



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:57 PM UTC

PDB ID : 4TT3 / pdb_00004tt3
Title : The Pathway of Binding of the Intrinsically Disordered Mitochondrial Inhibitor Protein to F1-ATPase
Authors : Bason, J.V.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2014-06-19
Resolution : 3.21 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

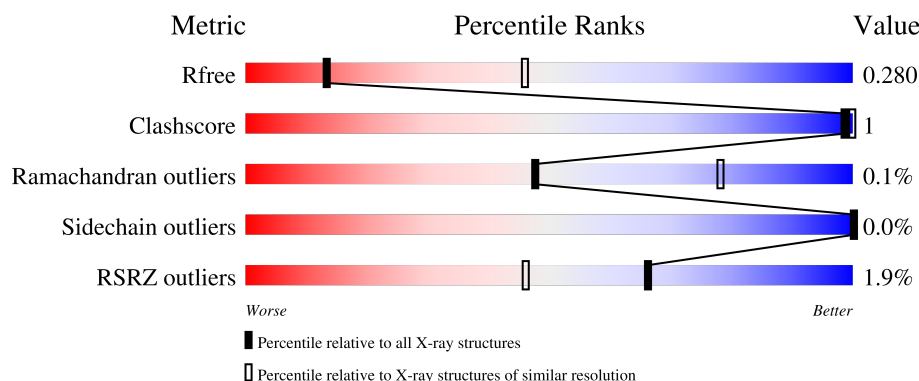
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	
1	B	510	
1	C	510	
2	D	480	
2	E	480	

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Mol	Chain	Length	Quality of chain
2	F	480	2% 96% ..
3	G	273	5% 67% 33%
4	H	66	2% 61% 39%
4	I	66	9% 42% 58%
4	J	66	26% .. 71%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24110 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	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	486	Total	C	N	O	S	0	0	0
			3701	2330	654	705	12			
1	C	483	Total	C	N	O	S	0	0	0
			3684	2323	651	698	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	see sequence details	UNP P19483
B	481	GLY	SER	see sequence details	UNP P19483
C	481	GLY	SER	see sequence details	UNP P19483

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			
2	E	470	Total	C	N	O	S	0	0	0
			3563	2257	606	689	11			
2	F	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	183	Total	C	N	O	S	0	0	0
			1430	894	260	269	7			

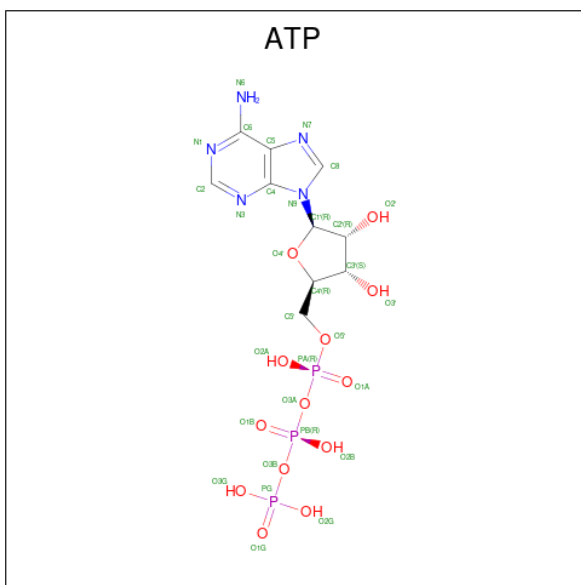
- Molecule 4 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	40	Total	C	N	O	0	0	0
			311	189	64	58			
4	I	28	Total	C	N	O	0	0	0
			236	144	49	43			
4	J	19	Total	C	N	O	0	0	0
			162	102	35	25			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	39	ALA	LYS	engineered mutation	UNP P01096
H	61	HIS	-	expression tag	UNP P01096
H	62	HIS	-	expression tag	UNP P01096
H	63	HIS	-	expression tag	UNP P01096
H	64	HIS	-	expression tag	UNP P01096
H	65	HIS	-	expression tag	UNP P01096
H	66	HIS	-	expression tag	UNP P01096
I	39	ALA	LYS	engineered mutation	UNP P01096
I	61	HIS	-	expression tag	UNP P01096
I	62	HIS	-	expression tag	UNP P01096
I	63	HIS	-	expression tag	UNP P01096
I	64	HIS	-	expression tag	UNP P01096
I	65	HIS	-	expression tag	UNP P01096
I	66	HIS	-	expression tag	UNP P01096
J	39	ALA	LYS	engineered mutation	UNP P01096
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

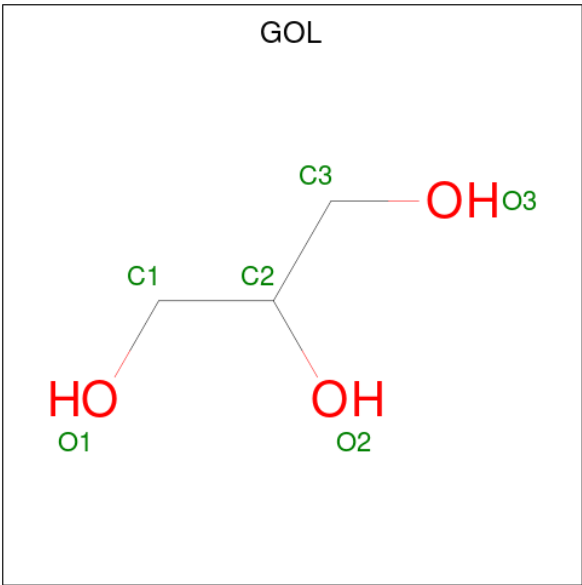


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	C	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

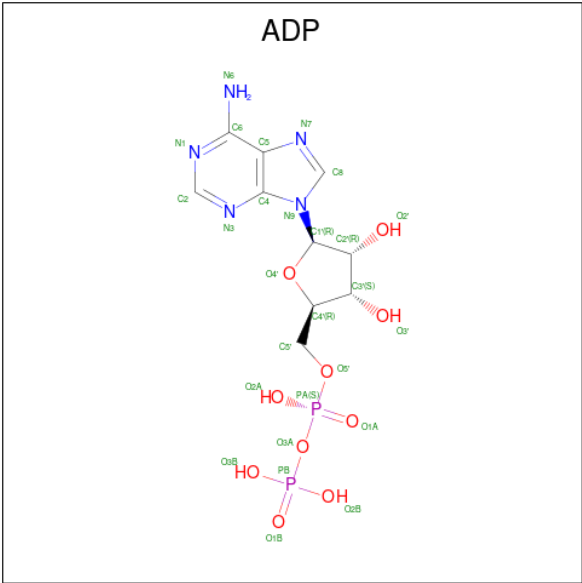
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

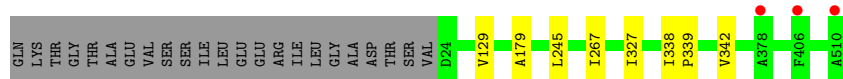
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total 3	O 3	0	0
9	B	3	Total 3	O 3	0	0
9	C	4	Total 4	O 4	0	0
9	D	5	Total 5	O 5	0	0
9	E	5	Total 5	O 5	0	0
9	F	8	Total 8	O 8	0	0

3 Residue-property plots [i](#)

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



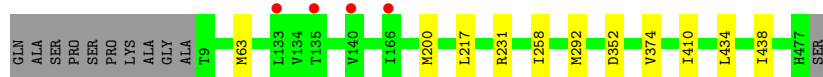
- Molecule 1: ATP synthase subunit alpha, mitochondrial



- Molecule 1: ATP synthase subunit alpha, mitochondrial



- Molecule 2: ATP synthase subunit beta, mitochondrial



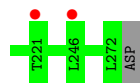
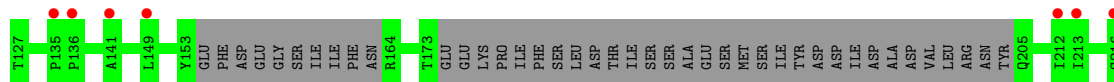
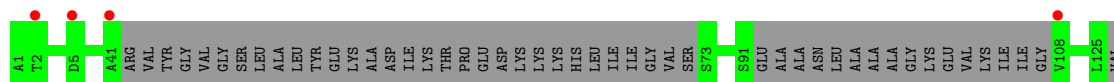
- Molecule 2: ATP synthase subunit beta, mitochondrial



- Molecule 2: ATP synthase subunit beta, mitochondrial



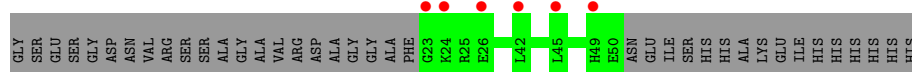
• Molecule 3: ATP synthase subunit gamma, mitochondrial



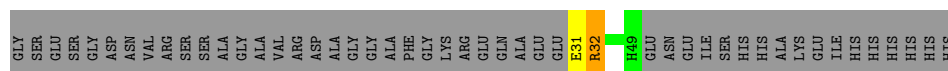
• Molecule 4: ATPase inhibitor, mitochondrial



• Molecule 4: ATPase inhibitor, mitochondrial



• Molecule 4: ATPase inhibitor, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.39Å 154.54Å 272.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	136.02 – 3.21 136.02 – 3.21	Depositor EDS
% Data completeness (in resolution range)	96.7 (136.02-3.21) 96.7 (136.02-3.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.242 , 0.283 0.242 , 0.280	Depositor DCC
R_{free} test set	3688 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	90.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24110	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

5.1 Standard geometry

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

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	0.38	0/3766	0.65	0/5080
1	B	0.38	0/3749	0.66	0/5057
1	C	0.39	0/3733	0.65	0/5035
2	D	0.39	0/3616	0.64	0/4906
2	E	0.39	0/3621	0.64	0/4913
2	F	0.40	0/3616	0.66	1/4906 (0.0%)
3	G	0.38	0/1441	0.65	0/1923
4	H	0.38	0/315	0.63	0/417
4	I	0.39	0/239	0.62	0/315
4	J	0.39	0/165	0.64	0/218
All	All	0.39	0/24261	0.65	1/32770 (0.0%)

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	F	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	477	HIS	CB-CA-C	6.70	122.83	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	477	HIS	CA

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	3715	0	3814	4	0
1	B	3701	0	3809	4	0
1	C	3684	0	3793	2	0
2	D	3558	0	3605	5	0
2	E	3563	0	3611	7	0
2	F	3558	0	3605	3	0
3	G	1430	0	1495	0	0
4	H	311	0	298	0	0
4	I	236	0	229	0	0
4	J	162	0	163	1	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
5	C	31	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	D	27	0	12	0	0
8	F	27	0	12	0	0
9	A	3	0	0	0	0
9	B	3	0	0	0	0
9	C	4	0	0	0	0
9	D	5	0	0	0	0
9	E	5	0	0	0	0
9	F	8	0	0	0	0
All	All	24110	0	24498	26	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 (26) 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:B:34:ILE:HD13	1:B:39:ALA:HB2	1.79	0.64
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.82	0.61
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.88	0.55
2:E:126:MET:HA	2:E:126:MET:HE2	1.91	0.53
2:E:97:VAL:HG13	2:E:98:ILE:HG23	1.92	0.52
2:D:258:ILE:HD11	2:D:292:MET:HE1	1.92	0.51
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.94	0.49
2:E:345:TYR:HA	2:E:346:PRO:C	2.39	0.48
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.96	0.47
1:C:327:ILE:HD11	1:C:342:VAL:HG21	1.97	0.46
1:A:129:VAL:HG21	1:A:245:LEU:HD11	1.99	0.45
2:E:121:PRO:HB2	2:E:126:MET:HE3	1.98	0.44
2:E:256:ASP:HA	2:E:257:ASN:HA	1.75	0.44
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.48	0.44
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.99	0.43
2:F:256:ASP:HA	2:F:257:ASN:HA	1.79	0.43
2:D:434:LEU:O	2:D:438:ILE:HD12	2.19	0.42
2:E:170:ILE:HG21	2:E:215:VAL:HG22	2.01	0.42
2:F:13:ILE:HD12	2:F:73:GLN:HB3	2.01	0.42
1:A:338:ILE:HB	1:A:339:PRO:HD3	2.00	0.42
1:B:383:MET:HG3	1:B:438:ILE:HD11	2.01	0.42
2:D:63:MET:HE1	2:D:231:ARG:HG3	2.01	0.41
2:F:237:LEU:C	2:F:237:LEU:HD23	2.45	0.41
4:J:31:GLU:O	4:J:32:ARG:C	2.63	0.41
1:B:258:ARG:NH1	1:B:308:ARG:O	2.54	0.41
1:C:294:TYR:HB3	1:C:298:VAL:HG11	2.03	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	485/510 (95%)	470 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	482/510 (94%)	463 (96%)	19 (4%)	0	100	100
1	C	479/510 (94%)	462 (96%)	17 (4%)	0	100	100
2	D	467/480 (97%)	442 (95%)	24 (5%)	1 (0%)	43	73
2	E	468/480 (98%)	445 (95%)	23 (5%)	0	100	100
2	F	467/480 (97%)	439 (94%)	26 (6%)	2 (0%)	30	61
3	G	171/273 (63%)	160 (94%)	11 (6%)	0	100	100
4	H	38/66 (58%)	38 (100%)	0	0	100	100
4	I	26/66 (39%)	26 (100%)	0	0	100	100
4	J	17/66 (26%)	16 (94%)	0	1 (6%)	1	9
All	All	3100/3441 (90%)	2961 (96%)	135 (4%)	4 (0%)	48	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	32	ARG
2	D	352	ASP
2	F	352	ASP
2	F	161	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%)	393 (100%)	0	100	100
1	B	393/412 (95%)	393 (100%)	0	100	100
1	C	390/412 (95%)	389 (100%)	1 (0%)	86	87
2	D	379/386 (98%)	379 (100%)	0	100	100
2	E	379/386 (98%)	379 (100%)	0	100	100
2	F	379/386 (98%)	379 (100%)	0	100	100
3	G	156/231 (68%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	26/49 (53%)	26 (100%)	0	100	100
4	I	21/49 (43%)	21 (100%)	0	100	100
4	J	14/49 (29%)	14 (100%)	0	100	100
All	All	2530/2772 (91%)	2529 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	416	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	A	475	GLN
1	B	70	ASN
1	B	186	GLN
1	B	475	GLN
1	B	503	ASN
1	C	48	GLN
1	C	263	HIS
2	D	24	GLN
2	D	411	GLN
2	E	194	ASN
2	E	198	HIS
2	E	249	GLN
2	E	361	ASN
2	F	117	HIS
2	F	477	HIS
4	H	48	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\# Z > 2$
8	ADP	F	600	6	28,29,29	1.46	5 (17%)	43,45,45	1.89	11 (25%)
8	ADP	D	600	6	28,29,29	1.43	4 (14%)	43,45,45	1.89	11 (25%)
5	ATP	A	601	6	32,33,33	1.43	4 (12%)	48,52,52	1.82	11 (22%)
7	GOL	B	603	-	5,5,5	0.27	0	5,5,5	0.34	0
7	GOL	A	603	-	5,5,5	0.30	0	5,5,5	0.19	0
5	ATP	B	601	6	32,33,33	1.43	4 (12%)	48,52,52	1.81	11 (22%)
5	ATP	C	600	6	32,33,33	1.47	6 (18%)	48,52,52	1.81	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	F	600	6	-	1/16/32/32	0/3/3/3
8	ADP	D	600	6	-	1/16/32/32	0/3/3/3
5	ATP	A	601	6	-	0/22/38/38	0/3/3/3
7	GOL	B	603	-	-	0/4/4/4	-
7	GOL	A	603	-	-	4/4/4/4	-
5	ATP	B	601	6	-	0/22/38/38	0/3/3/3
5	ATP	C	600	6	-	1/22/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	600	ATP	C5-C4	4.81	1.47	1.39
5	B	601	ATP	C5-C4	4.80	1.47	1.39
8	F	600	ADP	C5-C4	4.78	1.47	1.39
5	A	601	ATP	C5-C4	4.72	1.47	1.39
8	D	600	ADP	C5-C4	4.68	1.47	1.39
5	C	600	ATP	C5-C6	2.85	1.48	1.41
5	B	601	ATP	C5-C6	2.84	1.48	1.41
8	D	600	ADP	C5-C6	2.78	1.48	1.41
8	F	600	ADP	C5-C6	2.76	1.48	1.41
5	A	601	ATP	C5-C6	2.74	1.48	1.41
5	C	600	ATP	C8-N7	2.44	1.36	1.31
8	D	600	ADP	C8-N7	2.42	1.36	1.31
8	F	600	ADP	C8-N7	2.41	1.36	1.31
8	F	600	ADP	C5-N7	-2.40	1.34	1.39
5	A	601	ATP	C5-N7	-2.39	1.34	1.39
5	A	601	ATP	C8-N7	2.38	1.36	1.31
5	B	601	ATP	C8-N7	2.37	1.36	1.31
8	D	600	ADP	C5-N7	-2.34	1.34	1.39
5	B	601	ATP	C5-N7	-2.30	1.34	1.39
5	C	600	ATP	C5-N7	-2.25	1.35	1.39
8	F	600	ADP	PA-O3A	2.12	1.61	1.59
5	C	600	ATP	PA-O3A	2.09	1.61	1.59
5	C	600	ATP	PB-O3A	2.06	1.61	1.59

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	ATP	C5-C4-N3	-5.85	118.66	126.72
8	F	600	ADP	C5-C4-N3	-5.81	118.71	126.72
5	A	601	ATP	C5-C4-N3	-5.78	118.75	126.72
5	C	600	ATP	C5-C4-N3	-5.77	118.77	126.72
8	D	600	ADP	C5-C4-N3	-5.68	118.90	126.72
5	A	601	ATP	N3-C4-N9	4.65	135.07	127.17
8	F	600	ADP	N3-C4-N9	4.65	135.07	127.17
5	B	601	ATP	N3-C4-N9	4.63	135.04	127.17
5	C	600	ATP	N3-C4-N9	4.59	134.97	127.17
8	D	600	ADP	N3-C4-N9	4.48	134.79	127.17
5	B	601	ATP	C2-N3-C4	3.90	121.36	111.83
5	C	600	ATP	C2-N3-C4	3.90	121.36	111.83
5	A	601	ATP	C2-N3-C4	3.89	121.32	111.83
8	D	600	ADP	C2-N3-C4	3.87	121.29	111.83
8	F	600	ADP	C2-N3-C4	3.87	121.29	111.83
5	A	601	ATP	N3-C2-N1	-3.84	122.76	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	600	ADP	N3-C2-N1	-3.80	122.83	128.58
5	C	600	ATP	N3-C2-N1	-3.80	122.83	128.58
8	F	600	ADP	N3-C2-N1	-3.79	122.85	128.58
5	B	601	ATP	N3-C2-N1	-3.76	122.90	128.58
5	B	601	ATP	C4-C5-N7	-3.61	106.45	110.58
5	C	600	ATP	C4-C5-N7	-3.53	106.54	110.58
8	D	600	ADP	C4-C5-N7	-3.53	106.55	110.58
8	F	600	ADP	C4-C5-N7	-3.48	106.60	110.58
5	A	601	ATP	C4-C5-N7	-3.45	106.64	110.58
5	A	601	ATP	C4-N9-C8	2.84	108.72	105.74
5	C	600	ATP	C4-N9-C8	2.81	108.69	105.74
8	D	600	ADP	C4-N9-C8	2.77	108.65	105.74
5	B	601	ATP	C5-N7-C8	2.75	107.78	103.45
8	F	600	ADP	C4-N9-C8	2.75	108.63	105.74
5	B	601	ATP	C4-N9-C8	2.73	108.61	105.74
8	D	600	ADP	C5-N7-C8	2.72	107.72	103.45
5	C	600	ATP	C5-N7-C8	2.72	107.72	103.45
5	A	601	ATP	C5-N7-C8	2.69	107.68	103.45
8	F	600	ADP	C5-N7-C8	2.68	107.67	103.45
8	D	600	ADP	C3'-C2'-C1'	2.46	106.12	101.46
5	C	600	ATP	C3'-C2'-C1'	2.43	106.06	101.46
5	B	601	ATP	C3'-C2'-C1'	2.40	106.01	101.46
8	F	600	ADP	C3'-C2'-C1'	2.36	105.92	101.46
8	D	600	ADP	C6-C5-N7	2.29	136.50	132.09
5	B	601	ATP	C6-C5-N7	2.23	136.40	132.09
8	D	600	ADP	N9-C8-N7	-2.23	110.77	113.94
5	C	600	ATP	C6-C5-N7	2.23	136.39	132.09
5	A	601	ATP	N9-C8-N7	-2.22	110.79	113.94
5	C	600	ATP	N9-C8-N7	-2.22	110.79	113.94
5	B	601	ATP	N9-C8-N7	-2.17	110.86	113.94
8	F	600	ADP	C2-N1-C6	2.17	122.29	118.73
8	F	600	ADP	N9-C8-N7	-2.15	110.89	113.94
5	A	601	ATP	C2-N1-C6	2.13	122.23	118.73
8	F	600	ADP	C6-C5-N7	2.13	136.20	132.09
5	A	601	ATP	C6-C5-N7	2.13	136.19	132.09
5	C	600	ATP	C2-N1-C6	2.12	122.22	118.73
5	B	601	ATP	C2-N1-C6	2.08	122.14	118.73
8	D	600	ADP	C2-N1-C6	2.06	122.12	118.73
5	A	601	ATP	C3'-C2'-C1'	2.05	105.33	101.46

There are no chirality outliers.

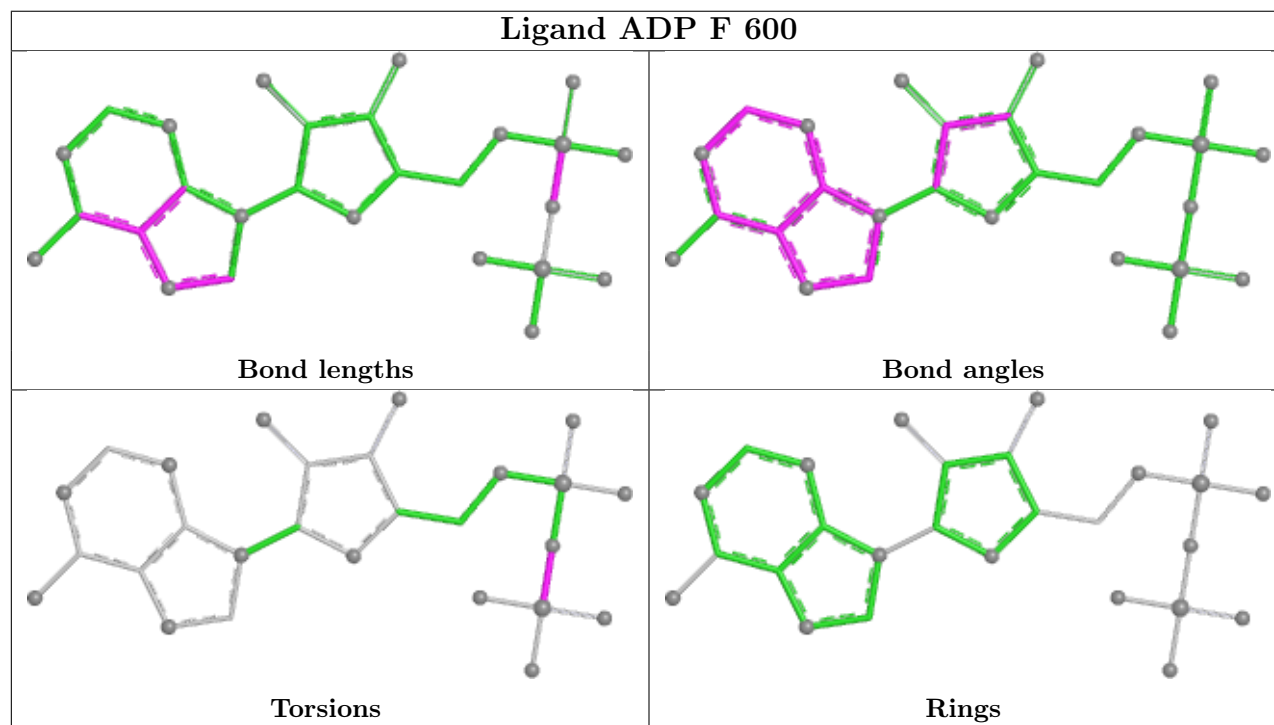
All (7) torsion outliers are listed below:

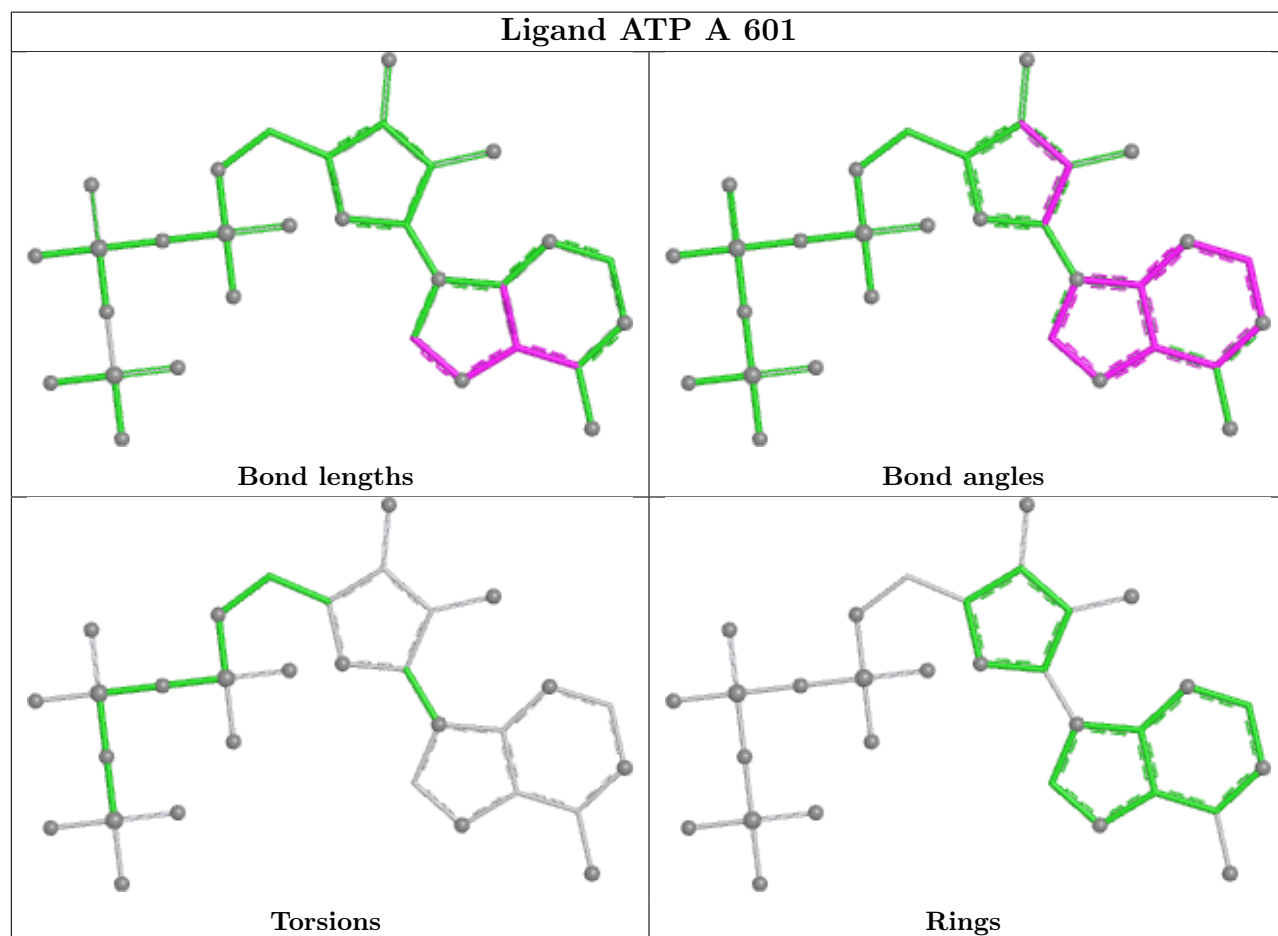
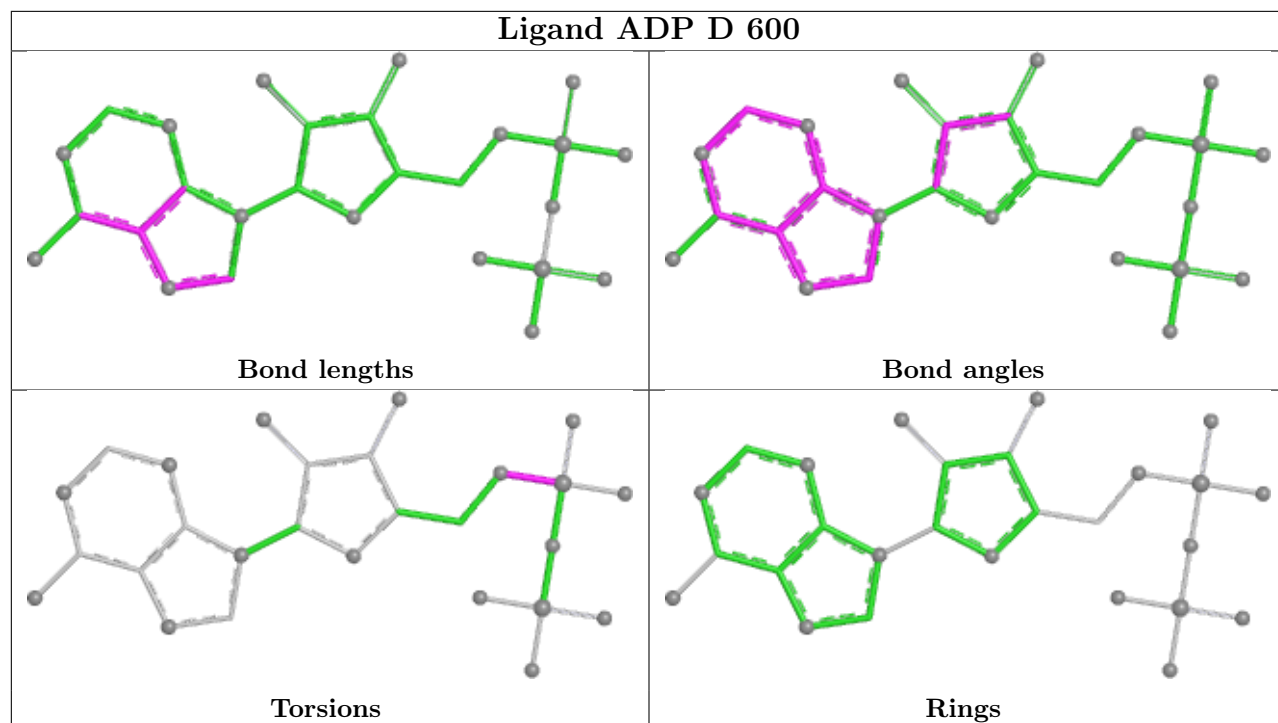
Mol	Chain	Res	Type	Atoms
7	A	603	GOL	O1-C1-C2-C3
8	D	600	ADP	C5'-O5'-PA-O1A
7	A	603	GOL	C1-C2-C3-O3
7	A	603	GOL	O1-C1-C2-O2
7	A	603	GOL	O2-C2-C3-O3
5	C	600	ATP	PB-O3A-PA-O2A
8	F	600	ADP	PA-O3A-PB-O1B

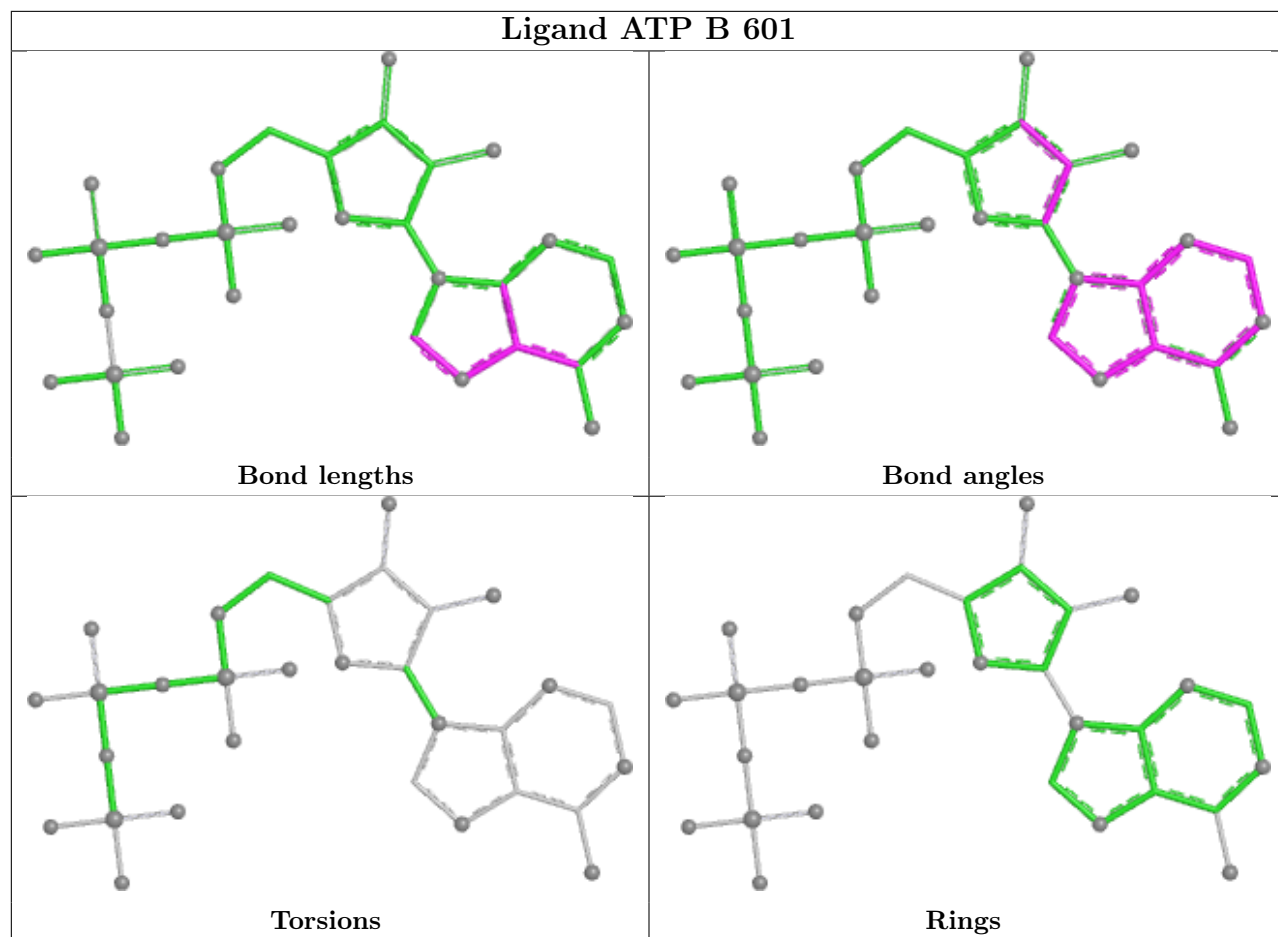
There are no ring outliers.

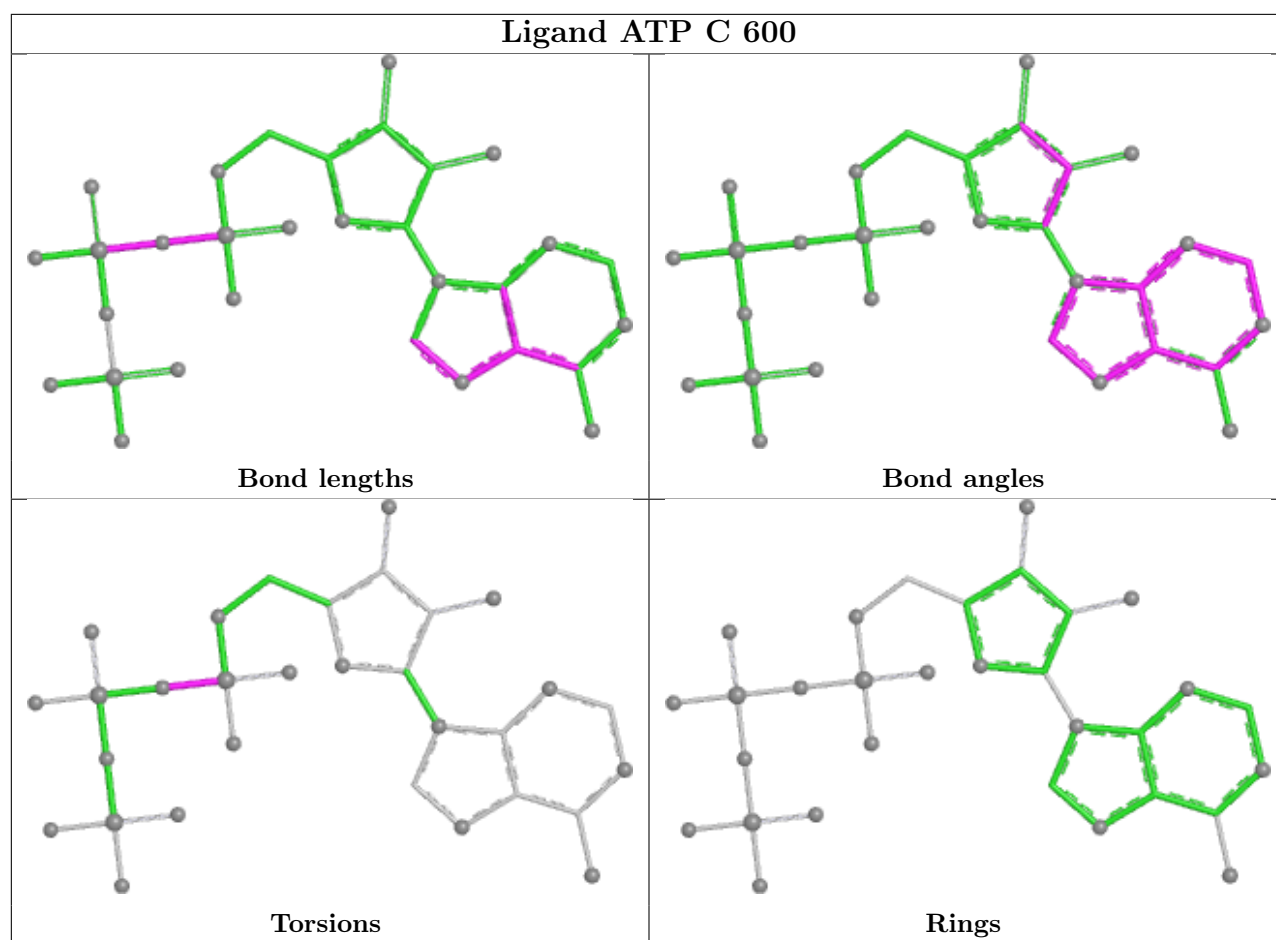
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	487/510 (95%)	0.15	3 (0%) 85 73	58, 80, 115, 164	0
1	B	486/510 (95%)	0.17	6 (1%) 76 58	55, 75, 107, 130	0
1	C	483/510 (94%)	0.35	8 (1%) 69 49	67, 97, 122, 151	0
2	D	469/480 (97%)	0.49	4 (0%) 81 64	74, 102, 131, 144	0
2	E	470/480 (97%)	0.17	10 (2%) 63 43	56, 78, 126, 164	0
2	F	469/480 (97%)	0.36	8 (1%) 69 49	66, 95, 118, 141	0
3	G	183/273 (67%)	0.76	13 (7%) 22 14	73, 135, 167, 178	0
4	H	40/66 (60%)	0.55	1 (2%) 58 39	92, 111, 132, 138	0
4	I	28/66 (42%)	1.22	6 (21%) 2 2	133, 140, 149, 153	0
4	J	19/66 (28%)	0.68	0 100 100	148, 151, 158, 159	0
All	All	3134/3441 (91%)	0.32	59 (1%) 66 46	55, 90, 140, 178	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	351	LEU	4.0
4	I	45	LEU	3.8
2	D	166	ILE	3.4
4	I	23	GLY	3.4
2	E	391	LEU	3.2
1	B	353	GLU	3.2
1	B	17	LEU	3.1
1	A	406	PHE	2.9
4	I	42	LEU	2.9
1	C	404	ALA	2.8
4	I	24	LYS	2.7
3	G	246	LEU	2.7
3	G	135	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
4	I	49	HIS	2.6
1	C	369	LEU	2.6
2	F	397	SER	2.6
3	G	136	PRO	2.6
1	C	402	ALA	2.6
3	G	212	ILE	2.6
1	C	100	GLY	2.6
2	E	392	GLY	2.6
3	G	213	ILE	2.5
2	F	215	VAL	2.5
3	G	149	LEU	2.4
1	C	370	SER	2.4
3	G	221	THR	2.4
3	G	216	SER	2.4
2	E	477	HIS	2.3
2	E	335	LEU	2.3
2	F	379	GLN	2.3
3	G	41	ALA	2.3
1	B	394	LEU	2.3
2	D	133	LEU	2.3
2	F	252	LEU	2.3
2	D	140	VAL	2.3
2	E	162	LYS	2.3
4	H	20	GLY	2.3
2	E	334	VAL	2.3
1	A	378	ALA	2.3
2	E	473	LEU	2.3
1	C	444	VAL	2.3
2	D	135	THR	2.2
2	F	396	LEU	2.2
1	C	142	VAL	2.2
1	B	401	ALA	2.2
2	F	236	GLY	2.2
2	F	403	THR	2.2
2	E	390	ILE	2.2
1	B	78	ASN	2.2
4	I	26	GLU	2.2
1	A	510	ALA	2.1
1	B	375	GLY	2.1
1	C	121	ILE	2.1
2	F	387	ILE	2.1
3	G	141	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	160	VAL	2.1
3	G	108	VAL	2.1
3	G	5	ASP	2.1
3	G	2	THR	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](#)

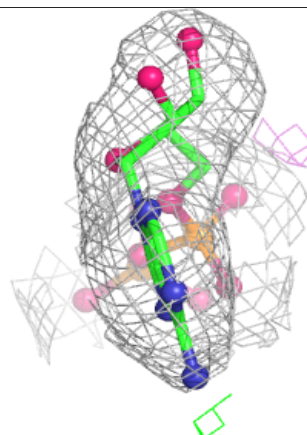
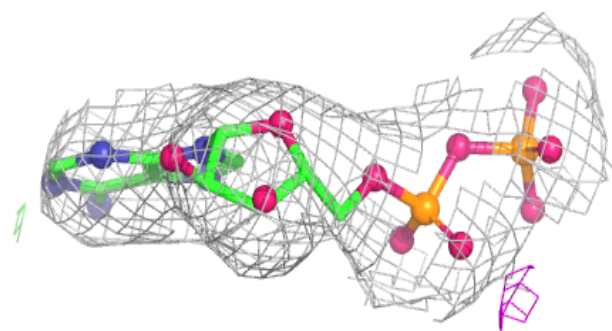
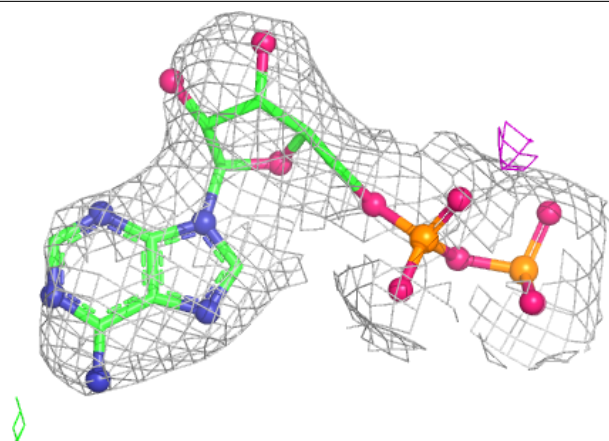
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	603	6/6	0.85	0.18	72,73,73,74	0
7	GOL	B	603	6/6	0.85	0.17	75,76,76,77	0
6	MG	D	601	1/1	0.91	0.10	88,88,88,88	0
8	ADP	D	600	27/27	0.93	0.10	85,88,90,91	0
5	ATP	A	601	31/31	0.94	0.09	72,74,76,76	4
8	ADP	F	600	27/27	0.94	0.10	76,82,86,86	0
5	ATP	C	600	31/31	0.95	0.08	83,93,100,101	4
5	ATP	B	601	31/31	0.96	0.07	63,72,78,78	0
6	MG	B	602	1/1	0.97	0.06	63,63,63,63	0
6	MG	A	602	1/1	0.97	0.06	75,75,75,75	0
6	MG	C	601	1/1	0.98	0.05	83,83,83,83	0
6	MG	F	601	1/1	0.98	0.05	78,78,78,78	0

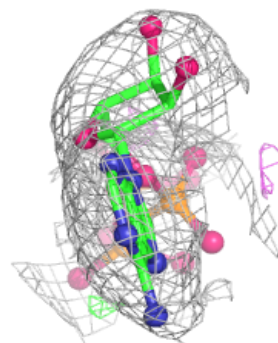
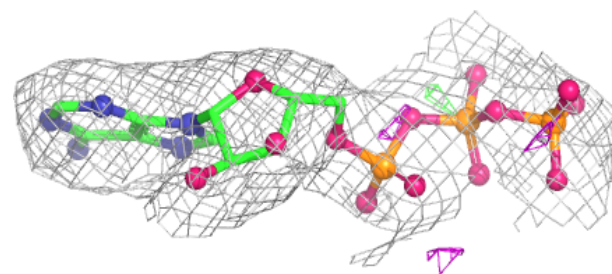
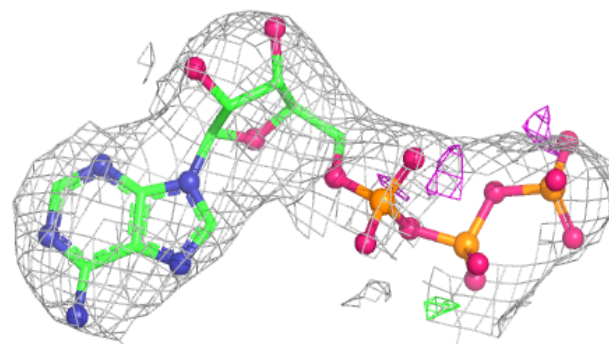
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP 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)

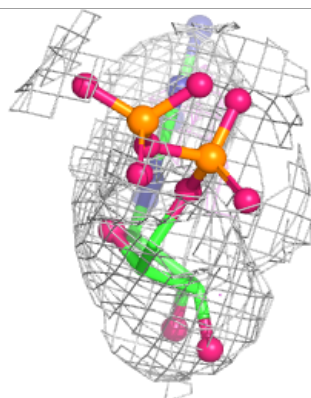
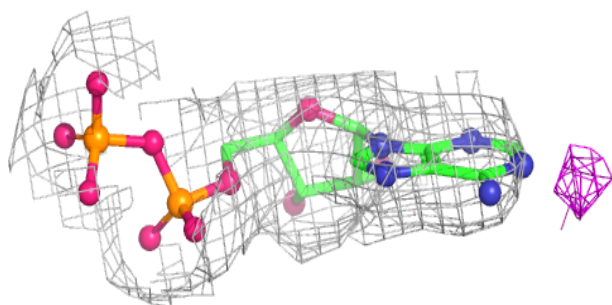
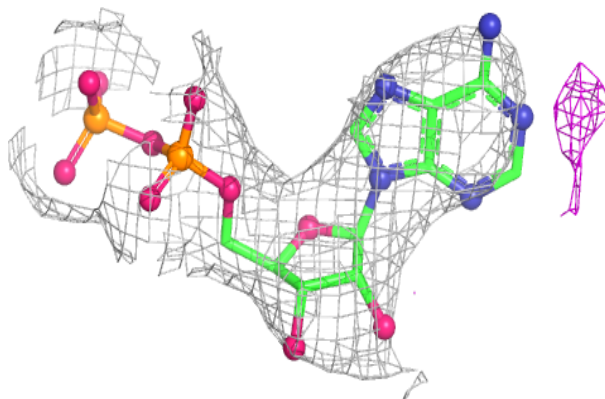
**Electron density around ATP A 601:**

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

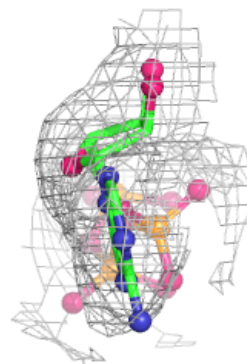
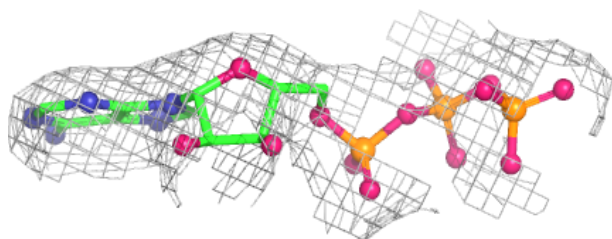
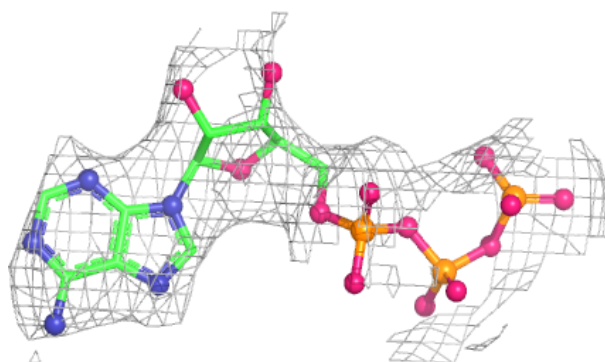


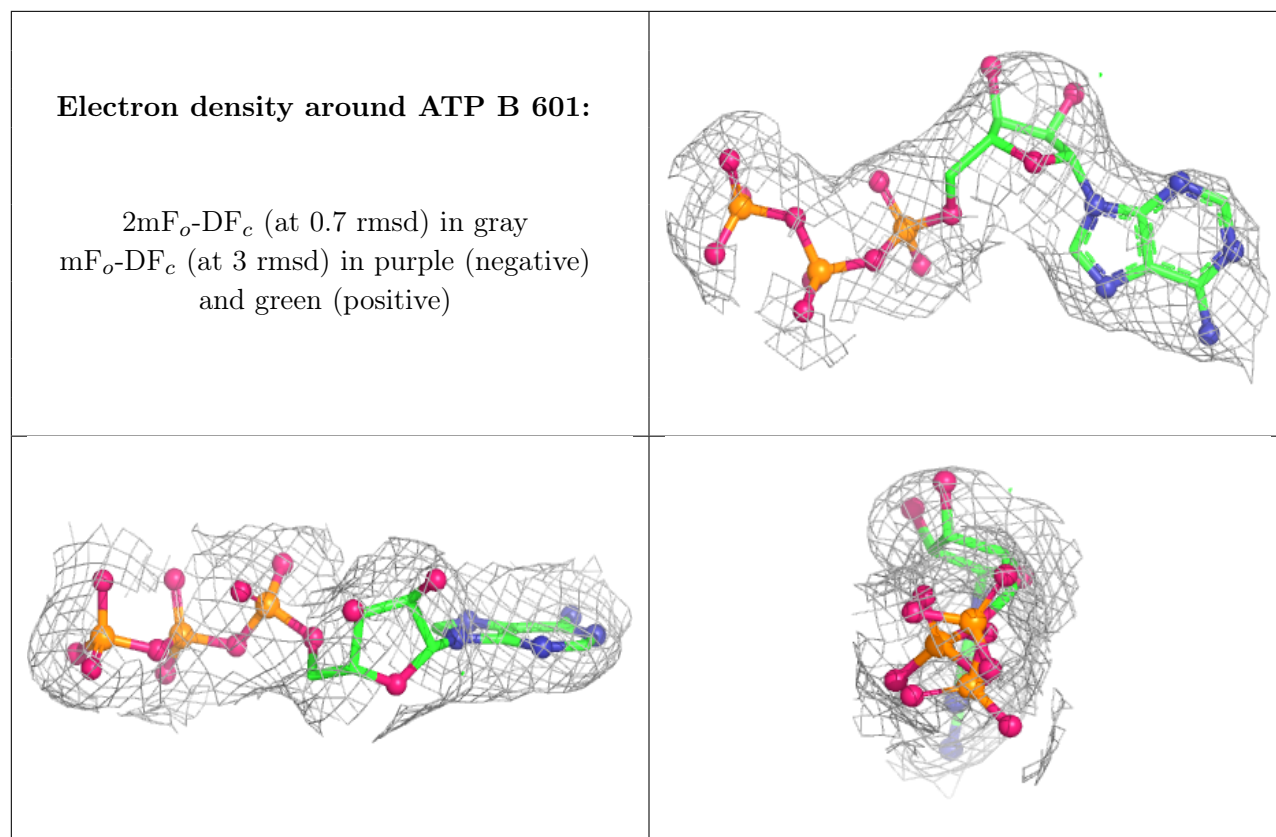
Electron density around ADP F 600:

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

**Electron density around ATP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.