



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 02:21 am BST

PDB ID : 1E79  
Title : Bovine F1-ATPase inhibited by DCCD (dicyclohexylcarbodiimide)  
Authors : Gibbons, C.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2000-08-25  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 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

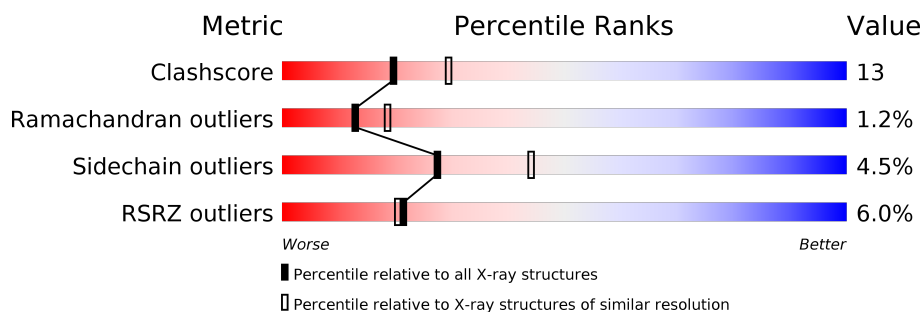
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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>4%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	B	510	<div> <div>5%</div> <div>70%</div> <div>24%</div> <div>• • •</div> </div>
1	C	510	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
2	D	482	<div> <div>2%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
2	E	482	<div> <div>8%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
2	F	482	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
3	G	272	<div> <div>16%</div> <div>58%</div> <div>33%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	H	146	<div><div></div><div>21%</div><div>51%</div><div>34%</div><div>•</div><div>10%</div></div>
5	I	50	<div><div></div><div>22%</div><div>58%</div><div>26%</div><div>8%</div><div>•</div><div>6%</div></div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26318 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 ALPHA CHAIN HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			
1	B	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	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	cloning artifact	UNP P19483
B	481	GLY	SER	cloning artifact	UNP P19483
C	481	GLY	SER	cloning artifact	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3538	2243	601	683	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 ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2051	1291	354	398	8			

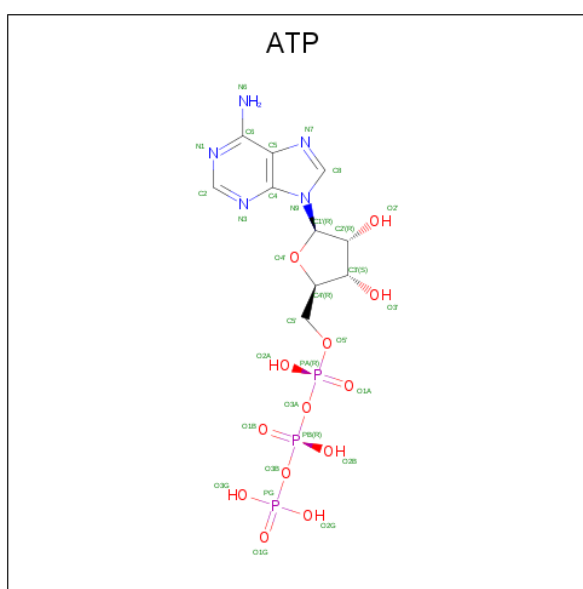
- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

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

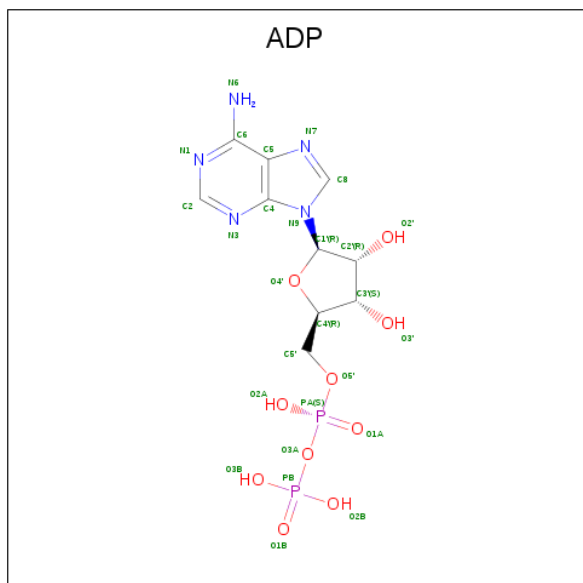
- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



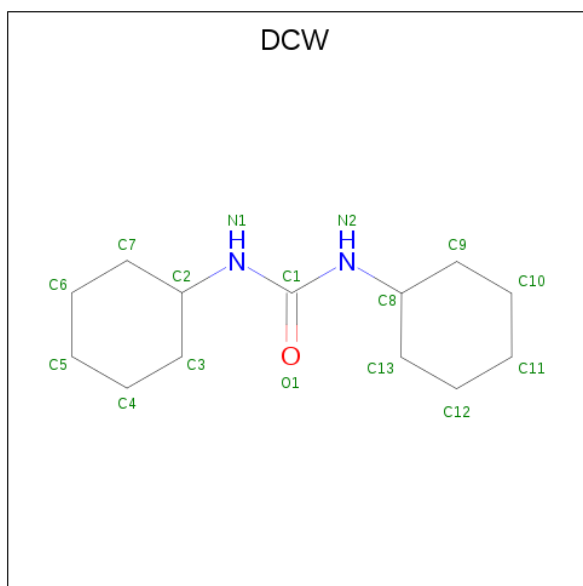
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 10 is DICYCLOHEXYLUREA (three-letter code: DCW) (formula:  $C_{13}H_{24}N_2O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			16	13	2	1		

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is water.

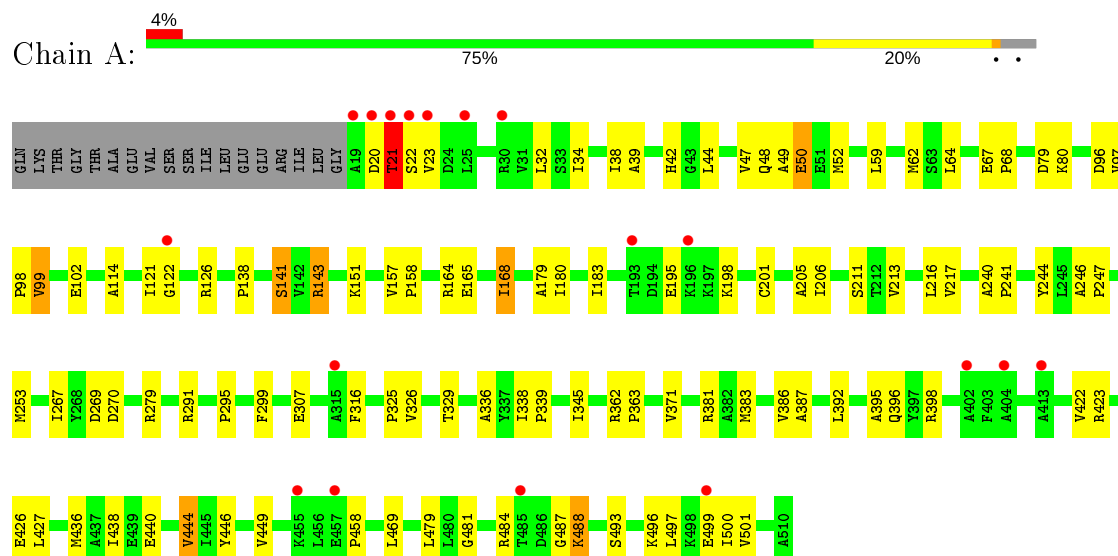
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	163	Total	O	0	0
			163	163		
12	B	140	Total	O	0	0
			140	140		
12	C	167	Total	O	0	0
			167	167		
12	D	148	Total	O	0	0
			148	148		
12	E	95	Total	O	0	0
			95	95		
12	F	164	Total	O	0	0
			164	164		
12	G	25	Total	O	0	0
			25	25		
12	H	5	Total	O	0	0
			5	5		
12	I	4	Total	O	0	0
			4	4		



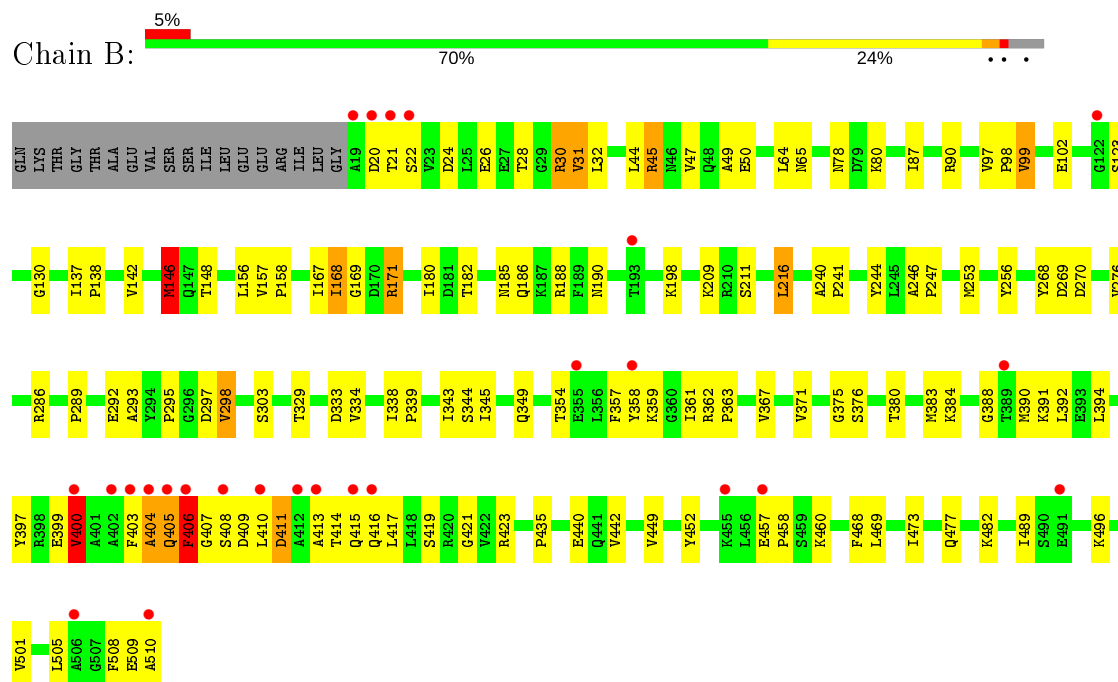
### 3 Residue-property plots

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.

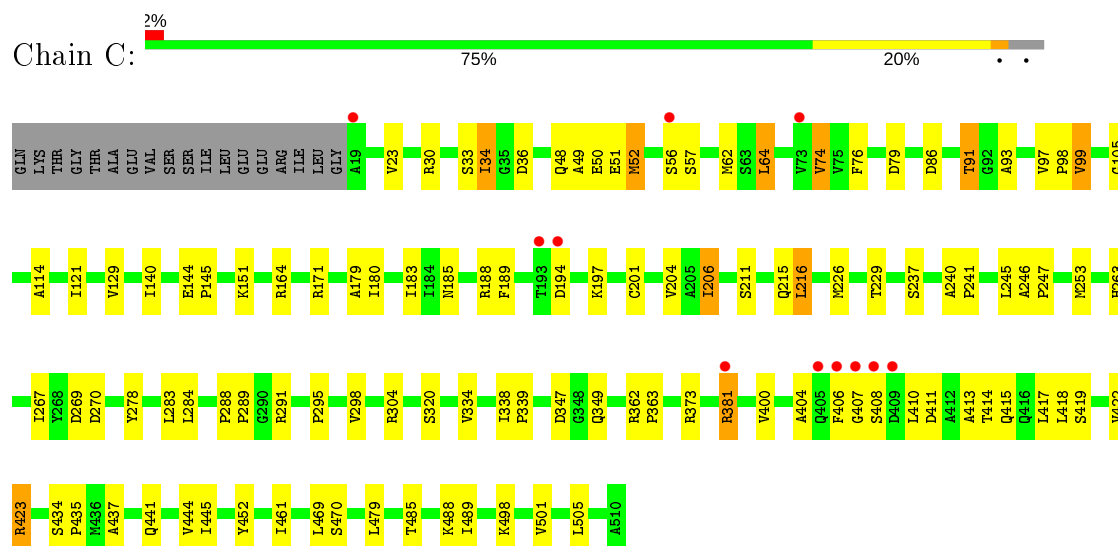
#### • Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM



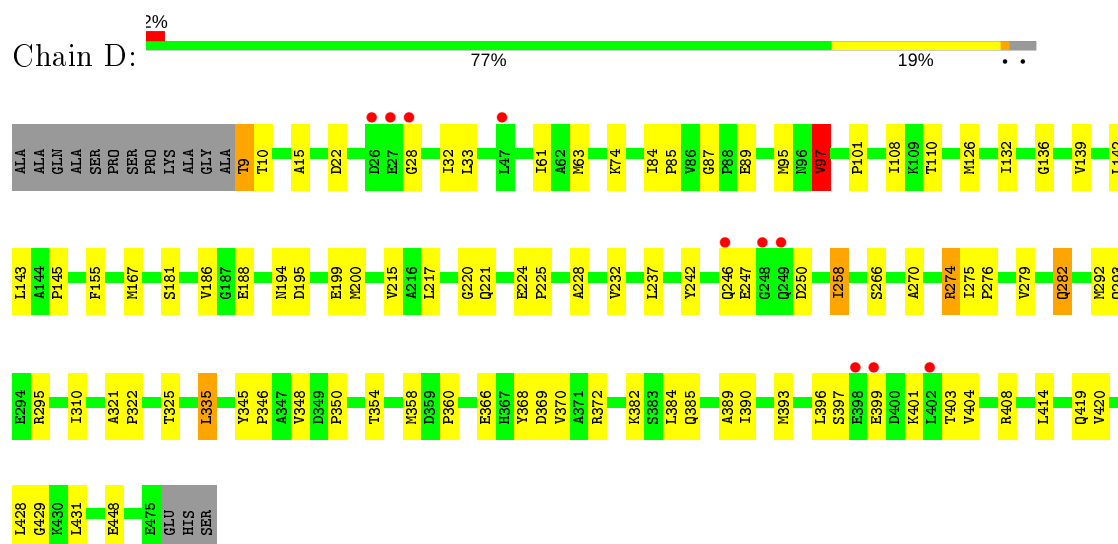
#### • Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM



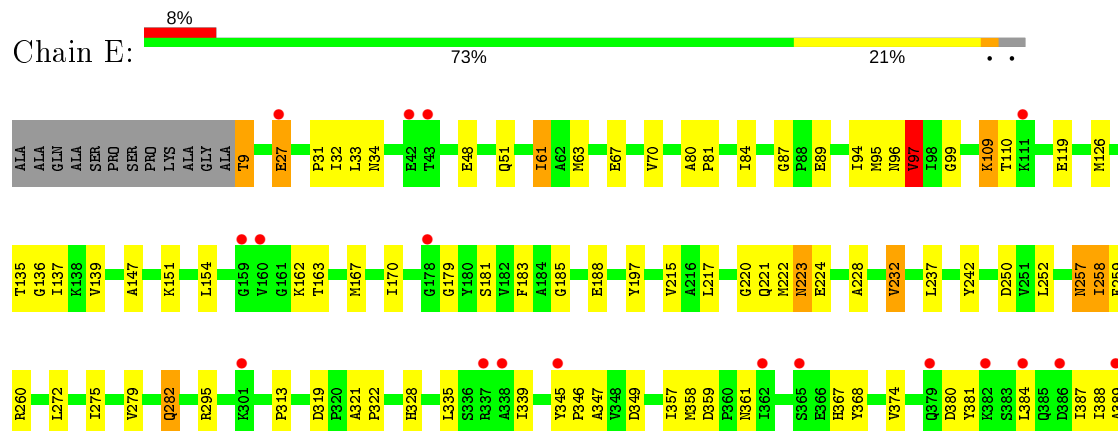
• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM

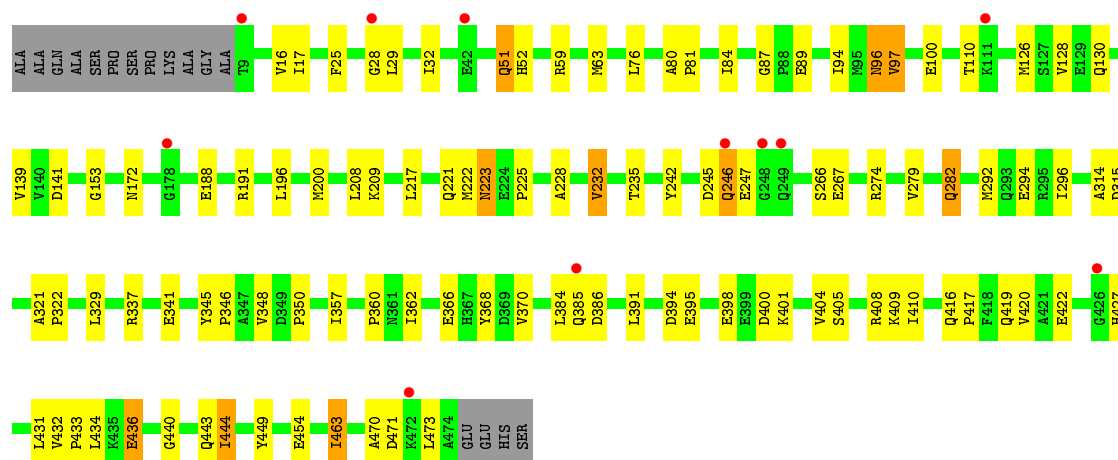


• Molecule 2: ATP SYNTHASE BETA CHAIN

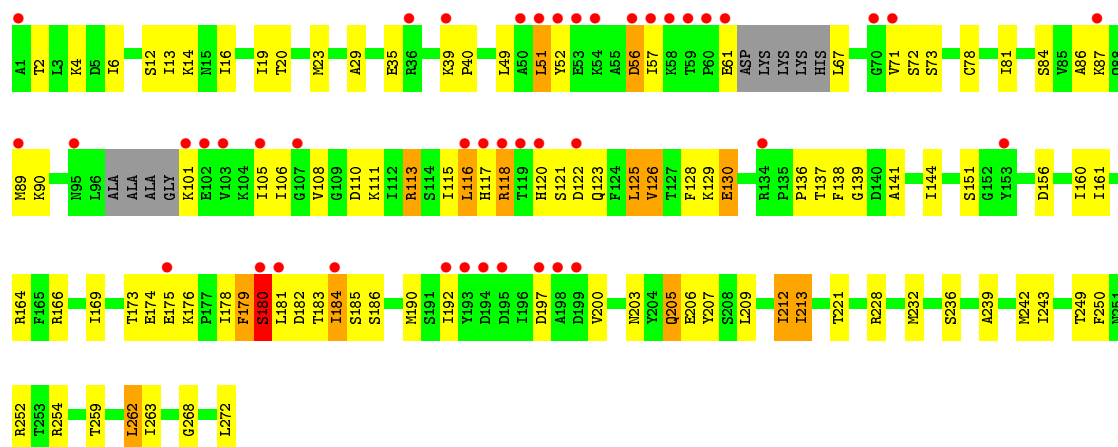


• Molecule 2: ATP SYNTHASE BETA CHAIN

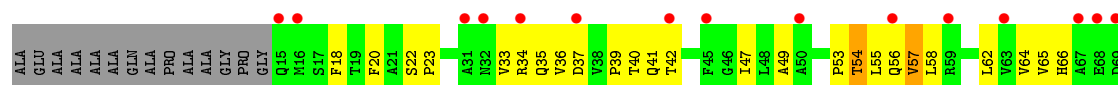


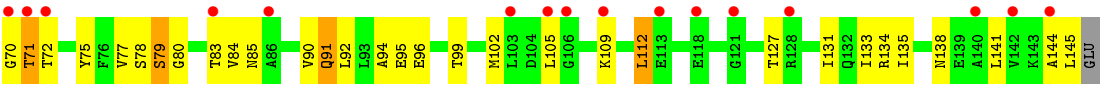


- Molecule 3: ATP SYNTHASE GAMMA CHAIN

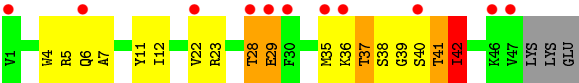


- Molecule 4: ATP SYNTHASE DELTA CHAIN





● Molecule 5: ATP SYNTHASE EPSILON CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	267.20 Å 107.20 Å 135.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.2 (20.00-2.40) 91.9 (19.98-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.41 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.225 , 0.281 0.204 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, MG, ADP, SO4, ATP, DCW

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	0/3799	0.78	0/5126
1	B	0.39	0/3799	0.81	2/5126 (0.0%)
1	C	0.40	0/3799	0.81	2/5126 (0.0%)
2	D	0.40	0/3595	0.81	2/4877 (0.0%)
2	E	0.38	0/3587	0.76	1/4867 (0.0%)
2	F	0.39	0/3587	0.79	1/4867 (0.0%)
3	G	0.35	0/2074	0.72	2/2785 (0.1%)
4	H	0.33	0/982	0.67	0/1337
5	I	0.34	0/374	0.71	0/501
All	All	0.38	0/25596	0.78	10/34612 (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	D	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	195	ASP	N-CA-CB	8.67	126.21	110.60
1	B	45	ARG	NE-CZ-NH2	-7.26	116.67	120.30
2	F	191	ARG	NE-CZ-NH2	-6.49	117.06	120.30
3	G	254	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	423	ARG	CD-NE-CZ	5.33	131.06	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	194	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	3748	0	3844	76	0
1	B	3748	0	3844	106	0
1	C	3748	0	3844	75	0
2	D	3538	0	3592	83	0
2	E	3530	0	3587	89	0
2	F	3530	0	3586	88	0
3	G	2051	0	2115	108	0
4	H	970	0	972	55	0
5	I	369	0	395	20	0
6	A	31	0	12	0	0
6	C	31	0	12	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	B	27	0	12	0	0
8	D	27	0	12	0	0
8	F	27	0	12	0	0
9	B	6	0	8	1	0
10	D	16	0	23	6	0
11	E	5	0	0	0	0
12	A	163	0	0	4	0
12	B	140	0	0	3	0
12	C	167	0	0	2	0
12	D	148	0	0	9	0
12	E	95	0	0	0	0
12	F	164	0	0	4	0
12	G	25	0	0	1	0
12	H	5	0	0	0	0
12	I	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	26318	0	25870	651	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 13.

The worst 5 of 651 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:GLU:HG2	10:D:700:DCW:H71C	1.32	1.08
2:D:199:GLU:CG	10:D:700:DCW:H71C	1.85	1.06
3:G:90:LYS:HB3	3:G:116:LEU:HD11	1.38	1.01
1:B:406:PHE:HB2	1:B:409:ASP:HB2	1.44	1.00
2:F:282:GLN:H	2:F:282:GLN:HE21	1.00	0.98

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	490/510 (96%)	468 (96%)	19 (4%)	3 (1%)	25	36
1	B	490/510 (96%)	451 (92%)	31 (6%)	8 (2%)	9	13
1	C	490/510 (96%)	468 (96%)	21 (4%)	1 (0%)	47	62
2	D	465/482 (96%)	437 (94%)	27 (6%)	1 (0%)	47	62
2	E	464/482 (96%)	434 (94%)	23 (5%)	7 (2%)	10	14
2	F	464/482 (96%)	433 (93%)	27 (6%)	4 (1%)	17	25
3	G	257/272 (94%)	223 (87%)	26 (10%)	8 (3%)	4	3
4	H	129/146 (88%)	118 (92%)	8 (6%)	3 (2%)	6	7
5	I	45/50 (90%)	36 (80%)	4 (9%)	5 (11%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3294/3444 (96%)	3068 (93%)	186 (6%)	40 (1%)	13	19

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	B	404	ALA
1	B	405	GLN
1	B	406	PHE
1	B	411	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	397/412 (96%)	380 (96%)	17 (4%)	29	46
1	B	397/412 (96%)	378 (95%)	19 (5%)	25	41
1	C	397/412 (96%)	374 (94%)	23 (6%)	20	32
2	D	377/386 (98%)	367 (97%)	10 (3%)	44	65
2	E	376/386 (97%)	359 (96%)	17 (4%)	27	44
2	F	376/386 (97%)	363 (96%)	13 (4%)	36	55
3	G	225/230 (98%)	210 (93%)	15 (7%)	16	26
4	H	104/109 (95%)	100 (96%)	4 (4%)	33	51
5	I	38/41 (93%)	35 (92%)	3 (8%)	12	19
All	All	2687/2774 (97%)	2566 (96%)	121 (4%)	27	44

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	434	SER
2	D	335	LEU
3	G	212	ILE
1	C	479	LEU

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Mol	Chain	Res	Type
2	D	97	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	282	GLN
2	E	194	ASN
4	H	91	GLN
2	D	411	GLN
2	E	223	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z  > 2$
11	SO4	E	630	-	4,4,4	0.64	0	6,6,6	0.08	0
6	ATP	A	600	7	26,33,33	0.81	0	31,52,52	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ATP	C	600	7	26,33,33	0.87	0	31,52,52	0.96	1 (3%)
9	GOL	B	701	-	5,5,5	0.26	0	5,5,5	0.38	0
8	ADP	D	600	7	24,29,29	0.91	0	29,45,45	0.96	1 (3%)
8	ADP	B	600	7	24,29,29	0.86	0	29,45,45	0.91	1 (3%)
10	DCW	D	700	2	17,17,17	1.14	1 (5%)	21,21,21	1.22	1 (4%)
8	ADP	F	600	7	24,29,29	0.84	0	29,45,45	0.98	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	A	600	7	-	7/18/38/38	0/3/3/3
6	ATP	C	600	7	-	4/18/38/38	0/3/3/3
9	GOL	B	701	-	-	2/4/4/4	-
8	ADP	D	600	7	-	3/12/32/32	0/3/3/3
8	ADP	B	600	7	-	2/12/32/32	0/3/3/3
10	DCW	D	700	2	-	3/8/24/24	0/2/2/2
8	ADP	F	600	7	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	700	DCW	C1-N1	2.48	1.40	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	700	DCW	C8-N2-C1	3.37	130.15	123.02
8	F	600	ADP	C5-C6-N6	2.78	124.58	120.35
8	B	600	ADP	C5-C6-N6	2.68	124.43	120.35
8	D	600	ADP	C5-C6-N6	2.37	123.95	120.35
6	C	600	ATP	C5-C6-N6	2.31	123.87	120.35

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

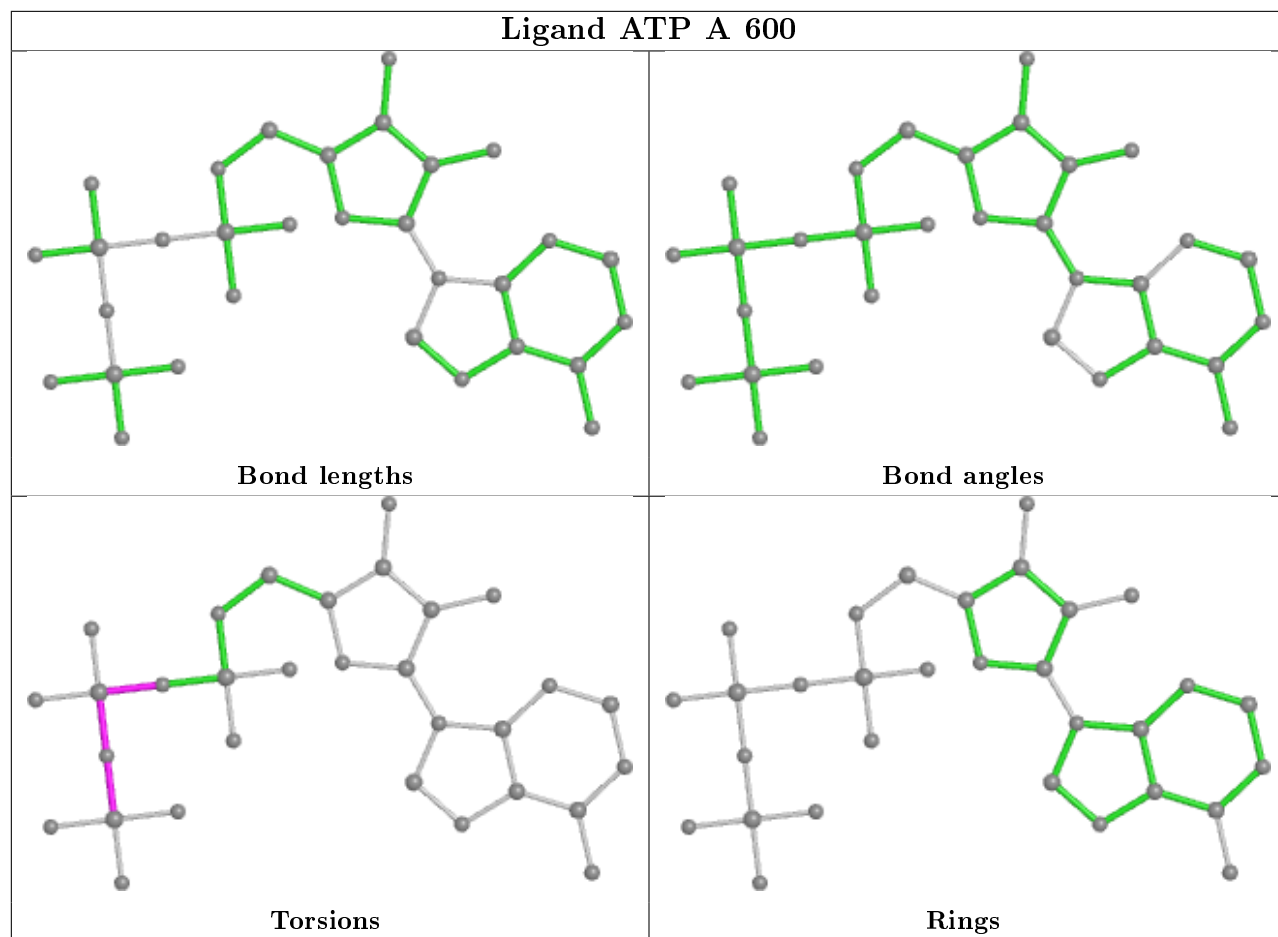
Mol	Chain	Res	Type	Atoms
6	A	600	ATP	PB-O3B-PG-O2G
6	C	600	ATP	PB-O3B-PG-O2G
9	B	701	GOL	C1-C2-C3-O3
9	B	701	GOL	O2-C2-C3-O3
8	D	600	ADP	PA-O3A-PB-O2B

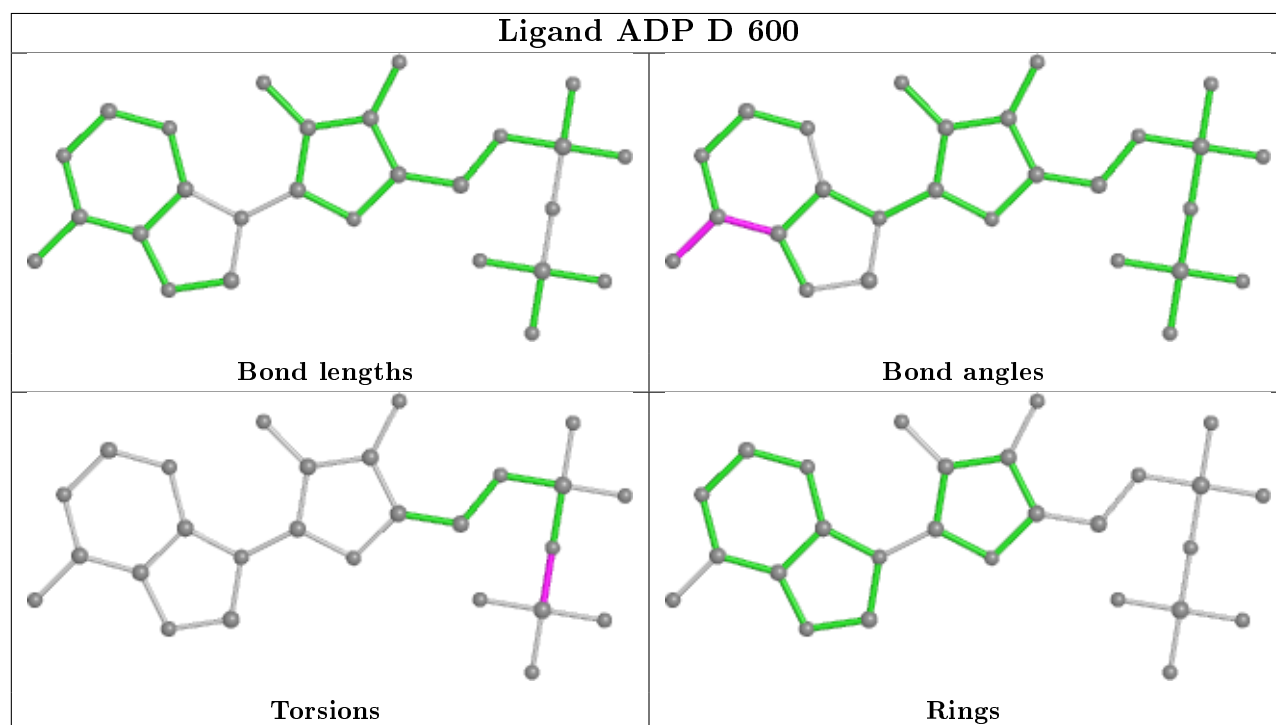
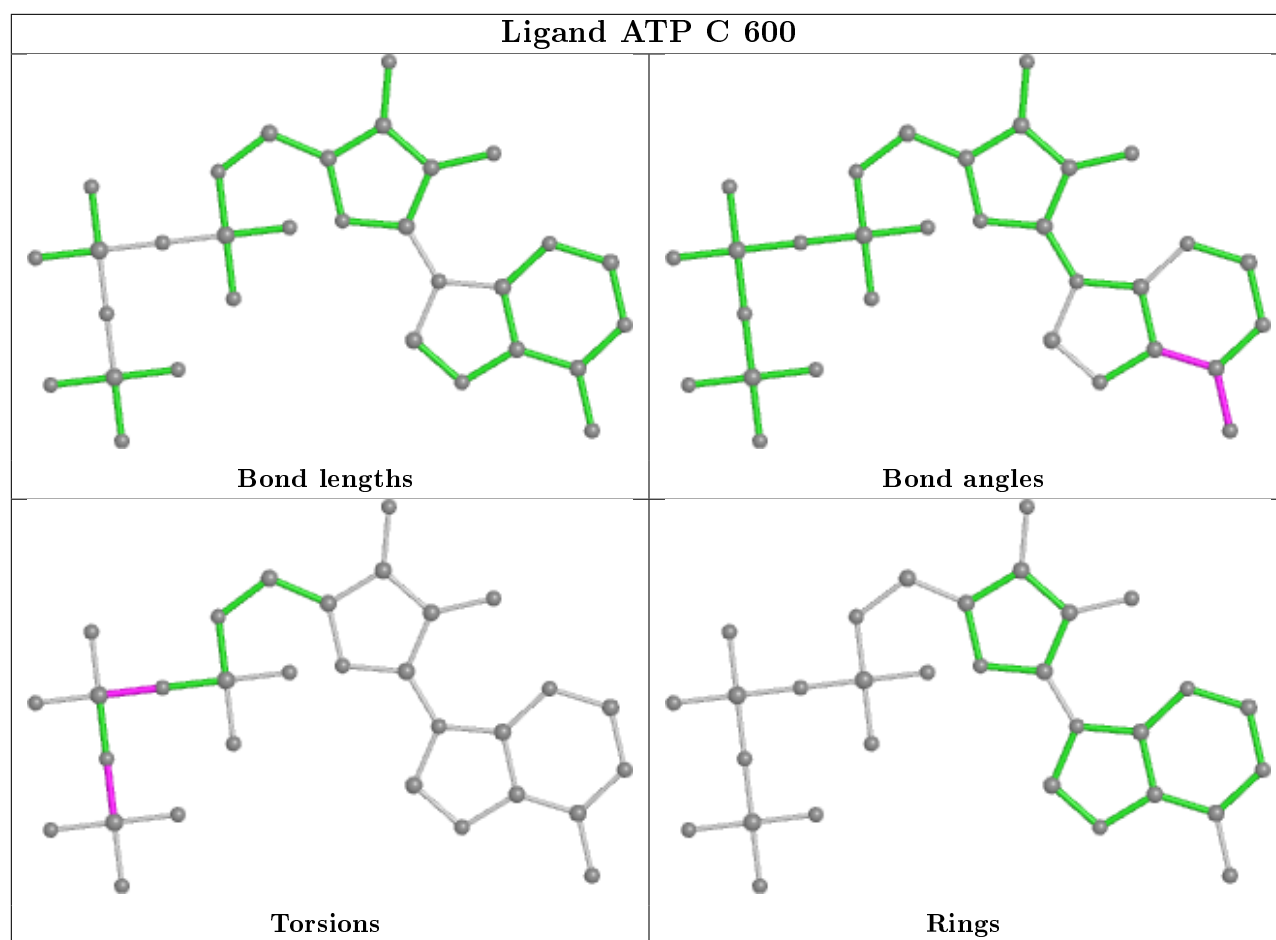
There are no ring outliers.

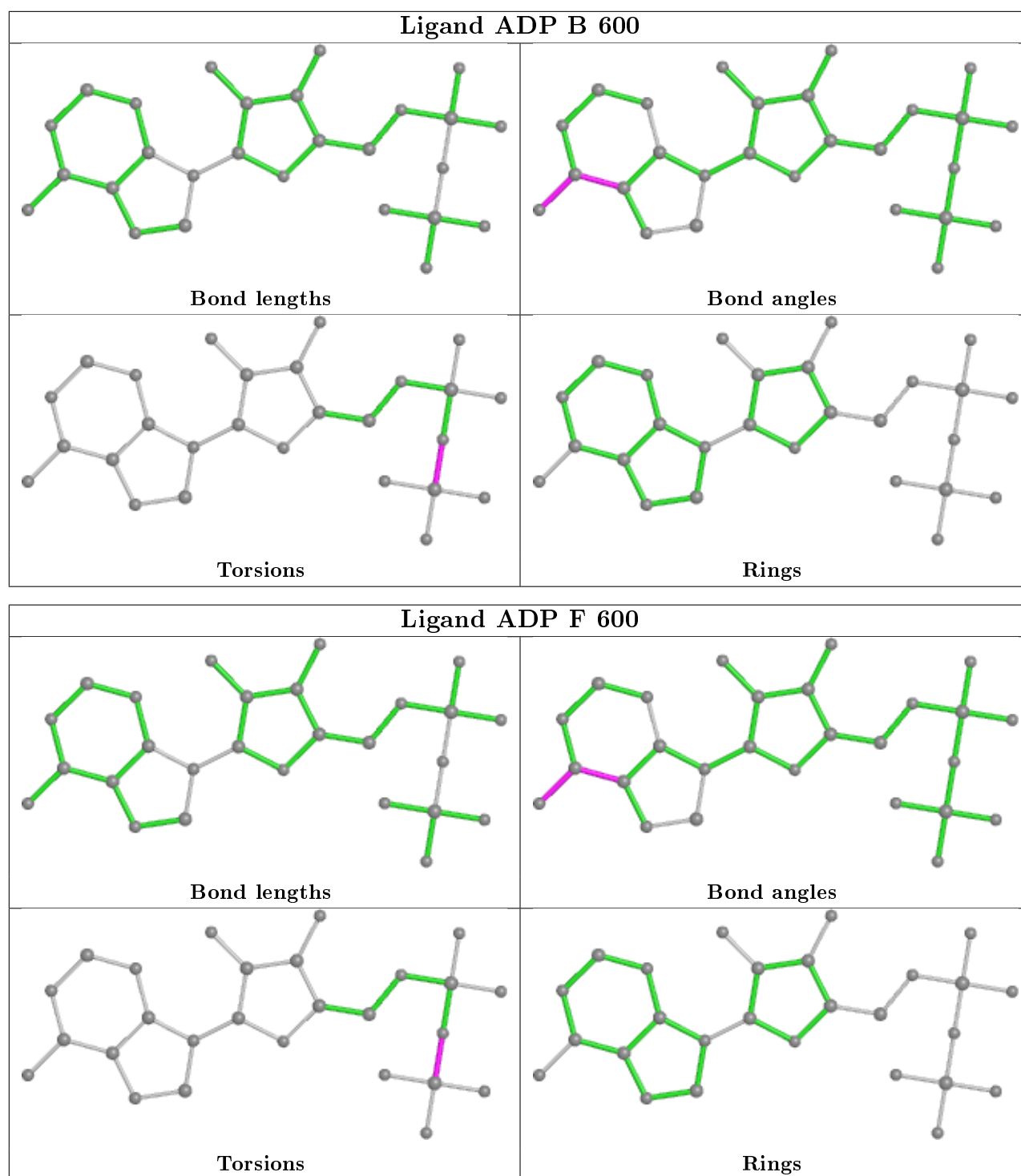
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	600	ATP	1	0
9	B	701	GOL	1	0
10	D	700	DCW	6	0

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







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	492/510 (96%)	-0.16	18 (3%)	41 41	32, 46, 74, 104	0
1	B	492/510 (96%)	0.02	26 (5%)	26 25	32, 48, 95, 143	0
1	C	492/510 (96%)	-0.25	11 (2%)	62 60	30, 44, 63, 102	0
2	D	467/482 (96%)	-0.24	10 (2%)	63 61	31, 45, 69, 100	0
2	E	466/482 (96%)	0.22	38 (8%)	11 10	34, 54, 101, 132	0
2	F	466/482 (96%)	-0.20	11 (2%)	59 57	32, 44, 74, 89	0
3	G	263/272 (96%)	0.67	43 (16%)	1 1	36, 68, 116, 133	0
4	H	131/146 (89%)	1.33	31 (23%)	0 0	67, 97, 131, 136	0
5	I	47/50 (94%)	1.33	11 (23%)	0 0	58, 91, 127, 129	0
All	All	3316/3444 (96%)	0.04	199 (6%)	21 20	30, 48, 102, 143	0

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	473	LEU	8.8
1	C	407	GLY	8.7
2	E	474	ALA	8.4
1	B	400	VAL	8.4
2	E	390	ILE	8.3

### 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

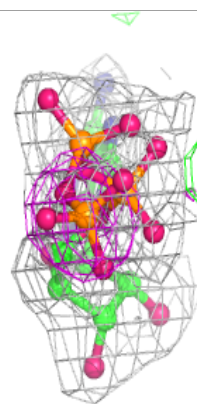
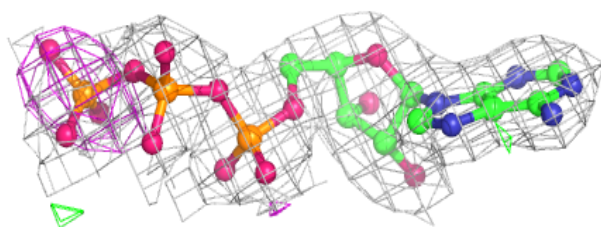
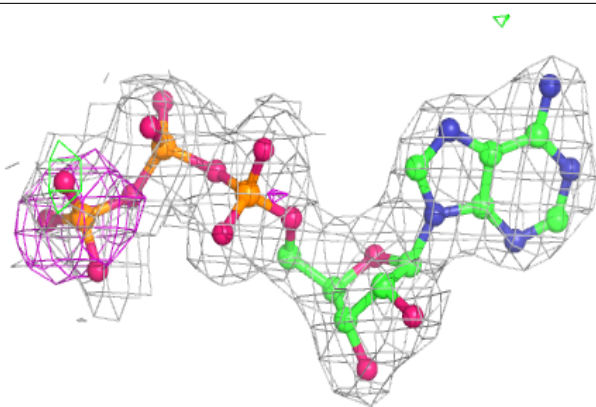
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	DCW	D	700	16/16	0.74	0.31	69,73,78,78	0
7	MG	A	601	1/1	0.77	0.12	44,44,44,44	0
11	SO4	E	630	5/5	0.83	0.45	100,100,100,100	0
7	MG	C	601	1/1	0.90	0.15	43,43,43,43	0
6	ATP	A	600	31/31	0.92	0.13	42,44,56,56	0
6	ATP	C	600	31/31	0.94	0.12	36,42,51,52	0
7	MG	F	601	1/1	0.95	0.08	34,34,34,34	0
9	GOL	B	701	6/6	0.97	0.12	39,43,44,45	0
7	MG	B	601	1/1	0.97	0.06	46,46,46,46	0
8	ADP	F	600	27/27	0.97	0.10	41,42,45,45	0
7	MG	D	601	1/1	0.97	0.18	35,35,35,35	0
8	ADP	D	600	27/27	0.98	0.11	35,37,38,39	0
8	ADP	B	600	27/27	0.98	0.10	44,52,56,56	0

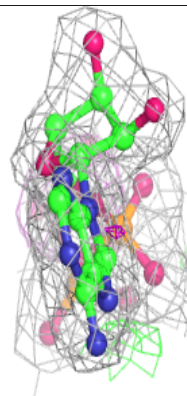
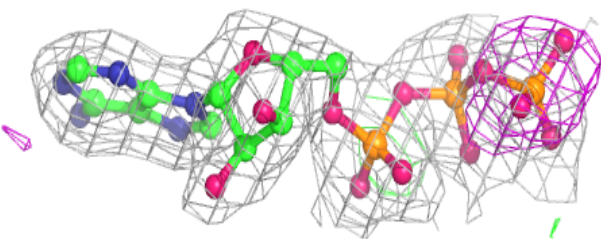
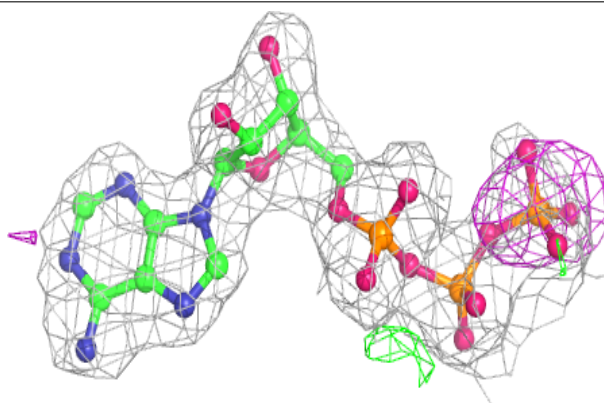
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 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)

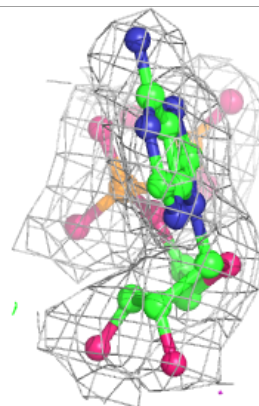
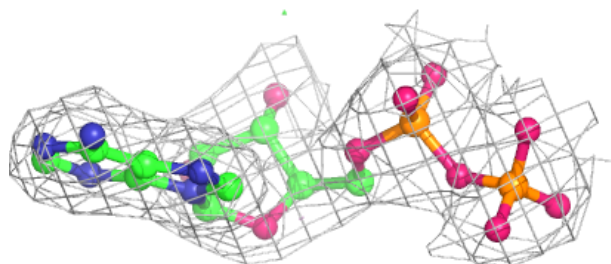
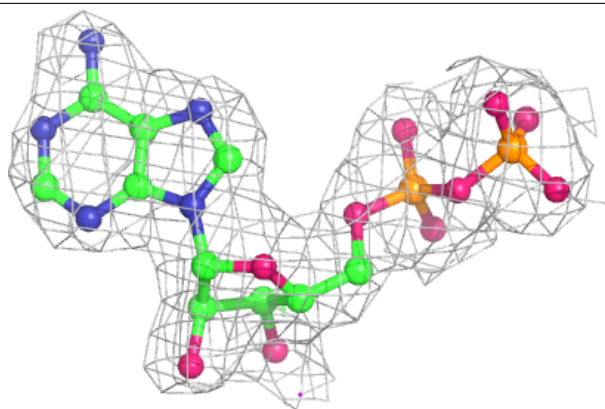
**Electron density around ATP C 600:**

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

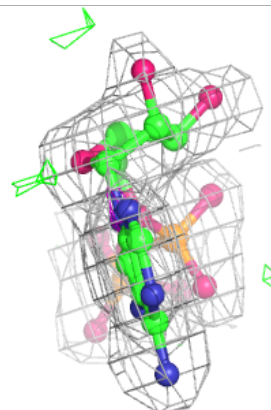
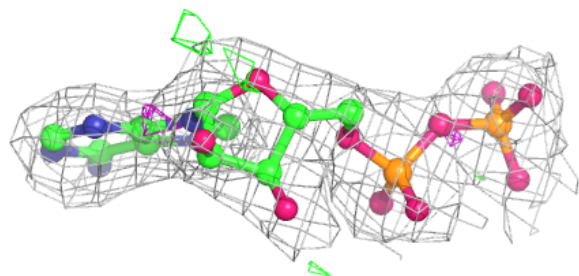
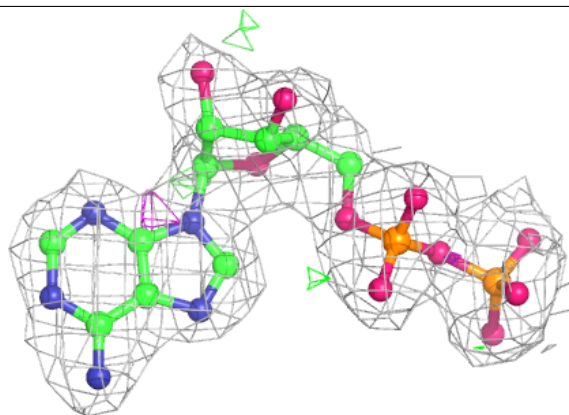


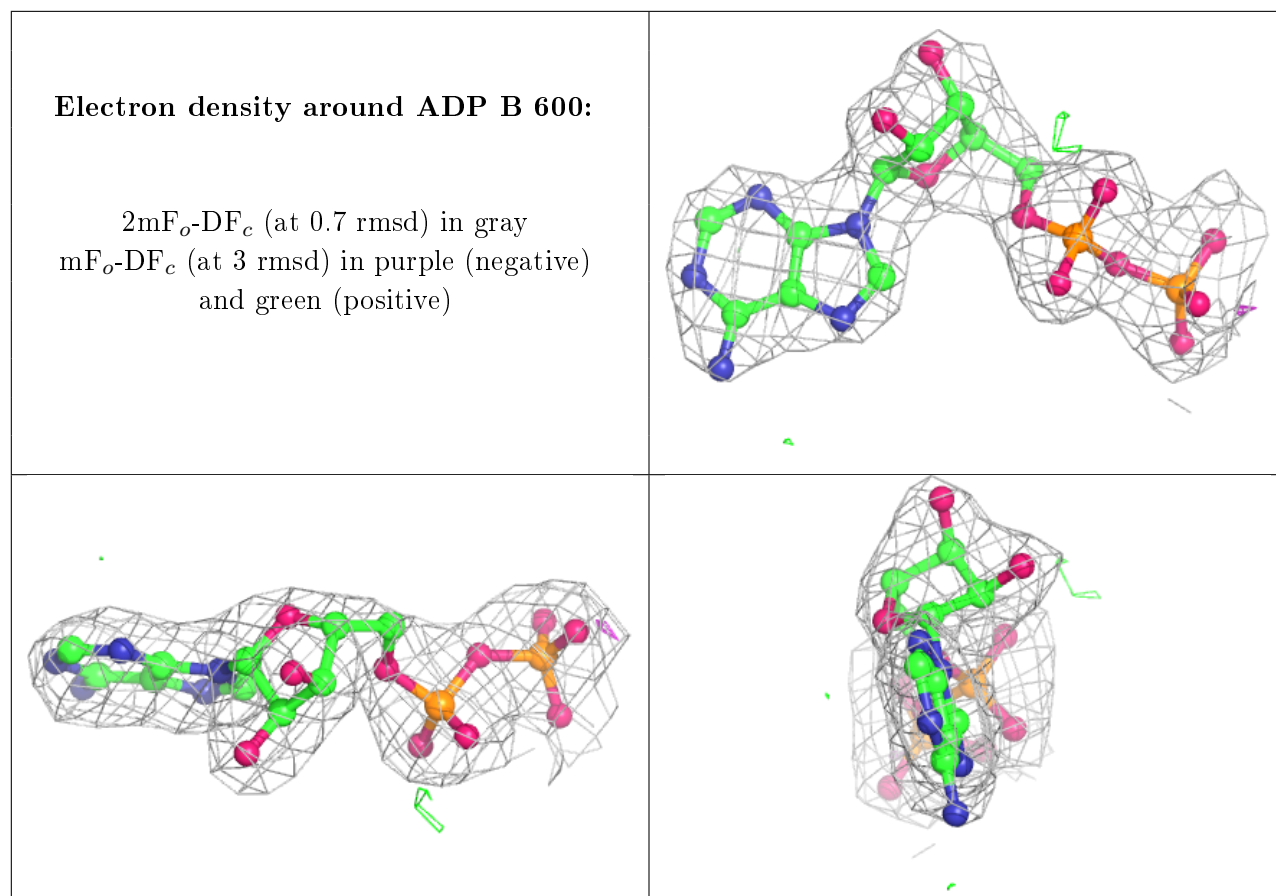
**Electron density around ADP F 600:**

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

**Electron density around ADP 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.