



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 02:00 PM BST

PDB ID : 6WEU
Title : Crystal structures of human E-NPP 1: bound to adenosine-5'-thio-monophosphate
Authors : Peat, T.S.; Dennis, M.; Newman, J.
Deposited on : 2020-04-03
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 ⓘ symbol.

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 : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

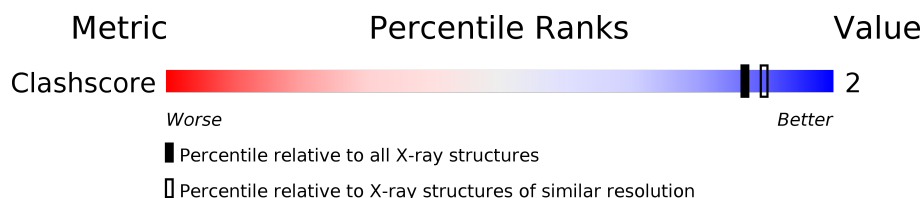
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1374 (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 on 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AbA	925	 88% 12%
1	BbB	925	 86% 14%
2	AcA	3	 100%
3	AfA	2	 50% 50%
3	BfB	2	 100%
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	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	AbA	1005	X	-	-	-

2 Entry composition [i](#)

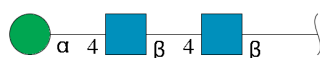
There are 9 unique types of molecules in this entry. The entry contains 13105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	C	N	O	S	0	3	0
			6564	4188	1111	1216	49			
1	BbB	799	Total	C	N	O	S	0	0	0
			6161	3921	1047	1147	46			

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

- Molecule 3 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
3	AfA	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	BfB	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.

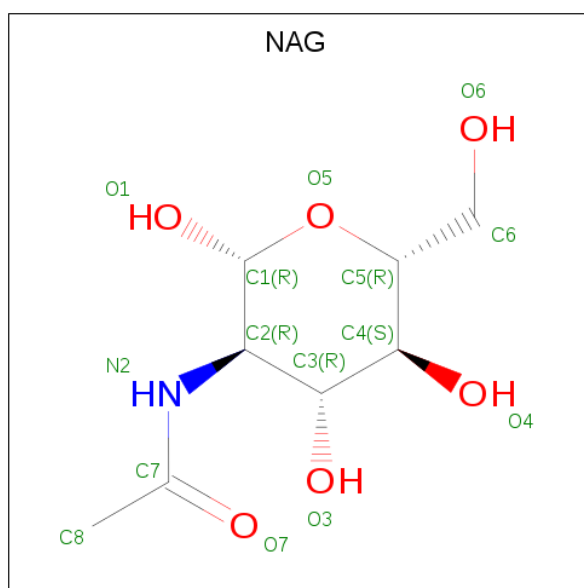


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	BcB	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



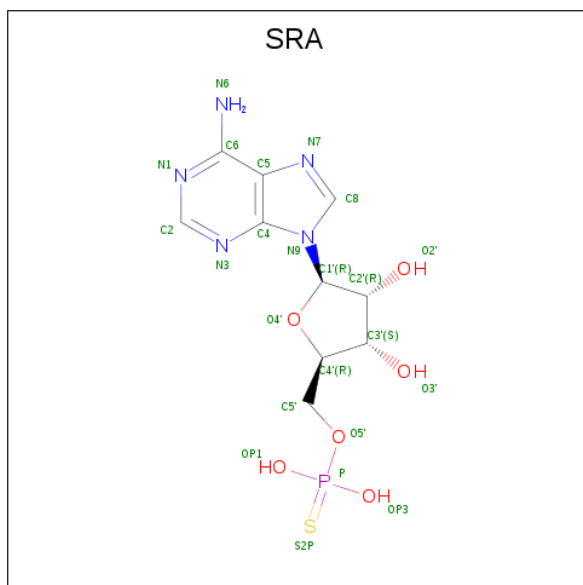
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AbA	1	Total	C	N	O	0	0
			14	8	1	5		
6	AbA	1	Total	C	N	O	0	0
			14	8	1	5		
6	AbA	1	Total	C	N	O	0	0
			14	8	1	5		
6	BbB	1	Total	C	N	O	0	0
			14	8	1	5		

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

- 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 author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	AbA	1	Total	C	N	O	P	S	0	0
			23	10	5	6	1	1		
7	BbB	1	Total	C	N	O	P	S	0	0
			23	10	5	6	1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AbA	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is water.

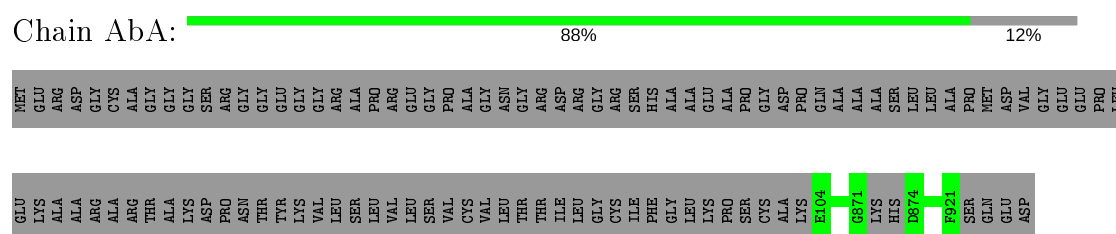
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AbA	86	Total	O	0	0
			86	86		
9	BbB	36	Total	O	0	0
			36	36		

3 Residue-property plots

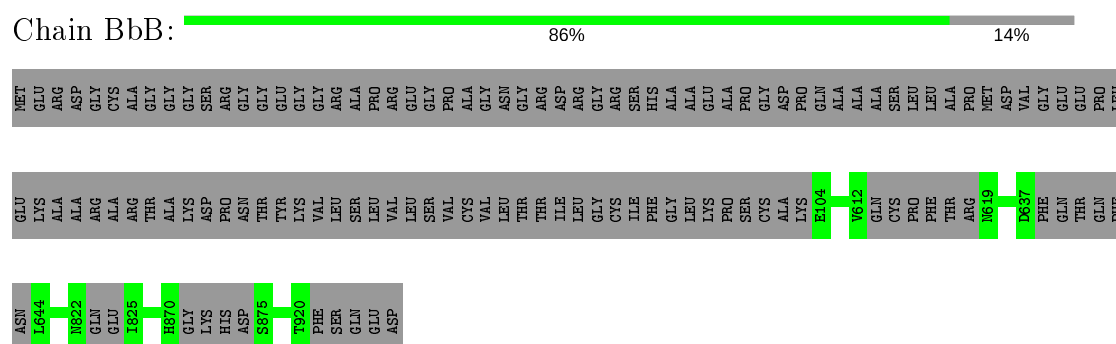
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 1



- 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



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



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

Chain BfB:  100%

MAG1
MAG2

- 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%

MAG1
MAG2
BfB3

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.01Å 160.14Å 209.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.65	Depositor
% Data completeness (in resolution range)	100.0 (47.57-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.207 , 0.239	Depositor
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.041	Xtriage
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
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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, EDO, SRA, 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	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

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

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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

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](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	AcA	1	1,2	14,14,15	0.77	1 (7%)	17,19,21	1.29	2 (11%)
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	1,4	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	1,2	-	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	1,4	-	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	Z	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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BfB	1	NAG	O7-C7-N2	-3.66	115.23	121.95
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	BfB	1	NAG	C8-C7-N2-C2
3	BfB	1	NAG	O7-C7-N2-C2
3	BfB	2	NAG	C8-C7-N2-C2
3	BfB	2	NAG	O7-C7-N2-C2
3	AfA	1	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.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	EDO	AbA	1007	-	3,3,3	0.06	0	2,2,2	0.16	0
6	NAG	AbA	1005	1	14,14,15	0.35	0	17,19,21	0.53	0
6	NAG	BbB	1003	1	14,14,15	0.63	0	17,19,21	1.79	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SRA	BbB	1005	-	22,25,25	5.11	10 (45%)	22,38,38	1.59	3 (13%)
6	NAG	BbB	1004	1	14,14,15	0.55	0	17,19,21	1.23	3 (17%)
7	SRA	AbA	1006	-	22,25,25	5.09	10 (45%)	22,38,38	1.65	3 (13%)
6	NAG	AbA	1004	1	14,14,15	0.49	0	17,19,21	1.21	3 (17%)
6	NAG	AbA	1003	1	14,14,15	0.45	0	17,19,21	1.28	1 (5%)

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

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

Mol	Chain	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	Z	Observed(°)	Ideal(°)
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

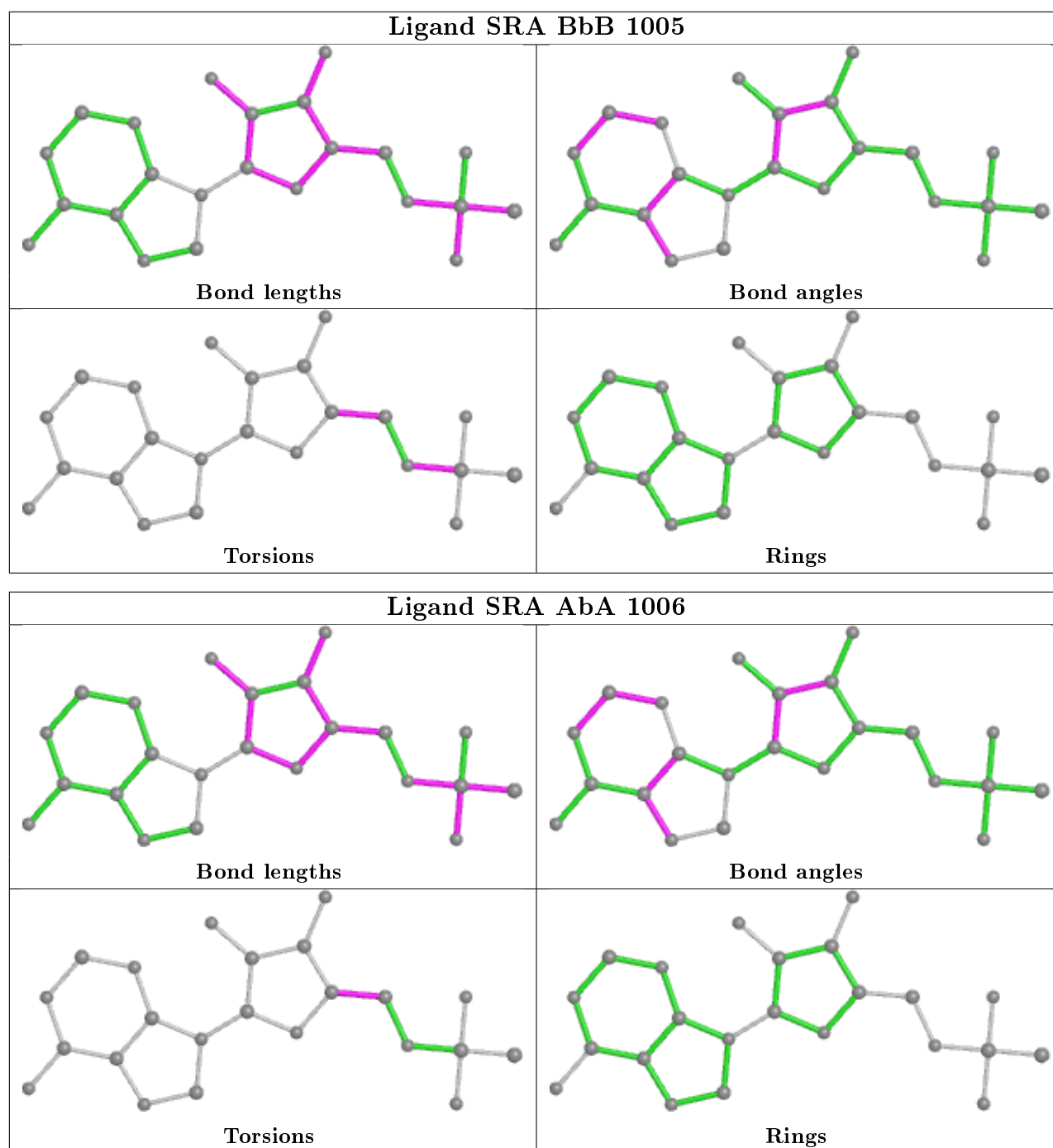
5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	BbB	1005	SRA	C3'-C4'-C5'-O5'
6	AbA	1003	NAG	C8-C7-N2-C2
6	AbA	1003	NAG	O7-C7-N2-C2
7	BbB	1005	SRA	O4'-C4'-C5'-O5'
7	AbA	1006	SRA	O4'-C4'-C5'-O5'

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 ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

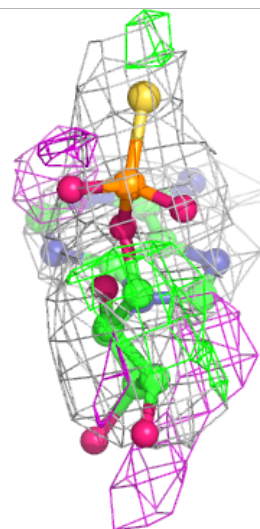
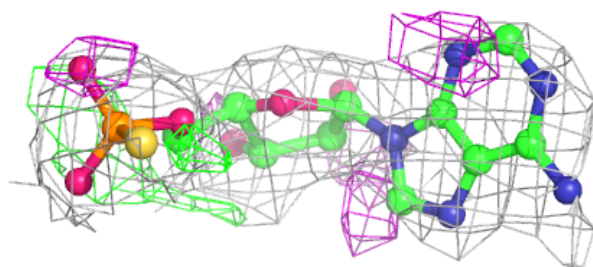
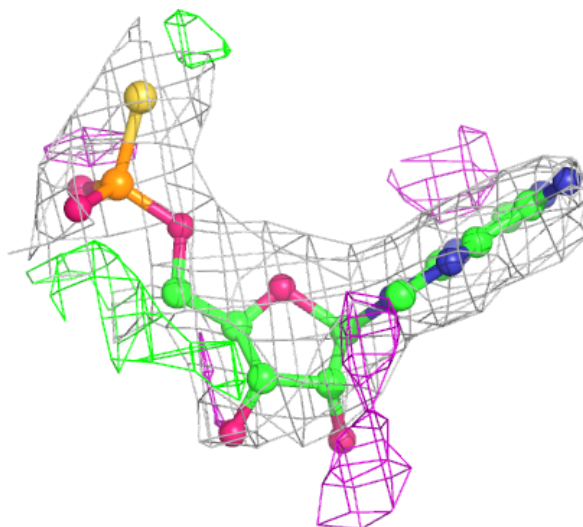
6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

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.

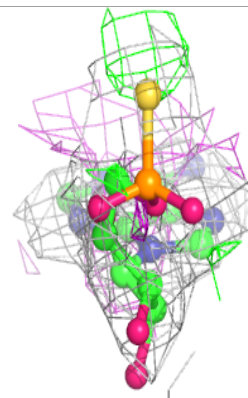
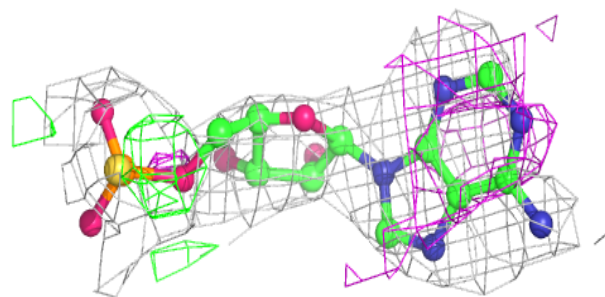
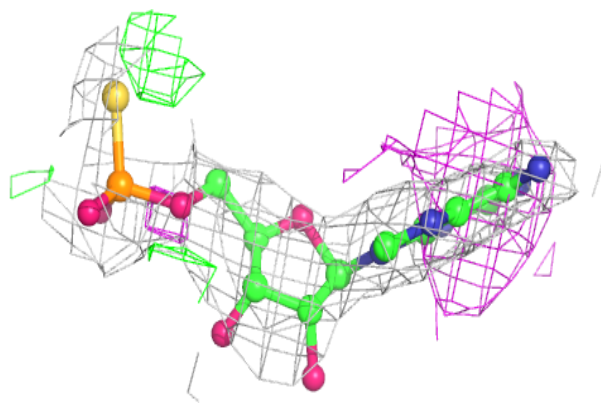
Electron density around SRA BbB 1005:

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



Electron density around SRA AbA 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](#)

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