Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 02:53 am GMT

PDB ID	:	6F5D
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 (i) 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 (i)) were used in the production of this report:

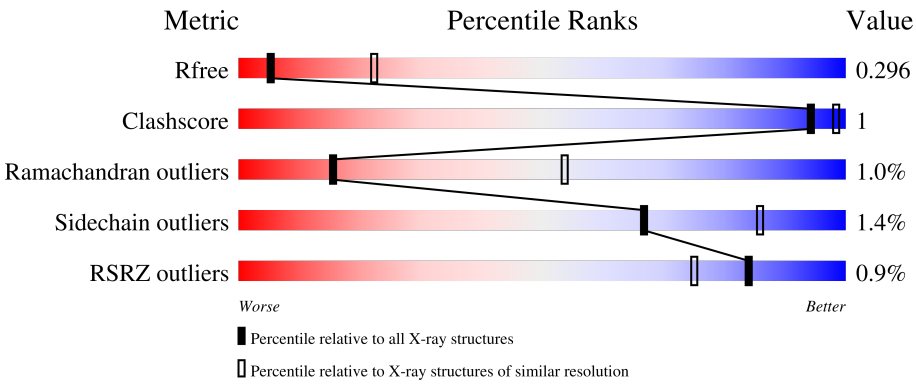
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 <=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	.% 88% 5% • 6%
1	B	560	2% 89% 5% 6%
1	C	560	89% • 7%
2	D	498	93% • •
2	E	498	.% 94% • •

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Mol	Chain	Length	Quality of chain
2	F	498	% 95%
3	G	304	% 87% 9%
4	H	165	83% 5% 12%
5	I	66	95% 5%
6	J	170	2% 85% 11%
6	K	170	3% 86% 8% 5%
6	L	170	% 86% 8%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	524	4046	2591	702	733	20	0	0	0
1	B	524	4046	2590	704	732	20	0	0	0
1	C	521	4022	2574	699	729	20	0	0	0

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

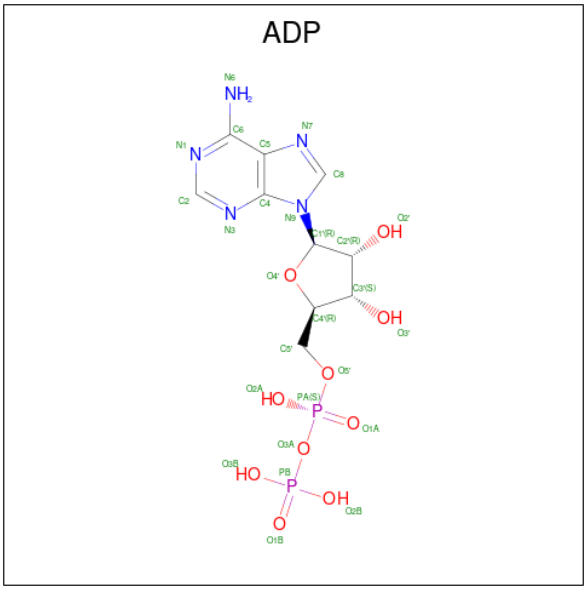
- Molecule 5 is a protein called ATP synthase subunit epsilon, mitochondrial.

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

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

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

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



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

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

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

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

- Molecule 9 is water.

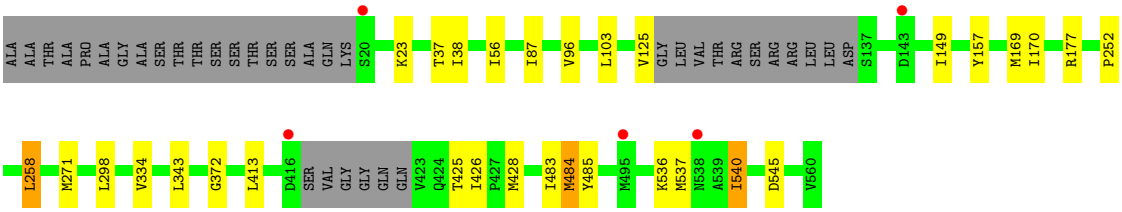
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	4	4	4	0	0
9	B	4	4	4	0	0
9	C	4	4	4	0	0
9	D	4	4	4	0	0
9	F	4	4	4	0	0

3 Residue-property plots (i)

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.

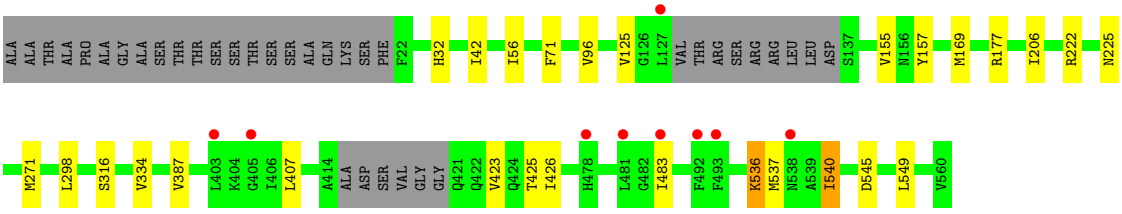
• Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain A:



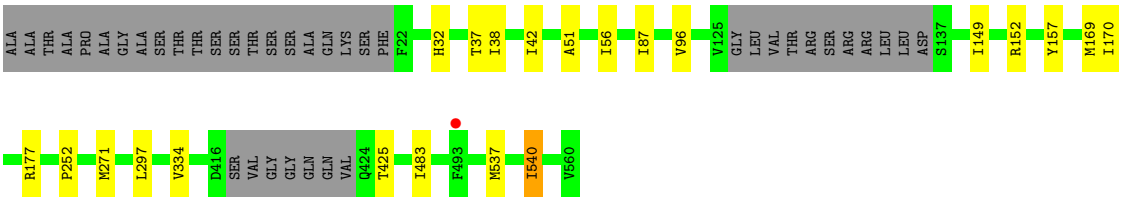
• Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain B:



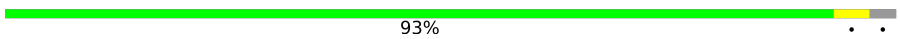
• Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C:



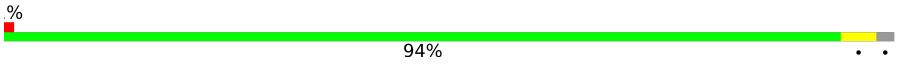
• Molecule 2: ATP synthase subunit beta, mitochondrial

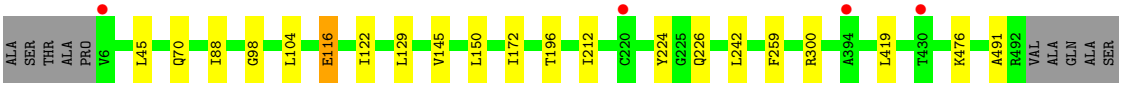
Chain D:



• Molecule 2: ATP synthase subunit beta, mitochondrial

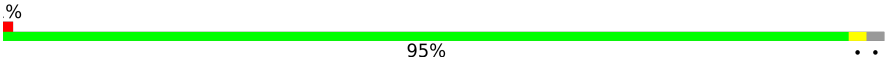
Chain E:

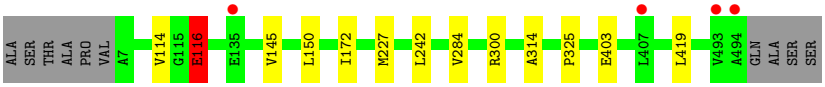




• Molecule 2: ATP synthase subunit beta, mitochondrial

Chain F:



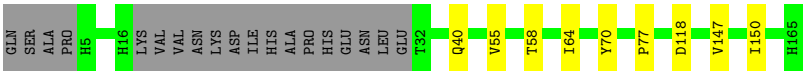


• Molecule 3: ATP synthase gamma subunit

Chain G:

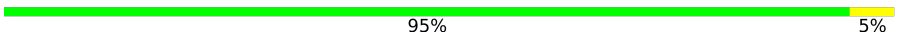
• Molecule 4: ATP synthase subunit delta, mitochondrial

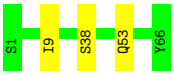
Chain H:



• Molecule 5: ATP synthase subunit epsilon, mitochondrial

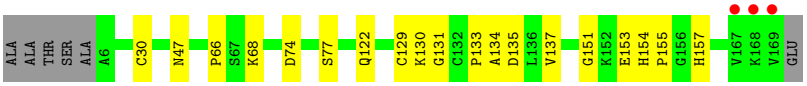
Chain I:





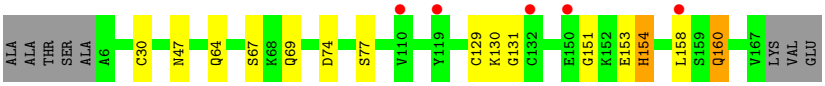
• Molecule 6: ATP synthase subunit p18, mitochondrial

Chain J:



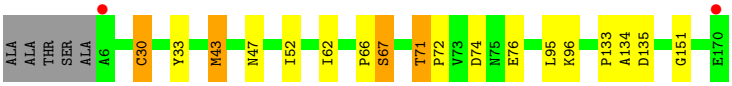
• Molecule 6: ATP synthase subunit p18, mitochondrial

Chain K:



• Molecule 6: ATP synthase subunit p18, mitochondrial

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 19.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	0/4120	0.53	0/5580
1	B	0.38	0/4119	0.54	0/5578
1	C	0.37	0/4095	0.53	0/5546
2	D	0.37	0/3695	0.54	0/5011
2	E	0.41	0/3745	0.58	2/5077 (0.0%)
2	F	0.38	0/3750	0.55	0/5084
3	G	0.37	0/2246	0.52	0/3025
4	H	0.36	0/1147	0.52	0/1555
5	I	0.39	0/552	0.56	0/746
6	J	0.41	0/1327	0.56	0/1791
6	K	0.43	0/1311	0.59	1/1770 (0.1%)
6	L	0.40	0/1336	0.59	2/1803 (0.1%)
All	All	0.38	0/31443	0.55	5/42566 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	30	CYS	CA-CB-SG	6.49	125.69	114.00
6	K	160	GLN	N-CA-C	5.67	126.30	111.00
6	L	43	MET	CA-CB-CG	5.65	122.90	113.30
2	E	224	TYR	CB-CG-CD1	5.61	124.37	121.00
2	E	224	TYR	CB-CG-CD2	-5.07	117.96	121.00

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	17	0
1	B	4046	0	4168	16	0
1	C	4022	0	4138	12	0
2	D	3639	0	3683	13	0
2	E	3689	0	3742	11	0
2	F	3694	0	3746	8	0
3	G	2210	0	2210	4	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	2	0
6	L	1309	0	1269	5	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	82	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 1.

All (82) 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
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
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
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:B:169:MET:CE	1:B:407:LEU:HD22	2.39	0.52
1:B:169:MET:HE3	1:B:407:LEU:HD22	1.92	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:206:ILE:O	6:J:68:LYS:NZ	2.41	0.49
6:J:133:PRO:O	6:J:135:ASP:N	2.47	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
2:E:88:ILE:O	2:E:122:ILE:HG12	2.20	0.41
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
1:B:536:LYS:HE3	1:B:549:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/560 (92%)	488 (94%)	27 (5%)	3 (1%)	25	64
1	B	518/560 (92%)	488 (94%)	28 (5%)	2 (0%)	34	69
1	C	515/560 (92%)	486 (94%)	28 (5%)	1 (0%)	47	79
2	D	479/498 (96%)	452 (94%)	26 (5%)	1 (0%)	47	79
2	E	485/498 (97%)	454 (94%)	29 (6%)	2 (0%)	34	69
2	F	486/498 (98%)	459 (94%)	26 (5%)	1 (0%)	47	79
3	G	273/304 (90%)	252 (92%)	16 (6%)	5 (2%)	8	41
4	H	142/165 (86%)	126 (89%)	12 (8%)	4 (3%)	5	29
5	I	64/66 (97%)	49 (77%)	13 (20%)	2 (3%)	4	26
6	J	162/170 (95%)	144 (89%)	12 (7%)	6 (4%)	3	22
6	K	160/170 (94%)	140 (88%)	12 (8%)	8 (5%)	2	16
6	L	163/170 (96%)	141 (86%)	17 (10%)	5 (3%)	4	26
All	All	3965/4219 (94%)	3679 (93%)	246 (6%)	40 (1%)	15	54

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

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Mol	Chain	Res	Type
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
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%)	428 (98%)	8 (2%)	59 82
1	B	436/462 (94%)	430 (99%)	6 (1%)	67 86
1	C	433/462 (94%)	428 (99%)	5 (1%)	71 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	394/405 (97%)	393 (100%)	1 (0%)	92	96
2	E	398/405 (98%)	394 (99%)	4 (1%)	76	90
2	F	398/405 (98%)	396 (100%)	2 (0%)	88	95
3	G	236/255 (92%)	234 (99%)	2 (1%)	81	93
4	H	123/140 (88%)	122 (99%)	1 (1%)	81	93
5	I	59/59 (100%)	58 (98%)	1 (2%)	60	83
6	J	144/147 (98%)	139 (96%)	5 (4%)	36	69
6	K	142/147 (97%)	137 (96%)	5 (4%)	36	69
6	L	145/147 (99%)	139 (96%)	6 (4%)	30	66
All	All	3344/3496 (96%)	3298 (99%)	46 (1%)	67	86

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	157	TYR
1	A	177	ARG
1	A	258	LEU
1	A	425	THR
1	A	426	ILE
1	A	536	LYS
1	A	537	MET
1	B	157	TYR
1	B	177	ARG
1	B	425	THR
1	B	426	ILE
1	B	536	LYS
1	B	537	MET
1	C	157	TYR
1	C	177	ARG
1	C	425	THR
1	C	537	MET
1	C	540	ILE
2	D	150	LEU
2	E	45	LEU
2	E	116	GLU
2	E	150	LEU
2	E	476	LYS
2	F	116	GLU

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Mol	Chain	Res	Type
2	F	150	LEU
3	G	17	PHE
3	G	131	LYS
4	H	70	TYR
5	I	53	GLN
6	J	30	CYS
6	J	74	ASP
6	J	153	GLU
6	J	155	PRO
6	J	157	HIS
6	K	30	CYS
6	K	64	GLN
6	K	74	ASP
6	K	153	GLU
6	K	154	HIS
6	L	30	CYS
6	L	43	MET
6	L	71	THR
6	L	74	ASP
6	L	76	GLU
6	L	96	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	268	GLN
3	G	171	ASN
3	G	267	GLN
6	J	60	GLN
6	J	90	GLN
6	J	122	GLN
6	J	145	GLN
6	K	145	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 monosaccharides 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	E	600	-	24,29,29	1.05	3 (12%)	29,45,45	1.46	4 (13%)
7	ADP	C	600	8	24,29,29	1.00	2 (8%)	29,45,45	1.38	4 (13%)
7	ADP	A	600	8	24,29,29	1.01	2 (8%)	29,45,45	1.42	5 (17%)
7	ADP	B	600	8	24,29,29	1.03	2 (8%)	29,45,45	1.34	4 (13%)
7	ADP	D	600	8	24,29,29	1.09	3 (12%)	29,45,45	1.44	4 (13%)
7	ADP	F	600	8	24,29,29	1.08	3 (12%)	29,45,45	1.35	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
7	ADP	E	600	-	-	0/12/32/32	0/3/3/3
7	ADP	C	600	8	-	0/12/32/32	0/3/3/3
7	ADP	A	600	8	-	0/12/32/32	0/3/3/3
7	ADP	B	600	8	-	0/12/32/32	0/3/3/3
7	ADP	D	600	8	-	3/12/32/32	0/3/3/3
7	ADP	F	600	8	-	3/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	600	ADP	C5-C4	2.70	1.48	1.40
7	D	600	ADP	C5-C4	2.64	1.47	1.40
7	F	600	ADP	C5-C4	2.63	1.47	1.40
7	A	600	ADP	C5-C4	2.59	1.47	1.40
7	B	600	ADP	C5-C4	2.58	1.47	1.40
7	C	600	ADP	C5-C4	2.54	1.47	1.40
7	F	600	ADP	O4'-C1'	2.37	1.44	1.41
7	D	600	ADP	C2-N3	2.26	1.35	1.32
7	D	600	ADP	O4'-C1'	2.21	1.44	1.41
7	A	600	ADP	C2-N3	2.20	1.35	1.32
7	F	600	ADP	C2-N3	2.17	1.35	1.32
7	B	600	ADP	C2-N3	2.14	1.35	1.32
7	E	600	ADP	C2-N3	2.10	1.35	1.32
7	C	600	ADP	C2-N3	2.10	1.35	1.32
7	E	600	ADP	O4'-C1'	2.02	1.43	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	600	ADP	N3-C2-N1	-3.79	122.75	128.68
7	C	600	ADP	N3-C2-N1	-3.76	122.80	128.68
7	F	600	ADP	N3-C2-N1	-3.67	122.94	128.68
7	B	600	ADP	N3-C2-N1	-3.65	122.97	128.68
7	D	600	ADP	N3-C2-N1	-3.64	122.98	128.68
7	E	600	ADP	N3-C2-N1	-3.62	123.02	128.68
7	D	600	ADP	C3'-C2'-C1'	3.59	106.38	100.98
7	E	600	ADP	C3'-C2'-C1'	3.52	106.28	100.98
7	F	600	ADP	C3'-C2'-C1'	3.08	105.61	100.98
7	E	600	ADP	C4-C5-N7	-3.01	106.26	109.40
7	C	600	ADP	PA-O3A-PB	-2.84	123.07	132.83
7	E	600	ADP	PA-O3A-PB	-2.78	123.28	132.83
7	D	600	ADP	C4-C5-N7	-2.76	106.53	109.40
7	B	600	ADP	PA-O3A-PB	-2.74	123.41	132.83
7	A	600	ADP	PA-O3A-PB	-2.72	123.49	132.83
7	A	600	ADP	C3'-C2'-C1'	2.65	104.97	100.98
7	B	600	ADP	C4-C5-N7	-2.65	106.64	109.40
7	F	600	ADP	C4-C5-N7	-2.58	106.71	109.40
7	A	600	ADP	C4-C5-N7	-2.55	106.74	109.40
7	C	600	ADP	C4-C5-N7	-2.48	106.81	109.40
7	C	600	ADP	C3'-C2'-C1'	2.44	104.65	100.98
7	D	600	ADP	PA-O3A-PB	-2.23	125.16	132.83
7	F	600	ADP	PA-O3A-PB	-2.19	125.30	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	600	ADP	C2-N1-C6	2.06	122.28	118.75
7	B	600	ADP	C2-N1-C6	2.06	122.28	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

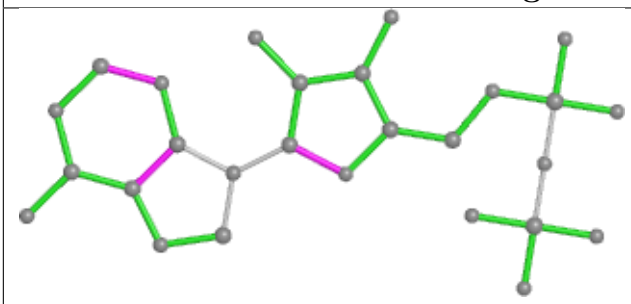
Mol	Chain	Res	Type	Atoms
7	D	600	ADP	O4'-C4'-C5'-O5'
7	D	600	ADP	C3'-C4'-C5'-O5'
7	F	600	ADP	O4'-C4'-C5'-O5'
7	F	600	ADP	C3'-C4'-C5'-O5'
7	F	600	ADP	PB-O3A-PA-O1A
7	D	600	ADP	PB-O3A-PA-O2A

There are no ring outliers.

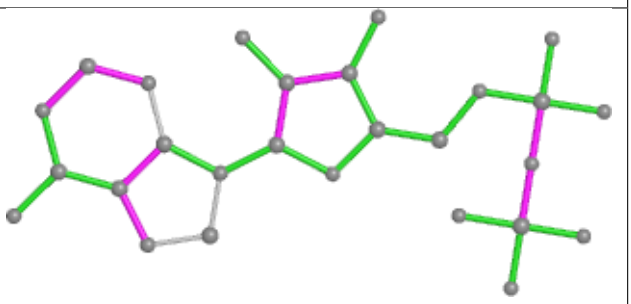
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

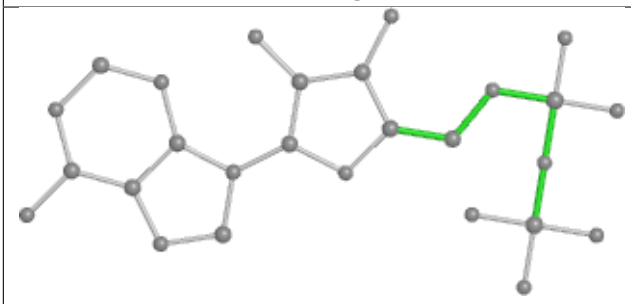
Ligand ADP E 600



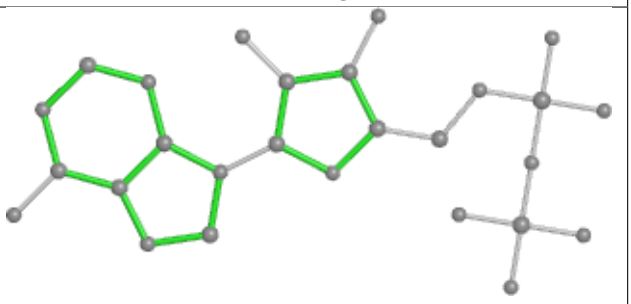
Bond lengths



Bond angles

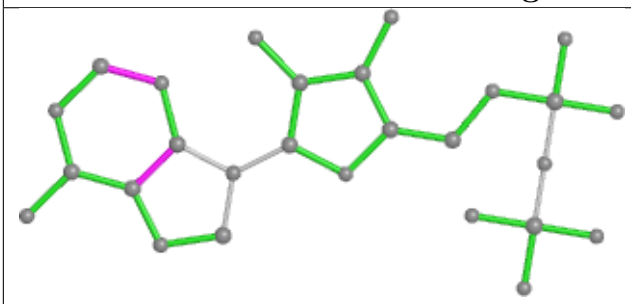


Torsions

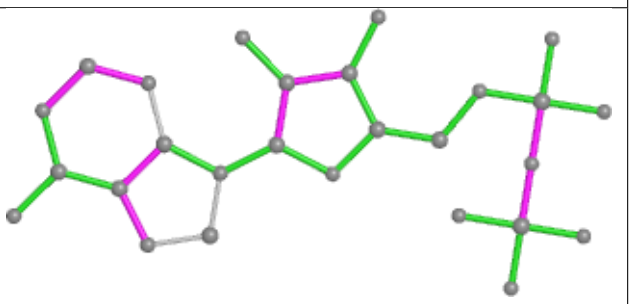


Rings

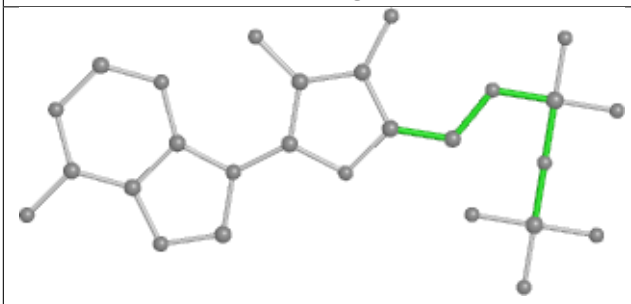
Ligand ADP C 600



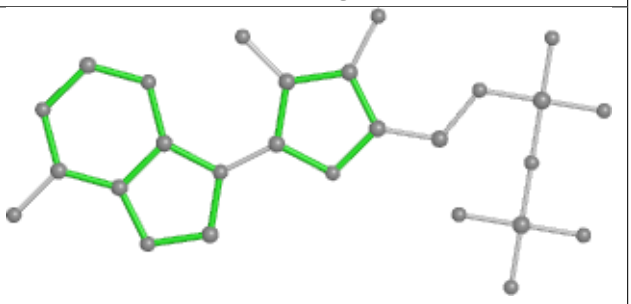
Bond lengths



Bond angles

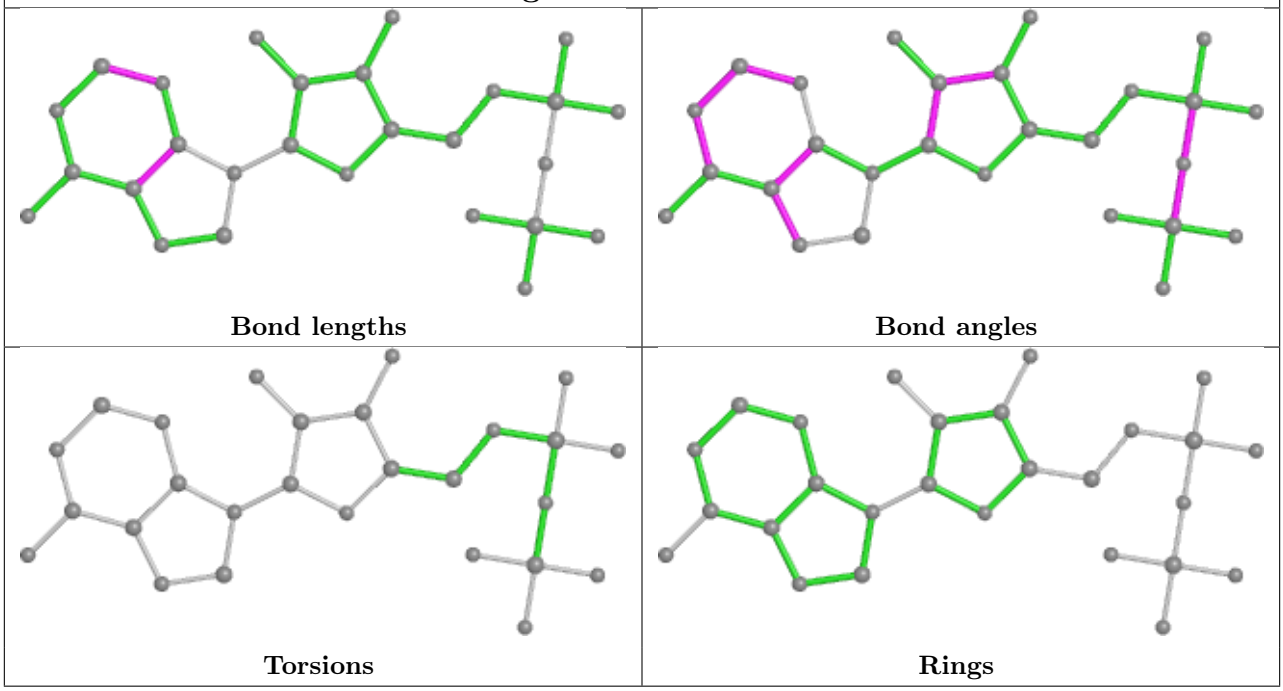


Torsions

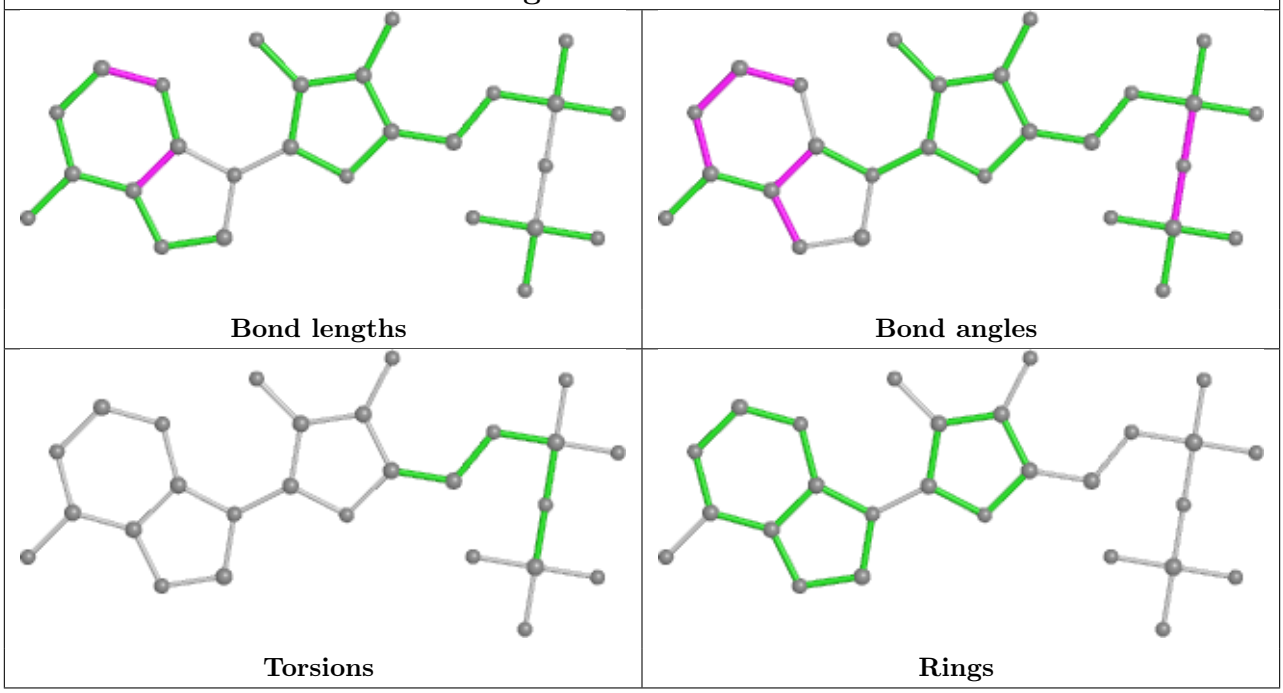


Rings

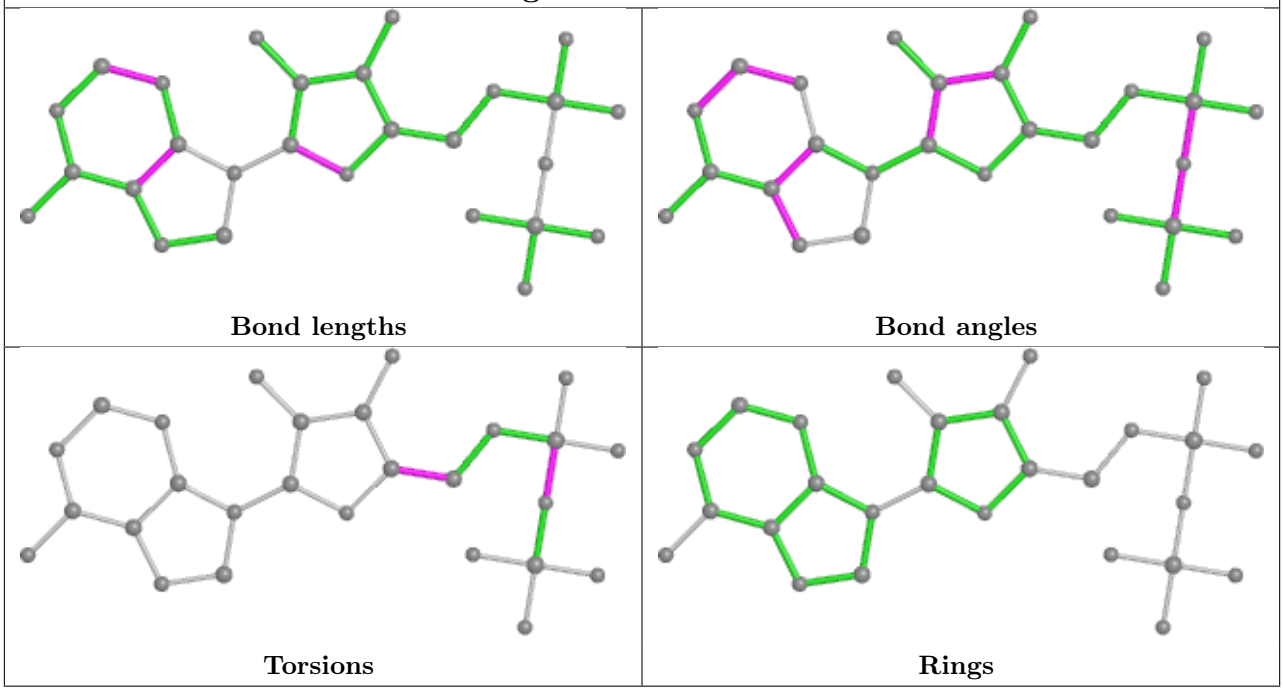
Ligand ADP A 600



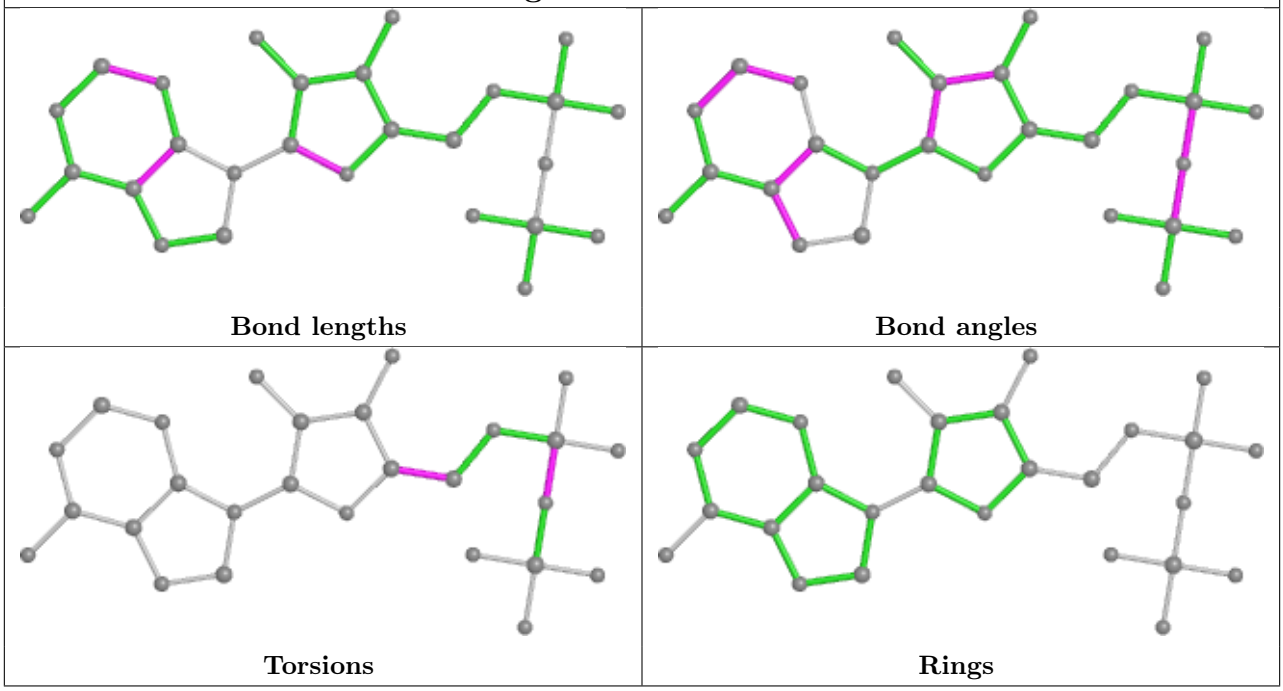
Ligand ADP B 600



Ligand ADP D 600



Ligand ADP F 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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, 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%)	0.06	5 (0%)	82	72	62, 94, 124, 163	0
1	B	524/560 (93%)	0.15	9 (1%)	70	57	47, 79, 119, 153	0
1	C	521/560 (93%)	0.04	1 (0%)	95	94	56, 86, 120, 154	0
2	D	481/498 (96%)	0.04	1 (0%)	95	94	60, 85, 113, 156	0
2	E	487/498 (97%)	0.09	4 (0%)	86	78	53, 86, 120, 148	0
2	F	488/498 (97%)	-0.02	4 (0%)	86	78	50, 77, 114, 165	0
3	G	277/304 (91%)	-0.07	2 (0%)	87	81	56, 88, 115, 133	0
4	H	146/165 (88%)	-0.09	0	100	100	70, 95, 119, 123	0
5	I	66/66 (100%)	-0.20	0	100	100	69, 89, 114, 116	0
6	J	164/170 (96%)	-0.00	3 (1%)	68	55	75, 96, 130, 138	0
6	K	162/170 (95%)	0.11	5 (3%)	49	32	95, 123, 140, 163	0
6	L	165/170 (97%)	0.00	2 (1%)	79	67	105, 126, 145, 150	0
All	All	4005/4219 (94%)	0.04	36 (0%)	84	75	47, 88, 128, 165	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	2	GLY	3.6
2	E	6	VAL	3.6
2	E	430	THR	3.5
1	B	481	LEU	3.3
2	E	394	ALA	3.2
1	B	483	ILE	2.9
2	E	220	CYS	2.9
6	K	150	GLU	2.8
6	K	132	CYS	2.8
3	G	149	VAL	2.7
6	L	6	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	494	ALA	2.6
1	A	416	ASP	2.5
6	K	110	VAL	2.5
1	A	20	SER	2.5
1	A	538	ASN	2.4
2	D	403	GLU	2.4
6	K	119	TYR	2.3
2	F	407	LEU	2.2
1	B	127	LEU	2.2
1	B	478	HIS	2.2
1	A	495	MET	2.2
6	J	167	VAL	2.2
1	A	143	ASP	2.1
1	B	492	PHE	2.1
1	B	403	LEU	2.1
6	L	170	GLU	2.1
1	B	405	GLY	2.1
2	F	493	VAL	2.1
6	J	169	VAL	2.1
1	B	538	ASN	2.0
2	F	135	GLU	2.0
6	K	158	LEU	2.0
1	B	493	PHE	2.0
1	C	493	PHE	2.0
6	J	168	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

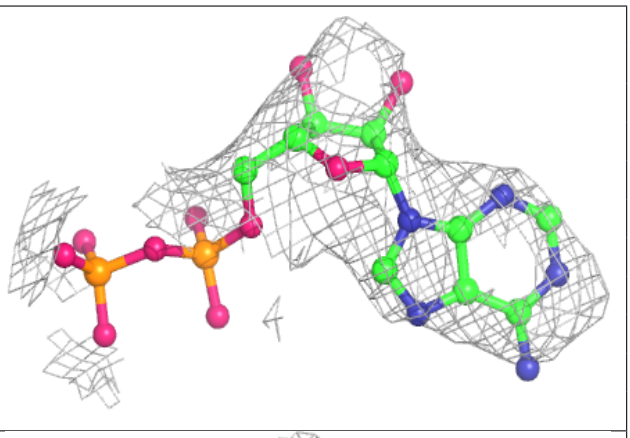
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

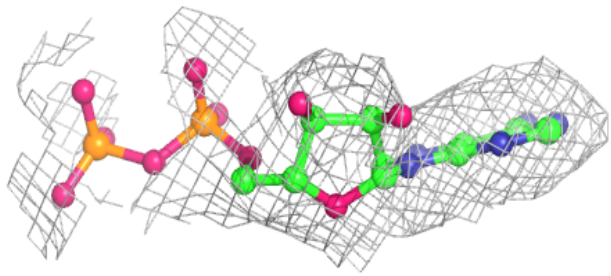
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	D	601	1/1	0.88	0.22	65,65,65,65	0
8	MG	F	601	1/1	0.88	0.11	73,73,73,73	0
7	ADP	E	600	27/27	0.89	0.19	116,122,125,126	0
8	MG	C	601	1/1	0.89	0.15	54,54,54,54	0
8	MG	A	601	1/1	0.91	0.13	64,64,64,64	0
8	MG	B	601	1/1	0.94	0.18	52,52,52,52	0
7	ADP	F	600	27/27	0.95	0.20	62,63,66,68	0
7	ADP	D	600	27/27	0.95	0.23	62,64,66,67	0
7	ADP	C	600	27/27	0.96	0.20	54,59,63,64	0
7	ADP	A	600	27/27	0.96	0.17	65,66,66,67	0
7	ADP	B	600	27/27	0.96	0.17	52,56,59,59	0

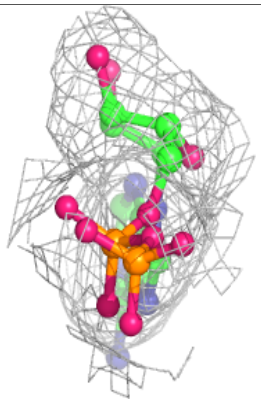
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP E 600:

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

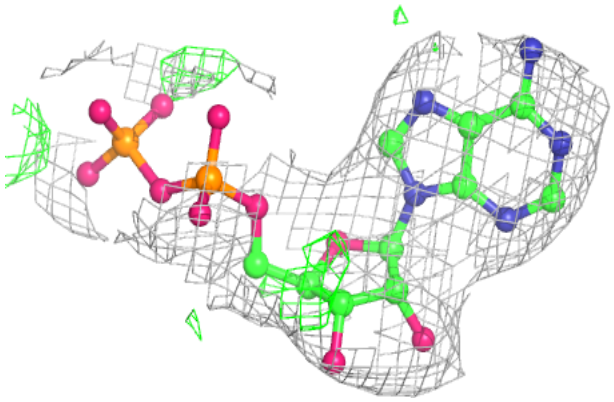


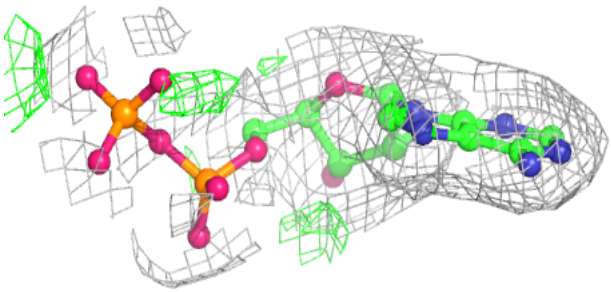


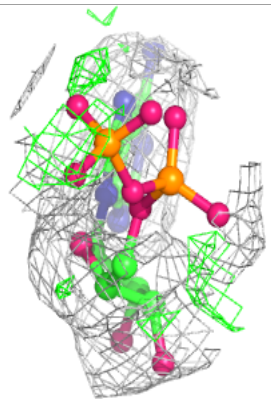


Electron density around ADP F 600:

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

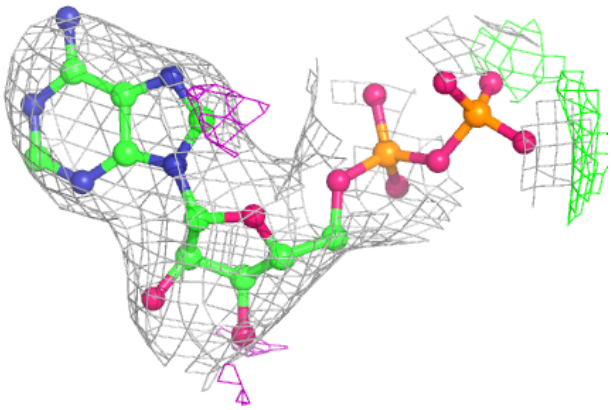


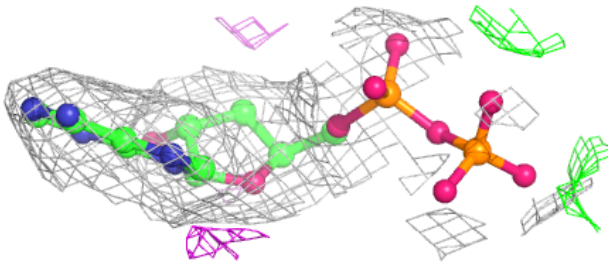




Electron density around ADP D 600:

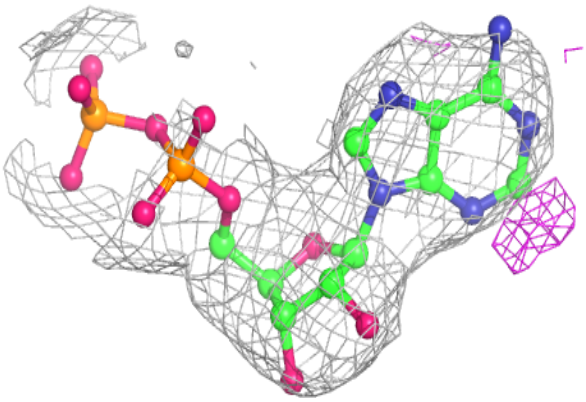
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

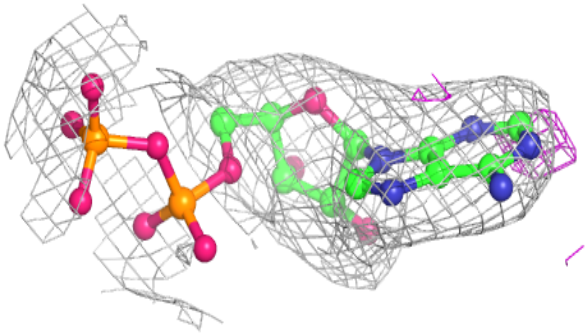


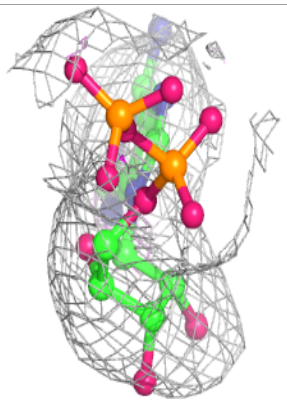


Electron density around ADP C 600:

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

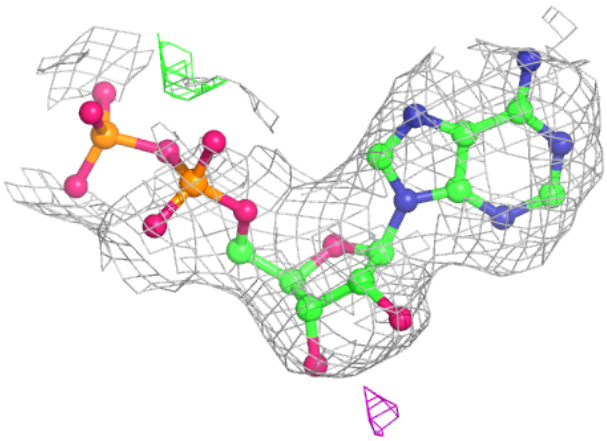


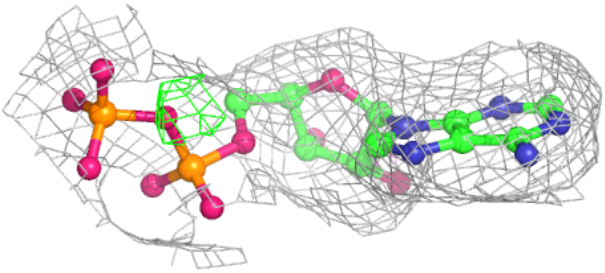


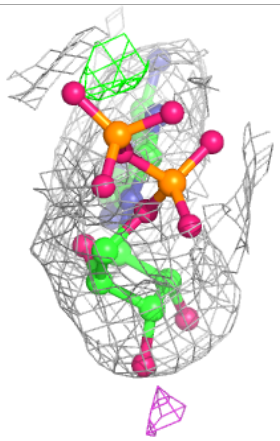


Electron density around ADP A 600:

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

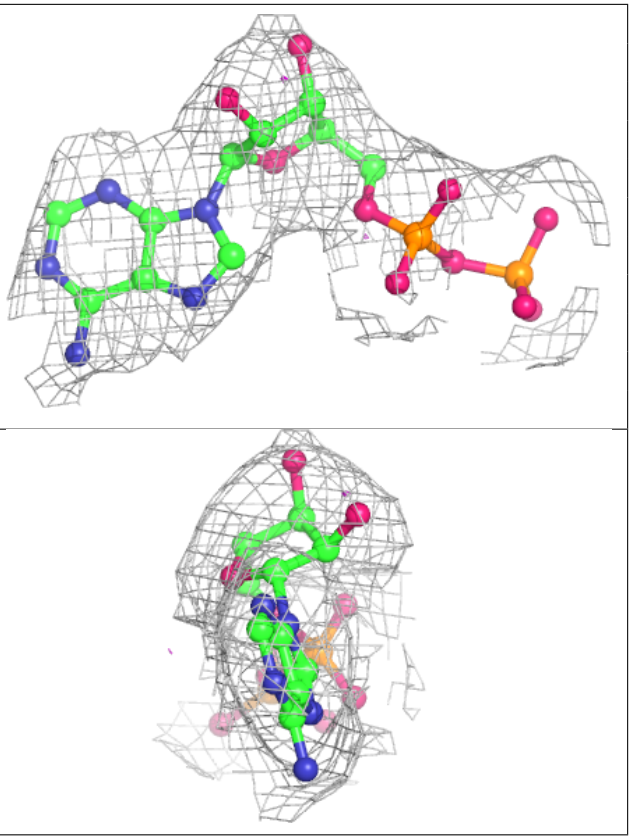


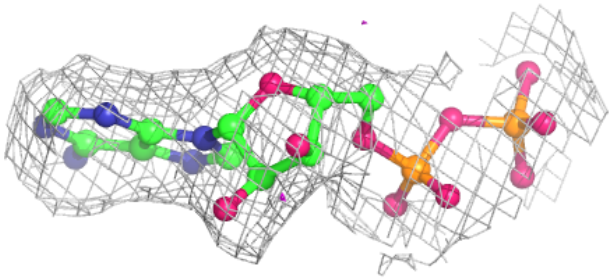




Electron density around ADP B 600:

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





6.5 Other polymers (i)

There are no such residues in this entry.