



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:30 AM UTC

PDB ID : 6WEW / pdb_00006wew
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 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

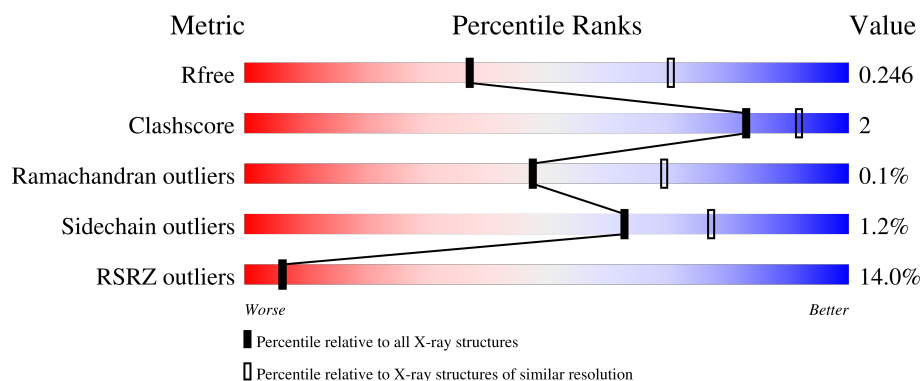
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



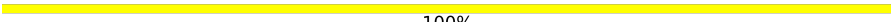
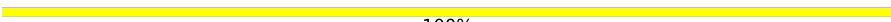
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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 $\leq 5\%$. 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	AbA	925	<div> <div>5%</div> <div>82%</div> <div>7%</div> <div>12%</div> </div>
1	BaB	925	<div> <div>20%</div> <div>80%</div> <div>5%</div> <div>14%</div> </div>
2	AdA	4	<div> <div>100%</div> </div>
3	AhA	3	<div> <div>100%</div> </div>
4	AlA	2	<div> <div>100%</div> </div>

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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	-	-	-

2 Entry composition [i](#)

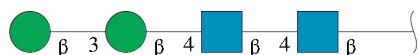
There are 11 unique types of molecules in this entry. The entry contains 13249 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

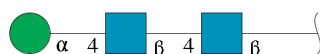
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AbA	817	Total	C	N	O	S	0	5	0
			6572	4194	1117	1211	50			
1	BaB	795	Total	C	N	O	S	0	2	0
			6180	3937	1049	1147	47			

- 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.



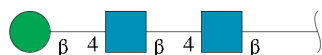
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AhA	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



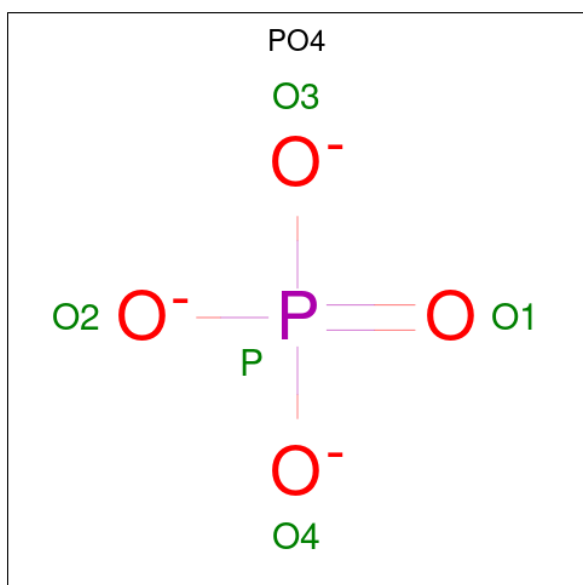
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AlA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	BeB	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 (CCD ID: PO4) (formula: O₄P).



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

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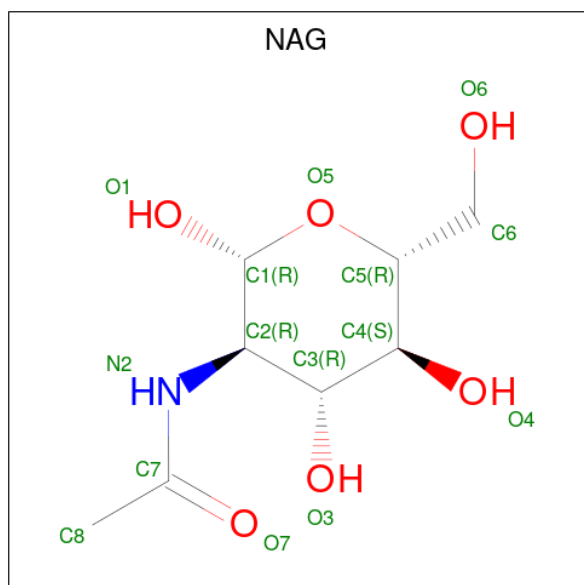
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BaB	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

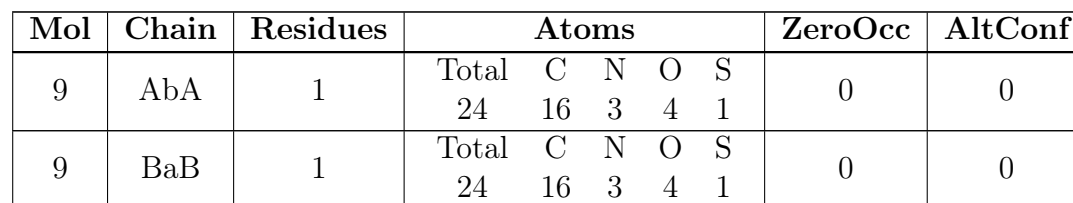
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AbA	2	Total	Zn	0	0
			2	2		
7	BaB	1	Total	Zn	0	0
			1	1		


- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is N-{4-[(7-methoxyquinolin-4-yl)oxy]phenyl}sulfuric diamide (CCD ID: TZV) (formula: C₁₆H₁₅N₃O₄S) (labeled as "Ligand of Interest" by depositor).



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



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

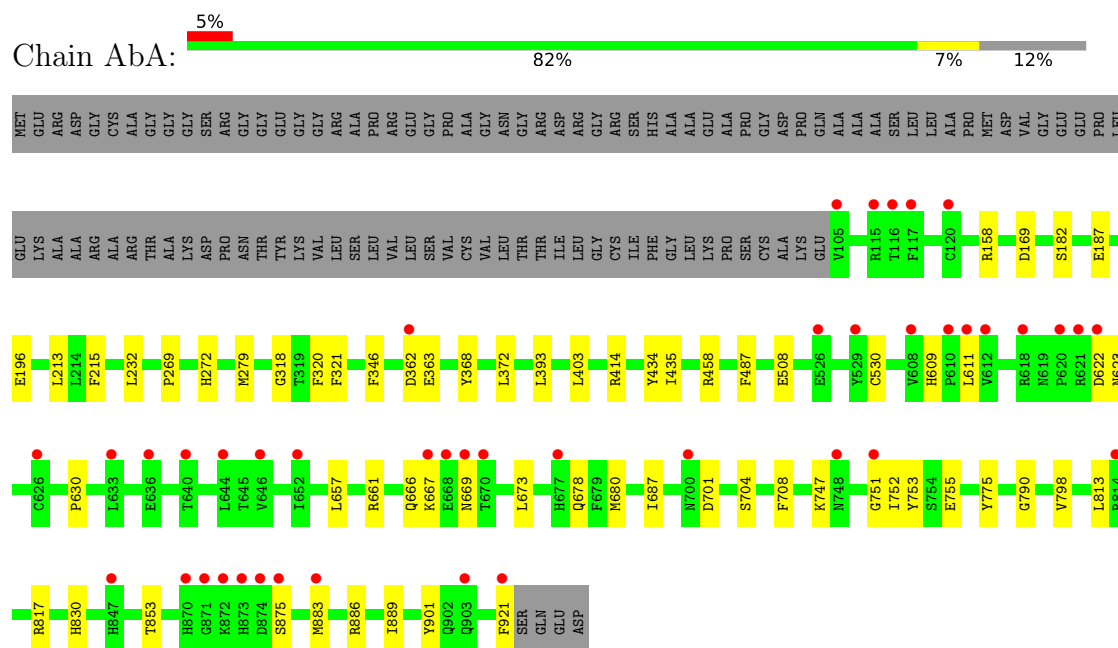
- Molecule 11 is water.

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

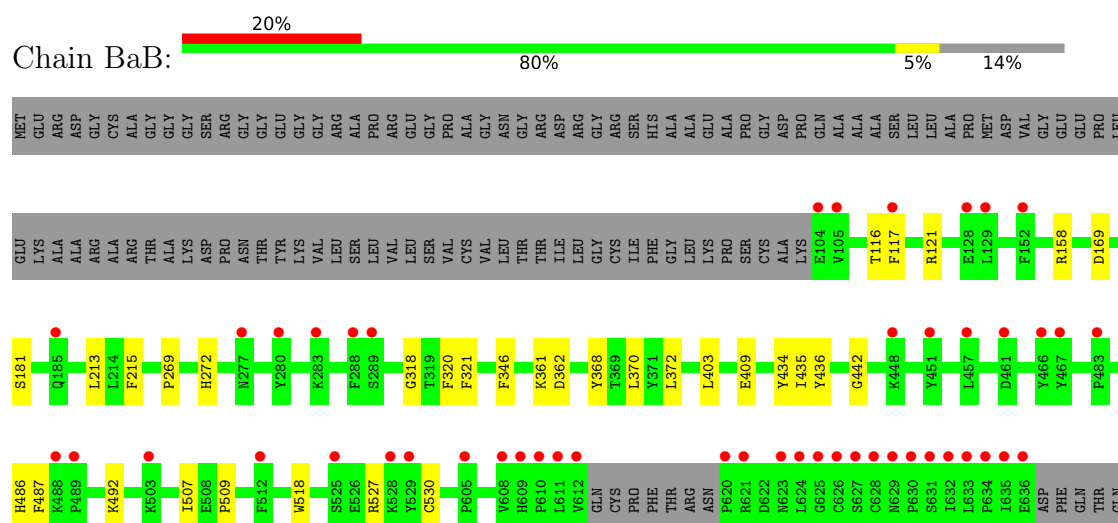
3 Residue-property plots

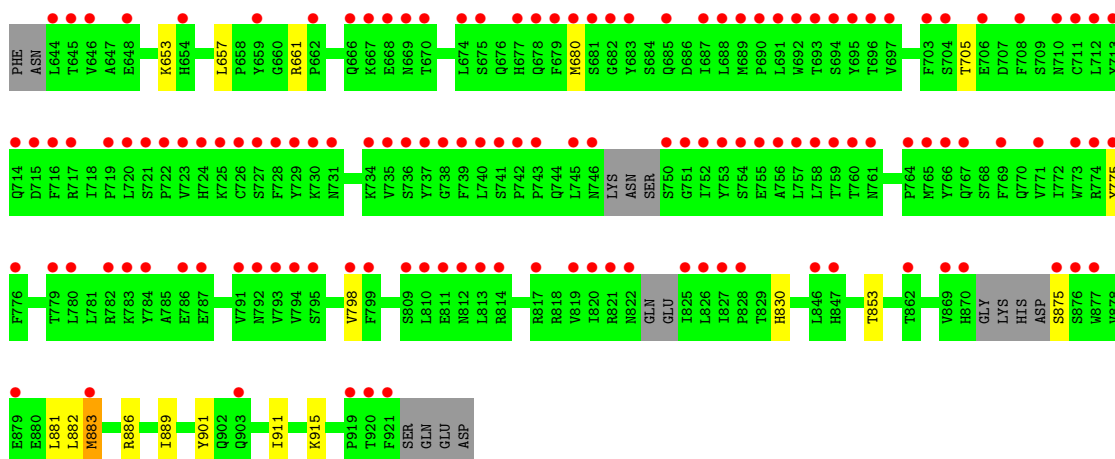
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 1



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 1





- 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: 100%



- 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: 100%



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

Chain AIA: 100%



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

Chain BeB: 100%



- 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: 100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.96%)	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)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, EDO, ZN, MAN, NAG, PO4, TZV

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	0.97	0/6759	1.33	3/9180 (0.0%)
1	BaB	0.99	0/6352	1.34	1/8645 (0.0%)
All	All	0.98	0/13111	1.33	4/17825 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AbA	790	GLY	CA-C-O	-5.31	118.57	122.23
1	AbA	630	PRO	CA-C-N	5.25	127.31	120.28
1	AbA	630	PRO	C-N-CA	5.25	127.31	120.28
1	BaB	442	GLY	CA-C-O	-5.10	117.28	122.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AbA	6572	0	6293	37	0
1	BaB	6180	0	5715	24	0
2	AdA	50	0	43	0	0
3	AhA	39	0	34	0	0
4	AlA	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	61	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.

The worst 5 of 61 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:AbA:883[A]:MET:SD	1:AbA:921:PHE:CE2	2.70	0.84
1:AbA:883[A]:MET:SD	1:AbA:921:PHE:CD2	2.72	0.83
1:BaB:117:PHE:O	1:BaB:121[A]:ARG:NH1	2.24	0.71
1:AbA:673:LEU:HD22	1:AbA:680:MET:HE3	1.76	0.66
1:AbA:708:PHE:HB3	1:AbA:752:ILE:HD13	1.78	0.65

There are no symmetry-related clashes.

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	AbA	820/925 (89%)	782 (95%)	37 (4%)	1 (0%)	48	69
1	BaB	785/925 (85%)	745 (95%)	39 (5%)	1 (0%)	48	69
All	All	1605/1850 (87%)	1527 (95%)	76 (5%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

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

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	AbA	733/824 (89%)	728 (99%)	5 (1%)	76	85
1	BaB	655/824 (80%)	644 (98%)	11 (2%)	53	71
All	All	1388/1648 (84%)	1372 (99%)	16 (1%)	63	77

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BaB	882	LEU
1	BaB	881	LEU
1	BaB	362	ASP
1	BaB	705	THR
1	BaB	361	LYS

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 ⓘ

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	0.60	0	17,19,21	1.36	2 (11%)
2	NAG	AdA	2	2	14,14,15	0.55	0	17,19,21	1.13	2 (11%)
2	BMA	AdA	3	2	11,11,12	1.01	1 (9%)	15,15,17	2.61	5 (33%)
2	BMA	AdA	4	2	11,11,12	0.31	0	15,15,17	1.53	1 (6%)
3	NAG	AhA	1	1,3	14,14,15	0.62	0	17,19,21	1.97	4 (23%)
3	NAG	AhA	2	3	14,14,15	0.43	0	17,19,21	0.98	1 (5%)
3	MAN	AhA	3	3	11,11,12	0.42	0	15,15,17	1.10	1 (6%)
4	NAG	AlA	1	1,4	14,14,15	0.55	0	17,19,21	1.13	2 (11%)
4	NAG	AlA	2	4	14,14,15	0.38	0	17,19,21	0.92	1 (5%)
5	NAG	BbB	1	5,1	14,14,15	0.71	0	17,19,21	1.55	2 (11%)
5	NAG	BbB	2	5	14,14,15	0.30	0	17,19,21	1.14	2 (11%)
5	BMA	BbB	3	5	11,11,12	0.48	0	15,15,17	0.98	1 (6%)
4	NAG	BeB	1	1,4	14,14,15	0.73	0	17,19,21	2.05	4 (23%)
4	NAG	BeB	2	4	14,14,15	0.99	1 (7%)	17,19,21	2.30	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,3	-	2/6/23/26	0/1/1/1
3	NAG	AhA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	AhA	3	3	-	2/2/19/22	0/1/1/1
4	NAG	AlA	1	1,4	-	4/6/23/26	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	-	1/6/23/26	0/1/1/1
5	BMA	BbB	3	5	-	0/2/19/22	0/1/1/1
4	NAG	BeB	1	1,4	-	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BeB	2	NAG	C1-C2	2.64	1.55	1.52
2	AdA	3	BMA	O5-C1	2.31	1.47	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AdA	3	BMA	C1-O5-C5	6.92	121.45	112.19
4	BeB	2	NAG	C1-O5-C5	6.56	120.98	112.19
3	AhA	1	NAG	O5-C1-C2	-5.72	102.45	111.29
2	AdA	4	BMA	C1-O5-C5	5.22	119.18	112.19
4	BeB	1	NAG	O7-C7-N2	-5.21	112.77	121.98

All (2) chirality outliers are listed below:

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

5 of 29 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

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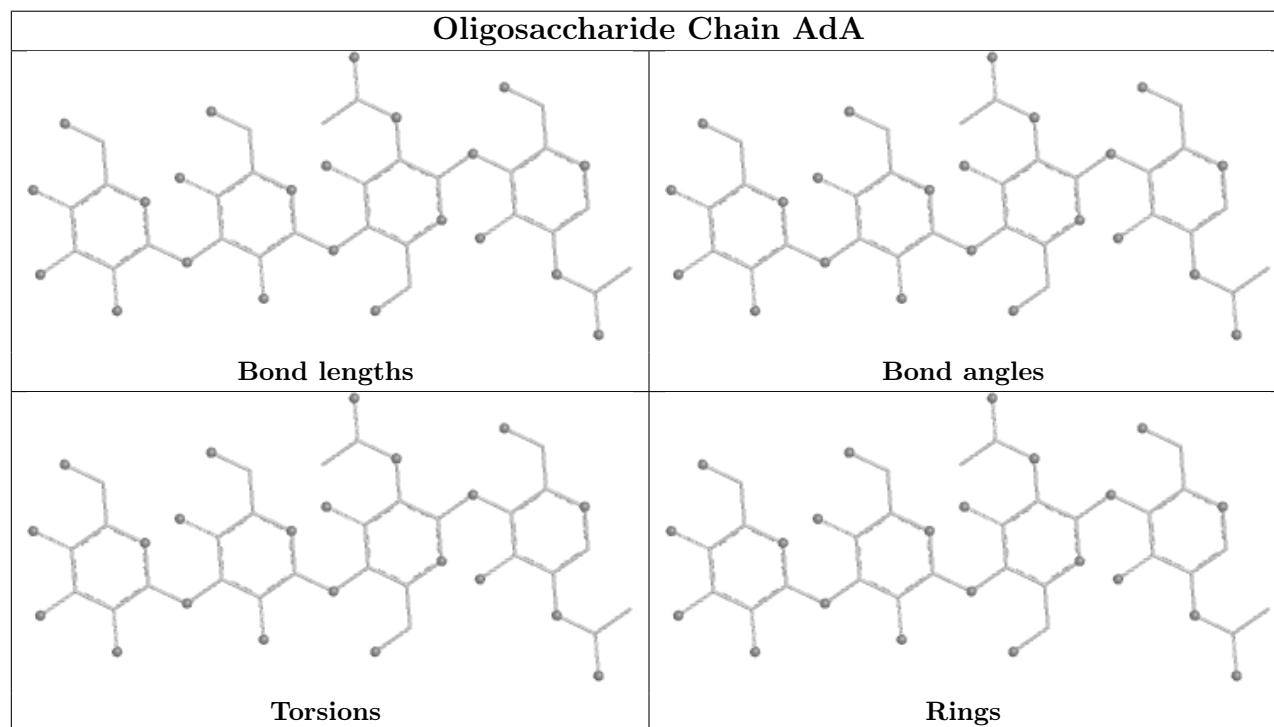
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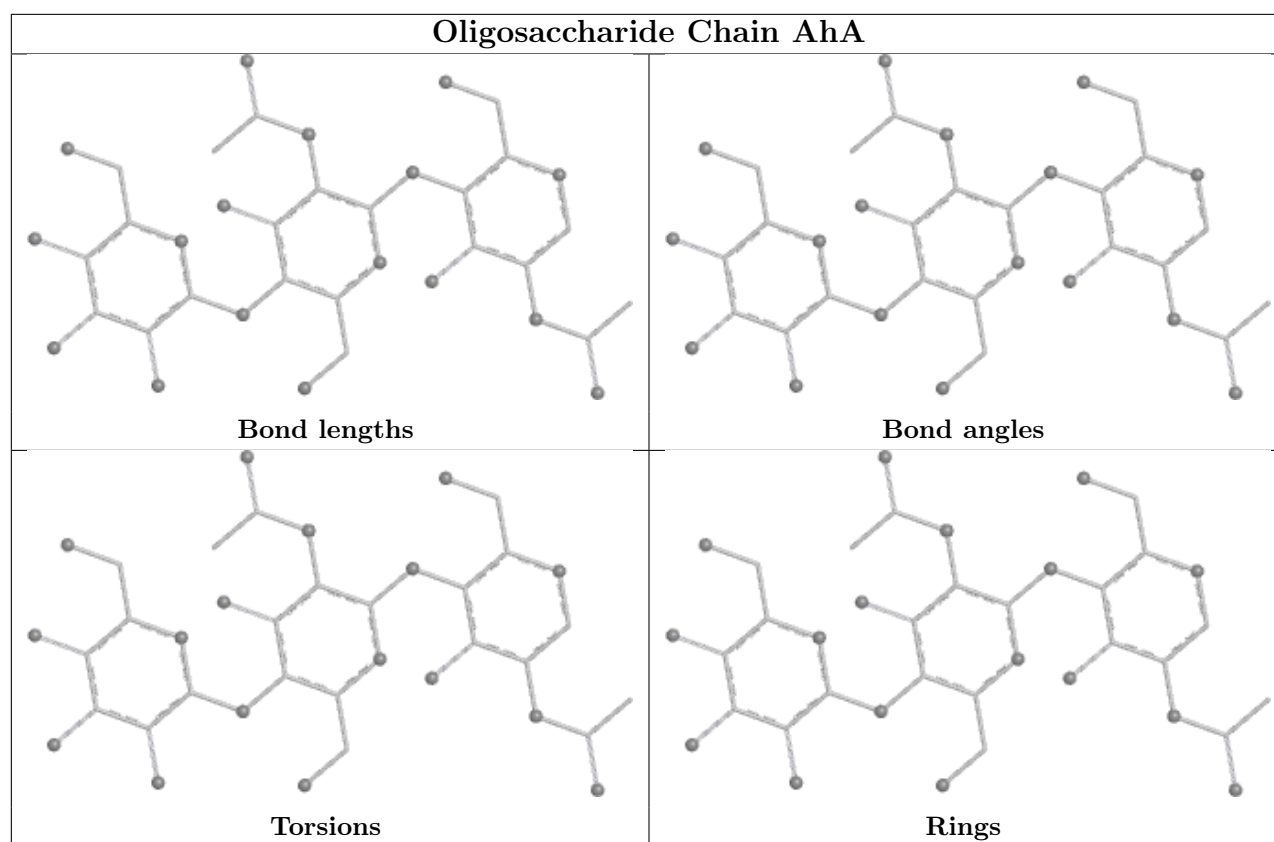
Mol	Chain	Res	Type	Atoms
4	BeB	2	NAG	C8-C7-N2-C2
4	BeB	2	NAG	O7-C7-N2-C2
3	AhA	3	MAN	C4-C5-C6-O6

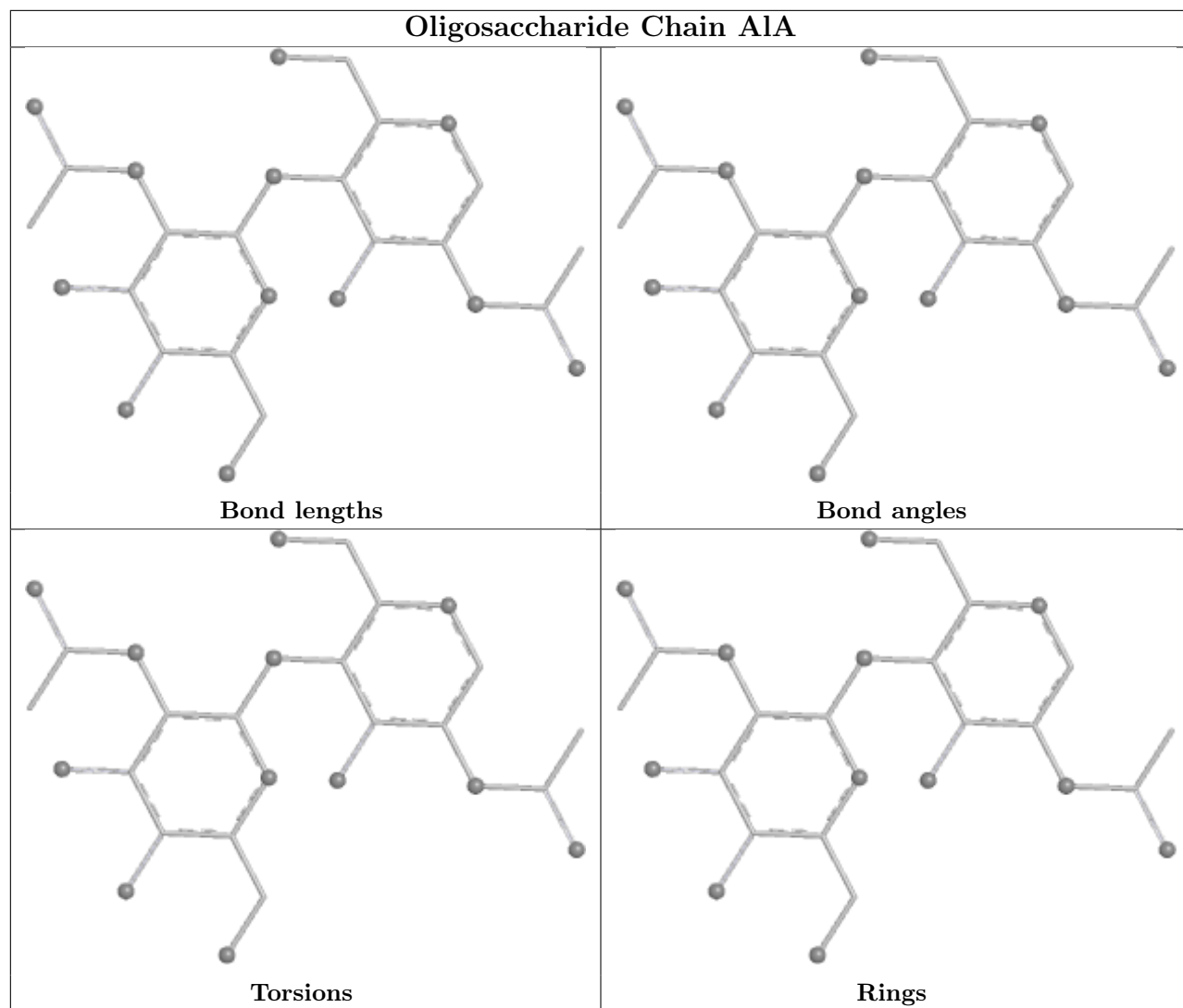
There are no ring outliers.

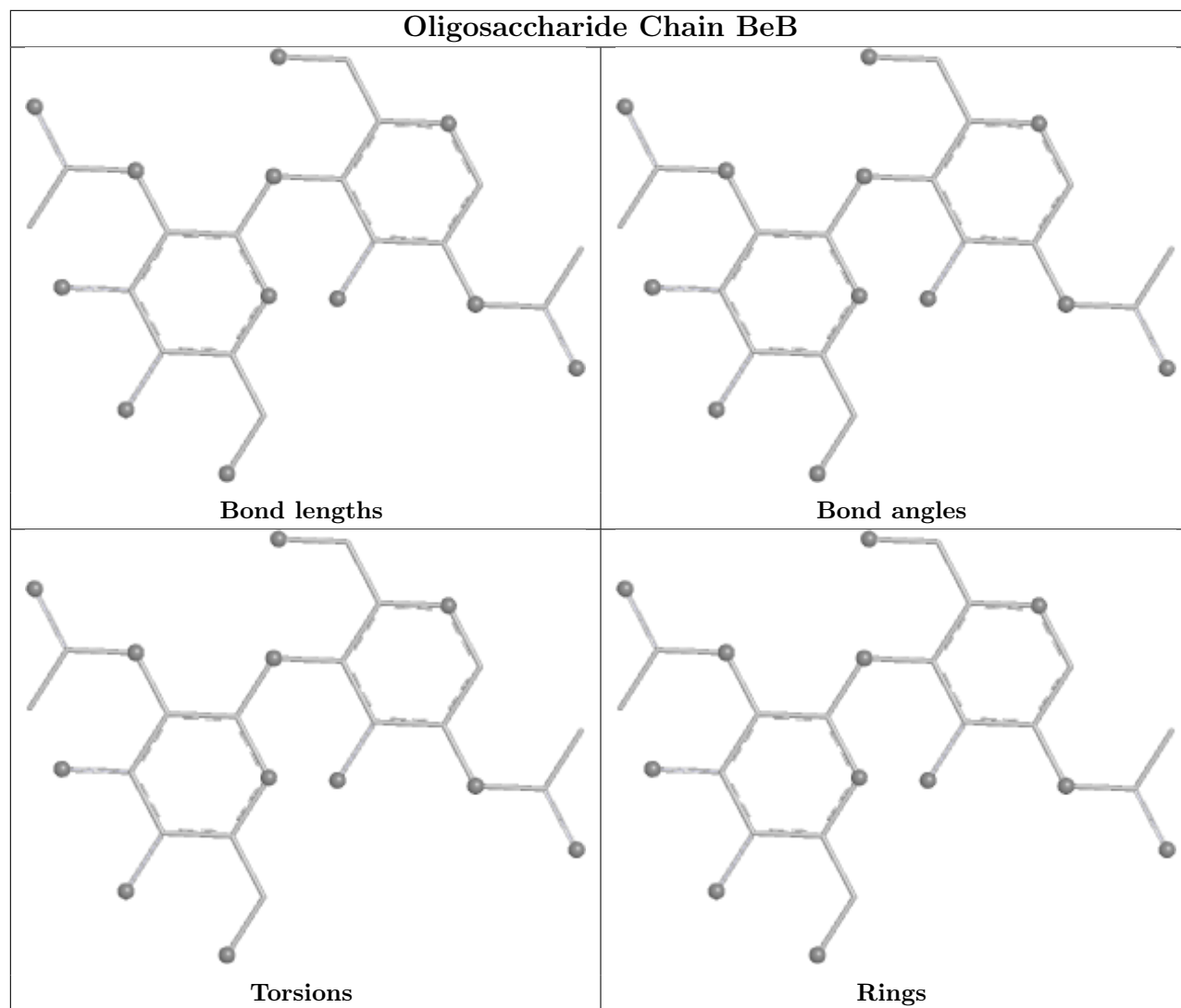
No monomer is involved in short contacts.

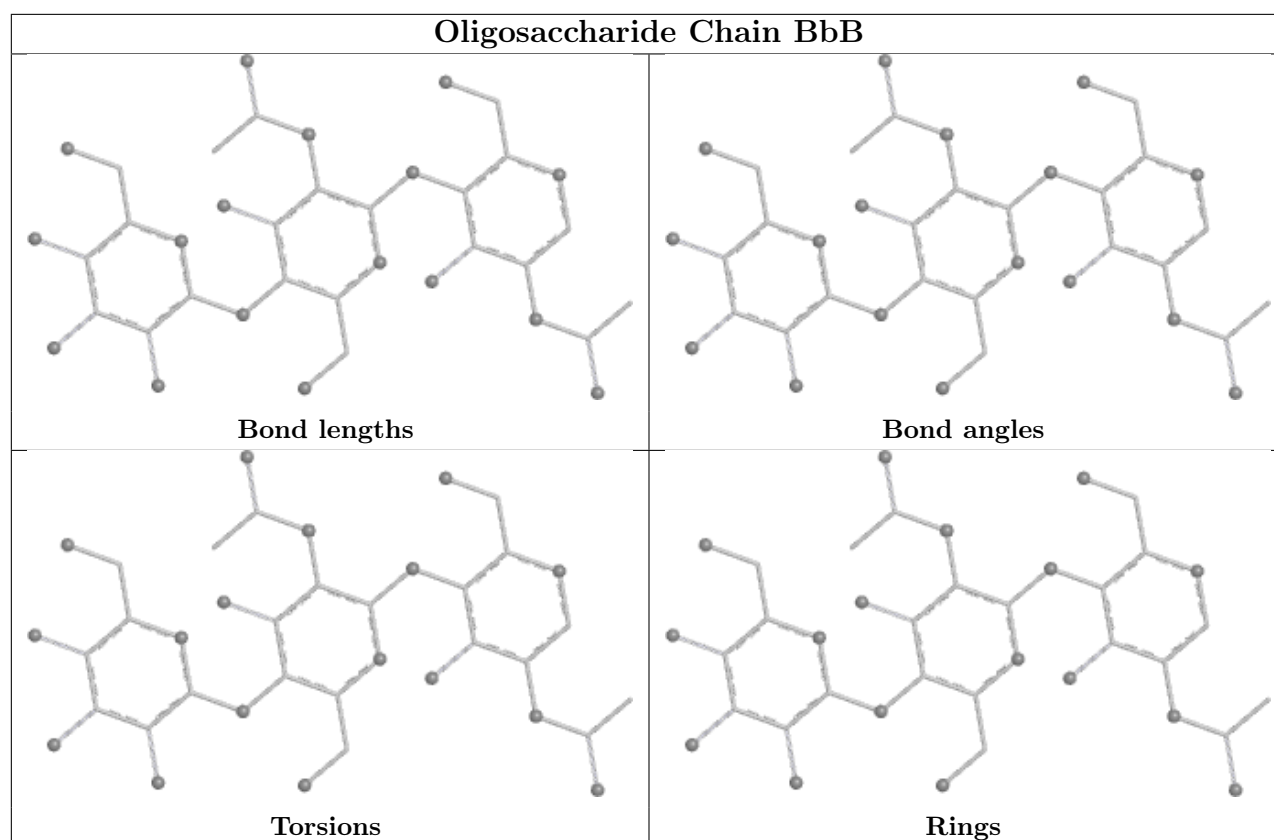
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
9	TZV	AbA	1006	-	24,26,26	1.12	1 (4%)	34,37,37	1.26	4 (11%)
9	TZV	BaB	1004	-	24,26,26	1.07	1 (4%)	34,37,37	1.34	4 (11%)
10	EDO	AbA	1007	-	3,3,3	0.05	0	2,2,2	0.10	0
8	NAG	AbA	1005	1	14,14,15	0.29	0	17,19,21	0.99	0
8	NAG	BaB	1003	1	14,14,15	0.44	0	17,19,21	1.14	2 (11%)
8	NAG	AbA	1004	1	14,14,15	0.65	0	17,19,21	1.63	3 (17%)
6	PO4	BaB	1005	7	4,4,4	0.73	0	6,6,6	0.47	0
10	EDO	AbA	1009	-	3,3,3	0.17	0	2,2,2	0.28	0
6	PO4	AbA	1001	1,7	0,3,4	-	-	0,3,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	BaB	1002	1	14,14,15	0.56	0	17,19,21	1.63	5 (29%)
10	EDO	AbA	1008	-	3,3,3	0.07	0	2,2,2	0.18	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
9	TZV	AbA	1006	-	-	6/10/11/11	0/3/3/3
9	TZV	BaB	1004	-	-	3/10/11/11	0/3/3/3
10	EDO	AbA	1007	-	-	1/1/1/1	-
8	NAG	AbA	1005	1	-	2/6/23/26	0/1/1/1
8	NAG	BaB	1003	1	-	1/6/23/26	0/1/1/1
8	NAG	AbA	1004	1	-	3/6/23/26	0/1/1/1
10	EDO	AbA	1009	-	-	1/1/1/1	-
8	NAG	BaB	1002	1	-	3/6/23/26	0/1/1/1
10	EDO	AbA	1008	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BaB	1004	TZV	C06-C11	-3.74	1.36	1.42
9	AbA	1006	TZV	C06-C11	-3.67	1.36	1.42

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AbA	1004	NAG	C1-C2-N2	-4.53	103.30	110.43
8	BaB	1002	NAG	C1-C2-N2	3.92	116.62	110.43
9	BaB	1004	TZV	C09-N10-C11	3.37	122.03	116.93
9	AbA	1006	TZV	C09-N10-C11	3.33	121.97	116.93
9	BaB	1004	TZV	C07-O13-C14	-3.28	111.36	118.79

There are no chirality outliers.

5 of 21 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

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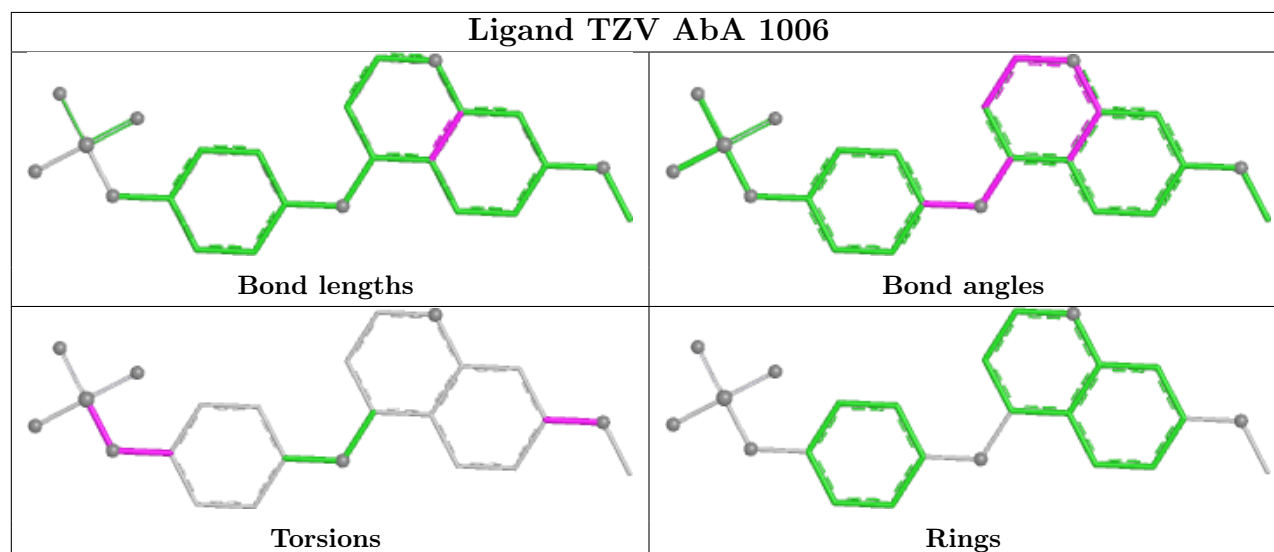
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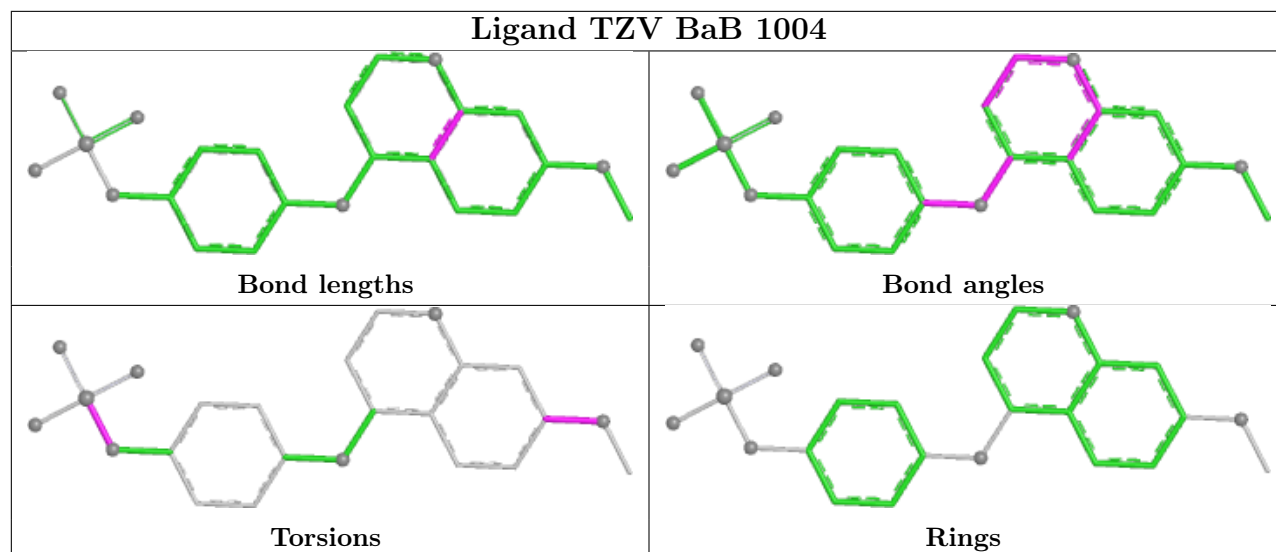
Mol	Chain	Res	Type	Atoms
9	BaB	1004	TZV	C17-N20-S21-O22
9	AbA	1006	TZV	C04-C03-O02-C01
9	AbA	1006	TZV	C12-C03-O02-C01

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	AbA	817/925 (88%)	0.16	42 (5%) 33 33	13, 41, 87, 150	5 (0%)
1	BaB	795/925 (85%)	1.05	183 (23%) 2 2	20, 63, 127, 152	2 (0%)
All	All	1612/1850 (87%)	0.60	225 (13%) 6 6	13, 48, 117, 152	7 (0%)

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BaB	678	GLN	6.2
1	AbA	529[A]	TYR	5.9
1	BaB	693	THR	5.7
1	BaB	722	PRO	5.6
1	BaB	723	VAL	5.6

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	-	-	31,34,37,46	0
2	NAG	AdA	2	14/15	-	-	52,59,66,83	0
2	BMA	AdA	3	11/12	-	-	86,93,99,111	0
2	BMA	AdA	4	11/12	-	-	119,137,143,152	0
3	NAG	AhA	1	14/15	-	-	50,65,72,75	0

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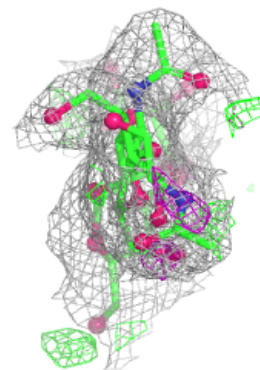
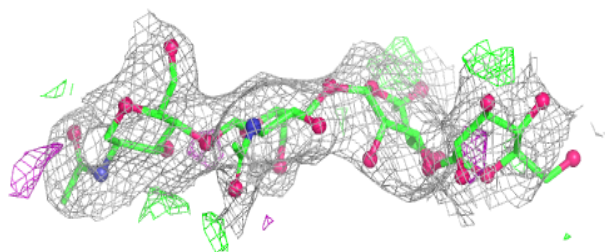
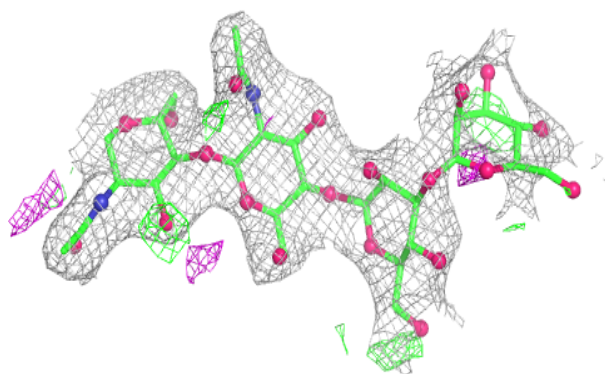
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	AhA	2	14/15	-	-	65,75,84,98	0
3	MAN	AhA	3	11/12	-	-	98,111,122,127	0
4	NAG	AlA	1	14/15	-	-	71,84,100,111	0
4	NAG	AlA	2	14/15	-	-	123,141,148,151	0
4	NAG	BeB	1	14/15	-	-	70,80,83,88	0
4	NAG	BeB	2	14/15	-	-	81,93,96,98	0
5	NAG	BbB	1	14/15	-	-	56,61,68,76	0
5	NAG	BbB	2	14/15	-	-	77,88,91,99	0
5	BMA	BbB	3	11/12	-	-	86,103,108,108	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.

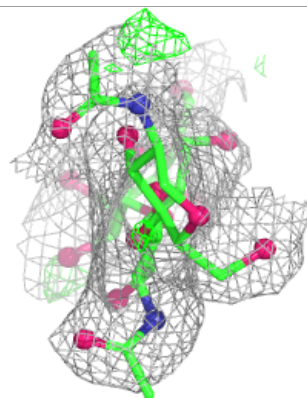
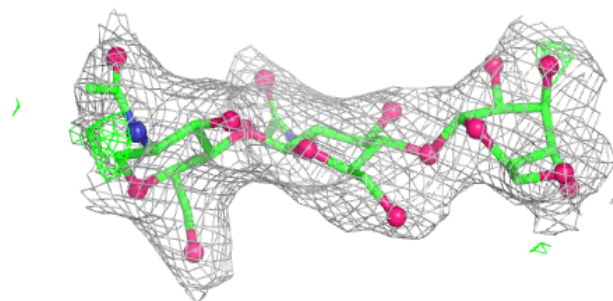
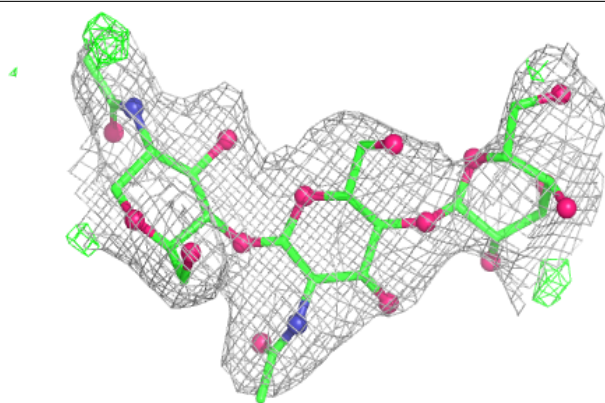
Electron density around Chain AdA:

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

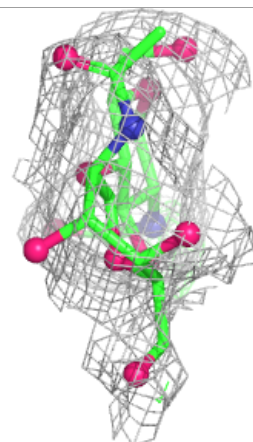
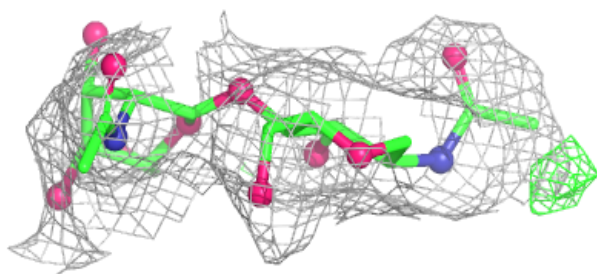
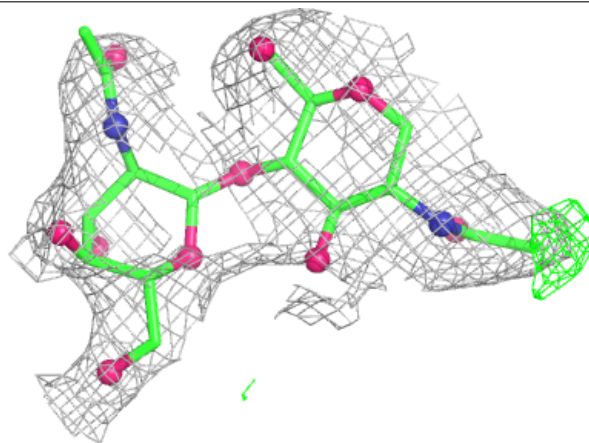


Electron density around Chain AhA:

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

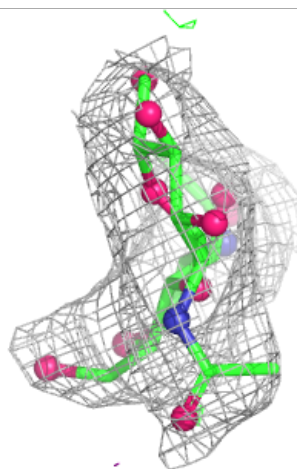
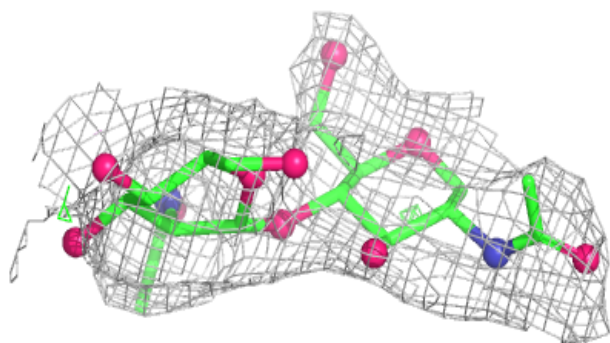
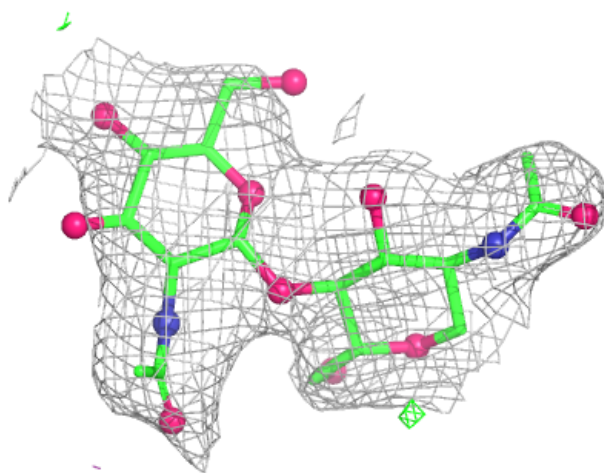
**Electron density around Chain A1A:**

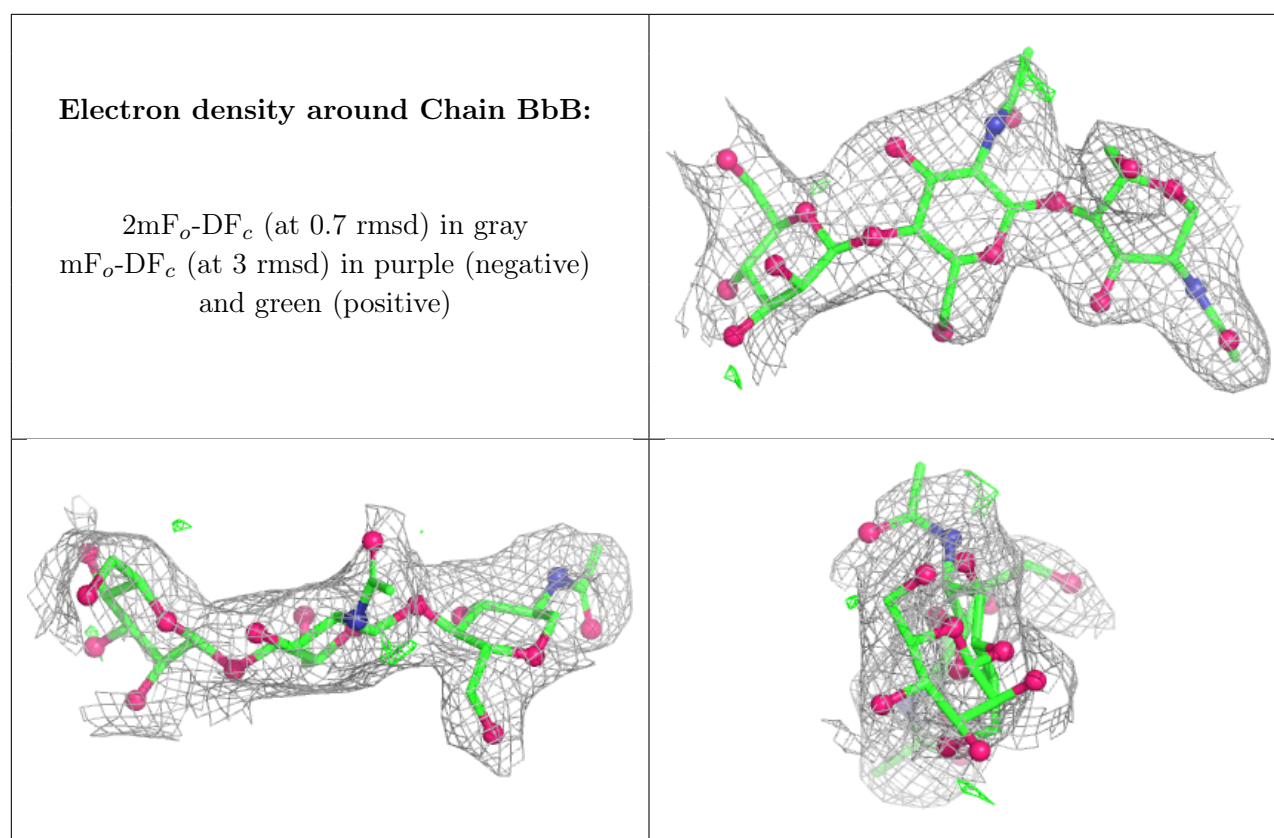
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

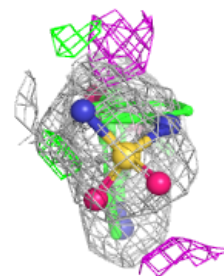
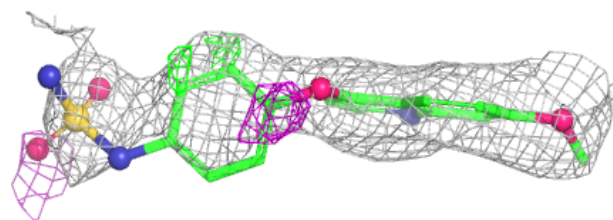
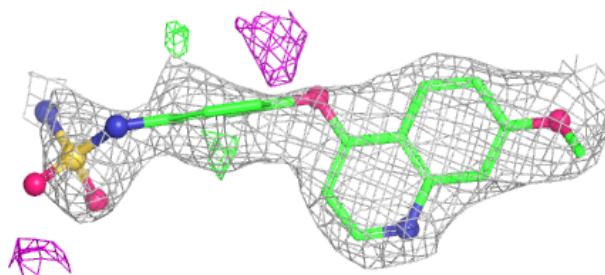
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	BaB	1002	14/15	0.45	0.22	118,134,143,151	0
8	NAG	AbA	1004	14/15	0.49	0.22	91,101,114,115	0
8	NAG	BaB	1003	14/15	0.70	0.16	99,106,110,115	0
6	PO4	AbA	1001	4/5	0.75	0.34	71,82,93,95	0
8	NAG	AbA	1005	14/15	0.80	0.14	67,86,93,95	0
10	EDO	AbA	1009	4/4	0.85	0.18	62,63,66,66	0
9	TZV	BaB	1004	24/24	0.87	0.17	48,61,112,123	0
9	TZV	AbA	1006	24/24	0.89	0.15	33,41,109,117	0
6	PO4	BaB	1005	5/5	0.89	0.16	49,49,52,52	5
7	ZN	AbA	1003	1/1	0.89	0.25	78,78,78,78	1
10	EDO	AbA	1008	4/4	0.90	0.16	58,60,61,62	0
10	EDO	AbA	1007	4/4	0.93	0.18	48,50,52,56	0
7	ZN	BaB	1001	1/1	0.99	0.04	54,54,54,54	0
7	ZN	AbA	1002	1/1	0.99	0.05	44,44,44,44	0

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

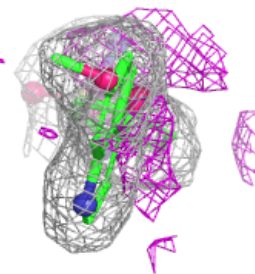
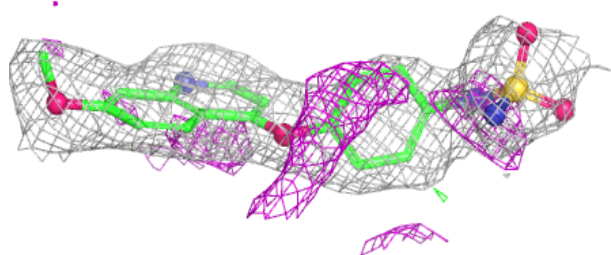
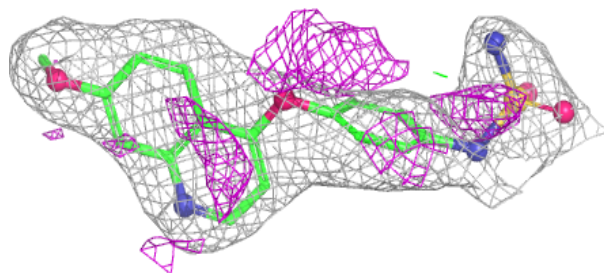
Electron density around TZV BaB 1004:

$2mF_o-DF_c$ (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.