Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2021 – 04:02 PM GMT

PDB ID	:	6YB5
Title	:	Orthorhombic crystal structure of a native BcsRQ complex crystallized in the presence of ADP
Authors	:	Caleechurn, M.; Abidi, W.; Zouhir, S.; Roche, S.; Krasteva, P.V.
Deposited on	:	2020-03-15
Resolution	:	1.59 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 following versions of software and data (see references ⓘ) were used in the production of this report:

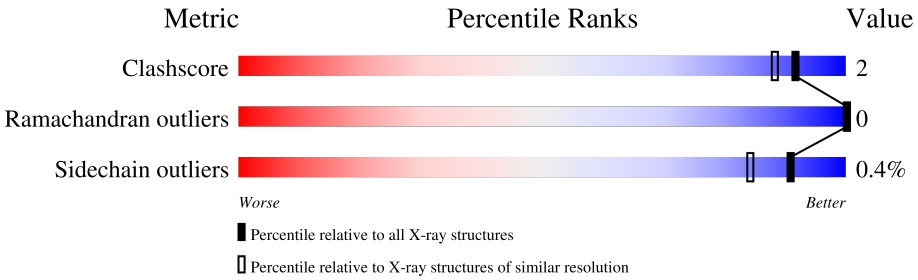
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17

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 1.59 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	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	261	89% . 7%
1	B	261	89% . 7%
1	H	261	. 97%
2	C	62	40% . 58%
2	D	62	55% . 44%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5084 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 Bacterial cellulose secretion regulator BcsQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	9	0
			1979	1241	357	370	11			
1	B	243	Total	C	N	O	S	0	15	0
			2031	1273	368	379	11			
1	H	8	Total	C	N	O		0	0	0
			77	47	20	10				

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ALA	-	expression tag	UNP A0A0B1KWQ0
A	252	ALA	-	expression tag	UNP A0A0B1KWQ0
A	253	ALA	-	expression tag	UNP A0A0B1KWQ0
A	254	LEU	-	expression tag	UNP A0A0B1KWQ0
A	255	GLU	-	expression tag	UNP A0A0B1KWQ0
A	256	HIS	-	expression tag	UNP A0A0B1KWQ0
A	257	HIS	-	expression tag	UNP A0A0B1KWQ0
A	258	HIS	-	expression tag	UNP A0A0B1KWQ0
A	259	HIS	-	expression tag	UNP A0A0B1KWQ0
A	260	HIS	-	expression tag	UNP A0A0B1KWQ0
A	261	HIS	-	expression tag	UNP A0A0B1KWQ0
B	251	ALA	-	expression tag	UNP A0A0B1KWQ0
B	252	ALA	-	expression tag	UNP A0A0B1KWQ0
B	253	ALA	-	expression tag	UNP A0A0B1KWQ0
B	254	LEU	-	expression tag	UNP A0A0B1KWQ0
B	255	GLU	-	expression tag	UNP A0A0B1KWQ0
B	256	HIS	-	expression tag	UNP A0A0B1KWQ0
B	257	HIS	-	expression tag	UNP A0A0B1KWQ0
B	258	HIS	-	expression tag	UNP A0A0B1KWQ0
B	259	HIS	-	expression tag	UNP A0A0B1KWQ0
B	260	HIS	-	expression tag	UNP A0A0B1KWQ0
B	261	HIS	-	expression tag	UNP A0A0B1KWQ0
H	256	ALA	-	expression tag	UNP A0A0B1KWQ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	257	ALA	-	expression tag	UNP A0A0B1KWQ0
H	258	ALA	-	expression tag	UNP A0A0B1KWQ0
H	259	LEU	-	expression tag	UNP A0A0B1KWQ0
H	260	GLU	-	expression tag	UNP A0A0B1KWQ0
H	261	HIS	-	expression tag	UNP A0A0B1KWQ0
H	262	HIS	-	expression tag	UNP A0A0B1KWQ0
H	263	HIS	-	expression tag	UNP A0A0B1KWQ0
H	264	HIS	-	expression tag	UNP A0A0B1KWQ0
H	265	HIS	-	expression tag	UNP A0A0B1KWQ0
H	266	HIS	-	expression tag	UNP A0A0B1KWQ0

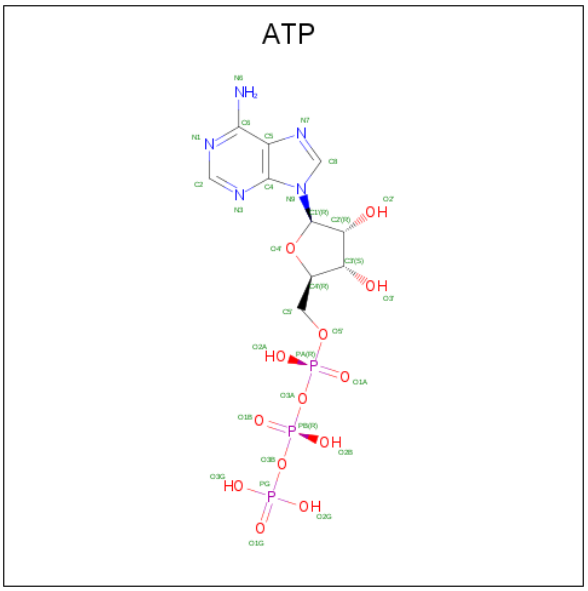
- Molecule 2 is a protein called Bacterial cellulose secretion regulator BcsR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	26	Total	C	N	O	0	0	0
			211	134	39	38			
2	D	35	Total	C	N	O	0	1	0
			294	189	52	53			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	190	Total	O	0	0
			190	190		
5	B	194	Total	O	0	0
			194	194		
5	C	14	Total	O	0	0
			14	14		
5	D	24	Total	O	0	0
			24	24		
5	H	6	Total	O	0	0
			6	6		

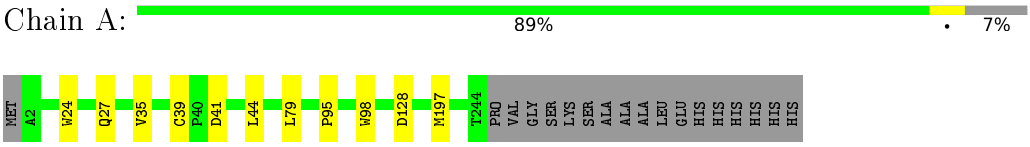
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

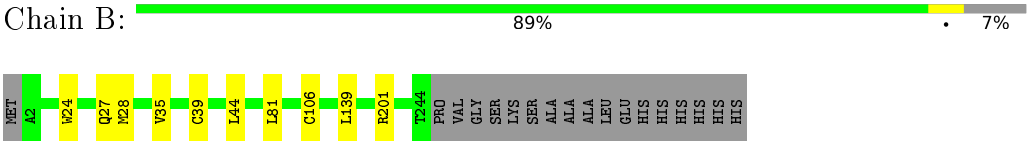
- Molecule 1: Bacterial cellulose secretion regulator BcsQ

Chain A:



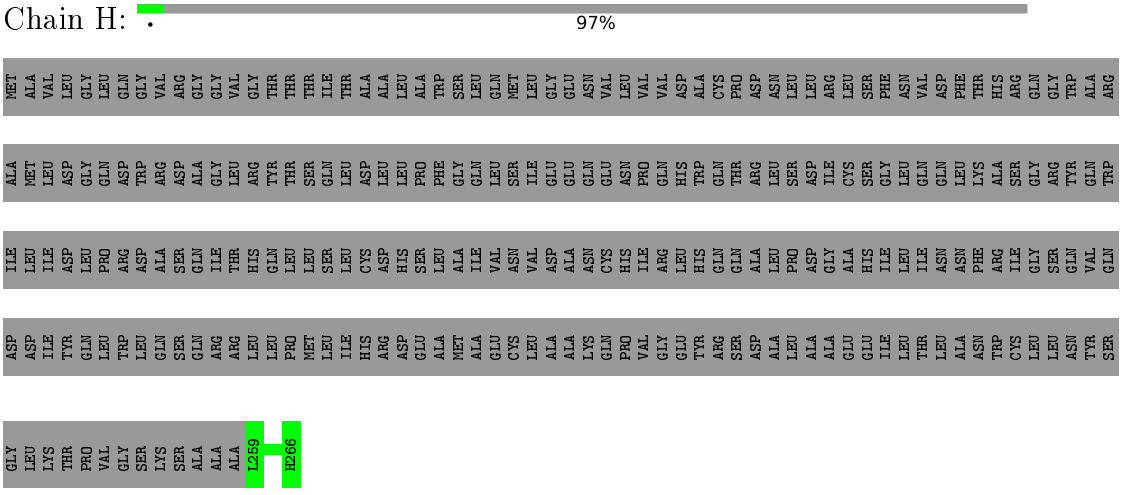
- Molecule 1: Bacterial cellulose secretion regulator BcsQ

Chain B:



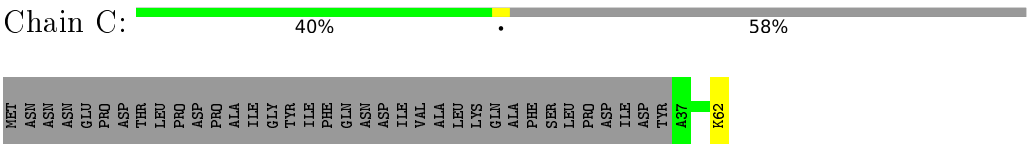
- Molecule 1: Bacterial cellulose secretion regulator BcsQ

Chain H:



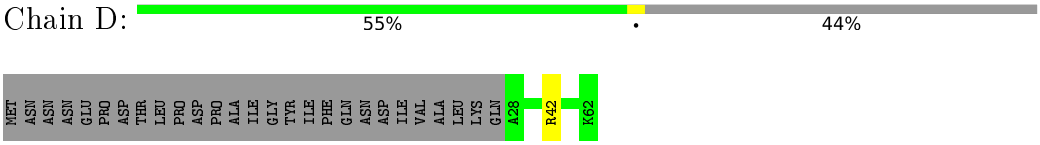
- Molecule 2: Bacterial cellulose secretion regulator BcsR

Chain C:



• Molecule 2: Bacterial cellulose secretion regulator BcsR

Chain D:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.11Å 73.16Å 140.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.23 – 1.59	Depositor
% Data completeness (in resolution range)	99.0 (45.23-1.59)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 1.59Å)	Xtriage
Refinement program	PHENIX 1.17rc2_3619	Depositor
R, R_{free}	0.160 , 0.184	Depositor
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.270	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5084	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.36	0/2016	0.54	0/2743
1	B	0.34	0/2068	0.53	0/2814
1	H	0.16	0/82	0.37	0/110
2	C	0.33	0/214	0.39	0/286
2	D	0.31	0/300	0.40	0/405
All	All	0.34	0/4680	0.52	0/6358

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	1979	0	1950	7	0
1	B	2031	0	2003	6	0
1	H	77	0	58	0	0
2	C	211	0	215	1	0
2	D	294	0	292	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	0	0
5	A	190	0	0	2	0
5	B	194	0	0	1	0
5	C	14	0	0	0	0
5	D	24	0	0	0	0
5	H	6	0	0	0	0
All	All	5084	0	4542	15	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 2.

All (15) 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:A:39[B]:CYS:SG	5:A:428:HOH:O	2.41	0.78
1:B:39[B]:CYS:SG	5:B:460:HOH:O	2.44	0.74
1:A:27:GLN:HG2	1:A:79[B]:LEU:HD12	1.83	0.59
1:A:35[A]:VAL:HG22	1:A:44:LEU:HD21	1.91	0.53
1:B:106:CYS:HA	1:B:139:LEU:HD11	1.93	0.49
1:B:35[A]:VAL:HG22	1:B:44:LEU:HD21	1.95	0.49
1:A:24:TRP:O	1:A:27:GLN:HG3	2.15	0.47
1:B:28:MET:HE2	1:B:28:MET:HA	1.99	0.45
1:B:24:TRP:O	1:B:27:GLN:HG3	2.17	0.44
1:B:35[B]:VAL:HG23	1:B:81:LEU:HA	2.02	0.41
1:A:95:PRO:HA	1:A:98:TRP:NE1	2.35	0.41
1:A:128:ASP:N	5:A:404:HOH:O	2.54	0.41
1:A:197:MET:HE3	1:A:197:MET:HB3	1.96	0.41
2:D:42:ARG:HA	2:D:42:ARG:HD3	1.92	0.40
2:C:62:LYS:HE3	2:C:62:LYS:HB3	1.86	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	250/261 (96%)	247 (99%)	3 (1%)	0	100	100
1	B	256/261 (98%)	252 (98%)	4 (2%)	0	100	100
1	H	6/261 (2%)	6 (100%)	0	0	100	100
2	C	24/62 (39%)	24 (100%)	0	0	100	100
2	D	34/62 (55%)	33 (97%)	1 (3%)	0	100	100
All	All	570/907 (63%)	562 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/219 (98%)	213 (100%)	1 (0%)	88	80
1	B	220/219 (100%)	219 (100%)	1 (0%)	88	80
1	H	8/219 (4%)	8 (100%)	0	100	100
2	C	20/52 (38%)	20 (100%)	0	100	100
2	D	29/52 (56%)	29 (100%)	0	100	100
All	All	491/761 (64%)	489 (100%)	2 (0%)	91	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	B	201	ARG

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

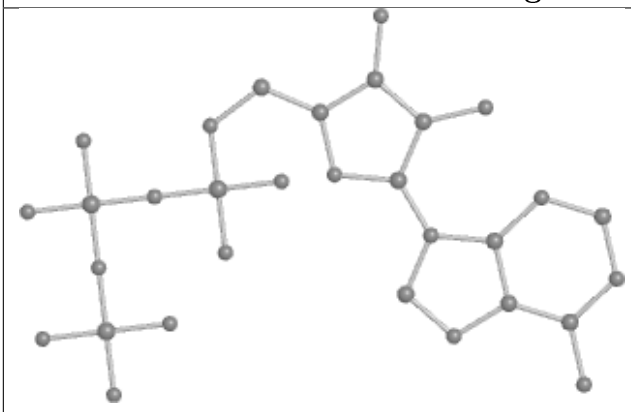
There are no torsion outliers.

There are no ring outliers.

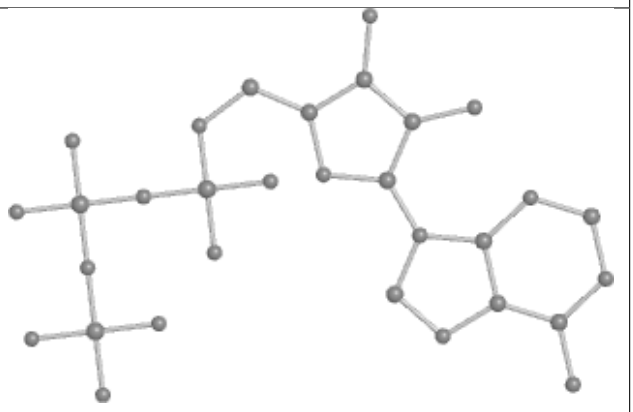
No monomer is involved in short contacts.

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.

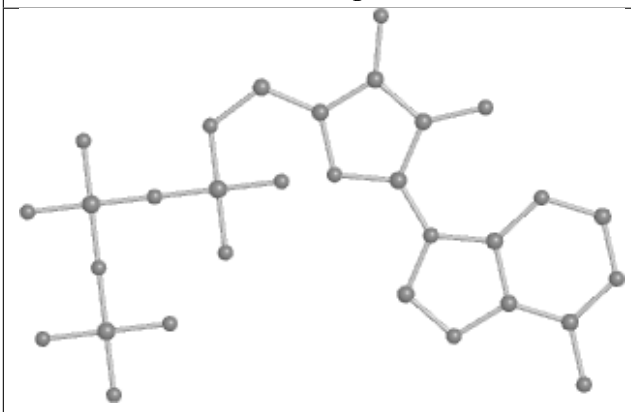
Ligand ATP A 302



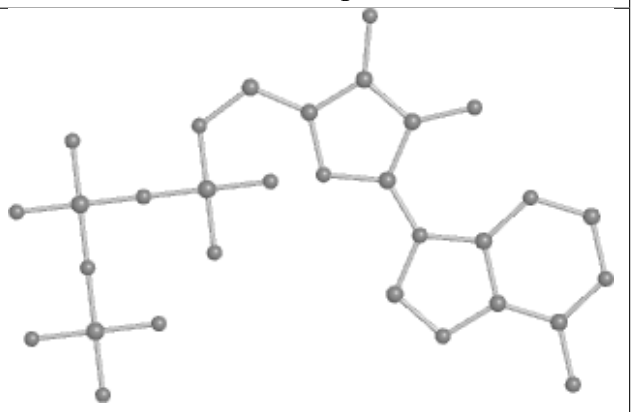
Bond lengths



Bond angles

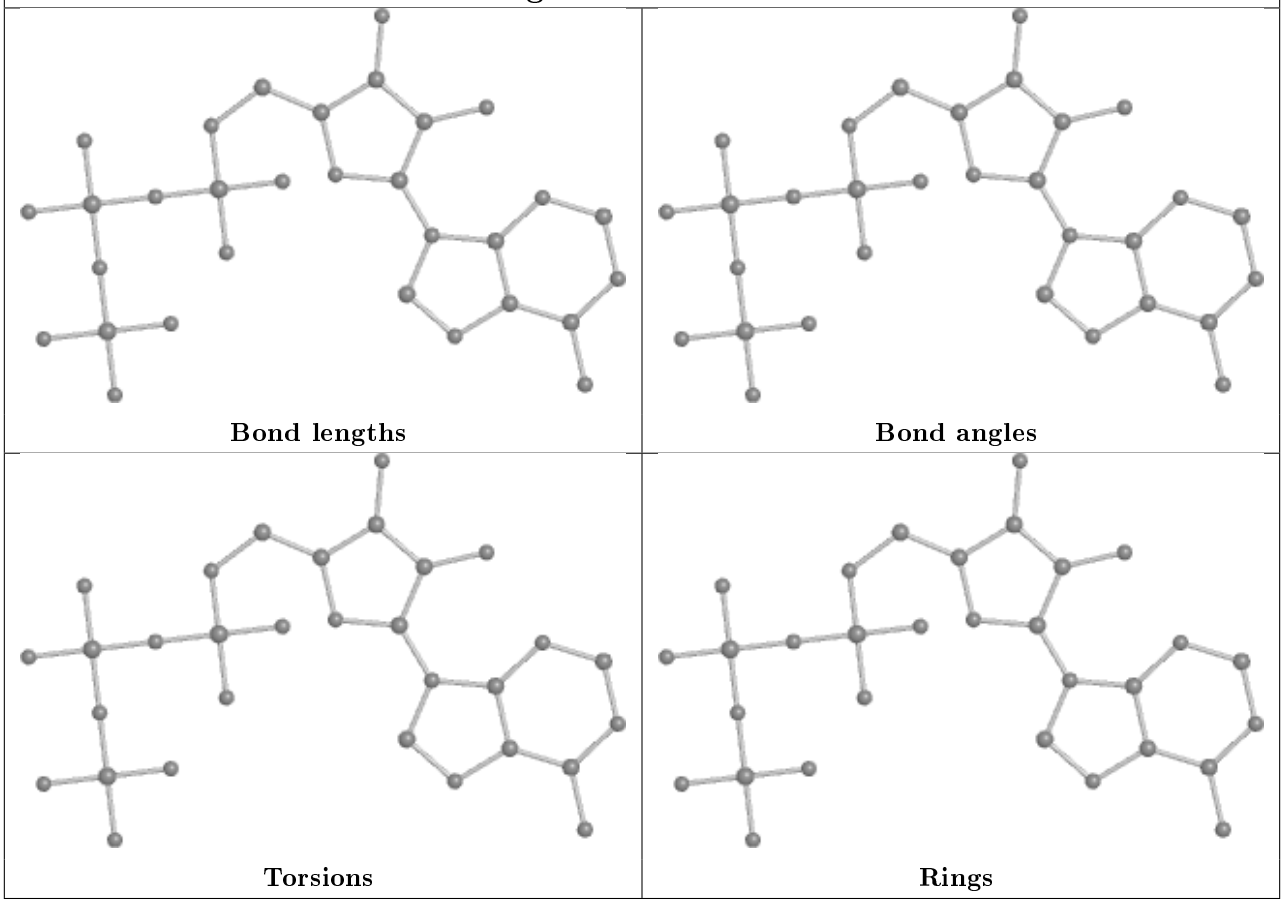


Torsions



Rings

Ligand ATP B 302



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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.