



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:14 AM UTC

PDB ID : 6F5D / pdb_00006f5d
Title : Trypanosoma brucei F1-ATPase
Authors : Montgomery, M.G.; Gahura, O.; Leslie, A.G.W.; Zikova, A.; Walker, J.E.
Deposited on : 2017-12-01
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

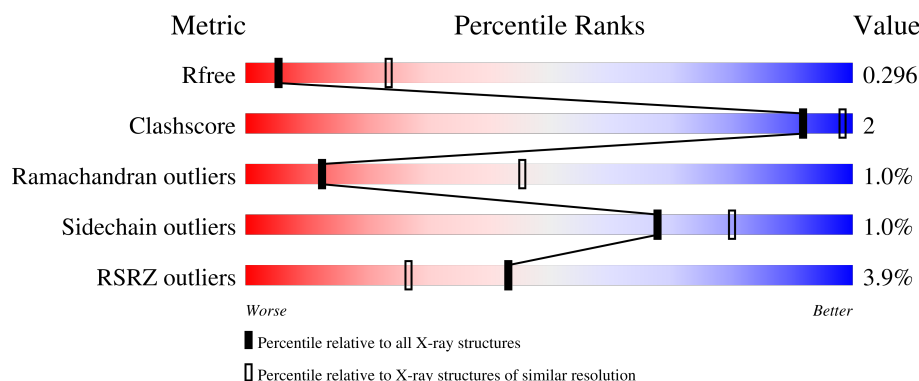
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	560	3% 88% 5% • 6%
1	B	560	2% 88% 5% • 6%
1	C	560	4% 89% • 7%
2	D	498	2% 92% • •
2	E	498	7% 93% • •

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Mol	Chain	Length	Quality of chain
2	F	498	5% 95%
3	G	304	2% 86% 5% 9%
4	H	165	% 84% 5% 12%
5	I	66	95% 5%
6	J	170	3% 85% 11%
6	K	170	6% 85% 9% 5%
6	L	170	9% 86% 9%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31092 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			4046	2591	702	733	20			
1	B	524	Total	C	N	O	S	0	0	0
			4046	2590	704	732	20			
1	C	521	Total	C	N	O	S	0	0	0
			4022	2574	699	729	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	481	Total	C	N	O	S	0	0	0
			3639	2300	616	704	19			
2	E	487	Total	C	N	O	S	0	0	0
			3689	2329	631	710	19			
2	F	488	Total	C	N	O	S	0	0	0
			3694	2332	632	711	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	277	Total	C	N	O	S	0	0	0
			2210	1399	386	417	8			

- Molecule 4 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	146	Total	C	N	O	S	0	0	0
			1128	712	188	224	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	32	THR	UNK	conflict	UNP P0DPG2

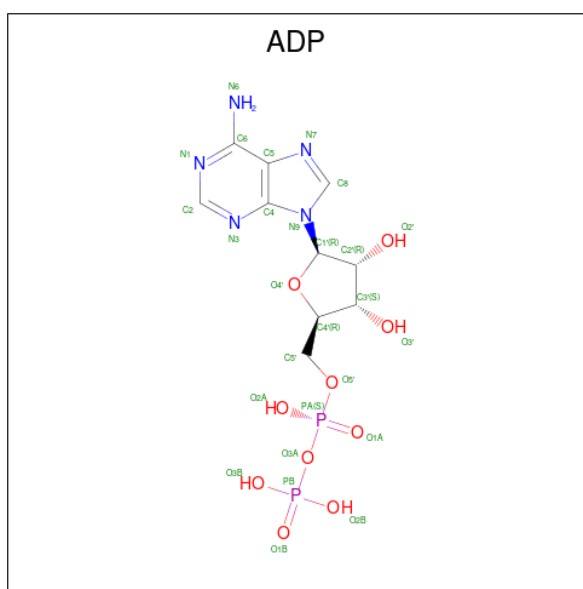
- Molecule 5 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	66	Total	C	N	O	S	0	0	0
			538	335	98	103	2			

- Molecule 6 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	164	Total	C	N	O	S	0	0	0
			1300	814	219	253	14			
6	K	162	Total	C	N	O	S	0	0	0
			1284	803	216	251	14			
6	L	165	Total	C	N	O	S	0	0	0
			1309	819	220	256	14			

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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

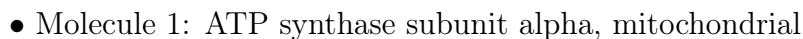
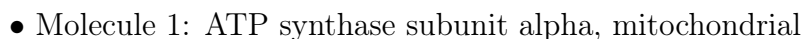
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

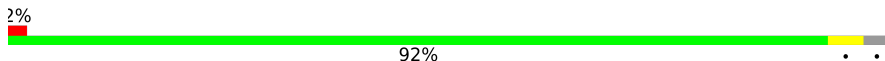
- Molecule 9 is water.

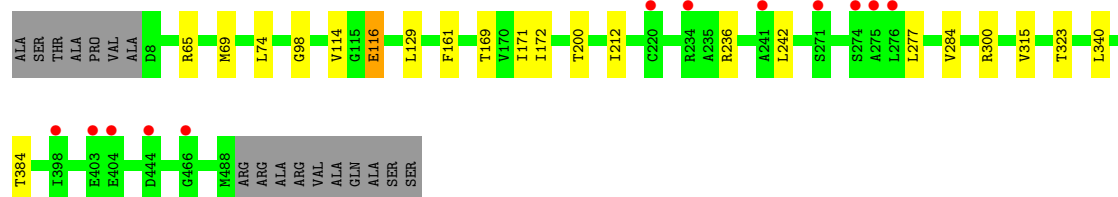
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	O	0	0
			4	4		
9	B	4	Total	O	0	0
			4	4		
9	C	4	Total	O	0	0
			4	4		
9	D	4	Total	O	0	0
			4	4		
9	F	4	Total	O	0	0
			4	4		

- Molecule 1: ATP synthase subunit alpha, mitochondrial

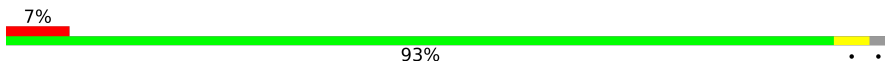


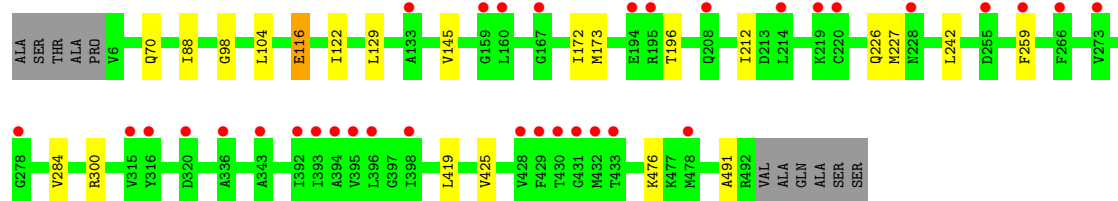
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain D: 

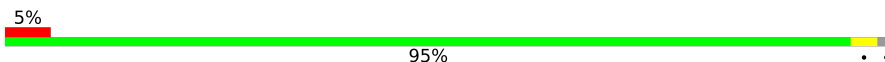


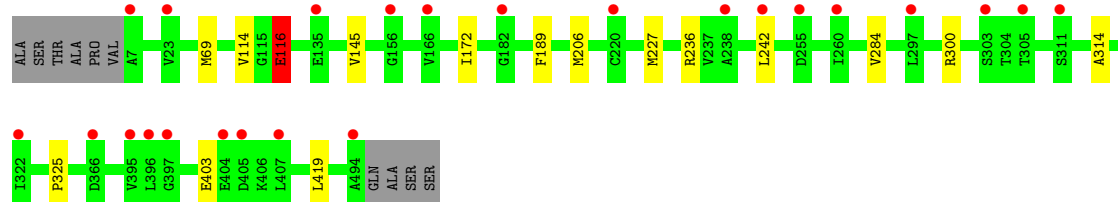
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain E: 

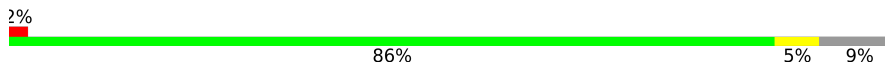


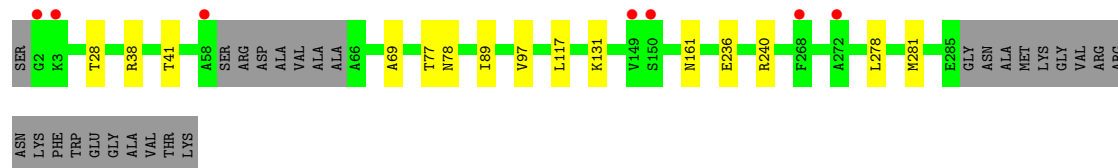
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain F: 



- Molecule 3: ATP synthase gamma subunit

Chain G: 

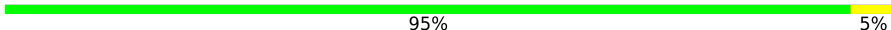


- Molecule 4: ATP synthase subunit delta, mitochondrial

Chain H: 



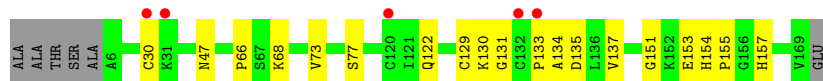
- Molecule 5: ATP synthase subunit epsilon, mitochondrial

Chain I:  95% 5%



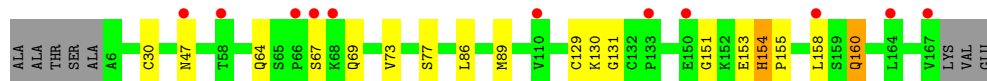
- Molecule 6: ATP synthase subunit p18, mitochondrial

Chain J:  3% 85% 11% .



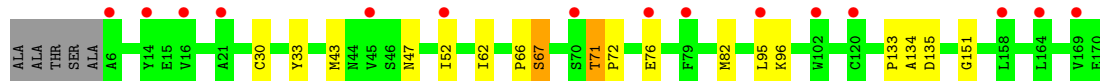
- Molecule 6: ATP synthase subunit p18, mitochondrial

Chain K:  6% 85% 9% • 5%



- Molecule 6: ATP synthase subunit p18, mitochondrial

Chain L:  9% 86% 9% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.22Å 206.35Å 130.21Å 90.00° 104.85° 90.00°	Depositor
Resolution (Å)	90.51 – 3.20 90.51 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (90.51-3.20) 95.6 (90.51-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0190	Depositor
R, R_{free}	0.272 , 0.297 0.271 , 0.296	Depositor DCC
R_{free} test set	4968 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 16.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	31092	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/4120	0.78	0/5580
1	B	0.57	0/4119	0.78	1/5578 (0.0%)
1	C	0.55	0/4095	0.76	0/5546
2	D	0.56	0/3695	0.78	0/5011
2	E	0.62	0/3745	0.81	0/5077
2	F	0.58	0/3750	0.78	0/5084
3	G	0.54	0/2246	0.81	0/3025
4	H	0.54	0/1147	0.77	0/1555
5	I	0.58	0/552	0.82	0/746
6	J	0.60	0/1327	0.88	0/1791
6	K	0.62	0/1311	0.93	2/1770 (0.1%)
6	L	0.60	0/1336	0.90	0/1803
All	All	0.58	0/31443	0.80	3/42566 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	160	GLN	N-CA-C	7.28	126.30	110.80
6	K	155	PRO	N-CA-C	5.81	119.75	110.40
1	B	543	GLU	N-CA-C	5.41	117.25	111.36

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	A	4046	0	4161	23	0
1	B	4046	0	4168	18	0
1	C	4022	0	4138	13	0
2	D	3639	0	3683	14	0
2	E	3689	0	3742	13	0
2	F	3694	0	3746	11	0
3	G	2210	0	2210	9	0
4	H	1128	0	1110	2	0
5	I	538	0	521	0	0
6	J	1300	0	1263	5	0
6	K	1284	0	1241	3	0
6	L	1309	0	1269	6	0
7	A	27	0	12	0	0
7	B	27	0	12	0	0
7	C	27	0	12	0	0
7	D	27	0	12	0	0
7	E	27	0	12	0	0
7	F	27	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	A	4	0	0	0	0
9	B	4	0	0	0	0
9	C	4	0	0	0	0
9	D	4	0	0	0	0
9	F	4	0	0	0	0
All	All	31092	0	31324	100	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 (100) 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:F:145:VAL:HG12	2:F:419:LEU:HD22	1.65	0.78
2:E:145:VAL:HG12	2:E:419:LEU:HD22	1.65	0.78
6:K:86:LEU:HA	6:K:89:MET:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ILE:O	2:D:200:THR:HG22	1.97	0.64
1:B:71:PHE:CE2	1:B:298:LEU:HD13	2.33	0.63
3:G:28:THR:HG21	3:G:240:ARG:HD2	1.80	0.63
2:F:189:PHE:CZ	2:F:206:MET:HE1	2.34	0.62
1:A:149:ILE:HD11	2:E:226:GLN:NE2	2.16	0.60
1:C:152:ARG:HB2	2:D:200:THR:HG21	1.83	0.60
1:A:125:VAL:HG22	2:D:129:LEU:HD22	1.84	0.59
1:B:540:ILE:HG23	1:B:545:ASP:HB3	1.86	0.57
6:L:33:TYR:HB2	6:L:62:ILE:HD13	1.85	0.57
1:A:343:LEU:HB3	2:D:323:THR:HG22	1.88	0.56
1:B:222:ARG:HG3	1:B:225:ASN:HB2	1.88	0.56
1:C:51:ALA:HB1	2:D:74:LEU:HA	1.88	0.55
2:D:169:THR:HA	2:D:172:ILE:HG12	1.88	0.54
1:A:302:PRO:CD	3:G:281:MET:HE1	2.37	0.54
1:B:116:VAL:HG21	1:B:266:MET:HE1	1.90	0.54
2:E:172:ILE:HG23	2:E:259:PHE:CD1	2.43	0.53
1:C:37:THR:HG22	1:C:87:ILE:HD13	1.90	0.53
1:A:37:THR:HG22	1:A:87:ILE:HD13	1.90	0.52
1:A:302:PRO:CG	3:G:281:MET:HE1	2.39	0.52
1:B:169:MET:CE	1:B:407:LEU:HD22	2.39	0.52
2:F:189:PHE:CE1	2:F:206:MET:HE1	2.45	0.51
2:F:172:ILE:HD11	2:F:314:ALA:HB2	1.93	0.50
2:F:145:VAL:HG12	2:F:419:LEU:CD2	2.40	0.49
1:B:169:MET:HE3	1:B:407:LEU:HD22	1.95	0.49
1:A:116:VAL:HG21	1:A:266:MET:HE1	1.94	0.48
6:J:133:PRO:O	6:J:135:ASP:N	2.47	0.46
1:C:116:VAL:HG21	1:C:266:MET:HE1	1.97	0.46
1:C:56:ILE:HD13	1:C:96:VAL:CG1	2.46	0.46
2:D:114:VAL:HG23	2:D:116:GLU:HG2	1.98	0.46
6:L:71:THR:HG22	6:L:72:PRO:HD2	1.98	0.45
1:A:56:ILE:HD13	1:A:96:VAL:CG1	2.46	0.45
1:B:56:ILE:HD13	1:B:96:VAL:CG1	2.46	0.45
1:B:206:ILE:O	6:J:68:LYS:NZ	2.41	0.45
4:H:147:VAL:HA	4:H:150:ILE:HD12	1.98	0.45
1:B:483:ILE:HD12	6:J:154:HIS:CD2	2.50	0.45
2:E:145:VAL:HG12	2:E:419:LEU:CD2	2.40	0.45
6:L:52:ILE:HD11	6:L:95:LEU:HD22	1.97	0.45
2:E:242:LEU:HD21	2:E:300:ARG:HB2	1.99	0.45
1:B:271:MET:HB2	1:B:334:VAL:HG23	1.98	0.45
1:C:32:HIS:HB2	1:C:42:ILE:HG12	2.00	0.45
1:C:38:ILE:HG12	1:C:297:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ILE:HD11	1:C:252:PRO:HG3	1.99	0.45
1:A:271:MET:HB2	1:A:334:VAL:HG23	1.99	0.44
1:A:483:ILE:HD12	1:A:484:MET:N	2.32	0.44
1:B:32:HIS:HB2	1:B:42:ILE:HG12	1.99	0.44
2:D:242:LEU:HD21	2:D:300:ARG:HB2	1.99	0.44
2:F:242:LEU:HD21	2:F:300:ARG:HB2	1.99	0.44
3:G:89:ILE:HD11	3:G:161:ASN:ND2	2.33	0.44
1:B:155:VAL:CG2	1:B:387:VAL:HG21	2.47	0.44
1:A:357:SER:O	2:E:227:MET:HE1	2.16	0.44
2:F:69:MET:HE1	2:F:236:ARG:HG3	2.00	0.44
1:A:540:ILE:HG23	1:A:545:ASP:HB3	1.99	0.43
1:A:87:ILE:HD11	1:A:252:PRO:HG3	2.00	0.43
2:F:403:GLU:HG2	3:G:117:LEU:HD21	1.99	0.43
6:L:133:PRO:O	6:L:135:ASP:N	2.50	0.43
1:C:271:MET:HB2	1:C:334:VAL:HG23	1.99	0.43
3:G:89:ILE:HD11	3:G:161:ASN:HD21	1.83	0.43
1:A:413:LEU:HD23	1:A:428:MET:CG	2.48	0.43
1:C:169:MET:HB2	1:C:170:ILE:HD12	2.01	0.43
2:E:70:GLN:HE22	2:E:104:LEU:HD11	1.84	0.43
1:A:103:LEU:HD23	1:A:258:LEU:HD21	2.00	0.43
2:D:69:MET:HE1	2:D:236:ARG:HG3	2.00	0.43
6:J:122:GLN:HE22	6:J:137:VAL:HG13	1.84	0.43
1:B:155:VAL:HG21	1:B:387:VAL:HG11	2.01	0.42
2:D:171:ILE:HD12	2:D:340:LEU:HD21	2.00	0.42
4:H:55:VAL:HG22	4:H:64:ILE:HD11	2.01	0.42
1:A:413:LEU:HD23	1:A:428:MET:HG3	2.00	0.42
1:A:540:ILE:HD12	1:A:545:ASP:HB3	2.01	0.42
6:J:129:CYS:O	6:J:131:GLY:N	2.51	0.42
6:L:82:MET:HE3	6:L:82:MET:HB2	1.92	0.42
1:A:302:PRO:HD2	3:G:281:MET:HE1	2.01	0.42
1:A:38:ILE:CG2	1:A:298:LEU:HD21	2.50	0.42
2:F:284:VAL:HG11	2:F:325:PRO:HD2	2.01	0.42
2:E:173:MET:HE2	2:E:425:VAL:HG21	2.02	0.42
3:G:77:THR:HG23	3:G:236:GLU:CD	2.45	0.42
6:K:129:CYS:O	6:K:131:GLY:N	2.53	0.42
2:E:172:ILE:HG23	2:E:259:PHE:CE1	2.55	0.41
1:C:56:ILE:HD13	1:C:96:VAL:HG13	2.02	0.41
1:A:169:MET:HB2	1:A:170:ILE:HD12	2.02	0.41
1:B:316:SER:HB2	2:F:227:MET:HB3	2.01	0.41
1:B:534:GLN:O	1:B:537:MET:HE2	2.20	0.41
2:E:88:ILE:O	2:E:122:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLY:HA2	2:D:384:THR:HG21	2.03	0.41
6:L:33:TYR:CE2	6:L:67:SER:HA	2.55	0.41
2:E:196:THR:HG23	2:E:226:GLN:HE21	1.85	0.41
1:A:56:ILE:HD13	1:A:96:VAL:HG13	2.02	0.41
2:E:98:GLY:HA2	2:E:212:ILE:HG23	2.02	0.41
2:F:114:VAL:HG13	2:F:116:GLU:HG2	2.02	0.41
1:B:56:ILE:HD13	1:B:96:VAL:HG13	2.03	0.40
2:D:65:ARG:HD3	2:D:277:LEU:HD23	2.04	0.40
2:D:161:PHE:CE2	2:D:315:VAL:HG11	2.56	0.40
1:B:125:VAL:HG13	2:E:129:LEU:HD22	2.03	0.40
2:D:98:GLY:HA2	2:D:212:ILE:HG23	2.02	0.40
1:C:483:ILE:HD12	6:K:158:LEU:HD13	2.04	0.40
3:G:278:LEU:HA	3:G:281:MET:HE3	2.02	0.40
1:A:483:ILE:HD12	1:A:483:ILE:C	2.47	0.40
1:B:536:LYS:HE3	1:B:549:LEU:HD13	2.04	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	518/560 (92%)	488 (94%)	27 (5%)	3 (1%)	21	56
1	B	518/560 (92%)	488 (94%)	28 (5%)	2 (0%)	30	62
1	C	515/560 (92%)	486 (94%)	28 (5%)	1 (0%)	43	73
2	D	479/498 (96%)	452 (94%)	26 (5%)	1 (0%)	43	73
2	E	485/498 (97%)	454 (94%)	29 (6%)	2 (0%)	30	62
2	F	486/498 (98%)	459 (94%)	26 (5%)	1 (0%)	43	73
3	G	273/304 (90%)	252 (92%)	16 (6%)	5 (2%)	6	34
4	H	142/165 (86%)	126 (89%)	12 (8%)	4 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	64/66 (97%)	49 (77%)	13 (20%)	2 (3%)	3	22
6	J	162/170 (95%)	144 (89%)	12 (7%)	6 (4%)	2	18
6	K	160/170 (94%)	140 (88%)	12 (8%)	8 (5%)	1	13
6	L	163/170 (96%)	141 (86%)	17 (10%)	5 (3%)	3	22
All	All	3965/4219 (94%)	3679 (93%)	246 (6%)	40 (1%)	12	45

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	116	GLU
3	G	97	VAL
6	J	130	LYS
6	K	130	LYS
6	K	160	GLN
1	A	484	MET
1	A	485	TYR
2	E	116	GLU
3	G	38	ARG
3	G	41	THR
4	H	118	ASP
6	K	67	SER
6	L	134	ALA
1	C	540	ILE
2	E	491	ALA
2	F	116	GLU
4	H	40	GLN
5	I	38	SER
6	J	47	ASN
6	J	66	PRO
6	J	77	SER
6	K	47	ASN
6	L	47	ASN
6	L	151	GLY
1	A	540	ILE
3	G	69	ALA
3	G	78	ASN
6	J	151	GLY
6	K	77	SER
6	L	67	SER
1	B	423	VAL
4	H	58	THR

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Mol	Chain	Res	Type
5	I	9	ILE
6	J	134	ALA
6	K	69	GLN
6	K	151	GLY
1	B	540	ILE
6	L	66	PRO
4	H	77	PRO
6	K	154	HIS

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	
1	A	436/462 (94%)	430 (99%)	6 (1%)	59	77
1	B	436/462 (94%)	432 (99%)	4 (1%)	70	81
1	C	433/462 (94%)	430 (99%)	3 (1%)	76	83
2	D	394/405 (97%)	393 (100%)	1 (0%)	86	88
2	E	398/405 (98%)	395 (99%)	3 (1%)	73	82
2	F	398/405 (98%)	397 (100%)	1 (0%)	86	88
3	G	236/255 (92%)	235 (100%)	1 (0%)	84	86
4	H	123/140 (88%)	123 (100%)	0	100	100
5	I	59/59 (100%)	58 (98%)	1 (2%)	53	75
6	J	144/147 (98%)	139 (96%)	5 (4%)	32	64
6	K	142/147 (97%)	137 (96%)	5 (4%)	32	64
6	L	145/147 (99%)	140 (97%)	5 (3%)	32	64
All	All	3344/3496 (96%)	3309 (99%)	35 (1%)	68	80

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	258	LEU

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Mol	Chain	Res	Type
1	A	425	THR
1	A	426	ILE
1	A	536	LYS
1	A	537	MET
1	B	425	THR
1	B	426	ILE
1	B	536	LYS
1	B	537	MET
1	C	425	THR
1	C	537	MET
1	C	540	ILE
2	D	284	VAL
2	E	116	GLU
2	E	284	VAL
2	E	476	LYS
2	F	116	GLU
3	G	131	LYS
5	I	53	GLN
6	J	30	CYS
6	J	73	VAL
6	J	153	GLU
6	J	155	PRO
6	J	157	HIS
6	K	30	CYS
6	K	64	GLN
6	K	73	VAL
6	K	153	GLU
6	K	154	HIS
6	L	30	CYS
6	L	43	MET
6	L	71	THR
6	L	76	GLU
6	L	96	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	531	GLN
1	B	94	GLN
1	B	422	GLN
1	B	531	GLN

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Mol	Chain	Res	Type
1	C	94	GLN
1	C	121	HIS
1	C	210	ASN
2	D	110	GLN
2	D	268	GLN
2	D	377	GLN
2	D	390	GLN
2	E	132	GLN
2	E	178	ASN
2	E	298	GLN
2	E	313	GLN
2	E	390	GLN
2	F	9	HIS
2	F	178	ASN
2	F	270	ASN
3	G	161	ASN
3	G	171	ASN
3	G	207	ASN
3	G	237	GLN
3	G	267	GLN
4	H	132	GLN
6	J	44	ASN
6	J	60	GLN
6	J	69	GLN
6	J	90	GLN
6	J	114	GLN
6	J	122	GLN
6	J	143	ASN
6	K	44	ASN
6	K	90	GLN
6	K	91	HIS
6	K	122	GLN
6	K	143	ASN
6	L	44	ASN
6	L	90	GLN
6	L	114	GLN
6	L	122	GLN

5.3.3 RNA ⓘ

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 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	$\# Z > 2$
7	ADP	F	600	8	28,29,29	1.55	5 (17%)	43,45,45	1.81	11 (25%)
7	ADP	B	600	8	28,29,29	1.50	5 (17%)	43,45,45	1.81	9 (20%)
7	ADP	E	600	-	28,29,29	1.50	5 (17%)	43,45,45	1.90	9 (20%)
7	ADP	D	600	8	28,29,29	1.56	5 (17%)	43,45,45	1.85	10 (23%)
7	ADP	A	600	8	28,29,29	1.50	5 (17%)	43,45,45	1.86	10 (23%)
7	ADP	C	600	8	28,29,29	1.48	5 (17%)	43,45,45	1.82	9 (20%)

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
7	ADP	F	600	8	-	4/16/32/32	0/3/3/3
7	ADP	B	600	8	-	0/16/32/32	0/3/3/3
7	ADP	E	600	-	-	0/16/32/32	0/3/3/3
7	ADP	D	600	8	-	3/16/32/32	0/3/3/3
7	ADP	A	600	8	-	0/16/32/32	0/3/3/3
7	ADP	C	600	8	-	0/16/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	600	ADP	C5-C4	5.04	1.48	1.39
7	D	600	ADP	C5-C4	4.95	1.47	1.39
7	F	600	ADP	C5-C4	4.93	1.47	1.39
7	A	600	ADP	C5-C4	4.87	1.47	1.39
7	B	600	ADP	C5-C4	4.86	1.47	1.39
7	C	600	ADP	C5-C4	4.80	1.47	1.39
7	E	600	ADP	C5-C6	2.98	1.49	1.41
7	D	600	ADP	C5-C6	2.91	1.49	1.41
7	B	600	ADP	C5-C6	2.83	1.48	1.41
7	F	600	ADP	C5-C6	2.80	1.48	1.41
7	F	600	ADP	PA-O3A	2.77	1.62	1.59
7	A	600	ADP	C5-C6	2.75	1.48	1.41
7	D	600	ADP	PA-O3A	2.75	1.62	1.59
7	C	600	ADP	C5-C6	2.69	1.48	1.41
7	C	600	ADP	C5-N7	-2.48	1.34	1.39
7	A	600	ADP	C5-N7	-2.45	1.34	1.39
7	E	600	ADP	C8-N7	2.45	1.36	1.31
7	F	600	ADP	C5-N7	-2.44	1.34	1.39
7	B	600	ADP	C5-N7	-2.42	1.34	1.39
7	D	600	ADP	C5-N7	-2.40	1.34	1.39
7	F	600	ADP	C8-N7	2.40	1.36	1.31
7	A	600	ADP	PA-O3A	2.39	1.62	1.59
7	A	600	ADP	C8-N7	2.39	1.36	1.31
7	C	600	ADP	PA-O3A	2.36	1.62	1.59
7	B	600	ADP	PA-O3A	2.32	1.62	1.59
7	C	600	ADP	C8-N7	2.30	1.36	1.31
7	D	600	ADP	C8-N7	2.27	1.36	1.31
7	E	600	ADP	C5-N7	-2.26	1.35	1.39
7	B	600	ADP	C8-N7	2.21	1.35	1.31
7	E	600	ADP	PA-O3A	2.05	1.61	1.59

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	600	ADP	C5-C4-N3	-6.00	118.46	126.72
7	D	600	ADP	C5-C4-N3	-5.88	118.62	126.72
7	C	600	ADP	C5-C4-N3	-5.73	118.82	126.72
7	F	600	ADP	C5-C4-N3	-5.69	118.89	126.72
7	A	600	ADP	C5-C4-N3	-5.67	118.92	126.72
7	B	600	ADP	C5-C4-N3	-5.66	118.92	126.72
7	A	600	ADP	N3-C4-N9	4.63	135.04	127.17
7	E	600	ADP	N3-C4-N9	4.59	134.97	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	ADP	N3-C4-N9	4.59	134.97	127.17
7	D	600	ADP	N3-C4-N9	4.57	134.93	127.17
7	C	600	ADP	N3-C4-N9	4.52	134.85	127.17
7	F	600	ADP	N3-C4-N9	4.43	134.70	127.17
7	E	600	ADP	C2-N3-C4	3.97	121.52	111.83
7	D	600	ADP	C2-N3-C4	3.88	121.31	111.83
7	C	600	ADP	C2-N3-C4	3.86	121.25	111.83
7	A	600	ADP	N3-C2-N1	-3.85	122.75	128.58
7	F	600	ADP	C2-N3-C4	3.83	121.18	111.83
7	A	600	ADP	C2-N3-C4	3.83	121.18	111.83
7	C	600	ADP	N3-C2-N1	-3.82	122.80	128.58
7	E	600	ADP	C4-C5-N7	-3.78	106.26	110.58
7	B	600	ADP	C2-N3-C4	3.76	121.02	111.83
7	F	600	ADP	N3-C2-N1	-3.73	122.94	128.58
7	B	600	ADP	N3-C2-N1	-3.71	122.97	128.58
7	D	600	ADP	N3-C2-N1	-3.70	122.98	128.58
7	E	600	ADP	N3-C2-N1	-3.67	123.02	128.58
7	D	600	ADP	C4-C5-N7	-3.55	106.53	110.58
7	B	600	ADP	C4-C5-N7	-3.45	106.64	110.58
7	F	600	ADP	C4-C5-N7	-3.38	106.71	110.58
7	A	600	ADP	C4-C5-N7	-3.36	106.74	110.58
7	C	600	ADP	C4-C5-N7	-3.30	106.81	110.58
7	A	600	ADP	C4-N9-C8	2.91	108.79	105.74
7	E	600	ADP	C5-N7-C8	2.76	107.78	103.45
7	B	600	ADP	C4-N9-C8	2.71	108.59	105.74
7	A	600	ADP	C5-N7-C8	2.63	107.59	103.45
7	D	600	ADP	C3'-C2'-C1'	2.60	106.38	101.46
7	B	600	ADP	C5-N7-C8	2.60	107.53	103.45
7	E	600	ADP	C3'-C2'-C1'	2.55	106.28	101.46
7	D	600	ADP	C5-N7-C8	2.44	107.28	103.45
7	C	600	ADP	C5-N7-C8	2.43	107.28	103.45
7	E	600	ADP	C4-N9-C8	2.39	108.25	105.74
7	F	600	ADP	C5-N7-C8	2.37	107.17	103.45
7	C	600	ADP	C4-N9-C8	2.36	108.21	105.74
7	E	600	ADP	C6-C5-N7	2.28	136.49	132.09
7	F	600	ADP	O4'-C1'-N9	2.25	112.42	108.09
7	F	600	ADP	C3'-C2'-C1'	2.19	105.61	101.46
7	A	600	ADP	N9-C8-N7	-2.18	110.85	113.94
7	F	600	ADP	C4-N9-C8	2.18	108.02	105.74
7	F	600	ADP	C6-C5-N7	2.17	136.27	132.09
7	A	600	ADP	C2-N1-C6	2.16	122.28	118.73
7	B	600	ADP	C2-N1-C6	2.16	122.28	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	600	ADP	C4-N9-C8	2.15	107.99	105.74
7	D	600	ADP	C6-C5-N7	2.10	136.14	132.09
7	C	600	ADP	C2-N1-C6	2.09	122.17	118.73
7	A	600	ADP	C6-C5-N7	2.09	136.12	132.09
7	D	600	ADP	C2-N1-C6	2.05	122.10	118.73
7	B	600	ADP	C6-C5-N7	2.05	136.04	132.09
7	F	600	ADP	C2-N1-C6	2.02	122.05	118.73
7	C	600	ADP	C6-C5-N7	2.02	135.99	132.09

There are no chirality outliers.

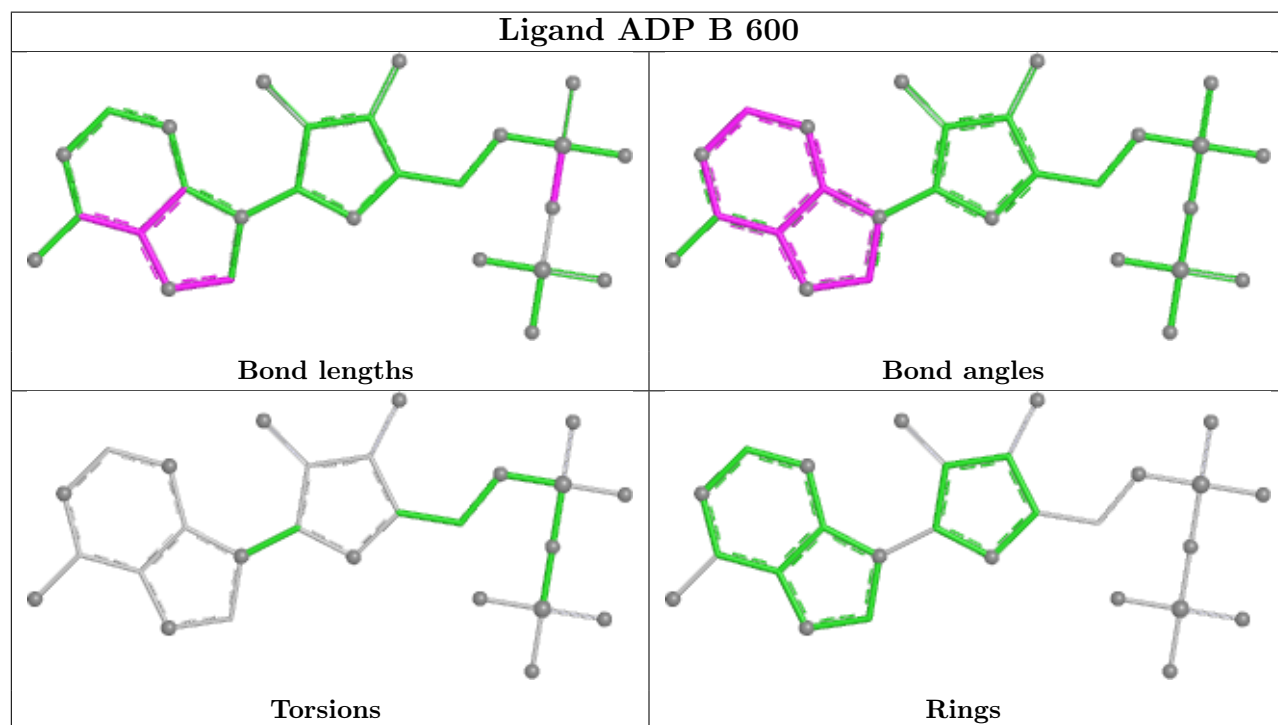
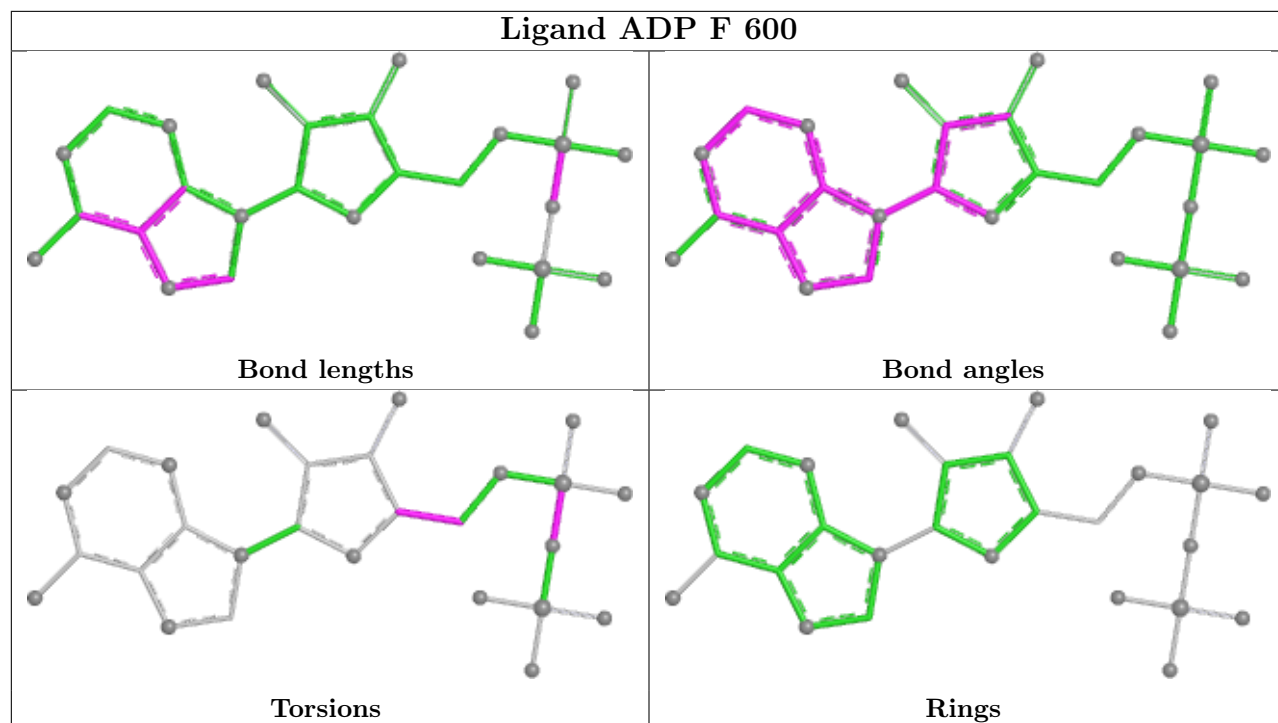
All (7) torsion outliers are listed below:

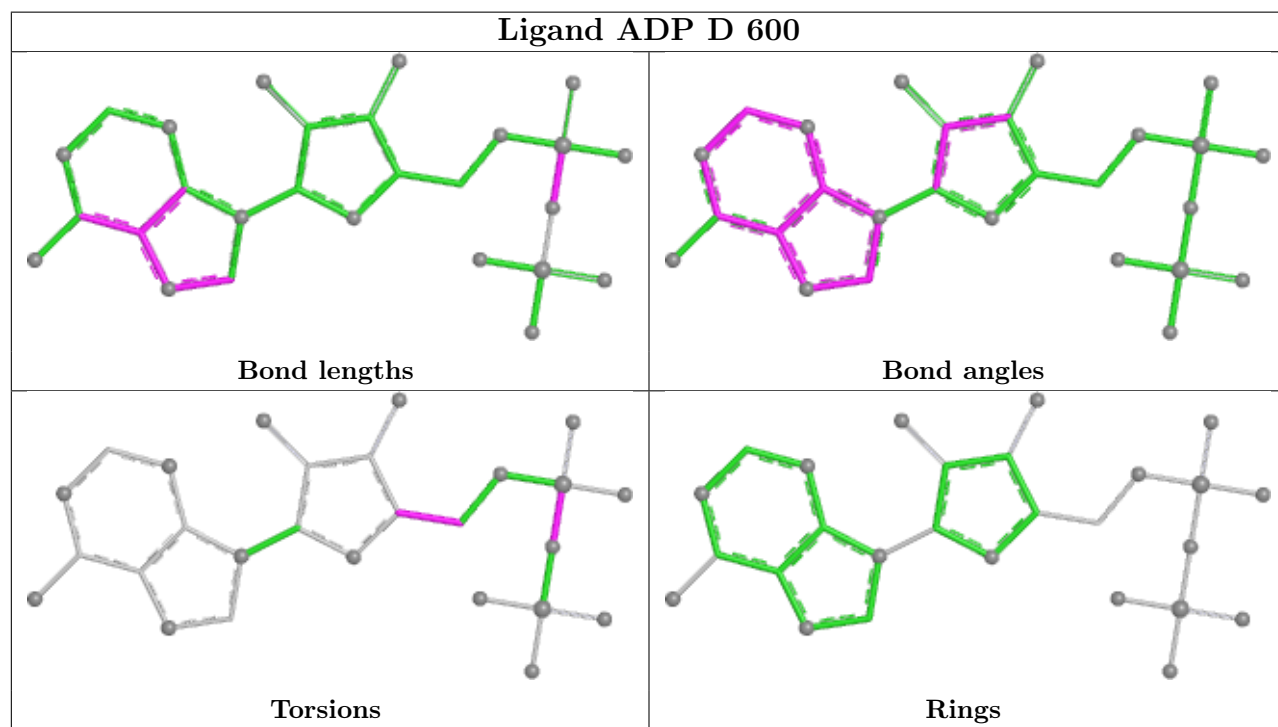
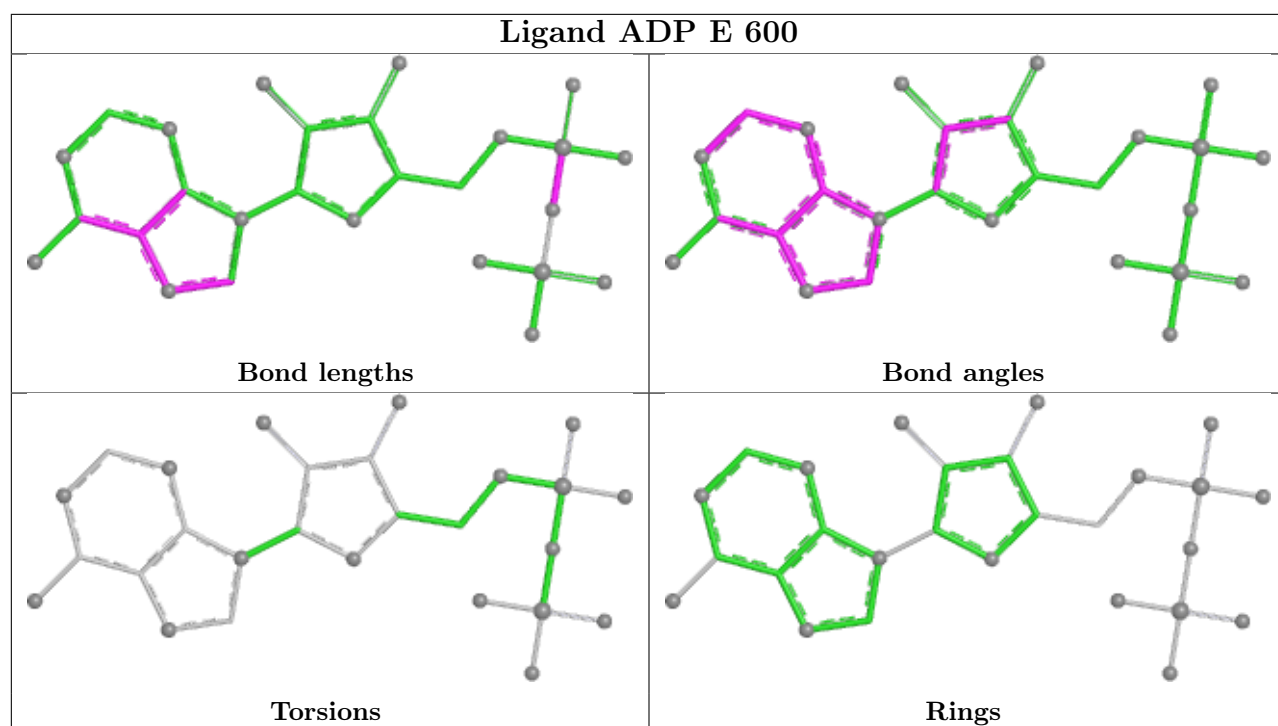
Mol	Chain	Res	Type	Atoms
7	D	600	ADP	O4'-C4'-C5'-O5'
7	D	600	ADP	C3'-C4'-C5'-O5'
7	F	600	ADP	O4'-C4'-C5'-O5'
7	F	600	ADP	C3'-C4'-C5'-O5'
7	F	600	ADP	PB-O3A-PA-O1A
7	D	600	ADP	PB-O3A-PA-O2A
7	F	600	ADP	PB-O3A-PA-O2A

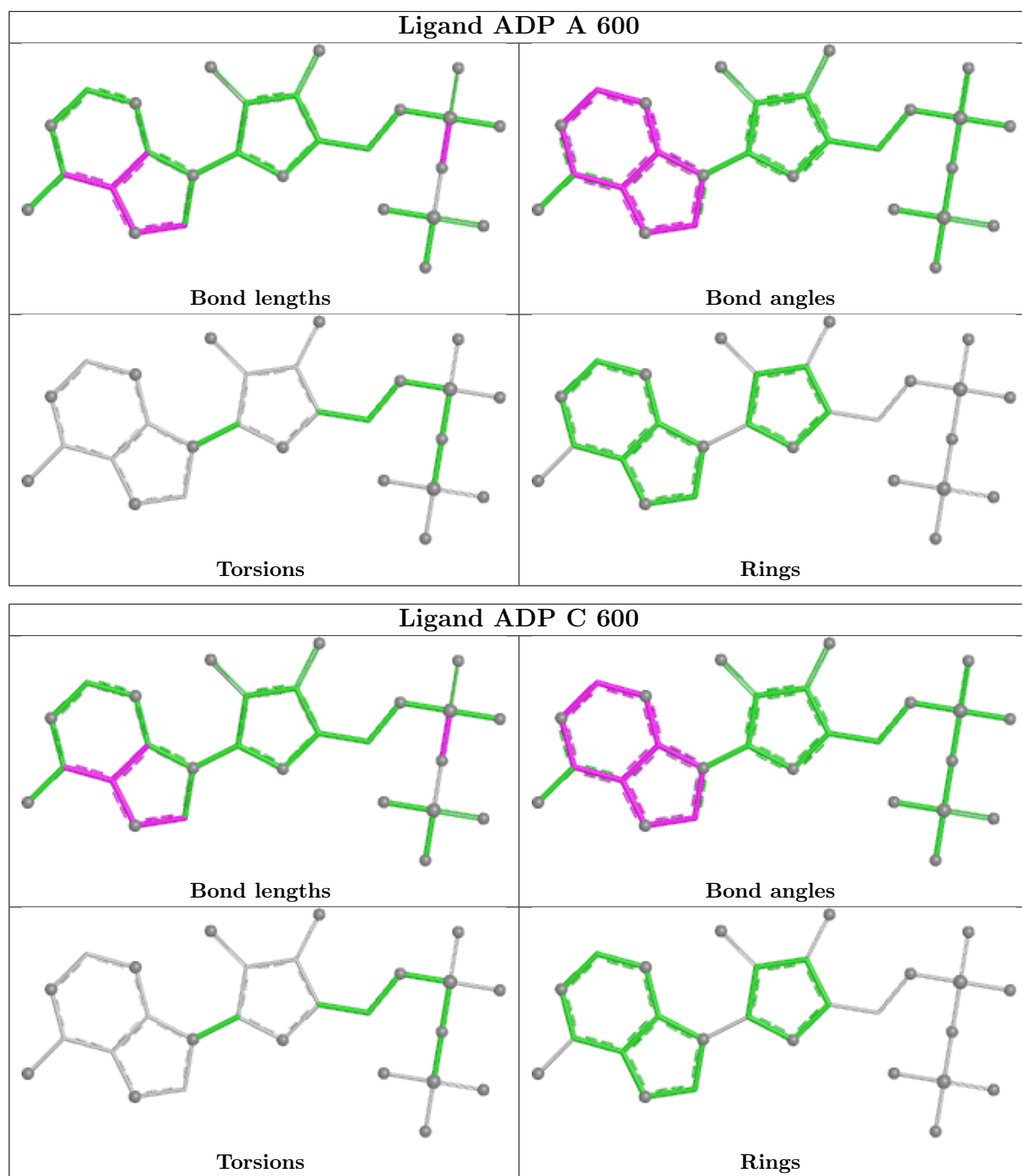
There are no ring outliers.

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	524/560 (93%)	0.66	15 (2%)	53	35	62, 94, 124, 162	0
1	B	524/560 (93%)	0.59	12 (2%)	61	41	47, 79, 119, 153	0
1	C	521/560 (93%)	0.69	22 (4%)	40	25	56, 86, 120, 154	0
2	D	481/498 (96%)	0.58	12 (2%)	58	39	60, 85, 113, 156	0
2	E	487/498 (97%)	0.76	34 (6%)	22	14	53, 86, 120, 148	0
2	F	488/498 (97%)	0.67	24 (4%)	35	22	50, 77, 114, 165	0
3	G	277/304 (91%)	0.32	7 (2%)	58	39	56, 88, 115, 133	0
4	H	146/165 (88%)	0.29	1 (0%)	84	69	70, 95, 119, 123	0
5	I	66/66 (100%)	0.44	0	100	100	69, 89, 114, 116	0
6	J	164/170 (96%)	0.55	5 (3%)	52	33	75, 96, 130, 138	0
6	K	162/170 (95%)	0.79	11 (6%)	23	15	95, 123, 140, 163	0
6	L	165/170 (97%)	0.84	15 (9%)	15	9	105, 126, 145, 150	0
All	All	4005/4219 (94%)	0.63	158 (3%)	43	27	47, 88, 128, 165	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	395	VAL	5.0
1	B	387	VAL	4.5
6	K	167	VAL	4.5
3	G	149	VAL	4.3
6	K	164	LEU	4.3
2	F	156	GLY	4.1
2	E	430	THR	3.8
1	B	560	VAL	3.6
2	D	276	LEU	3.6
1	C	387	VAL	3.5
2	E	219	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	194	GLU	3.4
2	F	407	LEU	3.4
2	E	220	CYS	3.3
2	D	234	ARG	3.3
1	B	71	PHE	3.2
1	C	560	VAL	3.2
2	F	404	GLU	3.1
3	G	2	GLY	3.1
2	F	396	LEU	3.1
2	F	135	GLU	3.1
2	E	395	VAL	3.0
1	C	424	GLN	3.0
2	F	397	GLY	3.0
2	D	398	ILE	3.0
2	E	316	TYR	3.0
2	F	305	THR	3.0
1	A	399	VAL	2.9
2	D	403	GLU	2.9
1	A	311	VAL	2.9
2	D	220	CYS	2.9
2	D	241	ALA	2.9
1	A	416	ASP	2.9
1	C	283	ASP	2.8
2	F	297	LEU	2.8
2	F	220	CYS	2.8
2	E	394	ALA	2.8
6	L	21	ALA	2.8
3	G	3	LYS	2.8
1	A	456	CYS	2.7
2	F	322	ILE	2.7
1	C	555	SER	2.7
6	L	14	TYR	2.7
1	C	536	LYS	2.7
2	E	396	LEU	2.7
2	F	303	SER	2.7
1	C	380	ILE	2.6
2	E	398	ILE	2.6
1	C	108	GLY	2.6
2	F	7	ALA	2.6
6	L	45	VAL	2.6
2	E	320	ASP	2.6
6	L	95	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	195	ARG	2.6
3	G	150	SER	2.6
2	E	259	PHE	2.6
2	E	315	VAL	2.6
2	E	432	MET	2.6
6	L	70	SER	2.6
2	E	159	GLY	2.6
2	F	405	ASP	2.6
1	A	374	GLN	2.5
1	B	22	PHE	2.5
1	C	396	MET	2.5
1	B	557	LYS	2.5
1	C	441	LYS	2.5
1	A	415	ALA	2.5
2	E	133	ALA	2.5
1	C	429	ILE	2.5
6	K	158	LEU	2.5
2	D	404	GLU	2.5
6	L	164	LEU	2.5
2	E	429	PHE	2.4
2	D	444	ASP	2.4
2	E	255	ASP	2.4
4	H	32	THR	2.4
6	L	102	TRP	2.4
2	E	336	ALA	2.4
1	C	540	ILE	2.4
2	E	392	ILE	2.4
6	K	150	GLU	2.4
2	E	228	ASN	2.4
1	B	554	TYR	2.4
1	C	309	GLY	2.4
2	D	275	ALA	2.4
1	A	315	HIS	2.4
6	L	79	PHE	2.4
2	E	160	LEU	2.4
6	K	110	VAL	2.4
2	F	260	ILE	2.3
6	K	133	PRO	2.3
1	B	127	LEU	2.3
1	C	557	LYS	2.3
1	C	87	ILE	2.3
2	F	23	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
6	J	133	PRO	2.3
2	E	278	GLY	2.3
2	D	271	SER	2.3
1	B	481	LEU	2.3
2	E	214	LEU	2.3
1	B	298	LEU	2.3
3	G	268	PHE	2.3
6	J	120	CYS	2.3
2	F	255	ASP	2.3
1	B	414	ALA	2.2
2	F	182	GLY	2.2
6	L	6	ALA	2.2
2	E	208	GLN	2.2
6	L	169	VAL	2.2
2	E	266	PHE	2.2
2	E	433	THR	2.2
6	K	58	THR	2.2
6	K	67	SER	2.2
1	B	328	GLY	2.2
2	F	238	ALA	2.2
6	L	120	CYS	2.2
1	C	310	ASP	2.2
6	K	68	LYS	2.2
1	B	442	GLN	2.2
1	A	345	ASN	2.2
2	F	311	SER	2.1
6	L	76	GLU	2.1
6	K	66	PRO	2.1
6	J	30	CYS	2.1
2	E	273	VAL	2.1
6	L	16	VAL	2.1
1	A	108	GLY	2.1
1	A	308	PRO	2.1
6	K	47	ASN	2.1
1	A	387	VAL	2.1
1	C	466	VAL	2.1
1	C	537	MET	2.1
2	D	466	GLY	2.1
6	J	31	LYS	2.1
6	L	158	LEU	2.1
1	C	245	MET	2.1
2	D	274	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	428	VAL	2.1
2	E	478	MET	2.1
2	F	366	ASP	2.1
6	J	132	CYS	2.1
2	E	343	ALA	2.1
1	C	303	GLY	2.1
2	E	167	GLY	2.1
1	A	148	ASN	2.0
2	F	494	ALA	2.0
3	G	272	ALA	2.0
2	E	431	GLY	2.0
1	A	423	VAL	2.0
2	F	242	LEU	2.0
1	C	351	ILE	2.0
2	E	393	ILE	2.0
1	C	243	THR	2.0
3	G	58	ALA	2.0
1	A	310	ASP	2.0
1	A	140	GLY	2.0
2	F	166	VAL	2.0
6	L	52	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

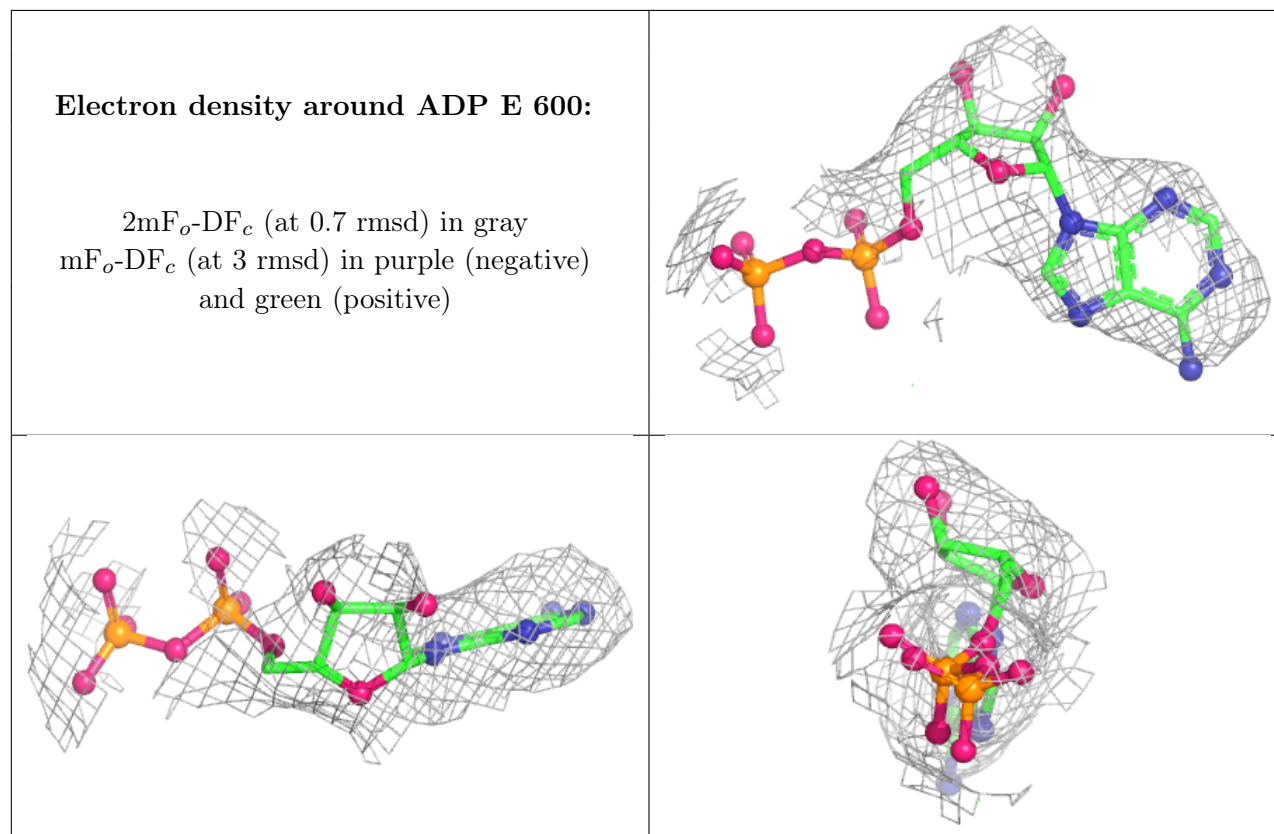
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ADP	E	600	27/27	0.87	0.11	116,122,125,126	0
7	ADP	F	600	27/27	0.93	0.09	62,63,66,68	0

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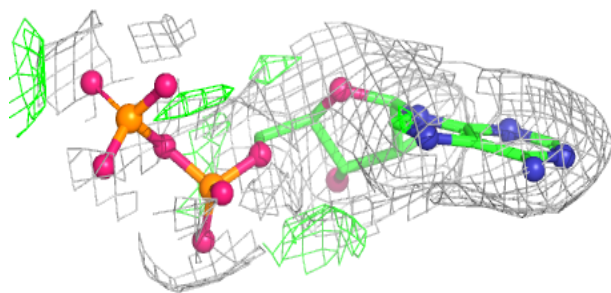
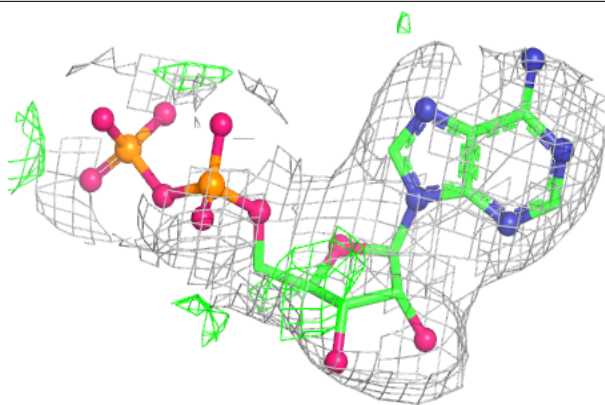
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ADP	A	600	27/27	0.94	0.08	65,66,66,67	0
7	ADP	D	600	27/27	0.95	0.08	62,64,66,67	0
7	ADP	C	600	27/27	0.96	0.08	54,59,63,64	0
7	ADP	B	600	27/27	0.96	0.07	52,56,59,59	0
8	MG	D	601	1/1	0.96	0.07	65,65,65,65	0
8	MG	F	601	1/1	0.98	0.06	73,73,73,73	0
8	MG	C	601	1/1	0.99	0.03	54,54,54,54	0
8	MG	A	601	1/1	0.99	0.03	64,64,64,64	0
8	MG	B	601	1/1	0.99	0.05	52,52,52,52	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.

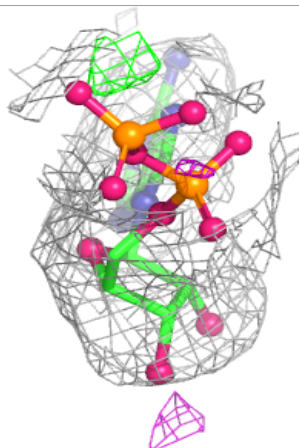
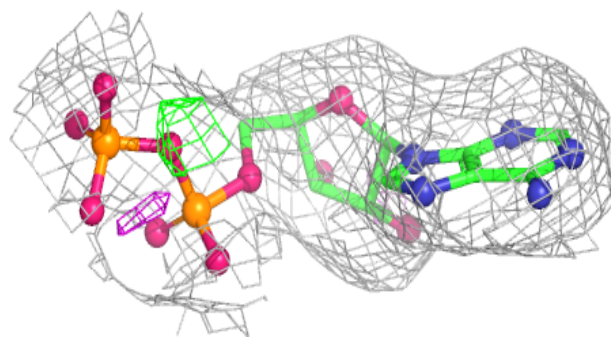
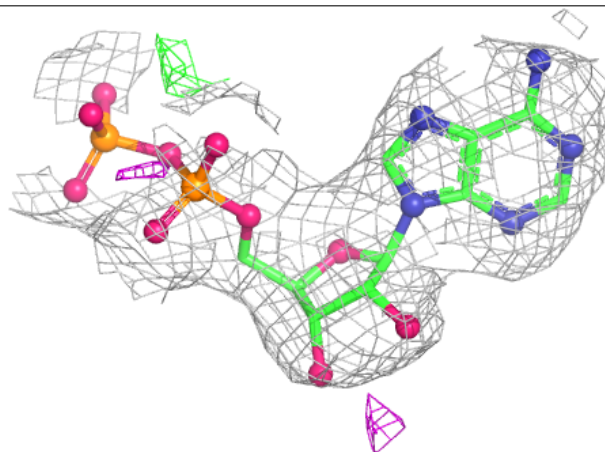


Electron density around ADP F 600:

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

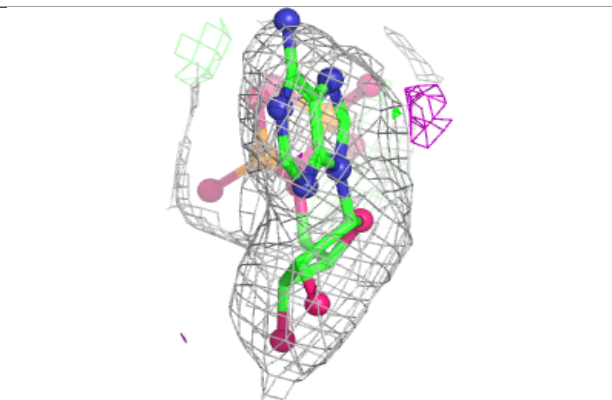
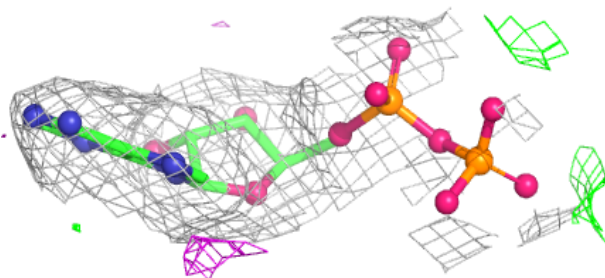
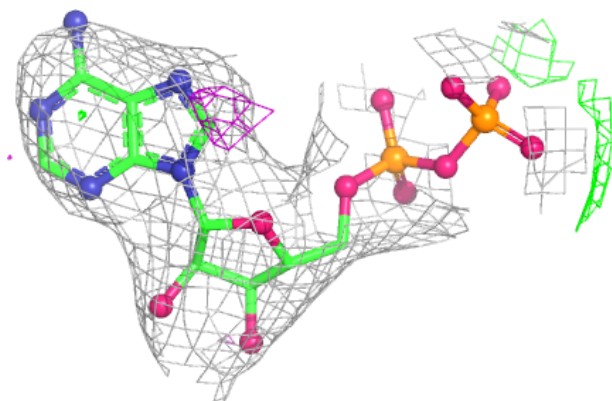
**Electron density around ADP A 600:**

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

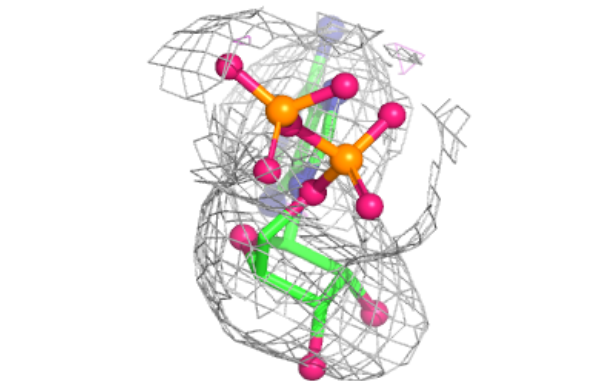
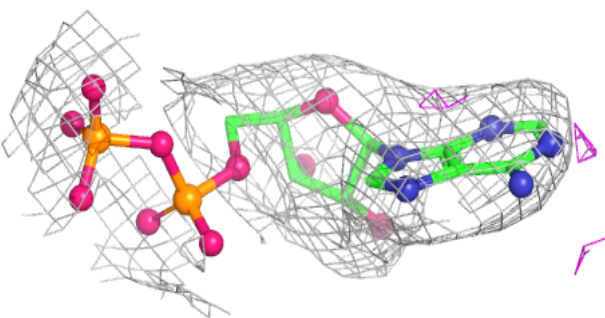
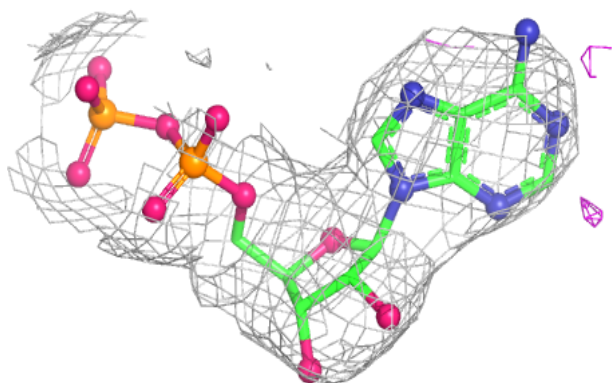


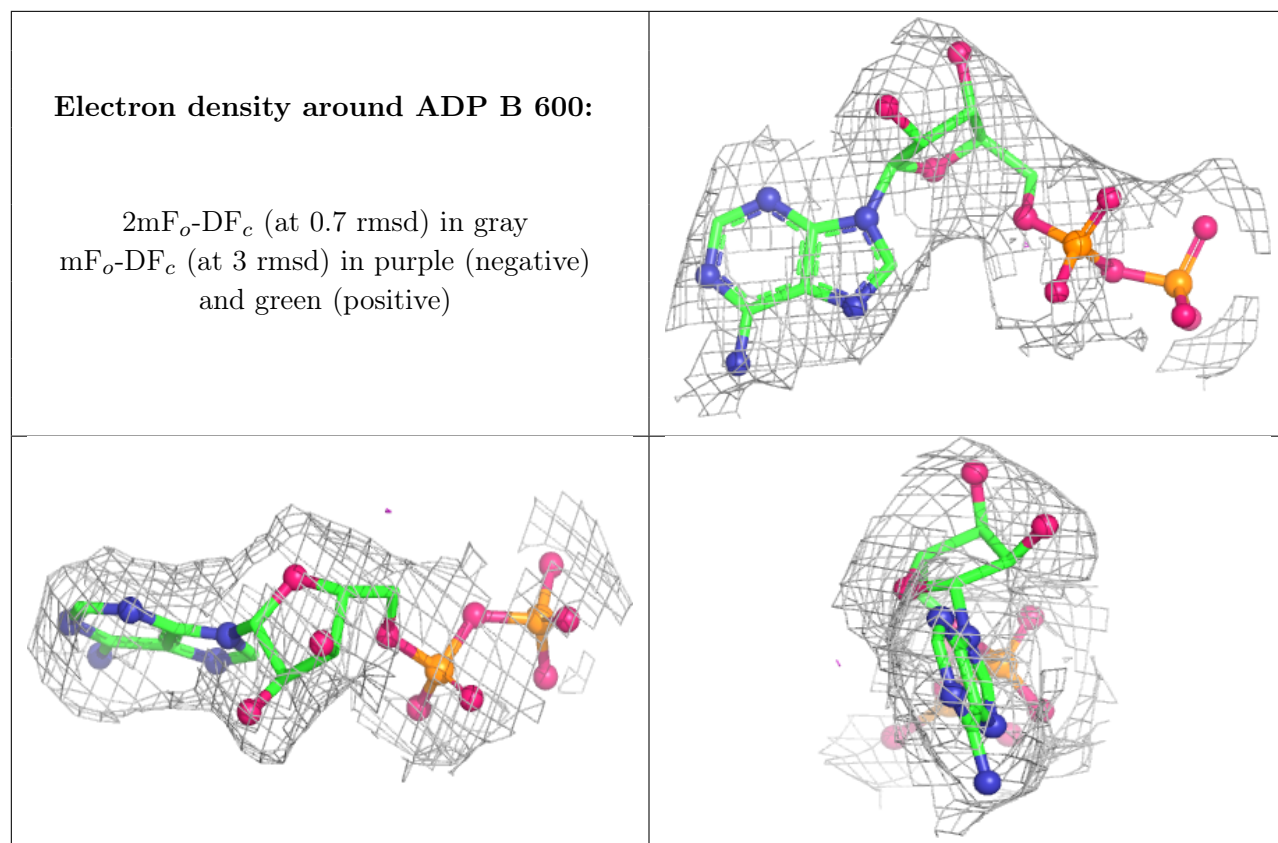
Electron density around ADP D 600:

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

**Electron density around ADP C 600:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.