



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:49 AM UTC

PDB ID : 6WFJ / pdb_00006wfj
Title : Crystal structures of human E-NPP 1: apo
Authors : Peat, T.S.; Dennis, M.; Newman, J.
Deposited on : 2020-04-03
Resolution : 2.50 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)
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

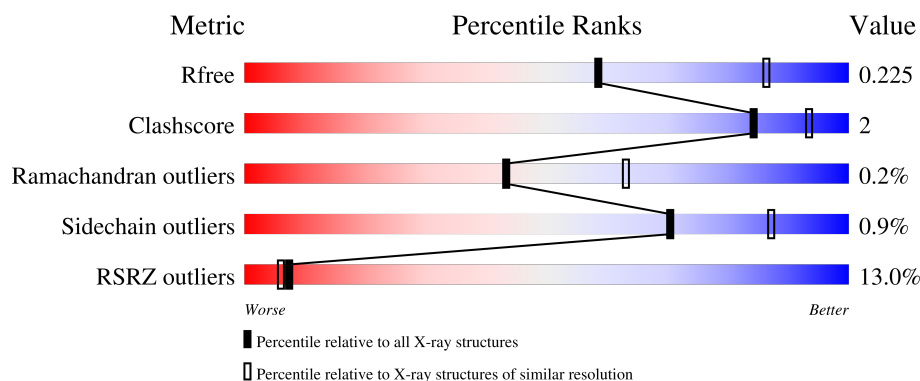
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	AcA	925	5% 82% 6% 12%
1	BcB	925	17% 80% 6% 14%
2	AeA	4	100%
3	AiA	3	100%
4	AmA	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	BgB	2	 100%
5	BdB	3	 67% 33%

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
4	NAG	BgB	2	X	-	-	-

2 Entry composition [i](#)

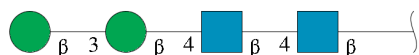
There are 12 unique types of molecules in this entry. The entry contains 13320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

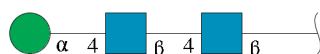
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AcA	817	Total	C	N	O	P	S	0	3	0
			6562	4181	1114	1217	1	49			
1	BcB	796	Total	C	N	O	P	S	0	2	0
			6233	3976	1053	1156	1	47			

- 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	AeA	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.



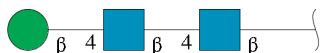
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AiA	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	AmA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	BgB	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	BdB	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AcA	2	Total	Zn	0	0
			2	2		
6	BcB	2	Total	Zn	0	0
			2	2		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

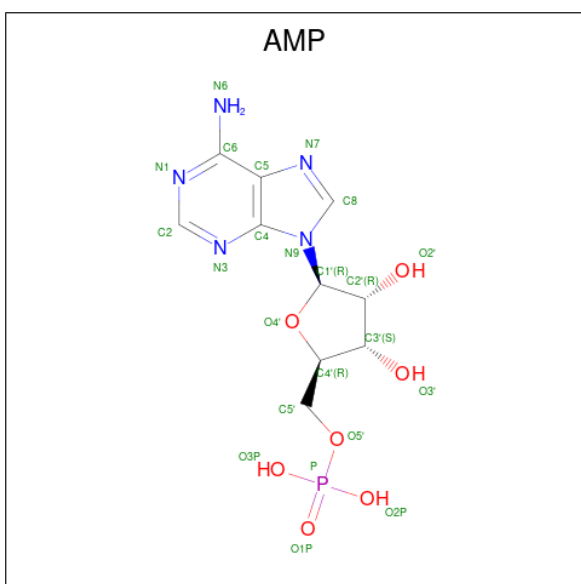
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AcA	1	Total	Ca	0	0
			1	1		
7	BcB	1	Total	Ca	0	0
			1	1		

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



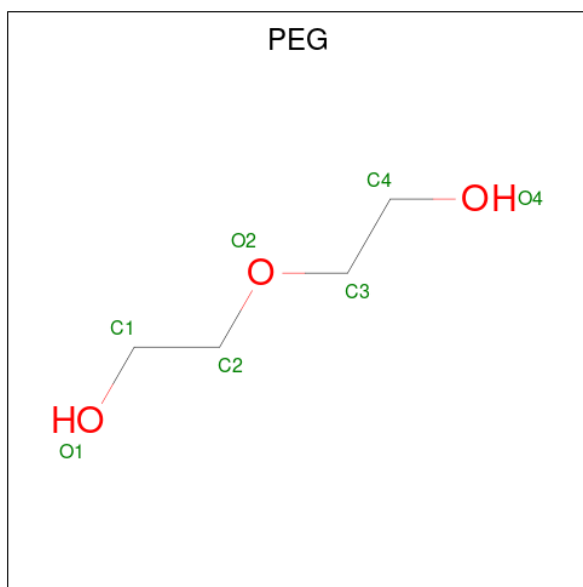
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	AcA	1	Total	C	N	O	0	0
			14	8	1	5		
8	AcA	1	Total	C	N	O	0	0
			14	8	1	5		
8	BcB	1	Total	C	N	O	0	0
			14	8	1	5		
8	BcB	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



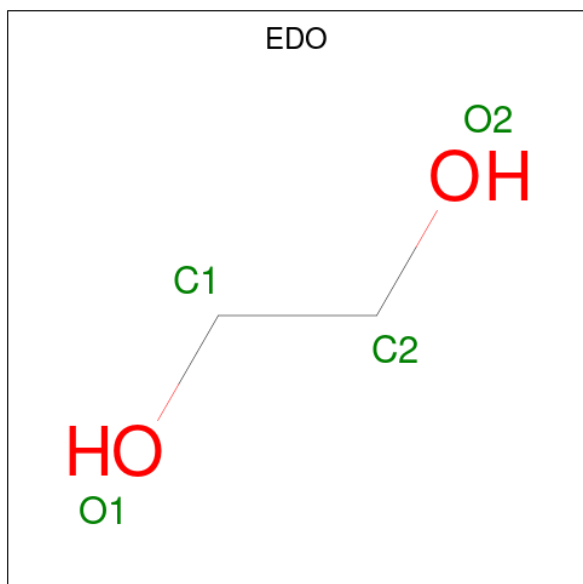
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AcA	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
9	BcB	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	AcA	1	Total	C	O	0	0
			7	4	3		

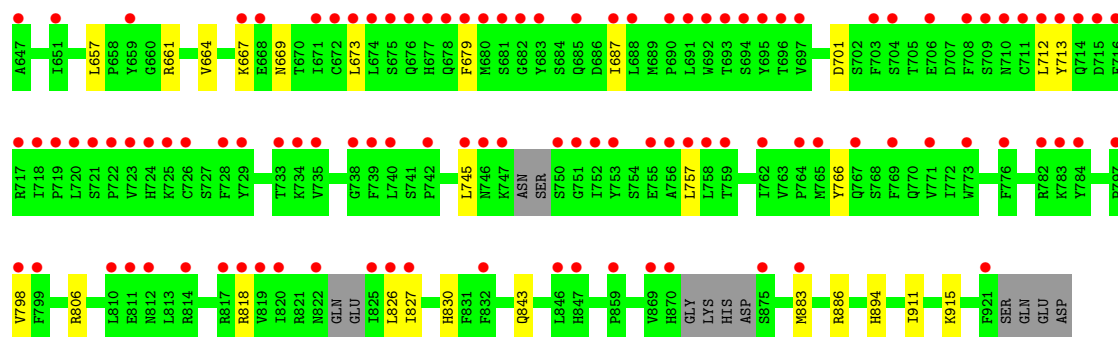
- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	AcA	1	Total C O 4 2 2	0	0
11	AcA	1	Total C O 4 2 2	0	0
11	BcB	1	Total C O 4 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	AcA	143	Total O 143 143	0	0
12	BcB	71	Total O 71 71	0	0



- 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 AeA:  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 AiA:  100%



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

Chain AmA:  100%



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

Chain BgB:  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 BdB:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.95Å 159.69Å 209.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.44 – 2.50 47.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.44-2.50) 99.9 (47.44-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.199 , 0.222 0.203 , 0.225	Depositor DCC
R_{free} test set	4841 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.6	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	0.94	EDS
Total number of atoms	13320	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: NEP, CA, ZN, EDO, PEG, MAN, NAG, AMP, BMA

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	AcA	0.96	0/6732	1.30	0/9142
1	BcB	0.98	0/6389	1.31	1/8691 (0.0%)
All	All	0.97	0/13121	1.31	1/17833 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BcB	818	ARG	CB-CA-C	5.31	119.80	109.33

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	AcA	6562	0	6282	29	0
1	BcB	6233	0	5825	30	0
2	AeA	50	0	43	0	0
3	AiA	39	0	34	0	0
4	AmA	28	0	25	0	0
4	BgB	28	0	25	0	0
5	BdB	39	0	34	0	0
6	AcA	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BcB	2	0	0	0	0
7	AcA	1	0	0	0	0
7	BcB	1	0	0	0	0
8	AcA	28	0	26	0	0
8	BcB	28	0	26	0	0
9	AcA	23	0	12	0	0
9	BcB	23	0	12	0	0
10	AcA	7	0	10	0	0
11	AcA	8	0	12	0	0
11	BcB	4	0	6	0	0
12	AcA	143	0	0	1	0
12	BcB	71	0	0	0	0
All	All	13320	0	12372	59	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 (59) 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:BcB:664:VAL:HG11	1:BcB:669:ASN:HD22	1.49	0.77
1:BcB:664:VAL:HG11	1:BcB:669:ASN:ND2	2.13	0.64
1:AcA:775:TYR:CZ	1:AcA:875:SER:HA	2.34	0.61
1:AcA:492:LYS:HD3	1:AcA:509:PRO:HA	1.82	0.61
1:AcA:701:ASP:OD2	1:AcA:747:LYS:HE2	2.01	0.60
1:AcA:435:ILE:HD13	1:AcA:487:PHE:CD1	2.37	0.59
1:AcA:700[B]:ASN:O	1:AcA:700[B]:ASN:CG	2.45	0.59
1:BcB:171:LYS:HD2	1:BcB:176:CYS:SG	2.43	0.58
1:AcA:158:ARG:NH2	1:AcA:169:ASP:OD1	2.37	0.57
1:BcB:158:ARG:NH2	1:BcB:169:ASP:OD1	2.37	0.57
1:AcA:237:LYS:NZ	12:AcA:1102:HOH:O	2.37	0.57
1:BcB:492:LYS:HG3	1:BcB:509:PRO:HA	1.88	0.56
1:AcA:708:PHE:HB3	1:AcA:752:ILE:HD13	1.89	0.55
1:AcA:492:LYS:HE3	1:AcA:502:ALA:O	2.07	0.54
1:AcA:622:ASP:OD1	1:AcA:623:ASN:N	2.40	0.54
1:AcA:109:LYS:NZ	1:AcA:154:CYS:O	2.38	0.53
1:BcB:611:LEU:HD22	1:BcB:673:LEU:HD12	1.90	0.53
1:BcB:435:ILE:HD13	1:BcB:487:PHE:CD1	2.44	0.53
1:AcA:178:ILE:HD12	1:AcA:402:MET:HE2	1.93	0.51
1:AcA:673:LEU:HD22	1:AcA:680:MET:HE3	1.93	0.51
1:AcA:678:GLN:HB2	1:AcA:753:TYR:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BcB:806:ARG:HH12	1:BcB:894:HIS:CD2	2.27	0.51
1:AcA:503:LYS:HE2	1:AcA:804:ASP:HB2	1.94	0.50
1:AcA:450:ILE:H	1:AcA:450:ILE:HD12	1.77	0.50
1:AcA:869:VAL:O	1:AcA:869:VAL:HG23	2.12	0.49
1:BcB:632:ILE:CG2	1:BcB:713:TYR:OH	2.60	0.49
1:BcB:798:VAL:HB	1:BcB:830:HIS:HB2	1.95	0.48
1:AcA:269:PRO:HA	1:AcA:272:HIS:CE1	2.48	0.48
1:BcB:492:LYS:HD3	1:BcB:507:ILE:O	2.14	0.48
1:BcB:269:PRO:HA	1:BcB:272:HIS:CE1	2.48	0.48
1:BcB:911:ILE:HG22	1:BcB:915:LYS:HE2	1.96	0.48
1:BcB:657:LEU:HD13	1:BcB:661:ARG:HB3	1.95	0.48
1:AcA:798:VAL:HB	1:AcA:830:HIS:HB2	1.95	0.47
1:AcA:753:TYR:CZ	1:AcA:755:GLU:HB2	2.49	0.47
1:BcB:213:LEU:HD23	1:BcB:403:LEU:HD21	1.96	0.46
1:AcA:171:LYS:O	1:AcA:172:ASP:C	2.59	0.46
1:AcA:657:LEU:HD13	1:AcA:661:ARG:HB3	1.97	0.46
1:AcA:423:ASP:CG	1:AcA:424:HIS:CD2	2.94	0.46
1:BcB:423:ASP:CG	1:BcB:424:HIS:CD2	2.94	0.46
1:BcB:687:ILE:HG23	1:BcB:826:LEU:HD23	1.98	0.46
1:BcB:766:TYR:CZ	1:BcB:827:ILE:HG21	2.52	0.45
1:BcB:712:LEU:HD23	1:BcB:757:LEU:O	2.16	0.45
1:BcB:318:GLY:O	1:BcB:368:TYR:HA	2.17	0.45
1:AcA:766:TYR:CZ	1:AcA:827:ILE:HG21	2.52	0.44
1:AcA:318:GLY:O	1:AcA:368:TYR:HA	2.17	0.44
1:BcB:883:MET:O	1:BcB:886:ARG:HD3	2.18	0.44
1:BcB:701:ASP:HB3	1:BcB:745:LEU:HD11	2.00	0.43
1:BcB:679:PHE:CD1	1:BcB:679:PHE:C	2.97	0.42
1:BcB:687:ILE:HG22	1:BcB:687:ILE:O	2.19	0.42
1:AcA:611:LEU:HD13	1:AcA:673:LEU:HG	2.02	0.42
1:BcB:609:HIS:NE2	1:BcB:667:LYS:O	2.49	0.42
1:BcB:632:ILE:HG21	1:BcB:713:TYR:OH	2.18	0.42
1:AcA:213:LEU:HD23	1:AcA:403:LEU:HD21	2.01	0.42
1:BcB:806:ARG:NH1	1:BcB:894:HIS:CD2	2.88	0.42
1:AcA:158:ARG:NH1	1:AcA:175:ASP:OD2	2.51	0.41
1:BcB:158:ARG:NH1	1:BcB:175:ASP:OD2	2.51	0.41
1:BcB:435:ILE:HD13	1:BcB:487:PHE:HD1	1.85	0.41
1:AcA:458:ARG:HB2	1:AcA:508:GLU:HG2	2.03	0.41
1:BcB:109:LYS:NZ	1:BcB:154:CYS:O	2.53	0.41

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	AcA	817/925 (88%)	779 (95%)	36 (4%)	2 (0%)	43	63
1	BcB	785/925 (85%)	746 (95%)	38 (5%)	1 (0%)	48	68
All	All	1602/1850 (87%)	1525 (95%)	74 (5%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AcA	119	ASN
1	AcA	321	PHE
1	BcB	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	AcA	734/823 (89%)	727 (99%)	7 (1%)	68	86
1	BcB	668/823 (81%)	662 (99%)	6 (1%)	70	87
All	All	1402/1646 (85%)	1389 (99%)	13 (1%)	70	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AcA	215	PHE
1	AcA	305	PRO
1	AcA	434	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AcA	530	CYS
1	AcA	669	ASN
1	AcA	676	GLN
1	AcA	843	GLN
1	BcB	215	PHE
1	BcB	305	PRO
1	BcB	311	LYS
1	BcB	434	TYR
1	BcB	530	CYS
1	BcB	843	GLN

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 ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	NEP	AcA	486	1	11,14,15	1.48	2 (18%)	8,20,22	0.37	0
1	NEP	BcB	486	1	11,14,15	1.42	2 (18%)	8,20,22	0.43	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
1	NEP	AcA	486	1	-	0/5/12/14	0/1/1/1
1	NEP	BcB	486	1	-	1/5/12/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AcA	486	NEP	P-O3P	3.99	1.52	1.46
1	BcB	486	NEP	P-O3P	3.52	1.51	1.46
1	AcA	486	NEP	P-O2P	-2.03	1.51	1.56
1	BcB	486	NEP	P-O1P	-2.01	1.51	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BcB	486	NEP	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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	AeA	1	1,2	14,14,15	0.55	0	17,19,21	1.23	1 (5%)
2	NAG	AeA	2	2	14,14,15	0.49	0	17,19,21	1.38	3 (17%)
2	BMA	AeA	3	2	11,11,12	0.42	0	15,15,17	1.50	4 (26%)
2	BMA	AeA	4	2	11,11,12	0.30	0	15,15,17	1.11	3 (20%)
3	NAG	AiA	1	3,1	14,14,15	0.49	0	17,19,21	1.45	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	AiA	2	3	14,14,15	0.64	0	17,19,21	1.30	1 (5%)
3	MAN	AiA	3	3	11,11,12	0.27	0	15,15,17	0.89	1 (6%)
4	NAG	AmA	1	1,4	14,14,15	0.49	0	17,19,21	1.61	4 (23%)
4	NAG	AmA	2	4	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
5	NAG	BdB	1	5,1	14,14,15	0.65	0	17,19,21	1.75	4 (23%)
5	NAG	BdB	2	5	14,14,15	0.37	0	17,19,21	0.85	0
5	BMA	BdB	3	5	11,11,12	0.30	0	15,15,17	0.49	0
4	NAG	BgB	1	1,4	14,14,15	0.73	0	17,19,21	2.59	4 (23%)
4	NAG	BgB	2	4	14,14,15	0.76	0	17,19,21	2.47	4 (23%)

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	AeA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	AeA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	AeA	3	2	-	2/2/19/22	0/1/1/1
2	BMA	AeA	4	2	-	2/2/19/22	1/1/1/1
3	NAG	AiA	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	AiA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	AiA	3	3	-	2/2/19/22	1/1/1/1
4	NAG	AmA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	AmA	2	4	-	2/6/23/26	0/1/1/1
5	NAG	BdB	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	BdB	2	5	-	0/6/23/26	0/1/1/1
5	BMA	BdB	3	5	-	0/2/19/22	0/1/1/1
4	NAG	BgB	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	BgB	2	4	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BgB	1	NAG	C8-C7-N2	-6.75	104.93	116.12
4	BgB	2	NAG	O5-C1-C2	6.72	121.69	111.29
4	BgB	1	NAG	O7-C7-N2	6.59	133.63	121.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BgB	2	NAG	C1-O5-C5	5.72	119.85	112.19
5	BdB	1	NAG	O5-C1-C2	-4.03	105.06	111.29
3	AiA	1	NAG	C8-C7-N2	-3.63	110.09	116.12
3	AiA	2	NAG	C4-C3-C2	3.49	116.13	111.02
5	BdB	1	NAG	C1-C2-N2	3.39	115.77	110.43
2	AeA	2	NAG	O5-C1-C2	-3.20	106.35	111.29
5	BdB	1	NAG	C3-C4-C5	3.12	115.90	110.23
4	BgB	2	NAG	O7-C7-N2	-2.99	116.70	121.98
4	BgB	1	NAG	C1-C2-N2	-2.97	105.76	110.43
4	AmA	1	NAG	O7-C7-N2	2.96	127.21	121.98
4	AmA	1	NAG	C8-C7-N2	-2.92	111.28	116.12
2	AeA	1	NAG	O5-C1-C2	-2.87	106.84	111.29
2	AeA	3	BMA	O2-C2-C1	2.86	115.78	109.22
4	AmA	1	NAG	C4-C3-C2	-2.80	106.92	111.02
4	AmA	1	NAG	C2-N2-C7	2.75	126.59	122.90
3	AiA	1	NAG	O7-C7-N2	2.58	126.54	121.98
4	BgB	2	NAG	C8-C7-N2	2.56	120.37	116.12
4	AmA	2	NAG	C1-O5-C5	2.54	115.59	112.19
3	AiA	3	MAN	C1-O5-C5	2.50	115.54	112.19
2	AeA	3	BMA	C1-O5-C5	-2.35	109.03	112.19
2	AeA	4	BMA	C1-O5-C5	2.31	115.29	112.19
2	AeA	4	BMA	C2-C3-C4	-2.23	106.93	110.86
2	AeA	3	BMA	C1-C2-C3	-2.23	106.40	109.64
3	AiA	1	NAG	C1-C2-N2	-2.13	107.08	110.43
2	AeA	3	BMA	C3-C4-C5	2.11	114.06	110.23
2	AeA	4	BMA	O5-C5-C6	2.10	111.76	107.66
2	AeA	2	NAG	O4-C4-C3	-2.08	105.47	110.38
4	BgB	1	NAG	C2-N2-C7	2.08	125.69	122.90
5	BdB	1	NAG	C4-C3-C2	2.07	114.05	111.02
2	AeA	2	NAG	C1-O5-C5	2.04	114.92	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	BgB	2	NAG	C1

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BgB	1	NAG	C3-C2-N2-C7
4	BgB	1	NAG	C8-C7-N2-C2
2	AeA	4	BMA	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	BgB	1	NAG	O7-C7-N2-C2
4	BgB	2	NAG	O7-C7-N2-C2
4	BgB	2	NAG	O5-C5-C6-O6
4	BgB	2	NAG	C8-C7-N2-C2
3	AiA	2	NAG	O5-C5-C6-O6
4	BgB	1	NAG	O5-C5-C6-O6
2	AeA	2	NAG	O5-C5-C6-O6
2	AeA	4	BMA	O5-C5-C6-O6
4	BgB	2	NAG	C4-C5-C6-O6
2	AeA	2	NAG	C4-C5-C6-O6
4	BgB	1	NAG	C4-C5-C6-O6
3	AiA	2	NAG	C4-C5-C6-O6
4	AmA	1	NAG	C8-C7-N2-C2
2	AeA	3	BMA	C4-C5-C6-O6
2	AeA	3	BMA	O5-C5-C6-O6
5	BdB	1	NAG	C8-C7-N2-C2
4	AmA	2	NAG	O5-C5-C6-O6
5	BdB	1	NAG	O5-C5-C6-O6
5	BdB	1	NAG	C4-C5-C6-O6
3	AiA	1	NAG	O5-C5-C6-O6
3	AiA	1	NAG	C8-C7-N2-C2
3	AiA	3	MAN	C4-C5-C6-O6
3	AiA	1	NAG	C4-C5-C6-O6
4	AmA	1	NAG	C3-C2-N2-C7
3	AiA	3	MAN	O5-C5-C6-O6
4	AmA	1	NAG	O7-C7-N2-C2
4	AmA	2	NAG	C4-C5-C6-O6
4	AmA	1	NAG	C1-C2-N2-C7

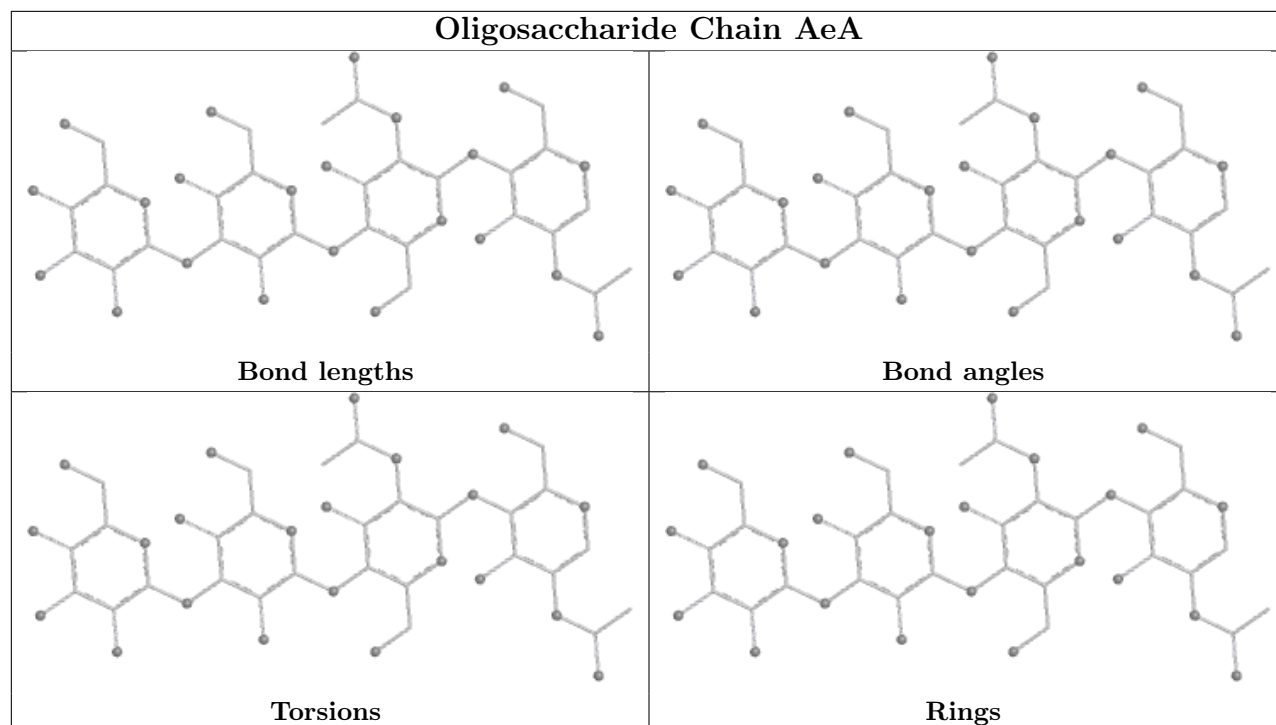
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AiA	3	MAN	C1-C2-C3-C4-C5-O5
2	AeA	4	BMA	C1-C2-C3-C4-C5-O5

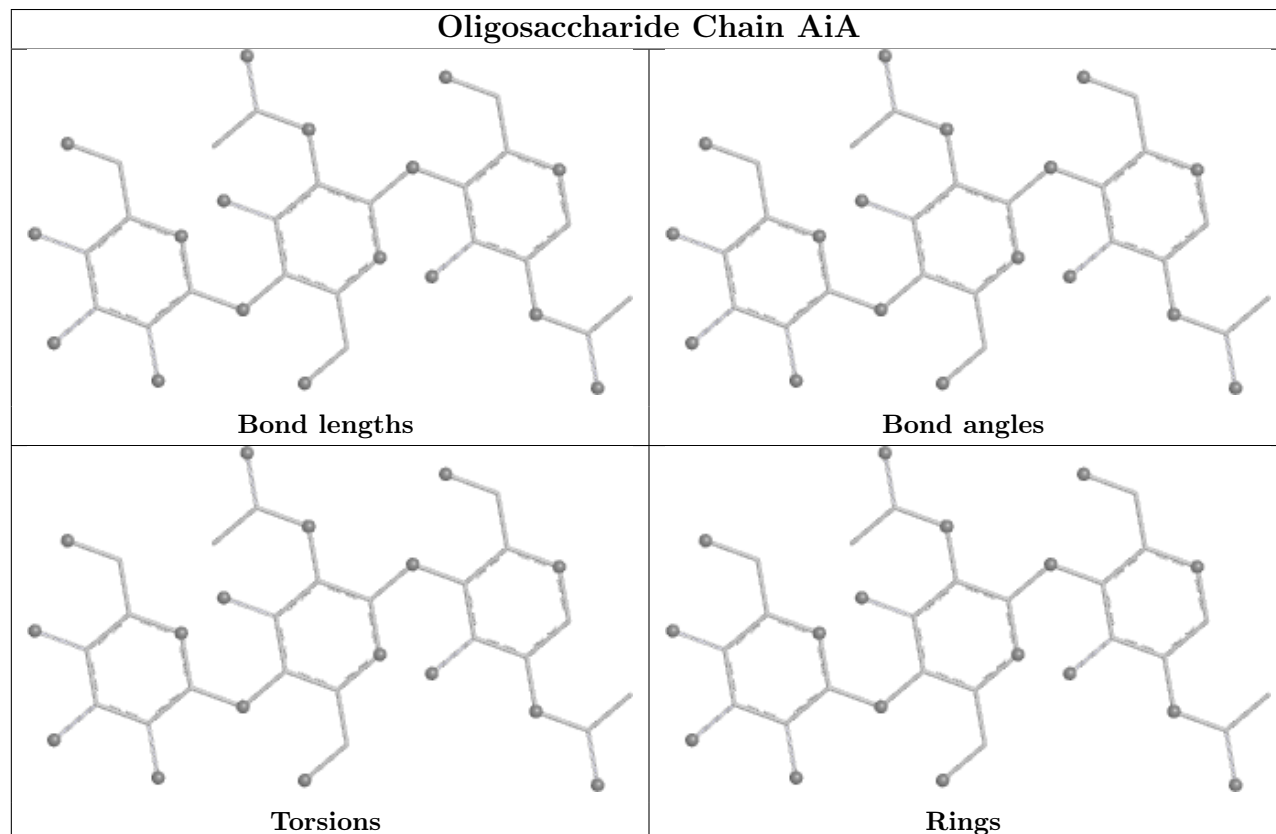
No monomer is involved in short contacts.

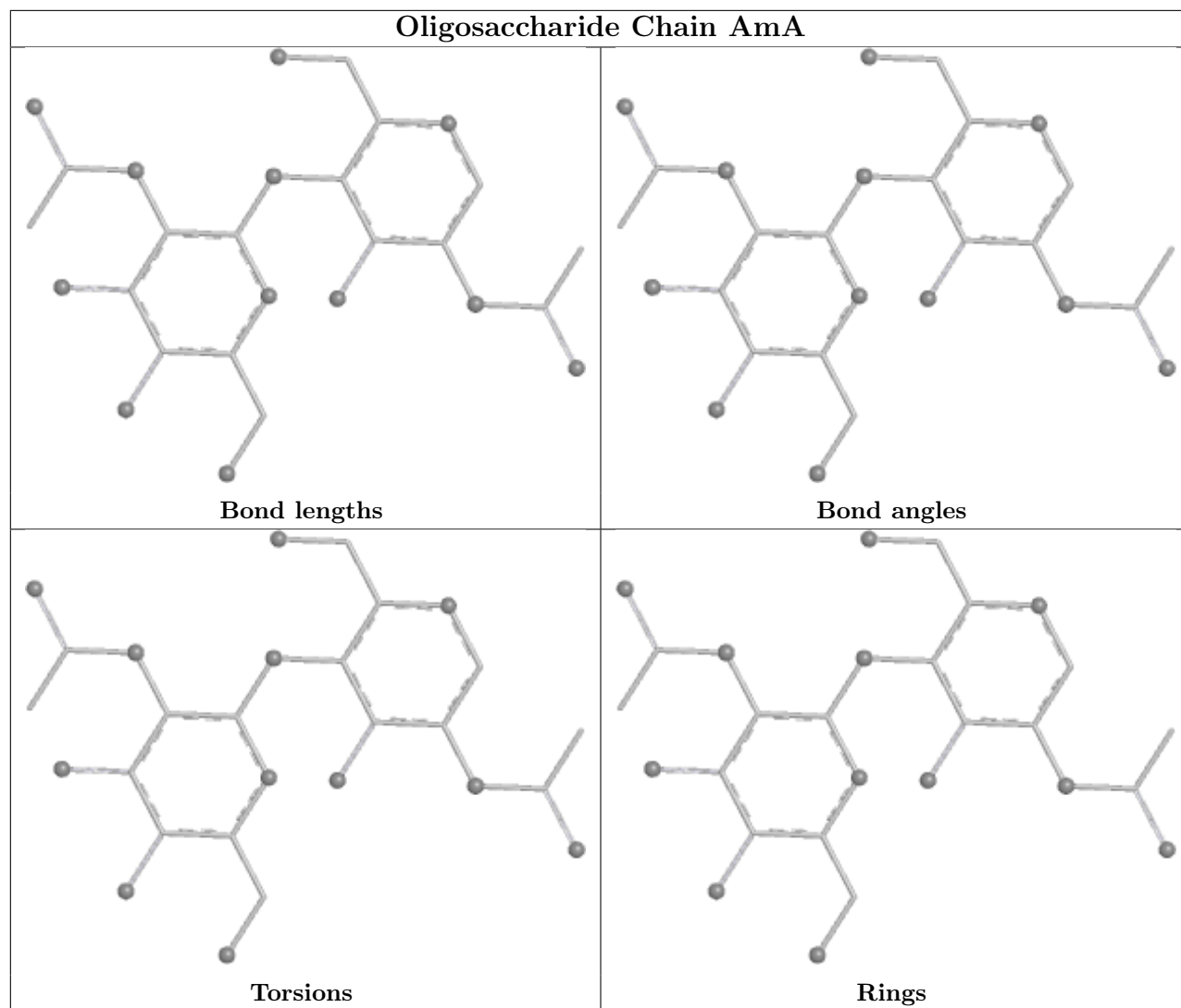
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

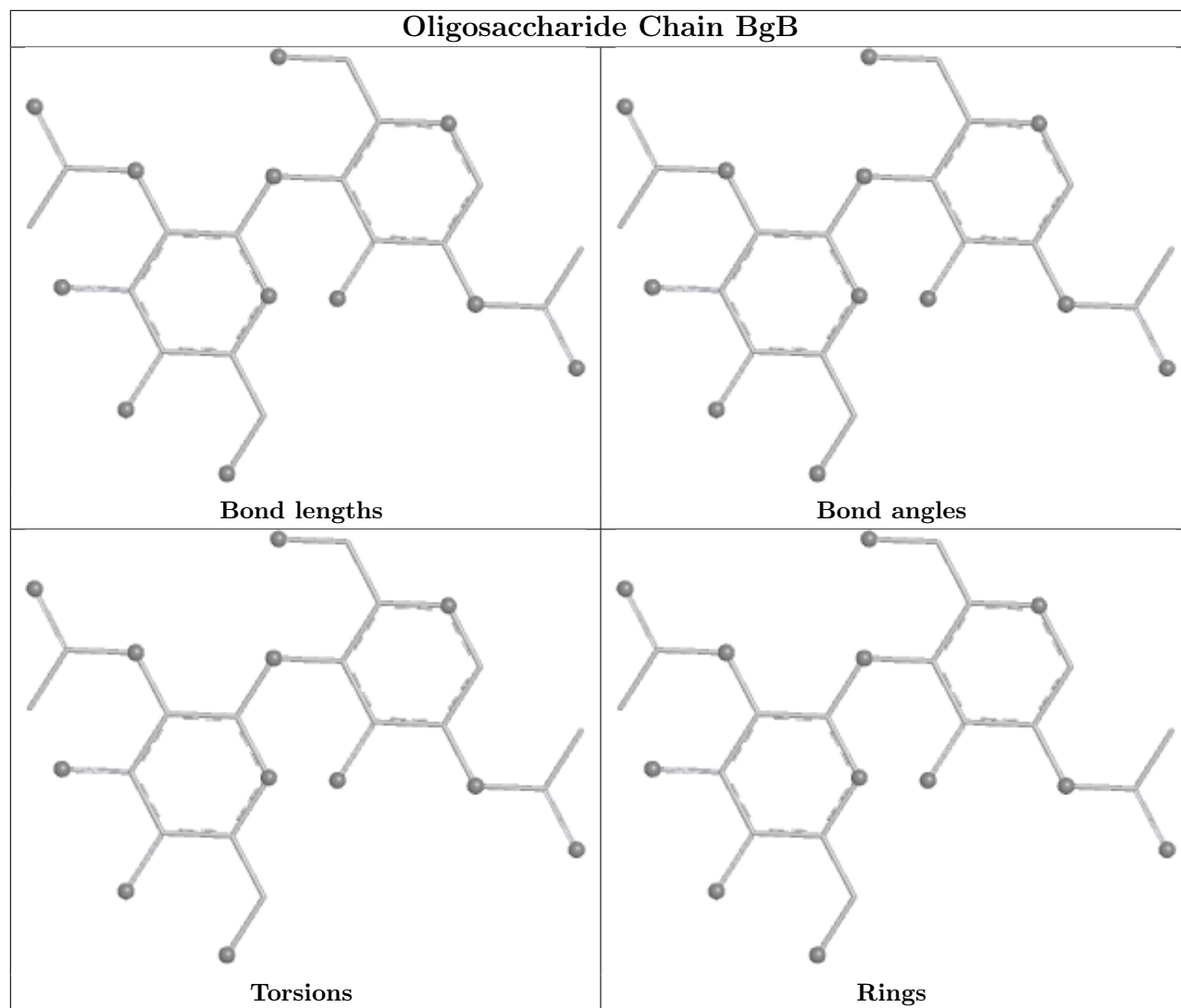
Oligosaccharide Chain AeA

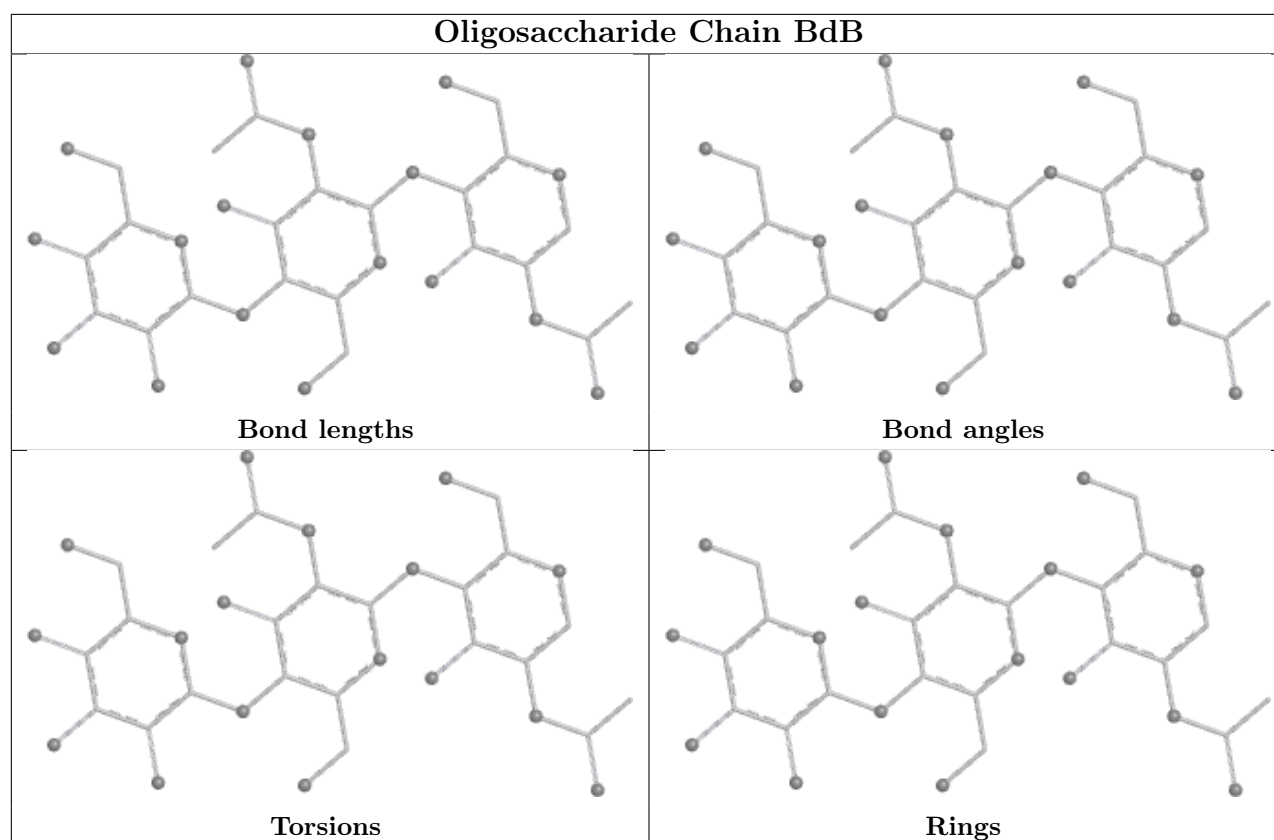


Oligosaccharide Chain AiA









5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\# Z > 2$
11	EDO	BcB	1007	-	3,3,3	0.05	0	2,2,2	0.12	0
8	NAG	BcB	1005	1	14,14,15	0.45	0	17,19,21	1.35	3 (17%)
11	EDO	AcA	1009	-	3,3,3	0.14	0	2,2,2	0.18	0
10	PEG	AcA	1007	-	6,6,6	0.21	0	5,5,5	0.21	0
8	NAG	AcA	1005	1	14,14,15	0.45	0	17,19,21	1.27	3 (17%)
9	AMP	BcB	1006	6	25,25,25	0.48	0	37,38,38	0.38	0
9	AMP	AcA	1006	6	25,25,25	0.39	0	37,38,38	0.45	0
8	NAG	BcB	1004	1	14,14,15	0.54	0	17,19,21	1.36	3 (17%)
8	NAG	AcA	1004	1	14,14,15	0.53	0	17,19,21	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	EDO	AcA	1008	-	3,3,3	0.06	0	2,2,2	0.17	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
11	EDO	BcB	1007	-	-	1/1/1/1	-
8	NAG	BcB	1005	1	-	2/6/23/26	0/1/1/1
11	EDO	AcA	1009	-	-	0/1/1/1	-
10	PEG	AcA	1007	-	-	1/4/4/4	-
8	NAG	AcA	1005	1	-	2/6/23/26	0/1/1/1
9	AMP	BcB	1006	6	-	0/10/26/26	0/3/3/3
9	AMP	AcA	1006	6	-	0/10/26/26	0/3/3/3
8	NAG	BcB	1004	1	-	3/6/23/26	0/1/1/1
8	NAG	AcA	1004	1	-	2/6/23/26	0/1/1/1
11	EDO	AcA	1008	-	-	1/1/1/1	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AcA	1004	NAG	C1-C2-N2	-3.41	105.06	110.43
8	BcB	1005	NAG	C1-C2-N2	3.19	115.46	110.43
8	BcB	1005	NAG	C8-C7-N2	-3.14	110.91	116.12
8	BcB	1004	NAG	C1-C2-N2	3.07	115.26	110.43
8	AcA	1004	NAG	C8-C7-N2	-2.47	112.02	116.12
8	AcA	1005	NAG	C8-C7-N2	2.45	120.18	116.12
8	AcA	1005	NAG	O5-C1-C2	-2.17	107.93	111.29
8	BcB	1004	NAG	C8-C7-N2	-2.14	112.56	116.12
8	BcB	1005	NAG	O5-C1-C2	-2.13	108.00	111.29
8	BcB	1004	NAG	O5-C1-C2	-2.09	108.06	111.29
8	AcA	1005	NAG	O7-C7-N2	-2.03	118.39	121.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AcA	1005	NAG	C8-C7-N2-C2

Continued on next page...

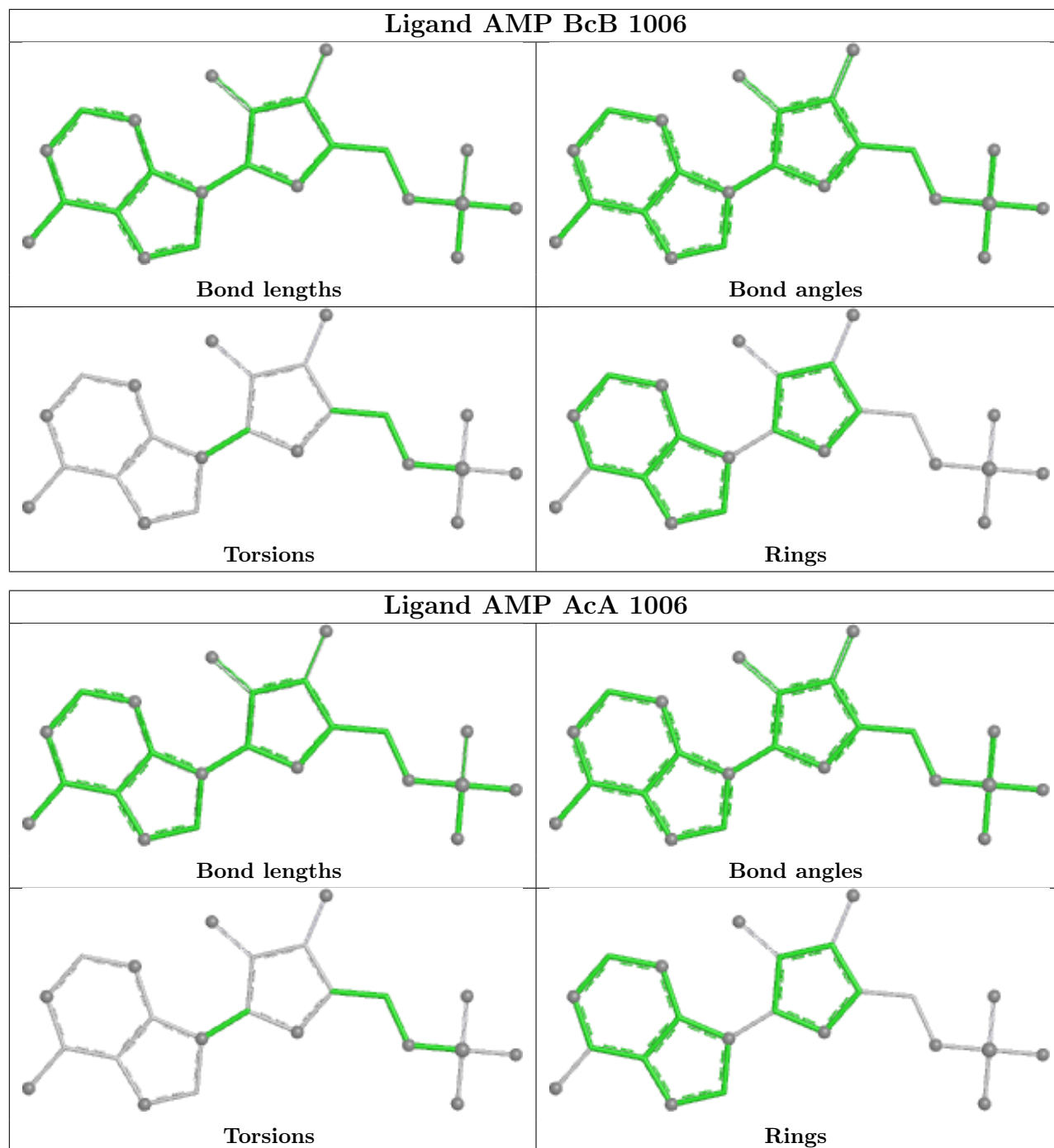
Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	AcA	1005	NAG	O7-C7-N2-C2
8	BcB	1004	NAG	C8-C7-N2-C2
8	BcB	1004	NAG	O7-C7-N2-C2
8	BcB	1005	NAG	C8-C7-N2-C2
8	BcB	1004	NAG	O5-C5-C6-O6
10	AcA	1007	PEG	O1-C1-C2-O2
8	AcA	1004	NAG	C8-C7-N2-C2
11	AcA	1008	EDO	O1-C1-C2-O2
8	BcB	1005	NAG	O7-C7-N2-C2
8	AcA	1004	NAG	O5-C5-C6-O6
11	BcB	1007	EDO	O1-C1-C2-O2

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	AcA	816/925 (88%)	0.22	49 (6%)	27 24	18, 51, 103, 152	3 (0%)
1	BcB	795/925 (85%)	0.95	160 (20%)	3 2	25, 70, 135, 156	2 (0%)
All	All	1611/1850 (87%)	0.58	209 (12%)	7 6	18, 58, 128, 156	5 (0%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BcB	678	GLN	6.7
1	BcB	870	HIS	6.6
1	BcB	753	TYR	6.2
1	BcB	921	PHE	5.7
1	BcB	822	ASN	5.7
1	BcB	611	LEU	5.2
1	BcB	722	PRO	5.1
1	BcB	820	ILE	5.1
1	AcA	105	VAL	5.0
1	AcA	921	PHE	5.0
1	AcA	677	HIS	4.9
1	BcB	826	LEU	4.9
1	BcB	289	SER	4.8
1	AcA	612	VAL	4.8
1	BcB	676	GLN	4.8
1	BcB	620	PRO	4.7
1	BcB	612	VAL	4.7
1	BcB	819	VAL	4.5
1	BcB	723	VAL	4.4
1	BcB	752	ILE	4.3
1	BcB	712	LEU	4.2
1	BcB	679	PHE	4.1
1	BcB	747	LYS	4.0
1	BcB	682	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AcA	611	LEU	4.0
1	BcB	693	THR	4.0
1	BcB	751	GLY	3.9
1	BcB	529	TYR	3.9
1	BcB	869	VAL	3.9
1	BcB	810	LEU	3.9
1	BcB	739	PHE	3.8
1	BcB	720	LEU	3.8
1	AcA	700[A]	ASN	3.8
1	BcB	694	SER	3.7
1	BcB	629	ASN	3.7
1	BcB	724	HIS	3.7
1	BcB	104	GLU	3.7
1	BcB	825	ILE	3.7
1	AcA	620	PRO	3.6
1	BcB	721	SER	3.6
1	BcB	668	GLU	3.6
1	BcB	105	VAL	3.5
1	BcB	762	ILE	3.5
1	AcA	873	HIS	3.5
1	BcB	784	TYR	3.5
1	BcB	677	HIS	3.5
1	BcB	713	TYR	3.4
1	AcA	119	ASN	3.4
1	AcA	608	VAL	3.4
1	BcB	633	LEU	3.4
1	BcB	644	LEU	3.4
1	BcB	691	LEU	3.4
1	BcB	621	ARG	3.4
1	BcB	626	CYS	3.4
1	AcA	872	LYS	3.4
1	AcA	626[A]	CYS	3.3
1	BcB	716	PHE	3.3
1	AcA	635	ILE	3.3
1	BcB	734	LYS	3.3
1	AcA	669	ASN	3.3
1	BcB	714	GLN	3.3
1	BcB	757	LEU	3.3
1	BcB	746	ASN	3.3
1	BcB	735	VAL	3.3
1	BcB	715	ASP	3.3
1	BcB	710	ASN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BcB	742	PRO	3.3
1	AcA	670	THR	3.3
1	BcB	875	SER	3.2
1	BcB	703	PHE	3.2
1	BcB	729	TYR	3.2
1	BcB	750	SER	3.2
1	AcA	362	ASP	3.2
1	AcA	649	GLU	3.2
1	BcB	726	CYS	3.1
1	BcB	530	CYS	3.1
1	AcA	610	PRO	3.1
1	BcB	728	PHE	3.1
1	BcB	764	PRO	3.1
1	BcB	708	PHE	3.0
1	BcB	758	LEU	3.0
1	BcB	799	PHE	3.0
1	BcB	827	ILE	3.0
1	BcB	685	GLN	3.0
1	BcB	636	GLU	3.0
1	BcB	673	LEU	3.0
1	BcB	518	TRP	3.0
1	BcB	695	TYR	3.0
1	BcB	756	ALA	2.9
1	BcB	745	LEU	2.9
1	BcB	674	LEU	2.9
1	BcB	812	ASN	2.9
1	BcB	651	ILE	2.9
1	BcB	814	ARG	2.9
1	BcB	487	PHE	2.9
1	BcB	623	ASN	2.9
1	BcB	503	LYS	2.8
1	BcB	671	ILE	2.8
1	BcB	687	ILE	2.8
1	BcB	798	VAL	2.8
1	BcB	680	MET	2.8
1	BcB	709	SER	2.8
1	BcB	608	VAL	2.8
1	BcB	630	PRO	2.8
1	BcB	769	PHE	2.8
1	BcB	646	VAL	2.8
1	BcB	521	ALA	2.8
1	AcA	621	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BcB	773	TRP	2.7
1	AcA	172	ASP	2.7
1	AcA	646	VAL	2.7
1	BcB	624	LEU	2.7
1	BcB	688	LEU	2.7
1	AcA	654	HIS	2.7
1	BcB	883	MET	2.6
1	AcA	526	GLU	2.6
1	AcA	636	GLU	2.6
1	AcA	668	GLU	2.6
1	BcB	675	SER	2.6
1	AcA	633	LEU	2.6
1	BcB	610	PRO	2.6
1	AcA	120	CYS	2.6
1	AcA	647	ALA	2.6
1	BcB	681	SER	2.6
1	BcB	733	THR	2.6
1	BcB	667	LYS	2.6
1	BcB	738	GLY	2.5
1	BcB	635	ILE	2.5
1	BcB	522	LEU	2.5
1	AcA	628	CYS	2.5
1	AcA	814	ARG	2.5
1	AcA	640	THR	2.5
1	BcB	797	PRO	2.5
1	BcB	440	TYR	2.5
1	AcA	644	LEU	2.5
1	BcB	528	LYS	2.5
1	BcB	847	HIS	2.5
1	BcB	494	PHE	2.4
1	BcB	776	PHE	2.4
1	AcA	618	ARG	2.4
1	BcB	632	ILE	2.4
1	AcA	117	PHE	2.4
1	BcB	647	ALA	2.4
1	AcA	733	THR	2.4
1	BcB	696	THR	2.4
1	BcB	627	SER	2.4
1	AcA	642	PHE	2.4
1	BcB	283	LYS	2.4
1	BcB	631	SER	2.3
1	BcB	704	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BcB	711	CYS	2.3
1	BcB	725	LYS	2.3
1	AcA	875	SER	2.3
1	BcB	765	MET	2.3
1	AcA	648	GLU	2.3
1	BcB	706	GLU	2.3
1	AcA	615	PRO	2.3
1	BcB	634	PRO	2.3
1	BcB	692	TRP	2.3
1	BcB	512	PHE	2.3
1	AcA	614	CYS	2.3
1	BcB	628	CYS	2.3
1	BcB	697	VAL	2.3
1	BcB	483	PRO	2.3
1	BcB	718	ILE	2.3
1	AcA	667	LYS	2.3
1	BcB	448	LYS	2.3
1	BcB	690	PRO	2.3
1	AcA	883	MET	2.2
1	BcB	431	CYS	2.2
1	BcB	672	CYS	2.2
1	AcA	870	HIS	2.2
1	BcB	441	LEU	2.2
1	BcB	435	ILE	2.2
1	BcB	811	GLU	2.2
1	AcA	613	GLN	2.2
1	BcB	759	THR	2.2
1	AcA	874	ASP	2.2
1	BcB	457	LEU	2.2
1	BcB	505	ASP	2.2
1	BcB	717	ARG	2.2
1	BcB	859	PRO	2.2
1	BcB	465	LYS	2.2
1	BcB	771	VAL	2.1
1	AcA	609	HIS	2.1
1	BcB	129	LEU	2.1
1	BcB	846	LEU	2.1
1	BcB	832	PHE	2.1
1	BcB	462	VAL	2.1
1	BcB	767	GLN	2.1
1	AcA	118	GLY	2.1
1	BcB	645	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BcB	740	LEU	2.1
1	AcA	651	ILE	2.1
1	BcB	683	TYR	2.1
1	BcB	755	GLU	2.1
1	BcB	782	ARG	2.1
1	BcB	817	ARG	2.1
1	BcB	451	TYR	2.1
1	BcB	783	LYS	2.1
1	BcB	152	PHE	2.0
1	BcB	818	ARG	2.0
1	BcB	478	LEU	2.0
1	BcB	488	LYS	2.0
1	BcB	659	TYR	2.0
1	BcB	517	GLN	2.0
1	BcB	449	VAL	2.0
1	BcB	719	PRO	2.0
1	AcA	753	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	NEP	BcB	486	14/15	0.77	0.19	85,105,130,132	0
1	NEP	AcA	486	14/15	0.84	0.17	53,75,99,102	0

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	AeA	1	14/15	-	-	41,44,48,56	0
2	NAG	AeA	2	14/15	-	-	62,73,83,101	0
2	BMA	AeA	3	11/12	-	-	111,122,132,142	0
2	BMA	AeA	4	11/12	-	-	128,149,152,153	0

Continued on next page...

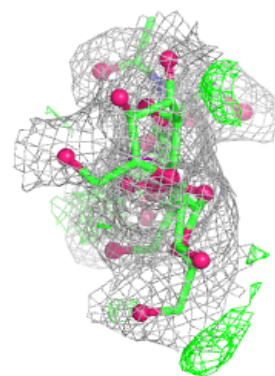
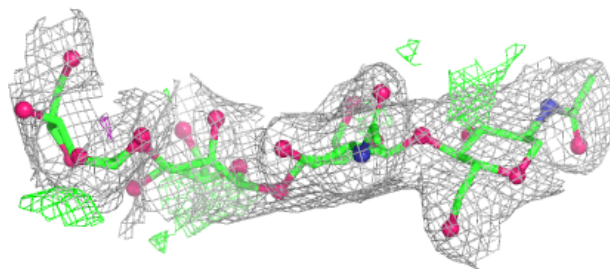
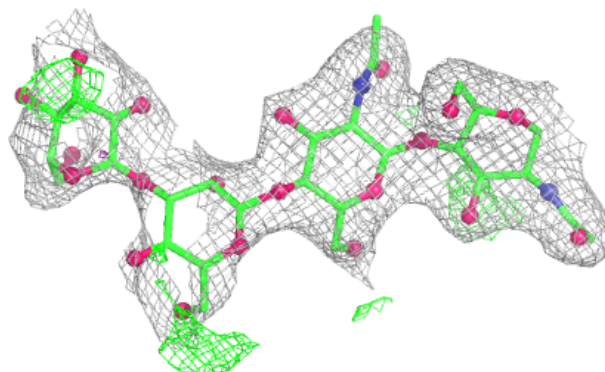
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	AiA	1	14/15	-	-	68,77,84,84	0
3	NAG	AiA	2	14/15	-	-	83,94,106,115	0
3	MAN	AiA	3	11/12	-	-	119,123,130,133	0
4	NAG	AmA	1	14/15	-	-	78,90,104,114	0
4	NAG	AmA	2	14/15	-	-	127,141,149,150	0
4	NAG	BgB	1	14/15	-	-	80,90,98,103	0
4	NAG	BgB	2	14/15	-	-	91,102,110,113	0
5	NAG	BdB	1	14/15	-	-	62,67,84,85	0
5	NAG	BdB	2	14/15	-	-	93,99,109,124	0
5	BMA	BdB	3	11/12	-	-	125,129,137,137	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.

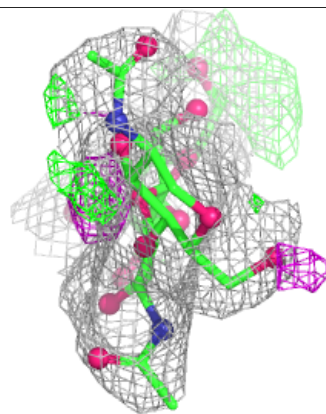
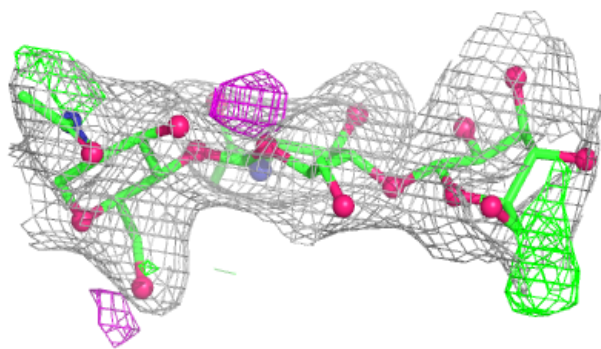
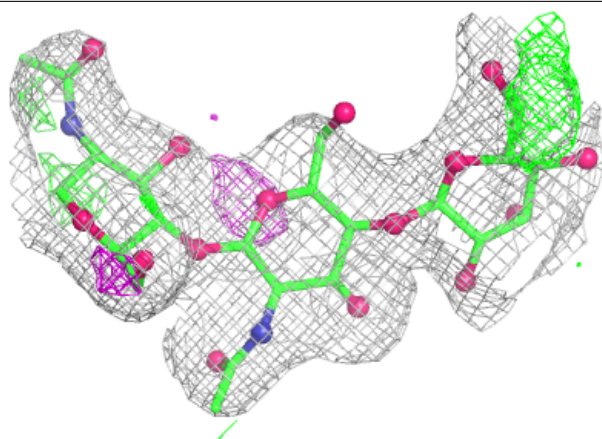
Electron density around Chain AeA:

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



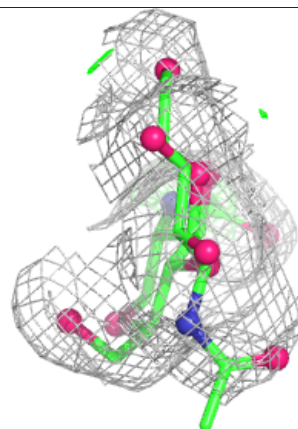
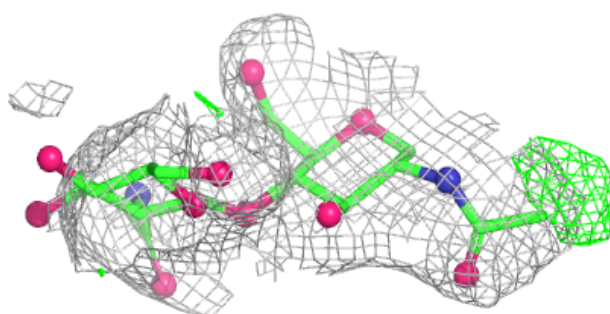
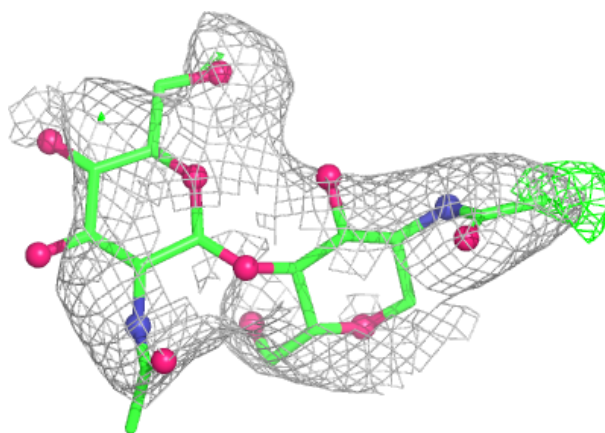
Electron density around Chain AiA:

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

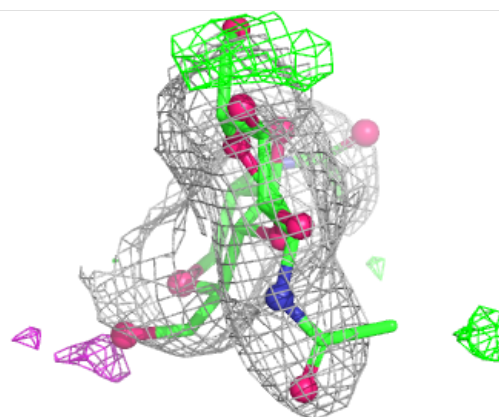
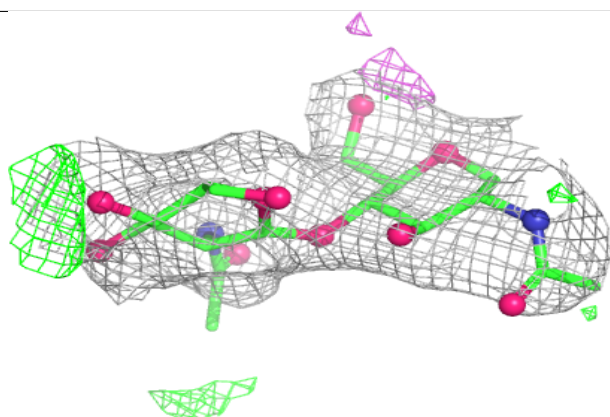
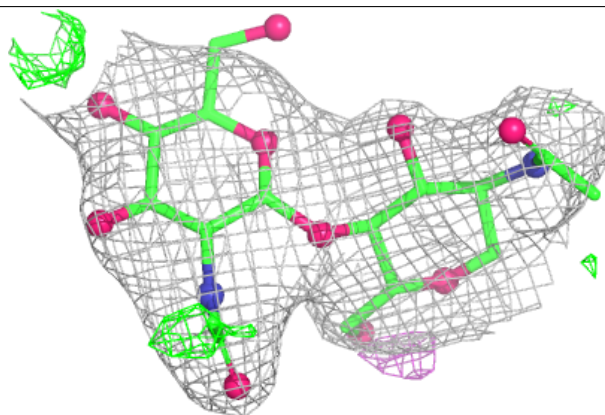


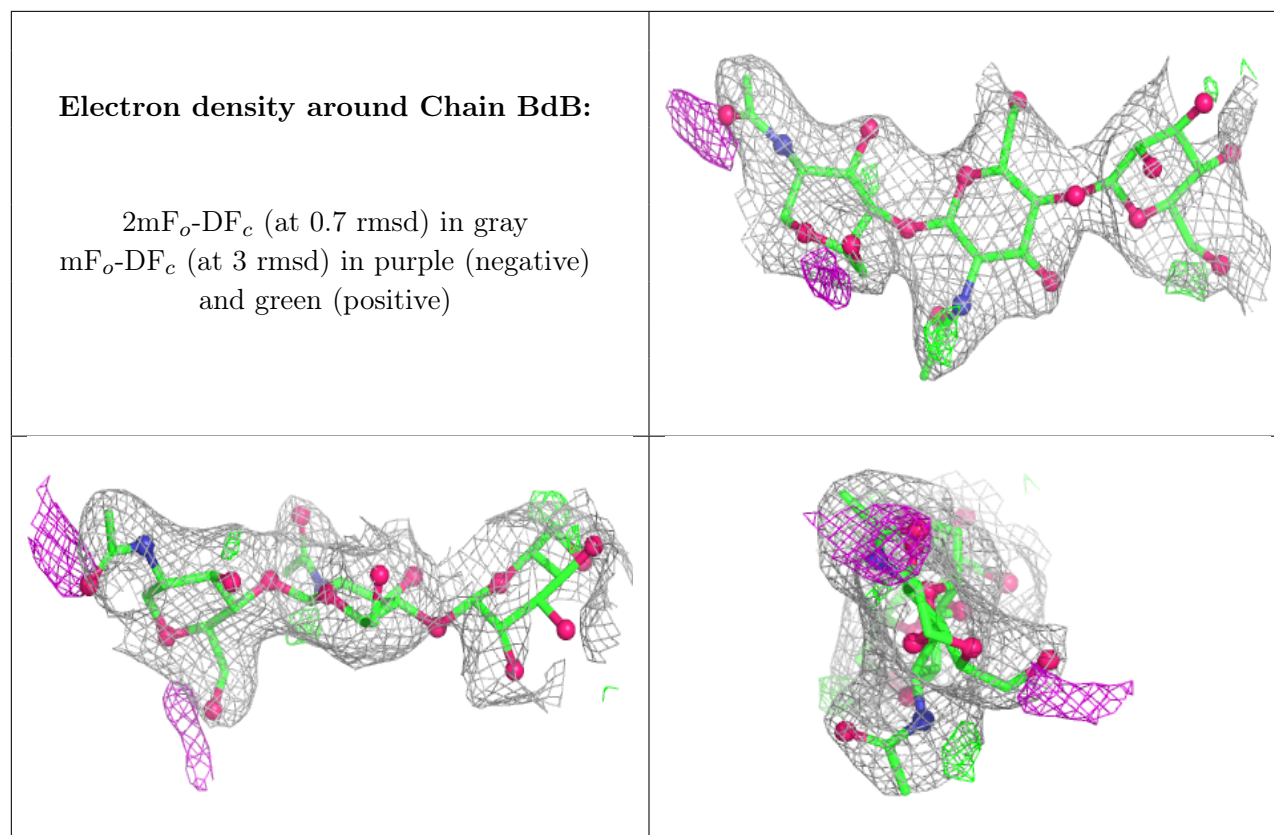
Electron density around Chain AmA:

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

**Electron density around Chain BgB:**

$2mF_o-DF_c$ (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.

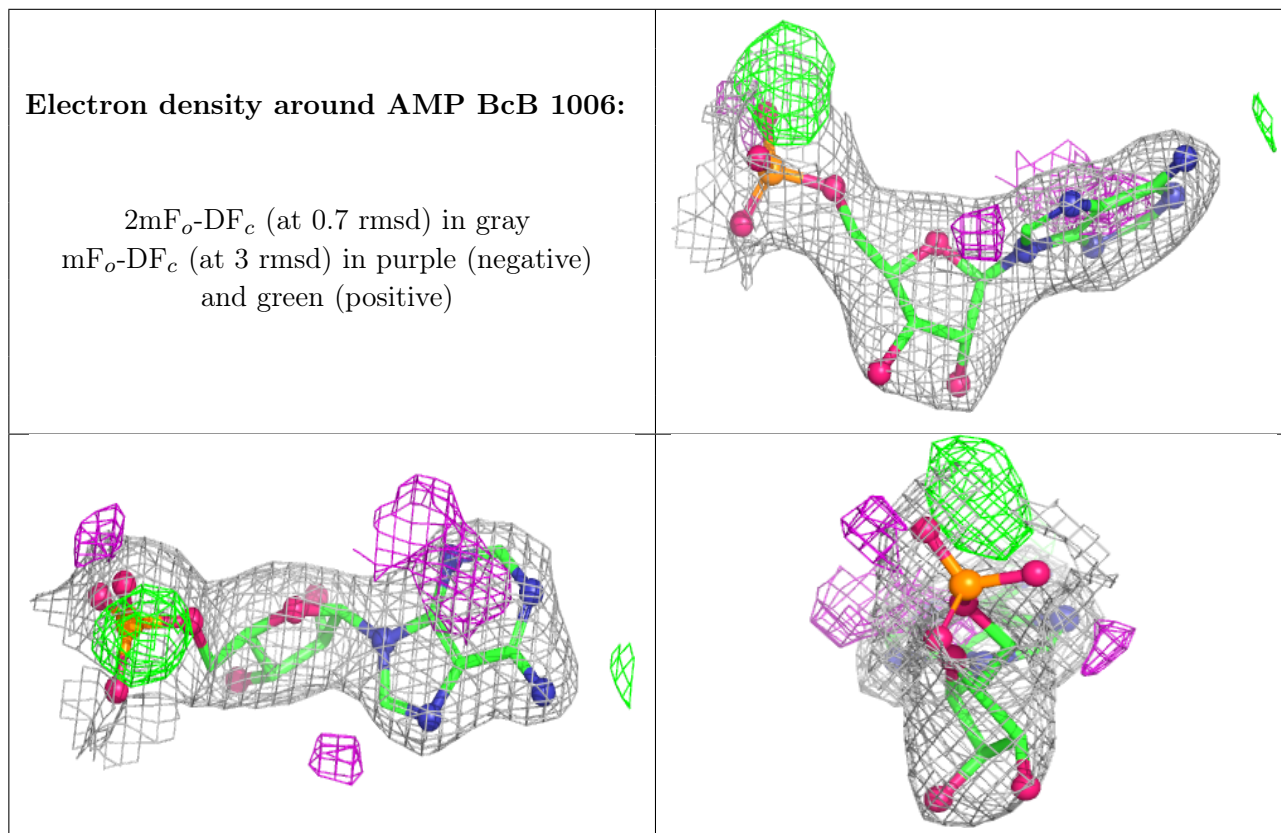
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	BcB	1004	14/15	0.38	0.20	124,140,145,145	0
8	NAG	AcA	1004	14/15	0.48	0.18	84,93,106,107	0
8	NAG	AcA	1005	14/15	0.67	0.19	97,104,110,116	0
8	NAG	BcB	1005	14/15	0.69	0.17	103,112,121,123	0
7	CA	BcB	1003	1/1	0.87	0.14	124,124,124,124	0
11	EDO	BcB	1007	4/4	0.88	0.17	78,83,85,87	0
11	EDO	AcA	1009	4/4	0.89	0.21	70,70,72,73	0
11	EDO	AcA	1008	4/4	0.91	0.21	72,72,72,73	0
7	CA	AcA	1003	1/1	0.92	0.12	85,85,85,85	0
9	AMP	BcB	1006	23/23	0.92	0.10	54,59,69,74	0
10	PEG	AcA	1007	7/7	0.92	0.14	75,79,84,86	0
9	AMP	AcA	1006	23/23	0.93	0.10	41,52,66,72	0
6	ZN	AcA	1001	1/1	1.00	0.01	37,37,37,37	0
6	ZN	AcA	1002	1/1	1.00	0.01	35,35,35,35	0

Continued on next page...

Continued from previous page...

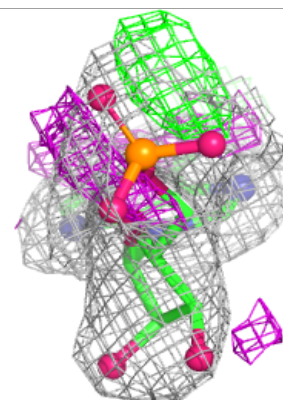
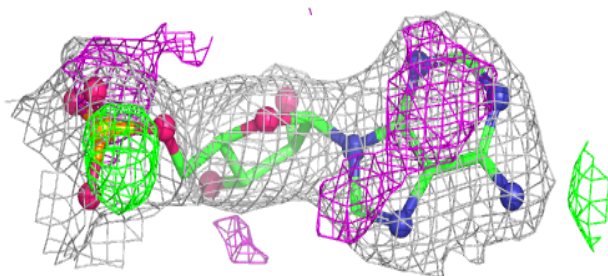
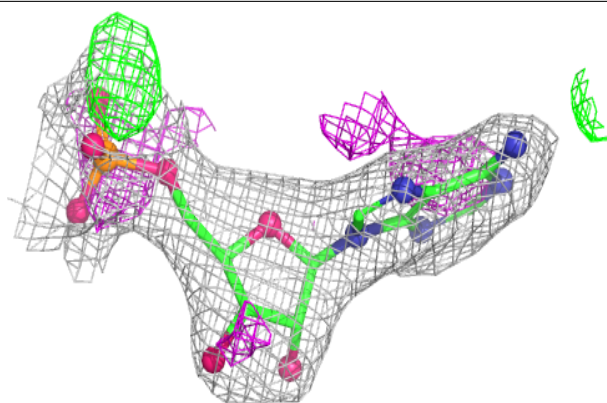
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ZN	BcB	1001	1/1	1.00	0.03	43,43,43,43	0
6	ZN	BcB	1002	1/1	1.00	0.01	42,42,42,42	0

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 AMP AcA 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.