (33%)	3,3,3	1.31	0
3	GOL	A	614	-	5,5,5	0.94	0	5,5,5	0.91	0
3	GOL	A	624	-	5,5,5	0.96	0	5,5,5	1.06	0
5	ACT	A	648	-	3,3,3	1.46	1 (33%)	3,3,3	1.37	0
5	ACT	A	640	-	3,3,3	1.46	1 (33%)	3,3,3	1.30	0
3	GOL	A	638	-	5,5,5	0.80	0	5,5,5	1.01	0
5	ACT	B	635	-	3,3,3	1.40	1 (33%)	3,3,3	1.36	0
6	PO4	B	644	-	4,4,4	0.91	0	6,6,6	0.47	0
3	GOL	B	602	-	5,5,5	0.93	0	5,5,5	1.11	0
3	GOL	A	626	-	5,5,5	1.04	0	5,5,5	0.97	0
3	GOL	B	620	-	5,5,5	0.89	0	5,5,5	1.01	0
3	GOL	B	605	-	5,5,5	0.91	0	5,5,5	0.90	0
3	GOL	A	623	-	5,5,5	1.08	1 (20%)	5,5,5	1.01	0
5	ACT	B	643	-	3,3,3	1.46	1 (33%)	3,3,3	1.33	0
6	PO4	B	608	-	4,4,4	0.93	0	6,6,6	0.45	0
5	ACT	A	635	-	3,3,3	1.32	0	3,3,3	1.40	0
3	GOL	A	602	-	5,5,5	0.84	0	5,5,5	1.07	0
3	GOL	B	627	-	5,5,5	1.08	1 (20%)	5,5,5	1.00	0
3	GOL	B	629	-	5,5,5	0.97	0	5,5,5	1.08	0
3	GOL	B	603	-	5,5,5	0.94	0	5,5,5	1.59	1 (20%)
5	ACT	A	639	-	3,3,3	1.35	0	3,3,3	1.34	0
6	PO4	A	647	-	4,4,4	0.96	0	6,6,6	0.47	0
3	GOL	A	620	-	5,5,5	0.95	0	5,5,5	1.02	0
3	GOL	A	605	-	5,5,5	0.92	0	5,5,5	1.16	1 (20%)
3	GOL	B	606	-	5,5,5	0.83	0	5,5,5	1.08	0
5	ACT	A	631	-	3,3,3	1.31	1 (33%)	3,3,3	1.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	634	-	5,5,5	0.88	0	5,5,5	1.14	1 (20%)
5	ACT	A	633	-	3,3,3	1.40	0	3,3,3	1.36	0
3	GOL	A	611	-	5,5,5	0.90	0	5,5,5	1.12	0
3	GOL	B	617	-	5,5,5	0.99	0	5,5,5	1.00	0
3	GOL	A	609	-	5,5,5	0.90	0	5,5,5	1.02	0
3	GOL	A	629	-	5,5,5	1.09	0	5,5,5	1.03	0
3	GOL	B	604	-	5,5,5	0.80	0	5,5,5	1.10	0
3	GOL	A	642	-	5,5,5	0.92	0	5,5,5	1.07	0
5	ACT	B	645	-	3,3,3	1.30	0	3,3,3	1.40	0
3	GOL	A	625	-	5,5,5	1.00	0	5,5,5	0.99	0
3	GOL	B	623	-	5,5,5	0.80	0	5,5,5	1.16	0
5	ACT	B	632	-	3,3,3	1.50	0	3,3,3	1.37	0
3	GOL	B	614	-	5,5,5	0.88	0	5,5,5	1.14	0
3	GOL	B	616	-	5,5,5	0.90	0	5,5,5	0.97	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
3	GOL	B	601	-	-	0/4/4/4	-
3	GOL	B	605	-	-	0/4/4/4	-
3	GOL	B	620	-	-	0/4/4/4	-
3	GOL	B	621	-	-	4/4/4/4	-
3	GOL	B	615	-	-	1/4/4/4	-
3	GOL	A	618	-	-	2/4/4/4	-
3	GOL	A	623	-	-	2/4/4/4	-
3	GOL	B	642	-	-	4/4/4/4	-
4	NGO	B	611	-	-	2/2/30/30	0/2/2/2
3	GOL	B	612	-	-	0/4/4/4	-
3	GOL	B	622	-	-	0/4/4/4	-
3	GOL	A	607	-	-	1/4/4/4	-
3	GOL	A	606	-	-	0/4/4/4	-
3	GOL	B	625	-	-	0/4/4/4	-
3	GOL	A	645	-	-	3/4/4/4	-
3	GOL	A	644	-	-	2/4/4/4	-
3	GOL	A	602	-	-	1/4/4/4	-
3	GOL	B	624	-	-	0/4/4/4	-
3	GOL	B	626	-	-	0/4/4/4	-
3	GOL	B	627	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	629	-	-	2/4/4/4	-
3	GOL	B	618	-	-	1/4/4/4	-
3	GOL	A	616	-	-	0/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	B	609	-	-	0/4/4/4	-
3	GOL	A	620	-	-	0/4/4/4	-
3	GOL	A	605	-	-	2/4/4/4	-
3	GOL	A	622	-	-	0/4/4/4	-
3	GOL	A	628	-	-	4/4/4/4	-
3	GOL	A	614	-	-	2/4/4/4	-
3	GOL	A	615	-	-	2/4/4/4	-
3	GOL	B	606	-	-	2/4/4/4	-
3	GOL	A	624	-	-	1/4/4/4	-
3	GOL	A	634	-	-	2/4/4/4	-
3	GOL	A	636	-	-	2/4/4/4	-
3	GOL	B	619	-	-	2/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	B	646	-	-	4/4/4/4	-
3	GOL	A	611	-	-	0/4/4/4	-
3	GOL	B	634	-	-	2/4/4/4	-
3	GOL	B	617	-	-	2/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-
3	GOL	A	609	-	-	2/4/4/4	-
3	GOL	A	612	-	-	0/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	A	629	-	-	0/4/4/4	-
3	GOL	B	604	-	-	0/4/4/4	-
3	GOL	B	637	-	-	2/4/4/4	-
4	NGO	A	610	-	-	0/2/30/30	0/2/2/2
3	GOL	B	607	-	-	0/4/4/4	-
3	GOL	A	642	-	-	2/4/4/4	-
3	GOL	A	617	-	-	4/4/4/4	-
3	GOL	A	619	-	-	2/4/4/4	-
3	GOL	A	638	-	-	4/4/4/4	-
3	GOL	B	640	-	-	2/4/4/4	-
3	GOL	A	608	-	-	3/4/4/4	-
3	GOL	A	621	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	625	-	-	0/4/4/4	-
3	GOL	A	637	-	-	3/4/4/4	-
3	GOL	B	623	-	-	2/4/4/4	-
3	GOL	B	602	-	-	4/4/4/4	-
3	GOL	A	613	-	-	1/4/4/4	-
3	GOL	B	613	-	-	2/4/4/4	-
3	GOL	B	633	-	-	3/4/4/4	-
3	GOL	B	610	-	-	0/4/4/4	-
3	GOL	B	614	-	-	0/4/4/4	-
3	GOL	A	626	-	-	1/4/4/4	-
3	GOL	B	616	-	-	3/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	GOL	O2-C2	-2.30	1.36	1.43
3	B	621	GOL	O1-C1	-2.28	1.32	1.42
3	B	619	GOL	O2-C2	-2.26	1.36	1.43
3	A	617	GOL	O1-C1	-2.23	1.33	1.42
5	B	643	ACT	CH3-C	2.15	1.57	1.49
5	A	648	ACT	CH3-C	2.13	1.57	1.49
5	B	641	ACT	CH3-C	2.11	1.57	1.49
5	A	640	ACT	CH3-C	2.10	1.57	1.49
5	B	636	ACT	CH3-C	2.08	1.57	1.49
5	B	628	ACT	CH3-C	2.07	1.57	1.49
3	B	627	GOL	O2-C2	-2.04	1.37	1.43
5	A	631	ACT	CH3-C	2.04	1.57	1.49
5	A	627	ACT	CH3-C	2.02	1.57	1.49
5	B	631	ACT	CH3-C	2.02	1.57	1.49
5	A	643	ACT	CH3-C	2.01	1.57	1.49
5	B	635	ACT	CH3-C	2.01	1.57	1.49
3	A	623	GOL	O2-C2	-2.00	1.37	1.43
5	B	638	ACT	CH3-C	2.00	1.57	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	NGO	C8-C7-N2	-4.29	120.86	127.05
4	B	611	NGO	C8-C7-N2	-4.15	121.07	127.05
4	A	610	NGO	C1-O5-C5	-3.44	107.00	113.72
4	A	610	NGO	C1-O1-C7	-2.72	103.12	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	611	NGO	O5-C1-O1	2.54	113.71	109.25
3	B	603	GOL	O2-C2-C3	2.26	118.55	109.18
3	B	610	GOL	C3-C2-C1	-2.26	103.52	111.80
3	B	613	GOL	C3-C2-C1	-2.23	103.60	111.80
3	A	634	GOL	C3-C2-C1	-2.21	103.68	111.80
3	A	605	GOL	C3-C2-C1	-2.13	103.99	111.80
3	A	616	GOL	C3-C2-C1	-2.10	104.08	111.80
3	A	606	GOL	C3-C2-C1	-2.07	104.20	111.80
3	B	609	GOL	C3-C2-C1	-2.06	104.24	111.80
3	B	618	GOL	C3-C2-C1	-2.05	104.27	111.80
3	A	615	GOL	C3-C2-C1	-2.05	104.28	111.80
3	B	625	GOL	C3-C2-C1	-2.02	104.37	111.80
3	B	612	GOL	C3-C2-C1	-2.01	104.41	111.80
3	A	645	GOL	C3-C2-C1	-2.00	104.44	111.80

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	608	GOL	C1-C2-C3-O3
3	A	608	GOL	O2-C2-C3-O3
3	A	609	GOL	O1-C1-C2-C3
3	A	614	GOL	O1-C1-C2-C3
3	A	617	GOL	O1-C1-C2-C3
3	A	618	GOL	C1-C2-C3-O3
3	A	619	GOL	O1-C1-C2-C3
3	A	623	GOL	O1-C1-C2-C3
3	A	628	GOL	O1-C1-C2-C3
3	A	634	GOL	C1-C2-C3-O3
3	A	634	GOL	O2-C2-C3-O3
3	A	642	GOL	O1-C1-C2-C3
3	A	645	GOL	C1-C2-C3-O3
3	B	602	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	C1-C2-C3-O3
3	B	603	GOL	O1-C1-C2-O2
3	B	603	GOL	O1-C1-C2-C3
3	B	613	GOL	O1-C1-C2-C3
3	B	616	GOL	C1-C2-C3-O3
3	B	621	GOL	O1-C1-C2-C3
3	B	623	GOL	O1-C1-C2-C3
3	B	627	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	634	GOL	C1-C2-C3-O3
3	B	634	GOL	O2-C2-C3-O3
3	B	640	GOL	O1-C1-C2-C3
3	B	642	GOL	O1-C1-C2-C3
3	B	642	GOL	C1-C2-C3-O3
3	B	646	GOL	O1-C1-C2-C3
3	B	646	GOL	C1-C2-C3-O3
3	A	614	GOL	O1-C1-C2-O2
3	A	628	GOL	O2-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
3	B	613	GOL	O1-C1-C2-O2
3	B	623	GOL	O1-C1-C2-O2
3	B	633	GOL	O2-C2-C3-O3
3	A	601	GOL	C1-C2-C3-O3
3	A	604	GOL	C1-C2-C3-O3
3	A	605	GOL	O1-C1-C2-C3
3	A	617	GOL	C1-C2-C3-O3
3	A	621	GOL	O1-C1-C2-C3
3	A	628	GOL	C1-C2-C3-O3
3	A	636	GOL	O1-C1-C2-C3
3	A	637	GOL	O1-C1-C2-C3
3	A	638	GOL	O1-C1-C2-C3
3	A	644	GOL	O1-C1-C2-C3
3	B	606	GOL	O1-C1-C2-C3
3	B	617	GOL	C1-C2-C3-O3
3	B	619	GOL	O1-C1-C2-C3
3	B	621	GOL	C1-C2-C3-O3
3	B	633	GOL	C1-C2-C3-O3
3	B	637	GOL	O1-C1-C2-C3
3	A	617	GOL	O1-C1-C2-O2
3	A	617	GOL	O2-C2-C3-O3
3	A	618	GOL	O2-C2-C3-O3
3	A	623	GOL	O1-C1-C2-O2
3	A	628	GOL	O1-C1-C2-O2
3	A	637	GOL	O1-C1-C2-O2
3	A	642	GOL	O1-C1-C2-O2
3	B	616	GOL	O2-C2-C3-O3
3	B	621	GOL	O1-C1-C2-O2
3	B	640	GOL	O1-C1-C2-O2
3	B	642	GOL	O1-C1-C2-O2
3	B	642	GOL	O2-C2-C3-O3
3	B	646	GOL	O1-C1-C2-O2

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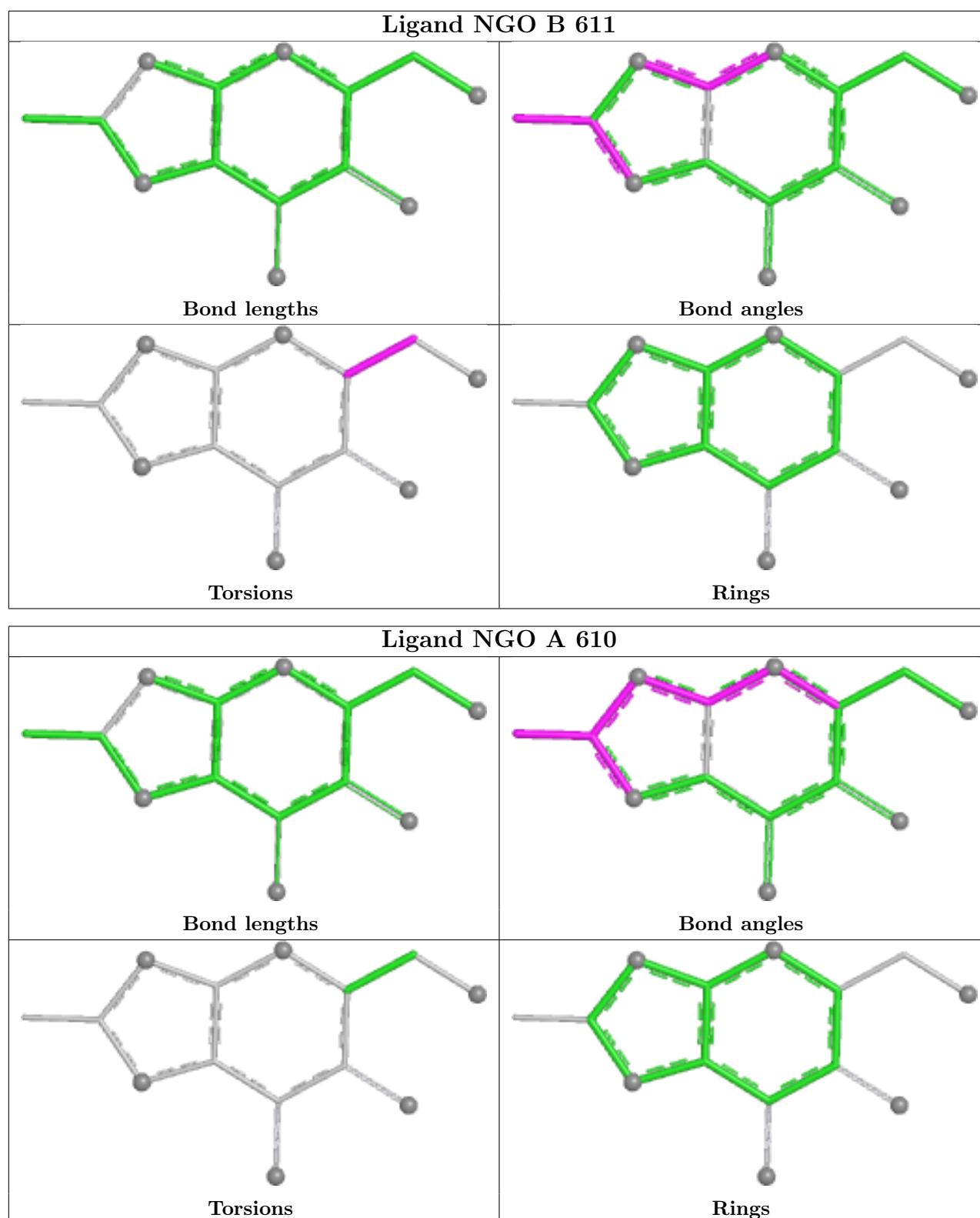
Mol	Chain	Res	Type	Atoms
3	B	646	GOL	O2-C2-C3-O3
3	A	601	GOL	O2-C2-C3-O3
3	A	609	GOL	O1-C1-C2-O2
3	A	619	GOL	O1-C1-C2-O2
3	A	645	GOL	O2-C2-C3-O3
3	B	606	GOL	O1-C1-C2-O2
3	B	621	GOL	O2-C2-C3-O3
3	B	627	GOL	O2-C2-C3-O3
3	B	616	GOL	O1-C1-C2-C3
3	A	644	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-O2
3	A	613	GOL	O2-C2-C3-O3
3	A	615	GOL	O2-C2-C3-O3
3	A	626	GOL	O1-C1-C2-O2
3	A	636	GOL	O1-C1-C2-O2
3	A	638	GOL	O1-C1-C2-O2
3	B	618	GOL	O1-C1-C2-O2
3	B	629	GOL	O1-C1-C2-O2
3	B	637	GOL	O1-C1-C2-O2
3	B	619	GOL	O1-C1-C2-O2
3	A	637	GOL	C1-C2-C3-O3
3	A	645	GOL	O1-C1-C2-C3
3	B	629	GOL	O1-C1-C2-C3
3	A	604	GOL	O2-C2-C3-O3
3	A	608	GOL	O1-C1-C2-O2
3	A	605	GOL	O1-C1-C2-O2
3	A	615	GOL	O1-C1-C2-O2
3	A	624	GOL	O2-C2-C3-O3
3	B	617	GOL	O2-C2-C3-O3
4	B	611	NGO	C4-C5-C6-O6
3	A	638	GOL	C1-C2-C3-O3
3	B	633	GOL	O1-C1-C2-C3
3	A	607	GOL	O1-C1-C2-O2
3	B	615	GOL	O2-C2-C3-O3
4	B	611	NGO	O5-C5-C6-O6
3	A	621	GOL	O1-C1-C2-O2
3	A	638	GOL	O2-C2-C3-O3

There are no ring outliers.

22 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	615	GOL	1	0
4	B	611	NGO	3	0
3	A	619	GOL	1	0
3	B	610	GOL	1	0
3	B	642	GOL	2	0
3	A	645	GOL	2	0
3	B	621	GOL	2	0
3	B	646	GOL	4	0
4	A	610	NGO	6	0
3	A	617	GOL	2	0
3	A	608	GOL	1	0
3	A	637	GOL	1	0
3	B	613	GOL	4	0
5	A	630	ACT	2	0
3	A	628	GOL	3	0
3	A	622	GOL	1	0
5	B	638	ACT	1	0
3	B	603	GOL	2	0
3	A	634	GOL	4	0
3	A	609	GOL	1	0
3	A	629	GOL	1	0
3	B	623	GOL	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	499/511 (97%)	-1.21	0 100 100	8, 21, 35, 62	48 (9%)
1	B	498/511 (97%)	-1.23	0 100 100	9, 21, 34, 64	49 (9%)
All	All	997/1022 (97%)	-1.22	0 100 100	8, 21, 35, 64	97 (9%)

There are no RSRZ outliers to report.

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](#)

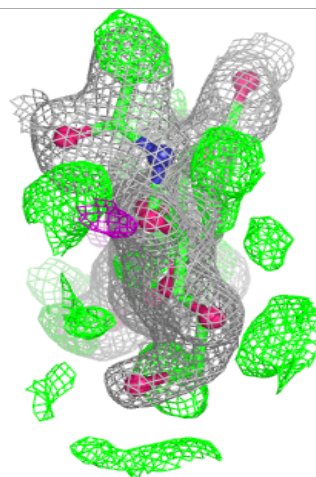
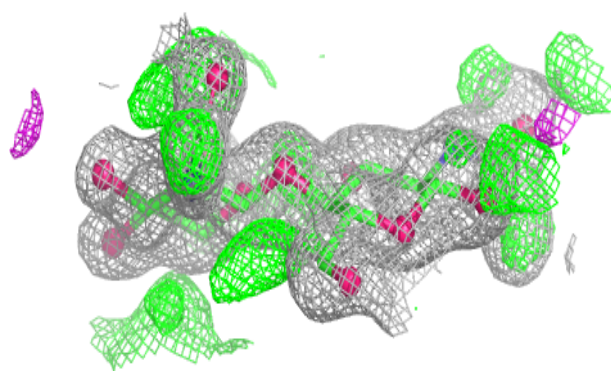
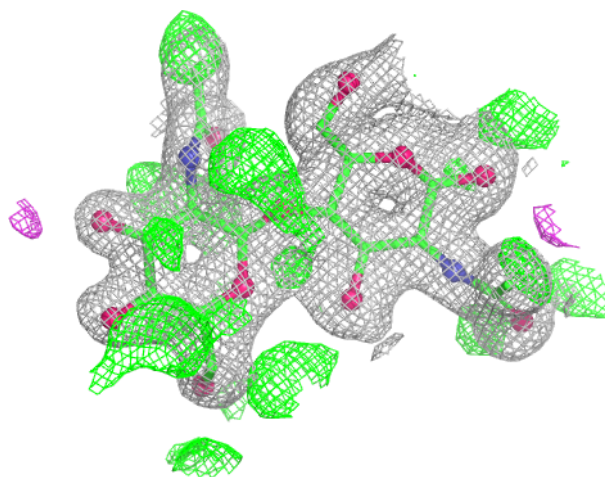
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

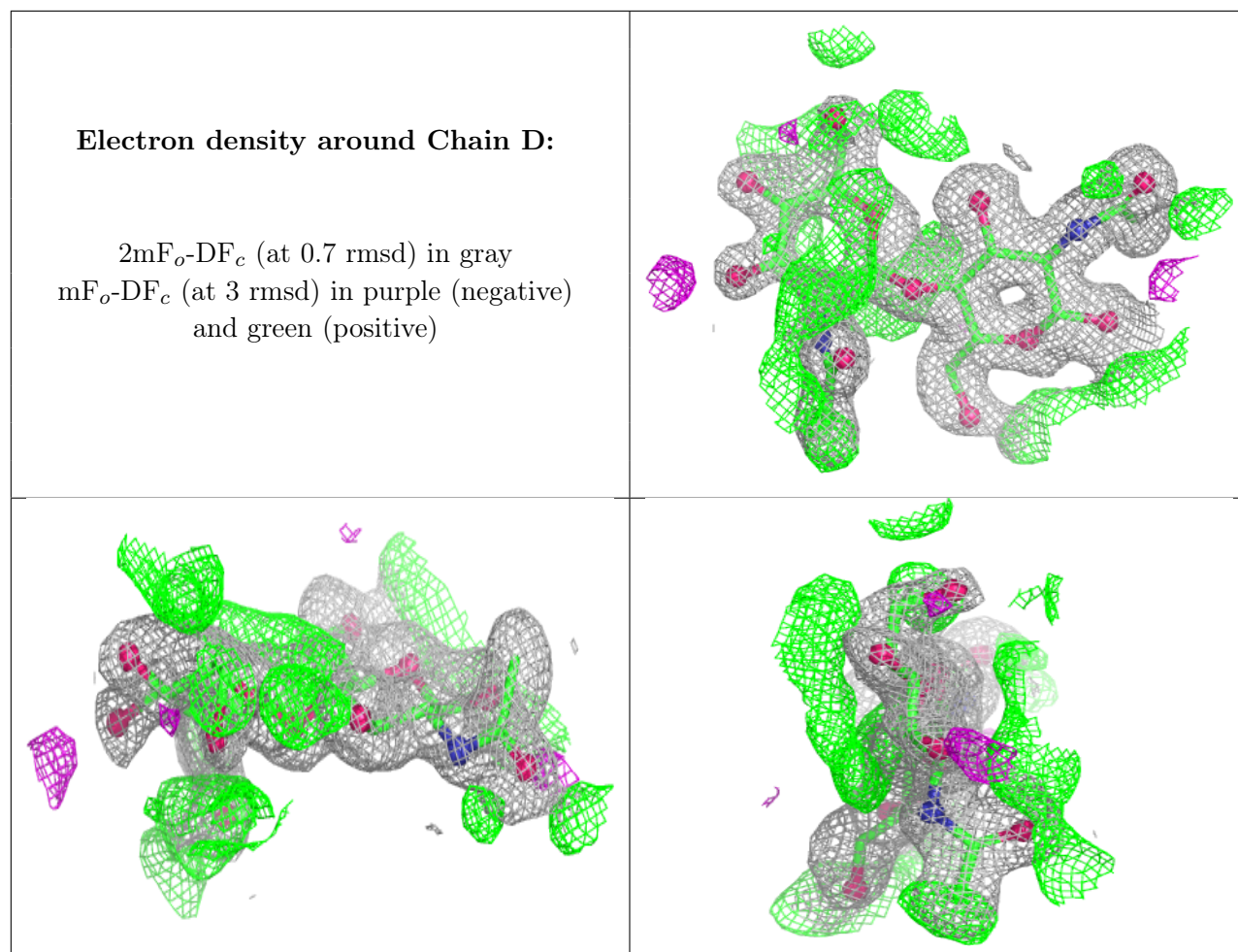
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.95	0.08	26,32,37,39	14
2	NAG	C	2	14/15	0.97	0.06	27,33,37,38	14
2	NAG	D	1	15/15	0.98	0.05	24,28,33,36	13
2	NAG	C	1	15/15	0.98	0.05	27,31,36,40	15

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 C:

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





6.4 Ligands [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(Å ²)	Q<0.9
3	GOL	A	611	6/6	0.88	0.21	55,57,58,58	6
5	ACT	A	635	4/4	0.90	0.16	54,55,56,56	0
3	GOL	A	628	6/6	0.92	0.15	50,52,53,55	6
5	ACT	A	648	4/4	0.92	0.13	53,54,54,56	0
5	ACT	A	627	4/4	0.93	0.11	83,84,84,84	0
5	ACT	B	641	4/4	0.94	0.11	54,56,56,56	0
3	GOL	B	627	6/6	0.95	0.12	48,52,52,52	6
3	GOL	A	626	6/6	0.95	0.13	52,55,56,56	6
3	GOL	A	638	6/6	0.95	0.10	70,71,71,71	0
5	ACT	A	640	4/4	0.95	0.13	60,61,61,61	4
3	GOL	B	623	6/6	0.95	0.14	72,74,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	625	6/6	0.95	0.12	53,56,56,57	0
5	ACT	B	643	4/4	0.95	0.10	65,66,66,66	4
5	ACT	A	639	4/4	0.96	0.10	68,68,69,69	0
5	ACT	B	631	4/4	0.96	0.12	56,58,59,59	0
5	ACT	B	638	4/4	0.96	0.10	58,58,58,59	4
3	GOL	B	629	6/6	0.96	0.08	73,73,74,75	0
5	ACT	A	641	4/4	0.96	0.08	67,67,67,68	0
3	GOL	B	624	6/6	0.97	0.12	58,63,64,64	0
3	GOL	A	622	6/6	0.97	0.09	58,59,60,62	0
3	GOL	A	629	6/6	0.97	0.09	29,40,44,45	6
3	GOL	A	637	6/6	0.97	0.10	51,52,53,54	6
5	ACT	B	628	4/4	0.97	0.07	82,83,83,84	0
3	GOL	B	633	6/6	0.97	0.09	47,49,50,51	6
3	GOL	B	646	6/6	0.97	0.14	46,49,50,51	6
5	ACT	B	639	4/4	0.97	0.09	69,70,70,70	0
3	GOL	A	624	6/6	0.97	0.12	57,64,65,66	0
3	GOL	A	601	6/6	0.97	0.07	34,40,41,41	0
5	ACT	B	645	4/4	0.97	0.10	67,67,68,68	0
6	PO4	A	647	5/5	0.97	0.13	77,78,78,78	5
6	PO4	B	608	5/5	0.97	0.09	65,66,67,67	5
3	GOL	A	634	6/6	0.98	0.07	32,37,38,39	6
3	GOL	B	634	6/6	0.98	0.07	51,53,54,55	6
3	GOL	B	637	6/6	0.98	0.06	42,47,49,50	6
3	GOL	B	642	6/6	0.98	0.06	52,54,55,57	6
3	GOL	A	602	6/6	0.98	0.06	29,39,40,43	0
4	NGO	A	610	14/14	0.98	0.10	30,44,47,47	14
4	NGO	B	611	14/14	0.98	0.09	32,45,47,48	14
3	GOL	A	623	6/6	0.98	0.07	34,37,41,44	6
5	ACT	A	630	4/4	0.98	0.09	83,83,83,83	0
5	ACT	A	632	4/4	0.98	0.06	69,70,70,70	0
3	GOL	A	642	6/6	0.98	0.07	58,60,61,61	0
3	GOL	A	645	6/6	0.98	0.08	71,72,73,74	0
3	GOL	B	602	6/6	0.98	0.08	72,73,74,75	0
3	GOL	B	612	6/6	0.98	0.07	42,46,48,50	6
5	ACT	A	643	4/4	0.98	0.08	70,70,70,70	0
3	GOL	B	613	6/6	0.98	0.06	32,38,39,40	6
3	GOL	B	614	6/6	0.98	0.07	49,52,54,55	6
5	ACT	B	630	4/4	0.98	0.05	69,70,70,70	0
3	GOL	B	621	6/6	0.98	0.06	29,31,34,35	6
5	ACT	B	635	4/4	0.98	0.07	74,75,75,76	0
5	ACT	B	636	4/4	0.98	0.07	70,70,70,71	4
3	GOL	B	622	6/6	0.98	0.06	40,44,47,47	0

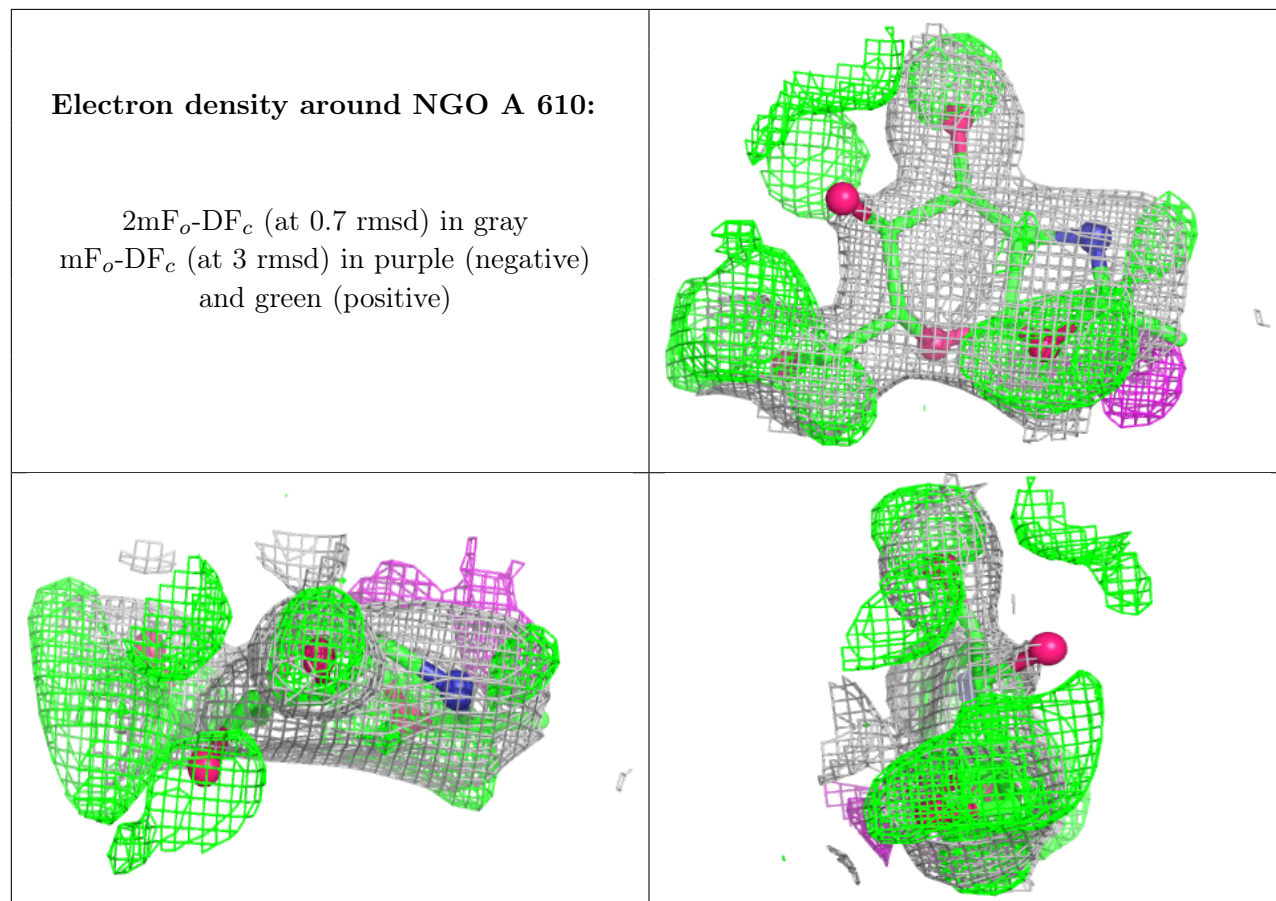
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	612	6/6	0.98	0.07	39,44,45,47	6
3	GOL	A	625	6/6	0.98	0.07	42,46,49,50	6
3	GOL	A	613	6/6	0.98	0.07	59,61,62,63	0
3	GOL	B	626	6/6	0.98	0.07	32,35,37,39	6
6	PO4	A	646	5/5	0.98	0.06	57,59,60,60	5
3	GOL	A	617	6/6	0.98	0.07	28,30,34,36	6
3	GOL	A	620	6/6	0.98	0.06	32,37,39,40	6
6	PO4	B	644	5/5	0.98	0.09	80,80,81,81	5
3	GOL	A	644	6/6	0.99	0.05	43,50,50,52	6
3	GOL	A	607	6/6	0.99	0.05	41,50,52,52	6
3	GOL	B	640	6/6	0.99	0.06	58,60,61,61	0
3	GOL	B	601	6/6	0.99	0.05	25,31,34,40	6
3	GOL	A	621	6/6	0.99	0.06	23,40,44,45	6
3	GOL	B	603	6/6	0.99	0.05	24,32,35,35	6
3	GOL	B	604	6/6	0.99	0.05	29,39,41,44	0
3	GOL	B	605	6/6	0.99	0.04	21,29,31,32	6
3	GOL	B	606	6/6	0.99	0.03	34,37,43,45	0
5	ACT	A	631	4/4	0.99	0.05	38,44,45,47	0
3	GOL	B	607	6/6	0.99	0.03	33,34,35,35	6
5	ACT	A	633	4/4	0.99	0.06	63,64,64,64	4
3	GOL	B	609	6/6	0.99	0.04	32,43,45,46	6
3	GOL	B	610	6/6	0.99	0.04	31,41,43,45	6
3	GOL	A	608	6/6	0.99	0.06	44,48,50,50	6
3	GOL	A	609	6/6	0.99	0.05	28,32,34,35	6
3	GOL	A	603	6/6	0.99	0.03	21,29,31,33	6
3	GOL	B	615	6/6	0.99	0.05	45,54,55,56	6
3	GOL	B	616	6/6	0.99	0.05	24,40,44,45	6
3	GOL	B	617	6/6	0.99	0.04	40,42,42,43	6
3	GOL	B	618	6/6	0.99	0.06	41,44,48,50	6
5	ACT	B	632	4/4	0.99	0.05	39,45,46,49	0
3	GOL	B	619	6/6	0.99	0.04	26,30,31,33	6
3	GOL	B	620	6/6	0.99	0.05	32,35,37,39	0
3	GOL	A	604	6/6	0.99	0.04	26,31,32,32	6
3	GOL	A	605	6/6	0.99	0.04	35,36,41,44	0
3	GOL	A	614	6/6	0.99	0.04	41,42,43,43	6
3	GOL	A	615	6/6	0.99	0.05	41,44,47,49	6
3	GOL	A	616	6/6	0.99	0.04	23,27,29,32	6
3	GOL	A	636	6/6	0.99	0.05	39,45,46,48	6
3	GOL	A	606	6/6	0.99	0.03	33,34,35,35	6
3	GOL	A	618	6/6	0.99	0.05	26,31,39,43	6
3	GOL	A	619	6/6	0.99	0.06	29,33,35,35	6

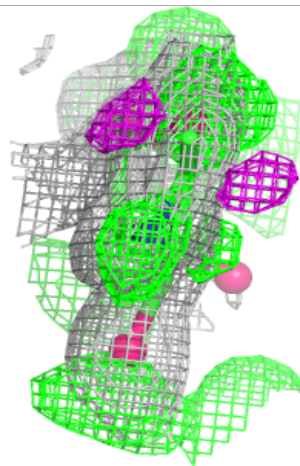
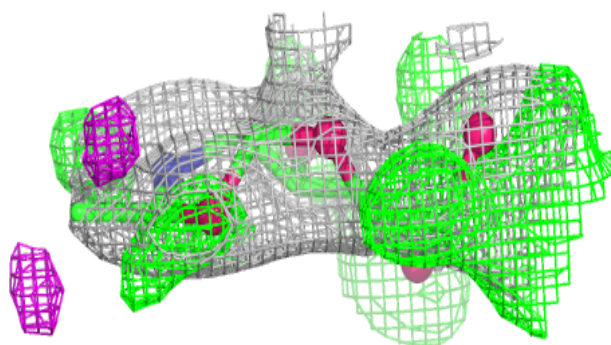
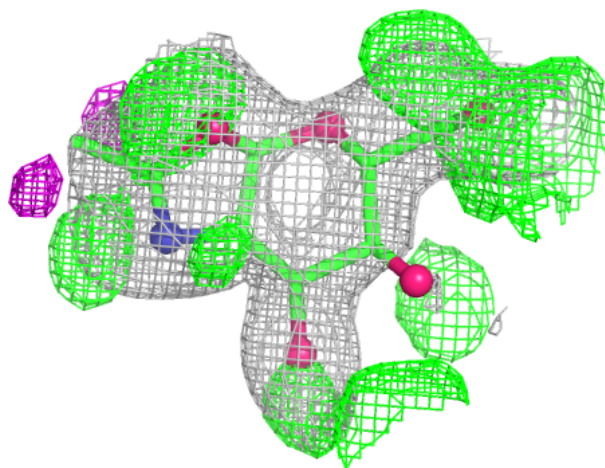
The following is a graphical depiction of the model fit to experimental electron density of all

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 NGO B 611:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.