



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 01:50 am BST

PDB ID : 1E1Q  
Title : BOVINE MITOCHONDRIAL F1-ATPASE AT 100K  
Authors : Braig, K.; Menz, R.I.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2000-05-10  
Resolution : 2.61 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

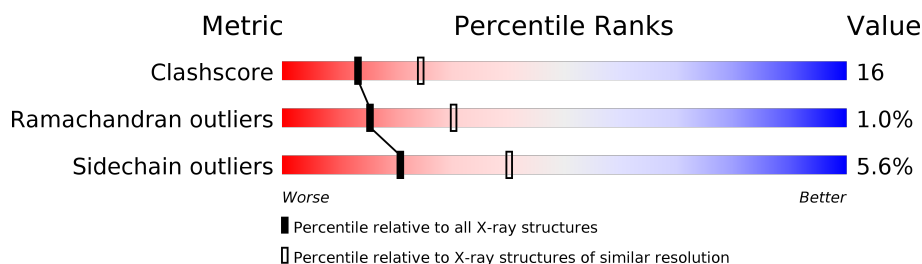
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	272	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23366 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

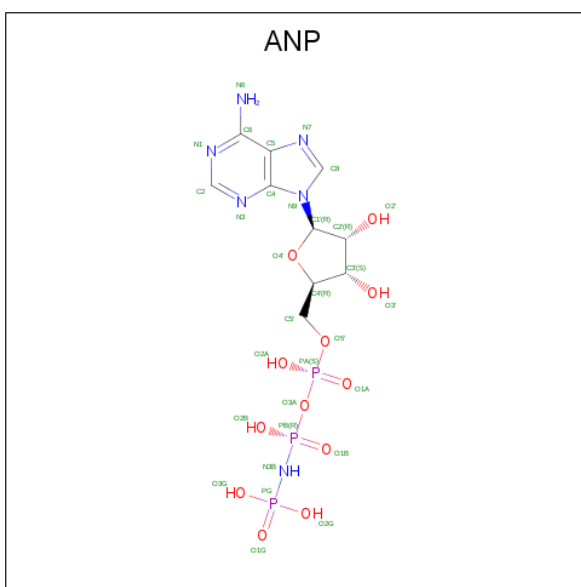
- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

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	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

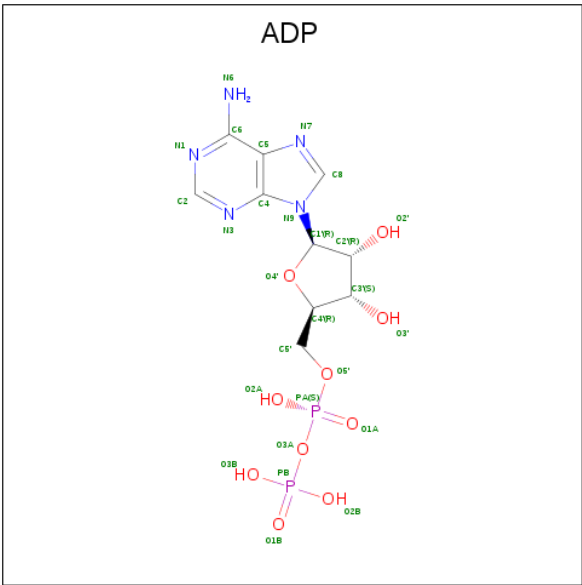


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	F	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

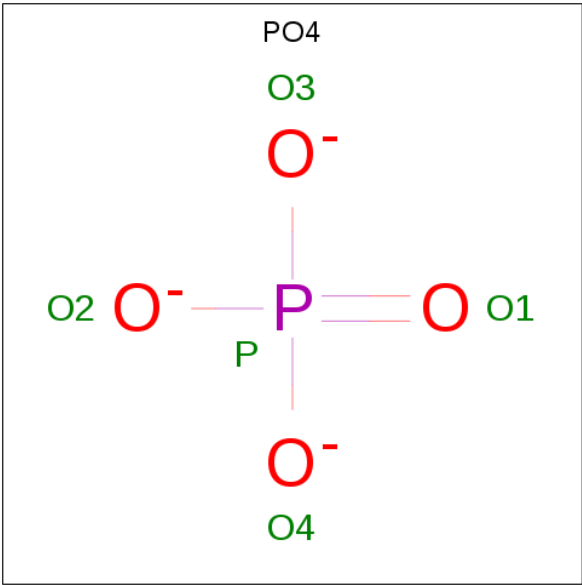
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

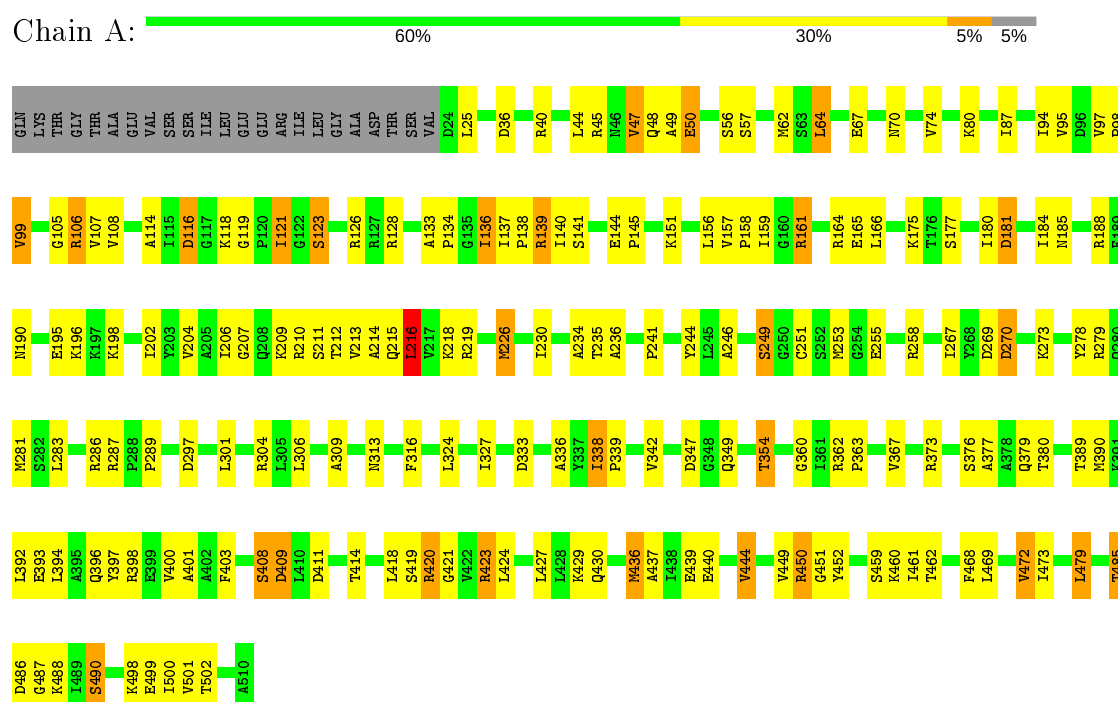
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	100	Total 100	O 100	0	0
8	B	83	Total 83	O 83	0	0
8	C	109	Total 109	O 109	0	0
8	D	92	Total 92	O 92	0	0
8	E	44	Total 44	O 44	0	0
8	F	107	Total 107	O 107	0	0
8	G	7	Total 7	O 7	0	0

### 3 Residue-property plots [i](#)

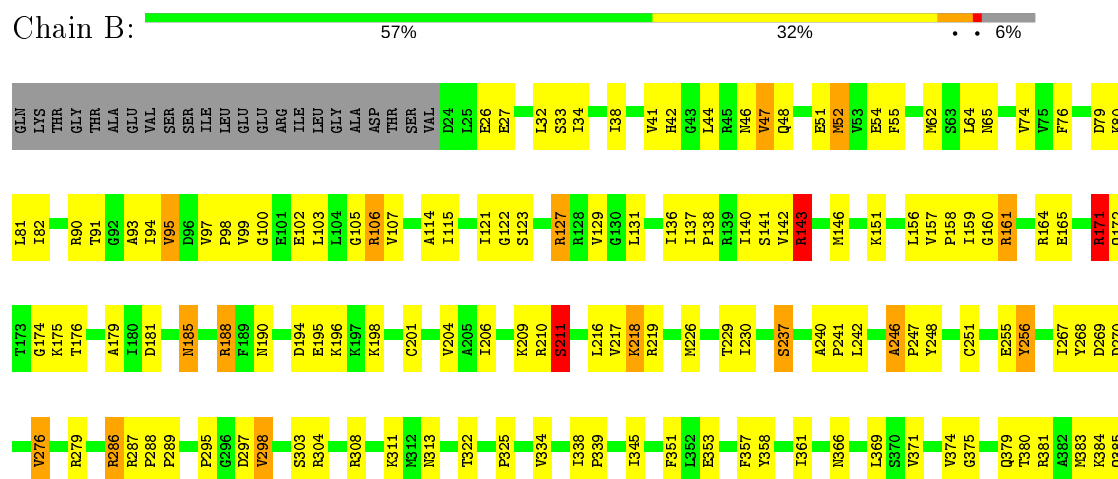
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

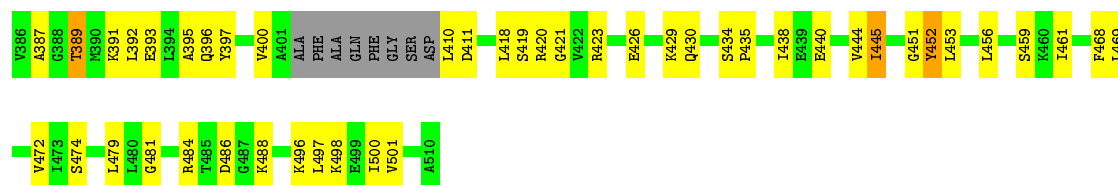
Note EDS was not executed.

#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



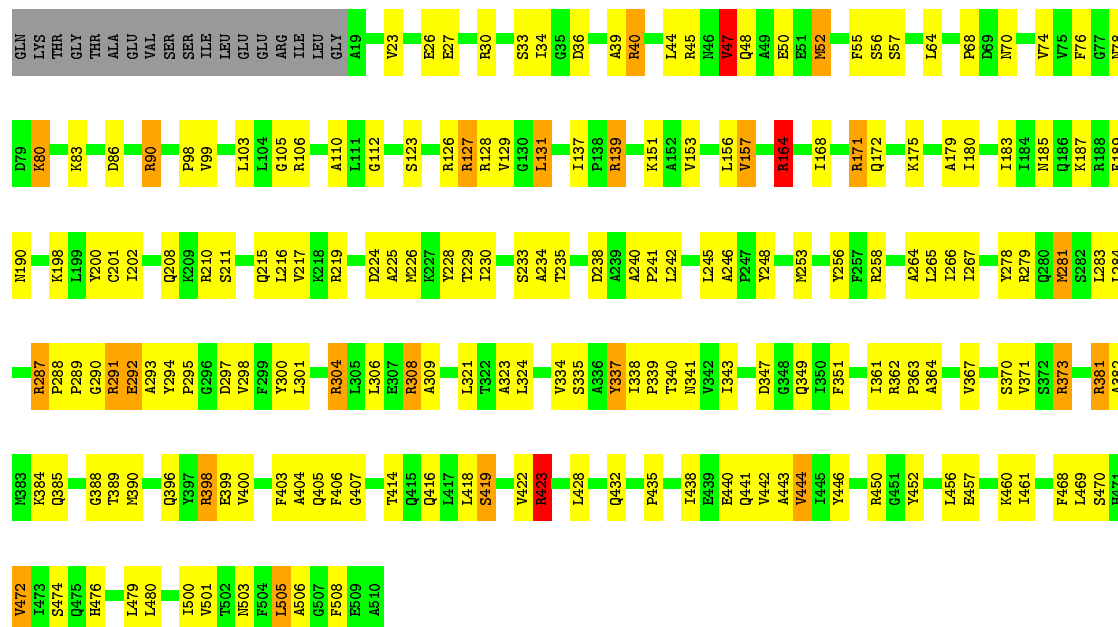
#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE





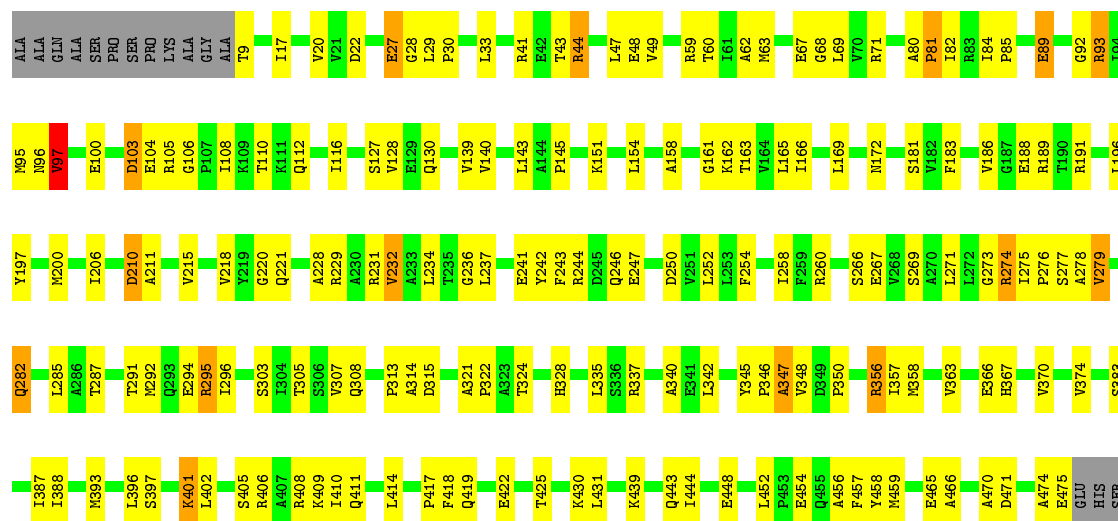
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

Chain C: 59% 32% 5%



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

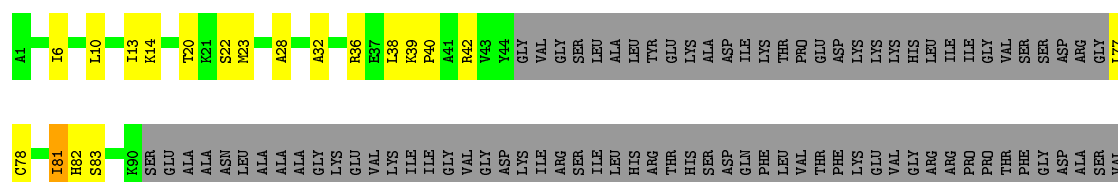
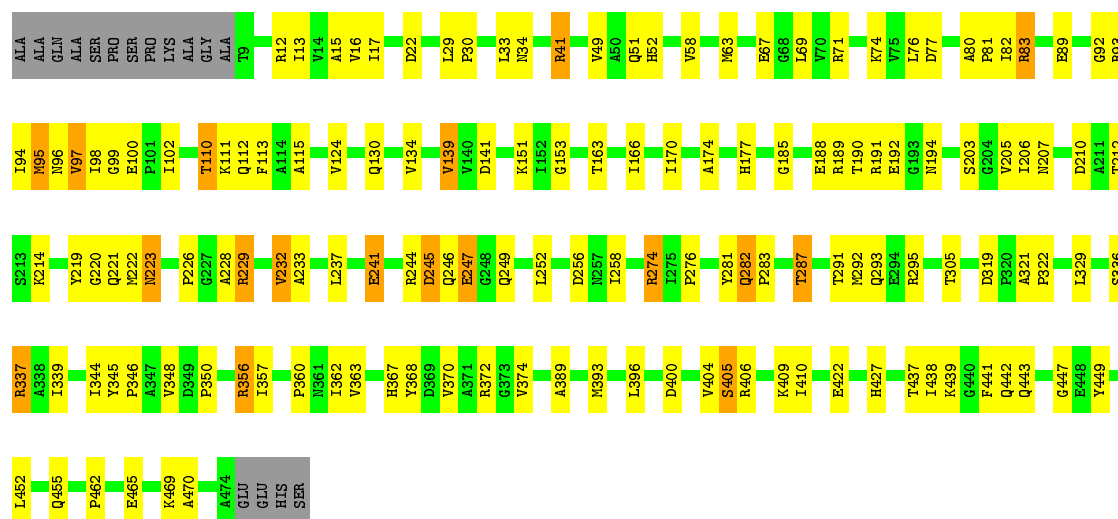
Chain D: 60% 34% 6%



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



I438	S355	T258	I170	R83	ALA
K439	R356	F259	A174	I84	GLN
M358	I357	Q263	F183	G87	ALA
G440	M358	Q263	A184	P88	SER
I444	P360	E267	G185	E89	PRO
Y449	M361	T275		R83	SER
L452	S365	P276	E188	I84	LVS
Q455	E366	S277	R189	M95	ALA
A456	H367	A278	T190	N96	GLY
M459	Y368	G280	A191	V97	ALA
I463	P369	Y281	E192		T9
A466	V370	Q282	M194	E100	T10
V467	V374	P283	D195	I102	G11
A468			I196	D103	R12
A474		D288	Y197	E104	
GLU	I377	M292	I201	R105	A15
GLU	L384	Q293	L208	T110	D22
HIS	I387	R295	K209	K111	V23
SER	I388	T296	D210	Q112	Q24
	A389	T297	A211	A115	F25
	I390	T298	T212	I116	
	I391	T299	S213	A120	L29
	G392	K300	K214	P121	I32
	K393		V215		L33
	D394	S303	A216	E125	L36
	L396	I304	L217	M126	R41
	V404	S306	Q221	S127	E42
	S405	V307	M222	V128	T43
		Q308	M223		
		A309	E224	I132	V46
		I310	P225		L47
				G136	E48
		P313	A228	I137	V49
		A314	R229	K138	
		D315	A230	V139	H52
			R231		
		D319	V232	L142	S56
		P320		L143	
		A321	T235	A144	T60
		P322		P145	
				Y146	D64
		F326	T238	A147	G65
				K148	T66
		L329	F243	G149	E67
		D330		G150	G68
		A331	Q246	K151	L69
				I152	V70
		V334	V251		R71
			L252	K162	
		R337	L253	T163	L76
			F254	V164	
		D352	T255	M167	A80
		S353	D256	P81	
		T354	M257	I52	



ILE	TYR
ALA	GLN
LEU	GLU
GLU	TYR
LEU	SER
LEU	L209
ASN	A210
SER	N211
GLY	
TYR	S220
GLU	E224
PHE	
ASP	
GLU	R228
GLY	N229
SER	
ILE	N232
ILE	
PHE	S236
ASN	K237
ARG	D238
PHE	A239
ARG	S240
SER	E241
VAL	N242
ILE	T243
SER	
TYR	L246
LYS	
THR	F250
GLU	
GLU	R254
LYS	
PRO	T259
ILE	
PHE	L262
SER	I263
LEU	
ASP	T266
THR	
ILE	L272
SER	
SER	
ALA	
GLU	
SER	
MET	
SER	
ILE	
TYR	
ASP	
ASP	
ILE	
ASP	
ALA	
ASP	
VAL	
LEU	
ARG	
ASN	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	280.80 Å   107.40 Å   139.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.61	Depositor
% Data completeness (in resolution range)	95.0 (20.00-2.61)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.232 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

## 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: PO4, ANP, MG, ADP

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	0.59	0/3766	1.24	28/5080 (0.6%)
1	B	0.60	0/3704	1.24	23/4995 (0.5%)
1	C	0.63	0/3799	1.33	28/5126 (0.5%)
2	D	0.59	0/3596	1.28	26/4879 (0.5%)
2	E	0.55	0/3587	1.18	20/4867 (0.4%)
2	F	0.63	0/3587	1.29	26/4867 (0.5%)
3	G	0.45	0/949	0.97	4/1266 (0.3%)
All	All	0.59	0/22988	1.25	155/31080 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	274	ARG	NE-CZ-NH1	14.94	127.77	120.30
1	C	304	ARG	NE-CZ-NH2	13.00	126.80	120.30
1	C	423	ARG	NE-CZ-NH2	-12.63	113.98	120.30
1	C	219	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	A	210	ARG	CD-NE-CZ	11.64	139.89	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	97	VAL	Mainchain
2	E	223	ASN	Mainchain

## 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	3715	0	3814	136	0
1	B	3656	0	3765	142	0
1	C	3748	0	3845	125	0
2	D	3539	0	3592	119	0
2	E	3530	0	3587	145	0
2	F	3530	0	3586	94	0
3	G	945	0	1019	30	0
4	A	31	0	13	1	0
4	B	31	0	13	2	0
4	C	31	0	13	2	0
4	F	31	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	D	27	0	12	1	0
7	E	5	0	0	1	0
8	A	100	0	0	6	0
8	B	83	0	0	6	0
8	C	109	0	0	3	0
8	D	92	0	0	4	0
8	E	44	0	0	4	0
8	F	107	0	0	3	0
8	G	7	0	0	0	0
All	All	23366	0	23272	741	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 16.

The worst 5 of 741 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:D:282:GLN:H	2:D:282:GLN:HE21	0.96	0.96
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.52	0.91
2:D:139:VAL:HB	8:D:2027:HOH:O	1.72	0.90
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.54	0.89
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.56	0.88

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	485/510 (95%)	452 (93%)	25 (5%)	8 (2%)	9	18
1	B	475/510 (93%)	434 (91%)	38 (8%)	3 (1%)	25	45
1	C	490/510 (96%)	457 (93%)	28 (6%)	5 (1%)	15	30
2	D	465/482 (96%)	429 (92%)	32 (7%)	4 (1%)	17	33
2	E	464/482 (96%)	419 (90%)	40 (9%)	5 (1%)	14	27
2	F	464/482 (96%)	431 (93%)	31 (7%)	2 (0%)	34	55
3	G	116/272 (43%)	107 (92%)	6 (5%)	3 (3%)	5	8
All	All	2959/3248 (91%)	2729 (92%)	200 (7%)	30 (1%)	15	30

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	ASP
2	E	211	ALA
1	B	452	TYR
1	C	337	TYR
1	C	388	GLY

### 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	393/412 (95%)	365 (93%)	28 (7%)	14	28
1	B	388/412 (94%)	371 (96%)	17 (4%)	28	52
1	C	397/412 (96%)	368 (93%)	29 (7%)	14	27
2	D	377/386 (98%)	358 (95%)	19 (5%)	24	46
2	E	376/386 (97%)	355 (94%)	21 (6%)	21	40
2	F	376/386 (97%)	359 (96%)	17 (4%)	27	50
3	G	102/230 (44%)	97 (95%)	5 (5%)	25	46
All	All	2409/2624 (92%)	2273 (94%)	136 (6%)	21	40

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	349	GLN
2	D	44	ARG
2	F	232	VAL
1	C	390	MET
1	C	470	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	282	GLN
2	E	263	GLN
2	F	282	GLN
2	E	223	ASN
2	E	246	GLN

### 5.3.3 RNA ⓘ

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 11 ligands modelled in this entry, 5 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$
4	ANP	F	600	5	29,33,33	1.48	5 (17%)	31,52,52	1.78	5 (16%)
6	ADP	D	600	5	24,29,29	0.92	2 (8%)	29,45,45	1.27	3 (10%)
7	PO4	E	602	-	4,4,4	0.76	0	6,6,6	0.51	0
4	ANP	B	600	5	29,33,33	1.63	7 (24%)	31,52,52	2.74	7 (22%)
4	ANP	A	600	5	29,33,33	1.46	5 (17%)	31,52,52	1.59	6 (19%)
4	ANP	C	600	5	29,33,33	1.59	6 (20%)	31,52,52	1.60	8 (25%)

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
4	ANP	F	600	5	-	4/14/38/38	0/3/3/3
4	ANP	A	600	5	-	3/14/38/38	0/3/3/3
6	ADP	D	600	5	-	5/12/32/32	0/3/3/3
4	ANP	B	600	5	-	3/14/38/38	0/3/3/3
4	ANP	C	600	5	-	3/14/38/38	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	ANP	PG-O3G	-4.32	1.45	1.56
4	C	600	ANP	PG-O3G	-3.98	1.46	1.56
4	F	600	ANP	PG-O3G	-3.67	1.46	1.56
4	C	600	ANP	PB-O3A	-3.61	1.54	1.59
4	A	600	ANP	PG-O3G	-3.44	1.47	1.56

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ANP	O1B-PB-N3B	12.61	130.33	111.77
4	F	600	ANP	C5-C6-N6	6.45	130.15	120.35
4	A	600	ANP	O2B-PB-O1B	4.58	119.52	109.92
4	B	600	ANP	O2G-PG-O1G	-4.17	102.97	113.45
4	A	600	ANP	C5-C6-N6	3.38	125.48	120.35

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	600	ANP	PB-N3B-PG-O1G
4	F	600	ANP	PG-N3B-PB-O1B
4	F	600	ANP	PA-O3A-PB-O1B
4	F	600	ANP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O2B

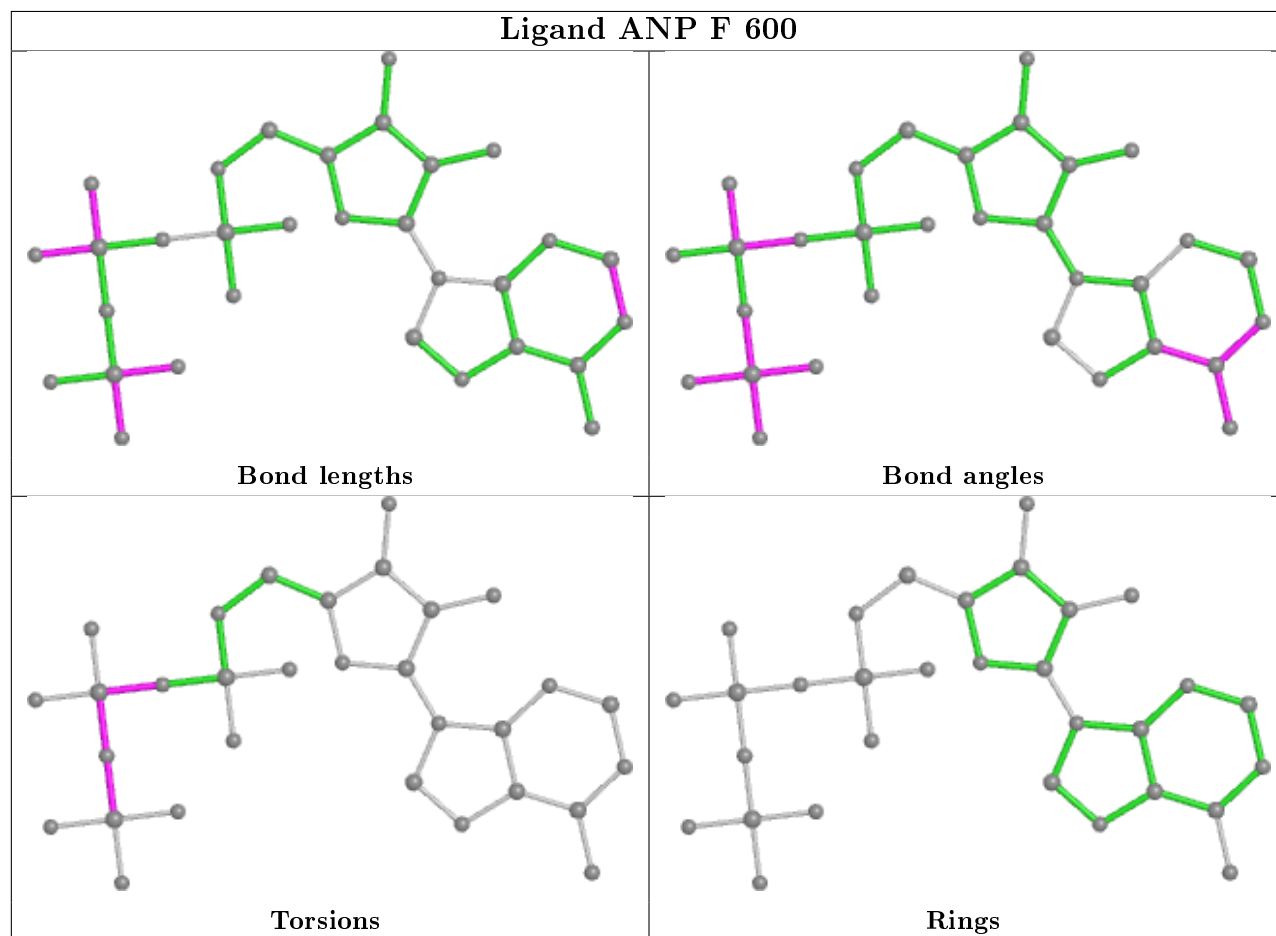
There are no ring outliers.

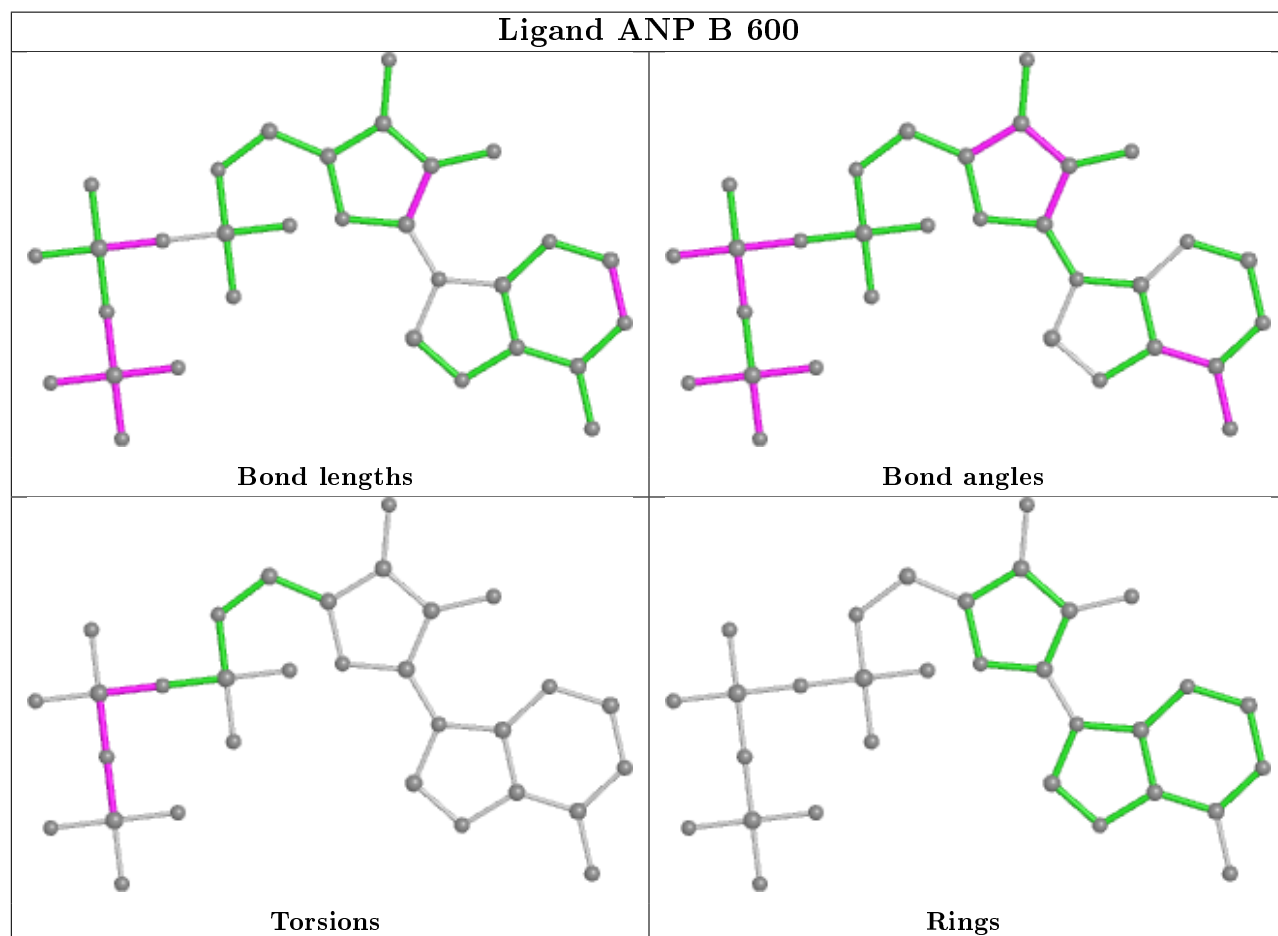
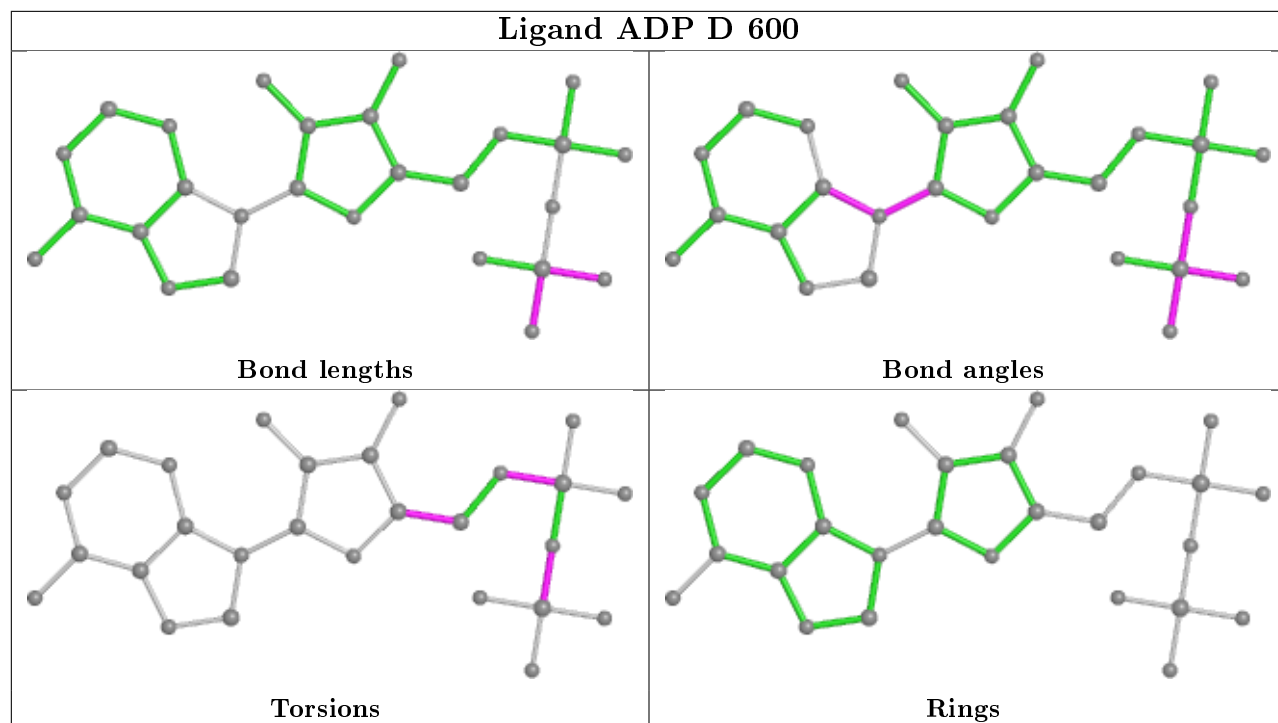
5 monomers are involved in 7 short contacts:

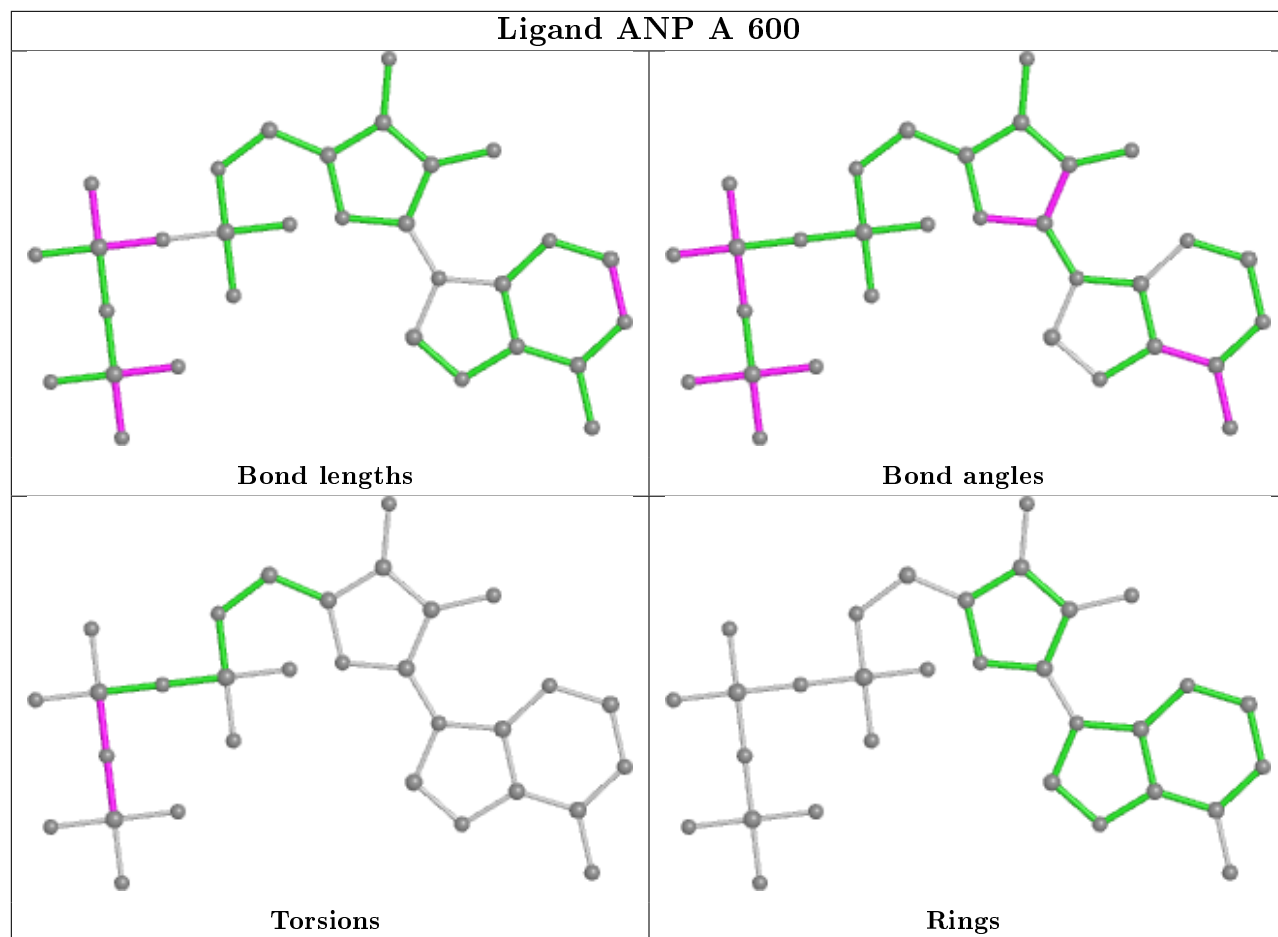
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	ADP	1	0
7	E	602	PO4	1	0
4	B	600	ANP	2	0
4	A	600	ANP	1	0
4	C	600	ANP	2	0

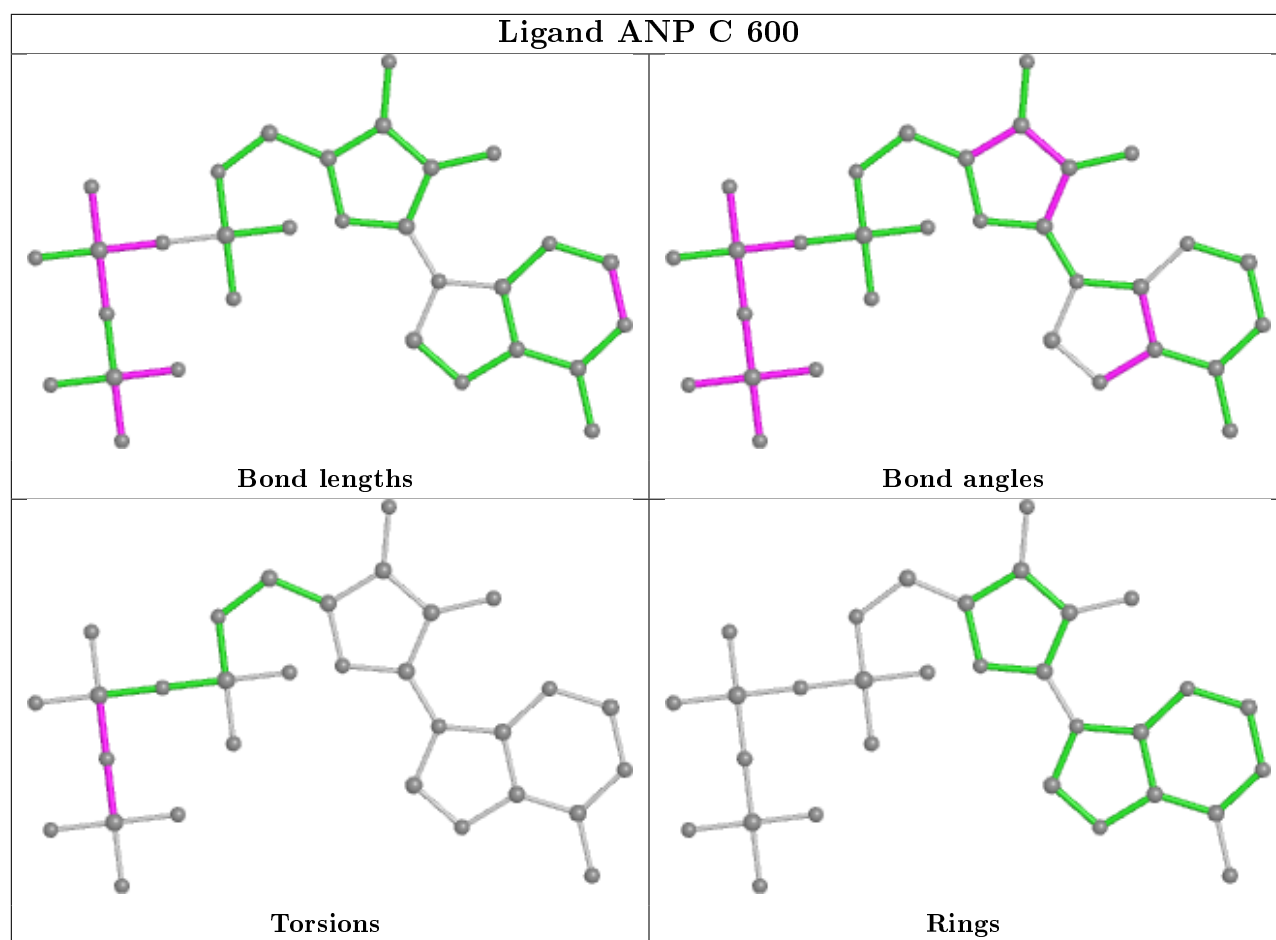
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.