



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:54 AM UTC

PDB ID : 5JM8 / pdb_00005jm8
Title : The structure of ATP-bound aerobactin synthetase IucA from a hypervirulent pathotype of *Klebsiella pneumoniae*
Authors : Bailey, D.C.; Drake, E.J.; Gulick, A.M.
Deposited on : 2016-04-28
Resolution : 2.20 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

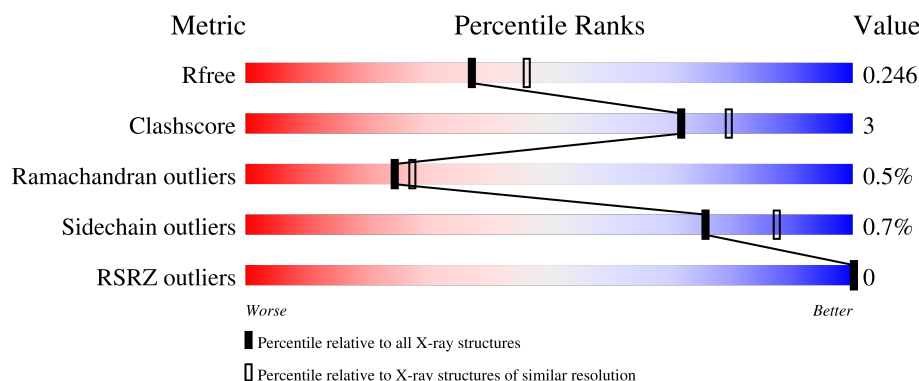
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	576	
1	B	576	
1	C	576	
1	D	576	
1	E	576	

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Mol	Chain	Length	Quality of chain
1	F	576	87% 8% . .
1	G	576	88% 8% .
1	H	576	84% 10% . 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35902 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 Aerobactin synthase IucA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4388	2803	776	792	17			
1	B	556	Total	C	N	O	S	0	0	0
			4383	2803	772	791	17			
1	C	552	Total	C	N	O	S	0	0	0
			4360	2779	770	794	17			
1	D	552	Total	C	N	O	S	0	0	0
			4338	2771	765	785	17			
1	E	552	Total	C	N	O	S	0	0	0
			4378	2798	773	790	17			
1	F	551	Total	C	N	O	S	0	0	0
			4248	2691	760	780	17			
1	G	552	Total	C	N	O	S	0	0	0
			4359	2780	772	790	17			
1	H	550	Total	C	N	O	S	0	0	0
			4258	2713	755	773	17			

There are 16 discrepancies between the modelled and reference sequences:

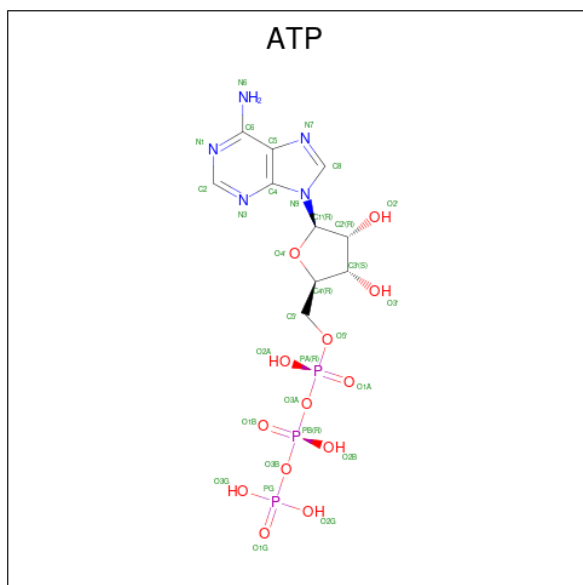
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0X9V8F4
A	0	HIS	-	expression tag	UNP A0A0X9V8F4
B	-1	GLY	-	expression tag	UNP A0A0X9V8F4
B	0	HIS	-	expression tag	UNP A0A0X9V8F4
C	-1	GLY	-	expression tag	UNP A0A0X9V8F4
C	0	HIS	-	expression tag	UNP A0A0X9V8F4
D	-1	GLY	-	expression tag	UNP A0A0X9V8F4
D	0	HIS	-	expression tag	UNP A0A0X9V8F4
E	-1	GLY	-	expression tag	UNP A0A0X9V8F4
E	0	HIS	-	expression tag	UNP A0A0X9V8F4
F	-1	GLY	-	expression tag	UNP A0A0X9V8F4
F	0	HIS	-	expression tag	UNP A0A0X9V8F4
G	-1	GLY	-	expression tag	UNP A0A0X9V8F4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A0X9V8F4
H	-1	GLY	-	expression tag	UNP A0A0X9V8F4
H	0	HIS	-	expression tag	UNP A0A0X9V8F4

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



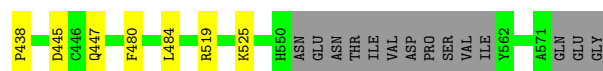
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

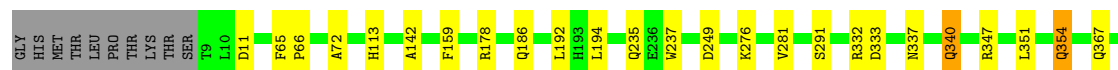
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	124	Total O 124 124	0	0
4	B	118	Total O 118 118	0	0
4	C	127	Total O 127 127	0	0
4	D	110	Total O 110 110	0	0
4	E	115	Total O 115 115	0	0
4	F	125	Total O 125 125	0	0
4	G	111	Total O 111 111	0	0
4	H	104	Total O 104 104	0	0



• Molecule 1: Aerobactin synthase IucA

Chain E: 89% 6% .



• Molecule 1: Aerobactin synthase IucA

Chain F: 87% 8% . .



• Molecule 1: Aerobactin synthase IucA

Chain G: 88% 8% .



• Molecule 1: Aerobactin synthase IucA

Chain H: 84% 10% . 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	170.85Å 96.63Å 173.23Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	49.57 – 2.20 49.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.57-2.20) 96.7 (49.57-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.214 , 0.249 0.214 , 0.246	Depositor DCC
R_{free} test set	14176 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 8.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.458 for h,-k,-l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	7 of 283617 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35902	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0085e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.35	0/4500	0.67	3/6133 (0.0%)
1	B	0.32	0/4496	0.66	1/6125 (0.0%)
1	C	0.31	0/4472	0.65	0/6095
1	D	0.31	0/4450	0.65	0/6066
1	E	0.31	0/4490	0.64	1/6117 (0.0%)
1	F	0.32	0/4354	0.67	1/5938 (0.0%)
1	G	0.33	0/4471	0.66	0/6094
1	H	0.34	1/4367 (0.0%)	0.67	2/5957 (0.0%)
All	All	0.32	1/35600 (0.0%)	0.66	8/48525 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	97	LEU	C-N	7.08	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	GLY	N-CA-C	8.07	122.33	110.63
1	A	34	GLN	C-N-CD	7.13	136.29	120.60
1	B	34	GLN	C-N-CD	7.13	136.28	120.60
1	H	97	LEU	CA-C-N	-5.86	114.26	120.94
1	H	97	LEU	C-N-CA	-5.86	114.26	120.94
1	A	74	GLY	CA-C-O	-5.43	116.34	121.87
1	F	96	LEU	CB-CA-C	-5.17	110.20	117.23
1	E	72	ALA	N-CA-C	-5.12	105.62	111.14

There are no chirality outliers.

There are no planarity outliers.

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	4388	0	4258	31	0
1	B	4383	0	4245	17	0
1	C	4360	0	4207	19	0
1	D	4338	0	4175	22	0
1	E	4378	0	4259	20	0
1	F	4248	0	3983	34	0
1	G	4359	0	4208	34	0
1	H	4258	0	4029	55	0
2	A	31	0	12	2	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	2	0
2	F	31	0	12	2	0
2	G	31	0	12	1	0
2	H	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	124	0	0	1	0
4	B	118	0	0	2	0
4	C	127	0	0	4	0
4	D	110	0	0	3	0
4	E	115	0	0	2	0
4	F	125	0	0	3	0
4	G	111	0	0	11	0
4	H	104	0	0	1	0
All	All	35902	0	33460	228	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 3.

All (228) 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)
1:D:100:THR:HA	1:D:103:GLU:OE2	1.25	1.29
1:H:42:LEU:HA	1:H:90:LYS:NZ	1.50	1.25
1:A:72:ALA:HB2	1:F:335:HIS:NE2	1.62	1.12
1:H:42:LEU:CA	1:H:90:LYS:HZ1	1.75	0.99
1:G:157:GLU:OE2	1:G:282:ARG:HD2	1.64	0.96
1:H:42:LEU:HA	1:H:90:LYS:HZ1	1.00	0.96
1:D:99:ALA:O	1:D:103:GLU:OE1	1.84	0.95
1:E:540:LYS:CB	4:E:789:HOH:O	2.14	0.94
1:H:92:GLN:NE2	1:H:99:ALA:HA	1.81	0.94
1:H:482:TYR:HB2	1:H:539:VAL:HG11	1.51	0.92
1:D:100:THR:CA	1:D:103:GLU:OE2	2.15	0.92
1:H:92:GLN:HE21	1:H:99:ALA:HA	1.30	0.92
1:A:69:LEU:O	1:A:75:SER:CB	2.22	0.88
1:G:10:LEU:HA	4:G:710:HOH:O	1.75	0.86
1:B:366:THR:OG1	1:B:426:GLN:OE1	1.95	0.83
1:A:178:ARG:NH2	1:A:249:ASP:OD2	2.13	0.82
1:A:366:THR:OG1	1:A:426:GLN:OE1	1.99	0.81
1:D:100:THR:HA	1:D:103:GLU:CD	2.05	0.80
1:H:92:GLN:HB3	1:H:99:ALA:HA	1.63	0.80
1:G:341:GLU:OE2	4:G:701:HOH:O	2.00	0.80
1:D:43:GLY:O	1:D:45:GLN:N	2.13	0.80
1:B:34:GLN:HA	1:B:35:PRO:C	2.10	0.76
1:A:34:GLN:HA	1:A:35:PRO:C	2.11	0.76
1:A:72:ALA:CB	1:F:335:HIS:NE2	2.48	0.76
1:G:178:ARG:NH2	1:G:249:ASP:OD2	2.20	0.74
1:G:519:ARG:O	1:G:525:LYS:NZ	2.20	0.74
1:B:70:VAL:O	1:B:71:THR:CB	2.36	0.72
1:F:41:PRO:HA	1:F:47:ALA:HB2	1.73	0.71
1:F:519:ARG:O	1:F:525:LYS:NZ	2.23	0.70
1:H:240:GLU:HB3	1:H:334:LEU:HD11	1.74	0.69
1:G:43:GLY:HA2	4:G:711:HOH:O	1.93	0.69
1:H:42:LEU:CA	1:H:90:LYS:NZ	2.38	0.69
1:B:178:ARG:NH2	1:B:249:ASP:OD2	2.27	0.68
1:C:297:ARG:NH2	1:C:468:GLU:OE2	2.26	0.68
1:E:415:GLU:OE2	4:E:701:HOH:O	2.12	0.68
1:G:24:GLU:CD	1:G:541:GLY:HA2	2.19	0.67
1:D:190:GLU:OE2	1:D:303:ARG:NH2	2.27	0.67
1:B:415:GLU:OE2	4:B:701:HOH:O	2.13	0.67
1:G:43:GLY:CA	4:G:711:HOH:O	2.42	0.67
1:G:233:LEU:O	1:G:239:GLN:NE2	2.29	0.66
1:H:91:LEU:CB	1:H:102:CYS:SG	2.84	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:GLN:NE2	1:H:99:ALA:CA	2.56	0.66
1:D:41:PRO:O	1:D:90:LYS:NZ	2.21	0.66
1:F:88:VAL:HG13	1:F:102:CYS:SG	2.35	0.66
1:F:11:ASP:OD2	1:F:113:HIS:NE2	2.23	0.65
1:H:241:LEU:HD23	1:H:334:LEU:CD2	2.25	0.65
1:F:41:PRO:HA	1:F:47:ALA:CB	2.27	0.65
1:E:186:GLN:NE2	1:E:332:ARG:O	2.29	0.65
1:G:326:ASP:OD2	4:G:702:HOH:O	2.15	0.64
1:B:168:LEU:O	4:B:702:HOH:O	2.15	0.64
1:H:92:GLN:HA	1:H:97:LEU:CB	2.28	0.64
1:B:45:GLN:O	1:B:71:THR:CB	2.47	0.62
1:A:265:SER:OG	2:A:600:ATP:O1G	2.16	0.62
1:F:157:GLU:HA	4:F:706:HOH:O	1.99	0.62
1:H:87:ILE:O	1:H:90:LYS:HG3	2.00	0.61
1:G:374:ASP:OD2	1:G:382:LYS:NZ	2.30	0.61
1:H:99:ALA:O	1:H:102:CYS:N	2.30	0.61
1:E:276:LYS:NZ	2:E:600:ATP:O1G	2.32	0.60
1:H:71:THR:HG22	1:H:72:ALA:N	2.16	0.60
1:H:11:ASP:OD2	1:H:113:HIS:NE2	2.29	0.60
1:D:332:ARG:NH1	1:D:336:GLY:O	2.33	0.60
1:B:519:ARG:O	1:B:525:LYS:NZ	2.35	0.59
1:H:235:GLN:OE1	1:H:237:TRP:NE1	2.32	0.59
1:A:68:ARG:HD3	1:A:76:HIS:O	2.02	0.59
1:F:333:ASP:OD1	1:F:334:LEU:N	2.35	0.59
1:F:190:GLU:OE2	1:F:303:ARG:NH2	2.34	0.59
1:H:567:ASN:OD1	1:H:569:LEU:N	2.36	0.58
1:A:519:ARG:O	1:A:525:LYS:NZ	2.36	0.58
1:A:538:ASN:ND2	1:A:564:ASP:OD1	2.37	0.58
1:F:41:PRO:O	1:F:90:LYS:NZ	2.31	0.58
1:D:519:ARG:O	1:D:525:LYS:NZ	2.37	0.57
1:G:92:GLN:O	1:G:97:LEU:N	2.37	0.57
1:H:241:LEU:HD23	1:H:334:LEU:HD21	1.86	0.57
1:H:98:PRO:O	1:H:99:ALA:HB3	2.05	0.56
1:H:519:ARG:O	1:H:525:LYS:NZ	2.36	0.56
1:A:321:ARG:NH1	4:A:709:HOH:O	2.39	0.55
1:A:385:SER:OG	1:A:390:ILE:O	2.19	0.55
1:C:519:ARG:O	1:C:525:LYS:NZ	2.39	0.55
1:F:385:SER:OG	1:F:390:ILE:O	2.19	0.55
1:F:88:VAL:CG1	1:F:102:CYS:SG	2.95	0.55
1:E:11:ASP:OD2	1:E:113:HIS:NE2	2.31	0.54
1:G:10:LEU:CA	4:G:710:HOH:O	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:534:ASN:ND2	1:G:536:TYR:O	2.41	0.54
1:G:357:SER:O	4:G:703:HOH:O	2.18	0.54
1:C:178:ARG:NH2	4:C:701:HOH:O	2.40	0.53
1:D:42:LEU:CB	1:D:46:GLN:HG3	2.38	0.53
1:E:235:GLN:OE1	1:E:237:TRP:NE1	2.41	0.53
1:C:190:GLU:OE2	1:C:303:ARG:NH2	2.38	0.53
1:H:46:GLN:HA	1:H:70:VAL:O	2.08	0.53
1:G:92:GLN:HA	1:G:97:LEU:CB	2.39	0.53
1:A:186:GLN:NE2	1:A:332:ARG:O	2.43	0.52
1:D:333:ASP:OD1	1:D:337:ASN:N	2.41	0.52
1:G:540:LYS:HA	1:G:562:TYR:CD2	2.44	0.52
1:A:276:LYS:NZ	2:A:600:ATP:O3G	2.40	0.51
1:A:459:LEU:HD23	1:A:464:GLU:O	2.10	0.51
1:G:43:GLY:N	4:G:711:HOH:O	2.40	0.51
1:B:535:PRO:HA	1:B:570:LEU:HD11	1.93	0.51
1:C:518:MET:HE3	1:C:528:LEU:HD21	1.93	0.51
1:H:42:LEU:CB	1:H:90:LYS:HZ1	2.22	0.51
1:H:71:THR:CG2	1:H:72:ALA:N	2.73	0.51
1:H:477:LEU:HD22	1:H:530:TYR:CB	2.40	0.51
1:F:130:ARG:NH1	4:F:714:HOH:O	2.44	0.51
1:A:46:GLN:HG2	1:A:71:THR:HA	1.93	0.50
1:F:186:GLN:NE2	1:F:332:ARG:O	2.44	0.50
1:E:178:ARG:NH2	1:E:249:ASP:OD2	2.44	0.50
1:D:34:GLN:HA	1:D:35:PRO:C	2.37	0.50
1:H:426:GLN:NE2	1:H:487:ASN:O	2.44	0.50
1:F:9:THR:O	1:F:65:PHE:HB2	2.12	0.50
1:D:438:PRO:O	4:D:701:HOH:O	2.19	0.49
1:G:161:GLN:NE2	4:G:704:HOH:O	2.42	0.49
1:C:409:LYS:HA	1:C:518:MET:SD	2.52	0.49
1:G:188:ALA:HB2	1:G:332:ARG:HE	1.76	0.49
1:E:333:ASP:OD1	1:E:337:ASN:N	2.46	0.49
1:H:92:GLN:CB	1:H:99:ALA:HA	2.40	0.49
1:H:240:GLU:HB3	1:H:334:LEU:CD1	2.41	0.49
1:A:297:ARG:NH2	1:A:468:GLU:OE2	2.37	0.49
1:D:285:ASN:HA	4:D:800:HOH:O	2.12	0.49
1:E:192:LEU:O	1:E:194:LEU:N	2.45	0.49
1:C:188:ALA:HB2	1:C:332:ARG:HE	1.77	0.49
1:H:291:SER:OG	1:H:294:GLU:HG3	2.13	0.49
1:A:293:LYS:NZ	1:A:468:GLU:HG3	2.28	0.48
1:H:519:ARG:HA	1:H:528:LEU:HD23	1.95	0.48
1:F:458:TRP:O	1:F:461:THR:OG1	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:PHE:HB3	1:F:66:PRO:HA	1.94	0.48
1:H:10:LEU:HA	4:H:786:HOH:O	2.14	0.47
1:H:47:ALA:O	1:H:70:VAL:N	2.46	0.47
1:E:426:GLN:NE2	1:E:491:ALA:CB	2.77	0.47
1:A:46:GLN:HA	1:A:70:VAL:O	2.14	0.47
1:F:132:LYS:NZ	4:F:702:HOH:O	2.25	0.47
1:D:43:GLY:C	1:D:45:GLN:N	2.73	0.47
1:H:374:ASP:OD2	1:H:382:LYS:NZ	2.34	0.47
1:C:321:ARG:NH2	4:C:716:HOH:O	2.48	0.47
1:D:18:LEU:HD21	1:D:83:LEU:HD21	1.97	0.47
1:G:11:ASP:N	4:G:710:HOH:O	2.40	0.47
1:A:68:ARG:HD3	1:A:76:HIS:C	2.39	0.46
1:G:540:LYS:HA	1:G:562:TYR:HD2	1.80	0.46
1:C:502:ASP:OD1	1:C:503:SER:N	2.46	0.46
1:E:142:ALA:O	1:E:367:GLN:NE2	2.41	0.46
1:A:192:LEU:O	1:A:194:LEU:N	2.48	0.46
1:F:276:LYS:NZ	2:F:600:ATP:O1G	2.49	0.46
1:D:235:GLN:OE1	1:D:237:TRP:NE1	2.44	0.46
1:H:92:GLN:NE2	1:H:99:ALA:CB	2.79	0.46
1:A:72:ALA:C	1:A:74:GLY:N	2.72	0.46
1:G:412:PHE:CD2	1:G:518:MET:HE1	2.51	0.46
1:H:88:VAL:HG11	1:H:106:HIS:HB2	1.97	0.46
1:A:460:ASP:OD1	1:A:465:ALA:HB2	2.16	0.46
1:B:192:LEU:O	1:B:194:LEU:N	2.48	0.46
1:G:258:LEU:HD12	1:G:258:LEU:O	2.16	0.46
1:C:65:PHE:HB3	1:C:66:PRO:HA	1.97	0.45
1:D:415:GLU:OE2	4:D:702:HOH:O	2.21	0.45
1:E:509:ALA:HA	1:E:512:ARG:NH1	2.31	0.45
1:A:534:ASN:ND2	1:A:536:TYR:O	2.46	0.45
1:G:235:GLN:OE1	1:G:237:TRP:NE1	2.44	0.45
1:F:285:ASN:O	1:F:286:SER:CB	2.64	0.45
1:F:347:ARG:NH1	1:F:444:ARG:HD2	2.32	0.45
1:H:69:LEU:O	1:H:75:SER:HA	2.16	0.45
1:D:30:LEU:HD11	1:D:55:PHE:CE1	2.52	0.45
1:F:333:ASP:OD1	1:F:335:HIS:N	2.38	0.45
1:F:426:GLN:NE2	1:F:491:ALA:CB	2.79	0.45
1:F:42:LEU:N	1:F:46:GLN:O	2.46	0.45
1:H:50:PHE:CE1	1:H:83:LEU:HD11	2.52	0.45
1:H:88:VAL:HG12	1:H:102:CYS:SG	2.57	0.45
1:E:347:ARG:NH1	1:E:444:ARG:HD2	2.33	0.44
1:G:24:GLU:CD	1:G:541:GLY:CA	2.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:PHE:HB3	1:D:66:PRO:HA	1.99	0.44
1:D:447:GLN:N	1:D:447:GLN:OE1	2.50	0.44
1:C:46:GLN:HG2	1:C:71:THR:HG22	1.99	0.44
1:H:42:LEU:HA	1:H:90:LYS:HZ3	1.65	0.44
1:H:241:LEU:HD23	1:H:334:LEU:HD23	1.97	0.44
1:H:291:SER:HG	1:H:294:GLU:HG3	1.82	0.44
1:C:510:ARG:NH2	4:C:722:HOH:O	2.50	0.44
1:B:65:PHE:HB3	1:B:66:PRO:HA	2.00	0.44
1:B:528:LEU:O	1:B:532:LEU:HD12	2.18	0.44
1:C:188:ALA:O	1:C:330:GLY:N	2.50	0.44
1:H:165:GLU:HG2	1:H:171:PHE:CE2	2.53	0.44
1:A:65:PHE:HB3	1:A:66:PRO:HA	2.00	0.44
1:H:18:LEU:HD21	1:H:83:LEU:HD21	1.98	0.44
1:H:477:LEU:HD22	1:H:530:TYR:CG	2.52	0.44
1:C:49:HIS:CE1	1:C:70:VAL:HG21	2.52	0.44
1:C:252:GLU:OE2	4:C:701:HOH:O	2.21	0.44
1:A:321:ARG:HD3	1:E:388:LEU:CD2	2.48	0.43
1:H:244:LYS:HE3	1:H:334:LEU:HD13	2.00	0.43
1:C:297:ARG:NE	1:C:468:GLU:OE2	2.51	0.43
1:E:65:PHE:HB3	1:E:66:PRO:HA	2.00	0.43
1:F:192:LEU:O	1:F:194:LEU:N	2.51	0.43
1:B:186:GLN:NE2	1:B:332:ARG:O	2.50	0.43
1:H:468:GLU:CD	1:H:468:GLU:C	2.85	0.43
1:H:53:ALA:CB	1:H:62:ARG:NH1	2.81	0.43
1:A:197:GLN:NE2	1:G:217:ASP:OD1	2.41	0.43
1:B:512:ARG:NE	1:B:569:LEU:O	2.47	0.43
1:A:10:LEU:HD21	1:A:372:GLY:HA3	2.00	0.43
1:F:177:LEU:HG	1:F:257:TRP:CD1	2.54	0.43
1:F:276:LYS:NZ	2:F:600:ATP:O1B	2.39	0.42
1:G:24:GLU:OE2	1:G:541:GLY:HA2	2.19	0.42
1:H:412:PHE:CD2	1:H:518:MET:HE1	2.54	0.42
1:E:276:LYS:NZ	2:E:600:ATP:O1B	2.51	0.42
1:F:11:ASP:HB3	1:F:65:PHE:CE2	2.54	0.42
1:F:473:ARG:NH1	1:F:526:THR:HG21	2.35	0.42
1:E:351:LEU:HA	1:E:354:GLN:OE1	2.19	0.42
1:F:11:ASP:HB3	1:F:65:PHE:HE2	1.85	0.42
1:C:452:MET:SD	1:C:476:LEU:HD22	2.60	0.42
1:C:50:PHE:CE1	1:C:67:ALA:HB2	2.55	0.42
1:F:23:ARG:NH2	1:F:58:THR:O	2.51	0.42
1:G:165:GLU:OE2	4:G:704:HOH:O	2.20	0.42
1:A:69:LEU:HD23	1:A:76:HIS:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ASN:HB3	1:C:546:TYR:HD1	1.84	0.41
1:F:92:GLN:HG2	1:F:102:CYS:SG	2.60	0.41
1:H:65:PHE:HB3	1:H:66:PRO:HA	2.02	0.41
1:A:244:LYS:HG3	1:A:246:LEU:HG	2.02	0.41
1:E:159:PHE:CZ	1:E:281:VAL:HG21	2.56	0.41
1:F:25:THR:O	1:F:28:TRP:NE1	2.51	0.41
1:G:276:LYS:NZ	2:G:600:ATP:O1B	2.50	0.41
1:G:65:PHE:HB3	1:G:66:PRO:HA	2.03	0.41
1:G:409:LYS:HD3	1:G:518:MET:HG2	2.03	0.41
1:H:409:LYS:HA	1:H:518:MET:HE3	2.03	0.41
1:E:409:LYS:HA	1:E:518:MET:HE3	2.03	0.41
1:A:72:ALA:C	1:A:74:GLY:H	2.29	0.40
1:B:378:VAL:HG12	1:B:382:LYS:HD2	2.03	0.40
1:D:480:PHE:CE2	1:D:484:LEU:HD22	2.56	0.40
1:H:69:LEU:HD23	1:H:76:HIS:CE1	2.56	0.40
1:H:92:GLN:HE21	1:H:92:GLN:HB3	1.63	0.40
1:E:291:SER:HA	1:E:340:GLN:HG2	2.04	0.40
1:H:536:TYR:O	1:H:537:TRP:HD1	2.04	0.40
1:B:46:GLN:HA	1:B:71:THR:CB	2.51	0.40
1:G:228:GLN:HG3	1:G:232:LEU:HD13	2.03	0.40
1:H:54:TYR:HB3	1:H:62:ARG:HG2	2.04	0.40
1:B:473:ARG:O	1:B:477:LEU:HD13	2.20	0.40
1:G:497:GLY:HA2	1:G:502:ASP:O	2.22	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	552/576 (96%)	535 (97%)	14 (2%)	3 (0%)	24 27
1	B	552/576 (96%)	530 (96%)	19 (3%)	3 (0%)	24 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	548/576 (95%)	528 (96%)	18 (3%)	2 (0%)	30	34
1	D	548/576 (95%)	524 (96%)	20 (4%)	4 (1%)	18	19
1	E	548/576 (95%)	531 (97%)	15 (3%)	2 (0%)	30	34
1	F	547/576 (95%)	522 (95%)	21 (4%)	4 (1%)	18	19
1	G	548/576 (95%)	533 (97%)	12 (2%)	3 (0%)	24	27
1	H	546/576 (95%)	512 (94%)	31 (6%)	3 (0%)	24	27
All	All	4389/4608 (95%)	4215 (96%)	150 (3%)	24 (0%)	24	27

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	GLU
1	D	286	SER
1	F	285	ASN
1	F	286	SER
1	H	93	HIS
1	A	488	SER
1	B	71	THR
1	B	488	SER
1	E	445	ASP
1	F	488	SER
1	G	284	THR
1	H	95	LEU
1	A	284	THR
1	D	98	PRO
1	D	445	ASP
1	E	488	SER
1	G	488	SER
1	C	284	THR
1	C	445	ASP
1	H	91	LEU
1	B	445	ASP
1	G	445	ASP
1	A	539	VAL
1	F	97	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	453/488 (93%)	450 (99%)	3 (1%)	76	87
1	B	450/488 (92%)	447 (99%)	3 (1%)	76	87
1	C	451/488 (92%)	449 (100%)	2 (0%)	84	92
1	D	443/488 (91%)	443 (100%)	0	100	100
1	E	454/488 (93%)	452 (100%)	2 (0%)	84	92
1	F	419/488 (86%)	413 (99%)	6 (1%)	59	75
1	G	449/488 (92%)	448 (100%)	1 (0%)	87	94
1	H	423/488 (87%)	416 (98%)	7 (2%)	53	69
All	All	3542/3904 (91%)	3518 (99%)	24 (1%)	76	87

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ARG
1	A	468	GLU
1	A	488	SER
1	B	367	GLN
1	B	488	SER
1	B	533	GLU
1	C	199	ARG
1	C	468	GLU
1	E	340	GLN
1	E	354	GLN
1	F	89	ASP
1	F	97	LEU
1	F	102	CYS
1	F	199	ARG
1	F	333	ASP
1	F	468	GLU
1	G	367	GLN
1	H	90	LYS
1	H	92	GLN
1	H	94	GLN
1	H	118	GLN
1	H	234	GLN
1	H	539	VAL

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Mol	Chain	Res	Type
1	H	540	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	92	GLN
1	A	106	HIS
1	A	156	HIS
1	A	360	ASN
1	A	447	GLN
1	B	49	HIS
1	B	337	ASN
1	B	406	GLN
1	C	49	HIS
1	C	141	GLN
1	C	360	ASN
1	C	534	ASN
1	D	115	HIS
1	D	186	GLN
1	D	239	GLN
1	D	337	ASN
1	D	393	GLN
1	E	107	GLN
1	E	124	HIS
1	E	337	ASN
1	F	193	HIS
1	F	234	GLN
1	F	285	ASN
1	F	306	GLN
1	F	337	ASN
1	F	349	ASN
1	G	161	GLN
1	G	360	ASN
1	G	548	ASN
1	H	92	GLN
1	H	141	GLN
1	H	360	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ATP	B	600	3	32,33,33	1.46	6 (18%)	48,52,52	1.81	10 (20%)
2	ATP	F	600	3	32,33,33	1.39	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	A	600	3	32,33,33	1.45	6 (18%)	48,52,52	1.83	9 (18%)
2	ATP	D	600	3	32,33,33	1.43	7 (21%)	48,52,52	1.83	10 (20%)
2	ATP	G	600	3	32,33,33	1.42	6 (18%)	48,52,52	1.80	8 (16%)
2	ATP	C	600	3	32,33,33	1.45	6 (18%)	48,52,52	1.80	9 (18%)
2	ATP	E	600	3	32,33,33	1.39	5 (15%)	48,52,52	1.86	8 (16%)
2	ATP	H	600	3	32,33,33	1.38	5 (15%)	48,52,52	1.84	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	600	3	-	1/22/38/38	0/3/3/3
2	ATP	F	600	3	-	2/22/38/38	0/3/3/3
2	ATP	A	600	3	-	4/22/38/38	0/3/3/3
2	ATP	D	600	3	-	5/22/38/38	0/3/3/3
2	ATP	G	600	3	-	3/22/38/38	0/3/3/3
2	ATP	C	600	3	-	1/22/38/38	0/3/3/3
2	ATP	E	600	3	-	2/22/38/38	0/3/3/3
2	ATP	H	600	3	-	7/22/38/38	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ATP	C5-C4	4.66	1.47	1.39
2	H	600	ATP	C5-C4	4.57	1.47	1.39
2	C	600	ATP	C5-C4	4.56	1.47	1.39
2	A	600	ATP	C5-C4	4.56	1.47	1.39
2	E	600	ATP	C5-C4	4.50	1.47	1.39
2	G	600	ATP	C5-C4	4.47	1.47	1.39
2	F	600	ATP	C5-C4	4.43	1.47	1.39
2	D	600	ATP	C5-C4	4.28	1.46	1.39
2	D	600	ATP	PB-O3B	2.77	1.62	1.59
2	A	600	ATP	PB-O3B	2.76	1.62	1.59
2	B	600	ATP	C5-C6	2.68	1.48	1.41
2	G	600	ATP	PB-O3B	2.59	1.62	1.59
2	A	600	ATP	C5-C6	2.57	1.48	1.41
2	C	600	ATP	C5-C6	2.54	1.48	1.41
2	D	600	ATP	C5-C6	2.53	1.48	1.41
2	E	600	ATP	C5-C6	2.52	1.48	1.41
2	H	600	ATP	C5-C6	2.49	1.47	1.41
2	G	600	ATP	C5-C6	2.49	1.47	1.41
2	F	600	ATP	C5-C6	2.47	1.47	1.41
2	B	600	ATP	C8-N7	2.44	1.36	1.31
2	C	600	ATP	PA-O3A	2.43	1.62	1.59
2	H	600	ATP	C5-N7	-2.42	1.34	1.39
2	G	600	ATP	C5-N7	-2.39	1.34	1.39
2	B	600	ATP	PB-O3B	2.39	1.62	1.59
2	C	600	ATP	C8-N7	2.39	1.36	1.31
2	F	600	ATP	C5-N7	-2.38	1.34	1.39
2	C	600	ATP	C5-N7	-2.37	1.34	1.39
2	E	600	ATP	C5-N7	-2.36	1.34	1.39
2	E	600	ATP	C8-N7	2.36	1.36	1.31
2	F	600	ATP	C8-N7	2.36	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	ATP	PB-O3B	2.34	1.62	1.59
2	G	600	ATP	C8-N7	2.31	1.36	1.31
2	A	600	ATP	C8-N7	2.31	1.36	1.31
2	A	600	ATP	C5-N7	-2.31	1.34	1.39
2	E	600	ATP	PB-O3B	2.29	1.62	1.59
2	D	600	ATP	C8-N7	2.26	1.36	1.31
2	B	600	ATP	C5-N7	-2.24	1.35	1.39
2	H	600	ATP	C8-N7	2.22	1.36	1.31
2	D	600	ATP	C5-N7	-2.20	1.35	1.39
2	F	600	ATP	PB-O3B	2.16	1.61	1.59
2	A	600	ATP	PB-O3A	2.15	1.61	1.59
2	B	600	ATP	PA-O3A	2.12	1.61	1.59
2	D	600	ATP	PA-O3A	2.09	1.61	1.59
2	D	600	ATP	PB-O3A	2.05	1.61	1.59
2	H	600	ATP	PB-O3B	2.03	1.61	1.59
2	G	600	ATP	C4-N9	-2.02	1.33	1.37

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	600	ATP	C5-C4-N3	-6.26	118.09	126.72
2	E	600	ATP	C5-C4-N3	-6.24	118.12	126.72
2	F	600	ATP	C5-C4-N3	-5.92	118.57	126.72
2	A	600	ATP	C5-C4-N3	-5.91	118.58	126.72
2	C	600	ATP	C5-C4-N3	-5.81	118.72	126.72
2	G	600	ATP	C5-C4-N3	-5.81	118.72	126.72
2	B	600	ATP	C5-C4-N3	-5.62	118.98	126.72
2	D	600	ATP	C5-C4-N3	-5.50	119.15	126.72
2	H	600	ATP	N3-C4-N9	5.43	136.40	127.17
2	E	600	ATP	N3-C4-N9	5.36	136.28	127.17
2	A	600	ATP	N3-C4-N9	5.03	135.72	127.17
2	G	600	ATP	N3-C4-N9	5.02	135.70	127.17
2	C	600	ATP	N3-C4-N9	4.90	135.50	127.17
2	F	600	ATP	N3-C4-N9	4.90	135.49	127.17
2	D	600	ATP	N3-C4-N9	4.86	135.44	127.17
2	B	600	ATP	N3-C4-N9	4.69	135.14	127.17
2	E	600	ATP	C2-N3-C4	4.03	121.67	111.83
2	H	600	ATP	C2-N3-C4	4.00	121.60	111.83
2	D	600	ATP	N3-C2-N1	-3.94	122.62	128.58
2	F	600	ATP	C2-N3-C4	3.92	121.40	111.83
2	D	600	ATP	C4-N9-C8	3.89	109.83	105.74
2	A	600	ATP	C2-N3-C4	3.87	121.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	ATP	C2-N3-C4	3.85	121.24	111.83
2	C	600	ATP	C2-N3-C4	3.83	121.18	111.83
2	G	600	ATP	C2-N3-C4	3.82	121.16	111.83
2	B	600	ATP	C2-N3-C4	3.77	121.05	111.83
2	B	600	ATP	N3-C2-N1	-3.76	122.90	128.58
2	C	600	ATP	N3-C2-N1	-3.74	122.92	128.58
2	F	600	ATP	N3-C2-N1	-3.73	122.94	128.58
2	E	600	ATP	N3-C2-N1	-3.72	122.95	128.58
2	A	600	ATP	N3-C2-N1	-3.72	122.96	128.58
2	H	600	ATP	N3-C2-N1	-3.67	123.03	128.58
2	G	600	ATP	N3-C2-N1	-3.64	123.07	128.58
2	G	600	ATP	C4-N9-C8	3.51	109.42	105.74
2	B	600	ATP	C4-C5-N7	-3.43	106.66	110.58
2	B	600	ATP	C4-N9-C8	3.33	109.23	105.74
2	E	600	ATP	C4-N9-C8	3.26	109.16	105.74
2	A	600	ATP	C4-N9-C8	3.22	109.12	105.74
2	C	600	ATP	C4-N9-C8	3.20	109.10	105.74
2	H	600	ATP	C4-N9-C8	3.19	109.09	105.74
2	C	600	ATP	C4-C5-N7	-3.17	106.96	110.58
2	A	600	ATP	C4-C5-N7	-3.15	106.98	110.58
2	D	600	ATP	C4-C5-N7	-3.08	107.06	110.58
2	F	600	ATP	C4-N9-C8	3.05	108.94	105.74
2	F	600	ATP	C4-C5-N7	-3.04	107.11	110.58
2	G	600	ATP	C4-C5-N7	-3.02	107.12	110.58
2	H	600	ATP	C4-C5-N7	-2.97	107.18	110.58
2	E	600	ATP	C4-C5-N7	-2.92	107.24	110.58
2	B	600	ATP	C5-N7-C8	2.70	107.70	103.45
2	D	600	ATP	N9-C8-N7	-2.69	110.12	113.94
2	D	600	ATP	C5-N7-C8	2.62	107.58	103.45
2	C	600	ATP	C5-N7-C8	2.58	107.51	103.45
2	G	600	ATP	C5-N7-C8	2.54	107.44	103.45
2	A	600	ATP	C5-N7-C8	2.53	107.43	103.45
2	E	600	ATP	C5-N7-C8	2.49	107.36	103.45
2	F	600	ATP	C5-N7-C8	2.48	107.34	103.45
2	G	600	ATP	N9-C8-N7	-2.47	110.44	113.94
2	H	600	ATP	C5-N7-C8	2.45	107.31	103.45
2	B	600	ATP	N9-C8-N7	-2.40	110.53	113.94
2	E	600	ATP	N9-C8-N7	-2.33	110.64	113.94
2	C	600	ATP	N9-C8-N7	-2.32	110.64	113.94
2	F	600	ATP	N9-C8-N7	-2.30	110.67	113.94
2	B	600	ATP	C2-N1-C6	2.27	122.47	118.73
2	A	600	ATP	N9-C8-N7	-2.24	110.76	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	ATP	C6-C5-N7	2.16	136.25	132.09
2	B	600	ATP	C6-C5-N7	2.14	136.21	132.09
2	H	600	ATP	N9-C8-N7	-2.13	110.92	113.94
2	H	600	ATP	N6-C6-N1	2.13	123.11	118.38
2	D	600	ATP	C2-N1-C6	2.11	122.19	118.73
2	C	600	ATP	C2-N1-C6	2.10	122.18	118.73
2	F	600	ATP	C3'-C2'-C1'	2.07	105.37	101.46
2	A	600	ATP	C2-N1-C6	2.03	122.07	118.73

There are no chirality outliers.

All (25) torsion outliers are listed below:

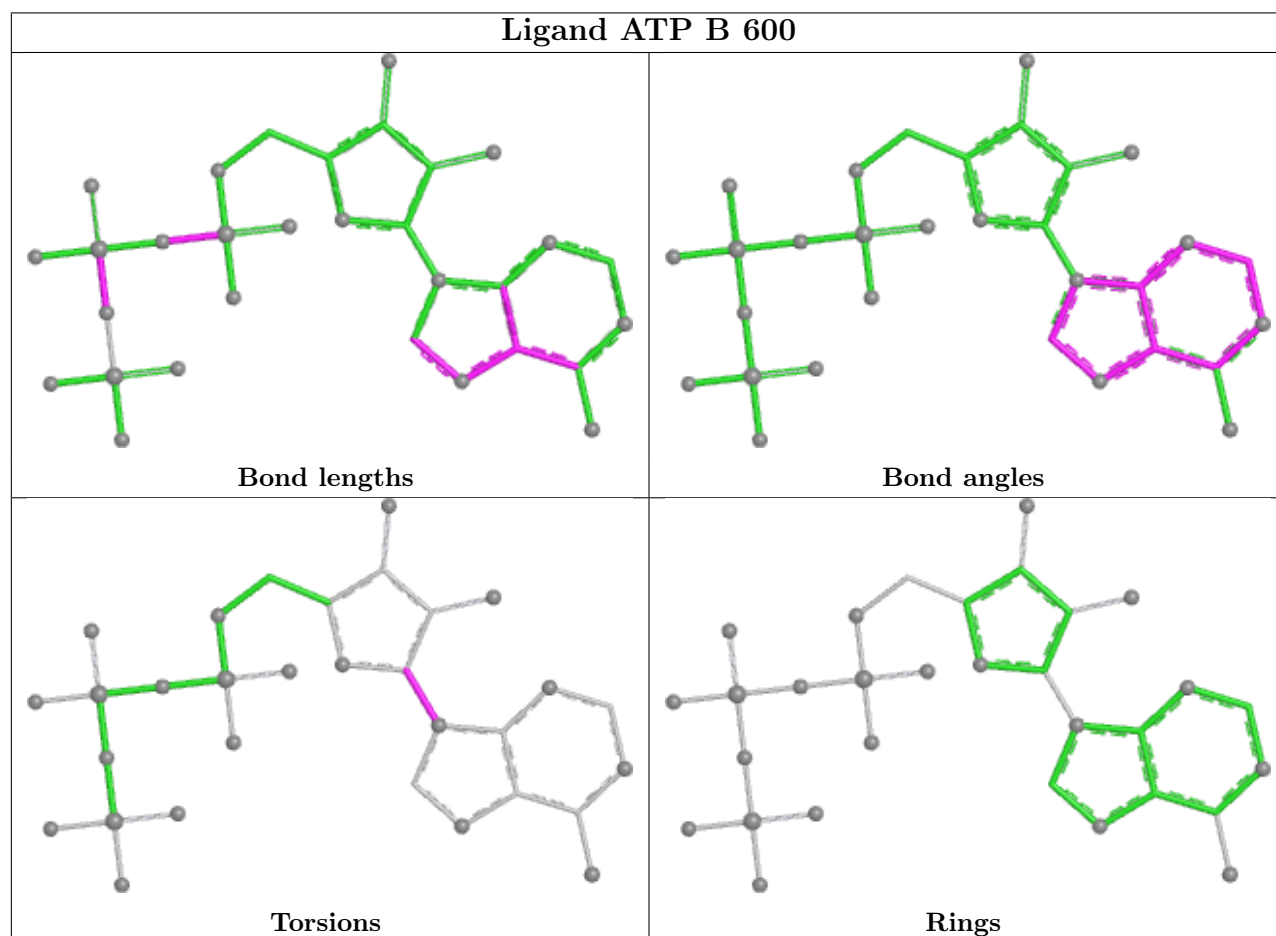
Mol	Chain	Res	Type	Atoms
2	A	600	ATP	PB-O3B-PG-O3G
2	D	600	ATP	C5'-O5'-PA-O2A
2	H	600	ATP	PB-O3B-PG-O2G
2	H	600	ATP	PB-O3B-PG-O1G
2	E	600	ATP	PB-O3A-PA-O1A
2	F	600	ATP	PB-O3A-PA-O1A
2	A	600	ATP	PG-O3B-PB-O1B
2	G	600	ATP	PB-O3A-PA-O2A
2	D	600	ATP	O4'-C4'-C5'-O5'
2	A	600	ATP	PG-O3B-PB-O2B
2	E	600	ATP	PB-O3A-PA-O2A
2	F	600	ATP	PB-O3A-PA-O2A
2	A	600	ATP	PB-O3B-PG-O1G
2	G	600	ATP	PB-O3A-PA-O1A
2	H	600	ATP	PG-O3B-PB-O1B
2	H	600	ATP	C4'-C5'-O5'-PA
2	H	600	ATP	O4'-C1'-N9-C8
2	D	600	ATP	C3'-C4'-C5'-O5'
2	H	600	ATP	O4'-C4'-C5'-O5'
2	G	600	ATP	O4'-C1'-N9-C8
2	B	600	ATP	O4'-C1'-N9-C8
2	D	600	ATP	O4'-C1'-N9-C8
2	C	600	ATP	PB-O3A-PA-O2A
2	D	600	ATP	PB-O3A-PA-O2A
2	H	600	ATP	PG-O3B-PB-O2B

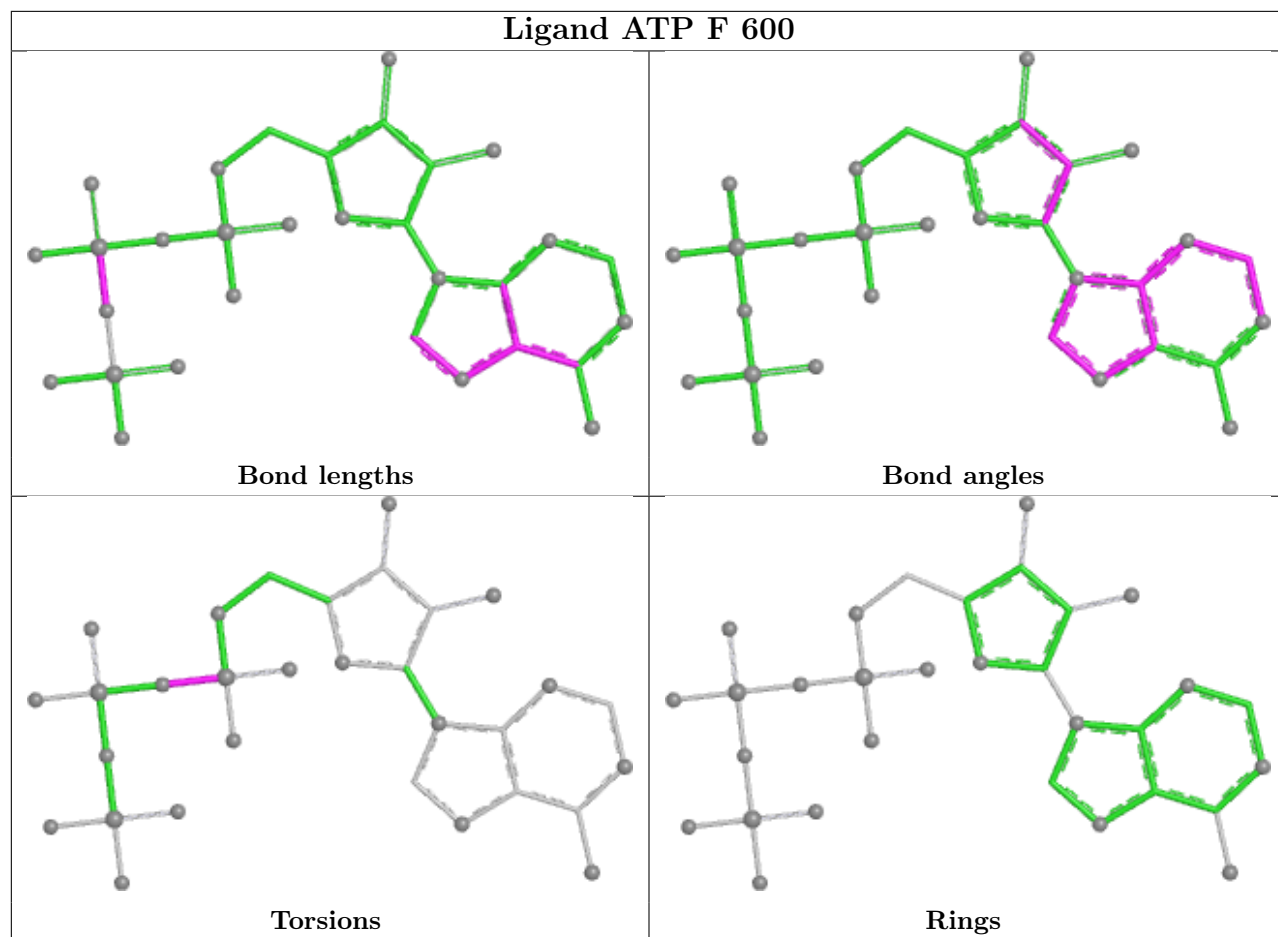
There are no ring outliers.

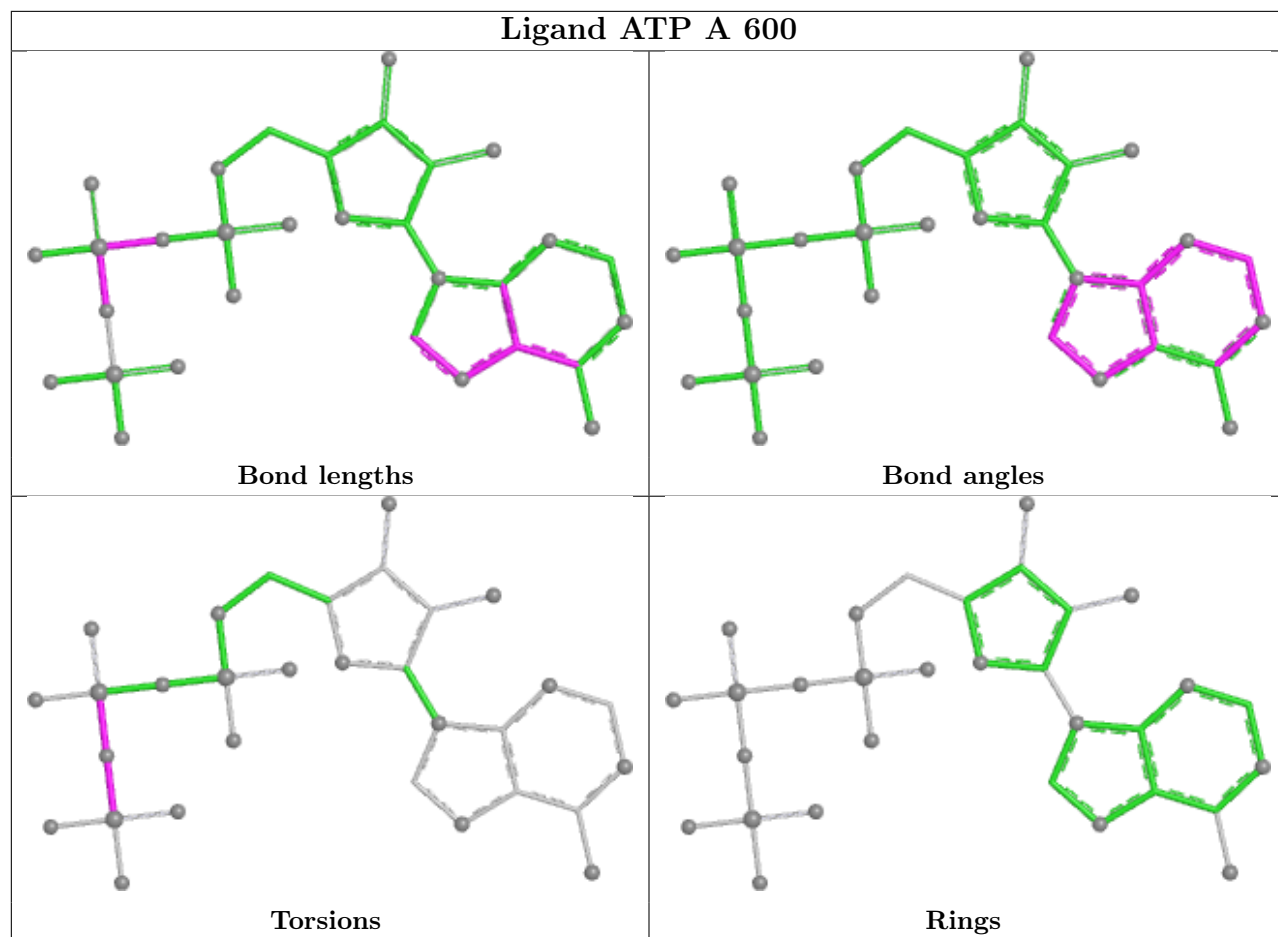
4 monomers are involved in 7 short contacts:

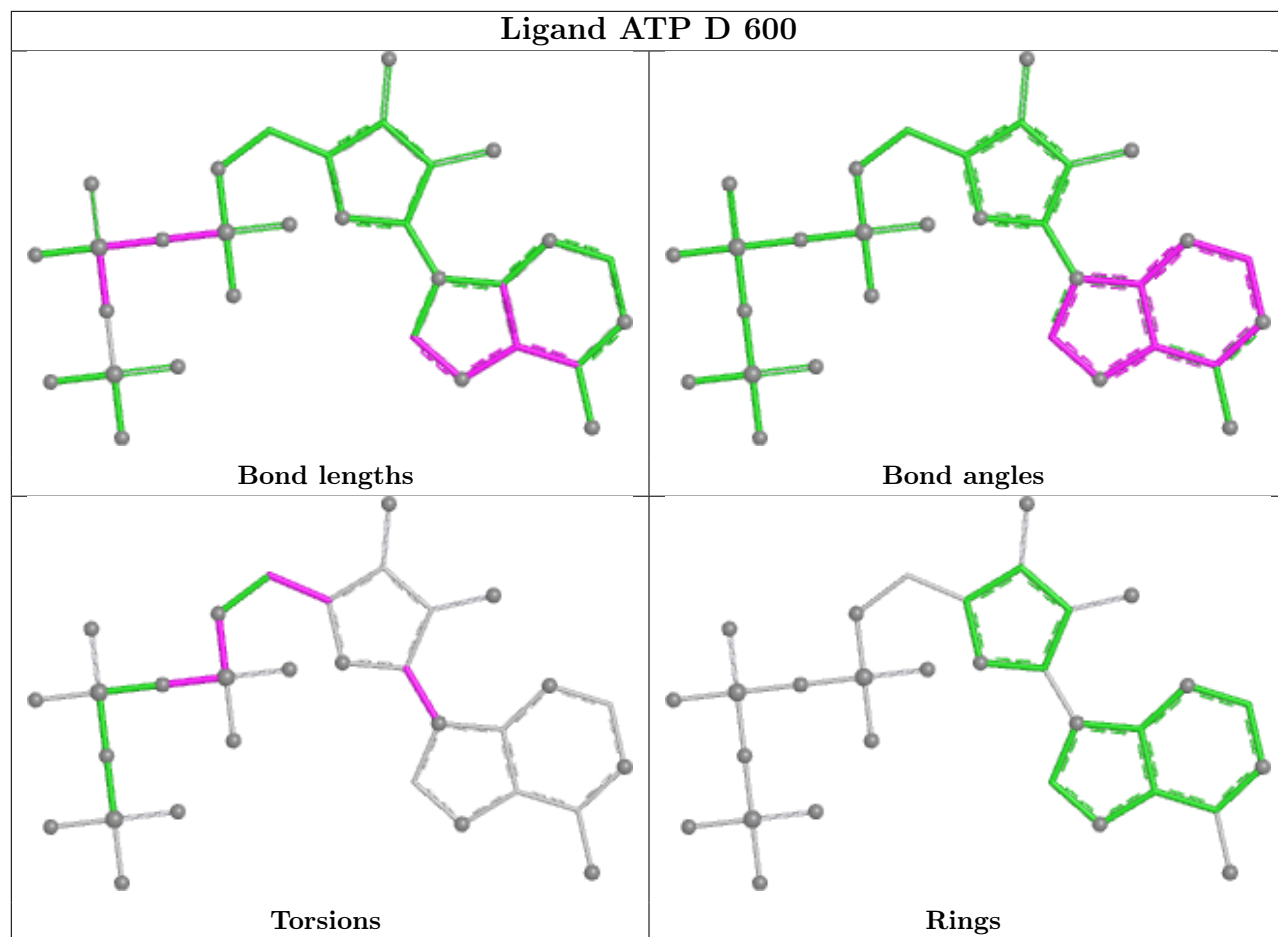
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	600	ATP	2	0
2	A	600	ATP	2	0
2	G	600	ATP	1	0
2	E	600	ATP	2	0

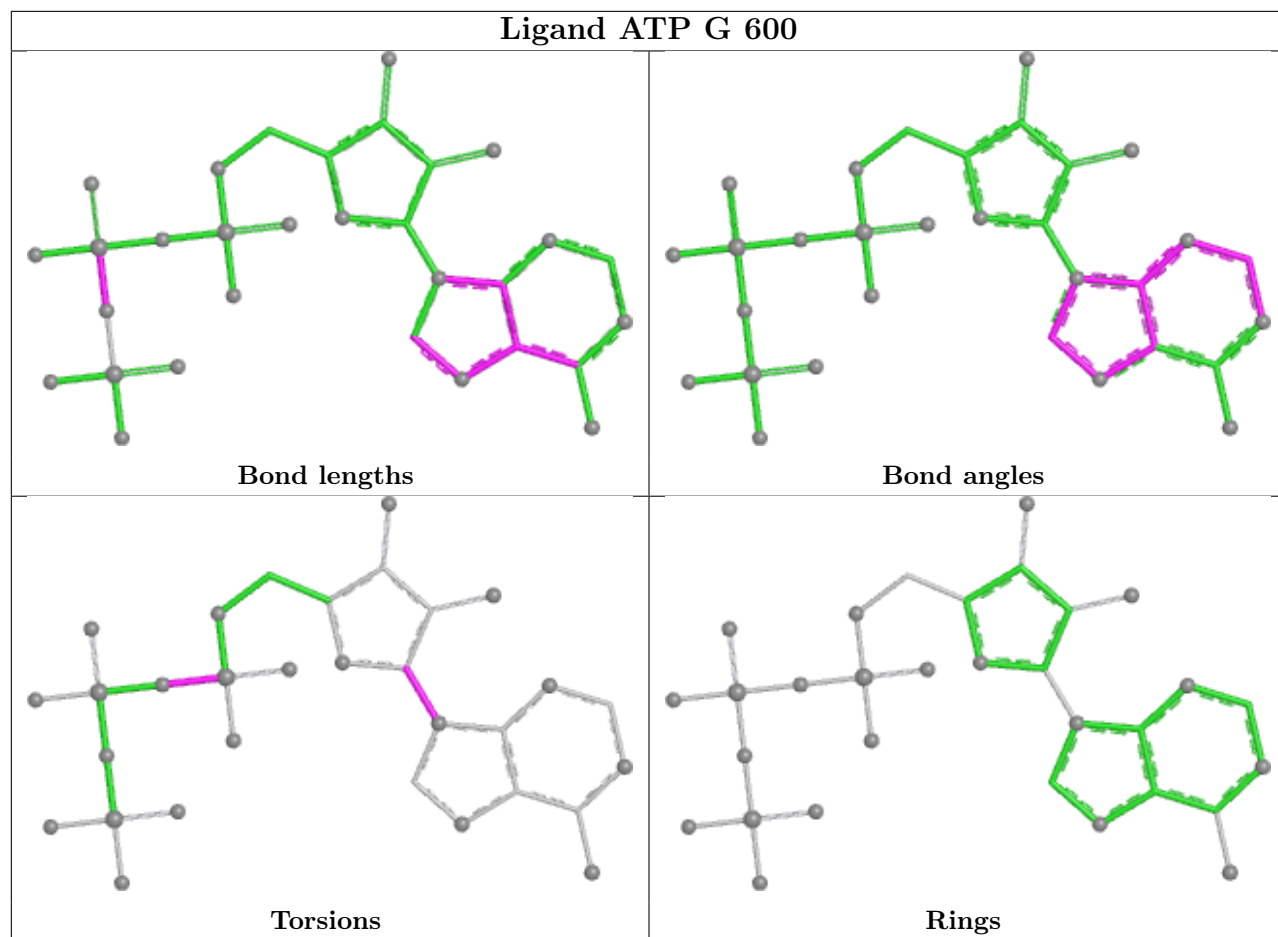
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

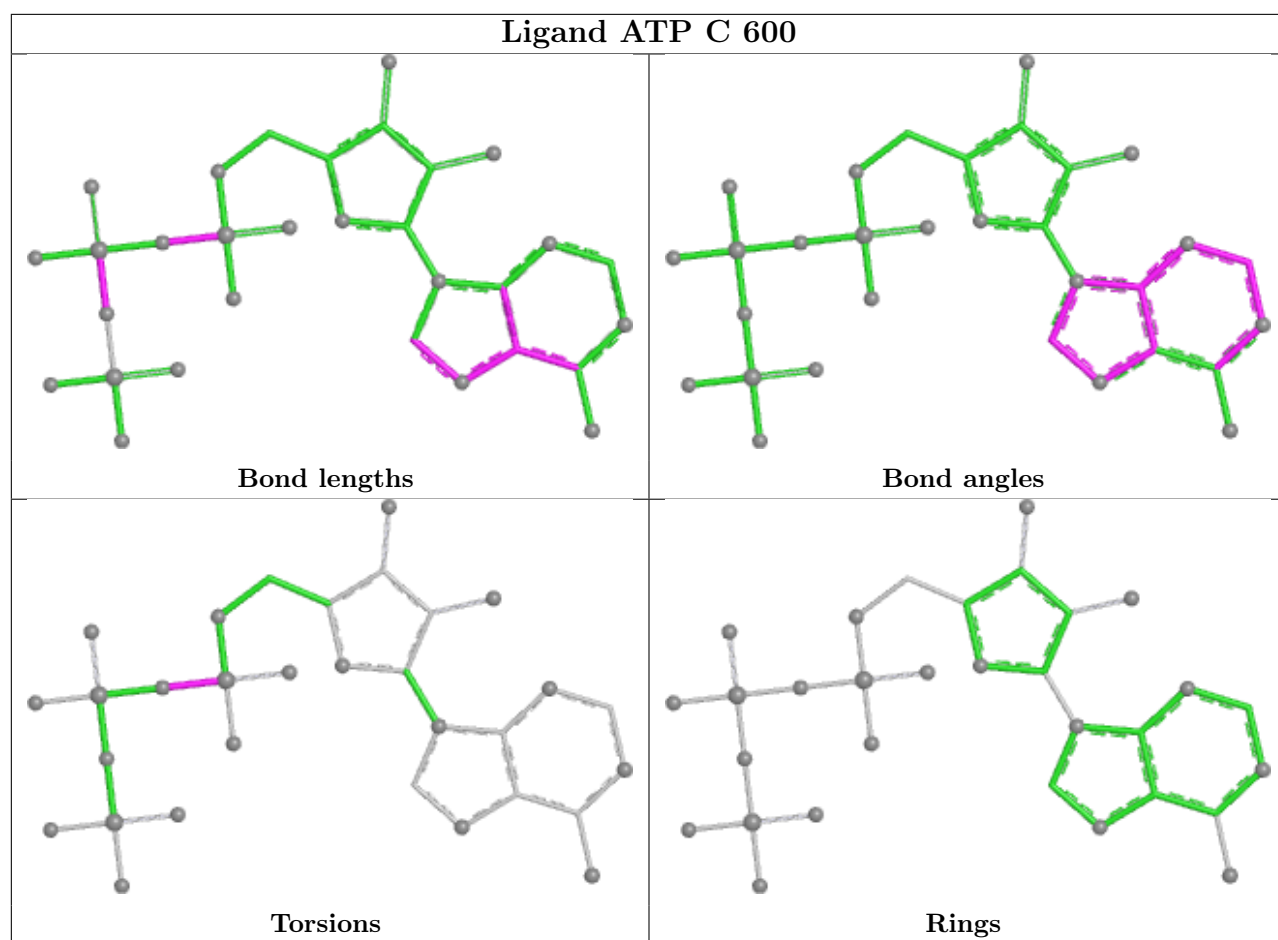


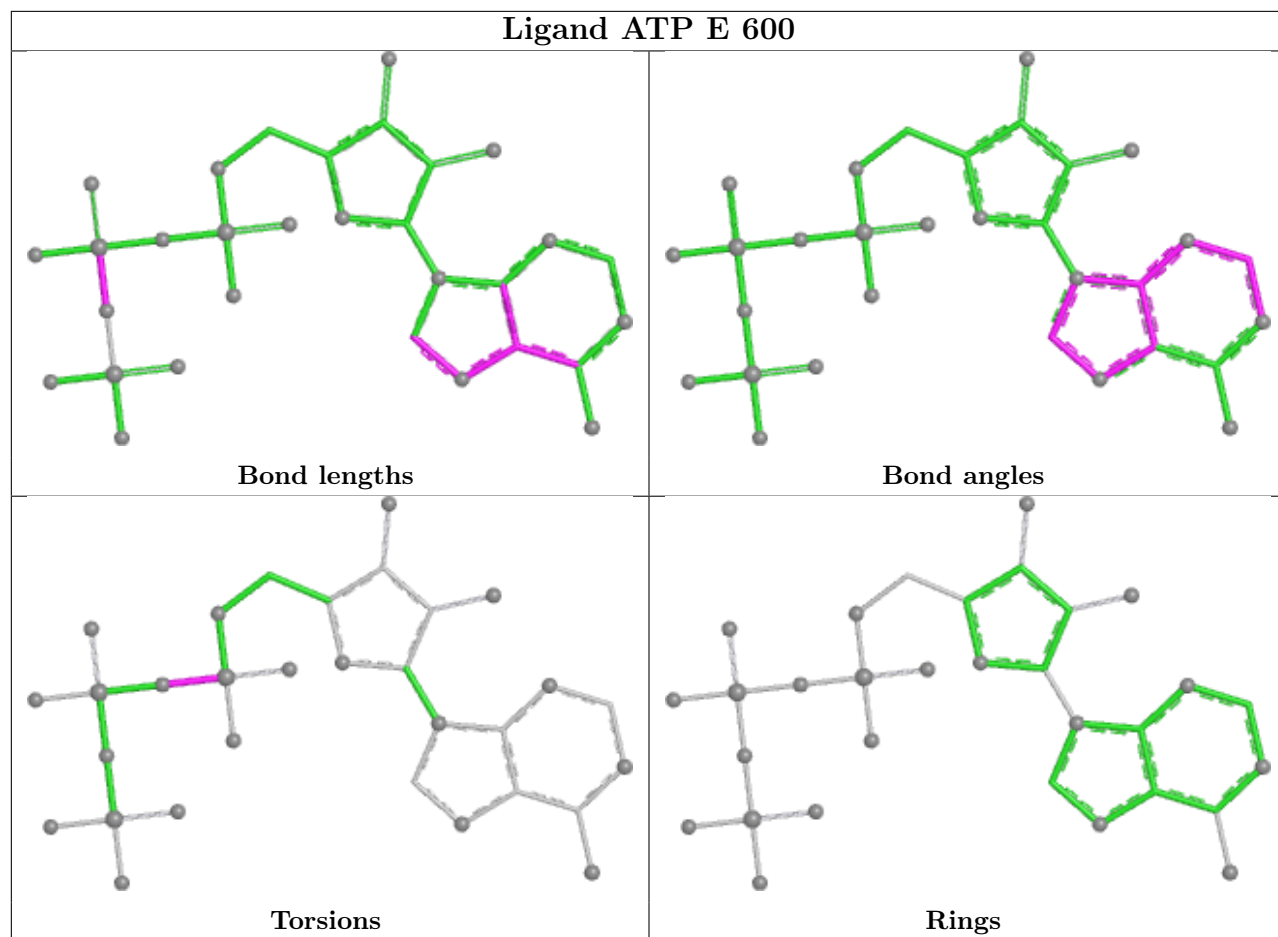


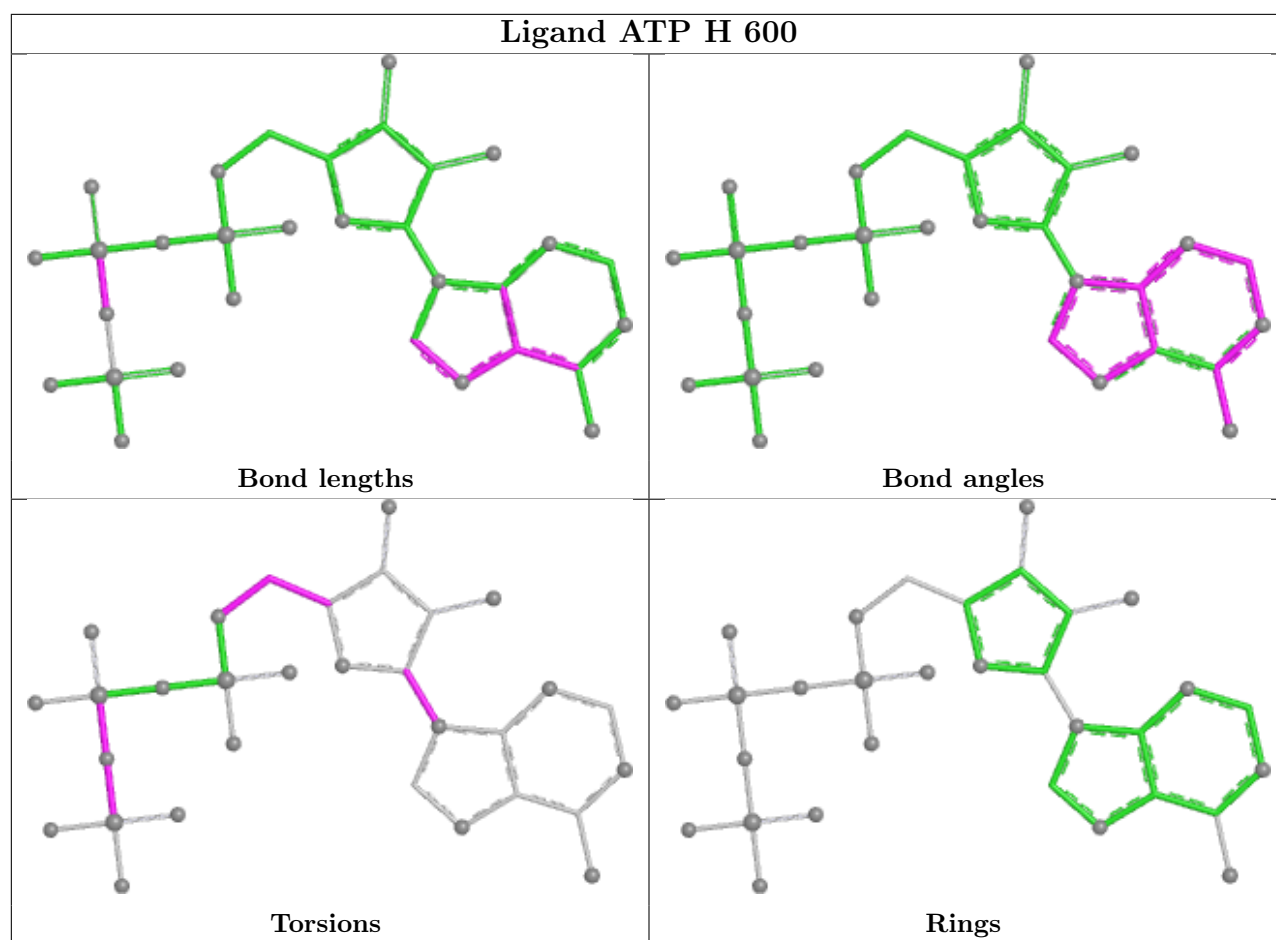












5.7 Other polymers [i](#)

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	556/576 (96%)	-1.50	0 100 100	12, 26, 47, 69	0
1	B	556/576 (96%)	-1.45	0 100 100	14, 29, 48, 68	0
1	C	552/576 (95%)	-1.52	0 100 100	11, 23, 44, 61	0
1	D	552/576 (95%)	-1.43	0 100 100	13, 27, 51, 71	0
1	E	552/576 (95%)	-1.52	0 100 100	11, 21, 41, 67	0
1	F	551/576 (95%)	-1.05	0 100 100	21, 40, 83, 114	0
1	G	552/576 (95%)	-1.58	0 100 100	8, 18, 36, 58	0
1	H	550/576 (95%)	-1.25	0 100 100	14, 32, 71, 90	0
All	All	4421/4608 (95%)	-1.41	0 100 100	8, 27, 58, 114	0

There are no RSRZ outliers to report.

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](#)

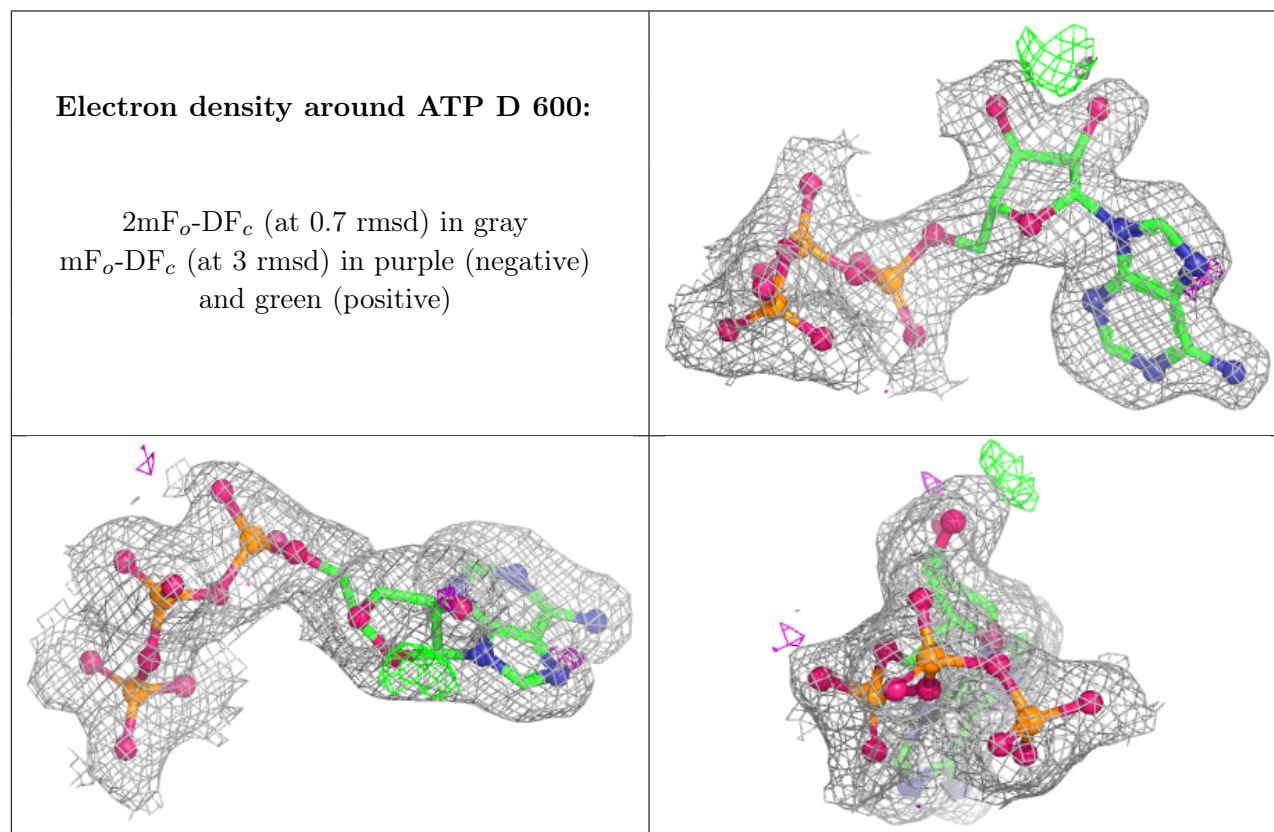
There are no oligosaccharides in this entry.

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.

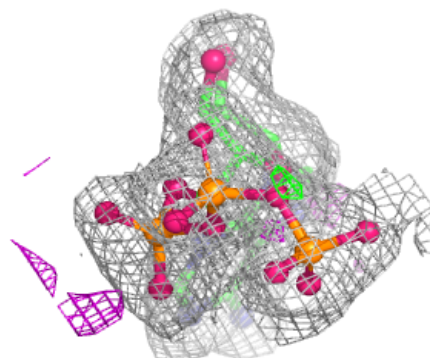
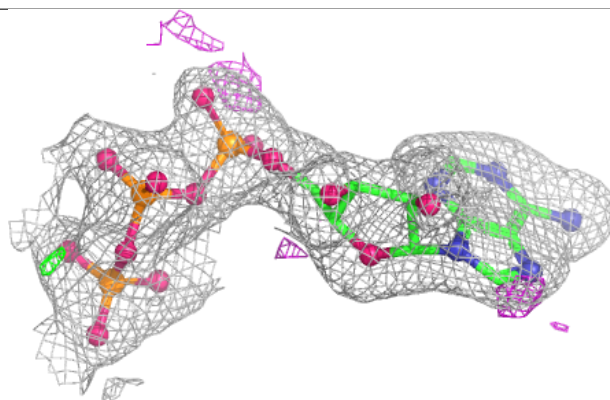
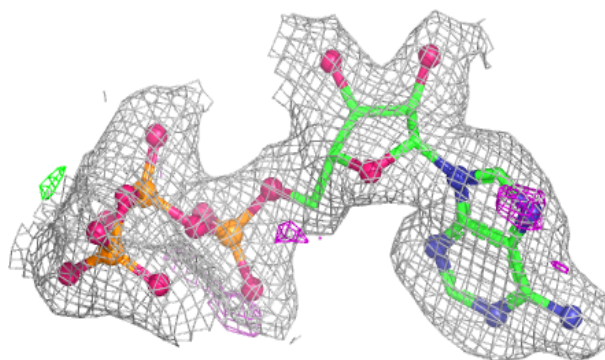
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	601	1/1	0.99	0.04	14,14,14,14	0
3	MG	D	601	1/1	0.99	0.05	21,21,21,21	0
3	MG	E	601	1/1	0.99	0.04	21,21,21,21	0
2	ATP	D	600	31/31	1.00	0.02	11,16,23,27	0
2	ATP	E	600	31/31	1.00	0.02	8,18,24,25	0
2	ATP	F	600	31/31	1.00	0.02	15,21,32,35	0
2	ATP	G	600	31/31	1.00	0.02	5,14,22,28	0
2	ATP	H	600	31/31	1.00	0.03	13,25,32,37	0
3	MG	A	601	1/1	1.00	0.01	19,19,19,19	0
3	MG	B	601	1/1	1.00	0.02	24,24,24,24	0
2	ATP	A	600	31/31	1.00	0.02	14,20,25,28	0
2	ATP	B	600	31/31	1.00	0.02	11,27,30,35	0
2	ATP	C	600	31/31	1.00	0.02	7,13,20,23	0
3	MG	F	601	1/1	1.00	0.03	27,27,27,27	0
3	MG	G	601	1/1	1.00	0.01	17,17,17,17	0
3	MG	H	601	1/1	1.00	0.05	30,30,30,30	0

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

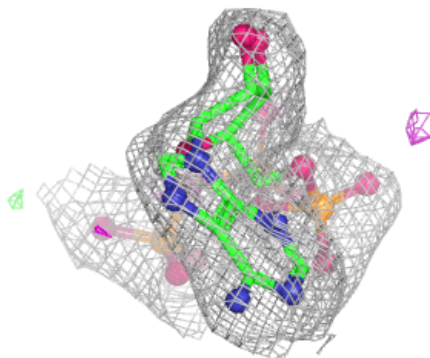
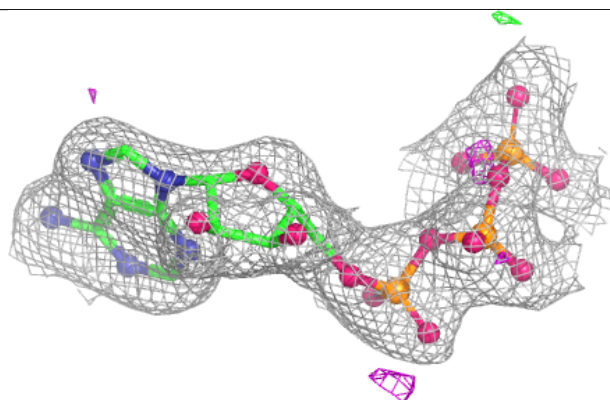
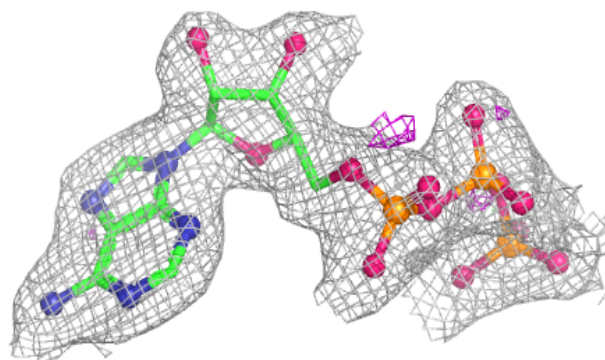


Electron density around ATP E 600:

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

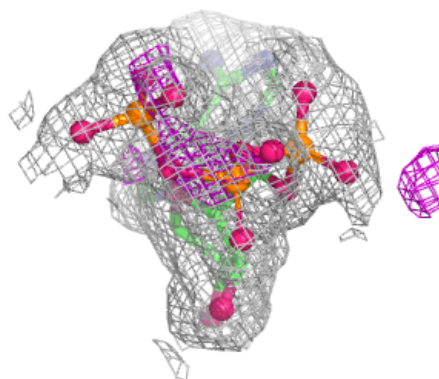
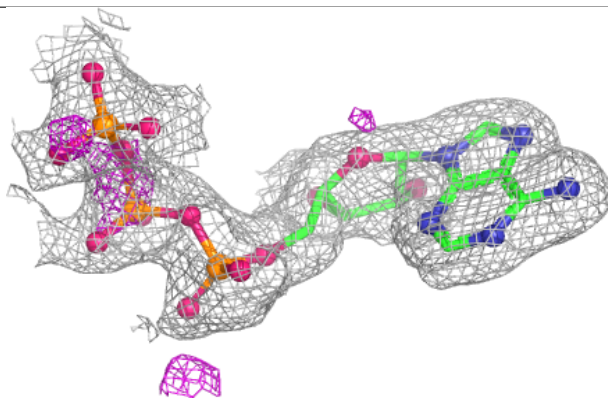
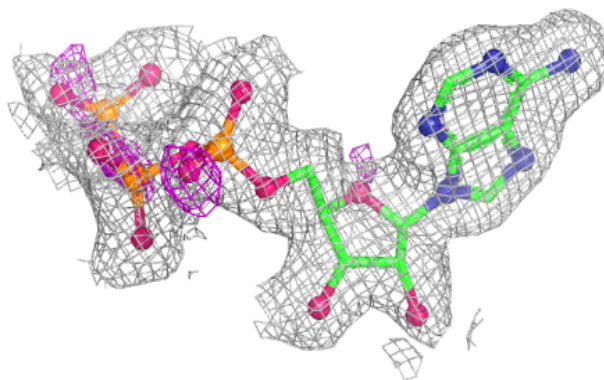
**Electron density around ATP F 600:**

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

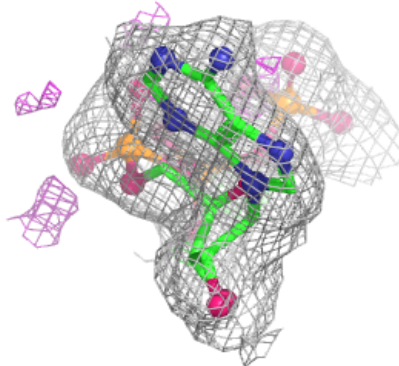
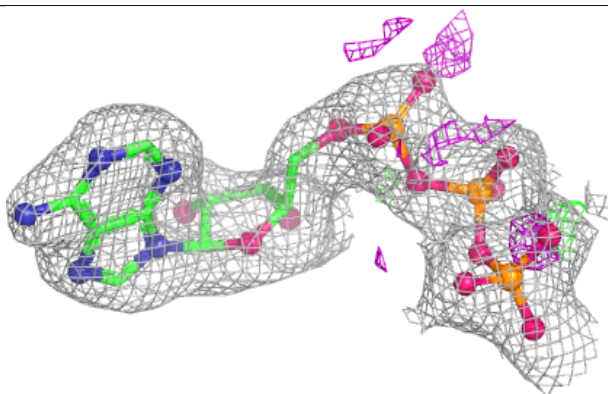
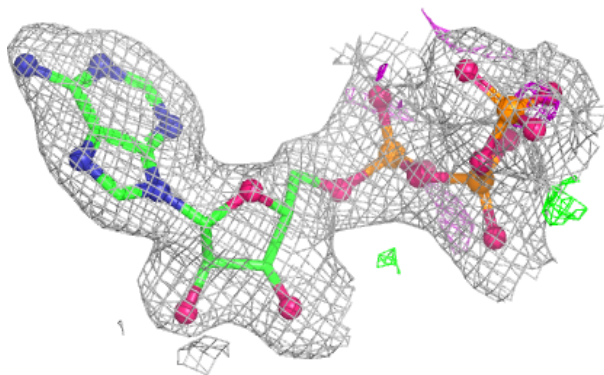


Electron density around ATP G 600:

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

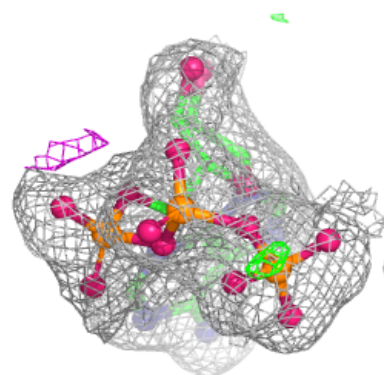
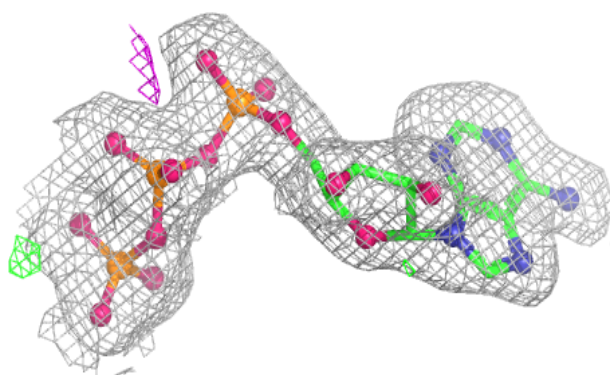
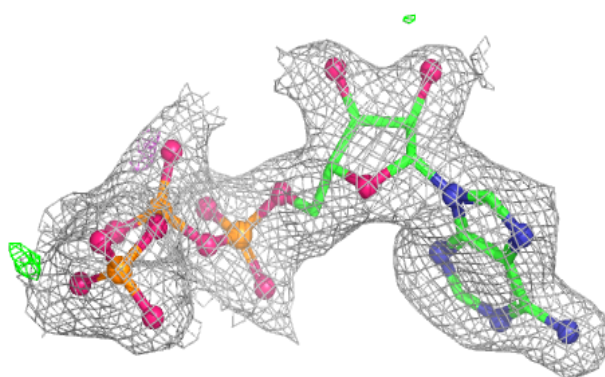
**Electron density around ATP H 600:**

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

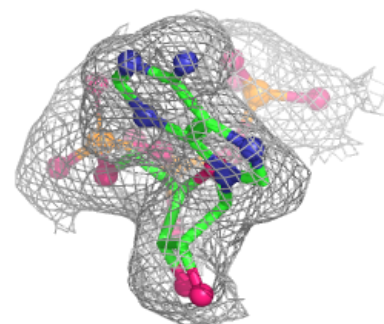
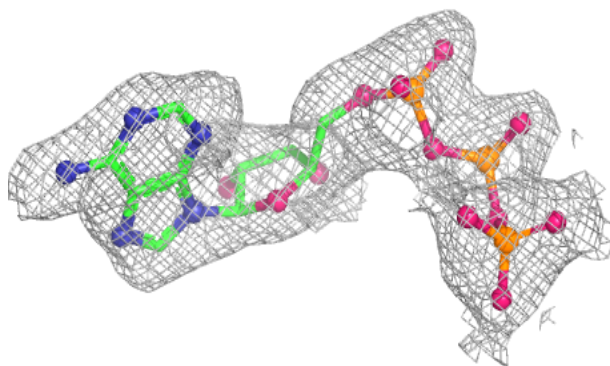
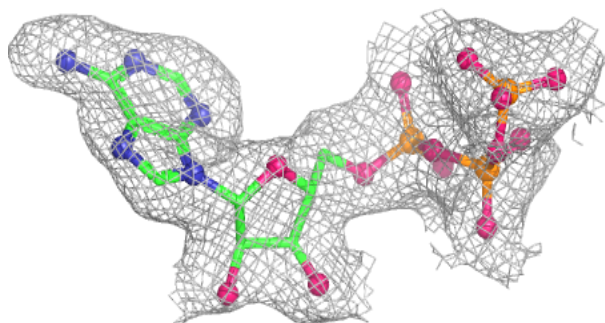


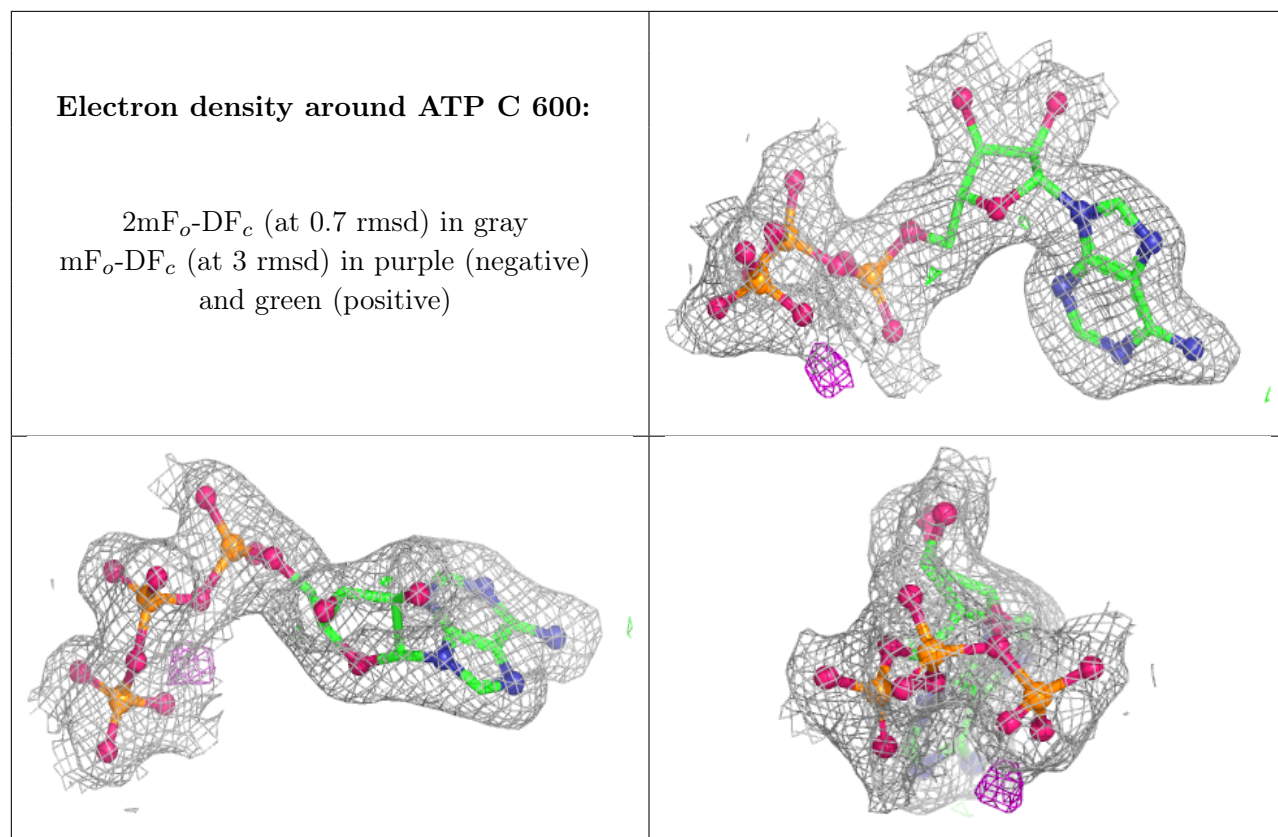
Electron density around ATP A 600:

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

**Electron density around ATP 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 ⓘ

There are no such residues in this entry.