



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 11:17 PM UTC

PDB ID : 5DN6 / pdb\_00005dn6  
Title : ATP synthase from *Paracoccus denitrificans*  
Authors : Morales-Rios, E.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2015-09-09  
Resolution : 3.98 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

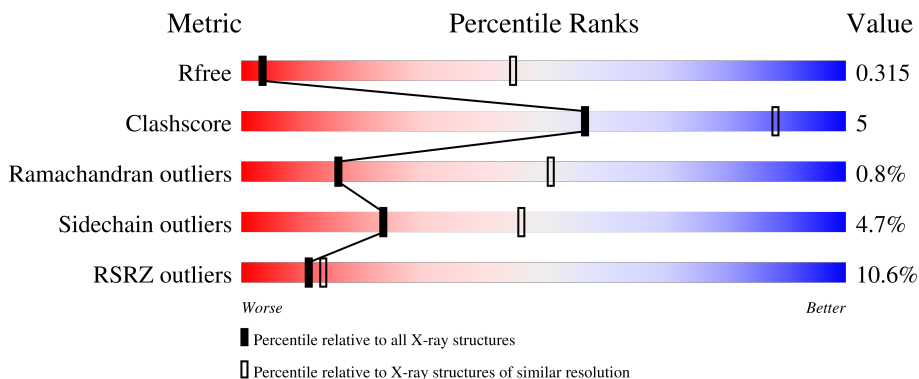
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.98 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	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)

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  $\geq 3$ , 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	1	20	100%
2	2	15	100%
3	3	19	100%
4	A	511	10% (red), 83% (green), 14% (yellow), .. (grey)
4	B	511	8% (red), 81% (green), 14% (yellow), .. (grey)

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Mol	Chain	Length	Quality of chain
4	C	511	 7% 76% 18% 5%
5	D	474	 8% 87% 11% ..
5	E	474	 8% 84% 13% ..
5	F	474	 5% 82% 14% ..
6	G	290	 10% 75% 13% 10%
7	H	188	 5% 53% .. 41%
8	I	148	 2% 49% . 49%
9	J	77	 25% 95% ..
9	K	77	 19% 95% ..
9	L	77	 18% 96% .
9	M	77	 9% 96% .
9	N	77	 22% 96% .
9	O	77	 17% 96% .
9	P	77	 23% 96% .
9	Q	77	 27% 96% .
9	R	77	 31% 96% .
9	S	77	 12% 96% .
9	T	77	 10% 95% ..
9	U	77	 16% 95% ..
10	V	78	 100%
11	W	124	 100%
12	X	283	 2% 34% 65%
13	Y	54	 100%
14	Z	104	 3% 45% 7% 48%

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31527 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 Chain A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	1	20	100	60	20	20	0	0	0

- Molecule 2 is a protein called Chain B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	2	15	75	45	15	15	0	0	0

- Molecule 3 is a protein called Chain C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	3	19	95	57	19	19	0	0	0

- Molecule 4 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	505	3811	2395	665	735	16	0	0	0
4	B	496	3754	2359	657	723	15	0	0	0
4	C	484	3652	2293	640	703	16	0	0	0

- Molecule 5 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	470	3508	2211	600	687	10	0	0	0
5	E	466	3490	2198	596	686	10	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	466	3489	2199	596	684	10	0	0	0

- Molecule 6 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	G	260	1978	1227	367	375	9	0	0	0

- Molecule 7 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	H	110	544	324	110	110	0	0	0

- Molecule 8 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	I	75	366	216	75	75	0	0	0

- Molecule 9 is a protein called ATP synthase F0 subcomplex C subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	J	74	358	210	74	74	0	0	0
9	K	74	358	210	74	74	0	0	0
9	L	74	358	210	74	74	0	0	0
9	M	74	358	210	74	74	0	0	0
9	N	74	358	210	74	74	0	0	0
9	O	74	358	210	74	74	0	0	0
9	P	74	358	210	74	74	0	0	0
9	Q	74	358	210	74	74	0	0	0
9	R	74	358	210	74	74	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	T	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	U	74	Total	C	N	O	0	0	0
			358	210	74	74			

- Molecule 10 is a protein called Chain V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	78	Total	C	N	O	0	0	0
			390	234	78	78			

- Molecule 11 is a protein called Chain W.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	W	124	Total	C	N	O	0	0	0
			620	372	124	124			

- Molecule 12 is a protein called ATP synthase subunit a,ATP synthase subunit a,ATP synthase subunit a,ATP synthase subunit a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	98	Total	C	N	O	0	0	0
			486	291	98	97			

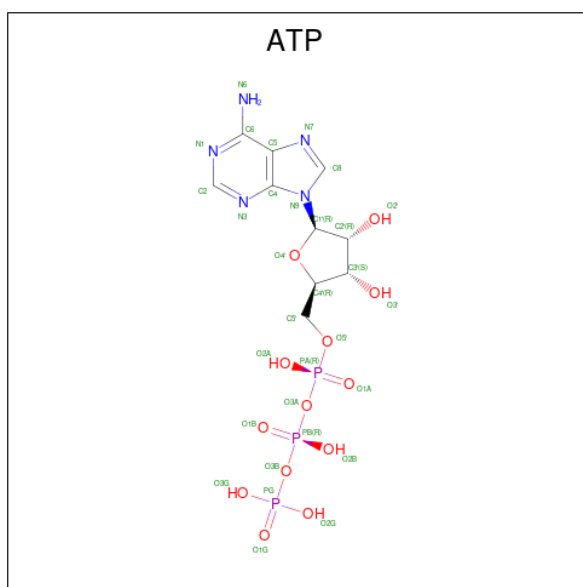
- Molecule 13 is a protein called Chain Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	Y	54	Total	C	N	O	0	0	0
			270	162	54	54			

- Molecule 14 is a protein called Zeta inhibitor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Z	54	Total	C	N	O	S	0	0	0
			447	274	88	84	1			

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

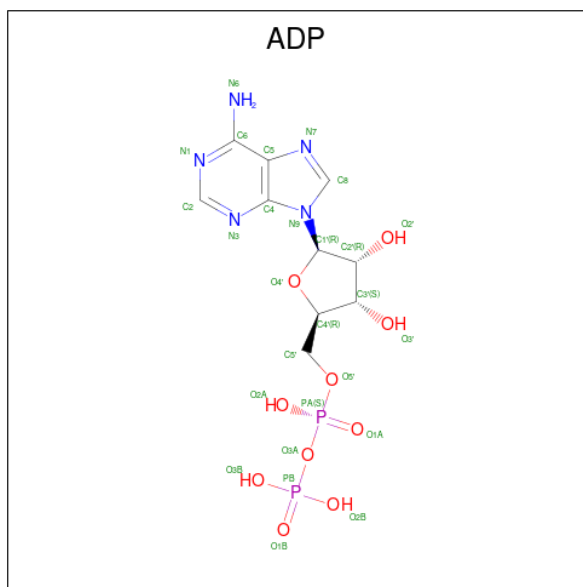


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
15	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
15	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
15	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
15	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

### 3 Residue-property plots

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

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Chain B

Chain 2:  100%


There are no outlier residues recorded for this chain.

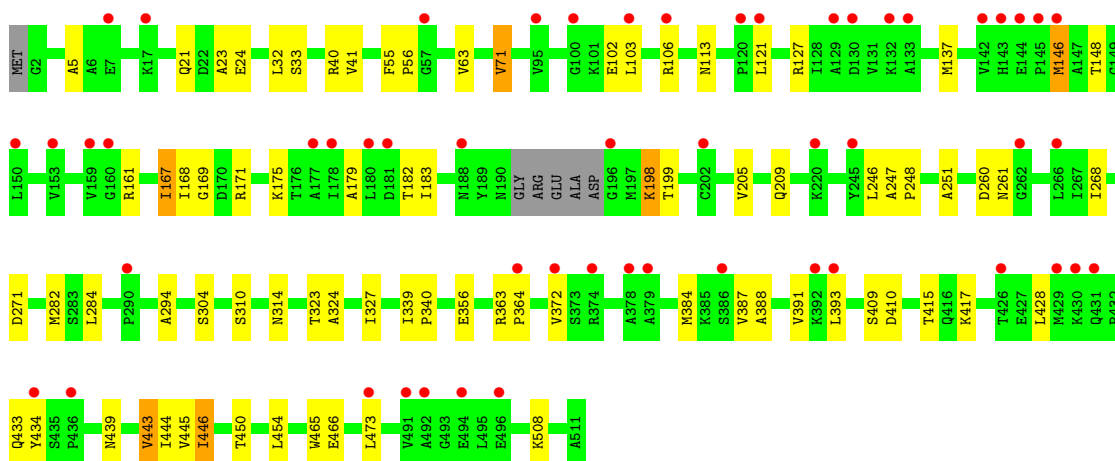
- Molecule 3: Chain C

Chain 3:  100%


There are no outlier residues recorded for this chain.

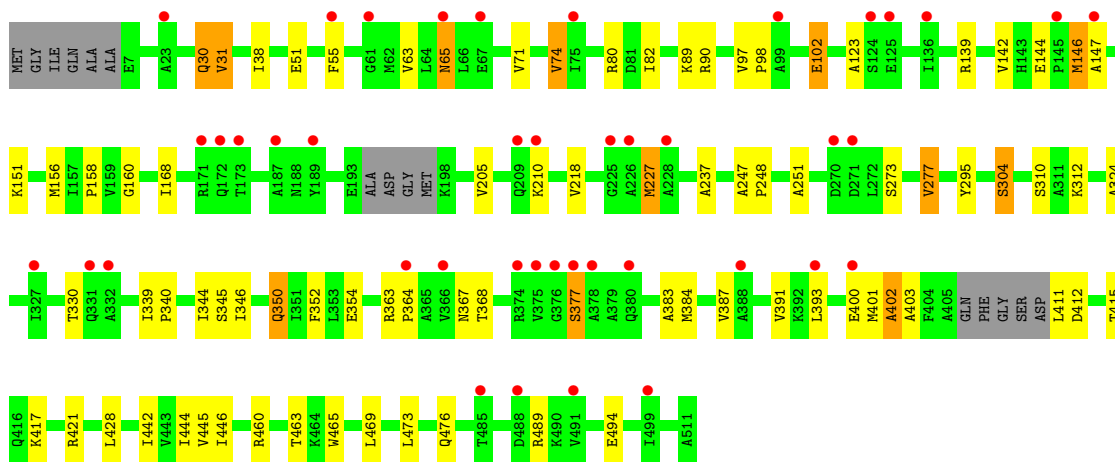
- Molecule 4: ATP synthase subunit alpha

Chain A:  10% 83% 14% ..

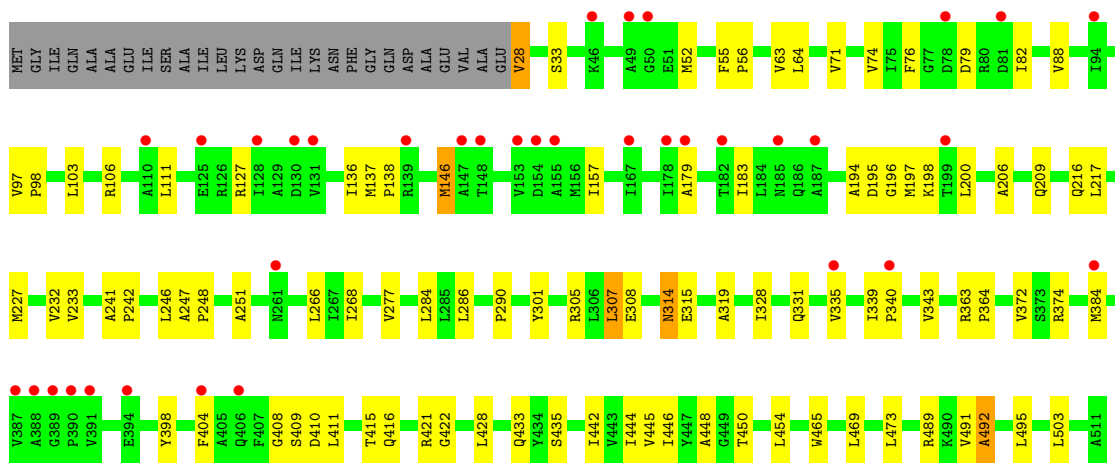
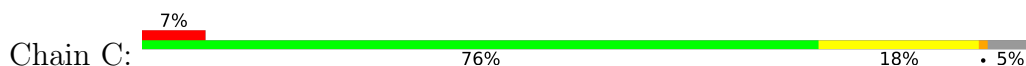


- Molecule 4: ATP synthase subunit alpha

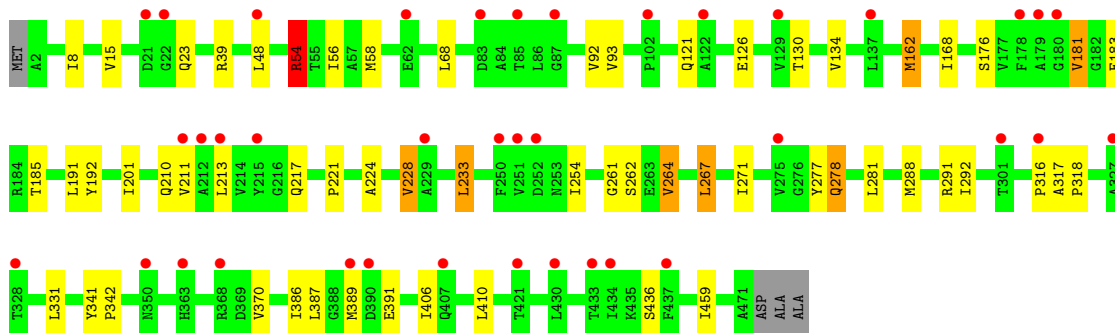
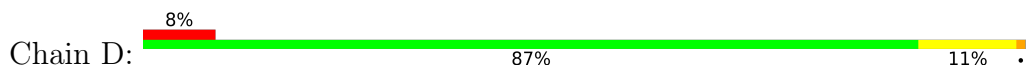
Chain B:  8% 81% 14% ..



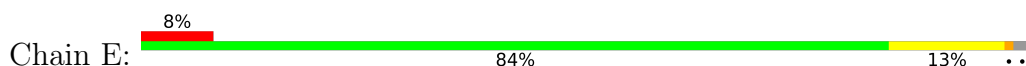
• Molecule 4: ATP synthase subunit alpha

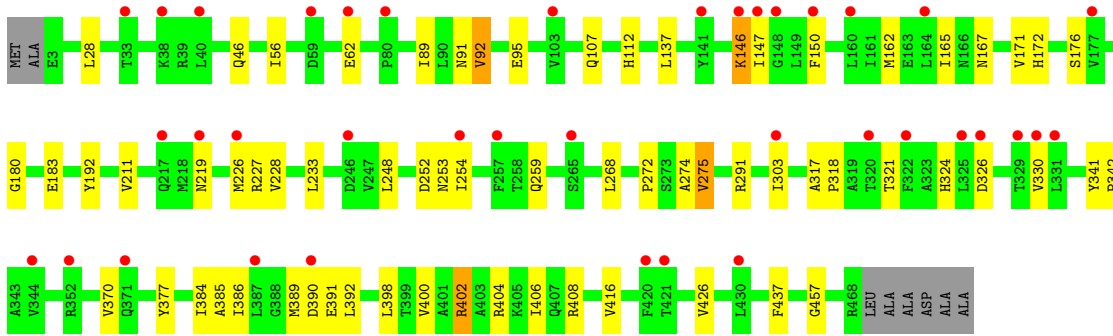


• Molecule 5: ATP synthase subunit beta



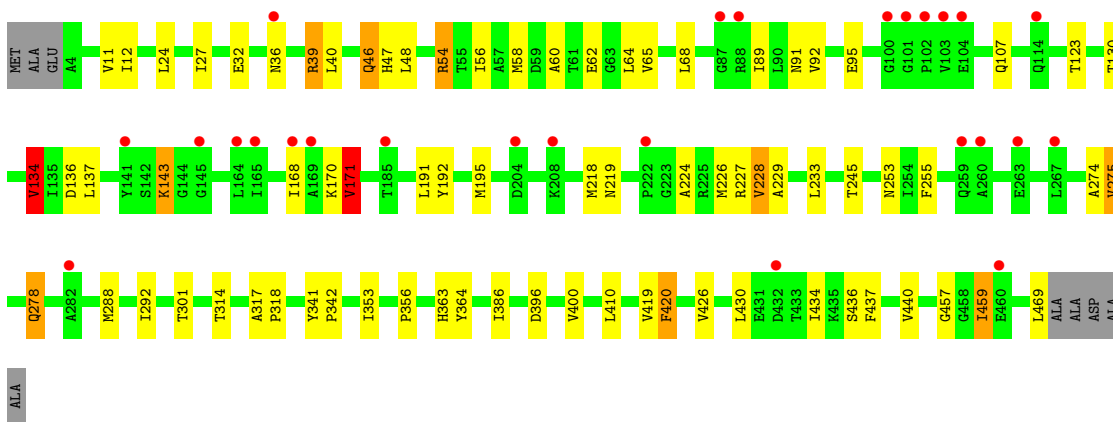
• Molecule 5: ATP synthase subunit beta





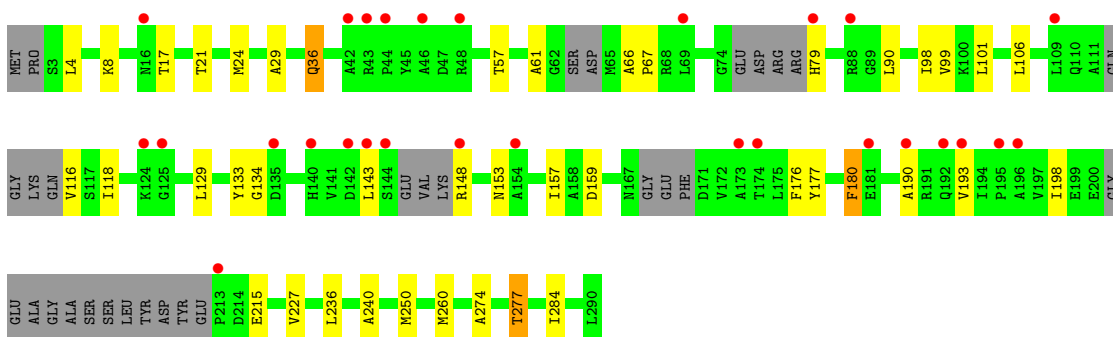
- Molecule 5: ATP synthase subunit beta

Chain F: 5% 82% 14% ..



- Molecule 6: ATP synthase gamma chain

Chain G: 10% 75% 13% 10%



- Molecule 7: ATP synthase subunit delta

Chain H: 5% 53% 41%



SER GLY LYS THR VAL LYS LEU ASN ALA ARG VAL ASP GLU LEU SER MET ILE LEU GLY LYS MET ILE VAL LYS LEU LYS SER GLY SER GLM MET ILE SER SER ILE ARG LYS LYS LEU ALA SER LEU GLN ALA ASN ARG MET LYS VAL GLY

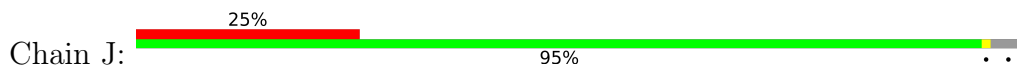
• Molecule 8: ATP synthase epsilon chain



MET ALA ASP THR MET GLN PHE ASP LEU V9 S10 V82 G55 T60 N73 R82 G83 HIS PRO GLY SER ARG ALA GLU MET THR GLN SER SER ILE VAL PHE ASN GLU MET MET ALA GLN ALA ARG ARG MET VAL GLU ALA LYS ARG GLU SER ALA

ALA VAL LYS LEU LEU ALA ASP MET ALA ALA GLY THR HIS ILE LEU ASP PRO ASN HIS

• Molecule 9: ATP synthase F0 subcomplex C subunit



MET GLU M3 A21 G22 A23 A24 M25 N29 V30 A31 G32 M33 S47 Q48 T49 F53 I54 A57 F58 A59 B60 A61 L62 F65 L68 L71 L74 F75 A76 VAL

• Molecule 9: ATP synthase F0 subcomplex C subunit



MET GLU M3 A21 G22 A23 A24 M25 N29 V30 A31 G32 M33 S47 Q48 T49 F53 I54 A57 F58 A59 B60 A61 L62 F65 L68 L71 A76 VAL

• Molecule 9: ATP synthase F0 subcomplex C subunit



MET GLU M3 V18 A31 L35 A36 G37 A38 N41 S43 S47 Q48 T49 F53 A57 L68 A76 VAL

• Molecule 9: ATP synthase F0 subcomplex C subunit



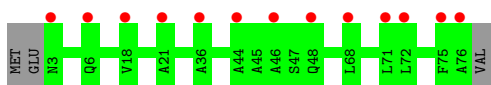
MET GLU M3 L15 V18 A31 V34 L35 A36 S43 L68 A76 VAL

• Molecule 9: ATP synthase F0 subcomplex C subunit

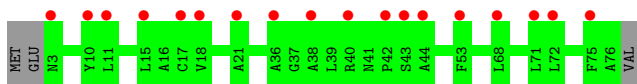


MET GLU M3 V18 G19 M20 A21 V30 A38 N41 P42 S43 A44 A45 A46 S47 Q48 T49 A61 L64 F65 L68 A76 VAL

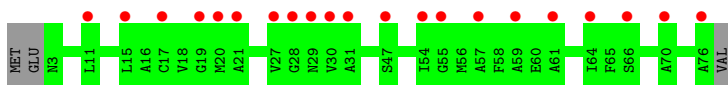
• Molecule 9: ATP synthase F0 subcomplex C subunit



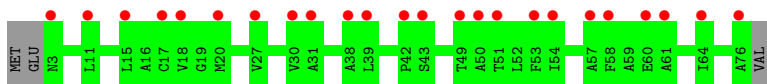
- Molecule 9: ATP synthase F0 subcomplex C subunit



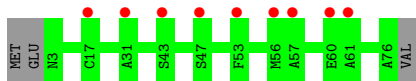
- Molecule 9: ATP synthase F0 subcomplex C subunit



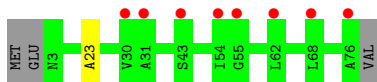
- Molecule 9: ATP synthase F0 subcomplex C subunit



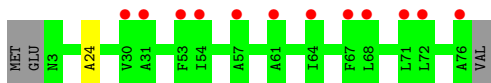
- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.00Å 187.94Å 164.72Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	36.84 – 3.98 36.84 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.84-3.98) 98.7 (36.84-3.98)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.99Å)	Xtrriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.295 , 0.324 0.292 , 0.315	Depositor DCC
$R_{free}$ test set	2791 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.8	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	31527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	156.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 i

### 5.1 Standard geometry i

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

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$
4	A	0.55	1/3864 (0.0%)	0.86	0/5227
4	B	0.53	0/3805	0.86	3/5146 (0.1%)
4	C	0.52	0/3705	0.88	4/5015 (0.1%)
5	D	0.51	0/3562	0.82	2/4840 (0.0%)
5	E	0.51	2/3544 (0.1%)	0.81	3/4815 (0.1%)
5	F	0.49	0/3543	0.80	1/4814 (0.0%)
6	G	0.57	0/1990	0.88	2/2674 (0.1%)
7	H	0.63	0/543	0.97	3/755 (0.4%)
8	I	0.52	0/365	0.86	2/504 (0.4%)
9	J	0.63	0/357	1.15	0/491
9	K	0.64	0/357	1.15	0/491
9	L	0.64	0/357	1.15	0/491
9	M	0.64	0/357	1.15	0/491
9	N	0.64	0/357	1.15	0/491
9	O	0.64	0/357	1.15	0/491
9	P	0.64	0/357	1.15	0/491
9	Q	0.64	0/357	1.15	0/491
9	R	0.63	0/357	1.15	0/491
9	S	0.63	0/357	1.15	0/491
9	T	0.63	0/357	1.14	0/491
9	U	0.63	0/357	1.15	0/491
12	X	0.53	0/309	1.30	2/428 (0.5%)
14	Z	0.67	0/450	0.93	0/599
All	All	0.54	3/29964 (0.0%)	0.90	22/40709 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	40	ARG	CZ-NH1	6.76	1.42	1.32
5	E	259	GLN	CD-OE1	6.51	1.35	1.23
5	E	326	ASP	CG-OD1	5.29	1.35	1.25

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	307	LEU	N-CA-C	-8.60	98.94	110.55
4	C	314	ASN	N-CA-CB	-7.62	99.20	110.17
7	H	49	ASP	N-CA-C	6.38	117.90	111.07
7	H	49	ASP	CB-CA-C	6.36	120.86	110.88
4	C	106	ARG	NE-CZ-NH2	6.32	124.89	119.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	1	100	0	23	0	0
2	2	75	0	17	0	0
3	3	95	0	21	0	0
4	A	3811	0	3875	35	0
4	B	3754	0	3822	42	0
4	C	3652	0	3709	54	0
5	D	3508	0	3532	36	0
5	E	3490	0	3513	38	0
5	F	3489	0	3517	48	0
6	G	1978	0	2035	26	0
7	H	544	0	277	4	0
8	I	366	0	176	0	0
9	J	358	0	209	1	0
9	K	358	0	209	1	0
9	L	358	0	209	0	0
9	M	358	0	209	0	0
9	N	358	0	209	0	0
9	O	358	0	209	0	0
9	P	358	0	209	0	0
9	Q	358	0	209	0	0
9	R	358	0	209	0	0
9	S	358	0	209	0	0
9	T	358	0	209	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	U	358	0	209	1	0
10	V	390	0	80	0	0
11	W	620	0	127	0	0
12	X	486	0	181	0	0
13	Y	270	0	58	0	0
14	Z	447	0	449	4	0
15	A	31	0	12	0	0
15	C	31	0	12	0	0
15	D	31	0	12	0	0
15	F	31	0	12	0	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	D	1	0	0	0	0
16	F	1	0	0	0	0
17	B	27	0	12	0	0
All	All	31527	0	27980	273	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 5.

The worst 5 of 273 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)
5:F:191:LEU:HD11	5:F:195:MET:HE3	1.59	0.84
5:F:278:GLN:H	5:F:278:GLN:HE21	1.24	0.83
5:D:386:ILE:HD11	6:G:17:THR:HG22	1.59	0.82
5:E:176:SER:HB2	5:E:211:VAL:HG12	1.62	0.80
14:Z:31:LEU:HD23	14:Z:91:LEU:HD22	1.64	0.80

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	
4	A	501/511 (98%)	470 (94%)	24 (5%)	7 (1%)	9	39
4	B	490/511 (96%)	459 (94%)	26 (5%)	5 (1%)	12	45
4	C	482/511 (94%)	463 (96%)	15 (3%)	4 (1%)	16	51
5	D	468/474 (99%)	448 (96%)	19 (4%)	1 (0%)	43	75
5	E	464/474 (98%)	439 (95%)	22 (5%)	3 (1%)	21	57
5	F	464/474 (98%)	439 (95%)	23 (5%)	2 (0%)	30	65
6	G	246/290 (85%)	233 (95%)	8 (3%)	5 (2%)	6	33
7	H	108/188 (57%)	90 (83%)	12 (11%)	6 (6%)	1	18
8	I	73/148 (49%)	66 (90%)	5 (7%)	2 (3%)	4	28
9	J	72/77 (94%)	72 (100%)	0	0	100	100
9	K	72/77 (94%)	72 (100%)	0	0	100	100
9	L	72/77 (94%)	72 (100%)	0	0	100	100
9	M	72/77 (94%)	72 (100%)	0	0	100	100
9	N	72/77 (94%)	72 (100%)	0	0	100	100
9	O	72/77 (94%)	72 (100%)	0	0	100	100
9	P	72/77 (94%)	72 (100%)	0	0	100	100
9	Q	72/77 (94%)	72 (100%)	0	0	100	100
9	R	72/77 (94%)	72 (100%)	0	0	100	100
9	S	72/77 (94%)	72 (100%)	0	0	100	100
9	T	72/77 (94%)	72 (100%)	0	0	100	100
9	U	72/77 (94%)	72 (100%)	0	0	100	100
12	X	59/283 (21%)	58 (98%)	1 (2%)	0	100	100
14	Z	50/104 (48%)	47 (94%)	2 (4%)	1 (2%)	6	33
All	All	4269/4892 (87%)	4076 (96%)	157 (4%)	36 (1%)	16	51

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	23	ALA
4	A	199	THR
4	B	402	ALA
4	C	197	MET

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Mol	Chain	Res	Type
4	C	492	ALA

### 5.3.2 Protein sidechains [i](#)

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	
4	A	396/401 (99%)	371 (94%)	25 (6%)	16	40
4	B	391/401 (98%)	370 (95%)	21 (5%)	20	44
4	C	379/401 (94%)	361 (95%)	18 (5%)	23	46
5	D	371/375 (99%)	354 (95%)	17 (5%)	24	47
5	E	372/375 (99%)	362 (97%)	10 (3%)	39	60
5	F	372/375 (99%)	354 (95%)	18 (5%)	23	46
6	G	203/227 (89%)	195 (96%)	8 (4%)	28	50
14	Z	45/81 (56%)	44 (98%)	1 (2%)	45	64
All	All	2529/2636 (96%)	2411 (95%)	118 (5%)	23	46

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	372	VAL
6	G	79	HIS
5	D	210	GLN
6	G	36	GLN
5	F	219	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	107	GLN
5	F	35	ASN
6	G	9	ASN
5	E	189	ASN

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Mol	Chain	Res	Type
5	E	304	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
15	ATP	C	600	16	32,33,33	1.51	6 (18%)	48,52,52	1.77	11 (22%)
17	ADP	B	600	16	28,29,29	1.49	5 (17%)	43,45,45	1.88	10 (23%)
15	ATP	D	600	16	32,33,33	1.44	5 (15%)	48,52,52	1.83	12 (25%)
15	ATP	A	600	16	32,33,33	1.50	4 (12%)	48,52,52	1.77	8 (16%)
15	ATP	F	600	16	32,33,33	1.51	5 (15%)	48,52,52	1.75	9 (18%)

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
15	ATP	C	600	16	-	2/22/38/38	0/3/3/3
17	ADP	B	600	16	-	0/16/32/32	0/3/3/3
15	ATP	D	600	16	-	0/22/38/38	0/3/3/3
15	ATP	A	600	16	-	0/22/38/38	0/3/3/3
15	ATP	F	600	16	-	7/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	600	ATP	C5-C4	5.12	1.48	1.39
15	F	600	ATP	C5-C4	4.92	1.47	1.39
17	B	600	ADP	C5-C4	4.88	1.47	1.39
15	C	600	ATP	C5-C4	4.83	1.47	1.39
15	D	600	ATP	C5-C4	4.74	1.47	1.39

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	600	ATP	C5-C4-N3	-5.97	118.50	126.72
15	F	600	ATP	C5-C4-N3	-5.95	118.52	126.72
17	B	600	ADP	C5-C4-N3	-5.82	118.71	126.72
15	D	600	ATP	C5-C4-N3	-5.62	118.98	126.72
15	C	600	ATP	C5-C4-N3	-5.57	119.05	126.72

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

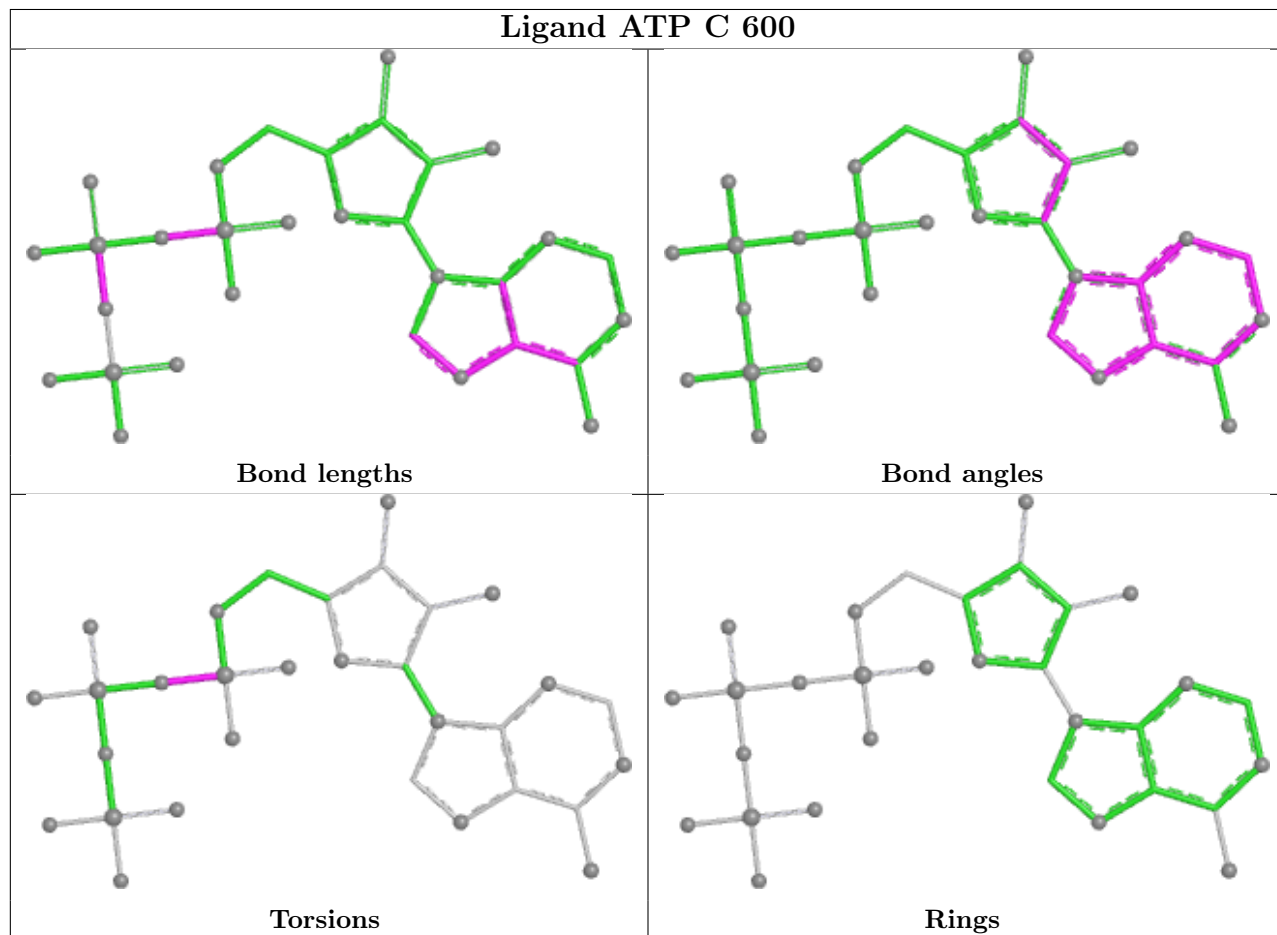
Mol	Chain	Res	Type	Atoms
15	F	600	ATP	C5'-O5'-PA-O2A
15	F	600	ATP	C5'-O5'-PA-O3A
15	F	600	ATP	O4'-C4'-C5'-O5'
15	F	600	ATP	C3'-C4'-C5'-O5'
15	C	600	ATP	PB-O3A-PA-O1A

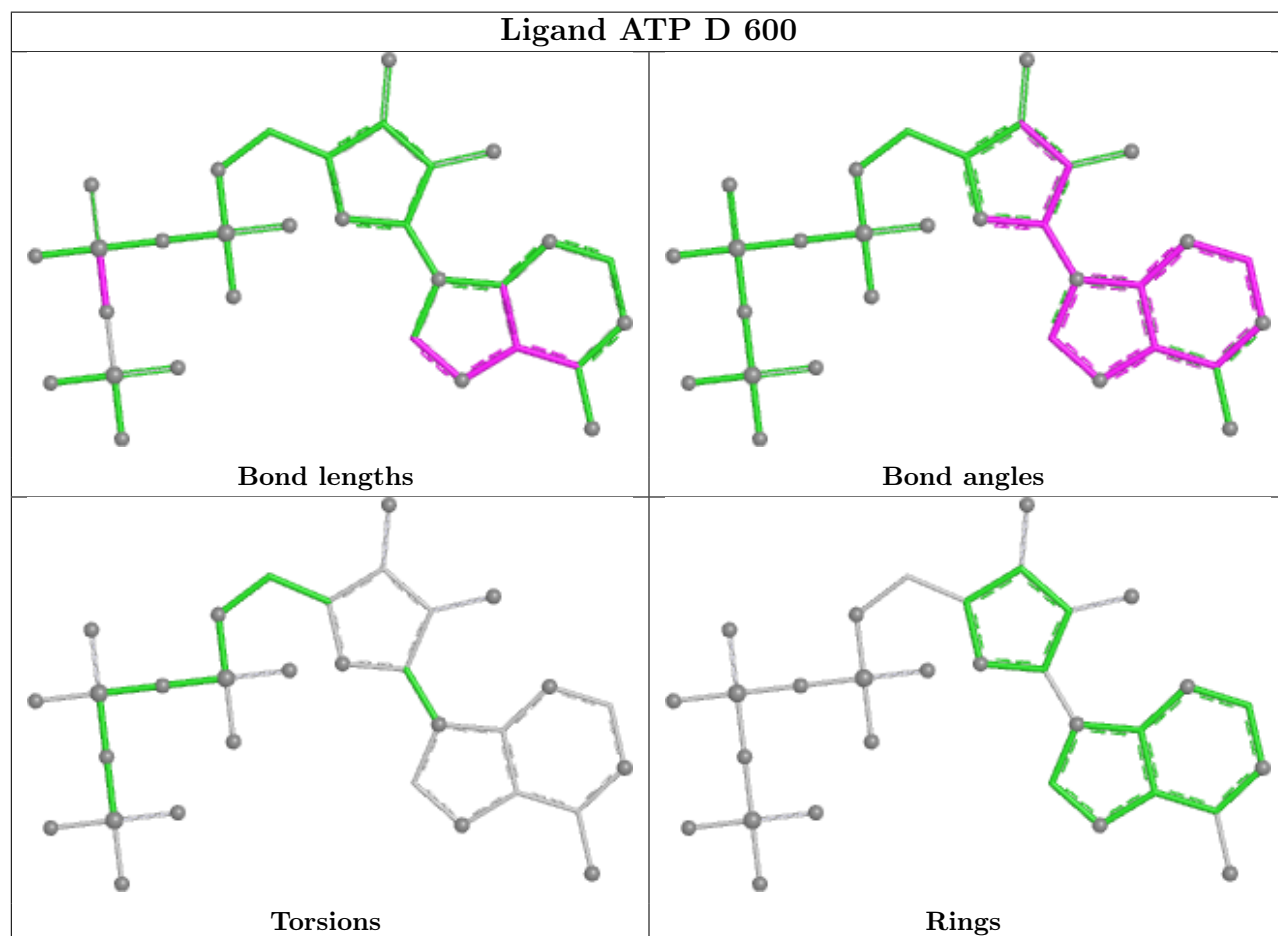
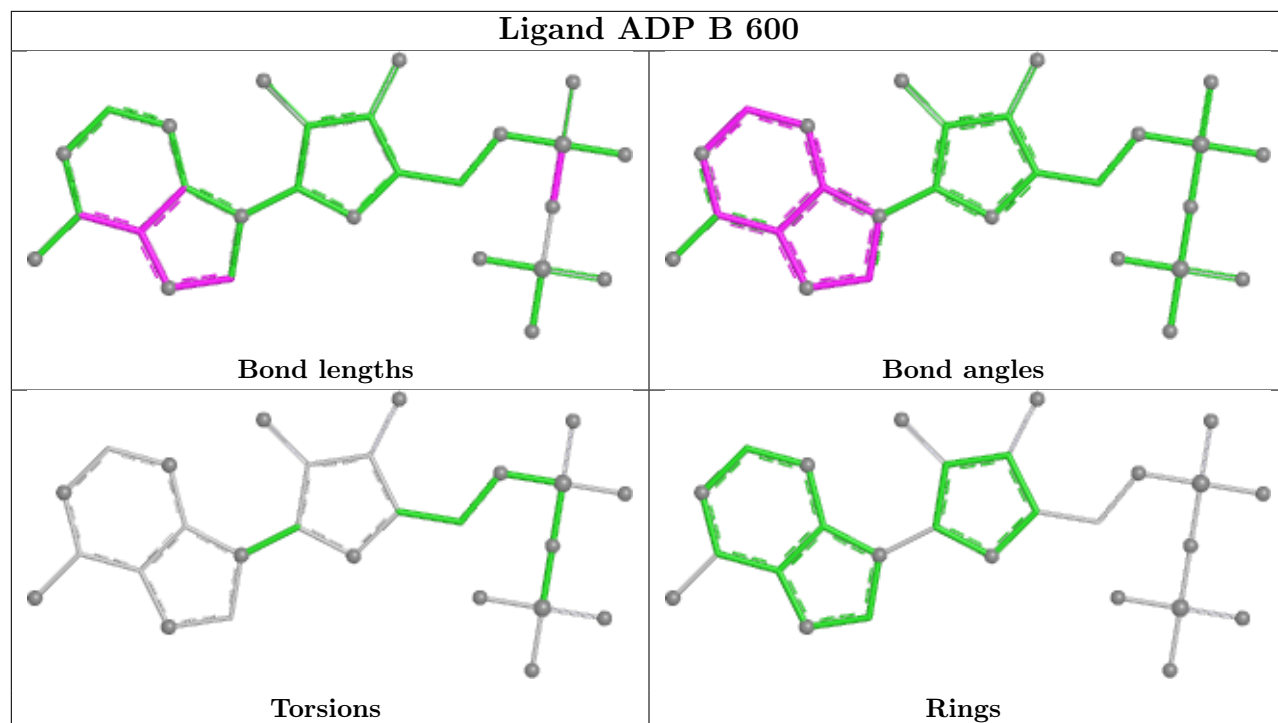
There are no ring outliers.

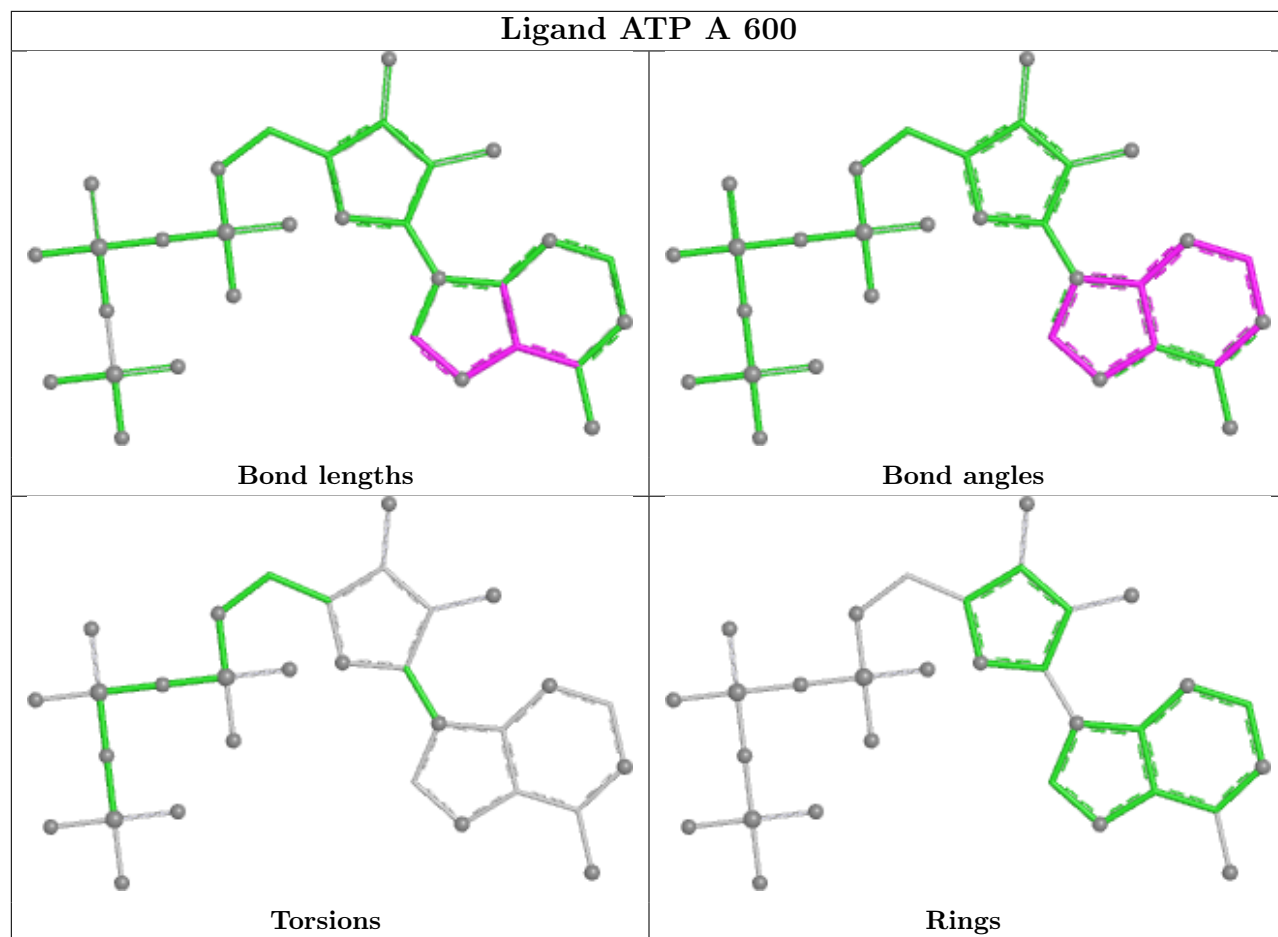
No monomer is involved in short contacts.

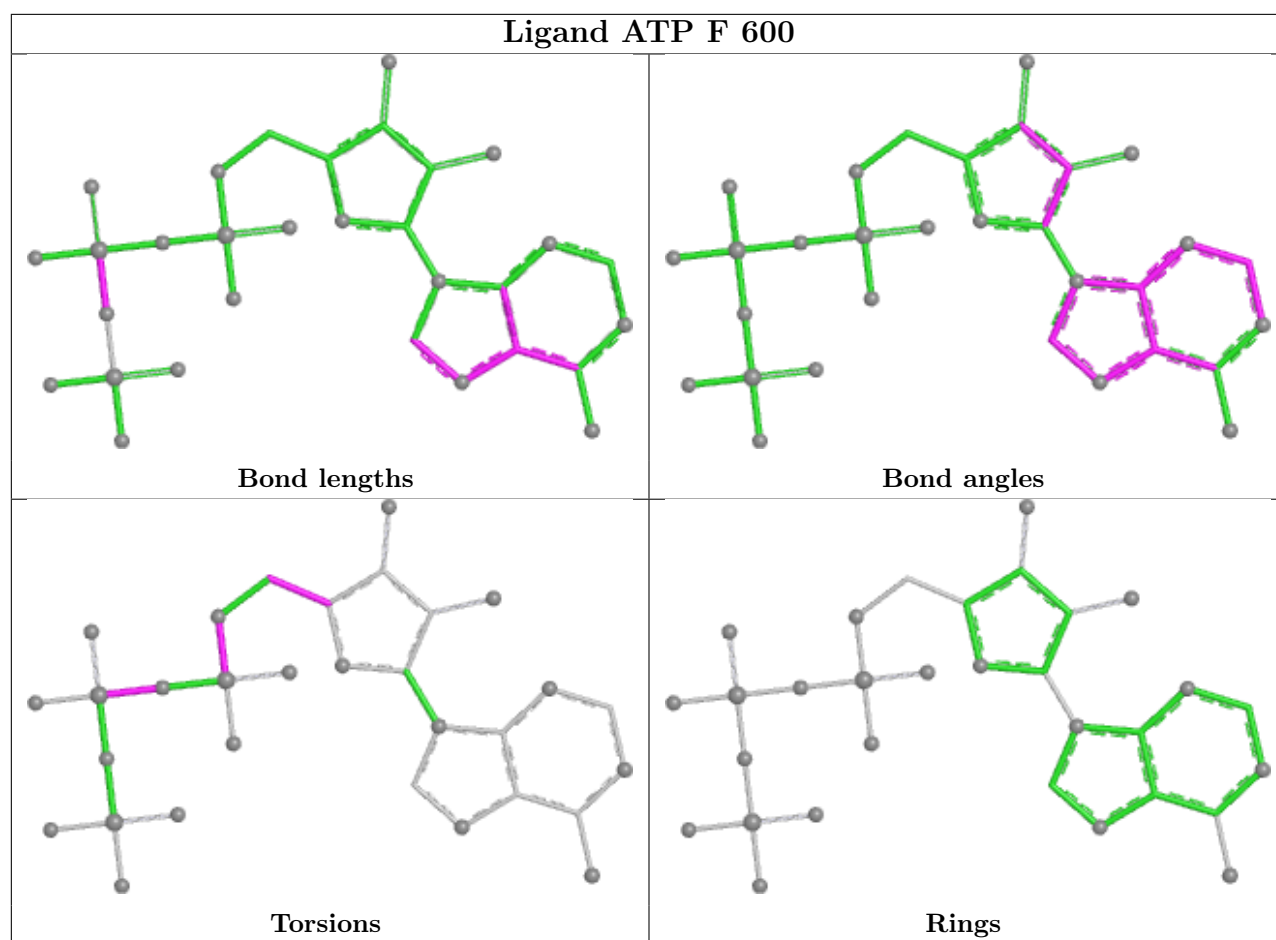
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	1	0/20	-	-	-	-
2	2	0/15	-	-	-	-
3	3	0/19	-	-	-	-
4	A	505/511 (98%)	0.70	53 (10%) 11 14	73, 123, 205, 249	0
4	B	496/511 (97%)	0.54	42 (8%) 16 18	59, 112, 185, 216	0
4	C	484/511 (94%)	0.58	36 (7%) 20 20	67, 107, 159, 206	0
5	D	470/474 (99%)	0.58	38 (8%) 18 18	73, 107, 156, 186	0
5	E	466/474 (98%)	0.53	38 (8%) 17 18	72, 131, 203, 247	0
5	F	466/474 (98%)	0.48	26 (5%) 30 25	58, 100, 153, 189	0
6	G	260/290 (89%)	0.66	28 (10%) 11 13	80, 143, 203, 224	0
7	H	110/188 (58%)	0.54	9 (8%) 17 18	110, 152, 185, 215	0
8	I	75/148 (50%)	0.58	3 (4%) 42 32	167, 207, 238, 241	0
9	J	74/77 (96%)	1.78	19 (25%) 1 4	217, 279, 383, 417	0
9	K	74/77 (96%)	2.05	15 (20%) 3 5	182, 295, 402, 415	0
9	L	74/77 (96%)	1.25	14 (18%) 3 6	224, 296, 463, 488	0
9	M	74/77 (96%)	0.88	7 (9%) 14 16	209, 279, 409, 418	0
9	N	74/77 (96%)	1.20	17 (22%) 2 4	214, 273, 401, 421	0
9	O	74/77 (96%)	1.21	13 (17%) 4 7	220, 287, 352, 363	0
9	P	74/77 (96%)	1.46	18 (24%) 2 4	222, 304, 397, 443	0
9	Q	74/77 (96%)	1.78	21 (28%) 1 3	266, 349, 427, 451	0
9	R	74/77 (96%)	1.64	24 (32%) 1 2	200, 315, 439, 449	0
9	S	74/77 (96%)	1.09	9 (12%) 8 12	239, 320, 445, 471	0
9	T	74/77 (96%)	0.79	8 (10%) 11 13	260, 317, 430, 437	0
9	U	74/77 (96%)	1.34	12 (16%) 4 8	231, 279, 431, 447	0
10	V	0/78	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
11	W	0/124	-	-	-	-
12	X	63/283 (22%)	0.68	6 (9%) 14 16	147, 201, 252, 268	0
13	Y	0/54	-	-	-	-
14	Z	54/104 (51%)	0.43	3 (5%) 30 25	135, 172, 218, 248	0
All	All	4337/5202 (83%)	0.74	459 (10%) 11 13	58, 131, 361, 488	0

The worst 5 of 459 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	K	61	ALA	24.4
9	K	64	ILE	20.9
9	Q	61	ALA	14.5
12	X	1205	ILE	13.0
9	K	68	LEU	11.6

## 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, 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.

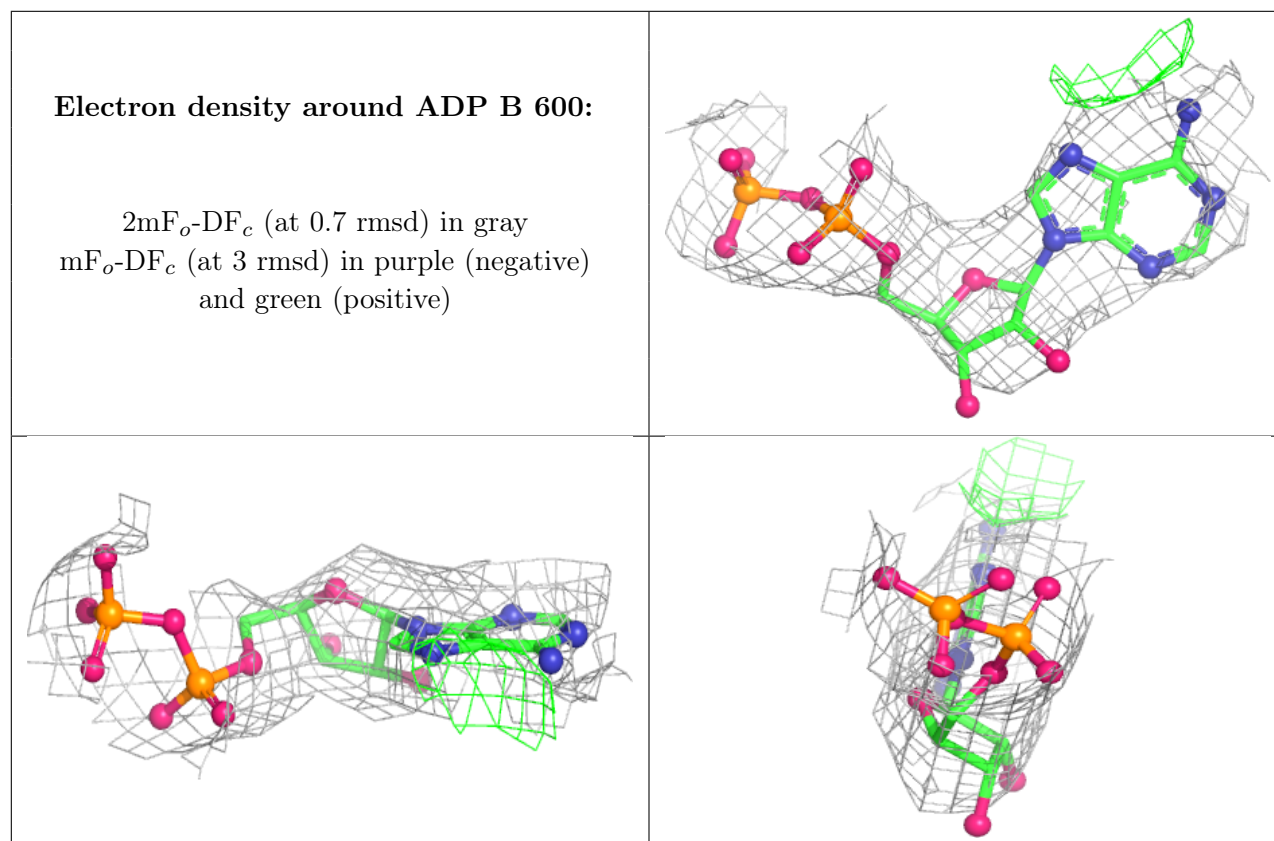
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
17	ADP	B	600	27/27	0.72	0.13	155,165,171,173	0
16	MG	A	601	1/1	0.92	0.16	78,78,78,78	0
15	ATP	A	600	31/31	0.93	0.11	96,98,105,106	0
15	ATP	D	600	31/31	0.93	0.10	90,96,152,153	0
15	ATP	C	600	31/31	0.94	0.08	103,110,115,118	0
15	ATP	F	600	31/31	0.95	0.10	69,74,109,110	0
16	MG	C	601	1/1	0.96	0.10	48,48,48,48	0
16	MG	B	601	1/1	0.96	0.15	72,72,72,72	0

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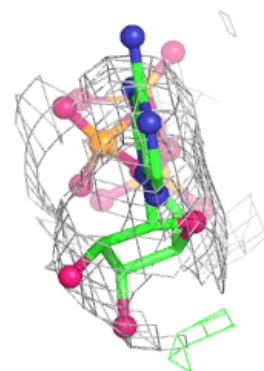
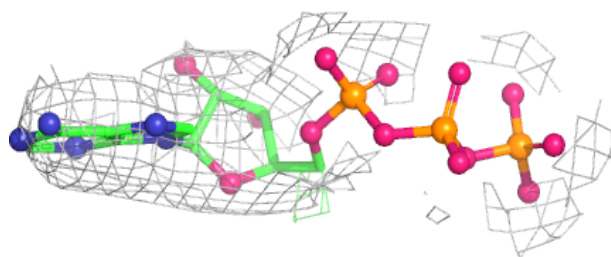
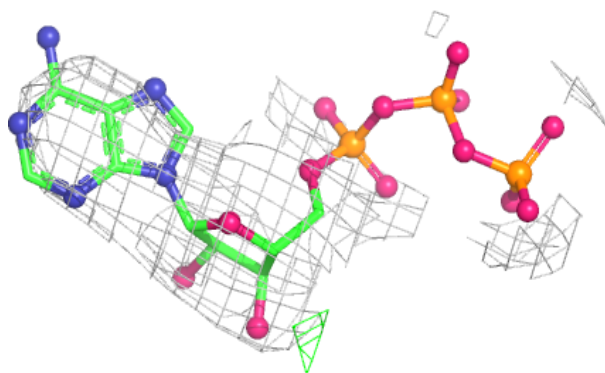
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	MG	F	601	1/1	0.99	0.07	35,35,35,35	0
16	MG	D	601	1/1	0.99	0.04	41,41,41,41	0

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.

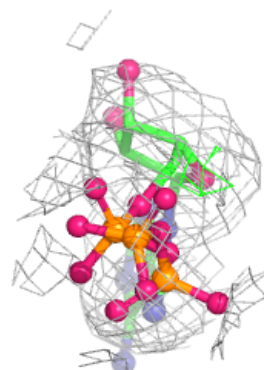
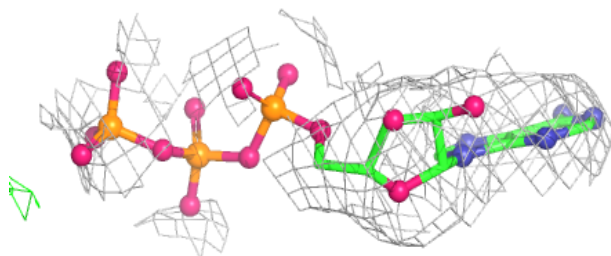
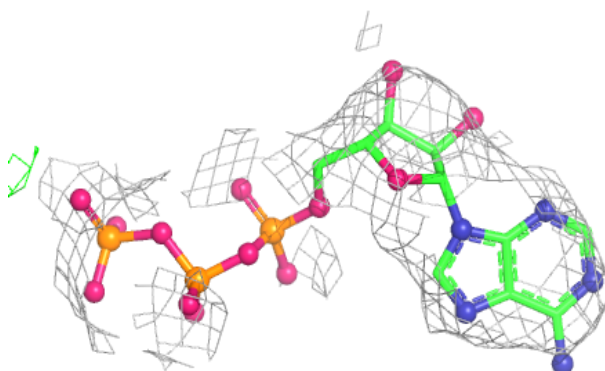


**Electron density around ATP A 600:**

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

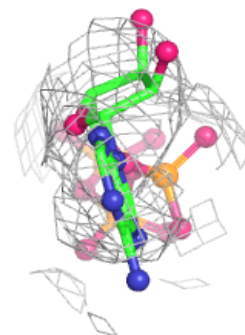
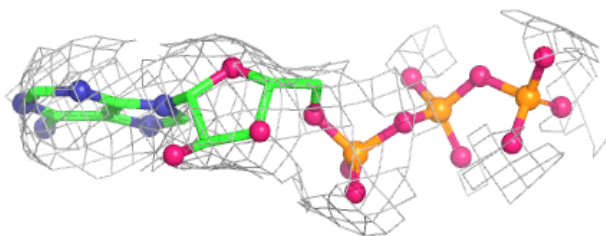
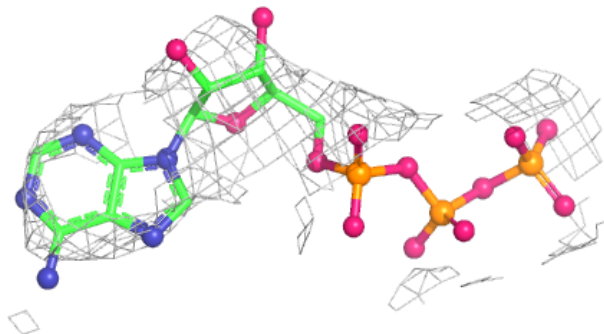
**Electron density around ATP D 600:**

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

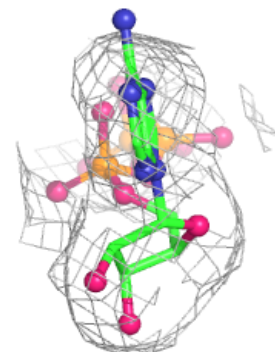
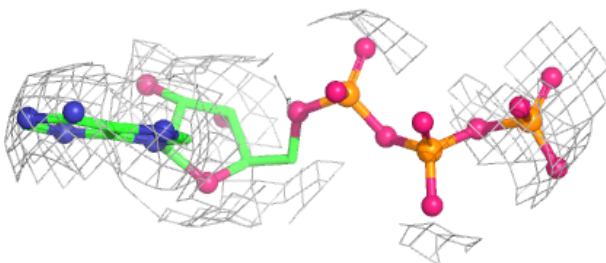
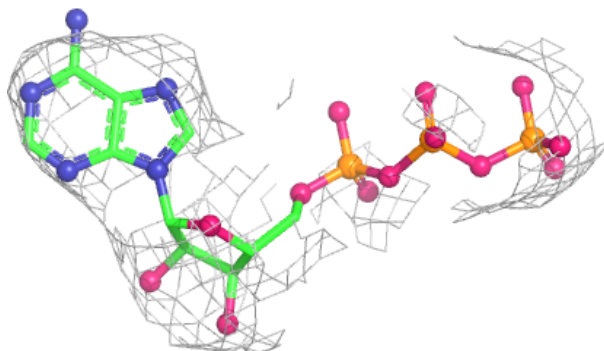


**Electron density around ATP C 600:**

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

**Electron density around ATP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.