



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:54 am BST

PDB ID : 6FOC  
Title : F1-ATPase from Mycobacterium smegmatis  
Authors : Zhang, T.; Montgomery, M.G.; Leslie, A.G.W.; Cook, G.M.; Walker, J.E.  
Deposited on : 2018-02-06  
Resolution : 4.00 Å(reported)

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

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

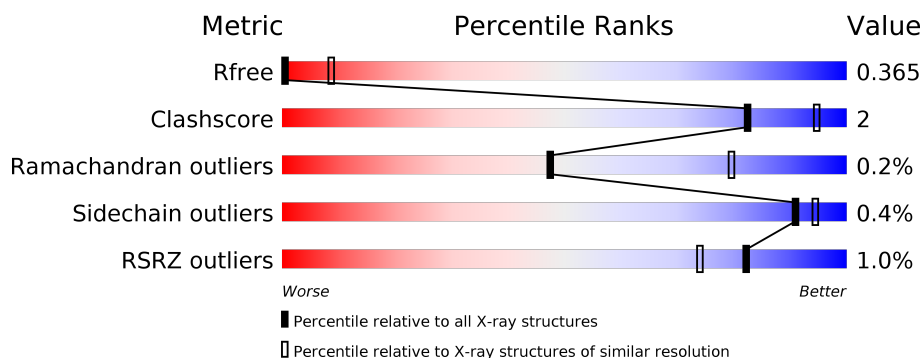
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	548	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>12%</div> </div> </div>
1	B	548	<div> <div></div> <div>80%</div> <div>15%</div> </div>
1	C	548	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>14%</div> </div> </div>
2	D	475	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>5%</div> </div> </div>
2	E	475	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>6%</div> </div> </div>
2	F	475	<div> <div></div> <div>91%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	307	
4	H	121	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PO4	E	602	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23579 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,ATP synthase subunit alpha,ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3609	2272	630	697	10			
1	B	464	Total	C	N	O	S	0	0	0
			3515	2213	613	679	10			
1	C	469	Total	C	N	O	S	0	0	0
			3552	2238	618	686	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	451	Total	C	N	O	S	0	0	0
			3459	2179	595	672	13			
2	E	448	Total	C	N	O	S	0	0	0
			3432	2164	589	666	13			
2	F	454	Total	C	N	O	S	0	0	0
			3485	2196	598	678	13			

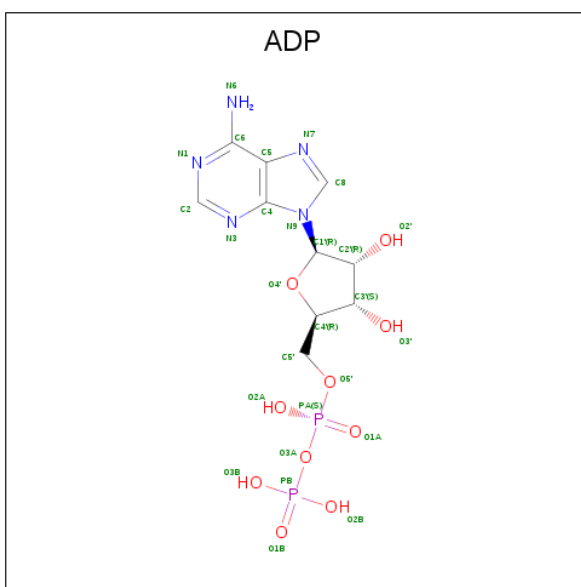
- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	193	Total	C	N	O	S	0	0	0
			1485	917	280	283	5			

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	113	Total	C	N	O	S	0	0	0
			877	543	155	178	1			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



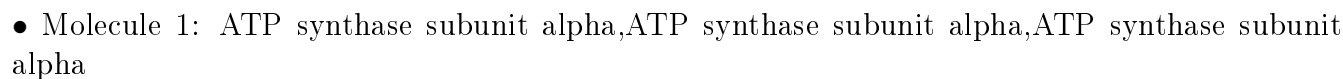
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	P	0	0
			5	4	1		

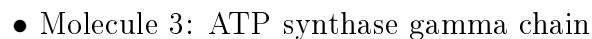
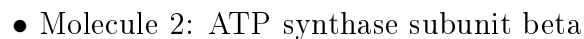
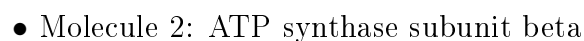
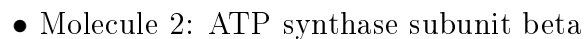
- Molecule 8 is water.

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

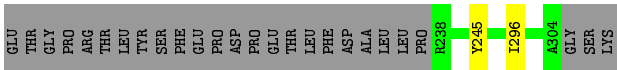


- Molecule 1: ATP synthase subunit alpha,ATP synthase subunit alpha,ATP synthase subunit alpha

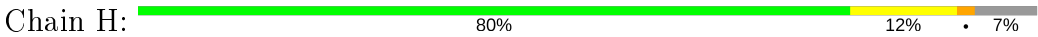








● Molecule 4: ATP synthase epsilon chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.19Å 105.19Å 628.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.59 – 4.00 45.55 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.59-4.00) 98.0 (45.55-4.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.331 , 0.367 0.330 , 0.365	Depositor DCC
$R_{free}$ test set	1666 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	146.3	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 86.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	23579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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: PO4, MG, ADP

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	0.30	0/3608	0.46	0/4881
1	B	0.29	0/3567	0.45	0/4823
1	C	0.30	0/3605	0.45	0/4875
2	D	0.30	0/3518	0.45	0/4768
2	E	0.31	0/3490	0.47	0/4729
2	F	0.29	0/3545	0.46	0/4805
3	G	0.29	0/1493	0.41	0/2000
4	H	0.28	0/888	0.50	0/1206
All	All	0.30	0/23714	0.46	0/32087

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	193	ARG	Sidechain

## 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	3609	0	3600	19	0
1	B	3515	0	3548	17	0
1	C	3552	0	3582	11	0
2	D	3459	0	3442	21	0
2	E	3432	0	3416	27	0
2	F	3485	0	3462	15	0
3	G	1485	0	1516	7	0
4	H	877	0	853	17	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
5	C	27	0	12	0	0
5	D	27	0	12	1	0
5	F	27	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	E	5	0	0	0	0
8	A	4	0	0	0	0
8	B	4	0	0	0	0
8	C	4	0	0	0	0
8	D	4	0	0	1	0
8	F	4	0	0	0	0
All	All	23579	0	23479	117	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 2.

All (117) 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)
4:H:63:ILE:HG13	4:H:114:LEU:HD22	1.69	0.71
2:F:246:GLY:HA2	2:F:300:ARG:HG3	1.72	0.71
2:F:157:ALA:CB	2:F:327:LEU:HD13	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:ALA:CB	2:D:327:LEU:HD13	2.27	0.65
2:F:407:ARG:NH1	2:F:450:LEU:O	2.31	0.64
1:B:65:VAL:HG11	1:B:98:LEU:HD11	1.81	0.63
4:H:22:PHE:CE1	4:H:53:VAL:HG21	2.33	0.63
2:E:151:VAL:HG22	2:E:355:ILE:HD12	1.79	0.63
1:B:82:PHE:O	2:E:32:LEU:HD12	1.99	0.62
3:G:53:MET:SD	4:H:70:LEU:HD22	2.41	0.60
1:B:52:THR:HG21	2:F:15:ILE:HG21	1.84	0.59
2:D:157:ALA:HB2	2:D:327:LEU:HD22	1.87	0.57
4:H:63:ILE:CG1	4:H:114:LEU:HD22	2.34	0.57
2:E:170:ILE:HG23	2:E:252:PHE:CE1	2.39	0.57
2:E:219:GLN:OE1	2:E:219:GLN:N	2.38	0.56
2:D:242:ARG:HG2	2:D:300:ARG:HD3	1.87	0.56
2:F:157:ALA:HB2	2:F:327:LEU:HD22	1.87	0.56
2:D:242:ARG:O	2:D:300:ARG:HG2	2.06	0.56
1:B:352:GLN:NE2	1:B:374:VAL:HG12	2.21	0.55
2:E:147:LEU:O	2:E:356:LEU:HD11	2.07	0.55
4:H:63:ILE:HD13	4:H:111:ARG:HG2	1.89	0.55
1:A:212:LYS:NZ	2:D:328:ASP:OD1	2.40	0.54
2:E:458:ILE:HD12	2:E:464:LEU:HD23	1.90	0.53
1:A:303:TYR:CZ	1:A:307:ARG:HD3	2.43	0.53
1:A:354:PHE:CD2	1:A:372:VAL:HG12	2.44	0.53
2:E:319:ALA:HB3	2:E:320:PRO:CD	2.39	0.53
2:F:319:ALA:HB3	2:F:320:PRO:CD	2.39	0.52
2:E:299:GLY:O	2:E:300:ARG:HG2	2.09	0.52
2:D:319:ALA:HB3	2:D:320:PRO:CD	2.40	0.51
1:B:269:ILE:HD11	1:B:312:CYS:SG	2.50	0.51
1:A:269:ILE:HD11	1:A:312:CYS:SG	2.50	0.51
2:D:209:VAL:O	2:D:209:VAL:HG12	2.11	0.50
1:C:269:ILE:HD11	1:C:312:CYS:SG	2.51	0.50
1:B:347:SER:O	2:F:193:ARG:NH2	2.44	0.50
2:E:170:ILE:HG23	2:E:252:PHE:CD1	2.47	0.50
2:E:454:ALA:O	2:E:458:ILE:HD12	2.11	0.50
2:D:168:VAL:HG21	5:D:600:ADP:H3'	1.94	0.49
3:G:147:TYR:CE1	4:H:11:VAL:HG22	2.48	0.49
1:A:35:ILE:HD11	1:A:45:GLU:HB2	1.93	0.49
1:B:65:VAL:CG1	1:B:98:LEU:HD11	2.41	0.49
2:E:155:LYS:CB	2:E:327:LEU:HD23	2.43	0.48
1:A:407:ALA:HB2	1:A:421:LEU:HD22	1.95	0.48
2:E:319:ALA:HB3	2:E:320:PRO:HD3	1.96	0.48
4:H:63:ILE:HD12	4:H:85:GLN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:LYS:HE2	2:D:294:ILE:O	2.14	0.47
1:B:47:LEU:O	2:F:75:ARG:NH2	2.48	0.47
1:C:31:ILE:HG23	1:C:90:GLN:HG3	1.95	0.47
2:E:151:VAL:CG2	2:E:355:ILE:HD12	2.45	0.46
4:H:69:PHE:C	4:H:70:LEU:HD23	2.35	0.46
1:A:338:SER:HB3	2:E:312:ALA:HB2	1.96	0.46
2:E:153:GLY:HA2	2:E:302:ILE:O	2.15	0.46
2:D:193:ARG:NH1	8:D:701:HOH:O	2.49	0.46
1:C:159:MET:CE	1:C:370:VAL:HG22	2.45	0.46
2:D:319:ALA:HB3	2:D:320:PRO:HD3	1.97	0.46
2:D:254:ASP:HA	2:D:255:ASN:HA	1.74	0.46
2:F:157:ALA:HB2	2:F:327:LEU:HD13	1.98	0.46
2:F:319:ALA:HB3	2:F:320:PRO:HD3	1.97	0.46
2:E:155:LYS:HB3	2:E:327:LEU:HD23	1.97	0.45
2:E:155:LYS:HB2	2:E:327:LEU:HA	1.99	0.45
4:H:61:LEU:HD12	4:H:61:LEU:O	2.16	0.45
4:H:63:ILE:HD12	4:H:85:GLN:CB	2.47	0.45
2:E:324:PHE:HA	2:E:327:LEU:HD12	1.99	0.44
1:B:209:ILE:HG21	1:B:277:GLN:HB2	2.00	0.44
2:D:175:ASN:O	2:D:179:ARG:HG2	2.17	0.44
1:A:296:ALA:HB2	3:G:296:ILE:HD13	2.00	0.44
1:B:249:ALA:HB3	1:B:250:PRO:HD3	2.00	0.44
2:D:157:ALA:HB2	2:D:327:LEU:HD13	1.99	0.44
1:C:249:ALA:HB3	1:C:250:PRO:HD3	1.99	0.43
1:C:330:ILE:HD11	1:C:345:VAL:HG21	2.00	0.43
2:E:153:GLY:HA3	2:E:296:SER:HB2	2.01	0.43
1:C:209:ILE:HG21	1:C:277:GLN:HB2	2.00	0.43
1:C:346:ILE:CG2	2:D:162:ALA:HB1	2.48	0.43
1:A:330:ILE:HD11	1:A:345:VAL:HG21	2.01	0.43
1:B:449:PHE:CD2	1:B:500:LEU:HD23	2.54	0.43
3:G:44:ARG:N	3:G:45:PRO:HD2	2.34	0.43
1:A:249:ALA:HB3	1:A:250:PRO:HD3	2.00	0.43
2:E:294:ILE:HG21	2:E:304:SER:HB2	2.00	0.43
2:E:355:ILE:HG23	2:E:360:ILE:HG21	2.01	0.43
3:G:53:MET:CE	4:H:42:VAL:HG13	2.48	0.43
1:A:102:VAL:HG11	1:A:259:HIS:HB2	2.01	0.43
1:A:98:LEU:HB3	1:A:132:LEU:HD12	2.00	0.43
1:C:346:ILE:HG22	2:D:162:ALA:HB1	2.00	0.43
2:E:323:THR:HG22	2:E:327:LEU:HD11	2.01	0.43
4:H:61:LEU:HB2	4:H:114:LEU:HD11	2.01	0.43
1:B:330:ILE:HD11	1:B:345:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:ALA:O	2:E:182:GLY:HA2	2.19	0.42
1:A:159:MET:CE	1:A:397:LEU:HD12	2.49	0.42
2:D:70:THR:HB	2:D:73:LEU:HD12	2.02	0.42
4:H:34:ILE:HG13	4:H:69:PHE:CE2	2.54	0.42
4:H:87:GLU:O	4:H:88:SER:C	2.58	0.42
2:E:49:LEU:CD2	2:E:73:LEU:HD11	2.50	0.42
1:B:63:LEU:HD12	1:B:114:LEU:HD13	2.01	0.41
2:E:70:THR:HB	2:E:73:LEU:HD12	2.01	0.41
2:D:49:LEU:CD2	2:D:73:LEU:HD11	2.51	0.41
4:H:70:LEU:N	4:H:70:LEU:HD23	2.35	0.41
4:H:87:GLU:O	4:H:89:GLU:N	2.53	0.41
1:B:110:VAL:HG11	2:E:127:PHE:CE1	2.55	0.41
1:C:98:LEU:HB3	1:C:132:LEU:HD12	2.03	0.41
1:A:171:ILE:HG23	1:A:354:PHE:CD1	2.56	0.41
1:B:58:PHE:HB3	1:B:59:PRO:HD2	2.02	0.41
1:C:352:GLN:HE22	1:C:376:ARG:HH21	1.68	0.41
2:F:49:LEU:CD2	2:F:73:LEU:HD11	2.50	0.41
1:A:310:GLU:HG2	2:E:221:ASP:HB3	2.03	0.41
1:A:341:ILE:HB	1:A:342:PRO:HD3	2.03	0.41
1:A:365:ARG:NH1	2:D:370:GLN:HE22	2.18	0.41
3:G:53:MET:HE3	4:H:42:VAL:HG13	2.02	0.41
1:A:58:PHE:HB3	1:A:59:PRO:HD2	2.03	0.41
2:D:155:LYS:NZ	2:D:294:ILE:O	2.51	0.41
1:A:169:LEU:HB3	1:A:352:GLN:HG3	2.03	0.41
2:F:62:VAL:HG23	2:F:62:VAL:O	2.21	0.41
2:F:277:VAL:HG23	2:F:279:TYR:CD1	2.56	0.41
1:B:65:VAL:HG22	1:B:98:LEU:HD21	2.02	0.40
1:C:169:LEU:HB3	1:C:352:GLN:HG3	2.03	0.40
2:D:167:THR:HA	2:D:170:ILE:HG22	2.02	0.40
1:B:51:MET:HG2	2:F:74:VAL:HG22	2.02	0.40
3:G:147:TYR:CZ	3:G:245:TYR:CZ	3.10	0.40
2:F:167:THR:HA	2:F:170:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	467/548 (85%)	446 (96%)	21 (4%)	0	100	100
1	B	458/548 (84%)	438 (96%)	20 (4%)	0	100	100
1	C	463/548 (84%)	443 (96%)	20 (4%)	0	100	100
2	D	445/475 (94%)	420 (94%)	24 (5%)	1 (0%)	47	79
2	E	440/475 (93%)	417 (95%)	20 (4%)	3 (1%)	22	61
2	F	448/475 (94%)	423 (94%)	24 (5%)	1 (0%)	47	79
3	G	181/307 (59%)	178 (98%)	3 (2%)	0	100	100
4	H	111/121 (92%)	100 (90%)	10 (9%)	1 (1%)	17	55
All	All	3013/3497 (86%)	2865 (95%)	142 (5%)	6 (0%)	47	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	26	ARG
4	H	88	SER
2	D	165	GLY
2	E	165	GLY
2	F	165	GLY
2	E	356	LEU

### 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	377/432 (87%)	376 (100%)	1 (0%)	92	95
1	B	374/432 (87%)	374 (100%)	0	100	100
1	C	377/432 (87%)	377 (100%)	0	100	100
2	D	373/388 (96%)	369 (99%)	4 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	370/388 (95%)	368 (100%)	2 (0%)	88	93
2	F	376/388 (97%)	376 (100%)	0	100	100
3	G	148/238 (62%)	148 (100%)	0	100	100
4	H	91/96 (95%)	89 (98%)	2 (2%)	52	71
All	All	2486/2794 (89%)	2477 (100%)	9 (0%)	91	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
2	D	155	LYS
2	D	300	ARG
2	D	377	GLN
2	D	392	ASP
2	E	328	ASP
2	E	392	ASP
4	H	48	ASP
4	H	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	352	GLN
2	F	377	GLN
3	G	286	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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ADP	B	600	6	24,29,29	1.00	2 (8%)	29,45,45	1.47	5 (17%)
5	ADP	C	600	6	24,29,29	1.01	2 (8%)	29,45,45	1.45	4 (13%)
5	ADP	D	600	6	24,29,29	1.06	3 (12%)	29,45,45	1.27	3 (10%)
7	PO4	E	602	-	4,4,4	0.92	0	6,6,6	0.44	0
5	ADP	A	1600	6	24,29,29	0.99	2 (8%)	29,45,45	1.54	5 (17%)
5	ADP	F	600	6	24,29,29	1.01	2 (8%)	29,45,45	1.46	4 (13%)

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
5	ADP	B	600	6	-	0/12/32/32	0/3/3/3
5	ADP	D	600	6	-	5/12/32/32	0/3/3/3
5	ADP	C	600	6	-	0/12/32/32	0/3/3/3
5	ADP	F	600	6	-	2/12/32/32	0/3/3/3
5	ADP	A	1600	6	-	1/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	600	ADP	C5-C4	2.59	1.47	1.40
5	C	600	ADP	C5-C4	2.56	1.47	1.40
5	A	1600	ADP	C5-C4	2.55	1.47	1.40
5	B	600	ADP	C5-C4	2.52	1.47	1.40
5	F	600	ADP	C5-C4	2.50	1.47	1.40
5	D	600	ADP	O4'-C1'	2.17	1.44	1.41
5	D	600	ADP	C2-N3	2.10	1.35	1.32
5	C	600	ADP	C2-N3	2.09	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1600	ADP	C2-N3	2.04	1.35	1.32
5	F	600	ADP	C2-N3	2.02	1.35	1.32
5	B	600	ADP	C2-N3	2.01	1.35	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	ADP	N3-C2-N1	-3.72	122.86	128.68
5	A	1600	ADP	N3-C2-N1	-3.71	122.88	128.68
5	F	600	ADP	N3-C2-N1	-3.71	122.88	128.68
5	D	600	ADP	N3-C2-N1	-3.64	122.99	128.68
5	C	600	ADP	N3-C2-N1	-3.63	123.01	128.68
5	A	1600	ADP	C3'-C2'-C1'	3.54	106.30	100.98
5	A	1600	ADP	PA-O3A-PB	-3.50	120.83	132.83
5	C	600	ADP	PA-O3A-PB	-3.32	121.44	132.83
5	B	600	ADP	C3'-C2'-C1'	3.22	105.83	100.98
5	F	600	ADP	PA-O3A-PB	-3.17	121.95	132.83
5	F	600	ADP	C3'-C2'-C1'	3.14	105.71	100.98
5	D	600	ADP	PA-O3A-PB	-3.06	122.34	132.83
5	B	600	ADP	PA-O3A-PB	-2.99	122.55	132.83
5	B	600	ADP	C4-C5-N7	-2.85	106.43	109.40
5	C	600	ADP	C3'-C2'-C1'	2.84	105.25	100.98
5	C	600	ADP	C4-C5-N7	-2.76	106.52	109.40
5	F	600	ADP	C4-C5-N7	-2.70	106.59	109.40
5	A	1600	ADP	C4-C5-N7	-2.59	106.70	109.40
5	D	600	ADP	C4-C5-N7	-2.34	106.96	109.40
5	A	1600	ADP	C2-N1-C6	2.03	122.22	118.75
5	B	600	ADP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

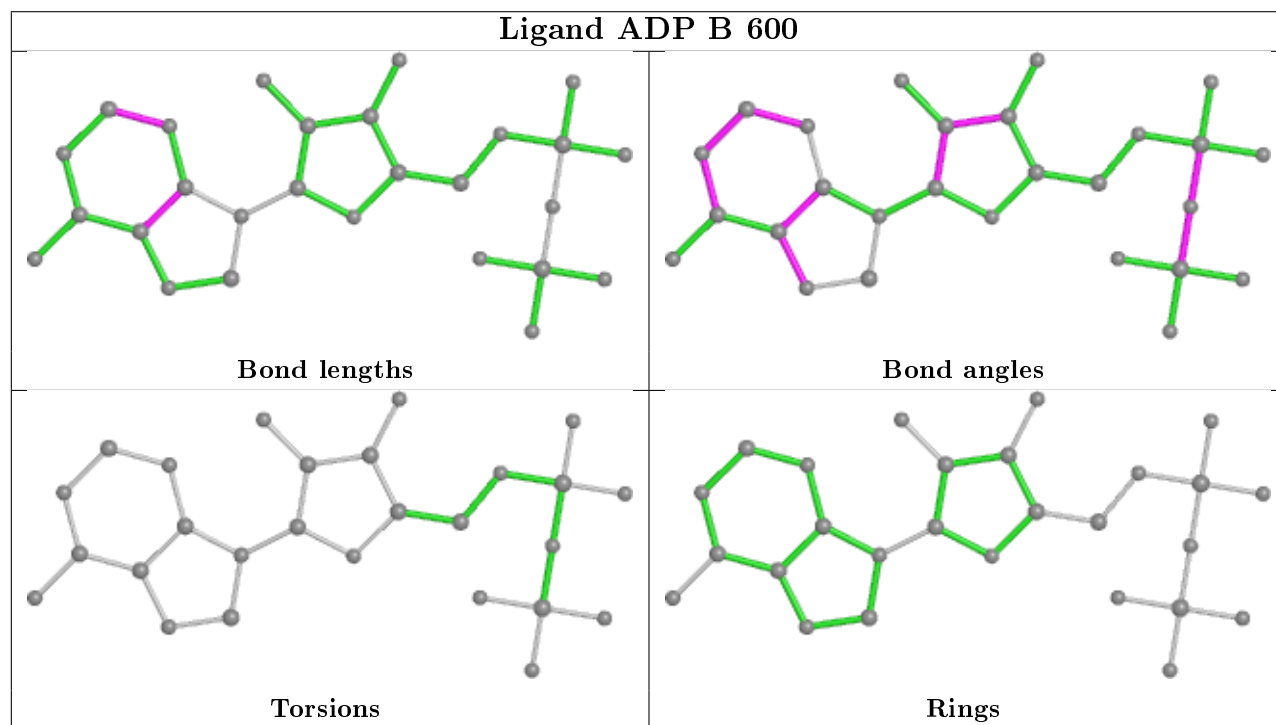
Mol	Chain	Res	Type	Atoms
5	D	600	ADP	C5'-O5'-PA-O1A
5	D	600	ADP	C5'-O5'-PA-O2A
5	D	600	ADP	C5'-O5'-PA-O3A
5	D	600	ADP	O4'-C4'-C5'-O5'
5	D	600	ADP	C3'-C4'-C5'-O5'
5	F	600	ADP	O4'-C4'-C5'-O5'
5	F	600	ADP	C3'-C4'-C5'-O5'
5	A	1600	ADP	O4'-C4'-C5'-O5'

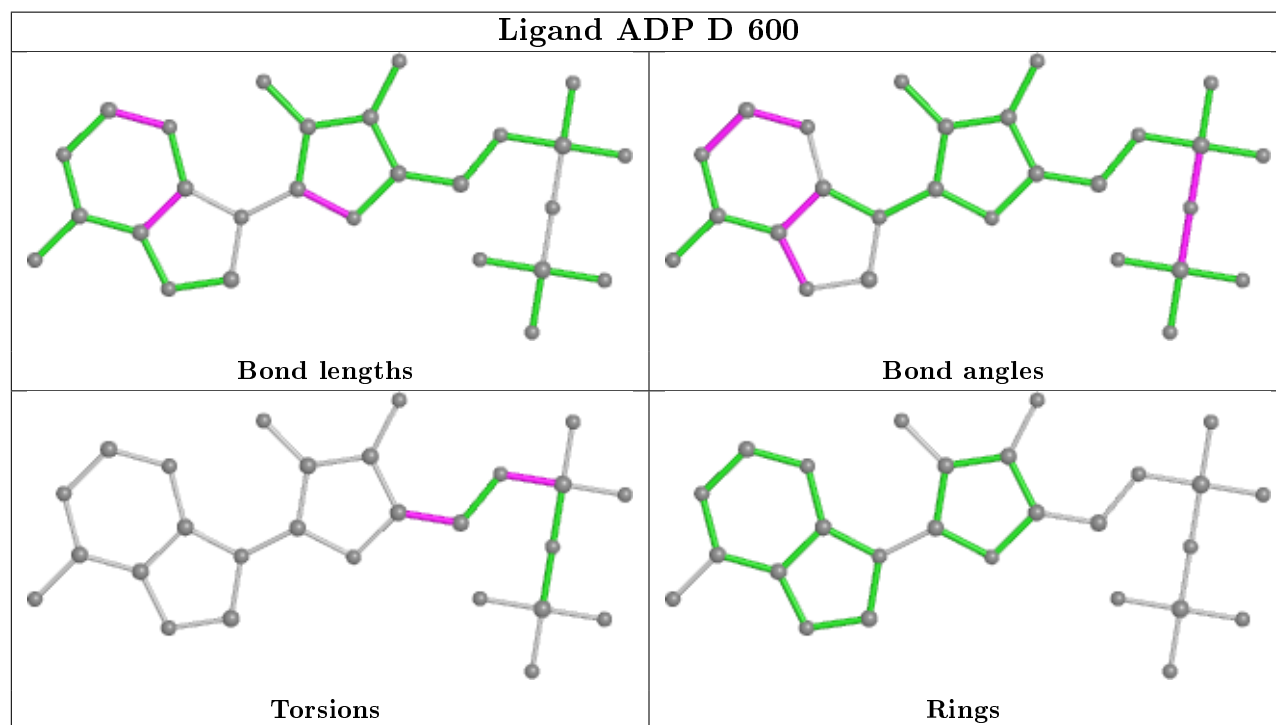
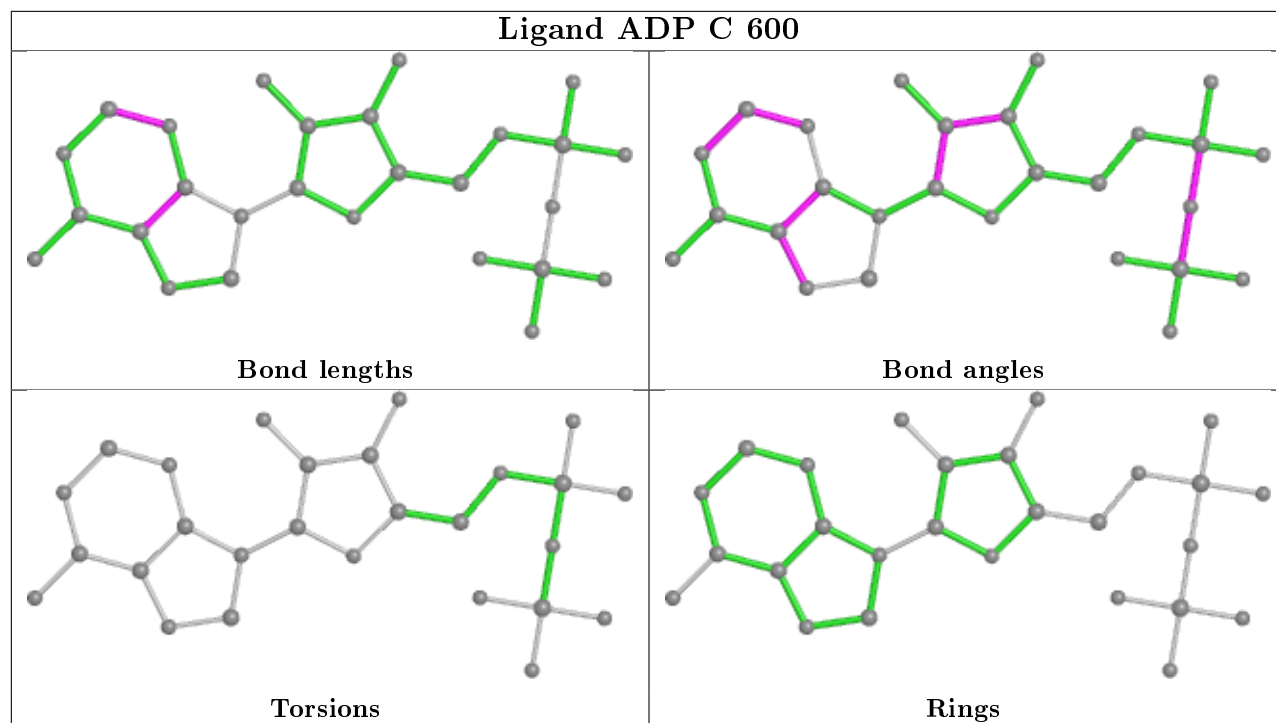
There are no ring outliers.

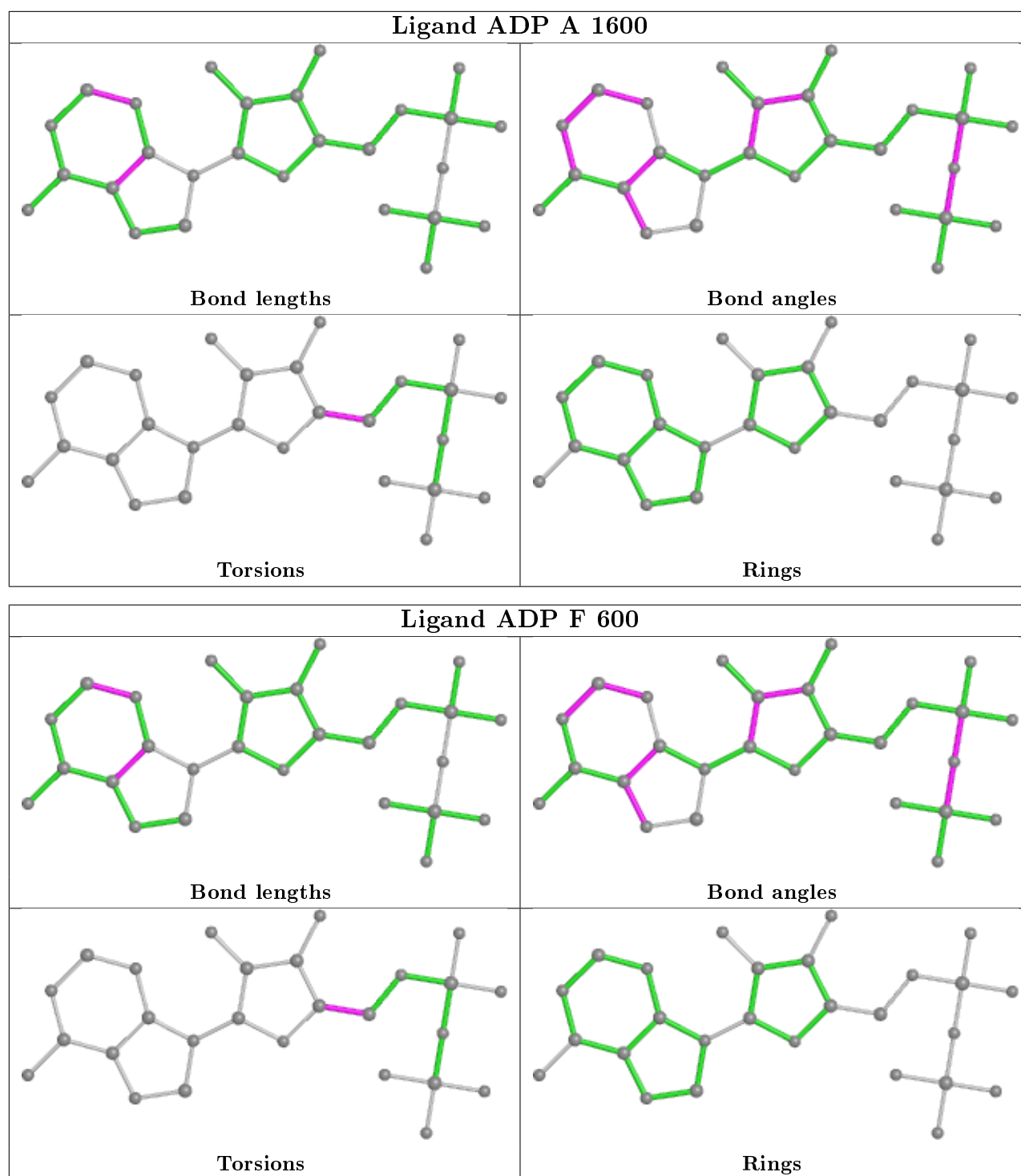
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	600	ADP	1	0

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







## 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 ⓘ

### 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, 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	470/548 (85%)	-0.15	4 (0%) 84 77	105, 156, 210, 242	0
1	B	464/548 (84%)	-0.12	1 (0%) 95 93	103, 178, 228, 286	0
1	C	469/548 (85%)	-0.14	3 (0%) 89 84	99, 158, 221, 241	0
2	D	451/475 (94%)	-0.01	10 (2%) 62 52	117, 188, 220, 242	0
2	E	448/475 (94%)	0.03	5 (1%) 80 72	102, 183, 235, 259	0
2	F	454/475 (95%)	-0.32	2 (0%) 92 87	89, 136, 177, 193	0
3	G	193/307 (62%)	-0.07	7 (3%) 42 34	81, 161, 243, 276	0
4	H	113/121 (93%)	0.02	0 100 100	162, 186, 219, 238	0
All	All	3062/3497 (87%)	-0.11	32 (1%) 82 74	81, 167, 224, 286	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	VAL	3.7
3	G	159	ASN	3.6
2	D	62	VAL	3.5
1	A	92	LYS	3.3
2	D	101	ALA	3.1
1	A	203	ARG	3.1
2	D	21	ASP	2.9
1	C	141	GLN	2.8
1	C	385	ALA	2.8
2	D	214	ALA	2.7
2	F	185	SER	2.7
3	G	127	PHE	2.7
1	B	44	VAL	2.6
1	A	90	GLN	2.6
3	G	157	LEU	2.5
2	D	188	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	158	VAL	2.4
2	D	305	MET	2.3
2	E	453	GLN	2.3
3	G	149	ASN	2.3
2	D	459	GLY	2.3
3	G	155	ASP	2.3
2	E	214	ALA	2.3
1	A	314	LYS	2.2
2	E	127	PHE	2.2
2	E	454	ALA	2.1
1	C	443	GLU	2.1
2	E	423	THR	2.1
2	D	189	GLY	2.1
3	G	156	THR	2.1
2	D	471	LEU	2.1
2	F	75	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 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.

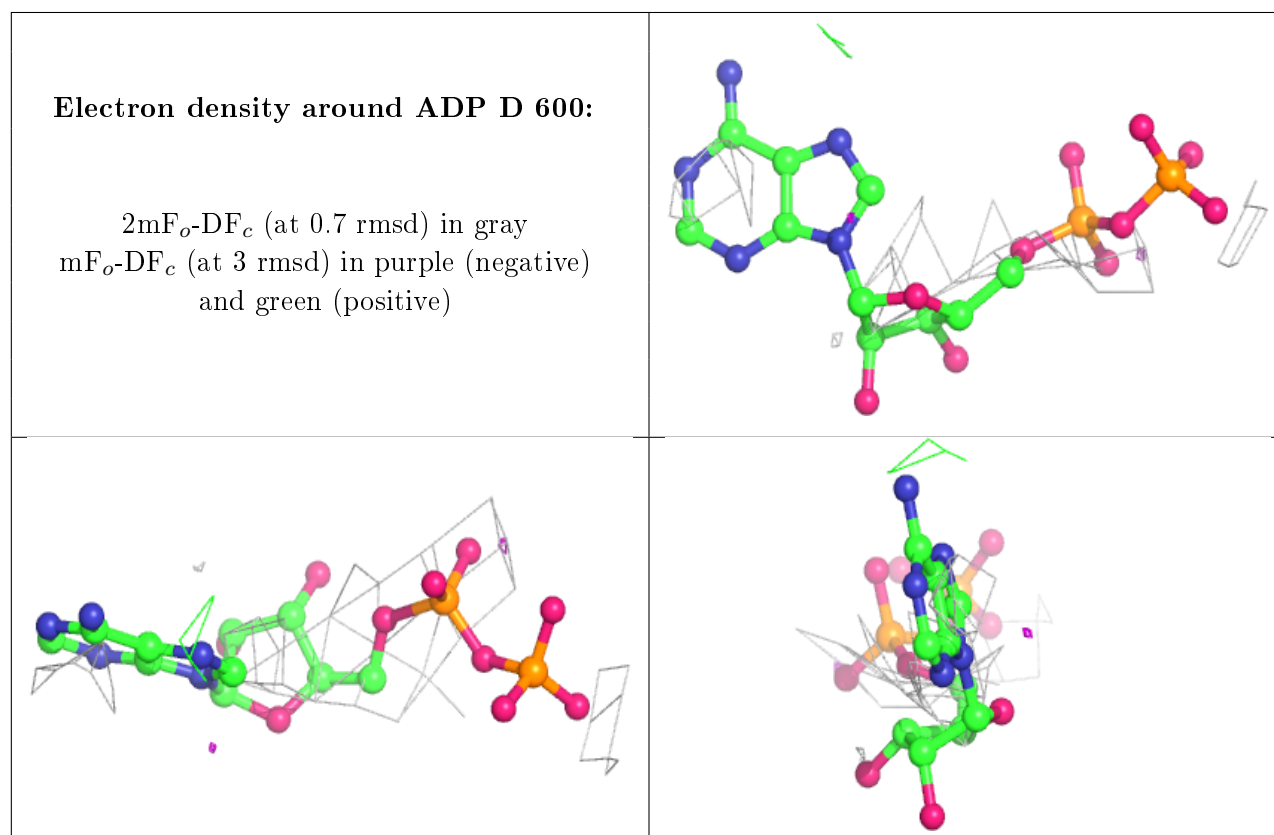
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PO4	E	602	5/5	0.48	0.73	172,173,173,175	0
6	MG	D	601	1/1	0.82	0.27	184,184,184,184	0
5	ADP	D	600	27/27	0.83	0.34	188,224,232,232	0
6	MG	B	601	1/1	0.88	0.19	138,138,138,138	0
5	ADP	C	600	27/27	0.88	0.26	120,127,129,131	0
6	MG	C	601	1/1	0.90	0.35	125,125,125,125	0
5	ADP	A	1600	27/27	0.91	0.25	123,128,133,133	0

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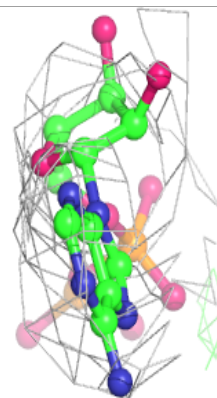
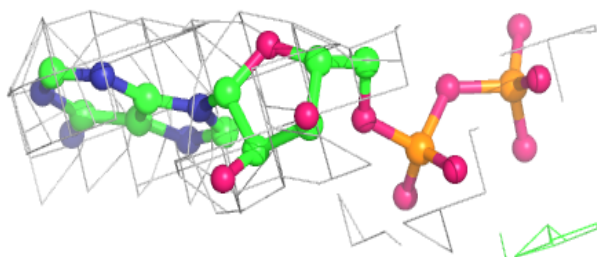
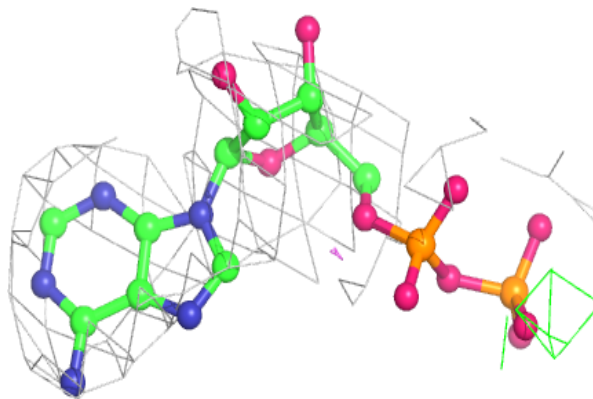
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ADP	B	600	27/27	0.93	0.16	135,145,150,151	0
5	ADP	F	600	27/27	0.93	0.20	105,112,112,113	0
6	MG	A	1601	1/1	0.94	0.26	133,133,133,133	0
6	MG	F	601	1/1	0.96	0.14	107,107,107,107	0

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.

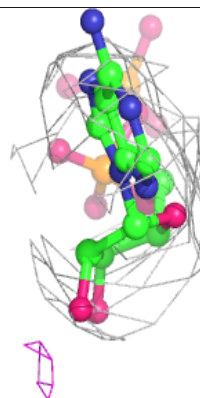
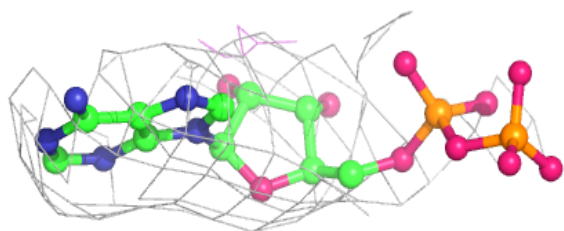
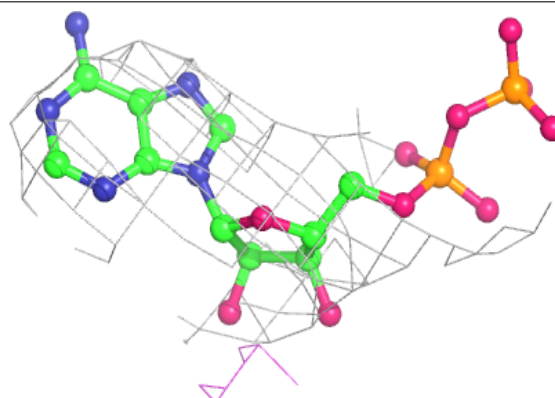


**Electron density around ADP C 600:**

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

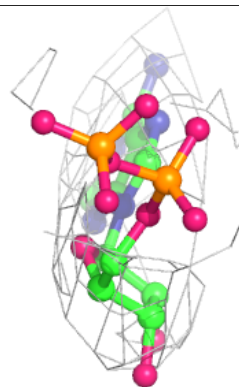
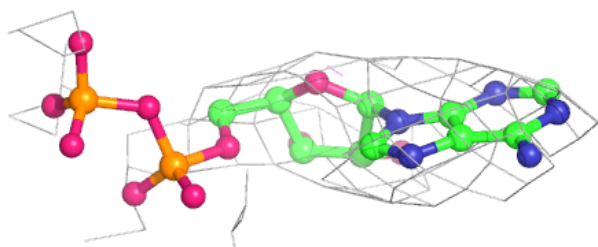
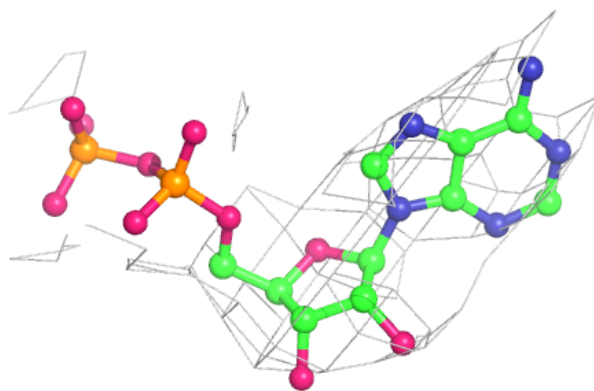
**Electron density around ADP A 1600:**

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

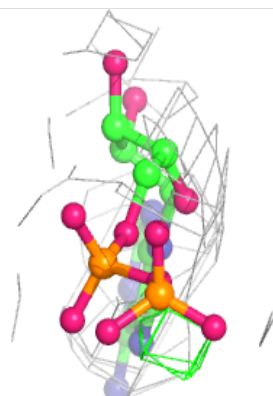
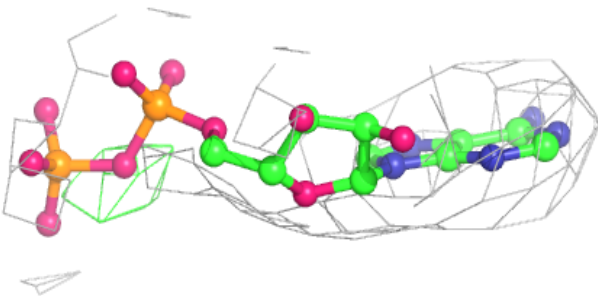
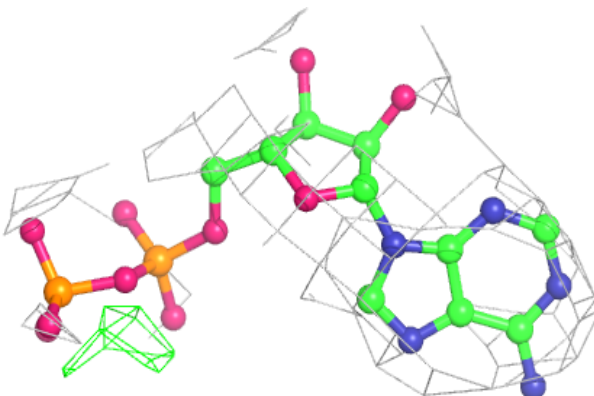


**Electron density around ADP B 600:**

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

**Electron density around ADP 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.