

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 05:02 AM EDT

PDB ID	:	6WEU
Title	:	Crystal structures of human E-NPP 1: bound to adenosine-5'-thio-monophos
		phate
Authors	:	Peat, T.S.; Dennis, M.; Newman, J.
Deposited on		
Resolution	:	2.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

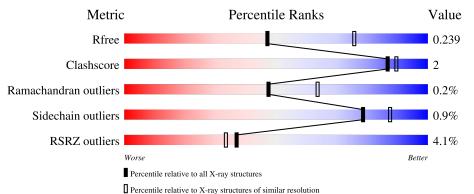
MolProbity	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.65 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374(2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	AbA	925	2%	20/
	ADA	920	87% · 12	2%
1	BbB	925	86% • 14	4%
2	AcA	3	100%	
3	AfA	2	50% 50%	
3	BfB	2	100%	



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Mol	Chain	Length	Quality of chain	
4	BcB	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
3	NAG	BfB	2	Х	-	-	-
6	NAG	AbA	1005	Х	-	-	-
6	NAG	BbB	1003	-	-	-	Х



6WEU

2 Entry composition (i)

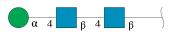
There are 9 unique types of molecules in this entry. The entry contains 13105 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	AbA	816	Total 6564	C 4188	N 1111	O 1216	S 49	0	3	0
1	BbB	799	Total 6161	C 3921	N 1047	0 1147	S 46	0	0	0

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



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

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	AfA	2	Total C N O 28 16 2 10	0	0	0
3	BfB	2	Total C N O 28 16 2 10	0	0	0

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



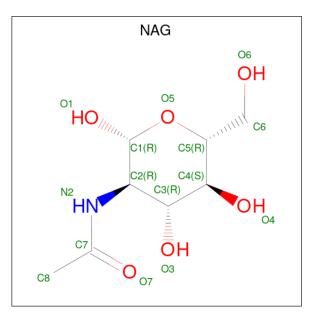


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
4	BcB	3	Total 39	C 22	N 2	O 15	0	0	0

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

I	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	5	AbA	2	Total Zn 2 2	0	0
	5	BbB	2	Total Zn 2 2	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



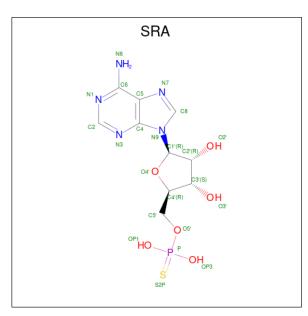
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AbA	1	Total C N O 14 8 1 5	0	0
6	AbA	1	Total C N O 14 8 1 5	0	0
6	AbA	1	Total C N O 14 8 1 5	0	0
6	BbB	1	Total C N O 14 8 1 5	0	0



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

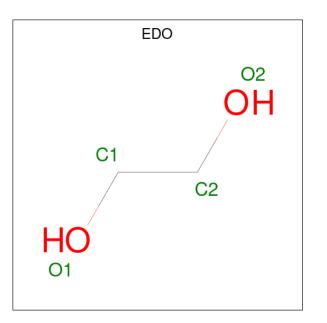
• Molecule 7 is ADENOSINE -5'-THIO-MONOPHOSPHATE (three-letter code: SRA) (formula: $C_{10}H_{14}N_5O_6PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
7	AbA	1	Total	С	Ν	0	Р	S	0	0
1	AUA	1	23	10	5	6	1	1	0	0
7	BbB	1	Total	С	Ν	0	Р	S	0	0
1	DOD	1	23	10	5	6	1	1	0	0

• Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
8	AbA	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 9 is water.

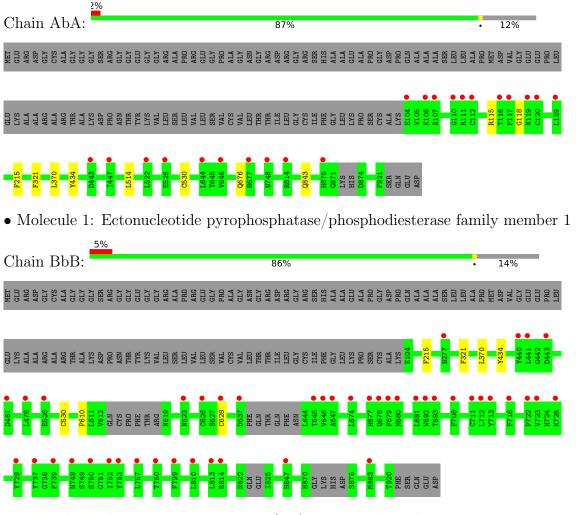
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AbA	86	Total O 86 86	0	0
9	BbB	36	Total O 36 36	0	0



3 Residue-property plots (i)

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

• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 1



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

Chain AcA:

100%

NAG1 NAG2 MAN3



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

50%

Chain AfA:

NAG1 NAG2

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

Chain BfB:

100%

NAG1 NAG2

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

Chain BcB: 67% 33%

50%

NAG1 NAG2 BMA3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	83.01Å 160.14Å 209.63Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 - 2.65	Depositor
Resolution (A)	47.57 - 2.65	EDS
% Data completeness	$100.0 \ (47.57-2.65)$	Depositor
(in resolution range)	$100.0 \ (47.57 - 2.65)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.46 (at 2.65 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D.	0.207 , 0.239	Depositor
R, R_{free}	0.210 , 0.239	DCC
R_{free} test set	4208 reflections $(5.14%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	53.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , 46.7	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	0.93	EDS
Total number of atoms	13105	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 2.54% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: SRA, ZN, EDO, BMA, NAG, 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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AbA	0.62	0/6749	0.74	0/9163	
1	BbB	0.64	0/6332	0.73	0/8619	
All	All	0.63	0/13081	0.73	0/17782	

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AbA	6564	0	6297	0	0
1	BbB	6161	0	5673	0	0
2	AcA	39	0	34	0	0
3	AfA	28	0	25	0	0
3	BfB	28	0	25	0	0
4	BcB	39	0	34	0	0
5	AbA	2	0	0	0	0
5	BbB	2	0	0	0	0
6	AbA	42	0	39	0	0
6	BbB	28	0	26	0	0
7	AbA	23	0	11	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BbB	23	0	11	0	0
8	AbA	4	0	6	0	0
9	AbA	86	0	0	0	0
9	BbB	36	0	0	0	0
All	All	13105	0	12181	0	0

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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	Perce	entiles
1	AbA	815/925~(88%)	774 (95%)	39~(5%)	2~(0%)	47	64
1	BbB	789/925~(85%)	746 (95%)	41 (5%)	2(0%)	41	56
All	All	1604/1850~(87%)	1520 (95%)	80~(5%)	4 (0%)	47	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AbA	118	GLY
1	AbA	321	PHE
1	BbB	321	PHE
1	BbB	610	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.



Mol	Chain Analysed		Rotameric	Outliers	Perce	ntiles
1	AbA	736/824~(89%)	728~(99%)	8 (1%)	73	85
1	BbB	648/824~(79%)	643 (99%)	5 (1%)	81	89
All	All	1384/1648~(84%)	1371 (99%)	13 (1%)	78	87

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

 $5~{\rm of}~13$ residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	AbA	843	GLN
1	BbB	215	PHE
1	BbB	628	CYS
1	BbB	434	TYR
1	BbB	530	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

10 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	Dog	Ros	Res	Link	Bo	ond leng	ths	В	ond ang	les
WIOI	Mol Type Chain Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2			
2	NAG	AcA	1	2,1	14,14,15	0.77	1 (7%)	17,19,21	1.29	2 (11%)	



Mol	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
MOI	Type	Ullaili	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	AcA	2	2	14,14,15	0.67	0	$17,\!19,\!21$	1.33	1 (5%)
2	MAN	AcA	3	2	11,11,12	0.30	0	$15,\!15,\!17$	1.35	2 (13%)
3	NAG	AfA	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	2.02	5 (29%)
3	NAG	AfA	2	3	14,14,15	0.43	0	17,19,21	0.85	0
4	NAG	BcB	1	4,1	14,14,15	0.53	0	$17,\!19,\!21$	1.30	2 (11%)
4	NAG	BcB	2	4	14,14,15	0.44	0	17,19,21	0.72	0
4	BMA	BcB	3	4	11,11,12	0.39	0	$15,\!15,\!17$	0.93	0
3	NAG	BfB	1	$1,\!3$	14,14,15	0.63	0	$17,\!19,\!21$	1.73	5 (29%)
3	NAG	BfB	2	3	14,14,15	0.38	0	17,19,21	1.60	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	AcA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AcA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	AcA	3	2	-	2/2/19/22	1/1/1/1
3	NAG	AfA	1	$1,\!3$	-	4/6/23/26	0/1/1/1
3	NAG	AfA	2	3	-	2/6/23/26	0/1/1/1
4	NAG	BcB	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	BcB	2	4	-	2/6/23/26	0/1/1/1
4	BMA	BcB	3	4	-	2/2/19/22	0/1/1/1
3	NAG	BfB	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	BfB	2	3	1/1/5/7	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
3	AfA	1	NAG	C1-C2	2.24	1.55	1.52
2	AcA	1	NAG	O5-C5	-2.12	1.39	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	AfA	1	NAG	O7-C7-N2	-4.62	113.46	121.95
3	AfA	1	NAG	C8-C7-N2	4.38	123.51	116.10
3	BfB	1	NAG	O7-C7-N2	-3.66	115.23	121.95



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	AcA	2	NAG	C3-C4-C5	3.43	116.35	110.24
3	BfB	2	NAG	C8-C7-N2	-3.42	110.32	116.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	BfB	2	NAG	C1

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AfA	1	NAG	C8-C7-N2-C2
3	AfA	1	NAG	O7-C7-N2-C2
3	BfB	1	NAG	C8-C7-N2-C2
3	BfB	1	NAG	O7-C7-N2-C2
3	BfB	2	NAG	C8-C7-N2-C2

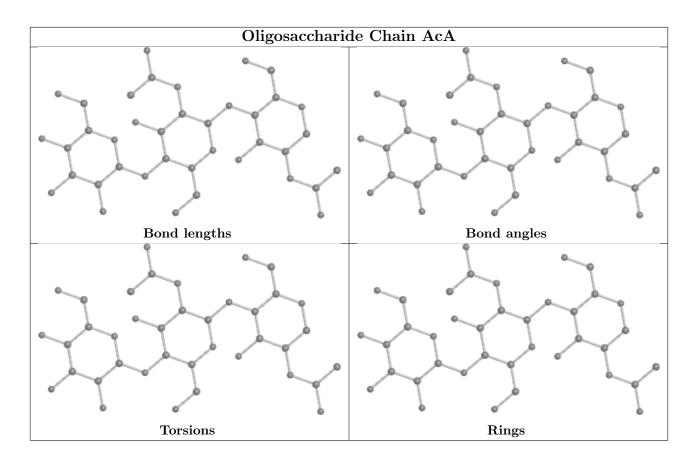
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AcA	3	MAN	C1-C2-C3-C4-C5-O5

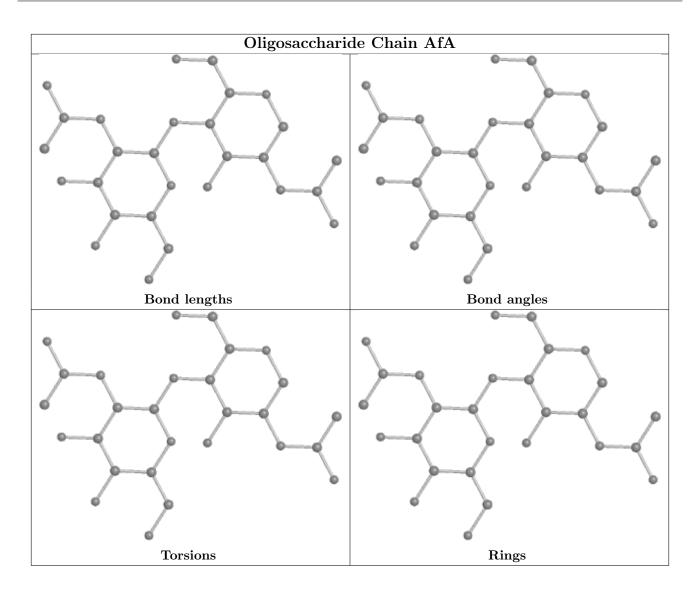
No monomer is involved in short contacts.

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

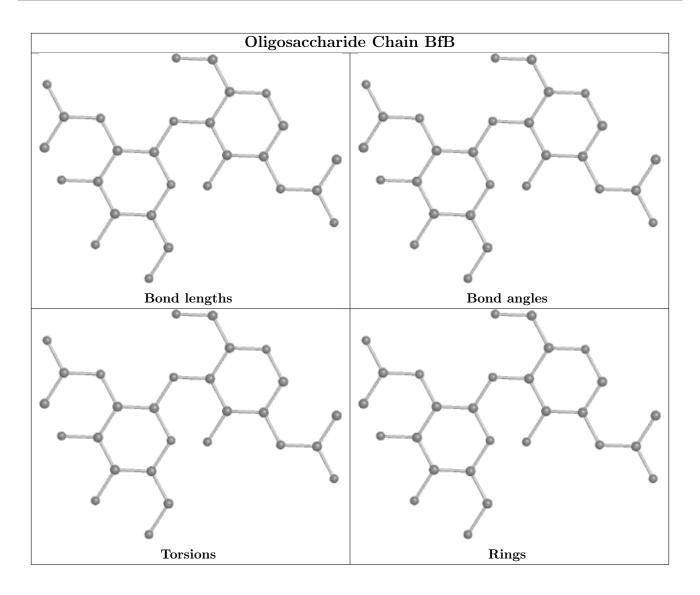




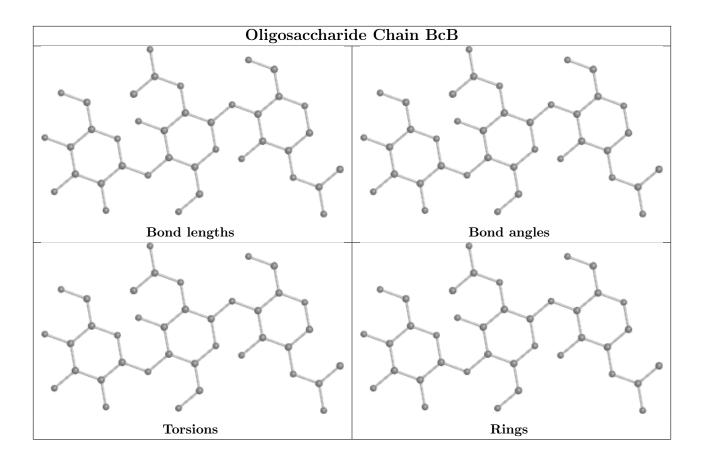












5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	Turne	Chain	Res	Link	B	ond leng	gths	Bond angles		
N101	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	BbB	1003	1	14,14,15	0.63	0	17,19,21	1.79	6 (35%)
7	SRA	BbB	1005	-	$22,\!25,\!25$	5.11	10 (45%)	22,38,38	1.59	3 (13%)
7	SRA	AbA	1006	-	$22,\!25,\!25$	<mark>5.09</mark>	10 (45%)	22,38,38	1.65	3 (13%)
8	EDO	AbA	1007	-	3,3,3	0.06	0	2,2,2	0.16	0
6	NAG	AbA	1003	1	$14,\!14,\!15$	0.45	0	17,19,21	1.28	1 (5%)
6	NAG	AbA	1005	1	14,14,15	0.35	0	17,19,21	0.53	0
6	NAG	AbA	1004	1	$14,\!14,\!15$	0.49	0	17,19,21	1.21	3 (17%)
6	NAG	BbB	1004	1	14,14,15	0.55	0	17,19,21	1.23	3 (17%)



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	BbB	1003	1	-	4/6/23/26	0/1/1/1
7	SRA	BbB	1005	-	-	4/6/26/26	0/3/3/3
7	SRA	AbA	1006	-	-	2/6/26/26	0/3/3/3
8	EDO	AbA	1007	-	-	1/1/1/1	-
6	NAG	AbA	1003	1	-	4/6/23/26	0/1/1/1
6	NAG	AbA	1005	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	AbA	1004	1	-	5/6/23/26	0/1/1/1
6	NAG	BbB	1004	1	-	4/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	BbB	1005	SRA	O4'-C1'	16.93	1.64	1.41
7	AbA	1006	SRA	O4'-C1'	16.59	1.64	1.41
7	AbA	1006	SRA	C2'-C1'	-12.45	1.34	1.53
7	BbB	1005	SRA	C2'-C1'	-12.35	1.35	1.53
7	AbA	1006	SRA	O4'-C4'	-7.88	1.27	1.45

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
7	AbA	1006	SRA	N3-C2-N1	-4.96	120.93	128.68
7	BbB	1005	SRA	N3-C2-N1	-4.92	120.98	128.68
6	BbB	1003	NAG	O5-C1-C2	-3.79	105.31	111.29
7	AbA	1006	SRA	C3'-C2'-C1'	3.69	106.53	100.98
7	BbB	1005	SRA	C3'-C2'-C1'	3.58	106.37	100.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	AbA	1005	NAG	C1

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AbA	1003	NAG	C8-C7-N2-C2



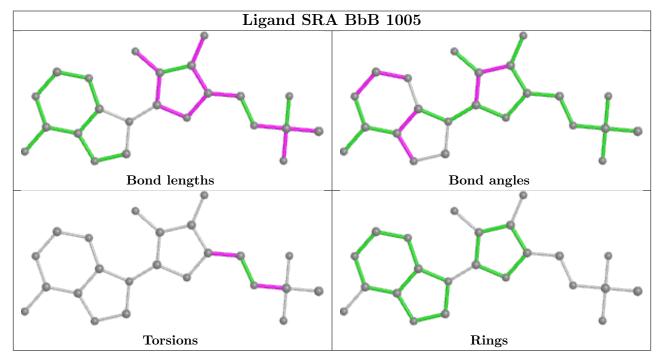
Mol	Chain	Res	Type	Atoms
6	AbA	1003	NAG	O7-C7-N2-C2
7	BbB	1005	SRA	C3'-C4'-C5'-O5'
7	AbA	1006	SRA	O4'-C4'-C5'-O5'
7	BbB	1005	SRA	O4'-C4'-C5'-O5'

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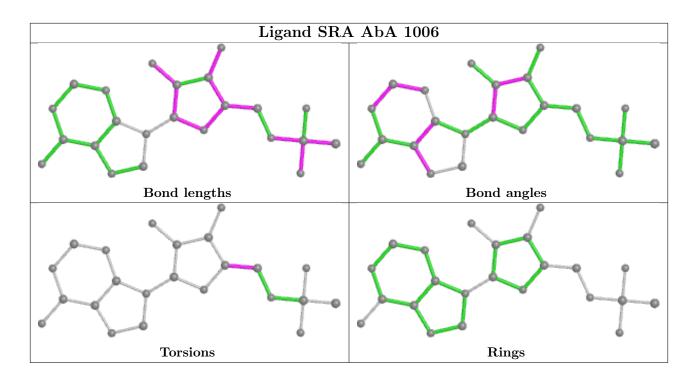
There are no ring outliers.

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 then 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2		$OWAB(A^2)$	Q<0.9
1	AbA	816/925~(88%)	-0.12	21 (2%)	56 52	30, 52, 100, 141	0
1	BbB	799/925~(86%)	0.15	45 (5%)	24 21	35, 73, 137, 166	0
All	All	1615/1850~(87%)	0.02	66 (4%)	37 33	30, 59, 128, 166	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BbB	723	VAL	5.0
1	BbB	739	PHE	4.4
1	BbB	637	ASP	4.3
1	AbA	104	GLU	4.2
1	BbB	443	ASP	4.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

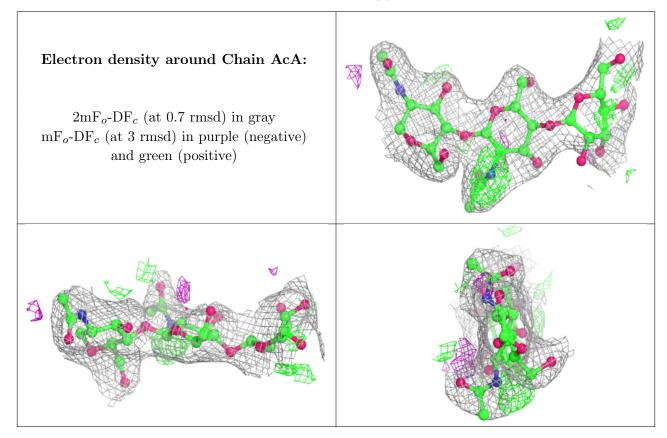
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	AcA	3	11/12	0.82	0.14	93,103,106,114	0
4	BMA	BcB	3	11/12	0.85	0.13	$105,\!114,\!120,\!123$	0
2	NAG	AcA	2	14/15	0.86	0.18	$62,\!72,\!80,\!93$	0
4	NAG	BcB	2	14/15	0.87	0.13	82,98,111,116	0
3	NAG	BfB	2	14/15	0.87	0.28	96,107,115,116	0



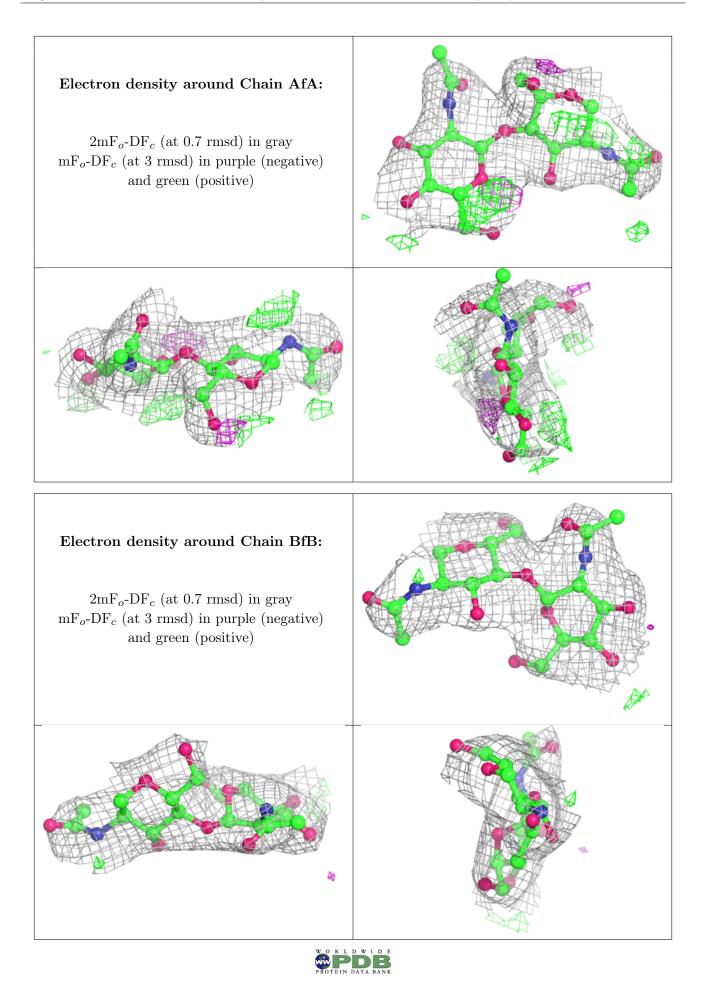
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	AfA	2	14/15	0.89	0.20	89,98,109,119	0
3	NAG	AfA	1	14/15	0.91	0.16	68,76,83,83	0
3	NAG	BfB	1	14/15	0.92	0.22	80,92,100,100	0
4	NAG	BcB	1	14/15	0.95	0.13	60,64,74,84	0
2	NAG	AcA	1	14/15	0.97	0.18	44,47,51,61	0

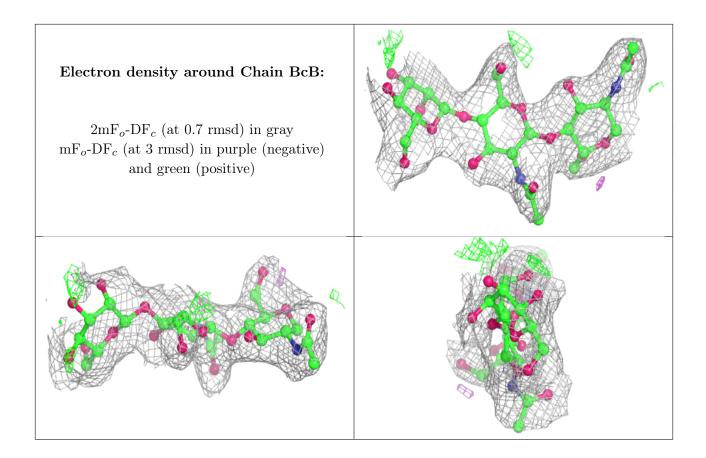
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The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.









6.4 Ligands (i)

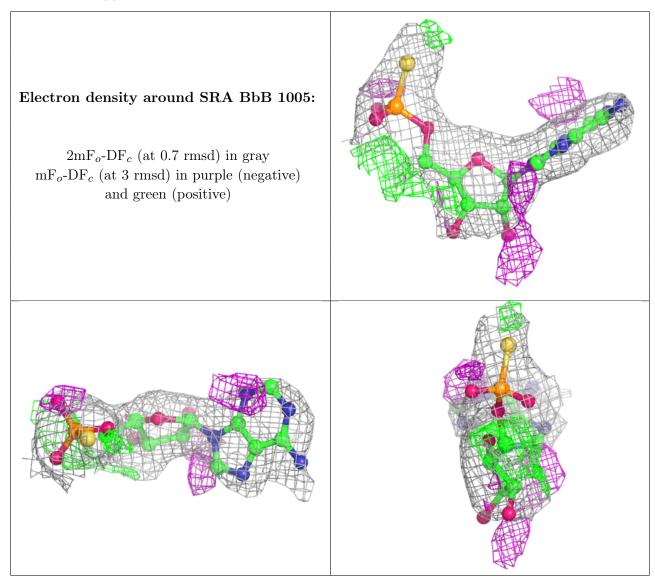
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
6	NAG	AbA	1005	14/15	0.70	0.38	113,122,129,130	0
6	NAG	BbB	1003	14/15	0.70	0.46	106,143,154,155	0
6	NAG	AbA	1004	14/15	0.79	0.17	82,105,117,118	0
6	NAG	BbB	1004	14/15	0.79	0.18	98,121,130,130	0
7	SRA	BbB	1005	23/23	0.89	0.27	71,82,91,99	0
6	NAG	AbA	1003	14/15	0.92	0.28	98,106,111,122	0
7	SRA	AbA	1006	23/23	0.93	0.24	67,87,103,107	0
5	ZN	BbB	1002	1/1	0.93	0.18	66,66,66,66	1
8	EDO	AbA	1007	4/4	0.95	0.31	$67,\!69,\!70,\!73$	0
5	ZN	AbA	1002	1/1	0.98	0.22	93,93,93,93	1
5	ZN	BbB	1001	1/1	0.99	0.12	$53,\!53,\!53,\!53$	0
5	ZN	AbA	1001	1/1	0.99	0.10	49,49,49,49	0

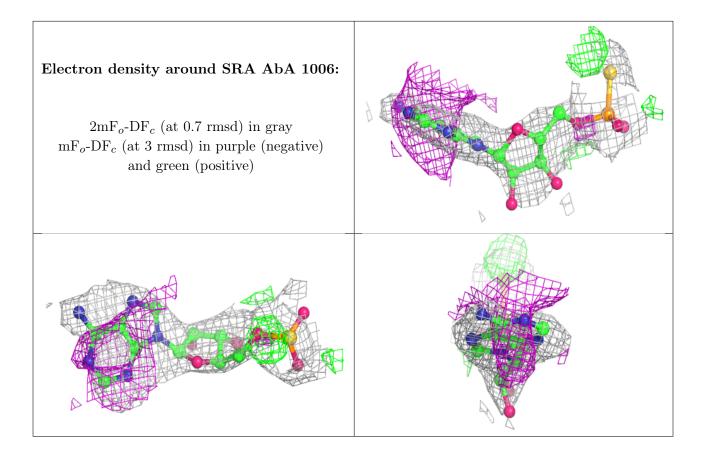
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

