



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:04 AM UTC

PDB ID : 7XZO / pdb_00007xzo
Title : Formate-tetrahydrofolate ligase in complex with ATP
Authors : Fang, C.L.; Zhang, Y.
Deposited on : 2022-06-03
Resolution : 2.31 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

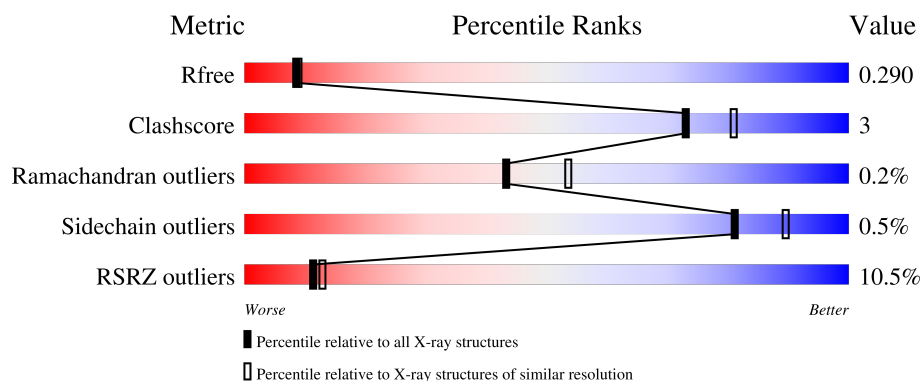
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	562	9% 89% 10%
1	B	562	12% 89% 10%
1	C	562	13% 91% 8%
1	D	562	8% 92% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17002 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 Formate--tetrahydrofolate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4170	2621	720	808	21			
1	B	556	Total	C	N	O	S	0	0	0
			4174	2625	721	807	21			
1	C	561	Total	C	N	O	S	0	0	0
			4216	2652	730	811	23			
1	D	560	Total	C	N	O	S	0	0	0
			4208	2644	729	812	23			

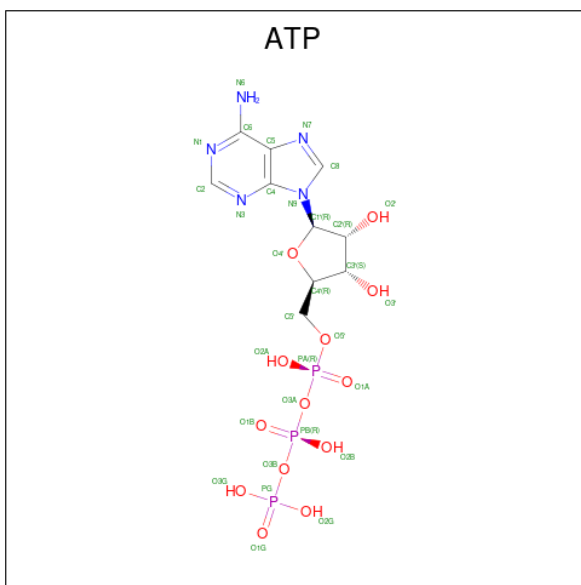
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A379CIH2
A	-2	SER	-	expression tag	UNP A0A379CIH2
A	-1	HIS	-	expression tag	UNP A0A379CIH2
A	0	MET	-	expression tag	UNP A0A379CIH2
B	-3	GLY	-	expression tag	UNP A0A379CIH2
B	-2	SER	-	expression tag	UNP A0A379CIH2
B	-1	HIS	-	expression tag	UNP A0A379CIH2
B	0	MET	-	expression tag	UNP A0A379CIH2
C	-3	GLY	-	expression tag	UNP A0A379CIH2
C	-2	SER	-	expression tag	UNP A0A379CIH2
C	-1	HIS	-	expression tag	UNP A0A379CIH2
C	0	MET	-	expression tag	UNP A0A379CIH2
D	-3	GLY	-	expression tag	UNP A0A379CIH2
D	-2	SER	-	expression tag	UNP A0A379CIH2
D	-1	HIS	-	expression tag	UNP A0A379CIH2
D	0	MET	-	expression tag	UNP A0A379CIH2

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

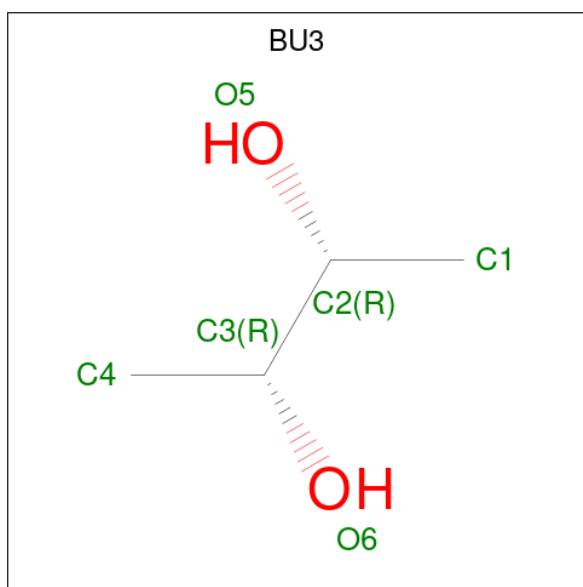
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

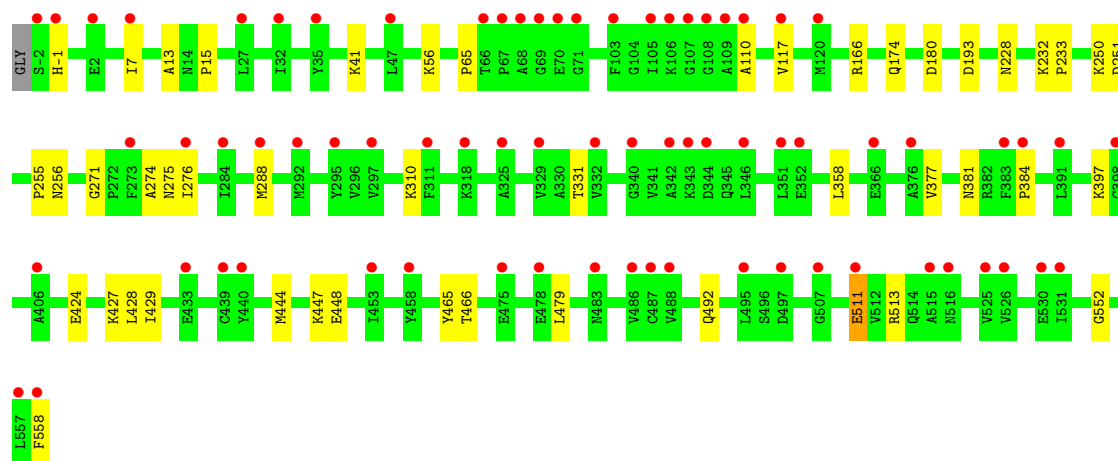
- Molecule 4 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: $C_4H_{10}O_2$).



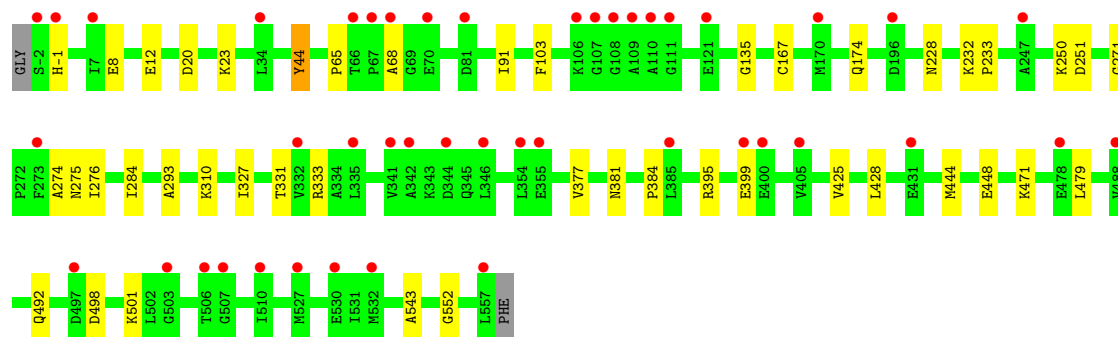
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	24	Total	O	0	0
			24	24		
5	C	16	Total	O	0	0
			16	16		
5	D	15	Total	O	0	0
			15	15		



- Molecule 1: Formate--tetrahydrofolate ligase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.28Å 115.10Å 106.53Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	30.03 – 2.31 30.03 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.03-2.31) 99.8 (30.03-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.252 , 0.290 0.253 , 0.290	Depositor DCC
R_{free} test set	1980 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17002	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 56.51 % 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 2.7075e-05. 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: ATP, K, BU3

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	0.10	0/4229	0.27	0/5724
1	B	0.09	0/4233	0.27	0/5730
1	C	0.09	0/4277	0.25	0/5788
1	D	0.08	0/4268	0.24	0/5776
All	All	0.09	0/17007	0.26	0/23018

There are no bond length outliers.

There are no bond angle outliers.

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	4170	0	4209	33	0
1	B	4174	0	4216	33	0
1	C	4216	0	4256	26	0
1	D	4208	0	4249	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	B	30	0	50	3	0
5	A	21	0	0	1	0
5	B	24	0	0	1	0
5	C	16	0	0	0	0
5	D	15	0	0	0	0
All	All	17002	0	17028	109	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 (109) 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:B:375:PRO:HD3	1:B:434:ASN:HB3	1.56	0.85
1:B:387:THR:HG22	1:B:389:ALA:H	1.56	0.70
1:A:332:VAL:HG12	1:A:336:LYS:HE2	1.79	0.64
1:A:41:LYS:NZ	1:A:256:ASN:OD1	2.30	0.64
1:B:41:LYS:NZ	1:B:256:ASN:OD1	2.33	0.62
1:D:44:TYR:HB3	1:D:284:ILE:HD11	1.84	0.59
1:D:331:THR:HG22	1:D:381:ASN:HB3	1.83	0.59
1:C:331:THR:HG22	1:C:381:ASN:HB3	1.82	0.59
1:A:444:MET:HE2	1:A:448:GLU:HB3	1.82	0.59
1:C:-1:HIS:HB3	1:C:384:PRO:HG3	1.85	0.58
1:B:355:GLU:HG2	1:B:393:LEU:HD21	1.86	0.58
1:B:39:LYS:NZ	1:B:122:ASP:OD2	2.34	0.58
1:C:444:MET:HE2	1:C:448:GLU:HB3	1.85	0.57
1:D:444:MET:HE2	1:D:448:GLU:HB3	1.87	0.57
1:B:553:LYS:HZ2	1:B:554:ILE:H	1.52	0.56
1:D:498:ASP:HB3	1:D:501:LYS:HD2	1.88	0.54
1:C:233:PRO:HG3	1:C:479:LEU:HD13	1.89	0.54
1:A:166:ARG:NH1	1:A:193:ASP:OD2	2.41	0.53
1:D:228:ASN:OD1	1:D:232:LYS:N	2.41	0.53
1:D:233:PRO:HG3	1:D:479:LEU:HD13	1.91	0.53
1:B:228:ASN:HD21	1:B:232:LYS:HB2	1.75	0.52
1:A:228:ASN:HD21	1:A:232:LYS:HB2	1.73	0.52
1:D:274:ALA:O	1:D:310:LYS:NZ	2.41	0.52
1:B:475:GLU:HB3	4:B:605:BU3:H43	1.90	0.52
1:C:41:LYS:NZ	1:C:256:ASN:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HA	1:A:120:MET:HE1	1.91	0.52
1:A:331:THR:HG22	1:A:381:ASN:HB3	1.92	0.51
1:B:7:ILE:O	1:B:11:GLN:HG2	2.10	0.51
1:D:20:ASP:HA	1:D:23:LYS:HE3	1.92	0.51
1:D:395:ARG:O	1:D:399:GLU:HG2	2.11	0.51
1:C:255:PRO:HG2	1:C:288:MET:HE3	1.93	0.51
1:B:56:LYS:HG2	1:B:294:ASP:O	2.10	0.50
1:A:382:ARG:HD3	1:A:407:LEU:HD21	1.93	0.50
1:A:99:MET:HE3	1:A:125:LEU:HD22	1.92	0.49
1:A:250:LYS:NZ	1:A:251:ASP:OD1	2.34	0.49
1:C:56:LYS:HG2	1:C:429:ILE:HG21	1.95	0.49
1:B:553:LYS:NZ	1:B:554:ILE:H	2.11	0.49
1:D:250:LYS:NZ	1:D:251:ASP:OD1	2.32	0.49
1:A:165:ARG:NH1	5:A:704:HOH:O	2.36	0.48
1:C:377:VAL:HB	1:C:428:LEU:HD11	1.93	0.48
1:B:227:TYR:CZ	4:B:605:BU3:H3	2.48	0.48
1:C:274:ALA:O	1:C:310:LYS:NZ	2.40	0.48
1:A:250:LYS:HD2	1:C:552:GLY:O	2.15	0.47
1:A:118:VAL:HG13	1:A:119:PRO:HA	1.97	0.47
1:C:65:PRO:HD2	1:C:492:GLN:O	2.15	0.47
1:B:471:LYS:NZ	1:B:475:GLU:OE2	2.40	0.47
1:B:318:LYS:HA	4:B:606:BU3:H43	1.96	0.46
1:A:423:ASN:O	1:A:427:LYS:HG2	2.15	0.46
1:B:18:ILE:HD11	1:B:257:LEU:HG	1.98	0.46
1:C:41:LYS:HE3	1:C:251:ASP:O	2.15	0.46
1:D:-1:HIS:HB3	1:D:384:PRO:HG3	1.98	0.45
1:B:354:LEU:HD12	1:B:393:LEU:HD23	1.97	0.45
1:D:68:ALA:O	1:D:333:ARG:NH2	2.50	0.45
1:A:445:THR:OG1	1:A:477:GLU:OE2	2.32	0.45
1:D:8:GLU:O	1:D:12:GLU:HG2	2.16	0.45
1:B:445:THR:HG23	1:B:448:GLU:H	1.82	0.45
1:C:288:MET:HE2	1:C:288:MET:HB2	1.80	0.45
1:B:445:THR:OG1	1:B:477:GLU:OE2	2.31	0.45
1:B:250:LYS:HD2	1:D:552:GLY:O	2.16	0.45
1:C:228:ASN:OD1	1:C:232:LYS:N	2.49	0.44
1:A:65:PRO:HA	1:A:70:GLU:OE2	2.16	0.44
1:A:349:GLU:HG3	1:A:387:THR:HG21	1.99	0.44
1:A:384:PRO:HB2	1:A:385:LEU:HD22	2.00	0.44
1:B:101:PRO:HA	1:B:171:ASN:HD21	1.82	0.44
1:B:444:MET:HE2	1:B:448:GLU:HB3	1.98	0.44
1:A:450:LEU:HD21	1:A:526:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ASP:HB2	1:D:174:GLN:O	2.16	0.44
1:A:19:ARG:O	1:A:23:LYS:HG2	2.18	0.44
1:A:497:ASP:HB2	1:A:528:THR:HG21	2.00	0.44
1:B:552:GLY:O	1:D:250:LYS:HD2	2.18	0.44
1:A:25:ILE:HG21	1:A:91:ILE:HD11	2.00	0.44
1:A:552:GLY:O	1:C:250:LYS:HD2	2.18	0.44
1:B:19:ARG:O	1:B:23:LYS:HG2	2.16	0.44
1:B:223:ILE:HG12	1:B:520:GLY:HA3	1.99	0.44
1:D:103:PHE:HB3	1:D:543:ALA:HB2	2.00	0.44
1:D:275:ASN:OD1	1:D:276:ILE:N	2.45	0.44
1:C:110:ALA:HB3	1:C:117:VAL:HB	2.00	0.43
1:D:377:VAL:HB	1:D:428:LEU:HD11	2.01	0.43
1:A:332:VAL:HG13	1:A:354:LEU:HD13	2.01	0.43
1:A:497:ASP:CB	1:A:528:THR:HG21	2.49	0.42
1:D:135:GLY:HA2	1:D:167:CYS:SG	2.59	0.42
1:A:445:THR:HG23	1:A:448:GLU:H	1.84	0.42
1:C:358:LEU:HD13	1:C:397:LYS:HG3	2.02	0.42
1:B:354:LEU:HD11	1:B:394:VAL:HG22	2.01	0.42
1:A:180:ASP:HB2	1:C:174:GLN:O	2.20	0.42
1:C:13:ALA:O	1:C:15:PRO:HD3	2.19	0.42
1:A:83:LEU:CB	1:A:90:VAL:HG21	2.49	0.42
1:B:311:PHE:HE1	1:B:323:PRO:HG3	1.84	0.42
1:C:466:THR:HG23	1:C:511:GLU:OE2	2.19	0.42
1:D:327:ILE:HD11	1:D:425:VAL:HG21	2.02	0.42
1:A:88:LYS:HD2	1:A:295:TYR:CE1	2.55	0.41
1:A:334:ALA:O	1:A:338:ASN:ND2	2.34	0.41
1:C:447:LYS:HE2	1:C:465:TYR:CZ	2.56	0.41
1:B:220:LEU:HD22	1:B:245:MET:HE2	2.02	0.41
1:A:174:GLN:O	1:C:180:ASP:HB2	2.19	0.41
1:A:322:ARG:HA	1:A:323:PRO:HD3	1.96	0.41
1:B:120:MET:HE2	1:B:558:PHE:CD1	2.56	0.41
1:B:498:ASP:OD2	1:B:500:THR:OG1	2.38	0.41
1:C:166:ARG:NH1	1:C:193:ASP:OD2	2.54	0.41
1:B:250:LYS:NZ	1:B:251:ASP:OD1	2.40	0.41
1:A:382:ARG:HB2	1:A:407:LEU:HD11	2.03	0.41
1:B:165:ARG:NH1	5:B:701:HOH:O	2.36	0.41
1:C:7:ILE:HD11	1:C:558:PHE:HB2	2.02	0.41
1:D:91:ILE:HG13	1:D:293:ALA:HB2	2.03	0.41
1:D:471:LYS:HE2	1:D:471:LYS:HB3	1.88	0.41
1:B:44:TYR:HA	1:B:288:MET:HE1	2.02	0.40
1:C:424:GLU:HA	1:C:427:LYS:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ASN:OD1	1:C:276:ILE:N	2.50	0.40
1:D:65:PRO:HD2	1:D:492:GLN: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	553/562 (98%)	529 (96%)	23 (4%)	1 (0%)	43	53
1	B	554/562 (99%)	533 (96%)	20 (4%)	1 (0%)	43	53
1	C	559/562 (100%)	538 (96%)	20 (4%)	1 (0%)	43	53
1	D	558/562 (99%)	537 (96%)	20 (4%)	1 (0%)	43	53
All	All	2224/2248 (99%)	2137 (96%)	83 (4%)	4 (0%)	43	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	GLY
1	D	271	GLY
1	C	271	GLY
1	B	271	GLY

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	437/447 (98%)	437 (100%)	0	100	100
1	B	437/447 (98%)	431 (99%)	6 (1%)	59	75
1	C	441/447 (99%)	439 (100%)	2 (0%)	81	89
1	D	441/447 (99%)	440 (100%)	1 (0%)	87	94
All	All	1756/1788 (98%)	1747 (100%)	9 (0%)	81	89

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

Mol	Chain	Res	Type
1	B	105	ILE
1	B	118	VAL
1	B	258	VAL
1	B	354	LEU
1	B	385	LEU
1	B	443	ASP
1	C	511	GLU
1	C	513	ARG
1	D	44	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	413	ASN
1	A	516	ASN
1	B	16	GLN
1	B	171	ASN
1	B	345	GLN
1	B	360	ASN
1	C	16	GLN
1	C	177	ASN
1	D	11	GLN
1	D	345	GLN
1	D	348	ASN
1	D	360	ASN

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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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$
4	BU3	B	606	-	4,5,5	0.32	0	6,6,6	0.32	0
4	BU3	B	603	-	4,5,5	0.32	0	6,6,6	0.30	0
4	BU3	B	604	-	4,5,5	0.31	0	6,6,6	0.30	0
3	ATP	B	602	-	32,33,33	1.42	5 (15%)	48,52,52	1.77	9 (18%)
3	ATP	D	602	-	32,33,33	1.45	6 (18%)	48,52,52	1.79	9 (18%)
4	BU3	B	607	-	4,5,5	0.36	0	6,6,6	0.39	0
3	ATP	A	602	-	32,33,33	1.41	5 (15%)	48,52,52	1.77	10 (20%)
3	ATP	C	602	-	32,33,33	1.44	6 (18%)	48,52,52	1.76	8 (16%)
4	BU3	B	605	-	4,5,5	0.27	0	6,6,6	0.37	0

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
4	BU3	B	606	-	-	0/4/4/4	-
4	BU3	B	603	-	-	4/4/4/4	-
4	BU3	B	604	-	-	0/4/4/4	-
3	ATP	B	602	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	D	602	-	-	9/22/38/38	0/3/3/3
4	BU3	B	607	-	-	3/4/4/4	-
3	ATP	A	602	-	-	1/22/38/38	0/3/3/3
3	ATP	C	602	-	-	2/22/38/38	0/3/3/3
4	BU3	B	605	-	-	3/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	ATP	C5-C4	4.79	1.47	1.39
3	B	602	ATP	C5-C4	4.75	1.47	1.39
3	C	602	ATP	C5-C4	4.72	1.47	1.39
3	A	602	ATP	C5-C4	4.72	1.47	1.39
3	D	602	ATP	C5-C6	2.81	1.48	1.41
3	A	602	ATP	C5-C6	2.79	1.48	1.41
3	C	602	ATP	C5-C6	2.78	1.48	1.41
3	B	602	ATP	C5-C6	2.74	1.48	1.41
3	C	602	ATP	C8-N7	2.39	1.36	1.31
3	B	602	ATP	C8-N7	2.39	1.36	1.31
3	D	602	ATP	C8-N7	2.38	1.36	1.31
3	A	602	ATP	C8-N7	2.36	1.36	1.31
3	C	602	ATP	PA-O3A	2.28	1.62	1.59
3	B	602	ATP	C5-N7	-2.24	1.35	1.39
3	C	602	ATP	PB-O3A	2.17	1.61	1.59
3	D	602	ATP	C5-N7	-2.17	1.35	1.39
3	A	602	ATP	PB-O3B	2.17	1.61	1.59
3	A	602	ATP	C5-N7	-2.17	1.35	1.39
3	C	602	ATP	C5-N7	-2.16	1.35	1.39
3	B	602	ATP	PB-O3B	2.14	1.61	1.59
3	D	602	ATP	PB-O3B	2.08	1.61	1.59
3	D	602	ATP	PA-O3A	2.03	1.61	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	ATP	C5-C4-N3	-5.82	118.70	126.72
3	A	602	ATP	C5-C4-N3	-5.81	118.71	126.72
3	B	602	ATP	C5-C4-N3	-5.77	118.77	126.72
3	C	602	ATP	C5-C4-N3	-5.76	118.78	126.72
3	D	602	ATP	N3-C4-N9	4.60	134.98	127.17
3	B	602	ATP	N3-C4-N9	4.55	134.91	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ATP	N3-C4-N9	4.54	134.89	127.17
3	C	602	ATP	N3-C4-N9	4.50	134.82	127.17
3	D	602	ATP	C2-N3-C4	3.71	120.89	111.83
3	A	602	ATP	C2-N3-C4	3.70	120.88	111.83
3	C	602	ATP	C2-N3-C4	3.70	120.86	111.83
3	B	602	ATP	C2-N3-C4	3.68	120.83	111.83
3	A	602	ATP	C4-C5-N7	-3.57	106.50	110.58
3	C	602	ATP	C4-C5-N7	-3.55	106.52	110.58
3	D	602	ATP	C4-C5-N7	-3.51	106.57	110.58
3	B	602	ATP	C4-C5-N7	-3.50	106.58	110.58
3	C	602	ATP	N3-C2-N1	-3.25	123.66	128.58
3	B	602	ATP	N3-C2-N1	-3.25	123.67	128.58
3	A	602	ATP	N3-C2-N1	-3.22	123.70	128.58
3	D	602	ATP	N3-C2-N1	-3.21	123.72	128.58
3	D	602	ATP	C4-N9-C8	2.66	108.53	105.74
3	B	602	ATP	C4-N9-C8	2.65	108.52	105.74
3	C	602	ATP	C4-N9-C8	2.63	108.50	105.74
3	A	602	ATP	C4-N9-C8	2.62	108.49	105.74
3	A	602	ATP	C5-N7-C8	2.59	107.53	103.45
3	B	602	ATP	C5-N7-C8	2.57	107.49	103.45
3	C	602	ATP	C5-N7-C8	2.56	107.47	103.45
3	D	602	ATP	C5-N7-C8	2.53	107.43	103.45
3	D	602	ATP	C3'-C2'-C1'	2.22	105.66	101.46
3	C	602	ATP	C6-C5-N7	2.17	136.27	132.09
3	D	602	ATP	C6-C5-N7	2.15	136.23	132.09
3	A	602	ATP	C6-C5-N7	2.14	136.21	132.09
3	B	602	ATP	C6-C5-N7	2.12	136.18	132.09
3	A	602	ATP	C3'-C2'-C1'	2.09	105.42	101.46
3	B	602	ATP	N9-C8-N7	-2.01	111.09	113.94
3	A	602	ATP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ATP	C5'-O5'-PA-O1A
3	D	602	ATP	C5'-O5'-PA-O1A
3	D	602	ATP	C5'-O5'-PA-O2A
3	D	602	ATP	C5'-O5'-PA-O3A
4	B	603	BU3	O5-C2-C3-O6
4	B	603	BU3	C1-C2-C3-O6
4	B	603	BU3	O5-C2-C3-C4

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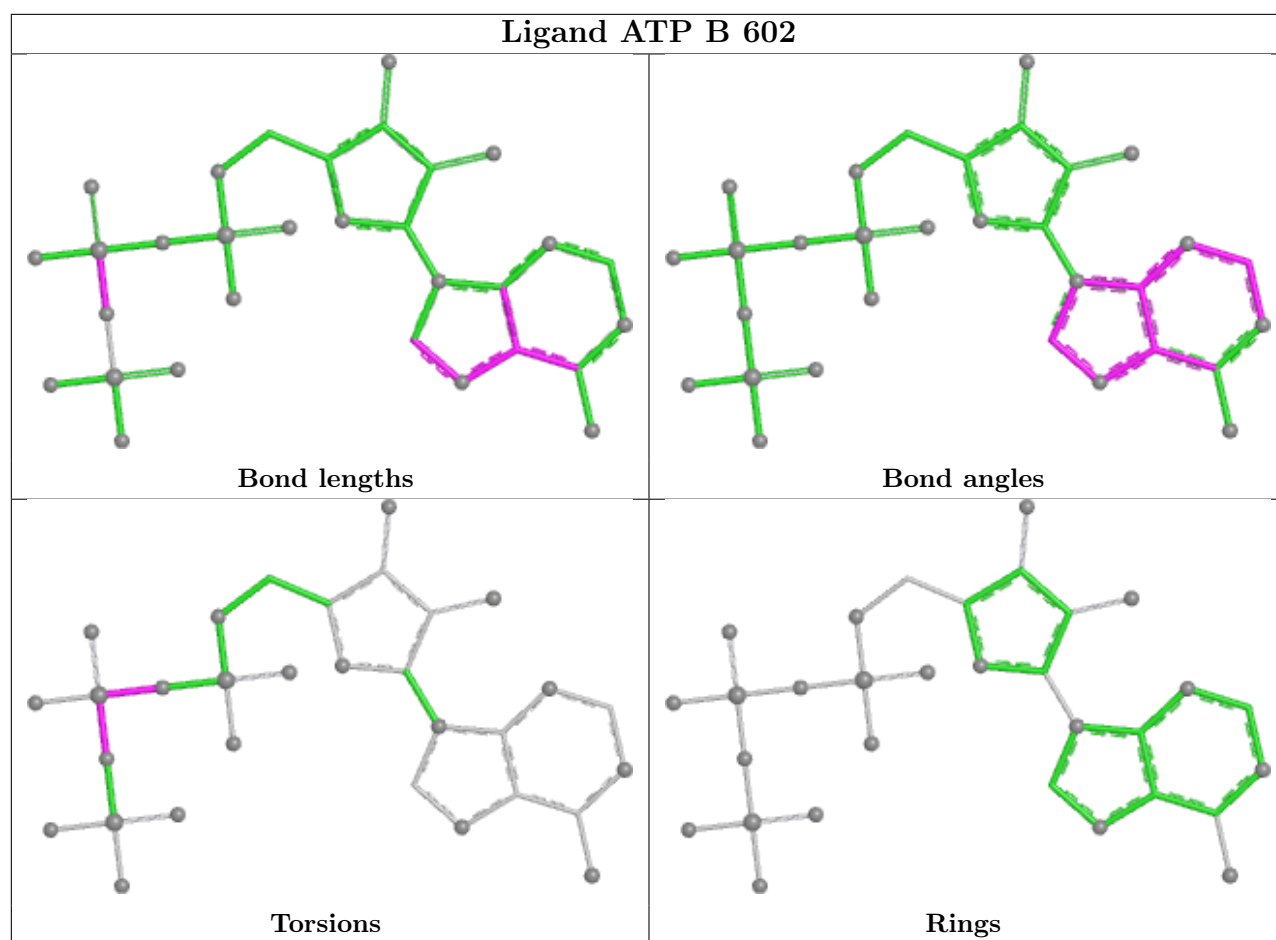
Mol	Chain	Res	Type	Atoms
4	B	603	BU3	C1-C2-C3-C4
4	B	607	BU3	C1-C2-C3-O6
4	B	607	BU3	O5-C2-C3-C4
4	B	607	BU3	C1-C2-C3-C4
3	D	602	ATP	PA-O3A-PB-O1B
4	B	605	BU3	O5-C2-C3-C4
3	B	602	ATP	PG-O3B-PB-O2B
3	B	602	ATP	PA-O3A-PB-O2B
3	D	602	ATP	PG-O3B-PB-O2B
3	D	602	ATP	PA-O3A-PB-O2B
3	D	602	ATP	O4'-C4'-C5'-O5'
3	B	602	ATP	PG-O3B-PB-O1B
3	B	602	ATP	PA-O3A-PB-O1B
3	C	602	ATP	PG-O3B-PB-O2B
3	D	602	ATP	PG-O3B-PB-O1B
4	B	605	BU3	C1-C2-C3-C4
4	B	605	BU3	O5-C2-C3-O6
3	C	602	ATP	PA-O3A-PB-O2B
3	D	602	ATP	PB-O3A-PA-O1A

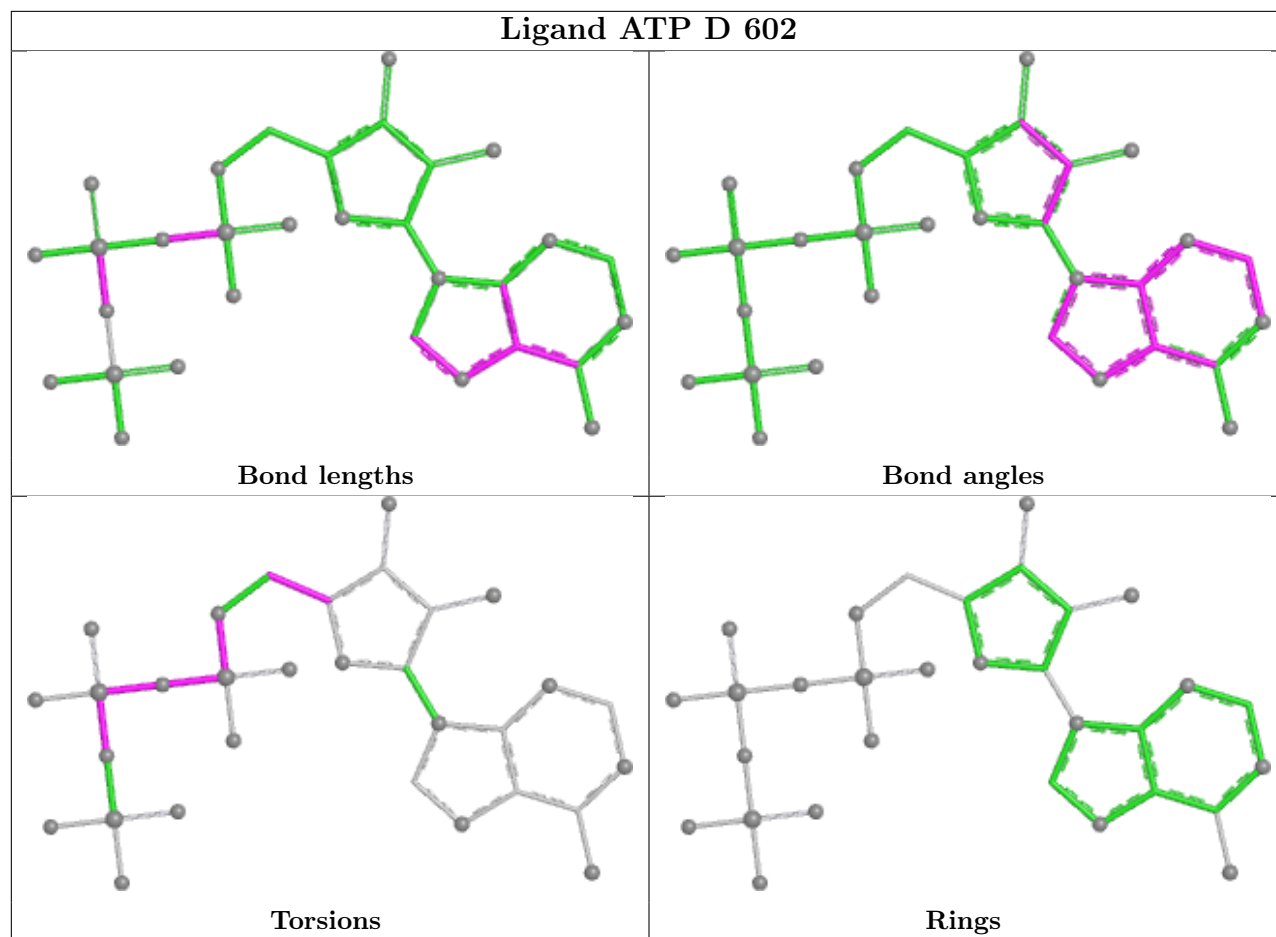
There are no ring outliers.

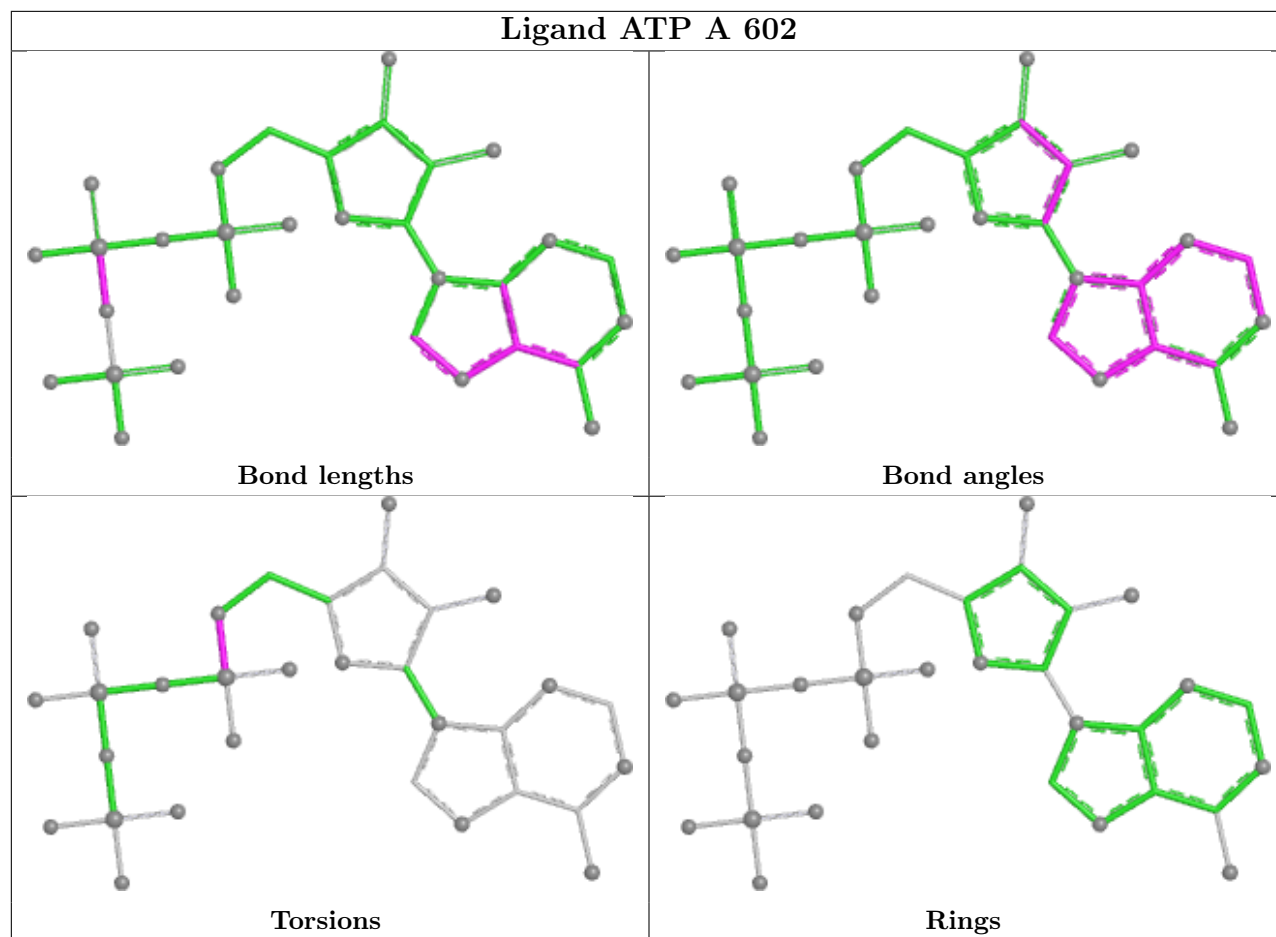
2 monomers are involved in 3 short contacts:

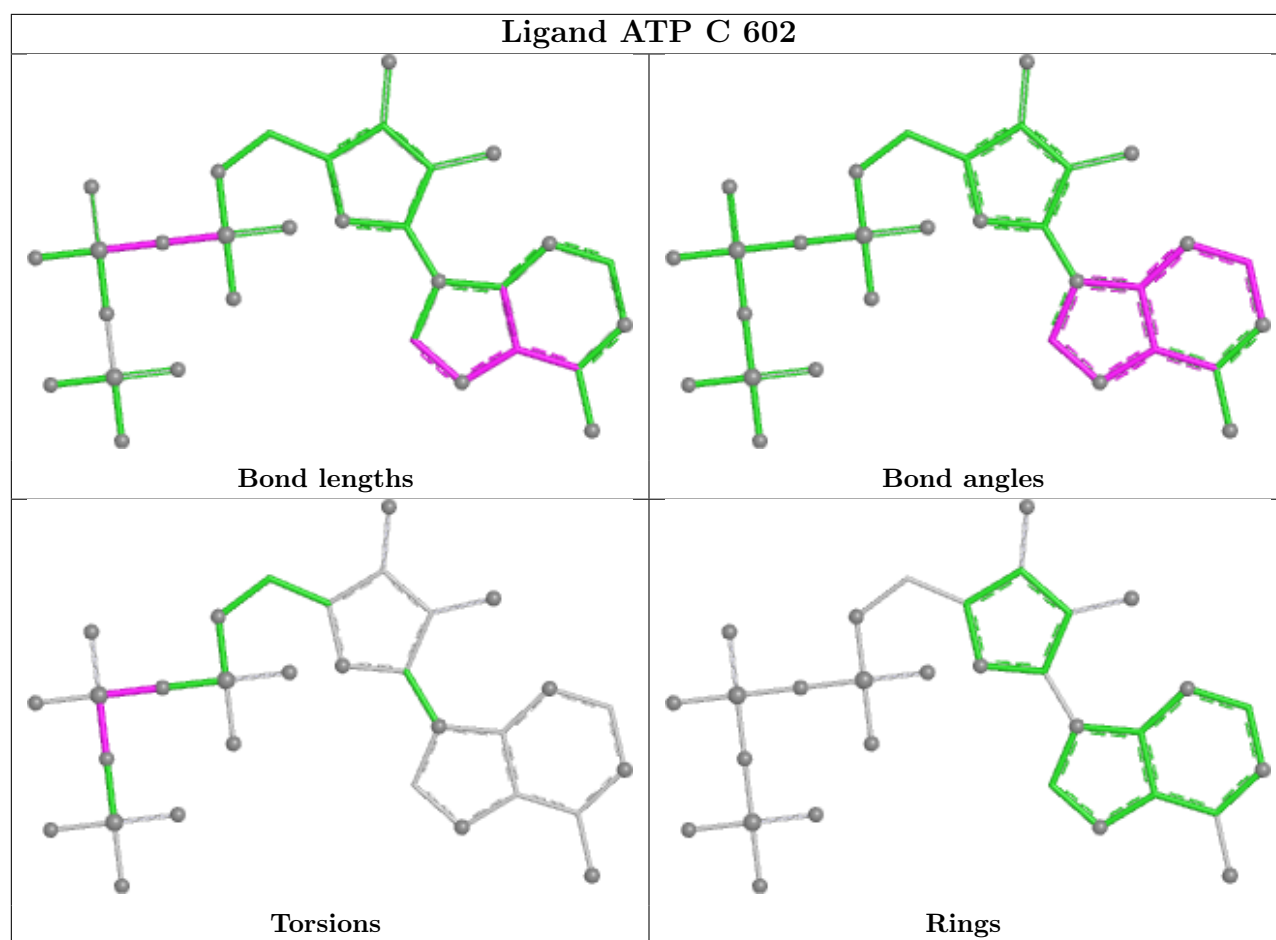
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	606	BU3	1	0
4	B	605	BU3	2	0

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

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	555/562 (98%)	0.95	53 (9%)	14 16	20, 41, 81, 98	0
1	B	556/562 (98%)	0.96	65 (11%)	9 10	22, 37, 62, 86	0
1	C	561/562 (99%)	1.06	72 (12%)	7 8	21, 40, 64, 81	0
1	D	560/562 (99%)	0.87	44 (7%)	18 21	21, 42, 67, 92	0
All	All	2232/2248 (99%)	0.96	234 (10%)	11 13	20, 40, 68, 98	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	CYS	6.9
1	D	273	PHE	5.9
1	D	110	ALA	5.5
1	A	394	VAL	5.1
1	C	70	GLU	5.1
1	D	66	THR	4.9
1	A	385	LEU	4.9
1	A	386	ASP	4.8
1	A	393	LEU	4.8
1	C	69	GLY	4.7
1	A	119	PRO	4.6
1	B	530	GLU	4.4
1	B	401	LEU	4.3
1	A	383	PHE	4.3
1	A	558	PHE	4.2
1	C	67	PRO	4.1
1	C	68	ALA	4.1
1	A	346	LEU	4.1
1	A	401	LEU	4.1
1	B	393	LEU	4.0
1	C	106	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	342	ALA	4.0
1	A	273	PHE	4.0
1	B	398	CYS	4.0
1	C	398	CYS	3.9
1	A	384	PRO	3.8
1	C	273	PHE	3.7
1	C	109	ALA	3.7
1	C	558	PHE	3.7
1	C	557	LEU	3.6
1	B	394	VAL	3.6
1	B	68	ALA	3.6
1	B	434	ASN	3.5
1	D	342	ALA	3.5
1	B	273	PHE	3.5
1	D	109	ALA	3.4
1	C	516	ASN	3.4
1	C	108	GLY	3.3
1	B	67	PRO	3.3
1	C	71	GLY	3.3
1	B	105	ILE	3.3
1	C	105	ILE	3.3
1	A	387	THR	3.3
1	A	357	GLY	3.2
1	D	557	LEU	3.2
1	B	343	LYS	3.2
1	C	525	VAL	3.2
1	A	402	GLY	3.2
1	D	107	GLY	3.2
1	B	107	GLY	3.2
1	B	347	ASN	3.2
1	D	344	ASP	3.2
1	C	120	MET	3.2
1	B	385	LEU	3.1
1	D	400	GLU	3.1
1	B	396	SER	3.1
1	B	387	THR	3.1
1	B	106	LYS	3.1
1	C	530	GLU	3.1
1	C	507	GLY	3.1
1	B	70	GLU	3.0
1	C	66	THR	3.0
1	B	3	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	391	LEU	3.0
1	B	268	LEU	2.9
1	C	344	ASP	2.9
1	D	510	ILE	2.9
1	C	458	TYR	2.9
1	C	110	ALA	2.9
1	B	120	MET	2.9
1	B	325	ALA	2.9
1	C	351	LEU	2.9
1	A	377	VAL	2.9
1	C	7	ILE	2.9
1	C	32	ILE	2.9
1	B	383	PHE	2.8
1	A	403	VAL	2.8
1	C	343	LYS	2.8
1	B	392	ALA	2.8
1	C	511	GLU	2.8
1	B	403	VAL	2.8
1	A	89	ASN	2.8
1	C	107	GLY	2.8
1	D	-2	SER	2.8
1	B	351	LEU	2.7
1	D	346	LEU	2.7
1	D	527	MET	2.7
1	C	284	ILE	2.7
1	A	399	GLU	2.7
1	A	337	TYR	2.7
1	C	342	ALA	2.7
1	D	506	THR	2.7
1	C	531	ILE	2.7
1	A	397	LYS	2.7
1	D	67	PRO	2.7
1	A	351	LEU	2.7
1	D	332	VAL	2.7
1	A	400	GLU	2.7
1	B	66	THR	2.7
1	D	108	GLY	2.7
1	C	325	ALA	2.6
1	B	433	GLU	2.6
1	A	358	LEU	2.6
1	B	431	GLU	2.6
1	C	384	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	507	GLY	2.6
1	C	433	GLU	2.6
1	D	170	MET	2.6
1	D	405	VAL	2.6
1	C	-2	SER	2.6
1	A	389	ALA	2.5
1	A	392	ALA	2.5
1	C	483	ASN	2.5
1	B	108	GLY	2.5
1	A	121	GLU	2.5
1	D	70	GLU	2.5
1	B	391	LEU	2.5
1	B	384	PRO	2.5
1	B	402	GLY	2.5
1	B	442	GLU	2.5
1	D	478	GLU	2.5
1	C	495	LEU	2.5
1	C	117	VAL	2.5
1	D	530	GLU	2.5
1	C	440	TYR	2.5
1	B	304	ALA	2.5
1	C	-1	HIS	2.5
1	B	288	MET	2.4
1	C	288	MET	2.4
1	B	81	ASP	2.4
1	A	530	GLU	2.4
1	D	121	GLU	2.4
1	C	329	VAL	2.4
1	D	7	ILE	2.4
1	D	354	LEU	2.4
1	C	35	TYR	2.4
1	B	381	ASN	2.4
1	A	70	GLU	2.4
1	B	119	PRO	2.4
1	B	390	GLU	2.4
1	D	81	ASP	2.4
1	C	376	ALA	2.4
1	C	486	VAL	2.4
1	C	526	VAL	2.4
1	B	479	LEU	2.4
1	C	475	GLU	2.4
1	A	547	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	493	TYR	2.3
1	B	526	VAL	2.3
1	C	488	VAL	2.3
1	D	488	VAL	2.3
1	C	47	LEU	2.3
1	B	397	LYS	2.3
1	B	524	VAL	2.3
1	C	297	VAL	2.3
1	A	360	ASN	2.3
1	D	-1	HIS	2.3
1	C	2	GLU	2.3
1	D	431	GLU	2.3
1	A	341	VAL	2.3
1	C	332	VAL	2.3
1	D	335	LEU	2.3
1	B	529	GLY	2.3
1	B	35	TYR	2.3
1	A	442	GLU	2.3
1	D	355	GLU	2.3
1	C	453	ILE	2.3
1	B	337	TYR	2.2
1	D	68	ALA	2.2
1	B	558	PHE	2.2
1	C	497	ASP	2.2
1	A	108	GLY	2.2
1	A	507	GLY	2.2
1	B	432	GLY	2.2
1	C	340	GLY	2.2
1	C	352	GLU	2.2
1	A	528	THR	2.2
1	B	389	ALA	2.2
1	B	474	ALA	2.2
1	C	346	LEU	2.2
1	B	329	VAL	2.2
1	A	516	ASN	2.2
1	B	60	THR	2.2
1	B	330	ALA	2.2
1	B	531	ILE	2.2
1	B	399	GLU	2.2
1	D	111	GLY	2.2
1	A	330	ALA	2.2
1	B	334	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	318	LYS	2.1
1	C	383	PHE	2.1
1	C	487	CYS	2.1
1	A	354	LEU	2.1
1	C	391	LEU	2.1
1	D	196	ASP	2.1
1	C	103	PHE	2.1
1	C	439	CYS	2.1
1	A	331	THR	2.1
1	A	334	ALA	2.1
1	A	376	ALA	2.1
1	C	292	MET	2.1
1	A	362	LEU	2.1
1	D	34	LEU	2.1
1	D	385	LEU	2.1
1	D	399	GLU	2.1
1	C	276	ILE	2.1
1	D	341	VAL	2.1
1	A	71	GLY	2.1
1	A	356	LYS	2.1
1	D	532	MET	2.1
1	C	478	GLU	2.1
1	D	497	ASP	2.1
1	B	117	VAL	2.1
1	D	503	GLY	2.1
1	B	528	THR	2.0
1	A	349	GLU	2.0
1	B	422	ALA	2.0
1	C	406	ALA	2.0
1	A	105	ILE	2.0
1	A	327	ILE	2.0
1	C	295	TYR	2.0
1	B	395	ARG	2.0
1	B	486	VAL	2.0
1	B	488	VAL	2.0
1	A	207	PHE	2.0
1	C	311	PHE	2.0
1	A	292	MET	2.0
1	A	396	SER	2.0
1	C	366	GLU	2.0
1	C	515	ALA	2.0
1	D	247	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	27	LEU	2.0
1	B	374	ILE	2.0
1	D	106	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

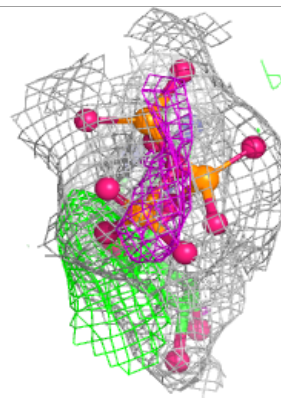
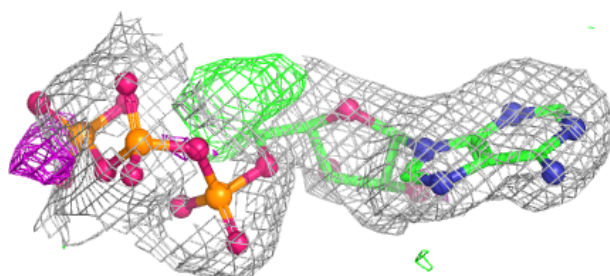
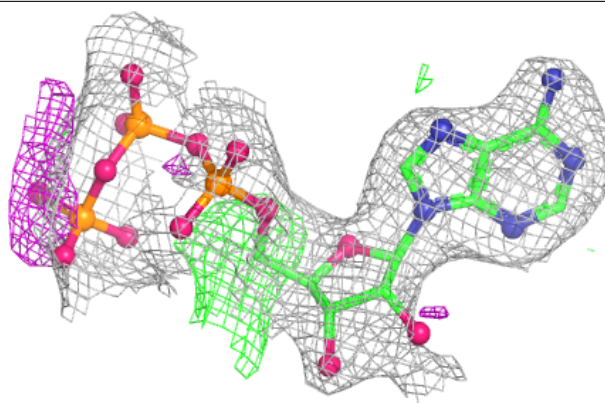
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BU3	B	604	6/6	0.41	0.24	42,47,54,55	0
4	BU3	B	606	6/6	0.50	0.25	45,50,54,55	0
4	BU3	B	603	6/6	0.65	0.15	40,50,56,61	0
4	BU3	B	607	6/6	0.70	0.20	37,44,47,48	0
3	ATP	C	602	31/31	0.72	0.14	40,56,81,91	0
3	ATP	D	602	31/31	0.73	0.13	41,55,79,80	0
4	BU3	B	605	6/6	0.73	0.21	40,43,46,46	0
3	ATP	A	602	31/31	0.81	0.13	52,65,86,95	0
3	ATP	B	602	31/31	0.82	0.12	44,54,68,79	0
2	K	D	601	1/1	0.96	0.04	30,30,30,30	0
2	K	B	601	1/1	0.96	0.05	34,34,34,34	0
2	K	A	601	1/1	0.97	0.04	38,38,38,38	0
2	K	C	601	1/1	0.98	0.07	33,33,33,33	0

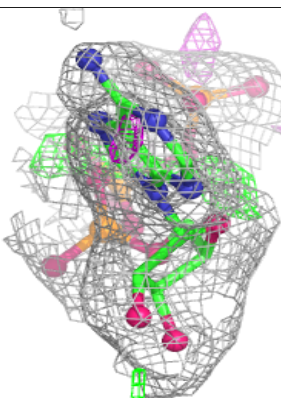
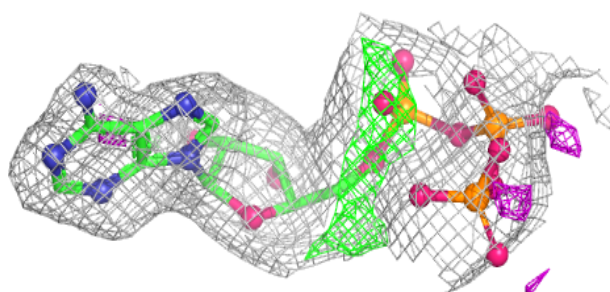
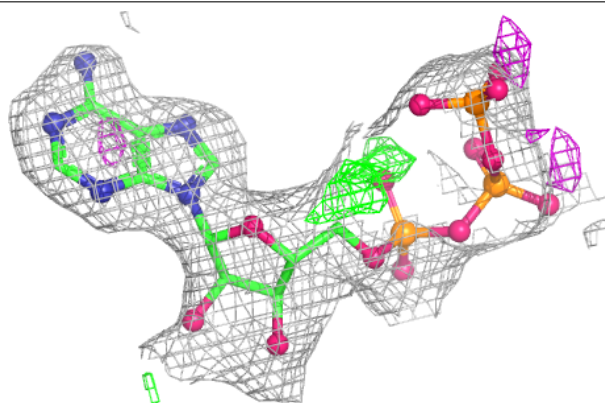
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 602:

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

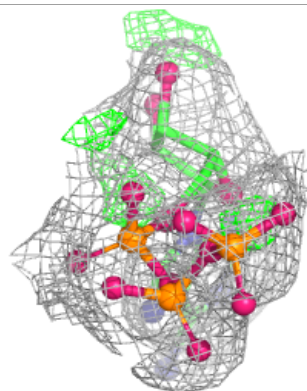
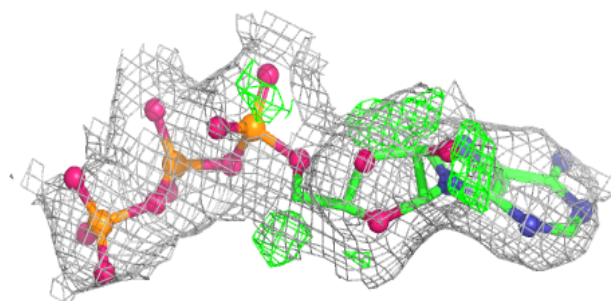
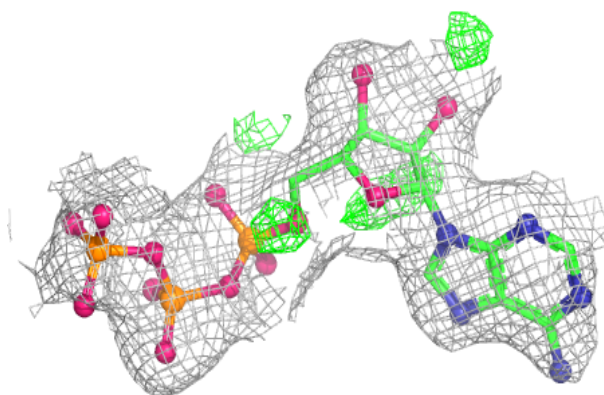
**Electron density around ATP D 602:**

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

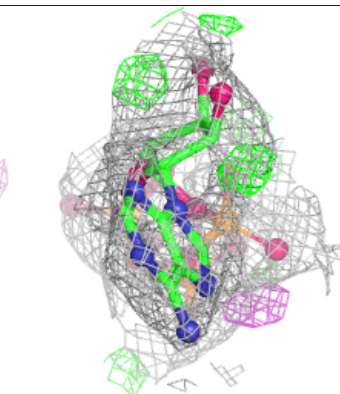
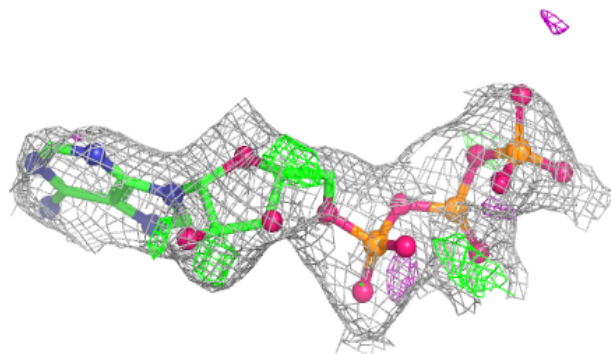
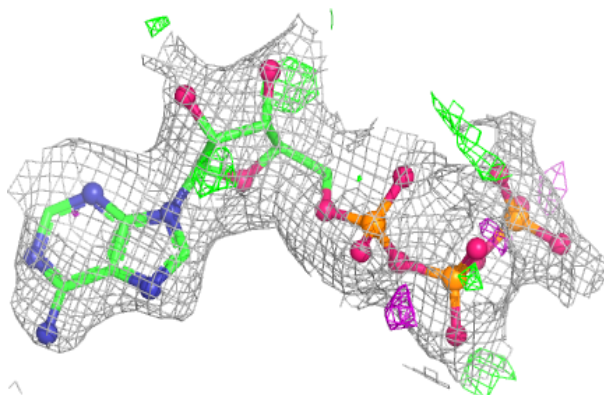


Electron density around ATP A 602:

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

**Electron density around ATP B 602:**

$2mF_o-DF_c$ (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.