wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 08:45 AM EDT

PDB ID	:	1L0O
Title	:	Crystal Structure of the Bacillus stearothermophilus Anti-Sigma Factor SpoIIAB with the Sporulation Sigma Factor SigmaF
Authors	:	Campbell, E.A.; Masuda, S.; Sun, J.L.; Muzzin, O.; Olson, C.A.; Wang, S.; Darst, S.A.
Deposited on	:	2002-02-12
Resolution	:	2.90 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 following versions of software and data (see references (1)) were used in the production of this report:

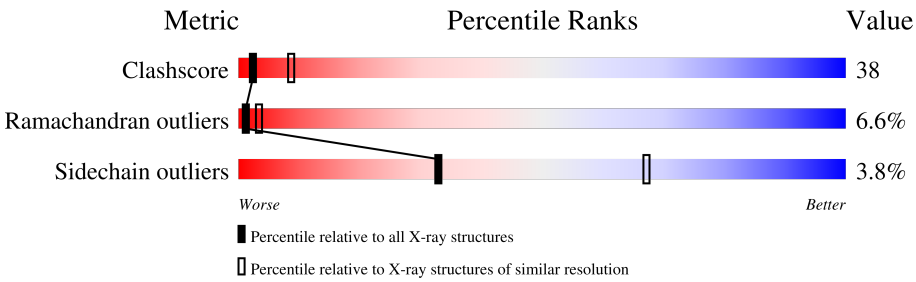
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	150	42% 49% • • 6%
1	B	150	33% 51% 10% 6%
2	C	243	11% 10% • 77%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2736 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 Anti-sigma F factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1097	688	184	219	6	0	0	0
1	B	141	1072	672	179	215	6	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	THR	SEE REMARK 999	UNP O32727
A	137	HIS	ALA	SEE REMARK 999	UNP O32727
A	138	ILE	TYR	SEE REMARK 999	UNP O32727
A	139	VAL	CYS	SEE REMARK 999	UNP O32727
A	140	LYS	GLU	SEE REMARK 999	UNP O32727
A	141	SER	LYS	SEE REMARK 999	UNP O32727
A	142	LYS	GLN	SEE REMARK 999	UNP O32727
A	143	ARG	-	cloning artifact	UNP O32727
A	144	TYR	-	cloning artifact	UNP O32727
A	145	LEU	-	cloning artifact	UNP O32727
A	146	GLU	-	cloning artifact	UNP O32727
A	147	GLY	-	cloning artifact	UNP O32727
A	148	SER	-	cloning artifact	UNP O32727
A	149	SER	-	cloning artifact	UNP O32727
A	150	PHE	-	cloning artifact	UNP O32727
B	34	MET	THR	SEE REMARK 999	UNP O32727
B	137	HIS	ALA	SEE REMARK 999	UNP O32727
B	138	ILE	TYR	SEE REMARK 999	UNP O32727
B	139	VAL	CYS	SEE REMARK 999	UNP O32727
B	140	LYS	GLU	SEE REMARK 999	UNP O32727
B	141	SER	LYS	SEE REMARK 999	UNP O32727
B	142	LYS	GLN	SEE REMARK 999	UNP O32727
B	143	ARG	-	cloning artifact	UNP O32727
B	144	TYR	-	cloning artifact	UNP O32727
B	145	LEU	-	cloning artifact	UNP O32727

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Chain	Residue	Modelled	Actual	Comment	Reference
B	146	GLU	-	cloning artifact	UNP O32727
B	147	GLY	-	cloning artifact	UNP O32727
B	148	SER	-	cloning artifact	UNP O32727
B	149	SER	-	cloning artifact	UNP O32727
B	150	PHE	-	cloning artifact	UNP O32727

- Molecule 2 is a protein called sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	57	428	262	82	83	1	0	0	0

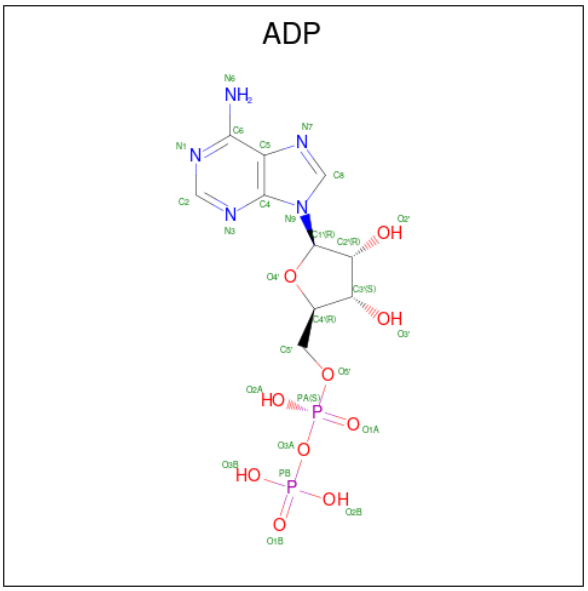
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	GLY	-	cloning artifact	UNP O32728
C	4	SER	-	cloning artifact	UNP O32728
C	5	HIS	-	cloning artifact	UNP O32728
C	6	MET	-	cloning artifact	UNP O32728
C	132	ALA	SER	SEE REMARK 999	UNP O32728
C	135	VAL	ILE	SEE REMARK 999	UNP O32728
C	215	LYS	ARG	SEE REMARK 999	UNP O32728
C	217	GLN	ARG	SEE REMARK 999	UNP O32728
C	233	MET	VAL	engineered mutation	UNP O32728

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	31	Total	O	0	0
			31	31		
5	C	11	Total	O	0	0
			11	11		

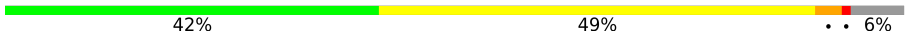
3 Residue-property plots (i)

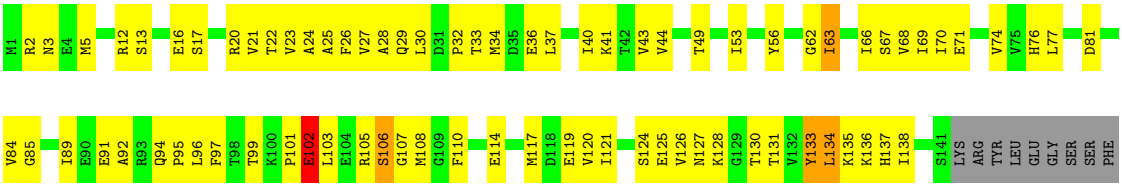
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 was not executed.

• Molecule 1: Anti-sigma F factor

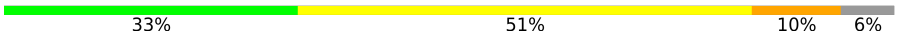
Chain A:





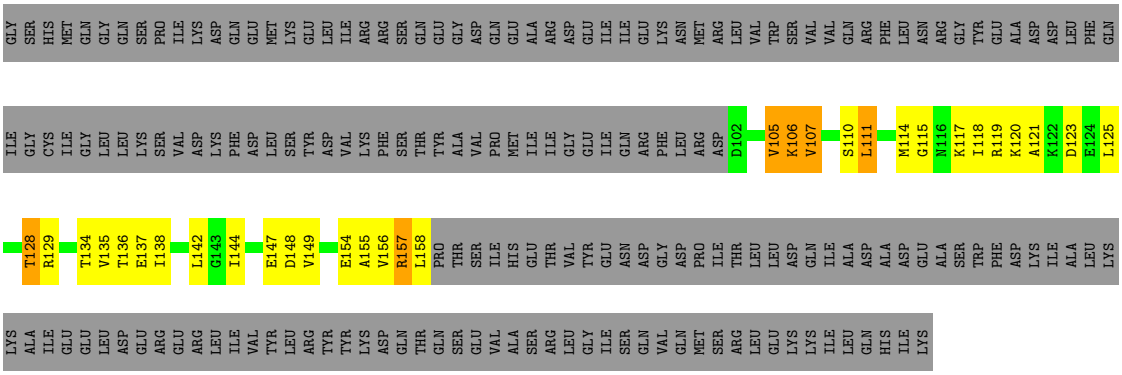
• Molecule 1: Anti-sigma F factor

Chain B:



• Molecule 2: sigma factor

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	97.31Å 97.31Å 262.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2736	wwPDB-VP
Average B, all atoms ($Å^2$)	56.0	wwPDB-VP

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: ADP, 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	0.44	0/1113	0.66	0/1508
1	B	0.38	0/1088	0.65	1/1479 (0.1%)
2	C	0.41	0/430	0.57	0/576
All	All	0.41	0/2631	0.64	1/3563 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	GLY	N-CA-C	-6.08	97.91	113.10

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	A	1097	0	1087	73	1
1	B	1072	0	1038	102	0
2	C	428	0	448	43	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	41	0	0	4	1
5	B	31	0	0	1	0
5	C	11	0	0	2	0
All	All	2736	0	2597	200	2

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 38.

The worst 5 of 200 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:21:VAL:HG21	2:C:147:GLU:HB3	1.40	1.02
1:A:3:ASN:HD22	1:A:29:GLN:HE22	1.13	0.90
1:B:92:ALA:HA	1:B:97:PHE:CD2	2.13	0.83
2:C:111:LEU:HD23	2:C:155:ALA:HB2	1.62	0.80
2:C:118:ILE:HD13	2:C:149:VAL:HG13	1.64	0.78

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:OG	1:A:106:SER:OG[11_555]	1.63	0.57
5:A:501:HOH:O	5:A:501:HOH:O[11_555]	1.92	0.28

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	139/150 (93%)	121 (87%)	13 (9%)	5 (4%)	3 14
1	B	139/150 (93%)	102 (73%)	23 (16%)	14 (10%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	55/243 (23%)	50 (91%)	2 (4%)	3 (6%)	2 5
All	All	333/543 (61%)	273 (82%)	38 (11%)	22 (7%)	1 3

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	ARG
1	B	126	VAL
1	A	102	GLU
1	B	133	TYR
2	C	106	LYS

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	124/133 (93%)	123 (99%)	1 (1%)	81 94
1	B	118/133 (89%)	111 (94%)	7 (6%)	19 49
2	C	46/216 (21%)	43 (94%)	3 (6%)	17 45
All	All	288/482 (60%)	277 (96%)	11 (4%)	33 67

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	115	ASN
2	C	111	LEU
2	C	157	ARG
2	C	128	THR
1	B	49	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	B	29	GLN
1	B	127	ASN
1	B	115	ASN
1	A	127	ASN

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 4 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
4	ADP	A	601	3	24,29,29	1.37	4 (16%)	29,45,45	0.97	0
4	ADP	B	701	3	24,29,29	1.88	5 (20%)	29,45,45	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	601	3	-	0/12/32/32	0/3/3/3
4	ADP	B	701	3	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ADP	O4'-C1'	5.12	1.48	1.41
4	A	601	ADP	C8-N7	-3.52	1.28	1.34
4	B	701	ADP	C8-N7	-3.24	1.28	1.34
4	B	701	ADP	C2-N3	3.19	1.37	1.32
4	B	701	ADP	O4'-C4'	2.68	1.51	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

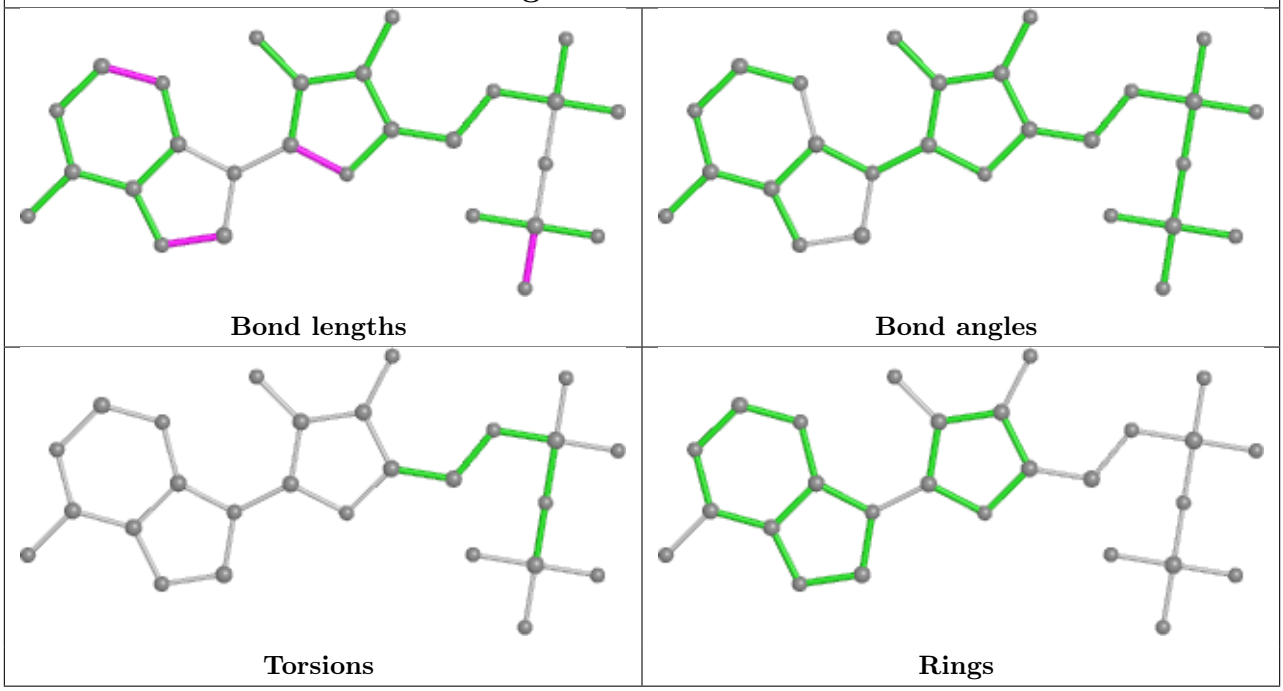
There are no ring outliers.

1 monomer is involved in 3 short contacts:

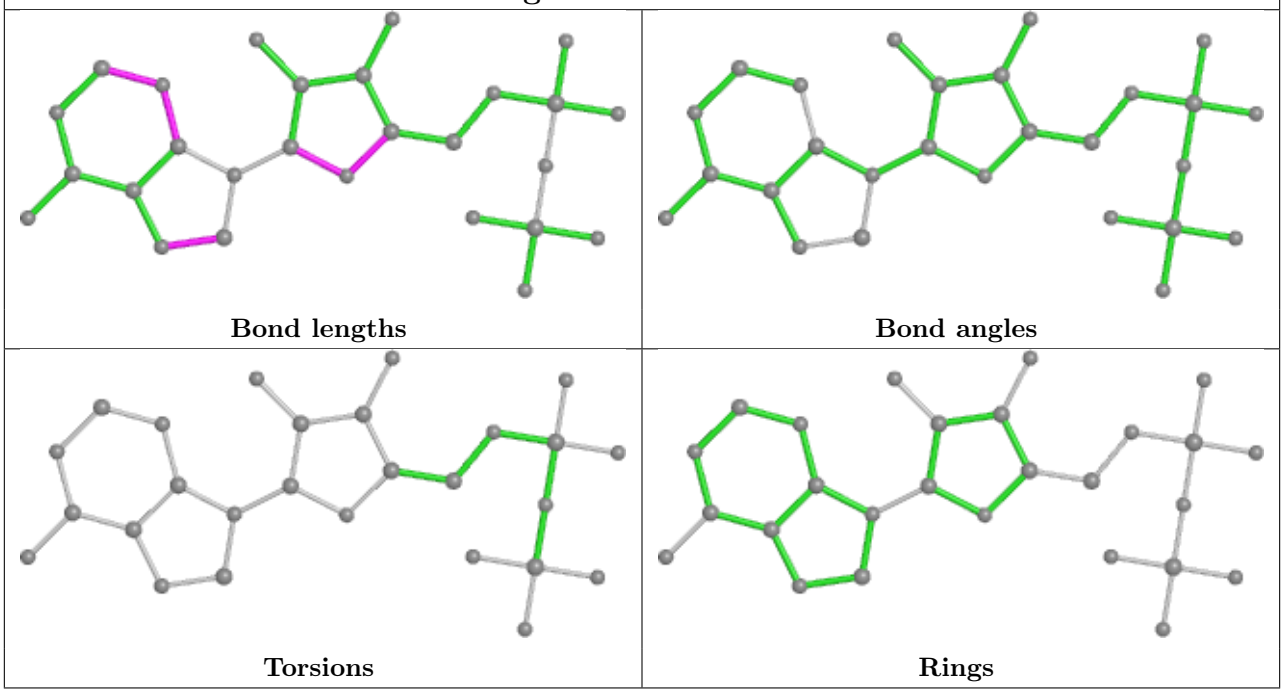
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	ADP	3	0

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 ADP A 601



Ligand ADP B 701



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.