



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:40 AM UTC

PDB ID : 1E1Q / pdb_00001e1q
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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

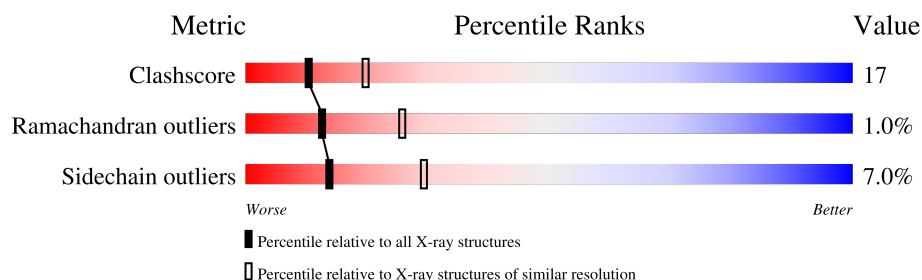
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (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 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 $\leq 5\%$.

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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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 (CCD ID: MG) (formula: Mg).

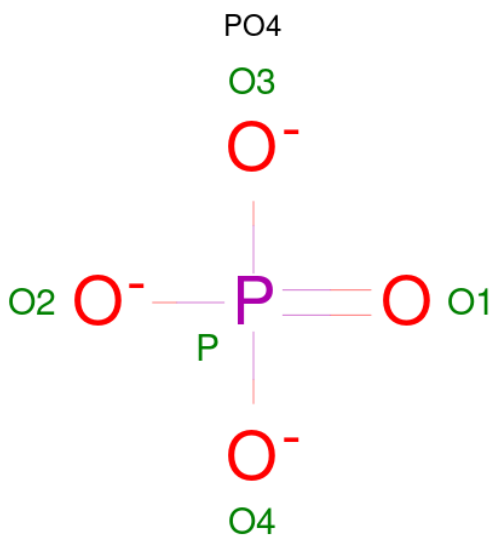
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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 (CCD ID: PO4) (formula: O_4P).



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

- Molecule 8 is water.

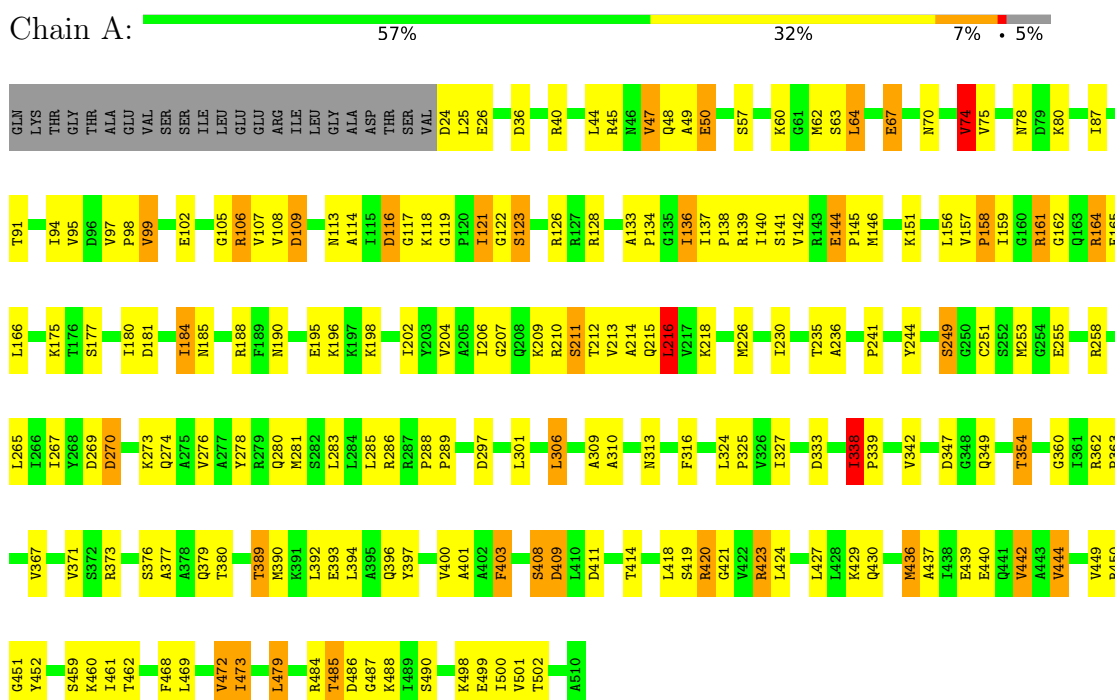
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	100	Total 100	O 100	0	0
8	B	83	Total 83	O 83	0	0
8	C	109	Total 109	O 109	0	0
8	D	92	Total 92	O 92	0	0
8	E	44	Total 44	O 44	0	0
8	F	107	Total 107	O 107	0	0
8	G	7	Total 7	O 7	0	0

3 Residue-property plots

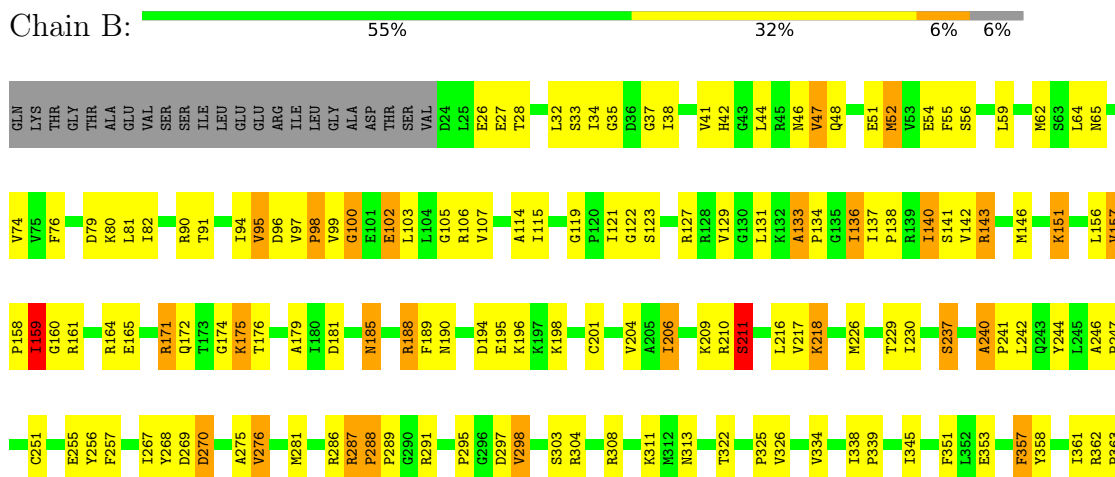
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

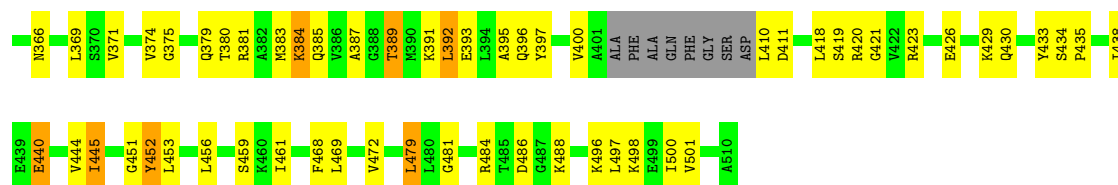
Note EDS was not executed.

• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



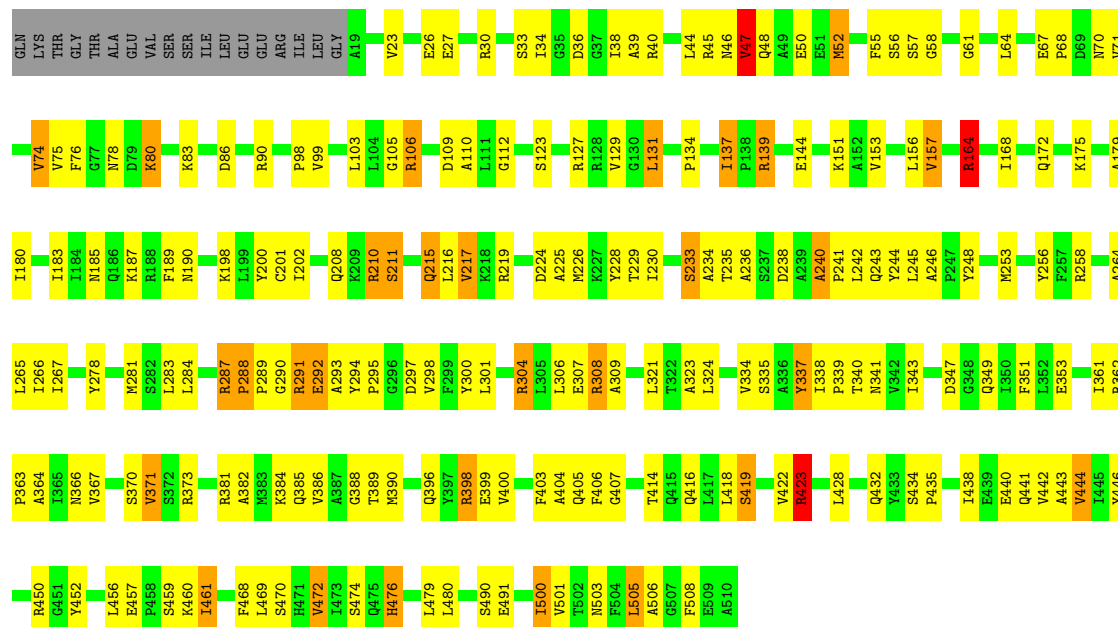
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE





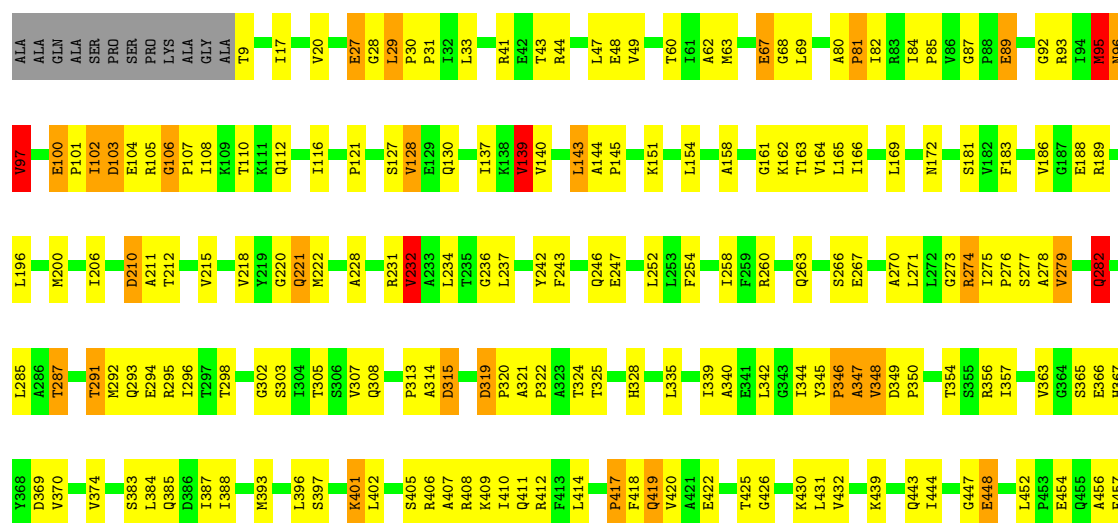
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

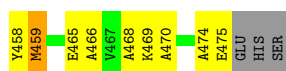
Chain C: 56% 34% 6% . .



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

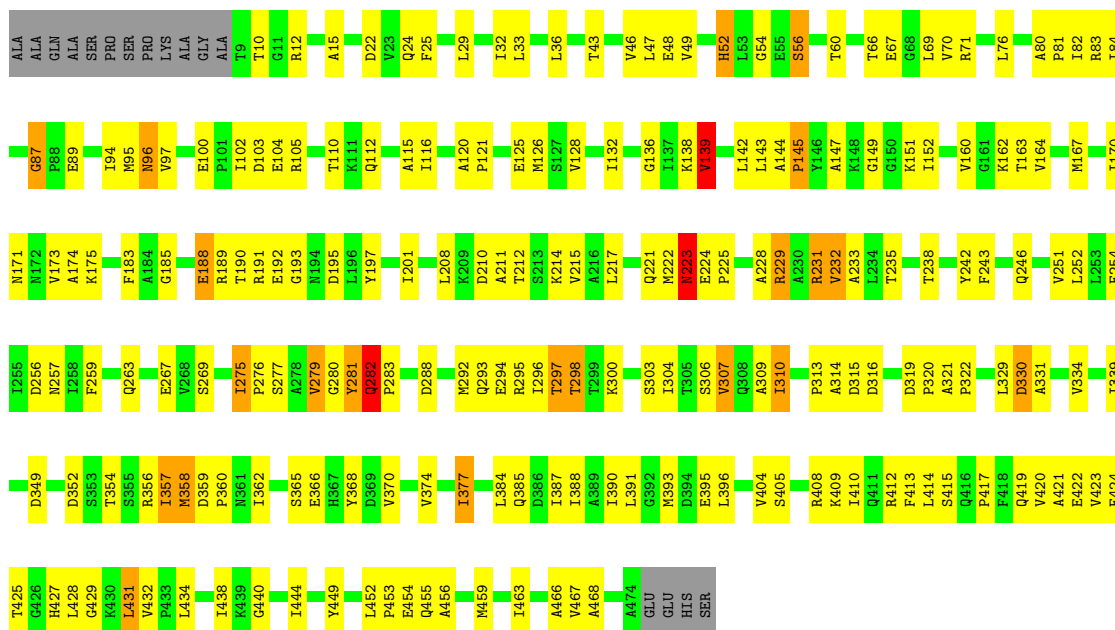
Chain D: 55% 35% 6% . .





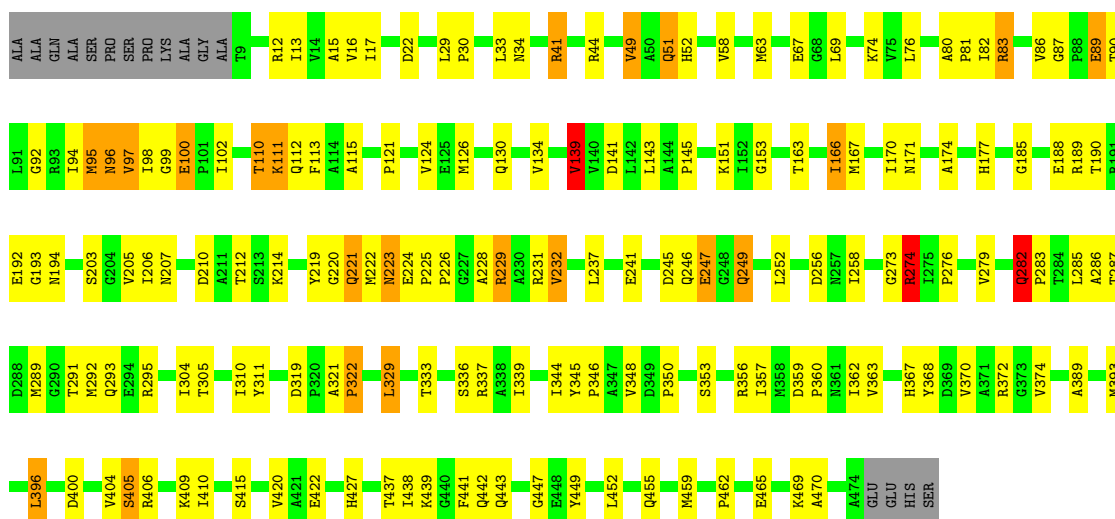
• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

Chain E: 53% 39% . . .



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

Chain F: 62% 29% 5% . . .



• Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE

Chain G: 29% 14% . 55%

TYR	ILE	C78	A1
GLN	ALA		
LEU	LEU	I81	I6
TYR	LEU	H82	
SER	LEU	S83	L10
L209	LEU		
A210	ASN	K89	I13
M211	SER	SER	K14
	GLY	GLU	
S220	TYR	ALA	T20
T221	GLU	ALA	K21
T222	PHE	ASN	S22
S223	ASP	LEU	M23
E224	GLU	ALA	
Q225	GLY	ALA	A28
S226	SER	ALA	
A227	ILE	GLY	A32
R228	ILE	LYS	
M229	PHE	GLU	R36
	ASN	VAL	E37
M232	ARG	LYS	L38
S236	PHE	ILE	K39
R238	ARG	ILE	P40
T237	SER	GLY	A41
A239	VAL	VAL	R42
S240	ILE	ASP	V43
E241	SER	GLY	Y44
M242	TYR	LYS	GLY
I243	LYS	ILE	VAL
	THR	ARG	GLY
L246	GLU	ILE	GLY
	GLU	ILE	SER
F250	LYS	LEU	LEU
	PRO	HIS	LEU
R254	PHE	THR	TVR
Q255	SER	HIS	GLU
	LEU	SER	LYS
T259	ASP	ASP	ALA
	THR	GLN	ASP
L262	ILE	PHE	ILE
I263	SER	LEU	LYS
	SER	VAL	THR
T266	ALA	THR	PHO
	GLU	PHE	GLU
L272	SER	LYS	ASP
	MET	GLU	LYS
	SER	VAL	LYS
	ILE	GLY	LYS
	TYR	ARG	HIS
	ASP	ARG	LEU
	ASP	PRO	ILE
	ILE	PRO	ILE
	ASP	THR	GLY
	ALA	PHE	VAL
	ASP	GLY	SER
	VAL	ASP	ASP
	LEU	ALA	ARG
	ARG	SER	GLY
	ASN	VAL	L77

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, α , β , γ	280.80Å 107.40Å 139.60Å 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 ²)	63.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MG, ADP, PO4

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	0.76	0/3766	1.59	44/5080 (0.9%)
1	B	0.78	0/3704	1.62	43/4995 (0.9%)
1	C	0.81	0/3799	1.70	54/5126 (1.1%)
2	D	0.78	0/3596	1.67	64/4879 (1.3%)
2	E	0.70	0/3587	1.58	42/4867 (0.9%)
2	F	0.82	0/3587	1.66	55/4867 (1.1%)
3	G	0.61	0/949	1.36	5/1266 (0.4%)
All	All	0.77	0/22988	1.63	307/31080 (1.0%)

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 307 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	CA-CB-CG	15.92	128.52	112.60
1	B	185	ASN	CA-CB-CG	14.48	127.08	112.60
2	D	97	VAL	CB-CA-C	-12.81	95.79	111.81
1	A	210	ARG	CD-NE-CZ	11.07	139.89	124.40
1	B	270	ASP	CA-CB-CG	10.82	123.42	112.60

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	141	0
1	B	3656	0	3765	152	0
1	C	3748	0	3845	130	0
2	D	3539	0	3592	126	0
2	E	3530	0	3587	154	0
2	F	3530	0	3586	101	0
3	G	945	0	1019	32	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	4	0
8	G	7	0	0	0	0
All	All	23366	0	23272	783	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 17.

The worst 5 of 783 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:A:390:MET:HE3	1:A:424:LEU:HD22	1.44	0.98
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

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%)	7	15
1	B	475/510 (93%)	434 (91%)	38 (8%)	3 (1%)	21	39
1	C	490/510 (96%)	457 (93%)	28 (6%)	5 (1%)	12	26
2	D	465/482 (96%)	429 (92%)	32 (7%)	4 (1%)	14	28
2	E	464/482 (96%)	419 (90%)	40 (9%)	5 (1%)	11	23
2	F	464/482 (96%)	431 (93%)	31 (7%)	2 (0%)	30	49
3	G	116/272 (43%)	107 (92%)	6 (5%)	3 (3%)	4	6
All	All	2959/3248 (91%)	2729 (92%)	200 (7%)	30 (1%)	12	26

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%)	359 (91%)	34 (9%)	9	20
1	B	388/412 (94%)	361 (93%)	27 (7%)	14	29
1	C	397/412 (96%)	366 (92%)	31 (8%)	11	25
2	D	377/386 (98%)	352 (93%)	25 (7%)	15	32
2	E	376/386 (97%)	352 (94%)	24 (6%)	16	33
2	F	376/386 (97%)	353 (94%)	23 (6%)	17	35
3	G	102/230 (44%)	97 (95%)	5 (5%)	22	44
All	All	2409/2624 (92%)	2240 (93%)	169 (7%)	14	29

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	420	VAL
2	F	67	GLU
2	E	112	GLN
2	E	277	SER
2	F	124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	293	GLN
2	F	282	GLN
2	E	308	GLN
2	E	455	GLN
2	F	411	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 oligosaccharides 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	A	600	5	33,33,33	1.47	5 (15%)	45,52,52	1.29	5 (11%)
7	PO4	E	602	-	4,4,4	0.81	0	6,6,6	0.55	0
4	ANP	C	600	5	33,33,33	1.66	8 (24%)	45,52,52	1.34	6 (13%)
4	ANP	B	600	5	33,33,33	1.65	7 (21%)	45,52,52	2.28	6 (13%)
4	ANP	F	600	5	33,33,33	1.55	7 (21%)	45,52,52	1.34	6 (13%)
6	ADP	D	600	5	28,29,29	1.25	3 (10%)	43,45,45	1.08	4 (9%)

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	A	600	5	-	3/18/38/38	0/3/3/3
4	ANP	C	600	5	-	3/18/38/38	0/3/3/3
4	ANP	B	600	5	-	3/18/38/38	0/3/3/3
4	ANP	F	600	5	-	4/18/38/38	0/3/3/3
6	ADP	D	600	5	-	5/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	ANP	PG-O3G	-4.40	1.45	1.56
4	C	600	ANP	PG-O3G	-4.06	1.46	1.56
6	D	600	ADP	PA-O3A	3.79	1.63	1.59
4	F	600	ANP	PG-O3G	-3.74	1.46	1.56
4	C	600	ANP	PB-O3A	-3.67	1.54	1.59

The worst 5 of 27 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	A	600	ANP	O2B-PB-O1B	4.50	119.52	109.87
4	B	600	ANP	O2G-PG-O1G	-4.18	102.97	113.45
4	C	600	ANP	O2B-PB-O3A	3.35	115.81	104.64
4	C	600	ANP	O2G-PG-O3G	3.30	116.45	107.59

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

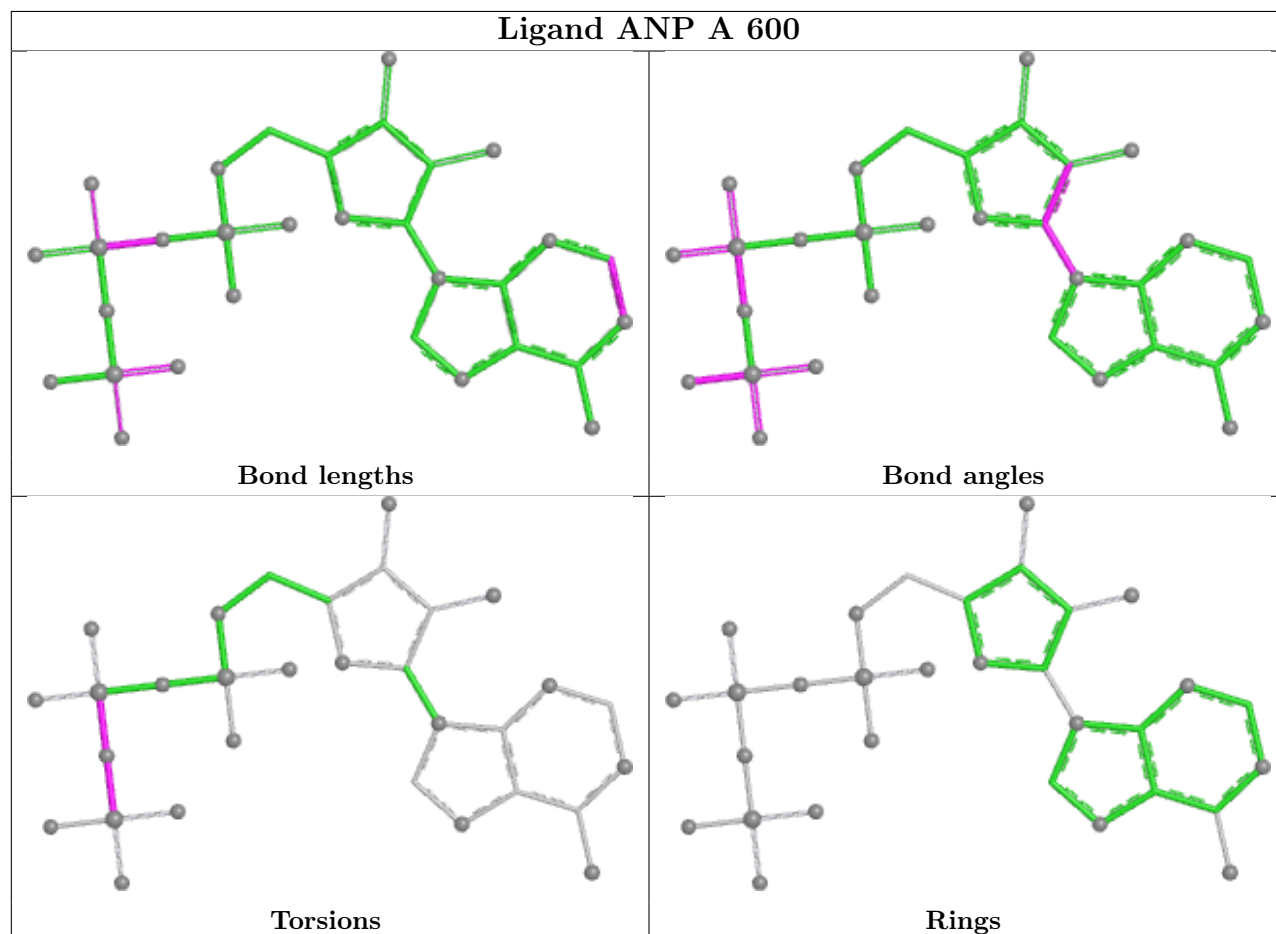
There are no ring outliers.

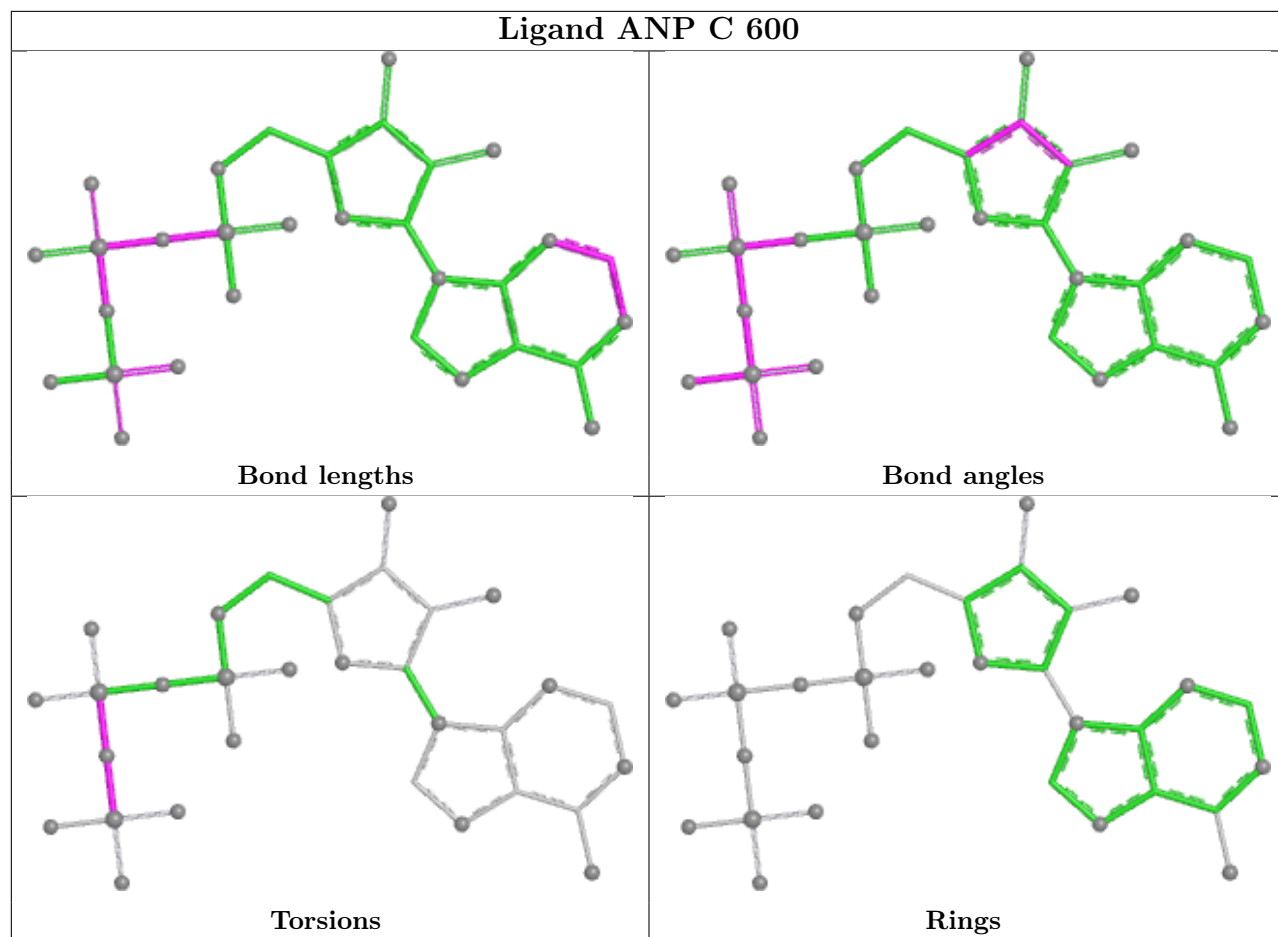
5 monomers are involved in 7 short contacts:

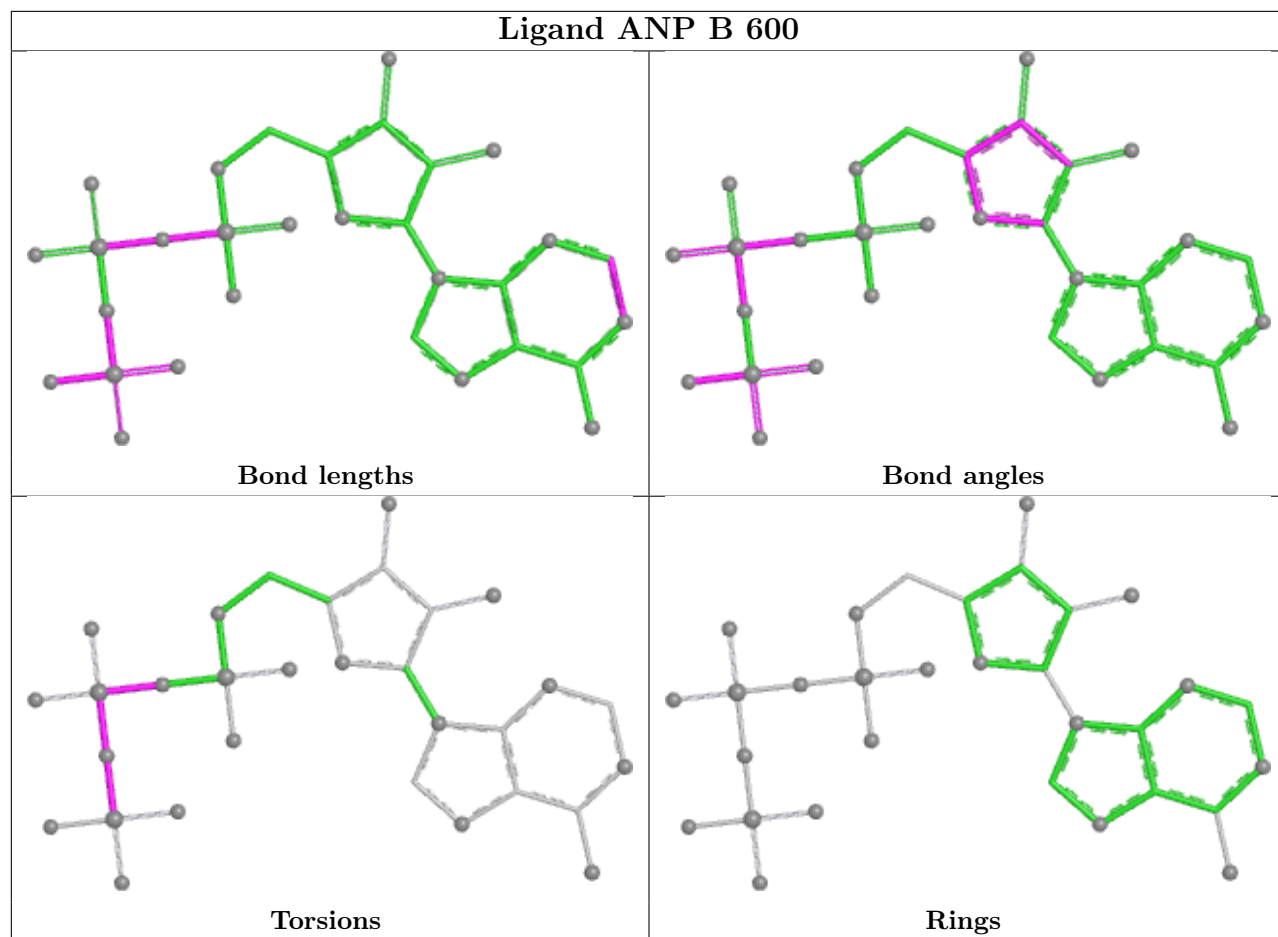
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	ANP	1	0
7	E	602	PO4	1	0
4	C	600	ANP	2	0
4	B	600	ANP	2	0
6	D	600	ADP	1	0

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

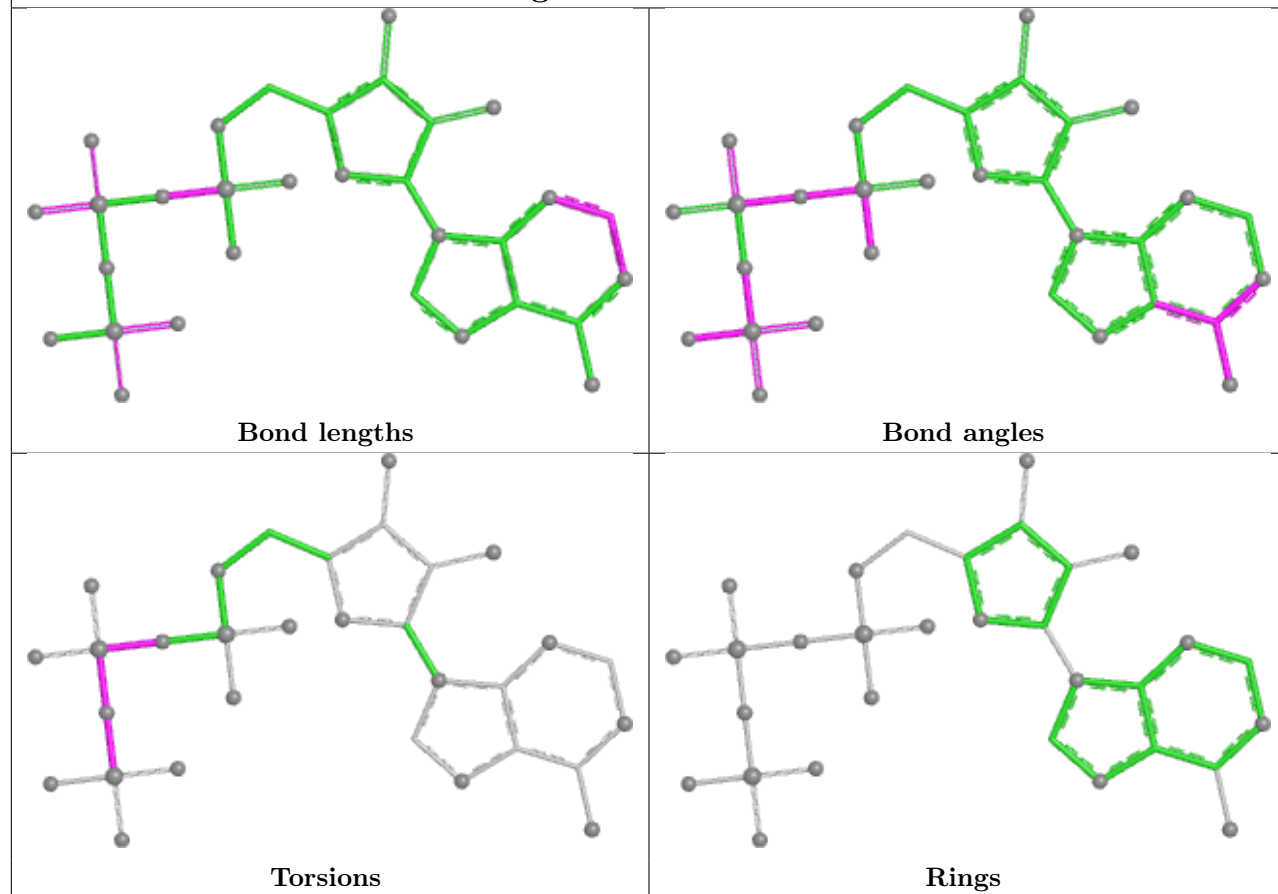
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



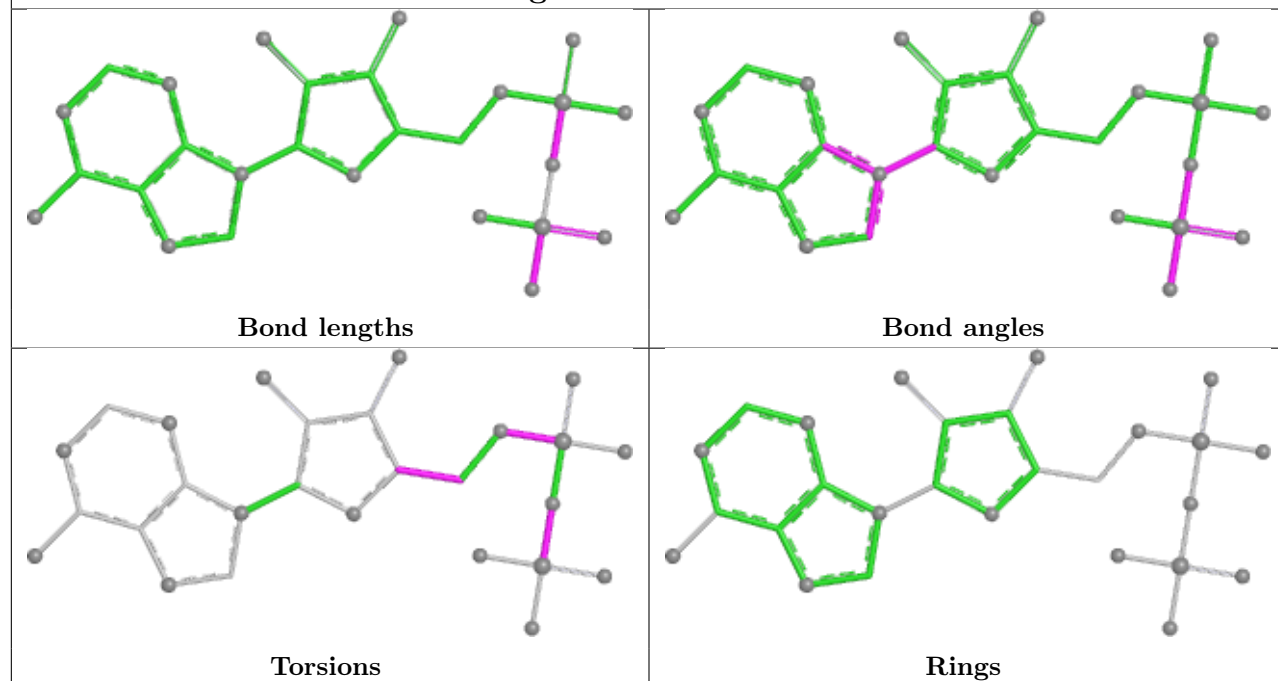




Ligand ANP F 600



Ligand ADP D 600



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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.