



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 11:45 pm BST

PDB ID : 3ZIA
Title : The structure of F1-ATPase from *Saccharomyces cerevisiae* inhibited by its regulatory protein IF1
Authors : Robinson, G.C.; Bason, J.V.; Montgomery, M.G.; Fearnley, I.M.; Mueller, D.M.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2013-01-07
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

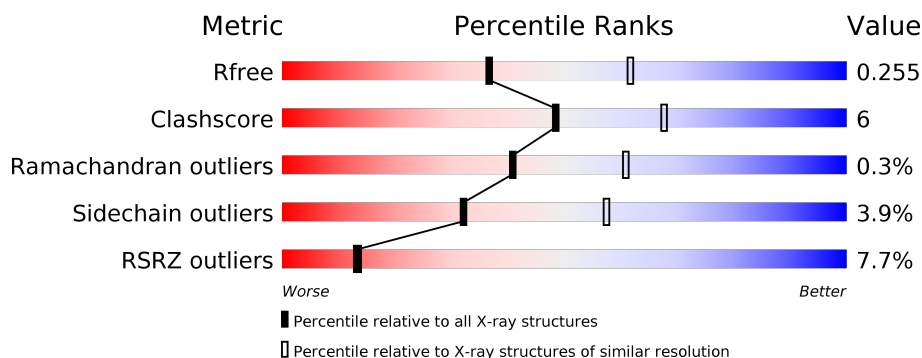
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	510	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div> </div>
1	C	510	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	K	510	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	L	510	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	M	510	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	478	
2	E	478	
2	F	478	
2	N	478	
2	O	478	
2	P	478	
3	G	278	
3	Q	278	
4	H	138	
4	R	138	
5	I	61	
5	S	61	
6	J	63	
6	T	63	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 51906 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	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	B	480	Total	C	N	O	S	0	1	0
			3655	2310	648	694	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	K	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	L	480	Total	C	N	O	S	0	1	0
			3655	2310	648	694	3			
1	M	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	469	Total	C	N	O	S	0	1	0
			3548	2251	603	687	7			
2	N	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	O	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	P	469	Total	C	N	O	S	0	3	0
			3559	2260	603	689	7			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total	C	N	O	S	0	0	0
			2057	1291	358	398	10			
3	Q	265	Total	C	N	O	S	0	1	0
			2063	1295	358	400	10			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	124	Total	C	N	O	S	0	0	0
			937	594	156	185	2			
4	R	124	Total	C	N	O	S	0	0	0
			937	594	156	185	2			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	58	Total	C	N	O	0	0	0
			450	283	79	88			
5	S	58	Total	C	N	O	0	0	0
			450	283	79	88			

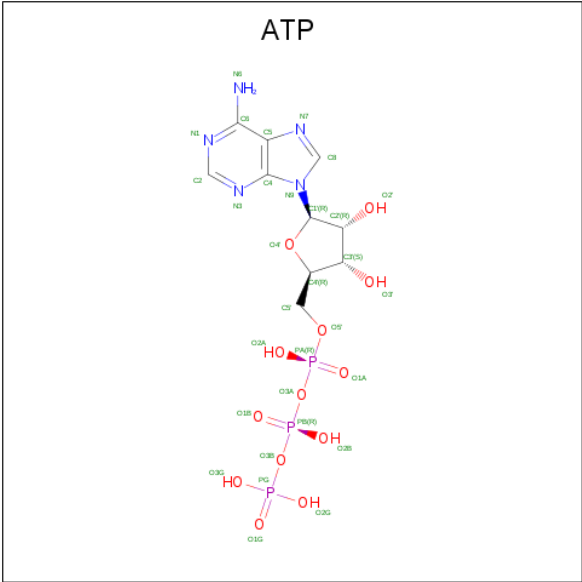
- Molecule 6 is a protein called ATPASE INHIBITOR, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	36	Total	C	N	O	0	0	0
			283	168	55	60			
6	T	36	Total	C	N	O	0	0	0
			283	168	55	60			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	21	ALA	GLU	engineered mutation	UNP P01097
T	21	ALA	GLU	engineered mutation	UNP P01097

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

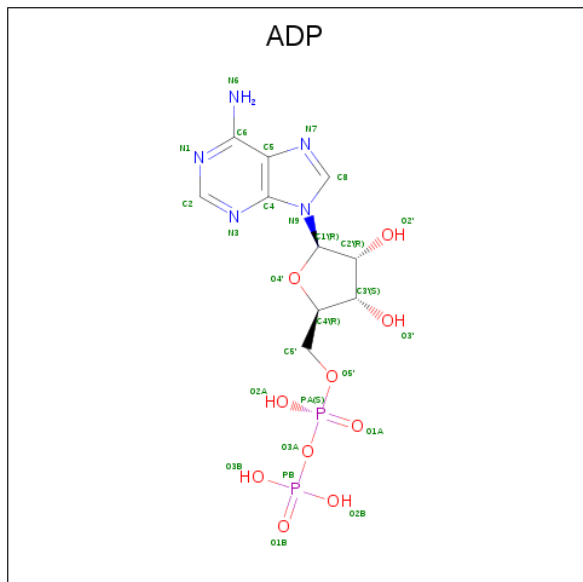


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

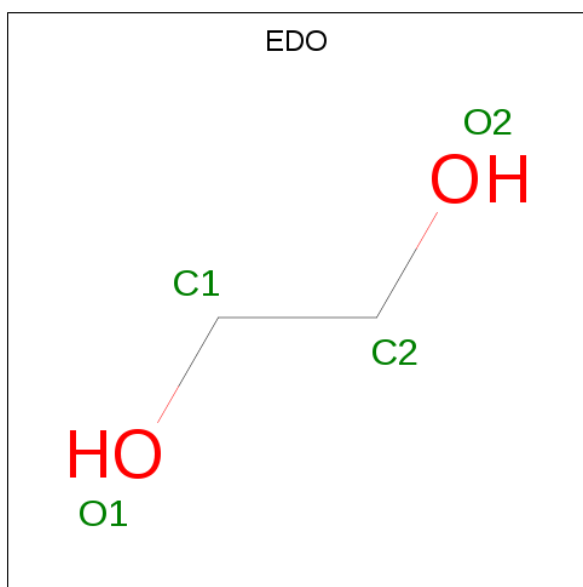
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	K	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		
8	N	1	Total	Mg	0	0
			1	1		
8	L	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		
8	M	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			4	2	2		
10	L	1	Total	C	O	0	0
			4	2	2		
10	L	1	Total	C	O	0	0
			4	2	2		
10	M	1	Total	C	O	0	0
			4	2	2		
10	O	1	Total	C	O	0	0
			4	2	2		
10	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	18	Total	O	0	0
			18	18		
11	B	90	Total	O	0	0
			90	90		
11	C	94	Total	O	0	0
			94	94		
11	D	37	Total	O	0	0
			37	37		
11	E	20	Total	O	0	0
			20	20		
11	F	81	Total	O	0	0
			81	81		

Continued on next page...

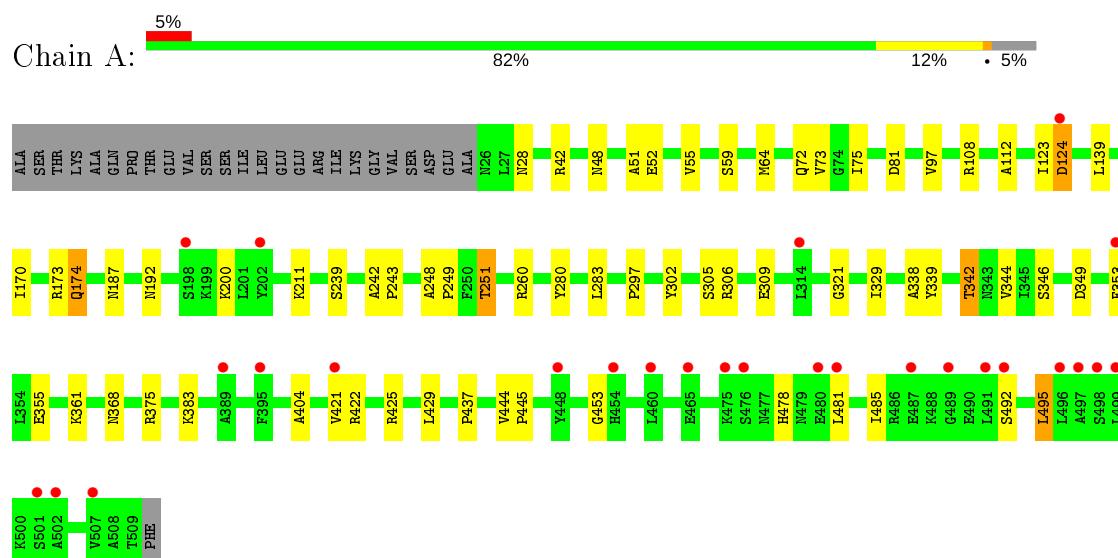
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	G	11	Total 11	O 11	0	0
11	H	1	Total 1	O 1	0	0
11	I	1	Total 1	O 1	0	0
11	K	27	Total 27	O 27	0	0
11	L	156	Total 156	O 156	0	0
11	M	76	Total 76	O 76	0	0
11	N	32	Total 32	O 32	0	0
11	O	52	Total 52	O 52	0	0
11	P	68	Total 68	O 68	0	0
11	Q	8	Total 8	O 8	0	0
11	R	1	Total 1	O 1	0	0

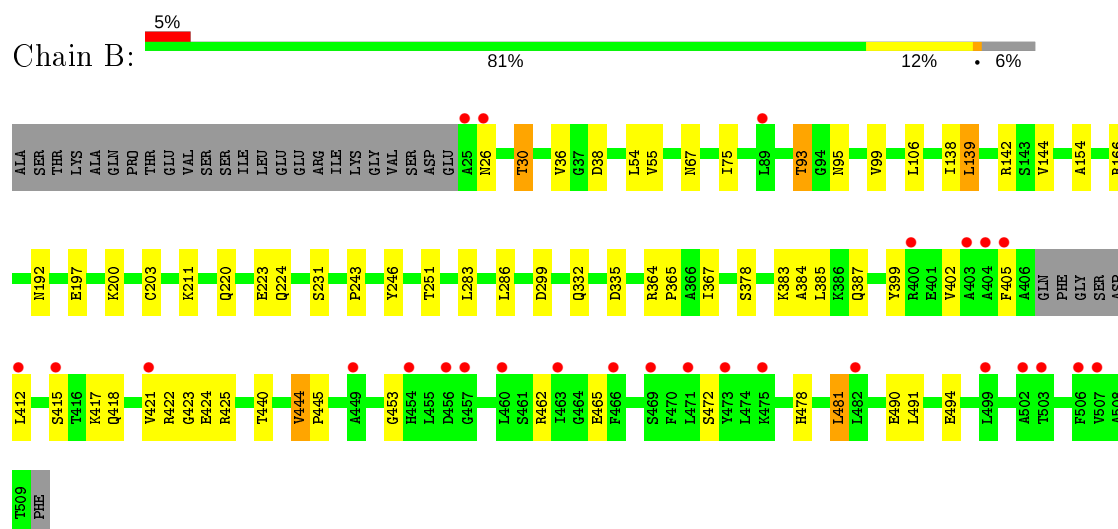
3 Residue-property plots [i](#)

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 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.

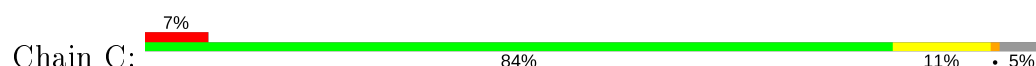
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

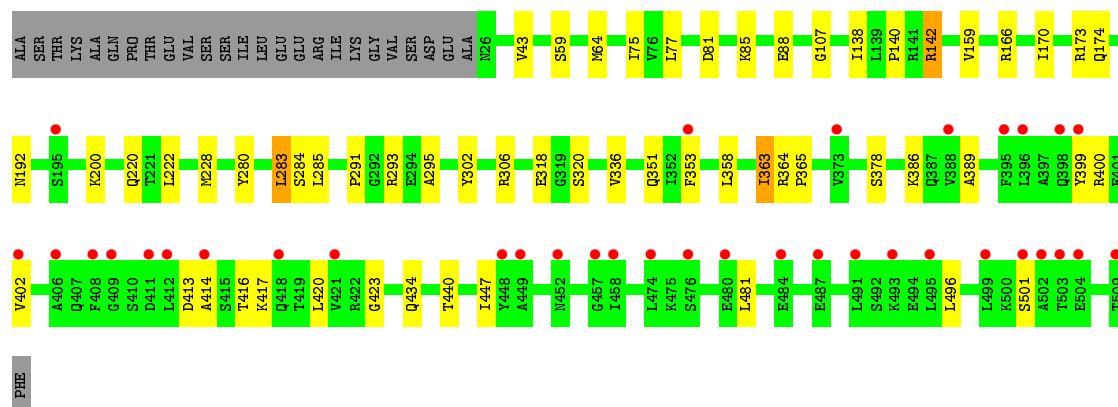


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



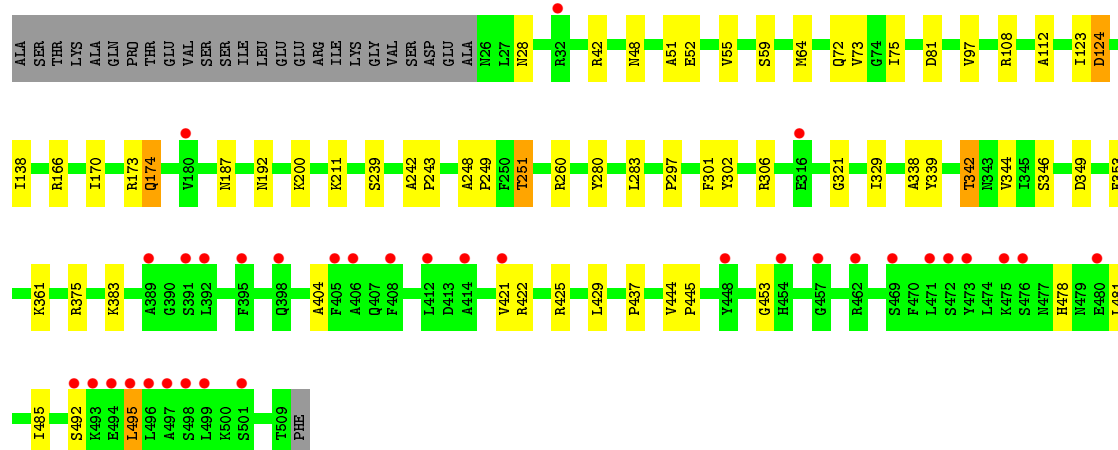
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL





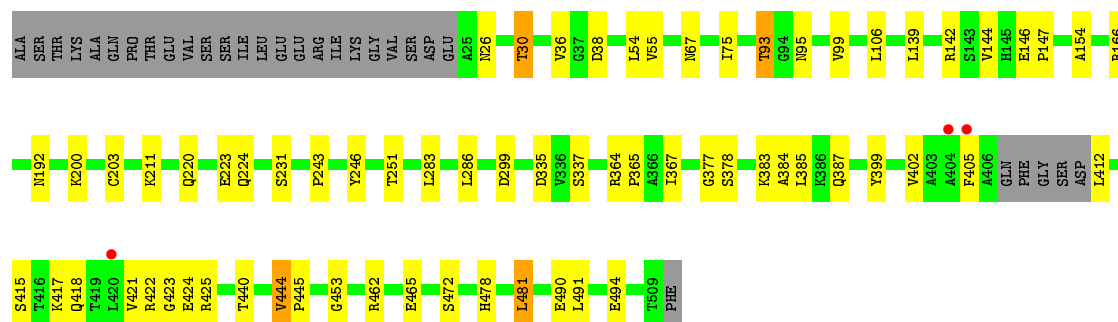
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain K: 7% 82% 12% • 5%



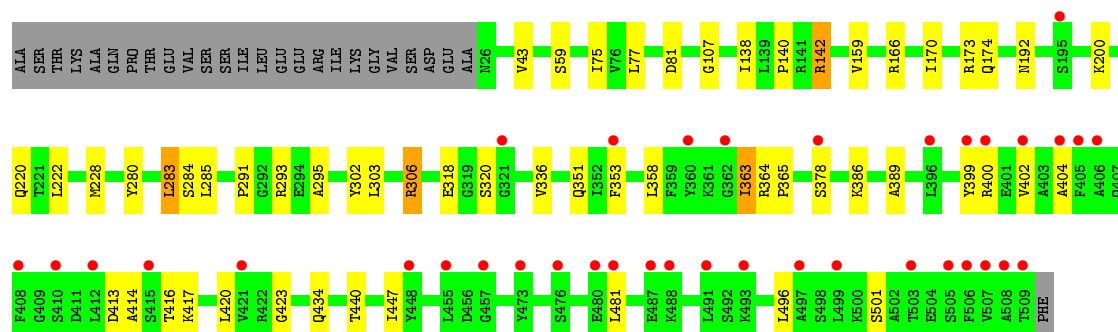
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain L: 1% 81% 13% • 6%

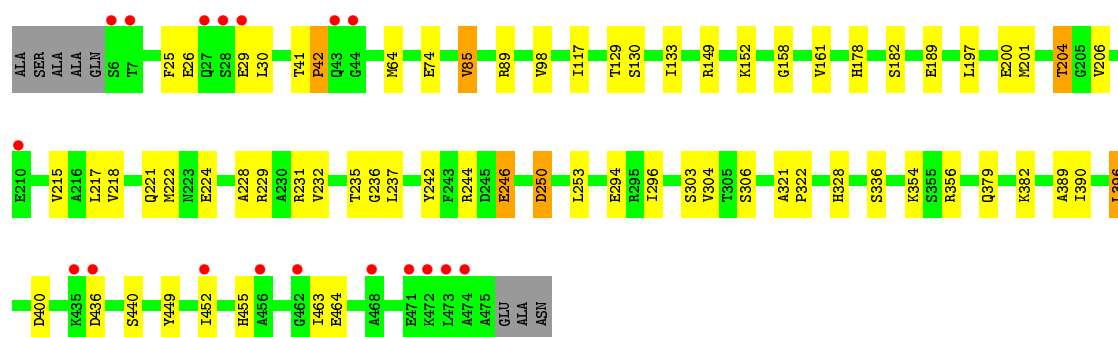
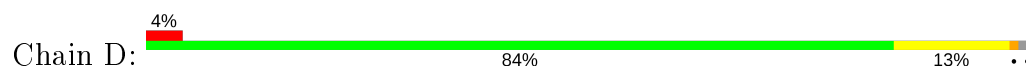


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

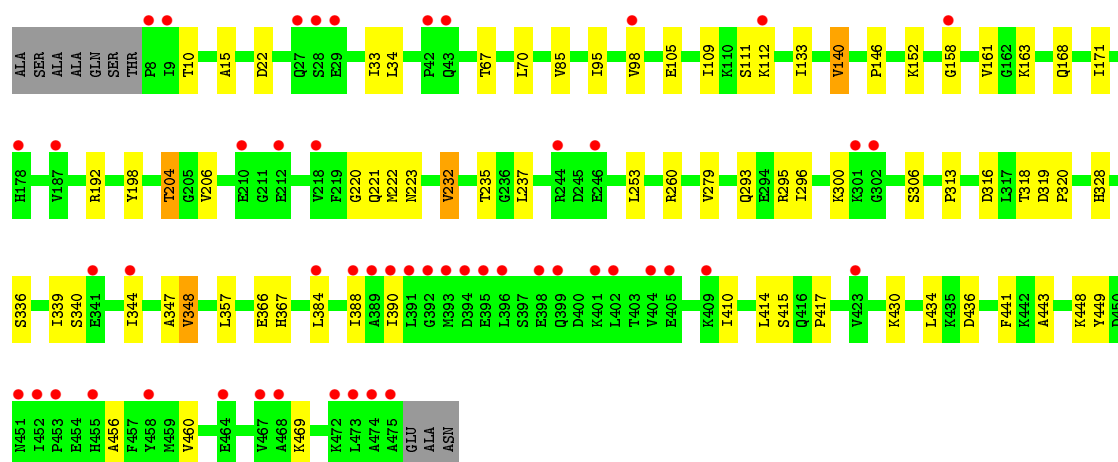
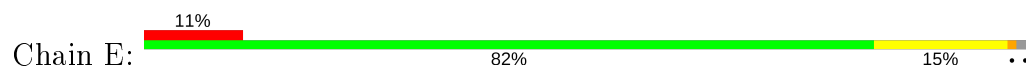
Chain M: 7% 84% 10% • 5%



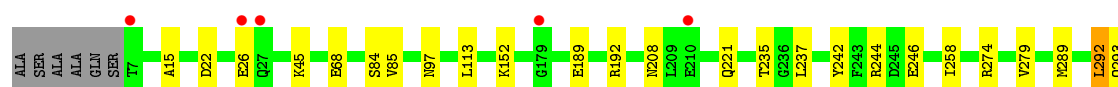
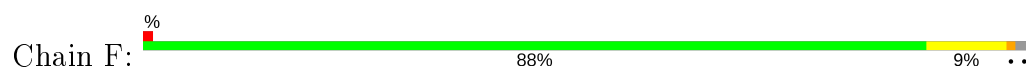
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

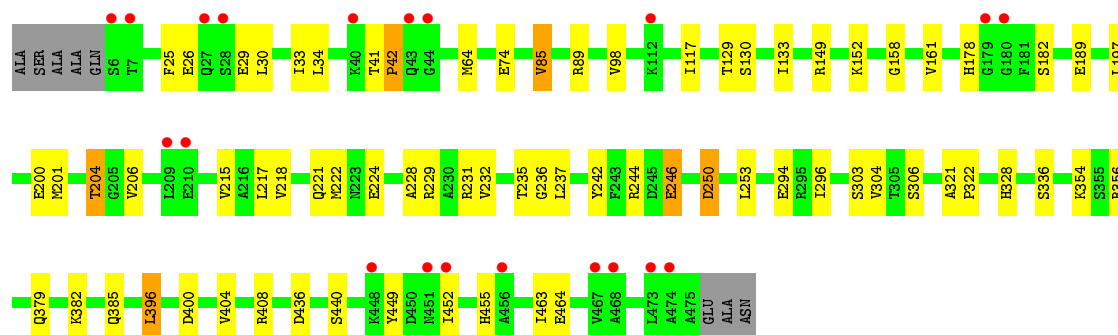
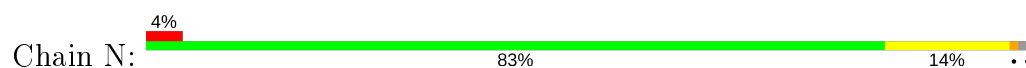


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

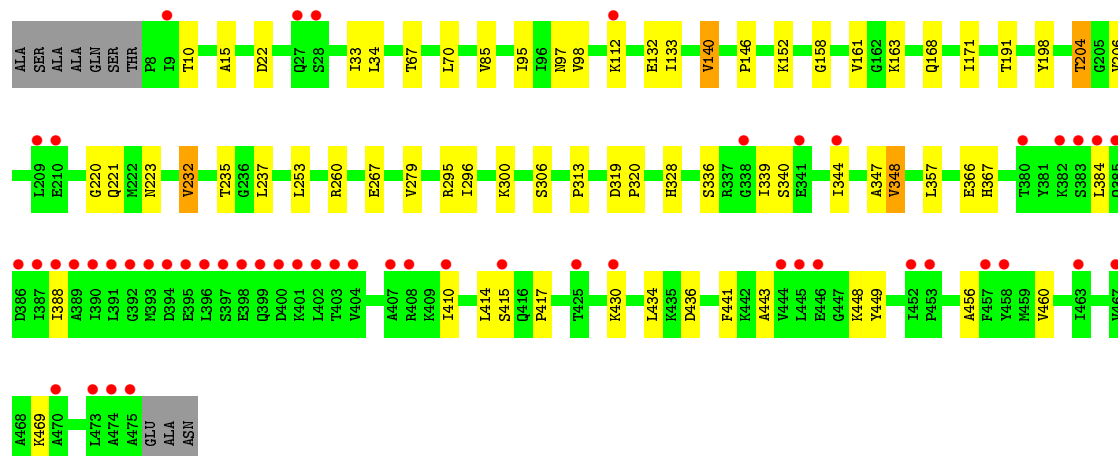
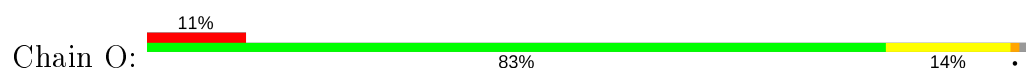




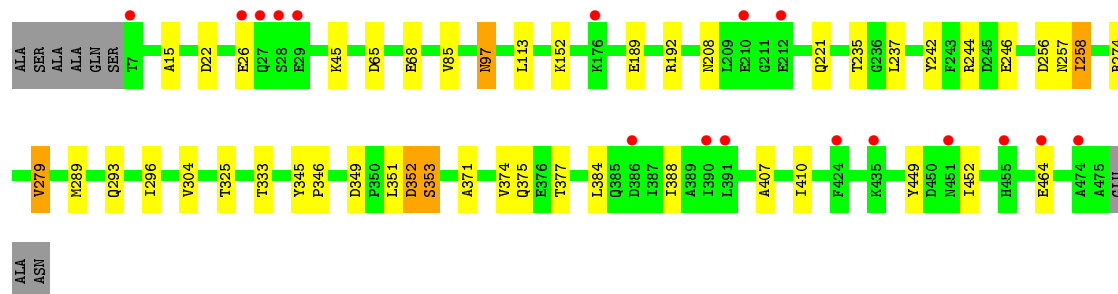
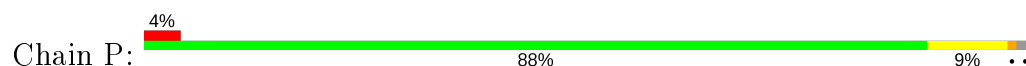
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



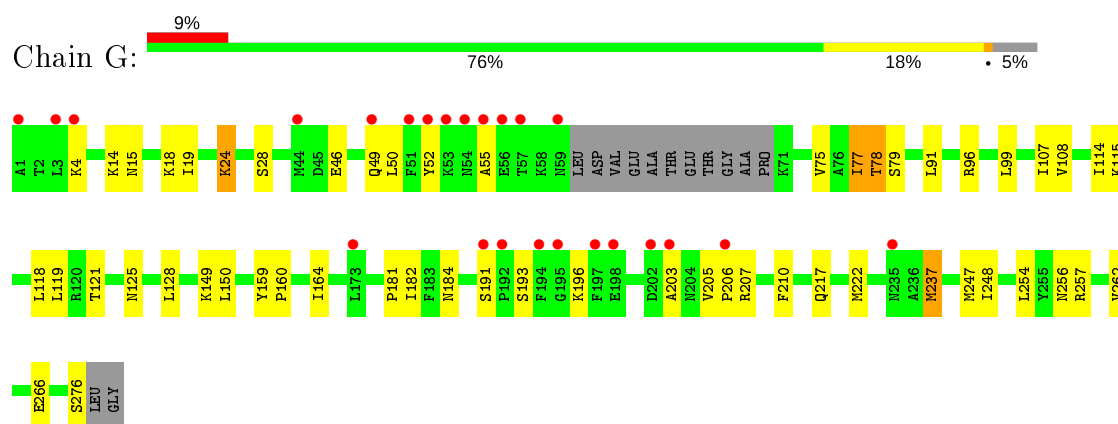
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



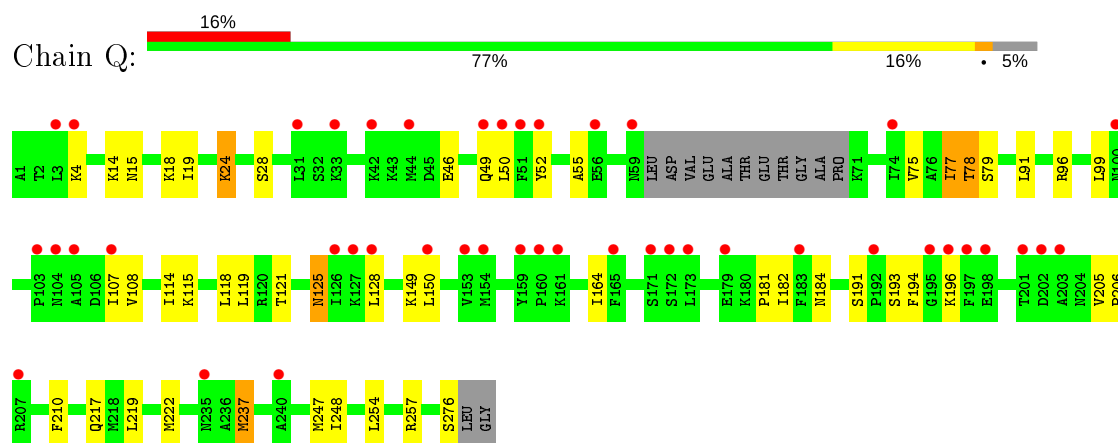
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



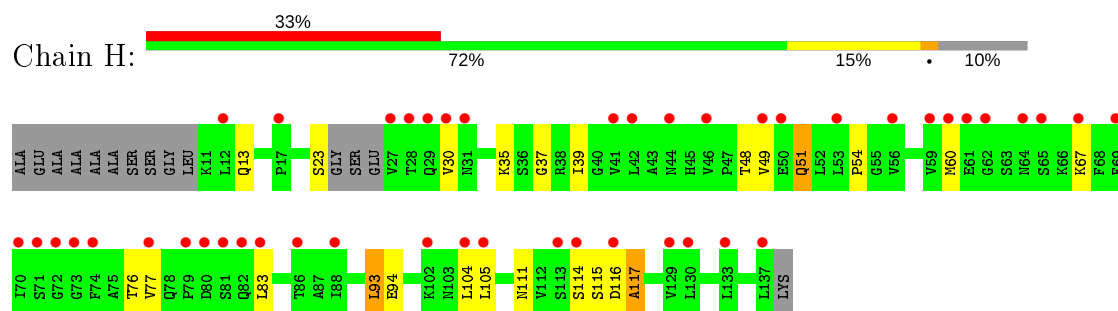
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



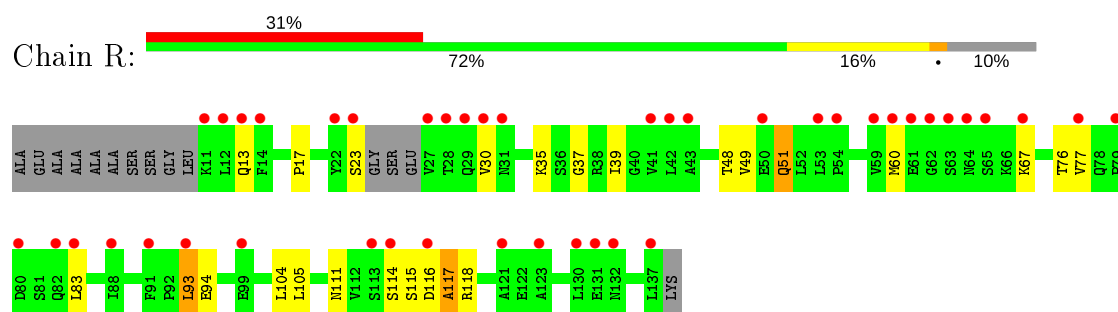
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



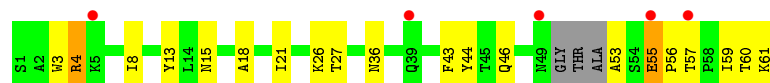
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



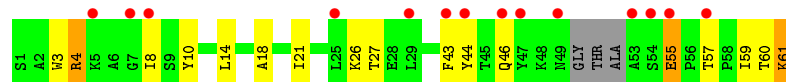
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



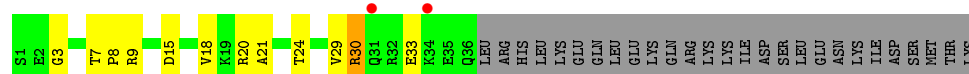
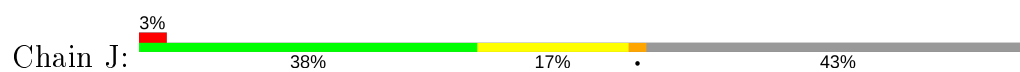
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



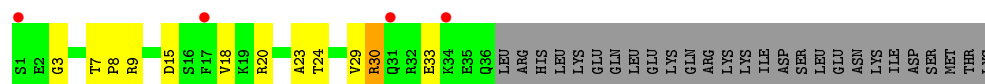
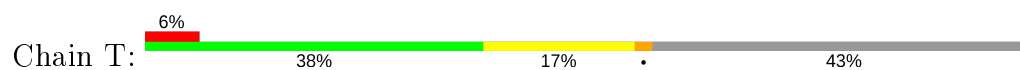
- Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



- Molecule 6: ATPASE INHIBITOR, MITOCHONDRIAL



- Molecule 6: ATPASE INHIBITOR, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.22Å 187.85Å 181.81Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	181.81 – 2.50 40.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (181.81-2.50) 98.3 (40.91-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.224 , 0.262 0.218 , 0.255	Depositor DCC
R_{free} test set	13570 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,-l,-k 0.004 for -h,l,k 0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51906	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: MG, ATP, ADP, EDO

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	0.39	0/3736	0.55	0/5057
1	B	0.50	0/3712	0.62	0/5023
1	C	0.47	0/3736	0.58	0/5057
1	K	0.39	0/3736	0.55	0/5057
1	L	0.53	0/3712	0.63	0/5023
1	M	0.46	0/3736	0.58	0/5057
2	D	0.42	0/3605	0.55	0/4889
2	E	0.42	0/3592	0.58	0/4870
2	F	0.50	0/3607	0.63	0/4891
2	N	0.41	0/3605	0.55	0/4889
2	O	0.45	0/3592	0.59	0/4870
2	P	0.49	0/3624	0.62	0/4914
3	G	0.38	0/2082	0.52	0/2800
3	Q	0.38	0/2091	0.52	0/2812
4	H	0.37	0/950	0.55	0/1288
4	R	0.38	0/950	0.55	0/1288
5	I	0.43	0/457	0.55	0/619
5	S	0.44	0/457	0.55	0/619
6	J	0.42	0/286	0.62	0/379
6	T	0.41	0/286	0.61	0/379
All	All	0.45	0/51552	0.58	0/69781

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 ⓘ

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	3680	0	3763	45	0
1	B	3655	0	3751	36	0
1	C	3680	0	3763	47	0
1	K	3680	0	3763	42	0
1	L	3655	0	3751	34	0
1	M	3680	0	3763	48	0
2	D	3549	0	3620	45	0
2	E	3536	0	3610	48	0
2	F	3548	0	3624	30	0
2	N	3549	0	3620	46	0
2	O	3536	0	3610	42	0
2	P	3559	0	3641	30	0
3	G	2057	0	2127	38	0
3	Q	2063	0	2133	32	0
4	H	937	0	947	18	0
4	R	937	0	947	22	0
5	I	450	0	452	20	0
5	S	450	0	452	20	0
6	J	283	0	267	11	0
6	T	283	0	267	12	0
7	A	31	0	12	0	0
7	K	31	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	P	1	0	0	0	0
9	B	27	0	12	0	0
9	C	27	0	12	1	0
9	D	27	0	12	0	0
9	E	27	0	12	0	0
9	F	27	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	27	0	12	0	0
9	M	27	0	12	1	0
9	N	27	0	12	0	0
9	O	27	0	12	0	0
9	P	27	0	12	0	0
10	C	4	0	6	0	0
10	L	8	0	12	0	0
10	M	4	0	6	2	0
10	O	4	0	6	0	0
10	P	4	0	6	1	0
11	A	18	0	0	0	0
11	B	90	0	0	4	0
11	C	94	0	0	1	0
11	D	37	0	0	0	0
11	E	20	0	0	0	0
11	F	81	0	0	3	0
11	G	11	0	0	1	0
11	H	1	0	0	1	0
11	I	1	0	0	1	0
11	K	27	0	0	0	0
11	L	156	0	0	3	0
11	M	76	0	0	0	0
11	N	32	0	0	0	0
11	O	52	0	0	2	0
11	P	68	0	0	0	0
11	Q	8	0	0	0	0
11	R	1	0	0	0	0
All	All	51906	0	52051	617	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 6.

The worst 5 of 617 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:O:85:VAL:HG11	2:O:235:THR:HG23	1.30	1.11
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.30	1.09
3:Q:96:ARG:HE	3:Q:121:THR:HG21	1.18	1.08
3:G:96:ARG:HE	3:G:121:THR:HG21	1.18	1.08
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.36	1.07

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	482/510 (94%)	462 (96%)	19 (4%)	1 (0%)	47	68
1	B	477/510 (94%)	464 (97%)	13 (3%)	0	100	100
1	C	482/510 (94%)	460 (95%)	22 (5%)	0	100	100
1	K	482/510 (94%)	460 (95%)	21 (4%)	1 (0%)	47	68
1	L	477/510 (94%)	463 (97%)	14 (3%)	0	100	100
1	M	482/510 (94%)	460 (95%)	22 (5%)	0	100	100
2	D	468/478 (98%)	449 (96%)	18 (4%)	1 (0%)	47	68
2	E	466/478 (98%)	444 (95%)	20 (4%)	2 (0%)	34	54
2	F	468/478 (98%)	445 (95%)	21 (4%)	2 (0%)	34	54
2	N	468/478 (98%)	449 (96%)	18 (4%)	1 (0%)	47	68
2	O	466/478 (98%)	445 (96%)	19 (4%)	2 (0%)	34	54
2	P	470/478 (98%)	446 (95%)	22 (5%)	2 (0%)	34	54
3	G	261/278 (94%)	251 (96%)	10 (4%)	0	100	100
3	Q	262/278 (94%)	252 (96%)	10 (4%)	0	100	100
4	H	120/138 (87%)	104 (87%)	14 (12%)	2 (2%)	9	16
4	R	120/138 (87%)	104 (87%)	14 (12%)	2 (2%)	9	16
5	I	54/61 (88%)	51 (94%)	2 (4%)	1 (2%)	8	13
5	S	54/61 (88%)	51 (94%)	2 (4%)	1 (2%)	8	13
6	J	34/63 (54%)	33 (97%)	1 (3%)	0	100	100
6	T	34/63 (54%)	33 (97%)	1 (3%)	0	100	100
All	All	6627/7008 (95%)	6326 (96%)	283 (4%)	18 (0%)	41	61

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	117	ALA
5	I	57	THR
4	R	117	ALA
5	S	57	THR
2	F	352	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/412 (95%)	381 (98%)	9 (2%)	50	76
1	B	387/412 (94%)	367 (95%)	20 (5%)	23	44
1	C	390/412 (95%)	376 (96%)	14 (4%)	35	61
1	K	390/412 (95%)	380 (97%)	10 (3%)	46	72
1	L	387/412 (94%)	366 (95%)	21 (5%)	22	42
1	M	390/412 (95%)	375 (96%)	15 (4%)	33	58
2	D	380/384 (99%)	365 (96%)	15 (4%)	32	57
2	E	378/384 (98%)	367 (97%)	11 (3%)	42	69
2	F	380/384 (99%)	369 (97%)	11 (3%)	42	69
2	N	380/384 (99%)	365 (96%)	15 (4%)	32	57
2	O	378/384 (98%)	366 (97%)	12 (3%)	39	65
2	P	382/384 (100%)	372 (97%)	10 (3%)	46	72
3	G	227/236 (96%)	215 (95%)	12 (5%)	22	43
3	Q	228/236 (97%)	215 (94%)	13 (6%)	20	39
4	H	105/112 (94%)	100 (95%)	5 (5%)	25	48
4	R	105/112 (94%)	100 (95%)	5 (5%)	25	48
5	I	47/48 (98%)	43 (92%)	4 (8%)	10	21
5	S	47/48 (98%)	43 (92%)	4 (8%)	10	21
6	J	30/57 (53%)	28 (93%)	2 (7%)	16	31
6	T	30/57 (53%)	28 (93%)	2 (7%)	16	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5431/5682 (96%)	5221 (96%)	210 (4%)	32 57

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	93	LEU
1	L	106	LEU
3	Q	181	PRO
5	I	4	ARG
1	K	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	103	ASN
1	K	174	GLN
3	Q	125	ASN
5	I	19	GLN
6	J	36	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 10 are monoatomic - leaving 18 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
9	ADP	O	600	-	24,29,29	1.43	3 (12%)	29,45,45	1.39	3 (10%)
9	ADP	M	600	8	24,29,29	1.14	2 (8%)	29,45,45	1.46	4 (13%)
9	ADP	N	600	8	24,29,29	1.29	2 (8%)	29,45,45	1.38	3 (10%)
9	ADP	C	600	8	24,29,29	1.16	2 (8%)	29,45,45	1.50	4 (13%)
9	ADP	L	600	8	24,29,29	1.18	2 (8%)	29,45,45	1.49	4 (13%)
7	ATP	A	600	8	26,33,33	1.10	2 (7%)	31,52,52	1.25	2 (6%)
9	ADP	P	600	8	24,29,29	1.21	2 (8%)	29,45,45	1.33	3 (10%)
10	EDO	P	603	-	3,3,3	0.69	0	2,2,2	0.44	0
10	EDO	C	603	-	3,3,3	0.33	0	2,2,2	0.45	0
10	EDO	M	602	-	3,3,3	0.38	0	2,2,2	0.30	0
10	EDO	L	602	-	3,3,3	0.59	0	2,2,2	0.21	0
10	EDO	O	602	-	3,3,3	0.46	0	2,2,2	0.40	0
9	ADP	B	600	8	24,29,29	1.37	3 (12%)	29,45,45	1.56	4 (13%)
9	ADP	E	600	-	24,29,29	1.31	2 (8%)	29,45,45	1.41	3 (10%)
9	ADP	F	600	8	24,29,29	1.16	3 (12%)	29,45,45	1.35	3 (10%)
7	ATP	K	600	8	26,33,33	1.03	1 (3%)	31,52,52	1.24	2 (6%)
9	ADP	D	600	8	24,29,29	1.33	3 (12%)	29,45,45	1.40	3 (10%)
10	EDO	L	604	-	3,3,3	0.52	0	2,2,2	0.27	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
9	ADP	O	600	-	-	0/12/32/32	0/3/3/3
9	ADP	M	600	8	-	4/12/32/32	0/3/3/3
9	ADP	N	600	8	-	1/12/32/32	0/3/3/3
9	ADP	C	600	8	-	4/12/32/32	0/3/3/3
9	ADP	L	600	8	-	0/12/32/32	0/3/3/3
7	ATP	A	600	8	-	2/18/38/38	0/3/3/3
9	ADP	P	600	8	-	1/12/32/32	0/3/3/3
10	EDO	P	603	-	-	0/1/1/1	-
10	EDO	C	603	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	M	602	-	-	0/1/1/1	-
10	EDO	L	602	-	-	0/1/1/1	-
10	EDO	O	602	-	-	0/1/1/1	-
9	ADP	B	600	8	-	0/12/32/32	0/3/3/3
9	ADP	E	600	-	-	0/12/32/32	0/3/3/3
9	ADP	F	600	8	-	1/12/32/32	0/3/3/3
7	ATP	K	600	8	-	2/18/38/38	0/3/3/3
9	ADP	D	600	8	-	1/12/32/32	0/3/3/3
10	EDO	L	604	-	-	0/1/1/1	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	600	ADP	PB-O1B	4.15	1.63	1.50
9	O	600	ADP	O4'-C1'	3.96	1.46	1.41
9	O	600	ADP	PB-O1B	3.83	1.62	1.50
9	E	600	ADP	O4'-C1'	3.83	1.46	1.41
9	D	600	ADP	O4'-C1'	3.81	1.46	1.41

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	600	ADP	N3-C2-N1	-4.89	121.03	128.68
9	F	600	ADP	N3-C2-N1	-4.88	121.04	128.68
9	P	600	ADP	N3-C2-N1	-4.81	121.16	128.68
9	D	600	ADP	N3-C2-N1	-4.63	121.44	128.68
9	M	600	ADP	N3-C2-N1	-4.60	121.49	128.68

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

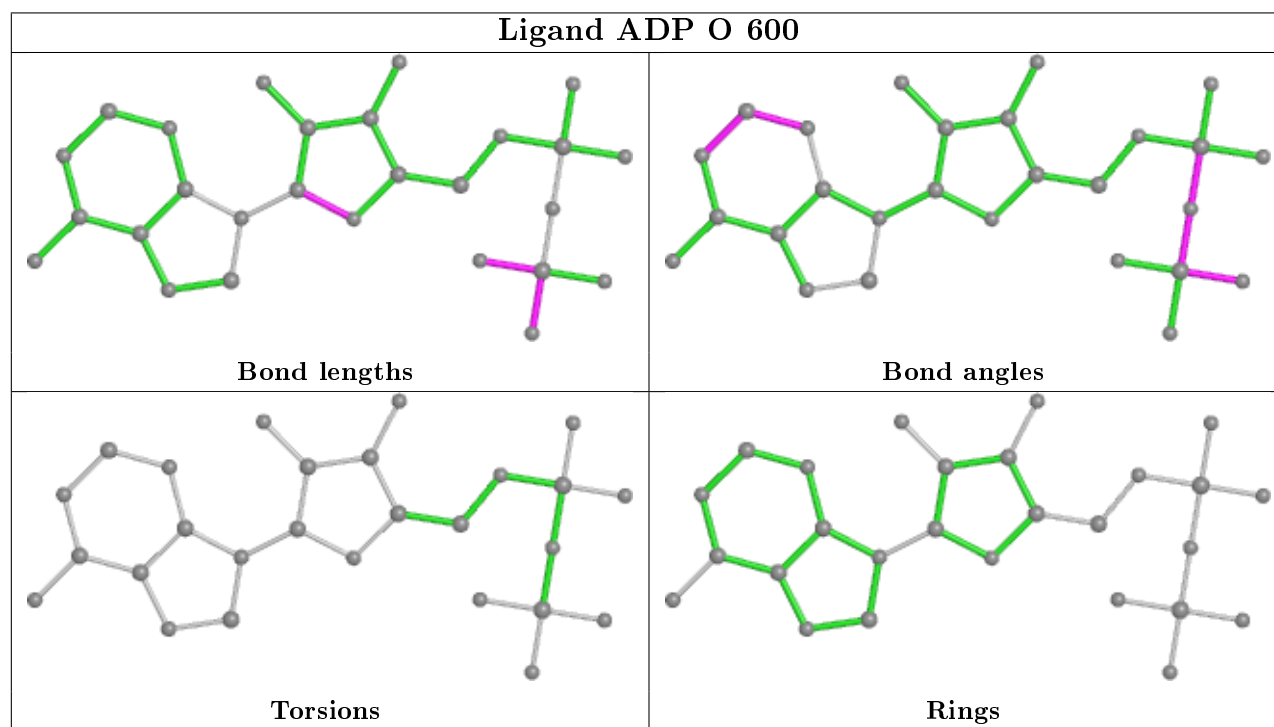
Mol	Chain	Res	Type	Atoms
7	A	600	ATP	PB-O3B-PG-O2G
9	M	600	ADP	C5'-O5'-PA-O1A
7	K	600	ATP	PB-O3B-PG-O2G
9	D	600	ADP	PA-O3A-PB-O2B
9	N	600	ADP	PA-O3A-PB-O2B

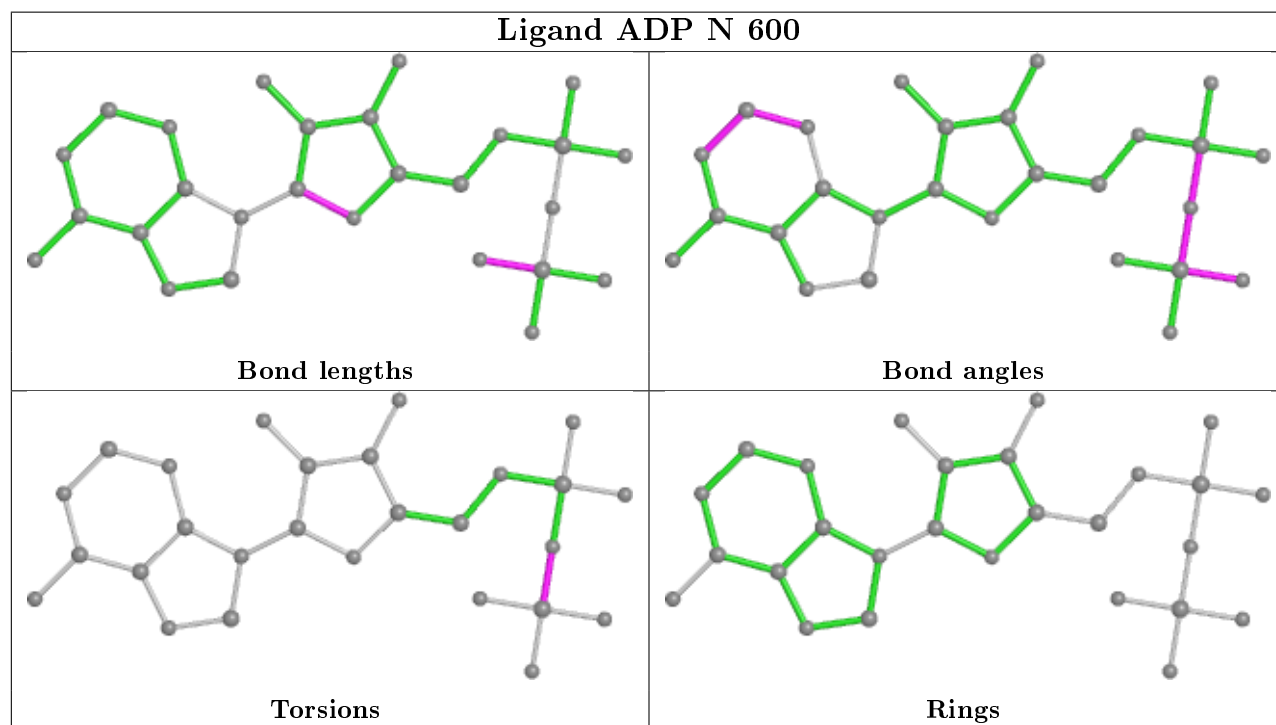
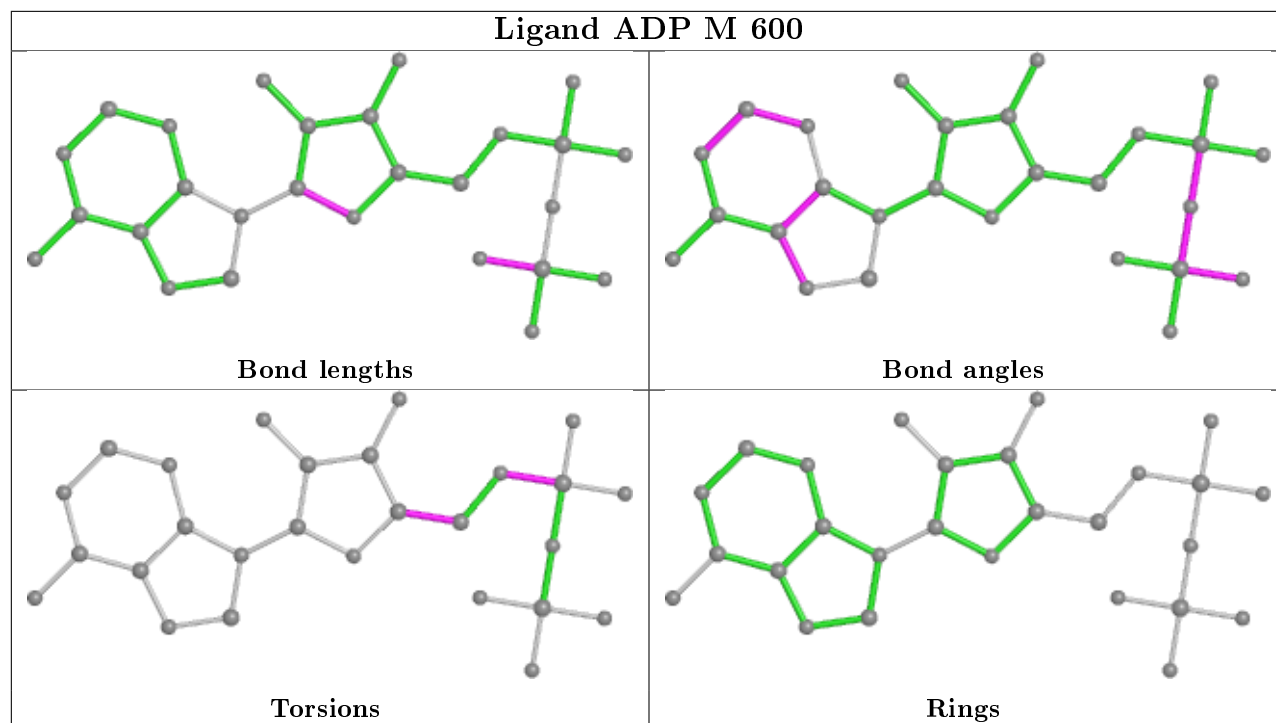
There are no ring outliers.

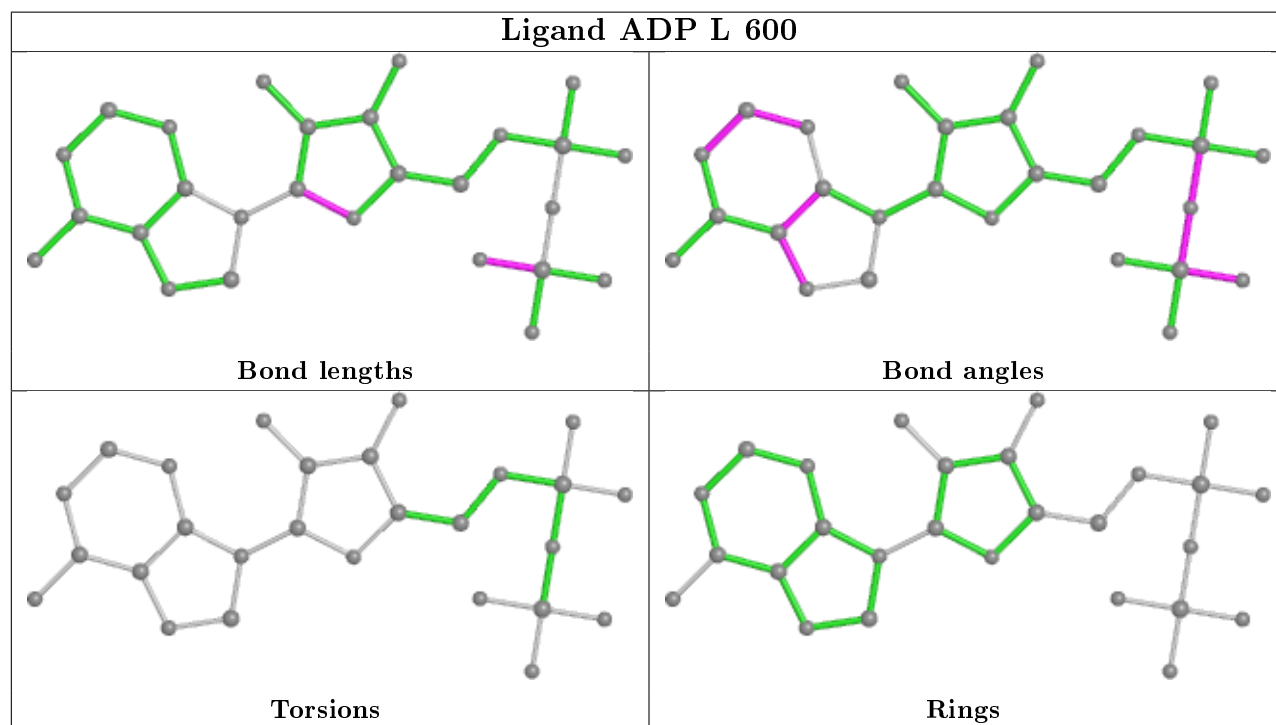
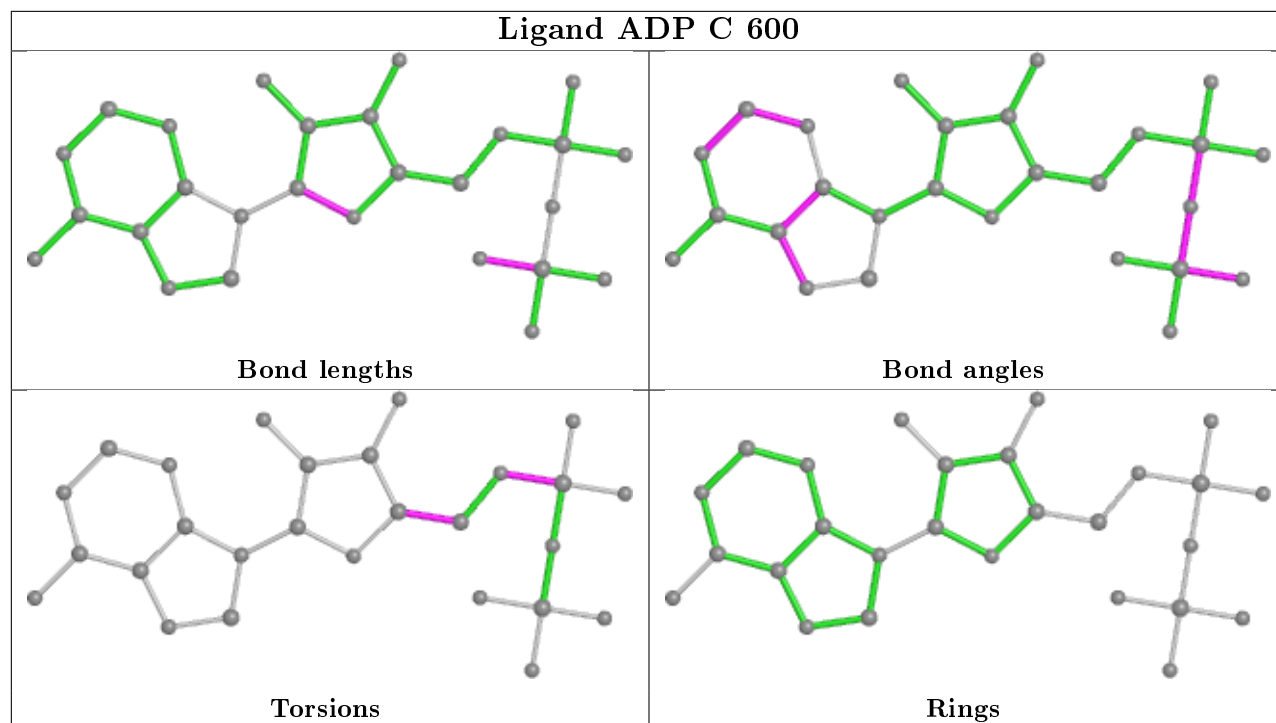
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	600	ADP	1	0
9	C	600	ADP	1	0
10	P	603	EDO	1	0
10	M	602	EDO	2	0

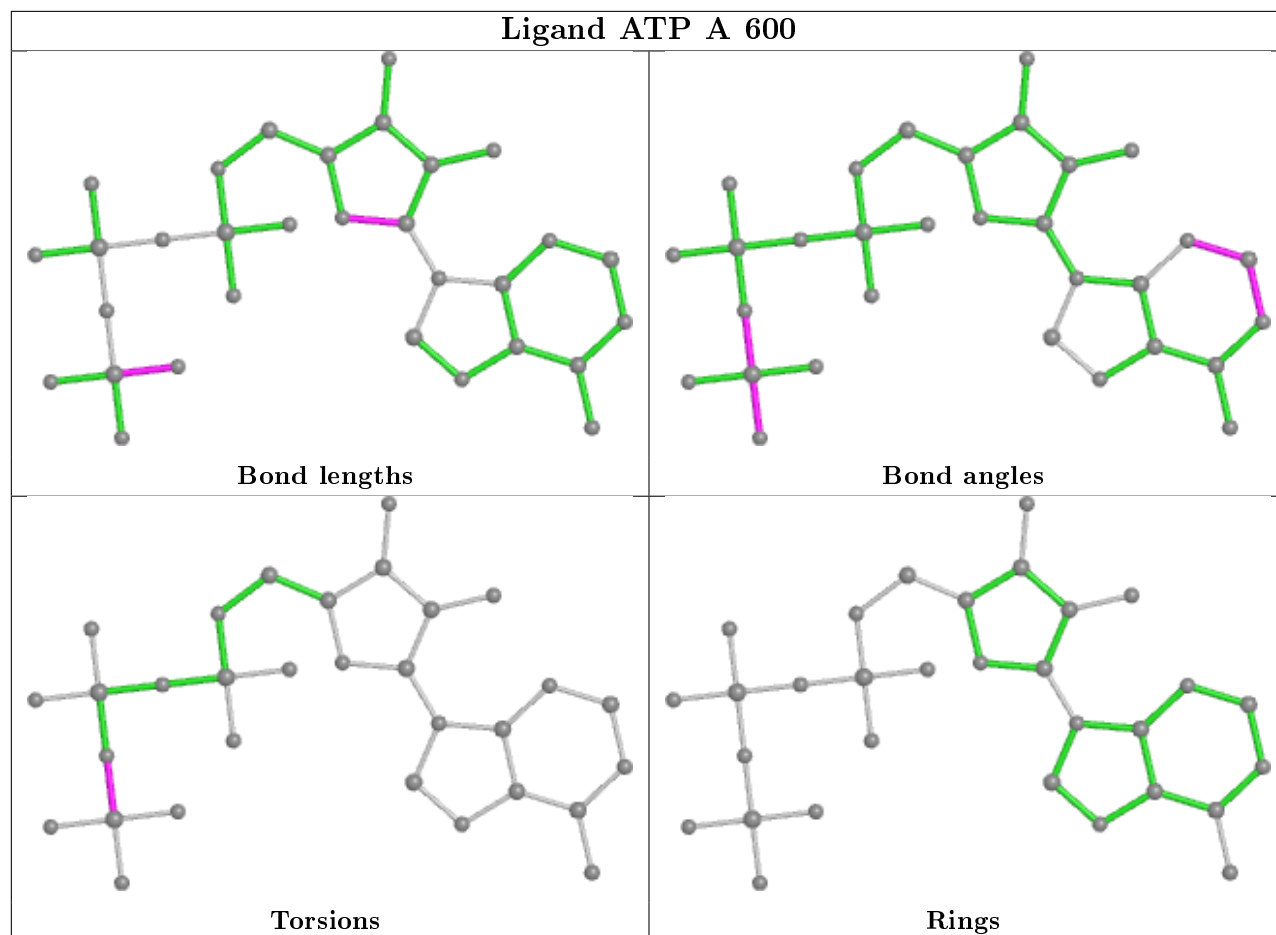
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



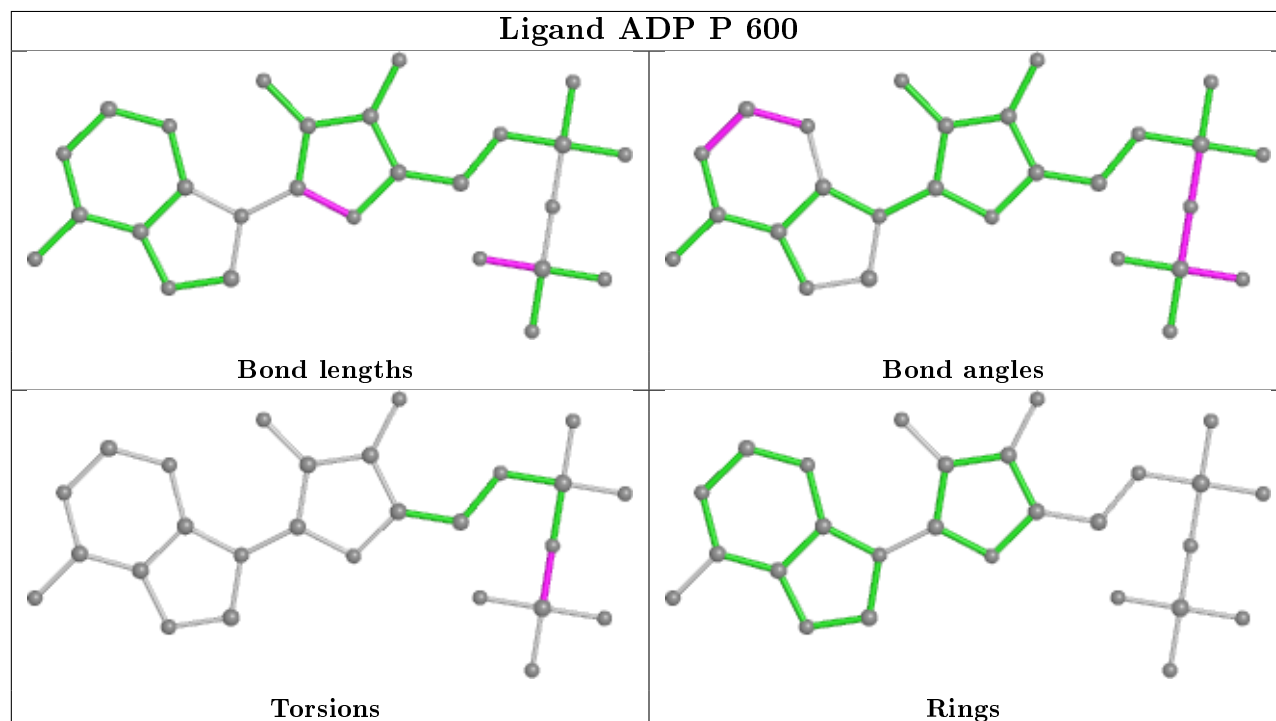


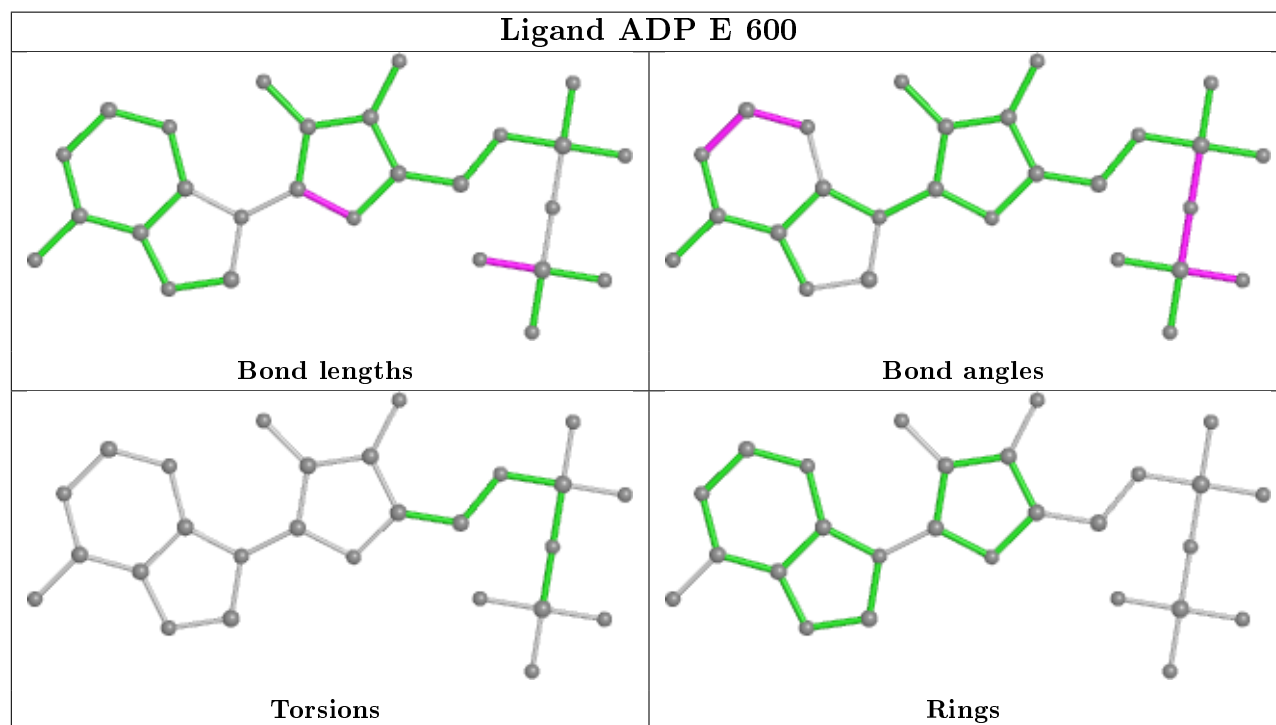
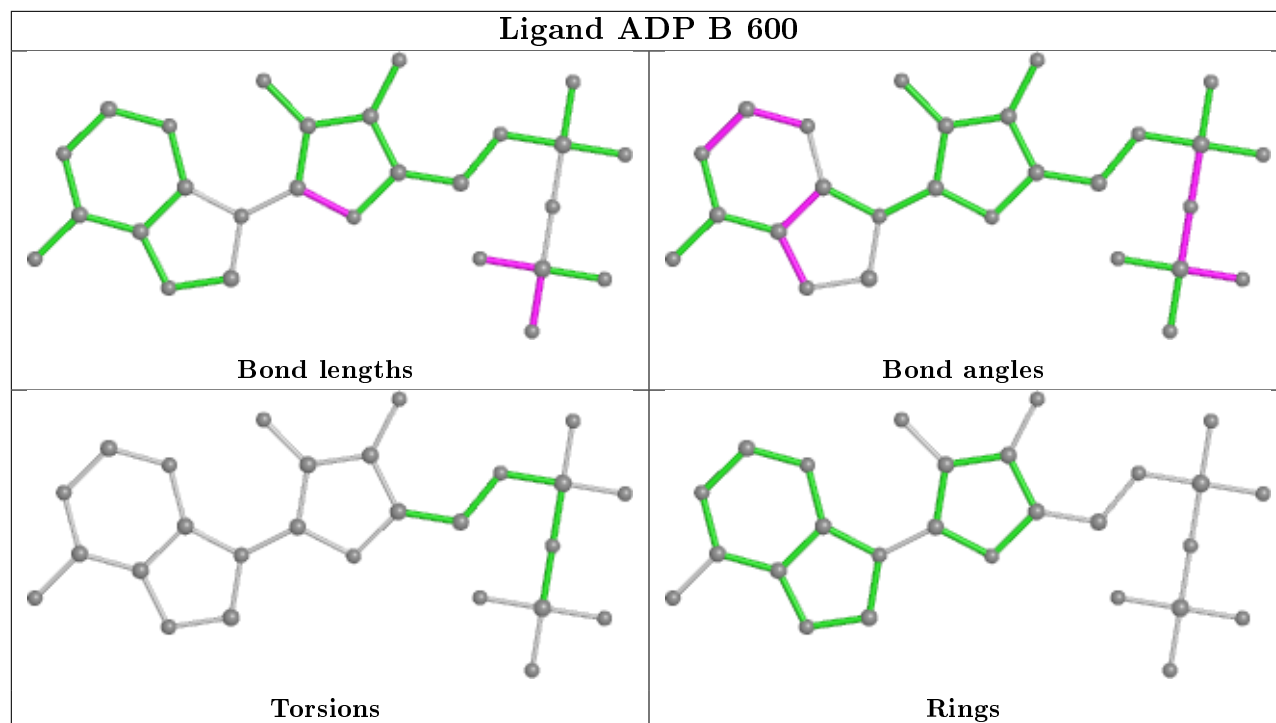


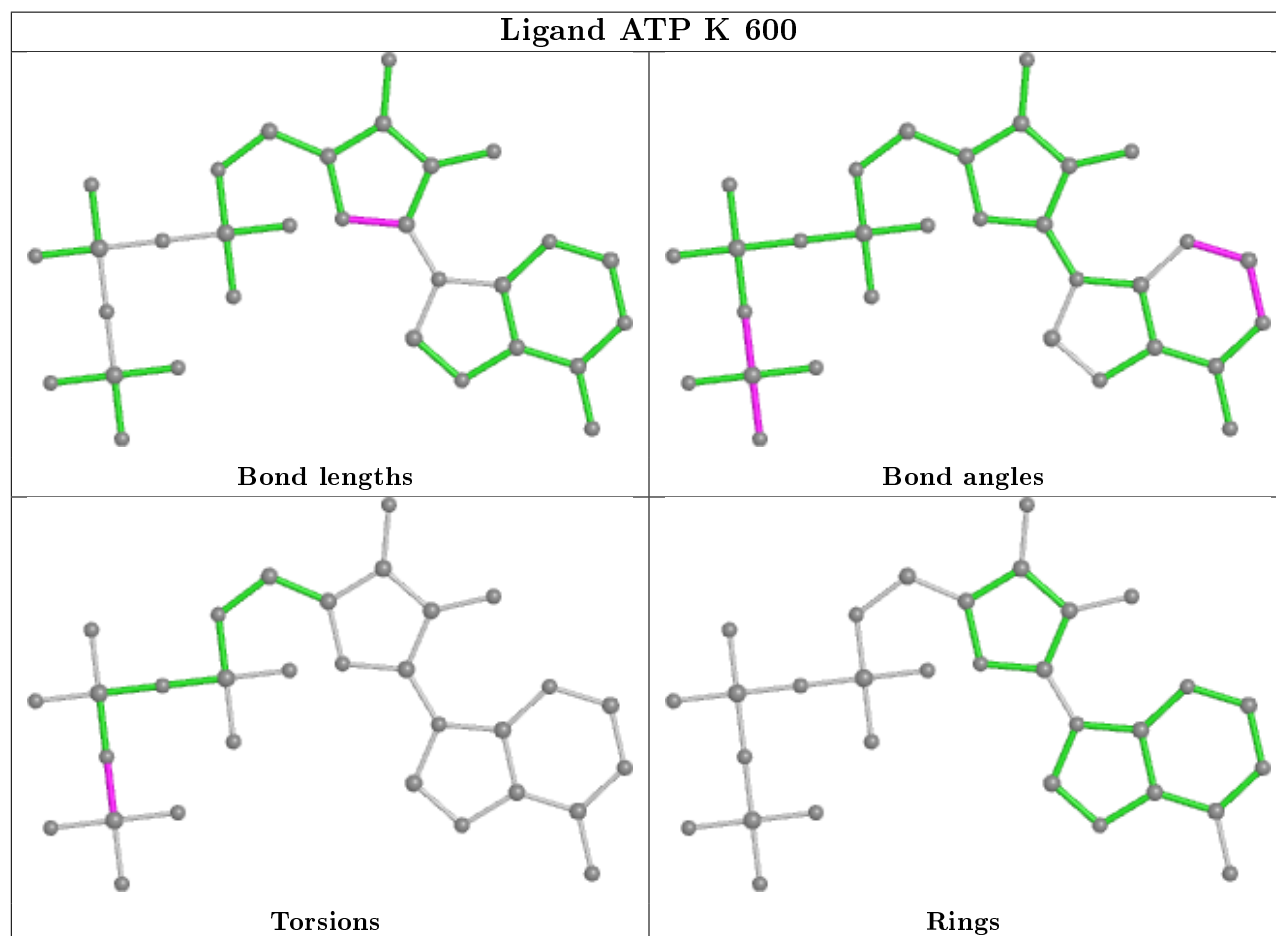
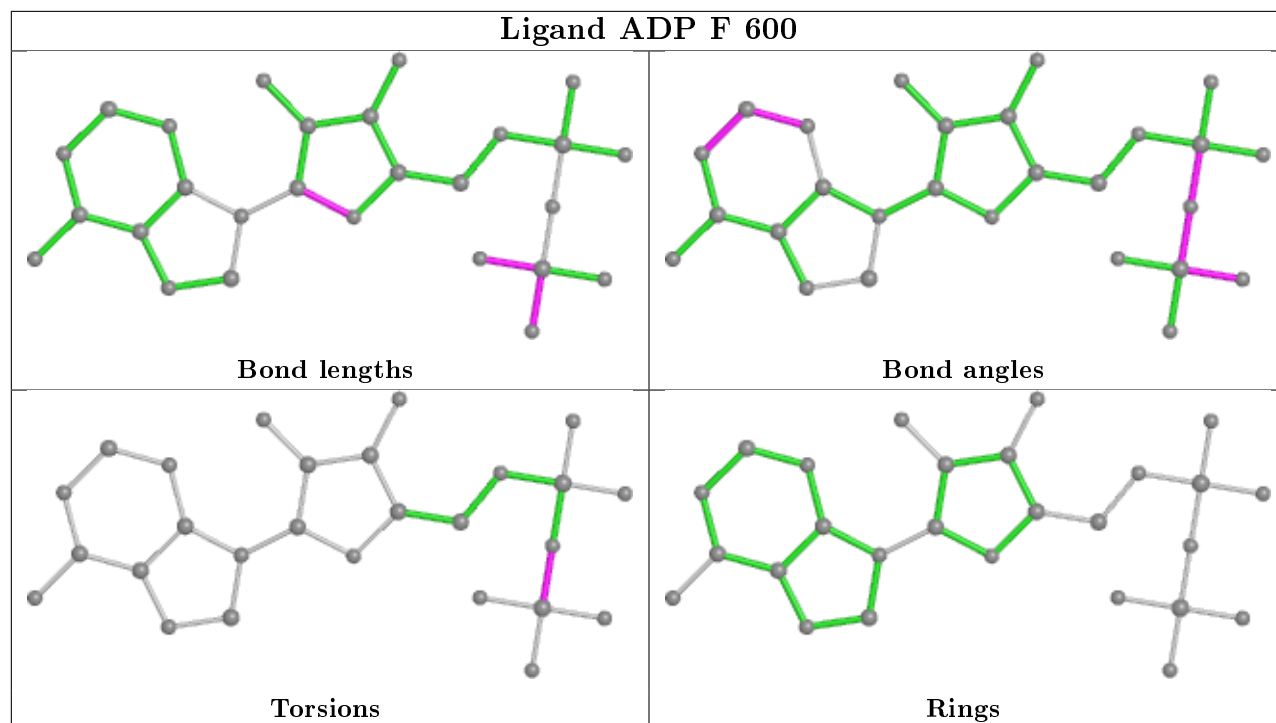
Ligand ATP A 600

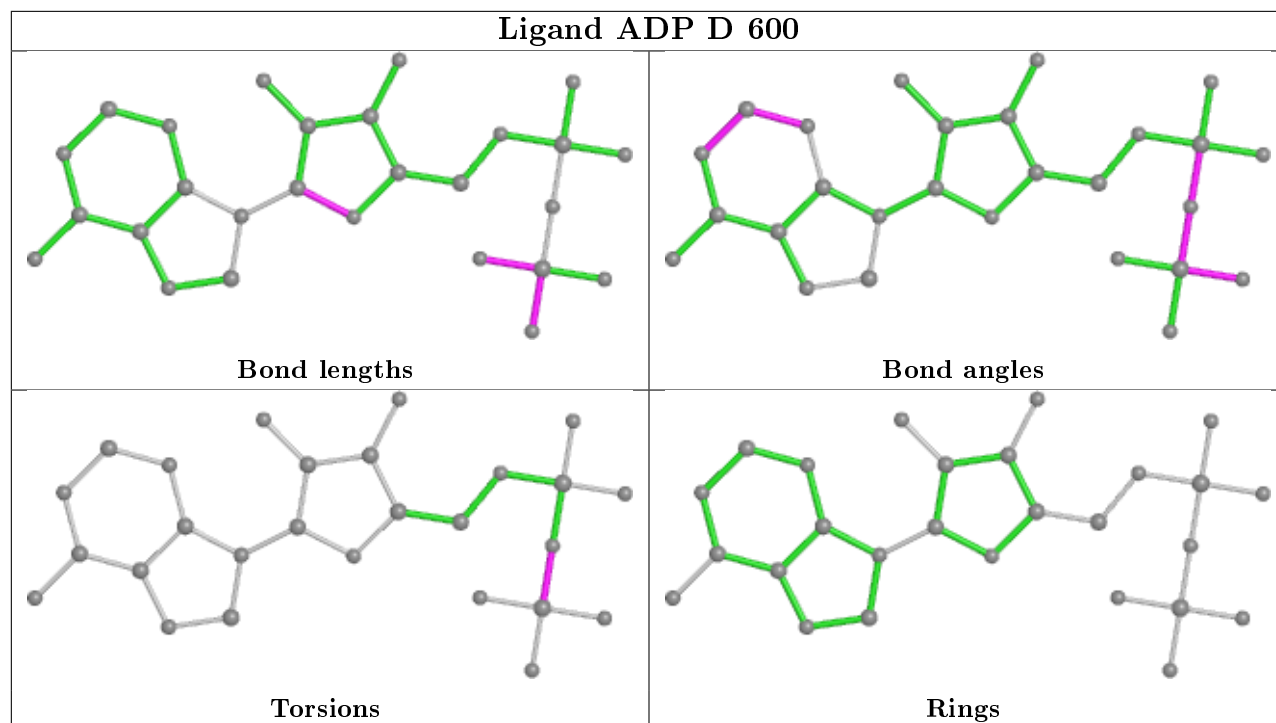


Ligand ADP P 600









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 ⓘ

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	484/510 (94%)	0.40	27 (5%) 24 25	34, 67, 108, 119	0
1	B	480/510 (94%)	0.16	27 (5%) 24 25	18, 42, 84, 104	0
1	C	484/510 (94%)	0.18	36 (7%) 14 15	22, 40, 112, 138	0
1	K	484/510 (94%)	0.43	34 (7%) 16 16	32, 60, 110, 119	0
1	L	480/510 (94%)	-0.18	3 (0%) 89 90	15, 31, 70, 100	0
1	M	484/510 (94%)	0.29	37 (7%) 13 14	23, 48, 116, 138	0
2	D	470/478 (98%)	0.21	18 (3%) 40 43	32, 55, 77, 100	0
2	E	468/478 (97%)	0.69	51 (10%) 5 5	34, 65, 118, 133	0
2	F	469/478 (98%)	-0.10	7 (1%) 73 75	19, 38, 64, 76	0
2	N	470/478 (98%)	0.29	20 (4%) 35 38	34, 60, 82, 103	0
2	O	468/478 (97%)	0.57	52 (11%) 5 5	20, 50, 119, 135	0
2	P	469/478 (98%)	0.07	17 (3%) 42 46	20, 43, 72, 79	0
3	G	265/278 (95%)	0.69	24 (9%) 9 9	36, 70, 120, 129	0
3	Q	265/278 (95%)	1.04	44 (16%) 1 1	30, 83, 122, 128	0
4	H	124/138 (89%)	1.77	46 (37%) 0 0	97, 110, 128, 133	0
4	R	124/138 (89%)	1.63	43 (34%) 0 0	96, 111, 127, 132	0
5	I	58/61 (95%)	0.98	5 (8%) 10 10	64, 84, 115, 117	0
5	S	58/61 (95%)	1.09	14 (24%) 0 0	65, 86, 121, 123	0
6	J	36/63 (57%)	0.62	2 (5%) 24 25	70, 84, 109, 110	0
6	T	36/63 (57%)	0.80	4 (11%) 5 5	76, 87, 112, 113	0
All	All	6676/7008 (95%)	0.37	511 (7%) 13 13	15, 57, 113, 138	0

The worst 5 of 511 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	389	ALA	10.0
2	O	396	LEU	9.0
2	O	386	ASP	8.5
2	O	387	ILE	8.2
2	O	404	VAL	8.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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.

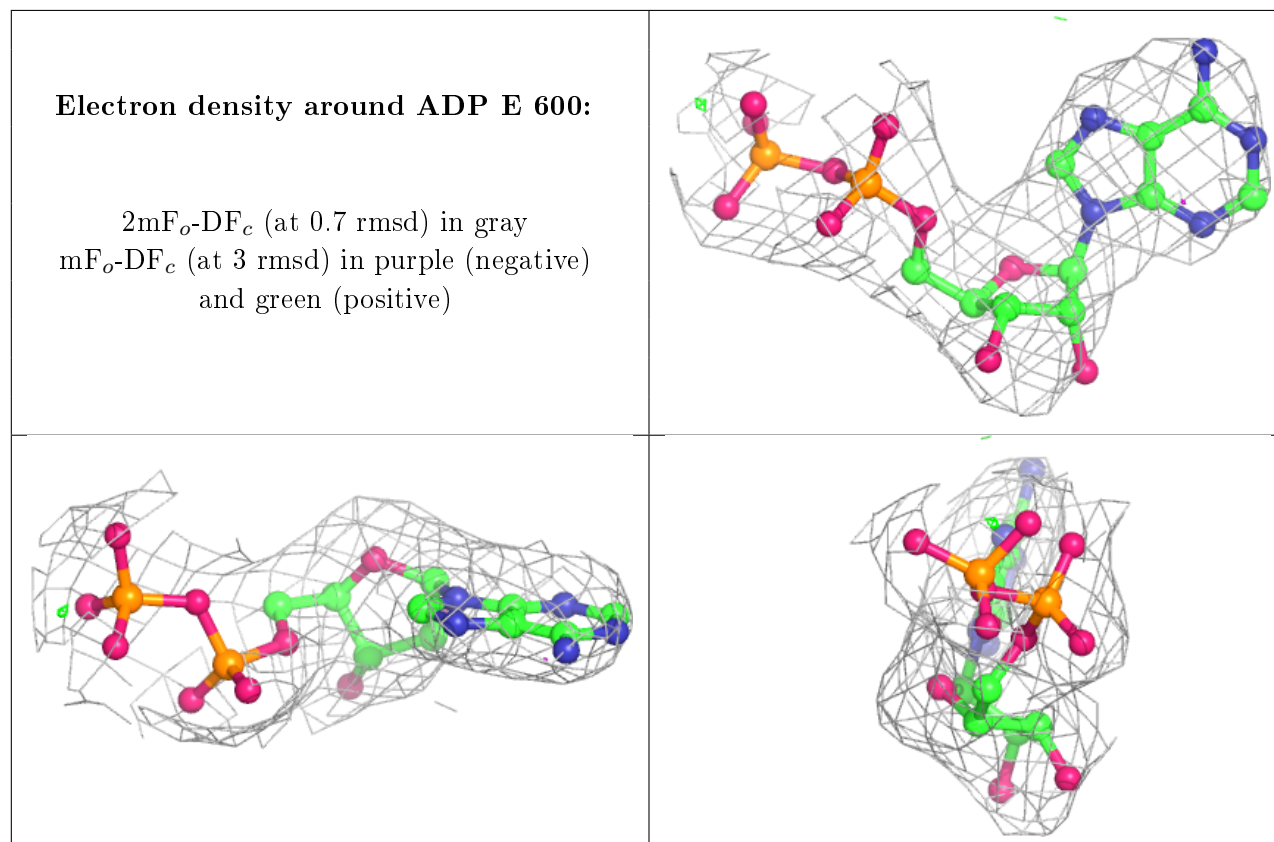
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	O	602	4/4	0.85	0.29	46,47,49,53	0
10	EDO	L	604	4/4	0.86	0.26	46,47,51,51	0
9	ADP	E	600	27/27	0.89	0.15	86,90,92,93	0
10	EDO	P	603	4/4	0.90	0.18	31,42,47,50	0
9	ADP	O	600	27/27	0.90	0.17	74,90,91,92	0
8	MG	A	601	1/1	0.92	0.18	50,50,50,50	0
8	MG	L	601	1/1	0.92	0.19	24,24,24,24	0
8	MG	B	601	1/1	0.93	0.15	40,40,40,40	0
8	MG	K	601	1/1	0.94	0.19	45,45,45,45	0
8	MG	P	601	1/1	0.95	0.22	25,25,25,25	0
9	ADP	M	600	27/27	0.96	0.13	36,65,72,73	0
9	ADP	N	600	27/27	0.96	0.15	37,46,55,57	0
9	ADP	C	600	27/27	0.96	0.16	28,53,65,65	0
10	EDO	L	602	4/4	0.96	0.12	28,28,31,32	0
7	ATP	A	600	31/31	0.96	0.16	45,53,57,58	4
7	ATP	K	600	31/31	0.96	0.19	38,54,59,60	4
10	EDO	C	603	4/4	0.97	0.20	33,35,36,39	0
9	ADP	B	600	27/27	0.97	0.14	29,48,55,57	0
9	ADP	D	600	27/27	0.98	0.16	33,46,55,58	0

Continued on next page...

Continued from previous page...

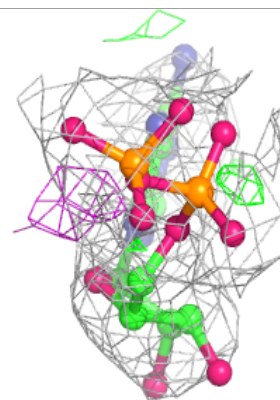
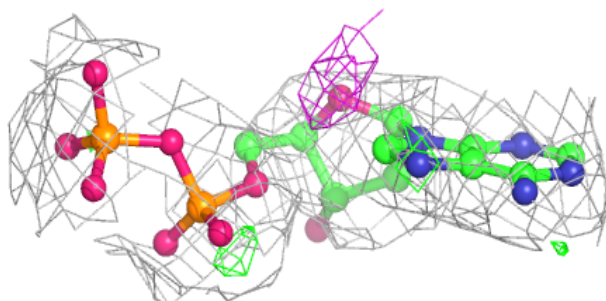
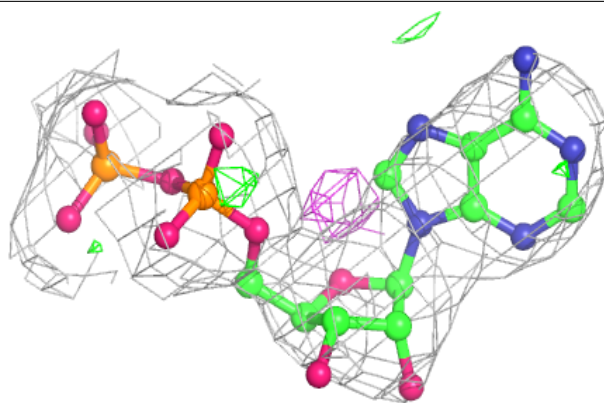
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MG	F	601	1/1	0.98	0.20	24,24,24,24	0
8	MG	C	601	1/1	0.98	0.15	27,27,27,27	0
8	MG	M	601	1/1	0.98	0.15	34,34,34,34	0
8	MG	D	601	1/1	0.98	0.18	35,35,35,35	0
9	ADP	L	600	27/27	0.98	0.14	18,32,41,43	0
10	EDO	M	602	4/4	0.98	0.20	32,39,42,45	0
9	ADP	F	600	27/27	0.98	0.17	24,29,32,39	0
9	ADP	P	600	27/27	0.99	0.16	22,33,36,41	0
8	MG	N	601	1/1	0.99	0.15	40,40,40,40	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.

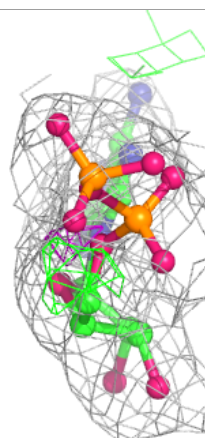
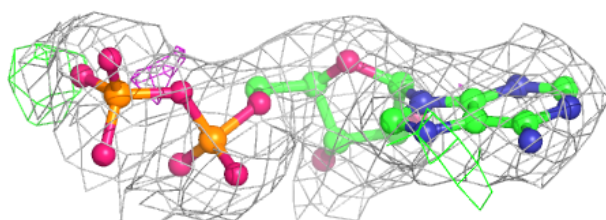
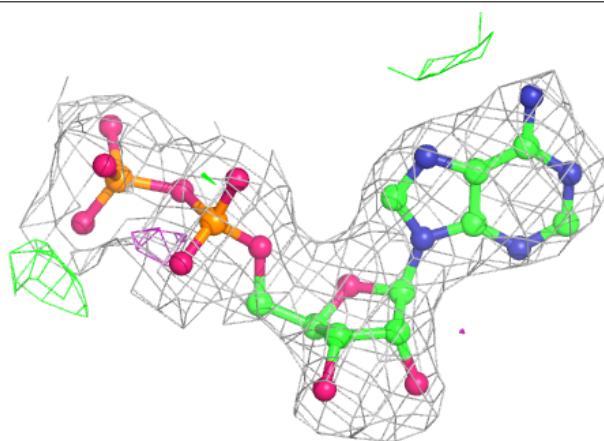


Electron density around ADP O 600:

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

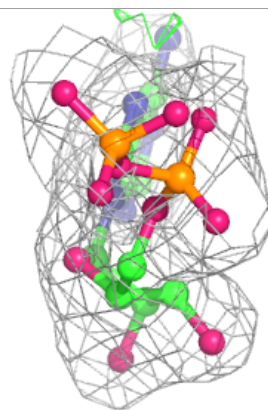
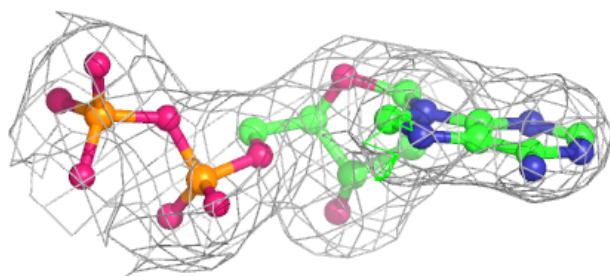
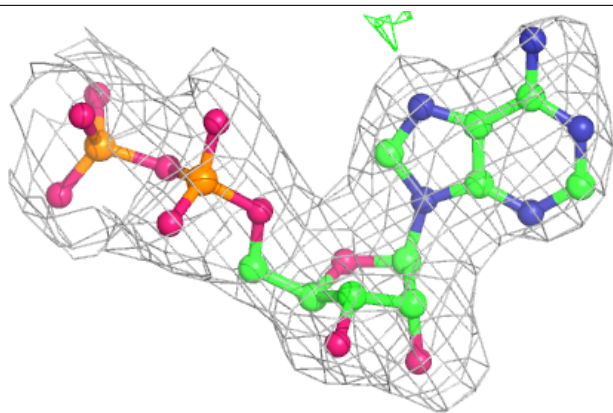
**Electron density around ADP M 600:**

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

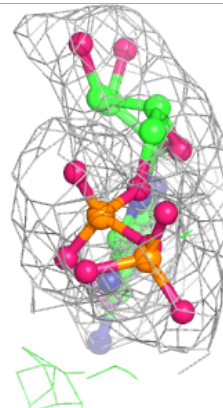
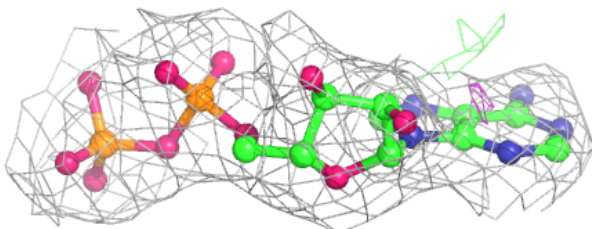
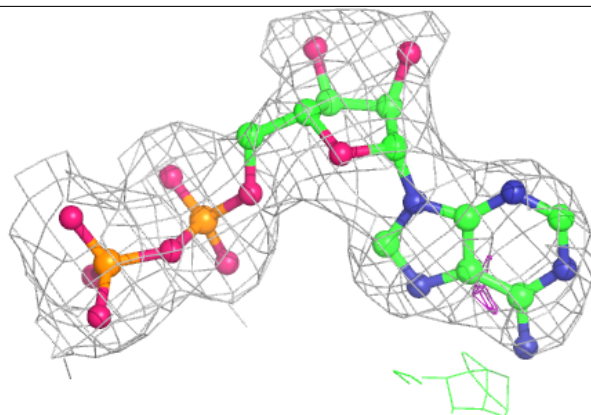


Electron density around ADP N 600:

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

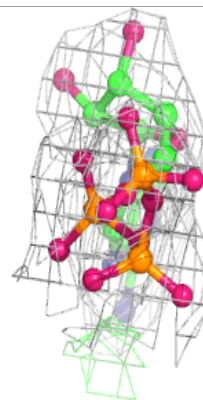
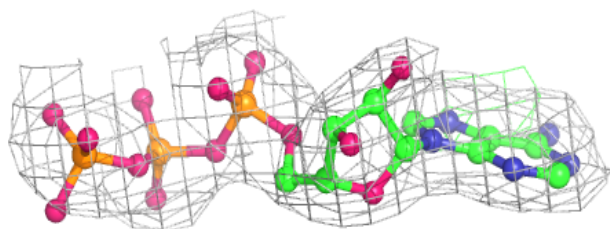
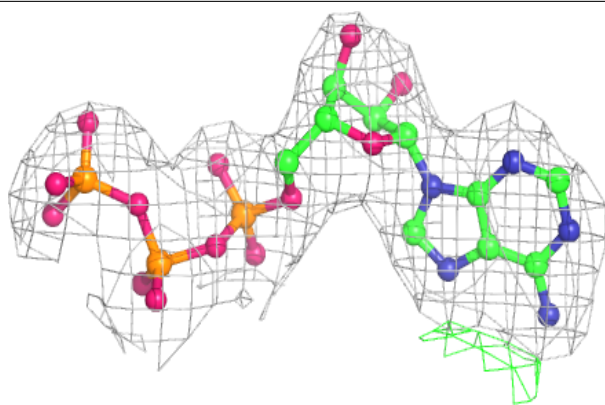
**Electron density around ADP C 600:**

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

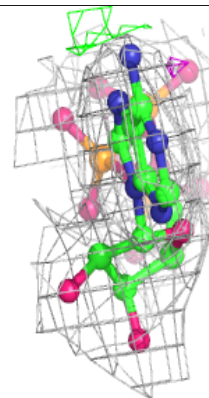
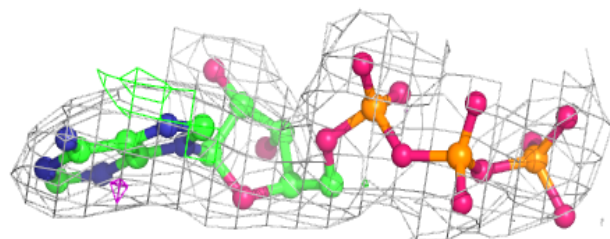
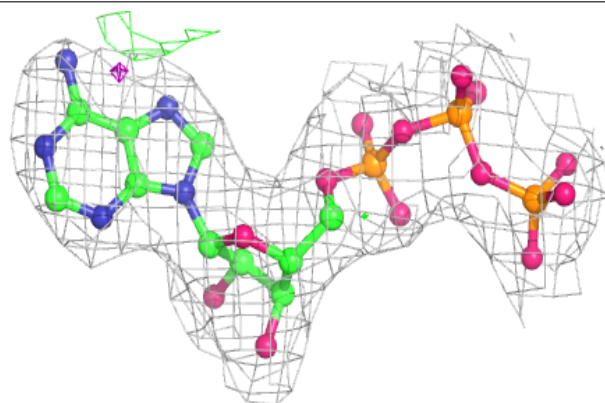


Electron density around ATP A 600:

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

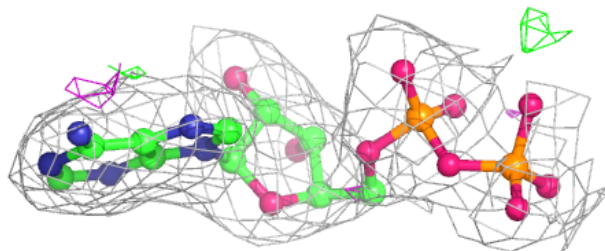
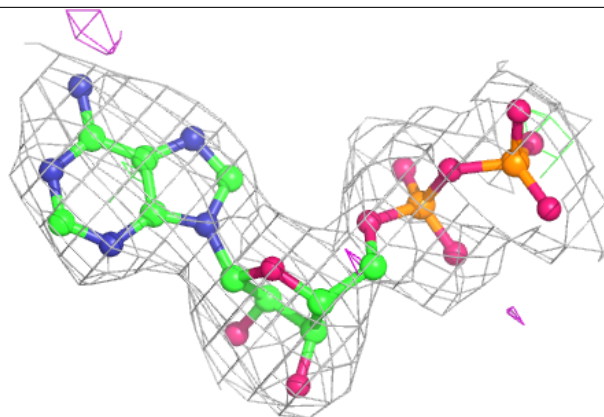
**Electron density around ATP K 600:**

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

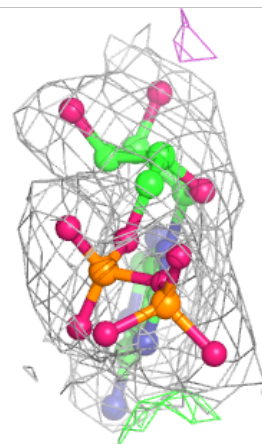
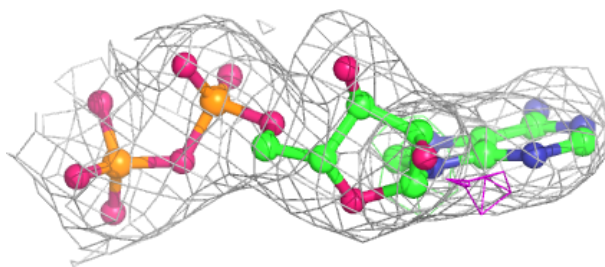
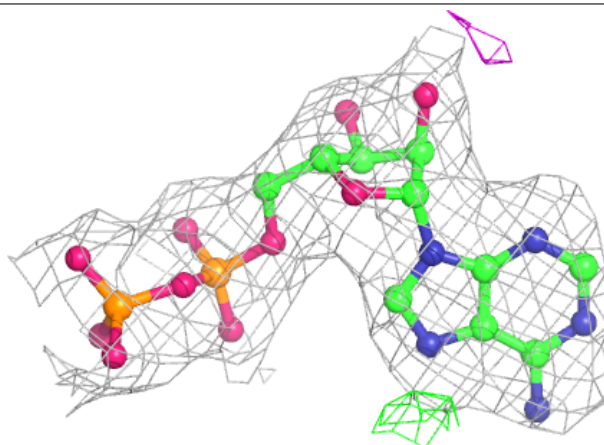


Electron density around ADP B 600:

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

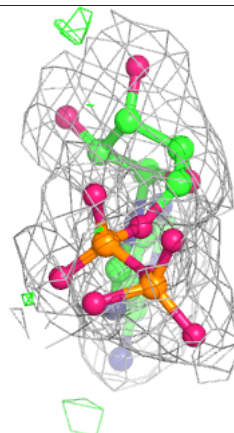
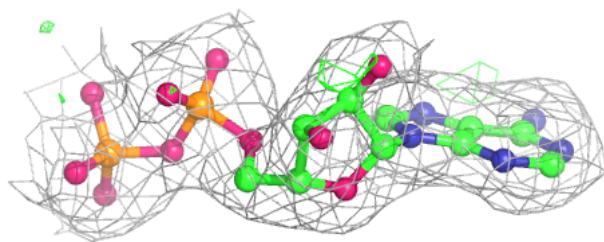
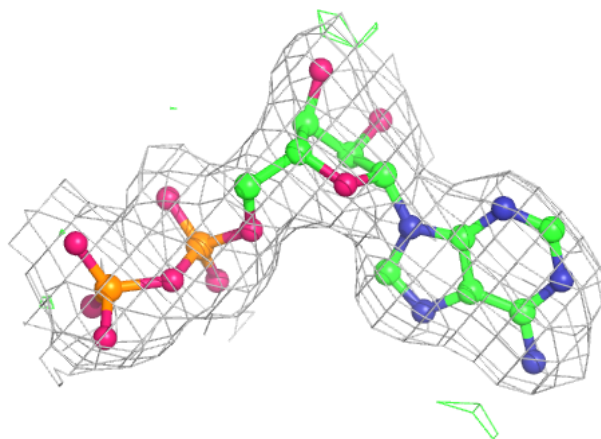
**Electron density around ADP D 600:**

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



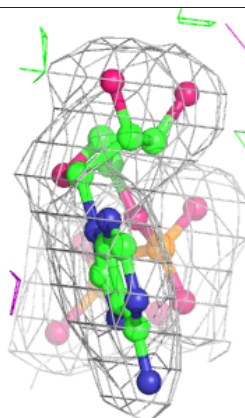
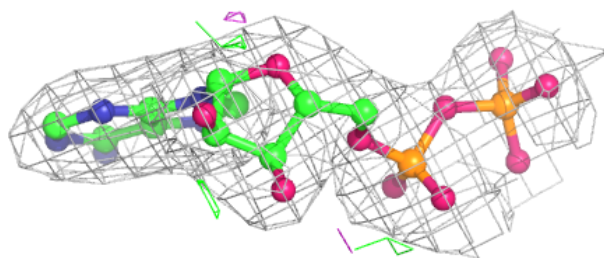
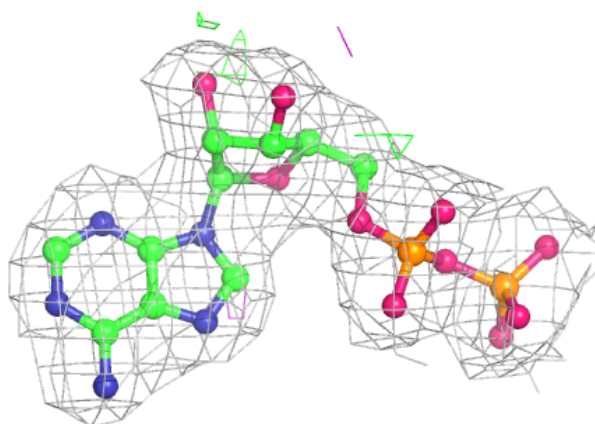
Electron density around ADP L 600:

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

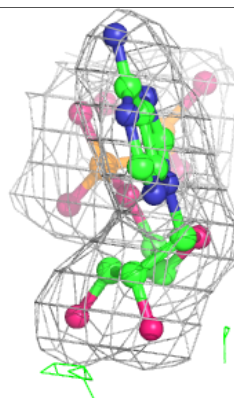
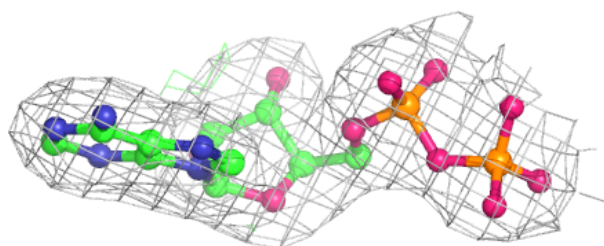
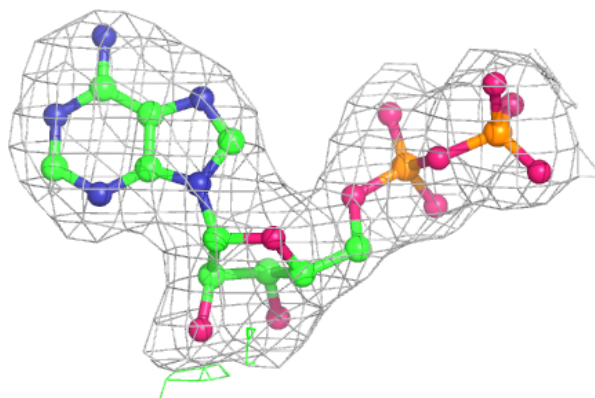


Electron density around ADP F 600:

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

**Electron density around ADP P 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.