wwPDB X-ray Structure Validation Summary Report (i)

Feb 6, 2024 – 02:46 PM EST

PDB ID	:	2FJB
Title	:	Adenosine-5'-phosphosulfate reductase im complex with products
Authors	:	Schiffer, A.; Fritz, G.; Kroneck, P.M.; Ermler, U.
Deposited on	:	2006-01-02
Resolution	:	1.70 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 (1)) were used in the production of this report:

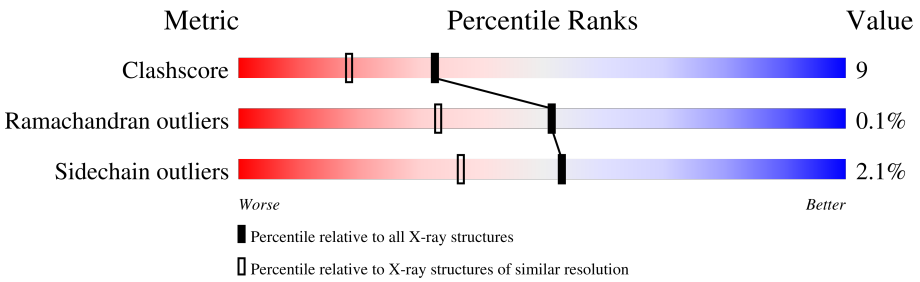
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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	643	85% 14% •
1	C	643	83% 15% •
2	B	150	85% 12% • •
2	D	150	85% 15% •

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SFD	A	1000	X	-	-	-
3	SFD	C	3000	X	-	-	-
4	AMP	A	1302	X	-	-	-
4	AMP	A	1303	X	-	-	-
4	AMP	C	1301	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14529 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.

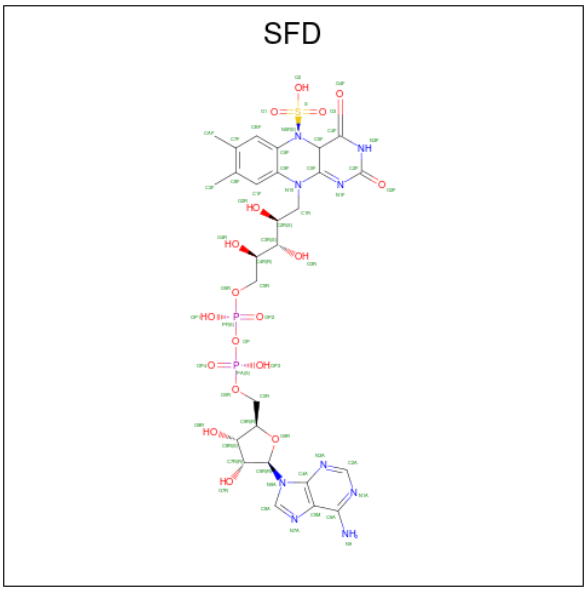
- Molecule 1 is a protein called adenylylsulfate reductase, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	642	5187	3358	851	948	30	0	6	0
1	C	642	5184	3355	851	949	29	0	6	0

- Molecule 2 is a protein called adenylylsulfate reductase, subunit B.

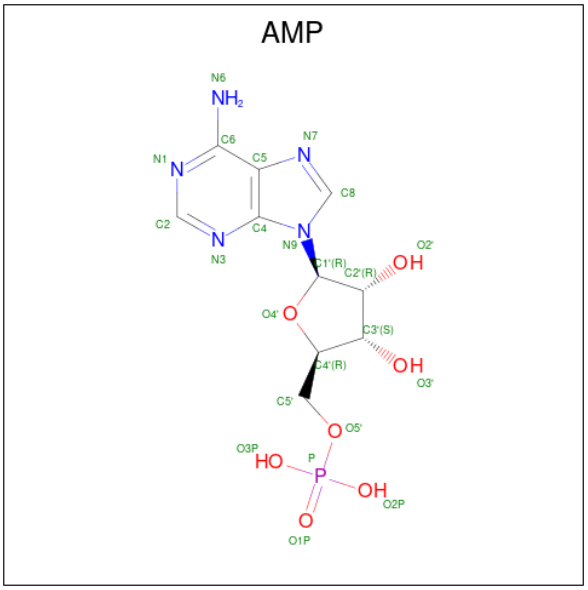
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	149	1175	747	193	219	16	0	1	0
2	D	149	1180	750	193	220	17	0	2	0

- Molecule 3 is (S)-10-((2S,3S,4R)-5-((S)-((S)-(((2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXY-TETRAHYDROFURAN-2-YL)METHOXY)(HYDROXY)PHOSPHORYLOXY)(HYDROXY)PHOSPHORYLOXY)-2,3,4-TRIHYDROXYPENTYL)-7,8-DIMETHYL-2,4-DIOXO-2,3,4,4A-TETRAHYDROBENZO[G]PTERIDINE-5(10H)-SULFONIC ACID (three-letter code: SFD) (formula: $C_{27}H_{35}N_9O_{18}P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	57	27	9	18	2	1	0	0
3	C	1	57	27	9	18	2	1	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	23	10	5	7	1	0	0
4	A	1	23	10	5	7	1	0	0

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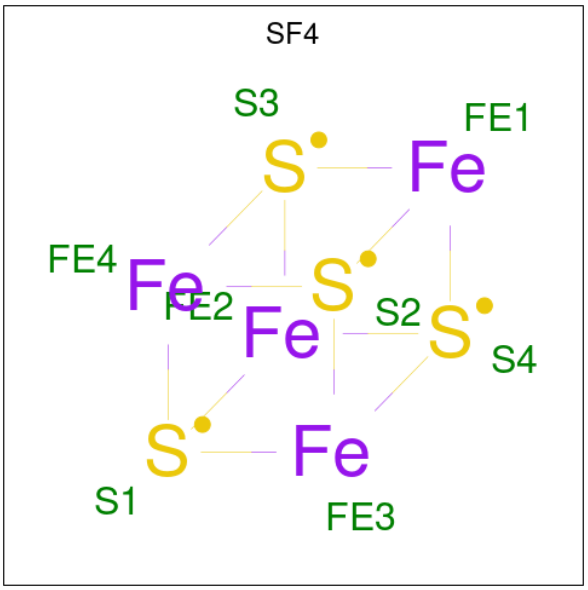
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	C	1	23	10	5	7	1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	C	1	1	1	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	B	1	8	4	4	0	0
			Total	Fe	S		
6	B	1	8	4	4	0	0
			Total	Fe	S		
6	D	1	8	4	4	0	0
			Total	Fe	S		
6	D	1	8	4	4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	579	579	579	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	C	635	635	635	0	0
			Total	O		
7	B	169	169	169	0	0
			Total	O		
7	D	204	204	204	0	0

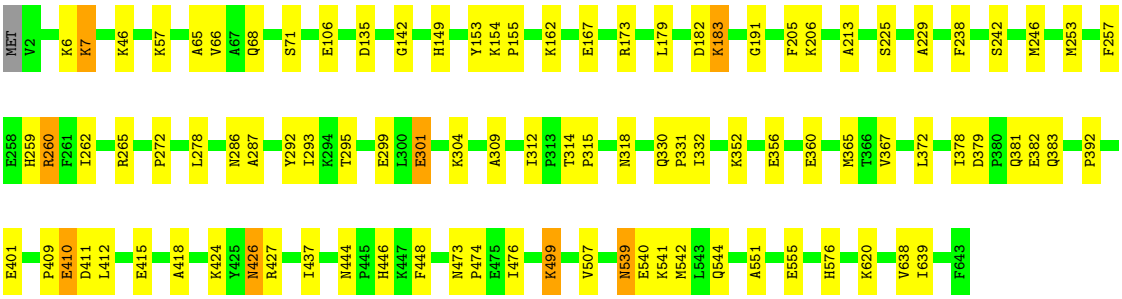
3 Residue-property plots (i)

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. 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: adenylylsulfate reductase, subunit A

Chain A: 85% 14%



• Molecule 1: adenylylsulfate reductase, subunit A

Chain C: 83% 15%

• Molecule 2: adenylylsulfate reductase, subunit B

Chain B: 85% 12%

• Molecule 2: adenylylsulfate reductase, subunit B

Chain D: 85% 15%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.60Å 113.50Å 193.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70	Depositor
% Data completeness (in resolution range)	90.8 (30.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.168 , 0.192	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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: SFD, SF4, AMP, NA

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	0.31	0/5352	0.58	0/7244
1	C	0.34	1/5349 (0.0%)	0.61	4/7241 (0.1%)
2	B	0.31	0/1209	0.63	0/1632
2	D	0.30	0/1218	0.64	0/1642
All	All	0.32	1/13128 (0.0%)	0.60	4/17759 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2330	GLN	C-N	-10.21	1.14	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2329	ASN	O-C-N	-8.68	108.82	122.70
1	C	2329	ASN	C-N-CA	6.83	138.78	121.70
1	C	2329	ASN	CA-C-N	5.97	130.33	117.20
1	C	2330	GLN	O-C-N	5.17	130.92	121.10

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	5187	0	5083	90	1
1	C	5184	0	5077	99	0
2	B	1175	0	1151	23	0
2	D	1180	0	1156	19	1
3	A	57	0	31	4	0
3	C	57	0	31	5	0
4	A	46	0	22	7	0
4	C	23	0	11	1	0
5	C	1	0	0	0	0
6	B	16	0	0	1	0
6	D	16	0	0	1	0
7	A	579	0	0	8	0
7	B	169	0	0	4	0
7	C	635	0	0	8	0
7	D	204	0	0	6	0
All	All	14529	0	12562	225	1

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 9.

The worst 5 of 225 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:A:1000:SFD:N5F	3:A:1000:SFD:S	1.97	1.35
3:C:3000:SFD:S	3:C:3000:SFD:N5F	2.09	1.24
2:B:713:CYS:HB3	2:B:716:LEU:HD21	1.25	1.08
1:C:2379:ASP:H	1:C:2383:GLN:HE21	1.03	0.95
1:C:2272:PRO:HG3	1:C:2365:MET:HE3	1.51	0.88

All (1) 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:182:ASP:OD1	2:D:2836:GLU:OE2[2_655]	2.11	0.09

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	646/643 (100%)	626 (97%)	20 (3%)	0	100	100
1	C	646/643 (100%)	627 (97%)	19 (3%)	0	100	100
2	B	148/150 (99%)	142 (96%)	5 (3%)	1 (1%)	22	8
2	D	149/150 (99%)	147 (99%)	2 (1%)	0	100	100
All	All	1589/1586 (100%)	1542 (97%)	46 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	714	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	531/526 (101%)	517 (97%)	14 (3%)	46	28
1	C	531/526 (101%)	520 (98%)	11 (2%)	53	36
2	B	130/130 (100%)	127 (98%)	3 (2%)	50	33
2	D	131/130 (101%)	130 (99%)	1 (1%)	81	74
All	All	1323/1312 (101%)	1294 (98%)	29 (2%)	53	34

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2007	LYS
2	B	794	ASN
1	C	2260	ARG
1	C	2624	GLU
1	C	2257	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2145	GLN
1	C	2310	GLN
1	C	2584	HIS
1	C	2286	ASN
1	C	2318	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 10 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
6	SF4	D	3110	2	0,12,12	-	-	-		
3	SFD	A	1000	-	54,62,62	5.31	33 (61%)	64,97,97	2.54	29 (45%)
4	AMP	C	1301	5	22,25,25	2.73	10 (45%)	25,38,38	3.02	14 (56%)
4	AMP	A	1303	-	22,25,25	2.92	11 (50%)	25,38,38	3.34	14 (56%)
6	SF4	B	1110	2	0,12,12	-	-	-		
4	AMP	A	1302	-	22,25,25	2.68	10 (45%)	25,38,38	2.95	13 (52%)
3	SFD	C	3000	-	54,62,62	5.27	33 (61%)	64,97,97	2.78	27 (42%)
6	SF4	B	1100	2	0,12,12	-	-	-		
6	SF4	D	3100	2	0,12,12	-	-	-		

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	SF4	D	3110	2	-	-	0/6/5/5
3	SFD	A	1000	-	1/1/16/17	3/34/88/88	0/5/6/6
4	AMP	C	1301	5	1/1/5/5	0/6/26/26	0/3/3/3
4	AMP	A	1303	-	1/1/5/5	1/6/26/26	0/3/3/3
6	SF4	B	1110	2	-	-	0/6/5/5
4	AMP	A	1302	-	1/1/5/5	0/6/26/26	0/3/3/3
3	SFD	C	3000	-	1/1/16/17	2/34/88/88	0/5/6/6
6	SF4	B	1100	2	-	-	0/6/5/5
6	SF4	D	3100	2	-	-	0/6/5/5

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	SFD	C5R-C4R	12.18	1.69	1.51
3	C	3000	SFD	C1F-C9F	12.11	1.59	1.39
3	A	1000	SFD	C1F-C9F	11.63	1.58	1.39
3	C	3000	SFD	C5R-C4R	11.40	1.67	1.51
3	C	3000	SFD	C7F-C8F	10.67	1.67	1.40

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3000	SFD	C5F-N5F-S	-11.27	97.23	117.50
4	A	1303	AMP	C1'-N9-C4	9.45	143.25	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1301	AMP	C1'-N9-C4	7.84	140.41	126.64
4	A	1302	AMP	C1'-N9-C4	7.31	139.49	126.64
3	C	3000	SFD	O9R-C6R-C7R	-7.18	96.44	106.93

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1000	SFD	C5F
3	C	3000	SFD	C5F
4	A	1302	AMP	C1'
4	A	1303	AMP	C1'
4	C	1301	AMP	C1'

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	SFD	C6F-N5F-S-O3
4	A	1303	AMP	O4'-C4'-C5'-O5'
3	A	1000	SFD	C5F-N5F-S-O3
3	C	3000	SFD	C5F-N5F-S-O1
3	A	1000	SFD	O0R-C0R-C9R-O9R

There are no ring outliers.

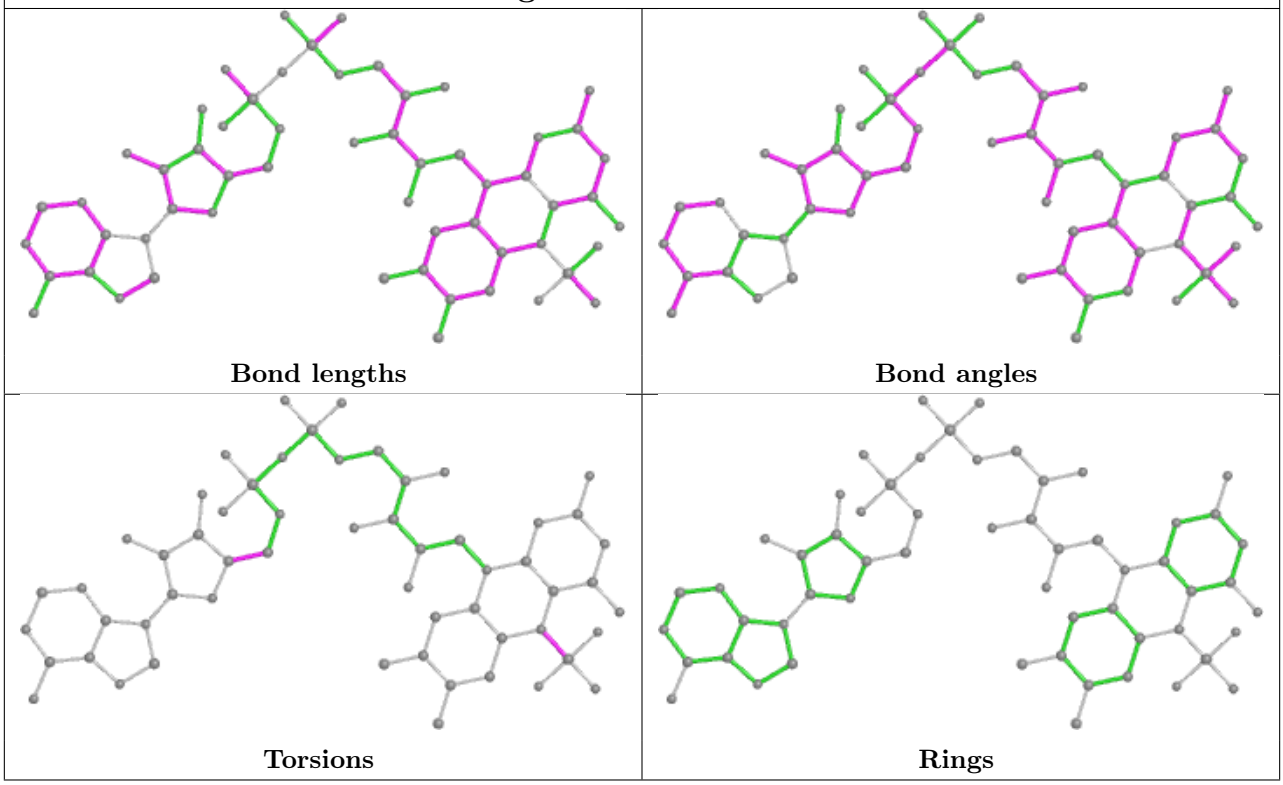
7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	3110	SF4	1	0
3	A	1000	SFD	4	0
4	C	1301	AMP	1	0
4	A	1303	AMP	5	0
6	B	1110	SF4	1	0
4	A	1302	AMP	4	0
3	C	3000	SFD	5	0

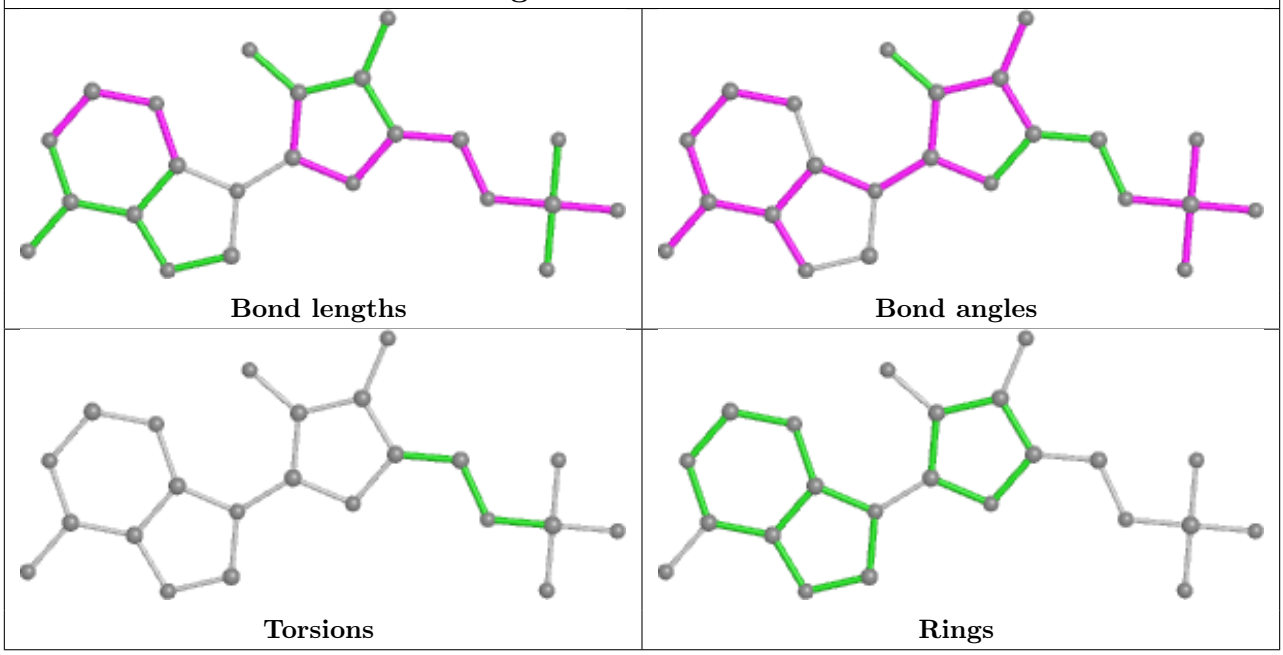
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

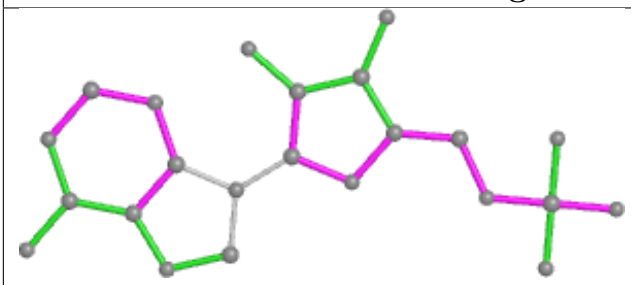
Ligand SFD A 1000



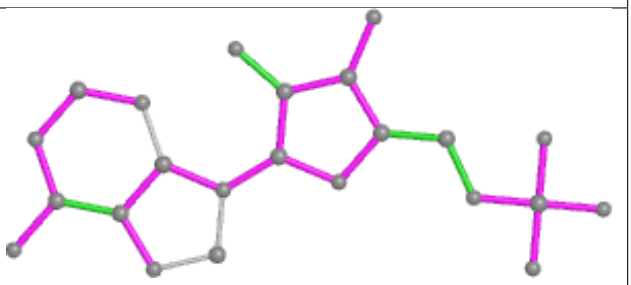
Ligand AMP C 1301



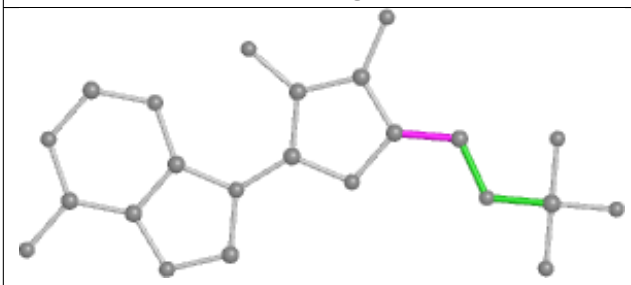
Ligand AMP A 1303



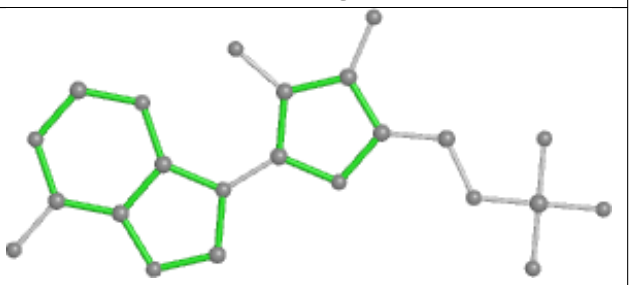
Bond lengths



Bond angles

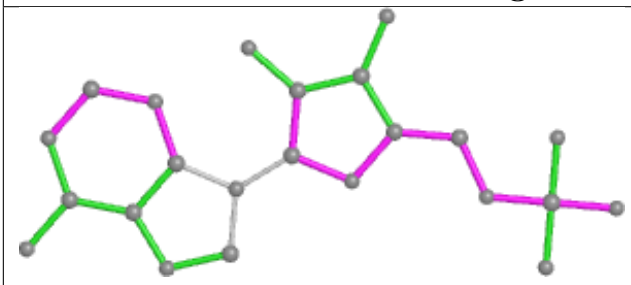


Torsions

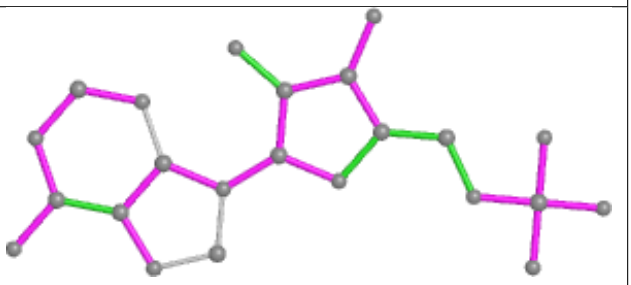


Rings

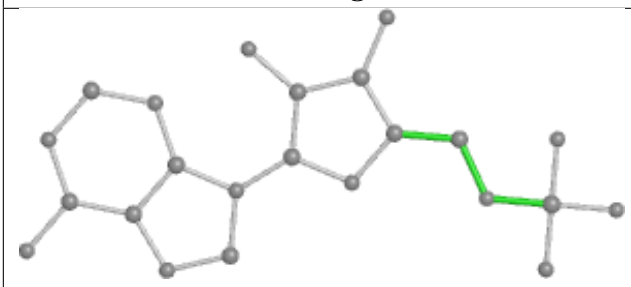
Ligand AMP A 1302



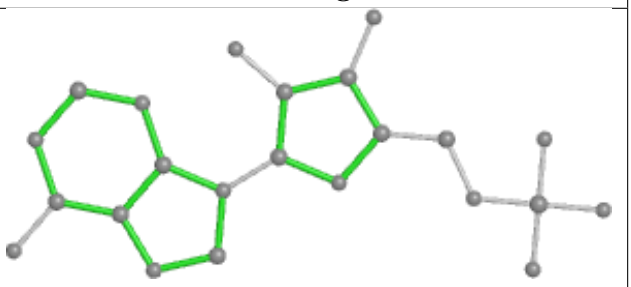
Bond lengths



Bond angles

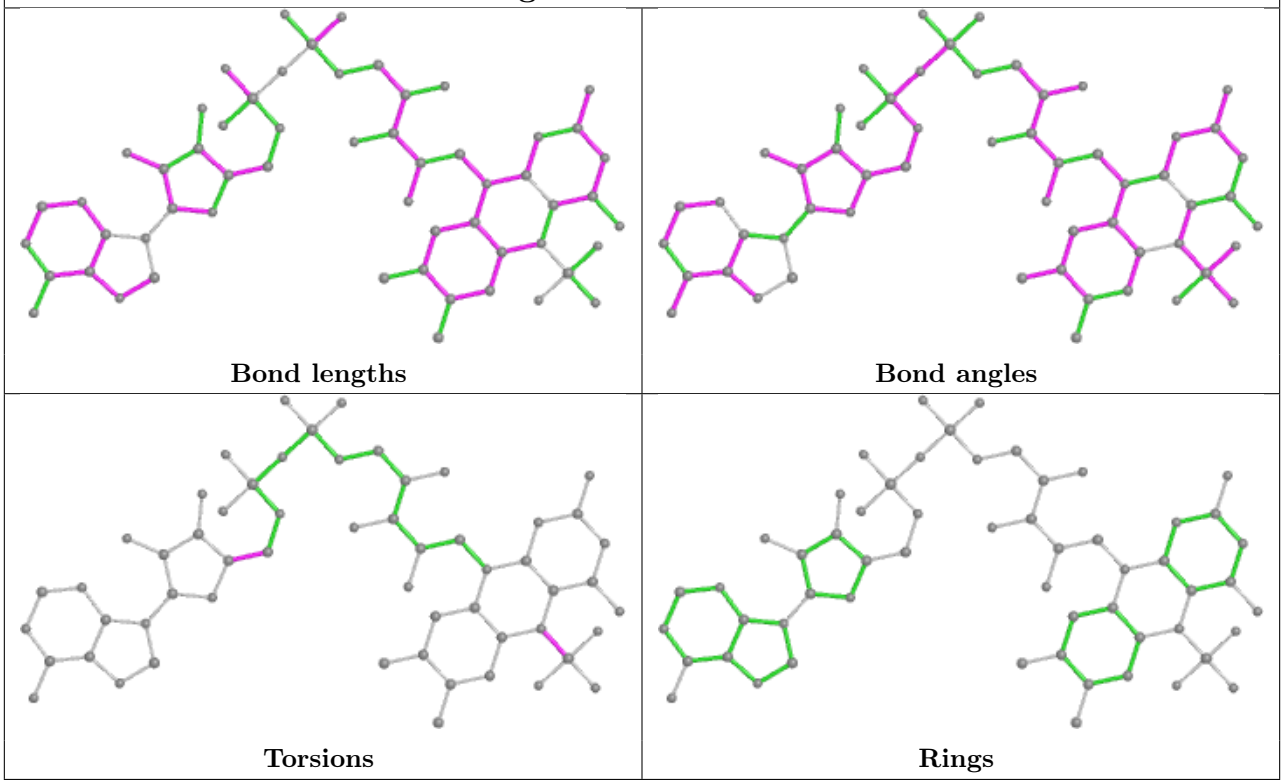


Torsions



Rings

Ligand SFD C 3000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2330:GLN	C	2331:PRO	N	1.14

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.