



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:36 AM UTC

PDB ID : 3B5Y / pdb_00003b5y
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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

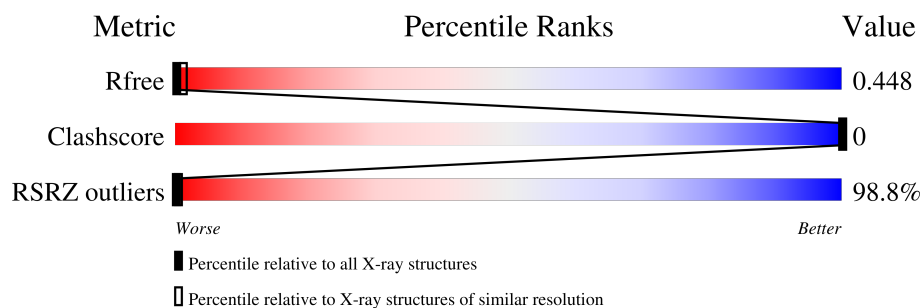
1 Overall quality at a glance

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}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
RSRZ outliers	180081	1122 (5.10-3.90)

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 $\leq 5\%$. 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	A	582	97% 98% .
1	B	582	97% 98% .
1	C	582	97% 98% .
1	D	582	97% 98% .

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
2	ANP	A	5002	-	-	-	X
2	ANP	B	5001	-	-	-	X
2	ANP	D	5003	-	-	-	X

2 Entry composition [i](#)

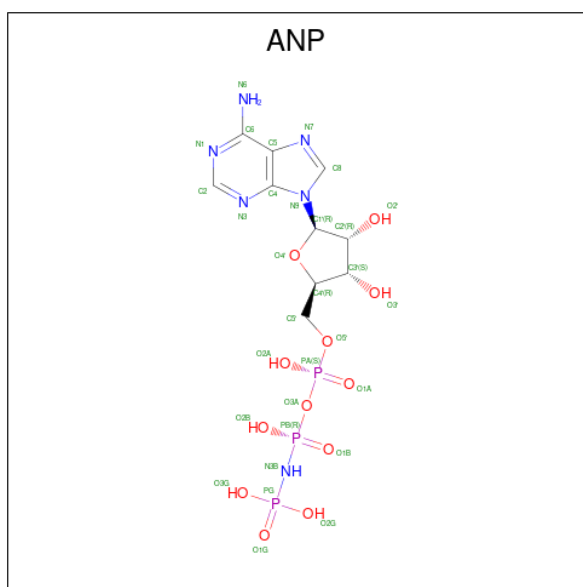
There are 2 unique types of molecules in this entry. The entry contains 2412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 572 572	0	0	572
1	B	572	Total C 572 572	0	0	572
1	C	572	Total C 572 572	0	0	572
1	D	572	Total C 572 572	0	0	572

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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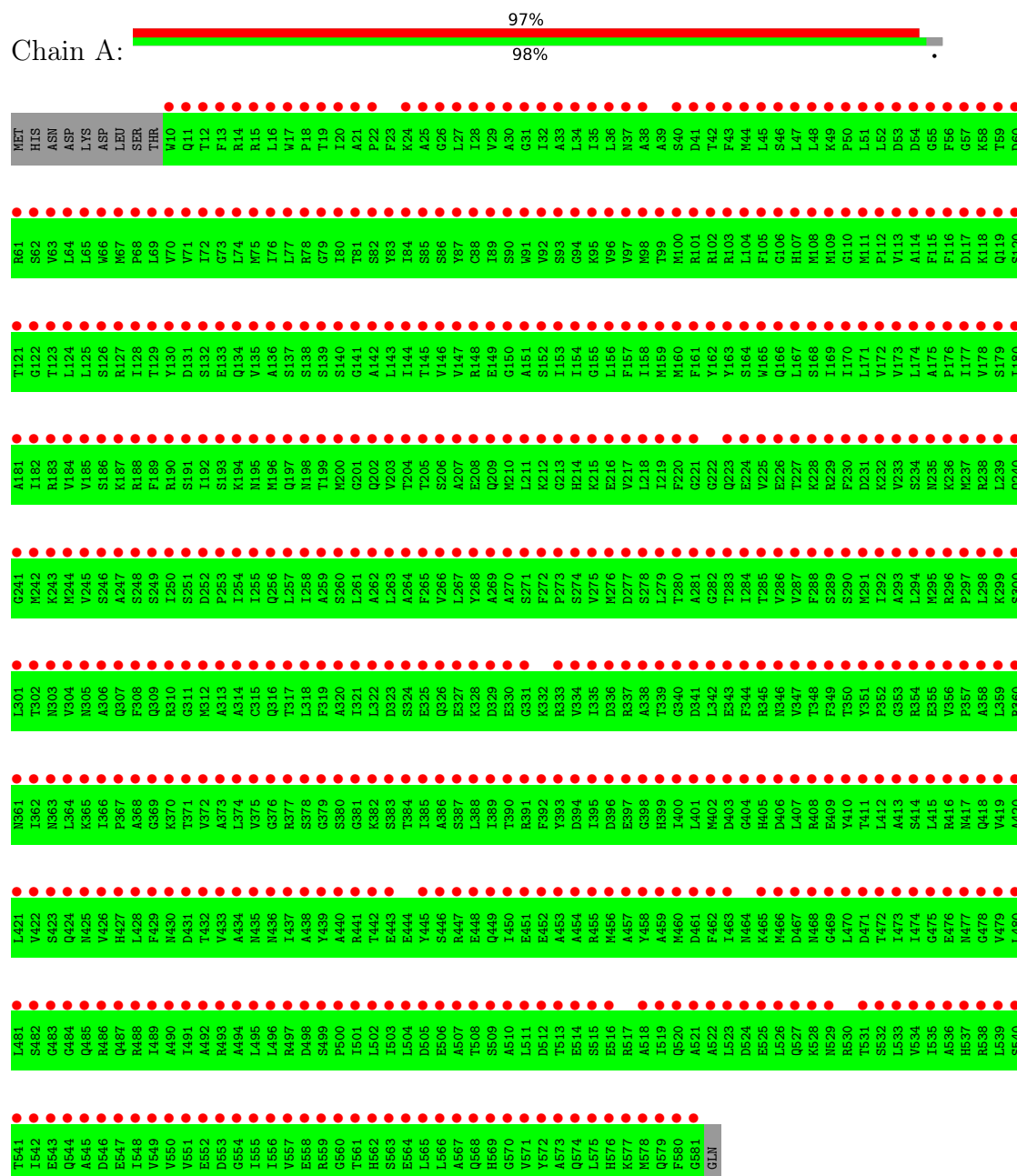
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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 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: Lipid A export ATP-binding/permease protein msbA



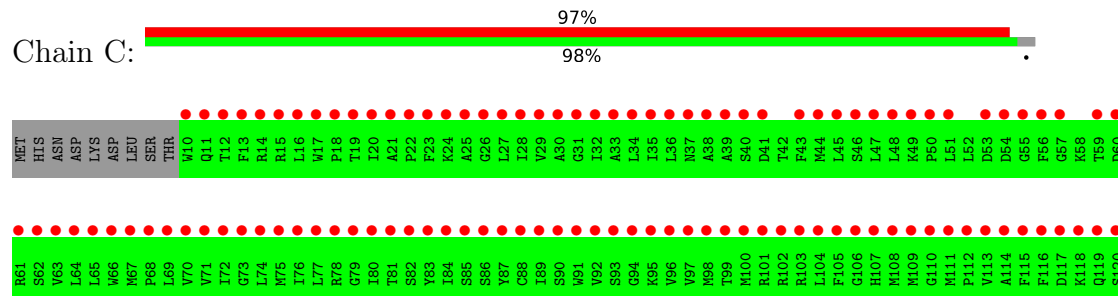
● Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain B:



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

Chain C:



T541	I542	L481	L482	V421	L421	N361	L301
T542	I543	L483	L484	V422	L422	I362	T302
E543	E544	G483	G484	S423	S423	R363	R303
Q544	A545	G485	G486	Q424	Q424	L364	N304
D546	D547	R486	R487	V426	V426	K365	V305
E547	E548	Q487	Q488	H427	H427	I366	A306
I549	I550	R488	R489	L428	L428	P367	Q307
V549	V550	I489	I490	F429	F429	A368	F308
V550	V551	A490	A491	M430	M430	G369	Q309
E552	E553	A492	A493	D431	D431	K370	R310
D553	D554	R493	R494	T432	T432	T371	G311
G554	G555	R493	R494	V433	V433	V372	M312
I555	I556	A494	A495	A434	A434	A373	A313
V557	V558	L495	L496	M435	M435	L374	A314
E558	E559	L497	L498	M436	M436	V375	C315
R559	R560	D498	D499	I437	I437	G376	Q316
G560	G561	P500	P501	R441	R441	R377	T317
T561	T562	I501	I502	T442	T442	S380	F319
S563	S564	L503	L504	E443	E443	G381	A320
E564	E565	L504	L505	E444	E444	K382	I321
L565	L566	D505	D506	Y445	Y445	L383	L322
L566	L567	E506	E507	S446	S446	T384	D323
A567	A568	A507	A508	R447	R447	I385	S324
Q568	Q569	T508	T509	E448	E448	A386	E325
H569	H570	S509	S510	Q449	Q449	S387	Q326
G570	G571	A510	A511	I450	I450	L388	E327
V571	V572	L511	L512	E451	E451	L389	K328
Y572	Y573	D512	D513	E452	E452	I390	D329
A573	A574	T513	T514	A453	A453	E391	E330
Q574	Q575	E514	E515	A454	A454	F392	G331
L575	L576	S515	S516	R455	R455	Y393	K332
H576	H577	E516	E517	M456	M456	D394	R333
Q577	Q578	R517	R518	A457	A457	I395	V334
M578	M579	A518	A519	Y458	Y458	D396	I335
Q579	Q580	I519	I520	A459	A459	E397	R337
F580	F581	T519	T520	M460	M460	G398	A338
GLN		Q520	Q521	D461	D461	H399	A338
		A521	A522	F462	F462	I400	T339
		E522	E523	I463	I463	L401	G340
		L523	L524	M464	M464	L401	D341
		D524	D525	K465	K465	M402	L342
		E525	E526	M466	M466	D403	E343
		Q527	Q528	D467	D467	G404	F344
		K528	K529	M468	M468	H405	R345
		N529	N530	G469	G469	D406	R346
		R530	R531	L470	L470	L407	N347
		T531	T532	D471	D471	R408	T348
		S532	S533	I472	I472	F349	T348
		L533	L534	T473	T473	E409	F349
		V534	V535	I474	I474	Y410	T350
		I535	I536	G475	G475	L411	Y351
		A536	A537	E476	E476	L412	P352
		H537	H538	M477	M477	A413	G353
		R538	R539	G478	G478	S414	R354
		L539	L540	V479	V479	L415	E355
		S540	S541	L480	L480	R416	V356
						M417	P357
						Q418	A358
						V419	L359
						A420	R360

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) 93.8 (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)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.295 , 0.343 0.447 , 0.448	Depositor DCC
R_{free} test set	2606 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	184.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	170.07 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	2412	wwPDB-VP
Average B, all atoms (Å ²)	219.0	wwPDB-VP

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

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 [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	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 oligosaccharides 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	C	5004	-	33,33,33	1.53	5 (15%)	45,52,52	1.84	10 (22%)
2	ANP	D	5003	-	33,33,33	1.53	5 (15%)	45,52,52	1.83	10 (22%)
2	ANP	A	5002	-	33,33,33	1.52	5 (15%)	45,52,52	1.83	10 (22%)
2	ANP	B	5001	-	33,33,33	2.67	15 (45%)	45,52,52	2.10	10 (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	C	5004	-	-	3/18/38/38	0/3/3/3
2	ANP	D	5003	-	-	3/18/38/38	0/3/3/3
2	ANP	A	5002	-	-	3/18/38/38	0/3/3/3
2	ANP	B	5001	-	-	3/18/38/38	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	PA-O3A	7.55	1.67	1.59
2	B	5001	ANP	PB-O1B	-5.13	1.38	1.46
2	B	5001	ANP	PB-O2B	-4.49	1.44	1.56
2	B	5001	ANP	PA-O1A	-4.48	1.35	1.50
2	C	5004	ANP	PB-O2B	-4.04	1.46	1.56

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	ANP	C4-N9-C8	-4.91	100.58	105.74
2	B	5001	ANP	O2B-PB-O1B	4.83	120.24	109.87
2	B	5001	ANP	O4'-C1'-C2'	-4.73	96.50	106.62
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

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

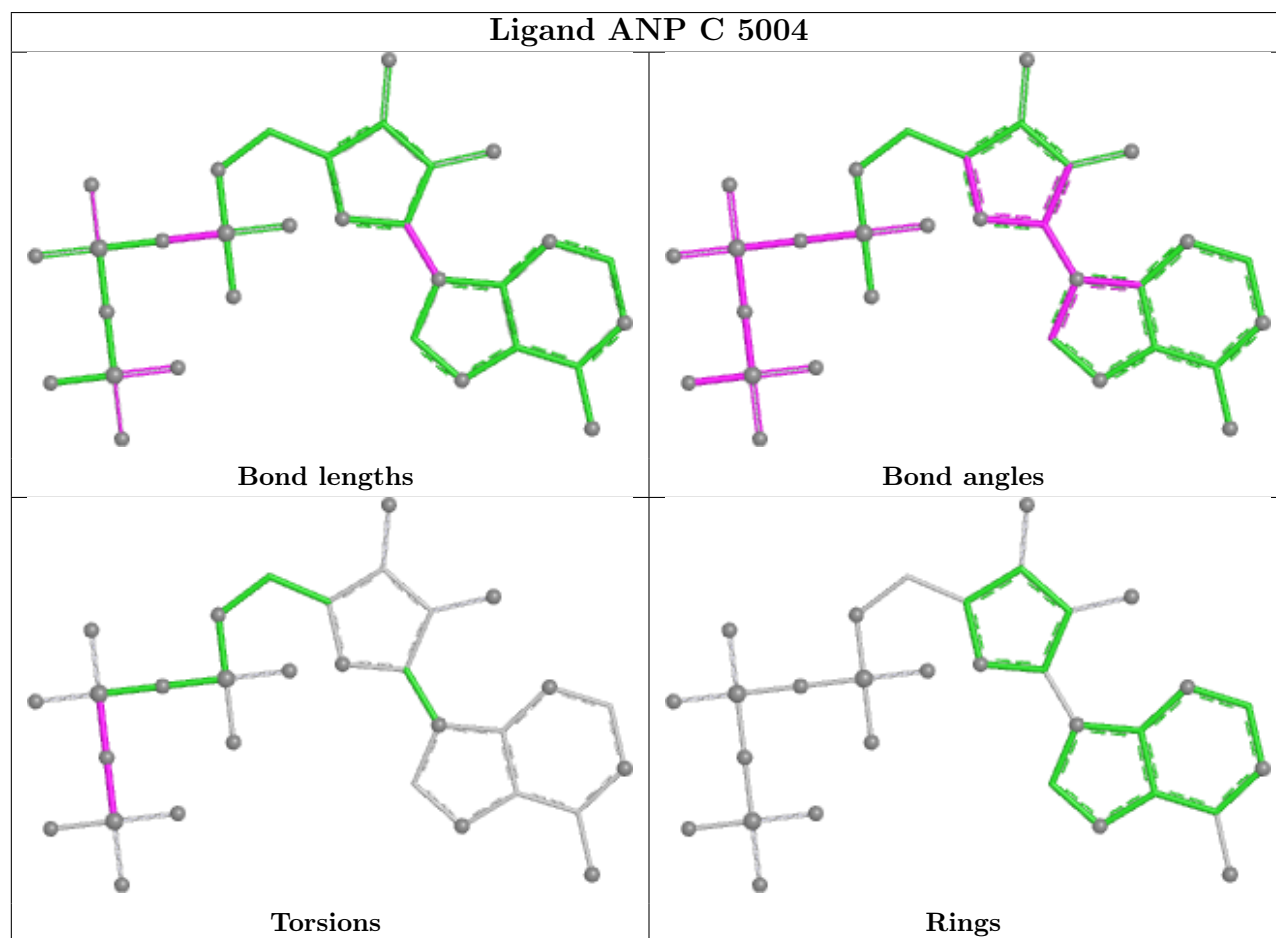
Mol	Chain	Res	Type	Atoms
2	A	5002	ANP	PB-N3B-PG-O1G
2	A	5002	ANP	PG-N3B-PB-O1B
2	A	5002	ANP	PG-N3B-PB-O3A
2	B	5001	ANP	PB-N3B-PG-O1G
2	B	5001	ANP	PG-N3B-PB-O1B

There are no ring outliers.

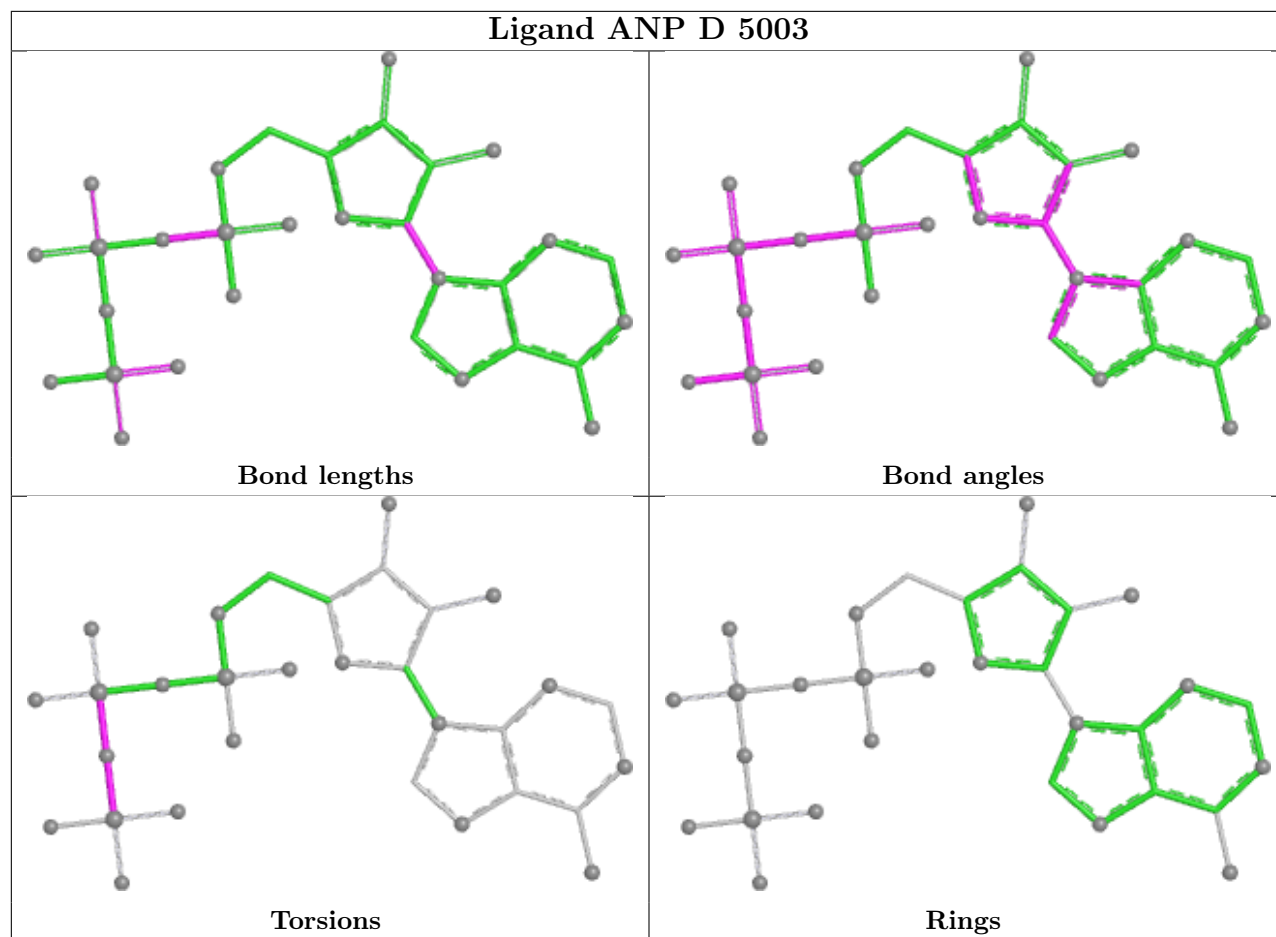
No monomer is involved in short contacts.

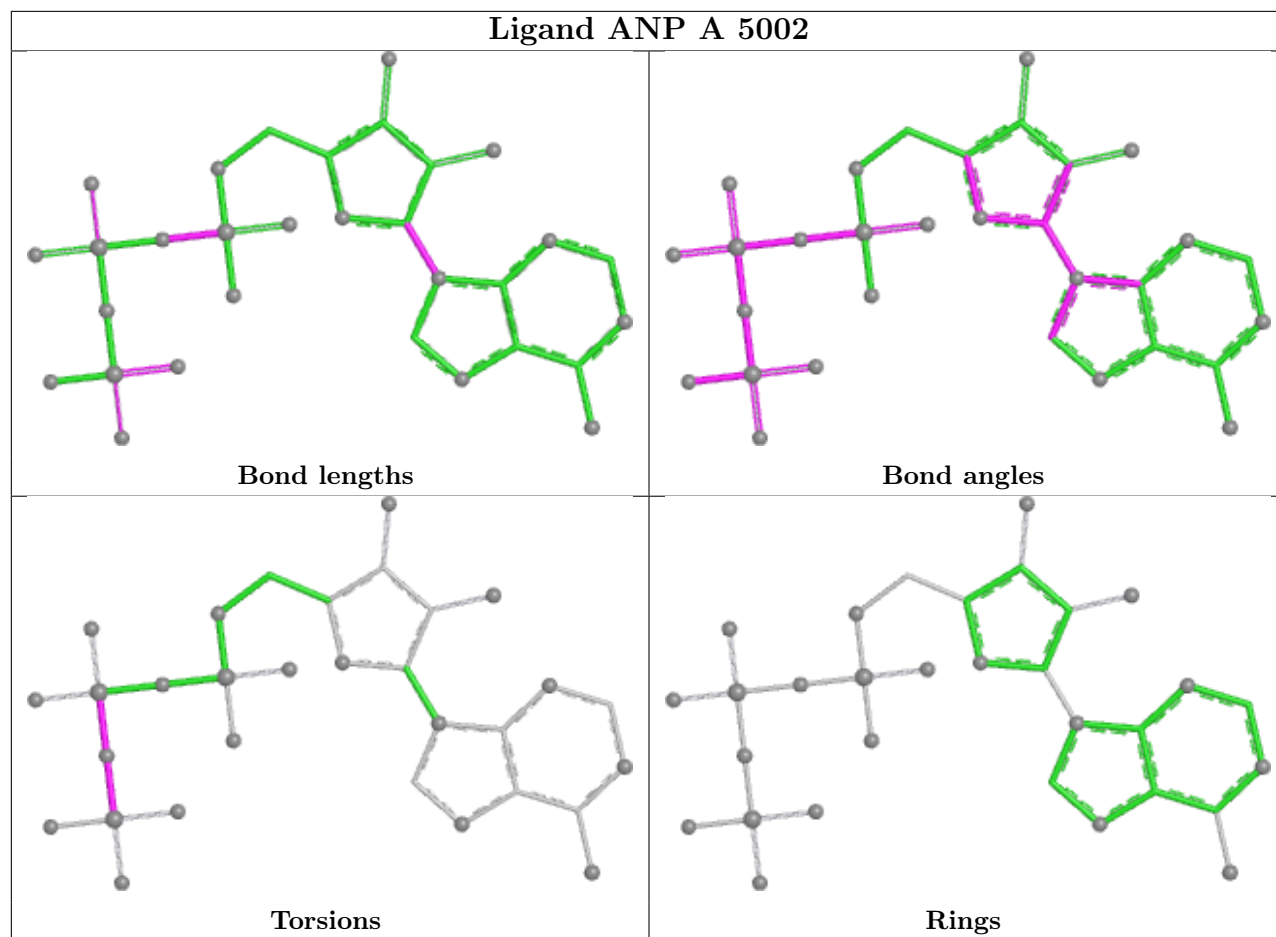
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

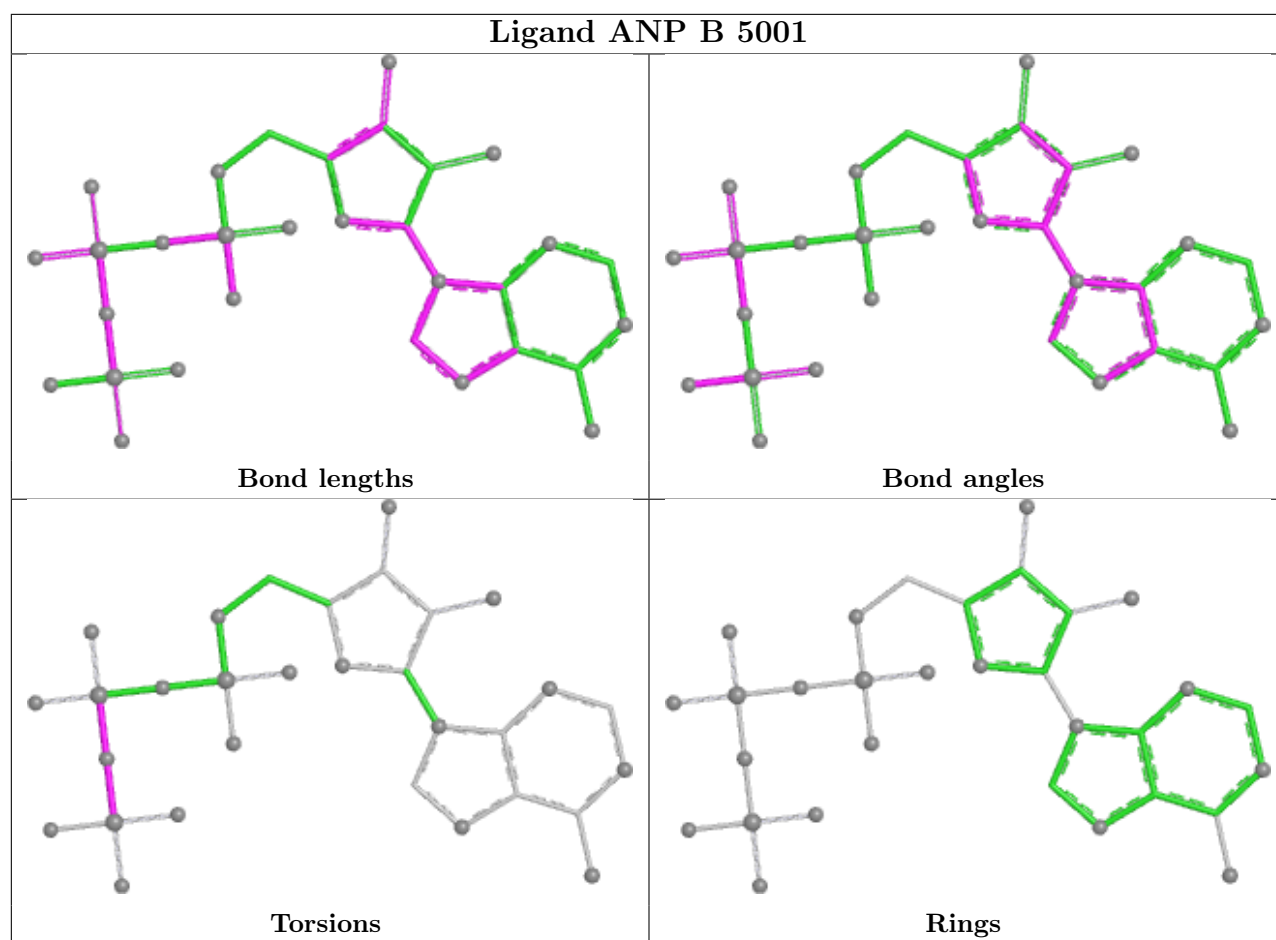
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



Ligand ANP D 5003







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, 95th 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 ²)	Q<0.9
1	A	572/582 (98%)	10.66	564 (98%) 0 0	142, 225, 277, 312	0
1	B	572/582 (98%)	10.59	566 (98%) 0 0	112, 212, 274, 321	0
1	C	572/582 (98%)	11.16	564 (98%) 0 0	130, 218, 271, 309	0
1	D	572/582 (98%)	10.16	566 (98%) 0 0	132, 220, 271, 314	0
All	All	2288/2328 (98%)	10.64	2260 (98%) 0 0	112, 219, 274, 321	0

The worst 5 of 2260 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	TRP	87.7
1	C	134	GLN	65.9
1	D	246	SER	59.1
1	A	417	ASN	56.0
1	A	414	SER	51.9

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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

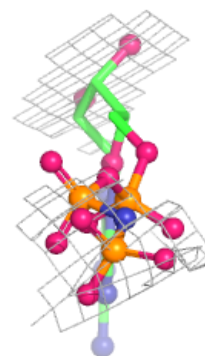
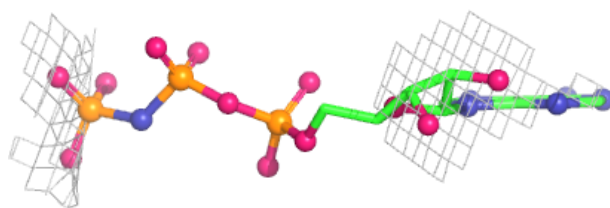
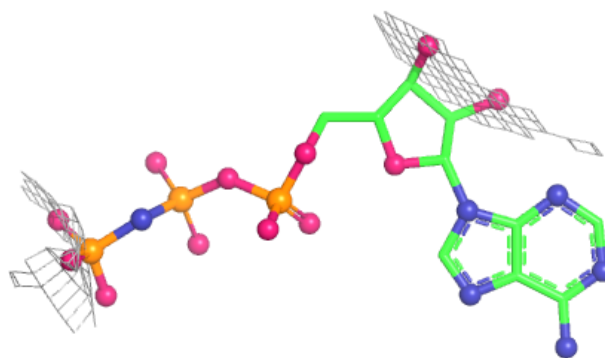
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	A	5002	31/31	0.36	0.91	219,219,219,219	0
2	ANP	B	5001	31/31	0.71	0.83	219,219,219,219	0
2	ANP	D	5003	31/31	0.78	0.72	219,219,219,219	0
2	ANP	C	5004	31/31	0.88	0.69	219,219,219,219	0

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

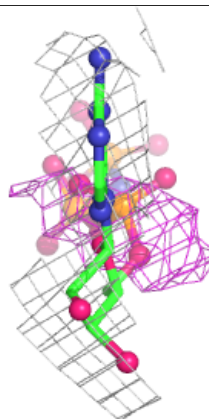
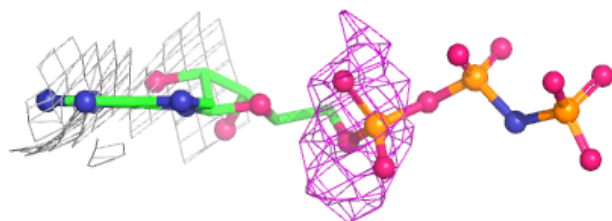
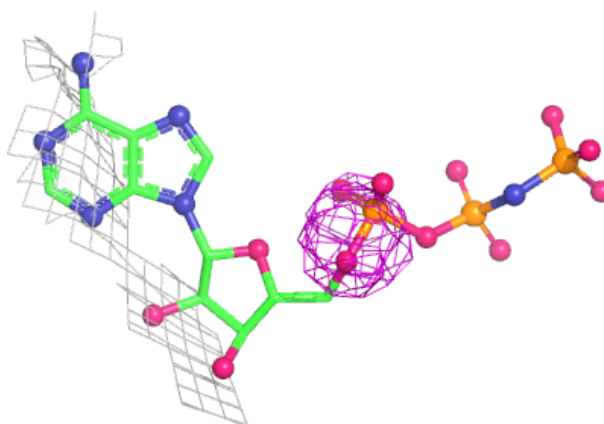
Electron density around ANP A 5002:

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

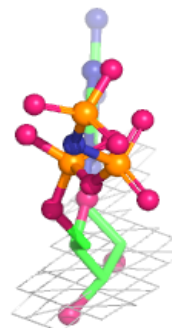
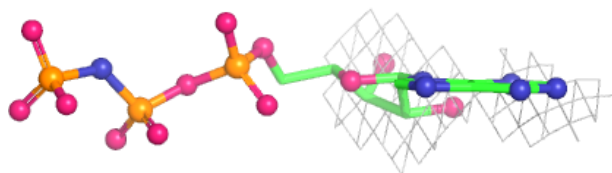
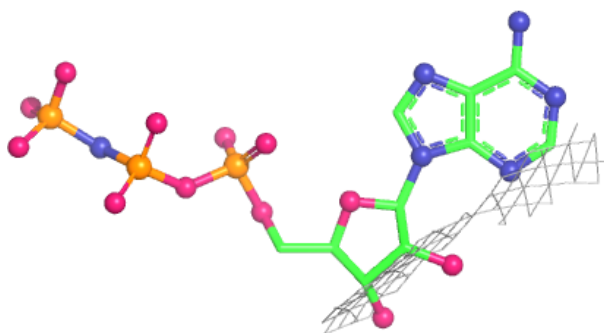


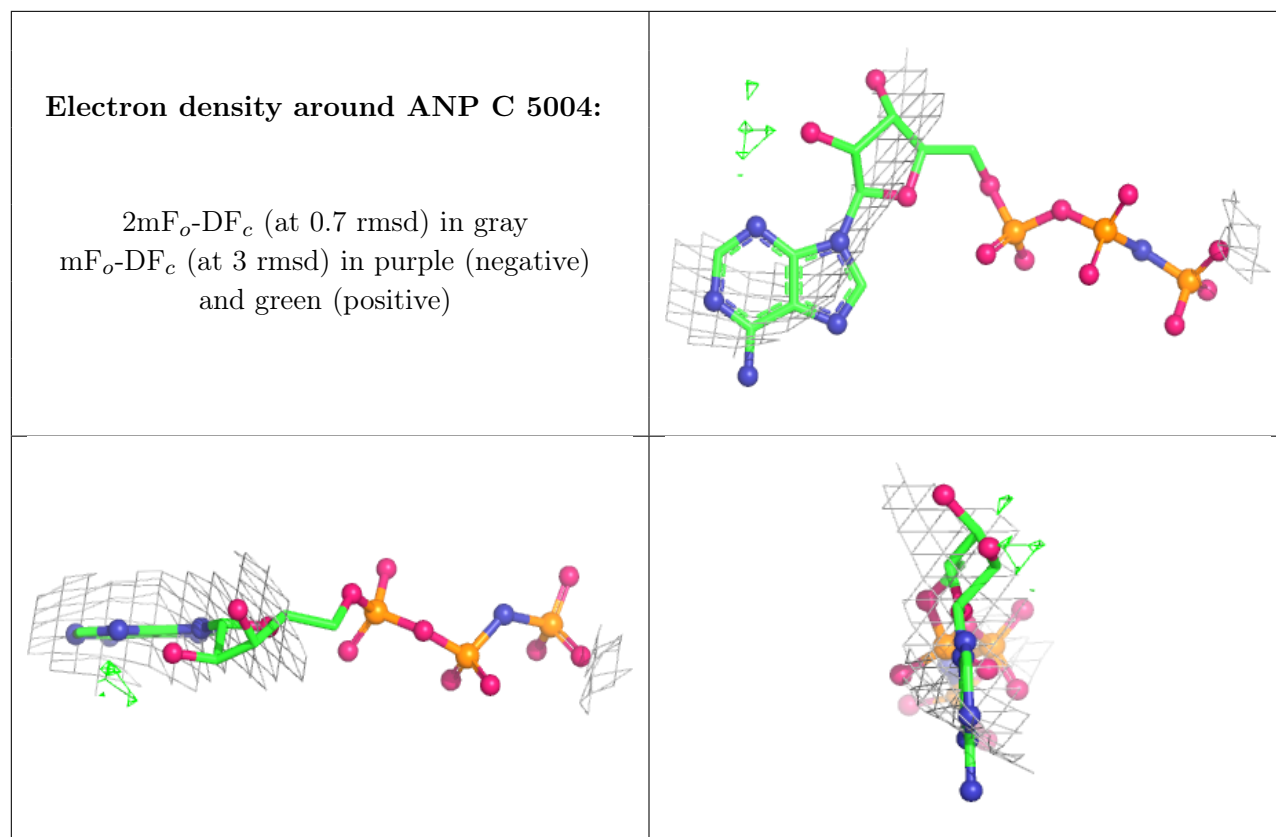
Electron density around ANP B 5001:

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

**Electron density around ANP D 5003:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.