Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 02:07 pm GMT

PDB ID	:	8AX3
Title	:	Structure of recombinant human beta-glucocerebrosidase in complex with L-carbaxylosyl fluoride
Authors	:	Rowland, R.J.; Davies, G.J.
Deposited on	:	2022-08-30
Resolution	:	1.59 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:

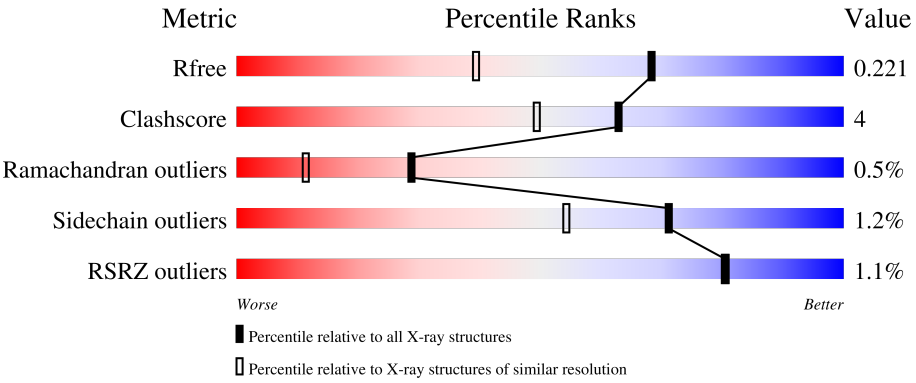
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	497	% 94% 6%
1	B	497	% 91% 9%
2	C	3	33% 67%
2	D	3	67% 33%
3	E	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
5	EDO	A	525	-	-	X	-

2 Entry composition

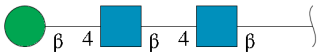
There are 11 unique types of molecules in this entry. The entry contains 17569 atoms, of which 8307 are hydrogens and 0 are deuteriums.

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 Lysosomal acid glucosylceramidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	497	Total	C	H	N	O	S	129	5	0
			7899	2562	3917	685	719	16			
1	B	497	Total	C	H	N	O	S	131	6	0
			7886	2561	3912	679	716	18			

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

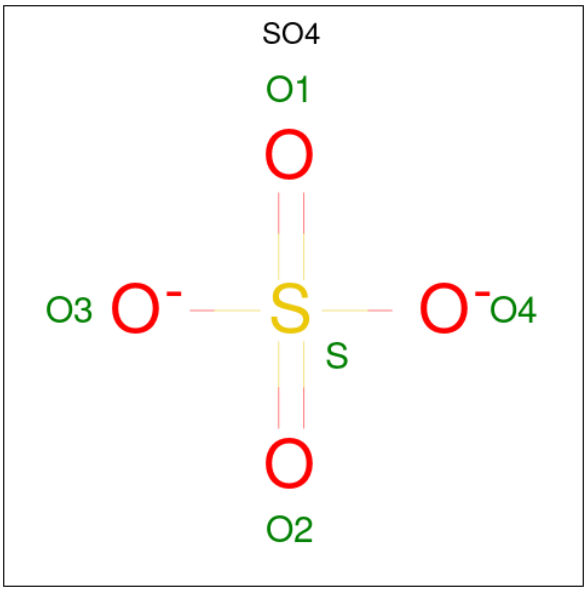


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	N	O	8	0	0
			78	22	39	2	15			
2	D	3	Total	C	H	N	O	8	0	0
			78	22	39	2	15			

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

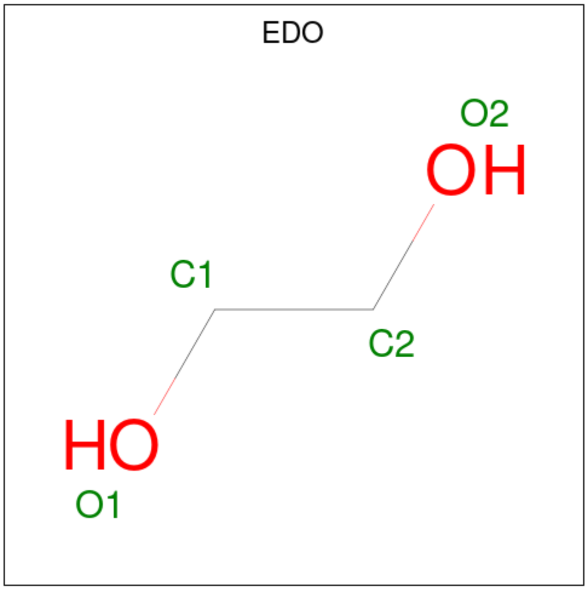
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	2	Total	C	H	N	O	5	0	0
			56	16	28	2	10			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 20 4 12 4	2	1
5	A	1	Total C H O 10 2 6 2	1	0
5	A	1	Total C H O 20 4 12 4	2	1
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0

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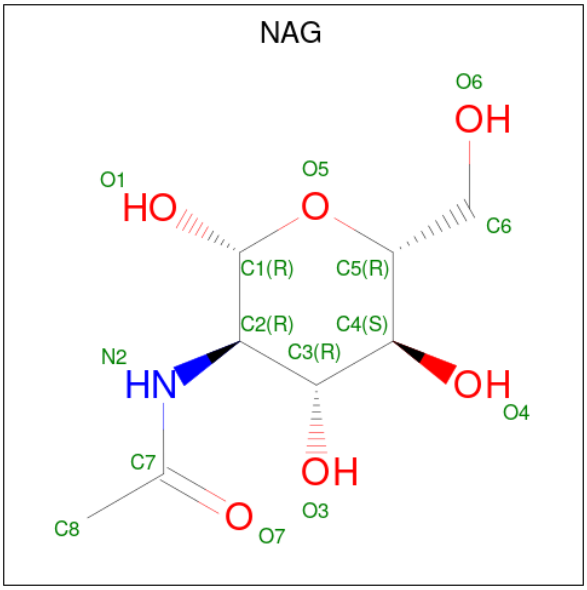
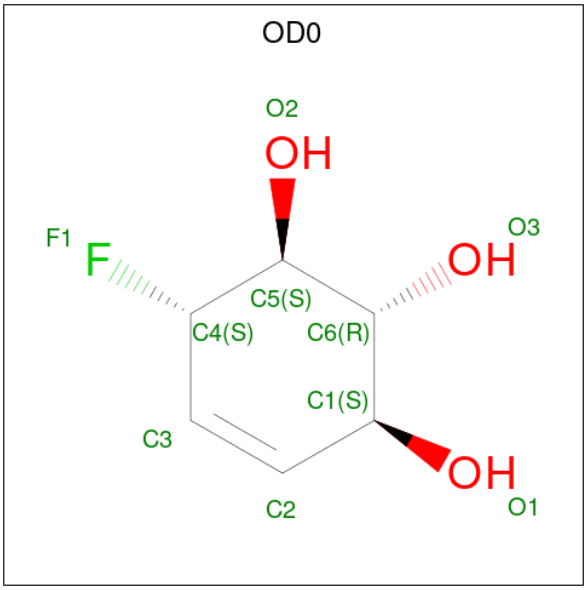
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 20 4 12 4	2	1
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0
5	B	1	Total C H O 10 2 6 2	1	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
6	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 7 is (1 {S},2 {R},3 {S},6 {S})-6-fluoranylcyclohex-4-ene-1,2,3-triol (three-letter code: OD0) (formula: $C_6H_9FO_3$) (labeled as "Ligand of Interest" by depositor).

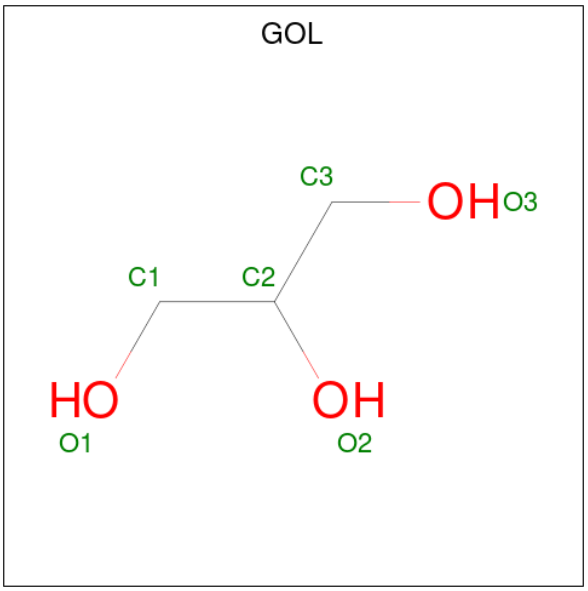


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	H	O	3	0
			19	6	1	9	3		
7	A	1	Total	C	F	H	O	3	0
			19	6	1	9	3		
7	B	1	Total	C	F	H	O	3	0
			19	6	1	9	3		
7	B	1	Total	C	F	H	O	3	0
			19	6	1	9	3		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C H O 14 3 8 3	2	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Ca 1 1	0	0

- Molecule 11 is water.

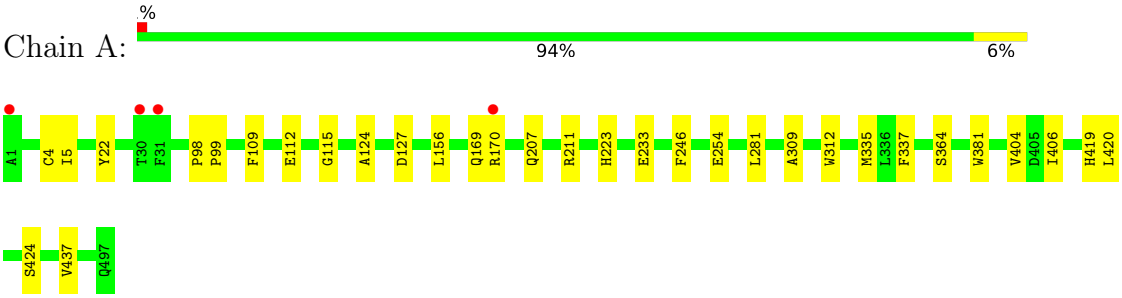
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	453	Total O 454 454	0	1
11	B	440	Total O 440 440	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

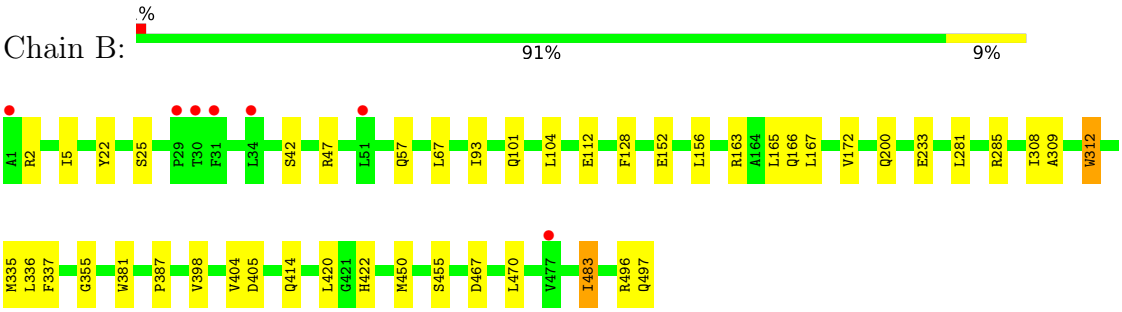
• Molecule 1: Lysosomal acid glucosylceramidase

Chain A:



• Molecule 1: Lysosomal acid glucosylceramidase

Chain B:



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

Chain C:

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

Chain D:

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

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.92Å 155.98Å 68.04Å 90.00° 101.96° 90.00°	Depositor
Resolution (Å)	51.82 – 1.59 51.77 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (51.82-1.59) 99.5 (51.77-1.59)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.212 0.193 , 0.221	Depositor DCC
R_{free} test set	7124 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17569	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, EDO, NA, SO4, NAG, OD0, GOL, CA

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	0.64	0/4102	0.76	0/5594
1	B	0.63	0/4094	0.77	1/5581 (0.0%)
All	All	0.64	0/8196	0.76	1/11175 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	285	ARG	NE-CZ-NH1	5.84	123.22	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3982	3917	3892	30	0
1	B	3974	3912	3882	37	0
2	C	39	39	34	2	0
2	D	39	39	34	0	0
3	E	28	28	25	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	100	150	150	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	100	150	150	7	0
6	A	14	14	13	0	0
6	B	14	14	13	0	0
7	A	20	18	0	0	0
7	B	20	18	0	0	0
8	A	1	0	0	0	0
9	B	6	8	8	0	0
10	B	1	0	0	0	0
11	A	454	0	0	11	0
11	B	440	0	0	11	0
All	All	9262	8307	8201	72	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 (72) 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:450[B]:MET:CE	1:B:450[B]:MET:HA	2.09	0.83
1:A:170[C]:ARG:NH1	1:A:424:SER:O	2.12	0.81
1:B:112:GLU:OE2	11:B:601:HOH:O	1.99	0.79
1:B:405:ASP:OD1	11:B:602:HOH:O	2.01	0.78
1:B:450[B]:MET:HA	1:B:450[B]:MET:HE3	1.67	0.75
1:B:2:ARG:HD2	5:B:528:EDO:H21	1.67	0.75
1:B:167:LEU:HG	5:B:521:EDO:H21	1.69	0.74
1:B:165[B]:LEU:O	11:B:603:HOH:O	2.07	0.72
1:B:42:SER:OG	1:B:422:HIS:HE1	1.71	0.72
1:B:166:GLN:OE1	11:B:604:HOH:O	2.13	0.66
1:A:109:PHE:O	5:A:525:EDO:H12	1.97	0.65
1:B:467:ASP:HB3	1:B:483:ILE:HD11	1.81	0.63
1:A:211:ARG:HD2	11:A:611:HOH:O	1.99	0.61
1:B:165[A]:LEU:O	11:B:603:HOH:O	2.16	0.60
1:A:223:HIS:HE1	11:A:965:HOH:O	1.85	0.60
1:B:167:LEU:HG	5:B:521:EDO:C2	2.33	0.58
5:A:508:EDO:H22	5:A:509:EDO:H11	1.86	0.57
1:B:450[B]:MET:HA	1:B:450[B]:MET:HE2	1.84	0.57
1:A:112:GLU:HG3	11:A:852:HOH:O	2.03	0.57
1:B:166:GLN:HG3	11:B:855:HOH:O	2.05	0.56
1:A:169:GLN:N	5:A:525:EDO:O2	2.34	0.55
1:B:355:GLY:H	1:B:414:GLN:HE21	1.56	0.52
1:A:211:ARG:NH1	11:A:611:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HG	1:B:470[A]:LEU:HD11	1.92	0.51
1:A:364:SER:OG	1:A:419:HIS:HD2	1.94	0.50
1:B:387:PRO:HD3	1:B:404:VAL:O	2.12	0.50
1:A:115:GLY:C	5:A:525:EDO:H11	2.32	0.49
1:B:165[A]:LEU:HD23	1:B:172:VAL:HB	1.94	0.49
1:A:254:GLU:HB2	5:A:524:EDO:H12	1.94	0.49
1:B:163:ARG:O	5:B:521:EDO:H21	2.13	0.48
1:B:2:ARG:HD2	5:B:528:EDO:C2	2.39	0.48
1:A:5[B]:ILE:HD12	1:A:22:TYR:CE1	2.49	0.48
1:B:200:GLN:NE2	11:B:625:HOH:O	2.47	0.47
1:A:5[B]:ILE:HD12	1:A:22:TYR:CD1	2.50	0.47
1:B:47:ARG:NE	11:B:622:HOH:O	2.47	0.47
1:A:207:GLN:HG3	11:A:888:HOH:O	2.14	0.47
1:A:5[B]:ILE:HD13	2:C:1:NAG:C6	2.45	0.47
1:B:450[B]:MET:HE2	1:B:455:SER:O	2.15	0.46
1:A:169:GLN:H	5:A:525:EDO:HO2	1.61	0.46
1:A:406:ILE:HG12	11:A:623:HOH:O	2.14	0.46
1:A:437:VAL:HG21	11:A:967:HOH:O	2.15	0.46
1:B:309:ALA:HA	1:B:337:PHE:O	2.16	0.46
1:A:406:ILE:CG1	11:A:623:HOH:O	2.64	0.46
1:B:57:GLN:HG3	11:B:660:HOH:O	2.15	0.46
1:B:308:ILE:HB	1:B:336:LEU:HD23	1.99	0.45
1:A:404:VAL:HG11	1:A:406:ILE:HD11	1.99	0.45
1:B:104:LEU:C	1:B:104:LEU:HD23	2.38	0.45
1:A:156:LEU:HD12	1:A:156:LEU:N	2.32	0.44
5:B:511:EDO:C2	11:B:613:HOH:O	2.64	0.44
1:B:152:GLU:O	1:B:156:LEU:HB2	2.18	0.43
5:A:522:EDO:C2	5:A:523:EDO:H11	2.48	0.43
1:B:25:SER:HB3	5:B:528:EDO:H22	2.00	0.43
1:B:67:LEU:HG	1:B:470[A]:LEU:CD1	2.48	0.43
1:B:450[B]:MET:HE1	1:B:496:ARG:HD2	2.01	0.42
1:A:207:GLN:CG	11:A:888:HOH:O	2.67	0.42
5:A:516:EDO:H12	11:A:867:HOH:O	2.18	0.42
1:A:98:PRO:HB2	1:A:99:PRO:HD3	2.01	0.42
1:A:404:VAL:CG1	1:A:406:ILE:CD1	2.98	0.42
1:A:404:VAL:CG1	1:A:406:ILE:HD13	2.50	0.42
5:A:522:EDO:H21	5:A:523:EDO:H11	2.01	0.42
1:A:404:VAL:HG12	1:A:406:ILE:HD13	2.01	0.42
1:B:165[A]:LEU:CD2	1:B:172:VAL:HB	2.50	0.42
1:A:309:ALA:HA	1:A:337:PHE:O	2.19	0.42
1:B:2:ARG:NH1	11:B:633:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PHE:CZ	1:B:398:VAL:HG22	2.56	0.41
1:B:312:TRP:CD1	1:B:312:TRP:C	2.94	0.41
1:A:5[B]:ILE:HD13	2:C:1:NAG:H62	2.01	0.41
1:A:207:GLN:CD	11:A:888:HOH:O	2.59	0.41
1:B:93:ILE:O	1:B:101:GLN:HG2	2.21	0.40
1:A:4:CYS:N	5:A:503:EDO:H11	2.36	0.40
1:B:5:ILE:HG12	1:B:22:TYR:CE1	2.57	0.40
1:A:127:ASP:HB3	1:A:246:PHE:CG	2.57	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	501/497 (101%)	486 (97%)	12 (2%)	3 (1%)	25 8
1	B	501/497 (101%)	482 (96%)	17 (3%)	2 (0%)	34 15
All	All	1002/994 (101%)	968 (97%)	29 (3%)	5 (0%)	29 11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	B	233	GLU
1	A	124	ALA
1	A	281	LEU
1	B	281	LEU

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	428/424 (101%)	424 (99%)	4 (1%)	78	65
1	B	427/424 (101%)	421 (99%)	6 (1%)	67	47
All	All	855/848 (101%)	845 (99%)	10 (1%)	71	54

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

Mol	Chain	Res	Type
1	A	312	TRP
1	A	335	MET
1	A	381	TRP
1	A	420	LEU
1	B	312	TRP
1	B	335	MET
1	B	381	TRP
1	B	420	LEU
1	B	483	ILE
1	B	497	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	223	HIS
1	A	362	GLN
1	A	365	HIS
1	A	419	HIS
1	B	166	GLN
1	B	200	GLN
1	B	207	GLN
1	B	223	HIS
1	B	414	GLN
1	B	422	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.60	0	17,19,21	0.76	0
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	1.35	2 (11%)
2	BMA	C	3	2	11,11,12	0.30	0	15,15,17	0.86	0
2	NAG	D	1	1,2	14,14,15	0.45	0	17,19,21	0.78	0
2	NAG	D	2	2	14,14,15	0.55	0	17,19,21	1.16	1 (5%)
2	BMA	D	3	2	11,11,12	0.35	0	15,15,17	0.93	0
3	NAG	E	1	1,3	14,14,15	0.47	0	17,19,21	0.83	0
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	1.07	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C1-O5-C5	3.78	117.31	112.19
3	E	2	NAG	O5-C5-C6	2.98	111.87	107.20
2	D	2	NAG	C1-O5-C5	2.79	115.97	112.19
2	C	2	NAG	O5-C1-C2	-2.04	108.06	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

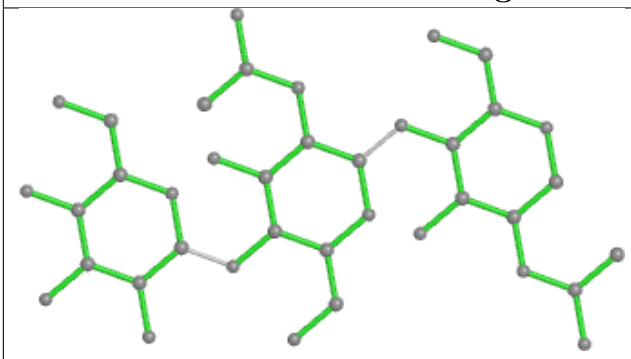
There are no ring outliers.

1 monomer is involved in 2 short contacts:

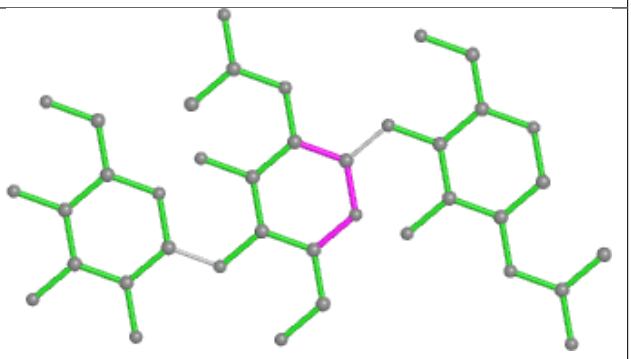
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0

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

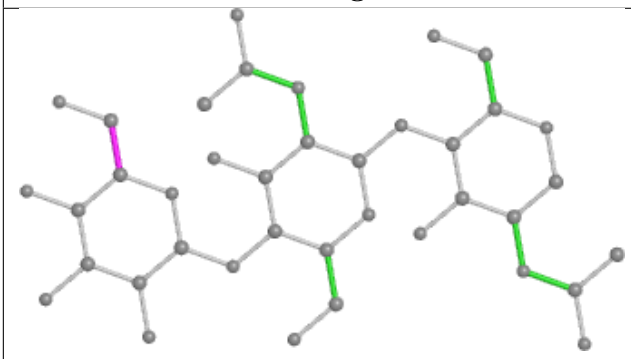
Oligosaccharide Chain C



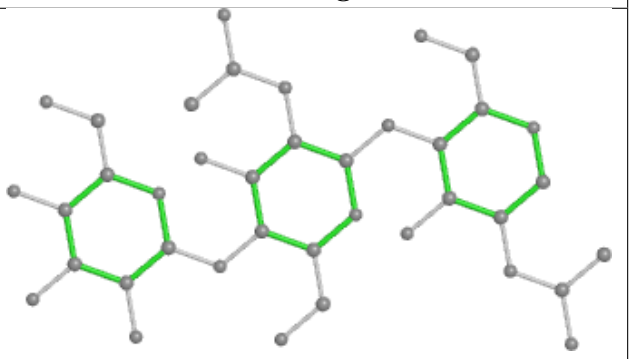
Bond lengths



Bond angles

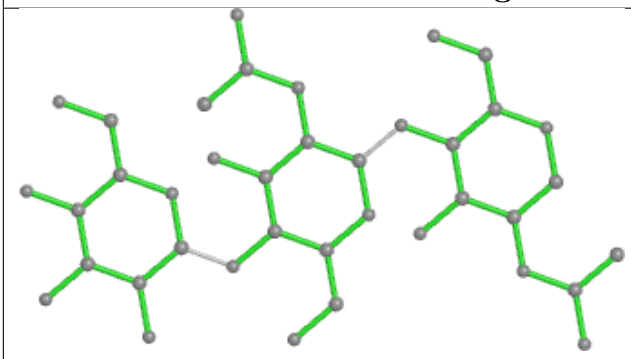


Torsions

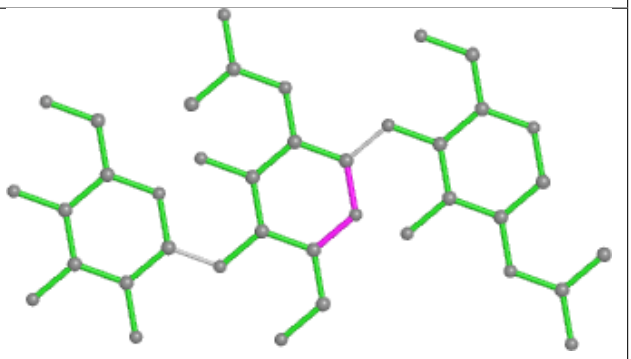


Rings

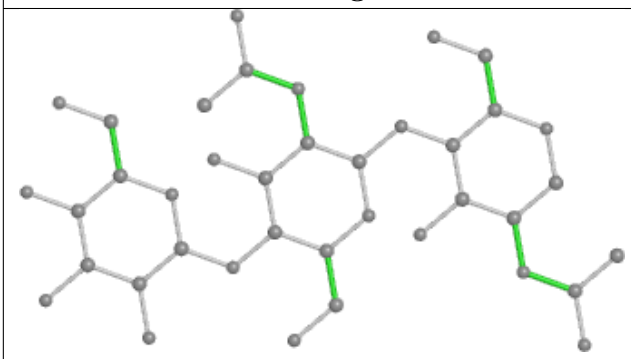
Oligosaccharide Chain D



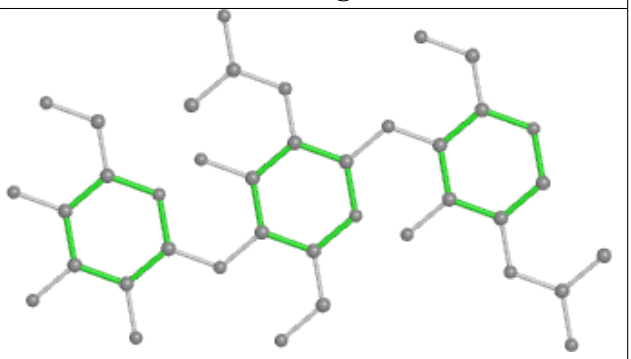
Bond lengths



Bond angles

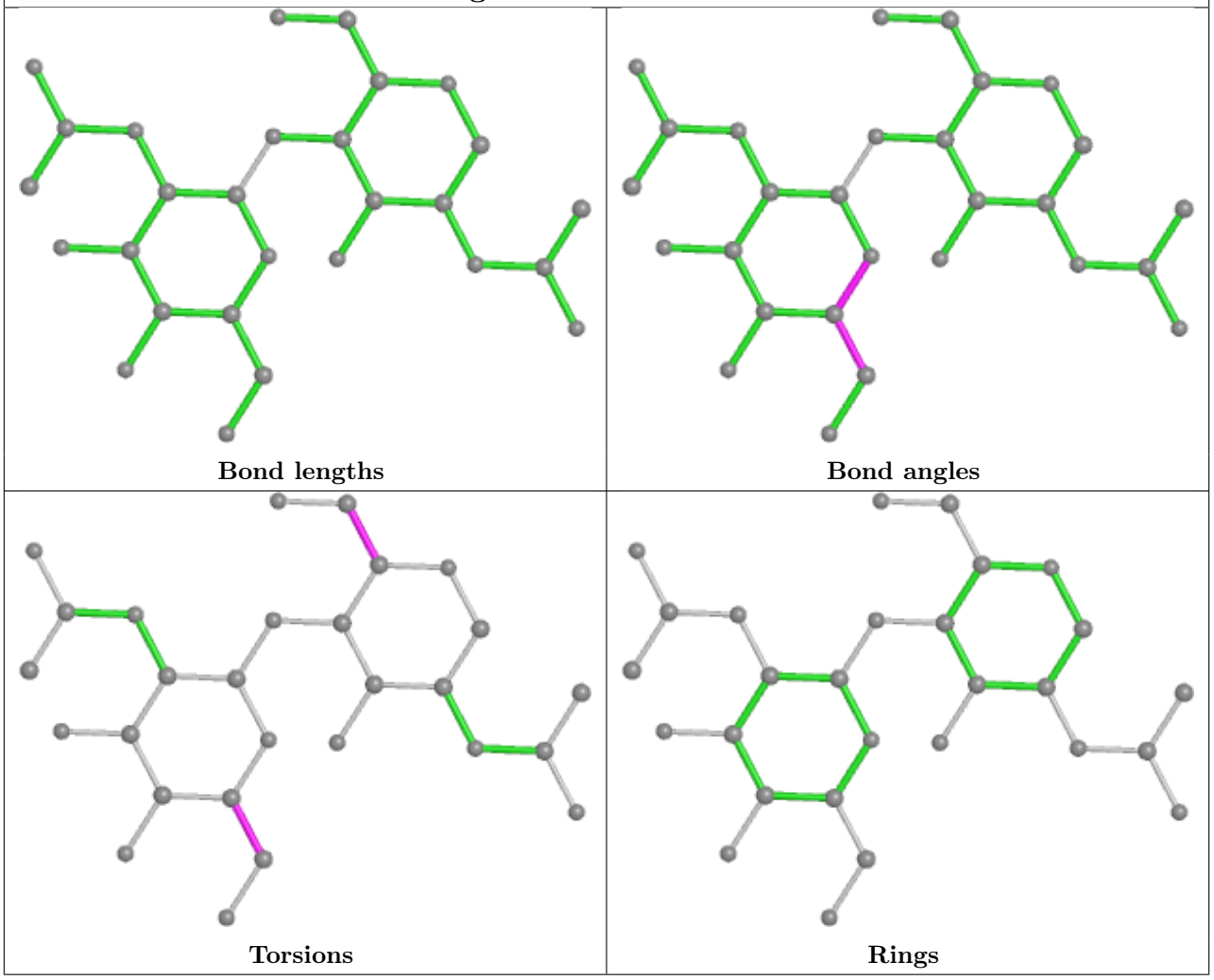


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 2 are monoatomic - leaving 63 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	510	1	14,14,15	0.60	0	17,19,21	1.01	2 (11%)
5	EDO	A	527[A]	-	3,3,3	0.09	0	2,2,2	0.10	0
7	OD0	B	516	-	7,10,10	0.28	0	10,14,14	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	501	-	4,4,4	0.32	0	6,6,6	0.21	0
5	EDO	A	511	-	3,3,3	0.12	0	2,2,2	0.27	0
5	EDO	B	507	-	3,3,3	0.11	0	2,2,2	0.16	0
5	EDO	A	523	-	3,3,3	0.16	0	2,2,2	0.32	0
7	OD0	A	518	-	7,10,10	0.46	0	10,14,14	0.73	0
5	EDO	A	508	-	3,3,3	0.05	0	2,2,2	0.41	0
5	EDO	A	506	-	3,3,3	0.30	0	2,2,2	0.26	0
4	SO4	B	504	-	4,4,4	0.46	0	6,6,6	0.12	0
5	EDO	A	524	-	3,3,3	0.09	0	2,2,2	0.32	0
5	EDO	B	511	-	3,3,3	0.27	0	2,2,2	0.29	0
5	EDO	A	529[B]	-	3,3,3	0.05	0	2,2,2	0.21	0
5	EDO	B	525	-	3,3,3	0.24	0	2,2,2	0.56	0
5	EDO	A	512	-	3,3,3	0.13	0	2,2,2	0.22	0
5	EDO	B	505	-	3,3,3	0.20	0	2,2,2	0.10	0
5	EDO	B	527	-	3,3,3	0.10	0	2,2,2	0.18	0
5	EDO	A	526	-	3,3,3	0.08	0	2,2,2	0.20	0
4	SO4	A	502	-	4,4,4	0.44	0	6,6,6	0.15	0
5	EDO	A	528	-	3,3,3	0.09	0	2,2,2	0.16	0
5	EDO	B	517	-	3,3,3	0.08	0	2,2,2	0.19	0
5	EDO	B	524	-	3,3,3	0.08	0	2,2,2	0.24	0
4	SO4	A	513	-	4,4,4	0.37	0	6,6,6	0.06	0
5	EDO	B	521	-	3,3,3	0.35	0	2,2,2	0.97	0
5	EDO	B	528	-	3,3,3	0.12	0	2,2,2	0.42	0
5	EDO	A	527[B]	-	3,3,3	0.09	0	2,2,2	0.14	0
6	NAG	B	513	1	14,14,15	0.47	0	17,19,21	0.72	0
5	EDO	B	526[A]	-	3,3,3	0.06	0	2,2,2	0.23	0
5	EDO	A	520	-	3,3,3	0.19	0	2,2,2	0.03	0
5	EDO	A	505	-	3,3,3	0.12	0	2,2,2	0.41	0
7	OD0	A	515	-	7,10,10	0.18	0	10,14,14	0.71	0
5	EDO	A	514	-	3,3,3	0.12	0	2,2,2	0.31	0
5	EDO	A	509	-	3,3,3	0.17	0	2,2,2	0.49	0
5	EDO	A	503	-	3,3,3	0.28	0	2,2,2	0.30	0
5	EDO	A	517	-	3,3,3	0.15	0	2,2,2	0.13	0
5	EDO	A	521	-	3,3,3	0.10	0	2,2,2	0.16	0
5	EDO	A	522	-	3,3,3	0.15	0	2,2,2	0.38	0
4	SO4	B	514	-	4,4,4	0.38	0	6,6,6	0.06	0
9	GOL	B	522	-	5,5,5	0.12	0	5,5,5	0.34	0
5	EDO	A	507	-	3,3,3	0.03	0	2,2,2	0.08	0
5	EDO	B	518	-	3,3,3	0.07	0	2,2,2	0.04	0
5	EDO	B	510	-	3,3,3	0.15	0	2,2,2	0.23	0
5	EDO	B	530	-	3,3,3	0.09	0	2,2,2	0.25	0
5	EDO	B	508	-	3,3,3	0.04	0	2,2,2	0.08	0
5	EDO	B	502	-	3,3,3	0.18	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	A	504	-	3,3,3	0.18	0	2,2,2	0.16	0
5	EDO	B	526[B]	-	3,3,3	0.07	0	2,2,2	0.18	0
5	EDO	B	529	-	3,3,3	0.07	0	2,2,2	0.12	0
5	EDO	B	519	-	3,3,3	0.18	0	2,2,2	0.40	0
5	EDO	A	525	-	3,3,3	0.17	0	2,2,2	0.27	0
5	EDO	A	529[A]	-	3,3,3	0.05	0	2,2,2	0.17	0
5	EDO	B	512	-	3,3,3	0.09	0	2,2,2	0.27	0
5	EDO	A	516	-	3,3,3	0.38	0	2,2,2	0.07	0
5	EDO	B	506	-	3,3,3	0.11	0	2,2,2	0.31	0
5	EDO	B	509	-	3,3,3	0.08	0	2,2,2	0.19	0
5	EDO	B	520	-	3,3,3	0.07	0	2,2,2	0.29	0
5	EDO	B	523	-	3,3,3	0.05	0	2,2,2	0.14	0
5	EDO	B	503	-	3,3,3	0.12	0	2,2,2	0.34	0
5	EDO	B	531	-	3,3,3	0.12	0	2,2,2	0.28	0
7	OD0	B	515	-	7,10,10	0.19	0	10,14,14	0.52	0
5	EDO	A	519	-	3,3,3	0.12	0	2,2,2	0.01	0
4	SO4	A	501	-	4,4,4	0.34	0	6,6,6	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	510	1	-	1/6/23/26	0/1/1/1
7	OD0	B	516	-	-	-	0/1/1/1
5	EDO	A	511	-	-	1/1/1/1	-
5	EDO	B	507	-	-	1/1/1/1	-
5	EDO	A	523	-	-	1/1/1/1	-
7	OD0	A	518	-	-	-	0/1/1/1
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	A	524	-	-	1/1/1/1	-
5	EDO	B	511	-	-	0/1/1/1	-
5	EDO	A	529[B]	-	-	1/1/1/1	-
5	EDO	B	525	-	-	1/1/1/1	-
5	EDO	A	512	-	-	0/1/1/1	-
5	EDO	B	505	-	-	1/1/1/1	-
5	EDO	B	527	-	-	1/1/1/1	-
5	EDO	A	526	-	-	1/1/1/1	-
5	EDO	B	517	-	-	0/1/1/1	-
5	EDO	A	528	-	-	0/1/1/1	-
5	EDO	B	524	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	521	-	-	1/1/1/1	-
5	EDO	B	528	-	-	0/1/1/1	-
5	EDO	A	527[B]	-	-	0/1/1/1	-
6	NAG	B	513	1	-	0/6/23/26	0/1/1/1
5	EDO	B	526[A]	-	-	1/1/1/1	-
5	EDO	A	520	-	-	1/1/1/1	-
5	EDO	A	505	-	-	1/1/1/1	-
7	OD0	A	515	-	-	-	0/1/1/1
5	EDO	A	514	-	-	0/1/1/1	-
5	EDO	A	509	-	-	1/1/1/1	-
5	EDO	A	503	-	-	1/1/1/1	-
5	EDO	A	517	-	-	1/1/1/1	-
5	EDO	A	521	-	-	0/1/1/1	-
5	EDO	A	522	-	-	1/1/1/1	-
9	GOL	B	522	-	-	0/4/4/4	-
5	EDO	A	507	-	-	1/1/1/1	-
5	EDO	B	518	-	-	1/1/1/1	-
5	EDO	B	510	-	-	1/1/1/1	-
5	EDO	B	530	-	-	0/1/1/1	-
5	EDO	B	508	-	-	0/1/1/1	-
5	EDO	B	502	-	-	0/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	B	526[B]	-	-	1/1/1/1	-
5	EDO	B	529	-	-	1/1/1/1	-
5	EDO	B	519	-	-	0/1/1/1	-
5	EDO	A	525	-	-	1/1/1/1	-
5	EDO	A	529[A]	-	-	0/1/1/1	-
5	EDO	B	512	-	-	1/1/1/1	-
5	EDO	A	516	-	-	0/1/1/1	-
5	EDO	B	506	-	-	1/1/1/1	-
5	EDO	B	509	-	-	0/1/1/1	-
5	EDO	B	520	-	-	0/1/1/1	-
5	EDO	B	523	-	-	1/1/1/1	-
5	EDO	B	503	-	-	0/1/1/1	-
5	EDO	B	531	-	-	1/1/1/1	-
7	OD0	B	515	-	-	-	0/1/1/1
5	EDO	A	519	-	-	1/1/1/1	-
5	EDO	A	527[A]	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	510	NAG	C1-O5-C5	2.14	115.09	112.19
6	A	510	NAG	O5-C5-C6	2.06	110.43	107.20

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	EDO	O1-C1-C2-O2
5	A	527[A]	EDO	O1-C1-C2-O2
5	A	519	EDO	O1-C1-C2-O2
5	A	522	EDO	O1-C1-C2-O2
5	A	524	EDO	O1-C1-C2-O2
5	B	505	EDO	O1-C1-C2-O2
5	B	507	EDO	O1-C1-C2-O2
5	B	531	EDO	O1-C1-C2-O2
5	B	521	EDO	O1-C1-C2-O2
5	B	526[A]	EDO	O1-C1-C2-O2
5	A	520	EDO	O1-C1-C2-O2
5	B	506	EDO	O1-C1-C2-O2
5	B	518	EDO	O1-C1-C2-O2
5	A	526	EDO	O1-C1-C2-O2
5	B	512	EDO	O1-C1-C2-O2
5	B	527	EDO	O1-C1-C2-O2
5	A	511	EDO	O1-C1-C2-O2
5	A	517	EDO	O1-C1-C2-O2
5	A	525	EDO	O1-C1-C2-O2
5	B	525	EDO	O1-C1-C2-O2
5	A	507	EDO	O1-C1-C2-O2
5	A	509	EDO	O1-C1-C2-O2
5	A	529[B]	EDO	O1-C1-C2-O2
5	B	510	EDO	O1-C1-C2-O2
5	A	503	EDO	O1-C1-C2-O2
5	A	523	EDO	O1-C1-C2-O2
5	B	523	EDO	O1-C1-C2-O2
5	B	526[B]	EDO	O1-C1-C2-O2
5	B	529	EDO	O1-C1-C2-O2
6	A	510	NAG	C4-C5-C6-O6

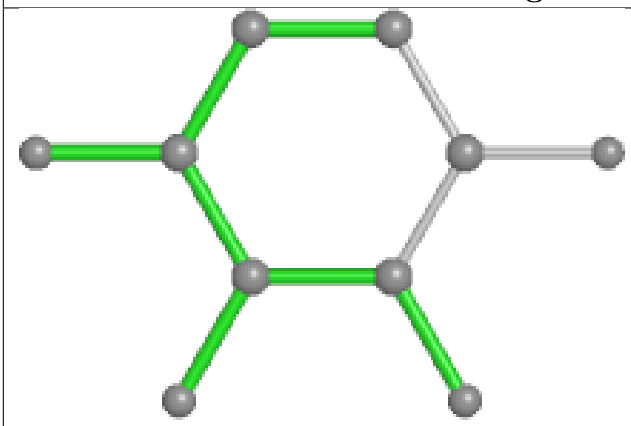
There are no ring outliers.

11 monomers are involved in 17 short contacts:

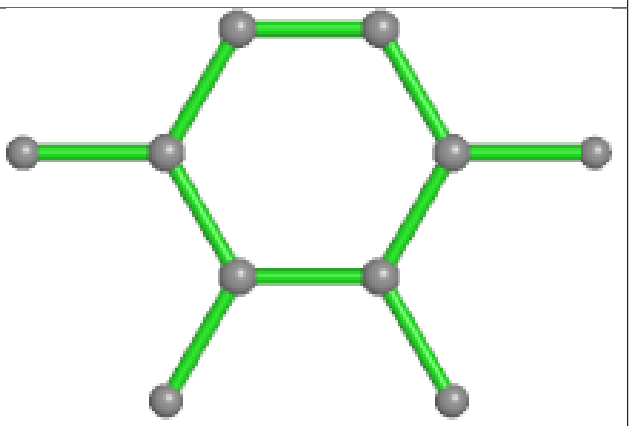
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	523	EDO	2	0
5	A	508	EDO	1	0
5	A	524	EDO	1	0
5	B	511	EDO	1	0
5	B	521	EDO	3	0
5	B	528	EDO	3	0
5	A	509	EDO	1	0
5	A	503	EDO	1	0
5	A	522	EDO	2	0
5	A	525	EDO	4	0
5	A	516	EDO	1	0

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 then 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.

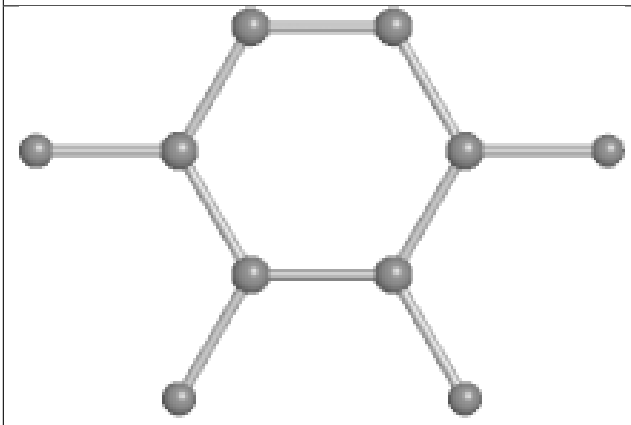
Ligand OD0 B 516



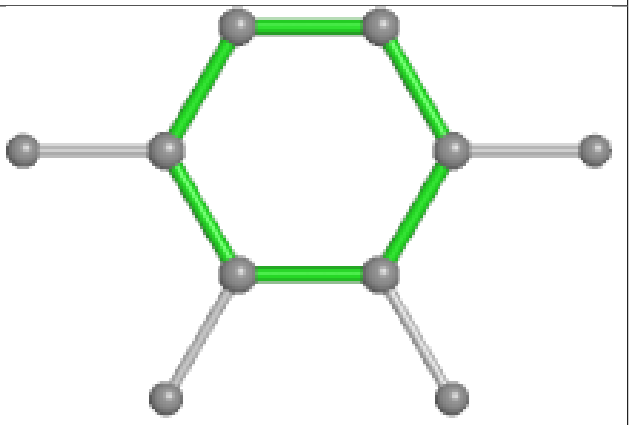
Bond lengths



Bond angles

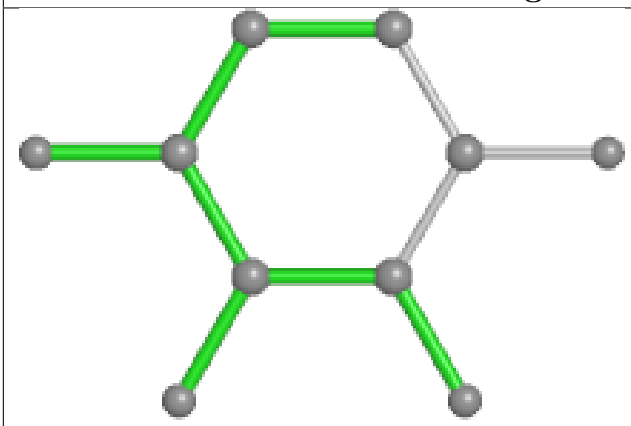


Torsions

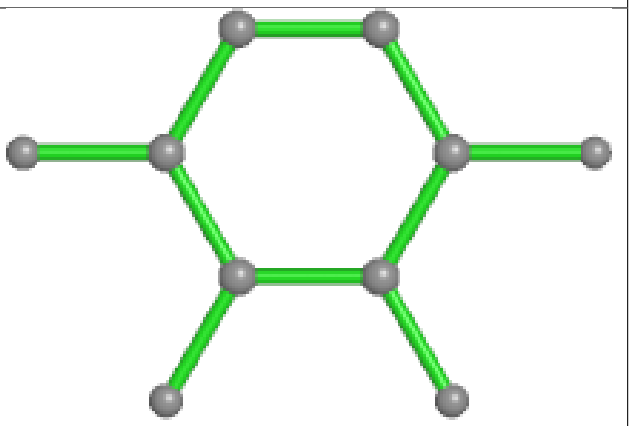


Rings

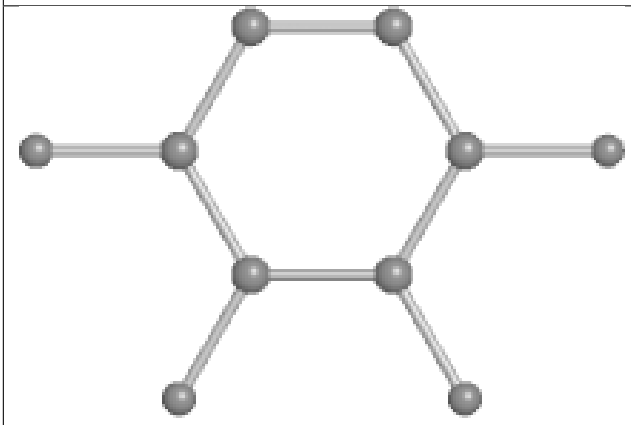
Ligand OD0 A 518



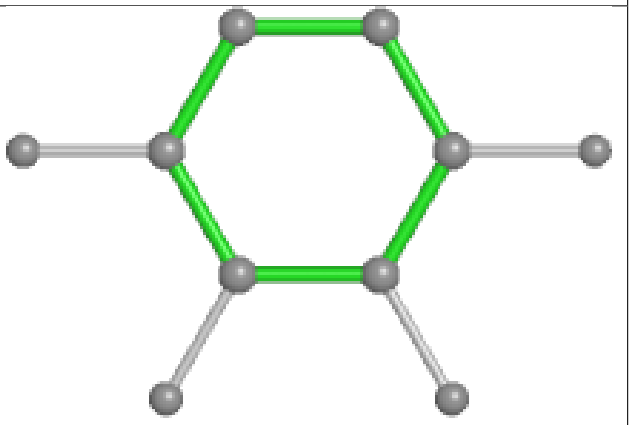
Bond lengths



Bond angles

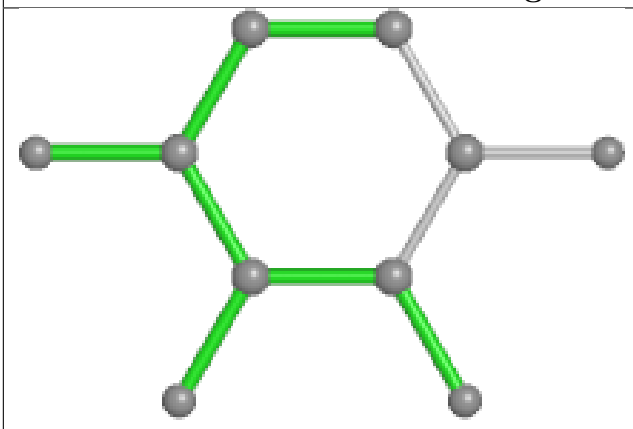


Torsions

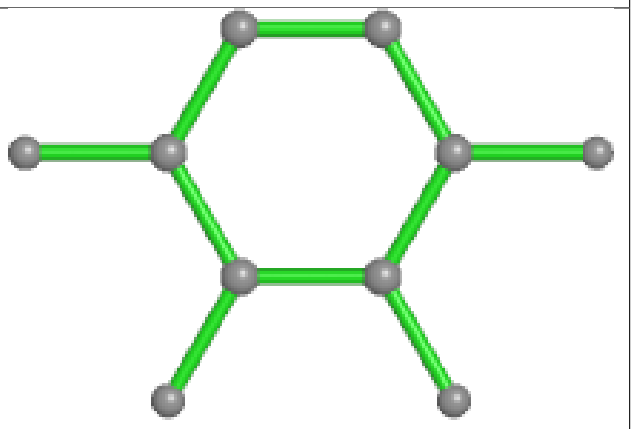


Rings

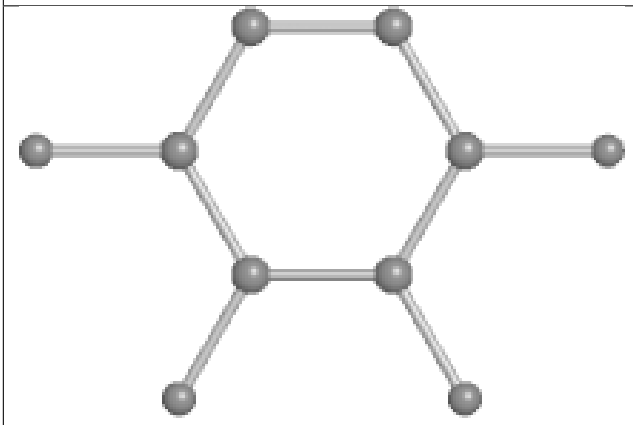
Ligand OD0 A 515



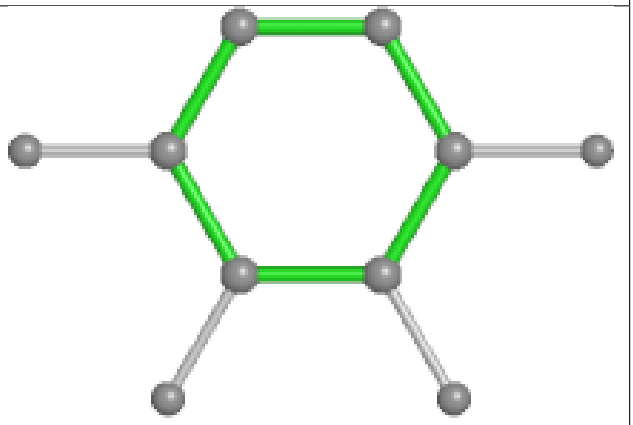
Bond lengths



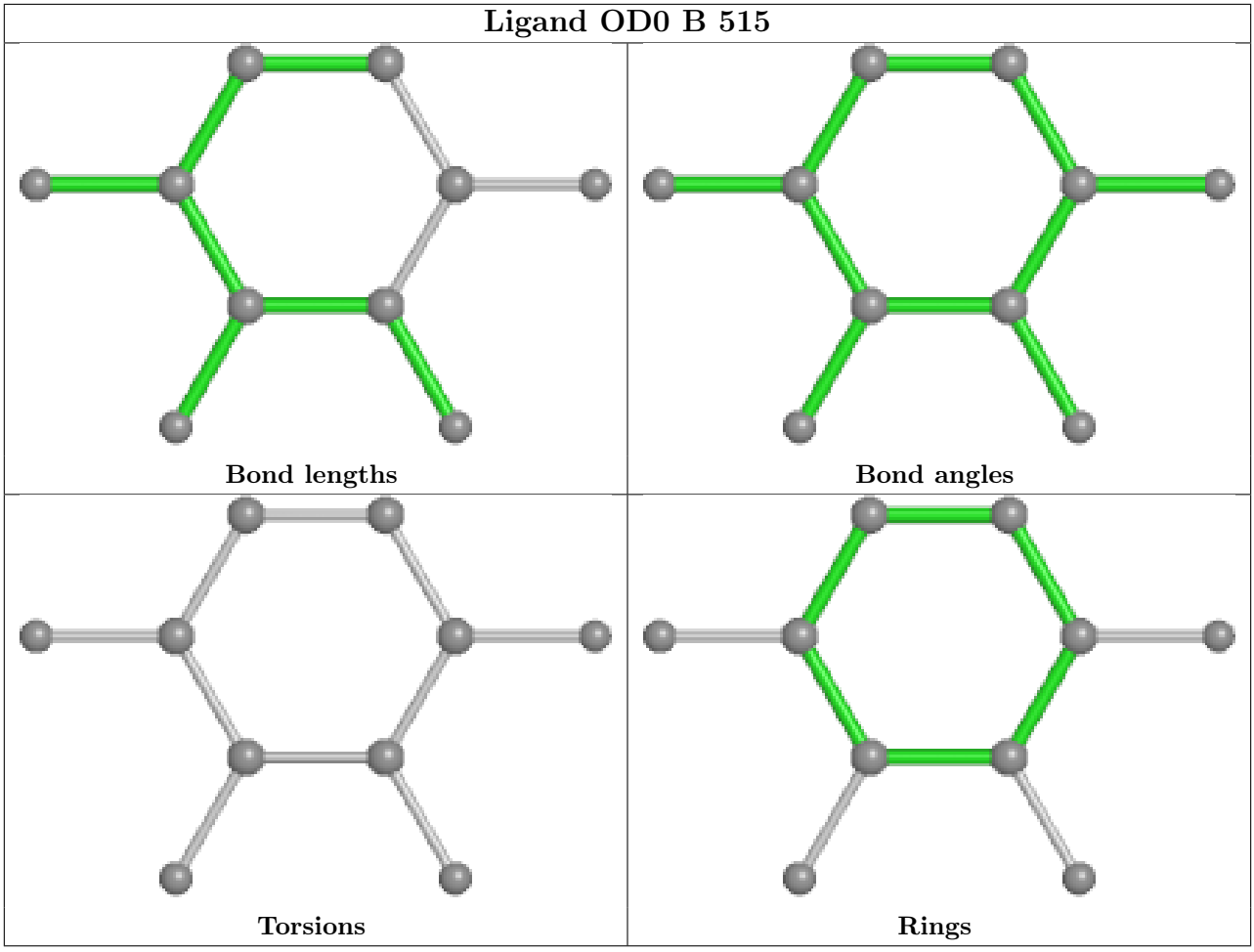
Bond angles



Torsions



Rings



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, 95^{th} 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	497/497 (100%)	-0.21	4 (0%)	86	86	12, 18, 29, 38	3 (0%)
1	B	497/497 (100%)	-0.19	7 (1%)	75	75	14, 20, 31, 48	4 (0%)
All	All	994/994 (100%)	-0.20	11 (1%)	80	80	12, 19, 31, 48	7 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	PHE	5.5
1	B	1	ALA	3.7
1	B	30	THR	2.3
1	B	51	LEU	2.3
1	B	477	VAL	2.3
1	A	31	PHE	2.2
1	A	170[A]	ARG	2.2
1	B	34	LEU	2.1
1	A	30	THR	2.1
1	A	1	ALA	2.1
1	B	29	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

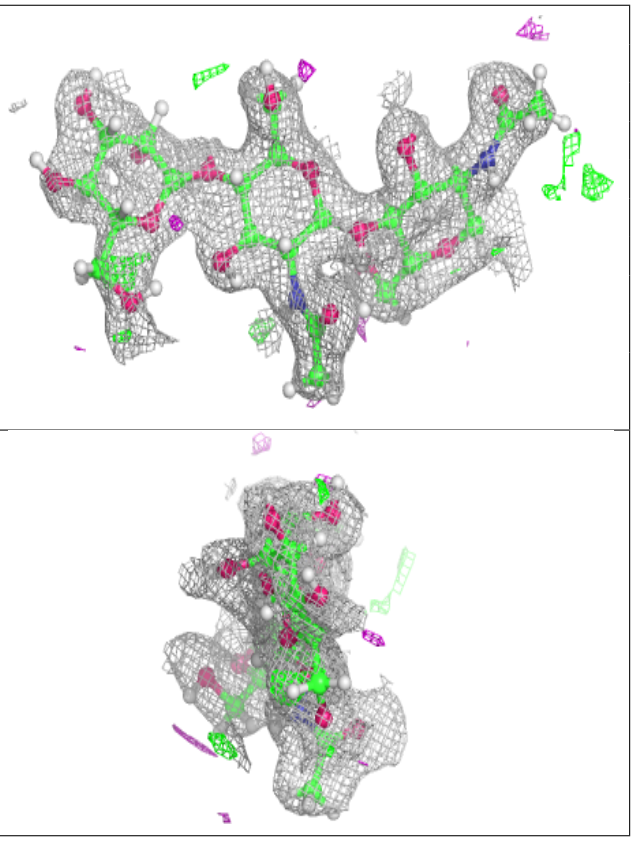
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

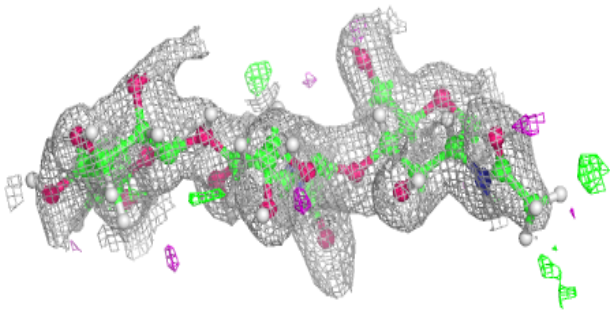
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	1	14/15	0.64	0.26	53,58,61,64	2
2	BMA	C	3	11/12	0.68	0.15	43,44,47,48	22
3	NAG	E	2	14/15	0.74	0.19	39,40,40,42	28
2	BMA	D	3	11/12	0.77	0.16	36,41,42,43	22
2	NAG	C	2	14/15	0.90	0.09	27,32,38,39	2
2	NAG	D	2	14/15	0.92	0.09	26,28,31,34	2
2	NAG	C	1	14/15	0.92	0.08	23,25,27,30	2
2	NAG	D	1	14/15	0.93	0.08	25,26,34,39	2

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:

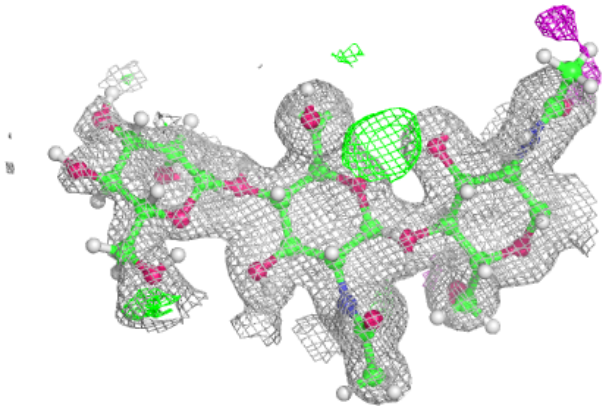
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

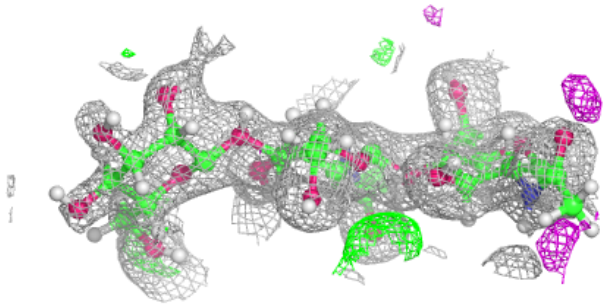


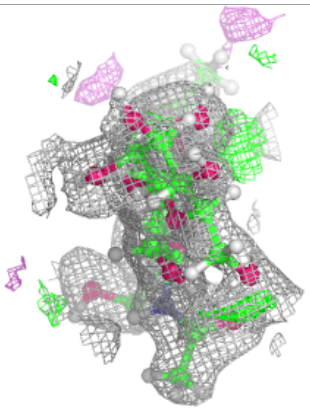


Electron density around Chain D:

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

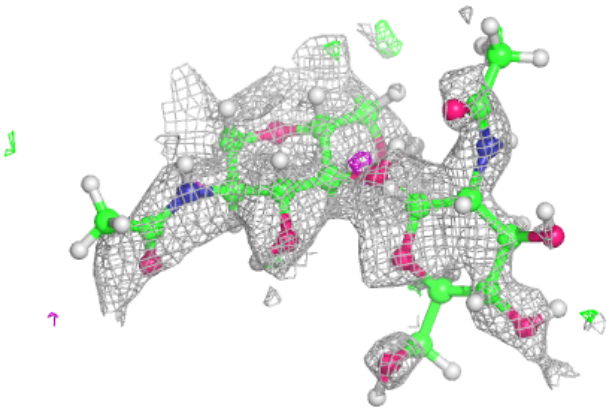


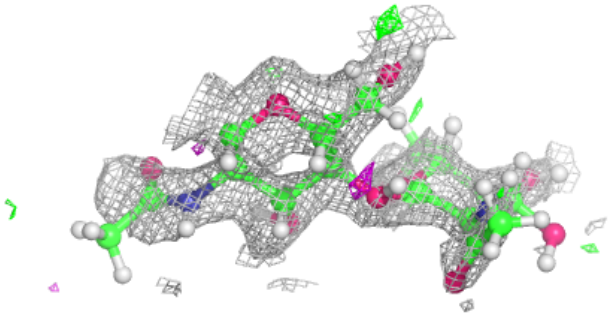


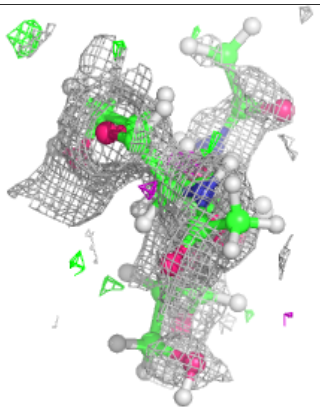


Electron density around Chain E:

$2mF_o$-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, 95^{th} 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	EDO	B	527	4/4	0.63	0.17	50,53,53,54	1
5	EDO	B	531	4/4	0.66	0.22	57,60,64,64	1
6	NAG	A	510	14/15	0.67	0.21	42,49,53,56	3
5	EDO	A	511	4/4	0.69	0.18	38,44,50,51	1
6	NAG	B	513	14/15	0.71	0.22	44,46,48,52	3
5	EDO	B	529	4/4	0.72	0.22	66,70,71,72	1
5	EDO	A	524	4/4	0.76	0.19	37,42,45,45	1
5	EDO	A	512	4/4	0.77	0.15	30,33,35,35	1
5	EDO	A	522	4/4	0.77	0.18	48,50,53,54	1
5	EDO	B	526[B]	4/4	0.79	0.17	43,45,47,48	10
5	EDO	B	503	4/4	0.79	0.14	33,39,42,43	1
5	EDO	B	526[A]	4/4	0.79	0.17	24,26,28,28	10
5	EDO	A	529[B]	4/4	0.80	0.29	25,26,28,28	10
5	EDO	A	521	4/4	0.80	0.18	38,40,42,42	1
5	EDO	A	529[A]	4/4	0.80	0.29	25,26,26,26	10
5	EDO	A	517	4/4	0.81	0.15	51,51,53,54	1
5	EDO	A	509	4/4	0.81	0.12	40,42,44,45	1
5	EDO	B	511	4/4	0.82	0.20	31,33,33,34	1
5	EDO	A	503	4/4	0.83	0.13	27,32,35,35	1
9	GOL	B	522	6/6	0.83	0.13	41,42,45,45	2
5	EDO	A	504	4/4	0.84	0.12	36,41,45,45	1
5	EDO	B	507	4/4	0.85	0.10	43,44,46,48	1
5	EDO	A	508	4/4	0.85	0.22	34,39,43,43	1
5	EDO	B	512	4/4	0.85	0.10	41,42,43,43	1
5	EDO	B	521	4/4	0.85	0.24	31,33,36,38	1
5	EDO	B	502	4/4	0.86	0.12	28,29,32,33	1
5	EDO	A	525	4/4	0.86	0.19	35,36,40,42	1
5	EDO	B	518	4/4	0.87	0.17	44,46,47,47	1
5	EDO	B	517	4/4	0.87	0.12	47,49,50,51	1
5	EDO	A	507	4/4	0.88	0.10	33,37,41,42	1
5	EDO	B	523	4/4	0.88	0.14	44,46,47,47	1
5	EDO	B	505	4/4	0.89	0.10	30,30,31,31	1
5	EDO	A	514	4/4	0.89	0.09	28,33,40,40	1
5	EDO	B	510	4/4	0.90	0.10	30,34,35,35	1
5	EDO	B	530	4/4	0.90	0.22	51,53,55,55	1
5	EDO	A	526	4/4	0.90	0.10	29,35,37,38	1
5	EDO	B	506	4/4	0.91	0.08	35,36,39,39	1

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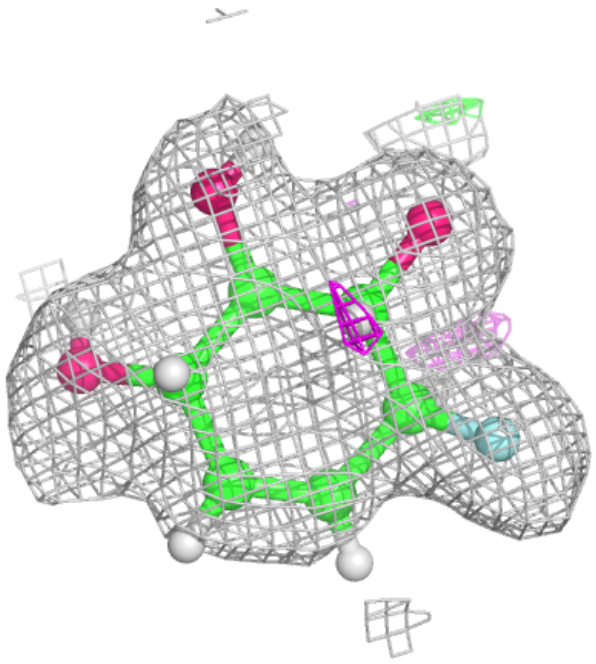
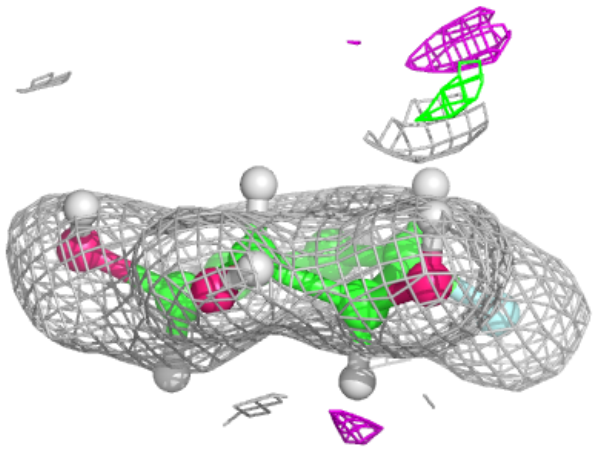
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	505	4/4	0.91	0.08	35,39,40,40	1
5	EDO	B	519	4/4	0.91	0.16	34,37,40,40	1
5	EDO	B	520	4/4	0.91	0.22	37,43,50,50	1
4	SO4	A	513	5/5	0.91	0.13	67,67,68,71	0
5	EDO	A	528	4/4	0.91	0.24	28,33,38,38	1
5	EDO	B	525	4/4	0.91	0.14	27,32,32,32	1
5	EDO	A	520	4/4	0.91	0.14	36,38,42,42	1
5	EDO	B	509	4/4	0.92	0.13	32,37,45,46	1
5	EDO	A	506	4/4	0.92	0.13	26,27,28,28	1
4	SO4	B	514	5/5	0.92	0.10	35,35,36,38	5
5	EDO	A	527[A]	4/4	0.92	0.23	36,37,38,38	10
7	OD0	B	515	10/10	0.92	0.17	31,34,36,36	3
5	EDO	A	527[B]	4/4	0.92	0.23	25,26,29,29	10
7	OD0	A	515	10/10	0.93	0.12	29,32,37,37	3
5	EDO	B	508	4/4	0.94	0.15	29,31,32,32	1
5	EDO	A	516	4/4	0.94	0.09	21,22,22,23	1
5	EDO	A	523	4/4	0.94	0.19	34,38,43,44	1
5	EDO	B	528	4/4	0.94	0.24	32,35,36,37	1
5	EDO	B	524	4/4	0.94	0.07	46,47,48,49	1
8	NA	A	530	1/1	0.94	0.05	33,33,33,33	0
5	EDO	A	519	4/4	0.94	0.07	32,35,36,36	1
10	CA	B	532	1/1	0.96	0.07	55,55,55,55	0
7	OD0	B	516	10/10	0.97	0.06	16,18,19,20	3
7	OD0	A	518	10/10	0.98	0.07	14,15,16,19	3
4	SO4	B	504	5/5	0.98	0.08	30,31,33,33	0
4	SO4	A	501	5/5	0.99	0.07	22,22,24,25	0
4	SO4	B	501	5/5	0.99	0.04	22,23,25,27	0
4	SO4	A	502	5/5	0.99	0.06	27,27,30,31	0

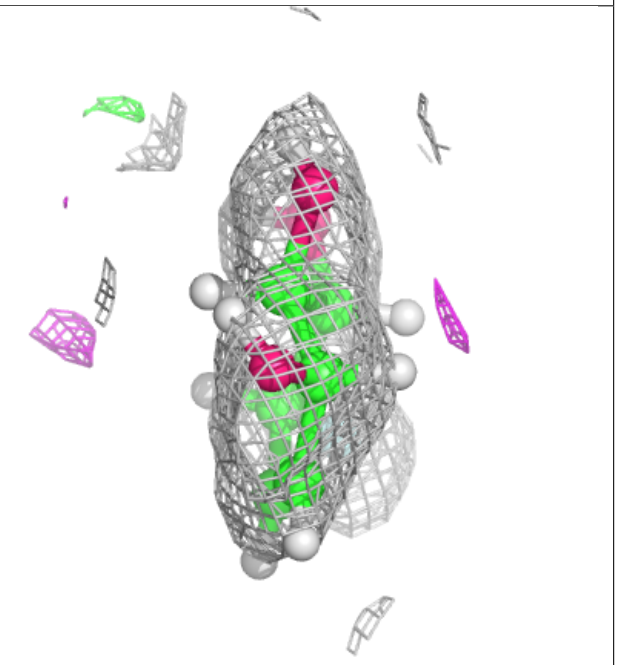
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OD0 B 515:

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

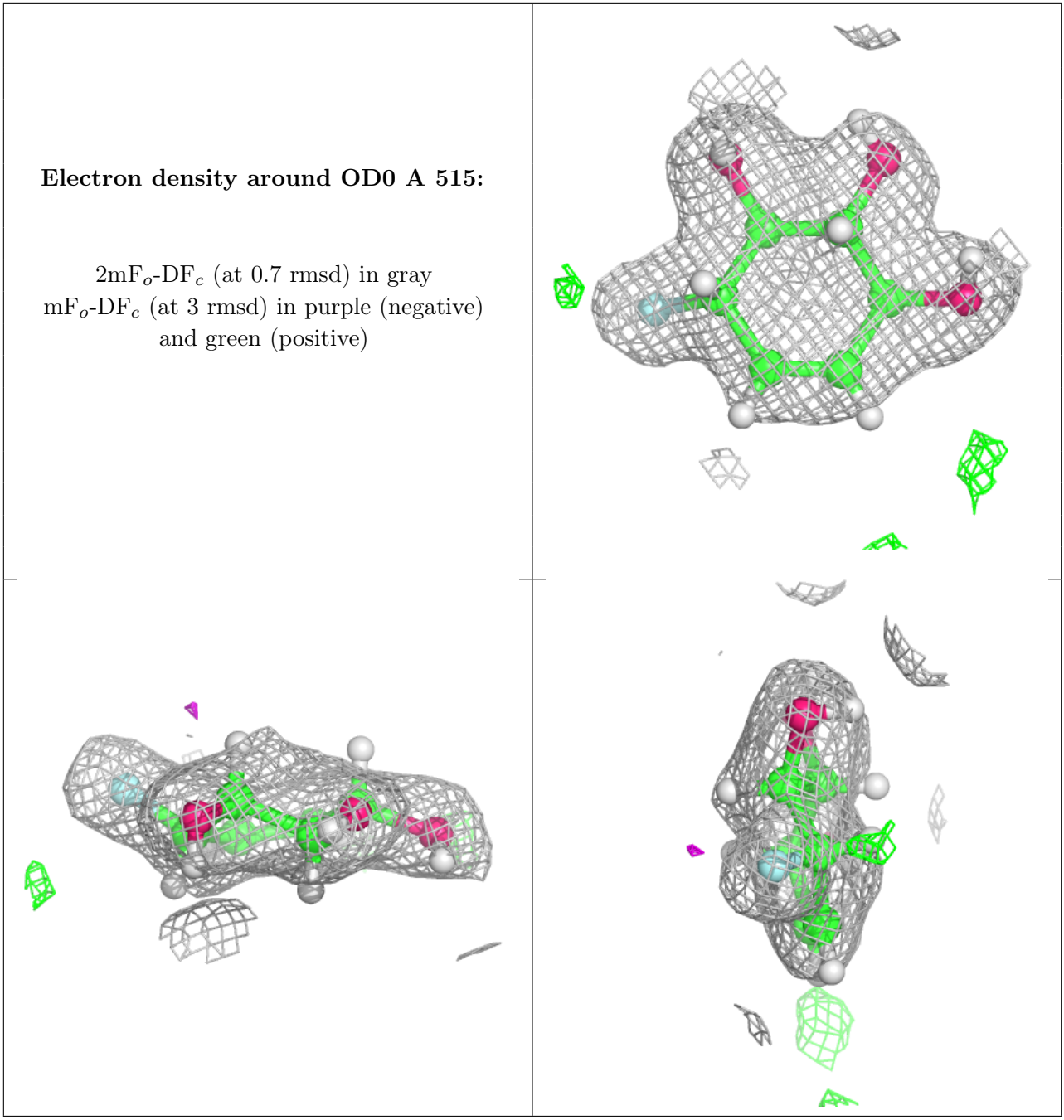






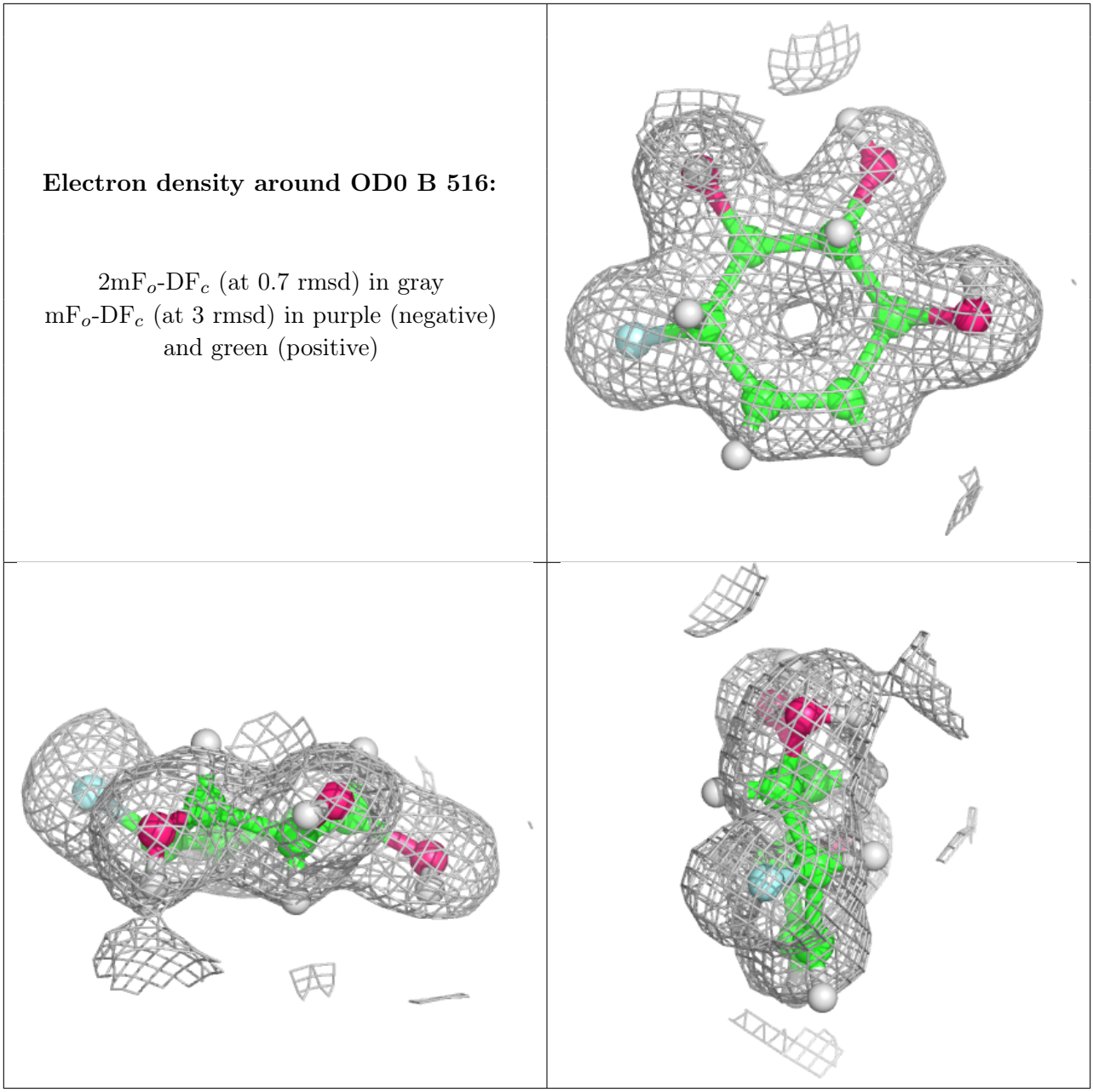
Electron density around OD0 A 515:

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



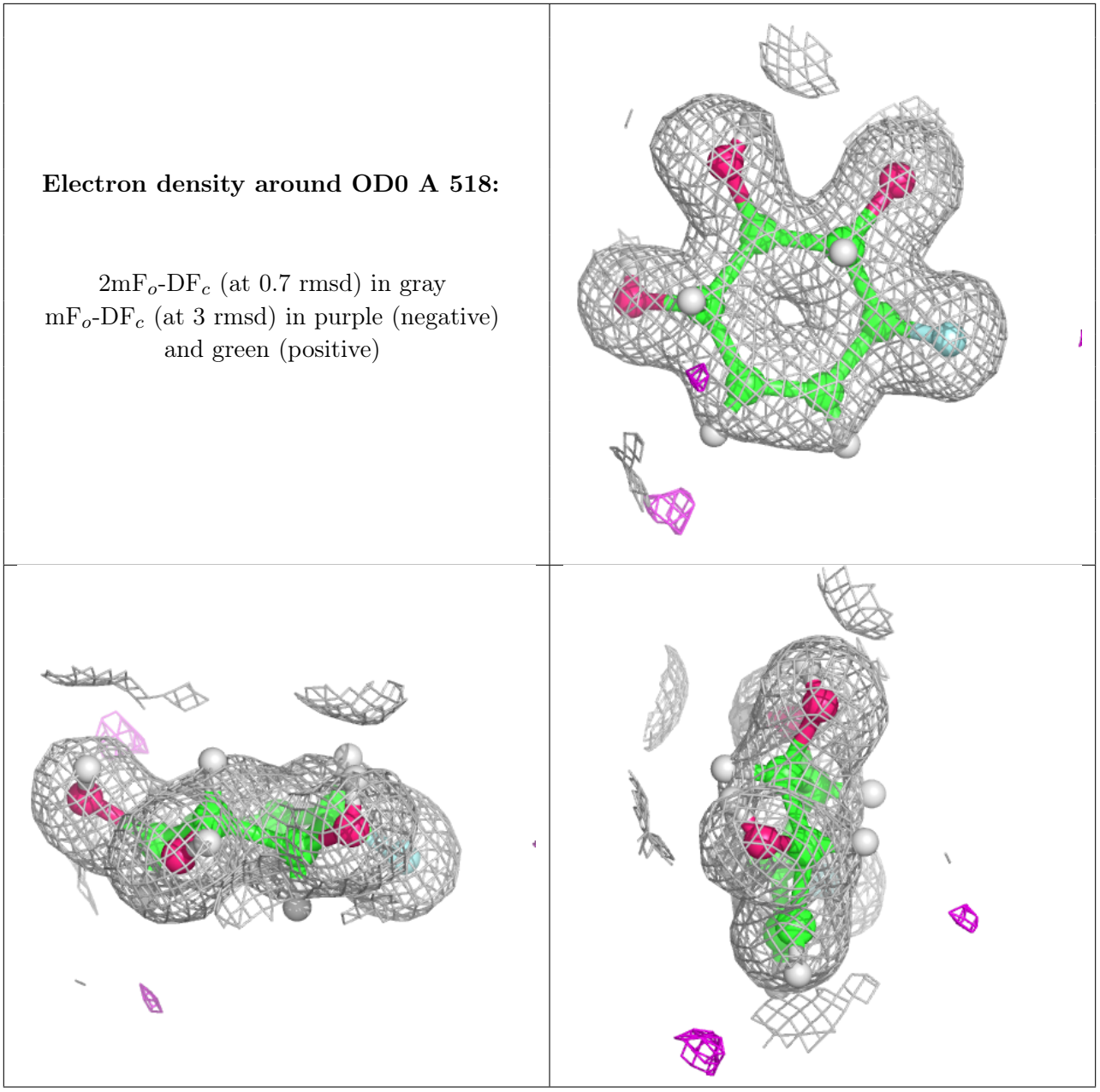
Electron density around OD0 B 516:

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



Electron density around OD0 A 518:

$2mF_o$-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.