



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 11:03 pm BST

PDB ID : 1JNZ
Title : Structure of adenylylsulfate reductase from the hyperthermophilic *Archaeoglobus fulgidus* at 1.6 resolution
Authors : Fritz, G.; Roth, A.; Schiffer, A.; Buechert, T.; Bourenkov, G.; Bartunik, H.D.; Huber, H.; Stetter, K.O.; Kroneck, P.M.; Ermler, U.
Deposited on : 2001-07-26
Resolution : 2.50 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 ⓘ symbol.

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)	:	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)	:	2.11

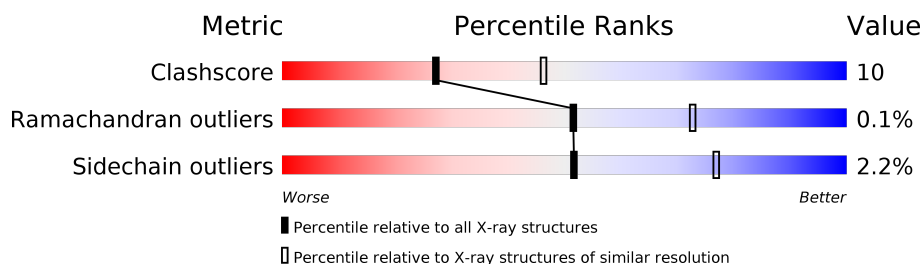
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	643	
1	C	643	
2	B	150	
2	D	150	

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	SO3	A	1001	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO3	C	3001	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14391 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5163	3336	851	950	26			
1	C	642	Total	C	N	O	S	0	0	0
			5163	3336	851	950	26			

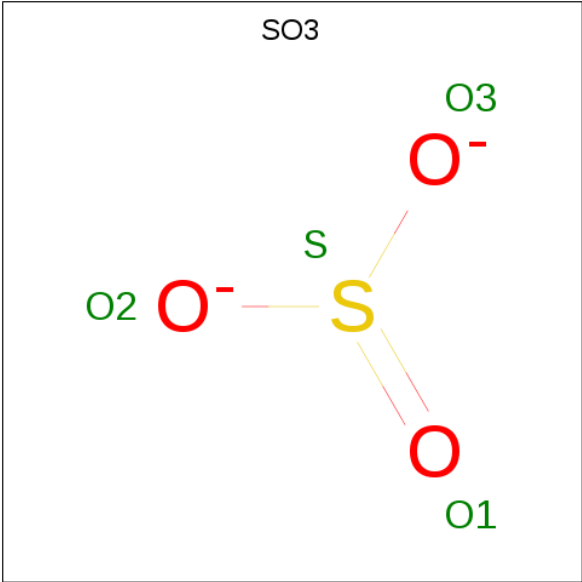
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	ASN	LYS	CONFLICT	GB 2648886
C	2183	ASN	LYS	CONFLICT	GB 2648886

- Molecule 2 is a protein called adenylylsulfate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	0	0
			1172	744	193	220	15			
2	D	149	Total	C	N	O	S	0	0	0
			1172	744	193	220	15			

- Molecule 3 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	S		0	0
			4	3	1			
3	C	1	Total	O	S		0	0
			4	3	1			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 6 is water.

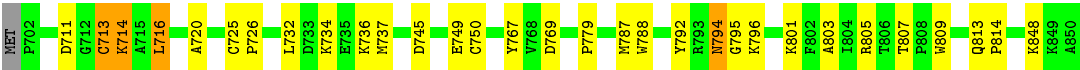
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	573	Total	O	0	0
			573	573		
6	B	163	Total	O	0	0
			163	163		
6	C	644	Total	O	0	0
			644	644		
6	D	195	Total	O	0	0
			195	195		

Chain B:

79%

18%

••



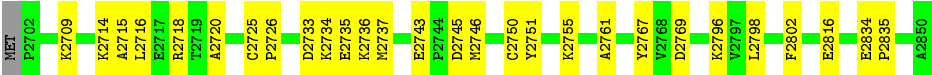
• Molecule 2: adenylylsulfate reductase

Chain D:

81%

19%

•



4 Data and refinement statistics

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	72.60 Å 113.50 Å 193.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.19 – 2.50	Depositor
% Data completeness (in resolution range)	95.2 (26.19-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.161 , 0.199	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14391	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: SF4, SO3, FAD

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	0.33	0/5304	0.58	0/7182
1	C	0.33	0/5304	0.58	0/7182
2	B	0.33	0/1202	0.63	0/1622
2	D	0.34	0/1202	0.65	0/1622
All	All	0.33	0/13012	0.59	0/17608

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 [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	5163	0	5042	106	0
1	C	5163	0	5042	108	0
2	B	1172	0	1146	32	0
2	D	1172	0	1146	21	0
3	A	4	0	0	3	0
3	C	4	0	0	2	0
4	A	53	0	31	7	0
4	C	53	0	29	6	0
5	B	16	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	16	0	0	1	0
6	A	573	0	0	8	0
6	B	163	0	0	4	0
6	C	644	0	0	7	0
6	D	195	0	0	3	0
All	All	14391	0	12436	252	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 10.

The worst 5 of 252 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)
2:B:713:CYS:HB3	2:B:716:LEU:HD21	1.30	1.10
1:C:2379:ASP:H	1:C:2383:GLN:NE2	1.63	0.96
1:C:2379:ASP:H	1:C:2383:GLN:HE21	0.95	0.93
1:C:2259:HIS:HD2	1:C:2401:GLU:H	1.22	0.86
3:C:3001:SO3:S	4:C:3000:FAD:C4X	2.63	0.86

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	640/643 (100%)	618 (97%)	22 (3%)	0	100	100
1	C	640/643 (100%)	616 (96%)	24 (4%)	0	100	100
2	B	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	22	39
2	D	147/150 (98%)	142 (97%)	5 (3%)	0	100	100
All	All	1574/1586 (99%)	1518 (96%)	55 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	714	LYS

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	525/526 (100%)	511 (97%)	14 (3%)	44	71
1	C	525/526 (100%)	515 (98%)	10 (2%)	57	80
2	B	129/130 (99%)	125 (97%)	4 (3%)	40	67
2	D	129/130 (99%)	128 (99%)	1 (1%)	81	93
All	All	1308/1312 (100%)	1279 (98%)	29 (2%)	52	77

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

Mol	Chain	Res	Type
1	A	539	ASN
2	B	769	ASP
1	C	2624	GLU
2	B	713	CYS
2	B	794	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	576	HIS
1	C	2068	GLN
1	C	2497	GLN
2	B	794	ASN
2	B	845	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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	FAD	A	1000	3	51,58,58	6.93	33 (64%)	60,89,89	3.55	28 (46%)
5	SF4	D	3110	2	0,12,12	0.00	-	-		
5	SF4	D	3100	2	0,12,12	0.00	-	-		
3	SO3	A	1001	4	1,3,3	0.01	0	0,3,3	0.00	-
3	SO3	C	3001	4	1,3,3	3.32	1 (100%)	0,3,3	0.00	-
4	FAD	C	3000	3	51,58,58	6.94	37 (72%)	60,89,89	3.83	34 (56%)
5	SF4	B	1110	2	0,12,12	0.00	-	-		
5	SF4	B	1100	2	0,12,12	0.00	-	-		

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	FAD	A	1000	3	-	1/30/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	D	3110	2	-	-	0/6/5/5
5	SF4	D	3100	2	-	-	0/6/5/5
4	FAD	C	3000	3	-	2/30/50/50	0/6/6/6
5	SF4	B	1110	2	-	-	0/6/5/5
5	SF4	B	1100	2	-	-	0/6/5/5

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3000	FAD	C1'-N10	-24.83	1.22	1.48
4	A	1000	FAD	C1'-N10	-23.25	1.24	1.48
4	A	1000	FAD	C9A-N10	17.02	1.61	1.38
4	A	1000	FAD	C4X-C10	15.94	1.54	1.38
4	C	3000	FAD	C9A-N10	15.53	1.59	1.38

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3000	FAD	C4-N3-C2	11.79	125.10	115.14
4	C	3000	FAD	C4X-N5-C5X	11.51	128.28	116.77
4	A	1000	FAD	C4X-N5-C5X	10.54	127.30	116.77
4	C	3000	FAD	P-O3P-PA	10.48	168.81	132.83
4	A	1000	FAD	C4-N3-C2	10.32	123.86	115.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3000	FAD	O4B-C4B-C5B-O5B
4	C	3000	FAD	C5'-O5'-P-O3P
4	A	1000	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 16 short contacts:

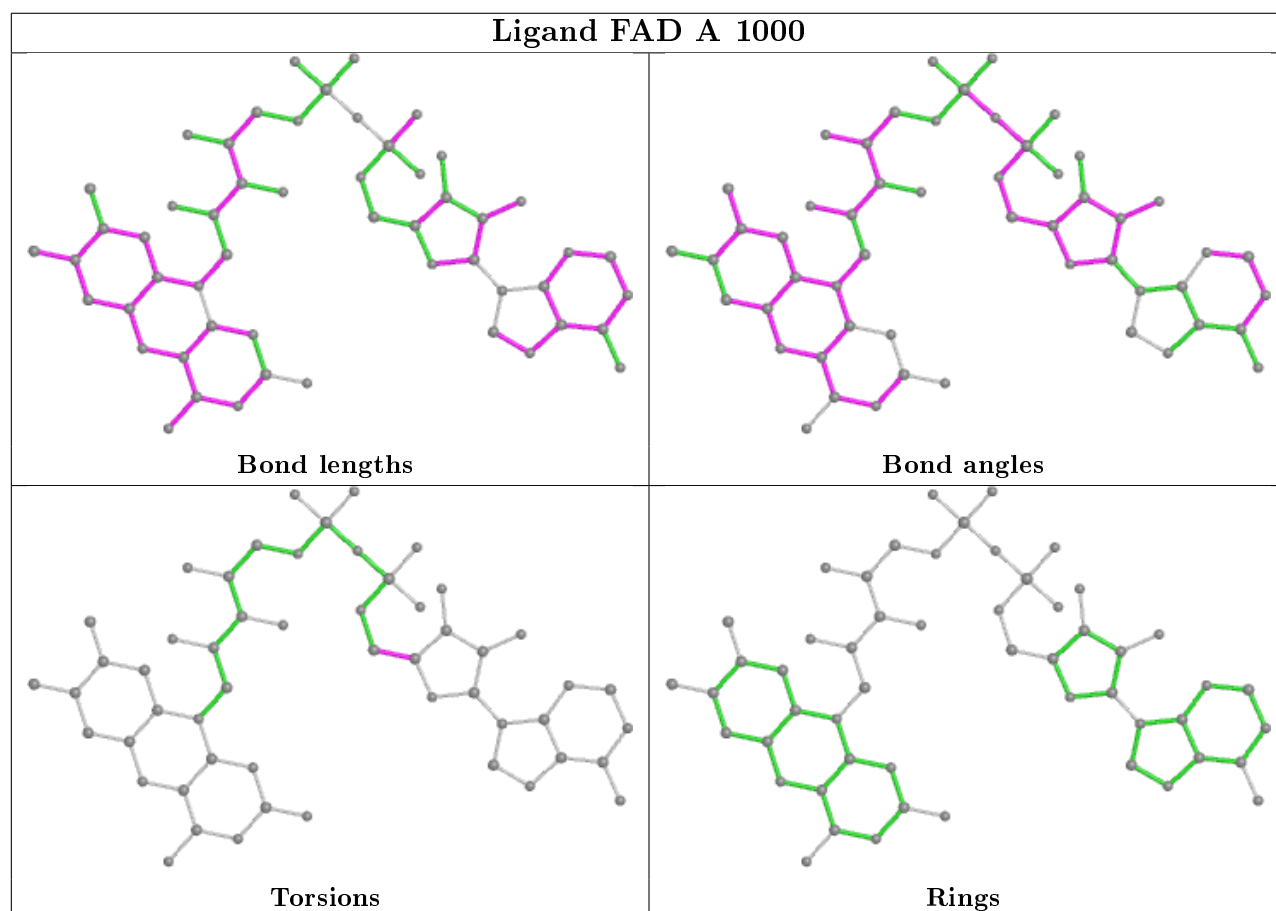
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	FAD	7	0
5	D	3110	SF4	1	0
3	A	1001	SO3	3	0
3	C	3001	SO3	2	0

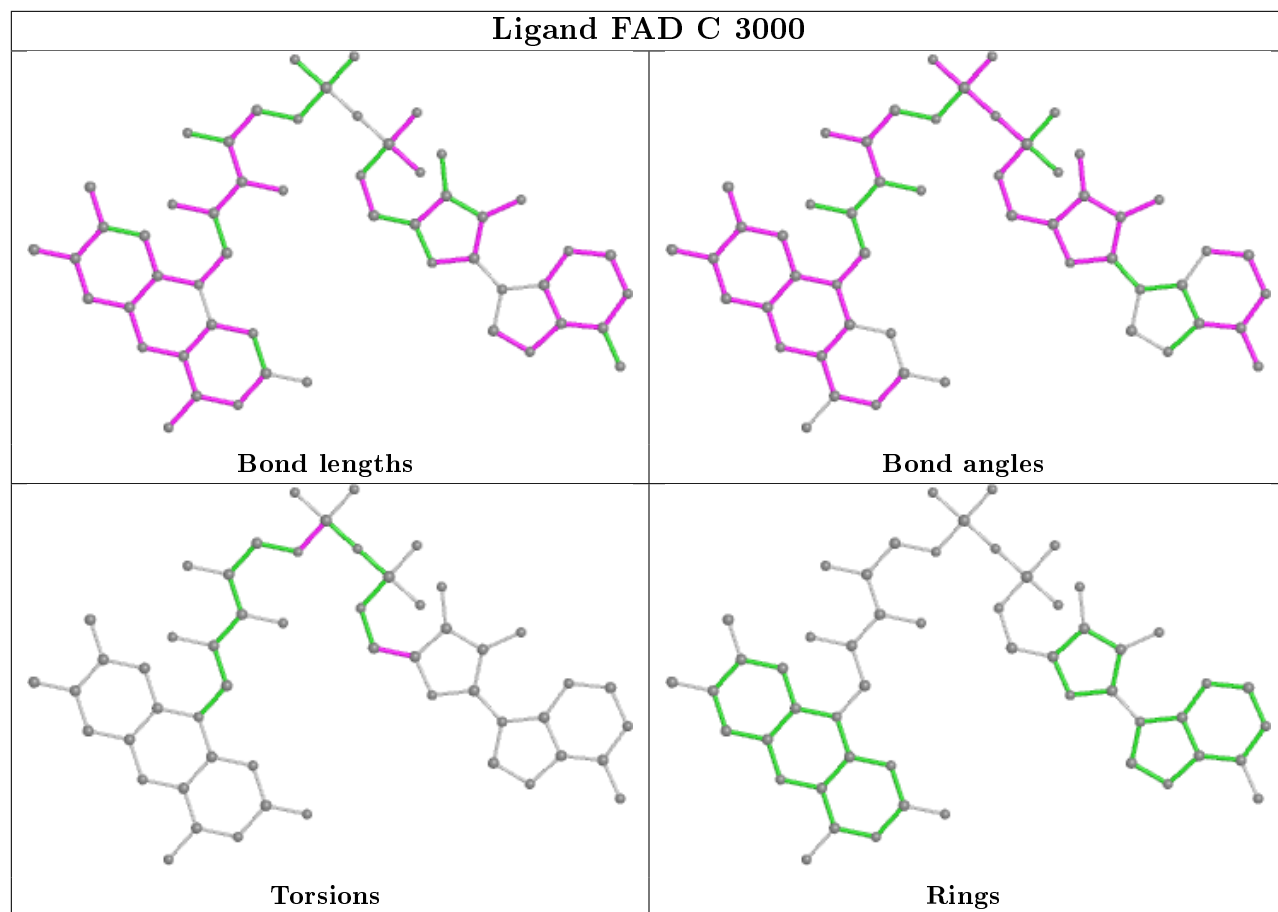
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3000	FAD	6	0
5	B	1110	SF4	1	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.