



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 09:48 PM UTC

PDB ID : 6YTR / pdb_00006ytr
Title : Structure of recombinant human beta-glucocerebrosidase in complex with cyclophellitol aziridine inhibitor
Authors : Rowland, R.J.; Davies, G.J.
Deposited on : 2020-04-24
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

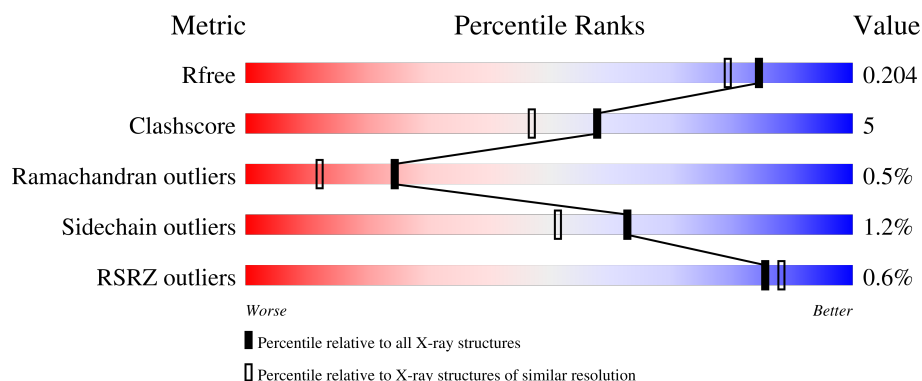
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

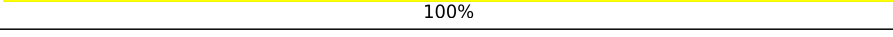
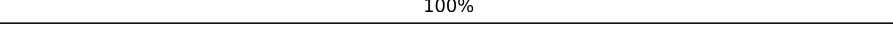
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	AAA	497	 89% 10% .
1	BBB	497	 90% 9% .
2	AdA	4	 50% 50%
3	BdB	3	 100%
4	BuB	2	 100%

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
6	SO4	AAA	521	-	-	X	-
8	EDO	BBB	2727	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17369 atoms, of which 8197 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.

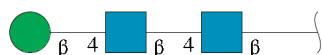
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	497	Total	C	H	N	O	S	208	8	0
			7906	2567	3915	684	724	16			
1	BBB	497	Total	C	H	N	O	S	205	3	0
			7808	2537	3868	672	715	16			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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	AdA	4	Total	C	H	N	O		11	0	0
			98	28	48	2	20				

- Molecule 3 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.



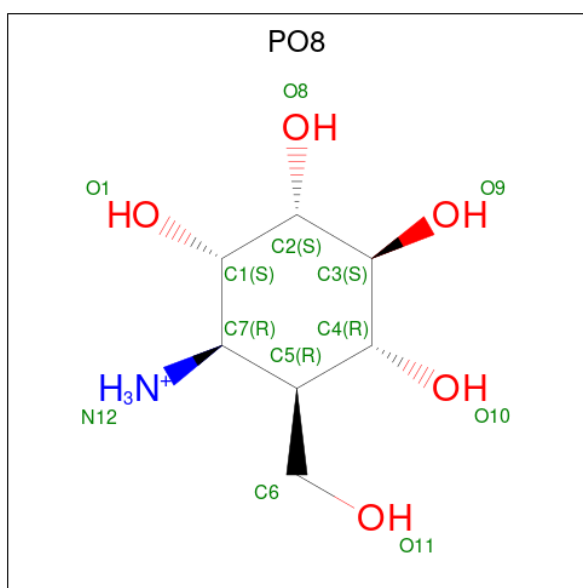
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	BdB	3	Total	C	H	N	O		8	0	0
			76	22	37	2	15				

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



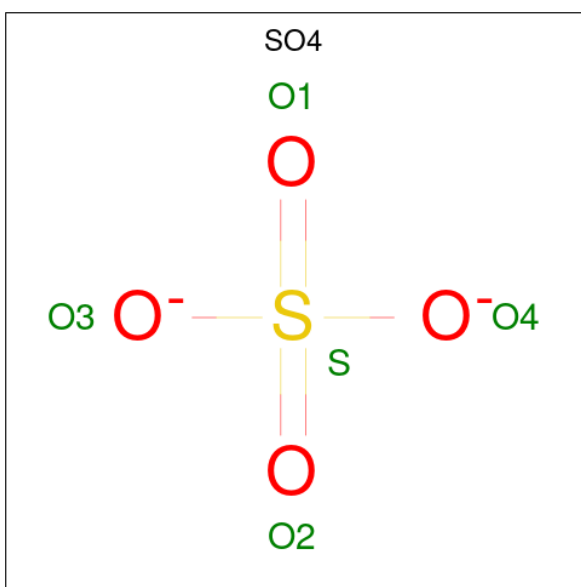
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BuB	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			

- Molecule 5 is (1 {R},2 {S},3 {S},4 {S},5 {R},6 {R})-5-azanyl-6-(hydroxymethyl)cyclohexane-1,2,3,4-tetrol (CCD ID: PO8) (formula: C₇H₁₆NO₅) (labeled as "Ligand of Interest" by depositor).



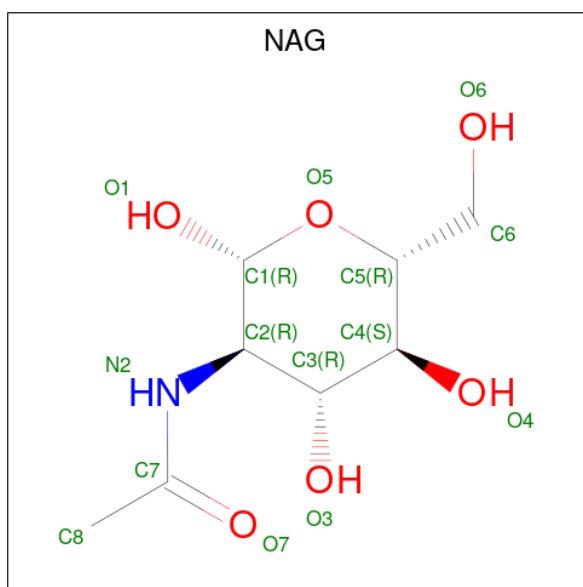
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	H	N	O	3	0
			27	7	15	1	4		
5	BBB	1	Total	C	H	N	O	3	0
			27	7	15	1	4		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



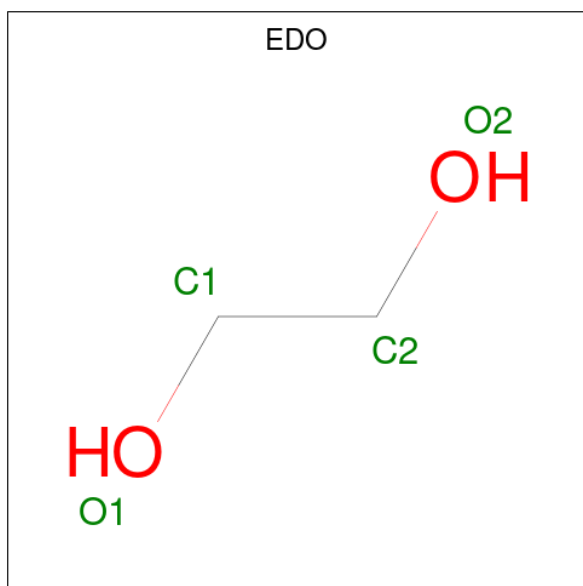
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	BBB	1	Total	O	S	0	0
			5	4	1		
6	BBB	1	Total	O	S	0	0
			5	4	1		
6	BBB	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
8	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
8	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	AAA	1	Total 10	C 2	H 6	O 2	1	0
8	BBB	1	Total 10	C 2	H 6	O 2	1	0
8	BBB	1	Total 10	C 2	H 6	O 2	1	0
8	BBB	1	Total 10	C 2	H 6	O 2	1	0
8	BBB	1	Total 10	C 2	H 6	O 2	1	0
8	BBB	1	Total 20	C 4	H 12	O 4	2	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
8	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	BBB	1	Total 1	Na 1	0	0

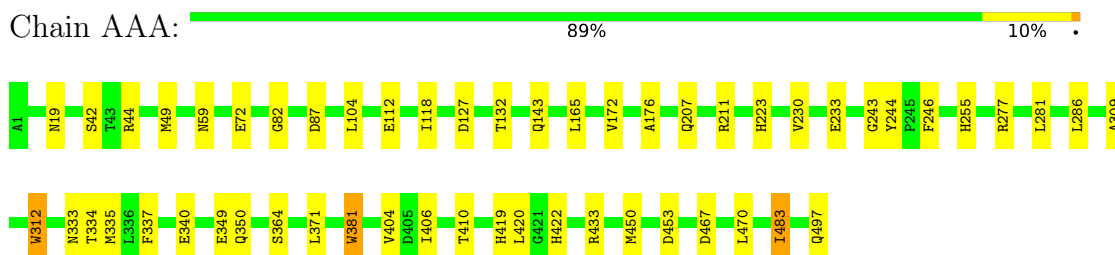
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	468	Total 468	O 468	0	0
10	BBB	409	Total 409	O 409	0	0

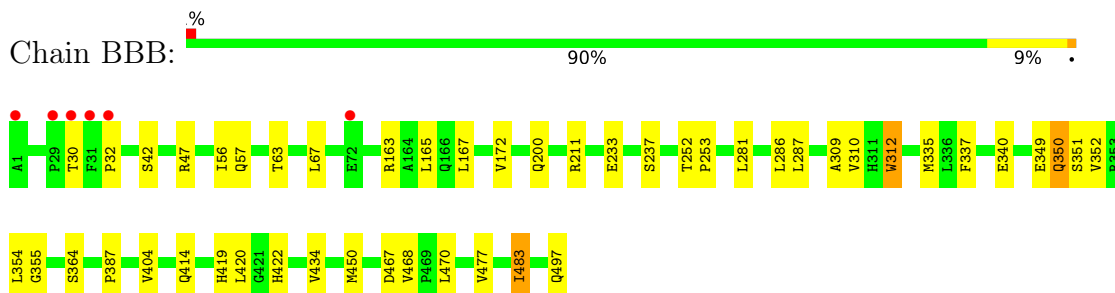
3 Residue-property plots [i](#)

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



- Molecule 1: Lysosomal acid glucosylceramidase



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



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



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

Chain BuB:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.16Å 156.78Å 68.23Å 90.00° 102.12° 90.00°	Depositor
Resolution (Å)	66.80 – 1.70 66.80 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.80-1.70) 99.9 (66.80-1.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.159 , 0.203 0.160 , 0.204	Depositor DCC
R_{free} test set	5927 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17369	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: NA, NAG, PO8, MAN, BMA, SO4, EDO

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	AAA	1.05	2/4111 (0.0%)	1.16	3/5607 (0.1%)
1	BBB	1.04	1/4059 (0.0%)	1.20	1/5538 (0.0%)
All	All	1.04	3/8170 (0.0%)	1.18	4/11145 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	340	GLU	CD-OE2	8.80	1.42	1.25
1	AAA	340	GLU	CD-OE2	8.13	1.40	1.25
1	AAA	49	MET	C-O	5.03	1.30	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	497	GLN	CA-C-O	-6.06	110.50	120.80
1	BBB	350	GLN	CB-CA-C	5.66	118.73	109.90
1	AAA	87	ASP	CA-CB-CG	5.08	117.68	112.60
1	AAA	453	ASP	CA-CB-CG	5.06	117.66	112.60

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	AAA	3991	3915	3882	37	0
1	BBB	3940	3868	3839	34	1
2	AdA	50	48	43	0	0
3	BdB	39	37	34	0	0
4	BuB	28	27	25	0	0
5	AAA	12	15	0	0	0
5	BBB	12	15	0	0	0
6	AAA	20	0	0	3	0
6	BBB	15	0	0	0	0
7	AAA	14	14	13	0	0
8	AAA	76	114	114	11	0
8	BBB	96	144	144	13	0
9	AAA	1	0	0	0	0
9	BBB	1	0	0	0	0
10	AAA	468	0	0	10	0
10	BBB	409	0	0	4	0
All	All	9172	8197	8094	74	1

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 5.

The worst 5 of 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:BBB:349:GLU:HA	8:BBB:2714:EDO:H12	1.63	0.79
1:BBB:56:ILE:HG21	1:BBB:477:VAL:HG12	1.69	0.74
1:BBB:237:SER:OG	8:BBB:2726:EDO:H11	1.88	0.73
1:AAA:165:LEU:HD22	1:AAA:172:VAL:HB	1.71	0.73
1:BBB:211:ARG:NH2	10:BBB:2801:HOH:O	2.20	0.71

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:63:THR:H	1:BBB:200:GLN:HE21[1_554]	1.17	0.43

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	AAA	503/497 (101%)	486 (97%)	14 (3%)	3 (1%)	21	9
1	BBB	498/497 (100%)	475 (95%)	21 (4%)	2 (0%)	30	16
All	All	1001/994 (101%)	961 (96%)	35 (4%)	5 (0%)	24	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	233	GLU
1	BBB	233	GLU
1	AAA	281	LEU
1	AAA	381	TRP
1	BBB	281	LEU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	AAA	428/424 (101%)	422 (99%)	6 (1%)	59	46
1	BBB	423/424 (100%)	419 (99%)	4 (1%)	70	62
All	All	851/848 (100%)	841 (99%)	10 (1%)	63	51

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	335	MET

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Mol	Chain	Res	Type
1	BBB	420	LEU
1	BBB	483	ILE
1	AAA	420	LEU
1	AAA	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

9 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	AdA	1	2,1	14,14,15	0.78	1 (7%)	17,19,21	0.71	0
2	NAG	AdA	2	2	14,14,15	0.60	0	17,19,21	1.47	3 (17%)
2	BMA	AdA	3	2	11,11,12	0.39	0	15,15,17	0.64	0
2	MAN	AdA	4	2	11,11,12	0.61	0	15,15,17	1.01	0
3	NAG	BdB	1	3,1	14,14,15	0.74	0	17,19,21	1.68	3 (17%)
3	NAG	BdB	2	3	14,14,15	0.66	0	17,19,21	1.73	5 (29%)
3	BMA	BdB	3	3	11,11,12	0.62	0	15,15,17	1.76	5 (33%)
4	NAG	BuB	1	1,4	14,14,15	0.60	0	17,19,21	1.13	2 (11%)
4	NAG	BuB	2	4	14,14,15	0.47	0	17,19,21	1.26	3 (17%)

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	AdA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AdA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	AdA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	AdA	4	2	-	0/2/19/22	0/1/1/1
3	NAG	BdB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BdB	2	3	-	0/6/23/26	0/1/1/1
3	BMA	BdB	3	3	-	2/2/19/22	0/1/1/1
4	NAG	BuB	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	BuB	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AdA	1	NAG	C1-C2	2.07	1.55	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BdB	2	NAG	C1-O5-C5	3.93	117.45	112.19
3	BdB	1	NAG	C1-O5-C5	3.91	117.43	112.19
2	AdA	2	NAG	C1-O5-C5	3.36	116.69	112.19
2	AdA	2	NAG	O3-C3-C2	-3.10	102.97	109.40
3	BdB	3	BMA	O5-C5-C4	-2.99	103.56	110.83

There are no chirality outliers.

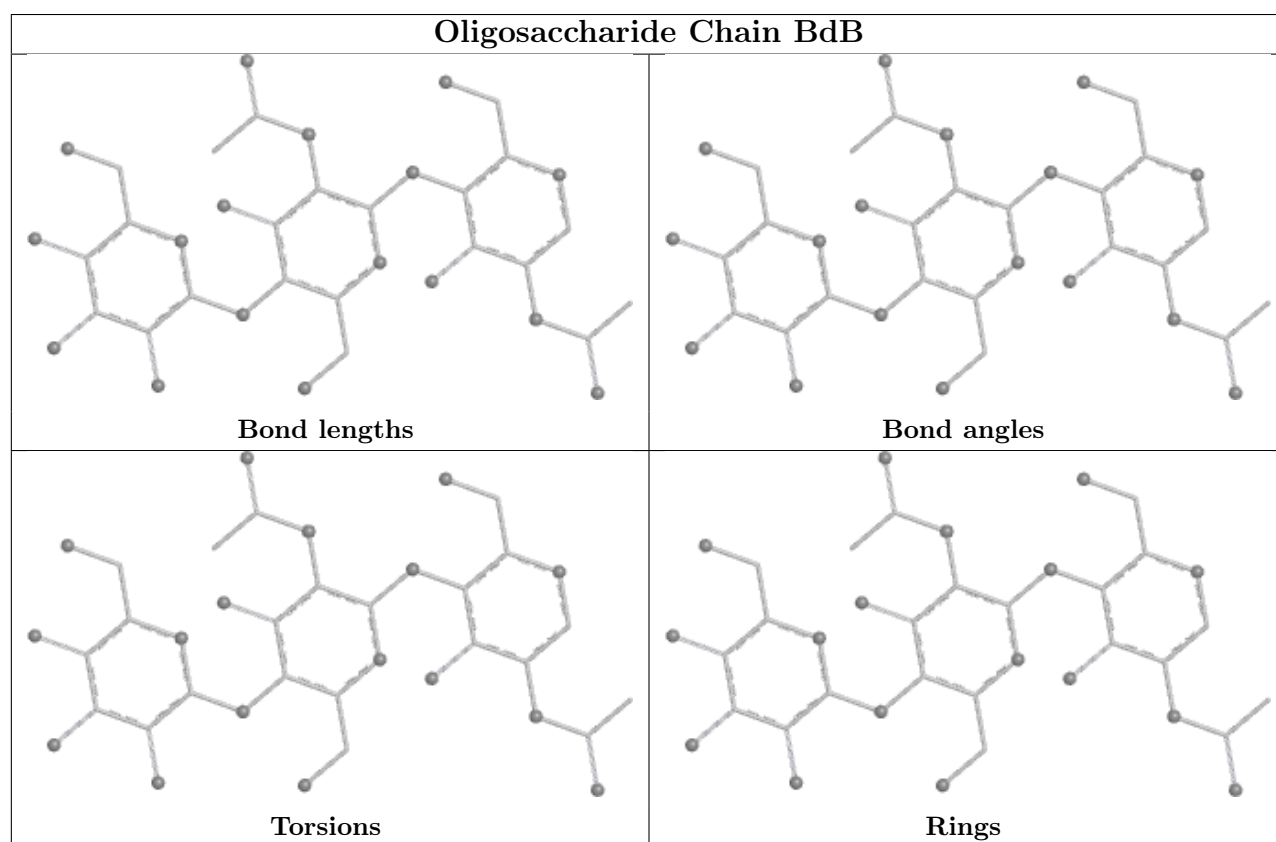
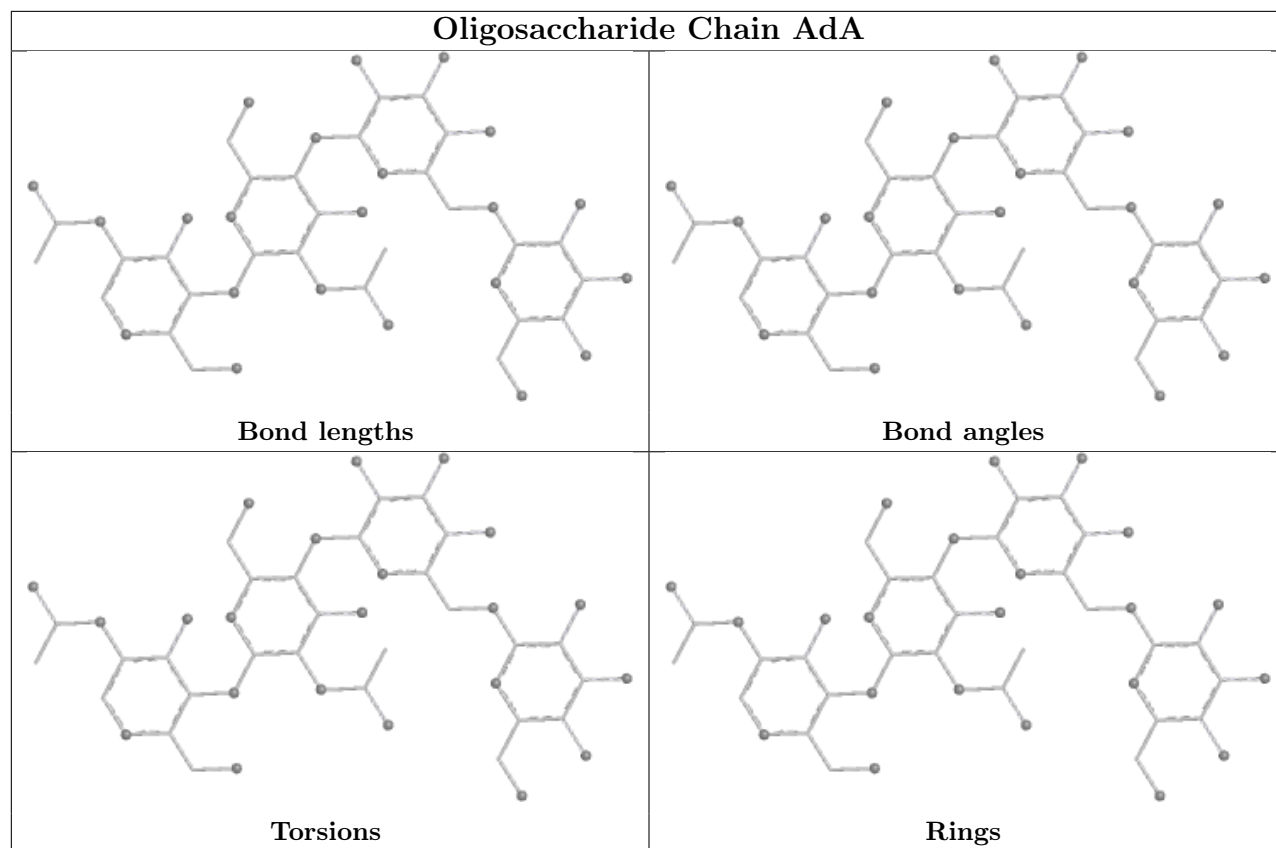
All (2) torsion outliers are listed below:

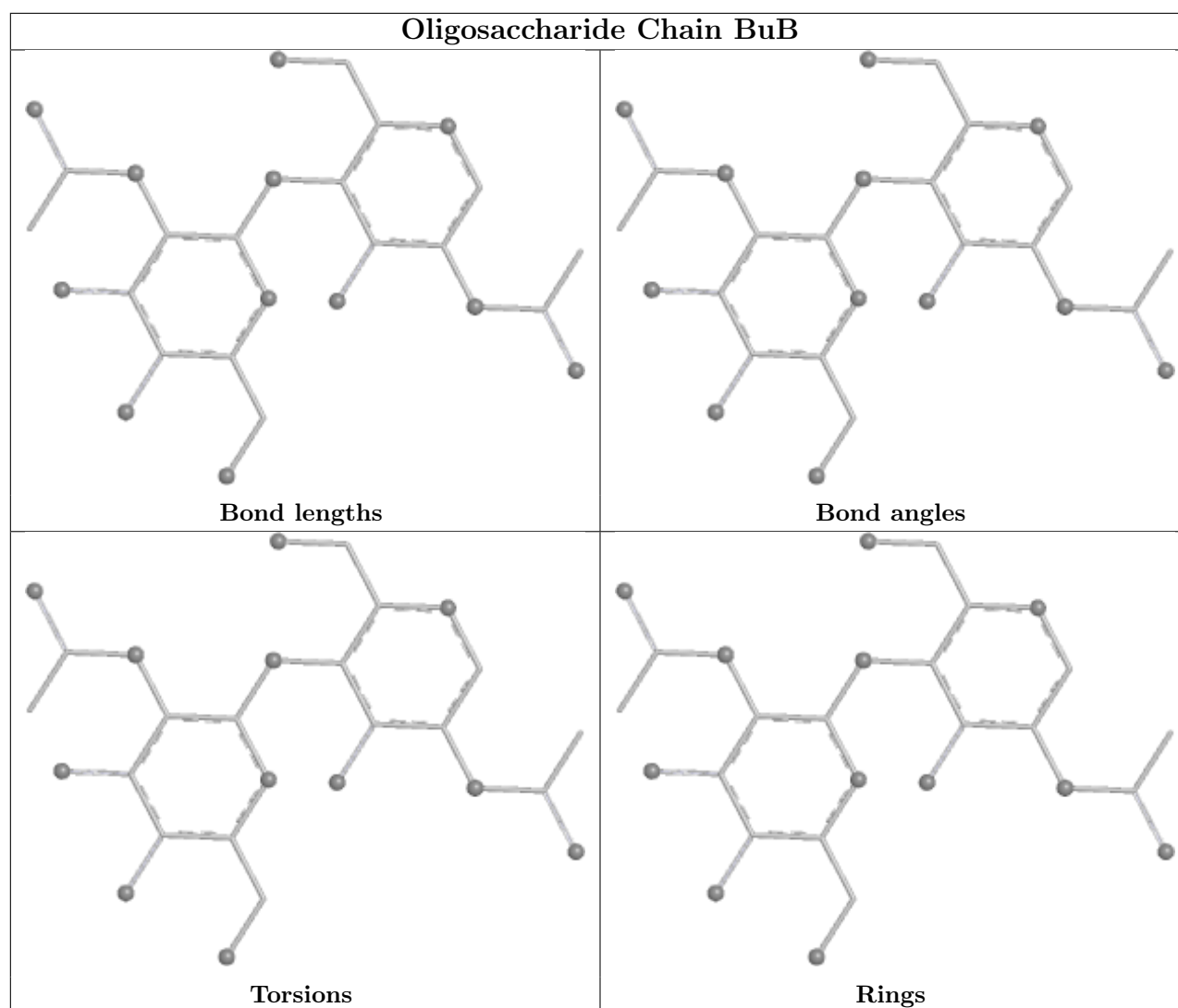
Mol	Chain	Res	Type	Atoms
3	BdB	3	BMA	O5-C5-C6-O6
3	BdB	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 2 are monoatomic - leaving 53 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	$\# Z > 2$
8	EDO	AAA	525	-	3,3,3	0.16	0	2,2,2	0.17	0
7	NAG	AAA	504	1	14,14,15	0.91	0	17,19,21	1.57	2 (11%)
8	EDO	BBB	2708[A]	-	3,3,3	0.21	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	AAA	508	-	3,3,3	0.08	0	2,2,2	0.29	0
8	EDO	AAA	520	-	3,3,3	0.07	0	2,2,2	0.20	0
8	EDO	BBB	2720	-	3,3,3	0.21	0	2,2,2	0.40	0
8	EDO	BBB	2725	-	3,3,3	0.06	0	2,2,2	0.15	0
8	EDO	AAA	513	-	3,3,3	0.14	0	2,2,2	0.17	0
8	EDO	AAA	517	-	3,3,3	0.15	0	2,2,2	0.19	0
6	SO4	BBB	2704	-	4,4,4	0.39	0	6,6,6	0.09	0
6	SO4	BBB	2703	-	4,4,4	0.23	0	6,6,6	0.24	0
8	EDO	BBB	2706	-	3,3,3	0.52	0	2,2,2	0.18	0
8	EDO	BBB	2724	-	3,3,3	0.47	0	2,2,2	0.28	0
8	EDO	BBB	2711	-	3,3,3	0.11	0	2,2,2	0.13	0
8	EDO	BBB	2727	-	3,3,3	0.19	0	2,2,2	0.37	0
8	EDO	AAA	526	-	3,3,3	0.34	0	2,2,2	0.26	0
6	SO4	AAA	521	-	4,4,4	0.45	0	6,6,6	0.18	0
8	EDO	BBB	2712	-	3,3,3	0.26	0	2,2,2	0.11	0
8	EDO	AAA	512	-	3,3,3	0.20	0	2,2,2	0.10	0
8	EDO	AAA	518	-	3,3,3	0.13	0	2,2,2	0.14	0
6	SO4	AAA	510	-	4,4,4	0.29	0	6,6,6	0.08	0
8	EDO	AAA	524	-	3,3,3	0.12	0	2,2,2	0.04	0
8	EDO	AAA	516	-	3,3,3	0.07	0	2,2,2	0.18	0
8	EDO	BBB	2708[B]	-	3,3,3	0.19	0	2,2,2	0.24	0
8	EDO	BBB	2709	-	3,3,3	0.46	0	2,2,2	0.29	0
8	EDO	BBB	2701	-	3,3,3	0.09	0	2,2,2	0.05	0
6	SO4	BBB	2721	-	4,4,4	0.29	0	6,6,6	0.12	0
8	EDO	AAA	515	-	3,3,3	0.52	0	2,2,2	0.60	0
8	EDO	AAA	514	-	3,3,3	0.26	0	2,2,2	0.61	0
5	PO8	BBB	2702	1	12,12,13	1.12	2 (16%)	14,17,19	1.12	1 (7%)
8	EDO	BBB	2717	-	3,3,3	0.06	0	2,2,2	0.18	0
8	EDO	BBB	2705	-	3,3,3	0.08	0	2,2,2	0.17	0
8	EDO	BBB	2728	-	3,3,3	0.10	0	2,2,2	0.18	0
8	EDO	BBB	2718	-	3,3,3	0.06	0	2,2,2	0.13	0
8	EDO	AAA	519	-	3,3,3	0.21	0	2,2,2	0.39	0
8	EDO	BBB	2715	-	3,3,3	0.05	0	2,2,2	0.11	0
8	EDO	BBB	2713	-	3,3,3	0.19	0	2,2,2	0.11	0
8	EDO	AAA	506	-	3,3,3	0.68	0	2,2,2	0.35	0
8	EDO	BBB	2716	-	3,3,3	0.19	0	2,2,2	0.10	0
5	PO8	AAA	501	1	12,12,13	0.91	0	14,17,19	1.30	1 (7%)
8	EDO	AAA	511	-	3,3,3	0.28	0	2,2,2	0.55	0
8	EDO	AAA	507	-	3,3,3	0.12	0	2,2,2	0.11	0
6	SO4	AAA	502	-	4,4,4	0.31	0	6,6,6	0.42	0
8	EDO	AAA	505	-	3,3,3	0.18	0	2,2,2	0.20	0
8	EDO	BBB	2723	-	3,3,3	0.10	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	AAA	523	-	3,3,3	0.17	0	2,2,2	0.10	0
8	EDO	BBB	2714	-	3,3,3	0.10	0	2,2,2	0.51	0
8	EDO	BBB	2719	-	3,3,3	0.17	0	2,2,2	0.09	0
8	EDO	BBB	2707	-	3,3,3	0.15	0	2,2,2	0.18	0
6	SO4	AAA	503	-	4,4,4	0.30	0	6,6,6	0.26	0
8	EDO	BBB	2710	-	3,3,3	0.14	0	2,2,2	0.10	0
8	EDO	AAA	509	-	3,3,3	0.21	0	2,2,2	0.21	0
8	EDO	BBB	2726	-	3,3,3	0.37	0	2,2,2	0.25	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
8	EDO	AAA	525	-	-	0/1/1/1	-
7	NAG	AAA	504	1	-	0/6/23/26	0/1/1/1
8	EDO	BBB	2708[A]	-	-	0/1/1/1	-
8	EDO	AAA	508	-	-	1/1/1/1	-
8	EDO	AAA	520	-	-	0/1/1/1	-
8	EDO	BBB	2720	-	-	0/1/1/1	-
8	EDO	BBB	2725	-	-	1/1/1/1	-
8	EDO	AAA	513	-	-	1/1/1/1	-
8	EDO	AAA	517	-	-	1/1/1/1	-
8	EDO	BBB	2706	-	-	0/1/1/1	-
8	EDO	BBB	2724	-	-	0/1/1/1	-
8	EDO	BBB	2711	-	-	0/1/1/1	-
8	EDO	BBB	2727	-	-	1/1/1/1	-
8	EDO	AAA	526	-	-	0/1/1/1	-
8	EDO	BBB	2712	-	-	1/1/1/1	-
8	EDO	AAA	512	-	-	0/1/1/1	-
8	EDO	AAA	518	-	-	1/1/1/1	-
8	EDO	AAA	524	-	-	1/1/1/1	-
8	EDO	AAA	516	-	-	0/1/1/1	-
8	EDO	BBB	2708[B]	-	-	1/1/1/1	-
8	EDO	BBB	2709	-	-	1/1/1/1	-
8	EDO	BBB	2701	-	-	0/1/1/1	-
8	EDO	AAA	515	-	-	1/1/1/1	-
8	EDO	AAA	514	-	-	1/1/1/1	-
5	PO8	BBB	2702	1	-	0/2/22/26	0/1/1/1
8	EDO	BBB	2717	-	-	0/1/1/1	-
8	EDO	BBB	2705	-	-	0/1/1/1	-
8	EDO	BBB	2728	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	BBB	2718	-	-	1/1/1/1	-
8	EDO	AAA	519	-	-	0/1/1/1	-
8	EDO	BBB	2715	-	-	1/1/1/1	-
8	EDO	BBB	2713	-	-	1/1/1/1	-
8	EDO	AAA	506	-	-	0/1/1/1	-
8	EDO	BBB	2716	-	-	1/1/1/1	-
5	PO8	AAA	501	1	-	0/2/22/26	0/1/1/1
8	EDO	AAA	511	-	-	1/1/1/1	-
8	EDO	AAA	507	-	-	1/1/1/1	-
8	EDO	AAA	505	-	-	1/1/1/1	-
8	EDO	BBB	2723	-	-	1/1/1/1	-
8	EDO	AAA	523	-	-	1/1/1/1	-
8	EDO	BBB	2714	-	-	1/1/1/1	-
8	EDO	BBB	2719	-	-	1/1/1/1	-
8	EDO	BBB	2707	-	-	1/1/1/1	-
8	EDO	BBB	2710	-	-	1/1/1/1	-
8	EDO	AAA	509	-	-	0/1/1/1	-
8	EDO	BBB	2726	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	BBB	2702	PO8	C5-C4	-2.36	1.50	1.53
5	BBB	2702	PO8	C1-C2	2.20	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AAA	504	NAG	C2-N2-C7	3.23	127.23	122.90
5	BBB	2702	PO8	C2-C1-C7	-3.03	106.44	112.65
5	AAA	501	PO8	C2-C1-C7	-2.93	106.66	112.65
7	AAA	504	NAG	C1-O5-C5	2.40	115.40	112.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AAA	511	EDO	O1-C1-C2-O2
8	AAA	513	EDO	O1-C1-C2-O2
8	BBB	2712	EDO	O1-C1-C2-O2
8	BBB	2714	EDO	O1-C1-C2-O2
8	AAA	507	EDO	O1-C1-C2-O2

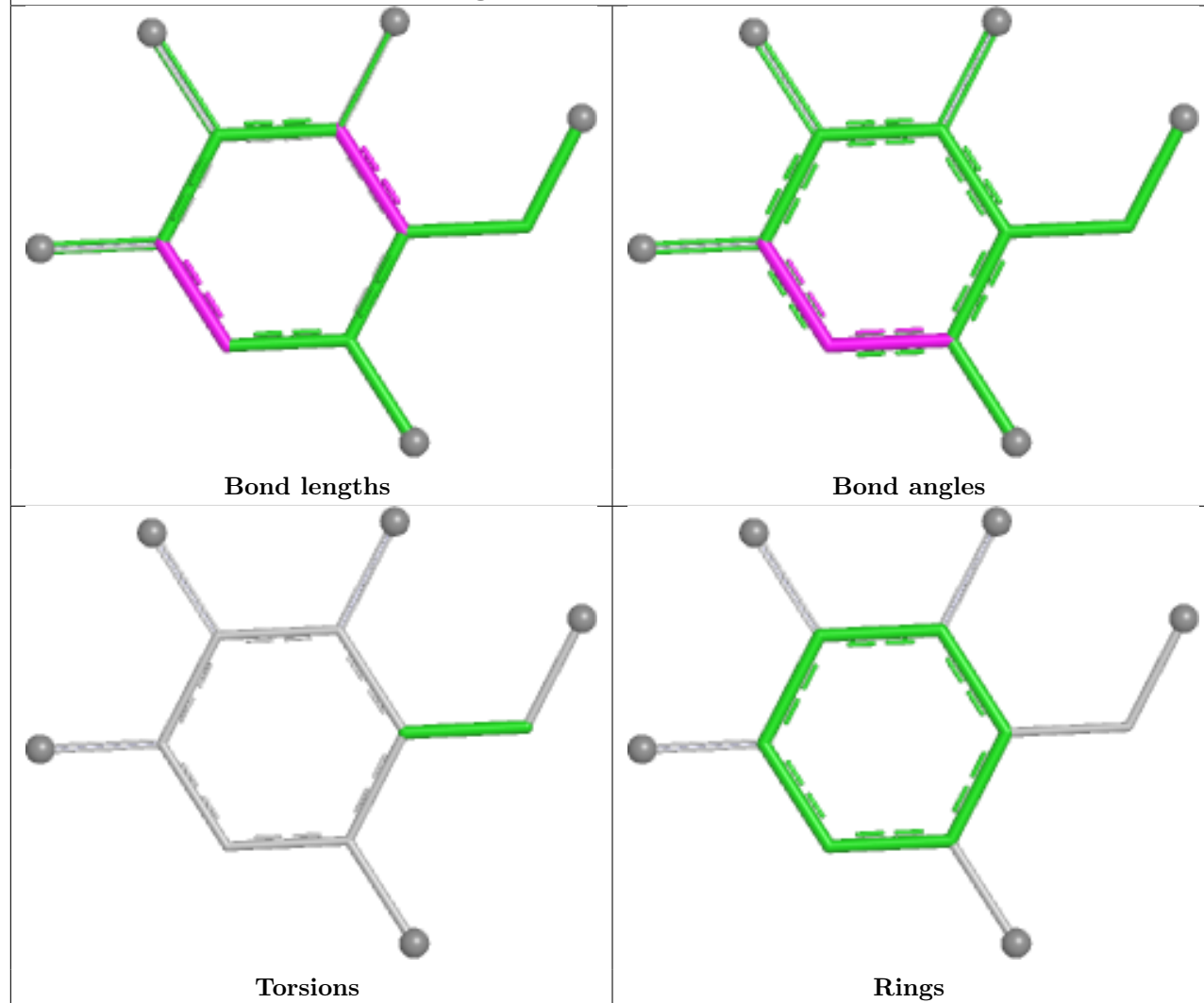
There are no ring outliers.

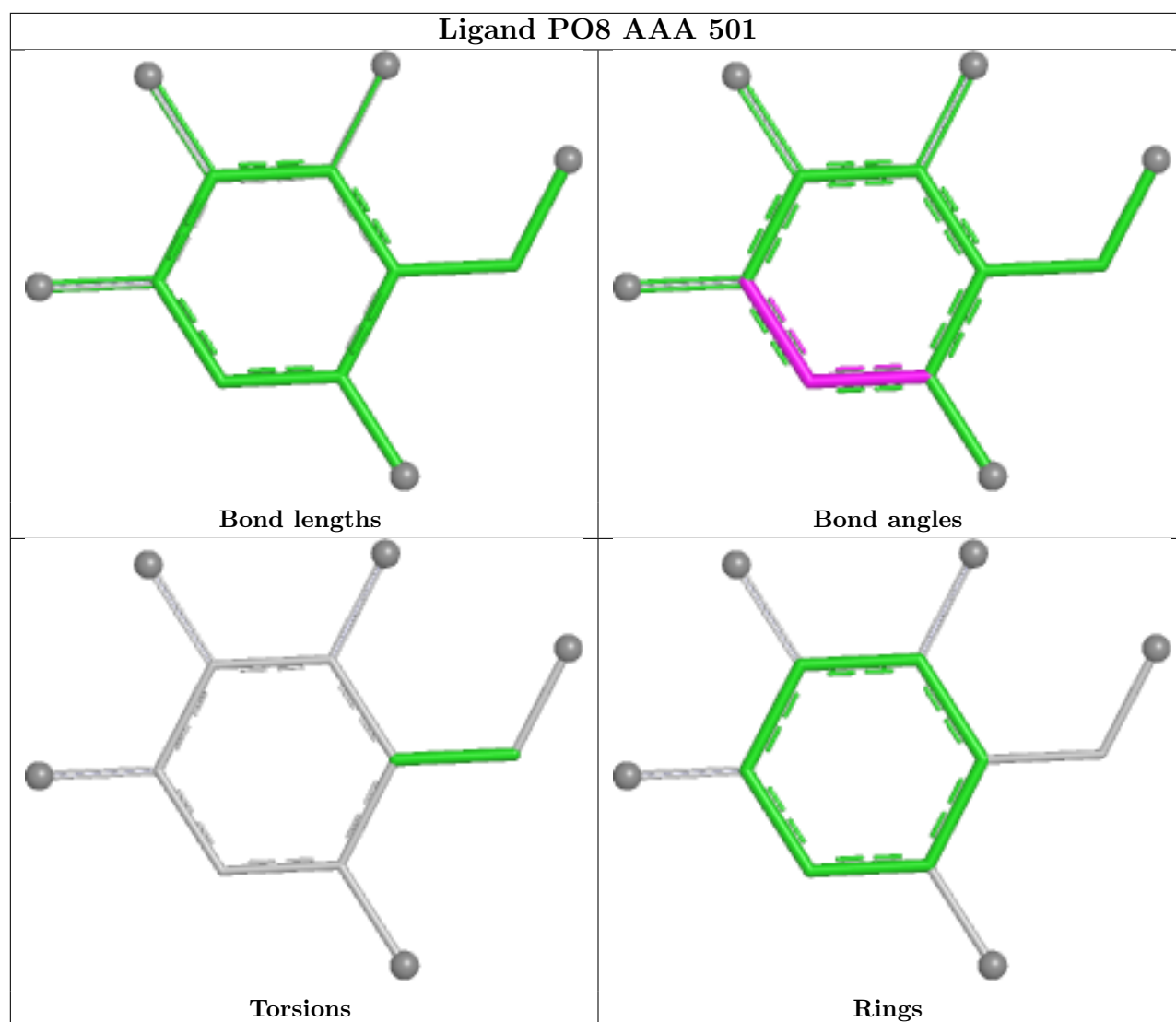
16 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	AAA	525	EDO	2	0
8	AAA	508	EDO	3	0
8	BBB	2706	EDO	1	0
8	BBB	2727	EDO	4	0
6	AAA	521	SO4	3	0
8	BBB	2712	EDO	1	0
8	AAA	518	EDO	1	0
8	BBB	2709	EDO	2	0
8	BBB	2701	EDO	1	0
8	AAA	514	EDO	1	0
8	AAA	519	EDO	1	0
8	AAA	506	EDO	1	0
8	AAA	505	EDO	2	0
8	BBB	2714	EDO	2	0
8	BBB	2719	EDO	1	0
8	BBB	2726	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 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 PO8 BBB 2702





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 [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	AAA	497/497 (100%)	-0.50	0 100 100	10, 21, 34, 47	9 (1%)
1	BBB	497/497 (100%)	-0.33	6 (1%) 76 80	13, 25, 38, 58	8 (1%)
All	All	994/994 (100%)	-0.42	6 (0%) 85 88	10, 23, 37, 58	17 (1%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	31	PHE	11.0
1	BBB	29	PRO	9.8
1	BBB	30	THR	5.2
1	BBB	32	PRO	3.3
1	BBB	1	ALA	2.5

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	AdA	1	14/15	-	-	25,29,31,33	2
2	NAG	AdA	2	14/15	-	-	31,36,42,48	2
2	BMA	AdA	3	11/12	-	-	58,63,65,67	3
2	MAN	AdA	4	11/12	-	-	62,72,79,81	4
3	NAG	BdB	1	14/15	-	-	28,31,40,44	2

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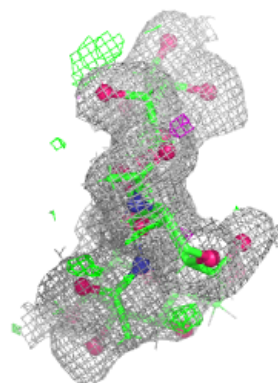
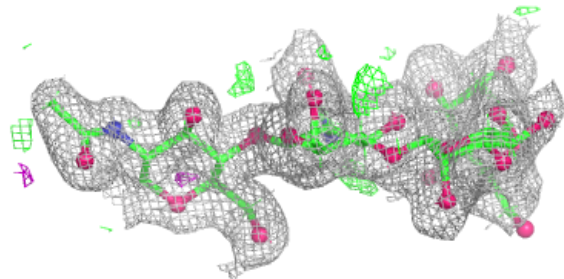
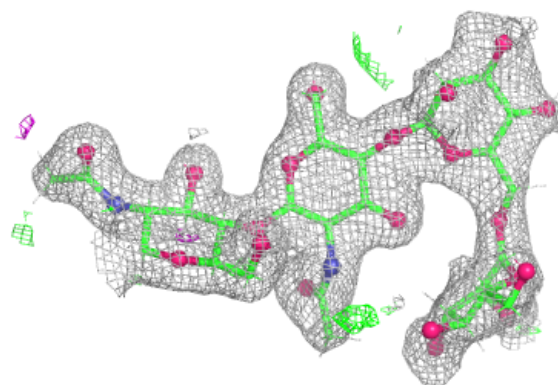
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	BdB	2	14/15	-	-	30,32,35,40	2
3	BMA	BdB	3	11/12	-	-	55,66,71,72	4
4	NAG	BuB	1	14/15	-	-	62,70,75,86	2
4	NAG	BuB	2	14/15	-	-	69,77,80,82	3

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.

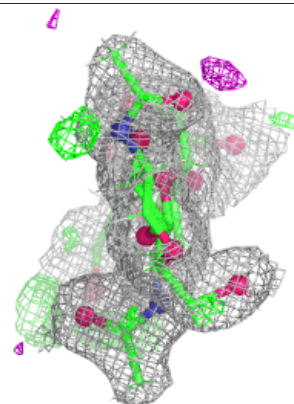
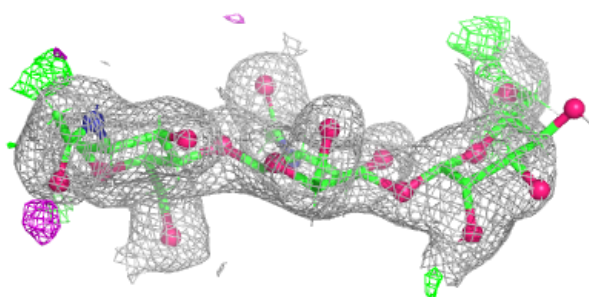
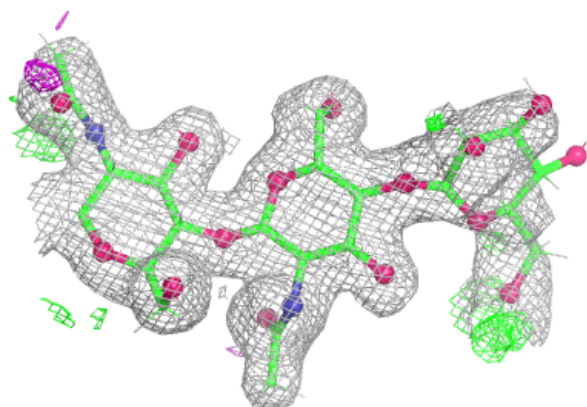
Electron density around Chain AdA:

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

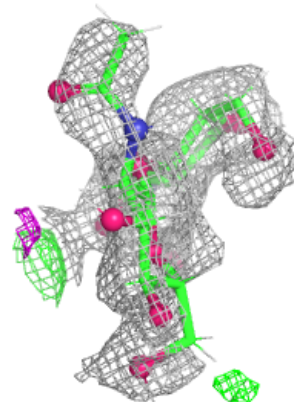
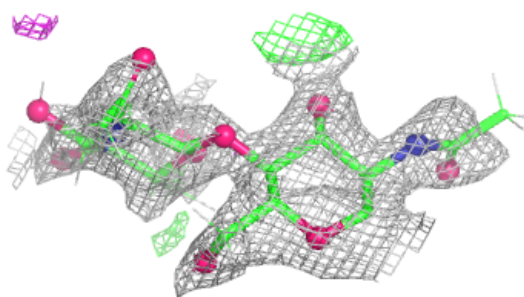
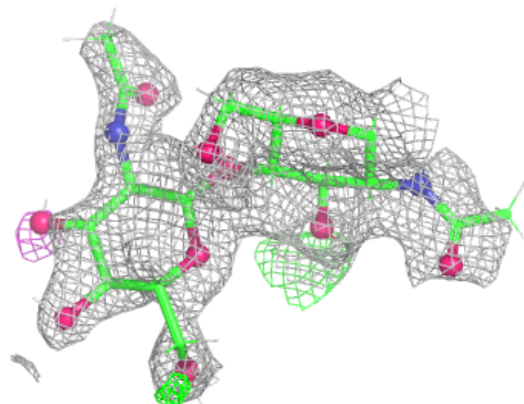


Electron density around Chain BdB:

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

**Electron density around Chain BuB:**

$2mF_o-DF_c$ (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
8	EDO	AAA	524	4/4	0.68	0.20	50,57,59,59	1
7	NAG	AAA	504	14/15	0.74	0.13	57,64,70,74	3
8	EDO	BBB	2714	4/4	0.76	0.15	47,48,50,52	1
8	EDO	BBB	2727	4/4	0.76	0.17	20,54,55,56	1
6	SO4	BBB	2721	5/5	0.77	0.12	55,69,80,82	0
6	SO4	AAA	510	5/5	0.77	0.10	74,75,82,88	0
8	EDO	AAA	511	4/4	0.77	0.20	48,55,59,59	1
8	EDO	AAA	507	4/4	0.78	0.16	56,60,61,61	1
8	EDO	BBB	2725	4/4	0.79	0.14	56,58,61,61	1
8	EDO	BBB	2723	4/4	0.80	0.11	60,65,68,69	1
8	EDO	BBB	2713	4/4	0.81	0.16	49,52,62,63	1
8	EDO	BBB	2719	4/4	0.82	0.13	56,56,58,58	1
8	EDO	AAA	525	4/4	0.83	0.15	52,56,59,59	1
8	EDO	BBB	2701	4/4	0.83	0.18	57,58,60,61	1
8	EDO	BBB	2710	4/4	0.84	0.17	45,48,53,54	1
8	EDO	BBB	2712	4/4	0.84	0.14	35,48,50,51	1
8	EDO	AAA	514	4/4	0.84	0.12	40,44,51,53	1
8	EDO	BBB	2705	4/4	0.84	0.13	47,51,52,54	1
8	EDO	AAA	513	4/4	0.85	0.13	53,55,59,62	1
8	EDO	BBB	2720	4/4	0.85	0.11	41,48,55,57	1
6	SO4	AAA	521	5/5	0.85	0.19	38,44,49,51	5
8	EDO	AAA	517	4/4	0.85	0.12	36,39,48,49	1
8	EDO	AAA	519	4/4	0.85	0.13	45,49,53,55	1
8	EDO	BBB	2707	4/4	0.86	0.15	47,53,55,56	1
8	EDO	AAA	523	4/4	0.87	0.13	50,53,58,59	1
8	EDO	BBB	2715	4/4	0.88	0.16	59,62,62,64	1
8	EDO	BBB	2716	4/4	0.88	0.14	55,56,58,58	1
8	EDO	AAA	516	4/4	0.88	0.12	42,47,49,50	1
8	EDO	AAA	512	4/4	0.88	0.12	35,42,48,48	1
8	EDO	AAA	526	4/4	0.88	0.11	20,46,47,52	1
8	EDO	AAA	508	4/4	0.88	0.12	45,51,52,52	1
8	EDO	AAA	505	4/4	0.88	0.11	47,48,49,50	1
8	EDO	BBB	2718	4/4	0.89	0.14	44,54,65,68	1
8	EDO	BBB	2706	4/4	0.89	0.19	29,35,38,38	1
8	EDO	AAA	506	4/4	0.89	0.12	22,26,27,27	1
8	EDO	BBB	2728	4/4	0.89	0.10	20,46,49,53	1
8	EDO	AAA	520	4/4	0.90	0.13	34,46,55,56	1

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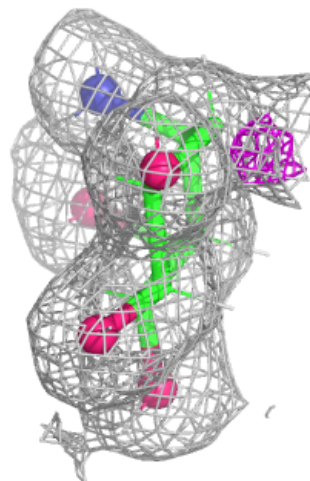
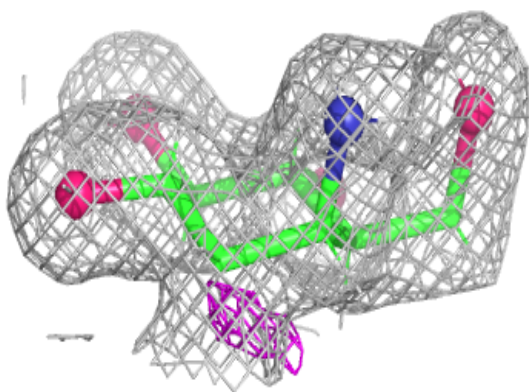
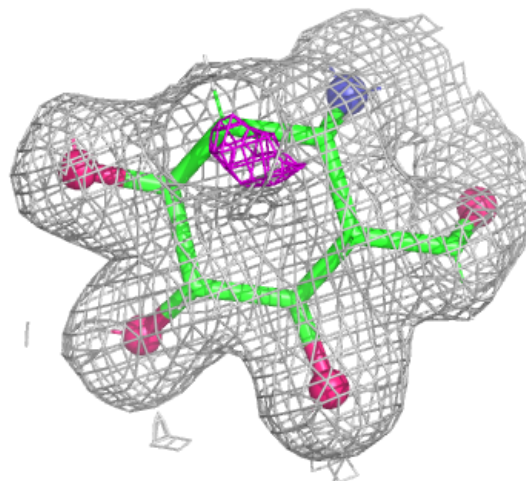
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	EDO	BBB	2717	4/4	0.90	0.11	41,47,48,48	1
8	EDO	BBB	2724	4/4	0.90	0.12	28,35,38,39	1
8	EDO	BBB	2726	4/4	0.91	0.11	20,43,47,48	1
8	EDO	AAA	518	4/4	0.91	0.12	36,45,53,53	1
8	EDO	AAA	509	4/4	0.91	0.12	36,43,51,51	1
8	EDO	BBB	2711	4/4	0.92	0.10	48,49,53,54	1
8	EDO	BBB	2708[A]	4/4	0.92	0.09	24,26,29,30	10
8	EDO	BBB	2708[B]	4/4	0.92	0.09	25,27,30,31	10
8	EDO	AAA	515	4/4	0.92	0.10	32,36,41,41	1
8	EDO	BBB	2709	4/4	0.93	0.16	32,34,38,39	1
6	SO4	BBB	2704	5/5	0.96	0.06	40,41,44,44	0
5	PO8	AAA	501	12/13	0.97	0.05	18,21,26,26	3
5	PO8	BBB	2702	12/13	0.97	0.05	20,24,27,28	3
6	SO4	AAA	503	5/5	0.98	0.05	33,34,35,35	0
6	SO4	BBB	2703	5/5	0.98	0.05	27,31,36,36	0
6	SO4	AAA	502	5/5	0.98	0.05	26,27,30,31	0
9	NA	BBB	2722	1/1	0.98	0.09	34,34,34,34	0
9	NA	AAA	522	1/1	0.99	0.10	34,34,34,34	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.

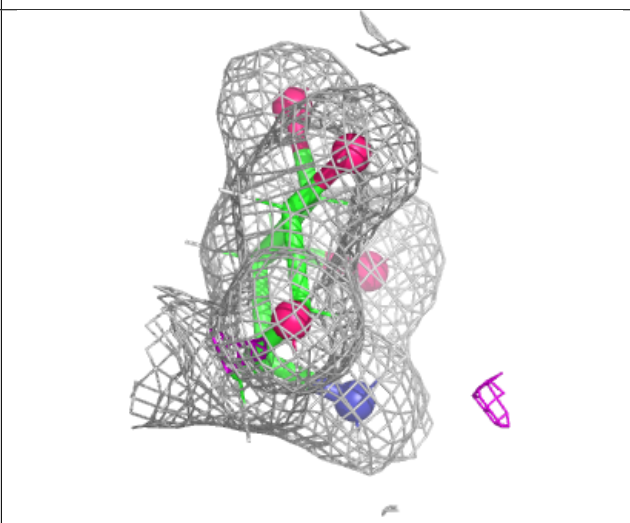
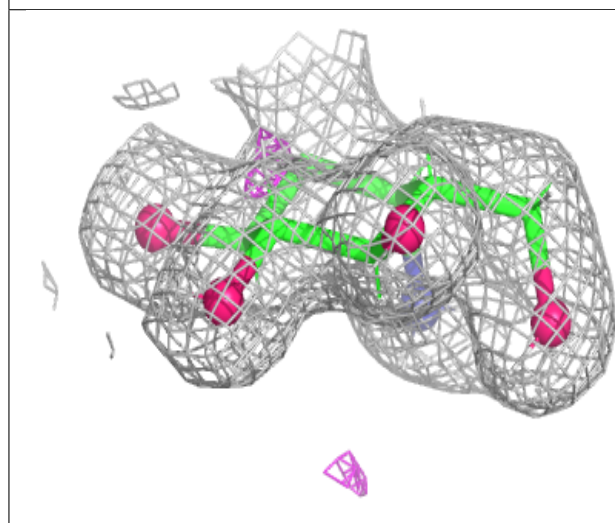
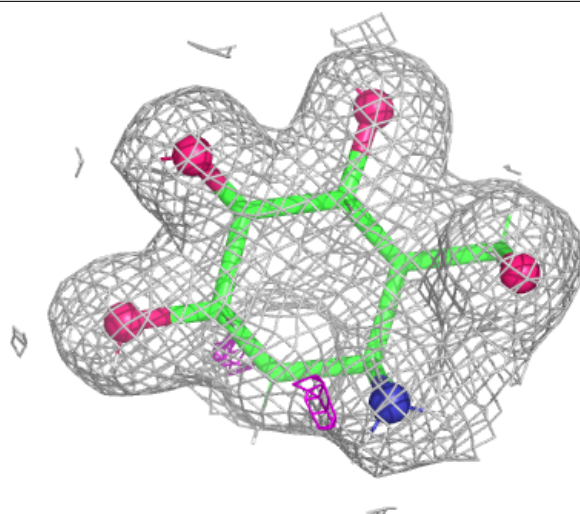
Electron density around PO8 AAA 501:

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



Electron density around PO8 BBB 2702:

$2mF_o-DF_c$ (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.