



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:04 AM UTC

PDB ID : 4YXW / pdb_00004yxw
Title : Bovine heart mitochondrial F1-ATPase inhibited by AMP-PNP and ADP in the presence of thiophosphate.
Authors : Bason, J.V.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2015-03-23
Resolution : 3.10 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 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

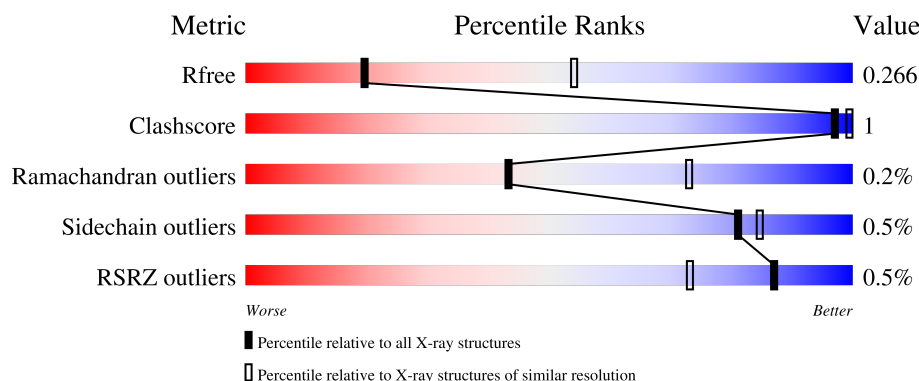
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	510	93%
1	B	510	92% 6%
1	C	510	93%
2	D	482	93%
2	E	482	91% 5%

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Mol	Chain	Length	Quality of chain
2	F	482	94%
3	G	273	2% 75% 22%
4	H	146	3% 85% 12%
5	I	50	90% 6%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24827 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 ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3728	2349	658	709	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	488	Total	C	N	O	S	0	0	0
			3722	2346	657	707	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	variant	UNP P19483
A	481	GLY	SER	variant	UNP P19483
B	1	GLU	GLN	variant	UNP P19483
B	481	GLY	SER	variant	UNP P19483
C	1	GLU	GLN	variant	UNP P19483
C	481	GLY	SER	variant	UNP P19483

- Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	458	Total	C	N	O	S	0	0	0
			3472	2201	592	669	10			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	213	Total	C	N	O	S	0	0	0
			1654	1039	298	310	7			

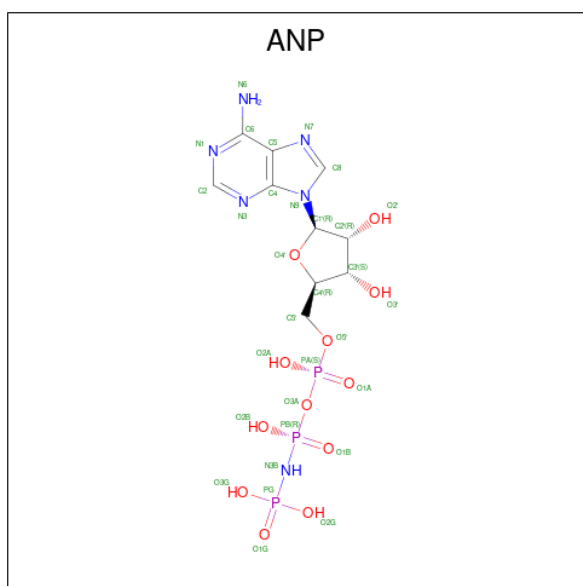
- Molecule 4 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	128	Total	C	N	O	S	0	0	0
			946	594	160	190	2			

- Molecule 5 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

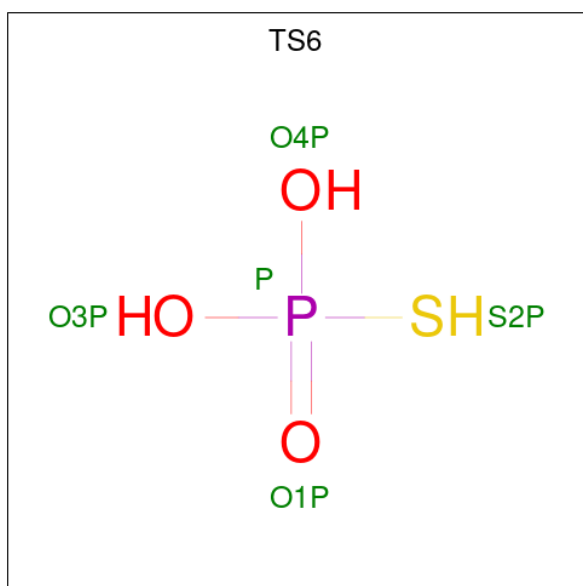
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Cl 1 1	0	0

- Molecule 9 is Monothiophosphate (CCD ID: TS6) (formula: H₃O₃PS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total O P S 5 3 1 1	0	0

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	1	Total	Na	0	0
			1	1		

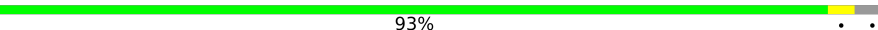
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	6	Total	O	0	0
			6	6		
11	B	7	Total	O	0	0
			7	7		
11	C	4	Total	O	0	0
			4	4		
11	D	8	Total	O	0	0
			8	8		
11	E	3	Total	O	0	0
			3	3		
11	F	9	Total	O	0	0
			9	9		

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: ATP synthase subunit alpha, mitochondrial

Chain A:  93%

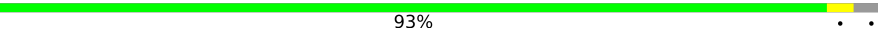


- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain B:  92% 6%



- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C:  93%



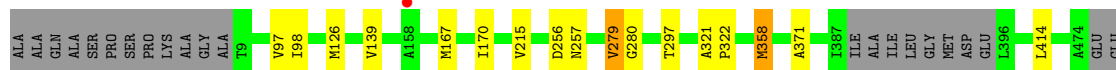
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain D:  93%



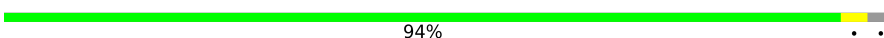
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain E:  91% 5%



HIS
SER

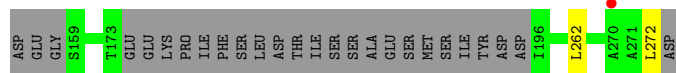
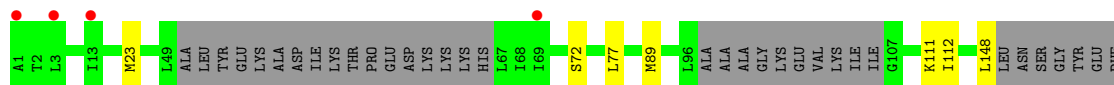
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain F:  94%



- Molecule 3: ATP synthase subunit gamma, mitochondrial

Chain G:  75%



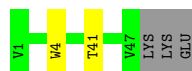
- Molecule 4: ATP synthase subunit delta, mitochondrial

Chain H:  85%



- Molecule 5: ATP synthase subunit epsilon, mitochondrial

Chain I:  90%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.35Å 123.05Å 261.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.50 – 3.10 76.50 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (76.50-3.10) 94.2 (76.50-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.226 , 0.273 0.224 , 0.266	Depositor DCC
R_{free} test set	3000 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.4	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	0.92	EDS
Total number of atoms	24827	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: MG, ANP, NA, TS6, CL

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	0.53	0/3779	0.77	0/5098
1	B	0.54	0/3711	0.77	0/5005
1	C	0.53	0/3773	0.78	0/5090
2	D	0.54	0/3596	0.77	0/4879
2	E	0.54	0/3528	0.76	0/4786
2	F	0.55	0/3587	0.77	0/4867
3	G	0.56	0/1668	0.82	0/2234
4	H	0.53	0/957	0.73	0/1301
5	I	0.61	0/374	0.82	0/501
All	All	0.54	0/24973	0.77	0/33761

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	3728	0	3828	6	0
1	B	3663	0	3774	4	0
1	C	3722	0	3823	7	0
2	D	3539	0	3592	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3472	0	3526	8	0
2	F	3530	0	3586	6	0
3	G	1654	0	1733	3	0
4	H	946	0	945	2	0
5	I	369	0	395	1	0
6	A	31	0	13	0	0
6	B	31	0	13	0	0
6	C	31	0	13	0	0
6	D	31	0	13	0	0
6	F	31	0	13	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	D	1	0	0	0	0
9	E	5	0	1	0	0
10	F	1	0	0	0	0
11	A	6	0	0	0	0
11	B	7	0	0	0	0
11	C	4	0	0	0	0
11	D	8	0	0	0	0
11	E	3	0	0	0	0
11	F	9	0	0	0	0
All	All	24827	0	25268	45	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 1.

All (45) 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)
2:F:139:VAL:HG12	2:F:414:LEU:HD22	1.55	0.89
4:H:21:ALA:HB2	4:H:26:VAL:HG23	1.83	0.60
2:E:358:MET:HE1	2:E:371:ALA:HB3	1.85	0.58
3:G:89:MET:HE1	3:G:112:ILE:HG23	1.85	0.58
2:F:84:ILE:HD11	2:F:238:THR:HB	1.90	0.54
2:D:393:MET:HE1	2:D:404:VAL:HG11	1.90	0.54
2:E:126:MET:HE1	2:E:297:THR:HG21	1.92	0.52
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.92	0.51
2:E:97:VAL:HG13	2:E:98:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ILE:HD13	1:B:429:LYS:HE2	1.93	0.50
1:C:392:LEU:HD13	2:D:459:MET:HE3	1.94	0.49
1:A:34:ILE:HD13	1:A:39:ALA:HB2	1.93	0.49
2:D:200:MET:CE	2:D:217:LEU:HD21	2.43	0.47
1:C:41:VAL:HG11	1:C:44:LEU:HD12	1.96	0.47
1:C:452:TYR:CE2	1:C:501:VAL:HG21	2.50	0.46
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.97	0.46
3:G:23:MET:HE1	3:G:77:LEU:HD12	1.98	0.46
1:A:44:LEU:O	1:A:47:VAL:HG22	2.17	0.44
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.46	0.44
1:C:152:ALA:HB3	1:C:365:ILE:HD12	2.00	0.44
1:A:99:VAL:HG13	1:A:253:MET:HA	2.00	0.44
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.53	0.43
2:D:298:THR:HG23	2:D:303:SER:HA	2.02	0.42
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.01	0.42
2:F:298:THR:HG23	2:F:303:SER:HA	2.01	0.42
2:E:167:MET:HA	2:E:170:ILE:HD12	2.01	0.42
2:E:256:ASP:HA	2:E:257:ASN:HA	1.89	0.42
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.50	0.42
2:D:200:MET:HE3	2:D:206:ILE:HD11	2.02	0.42
1:C:179:ALA:HB1	1:C:267:ILE:HD13	2.02	0.42
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.53	0.41
1:A:327:ILE:HD11	1:A:342:VAL:HG21	2.01	0.41
1:A:148:THR:HG21	1:A:153:VAL:HG11	2.02	0.41
2:F:359:ASP:O	2:F:363:VAL:HG22	2.21	0.40
1:B:258:ARG:NH1	1:B:308:ARG:O	2.55	0.40
1:C:306:LEU:HD12	1:C:345:ILE:HG21	2.03	0.40
2:D:377:ILE:HD11	2:D:406:ARG:HB2	2.02	0.40
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.52	0.40
1:B:38:ILE:CD1	1:B:285:LEU:HD21	2.51	0.40
2:D:84:ILE:HD12	2:D:95:MET:HE1	2.04	0.40
2:E:139:VAL:HG12	2:E:414:LEU:HD22	2.02	0.40
2:F:374:VAL:HG13	2:F:410:ILE:HG21	2.02	0.40
1:B:257:PHE:HB2	1:B:264:ALA:HB2	2.04	0.40
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.51	0.40
4:H:133:ILE:HD11	5:I:4:TRP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	487/510 (96%)	476 (98%)	9 (2%)	2 (0%)	30	61
1	B	476/510 (93%)	463 (97%)	13 (3%)	0	100	100
1	C	486/510 (95%)	474 (98%)	12 (2%)	0	100	100
2	D	465/482 (96%)	442 (95%)	22 (5%)	1 (0%)	43	73
2	E	454/482 (94%)	431 (95%)	21 (5%)	2 (0%)	30	61
2	F	464/482 (96%)	443 (96%)	21 (4%)	0	100	100
3	G	203/273 (74%)	191 (94%)	11 (5%)	1 (0%)	24	57
4	H	124/146 (85%)	116 (94%)	8 (6%)	0	100	100
5	I	45/50 (90%)	40 (89%)	5 (11%)	0	100	100
All	All	3204/3445 (93%)	3076 (96%)	122 (4%)	6 (0%)	43	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	407	GLY
2	E	358	MET
2	D	352	ASP
1	A	408	SER
3	G	72	SER
2	E	279	VAL

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	395/412 (96%)	395 (100%)	0	100	100
1	B	389/412 (94%)	388 (100%)	1 (0%)	86	87
1	C	394/412 (96%)	393 (100%)	1 (0%)	86	87
2	D	377/386 (98%)	376 (100%)	1 (0%)	86	87
2	E	370/386 (96%)	368 (100%)	2 (0%)	81	85
2	F	376/386 (97%)	374 (100%)	2 (0%)	81	85
3	G	180/231 (78%)	177 (98%)	3 (2%)	53	74
4	H	101/109 (93%)	100 (99%)	1 (1%)	68	79
5	I	38/41 (93%)	37 (97%)	1 (3%)	40	68
All	All	2620/2775 (94%)	2608 (100%)	12 (0%)	81	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	28	THR
1	C	99	VAL
2	D	237	LEU
2	E	215	VAL
2	E	279	VAL
2	F	279	VAL
2	F	395	GLU
3	G	111	LYS
3	G	148	LEU
3	G	272	LEU
4	H	84	VAL
5	I	41	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	476	HIS
1	B	186	GLN
1	B	466	ASN
1	C	186	GLN
1	C	396	GLN
1	C	405	GLN
1	C	441	GLN
2	D	171	ASN

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Mol	Chain	Res	Type
2	D	207	ASN
2	D	367	HIS
2	D	455	GLN
2	E	375	GLN
2	E	379	GLN
2	E	442	GLN
2	E	443	GLN
2	F	24	GLN
2	F	171	ASN
2	F	177	HIS
2	F	194	ASN
2	F	442	GLN
3	G	123	GLN
3	G	255	GLN
4	H	15	GLN
5	I	16	GLN

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](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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
6	ANP	B	600	7	33,33,33	2.01	12 (36%)	45,52,52	2.12	12 (26%)
6	ANP	C	600	7	33,33,33	2.03	13 (39%)	45,52,52	2.00	11 (24%)
6	ANP	D	600	7	33,33,33	2.03	11 (33%)	45,52,52	1.84	12 (26%)
6	ANP	F	600	7	33,33,33	2.03	14 (42%)	45,52,52	2.02	13 (28%)
6	ANP	A	600	7	33,33,33	2.04	11 (33%)	45,52,52	2.12	14 (31%)
9	TS6	E	603	-	3,4,4	4.45	2 (66%)	3,6,6	1.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	B	600	7	-	3/18/38/38	0/3/3/3
6	ANP	C	600	7	-	3/18/38/38	0/3/3/3
6	ANP	D	600	7	-	7/18/38/38	0/3/3/3
6	ANP	F	600	7	-	4/18/38/38	0/3/3/3
6	ANP	A	600	7	-	4/18/38/38	0/3/3/3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	603	TS6	P-O1P	6.75	1.61	1.46
6	C	600	ANP	C5-C4	5.06	1.48	1.39
6	F	600	ANP	C5-C4	4.93	1.47	1.39
6	A	600	ANP	C5-C4	4.90	1.47	1.39
6	B	600	ANP	C5-C4	4.79	1.47	1.39
6	D	600	ANP	C5-C4	4.76	1.47	1.39
6	D	600	ANP	PG-N3B	4.60	1.75	1.63
6	A	600	ANP	PB-N3B	4.54	1.75	1.63
6	D	600	ANP	PB-N3B	4.48	1.75	1.63
6	A	600	ANP	PG-N3B	4.37	1.74	1.63
6	B	600	ANP	PG-N3B	4.35	1.74	1.63
6	C	600	ANP	PG-N3B	4.34	1.74	1.63
6	C	600	ANP	PB-N3B	4.34	1.74	1.63
6	B	600	ANP	PB-N3B	4.32	1.74	1.63
6	F	600	ANP	PG-N3B	4.28	1.74	1.63
6	F	600	ANP	PB-N3B	4.15	1.74	1.63
6	A	600	ANP	PG-O1G	3.40	1.51	1.46
6	B	600	ANP	PG-O1G	3.38	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	600	ANP	PB-O1B	3.35	1.51	1.46
6	F	600	ANP	PG-O1G	3.30	1.51	1.46
9	E	603	TS6	P-O3P	-3.26	1.48	1.56
6	C	600	ANP	PG-O1G	3.18	1.51	1.46
6	D	600	ANP	PG-O1G	3.17	1.51	1.46
6	F	600	ANP	PB-O1B	3.07	1.50	1.46
6	B	600	ANP	PB-O1B	3.00	1.50	1.46
6	A	600	ANP	PB-O1B	2.91	1.50	1.46
6	A	600	ANP	C5-C6	2.88	1.49	1.41
6	F	600	ANP	C5-C6	2.84	1.48	1.41
6	B	600	ANP	C5-C6	2.83	1.48	1.41
6	C	600	ANP	C5-C6	2.82	1.48	1.41
6	C	600	ANP	PB-O1B	2.76	1.50	1.46
6	D	600	ANP	C5-C6	2.67	1.48	1.41
6	B	600	ANP	C5-N7	-2.53	1.34	1.39
6	F	600	ANP	C8-N7	2.46	1.36	1.31
6	C	600	ANP	C5-N7	-2.44	1.34	1.39
6	D	600	ANP	C5-N7	-2.42	1.34	1.39
6	A	600	ANP	C5-N7	-2.36	1.34	1.39
6	A	600	ANP	C8-N7	2.34	1.36	1.31
6	C	600	ANP	PA-O3A	2.34	1.62	1.59
6	F	600	ANP	C5-N7	-2.33	1.34	1.39
6	D	600	ANP	C8-N7	2.30	1.36	1.31
6	C	600	ANP	C8-N7	2.30	1.36	1.31
6	A	600	ANP	PA-O3A	2.29	1.62	1.59
6	B	600	ANP	C8-N7	2.26	1.36	1.31
6	F	600	ANP	PG-O2G	-2.25	1.50	1.56
6	D	600	ANP	PG-O2G	-2.23	1.50	1.56
6	F	600	ANP	PA-O3A	2.18	1.61	1.59
6	C	600	ANP	PG-O3G	-2.18	1.51	1.56
6	A	600	ANP	PB-O3A	2.17	1.61	1.59
6	D	600	ANP	PG-O3G	-2.15	1.51	1.56
6	F	600	ANP	PB-O3A	2.15	1.61	1.59
6	F	600	ANP	PG-O3G	-2.12	1.51	1.56
6	A	600	ANP	PB-O2B	-2.08	1.51	1.56
6	C	600	ANP	PB-O3A	2.06	1.61	1.59
6	D	600	ANP	PB-O2B	-2.06	1.51	1.56
6	F	600	ANP	PB-O2B	-2.06	1.51	1.56
6	B	600	ANP	PB-O3A	2.05	1.61	1.59
6	B	600	ANP	PG-O2G	-2.04	1.51	1.56
6	C	600	ANP	PB-O2B	-2.04	1.51	1.56
6	B	600	ANP	PB-O2B	-2.03	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ANP	PG-O2G	-2.03	1.51	1.56
6	B	600	ANP	PG-O3G	-2.02	1.51	1.56
6	F	600	ANP	C4-N9	-2.02	1.33	1.37

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	ANP	C5-C4-N3	-6.15	118.25	126.72
6	A	600	ANP	O1G-PG-N3B	-5.88	103.11	111.77
6	A	600	ANP	C5-C4-N3	-5.79	118.75	126.72
6	C	600	ANP	C5-C4-N3	-5.78	118.75	126.72
6	D	600	ANP	C5-C4-N3	-5.42	119.25	126.72
6	F	600	ANP	C5-C4-N3	-5.33	119.38	126.72
6	B	600	ANP	O1G-PG-N3B	-5.27	104.00	111.77
6	B	600	ANP	N3-C4-N9	4.89	135.48	127.17
6	C	600	ANP	N3-C4-N9	4.75	135.24	127.17
6	C	600	ANP	O1G-PG-N3B	-4.74	104.78	111.77
6	A	600	ANP	N3-C4-N9	4.73	135.22	127.17
6	F	600	ANP	O1G-PG-N3B	-4.38	105.31	111.77
6	F	600	ANP	O2B-PB-O1B	4.26	119.00	109.87
6	D	600	ANP	N3-C4-N9	4.23	134.36	127.17
6	F	600	ANP	N3-C4-N9	4.06	134.06	127.17
6	B	600	ANP	C2-N3-C4	4.02	121.66	111.83
6	A	600	ANP	C2-N3-C4	3.89	121.33	111.83
6	A	600	ANP	N3-C2-N1	-3.82	122.80	128.58
6	B	600	ANP	N3-C2-N1	-3.81	122.82	128.58
6	F	600	ANP	N3-C2-N1	-3.80	122.84	128.58
6	C	600	ANP	C2-N3-C4	3.77	121.03	111.83
6	B	600	ANP	O2B-PB-O1B	3.74	117.89	109.87
6	F	600	ANP	C2-N3-C4	3.73	120.94	111.83
6	D	600	ANP	C2-N3-C4	3.71	120.89	111.83
6	D	600	ANP	N3-C2-N1	-3.69	122.99	128.58
6	D	600	ANP	O2B-PB-O1B	3.68	117.75	109.87
6	C	600	ANP	N3-C2-N1	-3.64	123.07	128.58
6	F	600	ANP	C4-C5-N7	-3.54	106.53	110.58
6	A	600	ANP	O2B-PB-O1B	3.53	117.44	109.87
6	A	600	ANP	C4-C5-N7	-3.48	106.60	110.58
6	C	600	ANP	O2B-PB-O1B	3.48	117.33	109.87
6	B	600	ANP	C4-C5-N7	-3.44	106.65	110.58
6	C	600	ANP	C4-C5-N7	-3.36	106.73	110.58
6	D	600	ANP	C4-C5-N7	-3.29	106.82	110.58
6	F	600	ANP	O1B-PB-N3B	-3.11	107.19	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	ANP	O2G-PG-O3G	2.85	115.25	107.59
6	A	600	ANP	C4-N9-C8	2.83	108.71	105.74
6	F	600	ANP	O2G-PG-O3G	2.82	115.17	107.59
6	A	600	ANP	C5-N7-C8	2.71	107.71	103.45
6	C	600	ANP	C4-N9-C8	2.71	108.58	105.74
6	B	600	ANP	O1B-PB-N3B	-2.66	107.86	111.77
6	B	600	ANP	C5-N7-C8	2.65	107.61	103.45
6	A	600	ANP	O1B-PB-N3B	-2.62	107.91	111.77
6	C	600	ANP	C5-N7-C8	2.56	107.47	103.45
6	B	600	ANP	O2G-PG-O3G	2.50	114.30	107.59
6	F	600	ANP	C5-N7-C8	2.47	107.33	103.45
6	F	600	ANP	C4-N9-C8	2.43	108.29	105.74
6	D	600	ANP	C5-N7-C8	2.42	107.26	103.45
6	A	600	ANP	O2G-PG-O3G	2.41	114.07	107.59
6	C	600	ANP	O2G-PG-O3G	2.38	113.99	107.59
6	D	600	ANP	C4-N9-C8	2.35	108.20	105.74
6	F	600	ANP	C6-C5-N7	2.34	136.60	132.09
6	B	600	ANP	C4-N9-C8	2.34	108.19	105.74
6	B	600	ANP	C3'-C2'-C1'	2.33	105.86	101.46
6	F	600	ANP	C2-N1-C6	2.27	122.46	118.73
6	D	600	ANP	C2'-C1'-N9	-2.22	107.78	113.30
6	A	600	ANP	C6-C5-N7	2.21	136.36	132.09
6	D	600	ANP	C6-C5-N7	2.18	136.30	132.09
6	A	600	ANP	N9-C8-N7	-2.11	110.95	113.94
6	D	600	ANP	C2-N1-C6	2.09	122.17	118.73
6	C	600	ANP	C2-N1-C6	2.08	122.15	118.73
6	A	600	ANP	C2-N1-C6	2.08	122.14	118.73

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	A	600	ANP	PG-N3B-PB-O3A
6	B	600	ANP	PB-N3B-PG-O1G
6	B	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	PG-N3B-PB-O3A
6	C	600	ANP	PB-N3B-PG-O1G
6	C	600	ANP	PG-N3B-PB-O1B
6	C	600	ANP	PG-N3B-PB-O3A
6	D	600	ANP	PB-N3B-PG-O1G

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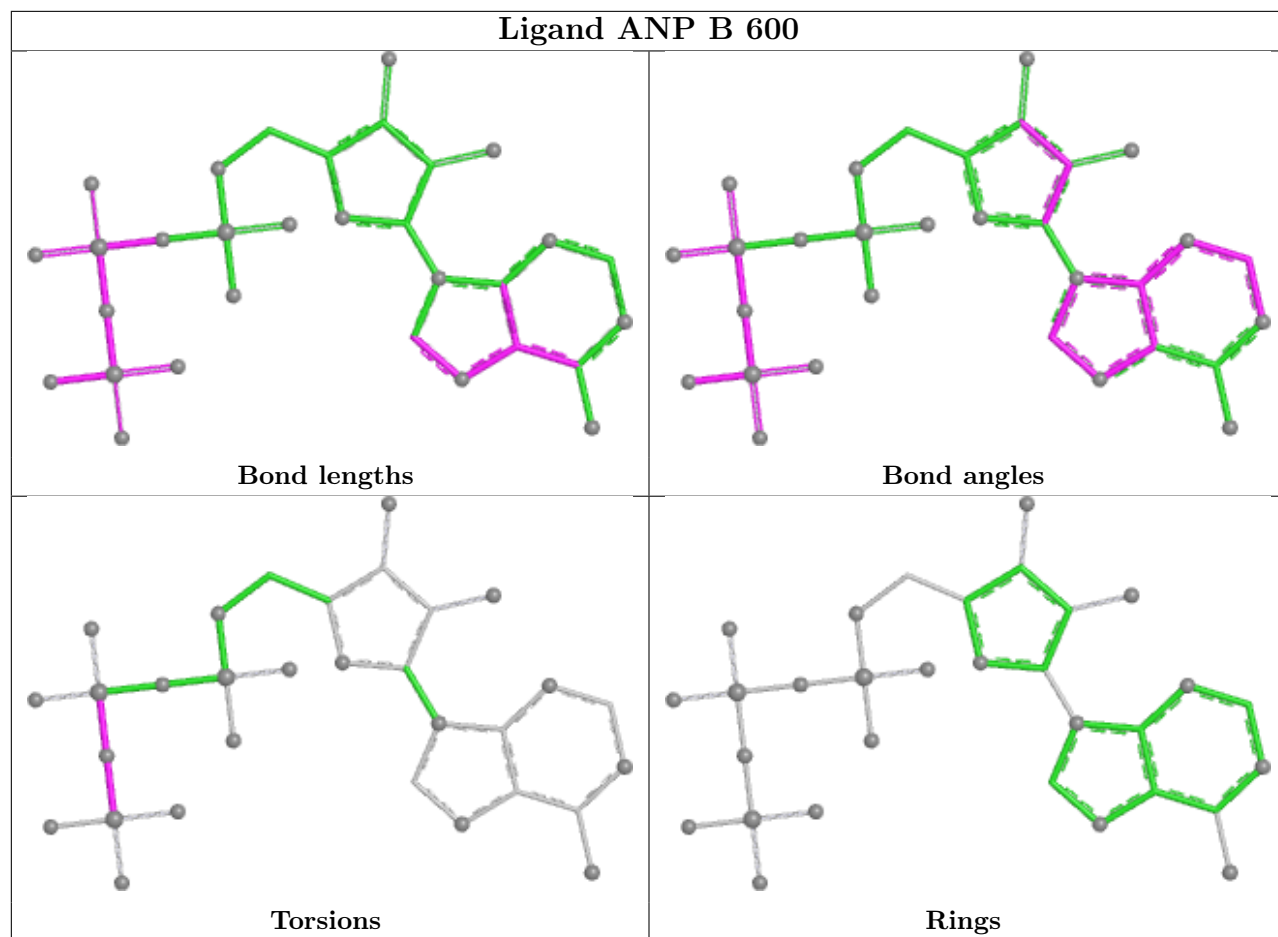
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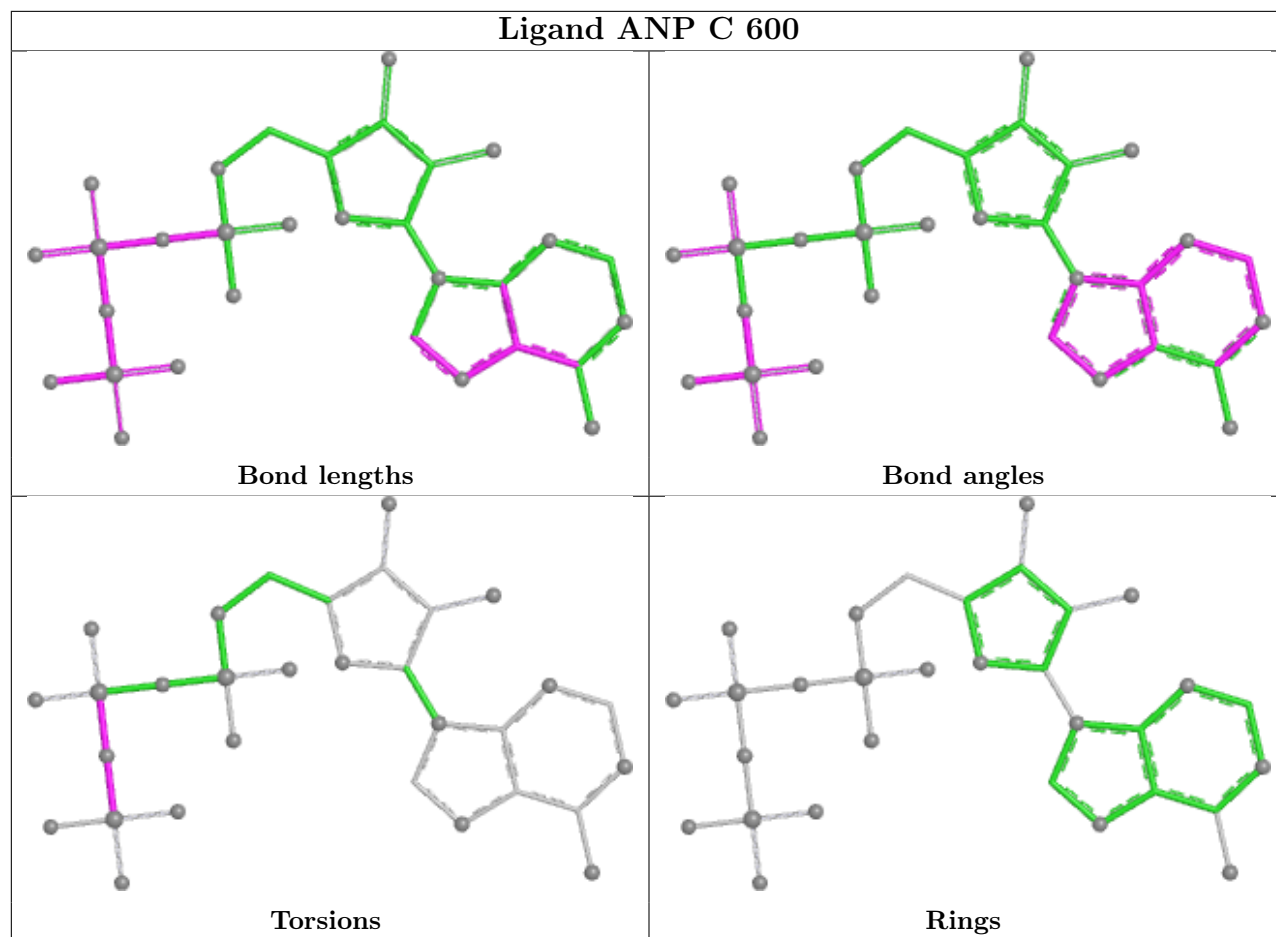
Mol	Chain	Res	Type	Atoms
6	D	600	ANP	PG-N3B-PB-O1B
6	D	600	ANP	PA-O3A-PB-O1B
6	F	600	ANP	PB-N3B-PG-O1G
6	F	600	ANP	PG-N3B-PB-O1B
6	F	600	ANP	PG-N3B-PB-O3A
6	F	600	ANP	C5'-O5'-PA-O1A
6	D	600	ANP	O4'-C4'-C5'-O5'
6	D	600	ANP	C3'-C4'-C5'-O5'
6	D	600	ANP	PA-O3A-PB-O2B
6	A	600	ANP	PA-O3A-PB-O1B
6	D	600	ANP	PG-N3B-PB-O3A

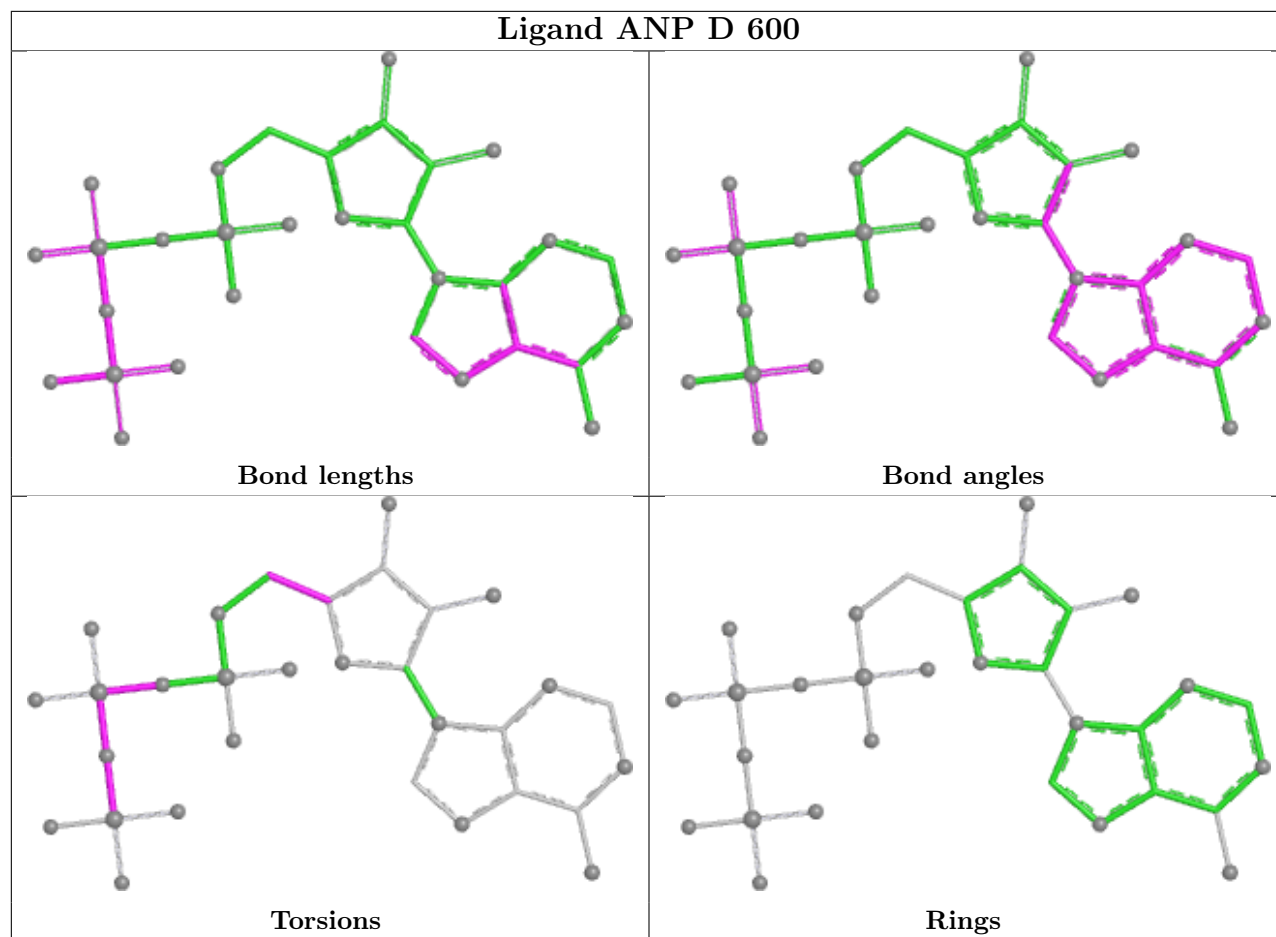
There are no ring outliers.

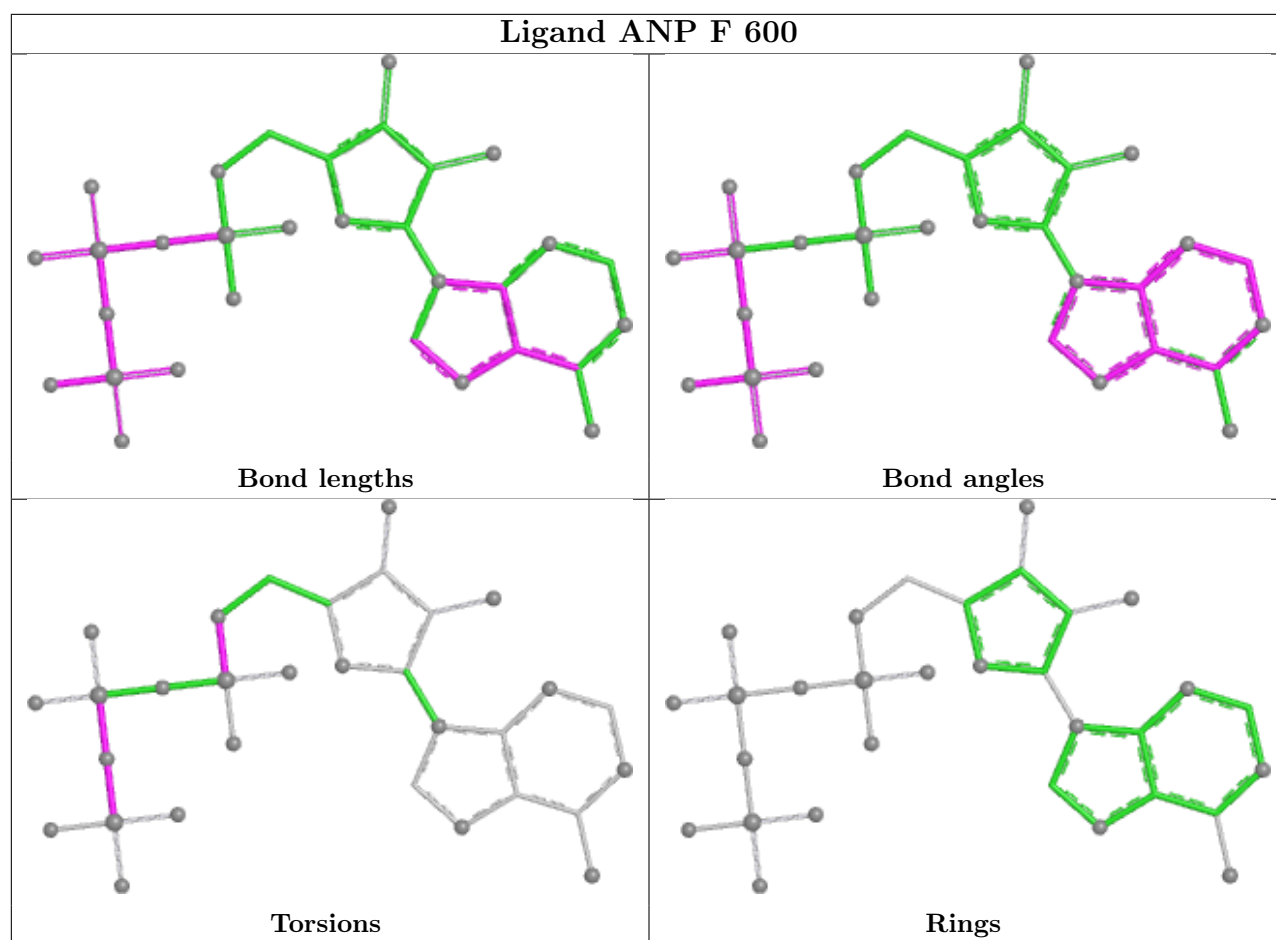
No monomer is involved in short contacts.

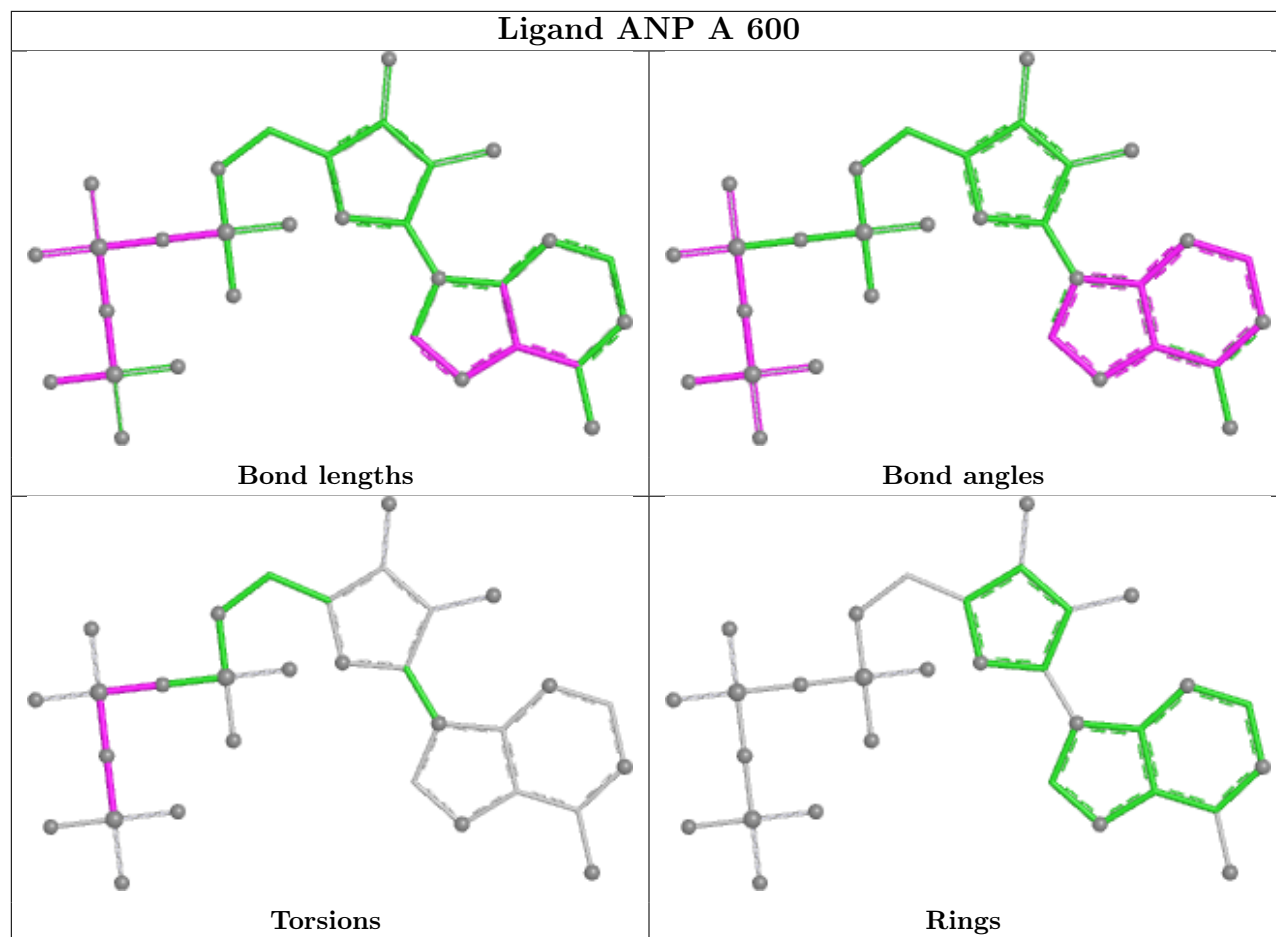
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

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	489/510 (95%)	-0.11	0 100 100	42, 66, 108, 144	0
1	B	480/510 (94%)	-0.18	1 (0%) 91 83	38, 59, 135, 163	0
1	C	488/510 (95%)	-0.10	1 (0%) 91 83	42, 61, 97, 142	0
2	D	467/482 (96%)	-0.21	1 (0%) 91 83	43, 61, 88, 109	0
2	E	458/482 (95%)	0.00	1 (0%) 91 83	37, 72, 139, 158	0
2	F	466/482 (96%)	-0.17	2 (0%) 88 76	39, 58, 97, 125	0
3	G	213/273 (78%)	0.41	5 (2%) 61 39	47, 115, 157, 174	0
4	H	128/146 (87%)	0.57	4 (3%) 51 30	92, 141, 175, 191	0
5	I	47/50 (94%)	0.37	0 100 100	90, 134, 161, 172	0
All	All	3236/3445 (93%)	-0.06	15 (0%) 87 73	37, 66, 139, 191	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	53	PRO	3.2
1	C	310	ALA	2.8
2	F	9	THR	2.8
3	G	270	ALA	2.5
4	H	101	ASP	2.4
1	B	451	GLY	2.3
4	H	112	LEU	2.3
4	H	105	LEU	2.3
2	F	474	ALA	2.2
3	G	3	LEU	2.2
3	G	69	ILE	2.1
2	D	343	GLY	2.1
3	G	1	ALA	2.1
2	E	158	ALA	2.0
3	G	13	ILE	2.0

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](#)

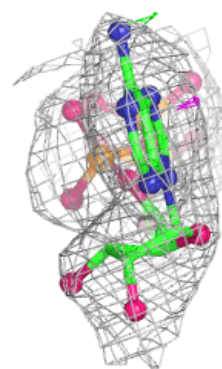
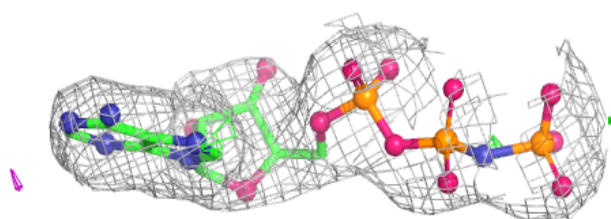
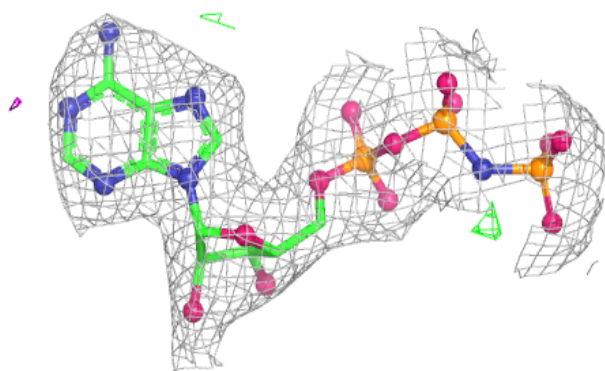
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
9	TS6	E	603	5/5	0.67	0.14	100,107,108,109	0
10	NA	F	503	1/1	0.75	0.23	61,61,61,61	0
8	CL	D	503	1/1	0.76	0.14	76,76,76,76	0
6	ANP	D	600	31/31	0.94	0.08	48,49,55,55	0
6	ANP	A	600	31/31	0.94	0.07	47,52,56,56	0
6	ANP	C	600	31/31	0.95	0.07	47,53,55,55	0
6	ANP	F	600	31/31	0.96	0.06	47,58,68,69	0
6	ANP	B	600	31/31	0.96	0.06	51,57,59,59	0
7	MG	C	601	1/1	0.98	0.08	49,49,49,49	0
7	MG	F	601	1/1	0.99	0.03	48,48,48,48	0
7	MG	B	601	1/1	0.99	0.03	53,53,53,53	0
7	MG	A	601	1/1	0.99	0.03	48,48,48,48	0
7	MG	D	601	1/1	0.99	0.04	55,55,55,55	0

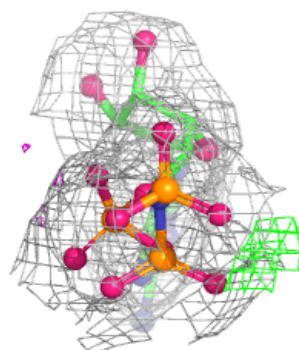
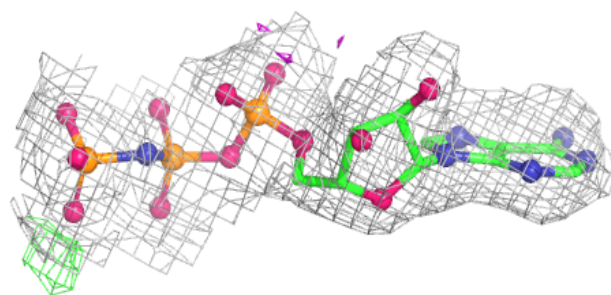
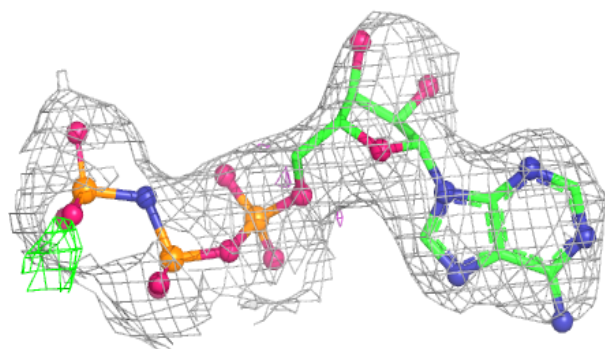
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP D 600:

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

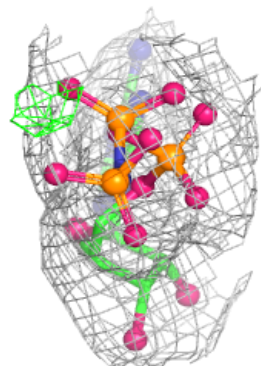
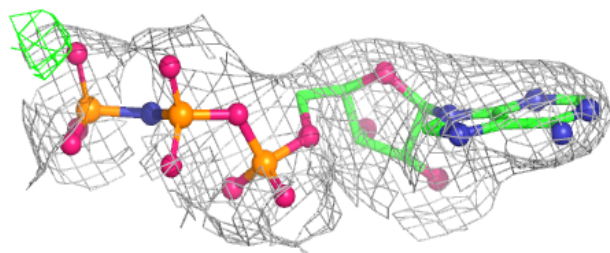
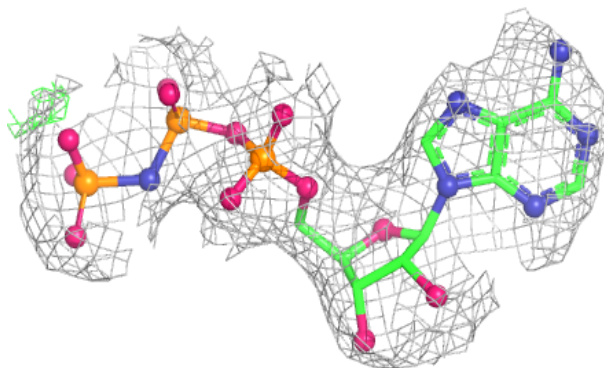
**Electron density around ANP A 600:**

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

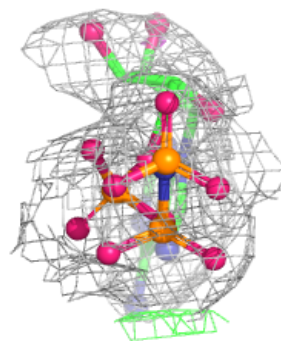
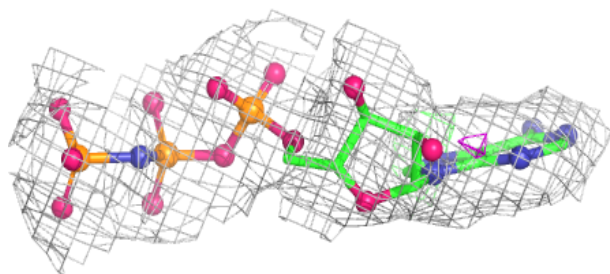
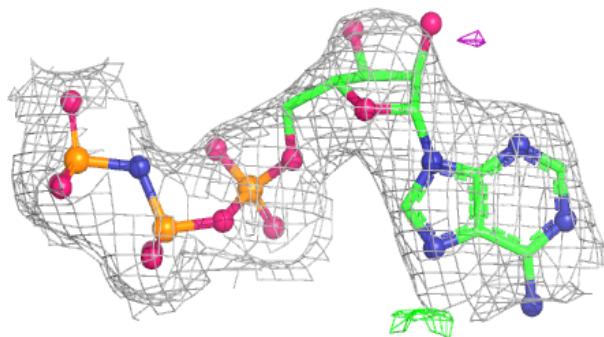


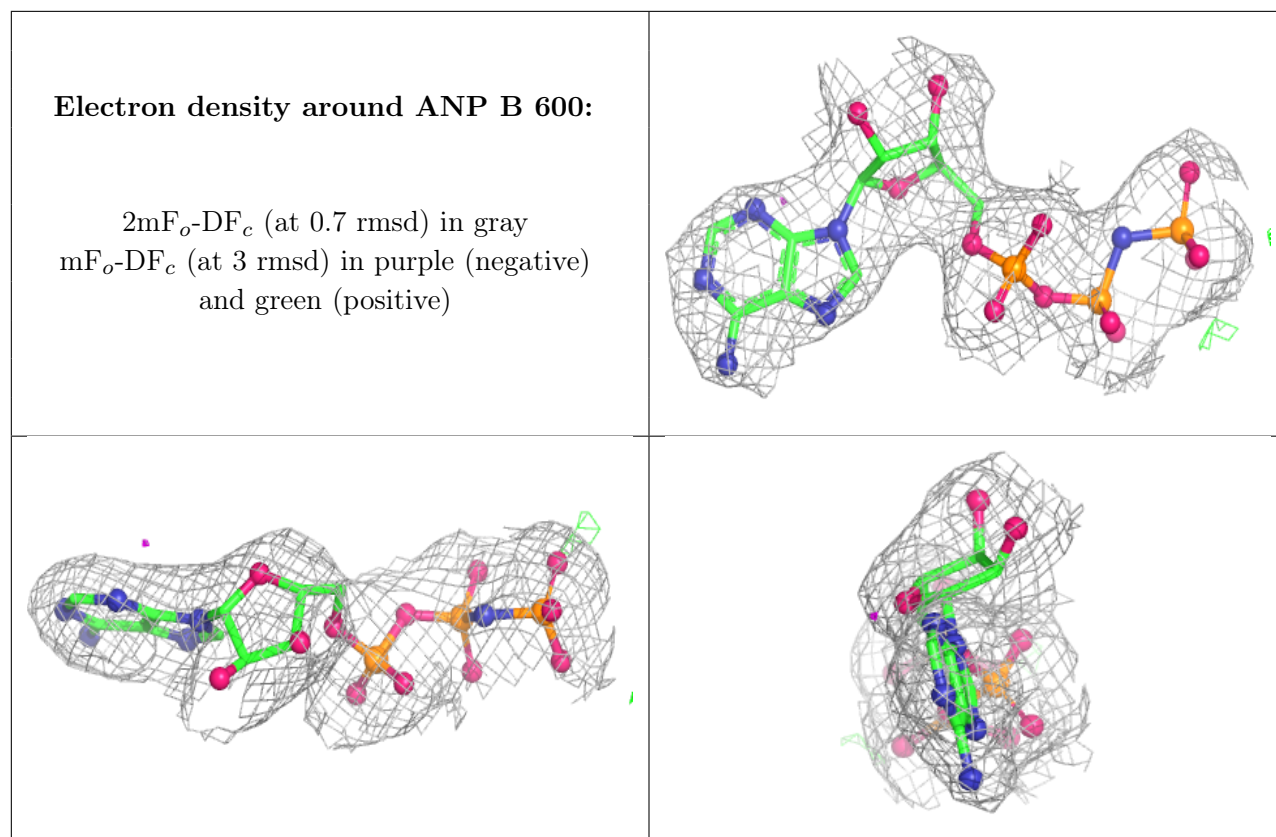
Electron density around ANP C 600:

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

**Electron density around ANP F 600:**

$2mF_o-DF_c$ (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.