



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:32 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

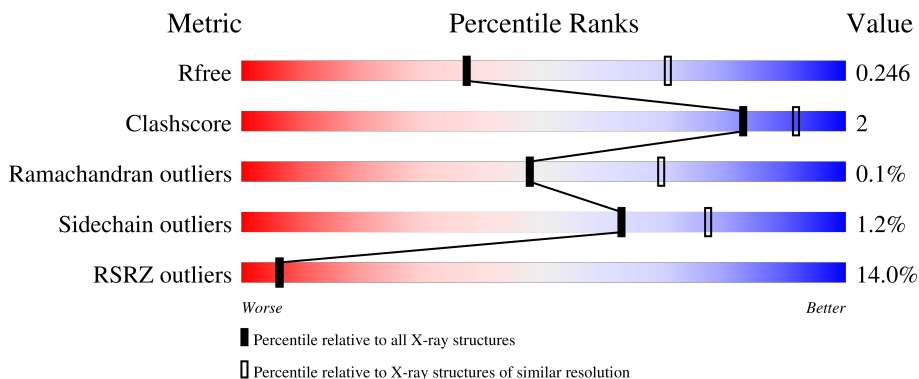
1 Overall quality at a glance

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.



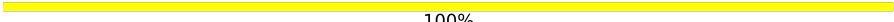
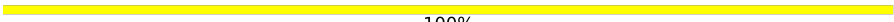
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	
1	BaB	925	
2	AdA	4	
3	AhA	3	
4	AlA	2	

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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.

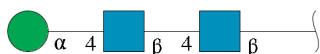
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AbA	817	6572	4194	1117	1211	50	0	5	0
1	BaB	795	6180	3937	1049	1147	47	0	2	0

- 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
			Total	C	N	O			
2	AdA	4	50	28	2	20	0	0	0

- 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.



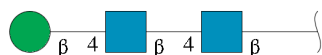
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	AhA	3	39	22	2	15	0	0	0

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



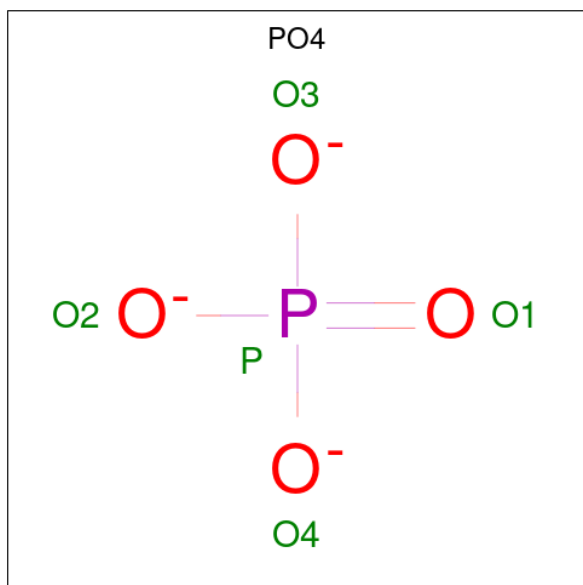
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AlA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	BeB	2	Total	C	N	O	0	0	0
			28	16	2	10			

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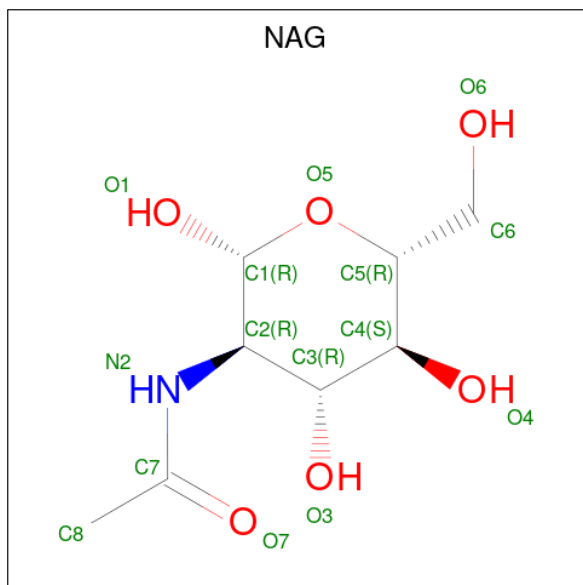
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BaB	1	Total	O	P	0	0
			5	4	1		

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

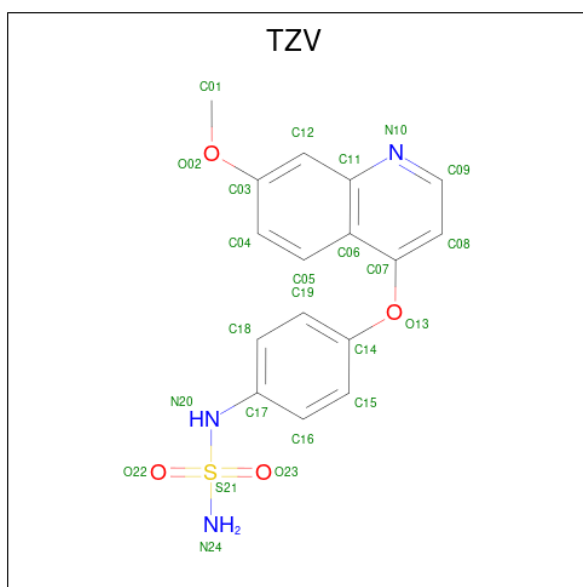
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AbA	2	Total	Zn	0	0
			2	2		
7	BaB	1	Total	Zn	0	0
			1	1		

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



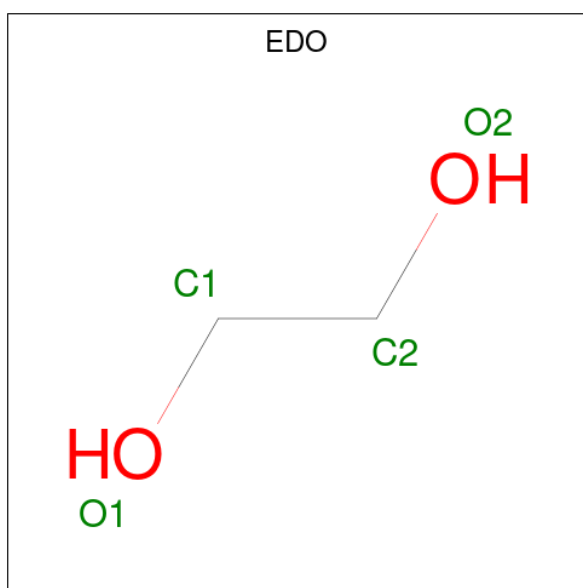
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	AbA	1	Total	C	N	O	0	0
			14	8	1	5		
8	AbA	1	Total	C	N	O	0	0
			14	8	1	5		
8	BaB	1	Total	C	N	O	0	0
			14	8	1	5		
8	BaB	1	Total	C	N	O	0	0
			14	8	1	5		

- 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).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



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	0	0
			4	2	2		

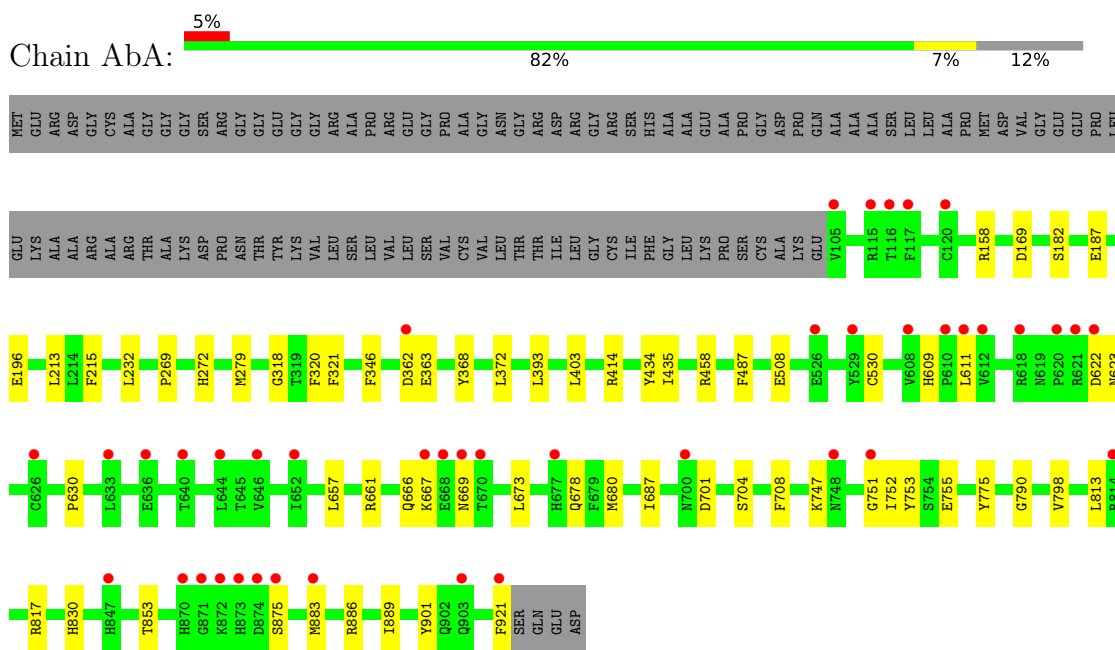
- Molecule 11 is water.

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

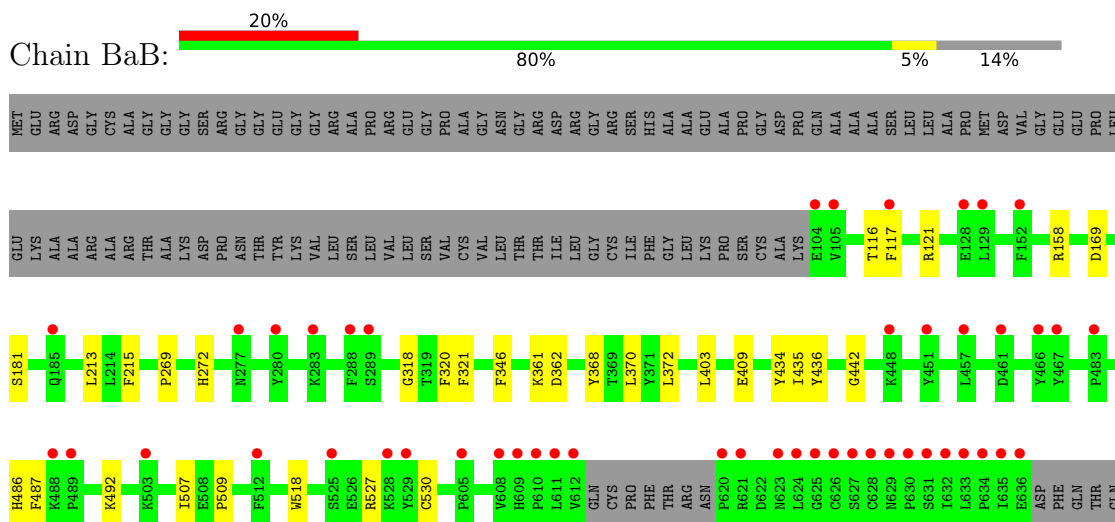
3 Residue-property plots [i](#)

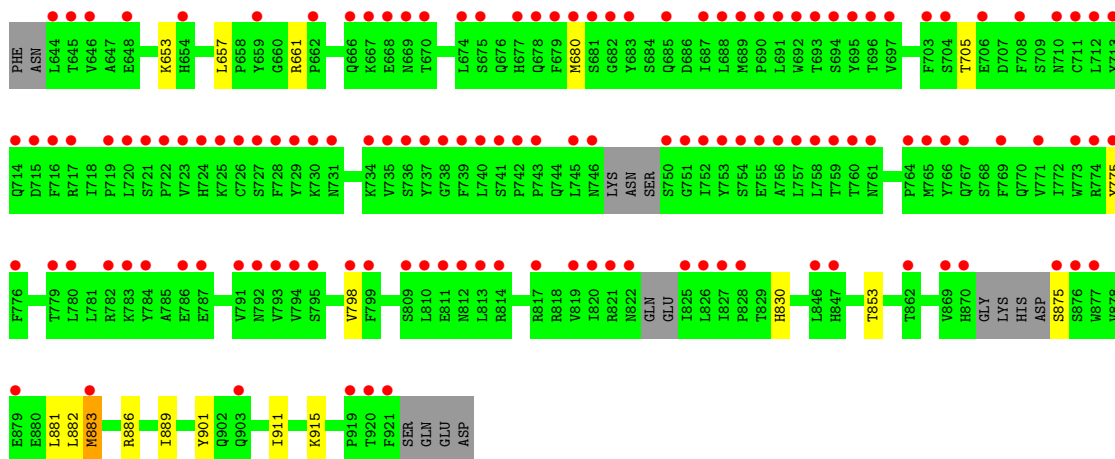
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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




- 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%

MAG1
MAG2
BNA3
BNA4

- 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%


MAG1
MAG2
MAN3

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

Chain AIA:  100%

MAG1
MAG2

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

Chain BeB:  100%

MAG1
MAG2

- 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)	Xtrriage
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	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.

All (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
1:BaB:486:HIS:ND1	1:BaB:518:TRP:CZ2	2.66	0.63
1:BaB:436:TYR:OH	1:BaB:527:ARG:NH1	2.33	0.61
1:AbA:666:GLN:HB2	1:AbA:669:ASN:HD22	1.67	0.58
1:BaB:435:ILE:HD13	1:BaB:487:PHE:CD1	2.38	0.58
1:AbA:609:HIS:NE2	1:AbA:667:LYS:O	2.38	0.57
1:AbA:435:ILE:HD13	1:AbA:487:PHE:CD1	2.41	0.55
1:BaB:158:ARG:NH2	1:BaB:169:ASP:OD1	2.40	0.55
1:AbA:883[A]:MET:SD	1:AbA:921:PHE:HE2	2.30	0.55
1:BaB:492:LYS:HG3	1:BaB:509:PRO:HA	1.89	0.55
1:BaB:492:LYS:HD3	1:BaB:507:ILE:O	2.08	0.54
1:AbA:883[A]:MET:O	1:AbA:886:ARG:HD3	2.07	0.53
1:BaB:775:TYR:CE2	1:BaB:875:SER:HB2	2.43	0.53
1:BaB:653:LYS:HA	1:BaB:680:MET:HE3	1.89	0.53
1:BaB:883:MET:O	1:BaB:886:ARG:HD3	2.08	0.52
1:AbA:883[B]:MET:O	1:AbA:886:ARG:HD3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AbA:158:ARG:NH2	1:AbA:169:ASP:OD1	2.43	0.52
1:AbA:687:ILE:HG22	1:AbA:817[A]:ARG:HH21	1.75	0.52
1:AbA:883[A]:MET:SD	1:AbA:921:PHE:HD2	2.32	0.52
1:AbA:753:TYR:CZ	1:AbA:755:GLU:HB2	2.45	0.51
1:AbA:701:ASP:OD2	1:AbA:747:LYS:HE2	2.11	0.50
1:AbA:666:GLN:CB	1:AbA:669:ASN:HD22	2.24	0.50
1:AbA:657:LEU:HD13	1:AbA:661:ARG:HB3	1.93	0.49
1:BaB:657:LEU:HD13	1:BaB:661:ARG:HB3	1.95	0.48
1:AbA:775:TYR:CZ	1:AbA:875:SER:HA	2.49	0.48
1:BaB:486:HIS:CE1	1:BaB:518:TRP:CZ2	3.02	0.47
1:AbA:458:ARG:HB2	1:AbA:508:GLU:HG2	1.96	0.47
1:BaB:911:ILE:HG22	1:BaB:915:LYS:HE2	1.97	0.46
1:AbA:853:THR:HB	1:AbA:889:ILE:HD11	1.97	0.46
1:AbA:775:TYR:CE1	1:AbA:875:SER:HA	2.50	0.46
1:BaB:853:THR:HB	1:BaB:889:ILE:HD11	1.99	0.45
1:AbA:362:ASP:OD1	1:AbA:363:GLU:HG2	2.17	0.44
1:AbA:798:VAL:HB	1:AbA:830:HIS:HB2	1.98	0.44
1:AbA:687:ILE:HG22	1:AbA:817[A]:ARG:NH2	2.32	0.44
1:AbA:182:SER:HA	1:AbA:187:GLU:O	2.18	0.44
1:BaB:318:GLY:O	1:BaB:368:TYR:HA	2.18	0.44
1:AbA:678:GLN:HB2	1:AbA:753:TYR:CE2	2.52	0.44
1:BaB:181:SER:HB2	1:BaB:409:GLU:OE1	2.17	0.44
1:BaB:213:LEU:HD23	1:BaB:403:LEU:HD21	2.00	0.43
1:BaB:889:ILE:HD13	1:BaB:901:TYR:HE2	1.84	0.43
1:AbA:318:GLY:O	1:AbA:368:TYR:HA	2.18	0.43
1:AbA:269:PRO:HA	1:AbA:272:HIS:CE1	2.54	0.42
1:BaB:269:PRO:HA	1:BaB:272:HIS:CE1	2.54	0.42
1:BaB:798:VAL:HB	1:BaB:830:HIS:HB2	2.02	0.42
1:AbA:889:ILE:HD13	1:AbA:901:TYR:HE2	1.84	0.42
1:AbA:704:SER:HB2	1:AbA:751:GLY:O	2.19	0.42
1:BaB:116:THR:O	1:BaB:121[A]:ARG:NH2	2.52	0.42
1:AbA:213:LEU:HD23	1:AbA:403:LEU:HD21	2.01	0.42
1:AbA:813:LEU:HD23	1:AbA:813:LEU:HA	1.96	0.41
1:AbA:196:GLU:HG3	1:AbA:414:ARG:NH1	2.35	0.41
1:BaB:775:TYR:CD2	1:BaB:875:SER:HB2	2.55	0.41
1:AbA:346:PHE:CD1	1:AbA:372:LEU:HD22	2.56	0.41
1:AbA:232:LEU:HD21	1:AbA:393:LEU:HB3	2.02	0.41
1:AbA:622:ASP:OD1	1:AbA:623:ASN:N	2.53	0.41
1:BaB:346:PHE:CD1	1:BaB:372:LEU:HD22	2.55	0.41
1:BaB:653:LYS:CA	1:BaB:680:MET:HE3	2.52	0.40
1:AbA:611:LEU:HD11	1:AbA:661:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	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 [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%)	76 85
1	BaB	655/824 (80%)	644 (98%)	11 (2%)	53 71
All	All	1388/1648 (84%)	1372 (99%)	16 (1%)	63 77

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

Mol	Chain	Res	Type
1	AbA	215	PHE

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Mol	Chain	Res	Type
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	0.60	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

All (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
2	AdA	3	BMA	O2-C2-C1	5.16	121.03	109.22
4	BeB	1	NAG	C8-C7-N2	4.86	124.17	116.12
5	BbB	1	NAG	C3-C4-C5	3.79	117.10	110.23
5	BbB	1	NAG	O5-C1-C2	-3.60	105.72	111.29
3	AhA	1	NAG	C8-C7-N2	-3.57	110.20	116.12
4	BeB	2	NAG	O5-C1-C2	3.33	116.44	111.29
2	AdA	1	NAG	O4-C4-C3	-2.97	103.37	110.38
4	BeB	2	NAG	O5-C5-C6	2.93	113.37	107.66
2	AdA	3	BMA	O2-C2-C3	-2.90	104.14	110.15
2	AdA	1	NAG	O5-C1-C2	-2.88	106.83	111.29
4	BeB	2	NAG	C8-C7-N2	2.83	120.81	116.12
4	AlA	2	NAG	C1-O5-C5	2.77	115.89	112.19
4	BeB	1	NAG	C1-C2-N2	-2.76	106.09	110.43
4	BeB	1	NAG	O5-C1-C2	-2.62	107.24	111.29
2	AdA	3	BMA	O5-C1-C2	2.59	116.96	110.79
3	AhA	3	MAN	C1-C2-C3	2.57	113.39	109.64
5	BbB	2	NAG	O5-C5-C4	-2.42	104.95	110.83
3	AhA	1	NAG	O7-C7-N2	2.29	126.03	121.98
2	AdA	2	NAG	C1-C2-N2	2.28	114.03	110.43
2	AdA	2	NAG	C1-O5-C5	2.22	115.16	112.19
4	BeB	2	NAG	O7-C7-N2	-2.20	118.10	121.98
3	AhA	1	NAG	C4-C3-C2	-2.16	107.86	111.02
5	BbB	3	BMA	C3-C4-C5	2.15	114.13	110.23
5	BbB	2	NAG	C4-C3-C2	-2.08	107.97	111.02
4	AlA	1	NAG	O7-C7-N2	2.07	125.64	121.98
2	AdA	3	BMA	O3-C3-C2	-2.06	105.85	110.05
3	AhA	2	NAG	C3-C4-C5	-2.05	106.51	110.23
4	AlA	1	NAG	C8-C7-N2	-2.01	112.78	116.12

All (2) chirality outliers are listed below:

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

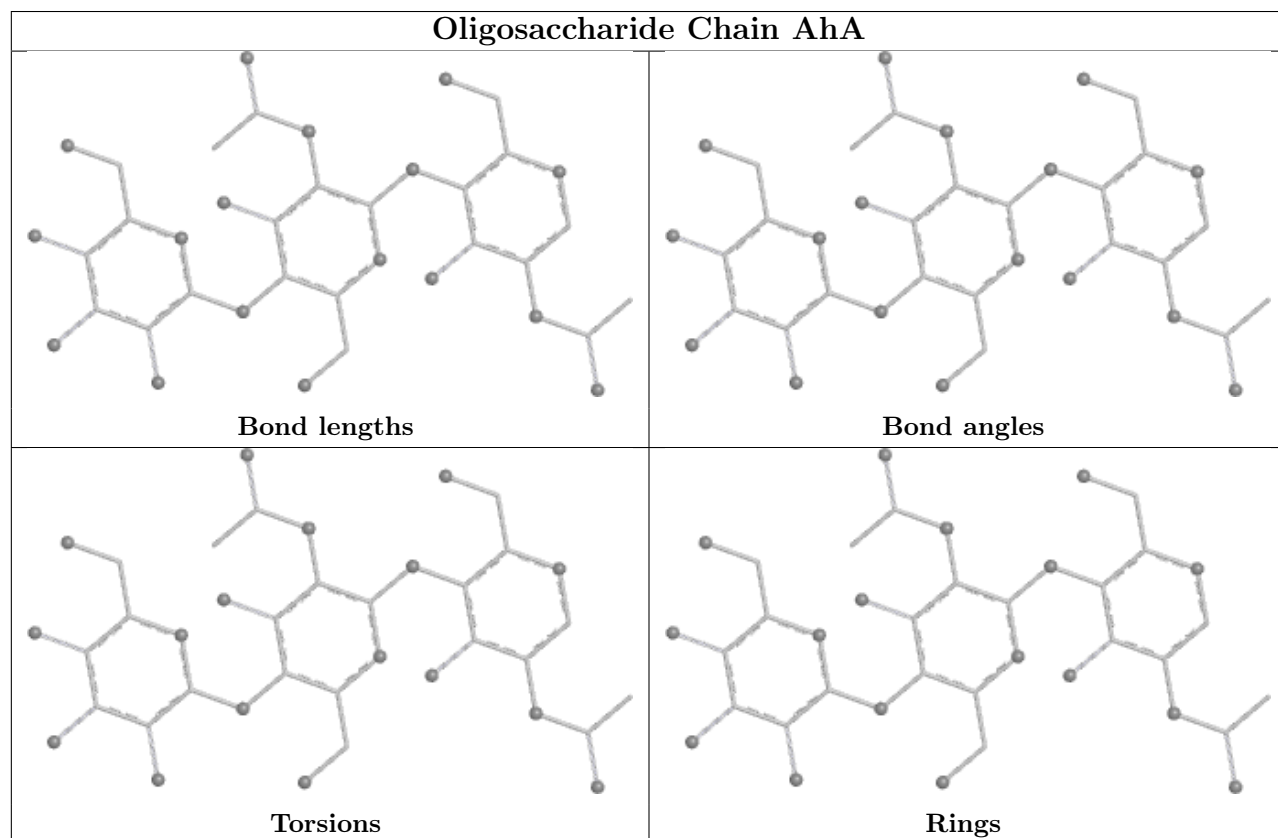
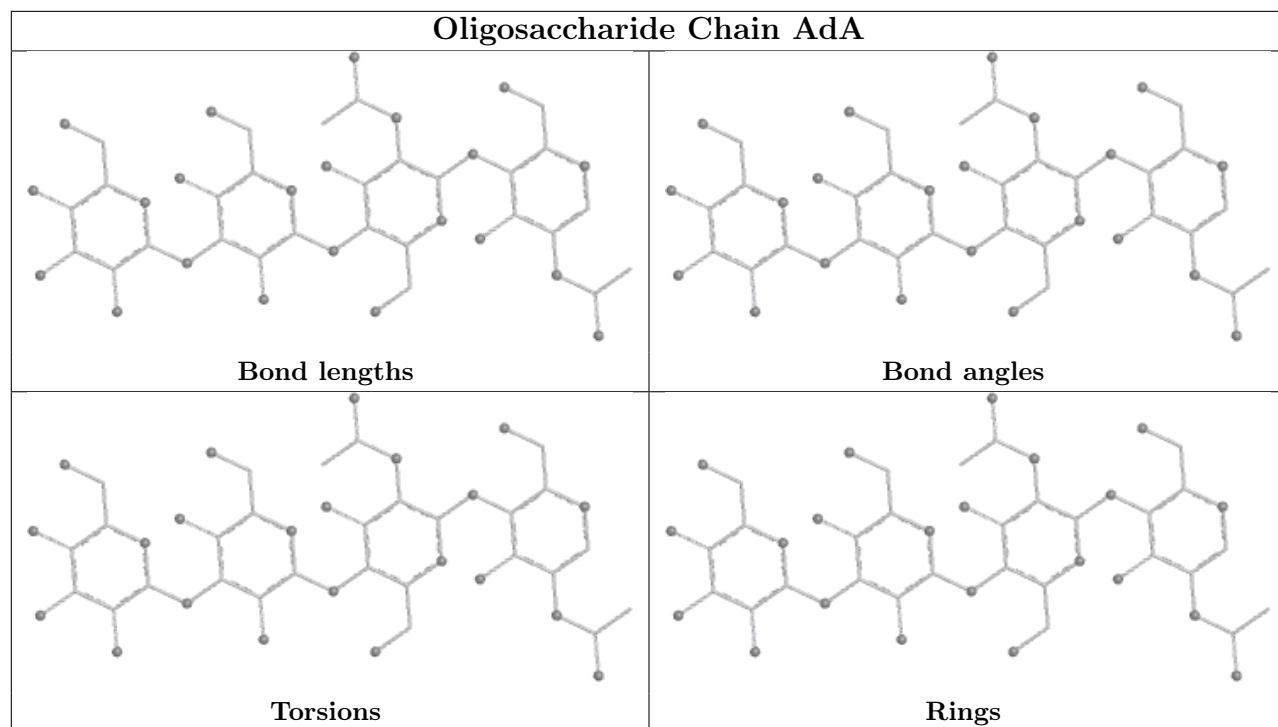
All (29) torsion outliers are listed below:

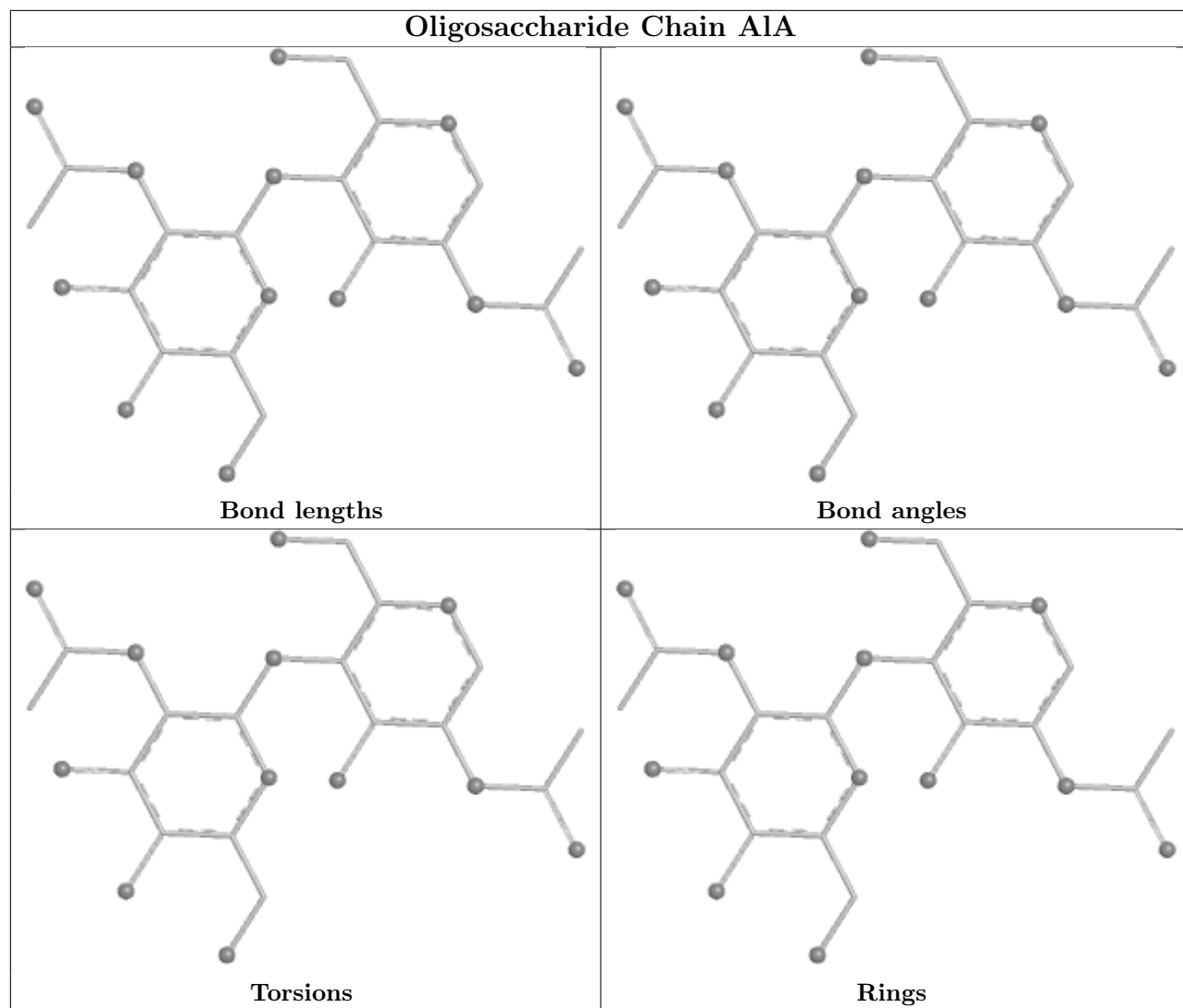
Mol	Chain	Res	Type	Atoms
4	BeB	1	NAG	C8-C7-N2-C2
4	BeB	1	NAG	O7-C7-N2-C2
4	BeB	2	NAG	C8-C7-N2-C2
4	BeB	2	NAG	O7-C7-N2-C2
3	AhA	3	MAN	C4-C5-C6-O6
3	AhA	3	MAN	O5-C5-C6-O6
4	AlA	2	NAG	C4-C5-C6-O6
2	AdA	4	BMA	O5-C5-C6-O6
4	BeB	2	NAG	O5-C5-C6-O6
2	AdA	3	BMA	O5-C5-C6-O6
3	AhA	2	NAG	O5-C5-C6-O6
4	AlA	2	NAG	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
5	BbB	1	NAG	C4-C5-C6-O6
2	AdA	4	BMA	C4-C5-C6-O6
4	BeB	2	NAG	C4-C5-C6-O6
4	AlA	1	NAG	C8-C7-N2-C2
3	AhA	2	NAG	C4-C5-C6-O6
2	AdA	2	NAG	C4-C5-C6-O6
3	AhA	1	NAG	C1-C2-N2-C7
2	AdA	2	NAG	O5-C5-C6-O6
4	AlA	1	NAG	C1-C2-N2-C7
3	AhA	1	NAG	C3-C2-N2-C7
4	AlA	1	NAG	C3-C2-N2-C7
4	AlA	1	NAG	O7-C7-N2-C2
5	BbB	2	NAG	O5-C5-C6-O6

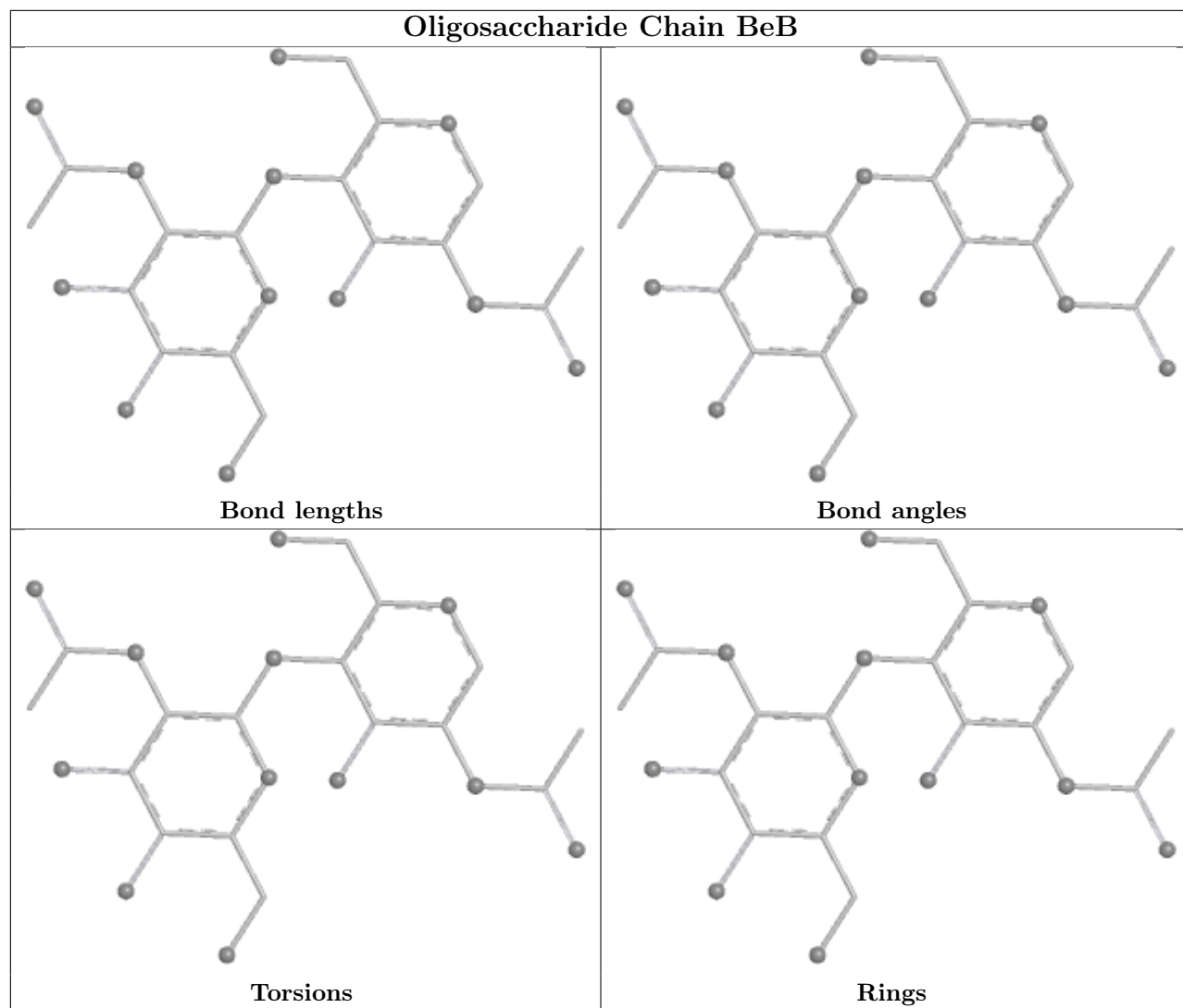
There are no ring outliers.

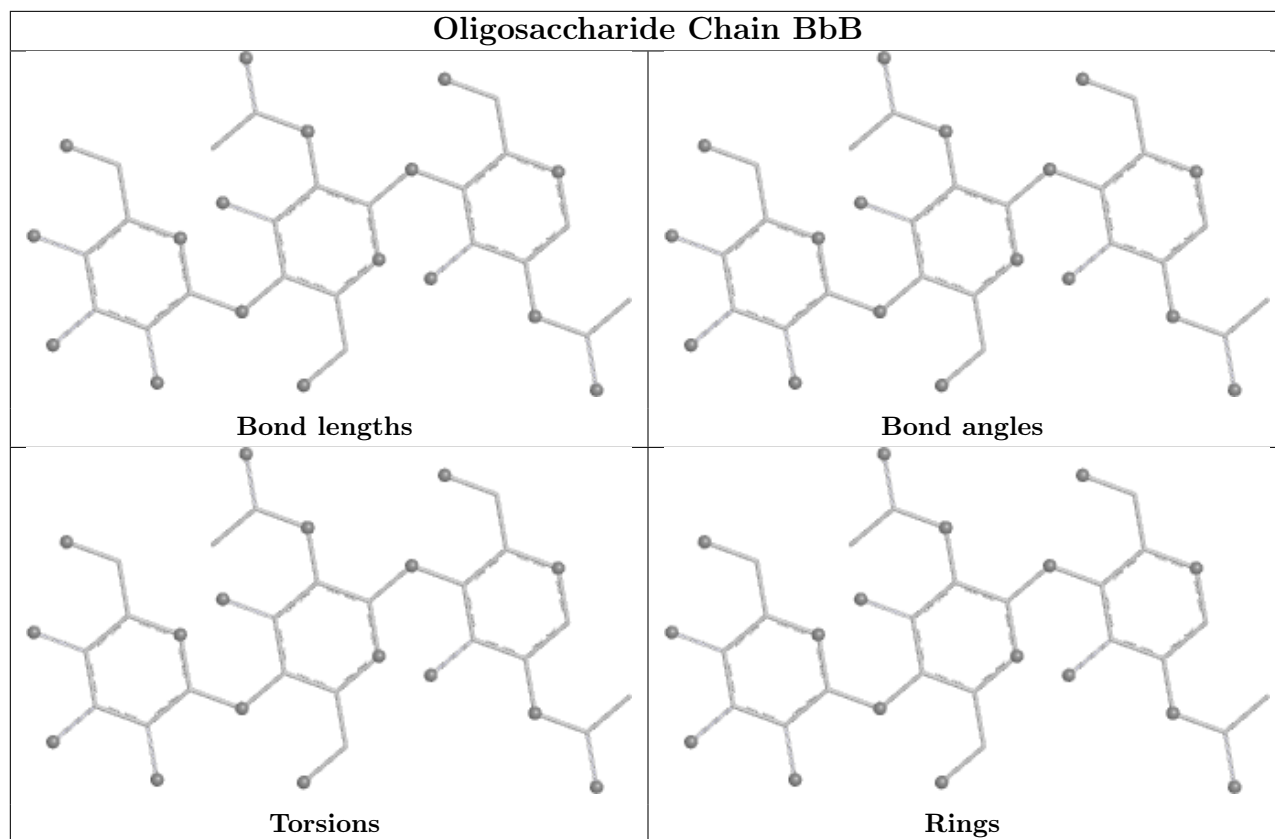
No monomer is involved in short contacts.

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

All (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
8	BaB	1003	NAG	C1-C2-N2	2.95	115.07	110.43
9	BaB	1004	TZV	C08-C09-N10	-2.89	120.31	124.60
9	AbA	1006	TZV	C08-C09-N10	-2.78	120.46	124.60
8	BaB	1002	NAG	O5-C1-C2	-2.60	107.26	111.29
8	AbA	1004	NAG	C8-C7-N2	-2.54	111.91	116.12
9	AbA	1006	TZV	C07-O13-C14	-2.43	113.30	118.79
8	BaB	1002	NAG	C2-N2-C7	-2.33	119.78	122.90
8	BaB	1003	NAG	O5-C1-C2	-2.30	107.73	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BaB	1004	TZV	C06-C11-N10	-2.16	120.53	122.82
9	AbA	1006	TZV	C06-C11-N10	-2.16	120.54	122.82
8	BaB	1002	NAG	C4-C3-C2	2.11	114.11	111.02
8	AbA	1004	NAG	O7-C7-N2	2.08	125.67	121.98
8	BaB	1002	NAG	C8-C7-N2	-2.02	112.77	116.12

There are no chirality outliers.

All (21) torsion outliers are listed below:

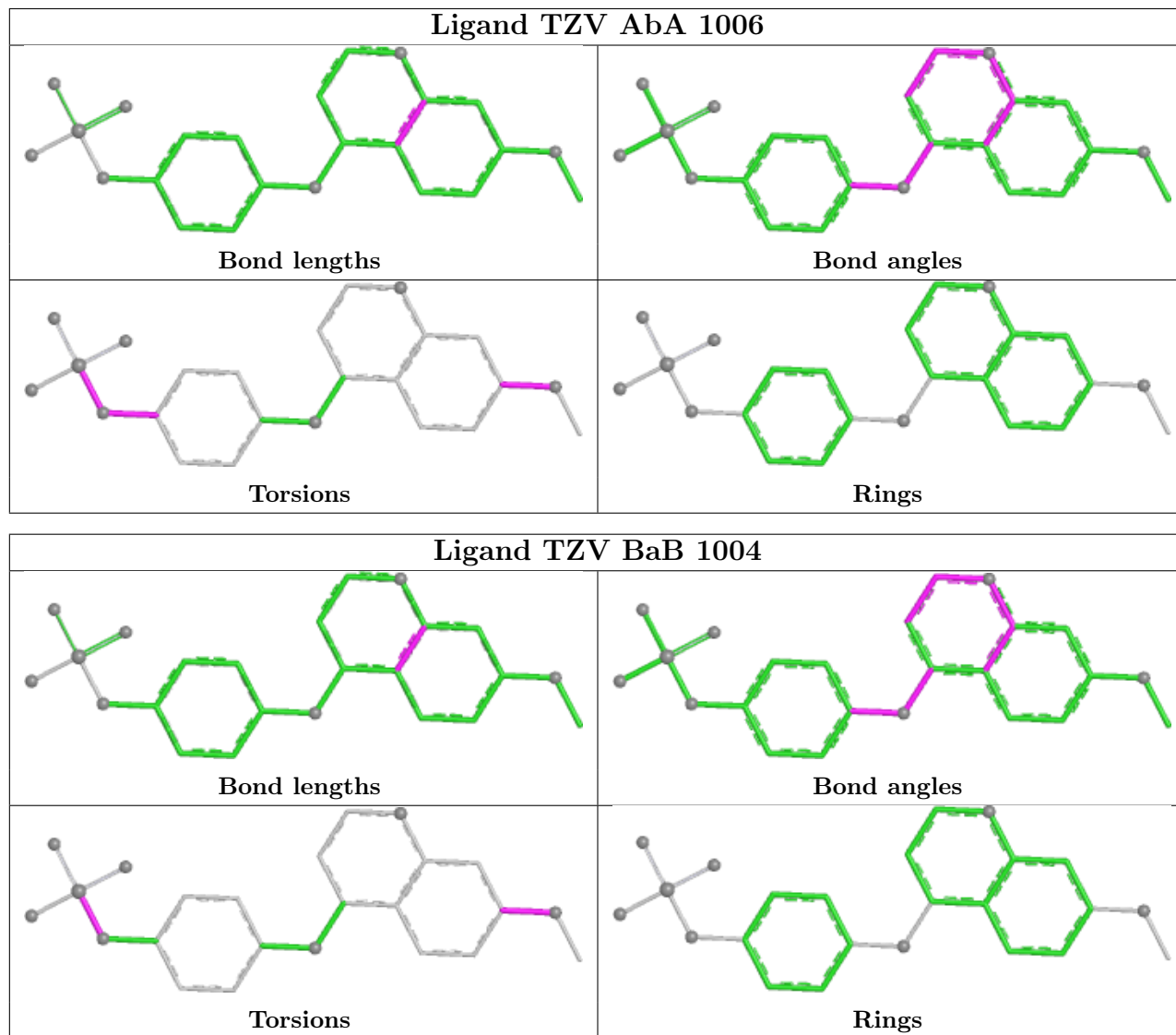
Mol	Chain	Res	Type	Atoms
9	AbA	1006	TZV	C17-N20-S21-O22
9	AbA	1006	TZV	C17-N20-S21-O23
9	BaB	1004	TZV	C17-N20-S21-O22
9	AbA	1006	TZV	C04-C03-O02-C01
9	AbA	1006	TZV	C12-C03-O02-C01
8	BaB	1002	NAG	C8-C7-N2-C2
9	BaB	1004	TZV	C04-C03-O02-C01
9	BaB	1004	TZV	C12-C03-O02-C01
8	AbA	1005	NAG	C8-C7-N2-C2
8	AbA	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
9	AbA	1006	TZV	C16-C17-N20-S21
9	AbA	1006	TZV	C18-C17-N20-S21
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 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

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, 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%)

All (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
1	BaB	289	SER	5.6
1	BaB	746	ASN	5.5
1	BaB	822	ASN	5.3
1	BaB	612	VAL	5.2
1	BaB	819	VAL	5.2
1	BaB	729	TYR	5.1
1	AbA	526	GLU	5.1
1	BaB	623	ASN	5.1
1	BaB	870	HIS	5.1
1	BaB	679	PHE	5.1
1	AbA	921	PHE	5.0
1	BaB	620	PRO	5.0
1	BaB	712	LEU	5.0
1	BaB	921	PHE	5.0
1	BaB	629	ASN	4.9
1	BaB	104	GLU	4.9
1	BaB	728	PHE	4.9
1	BaB	724	HIS	4.7
1	BaB	739	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	BaB	820	ILE	4.6
1	BaB	692	TRP	4.5
1	BaB	869	VAL	4.5
1	BaB	726	CYS	4.4
1	BaB	716	PHE	4.3
1	AbA	105	VAL	4.3
1	AbA	669	ASN	4.3
1	BaB	753	TYR	4.2
1	BaB	621	ARG	4.2
1	BaB	631	SER	4.2
1	BaB	697	VAL	4.2
1	BaB	710	ASN	4.2
1	BaB	105	VAL	4.2
1	BaB	626	CYS	4.1
1	BaB	633	LEU	4.1
1	BaB	451	TYR	4.0
1	BaB	674	LEU	4.0
1	BaB	668	GLU	4.0
1	BaB	826	LEU	3.9
1	BaB	767	GLN	3.9
1	BaB	730	LYS	3.9
1	BaB	740	LEU	3.9
1	BaB	810	LEU	3.9
1	BaB	825	ILE	3.9
1	BaB	646	VAL	3.9
1	BaB	713	TYR	3.9
1	BaB	759	THR	3.9
1	AbA	872	LYS	3.9
1	BaB	708	PHE	3.9
1	BaB	711	CYS	3.9
1	BaB	756	ALA	3.8
1	BaB	703	PHE	3.8
1	BaB	704	SER	3.8
1	BaB	795	SER	3.8
1	AbA	670	THR	3.8
1	BaB	751	GLY	3.8
1	BaB	920	THR	3.7
1	BaB	695	TYR	3.7
1	BaB	757	LEU	3.7
1	BaB	827	ILE	3.7
1	AbA	612	VAL	3.7
1	AbA	700	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	BaB	714	GLN	3.6
1	BaB	743	PRO	3.6
1	BaB	690	PRO	3.6
1	BaB	875	SER	3.6
1	BaB	682	GLY	3.6
1	BaB	735	VAL	3.6
1	BaB	787	GLU	3.6
1	BaB	780	LEU	3.5
1	BaB	814	ARG	3.5
1	BaB	731	ASN	3.5
1	BaB	758	LEU	3.5
1	BaB	742	PRO	3.5
1	BaB	630	PRO	3.4
1	BaB	771	VAL	3.4
1	BaB	727	SER	3.4
1	BaB	632	ILE	3.4
1	BaB	745	LEU	3.4
1	BaB	715	ASP	3.4
1	BaB	529	TYR	3.3
1	AbA	870	HIS	3.3
1	AbA	621	ARG	3.3
1	BaB	680	MET	3.3
1	BaB	773	TRP	3.3
1	AbA	677	HIS	3.3
1	BaB	750	SER	3.2
1	BaB	720	LEU	3.2
1	BaB	755	GLU	3.2
1	BaB	779	THR	3.2
1	BaB	512	PHE	3.2
1	BaB	677	HIS	3.2
1	BaB	721	SER	3.2
1	BaB	667	LYS	3.2
1	BaB	783	LYS	3.2
1	BaB	741	SER	3.2
1	BaB	734	LYS	3.1
1	BaB	611	LEU	3.1
1	BaB	817	ARG	3.1
1	BaB	717	ARG	3.0
1	AbA	875	SER	3.0
1	AbA	636	GLU	3.0
1	BaB	786	GLU	3.0
1	AbA	608	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	BaB	691	LEU	2.9
1	BaB	876	SER	2.9
1	BaB	628	CYS	2.9
1	BaB	466	TYR	2.9
1	BaB	689	MET	2.9
1	BaB	752	ILE	2.9
1	BaB	627	SER	2.9
1	AbA	626[A]	CYS	2.9
1	BaB	784	TYR	2.9
1	BaB	645	THR	2.9
1	BaB	792	ASN	2.9
1	BaB	670	THR	2.9
1	BaB	883	MET	2.9
1	BaB	461	ASP	2.9
1	BaB	634	PRO	2.8
1	BaB	725	LYS	2.8
1	AbA	620	PRO	2.8
1	BaB	809	SER	2.8
1	BaB	624	LEU	2.8
1	BaB	769	PHE	2.8
1	BaB	685	GLN	2.8
1	BaB	706	GLU	2.8
1	BaB	669	ASN	2.7
1	BaB	877	TRP	2.7
1	BaB	609	HIS	2.7
1	BaB	636	GLU	2.7
1	BaB	879	GLU	2.7
1	AbA	611	LEU	2.7
1	BaB	608	VAL	2.7
1	BaB	794	VAL	2.7
1	BaB	799	PHE	2.7
1	BaB	821	ARG	2.7
1	BaB	754	SER	2.7
1	AbA	646	VAL	2.7
1	BaB	610	PRO	2.7
1	BaB	765	MET	2.6
1	AbA	117	PHE	2.6
1	BaB	644	LEU	2.6
1	BaB	738	GLY	2.6
1	BaB	683	TYR	2.6
1	BaB	277	ASN	2.6
1	AbA	873	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	BaB	737	TYR	2.5
1	BaB	648	GLU	2.5
1	BaB	761	ASN	2.5
1	BaB	903	GLN	2.5
1	BaB	503	LYS	2.5
1	AbA	871	GLY	2.5
1	BaB	791	VAL	2.5
1	BaB	696	THR	2.5
1	BaB	681	SER	2.5
1	BaB	128	GLU	2.5
1	BaB	666	GLN	2.5
1	BaB	635	ILE	2.4
1	BaB	688	LEU	2.4
1	BaB	811	GLU	2.4
1	BaB	483	PRO	2.4
1	AbA	668	GLU	2.4
1	AbA	667	LYS	2.4
1	BaB	525	SER	2.4
1	AbA	120	CYS	2.4
1	BaB	793	VAL	2.4
1	BaB	846	LEU	2.3
1	AbA	652	ILE	2.3
1	BaB	662	PRO	2.3
1	BaB	694	SER	2.3
1	BaB	774	ARG	2.3
1	BaB	687	ILE	2.3
1	BaB	812	ASN	2.3
1	BaB	675	SER	2.3
1	AbA	115	ARG	2.3
1	BaB	782	ARG	2.3
1	AbA	633	LEU	2.3
1	BaB	847	HIS	2.3
1	AbA	640	THR	2.3
1	BaB	659	TYR	2.3
1	BaB	185	GLN	2.3
1	BaB	457	LEU	2.3
1	AbA	847	HIS	2.2
1	BaB	488	LYS	2.2
1	BaB	828	PRO	2.2
1	AbA	362	ASP	2.2
1	AbA	622	ASP	2.2
1	BaB	625	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	BaB	862	THR	2.2
1	AbA	618	ARG	2.2
1	BaB	467	TYR	2.2
1	BaB	719	PRO	2.2
1	BaB	798	VAL	2.2
1	BaB	776	PHE	2.2
1	BaB	760	THR	2.2
1	AbA	748	ASN	2.2
1	BaB	605	PRO	2.2
1	BaB	766	TYR	2.2
1	BaB	775	TYR	2.2
1	BaB	283	LYS	2.2
1	BaB	528	LYS	2.2
1	BaB	448	LYS	2.1
1	AbA	644	LEU	2.1
1	BaB	129	LEU	2.1
1	BaB	152	PHE	2.1
1	BaB	489	PRO	2.1
1	BaB	764	PRO	2.1
1	BaB	813	LEU	2.1
1	BaB	117	PHE	2.1
1	BaB	736	SER	2.1
1	AbA	610	PRO	2.1
1	AbA	883[A]	MET	2.1
1	BaB	280	TYR	2.1
1	BaB	288	PHE	2.1
1	AbA	116	THR	2.1
1	AbA	903	GLN	2.1
1	BaB	654	HIS	2.1
1	AbA	874	ASP	2.0
1	AbA	814	ARG	2.0
1	BaB	919	PRO	2.0
1	AbA	751	GLY	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

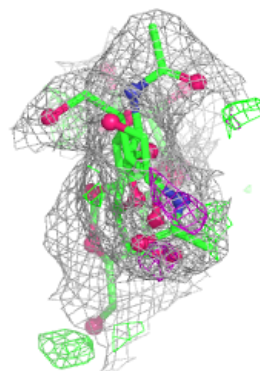
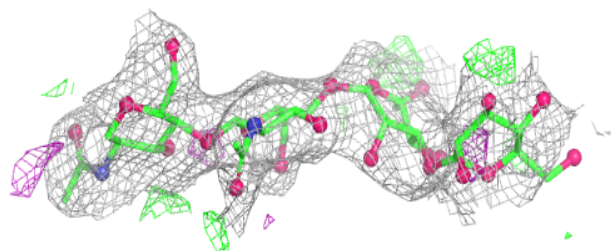
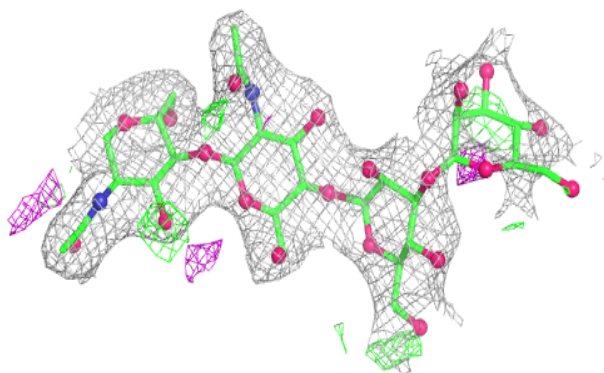
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

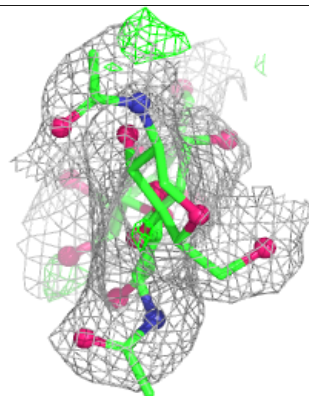
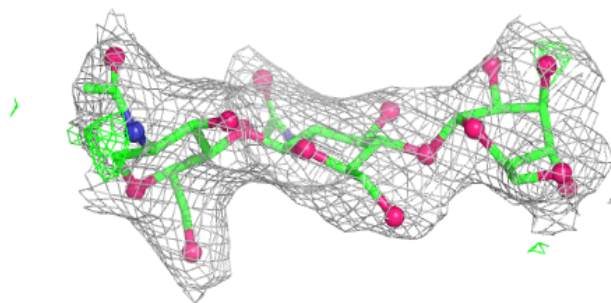
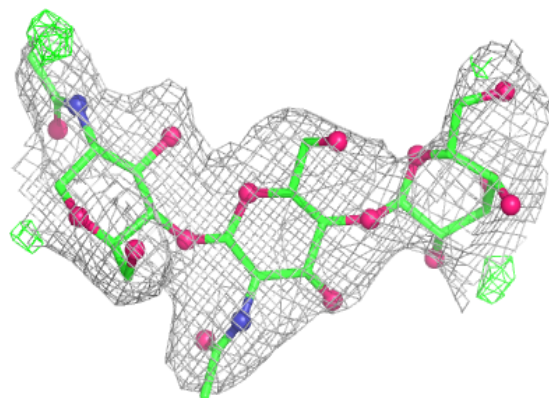
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

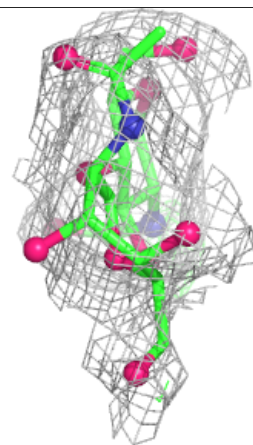
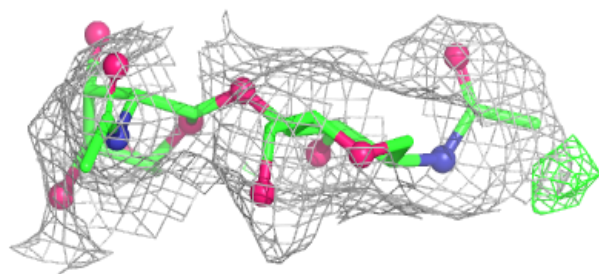
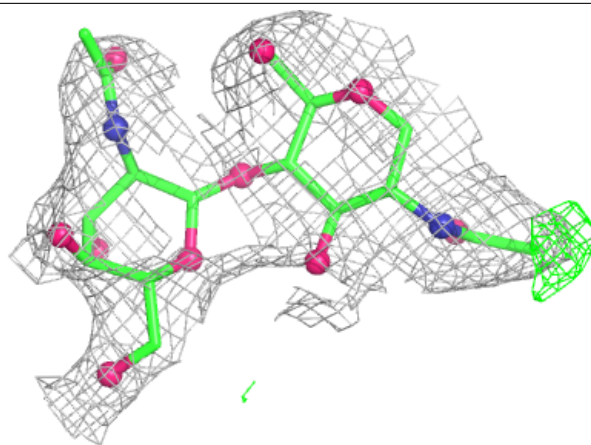
**Electron density around Chain AhA:**

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



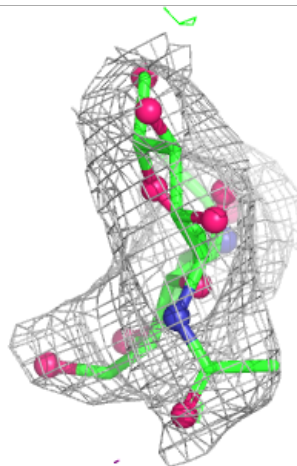
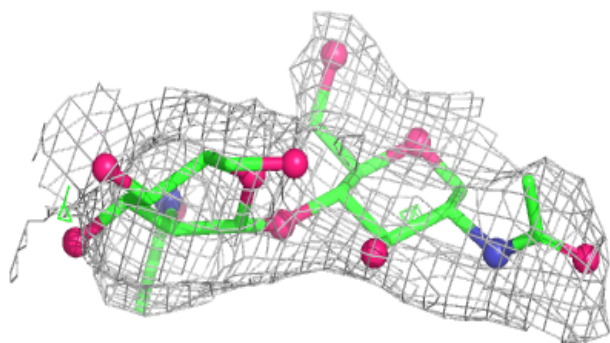
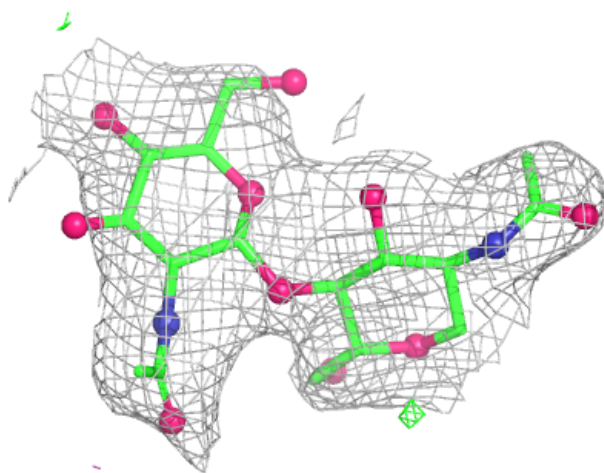
Electron density around Chain A1A:

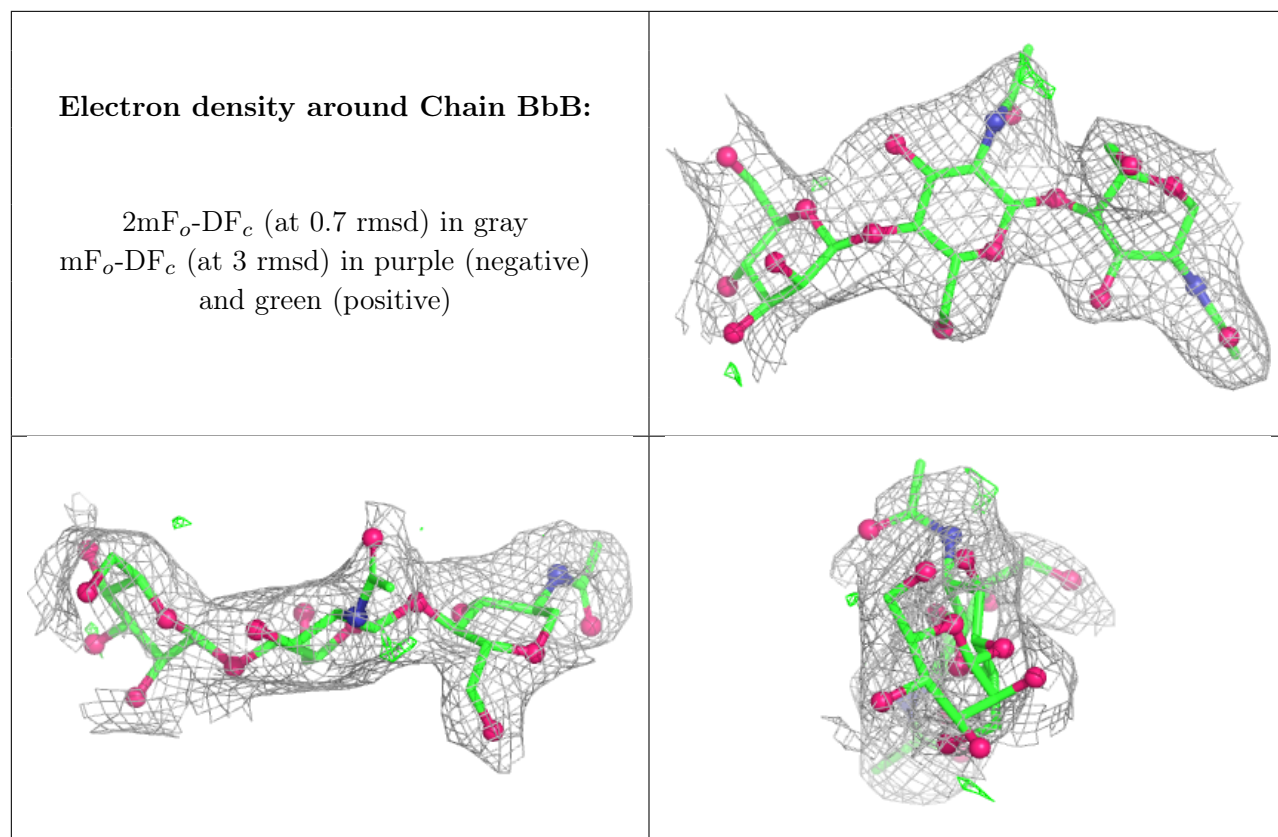
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)



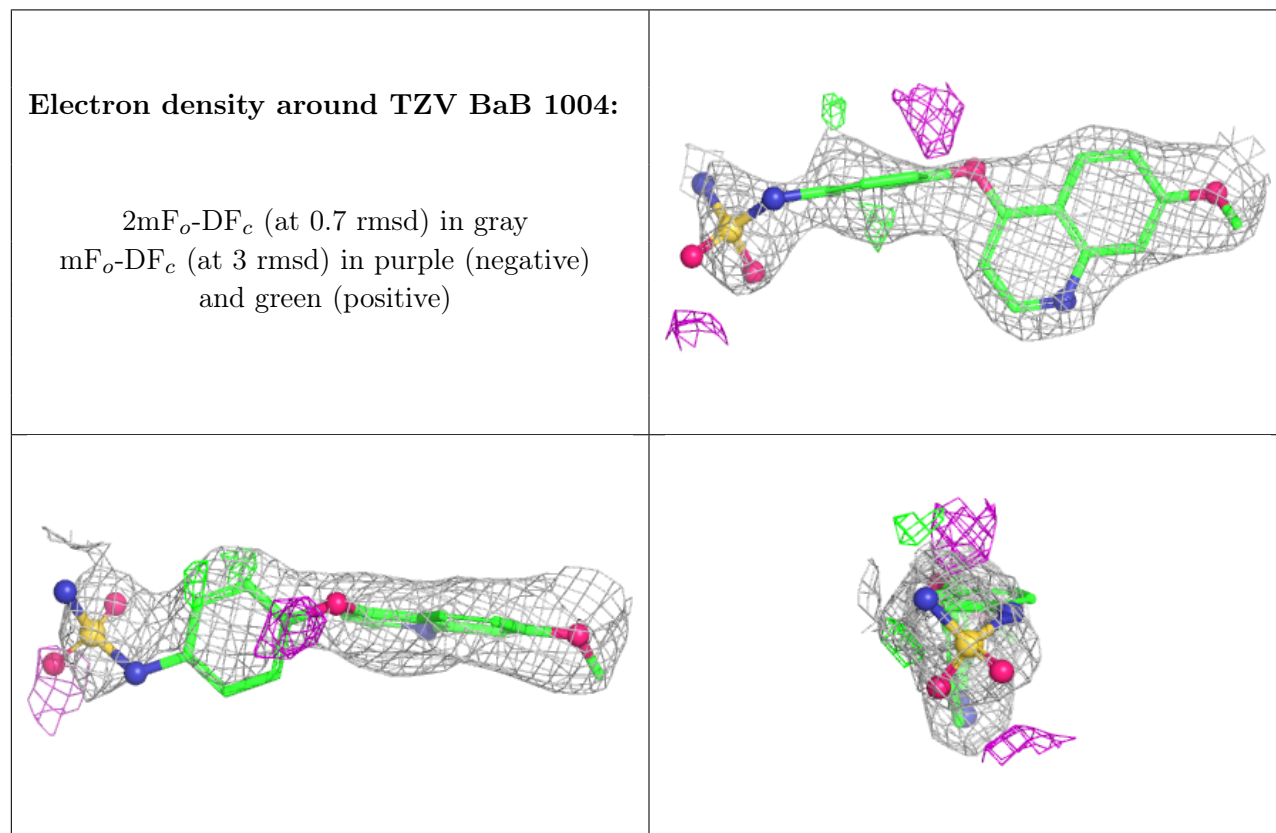


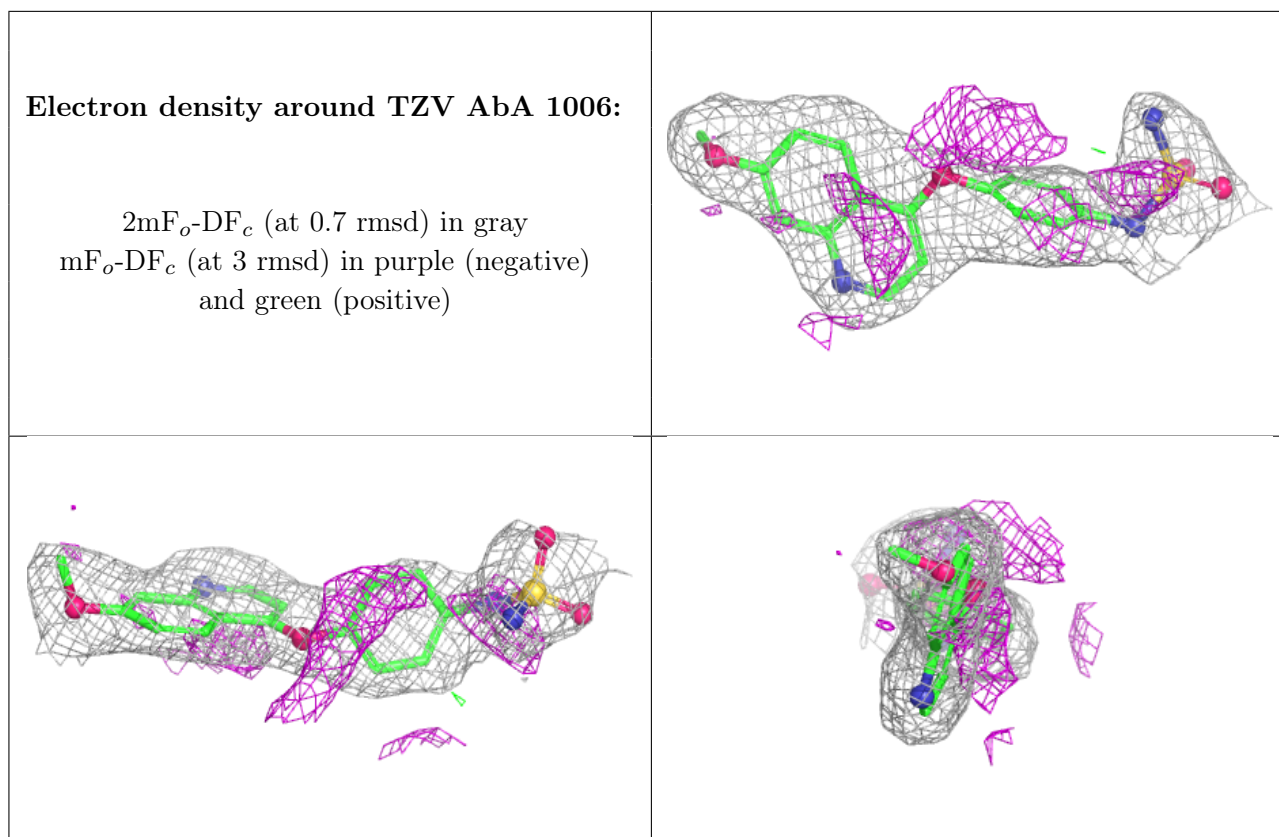
6.4 Ligands [i](#)

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(Å 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.





6.5 Other polymers [i](#)

There are no such residues in this entry.