Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:58 PM JST

PDB ID	:	7XZO
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:

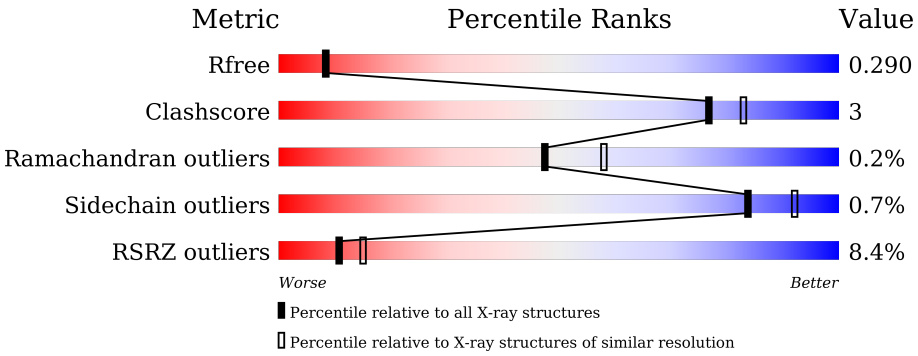
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 <=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% 90% 9%
1	B	562	6% 90% 9%
1	C	562	10% 91% 9%
1	D	562	9% 92% 8%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BU3	B	606	-	-	-	X

2 Entry composition (i)

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			

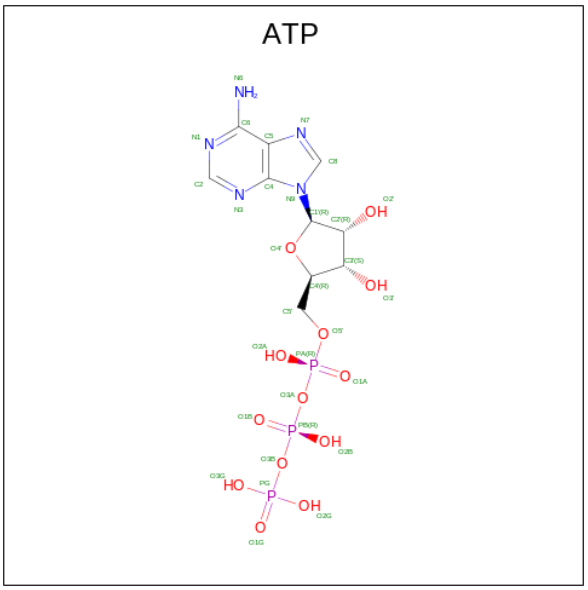
There are 16 discrepancies between the modelled and reference sequences:

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 (three-letter code: K) (formula: K).

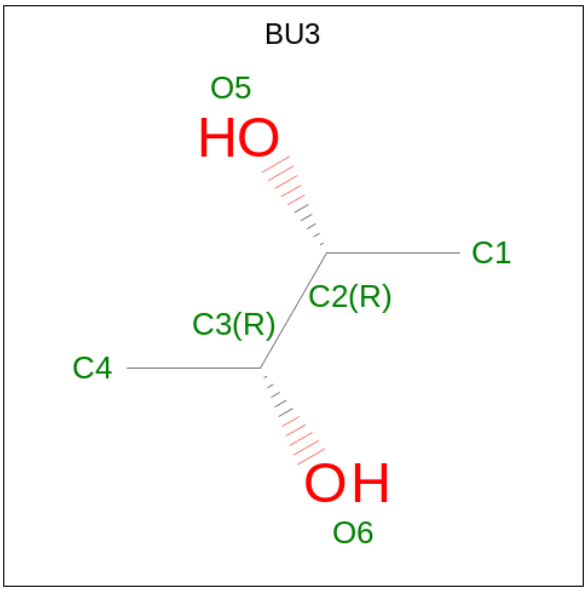
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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 (three-letter code: BU3) (formula: $C_4H_{10}O_2$).



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

- Molecule 5 is water.

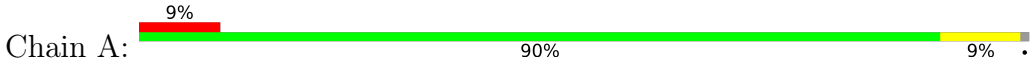
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	21	Total O 21 21	0	0
5	B	24	Total O 24 24	0	0
5	C	16	Total O 16 16	0	0
5	D	15	Total O 15 15	0	0

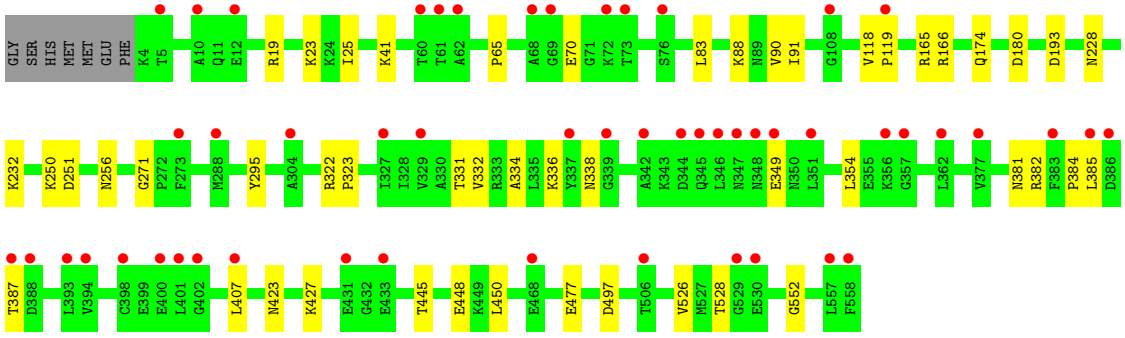
3 Residue-property plots (i)

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: Formate--tetrahydrofolate ligase

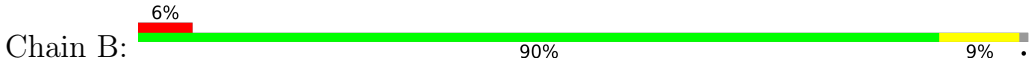
Chain A:

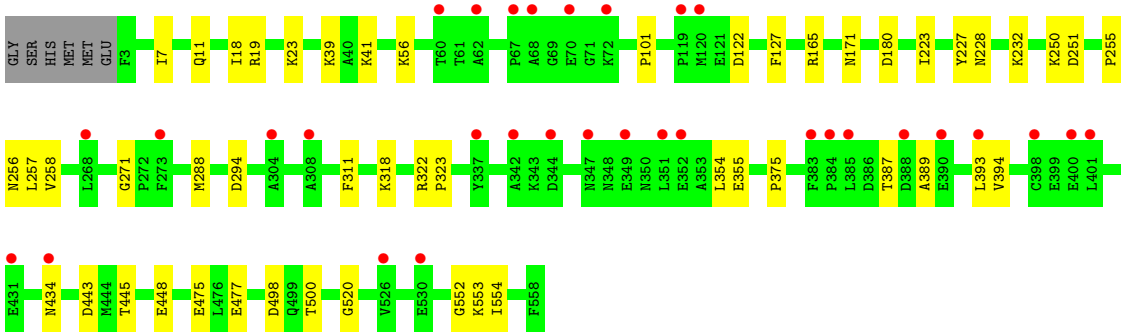




• Molecule 1: Formate--tetrahydrofolate ligase

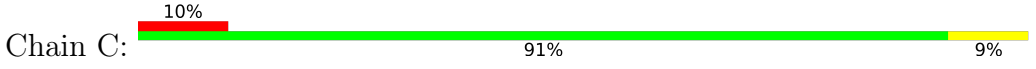
Chain B:

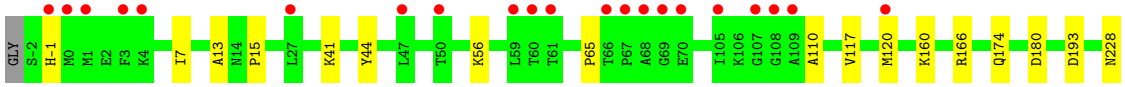


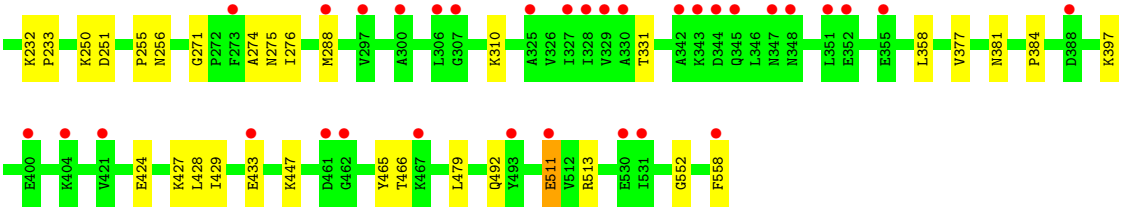


• Molecule 1: Formate--tetrahydrofolate ligase

Chain C:

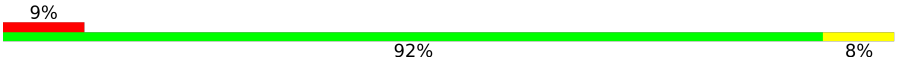


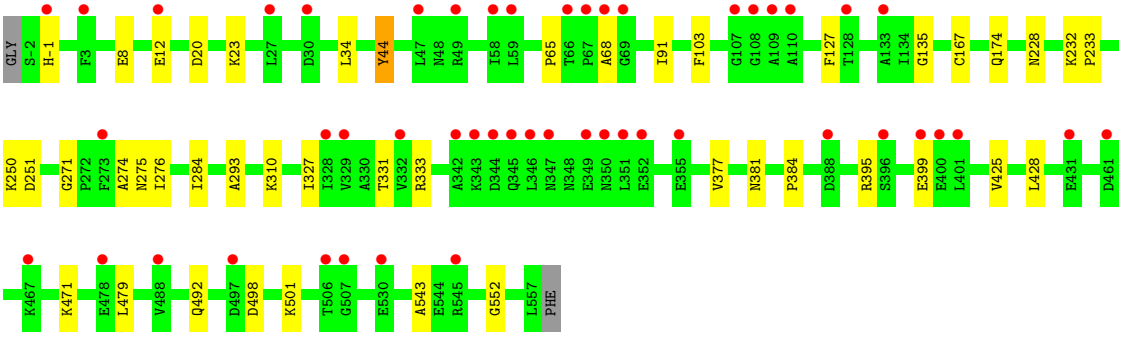




• Molecule 1: Formate--tetrahydrofolate ligase

Chain D:





4 Data and refinement statistics (i)

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 32.48 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.03-2.31) 99.9 (32.48-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.252 , 0.290 0.252 , 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 , 33.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	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.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BU3, ATP, K

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	0.24	0/4229	0.42	0/5724
1	B	0.24	0/4233	0.43	0/5730
1	C	0.24	0/4277	0.42	0/5788
1	D	0.24	0/4268	0.41	0/5776
All	All	0.24	0/17007	0.42	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	30	0
1	B	4174	0	4216	29	0
1	C	4216	0	4256	26	0
1	D	4208	0	4249	23	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	101	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 (101) 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:C:255:PRO:HG2	1:C:288:MET:HE3	1.82	0.61
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: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: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:250:LYS:NZ	1:B:251:ASP:OD1	2.40	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:ALA:O	1:D:310:LYS:NZ	2.41	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: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: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:250:LYS:NZ	1:C:251:ASP:OD1	2.44	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: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:B:255:PRO:HG2	1:B:288:MET:HE2	1.98	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: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:274:ALA:O	1:C:310:LYS:NZ	2.40	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:A:450:LEU:HD21	1:A:526:VAL:HG21	1.99	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:166:ARG:NH1	1:C:193:ASP:OD2	2.54	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:498:ASP:OD2	1:B:500:THR:OG1	2.38	0.41
1:C:424:GLU:HA	1:C:427:LYS:HE2	2.02	0.40
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
1:C:7:ILE:HG12	1:C:120:MET:HE1	2.03	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%)	47	58
1	B	554/562 (99%)	533 (96%)	20 (4%)	1 (0%)	47	58
1	C	559/562 (100%)	538 (96%)	20 (4%)	1 (0%)	47	58
1	D	558/562 (99%)	537 (96%)	20 (4%)	1 (0%)	47	58
All	All	2224/2248 (99%)	2137 (96%)	83 (4%)	4 (0%)	47	58

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%)	433 (99%)	4 (1%)	78	89
1	C	441/447 (99%)	436 (99%)	5 (1%)	73	85
1	D	441/447 (99%)	438 (99%)	3 (1%)	84	92
All	All	1756/1788 (98%)	1744 (99%)	12 (1%)	84	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	PHE
1	B	258	VAL
1	B	322	ARG
1	B	443	ASP
1	C	44	TYR
1	C	160	LYS
1	C	433	GLU
1	C	511	GLU
1	C	513	ARG
1	D	34	LEU
1	D	44	TYR
1	D	127	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
3	ATP	A	602	-	26,33,33	0.93	1 (3%)	31,52,52	1.52	5 (16%)
4	BU3	B	603	-	4,5,5	0.31	0	6,6,6	0.31	0
4	BU3	B	606	-	4,5,5	0.31	0	6,6,6	0.32	0
4	BU3	B	604	-	4,5,5	0.30	0	6,6,6	0.30	0
4	BU3	B	607	-	4,5,5	0.34	0	6,6,6	0.37	0
3	ATP	D	602	-	26,33,33	0.94	1 (3%)	31,52,52	1.50	5 (16%)
4	BU3	B	605	-	4,5,5	0.25	0	6,6,6	0.38	0
3	ATP	B	602	-	26,33,33	0.93	1 (3%)	31,52,52	1.49	5 (16%)
3	ATP	C	602	-	26,33,33	0.93	1 (3%)	31,52,52	1.49	5 (16%)

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
3	ATP	A	602	-	-	3/18/38/38	0/3/3/3
4	BU3	B	603	-	-	4/4/4/4	-
4	BU3	B	606	-	-	0/4/4/4	-
4	BU3	B	604	-	-	0/4/4/4	-
4	BU3	B	607	-	-	3/4/4/4	-
3	ATP	D	602	-	-	8/18/38/38	0/3/3/3
4	BU3	B	605	-	-	3/4/4/4	-
3	ATP	B	602	-	-	4/18/38/38	0/3/3/3
3	ATP	C	602	-	-	1/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	ATP	C5-C4	2.54	1.47	1.40
3	B	602	ATP	C5-C4	2.51	1.47	1.40
3	C	602	ATP	C5-C4	2.49	1.47	1.40
3	A	602	ATP	C5-C4	2.48	1.47	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	ATP	PA-O3A-PB	-3.58	120.54	132.83
3	C	602	ATP	PB-O3B-PG	-3.50	120.83	132.83
3	C	602	ATP	N3-C2-N1	-3.21	123.66	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	ATP	N3-C2-N1	-3.20	123.67	128.68
3	A	602	ATP	N3-C2-N1	-3.18	123.70	128.68
3	B	602	ATP	PA-O3A-PB	-3.18	121.93	132.83
3	D	602	ATP	N3-C2-N1	-3.17	123.72	128.68
3	D	602	ATP	C3'-C2'-C1'	3.11	105.66	100.98
3	B	602	ATP	PB-O3B-PG	-3.05	122.37	132.83
3	A	602	ATP	C3'-C2'-C1'	2.95	105.42	100.98
3	D	602	ATP	PB-O3B-PG	-2.90	122.88	132.83
3	D	602	ATP	PA-O3A-PB	-2.87	122.96	132.83
3	C	602	ATP	C3'-C2'-C1'	2.83	105.25	100.98
3	B	602	ATP	C3'-C2'-C1'	2.79	105.18	100.98
3	A	602	ATP	PB-O3B-PG	-2.79	123.25	132.83
3	A	602	ATP	C4-C5-N7	-2.78	106.50	109.40
3	C	602	ATP	C4-C5-N7	-2.76	106.52	109.40
3	D	602	ATP	C4-C5-N7	-2.72	106.57	109.40
3	B	602	ATP	C4-C5-N7	-2.71	106.58	109.40
3	C	602	ATP	PA-O3A-PB	-2.15	125.45	132.83

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
4	B	603	BU3	O5-C2-C3-O6
4	B	603	BU3	C1-C2-C3-O6
4	B	603	BU3	O5-C2-C3-C4
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
3	D	602	ATP	O4'-C4'-C5'-O5'
4	B	605	BU3	O5-C2-C3-C4
3	B	602	ATP	PG-O3B-PB-O2B
4	B	605	BU3	O5-C2-C3-O6
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	A	602	ATP	C5'-O5'-PA-O3A
3	D	602	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
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
3	A	602	ATP	C5'-O5'-PA-O2A
4	B	605	BU3	C1-C2-C3-C4

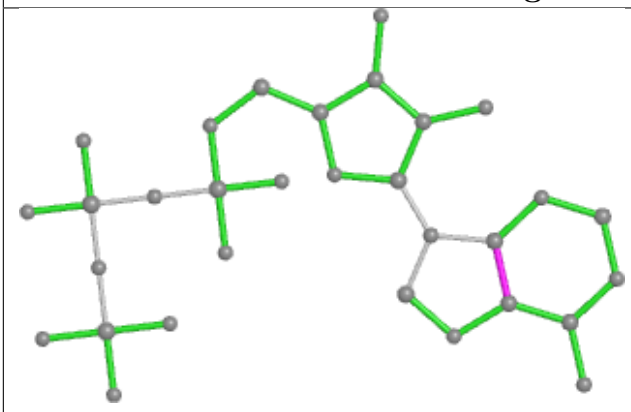
There are no ring outliers.

2 monomers are involved in 3 short contacts:

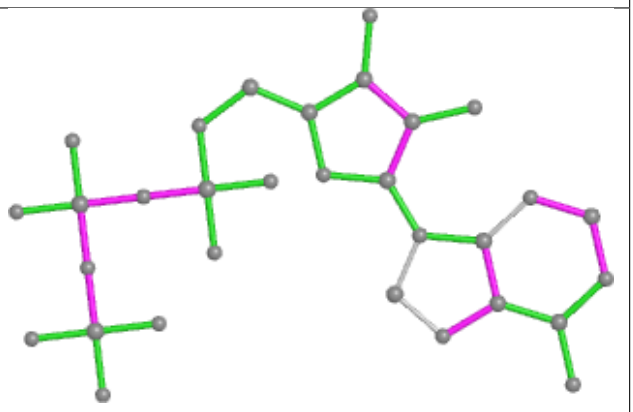
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	606	BU3	1	0
4	B	605	BU3	2	0

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 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.

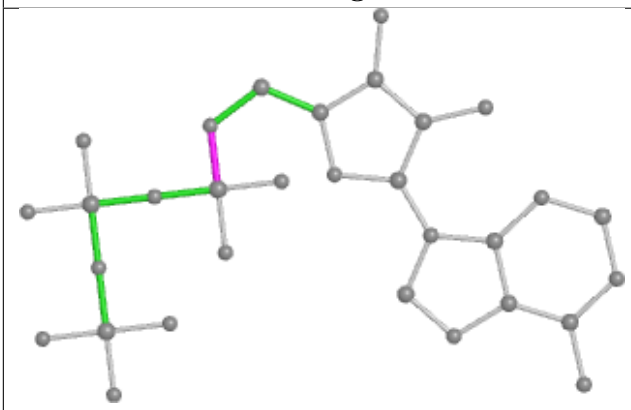
Ligand ATP A 602



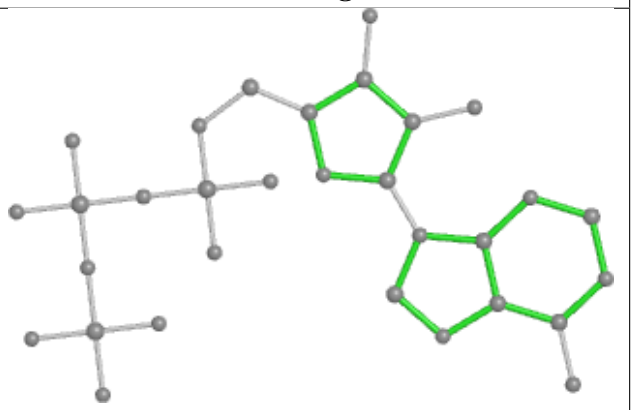
Bond lengths



Bond angles

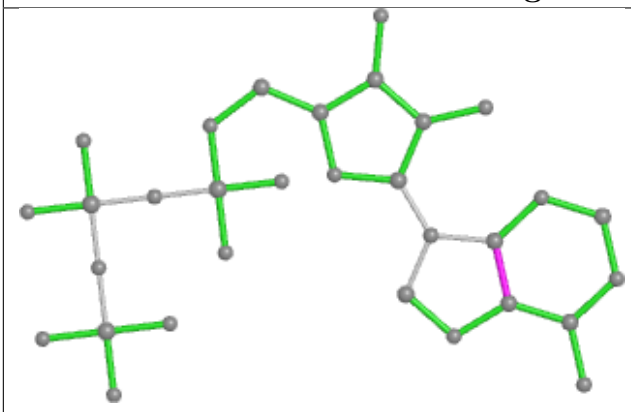


Torsions

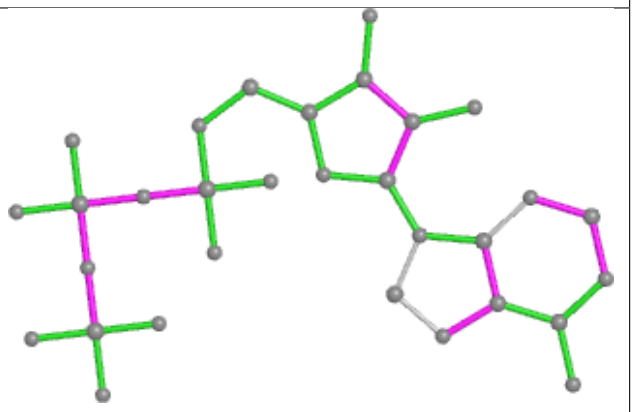


Rings

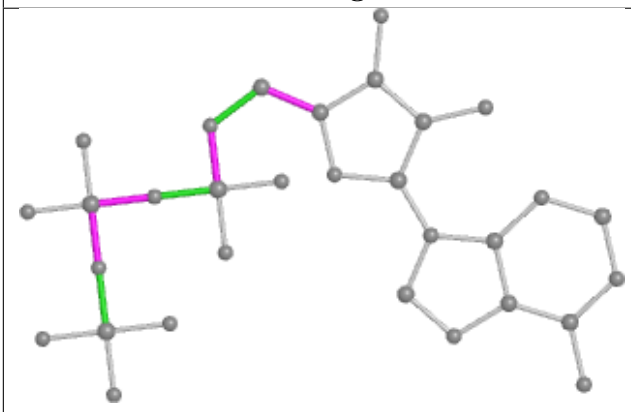
Ligand ATP D 602



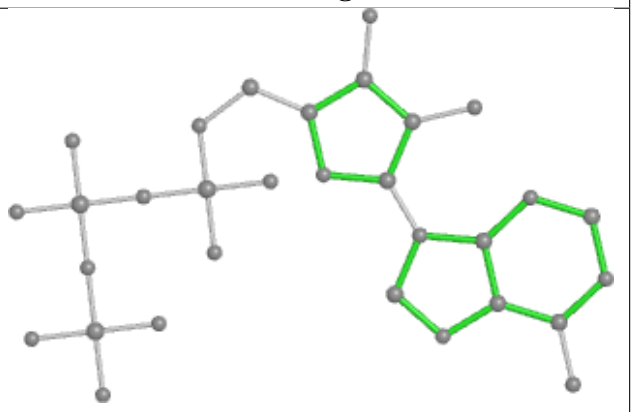
Bond lengths



Bond angles

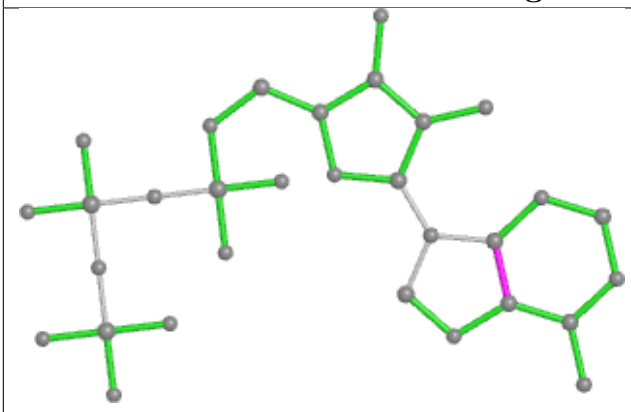


Torsions

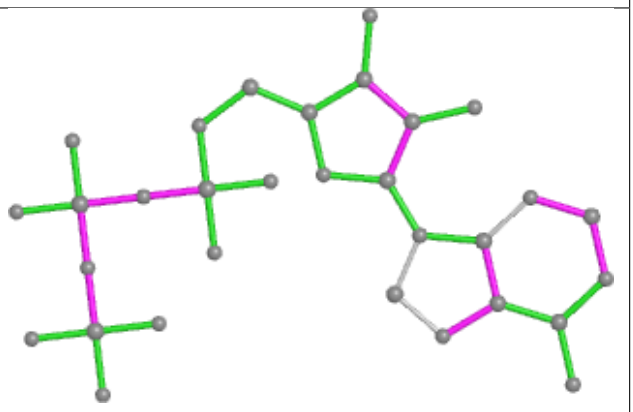


Rings

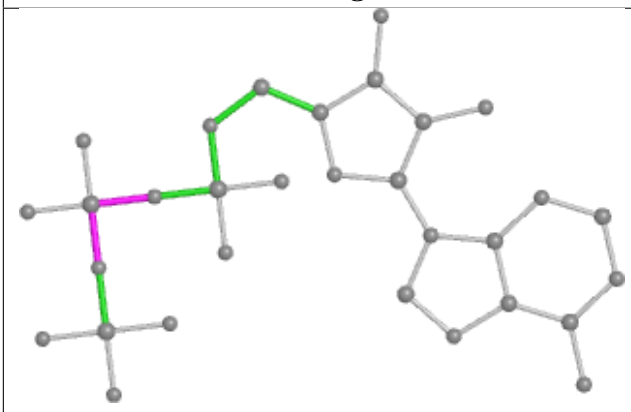
Ligand ATP B 602



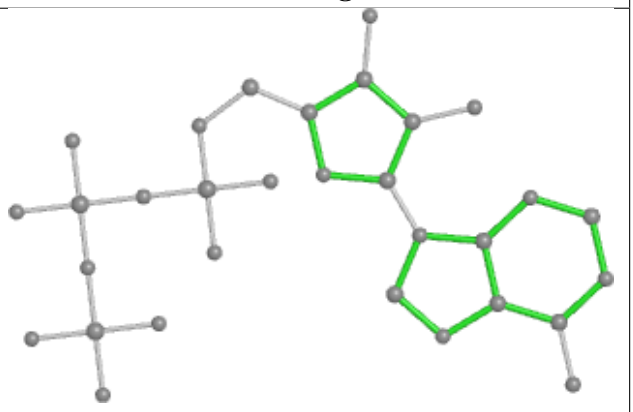
Bond lengths



Bond angles

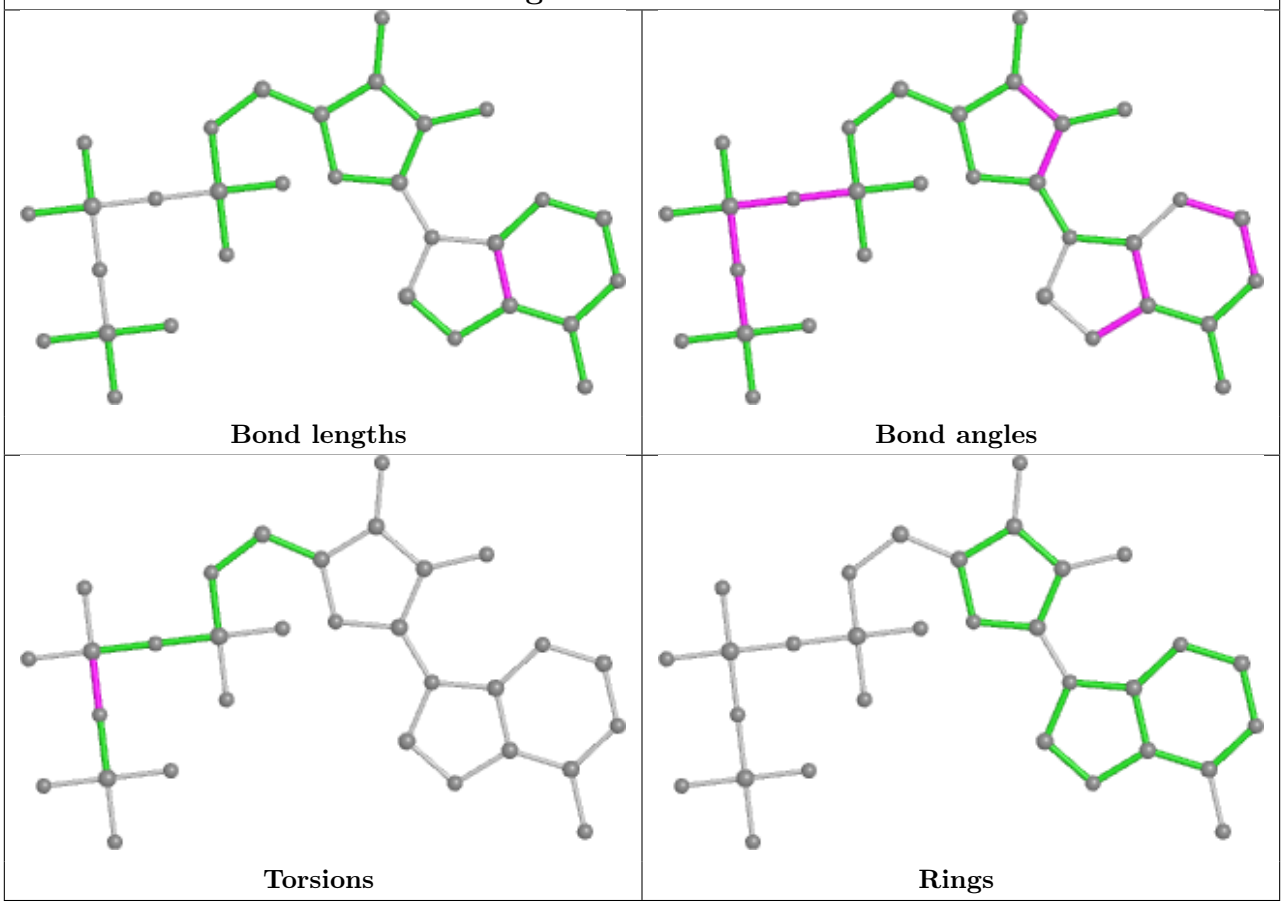


Torsions



Rings

Ligand ATP C 602



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, 95^{th} 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%)	0.58	52 (9%)	8 11	20, 41, 81, 98	0
1	B	556/562 (98%)	0.47	32 (5%)	23 29	22, 37, 62, 86	0
1	C	561/562 (99%)	0.67	54 (9%)	8 11	21, 40, 64, 81	0
1	D	560/562 (99%)	0.60	49 (8%)	10 14	21, 42, 67, 92	0
All	All	2232/2248 (99%)	0.58	187 (8%)	11 15	20, 40, 68, 98	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	344	ASP	8.2
1	B	68	ALA	8.0
1	A	398	CYS	7.6
1	D	67	PRO	7.5
1	D	273	PHE	6.7
1	C	69	GLY	6.2
1	A	383	PHE	6.1
1	C	351	LEU	5.9
1	B	401	LEU	5.7
1	A	394	VAL	5.5
1	B	67	PRO	5.5
1	C	67	PRO	5.4
1	A	558	PHE	5.2
1	A	349	GLU	5.2
1	A	346	LEU	5.0
1	D	109	ALA	4.9
1	A	402	GLY	4.8
1	C	70	GLU	4.5
1	B	530	GLU	4.5
1	A	388	ASP	4.3
1	C	352	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	393	LEU	4.2
1	D	108	GLY	4.1
1	C	68	ALA	4.0
1	A	351	LEU	4.0
1	C	47	LEU	4.0
1	C	343	LYS	4.0
1	D	66	THR	4.0
1	C	273	PHE	3.9
1	C	329	VAL	3.9
1	D	110	ALA	3.9
1	D	530	GLU	3.9
1	A	386	ASP	3.9
1	D	506	THR	3.8
1	C	120	MET	3.8
1	C	3	PHE	3.7
1	A	119	PRO	3.7
1	A	433	GLU	3.7
1	A	401	LEU	3.6
1	C	342	ALA	3.6
1	B	349	GLU	3.5
1	A	385	LEU	3.5
1	B	351	LEU	3.5
1	A	5	THR	3.5
1	C	530	GLU	3.4
1	C	109	ALA	3.4
1	B	347	ASN	3.4
1	D	12	GLU	3.3
1	C	404	LYS	3.3
1	D	68	ALA	3.3
1	A	62	ALA	3.3
1	C	400	GLU	3.3
1	D	347	ASN	3.2
1	A	530	GLU	3.2
1	B	352	GLU	3.2
1	D	351	LEU	3.2
1	C	288	MET	3.1
1	A	273	PHE	3.1
1	A	60	THR	3.1
1	C	347	ASN	3.1
1	A	345	GLN	3.1
1	C	-1	HIS	3.0
1	C	108	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	343	LYS	3.0
1	D	329	VAL	3.0
1	D	49	ARG	3.0
1	A	357	GLY	3.0
1	C	107	GLY	3.0
1	D	431	GLU	3.0
1	C	1	MET	3.0
1	D	507	GLY	3.0
1	B	273	PHE	3.0
1	B	342	ALA	2.9
1	C	558	PHE	2.9
1	D	-1	HIS	2.9
1	C	60	THR	2.9
1	C	297	VAL	2.9
1	C	345	GLN	2.9
1	A	72	LYS	2.8
1	D	355	GLU	2.8
1	B	388	ASP	2.8
1	C	325	ALA	2.8
1	A	327	ILE	2.8
1	A	344	ASP	2.8
1	D	30	ASP	2.8
1	A	68	ALA	2.8
1	D	47	LEU	2.8
1	D	461	ASP	2.8
1	A	69	GLY	2.8
1	D	400	GLU	2.8
1	D	478	GLU	2.8
1	D	69	GLY	2.8
1	B	400	GLU	2.8
1	C	105	ILE	2.8
1	A	342	ALA	2.7
1	C	433	GLU	2.8
1	B	60	THR	2.7
1	B	398	CYS	2.7
1	B	304	ALA	2.7
1	A	73	THR	2.7
1	C	61	THR	2.7
1	B	384	PRO	2.6
1	A	377	VAL	2.6
1	D	399	GLU	2.6
1	D	342	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	400	GLU	2.6
1	A	329	VAL	2.6
1	A	337	TYR	2.6
1	A	506	THR	2.6
1	D	467	LYS	2.6
1	C	531	ILE	2.5
1	B	434	ASN	2.5
1	B	62	ALA	2.5
1	D	388	ASP	2.5
1	A	557	LEU	2.5
1	B	393	LEU	2.5
1	D	352	GLU	2.5
1	C	461	ASP	2.5
1	C	66	THR	2.5
1	D	3	PHE	2.5
1	D	349	GLU	2.5
1	B	268	LEU	2.4
1	C	0	MET	2.4
1	C	348	ASN	2.4
1	C	511	GLU	2.4
1	C	327	ILE	2.4
1	D	345	GLN	2.4
1	C	328	ILE	2.4
1	C	307	GLY	2.4
1	A	61	THR	2.4
1	A	347	ASN	2.4
1	C	462	GLY	2.3
1	C	493	TYR	2.3
1	A	10	ALA	2.3
1	C	50	THR	2.3
1	B	120	MET	2.3
1	C	4	LYS	2.3
1	D	488	VAL	2.3
1	D	133	ALA	2.3
1	B	344	ASP	2.3
1	A	362	LEU	2.3
1	A	12	GLU	2.3
1	D	346	LEU	2.2
1	A	288	MET	2.2
1	B	70	GLU	2.2
1	B	431	GLU	2.2
1	A	304	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	300	ALA	2.2
1	C	306	LEU	2.2
1	B	526	VAL	2.2
1	D	401	LEU	2.2
1	D	107	GLY	2.2
1	A	468	GLU	2.2
1	C	467	LYS	2.2
1	B	337	TYR	2.2
1	D	128	THR	2.2
1	A	356	LYS	2.2
1	A	407	LEU	2.2
1	A	529	GLY	2.2
1	D	350	ASN	2.1
1	B	383	PHE	2.1
1	B	308	ALA	2.1
1	D	27	LEU	2.1
1	D	59	LEU	2.1
1	D	328	ILE	2.1
1	B	385	LEU	2.1
1	C	59	LEU	2.1
1	A	108	GLY	2.1
1	B	119	PRO	2.1
1	C	344	ASP	2.1
1	C	388	ASP	2.1
1	A	431	GLU	2.1
1	D	58	ILE	2.1
1	D	497	ASP	2.1
1	B	72	LYS	2.1
1	A	339	GLY	2.1
1	C	355	GLU	2.0
1	C	27	LEU	2.0
1	A	76	SER	2.0
1	C	421	VAL	2.0
1	D	332	VAL	2.0
1	A	348	ASN	2.0
1	B	390	GLU	2.0
1	A	387	THR	2.0
1	D	396	SER	2.0
1	D	545	ARG	2.0
1	C	330	ALA	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)

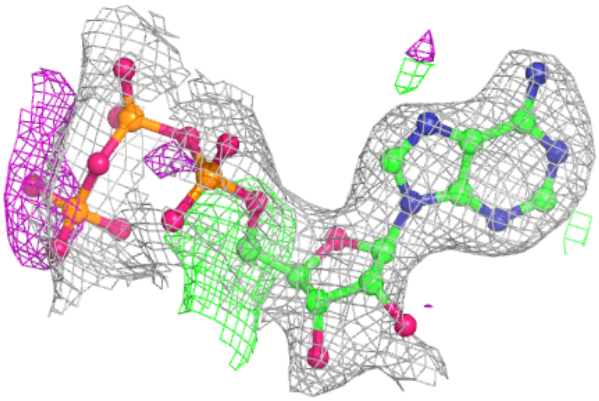
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

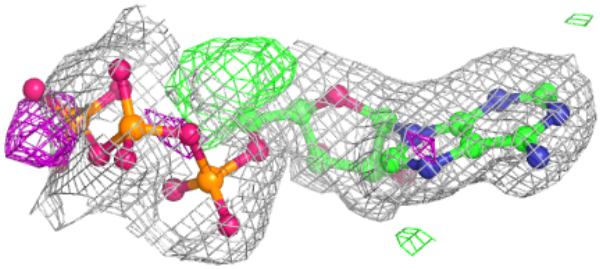
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BU3	B	607	6/6	0.66	0.38	37,44,47,48	0
4	BU3	B	606	6/6	0.68	0.42	45,50,54,55	0
4	BU3	B	604	6/6	0.69	0.22	42,47,54,55	0
4	BU3	B	603	6/6	0.78	0.26	40,50,56,61	0
3	ATP	C	602	31/31	0.83	0.16	40,56,81,91	0
3	ATP	A	602	31/31	0.85	0.17	52,65,86,95	0
3	ATP	D	602	31/31	0.85	0.15	41,55,79,80	0
4	BU3	B	605	6/6	0.86	0.32	40,43,46,46	0
3	ATP	B	602	31/31	0.87	0.17	44,54,68,79	0
2	K	B	601	1/1	0.96	0.08	34,34,34,34	0
2	K	D	601	1/1	0.97	0.08	30,30,30,30	0
2	K	A	601	1/1	0.98	0.08	38,38,38,38	0
2	K	C	601	1/1	0.98	0.04	33,33,33,33	0

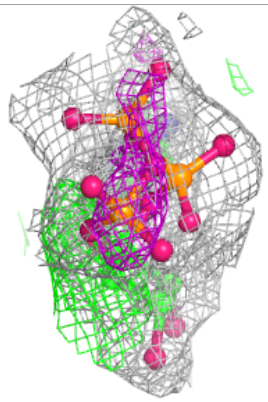
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

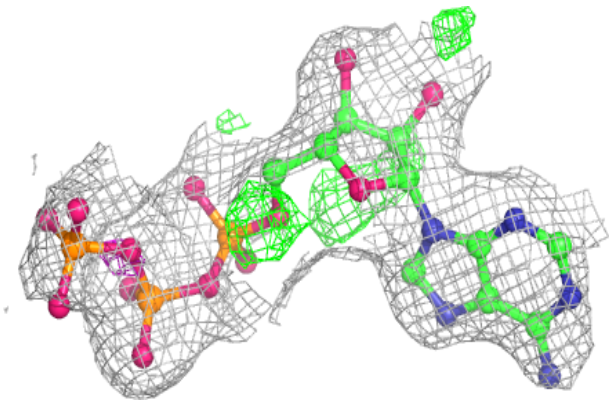


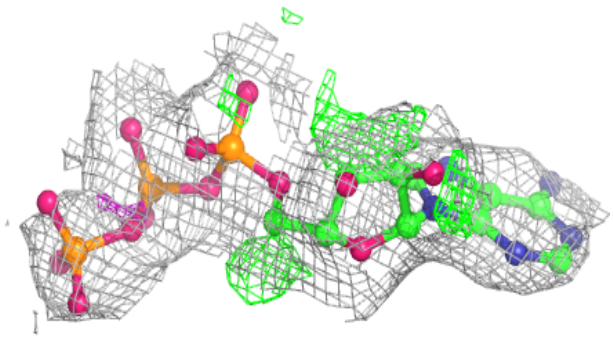


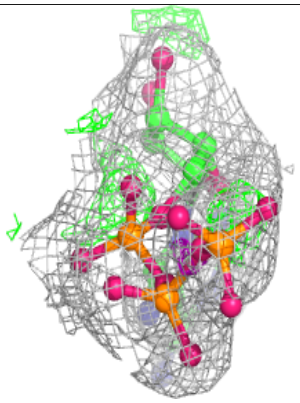


Electron density around ATP A 602:

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

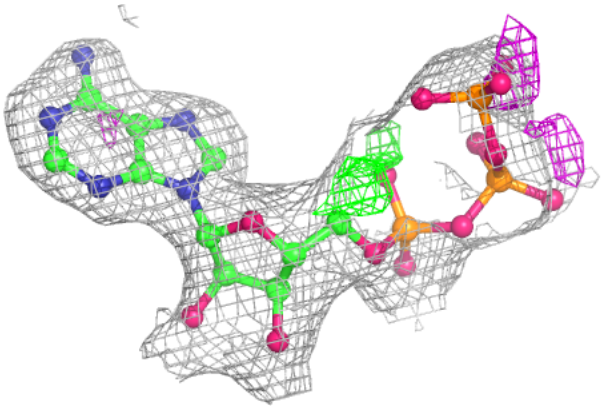


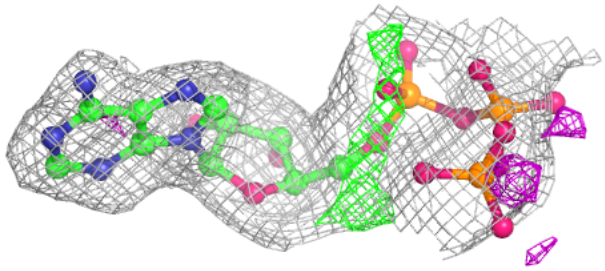


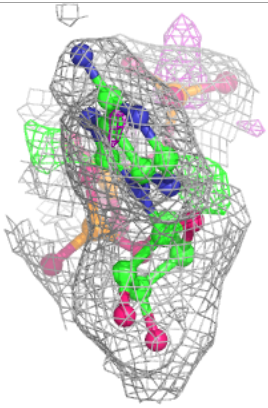


Electron density around ATP D 602:

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

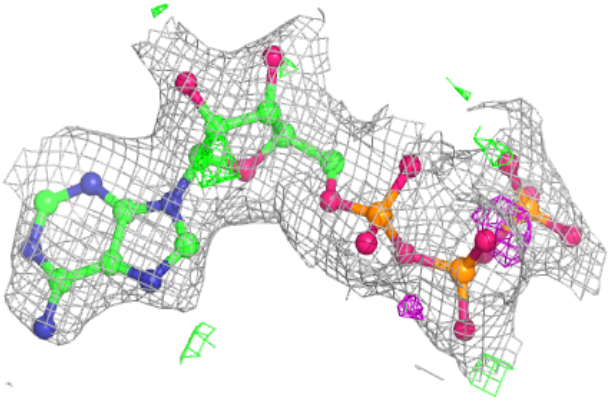


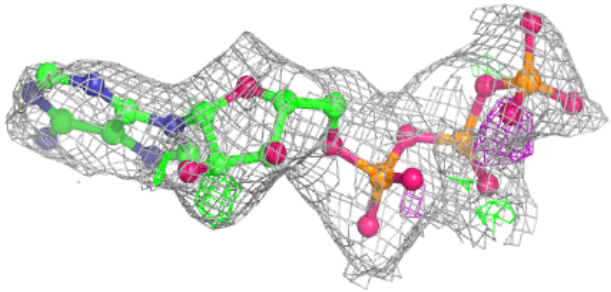


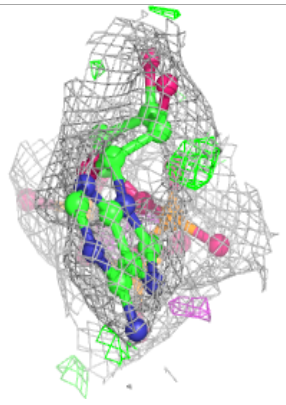


Electron density around ATP B 602:

$2mF_o$-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.