



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 09:48 AM EDT

PDB ID : 1MIW
Title : Crystal structure of Bacillus stearothermophilus CCA-adding enzyme in complex with ATP
Authors : Li, F.; Xiong, Y.; Wang, J.; Cho, H.D.; Weiner, A.M.; Steitz, T.A.
Deposited on : 2002-08-23
Resolution : 3.00 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	:	2.36.2
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)	:	2.36.2

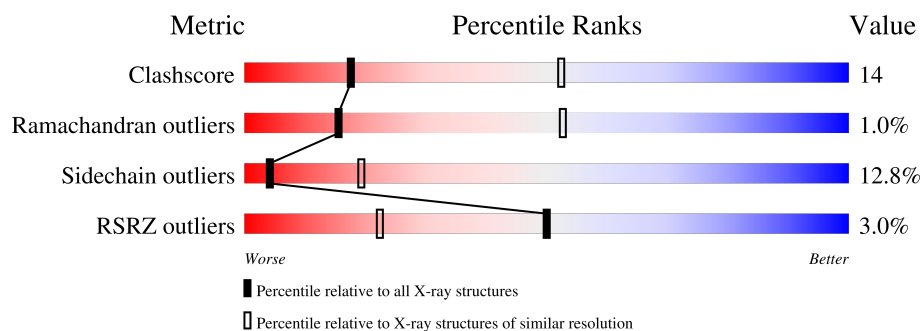
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	404	<div> <div>3%</div> <div>65%</div> <div>28%</div> <div>• •</div> </div>
1	B	404	<div> <div>3%</div> <div>67%</div> <div>27%</div> <div>• •</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6334 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.

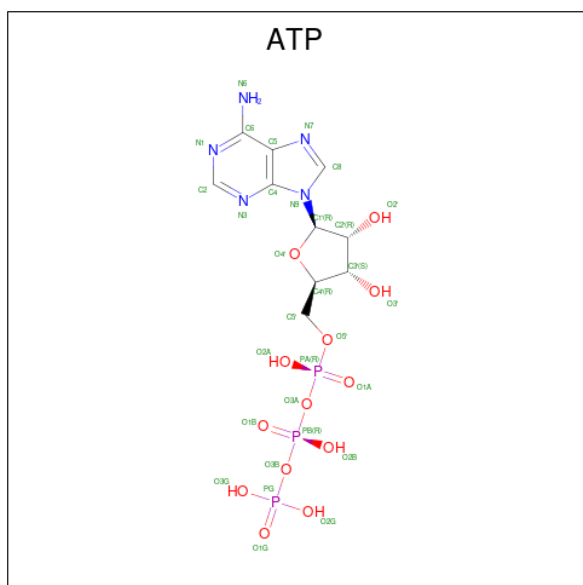
- Molecule 1 is a protein called tRNA CCA-adding enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	Se	0	0	0
			3113	1986	560	555	2	10			
1	B	395	Total	C	N	O	S	Se	0	0	0
			3113	1986	560	555	2	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- 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	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

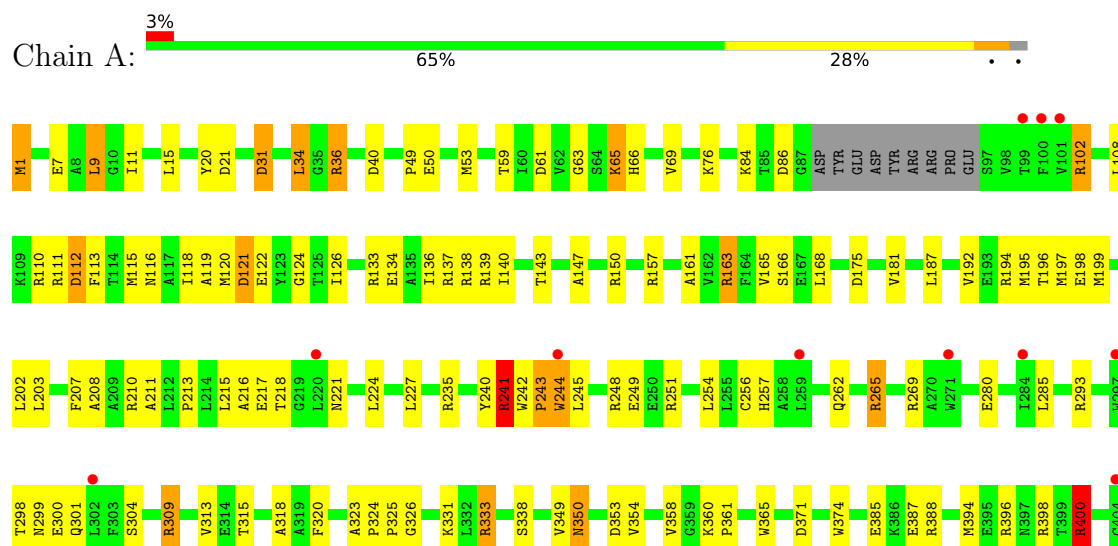
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	21	Total	O	0	0
			21	21		

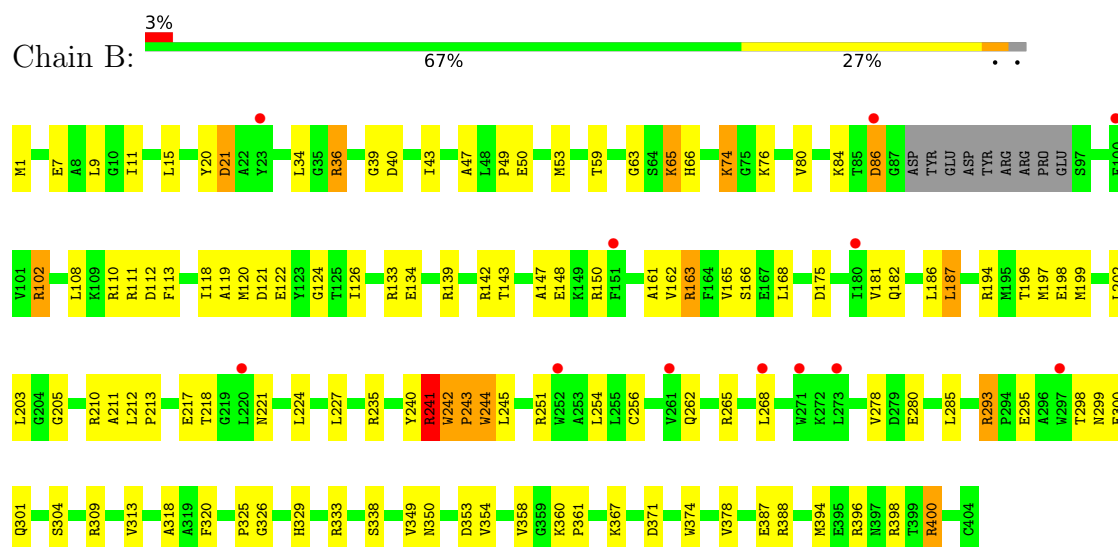
3 Residue-property plots

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: tRNA CCA-adding enzyme



• Molecule 1: tRNA CCA-adding enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.63Å 105.63Å 184.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.65 – 3.00 92.08 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (81.65-3.00) 90.5 (92.08-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.17	Depositor
R, R_{free}	0.228 , 0.263 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	116.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 96.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6334	wwPDB-VP
Average B, all atoms (Å ²)	88.0	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 40.54 % 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 2.6947e-04. 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, MG

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	0.89	2/3172 (0.1%)	0.97	11/4278 (0.3%)
1	B	0.84	3/3172 (0.1%)	0.92	7/4278 (0.2%)
All	All	0.86	5/6344 (0.1%)	0.94	18/8556 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	TRP	CB-CG	15.37	1.77	1.50
1	A	244	TRP	CB-CG	11.78	1.71	1.50
1	B	241	ARG	CG-CD	6.90	1.69	1.51
1	B	242	TRP	CB-CG	-5.41	1.40	1.50
1	A	241	ARG	CG-CD	5.09	1.64	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	241	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	40	ASP	CB-CG-OD2	7.61	125.15	118.30
1	A	121	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	40	ASP	CB-CA-C	6.30	122.99	110.40
1	A	31	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	40	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	112	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	309	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	112	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	353	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	243	PRO	CA-C-N	5.45	129.18	117.20
1	A	248	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	B	121	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	86	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	61	ASP	CB-CG-OD2	5.00	122.80	118.30
1	A	34	LEU	CB-CG-CD2	-5.00	102.50	111.00

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	3113	0	3161	84	0
1	B	3113	0	3161	78	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	12	6	0
3	B	31	0	12	7	0
4	A	21	0	0	0	0
4	B	21	0	0	0	0
All	All	6334	0	6346	173	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 14.

All (173) 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:244:TRP:CB	1:B:244:TRP:CG	1.77	1.62
1:B:241:ARG:HH22	1:B:244:TRP:CB	1.61	1.14
1:A:241:ARG:HH22	1:A:244:TRP:HB2	1.02	1.11
1:B:241:ARG:HH22	1:B:244:TRP:HB2	0.99	1.11
1:A:241:ARG:HH22	1:A:244:TRP:CB	1.68	1.05
1:A:163:ARG:HD3	1:A:198:GLU:OE2	1.62	0.99
1:A:241:ARG:NH2	1:A:244:TRP:CB	2.29	0.95
1:A:241:ARG:NH2	1:A:244:TRP:HB2	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:HD3	1:B:198:GLU:OE2	1.65	0.95
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.31	0.93
1:B:241:ARG:NH2	1:B:244:TRP:CB	2.30	0.92
1:B:241:ARG:NH2	1:B:244:TRP:HB2	1.83	0.92
1:B:400:ARG:HG2	1:B:400:ARG:HH11	1.39	0.87
1:A:298:THR:HB	1:A:301:GLN:HG3	1.58	0.84
1:B:120:MSE:HE3	1:B:126:ILE:HD11	1.60	0.82
1:A:199:MSE:HA	1:A:199:MSE:HE3	1.63	0.81
1:A:358:VAL:O	1:A:358:VAL:HG12	1.81	0.80
1:B:240:TYR:CE2	1:B:320:PHE:HD1	1.99	0.79
1:B:241:ARG:NH2	1:B:244:TRP:HB3	1.98	0.78
1:A:241:ARG:NH2	1:A:244:TRP:HB3	1.99	0.78
3:B:6501:ATP:C5'	3:B:6501:ATP:H8	1.97	0.77
1:B:199:MSE:HE3	1:B:199:MSE:HA	1.68	0.76
1:B:298:THR:HB	1:B:301:GLN:HG3	1.66	0.75
3:B:6501:ATP:H8	3:B:6501:ATP:H5'2	1.52	0.75
1:B:194:ARG:HA	1:B:197:MSE:HE2	1.68	0.73
1:A:240:TYR:CE2	1:A:320:PHE:HD1	2.07	0.73
3:B:6501:ATP:C5'	3:B:6501:ATP:C8	2.72	0.72
1:A:194:ARG:HA	1:A:197:MSE:HE2	1.72	0.71
1:A:400:ARG:HG2	1:A:400:ARG:NH1	1.99	0.69
1:B:20:TYR:O	1:B:21:ASP:CB	2.41	0.69
1:B:358:VAL:O	1:B:358:VAL:HG12	1.93	0.68
1:A:242:TRP:HB2	1:A:243:PRO:HD3	1.75	0.67
1:B:298:THR:HG22	1:B:300:GLU:H	1.59	0.67
1:B:242:TRP:HB2	1:B:243:PRO:HD3	1.78	0.66
1:A:120:MSE:HE3	1:A:126:ILE:HD11	1.78	0.66
1:A:199:MSE:CE	1:A:202:LEU:HB3	2.26	0.65
1:A:20:TYR:O	1:A:21:ASP:CB	2.43	0.65
1:A:298:THR:HG22	1:A:300:GLU:H	1.60	0.65
3:A:5501:ATP:C8	3:A:5501:ATP:H5'1	2.32	0.65
1:B:298:THR:H	1:B:301:GLN:HE21	1.43	0.64
1:A:298:THR:H	1:A:301:GLN:HE21	1.44	0.64
3:B:6501:ATP:H5'2	3:B:6501:ATP:C8	2.32	0.63
1:B:360:LYS:HG3	1:B:361:PRO:HD2	1.79	0.63
1:A:63:GLY:HA2	1:A:65:LYS:HE2	1.81	0.63
1:A:20:TYR:O	1:A:21:ASP:HB3	1.98	0.62
3:A:5501:ATP:C5'	3:A:5501:ATP:H8	2.13	0.62
1:A:360:LYS:HG3	1:A:361:PRO:HD2	1.81	0.62
1:B:108:LEU:O	1:B:111:ARG:HG3	1.99	0.62
1:B:199:MSE:CE	1:B:202:LEU:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:MSE:HE2	1:A:202:LEU:HB3	1.82	0.61
1:B:20:TYR:O	1:B:21:ASP:HB3	2.00	0.61
1:B:120:MSE:HE2	1:B:124:GLY:O	2.00	0.61
1:A:333:ARG:HH11	1:A:333:ARG:HG2	1.64	0.61
1:A:309:ARG:O	1:A:313:VAL:HG23	2.01	0.61
1:A:111:ARG:HD3	3:A:5501:ATP:O2'	2.01	0.61
3:A:5501:ATP:H5'1	3:A:5501:ATP:H8	1.65	0.60
1:B:49:PRO:O	1:B:53:MSE:HG3	2.02	0.60
1:A:49:PRO:O	1:A:53:MSE:HG3	2.02	0.59
1:B:120:MSE:HE3	1:B:126:ILE:CD1	2.32	0.59
1:B:166:SER:HB2	1:B:211:ALA:CB	2.32	0.59
1:A:118:ILE:HG22	1:A:119:ALA:H	1.66	0.59
1:B:318:ALA:CB	1:B:325:PRO:HG3	2.33	0.59
1:A:358:VAL:O	1:A:358:VAL:CG1	2.51	0.58
1:A:333:ARG:HH11	1:A:333:ARG:CG	2.16	0.58
1:A:298:THR:N	1:A:301:GLN:HE21	2.01	0.58
3:B:6501:ATP:C8	3:B:6501:ATP:H5'1	2.37	0.58
3:A:5501:ATP:C8	3:A:5501:ATP:C5'	2.87	0.58
1:B:15:LEU:O	1:B:20:TYR:HB2	2.03	0.58
1:B:210:ARG:C	1:B:213:PRO:HD2	2.24	0.58
1:B:309:ARG:O	1:B:313:VAL:HG23	2.04	0.58
1:A:400:ARG:HH11	1:A:400:ARG:CG	2.12	0.58
1:B:400:ARG:HG2	1:B:400:ARG:NH1	2.07	0.58
3:B:6501:ATP:H8	3:B:6501:ATP:H5'1	1.70	0.57
1:B:118:ILE:HG22	1:B:119:ALA:H	1.70	0.56
1:B:333:ARG:HG2	1:B:333:ARG:HH11	1.70	0.56
1:B:221:ASN:ND2	1:B:227:LEU:O	2.39	0.56
1:A:15:LEU:O	1:A:20:TYR:HB2	2.07	0.55
1:B:199:MSE:HE1	1:B:202:LEU:HD22	1.89	0.55
1:A:318:ALA:CB	1:A:325:PRO:HG3	2.38	0.54
1:B:199:MSE:HE3	1:B:202:LEU:HB3	1.89	0.54
1:B:111:ARG:HD3	3:B:6501:ATP:O2'	2.08	0.54
1:B:118:ILE:HG22	1:B:119:ALA:N	2.23	0.53
1:A:224:LEU:HB2	1:A:227:LEU:HD12	1.90	0.53
1:B:400:ARG:HH11	1:B:400:ARG:CG	2.17	0.53
1:B:224:LEU:HB2	1:B:227:LEU:HD12	1.89	0.53
1:B:298:THR:O	1:B:299:ASN:C	2.47	0.53
1:B:181:VAL:HG22	1:B:218:THR:HA	1.90	0.53
1:A:108:LEU:O	1:A:111:ARG:HG3	2.09	0.53
1:A:221:ASN:ND2	1:A:227:LEU:HB3	2.23	0.53
1:B:242:TRP:CE3	1:B:254:LEU:HD23	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ASN:ND2	1:B:227:LEU:HB3	2.24	0.52
1:B:34:LEU:HD23	1:B:36:ARG:HD2	1.92	0.52
1:A:166:SER:HB2	1:A:211:ALA:CB	2.40	0.51
1:B:298:THR:N	1:B:301:GLN:HE21	2.08	0.51
1:B:161:ALA:O	1:B:165:VAL:HG23	2.11	0.51
1:A:216:ALA:O	1:A:218:THR:O	2.29	0.51
1:A:118:ILE:HG22	1:A:119:ALA:N	2.25	0.51
1:B:50:GLU:H	1:B:50:GLU:CD	2.14	0.51
1:A:181:VAL:HG22	1:A:218:THR:HA	1.93	0.50
1:A:199:MSE:HA	1:A:199:MSE:CE	2.40	0.50
1:A:1:MSE:HE3	1:A:9:LEU:HD13	1.93	0.50
1:B:242:TRP:CZ3	1:B:254:LEU:HD23	2.46	0.50
1:A:34:LEU:HD23	1:A:36:ARG:HD2	1.93	0.50
1:B:166:SER:HB2	1:B:211:ALA:HB2	1.94	0.50
1:A:245:LEU:HD11	1:A:254:LEU:HD22	1.93	0.50
1:A:280:GLU:HA	1:A:280:GLU:OE1	2.13	0.49
1:A:298:THR:O	1:A:299:ASN:C	2.51	0.49
1:B:244:TRP:CG	1:B:244:TRP:CA	2.83	0.49
1:A:199:MSE:HE1	1:A:202:LEU:HD13	1.94	0.49
1:B:199:MSE:CE	1:B:202:LEU:HD22	2.43	0.49
1:A:143:THR:HG21	1:A:147:ALA:HA	1.95	0.49
1:B:280:GLU:OE1	1:B:280:GLU:HA	2.12	0.48
1:A:34:LEU:CD1	1:A:136:ILE:HG23	2.43	0.48
1:A:34:LEU:HD13	1:A:136:ILE:HG23	1.96	0.47
1:A:242:TRP:CE3	1:A:254:LEU:HD23	2.48	0.47
1:A:166:SER:HB2	1:A:211:ALA:HB2	1.97	0.47
1:B:63:GLY:HA2	1:B:65:LYS:HE2	1.96	0.47
1:B:102:ARG:HB2	1:B:102:ARG:CZ	2.45	0.47
1:B:113:PHE:CZ	1:B:161:ALA:HB2	2.50	0.47
1:A:102:ARG:CZ	1:A:102:ARG:HB2	2.46	0.46
1:A:1:MSE:HE3	1:A:9:LEU:CD1	2.45	0.46
1:B:203:LEU:HB3	1:B:251:ARG:HG2	1.98	0.46
1:A:333:ARG:CG	1:A:333:ARG:NH1	2.77	0.46
1:A:350:ASN:HB3	1:A:353:ASP:OD2	2.16	0.46
1:B:143:THR:HG21	1:B:147:ALA:HA	1.98	0.46
1:A:360:LYS:HG2	1:A:365:TRP:NE1	2.31	0.46
1:A:207:PHE:O	1:A:208:ALA:C	2.53	0.45
1:B:162:VAL:HG12	1:B:202:LEU:HD11	1.98	0.45
1:A:161:ALA:O	1:A:165:VAL:HG23	2.17	0.45
1:A:115:MSE:HG3	1:A:116:ASN:N	2.31	0.45
1:B:43:ILE:HB	1:B:80:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:HD11	1:B:254:LEU:HD22	1.99	0.45
1:A:210:ARG:C	1:A:213:PRO:HD2	2.37	0.45
1:A:59:THR:HG22	1:A:69:VAL:HG13	1.98	0.44
1:A:256:CYS:CB	1:A:285:LEU:HD11	2.47	0.44
1:B:325:PRO:HB2	1:B:329:HIS:CE1	2.53	0.44
1:A:31:ASP:OD1	1:A:36:ARG:HD3	2.17	0.44
1:B:166:SER:OG	1:B:205:GLY:HA3	2.17	0.44
1:A:256:CYS:O	1:A:257:HIS:C	2.55	0.44
1:B:299:ASN:HB3	1:B:378:VAL:HG12	2.00	0.44
1:B:268:LEU:HB2	1:B:278:VAL:HG13	2.00	0.43
1:B:194:ARG:HA	1:B:197:MSE:CE	2.44	0.43
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.82	0.43
1:A:50:GLU:CD	1:A:50:GLU:H	2.23	0.43
1:A:244:TRP:HD1	1:A:315:THR:HG23	1.83	0.43
1:B:256:CYS:CB	1:B:285:LEU:HD11	2.49	0.43
1:A:120:MSE:HE2	1:A:124:GLY:O	2.19	0.42
1:A:323:ALA:HA	1:A:324:PRO:HD3	1.88	0.42
1:A:138:ARG:HB3	1:A:140:ILE:HD12	2.01	0.42
1:B:74:LYS:HB3	1:B:74:LYS:HE3	1.75	0.42
1:B:212:LEU:N	1:B:213:PRO:CD	2.82	0.42
1:B:217:GLU:HG3	1:B:235:ARG:HH21	1.84	0.42
1:B:333:ARG:HH11	1:B:333:ARG:CG	2.33	0.42
1:B:358:VAL:O	1:B:358:VAL:CG1	2.63	0.42
1:A:199:MSE:CE	1:A:202:LEU:HD13	2.50	0.41
1:B:293:ARG:NH1	1:B:295:GLU:OE1	2.54	0.41
1:A:9:LEU:HD12	1:A:9:LEU:HA	1.79	0.41
1:B:143:THR:HG23	1:B:150:ARG:HG3	2.02	0.41
1:A:192:VAL:HA	1:A:195:MSE:CE	2.51	0.41
1:A:121:ASP:OD1	1:A:121:ASP:C	2.59	0.41
1:A:265:ARG:O	1:A:269:ARG:HB2	2.21	0.41
1:A:385:GLU:OE2	1:A:387:GLU:HB3	2.21	0.41
3:A:5501:ATP:H8	3:A:5501:ATP:H5'2	1.86	0.41
1:A:143:THR:HG23	1:A:150:ARG:HG3	2.03	0.41
1:B:20:TYR:CG	1:B:47:ALA:HB2	2.56	0.41
1:A:112:ASP:OD1	1:A:113:PHE:N	2.50	0.40
1:B:148:GLU:OE2	1:B:182:GLN:NE2	2.53	0.40
1:A:203:LEU:HB3	1:A:251:ARG:HG2	2.03	0.40
1:A:150:ARG:HE	1:A:157:ARG:NH1	2.20	0.40
1:A:217:GLU:HG3	1:A:235:ARG:HH21	1.87	0.40
1:A:221:ASN:ND2	1:A:227:LEU:O	2.55	0.40
1:A:249:GLU:H	1:A:249:GLU:CD	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LEU:HD23	1:B:285:LEU:HA	1.98	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	391/404 (97%)	357 (91%)	31 (8%)	3 (1%)	19	57
1	B	391/404 (97%)	357 (91%)	29 (7%)	5 (1%)	12	45
All	All	782/808 (97%)	714 (91%)	60 (8%)	8 (1%)	15	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	B	86	ASP
1	B	326	GLY
1	A	326	GLY
1	B	39	GLY
1	B	186	LEU
1	A	243	PRO
1	B	21	ASP

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	316/315 (100%)	276 (87%)	40 (13%)	4	19
1	B	316/315 (100%)	275 (87%)	41 (13%)	4	19
All	All	632/630 (100%)	551 (87%)	81 (13%)	4	19

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	7	GLU
1	A	9	LEU
1	A	11	ILE
1	A	36	ARG
1	A	65	LYS
1	A	66	HIS
1	A	76	LYS
1	A	84	LYS
1	A	102	ARG
1	A	110	ARG
1	A	122	GLU
1	A	133	ARG
1	A	134	GLU
1	A	137	ARG
1	A	139	ARG
1	A	163	ARG
1	A	168	LEU
1	A	175	ASP
1	A	187	LEU
1	A	196	THR
1	A	215	LEU
1	A	241	ARG
1	A	262	GLN
1	A	265	ARG
1	A	293	ARG
1	A	304	SER
1	A	331	LYS
1	A	333	ARG
1	A	338	SER
1	A	349	VAL
1	A	350	ASN
1	A	354	VAL
1	A	371	ASP
1	A	374	TRP

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Mol	Chain	Res	Type
1	A	388	ARG
1	A	394	MSE
1	A	396	ARG
1	A	398	ARG
1	A	400	ARG
1	B	1	MSE
1	B	7	GLU
1	B	9	LEU
1	B	11	ILE
1	B	36	ARG
1	B	59	THR
1	B	65	LYS
1	B	66	HIS
1	B	74	LYS
1	B	76	LYS
1	B	84	LYS
1	B	102	ARG
1	B	110	ARG
1	B	122	GLU
1	B	133	ARG
1	B	134	GLU
1	B	139	ARG
1	B	142	ARG
1	B	163	ARG
1	B	168	LEU
1	B	175	ASP
1	B	187	LEU
1	B	196	THR
1	B	241	ARG
1	B	262	GLN
1	B	265	ARG
1	B	293	ARG
1	B	304	SER
1	B	338	SER
1	B	349	VAL
1	B	350	ASN
1	B	354	VAL
1	B	367	LYS
1	B	371	ASP
1	B	374	TRP
1	B	387	GLU
1	B	388	ARG

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Mol	Chain	Res	Type
1	B	394	MSE
1	B	396	ARG
1	B	398	ARG
1	B	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	178	GLN
1	A	182	GLN
1	A	221	ASN
1	A	301	GLN
1	B	6	GLN
1	B	178	GLN
1	B	182	GLN
1	B	221	ASN
1	B	301	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	5501	2	26,33,33	1.30	3 (11%)	31,52,52	2.06	9 (29%)
3	ATP	B	6501	2	26,33,33	1.40	3 (11%)	31,52,52	1.95	6 (19%)

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	5501	2	-	5/18/38/38	0/3/3/3
3	ATP	B	6501	2	-	5/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	6501	ATP	C2-N3	4.48	1.39	1.32
3	A	5501	ATP	C2-N3	3.54	1.37	1.32
3	A	5501	ATP	O4'-C4'	-2.68	1.39	1.45
3	B	6501	ATP	C2-N1	2.40	1.38	1.33
3	A	5501	ATP	O5'-C5'	-2.31	1.35	1.44
3	B	6501	ATP	C2'-C1'	-2.07	1.50	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6501	ATP	N3-C2-N1	-6.29	118.84	128.68
3	A	5501	ATP	N3-C2-N1	-5.56	119.98	128.68
3	A	5501	ATP	PB-O3B-PG	-4.35	117.90	132.83
3	A	5501	ATP	PA-O3A-PB	-4.10	118.77	132.83
3	B	6501	ATP	PB-O3B-PG	-3.68	120.20	132.83
3	A	5501	ATP	O4'-C1'-C2'	-3.47	101.85	106.93
3	B	6501	ATP	PA-O3A-PB	-3.43	121.07	132.83
3	A	5501	ATP	O3G-PG-O3B	3.27	115.60	104.64
3	B	6501	ATP	O4'-C1'-C2'	-3.23	102.21	106.93
3	A	5501	ATP	O4'-C4'-C5'	-2.89	99.87	109.37
3	A	5501	ATP	C5'-C4'-C3'	-2.69	105.11	115.18
3	B	6501	ATP	O3G-PG-O3B	2.65	113.54	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6501	ATP	C5'-C4'-C3'	-2.64	105.30	115.18
3	A	5501	ATP	O2B-PB-O1B	-2.27	101.02	112.24
3	A	5501	ATP	O5'-C5'-C4'	-2.13	101.67	108.99

There are no chirality outliers.

All (10) torsion outliers are listed below:

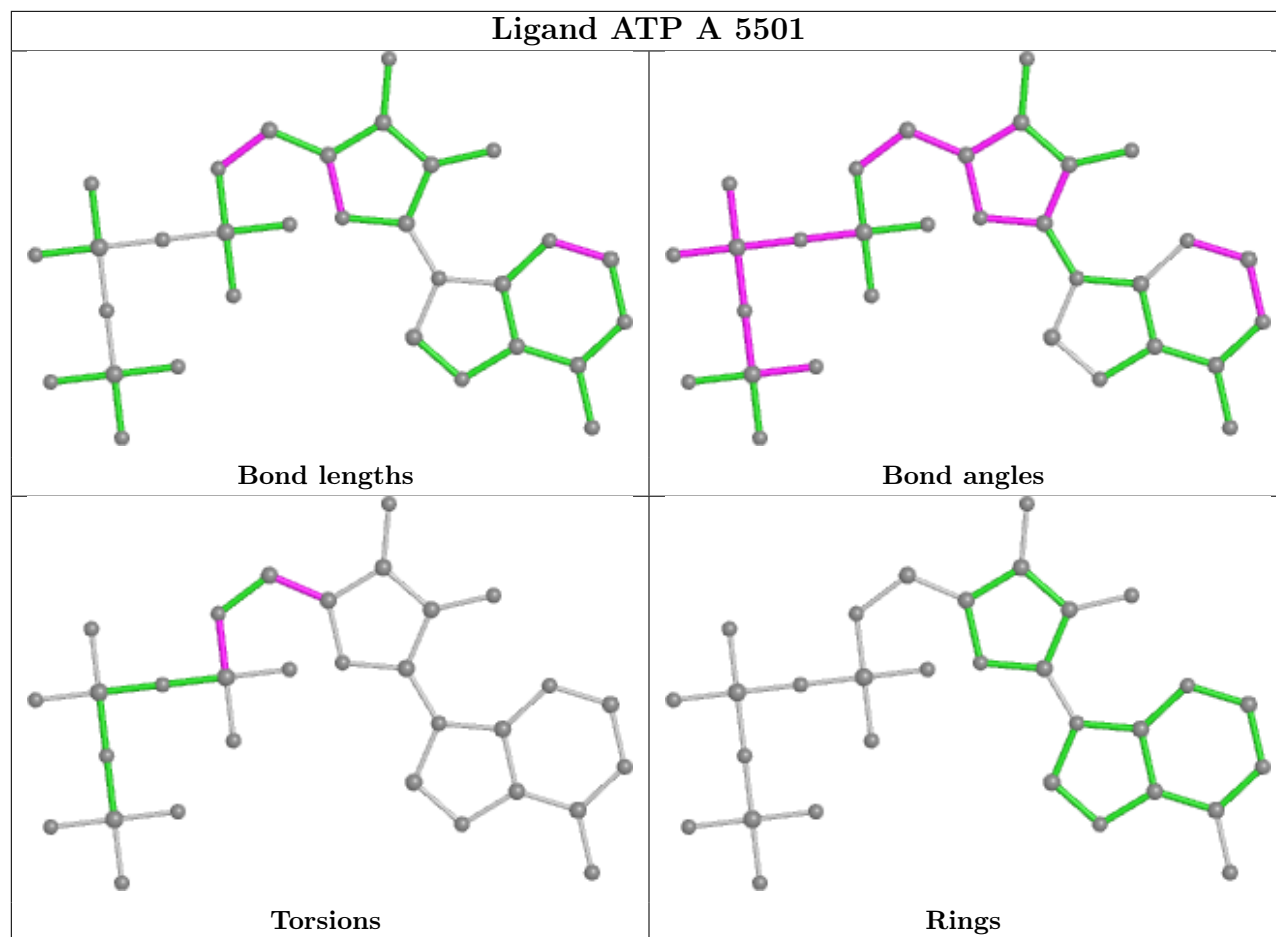
Mol	Chain	Res	Type	Atoms
3	A	5501	ATP	C5'-O5'-PA-O1A
3	A	5501	ATP	C5'-O5'-PA-O2A
3	A	5501	ATP	C5'-O5'-PA-O3A
3	B	6501	ATP	C5'-O5'-PA-O2A
3	A	5501	ATP	O4'-C4'-C5'-O5'
3	A	5501	ATP	C3'-C4'-C5'-O5'
3	B	6501	ATP	O4'-C4'-C5'-O5'
3	B	6501	ATP	C3'-C4'-C5'-O5'
3	B	6501	ATP	C5'-O5'-PA-O1A
3	B	6501	ATP	C5'-O5'-PA-O3A

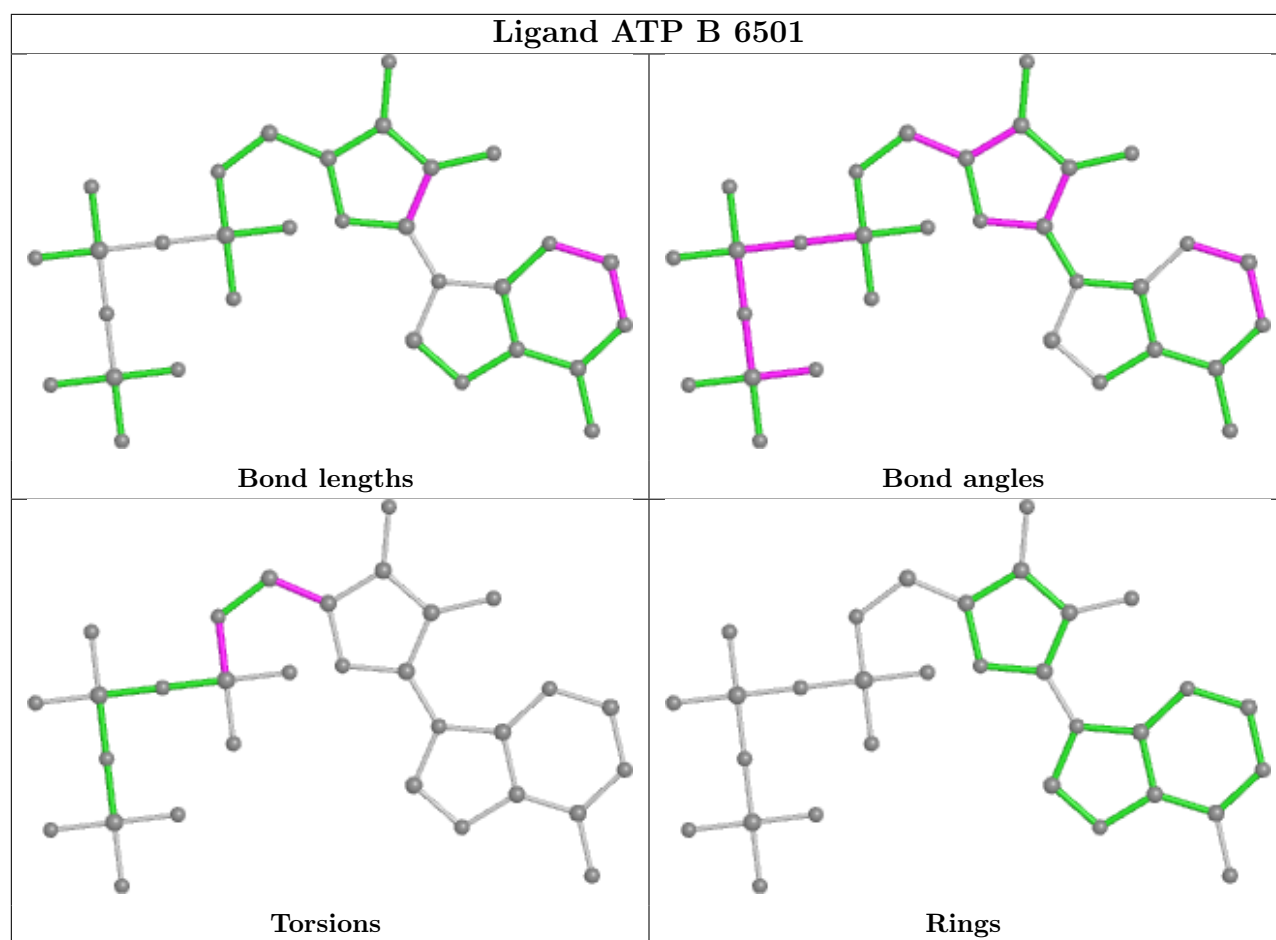
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5501	ATP	6	0
3	B	6501	ATP	7	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	385/404 (95%)	0.15	11 (2%)	51	23	58, 83, 121, 134	0
1	B	385/404 (95%)	0.19	12 (3%)	49	21	58, 83, 121, 134	0
All	All	770/808 (95%)	0.17	23 (2%)	50	22	58, 83, 121, 134	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	PHE	5.3
1	B	268	LEU	4.2
1	B	271	TRP	3.7
1	A	220	LEU	3.5
1	B	86	ASP	3.1
1	B	100	PHE	3.0
1	A	404	CYS	3.0
1	A	271	TRP	3.0
1	B	220	LEU	2.9
1	B	151	PHE	2.8
1	B	180	ILE	2.7
1	A	297	TRP	2.6
1	B	261	VAL	2.6
1	A	302	LEU	2.4
1	A	259	LEU	2.3
1	B	23	TYR	2.3
1	B	252	TRP	2.3
1	B	297	TRP	2.2
1	A	99	THR	2.2
1	A	284	ILE	2.1
1	A	101	VAL	2.1
1	A	244	TRP	2.1
1	B	273	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

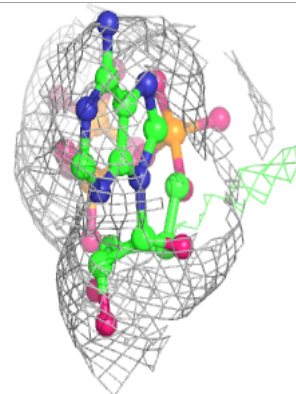
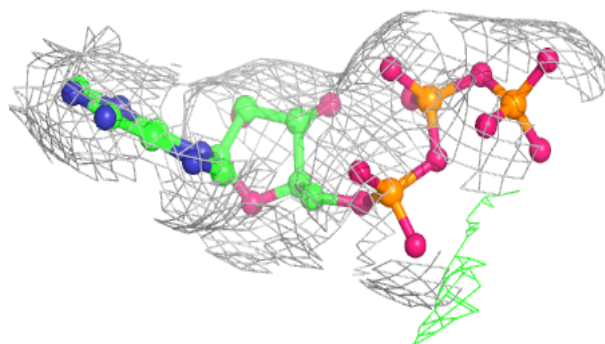
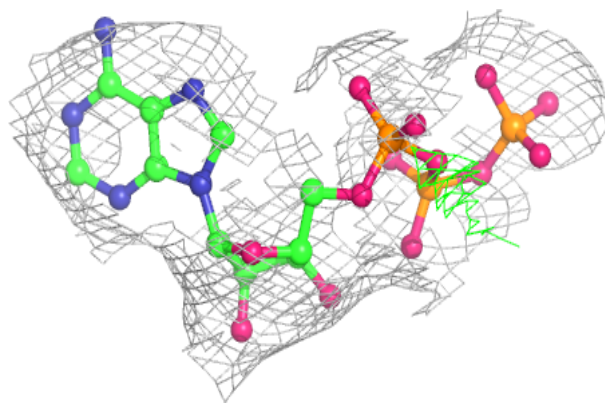
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	5611	1/1	0.85	0.29	69,69,69,69	0
2	MG	B	6611	1/1	0.87	0.33	69,69,69,69	0
2	MG	A	5601	1/1	0.95	0.31	62,62,62,62	0
3	ATP	A	5501	31/31	0.95	0.20	68,77,83,84	0
3	ATP	B	6501	31/31	0.95	0.20	69,77,83,84	0
2	MG	B	6601	1/1	0.99	0.25	62,62,62,62	0

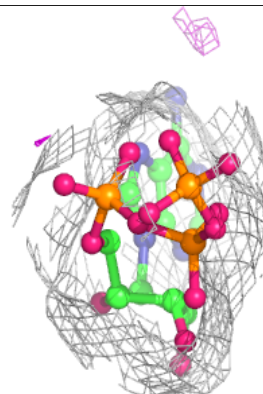
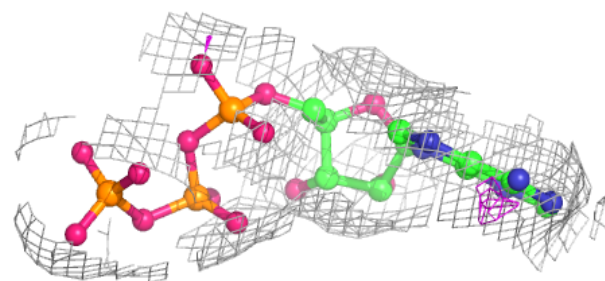
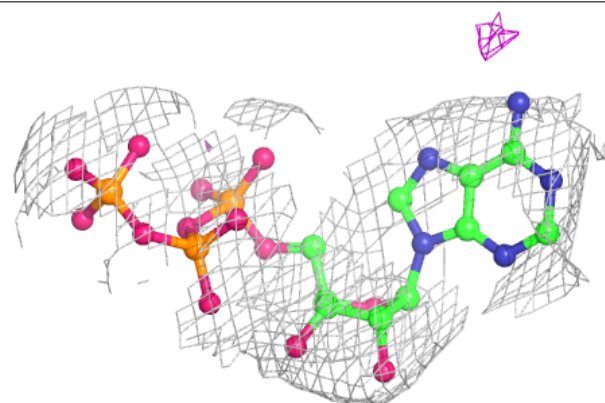
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 5501:

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

**Electron density around ATP B 6501:**

$2mF_o-DF_c$ (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.