



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:26 am BST

PDB ID : 3B5Y
Title : Crystal Structure of MsbA from Salmonella typhimurium with AMPPNP
Authors : Ward, A.; Reyes, C.L.; Yu, J.; Roth, C.B.; Chang, G.
Deposited on : 2007-10-26
Resolution : 4.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

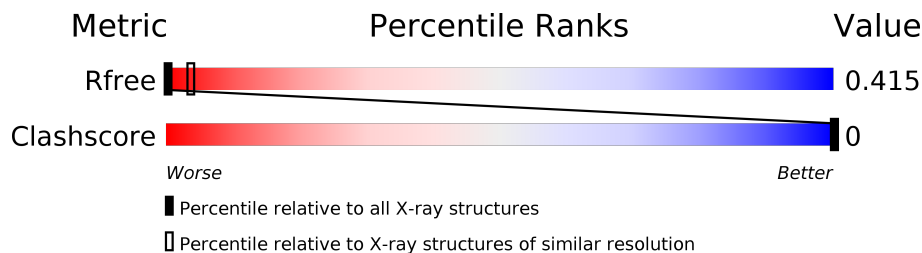
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

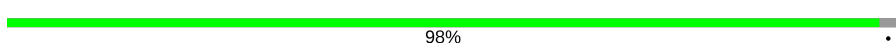
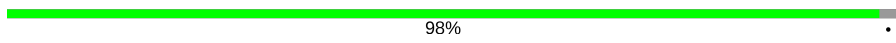
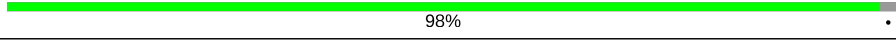
The reported resolution of this entry is 4.50 Å.

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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	582	 98%
1	B	582	 98%
1	C	582	 98%
1	D	582	 98%

2 Entry composition i

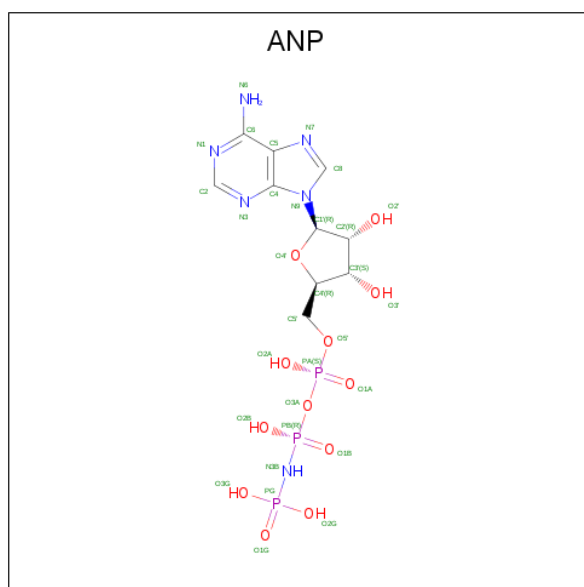
There are 2 unique types of molecules in this entry. The entry contains 2412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lipid A export ATP-binding/permease protein msbA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	572	Total	C	0	0	572
			572	572			
1	B	572	Total	C	0	0	572
			572	572			
1	C	572	Total	C	0	0	572
			572	572			
1	D	572	Total	C	0	0	572
			572	572			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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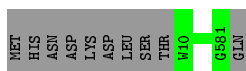
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	Total 31	10	6	12	3	0	0
2	D	1	Total 31	10	6	12	3	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

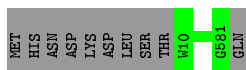
- Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain A:  98%



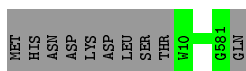
- Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain B:  98%



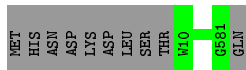
- Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain C:  98%



- Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain D:  98%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.93Å 121.24Å 173.12Å 90.00° 121.89° 90.00°	Depositor
Resolution (Å)	19.98 – 4.50 19.98 – 4.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (19.98-4.50) 95.0 (19.98-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 4.54Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.295 , 0.343 0.402 , 0.415	Depositor DCC
R_{free} test set	2606 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	184.2	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.65 , -8.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2412	wwPDB-VP
Average B, all atoms (Å ²)	219.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: ANP

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	572	0	0	0	0
1	B	572	0	0	0	0
1	C	572	0	0	0	0
1	D	572	0	0	0	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
All	All	2412	0	52	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 0.

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	ANP	A	5002	-	29,33,33	1.42	2 (6%)	31,52,52	2.10	7 (22%)
2	ANP	B	5001	-	29,33,33	2.11	9 (31%)	31,52,52	2.29	7 (22%)
2	ANP	C	5004	-	29,33,33	1.46	3 (10%)	31,52,52	2.12	7 (22%)
2	ANP	D	5003	-	29,33,33	1.43	2 (6%)	31,52,52	2.11	7 (22%)

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	ANP	A	5002	-	-	3/14/38/38	0/3/3/3
2	ANP	B	5001	-	-	3/14/38/38	0/3/3/3
2	ANP	C	5004	-	-	3/14/38/38	0/3/3/3
2	ANP	D	5003	-	-	3/14/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	PB-O1B	-4.86	1.38	1.46
2	B	5001	ANP	PB-O2B	-4.41	1.44	1.56
2	B	5001	ANP	PA-O1A	-4.40	1.35	1.50
2	C	5004	ANP	PB-O2B	-3.96	1.46	1.56
2	A	5002	ANP	PB-O2B	-3.91	1.46	1.56
2	D	5003	ANP	PB-O2B	-3.88	1.46	1.56
2	C	5004	ANP	PG-O2G	-3.61	1.47	1.56
2	D	5003	ANP	PG-O2G	-3.57	1.47	1.56
2	A	5002	ANP	PG-O2G	-3.56	1.47	1.56
2	B	5001	ANP	C3'-C4'	-3.48	1.44	1.53
2	B	5001	ANP	O4'-C1'	-3.10	1.36	1.41
2	B	5001	ANP	O3'-C3'	3.08	1.50	1.43
2	B	5001	ANP	PG-O2G	-2.71	1.49	1.56
2	B	5001	ANP	PB-N3B	2.39	1.69	1.63
2	C	5004	ANP	C2-N3	2.05	1.35	1.32
2	B	5001	ANP	PG-N3B	2.03	1.68	1.63

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	ANP	O4'-C1'-C2'	-7.14	96.50	106.93
2	C	5004	ANP	O4'-C1'-C2'	-6.67	97.18	106.93
2	A	5002	ANP	O4'-C1'-C2'	-6.63	97.24	106.93
2	D	5003	ANP	O4'-C1'-C2'	-6.63	97.24	106.93
2	B	5001	ANP	O2B-PB-O1B	4.92	120.24	109.92
2	C	5004	ANP	O1B-PB-N3B	-4.69	104.87	111.77
2	A	5002	ANP	O1B-PB-N3B	-4.65	104.92	111.77
2	D	5003	ANP	O1B-PB-N3B	-4.64	104.94	111.77
2	B	5001	ANP	C4-C5-N7	4.51	114.10	109.40
2	C	5004	ANP	O1G-PG-N3B	-4.36	105.34	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5002	ANP	O1G-PG-N3B	-4.34	105.37	111.77
2	D	5003	ANP	O1G-PG-N3B	-4.34	105.38	111.77
2	B	5001	ANP	O1B-PB-N3B	-4.02	105.85	111.77
2	C	5004	ANP	O2B-PB-O1B	3.73	117.74	109.92
2	D	5003	ANP	O2B-PB-O1B	3.73	117.74	109.92
2	A	5002	ANP	O2B-PB-O1B	3.70	117.67	109.92
2	B	5001	ANP	C1'-N9-C4	3.24	132.33	126.64
2	B	5001	ANP	O3G-PG-O1G	-2.93	106.10	113.45
2	D	5003	ANP	C4-C5-N7	2.60	112.11	109.40
2	D	5003	ANP	O3G-PG-O2G	2.57	114.47	107.64
2	C	5004	ANP	O3G-PG-O2G	2.56	114.46	107.64
2	A	5002	ANP	O3G-PG-O2G	2.54	114.41	107.64
2	C	5004	ANP	C4-C5-N7	2.47	111.97	109.40
2	A	5002	ANP	C4-C5-N7	2.39	111.89	109.40
2	C	5004	ANP	O2B-PB-O3A	2.35	112.49	104.64
2	A	5002	ANP	O2B-PB-O3A	2.34	112.44	104.64
2	D	5003	ANP	O2B-PB-O3A	2.33	112.40	104.64
2	B	5001	ANP	C3'-C2'-C1'	-2.27	97.56	100.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

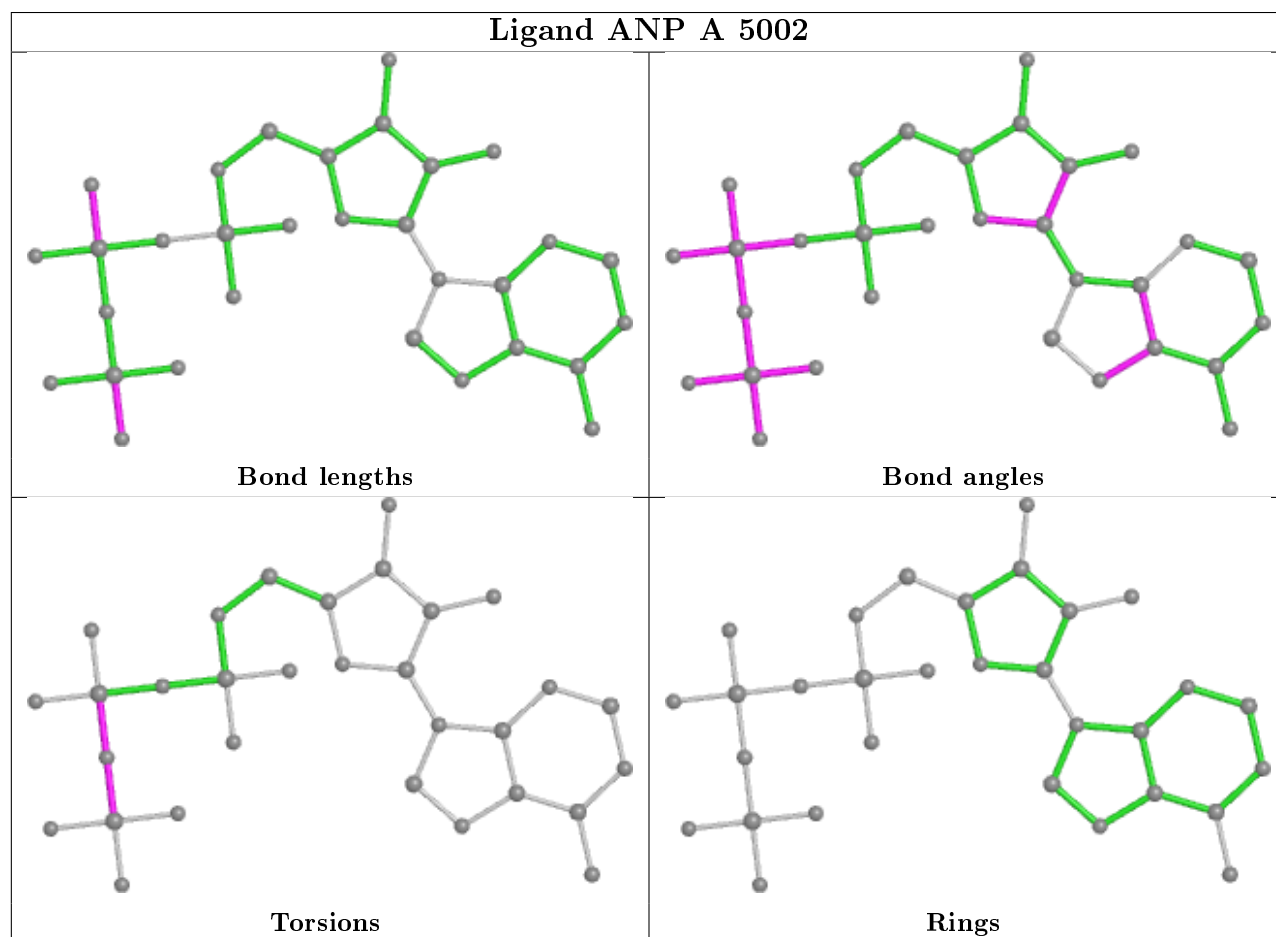
Mol	Chain	Res	Type	Atoms
2	A	5002	ANP	PB-N3B-PG-O1G
2	A	5002	ANP	PG-N3B-PB-O1B
2	A	5002	ANP	PG-N3B-PB-O3A
2	B	5001	ANP	PB-N3B-PG-O1G
2	B	5001	ANP	PG-N3B-PB-O1B
2	B	5001	ANP	PG-N3B-PB-O3A
2	C	5004	ANP	PB-N3B-PG-O1G
2	C	5004	ANP	PG-N3B-PB-O1B
2	C	5004	ANP	PG-N3B-PB-O3A
2	D	5003	ANP	PB-N3B-PG-O1G
2	D	5003	ANP	PG-N3B-PB-O1B
2	D	5003	ANP	PG-N3B-PB-O3A

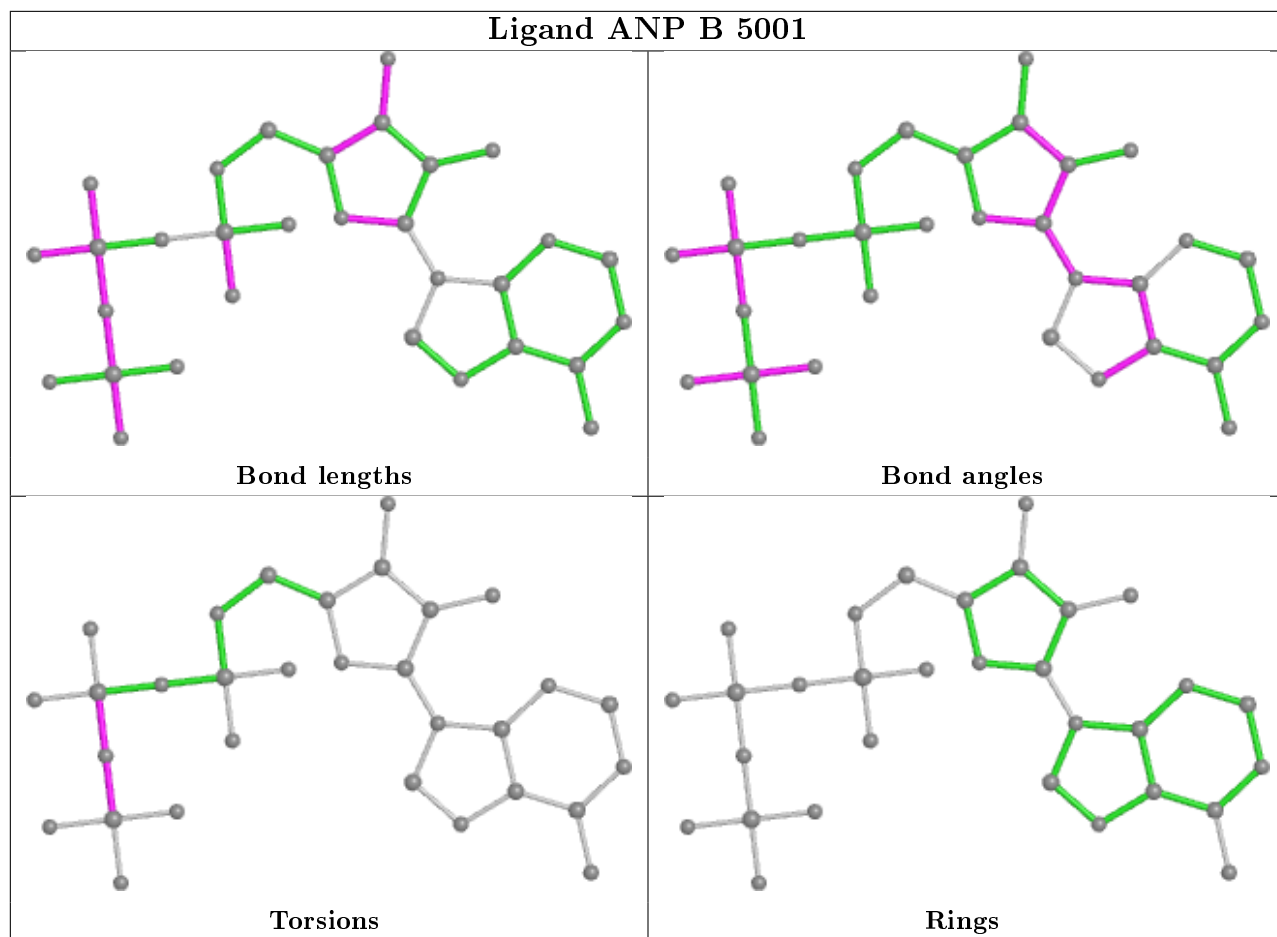
There are no ring outliers.

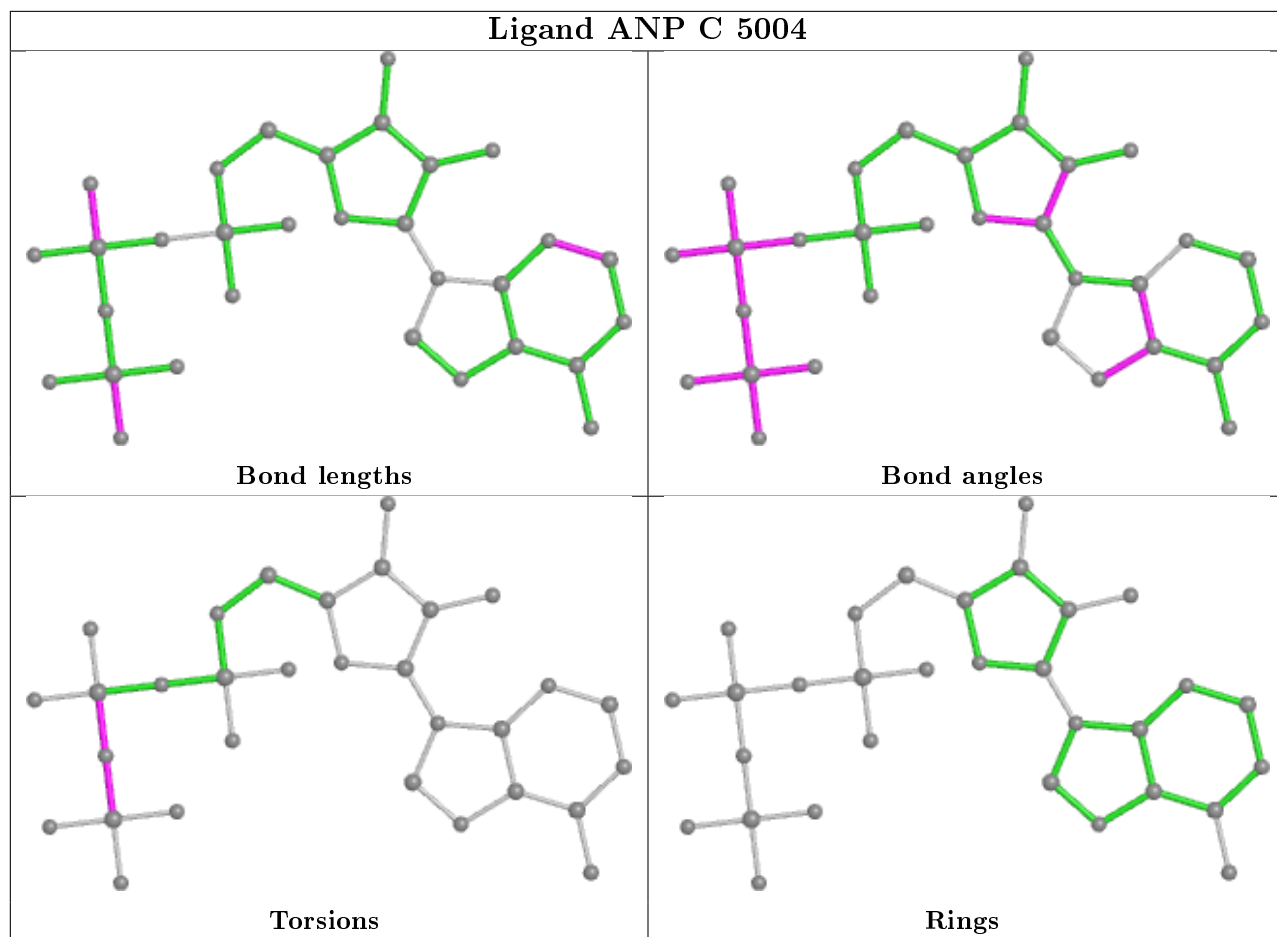
No monomer is involved in short contacts.

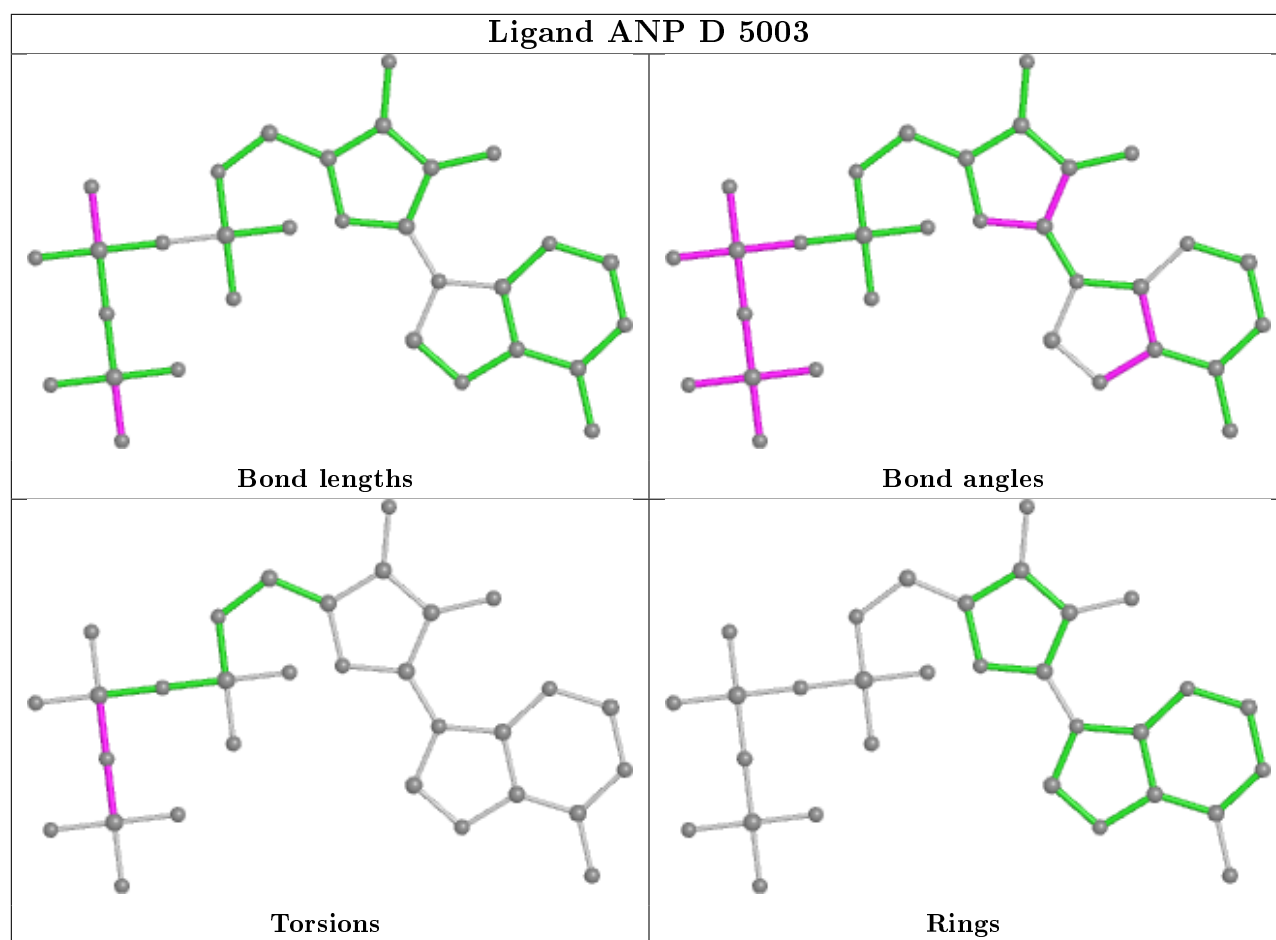
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

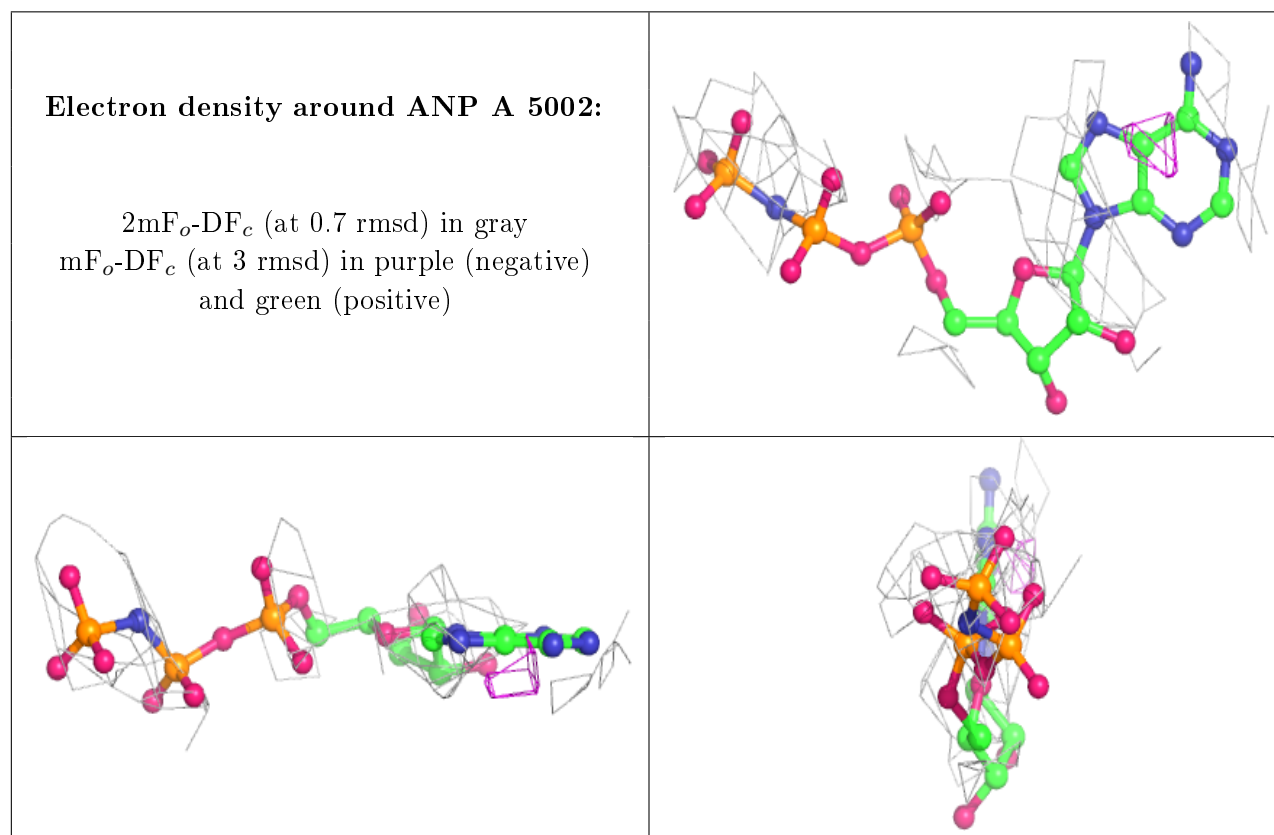
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

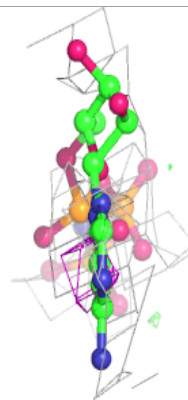
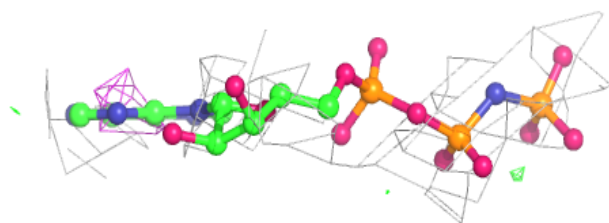
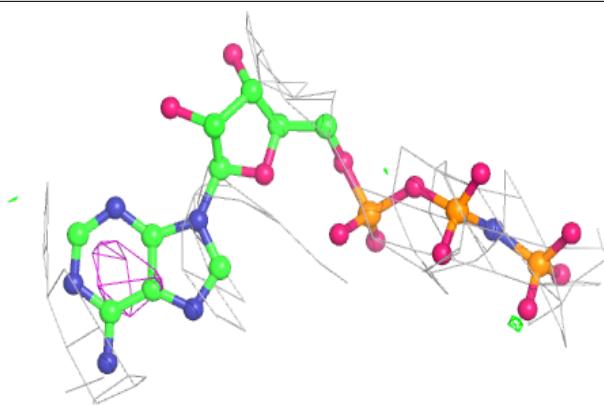
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

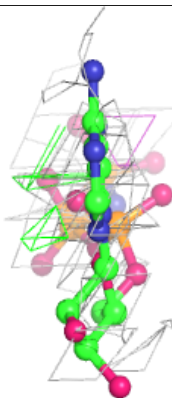
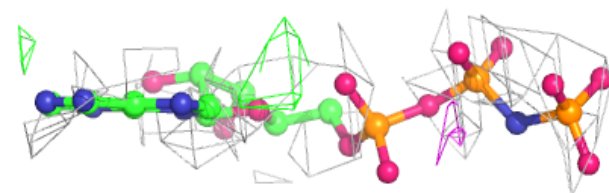
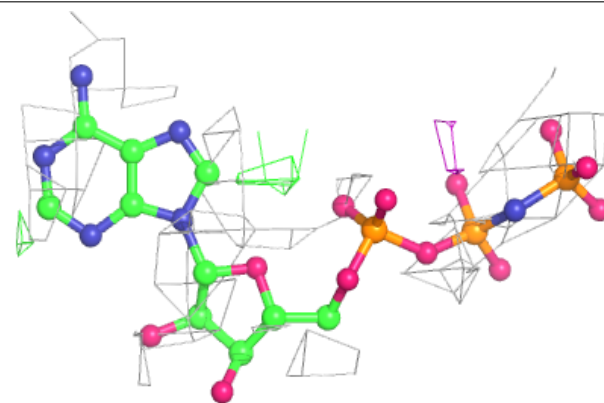


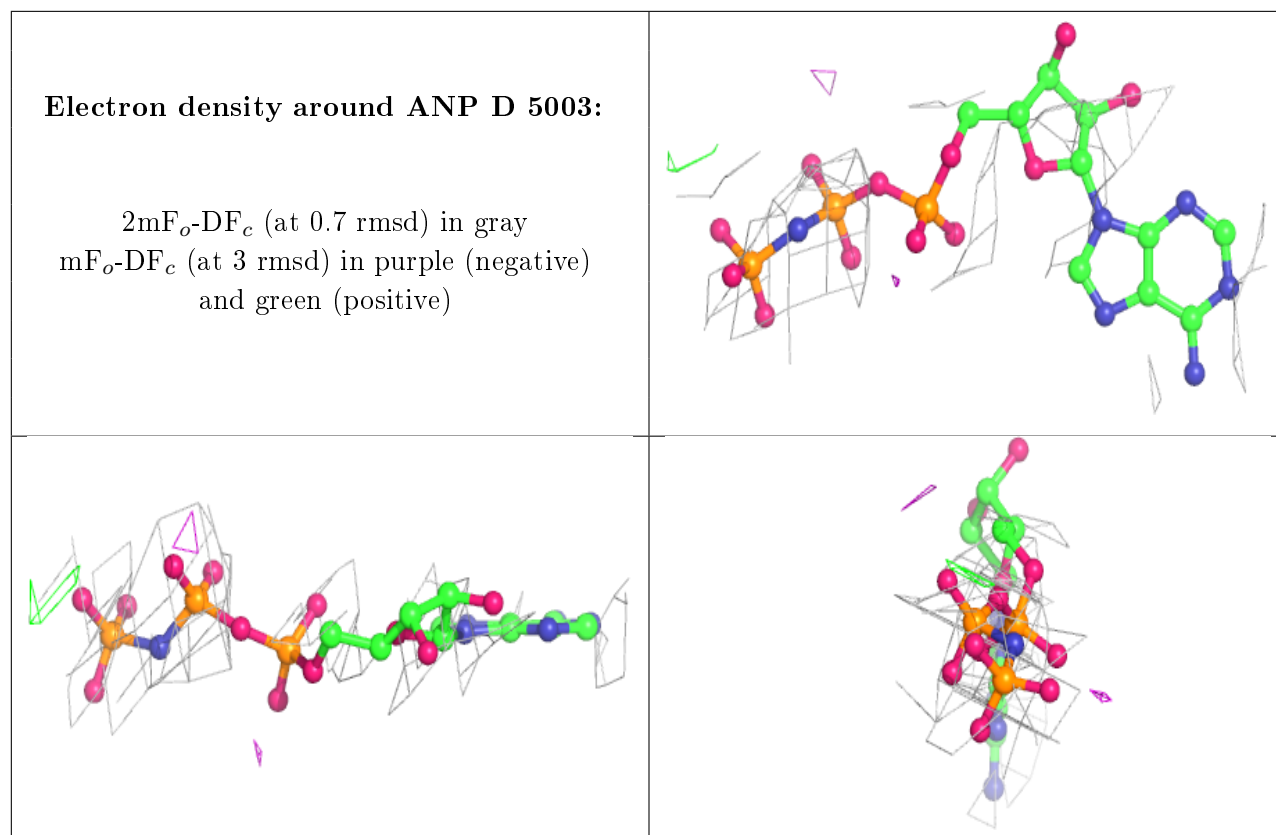
Electron density around ANP B 5001:

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

**Electron density around ANP C 5004:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.