



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 02:28 PM BST

PDB ID : 6WFJ  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

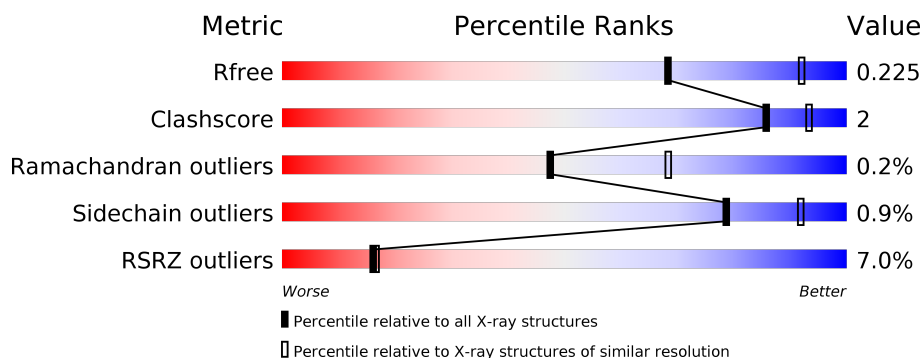
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>4%</div> <div>87%</div> <div>12%</div> </div>
1	BcB	925	<div> <div>8%</div> <div>85%</div> <div>14%</div> </div>
2	AeA	4	<div> <div>100%</div> </div>
3	AiA	3	<div> <div>100%</div> </div>
4	AmA	2	<div> <div>100%</div> </div>
4	BgB	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	BdB	3	 <div>67% 33%</div>

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	-	-	-
8	NAG	BcB	1004	-	-	-	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.

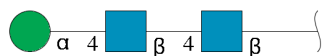
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AcA	817	Total	C	N	O	P	S	0	3	0
			6562	4181	1114	1217	1	49			
1	BcB	796	Total	C	N	O	P	S	0	2	0
			6233	3976	1053	1156	1	47			

- 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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

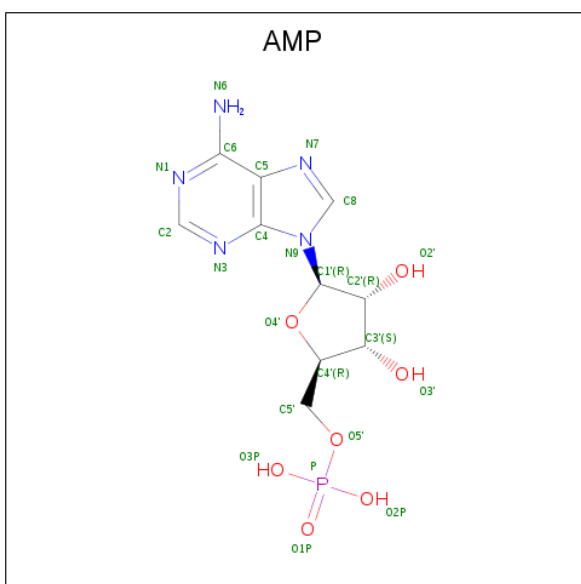
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	BcB	1	Total	Ca	0	0
			1	1		
7	AcA	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



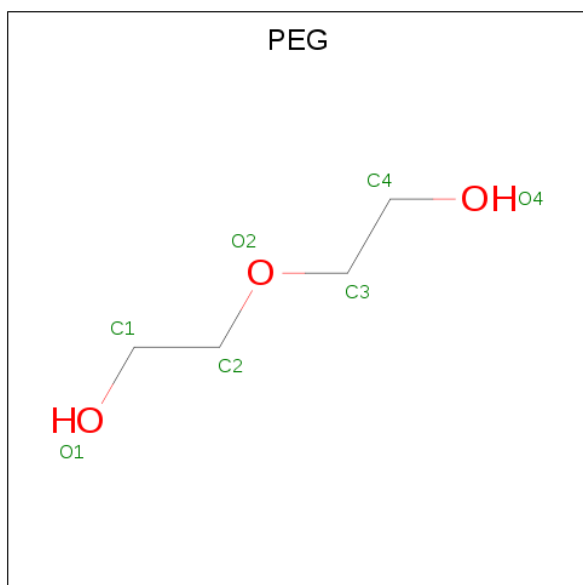
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	AcA	1	Total	C	N	O	0	0
			14	8	1	5		
8	AcA	1	Total	C	N	O	0	0
			14	8	1	5		
8	BcB	1	Total	C	N	O	0	0
			14	8	1	5		
8	BcB	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ) (labeled as "Ligand of Interest" by author).



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 (three-letter code: 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 (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 12 is water.

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






Chain AeA:  100%


NAG1  
NAG2  
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 AiA:  100%


NAG1  
NAG2  
NAG3

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

Chain AmA:  100%

NAG1  
NAG2

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

Chain BgB:  100%

NAG1  
NAG2

- 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%

NAG1  
NAG2  
BNA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CA, EDO, AMP, PEG, NEP, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AcA	0.61	0/6732	0.73	0/9142
1	BcB	0.63	0/6389	0.73	0/8691
All	All	0.62	0/13121	0.73	0/17833

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AcA	6562	0	6282	0	0
1	BcB	6233	0	5825	0	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
6	BcB	2	0	0	0	0
7	AcA	1	0	0	0	0
7	BcB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
12	BcB	71	0	0	0	0
All	All	13320	0	12372	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AcA	817/925 (88%)	779 (95%)	36 (4%)	2 (0%)	47	68
1	BcB	785/925 (85%)	746 (95%)	38 (5%)	1 (0%)	51	73
All	All	1602/1850 (87%)	1525 (95%)	74 (5%)	3 (0%)	47	68

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 [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	AcA	734/823 (89%)	727 (99%)	7 (1%)	76	90
1	BcB	668/823 (81%)	662 (99%)	6 (1%)	78	92
All	All	1402/1646 (85%)	1389 (99%)	13 (1%)	78	92

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
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

Some 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](#)

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	10,14,15	2.05	2 (20%)	5,20,22	0.88	0
1	NEP	BcB	486	1	10,14,15	1.87	2 (20%)	5,20,22	0.92	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	-	1/5/12/14	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	5.65	1.52	1.47
1	BcB	486	NEP	P-O3P	4.84	1.51	1.47
1	AcA	486	NEP	CE1-ND1	-2.20	1.31	1.35
1	BcB	486	NEP	CE1-ND1	-2.15	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BcB	486	NEP	O-C-CA-CB
1	AcA	486	NEP	CA-CB-CG-ND1

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	0.56	0	17,19,21	1.22	1 (5%)
2	NAG	AeA	2	2	14,14,15	0.51	0	17,19,21	1.35	3 (17%)
2	BMA	AeA	3	2	11,11,12	0.43	0	15,15,17	1.73	5 (33%)
2	BMA	AeA	4	2	11,11,12	0.30	0	15,15,17	1.25	3 (20%)
3	NAG	AiA	1	1,3	14,14,15	0.48	0	17,19,21	1.44	2 (11%)
3	NAG	AiA	2	3	14,14,15	0.64	0	17,19,21	1.31	1 (5%)
3	MAN	AiA	3	3	11,11,12	0.27	0	15,15,17	0.95	1 (6%)
4	NAG	AmA	1	1,4	14,14,15	0.49	0	17,19,21	1.58	5 (29%)
4	NAG	AmA	2	4	14,14,15	0.38	0	17,19,21	0.91	1 (5%)
5	NAG	BdB	1	1,5	14,14,15	0.66	0	17,19,21	1.70	4 (23%)
5	NAG	BdB	2	5	14,14,15	0.38	0	17,19,21	0.85	0
5	BMA	BdB	3	5	11,11,12	0.30	0	15,15,17	0.62	0
4	NAG	BgB	1	1,4	14,14,15	0.70	0	17,19,21	2.52	3 (17%)
4	NAG	BgB	2	4	14,14,15	0.74	0	17,19,21	2.45	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	1,3	-	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	-	3/6/23/26	0/1/1/1
4	NAG	AmA	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	BdB	1	1,5	-	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	-6.60	104.93	116.10
4	BgB	2	NAG	O5-C1-C2	6.59	121.69	111.29
4	BgB	1	NAG	O7-C7-N2	6.35	133.63	121.95
4	BgB	2	NAG	C1-O5-C5	5.65	119.85	112.19
5	BdB	1	NAG	O5-C1-C2	-3.95	105.06	111.29
3	AiA	1	NAG	C8-C7-N2	-3.55	110.09	116.10
3	AiA	2	NAG	C4-C3-C2	3.49	116.13	111.02
2	AeA	3	BMA	O2-C2-C1	3.24	115.78	109.15
5	BdB	1	NAG	C3-C4-C5	3.17	115.90	110.24
2	AeA	2	NAG	O5-C1-C2	-3.13	106.35	111.29
5	BdB	1	NAG	C1-C2-N2	3.09	115.77	110.49
2	AeA	3	BMA	O5-C1-C2	-3.07	106.03	110.77
2	AeA	4	BMA	O5-C5-C6	2.90	111.76	107.20
4	AmA	1	NAG	O7-C7-N2	2.86	127.21	121.95
4	BgB	2	NAG	O7-C7-N2	-2.85	116.70	121.95
4	AmA	1	NAG	C8-C7-N2	-2.85	111.28	116.10
2	AeA	1	NAG	O5-C1-C2	-2.81	106.84	111.29
4	AmA	1	NAG	C4-C3-C2	-2.80	106.92	111.02
4	BgB	1	NAG	C1-C2-N2	-2.77	105.76	110.49
2	AeA	3	BMA	C1-C2-C3	-2.66	106.40	109.67
4	AmA	1	NAG	C2-N2-C7	2.59	126.59	122.90
4	BgB	2	NAG	C8-C7-N2	2.52	120.37	116.10
4	AmA	2	NAG	C1-O5-C5	2.51	115.59	112.19
3	AiA	1	NAG	O7-C7-N2	2.50	126.54	121.95
3	AiA	3	MAN	C1-O5-C5	2.47	115.54	112.19
2	AeA	3	BMA	C1-O5-C5	-2.33	109.03	112.19
2	AeA	4	BMA	C2-C3-C4	-2.29	106.93	110.89
2	AeA	4	BMA	C1-O5-C5	2.28	115.29	112.19
2	AeA	3	BMA	C3-C4-C5	2.14	114.06	110.24
2	AeA	2	NAG	O4-C4-C3	-2.11	105.47	110.35
4	AmA	1	NAG	O5-C5-C6	-2.08	103.94	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	BdB	1	NAG	C4-C3-C2	2.07	114.05	111.02
2	AeA	2	NAG	C1-O5-C5	2.01	114.92	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	BgB	2	NAG	C1

All (30) 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
4	BgB	2	NAG	C8-C7-N2-C2
4	BgB	2	NAG	O7-C7-N2-C2
4	BgB	1	NAG	O7-C7-N2-C2
4	BgB	2	NAG	O5-C5-C6-O6
3	AiA	2	NAG	O5-C5-C6-O6
2	AeA	4	BMA	O5-C5-C6-O6
4	BgB	1	NAG	O5-C5-C6-O6
2	AeA	2	NAG	O5-C5-C6-O6
4	BgB	2	NAG	C4-C5-C6-O6
4	AmA	1	NAG	C8-C7-N2-C2
4	BgB	1	NAG	C4-C5-C6-O6
2	AeA	2	NAG	C4-C5-C6-O6
2	AeA	3	BMA	C4-C5-C6-O6
3	AiA	2	NAG	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
3	AiA	1	NAG	O5-C5-C6-O6
5	BdB	1	NAG	C4-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
3	AiA	3	MAN	O5-C5-C6-O6
4	AmA	1	NAG	C3-C2-N2-C7
4	AmA	1	NAG	O7-C7-N2-C2
4	AmA	2	NAG	C4-C5-C6-O6

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.

## 5.6 Ligand geometry

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	0.19	0
8	NAG	BcB	1004	1	14,14,15	0.53	0	17,19,21	1.33	3 (17%)
8	NAG	AcA	1005	1	14,14,15	0.43	0	17,19,21	1.27	2 (11%)
10	PEG	AcA	1007	-	6,6,6	0.21	0	5,5,5	0.21	0
11	EDO	AcA	1008	-	3,3,3	0.06	0	2,2,2	0.25	0
8	NAG	AcA	1004	1	14,14,15	0.51	0	17,19,21	1.23	2 (11%)
9	AMP	BcB	1006	6	22,25,25	0.72	0	25,38,38	0.73	1 (4%)
9	AMP	AcA	1006	6	22,25,25	0.64	0	25,38,38	0.80	1 (4%)
8	NAG	BcB	1005	1	14,14,15	0.43	0	17,19,21	1.31	3 (17%)
11	EDO	AcA	1009	-	3,3,3	0.14	0	2,2,2	0.26	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	-	-	0/1/1/1	-
8	NAG	BcB	1004	1	-	3/6/23/26	0/1/1/1
8	NAG	AcA	1005	1	-	2/6/23/26	0/1/1/1
10	PEG	AcA	1007	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	AcA	1008	-	-	1/1/1/1	-
8	NAG	AcA	1004	1	-	2/6/23/26	0/1/1/1
9	AMP	BcB	1006	6	-	0/6/26/26	0/3/3/3
9	AMP	AcA	1006	6	-	0/6/26/26	0/3/3/3
8	NAG	BcB	1005	1	-	2/6/23/26	0/1/1/1
11	EDO	AcA	1009	-	-	0/1/1/1	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AcA	1004	NAG	C1-C2-N2	-3.18	105.06	110.49
8	BcB	1005	NAG	C8-C7-N2	-3.06	110.91	116.10
8	BcB	1005	NAG	C1-C2-N2	2.91	115.46	110.49
8	BcB	1004	NAG	C1-C2-N2	2.80	115.26	110.49
8	AcA	1005	NAG	C8-C7-N2	2.41	120.18	116.10
8	AcA	1004	NAG	C8-C7-N2	-2.41	112.02	116.10
9	BcB	1006	AMP	C5-C6-N6	2.13	123.59	120.35
8	AcA	1005	NAG	O5-C1-C2	-2.13	107.93	111.29
9	AcA	1006	AMP	C5-C6-N6	2.10	123.54	120.35
8	BcB	1004	NAG	C8-C7-N2	-2.09	112.56	116.10
8	BcB	1005	NAG	O5-C1-C2	-2.08	108.00	111.29
8	BcB	1004	NAG	O5-C1-C2	-2.05	108.06	111.29

There are no chirality outliers.

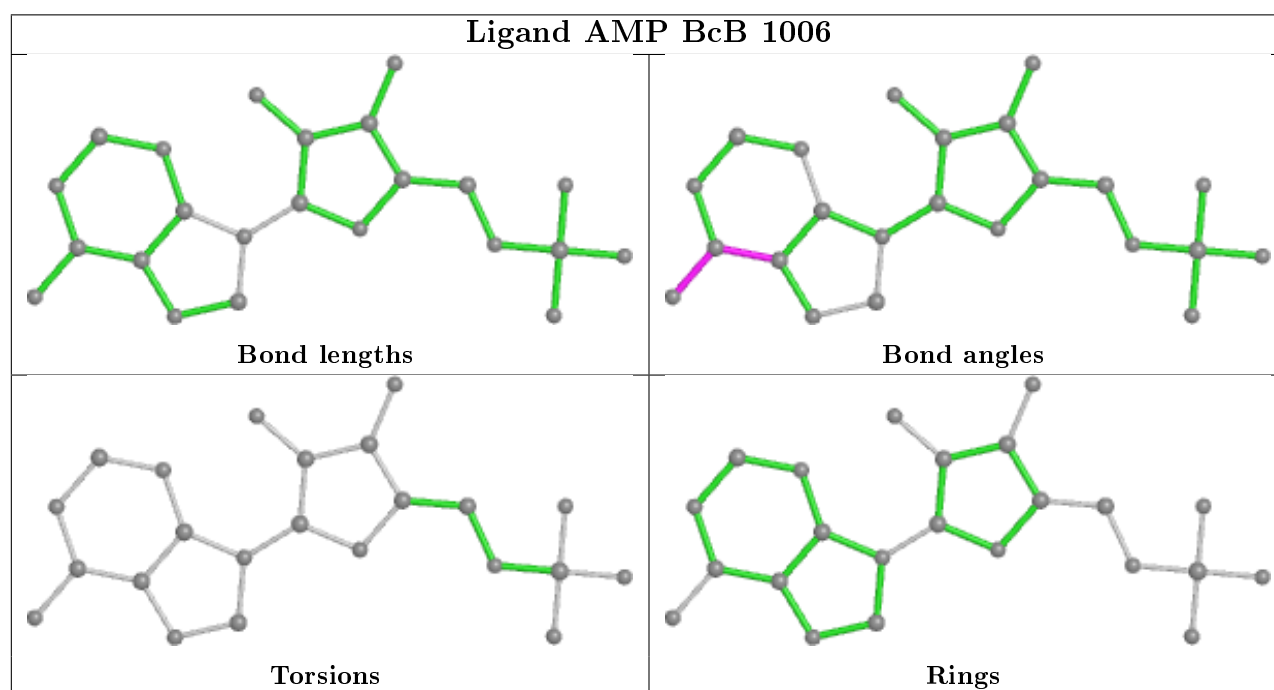
All (11) torsion outliers are listed below:

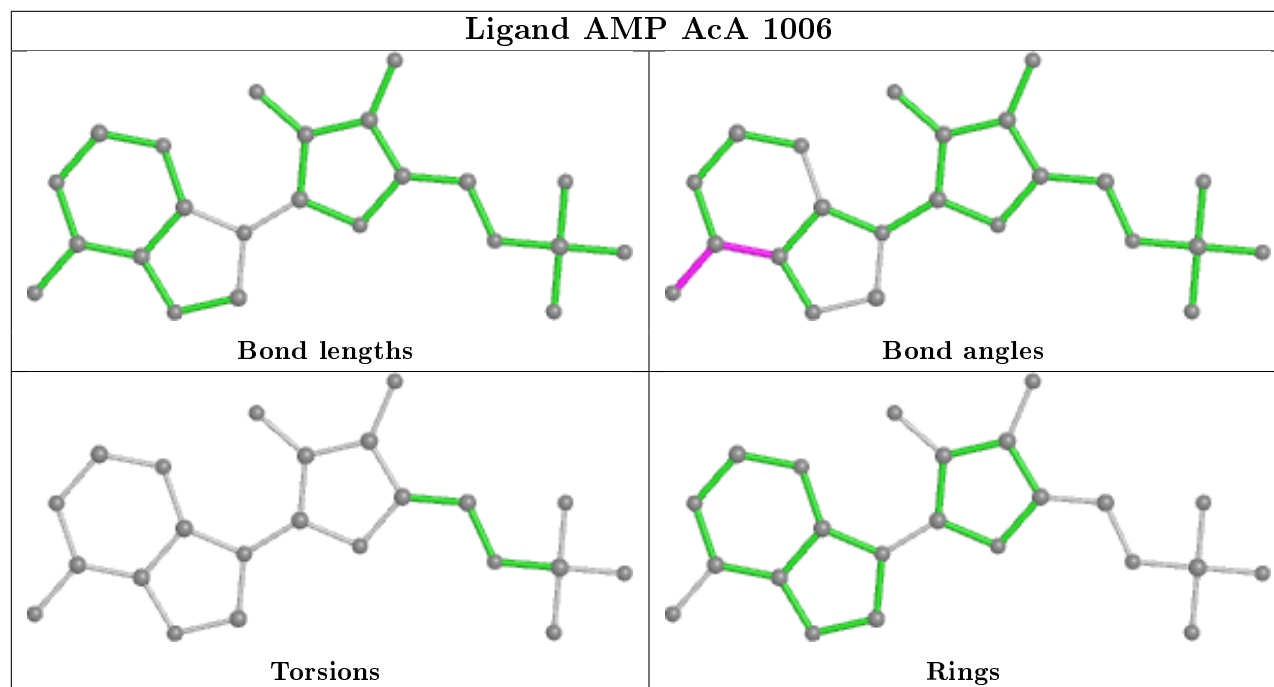
Mol	Chain	Res	Type	Atoms
8	BcB	1004	NAG	C8-C7-N2-C2
8	AcA	1005	NAG	C8-C7-N2-C2
8	AcA	1005	NAG	O7-C7-N2-C2
8	BcB	1004	NAG	O7-C7-N2-C2
8	BcB	1005	NAG	C8-C7-N2-C2
8	BcB	1004	NAG	O5-C5-C6-O6
10	AcA	1007	PEG	O1-C1-C2-O2
8	AcA	1004	NAG	C8-C7-N2-C2
11	AcA	1008	EDO	O1-C1-C2-O2
8	BcB	1005	NAG	O7-C7-N2-C2
8	AcA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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AcA	816/925 (88%)	0.11	37 (4%)	33 36	30, 51, 103, 152	0
1	BcB	795/925 (85%)	0.40	76 (9%)	8 7	34, 70, 135, 156	0
All	All	1611/1850 (87%)	0.25	113 (7%)	16 16	30, 58, 128, 156	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BcB	712	LEU	6.0
1	AcA	646	VAL	6.0
1	BcB	626	CYS	5.6
1	AcA	640	THR	5.3
1	BcB	739	PHE	4.6
1	BcB	810	LEU	4.6
1	BcB	722	PRO	4.6
1	BcB	529	TYR	4.5
1	AcA	677	HIS	4.3
1	BcB	678	GLN	4.3
1	BcB	713	TYR	4.2
1	BcB	441	LEU	4.1
1	AcA	119	ASN	4.0
1	BcB	443	ASP	3.9
1	BcB	440	TYR	3.9
1	BcB	812	ASN	3.9
1	BcB	826	LEU	3.8
1	AcA	639	GLN	3.7
1	AcA	873	HIS	3.7
1	AcA	642	PHE	3.7
1	BcB	723	VAL	3.7
1	BcB	646	VAL	3.6
1	BcB	623	ASN	3.6
1	BcB	644	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	BcB	611	LEU	3.5
1	BcB	847	HIS	3.4
1	AcA	870	HIS	3.4
1	BcB	674	LEU	3.4
1	BcB	708	PHE	3.4
1	BcB	628	CYS	3.4
1	AcA	668	GLU	3.4
1	AcA	643	ASN	3.3
1	BcB	729	TYR	3.3
1	AcA	649	GLU	3.3
1	BcB	754	SER	3.3
1	AcA	117	PHE	3.3
1	AcA	871	GLY	3.2
1	AcA	814	ARG	3.2
1	AcA	654	HIS	3.2
1	AcA	159	LEU	3.1
1	AcA	120	CYS	3.1
1	BcB	679	PHE	3.0
1	AcA	116	THR	3.0
1	BcB	105	VAL	3.0
1	AcA	111	ARG	2.9
1	BcB	624	LEU	2.9
1	AcA	526	GLU	2.9
1	AcA	645	THR	2.9
1	BcB	669	ASN	2.9
1	AcA	112	CYS	2.8
1	BcB	530	CYS	2.8
1	BcB	461	ASP	2.8
1	BcB	688	LEU	2.8
1	BcB	733	THR	2.8
1	BcB	608	VAL	2.8
1	BcB	622	ASP	2.8
1	BcB	635	ILE	2.8
1	BcB	521	ALA	2.7
1	BcB	707	ASP	2.7
1	BcB	487	PHE	2.7
1	BcB	632	ILE	2.7
1	BcB	645	THR	2.7
1	BcB	753	TYR	2.6
1	AcA	636	GLU	2.6
1	AcA	644	LEU	2.6
1	AcA	106	LYS	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BcB	612	VAL	2.6
1	BcB	680	MET	2.6
1	BcB	735	VAL	2.5
1	BcB	711	CYS	2.5
1	AcA	875	SER	2.5
1	BcB	759	THR	2.5
1	BcB	630	PRO	2.5
1	BcB	716	PHE	2.5
1	BcB	694	SER	2.4
1	AcA	443	ASP	2.4
1	AcA	484	ASN	2.4
1	AcA	616	PHE	2.4
1	AcA	637	ASP	2.4
1	BcB	814	ARG	2.4
1	AcA	613	GLN	2.4
1	BcB	815	GLN	2.4
1	BcB	671	ILE	2.4
1	BcB	756	ALA	2.4
1	BcB	636	GLU	2.4
1	BcB	693	THR	2.3
1	BcB	921	PHE	2.3
1	BcB	609	HIS	2.3
1	AcA	618	ARG	2.3
1	AcA	638	PHE	2.3
1	BcB	625	GLY	2.3
1	BcB	737	TYR	2.3
1	AcA	847	HIS	2.3
1	BcB	710	ASN	2.3
1	BcB	289	SER	2.3
1	BcB	505	ASP	2.2
1	BcB	655	GLU	2.2
1	AcA	114	GLU	2.2
1	BcB	673	LEU	2.2
1	BcB	820	ILE	2.1
1	BcB	633	LEU	2.1
1	BcB	518	TRP	2.1
1	BcB	621	ARG	2.1
1	BcB	844	THR	2.1
1	BcB	725	LYS	2.1
1	BcB	670	THR	2.1
1	BcB	648	GLU	2.1
1	BcB	849	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	BcB	687	ILE	2.0
1	BcB	437	LEU	2.0
1	BcB	649	GLU	2.0
1	AcA	110	GLY	2.0
1	AcA	113	PHE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	NEP	BcB	486	14/15	0.77	0.24	85,105,130,132	0
1	NEP	AcA	486	14/15	0.81	0.21	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BMA	AeA	4	11/12	0.65	0.29	128,149,152,153	0
2	BMA	AeA	3	11/12	0.68	0.24	111,122,132,142	0
3	MAN	AiA	3	11/12	0.69	0.25	119,123,130,133	0
5	BMA	BdB	3	11/12	0.70	0.21	125,129,137,137	0
4	NAG	AmA	2	14/15	0.80	0.34	127,141,149,150	0
4	NAG	BgB	2	14/15	0.84	0.28	91,102,110,113	0
3	NAG	AiA	2	14/15	0.85	0.18	83,94,106,115	0
5	NAG	BdB	2	14/15	0.87	0.19	93,99,109,124	0
4	NAG	AmA	1	14/15	0.88	0.17	78,90,104,114	0
3	NAG	AiA	1	14/15	0.89	0.17	68,77,84,84	0
4	NAG	BgB	1	14/15	0.91	0.26	80,90,98,103	0
5	NAG	BdB	1	14/15	0.91	0.15	62,67,84,85	0
2	NAG	AeA	2	14/15	0.94	0.14	62,73,83,101	0
2	NAG	AeA	1	14/15	0.97	0.21	41,44,48,56	0

## 6.4 Ligands ⓘ

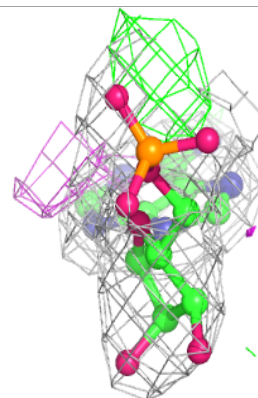
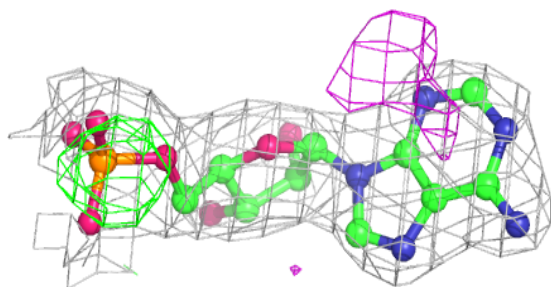
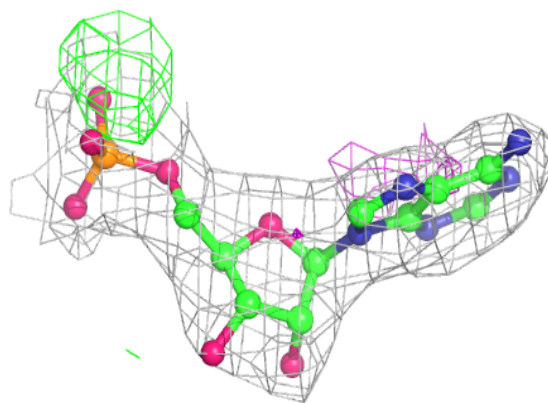
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	BcB	1004	14/15	0.77	0.46	124,140,145,145	0
7	CA	BcB	1003	1/1	0.77	0.18	124,124,124,124	0
8	NAG	AcA	1004	14/15	0.82	0.28	84,93,106,107	0
8	NAG	AcA	1005	14/15	0.83	0.33	97,104,110,116	0
11	EDO	AcA	1009	4/4	0.84	0.23	70,70,72,73	0
7	CA	AcA	1003	1/1	0.85	0.10	85,85,85,85	0
10	PEG	AcA	1007	7/7	0.87	0.23	75,79,84,86	0
8	NAG	BcB	1005	14/15	0.87	0.18	103,112,121,123	0
11	EDO	AcA	1008	4/4	0.92	0.43	72,72,72,73	0
11	EDO	BcB	1007	4/4	0.92	0.24	78,83,85,87	0
9	AMP	BcB	1006	23/23	0.94	0.18	54,59,69,74	0
9	AMP	AcA	1006	23/23	0.95	0.14	41,52,66,72	0
6	ZN	AcA	1001	1/1	0.99	0.12	37,37,37,37	0
6	ZN	BcB	1002	1/1	1.00	0.13	42,42,42,42	0
6	ZN	AcA	1002	1/1	1.00	0.12	35,35,35,35	0
6	ZN	BcB	1001	1/1	1.00	0.11	43,43,43,43	0

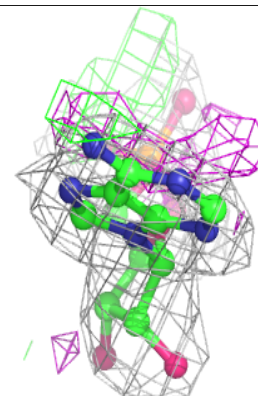
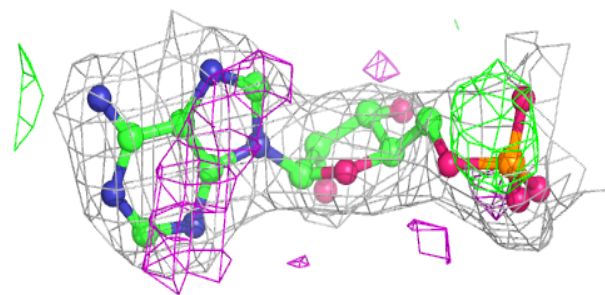
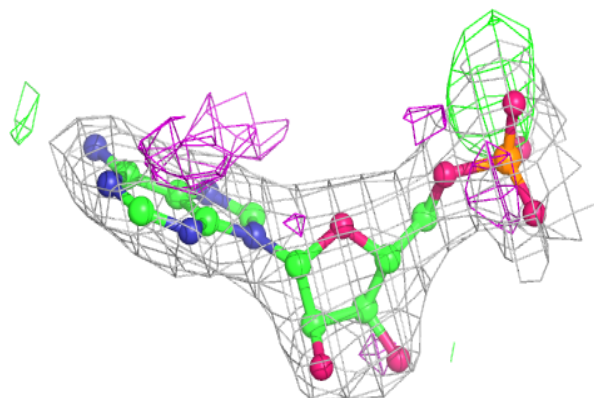
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AMP BcB 1006:**

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

**Electron density around 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.