wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 06:50 AM EDT

PDB ID	:	2HVY
Title	:	Crystal structure of an H/ACA box RNP from Pyrococcus furiosus
Authors	:	Ye, K.
Deposited on	:	2006-07-31
Resolution	:	2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

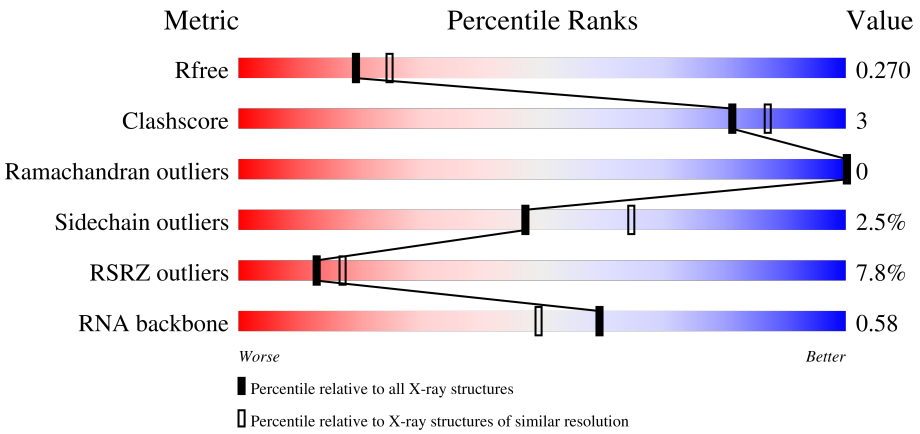
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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	E	65	23% 69% 14% 9% • 6%
2	A	346	5% 84% 8% • 8%
3	B	104	4% 60% 11% • 29%
4	C	60	10% 85% • 12%

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Mol	Chain	Length	Quality of chain
5	D	130	5% 84% 9% 7%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5897 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 RNA chain called H/ACA RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	61	1235	544	223	407	61	0	0	0

- Molecule 2 is a protein called Probable tRNA pseudouridine synthase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	320	2543	1645	435	453	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	HIS	-	expression tag	UNP Q7LWY0
A	345	HIS	-	expression tag	UNP Q7LWY0
A	346	HIS	-	expression tag	UNP Q7LWY0
A	347	HIS	-	expression tag	UNP Q7LWY0
A	348	HIS	-	expression tag	UNP Q7LWY0
A	349	HIS	-	expression tag	UNP Q7LWY0

- Molecule 3 is a protein called Small nucleolar rnp similar to gar1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	74	600	396	102	100	2	0	0	0

- Molecule 4 is a protein called Ribosome biogenesis protein Nop10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	53	444	283	86	71	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	ARG	engineered mutation	UNP Q8U1R4

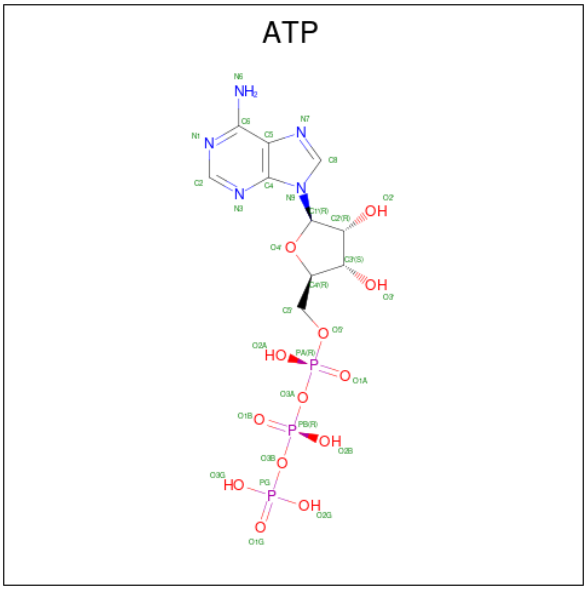
- Molecule 5 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	121	925	591	153	178	3	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP Q8U160
D	2	ALA	MET	engineered mutation	UNP Q8U160
D	125	HIS	-	expression tag	UNP Q8U160
D	126	HIS	-	expression tag	UNP Q8U160
D	127	HIS	-	expression tag	UNP Q8U160
D	128	HIS	-	expression tag	UNP Q8U160
D	129	HIS	-	expression tag	UNP Q8U160
D	130	HIS	-	expression tag	UNP Q8U160

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	C	1	1	1	0	0

- Molecule 8 is water.

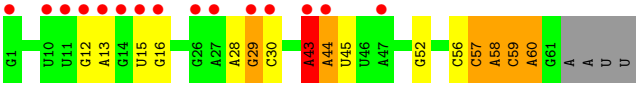
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	E	25	25	25	0	0
			Total	O		
8	A	61	61	61	0	0
			Total	O		
8	B	16	16	16	0	0
			Total	O		
8	C	10	10	10	0	0
			Total	O		
8	D	6	6	6	0	0

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.

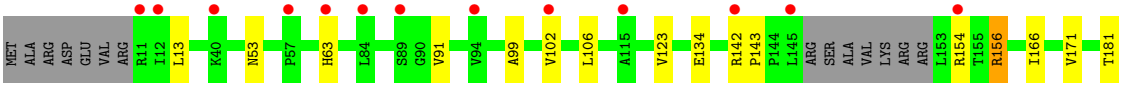
• Molecule 1: H/ACA RNA

Chain E:



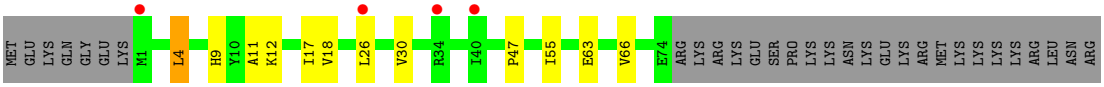
• Molecule 2: Probable tRNA pseudouridine synthase B

Chain A:



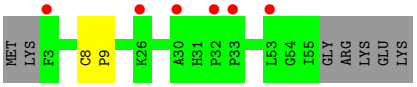
• Molecule 3: Small nucleolar rnp similar to gar1

Chain B:



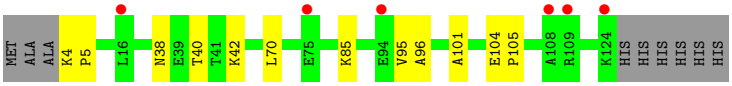
• Molecule 4: Ribosome biogenesis protein Nop10

Chain C:



• Molecule 5: 50S ribosomal protein L7Ae

Chain D:


MET
ALA
ALA
K4
P5
L16
N38
E39
T40
T41
K42
L70
E75
K85
E94
V95
A96
A101
E104
P105
A108
R109
K124
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.03Å 90.95Å 114.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 39.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.30) 99.7 (39.01-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.41 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.278 0.230 , 0.270	Depositor DCC
R_{free} test set	1917 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5897	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	E	0.62	0/1376	1.15	7/2137 (0.3%)
2	A	0.32	0/2602	0.49	0/3523
3	B	0.33	0/614	0.50	0/831
4	C	0.32	0/457	0.44	0/613
5	D	0.31	0/937	0.48	0/1264
All	All	0.41	0/5986	0.71	7/8368 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	43	A	O3'-P-O5'	-10.46	84.13	104.00
1	E	43	A	OP1-P-O3'	-9.09	85.21	105.20
1	E	43	A	P-O3'-C3'	8.14	129.46	119.70
1	E	57	C	P-O3'-C3'	8.03	129.33	119.70
1	E	44	A	OP1-P-OP2	6.42	129.23	119.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1235	0	617	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2543	0	2613	15	0
3	B	600	0	637	5	0
4	C	444	0	451	1	0
5	D	925	0	977	6	0
6	A	31	0	12	0	0
7	C	1	0	0	0	0
8	A	61	0	0	0	0
8	B	16	0	0	0	0
8	C	10	0	0	0	0
8	D	6	0	0	0	0
8	E	25	0	0	0	0
All	All	5897	0	5307	29	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.

The worst 5 of 29 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)
3:B:30:VAL:HG21	3:B:55:ILE:HD12	1.72	0.71
2:A:156:ARG:HG2	2:A:181:THR:OG1	1.94	0.67
5:D:40:THR:HG23	5:D:101:ALA:HB2	1.81	0.61
5:D:4:LYS:HB2	5:D:5:PRO:HD2	1.84	0.60
5:D:38:ASN:O	5:D:42:LYS:HG2	2.05	0.56

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
2	A	316/346 (91%)	310 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	72/104 (69%)	70 (97%)	2 (3%)	0	100	100
4	C	51/60 (85%)	48 (94%)	3 (6%)	0	100	100
5	D	119/130 (92%)	119 (100%)	0	0	100	100
All	All	558/640 (87%)	547 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	271/295 (92%)	265 (98%)	6 (2%)	52	69
3	B	67/96 (70%)	63 (94%)	4 (6%)	19	26
4	C	48/54 (89%)	48 (100%)	0	100	100
5	D	98/105 (93%)	96 (98%)	2 (2%)	55	72
All	All	484/550 (88%)	472 (98%)	12 (2%)	47	65

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	9	HIS
3	B	12	LYS
5	D	85	LYS
3	B	26	LEU
2	A	156	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	36	GLN
4	C	31	HIS
5	D	22	GLN

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Mol	Chain	Res	Type
2	A	80	HIS
2	A	221	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	53/65 (81%)	12 (22%)	6 (11%)

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	13	A
1	E	16	G
1	E	28	A
1	E	29	G
1	E	30	C

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	57	C
1	E	58	A
1	E	59	C
1	E	29	G
1	E	12	G

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
6	ATP	A	501	-	26,33,33	0.99	2 (7%)	31,52,52	1.48	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
6	ATP	A	501	-	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	ATP	C5-C4	2.61	1.47	1.40
6	A	501	ATP	C2-N3	2.04	1.35	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	501	ATP	N3-C2-N1	-3.31	123.51	128.68
6	A	501	ATP	PA-O3A-PB	-3.28	121.57	132.83
6	A	501	ATP	C3'-C2'-C1'	3.26	105.88	100.98
6	A	501	ATP	PB-O3B-PG	-2.89	122.91	132.83
6	A	501	ATP	C4-C5-N7	-2.68	106.61	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

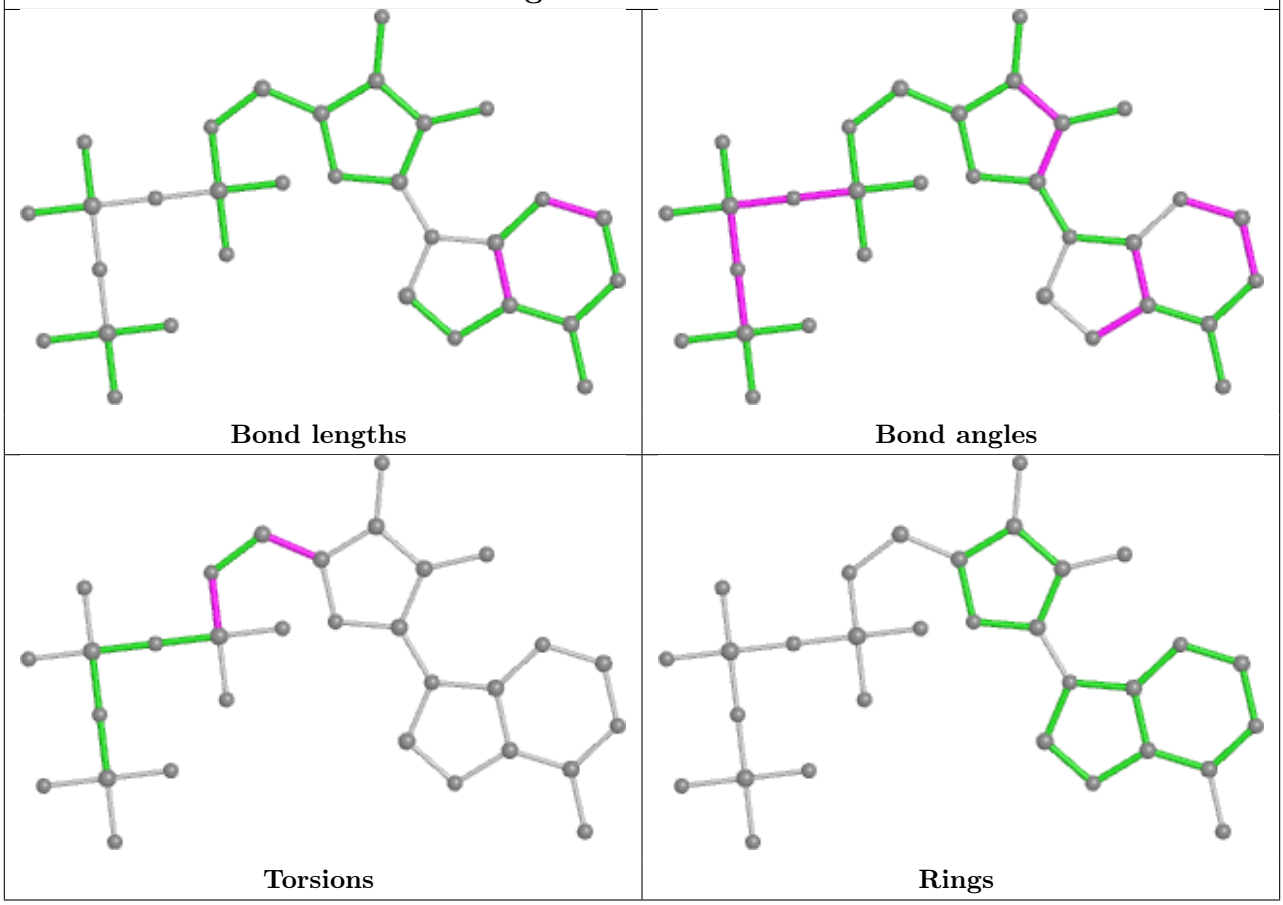
Mol	Chain	Res	Type	Atoms
6	A	501	ATP	C5'-O5'-PA-O3A
6	A	501	ATP	O4'-C4'-C5'-O5'
6	A	501	ATP	C3'-C4'-C5'-O5'
6	A	501	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	E	61/65 (93%)	1.19	15 (24%)	0	0	39, 43, 47, 53	0
2	A	320/346 (92%)	0.65	18 (5%)	24	30	37, 43, 49, 54	0
3	B	74/104 (71%)	0.32	4 (5%)	25	32	40, 43, 47, 48	0
4	C	53/60 (88%)	0.84	6 (11%)	5	7	41, 43, 46, 46	0
5	D	121/130 (93%)	0.56	6 (4%)	28	35	40, 43, 46, 47	0
All	All	629/705 (89%)	0.66	49 (7%)	13	17	37, 43, 48, 54	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	12	ILE	6.0
1	E	27	A	5.6
1	E	12	G	5.5
1	E	29	G	4.7
2	A	11	ARG	4.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

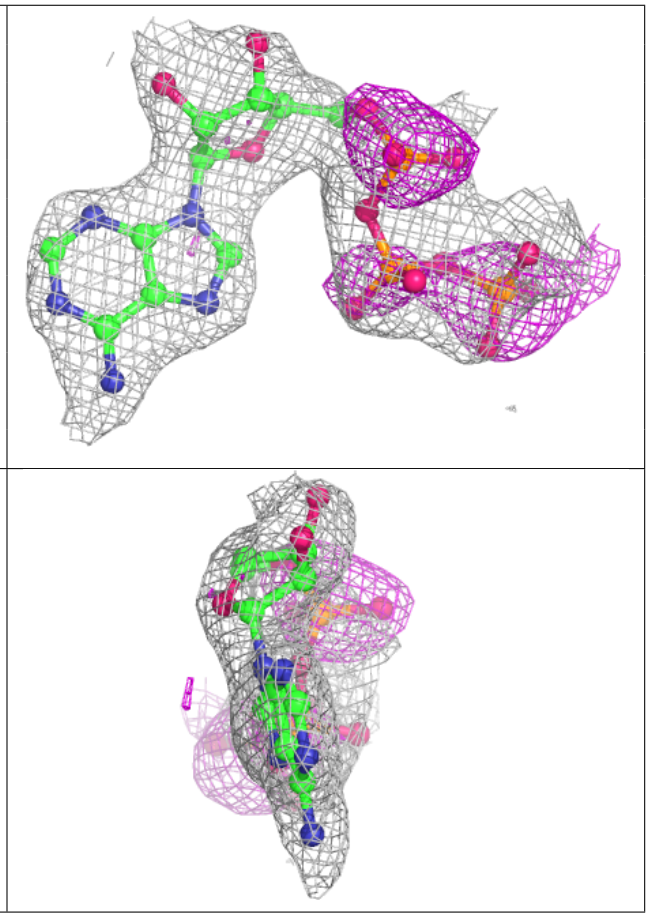
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ATP	A	501	31/31	0.78	0.33	61,64,74,75	0
7	ZN	C	201	1/1	0.97	0.13	64,64,64,64	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 501:

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.