



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 09:51 pm BST

PDB ID : 2D3B
Title : Crystal Structure of the Maize Glutamine Synthetase complexed with AMPPNP and Methionine sulfoximine
Authors : Unno, H.; Uchida, T.; Sugawara, H.; Kurisu, G.; Sugiyama, T.; Yamaya, T.; Sakakibara, H.; Hase, T.; Kusunoki, M.
Deposited on : 2005-09-26
Resolution : 3.50 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 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

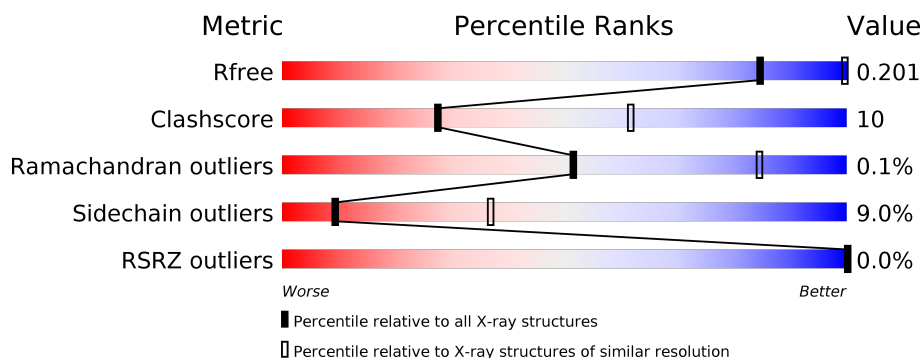
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 $\leq 5\%$. 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	356	<div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	B	356	<div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	C	356	<div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
1	D	356	<div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
1	E	356	<div> <div>76%</div> <div>21%</div> <div>• •</div> </div>
1	F	356	<div> <div>76%</div> <div>20%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	356	 74% 22% ..
1	H	356	 79% 17% ..
1	I	356	 79% 17% ..
1	J	356	 80% 16% ..

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	ANP	A	6001	X	-	-	-
3	ANP	B	6002	X	-	-	-
3	ANP	C	6003	X	-	-	-
3	ANP	D	6004	X	-	-	-
3	ANP	E	6005	X	-	-	-
3	ANP	F	6006	X	-	-	-
3	ANP	G	6007	X	-	-	-
3	ANP	H	6008	X	-	-	-
3	ANP	I	6009	X	-	-	-
3	ANP	J	6010	X	-	-	-
4	MSL	C	5002	-	-	X	-
4	MSL	C	5005	-	-	X	-
4	MSL	C	5007	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28277 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 glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	B	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	C	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	D	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	E	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	F	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	G	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	H	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	I	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	J	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

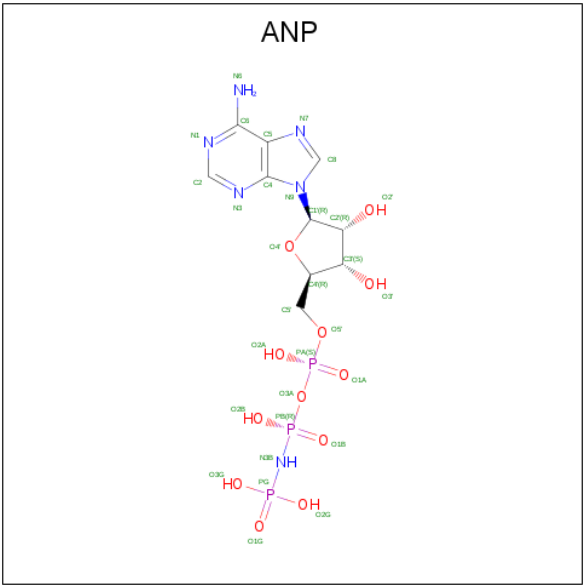
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Mn	0	0
			3	3		
2	J	3	Total	Mn	0	0
			3	3		
2	D	3	Total	Mn	0	0
			3	3		
2	E	3	Total	Mn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		
2	I	3	Total	Mn	0	0
			3	3		
2	C	3	Total	Mn	0	0
			3	3		
2	A	3	Total	Mn	0	0
			3	3		
2	F	3	Total	Mn	0	0
			3	3		

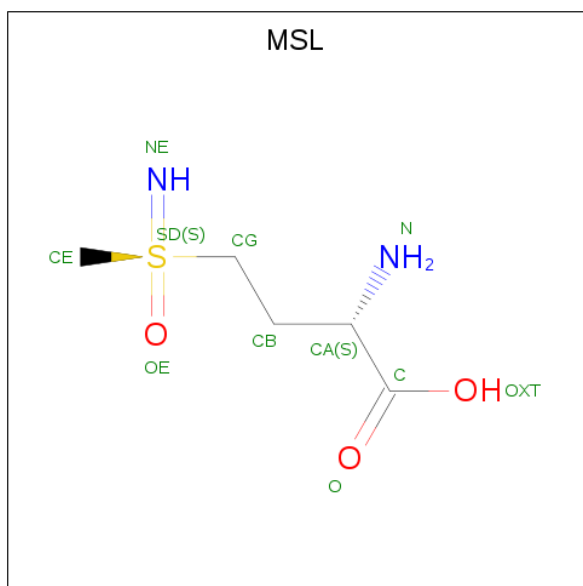
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is (2S)-2-AMINO-4-(METHYLSULFONIMIDOYL)BUTANOIC ACID (three-letter code: MSL) (formula: C₅H₁₂N₂O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			11	5	2	3	1		

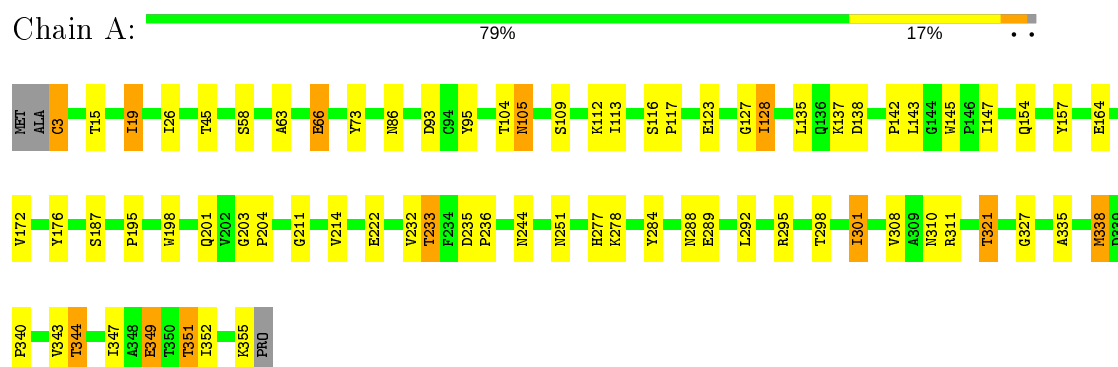
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	36	Total	O	0	0
			36	36		
5	C	40	Total	O	0	0
			40	40		
5	D	42	Total	O	0	0
			42	42		
5	E	41	Total	O	0	0
			41	41		
5	F	39	Total	O	0	0
			39	39		
5	G	40	Total	O	0	0
			40	40		
5	H	32	Total	O	0	0
			32	32		
5	I	37	Total	O	0	0
			37	37		
5	J	38	Total	O	0	0
			38	38		

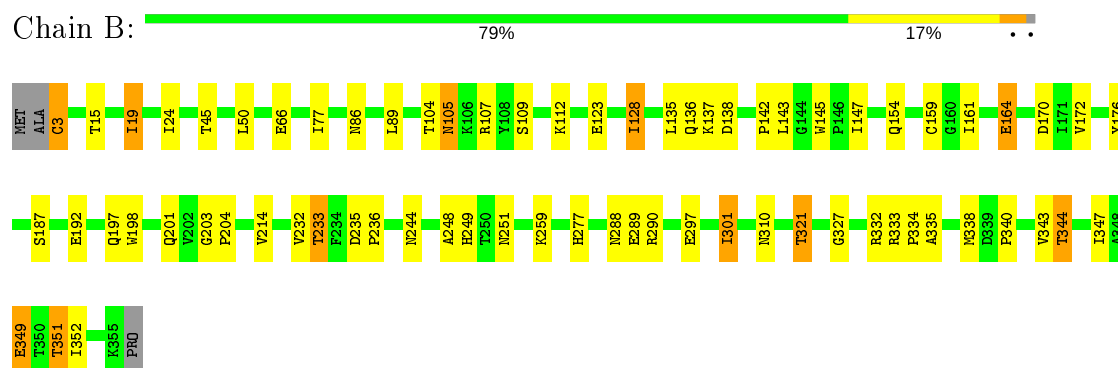
3 Residue-property plots

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 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.

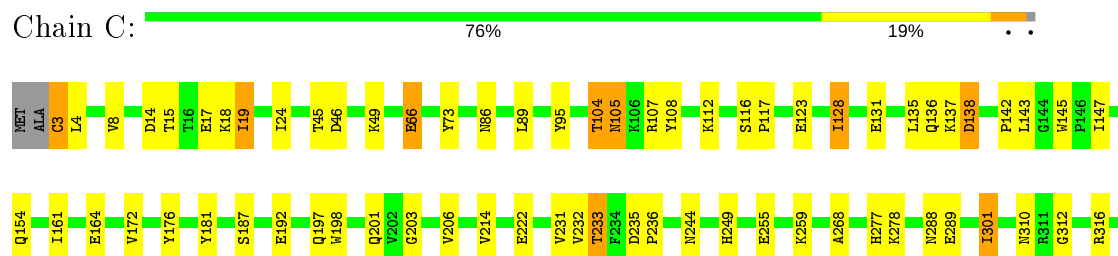
- Molecule 1: glutamine synthetase



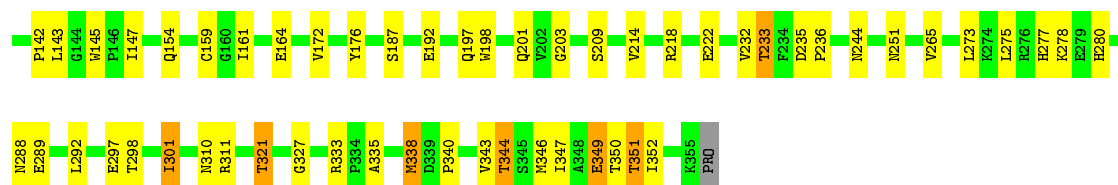
- Molecule 1: glutamine synthetase



- Molecule 1: glutamine synthetase

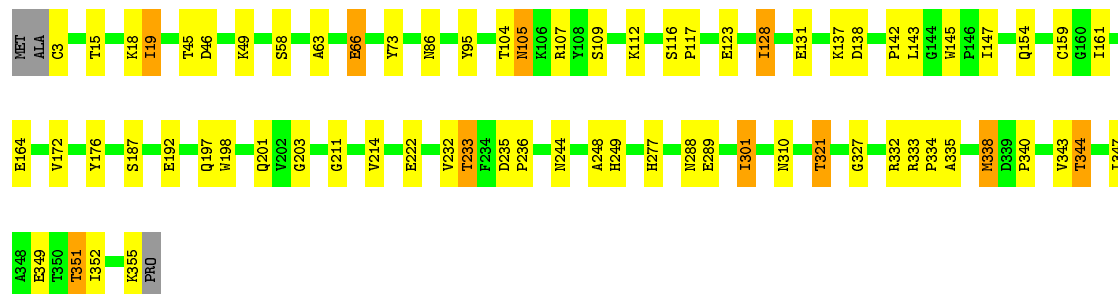






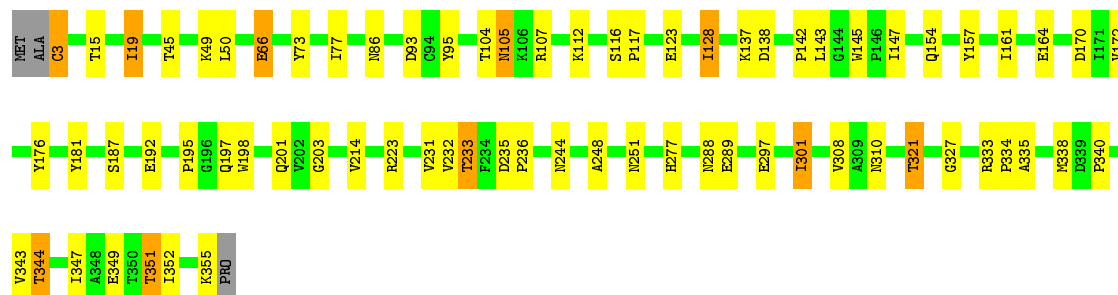
- Molecule 1: glutamine synthetase

Chain H: 79% 17% . .



- Molecule 1: glutamine synthetase

Chain I: 79% 17% . .



- Molecule 1: glutamine synthetase

Chain J: 80% 16% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.88Å 190.94Å 117.90Å 90.00° 101.23° 90.00°	Depositor
Resolution (Å)	33.50 – 3.50 33.50 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.1 (33.50-3.50) 83.1 (33.50-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.209 0.159 , 0.201	Depositor DCC
R_{free} test set	2227 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 44.1	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	0.95	EDS
Total number of atoms	28277	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: MSL, ANP, MN

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	A	0.67	0/2819	0.70	0/3834
1	B	0.69	1/2819 (0.0%)	0.70	0/3834
1	C	0.67	0/2819	0.70	0/3834
1	D	0.75	0/2819	0.72	0/3834
1	E	0.71	0/2819	0.70	0/3834
1	F	0.73	0/2819	0.72	0/3834
1	G	0.74	1/2819 (0.0%)	0.71	1/3834 (0.0%)
1	H	0.70	1/2819 (0.0%)	0.70	0/3834
1	I	0.66	0/2819	0.69	0/3834
1	J	0.67	0/2819	0.70	0/3834
All	All	0.70	3/28190 (0.0%)	0.70	1/38340 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	CYS	CB-SG	-5.96	1.72	1.81
1	H	159	CYS	CB-SG	-5.62	1.72	1.81
1	G	159	CYS	CB-SG	-5.14	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	218	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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	2745	0	2653	48	0
1	B	2745	0	2653	49	0
1	C	2745	0	2653	59	0
1	D	2745	0	2653	73	0
1	E	2745	0	2653	57	0
1	F	2745	0	2653	64	0
1	G	2745	0	2653	63	0
1	H	2745	0	2653	45	0
1	I	2745	0	2653	48	0
1	J	2745	0	2653	43	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	31	0	10	7	0
3	B	31	0	11	3	0
3	C	31	0	10	4	0
3	D	31	0	11	6	0
3	E	31	0	11	6	0
3	F	31	0	11	4	0
3	G	31	0	10	4	0
3	H	31	0	10	3	0
3	I	31	0	10	3	0
3	J	31	0	10	3	0
4	C	110	0	100	37	0
5	A	32	0	0	7	0
5	B	36	0	0	11	0
5	C	40	0	0	12	0
5	D	42	0	0	27	0
5	E	41	0	0	14	0
5	F	39	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	40	0	0	19	0
5	H	32	0	0	9	0
5	I	37	0	0	7	0
5	J	38	0	0	11	0
All	All	28277	0	26734	546	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 10.

The worst 5 of 546 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:LEU:HD23	5:G:6047:HOH:O	1.47	1.11
4:C:5010:MSL:NE	3:H:6008:ANP:PG	2.25	1.09
1:E:354:TRP:HA	5:E:6026:HOH:O	1.56	1.05
1:G:346:MET:SD	5:G:6041:HOH:O	2.14	1.03
1:E:255:GLU:HG2	5:E:6019:HOH:O	1.58	1.02

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	A	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	B	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	C	351/356 (99%)	334 (95%)	16 (5%)	1 (0%)	41	75
1	D	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	E	351/356 (99%)	328 (93%)	23 (7%)	0	100	100
1	F	351/356 (99%)	331 (94%)	20 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	351/356 (99%)	332 (95%)	18 (5%)	1 (0%)	41	75
1	H	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	I	351/356 (99%)	330 (94%)	21 (6%)	0	100	100
1	J	351/356 (99%)	332 (95%)	19 (5%)	0	100	100
All	All	3510/3560 (99%)	3316 (94%)	192 (6%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	84	ARG
1	C	138	ASP

5.3.2 Protein sidechains ⓘ

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	A	288/290 (99%)	261 (91%)	27 (9%)	8	35
1	B	288/290 (99%)	264 (92%)	24 (8%)	11	40
1	C	288/290 (99%)	262 (91%)	26 (9%)	9	37
1	D	288/290 (99%)	262 (91%)	26 (9%)	9	37
1	E	288/290 (99%)	262 (91%)	26 (9%)	9	37
1	F	288/290 (99%)	262 (91%)	26 (9%)	9	37
1	G	288/290 (99%)	262 (91%)	26 (9%)	9	37
1	H	288/290 (99%)	262 (91%)	26 (9%)	9	37
1	I	288/290 (99%)	264 (92%)	24 (8%)	11	40
1	J	288/290 (99%)	261 (91%)	27 (9%)	8	35
All	All	2880/2900 (99%)	2622 (91%)	258 (9%)	9	37

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	147	ILE
1	F	201	GLN
1	J	109	SER
1	E	232	VAL
1	F	19	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	288	ASN
1	F	277	HIS
1	J	154	GLN
1	E	296	HIS
1	F	190	ASN

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](#)

Of 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 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
3	ANP	J	6010	2	29,33,33	2.59	11 (37%)	31,52,52	3.37	17 (54%)
3	ANP	E	6005	2	29,33,33	2.82	12 (41%)	31,52,52	3.71	18 (58%)
3	ANP	A	6001	2	29,33,33	2.52	11 (37%)	31,52,52	3.03	16 (51%)
4	MSL	C	5004	2	5,10,10	0.84	0	4,14,14	4.11	4 (100%)
3	ANP	H	6008	2	29,33,33	2.50	13 (44%)	31,52,52	3.96	15 (48%)
4	MSL	C	5003	2	5,10,10	0.82	0	4,14,14	3.65	3 (75%)
3	ANP	C	6003	2	29,33,33	2.52	10 (34%)	31,52,52	3.40	14 (45%)
3	ANP	F	6006	2	29,33,33	2.92	11 (37%)	31,52,52	3.05	12 (38%)
4	MSL	C	5007	2	5,10,10	1.31	1 (20%)	4,14,14	6.52	4 (100%)
4	MSL	C	5009	2	5,10,10	0.81	0	4,14,14	3.26	3 (75%)
3	ANP	B	6002	2	29,33,33	2.72	12 (41%)	31,52,52	3.18	16 (51%)
3	ANP	G	6007	2	29,33,33	2.45	10 (34%)	31,52,52	2.98	15 (48%)
4	MSL	C	5002	2	5,10,10	0.85	0	4,14,14	7.86	2 (50%)
4	MSL	C	5005	2	5,10,10	0.79	0	4,14,14	4.01	3 (75%)
3	ANP	I	6009	2	29,33,33	2.55	11 (37%)	31,52,52	3.13	14 (45%)
4	MSL	C	5008	2	5,10,10	0.96	0	4,14,14	3.87	1 (25%)
4	MSL	C	5001	2	5,10,10	1.46	1 (20%)	4,14,14	2.82	3 (75%)
4	MSL	C	5010	2	5,10,10	1.05	0	4,14,14	5.23	3 (75%)
3	ANP	D	6004	2	29,33,33	2.87	10 (34%)	31,52,52	3.34	15 (48%)
4	MSL	C	5006	2	5,10,10	1.52	1 (20%)	4,14,14	3.09	3 (75%)

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
3	ANP	J	6010	2	2/2/7/8	10/14/38/38	0/3/3/3
4	MSL	C	5008	2	-	2/5/10/10	-
3	ANP	I	6009	2	2/2/7/8	8/14/38/38	0/3/3/3
3	ANP	E	6005	2	2/2/7/8	7/14/38/38	0/3/3/3
4	MSL	C	5004	2	-	0/5/10/10	-
4	MSL	C	5003	2	-	5/5/10/10	-
3	ANP	C	6003	2	2/2/7/8	8/14/38/38	0/3/3/3
3	ANP	F	6006	2	2/2/7/8	3/14/38/38	0/3/3/3
4	MSL	C	5007	2	-	4/5/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MSL	C	5009	2	-	3/5/10/10	-
3	ANP	B	6002	2	2/2/7/8	5/14/38/38	0/3/3/3
3	ANP	G	6007	2	2/2/7/8	5/14/38/38	0/3/3/3
4	MSL	C	5002	2	-	5/5/10/10	-
4	MSL	C	5005	2	-	5/5/10/10	-
3	ANP	A	6001	2	2/2/7/8	8/14/38/38	0/3/3/3
3	ANP	D	6004	2	2/2/7/8	5/14/38/38	0/3/3/3
4	MSL	C	5001	2	-	1/5/10/10	-
4	MSL	C	5010	2	-	2/5/10/10	-
3	ANP	H	6008	2	2/2/7/8	8/14/38/38	0/3/3/3
4	MSL	C	5006	2	-	0/5/10/10	-

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6004	ANP	PB-O3A	8.27	1.69	1.59
3	E	6005	ANP	PB-O3A	7.52	1.68	1.59
3	F	6006	ANP	PB-O3A	6.88	1.67	1.59
3	H	6008	ANP	C5'-C4'	-6.25	1.32	1.51
3	F	6006	ANP	PG-O2G	6.11	1.73	1.56

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5002	MSL	OE-SD-CG	13.85	119.32	108.39
3	E	6005	ANP	C2'-C3'-C4'	-11.81	79.70	102.64
3	H	6008	ANP	C2'-C3'-C4'	-11.33	80.62	102.64
3	C	6003	ANP	C2'-C3'-C4'	-11.05	81.18	102.64
3	J	6010	ANP	C2'-C3'-C4'	-10.53	82.19	102.64

5 of 20 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	J	6010	ANP	C4'
3	J	6010	ANP	C1'
3	E	6005	ANP	C4'
3	E	6005	ANP	C1'
3	H	6008	ANP	C4'

5 of 94 torsion outliers are listed below:

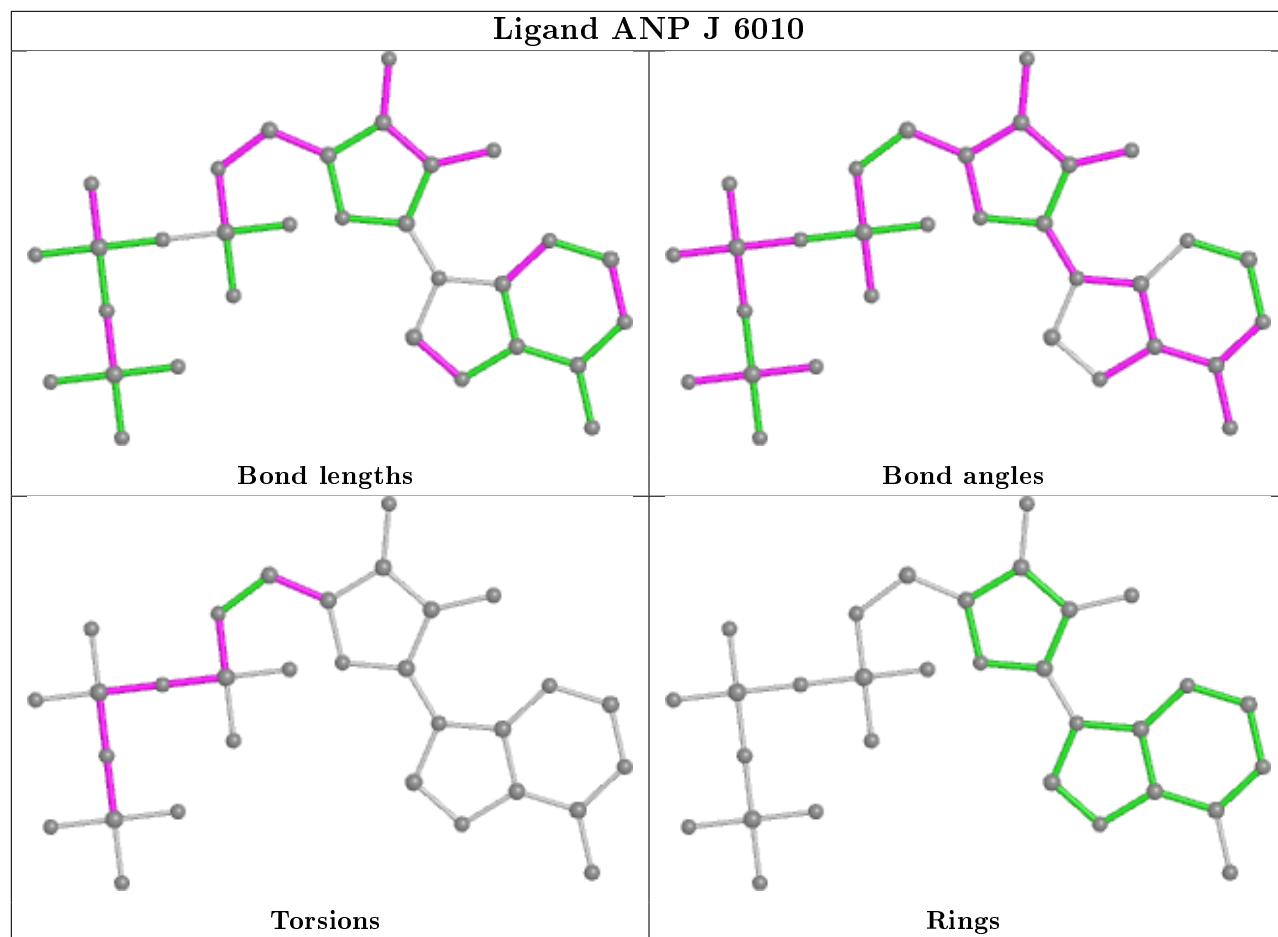
Mol	Chain	Res	Type	Atoms
3	J	6010	ANP	PB-N3B-PG-O1G
3	J	6010	ANP	PG-N3B-PB-O1B
3	J	6010	ANP	PA-O3A-PB-O1B
3	J	6010	ANP	C5'-O5'-PA-O2A
3	J	6010	ANP	C5'-O5'-PA-O3A

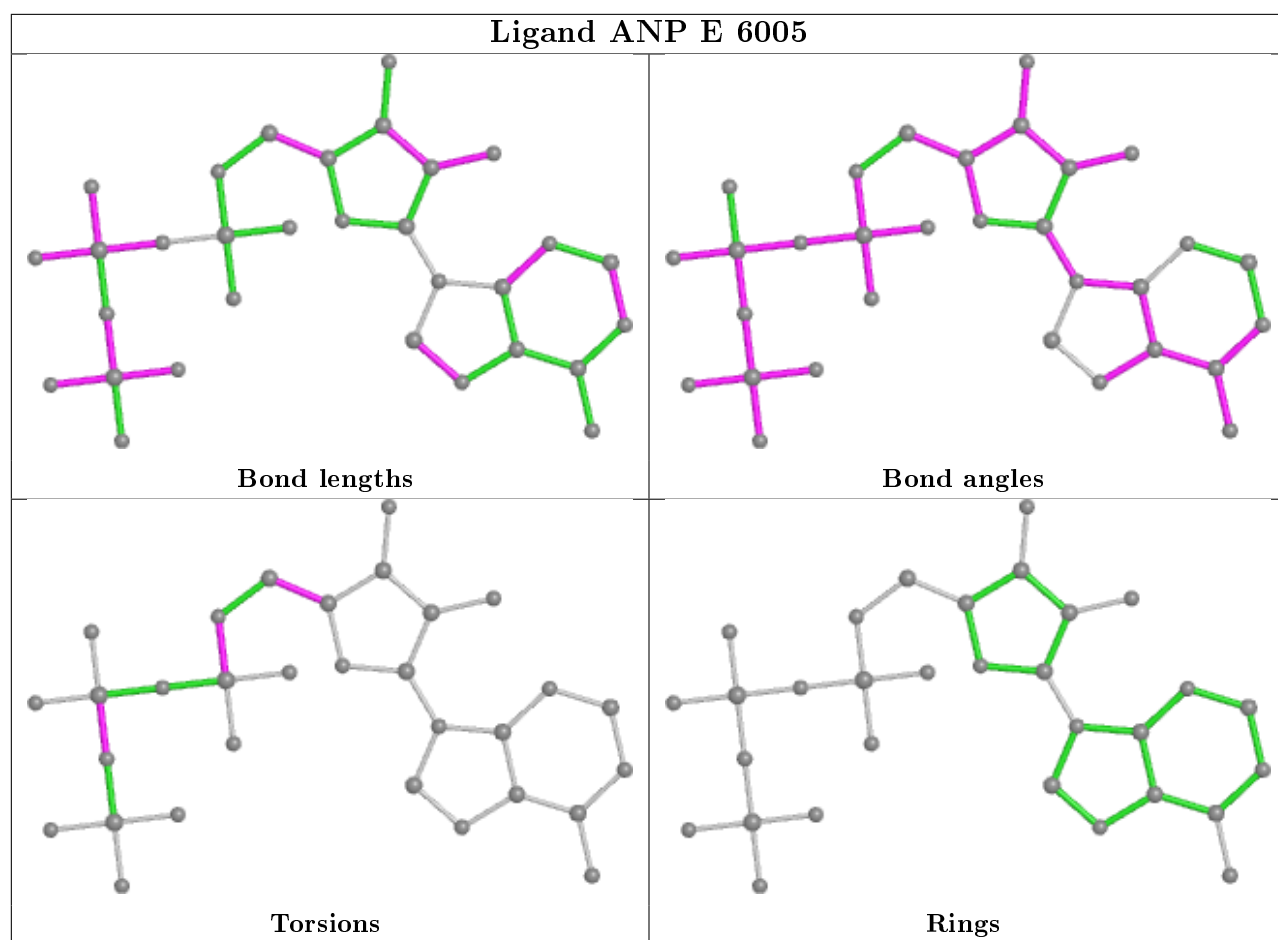
There are no ring outliers.

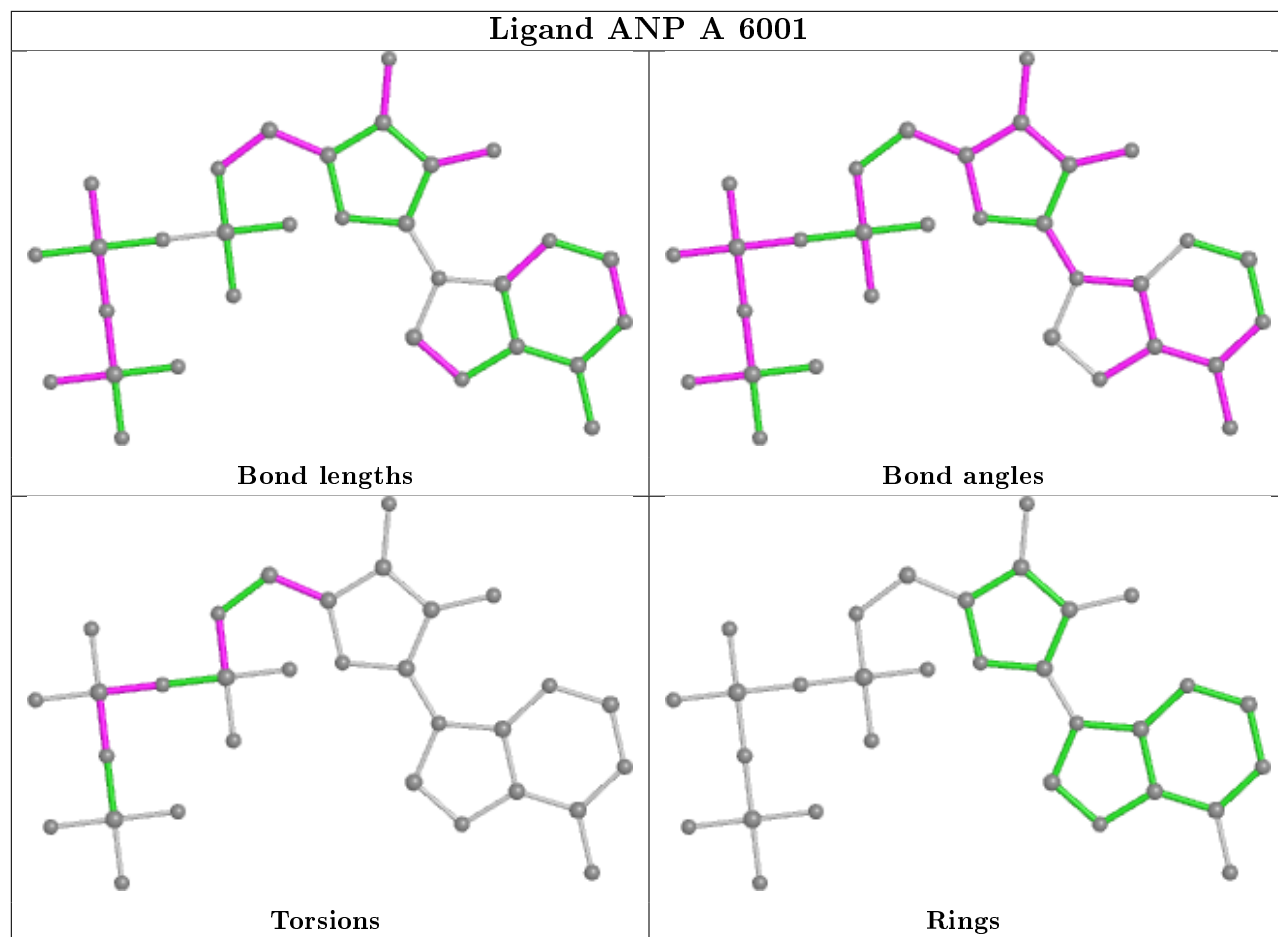
20 monomers are involved in 63 short contacts:

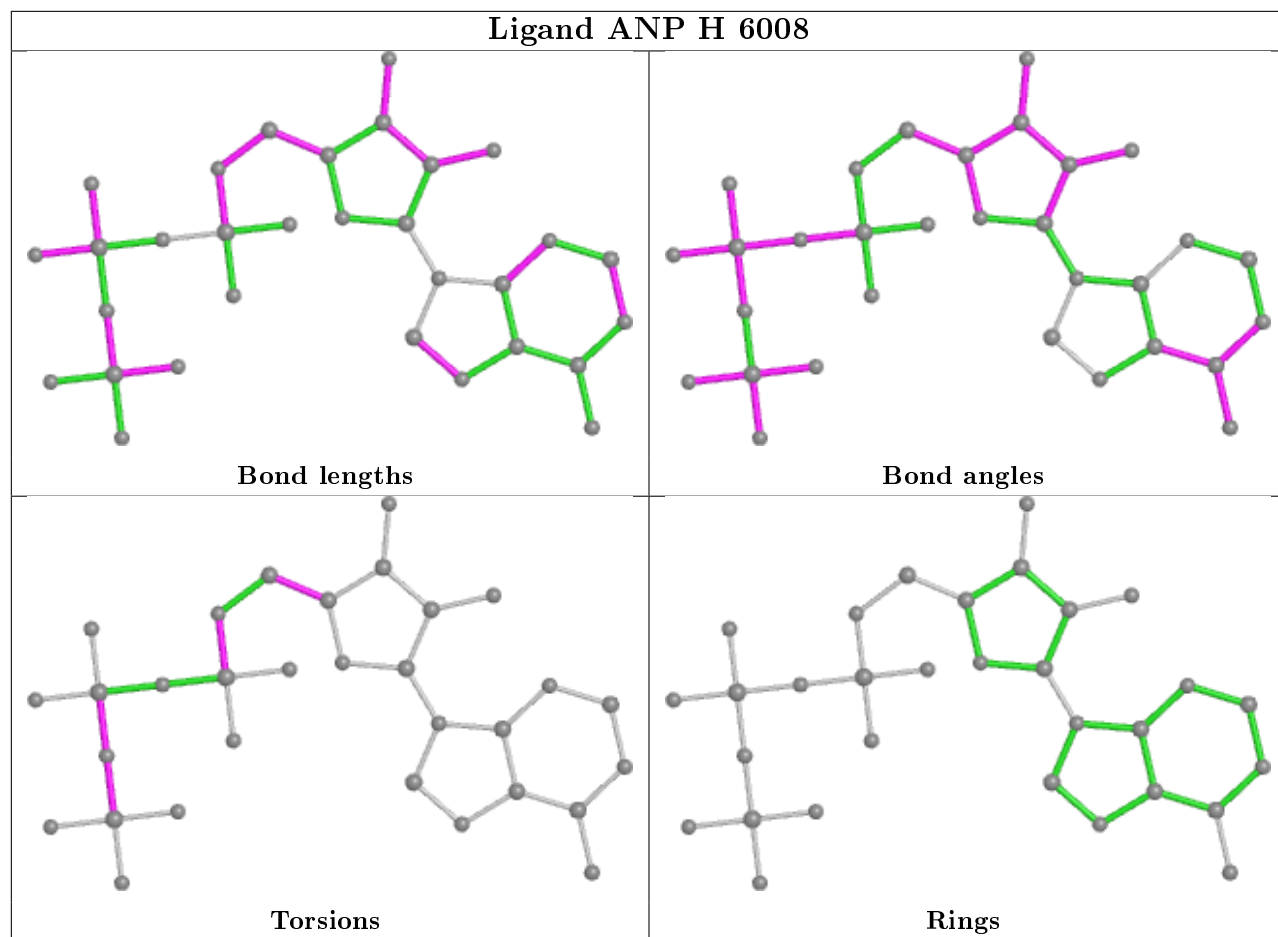
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	6010	ANP	3	0
3	E	6005	ANP	6	0
3	A	6001	ANP	7	0
4	C	5004	MSL	2	0
3	H	6008	ANP	3	0
4	C	5003	MSL	5	0
3	C	6003	ANP	4	0
3	F	6006	ANP	4	0
4	C	5007	MSL	6	0
4	C	5009	MSL	3	0
3	B	6002	ANP	3	0
3	G	6007	ANP	4	0
4	C	5002	MSL	6	0
4	C	5005	MSL	7	0
3	I	6009	ANP	3	0
4	C	5008	MSL	2	0
4	C	5001	MSL	2	0
4	C	5010	MSL	2	0
3	D	6004	ANP	6	0
4	C	5006	MSL	2	0

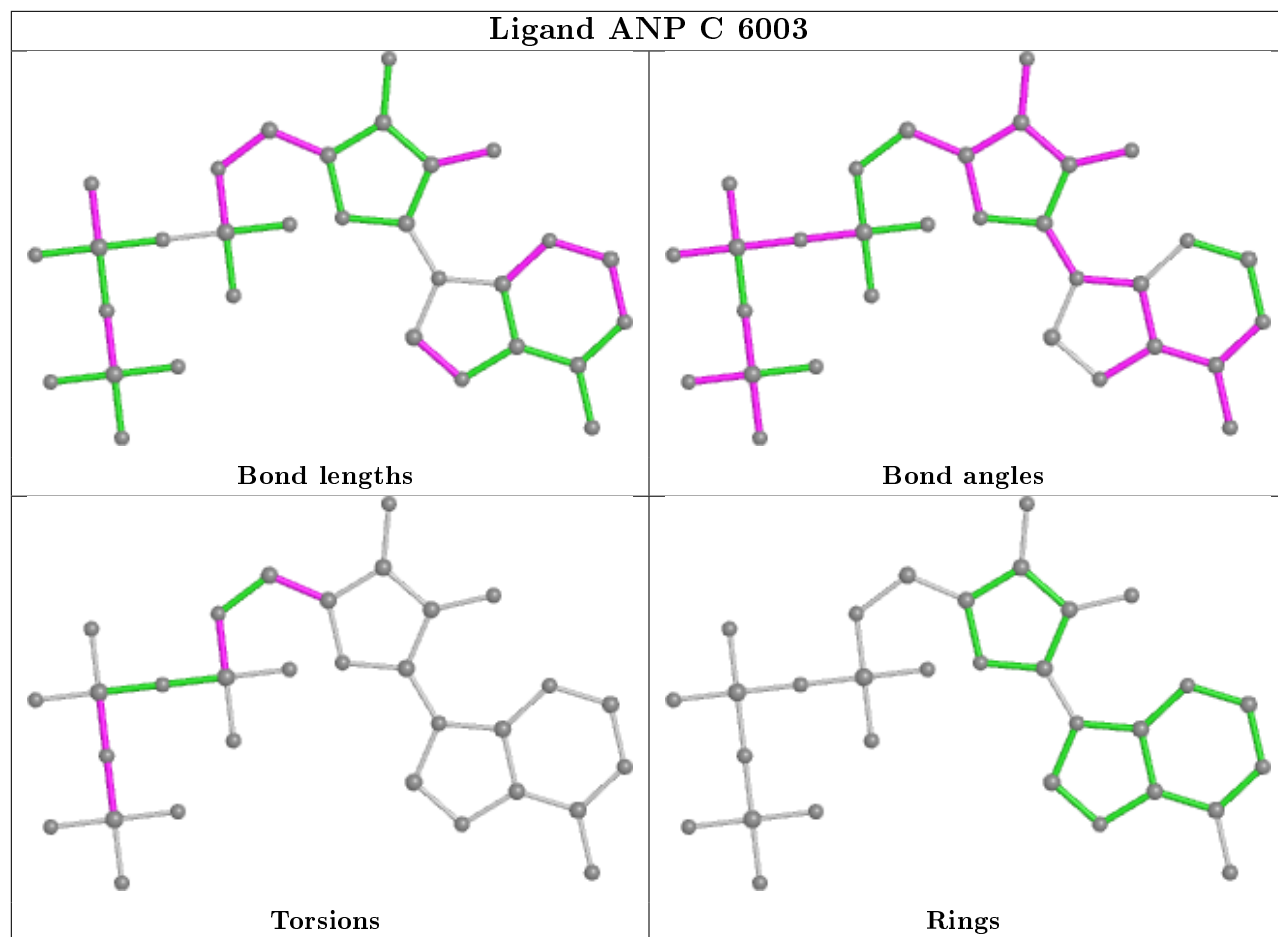
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

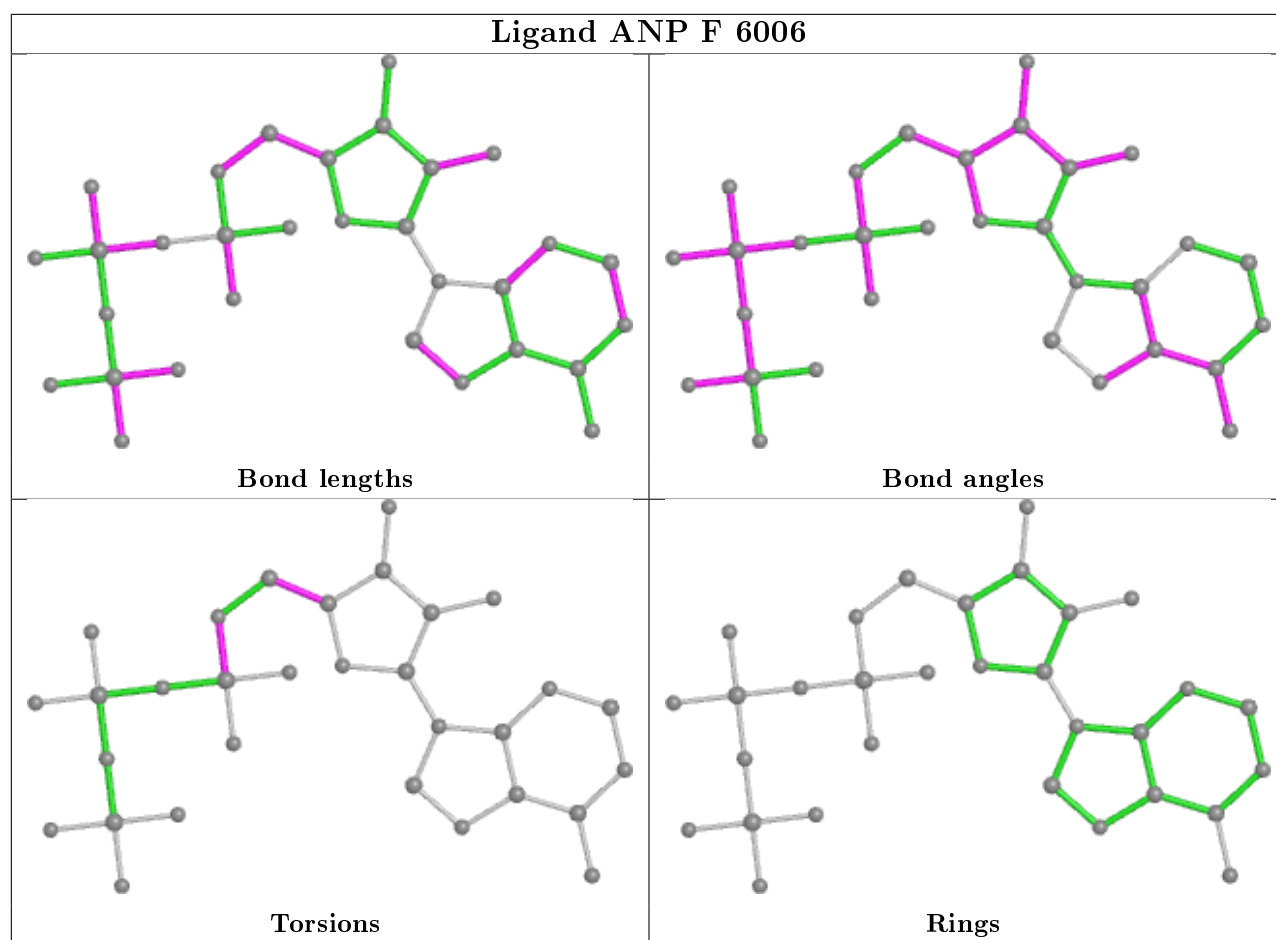


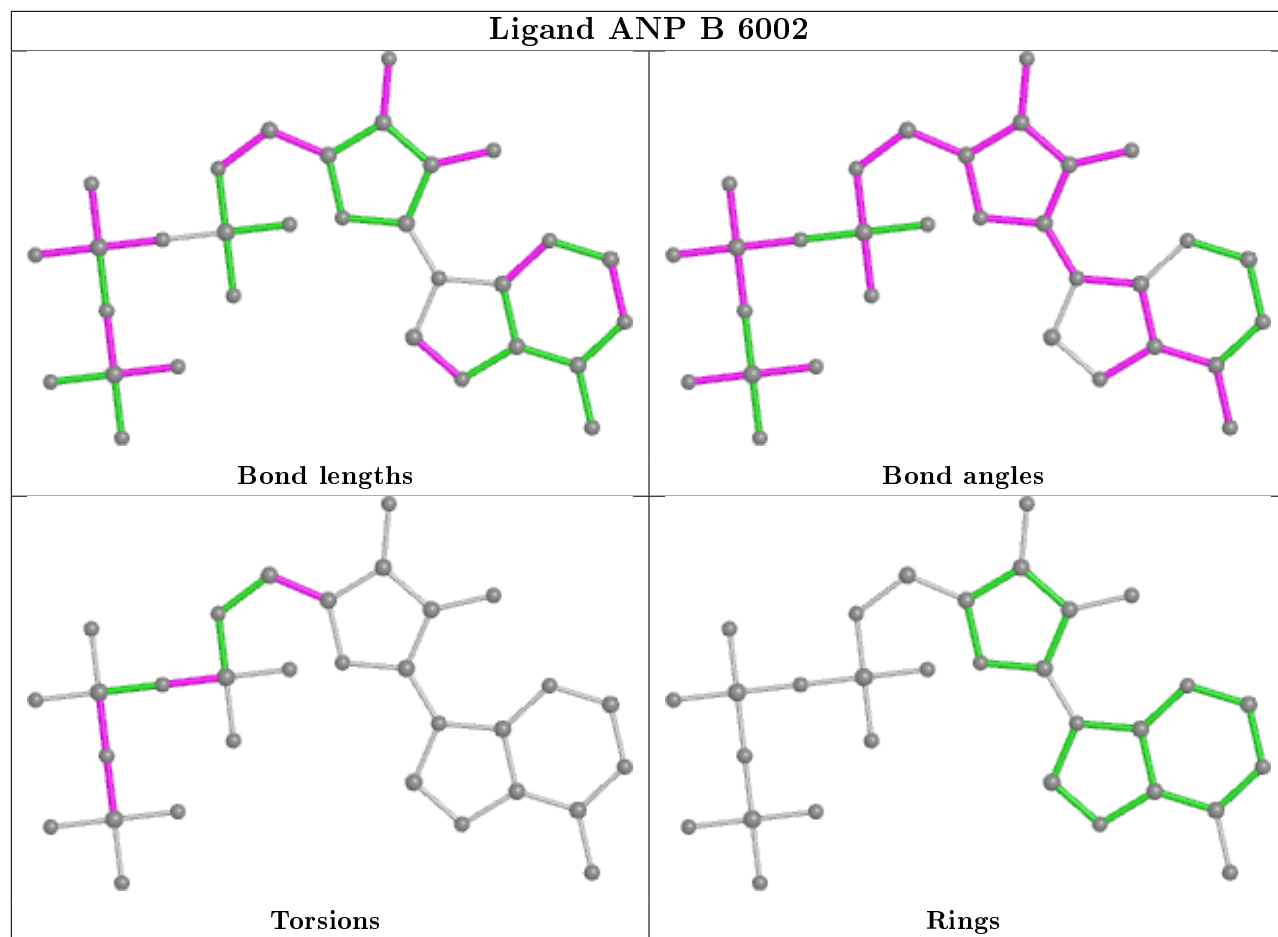


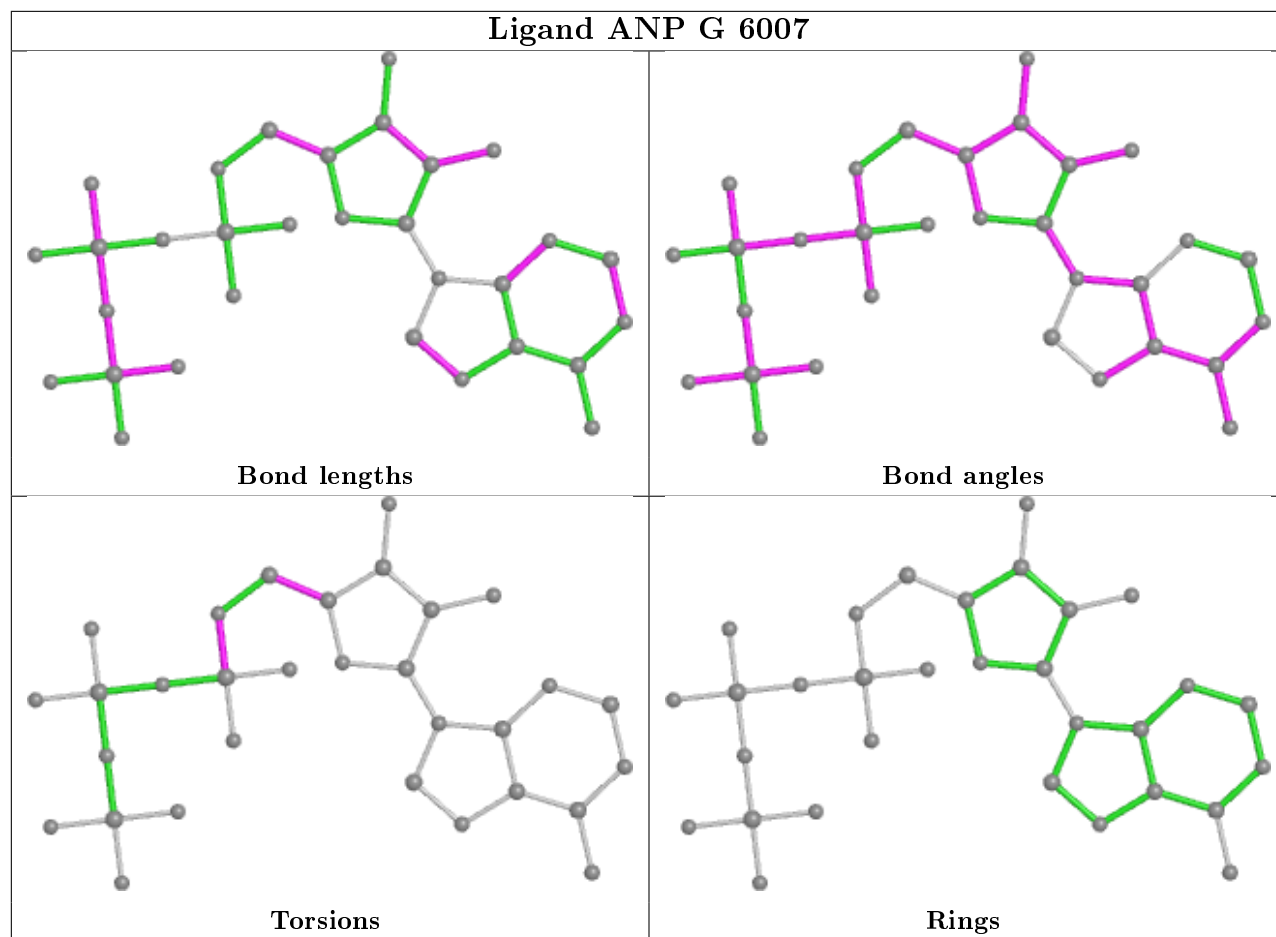


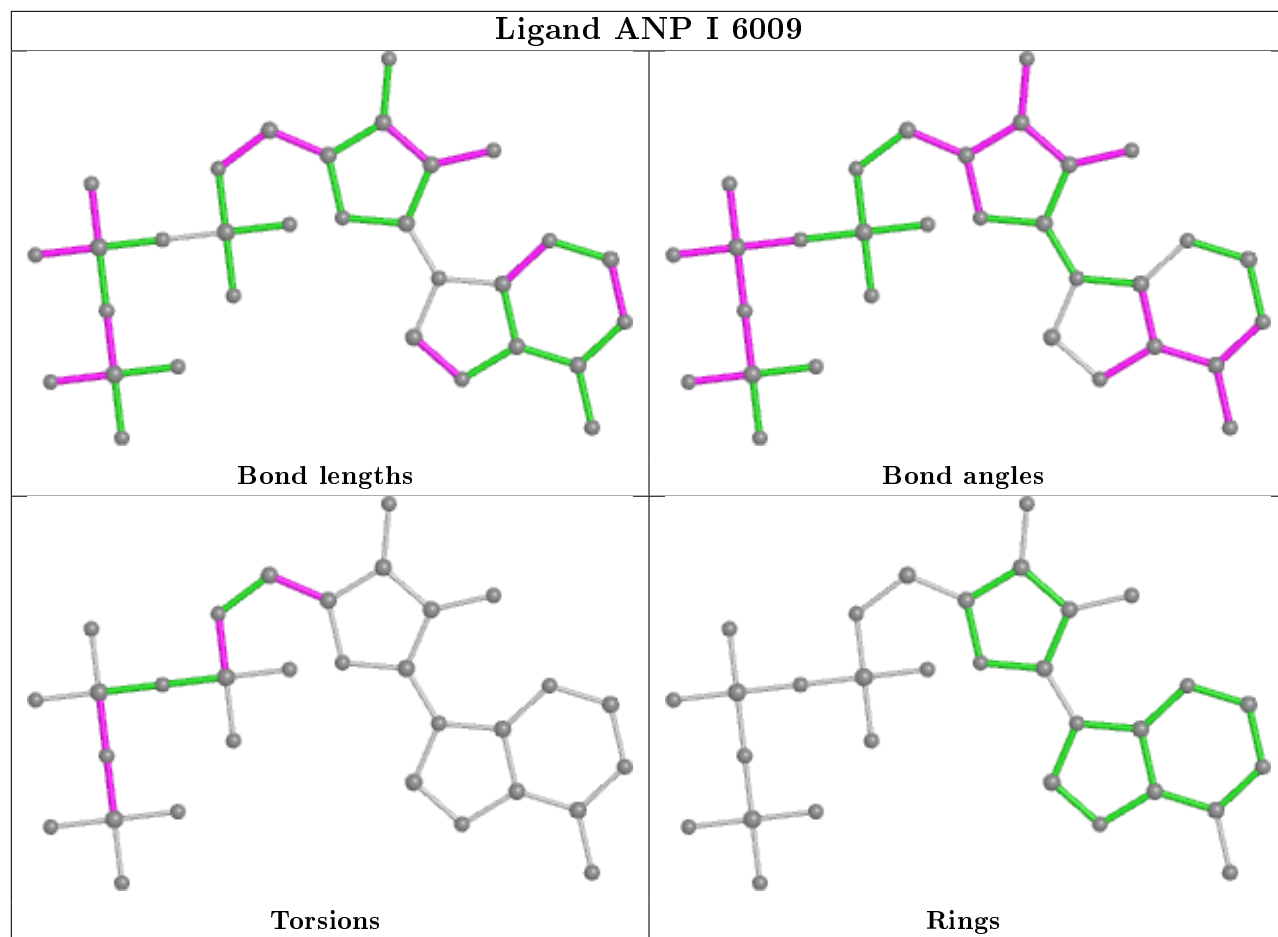


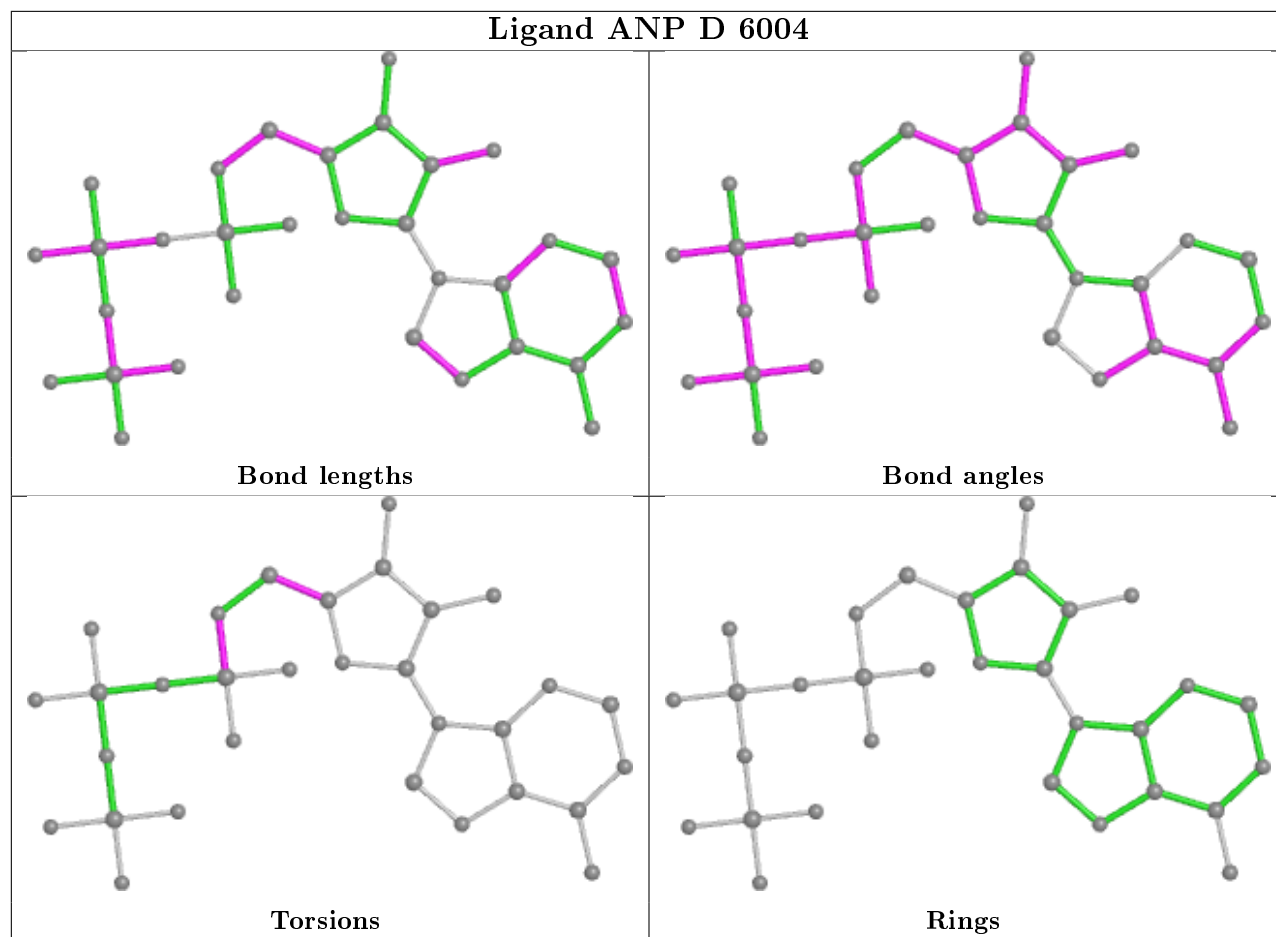












5.7 Other polymers [i](#)

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](#)

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	353/356 (99%)	-0.77	0 100 100	55, 73, 96, 108	0
1	B	353/356 (99%)	-0.72	0 100 100	55, 73, 96, 108	0
1	C	353/356 (99%)	-0.81	0 100 100	55, 73, 96, 108	0
1	D	353/356 (99%)	-0.75	0 100 100	55, 73, 96, 108	0
1	E	353/356 (99%)	-0.78	1 (0%) 94 91	55, 73, 96, 108	0
1	F	353/356 (99%)	-0.77	0 100 100	55, 73, 96, 108	0
1	G	353/356 (99%)	-0.70	0 100 100	55, 73, 96, 108	0
1	H	353/356 (99%)	-0.74	0 100 100	55, 73, 96, 108	0
1	I	353/356 (99%)	-0.78	0 100 100	55, 73, 96, 108	0
1	J	353/356 (99%)	-0.78	0 100 100	55, 73, 96, 108	0
All	All	3530/3560 (99%)	-0.76	1 (0%) 100 100	55, 73, 96, 108	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	CYS	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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.

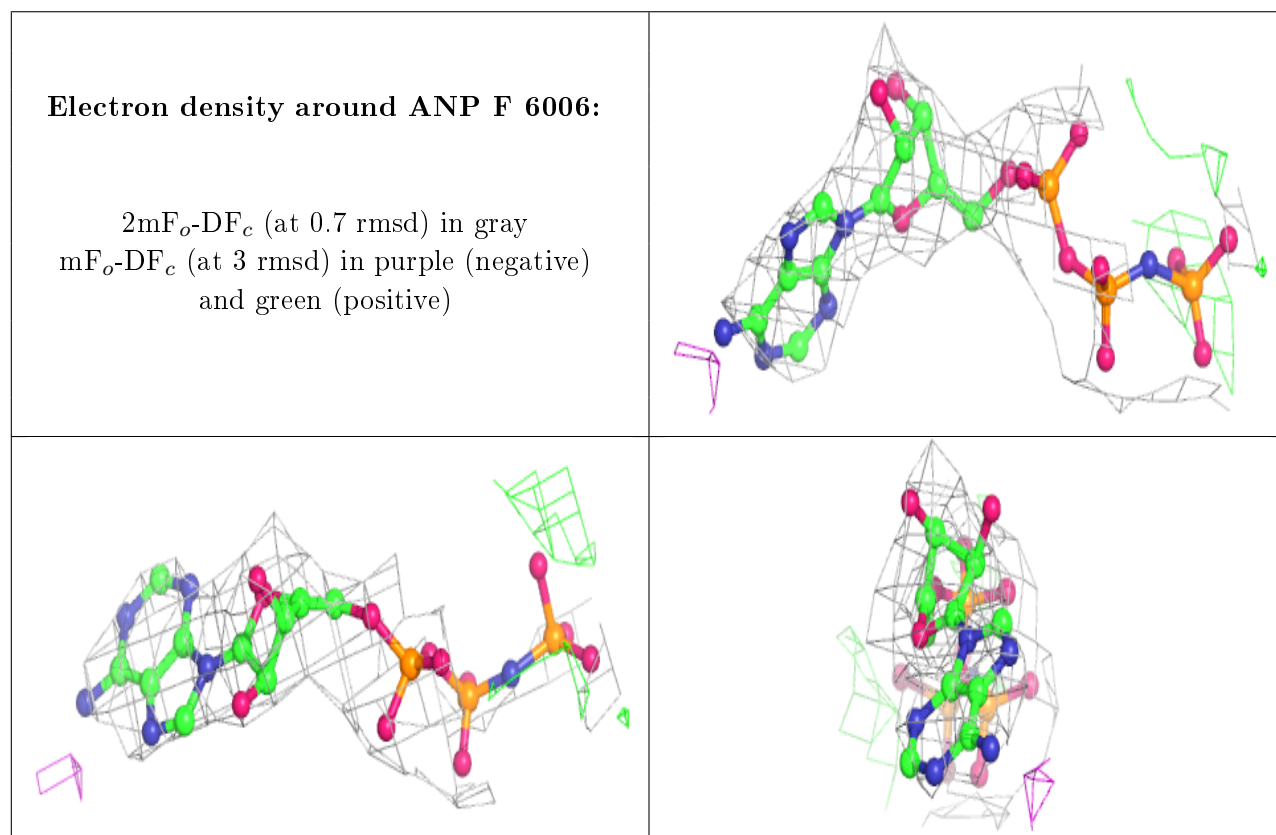
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	F	1053	1/1	0.87	0.14	69,69,69,69	0
2	MN	E	1043	1/1	0.89	0.17	61,61,61,61	0
2	MN	J	1091	1/1	0.91	0.24	62,62,62,62	0
3	ANP	F	6006	31/31	0.94	0.28	78,91,100,101	0
2	MN	C	1021	1/1	0.95	0.17	66,66,66,66	0
3	ANP	J	6010	31/31	0.95	0.19	47,58,64,67	0
3	ANP	C	6003	31/31	0.95	0.25	64,76,92,93	0
3	ANP	G	6007	31/31	0.95	0.26	65,86,95,96	0
3	ANP	B	6002	31/31	0.95	0.20	42,50,60,65	0
3	ANP	A	6001	31/31	0.95	0.22	60,76,82,82	0
3	ANP	E	6005	31/31	0.95	0.25	79,95,105,106	0
2	MN	G	1063	1/1	0.95	0.20	63,63,63,63	0
2	MN	B	1011	1/1	0.95	0.19	62,62,62,62	0
3	ANP	D	6004	31/31	0.96	0.23	83,95,105,106	0
2	MN	C	1023	1/1	0.96	0.21	63,63,63,63	0
3	ANP	H	6008	31/31	0.96	0.20	40,48,59,67	0
2	MN	F	1051	1/1	0.96	0.19	69,69,69,69	0
3	ANP	I	6009	31/31	0.96	0.23	69,78,84,85	0
4	MSL	C	5005	11/11	0.96	0.19	75,78,79,79	0
2	MN	E	1041	1/1	0.96	0.23	73,73,73,73	0
4	MSL	C	5007	11/11	0.97	0.21	62,68,77,77	0
2	MN	A	1001	1/1	0.97	0.23	68,68,68,68	0
2	MN	I	1083	1/1	0.97	0.18	62,62,62,62	0
2	MN	F	1052	1/1	0.97	0.17	70,70,70,70	0
4	MSL	C	5003	11/11	0.97	0.23	63,64,66,66	0
2	MN	E	1042	1/1	0.97	0.15	65,65,65,65	0
4	MSL	C	5008	11/11	0.97	0.23	63,65,66,67	0
2	MN	H	1072	1/1	0.97	0.19	57,57,57,57	0
2	MN	D	1033	1/1	0.98	0.18	56,56,56,56	0
2	MN	G	1062	1/1	0.98	0.21	65,65,65,65	0
2	MN	C	1022	1/1	0.98	0.17	66,66,66,66	0
2	MN	I	1082	1/1	0.98	0.17	67,67,67,67	0
2	MN	D	1032	1/1	0.98	0.16	70,70,70,70	0
2	MN	H	1071	1/1	0.98	0.24	57,57,57,57	0
2	MN	A	1002	1/1	0.98	0.17	62,62,62,62	0
2	MN	I	1081	1/1	0.98	0.22	68,68,68,68	0
2	MN	G	1061	1/1	0.98	0.17	66,66,66,66	0

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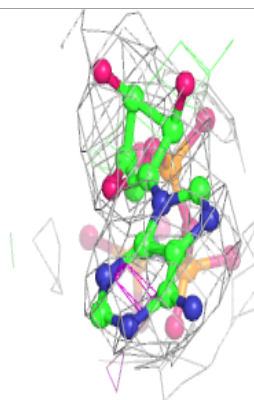
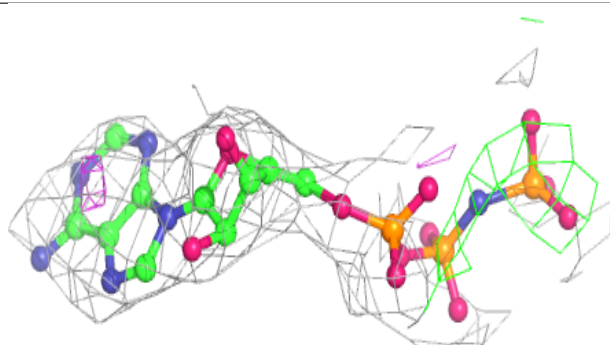
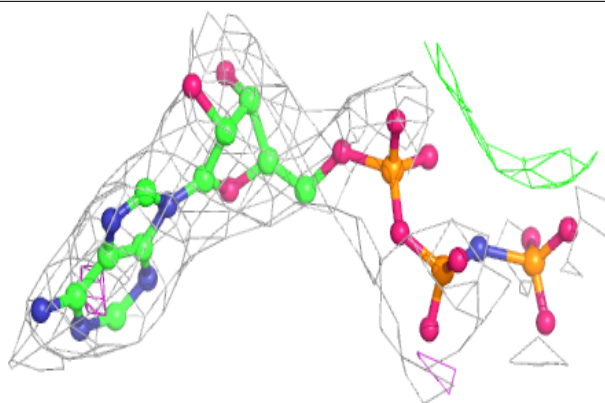
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MSL	C	5002	11/11	0.98	0.20	37,41,46,48	0
4	MSL	C	5001	11/11	0.98	0.18	51,54,57,58	0
4	MSL	C	5006	11/11	0.98	0.23	73,79,85,85	0
4	MSL	C	5004	11/11	0.99	0.17	71,73,75,77	0
4	MSL	C	5010	11/11	0.99	0.16	38,42,49,49	0
2	MN	H	1073	1/1	0.99	0.23	48,48,48,48	0
2	MN	J	1092	1/1	0.99	0.12	62,62,62,62	0
2	MN	J	1093	1/1	0.99	0.21	57,57,57,57	0
2	MN	B	1013	1/1	0.99	0.16	56,56,56,56	0
4	MSL	C	5009	11/11	0.99	0.17	53,56,64,65	0
2	MN	D	1031	1/1	0.99	0.24	65,65,65,65	0
2	MN	B	1012	1/1	0.99	0.17	60,60,60,60	0
2	MN	A	1003	1/1	0.99	0.22	57,57,57,57	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.

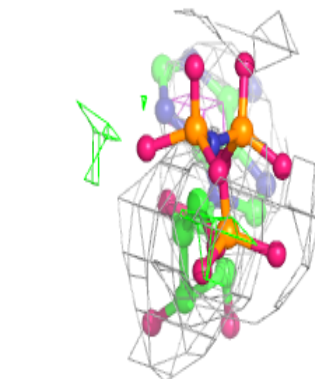
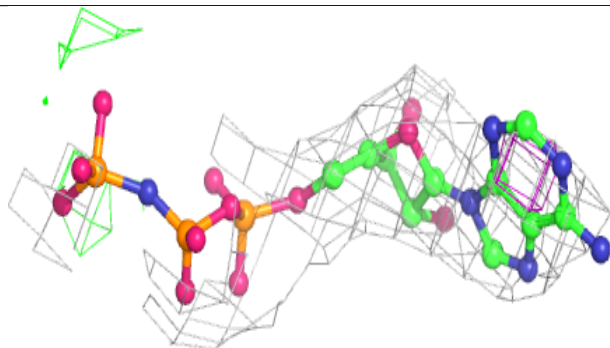
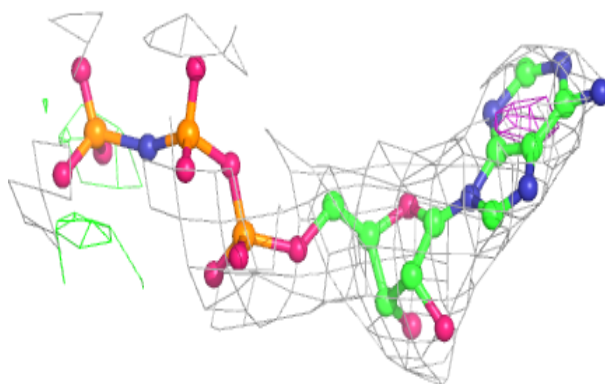


Electron density around ANP J 6010:

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

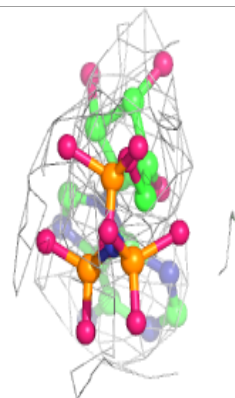
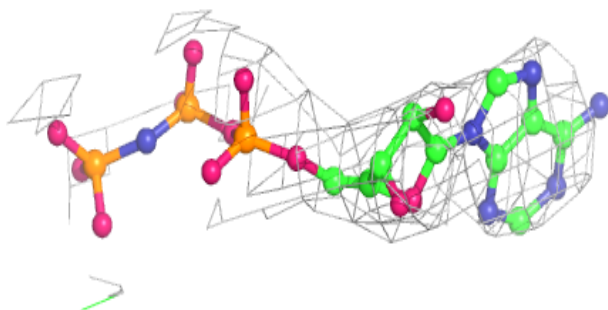
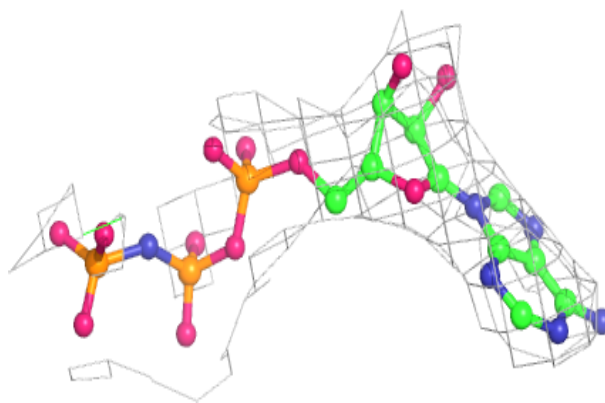
**Electron density around ANP C 6003:**

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

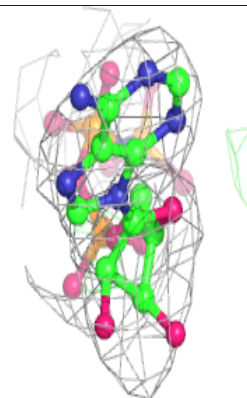
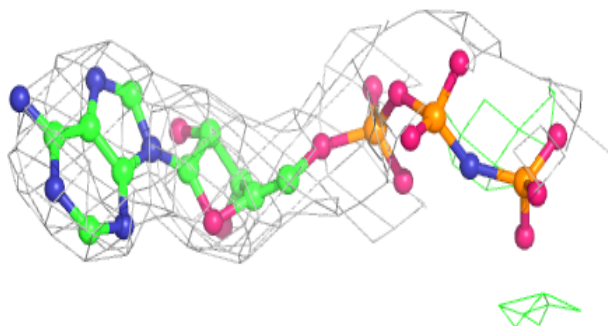
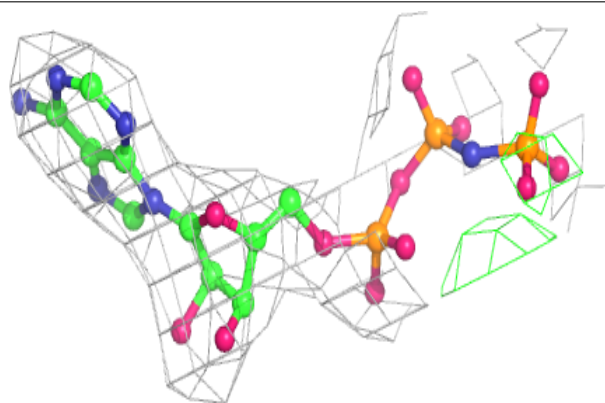


Electron density around ANP G 6007:

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

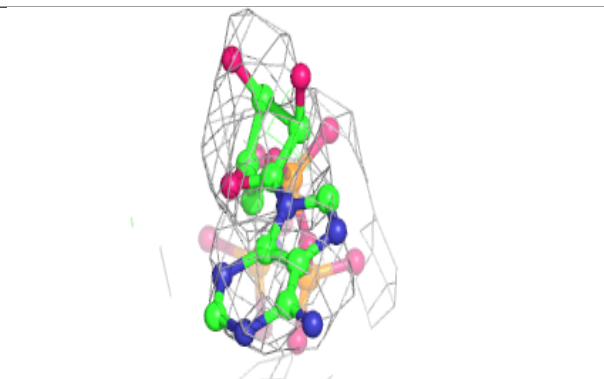
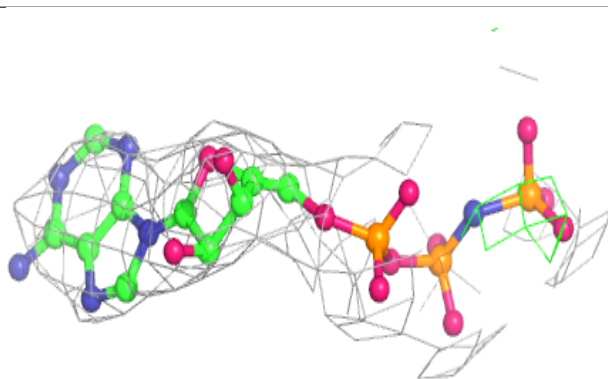
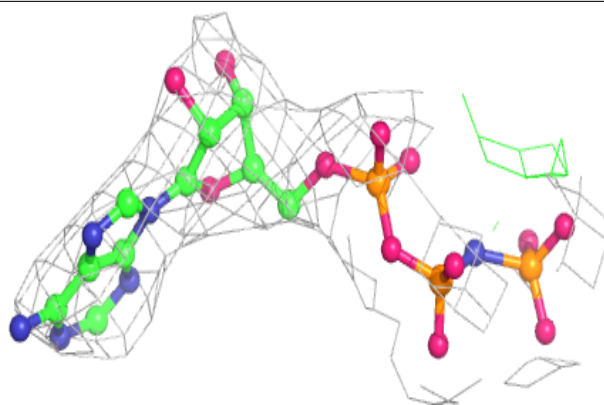
**Electron density around ANP B 6002:**

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

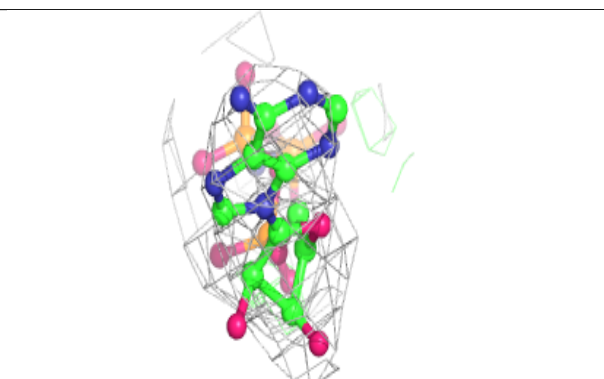
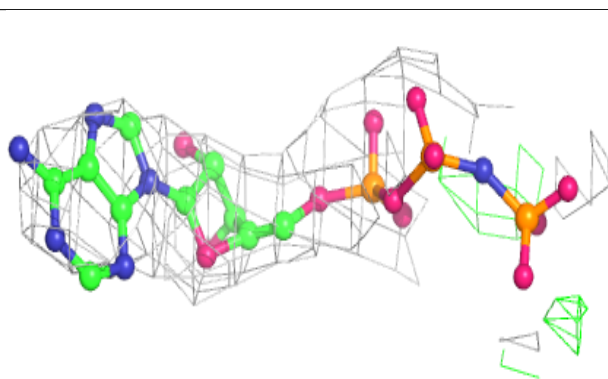
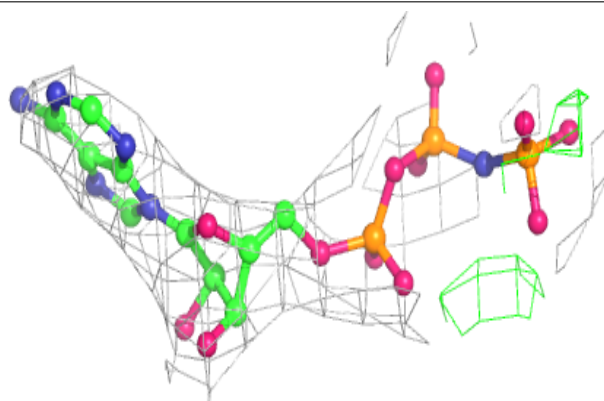


Electron density around ANP A 6001:

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

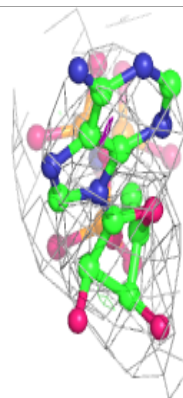
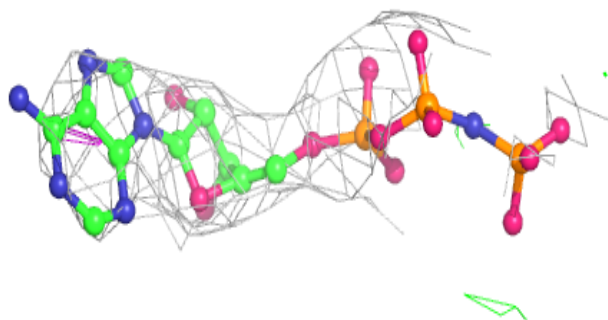
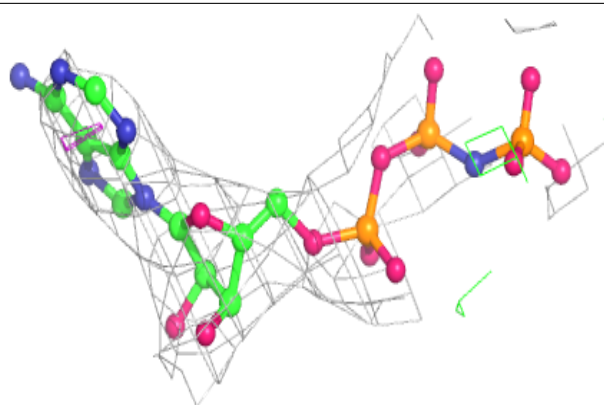
**Electron density around ANP E 6005:**

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

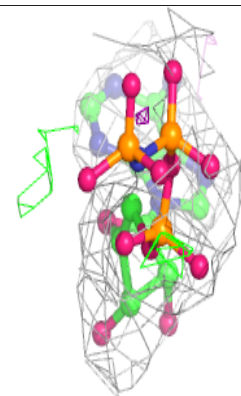
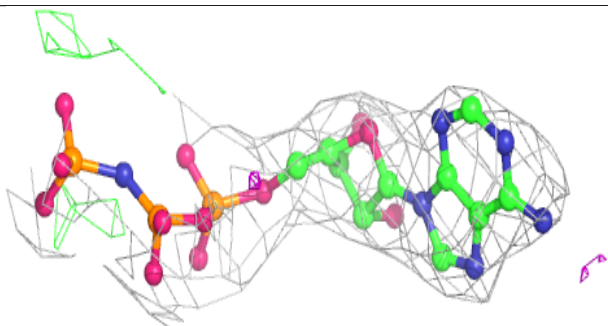
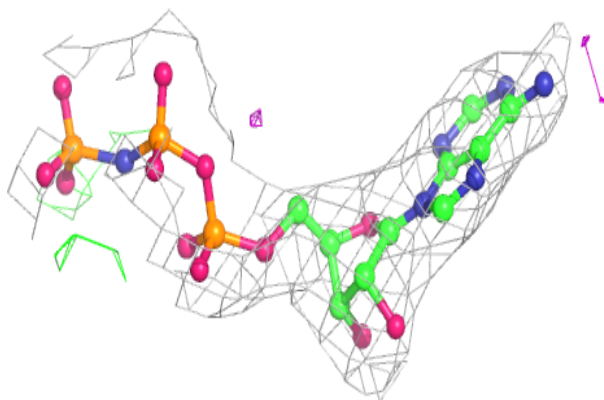


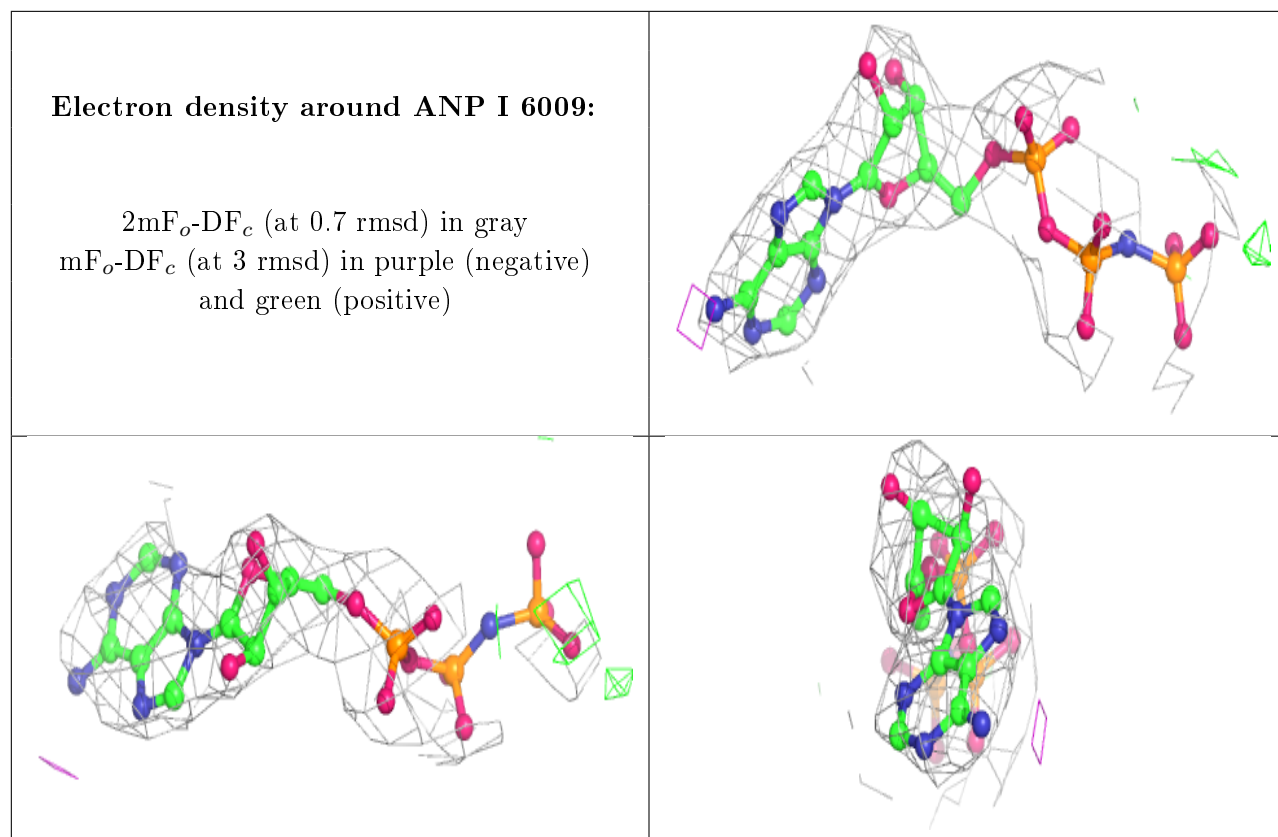
Electron density around ANP D 6004:

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

**Electron density around ANP H 6008:**

$2mF_o-DF_c$ (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.