



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 01:59 PM BST

PDB ID : 6WET  
Title : Crystal structures of human E-NPP 1: apo  
Authors : Peat, T.S.; Dennis, M.; Newman, J.  
Deposited on : 2020-04-02  
Resolution : 2.60 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  
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

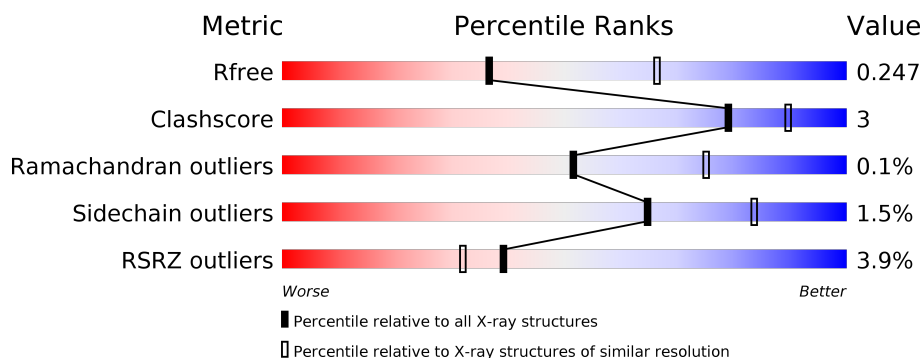
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	AaA	925	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
1	BaB	925	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>
2	AcA	3	<div> <div></div> <div>100%</div> </div>
2	BbB	3	<div> <div></div> <div>100%</div> </div>
3	AfA	3	<div> <div></div> <div>100%</div> </div>
4	BeB	2	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition [i](#)

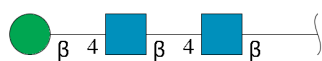
There are 8 unique types of molecules in this entry. The entry contains 12977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

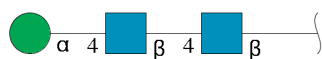
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AaA	814	Total	C	N	O	P	S	0	2	0
			6536	4168	1103	1215	1	49			
1	BaB	795	Total	C	N	O	P	S	0	0	0
			6132	3904	1039	1142	1	46			

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

- 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	AfA	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.

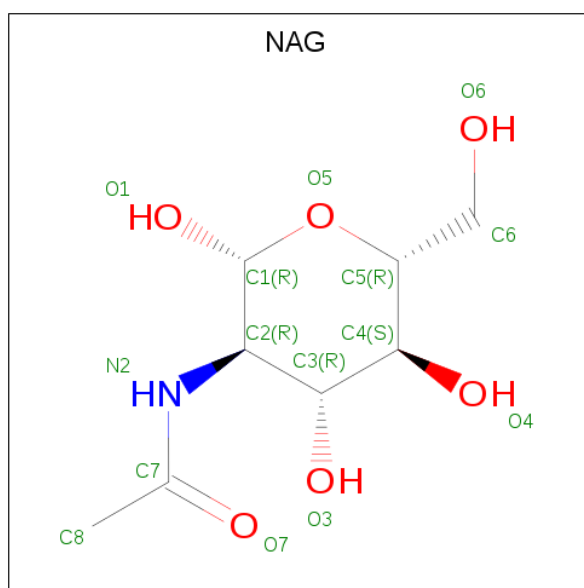


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	BeB	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	BaB	1	Total	Zn	0	0
			1	1		
5	AaA	1	Total	Zn	0	0
			1	1		

- Molecule 6 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
6	AaA	1	Total	C	N	O	0	0
			14	8	1	5		
6	AaA	1	Total	C	N	O	0	0
			14	8	1	5		
6	AaA	1	Total	C	N	O	0	0
			14	8	1	5		
6	BaB	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AaA	1	Total	C	O	0	0
			4	2	2		
7	AaA	1	Total	C	O	0	0
			4	2	2		
7	AaA	1	Total	C	O	0	0
			4	2	2		
7	AaA	1	Total	C	O	0	0
			4	2	2		
7	BaB	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AaA	50	Total	O	0	0
			50	50		
8	BaB	22	Total	O	0	0
			22	22		


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 2: 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

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

Chain AfA:  100%

MAG1  
MAG2  
MAN3

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

Chain BeB:  100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.11Å 158.88Å 209.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 2.60 44.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.40-2.60) 100.0 (44.38-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.210 , 0.244 0.213 , 0.247	Depositor DCC
$R_{free}$ test set	4461 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 35.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, TPO, EDO, 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	AaA	0.62	0/6707	0.74	0/9105
1	BaB	0.64	0/6290	0.74	0/8560
All	All	0.63	0/12997	0.74	0/17665

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	AaA	6536	0	6267	0	0
1	BaB	6132	0	5642	0	0
2	AcA	39	0	34	0	0
2	BbB	39	0	34	0	0
3	AfA	39	0	34	0	0
4	BeB	28	0	25	0	0
5	AaA	1	0	0	0	0
5	BaB	1	0	0	0	0
6	AaA	42	0	39	0	0
6	BaB	28	0	26	0	0
7	AaA	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BaB	4	0	6	0	0
8	AaA	50	0	0	0	0
8	BaB	22	0	0	0	0
All	All	12977	0	12131	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 3.

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	AaA	811/925 (88%)	775 (96%)	36 (4%)	0	100	100
1	BaB	782/925 (84%)	741 (95%)	39 (5%)	2 (0%)	41	64
All	All	1593/1850 (86%)	1516 (95%)	75 (5%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BaB	610	PRO
1	BaB	483	PRO

### 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	AaA	732/823 (89%)	722 (99%)	10 (1%)	67	85
1	BaB	643/823 (78%)	633 (98%)	10 (2%)	62	82
All	All	1375/1646 (84%)	1355 (98%)	20 (2%)	65	83

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AaA	161	ARG
1	AaA	215	PHE
1	AaA	257	PHE
1	AaA	317	SER
1	AaA	370	LEU
1	AaA	434	TYR
1	AaA	530	CYS
1	AaA	663	ARG
1	AaA	676	GLN
1	AaA	843	GLN
1	BaB	215	PHE
1	BaB	257	PHE
1	BaB	377	SER
1	BaB	434	TYR
1	BaB	503	LYS
1	BaB	530	CYS
1	BaB	612	VAL
1	BaB	806	ARG
1	BaB	843	GLN
1	BaB	886	ARG

Some 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	TPO	AaA	256	1	8,10,11	1.73	1 (12%)	10,14,16	1.16	1 (10%)
1	TPO	BaB	256	1,5	8,10,11	1.69	1 (12%)	10,14,16	1.20	1 (10%)

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	TPO	AaA	256	1	-	1/9/11/13	-
1	TPO	BaB	256	1,5	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AaA	256	TPO	P-OG1	4.64	1.68	1.59
1	BaB	256	TPO	P-OG1	4.55	1.67	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AaA	256	TPO	O-C-CA	-3.12	116.59	124.78
1	BaB	256	TPO	O-C-CA	-3.01	116.90	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BaB	256	TPO	CB-OG1-P-O2P
1	AaA	256	TPO	O-C-CA-CB
1	BaB	256	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

11 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	AcA	1	1,2	14,14,15	0.78	0	17,19,21	1.20	2 (11%)
2	NAG	AcA	2	2	14,14,15	0.54	0	17,19,21	1.10	1 (5%)
2	BMA	AcA	3	2	11,11,12	0.38	0	15,15,17	1.16	1 (6%)
3	NAG	AfA	1	1,3	14,14,15	0.86	1 (7%)	17,19,21	1.81	3 (17%)
3	NAG	AfA	2	3	14,14,15	0.45	0	17,19,21	1.21	2 (11%)
3	MAN	AfA	3	3	11,11,12	0.55	0	15,15,17	1.71	4 (26%)
2	NAG	BbB	1	1,2	14,14,15	0.46	0	17,19,21	1.61	4 (23%)
2	NAG	BbB	2	2	14,14,15	0.40	0	17,19,21	1.18	1 (5%)
2	BMA	BbB	3	2	11,11,12	0.29	0	15,15,17	1.07	1 (6%)
4	NAG	BeB	1	1,4	14,14,15	0.54	0	17,19,21	1.42	3 (17%)
4	NAG	BeB	2	4	14,14,15	0.53	0	17,19,21	1.12	2 (11%)

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	AcA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	AcA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	AcA	3	2	-	0/2/19/22	0/1/1/1
3	NAG	AfA	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	AfA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	AfA	3	3	-	2/2/19/22	0/1/1/1
2	NAG	BbB	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	BbB	2	2	-	0/6/23/26	0/1/1/1
2	BMA	BbB	3	2	-	0/2/19/22	0/1/1/1
4	NAG	BeB	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	BeB	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AfA	1	NAG	C1-C2	2.36	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AfA	3	MAN	C1-C2-C3	5.14	115.99	109.67
3	AfA	1	NAG	C8-C7-N2	-4.91	107.79	116.10
2	BbB	1	NAG	O5-C1-C2	-3.95	105.06	111.29
3	AfA	1	NAG	O7-C7-N2	3.77	128.89	121.95
2	AcA	1	NAG	C3-C4-C5	3.59	116.65	110.24
2	AcA	3	BMA	C1-C2-C3	3.03	113.39	109.67
3	AfA	2	NAG	C1-O5-C5	3.03	116.30	112.19
3	AfA	1	NAG	O5-C1-C2	-2.92	106.67	111.29
4	BeB	1	NAG	C8-C7-N2	2.80	120.83	116.10
2	BbB	2	NAG	C1-O5-C5	2.73	115.89	112.19
2	BbB	1	NAG	C1-C2-N2	2.57	114.88	110.49
2	BbB	3	BMA	C1-C2-C3	2.56	112.81	109.67
2	BbB	1	NAG	C3-C4-C5	2.48	114.65	110.24
4	BeB	2	NAG	O5-C5-C6	2.42	111.00	107.20
2	BbB	1	NAG	C4-C3-C2	2.24	114.30	111.02
4	BeB	1	NAG	C1-O5-C5	2.23	115.22	112.19
3	AfA	3	MAN	C2-C3-C4	2.18	114.67	110.89
3	AfA	2	NAG	O5-C5-C4	-2.18	105.52	110.83
3	AfA	3	MAN	O5-C5-C6	2.16	110.60	107.20
3	AfA	3	MAN	O5-C5-C4	-2.14	105.61	110.83
2	AcA	2	NAG	O7-C7-C8	-2.14	118.09	122.06
4	BeB	2	NAG	C1-O5-C5	2.04	114.95	112.19
4	BeB	1	NAG	C2-N2-C7	-2.03	120.02	122.90
2	AcA	1	NAG	O5-C1-C2	-2.02	108.10	111.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BeB	1	NAG	C8-C7-N2-C2
4	BeB	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	AfA	3	MAN	C4-C5-C6-O6
3	AfA	3	MAN	O5-C5-C6-O6
3	AfA	1	NAG	C8-C7-N2-C2
3	AfA	2	NAG	O5-C5-C6-O6
3	AfA	2	NAG	C4-C5-C6-O6
2	AcA	1	NAG	O5-C5-C6-O6
2	BbB	1	NAG	O5-C5-C6-O6
2	BbB	1	NAG	C8-C7-N2-C2
2	BbB	1	NAG	C4-C5-C6-O6
2	AcA	1	NAG	C4-C5-C6-O6
3	AfA	1	NAG	O7-C7-N2-C2
3	AfA	1	NAG	C1-C2-N2-C7
3	AfA	1	NAG	C4-C5-C6-O6
3	AfA	1	NAG	O5-C5-C6-O6
2	BbB	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 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	$\# Z  > 2$
6	NAG	AaA	1002	1	14,14,15	0.35	0	17,19,21	1.12	2 (11%)
6	NAG	BaB	1003	1	14,14,15	0.48	0	17,19,21	1.42	4 (23%)
7	EDO	AaA	1005	-	3,3,3	0.20	0	2,2,2	0.37	0
7	EDO	BaB	1004	-	3,3,3	0.13	0	2,2,2	0.35	0
7	EDO	AaA	1006	-	3,3,3	0.12	0	2,2,2	0.22	0
7	EDO	AaA	1008	-	3,3,3	0.12	0	2,2,2	0.20	0
7	EDO	AaA	1007	-	3,3,3	0.17	0	2,2,2	0.34	0
6	NAG	BaB	1002	1	14,14,15	0.58	0	17,19,21	2.09	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	AaA	1004	1	14,14,15	0.47	0	17,19,21	1.41	3 (17%)
6	NAG	AaA	1003	1	14,14,15	0.44	0	17,19,21	1.32	2 (11%)

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
6	NAG	AaA	1002	1	-	3/6/23/26	0/1/1/1
6	NAG	BaB	1003	1	-	5/6/23/26	0/1/1/1
7	EDO	AaA	1005	-	-	1/1/1/1	-
7	EDO	BaB	1004	-	-	0/1/1/1	-
7	EDO	AaA	1006	-	-	1/1/1/1	-
7	EDO	AaA	1008	-	-	1/1/1/1	-
7	EDO	AaA	1007	-	-	0/1/1/1	-
6	NAG	BaB	1002	1	-	6/6/23/26	0/1/1/1
6	NAG	AaA	1004	1	-	5/6/23/26	0/1/1/1
6	NAG	AaA	1003	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	BaB	1002	NAG	O5-C1-C2	-4.70	103.87	111.29
6	BaB	1002	NAG	C4-C3-C2	4.22	117.20	111.02
6	BaB	1002	NAG	C3-C4-C5	3.82	117.06	110.24
6	AaA	1004	NAG	O7-C7-N2	2.79	127.08	121.95
6	BaB	1002	NAG	C8-C7-N2	-2.76	111.43	116.10
6	BaB	1003	NAG	O7-C7-N2	2.73	126.97	121.95
6	AaA	1004	NAG	C8-C7-N2	-2.70	111.53	116.10
6	AaA	1002	NAG	C1-C2-N2	2.59	114.91	110.49
6	AaA	1004	NAG	C2-N2-C7	2.54	126.53	122.90
6	BaB	1003	NAG	C8-C7-N2	-2.51	111.84	116.10
6	AaA	1002	NAG	O5-C1-C2	-2.51	107.33	111.29
6	BaB	1003	NAG	C2-N2-C7	2.42	126.35	122.90
6	BaB	1003	NAG	O5-C5-C6	2.33	110.86	107.20
6	AaA	1003	NAG	O7-C7-N2	-2.20	117.90	121.95
6	AaA	1003	NAG	C8-C7-N2	2.05	119.58	116.10
6	BaB	1002	NAG	O7-C7-N2	2.03	125.68	121.95



There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AaA	1003	NAG	C8-C7-N2-C2
6	AaA	1003	NAG	O7-C7-N2-C2
6	BaB	1003	NAG	O5-C5-C6-O6
6	BaB	1002	NAG	O5-C5-C6-O6
6	BaB	1003	NAG	C4-C5-C6-O6
6	BaB	1003	NAG	C8-C7-N2-C2
6	AaA	1004	NAG	C8-C7-N2-C2
6	BaB	1002	NAG	C8-C7-N2-C2
6	BaB	1002	NAG	C4-C5-C6-O6
6	AaA	1002	NAG	C8-C7-N2-C2
6	AaA	1004	NAG	O5-C5-C6-O6
7	AaA	1005	EDO	O1-C1-C2-O2
7	AaA	1006	EDO	O1-C1-C2-O2
6	BaB	1002	NAG	C1-C2-N2-C7
6	BaB	1003	NAG	C3-C2-N2-C7
6	AaA	1004	NAG	O7-C7-N2-C2
6	BaB	1002	NAG	O7-C7-N2-C2
6	BaB	1003	NAG	O7-C7-N2-C2
6	AaA	1004	NAG	C4-C5-C6-O6
7	AaA	1008	EDO	O1-C1-C2-O2
6	AaA	1002	NAG	O7-C7-N2-C2
6	AaA	1002	NAG	C4-C5-C6-O6
6	AaA	1003	NAG	C4-C5-C6-O6
6	AaA	1004	NAG	C3-C2-N2-C7
6	BaB	1002	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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	AaA	813/925 (87%)	-0.07	20 (2%) 57 51	37, 60, 109, 139	0
1	BaB	794/925 (85%)	0.14	43 (5%) 25 20	41, 83, 147, 181	0
All	All	1607/1850 (86%)	0.03	63 (3%) 39 32	37, 68, 135, 181	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BaB	729	TYR	4.9
1	BaB	623	ASN	4.4
1	BaB	723	VAL	4.4
1	AaA	443	ASP	4.2
1	BaB	478	LEU	3.7
1	AaA	642	PHE	3.6
1	BaB	710	ASN	3.6
1	AaA	522	LEU	3.5
1	BaB	847	HIS	3.5
1	AaA	640	THR	3.3
1	AaA	702	SER	3.3
1	BaB	727	SER	3.3
1	AaA	111	ARG	3.2
1	BaB	870	HIS	3.2
1	BaB	810	LEU	3.2
1	BaB	635	ILE	3.2
1	AaA	748	ASN	3.2
1	BaB	628	CYS	3.1
1	BaB	722	PRO	3.1
1	BaB	624	LEU	3.1
1	BaB	714	GLN	3.0
1	BaB	724	HIS	3.0
1	BaB	619	ASN	2.9
1	AaA	814	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	AaA	874	ASP	2.8
1	BaB	622	ASP	2.7
1	BaB	529	TYR	2.7
1	BaB	696	THR	2.6
1	BaB	651	ILE	2.6
1	BaB	636	GLU	2.6
1	BaB	441	LEU	2.5
1	BaB	843	GLN	2.5
1	BaB	725	LYS	2.5
1	AaA	117	PHE	2.5
1	BaB	626	CYS	2.5
1	BaB	443	ASP	2.5
1	BaB	719	PRO	2.5
1	BaB	844	THR	2.4
1	BaB	674	LEU	2.4
1	BaB	673	LEU	2.4
1	BaB	814	ARG	2.4
1	BaB	700	ASN	2.4
1	BaB	612	VAL	2.4
1	AaA	750	SER	2.4
1	AaA	159	LEU	2.3
1	BaB	648	GLU	2.3
1	AaA	484	ASN	2.3
1	AaA	526	GLU	2.3
1	BaB	627	SER	2.2
1	AaA	651	ILE	2.2
1	AaA	749	SER	2.2
1	BaB	691	LEU	2.2
1	BaB	678	GLN	2.1
1	BaB	527	ARG	2.1
1	AaA	677	HIS	2.1
1	AaA	105	VAL	2.1
1	BaB	287	SER	2.1
1	AaA	112	CYS	2.1
1	AaA	746	ASN	2.1
1	BaB	512	PHE	2.1
1	BaB	637	ASP	2.1
1	BaB	434	TYR	2.0
1	BaB	288	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	TPO	BaB	256	11/12	0.88	0.18	55,64,129,136	0
1	TPO	AaA	256	11/12	0.91	0.20	42,51,127,127	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
3	MAN	AfA	3	11/12	0.60	0.21	90,98,101,105	11
2	BMA	AcA	3	11/12	0.76	0.16	116,130,137,141	0
2	BMA	BbB	3	11/12	0.85	0.14	121,128,132,133	0
4	NAG	BeB	1	14/15	0.85	0.30	101,117,124,130	0
3	NAG	AfA	1	14/15	0.87	0.16	74,88,97,101	0
4	NAG	BeB	2	14/15	0.88	0.39	110,142,154,156	0
2	NAG	BbB	2	14/15	0.92	0.12	88,97,114,125	0
3	NAG	AfA	2	14/15	0.92	0.17	97,103,118,124	0
2	NAG	BbB	1	14/15	0.94	0.17	76,83,94,96	0
2	NAG	AcA	2	14/15	0.94	0.14	70,82,91,97	0
2	NAG	AcA	1	14/15	0.96	0.20	49,52,62,64	0

## 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, 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
6	NAG	AaA	1002	14/15	0.81	0.35	115,139,151,170	0
6	NAG	BaB	1002	14/15	0.81	0.20	84,98,105,106	14
6	NAG	BaB	1003	14/15	0.83	0.20	109,125,132,133	0
7	EDO	BaB	1004	4/4	0.88	0.25	86,87,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	AaA	1003	14/15	0.88	0.28	109,114,120,133	0
7	EDO	AaA	1005	4/4	0.91	0.13	70,70,75,76	0
6	NAG	AaA	1004	14/15	0.91	0.13	89,112,123,124	0
7	EDO	AaA	1008	4/4	0.93	0.31	75,79,81,83	0
7	EDO	AaA	1006	4/4	0.94	0.29	69,70,74,77	0
7	EDO	AaA	1007	4/4	0.94	0.22	65,66,70,72	0
5	ZN	BaB	1001	1/1	0.99	0.06	67,67,67,67	0
5	ZN	AaA	1001	1/1	0.99	0.09	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.