Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 07:27 PM EDT

PDB ID	:	6WEW
Title	:	Crystal structures of human E-NPP 1: bound to N-{4-[(7-methoxyquinolin-4-yl)oxy]phenyl}sulfuric diamide
Authors	:	Peat, T.S.; Dennis, M.; Newman, J.
Deposited on	:	2020-04-03
Resolution	:	2.73 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:

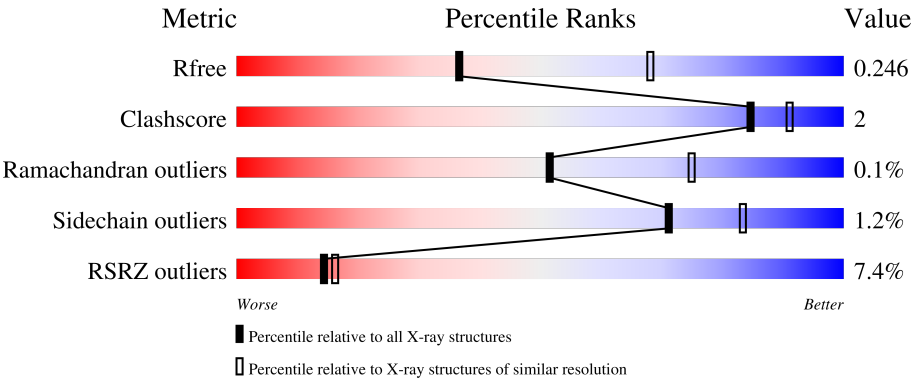
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	AbA	925	4% 88% 12%
1	BaB	925	9% 85% 14%
2	AdA	4	100%
3	AhA	3	100%
4	AlA	2	100%

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Mol	Chain	Length	Quality of chain
4	BeB	2	100%
5	BbB	3	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
2	BMA	AdA	4	X	-	-	-
4	NAG	BeB	2	X	-	-	-
8	NAG	BaB	1002	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 13249 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AbA	817	Total	C	N	O	S	0	5	0
			6572	4194	1117	1211	50			
1	BaB	795	Total	C	N	O	S	0	2	0
			6180	3937	1049	1147	47			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-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	N	O	0	0	0
			50	28	2	20			

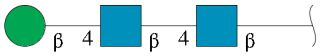
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

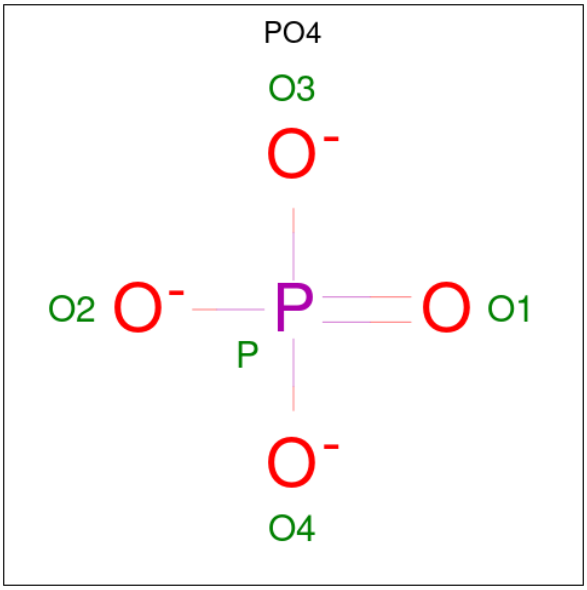
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AlA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	BeB	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	BbB	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AbA	1	Total	O	P	0	0
			4	3	1		

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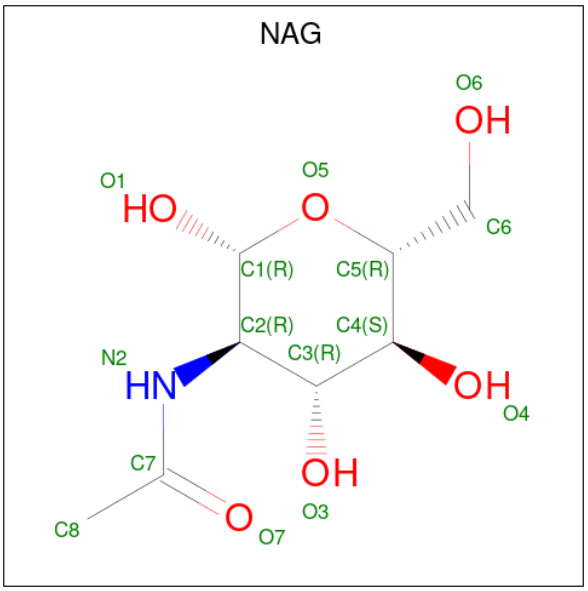
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BaB	1	Total O P 5 4 1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

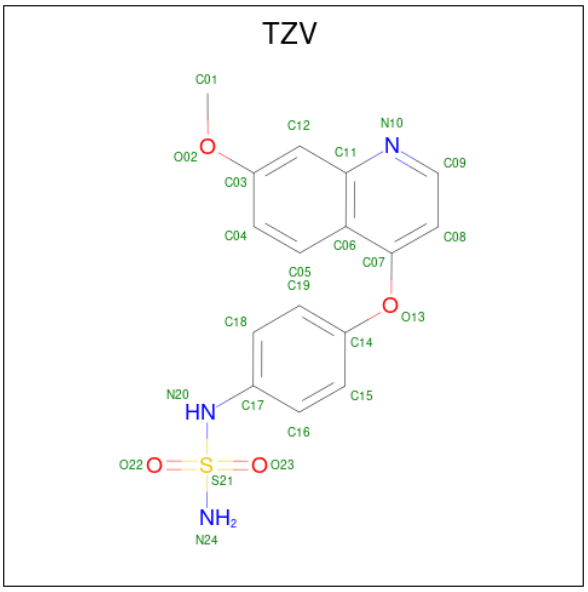
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AbA	2	Total Zn 2 2	0	0
7	BaB	1	Total Zn 1 1	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



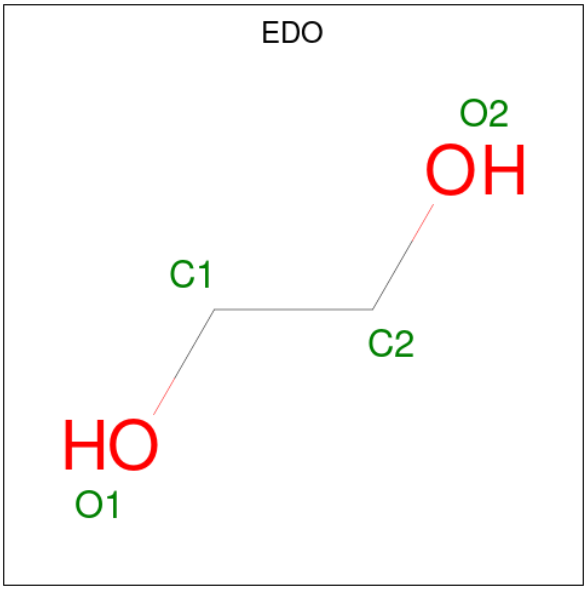
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AbA	1	Total C N O 14 8 1 5	0	0
8	AbA	1	Total C N O 14 8 1 5	0	0
8	BaB	1	Total C N O 14 8 1 5	0	0
8	BaB	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is N-{4-[(7-methoxyquinolin-4-yl)oxy]phenyl}sulfuric diamide (three-letter code: TZV) (formula: $C_{16}H_{15}N_3O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AbA	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
9	BaB	1	Total	C	N	O	S	0	0
			24	16	3	4	1		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	AbA	1	Total	C	O	0	0
			4	2	2		
10	AbA	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AbA	1	Total C O 4 2 2	0	0

- Molecule 11 is water.

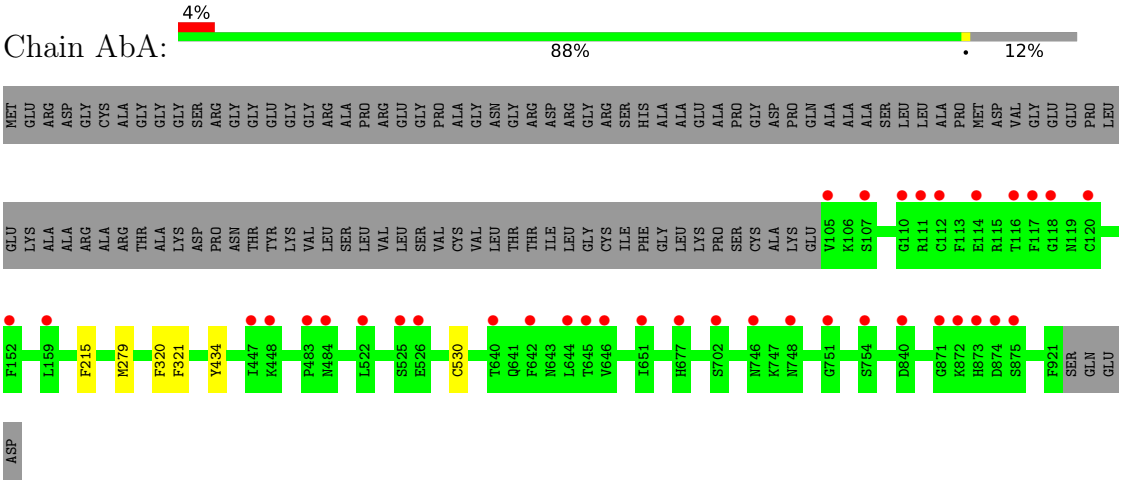
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	AbA	126	Total O 126 126	0	0
11	BaB	59	Total O 59 59	0	0

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.

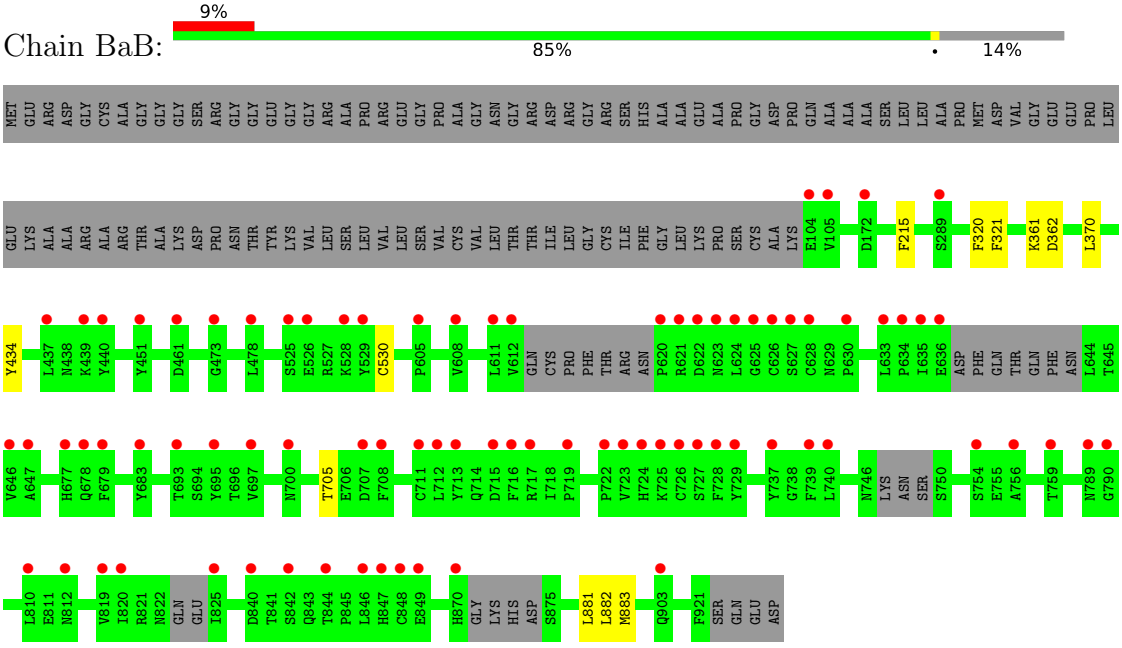
• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 1

Chain AbA:



• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 1

Chain BaB:



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

Chain AdA:

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

Chain AhA:

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

Chain AlA:

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

Chain BeB:

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

Chain BbB:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.13Å 161.58Å 209.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.73 47.92 – 2.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.92-2.73) 100.0 (47.92-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.241 0.217 , 0.246	Depositor DCC
R_{free} test set	3771 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13249	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: ZN, BMA, NAG, EDO, TZV, PO4, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AbA	0.63	0/6759	0.75	0/9180
1	BaB	0.64	0/6352	0.74	0/8645
All	All	0.63	0/13111	0.75	0/17825

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AbA	6572	0	6293	0	0
1	BaB	6180	0	5715	0	0
2	AdA	50	0	43	0	0
3	AhA	39	0	34	0	0
4	AlA	28	0	25	0	0
4	BeB	28	0	25	0	0
5	BbB	39	0	34	0	0
6	AbA	4	0	0	0	0
6	BaB	5	0	0	0	0
7	AbA	2	0	0	0	0
7	BaB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AbA	28	0	26	0	0
8	BaB	28	0	26	0	0
9	AbA	24	0	0	0	0
9	BaB	24	0	0	0	0
10	AbA	12	0	18	0	0
11	AbA	126	0	0	0	0
11	BaB	59	0	0	0	0
All	All	13249	0	12239	0	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 2.

There are no clashes within the asymmetric unit.

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	AbA	820/925 (89%)	782 (95%)	37 (4%)	1 (0%)	51 75
1	BaB	785/925 (85%)	745 (95%)	39 (5%)	1 (0%)	51 75
All	All	1605/1850 (87%)	1527 (95%)	76 (5%)	2 (0%)	51 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AbA	321	PHE
1	BaB	321	PHE

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	AbA	733/824 (89%)	728 (99%)	5 (1%)	84 90
1	BaB	655/824 (80%)	644 (98%)	11 (2%)	60 76
All	All	1388/1648 (84%)	1372 (99%)	16 (1%)	71 83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AbA	215	PHE
1	AbA	279	MET
1	AbA	320	PHE
1	AbA	434	TYR
1	AbA	530	CYS
1	BaB	215	PHE
1	BaB	320	PHE
1	BaB	361	LYS
1	BaB	362	ASP
1	BaB	370	LEU
1	BaB	434	TYR
1	BaB	530	CYS
1	BaB	705	THR
1	BaB	881	LEU
1	BaB	882	LEU
1	BaB	883	MET

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

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)

14 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	0.58	0	17,19,21	1.35	2 (11%)
2	NAG	AdA	2	2	14,14,15	0.56	0	17,19,21	1.10	2 (11%)
2	BMA	AdA	3	2	11,11,12	1.05	2 (18%)	15,15,17	2.83	5 (33%)
2	BMA	AdA	4	2	11,11,12	0.31	0	15,15,17	1.53	1 (6%)
3	NAG	AhA	1	3,1	14,14,15	0.62	0	17,19,21	1.93	4 (23%)
3	NAG	AhA	2	3	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
3	MAN	AhA	3	3	11,11,12	0.43	0	15,15,17	1.25	1 (6%)
4	NAG	AlA	1	4,1	14,14,15	0.55	0	17,19,21	1.09	1 (5%)
4	NAG	AlA	2	4	14,14,15	0.37	0	17,19,21	0.92	1 (5%)
5	NAG	BbB	1	5,1	14,14,15	0.72	0	17,19,21	1.54	2 (11%)
5	NAG	BbB	2	5	14,14,15	0.31	0	17,19,21	1.16	2 (11%)
5	BMA	BbB	3	5	11,11,12	0.48	0	15,15,17	1.12	1 (6%)
4	NAG	BeB	1	4,1	14,14,15	0.73	0	17,19,21	2.01	4 (23%)
4	NAG	BeB	2	4	14,14,15	0.96	2 (14%)	17,19,21	2.36	5 (29%)

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	-	2/6/23/26	0/1/1/1
2	BMA	AdA	3	2	-	2/2/19/22	0/1/1/1
2	BMA	AdA	4	2	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	AhA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	AhA	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	AhA	3	3	-	2/2/19/22	0/1/1/1
4	NAG	AlA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	AlA	2	4	-	2/6/23/26	0/1/1/1
5	NAG	BbB	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	BbB	2	5	-	0/6/23/26	0/1/1/1
5	BMA	BbB	3	5	-	0/2/19/22	0/1/1/1
4	NAG	BeB	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	BeB	2	4	1/1/5/7	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AdA	3	BMA	O5-C1	2.41	1.47	1.43
4	BeB	2	NAG	C1-C2	2.41	1.55	1.52
2	AdA	3	BMA	C1-C2	2.08	1.56	1.52
4	BeB	2	NAG	O5-C1	2.02	1.46	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AdA	3	BMA	C1-O5-C5	6.84	121.45	112.19
4	BeB	2	NAG	C1-O5-C5	6.48	120.98	112.19
2	AdA	3	BMA	O2-C2-C1	5.80	121.03	109.15
3	AhA	1	NAG	O5-C1-C2	-5.60	102.45	111.29
2	AdA	4	BMA	C1-O5-C5	5.16	119.18	112.19
4	BeB	1	NAG	O7-C7-N2	-4.99	112.77	121.95
4	BeB	1	NAG	C8-C7-N2	4.77	124.17	116.10
2	AdA	3	BMA	O5-C1-C2	4.01	116.96	110.77
4	BeB	2	NAG	O5-C5-C6	3.94	113.37	107.20
5	BbB	1	NAG	C3-C4-C5	3.85	117.10	110.24
5	BbB	1	NAG	O5-C1-C2	-3.53	105.72	111.29
3	AhA	1	NAG	C8-C7-N2	-3.48	110.20	116.10
4	BeB	2	NAG	O5-C1-C2	3.26	116.44	111.29
3	AhA	3	MAN	C1-C2-C3	3.03	113.39	109.67
2	AdA	1	NAG	O4-C4-C3	-3.02	103.37	110.35
2	AdA	3	BMA	O2-C2-C3	-2.99	104.14	110.14
2	AdA	1	NAG	O5-C1-C2	-2.82	106.83	111.29
4	BeB	2	NAG	C8-C7-N2	2.78	120.81	116.10
4	AlA	2	NAG	C1-O5-C5	2.73	115.89	112.19
4	BeB	1	NAG	C1-C2-N2	-2.57	106.09	110.49
4	BeB	1	NAG	O5-C1-C2	-2.56	107.24	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BbB	2	NAG	O5-C5-C4	-2.42	104.95	110.83
3	AhA	1	NAG	O7-C7-N2	2.22	126.03	121.95
2	AdA	2	NAG	C1-O5-C5	2.19	115.16	112.19
5	BbB	3	BMA	C3-C4-C5	2.18	114.13	110.24
2	AdA	3	BMA	O3-C3-C2	-2.16	105.85	109.99
3	AhA	1	NAG	C4-C3-C2	-2.16	107.86	111.02
4	BeB	2	NAG	O7-C7-N2	-2.10	118.10	121.95
3	AhA	2	NAG	C3-C4-C5	-2.09	106.51	110.24
5	BbB	2	NAG	C4-C3-C2	-2.08	107.97	111.02
2	AdA	2	NAG	C1-C2-N2	2.07	114.03	110.49
4	AlA	1	NAG	O7-C7-N2	2.01	125.64	121.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AdA	4	BMA	C1
4	BeB	2	NAG	C1

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BeB	1	NAG	C8-C7-N2-C2
4	BeB	1	NAG	O7-C7-N2-C2
4	BeB	2	NAG	C8-C7-N2-C2
4	BeB	2	NAG	O7-C7-N2-C2
3	AhA	3	MAN	C4-C5-C6-O6
3	AhA	3	MAN	O5-C5-C6-O6
4	AlA	2	NAG	C4-C5-C6-O6
2	AdA	4	BMA	O5-C5-C6-O6
2	AdA	3	BMA	O5-C5-C6-O6
3	AhA	2	NAG	O5-C5-C6-O6
4	BeB	2	NAG	O5-C5-C6-O6
4	AlA	2	NAG	O5-C5-C6-O6
2	AdA	3	BMA	C4-C5-C6-O6
4	BeB	1	NAG	O5-C5-C6-O6
4	BeB	1	NAG	C4-C5-C6-O6
5	BbB	1	NAG	O5-C5-C6-O6
4	BeB	2	NAG	C4-C5-C6-O6
5	BbB	1	NAG	C4-C5-C6-O6
2	AdA	4	BMA	C4-C5-C6-O6
4	AlA	1	NAG	C8-C7-N2-C2
3	AhA	2	NAG	C4-C5-C6-O6

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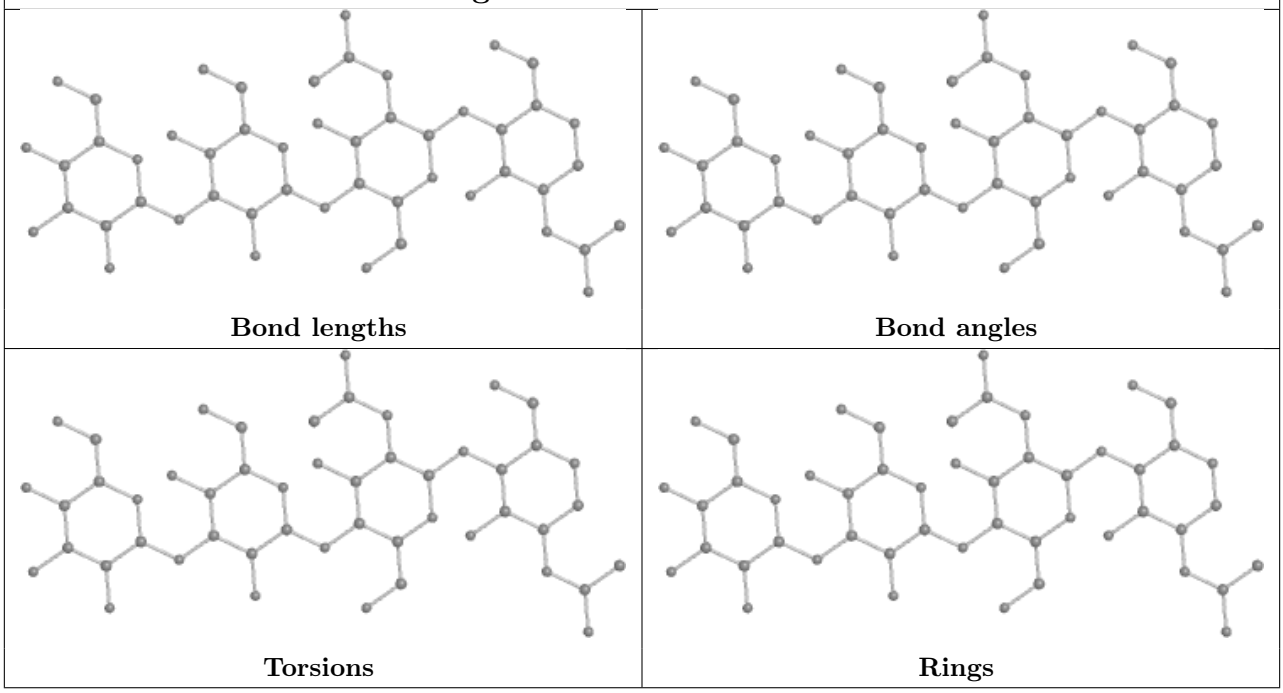
Mol	Chain	Res	Type	Atoms
2	AdA	2	NAG	C4-C5-C6-O6
2	AdA	2	NAG	O5-C5-C6-O6
3	AhA	1	NAG	C3-C2-N2-C7
4	AlA	1	NAG	C3-C2-N2-C7

There are no ring outliers.

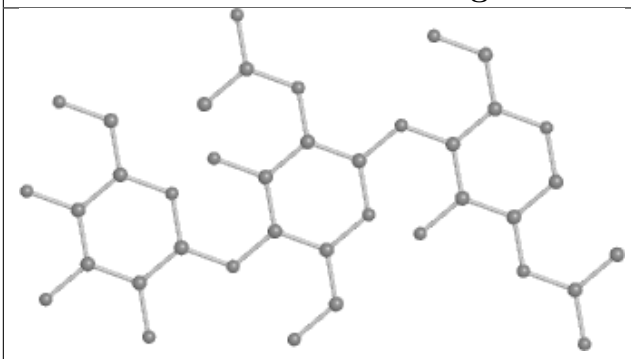
No monomer is involved in short contacts.

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

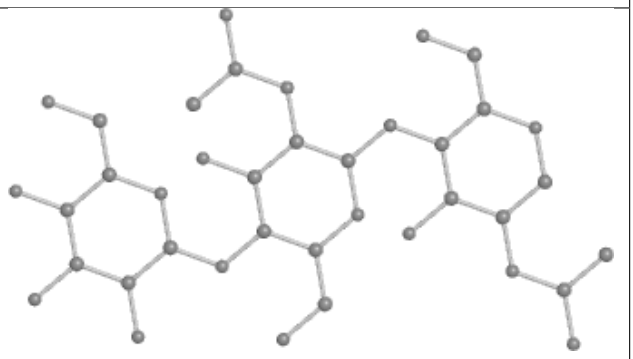
Oligosaccharide Chain AdA



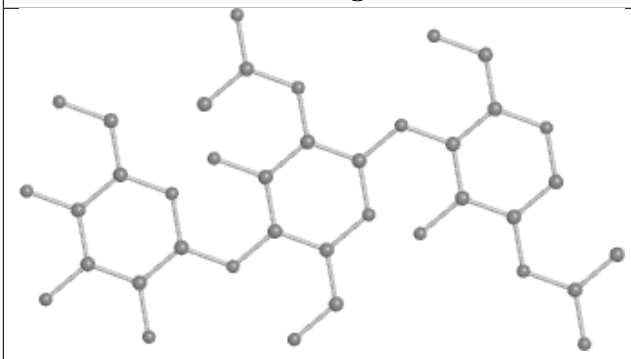
Oligosaccharide Chain AhA



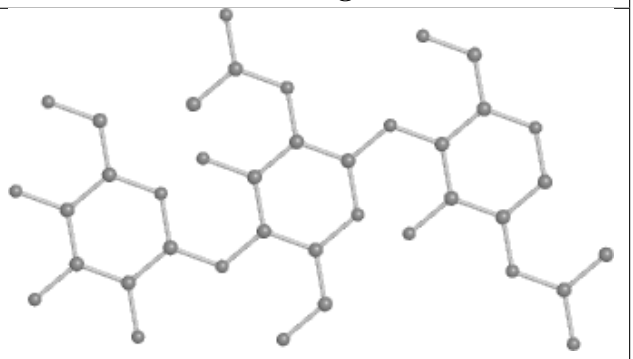
Bond lengths



Bond angles

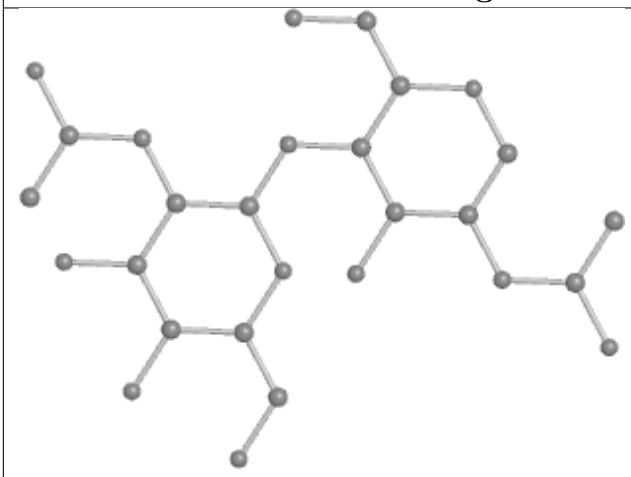


Torsions

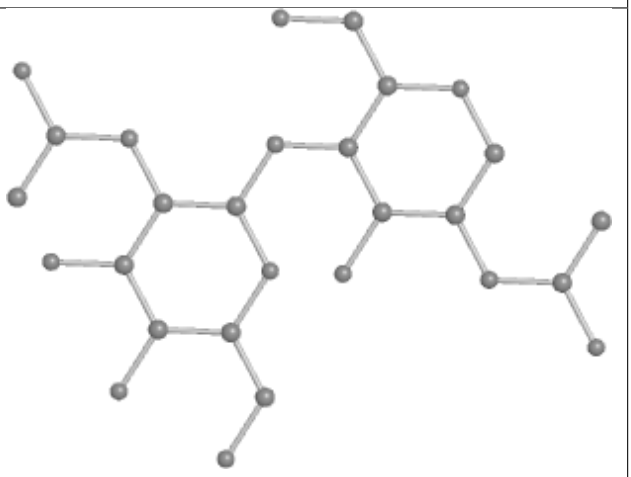


Rings

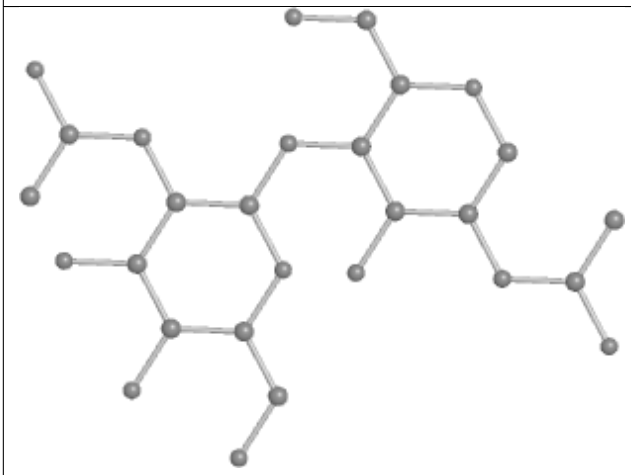
Oligosaccharide Chain AlA



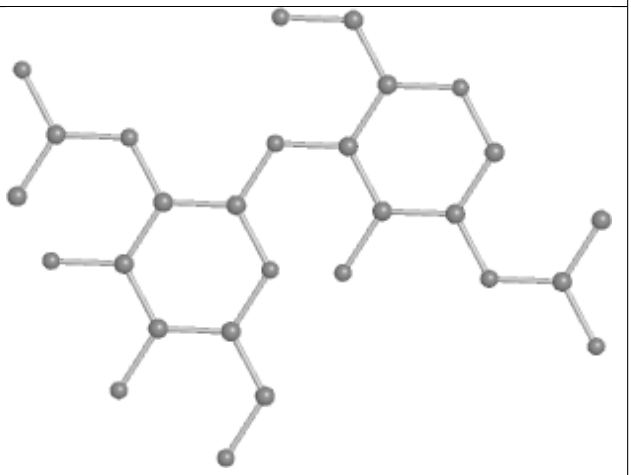
Bond lengths



Bond angles

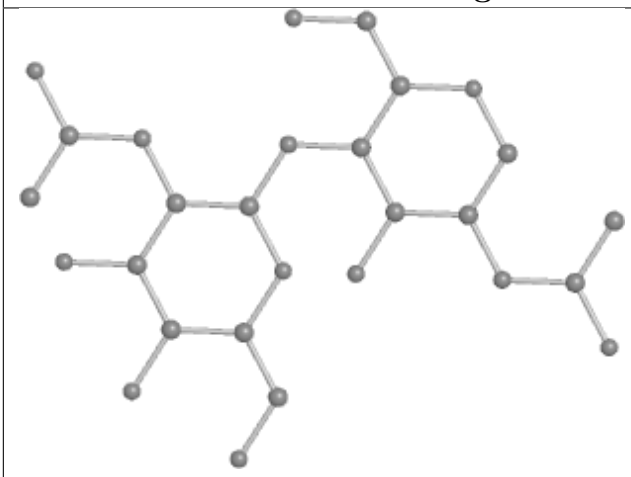


Torsions

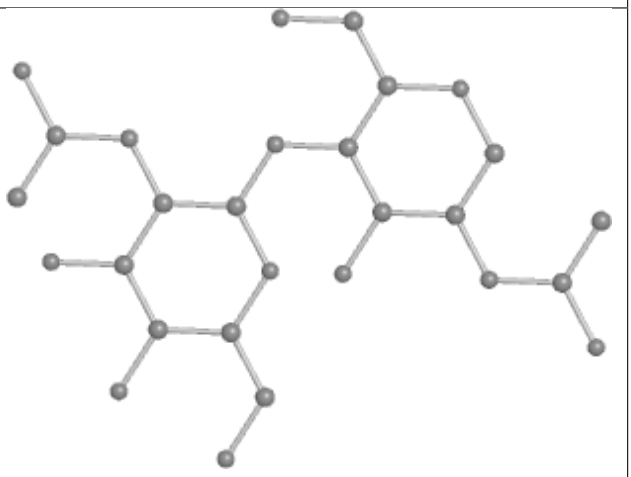


Rings

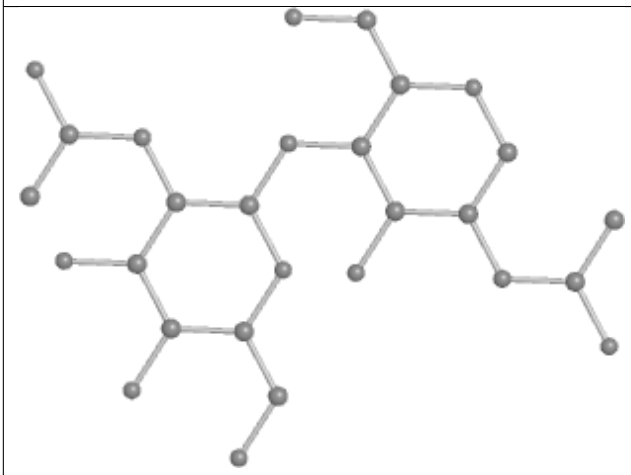
Oligosaccharide Chain BeB



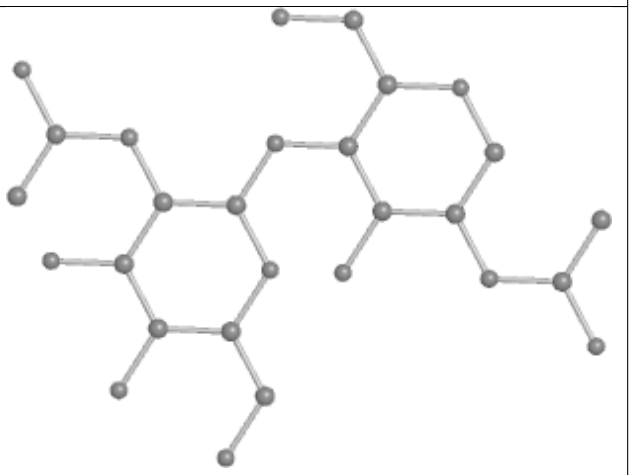
Bond lengths



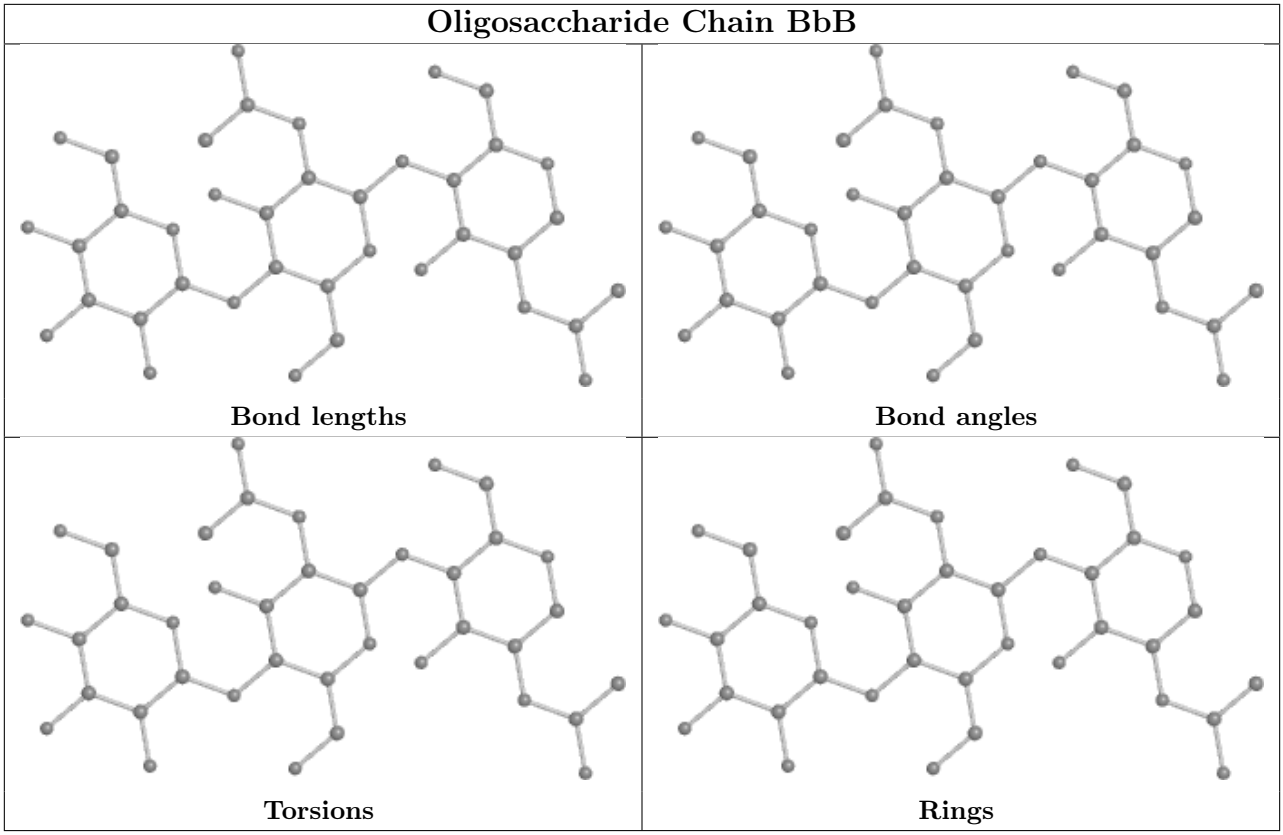
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PO4	AbA	1001	7,1	0,3,4	-	-	0,3,6	-	-
10	EDO	AbA	1007	-	3,3,3	0.05	0	2,2,2	0.17	0
9	TZV	AbA	1006	-	25,26,26	1.12	1 (4%)	35,37,37	1.87	5 (14%)
8	NAG	AbA	1004	1	14,14,15	0.62	0	17,19,21	1.62	4 (23%)
9	TZV	BaB	1004	-	25,26,26	1.06	1 (4%)	35,37,37	1.95	5 (14%)
10	EDO	AbA	1008	-	3,3,3	0.08	0	2,2,2	0.26	0
10	EDO	AbA	1009	-	3,3,3	0.18	0	2,2,2	0.36	0
8	NAG	BaB	1003	1	14,14,15	0.43	0	17,19,21	1.14	2 (11%)
8	NAG	BaB	1002	1	14,14,15	0.55	0	17,19,21	1.60	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PO4	BaB	1005	7	4,4,4	0.68	0	6,6,6	0.44	0
8	NAG	AbA	1005	1	14,14,15	0.28	0	17,19,21	0.99	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
10	EDO	AbA	1007	-	-	1/1/1/1	-
8	NAG	AbA	1004	1	-	3/6/23/26	0/1/1/1
9	TZV	BaB	1004	-	-	3/10/11/11	0/3/3/3
10	EDO	AbA	1008	-	-	1/1/1/1	-
10	EDO	AbA	1009	-	-	1/1/1/1	-
8	NAG	BaB	1003	1	-	1/6/23/26	0/1/1/1
8	NAG	BaB	1002	1	-	3/6/23/26	0/1/1/1
9	TZV	AbA	1006	-	-	4/10/11/11	0/3/3/3
8	NAG	AbA	1005	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BaB	1004	TZV	C06-C11	-3.57	1.36	1.42
9	AbA	1006	TZV	C06-C11	-3.50	1.36	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	BaB	1004	TZV	O23-S21-O22	-8.17	101.25	119.96
9	AbA	1006	TZV	O23-S21-O22	-8.09	101.45	119.96
8	AbA	1004	NAG	C1-C2-N2	-4.21	103.30	110.49
9	BaB	1004	TZV	C07-O13-C14	-3.73	111.36	118.52
8	BaB	1002	NAG	C1-C2-N2	3.59	116.62	110.49
9	BaB	1004	TZV	C09-N10-C11	3.29	122.03	116.93
9	AbA	1006	TZV	C09-N10-C11	3.26	121.97	116.93
9	BaB	1004	TZV	C08-C09-N10	-2.76	120.31	124.58
9	AbA	1006	TZV	C07-O13-C14	-2.72	113.30	118.52
8	BaB	1003	NAG	C1-C2-N2	2.68	115.07	110.49
9	AbA	1006	TZV	C08-C09-N10	-2.66	120.46	124.58
8	BaB	1002	NAG	O5-C1-C2	-2.55	107.26	111.29
8	AbA	1004	NAG	O5-C5-C6	2.50	111.13	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AbA	1004	NAG	C8-C7-N2	-2.47	111.91	116.10
8	BaB	1003	NAG	O5-C1-C2	-2.25	107.73	111.29
8	BaB	1002	NAG	C2-N2-C7	-2.19	119.78	122.90
9	BaB	1004	TZV	C06-C11-N10	-2.16	120.53	122.83
9	AbA	1006	TZV	C06-C11-N10	-2.16	120.54	122.83
8	BaB	1002	NAG	C4-C3-C2	2.11	114.11	111.02
8	BaB	1002	NAG	O5-C5-C6	2.02	110.38	107.20
8	AbA	1004	NAG	O7-C7-N2	2.02	125.67	121.95

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	AbA	1006	TZV	C17-N20-S21-O22
9	AbA	1006	TZV	C17-N20-S21-O23
9	BaB	1004	TZV	C17-N20-S21-O22
9	AbA	1006	TZV	C04-C03-O02-C01
9	AbA	1006	TZV	C12-C03-O02-C01
8	BaB	1002	NAG	C8-C7-N2-C2
9	BaB	1004	TZV	C04-C03-O02-C01
9	BaB	1004	TZV	C12-C03-O02-C01
8	AbA	1005	NAG	C8-C7-N2-C2
8	AbA	1005	NAG	O7-C7-N2-C2
8	BaB	1002	NAG	O7-C7-N2-C2
8	AbA	1004	NAG	C8-C7-N2-C2
8	BaB	1002	NAG	O5-C5-C6-O6
10	AbA	1007	EDO	O1-C1-C2-O2
8	AbA	1004	NAG	O5-C5-C6-O6
10	AbA	1009	EDO	O1-C1-C2-O2
8	BaB	1003	NAG	C8-C7-N2-C2
10	AbA	1008	EDO	O1-C1-C2-O2
8	AbA	1004	NAG	O7-C7-N2-C2

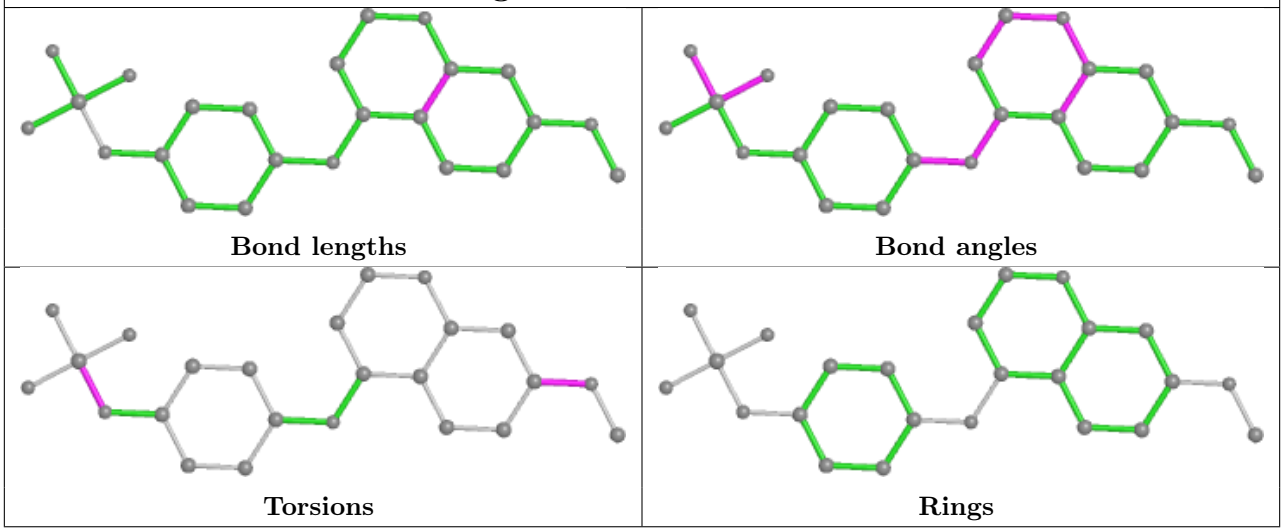
There are no ring outliers.

No monomer is involved in short contacts.

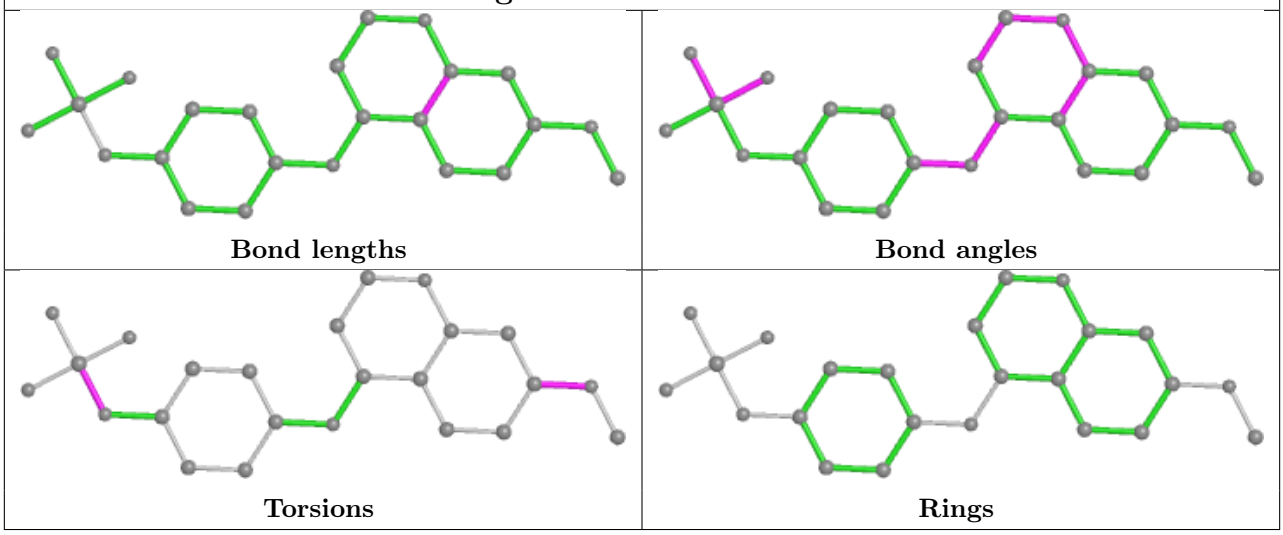
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 TZV AbA 1006



Ligand TZV BaB 1004



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	AbA	817/925 (88%)	0.18	37 (4%)	33	36	22, 41, 87, 150	0
1	BaB	795/925 (85%)	0.54	82 (10%)	6	6	25, 63, 127, 152	0
All	All	1612/1850 (87%)	0.36	119 (7%)	14	16	22, 48, 117, 152	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BaB	716	PHE	8.4
1	BaB	712	LEU	6.9
1	BaB	626	CYS	5.6
1	BaB	624	LEU	5.2
1	BaB	729	TYR	5.1
1	AbA	873	HIS	5.1
1	BaB	623	ASN	5.0
1	BaB	739	PHE	4.9
1	BaB	461	ASP	4.6
1	BaB	728	PHE	4.6
1	AbA	526	GLU	4.6
1	AbA	117	PHE	4.2
1	BaB	713	TYR	4.2
1	BaB	635	ILE	4.2
1	BaB	679	PHE	4.1
1	BaB	628	CYS	4.1
1	BaB	708	PHE	4.0
1	AbA	484	ASN	3.9
1	BaB	725	LYS	3.8
1	BaB	711	CYS	3.7
1	AbA	871	GLY	3.6
1	BaB	707	ASP	3.6
1	BaB	717	ARG	3.6
1	BaB	289	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	BaB	759	THR	3.6
1	AbA	118	GLY	3.5
1	BaB	737	TYR	3.5
1	BaB	722	PRO	3.5
1	BaB	724	HIS	3.4
1	BaB	440	TYR	3.4
1	AbA	651	ILE	3.4
1	AbA	640	THR	3.3
1	BaB	848	CYS	3.3
1	BaB	727	SER	3.3
1	BaB	723	VAL	3.3
1	BaB	526	GLU	3.3
1	BaB	630	PRO	3.2
1	BaB	647	ALA	3.2
1	BaB	528	LYS	3.1
1	BaB	810	LEU	3.1
1	AbA	111	ARG	3.1
1	BaB	451	TYR	3.1
1	AbA	677	HIS	3.1
1	BaB	608	VAL	3.0
1	BaB	756	ALA	3.0
1	AbA	875	SER	3.0
1	AbA	522	LEU	3.0
1	BaB	646	VAL	3.0
1	BaB	636	GLU	2.9
1	BaB	820	ILE	2.9
1	BaB	678	GLN	2.9
1	BaB	844	THR	2.9
1	BaB	847	HIS	2.9
1	BaB	439	LYS	2.8
1	BaB	719	PRO	2.8
1	BaB	790	GLY	2.8
1	AbA	646	VAL	2.8
1	BaB	789	ASN	2.8
1	BaB	621	ARG	2.8
1	AbA	110	GLY	2.7
1	BaB	611	LEU	2.7
1	BaB	697	VAL	2.7
1	BaB	473	GLY	2.7
1	BaB	104	GLU	2.7
1	BaB	677	HIS	2.6
1	AbA	874	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	BaB	529	TYR	2.6
1	BaB	700	ASN	2.6
1	AbA	644	LEU	2.6
1	BaB	525	SER	2.6
1	BaB	620	PRO	2.5
1	AbA	748	ASN	2.5
1	AbA	112	CYS	2.5
1	BaB	812	ASN	2.5
1	AbA	447	ILE	2.5
1	AbA	642	PHE	2.5
1	BaB	842	SER	2.5
1	BaB	478	LEU	2.4
1	AbA	746	ASN	2.4
1	BaB	726	CYS	2.4
1	BaB	633	LEU	2.4
1	BaB	840	ASP	2.4
1	AbA	702	SER	2.4
1	BaB	754	SER	2.4
1	AbA	872	LYS	2.4
1	BaB	627	SER	2.3
1	AbA	525	SER	2.3
1	BaB	105	VAL	2.3
1	BaB	634	PRO	2.3
1	BaB	849	GLU	2.3
1	AbA	840	ASP	2.3
1	AbA	107	SER	2.3
1	BaB	870	HIS	2.3
1	BaB	903	GLN	2.3
1	BaB	825	ILE	2.3
1	AbA	152	PHE	2.3
1	BaB	612	VAL	2.3
1	AbA	116	THR	2.2
1	AbA	645	THR	2.2
1	BaB	715	ASP	2.2
1	AbA	120	CYS	2.2
1	BaB	693	THR	2.2
1	BaB	695	TYR	2.2
1	BaB	683	TYR	2.1
1	AbA	105	VAL	2.1
1	AbA	754	SER	2.1
1	AbA	751	GLY	2.1
1	BaB	625	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	BaB	740	LEU	2.1
1	BaB	622	ASP	2.1
1	BaB	819	VAL	2.1
1	BaB	846	LEU	2.1
1	AbA	483	PRO	2.1
1	BaB	437	LEU	2.1
1	BaB	605	PRO	2.1
1	BaB	172	ASP	2.0
1	AbA	114	GLU	2.0
1	AbA	159	LEU	2.0
1	AbA	448	LYS	2.0

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

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

6.3 Carbohydrates (i)

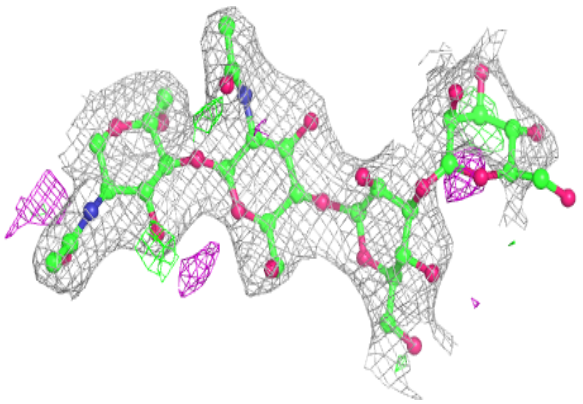
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

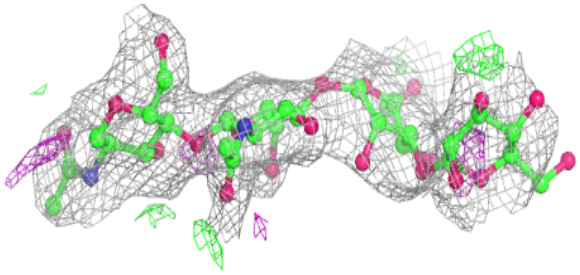
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	AdA	4	11/12	0.52	0.33	119,137,143,152	0
2	BMA	AdA	3	11/12	0.74	0.19	86,93,99,111	0
5	BMA	BbB	3	11/12	0.76	0.28	86,103,108,108	0
3	MAN	AhA	3	11/12	0.77	0.28	98,111,122,127	0
4	NAG	AlA	2	14/15	0.84	0.40	123,141,148,151	0
4	NAG	BeB	2	14/15	0.87	0.31	81,93,96,98	0
3	NAG	AhA	1	14/15	0.89	0.18	50,65,72,75	0
3	NAG	AhA	2	14/15	0.89	0.20	65,75,84,98	0
5	NAG	BbB	2	14/15	0.90	0.17	77,88,91,99	0
2	NAG	AdA	2	14/15	0.90	0.15	52,59,66,83	0
4	NAG	BeB	1	14/15	0.91	0.30	70,80,83,88	0
4	NAG	AlA	1	14/15	0.91	0.20	71,84,100,111	0
5	NAG	BbB	1	14/15	0.92	0.15	56,61,68,76	0
2	NAG	AdA	1	14/15	0.96	0.19	31,34,37,46	0

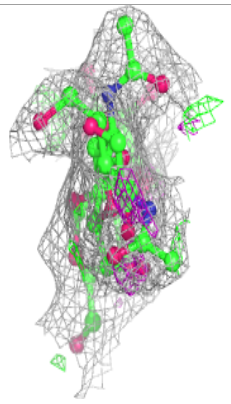
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain AdA:

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

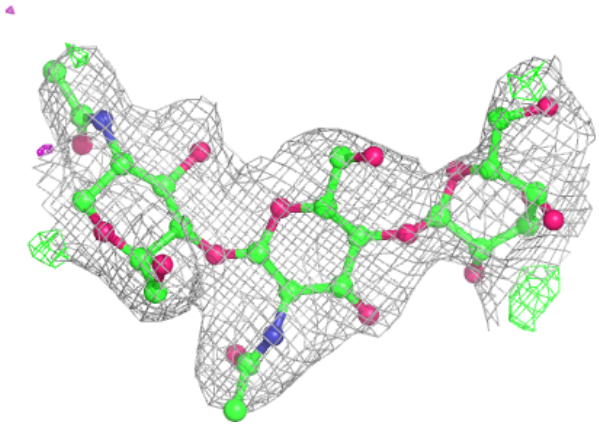


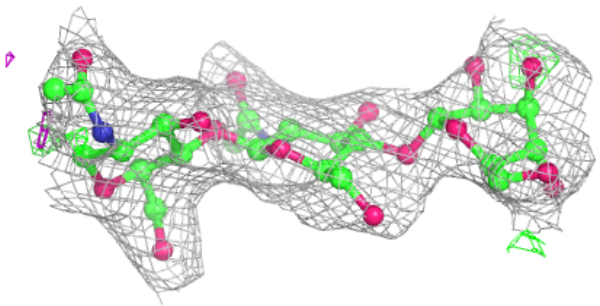


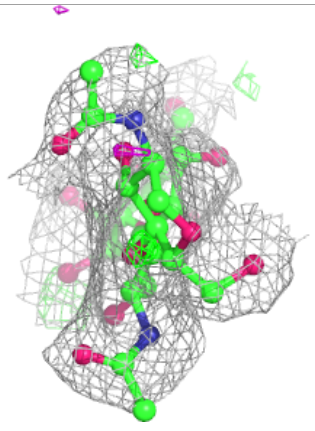


Electron density around Chain AhA:

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

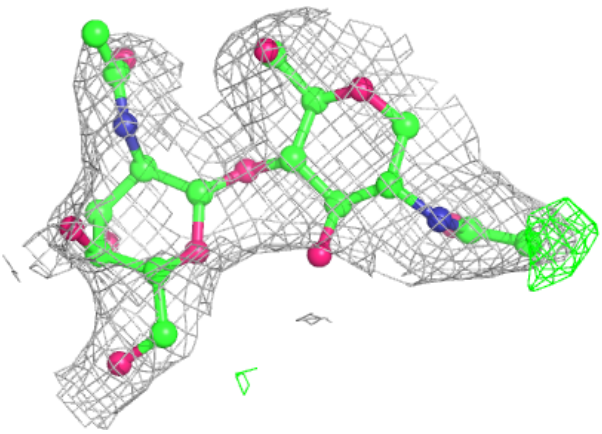


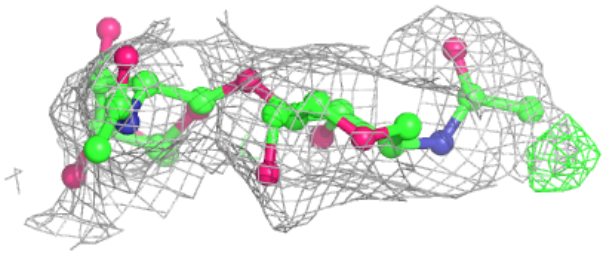


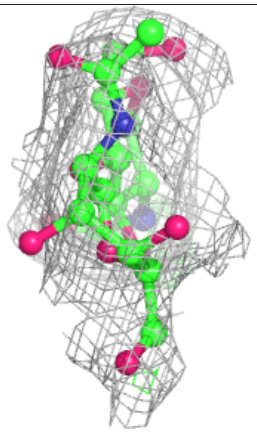


Electron density around Chain A1A:

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

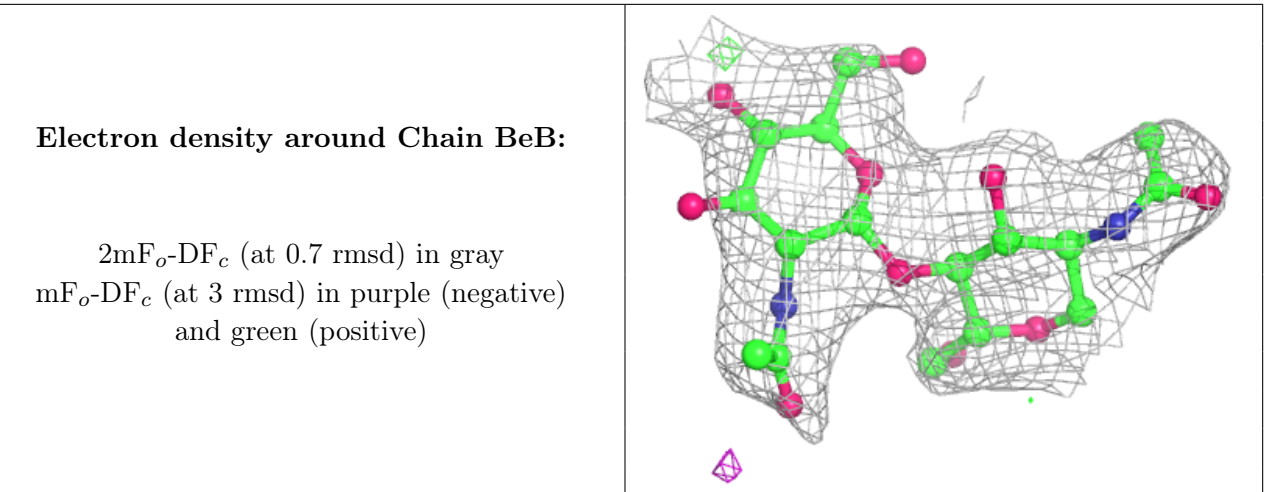


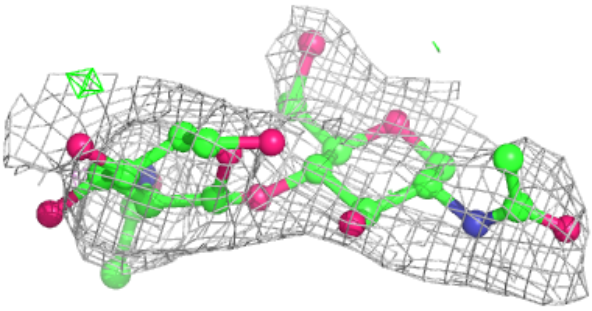


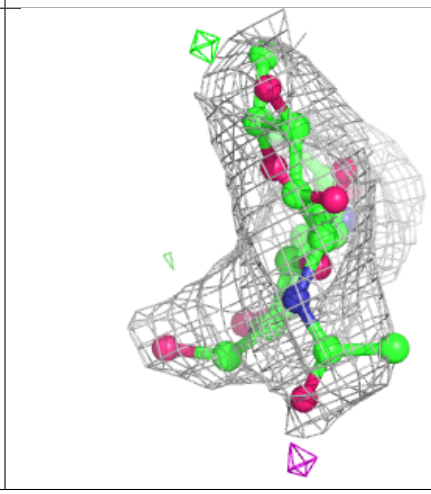


Electron density around Chain BeB:

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

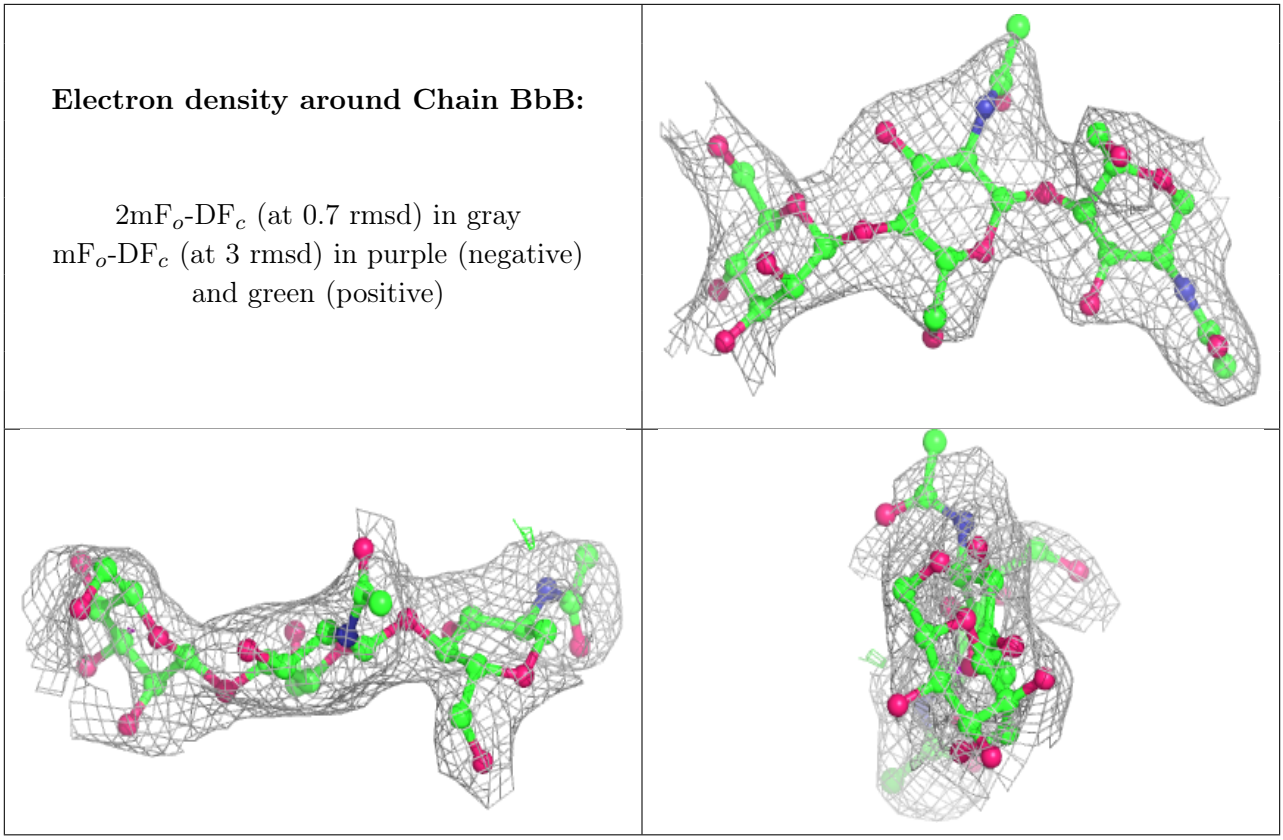






Electron density around Chain BbB:

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



6.4 Ligands

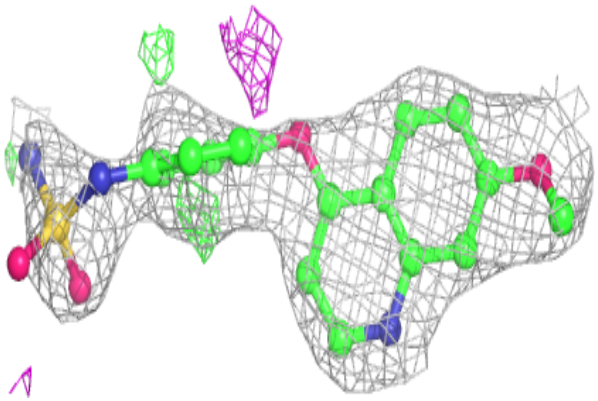
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

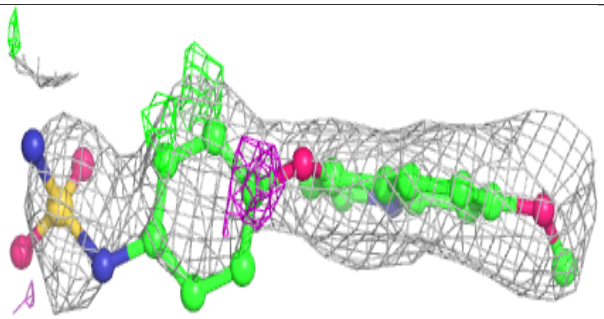
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	BaB	1002	14/15	0.73	0.42	118,134,143,151	0
8	NAG	AbA	1004	14/15	0.77	0.39	91,101,114,115	0
6	PO4	AbA	1001	4/5	0.82	0.28	71,82,93,95	0
10	EDO	AbA	1009	4/4	0.84	0.23	62,63,66,66	0
9	TZV	BaB	1004	24/24	0.88	0.31	48,61,112,123	0
9	TZV	AbA	1006	24/24	0.89	0.29	33,41,109,117	0
8	NAG	AbA	1005	14/15	0.89	0.30	67,86,93,95	0
8	NAG	BaB	1003	14/15	0.89	0.24	99,106,110,115	0
7	ZN	AbA	1003	1/1	0.90	0.26	78,78,78,78	1
10	EDO	AbA	1008	4/4	0.90	0.26	58,60,61,62	0
6	PO4	BaB	1005	5/5	0.90	0.20	49,49,52,52	5
10	EDO	AbA	1007	4/4	0.91	0.43	48,50,52,56	0
7	ZN	AbA	1002	1/1	0.98	0.08	44,44,44,44	0
7	ZN	BaB	1001	1/1	0.99	0.06	54,54,54,54	0

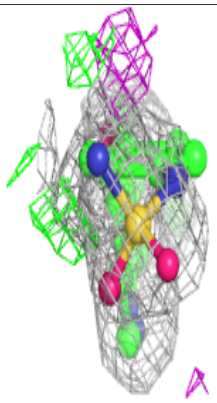
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TZV BaB 1004:

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

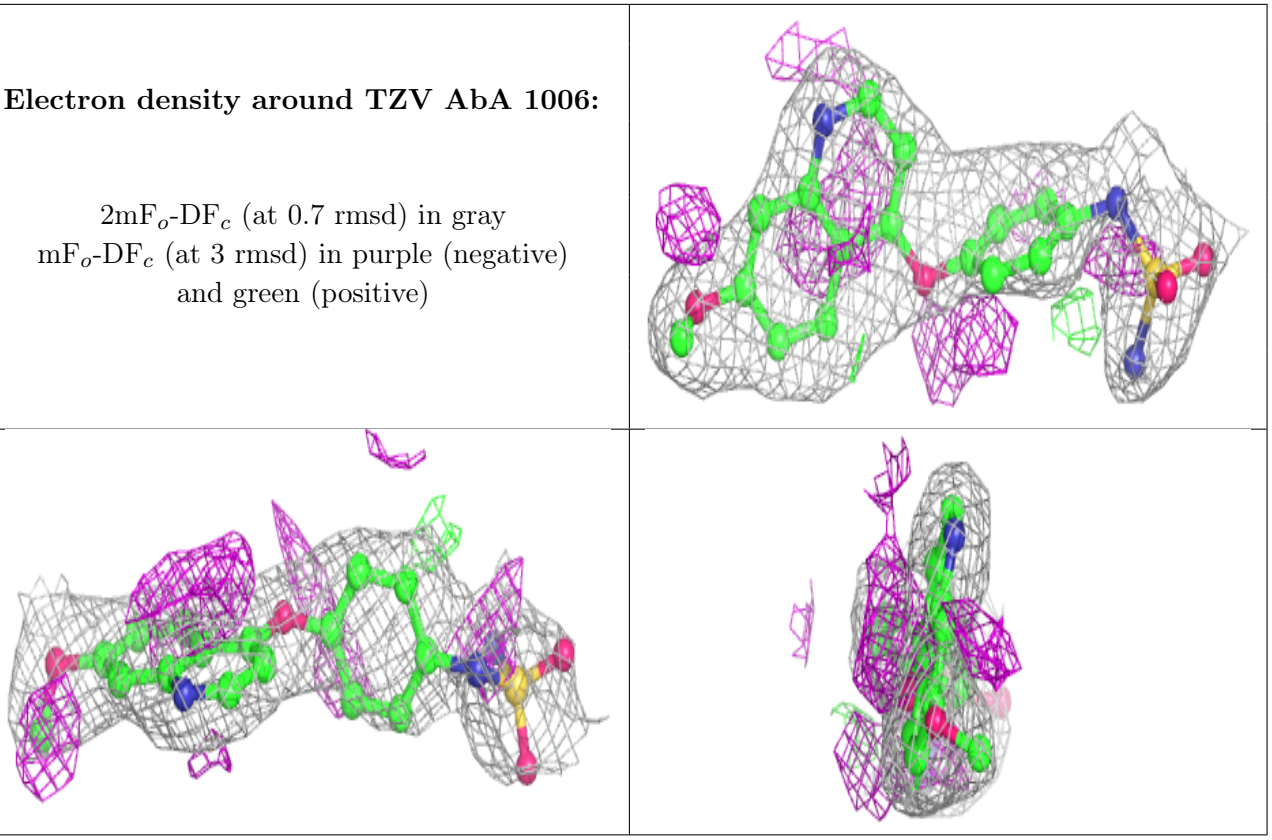






Electron density around TZV AbA 1006:

$2mF_o$-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.