



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2017 – 10:33 AM EDT

PDB ID : 2FJD
Title : adenosine-5-phosphosulfate reductase in complex with sulfite (covalent adduct)
Authors : Schiffer, A.; Fritz, G.; Kroneck, P.M.; Ermler, U.
Deposited on : unknown
Resolution : 1.84 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

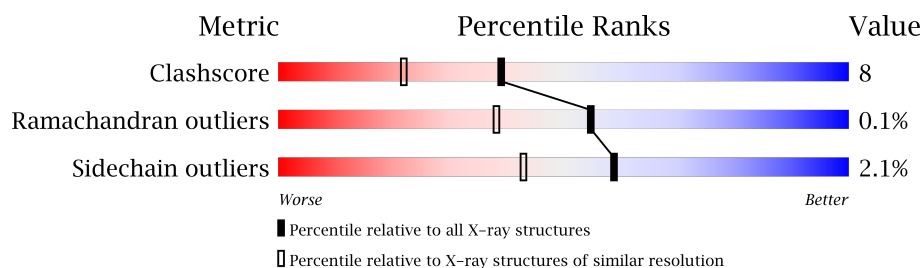
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)

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. 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 $\leq 5\%$. 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.

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	SFD	A	1000	X	-	-	-
3	SFD	C	3000	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14488 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.

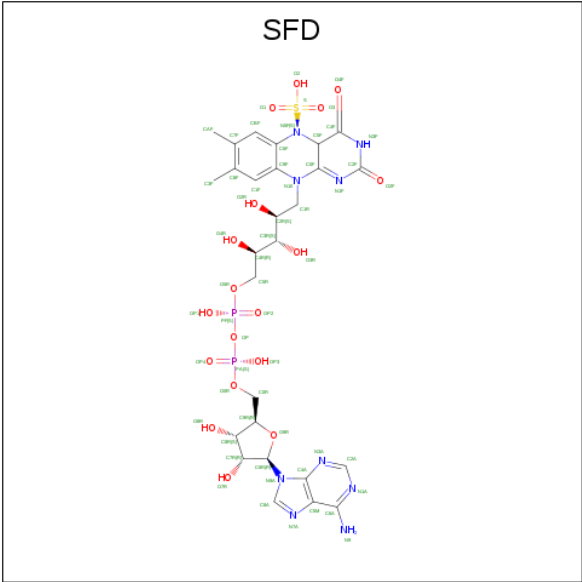
- Molecule 1 is a protein called adenylylsulfate reductase, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	7	0
			5190	3360	851	948	31			
1	C	642	Total	C	N	O	S	0	7	0
			5194	3361	854	948	31			

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

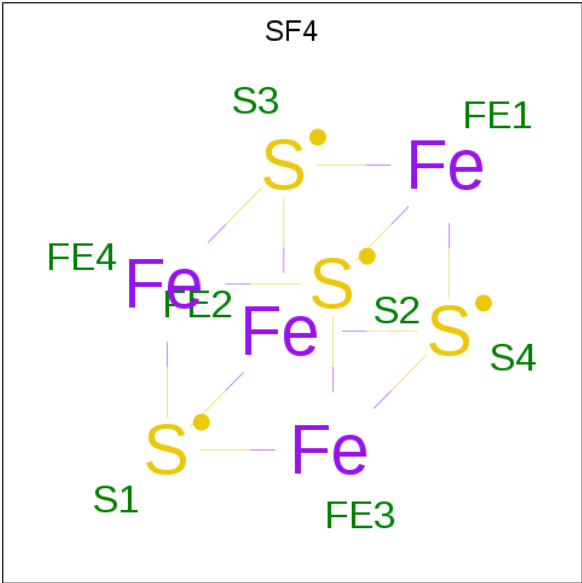
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	1	0
			1175	747	193	219	16			
2	D	149	Total	C	N	O	S	0	1	0
			1176	747	193	220	16			

- 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: C₂₇H₃₅N₉O₁₈P₂S).



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

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

- Molecule 5 is water.

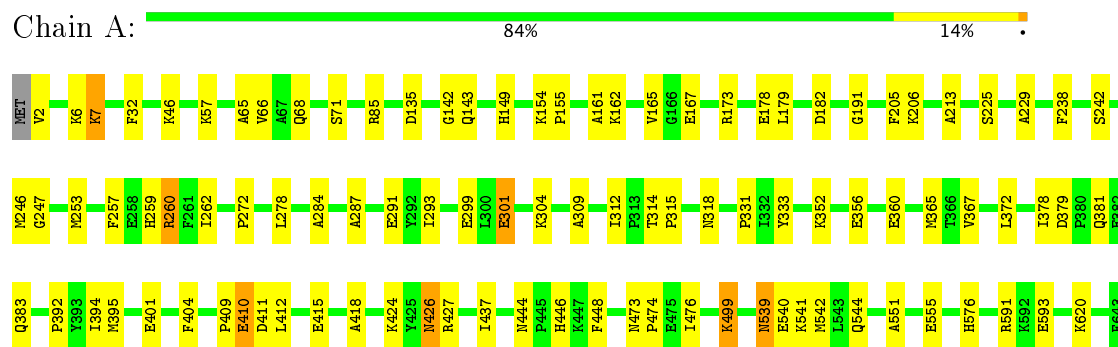
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	578	Total	O	0	0
			578	578		
5	C	652	Total	O	0	0
			652	652		
5	B	175	Total	O	0	0
			175	175		
5	D	202	Total	O	0	0
			202	202		

3 Residue-property plots

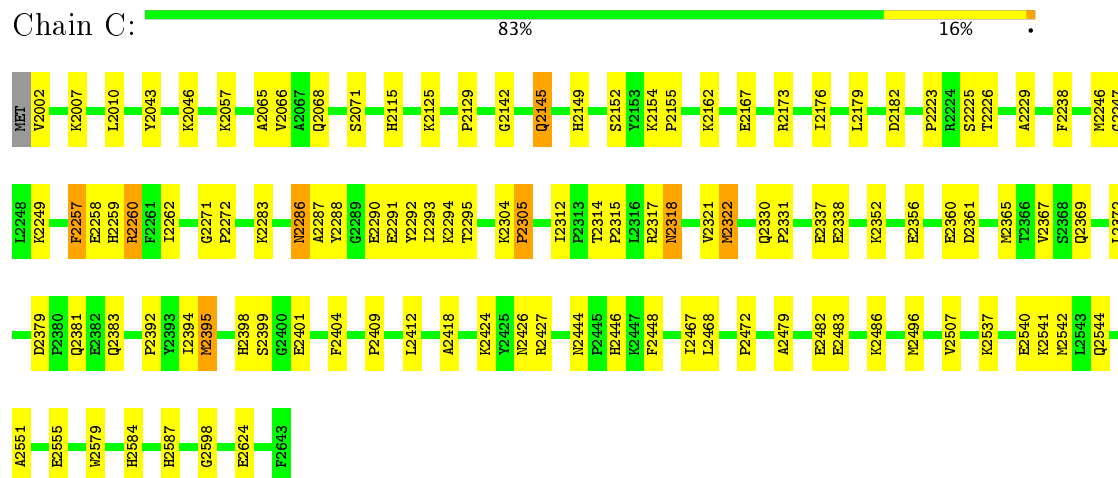
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

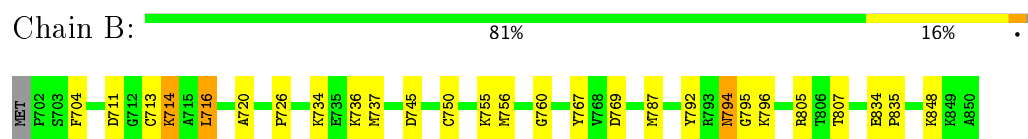
- Molecule 1: adenylylsulfate reductase, subunit A



- Molecule 1: adenylylsulfate reductase, subunit A



- Molecule 2: adenylylsulfate reductase, subunit B

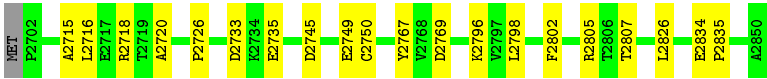


- Molecule 2: adenylylsulfate reductase, subunit B

Chain D:

86%

13%



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)	30.00 – 1.84	Depositor
% Data completeness (in resolution range)	86.8 (30.00-1.84)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.157 , 0.182	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14488	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, SFD

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	1/5359 (0.0%)	0.59	0/7253
1	C	0.36	1/5363 (0.0%)	0.59	0/7257
2	B	0.29	0/1209	0.63	0/1632
2	D	0.29	0/1210	0.63	0/1632
All	All	0.35	2/13141 (0.0%)	0.60	0/17774

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	ASP	C-N	-12.99	1.04	1.34
1	C	2182	ASP	C-N	-12.46	1.05	1.34

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	5190	0	5085	88	0
1	C	5194	0	5089	96	0
2	B	1175	0	1151	28	0
2	D	1176	0	1151	17	0
3	A	57	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	57	0	31	4	0
4	B	16	0	0	1	0
4	D	16	0	0	1	0
5	A	578	0	0	7	0
5	B	175	0	0	5	0
5	C	652	0	0	8	0
5	D	202	0	0	3	0
All	All	14488	0	12538	216	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 8.

The worst 5 of 216 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:S	3:A:1000:SFD:N5F	2.02	1.30
3:C:3000:SFD:S	3:C:3000:SFD:N5F	2.05	1.27
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	0.99
1:C:2379:ASP:H	1:C:2383:GLN:NE2	1.69	0.88

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	647/643 (101%)	626 (97%)	21 (3%)	0	100	100
1	C	647/643 (101%)	624 (96%)	23 (4%)	0	100	100
2	B	148/150 (99%)	142 (96%)	5 (3%)	1 (1%)	25	10
2	D	148/150 (99%)	144 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1590/1586 (100%)	1536 (97%)	53 (3%)	1 (0%)	55 38

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	532/526 (101%)	520 (98%)	12 (2%)	56 38
1	C	532/526 (101%)	519 (98%)	13 (2%)	54 37
2	B	130/130 (100%)	127 (98%)	3 (2%)	56 38
2	D	130/130 (100%)	129 (99%)	1 (1%)	85 79
All	All	1324/1312 (101%)	1295 (98%)	29 (2%)	59 40

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

Mol	Chain	Res	Type
1	C	2145	GLN
1	C	2286	ASN
2	B	769	ASP
1	C	2257	PHE
1	C	2305	PRO

Some 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	2074	ASN
1	C	2259	HIS
1	C	2584	HIS
1	C	2115	HIS

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Mol	Chain	Res	Type
1	A	318	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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$
3	SFD	A	1000	-	52,62,62	5.16	30 (57%)	58,97,97	2.47	22 (37%)
4	SF4	B	1100	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1110	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SFD	C	3000	-	52,62,62	5.11	30 (57%)	58,97,97	2.45	19 (32%)
4	SF4	D	3100	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	D	3110	2	0,12,12	0.00	-	0,24,24	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
3	SFD	A	1000	-	1/1/16/17	0/34/88/88	0/5/6/6
4	SF4	B	1100	2	-	0/0/48/48	0/6/5/5
4	SF4	B	1110	2	-	0/0/48/48	0/6/5/5
3	SFD	C	3000	-	1/1/16/17	0/34/88/88	0/5/6/6
4	SF4	D	3100	2	-	0/0/48/48	0/6/5/5
4	SF4	D	3110	2	-	0/0/48/48	0/6/5/5

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3000	SFD	C1R-N10	-8.64	1.24	1.48
3	A	1000	SFD	C1R-N10	-8.49	1.25	1.48
3	A	1000	SFD	O2F-C2F	-4.32	1.16	1.24
3	C	3000	SFD	O2F-C2F	-4.15	1.16	1.24
3	A	1000	SFD	PA-OP3	-4.02	1.34	1.55

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3000	SFD	N3A-C2A-N1A	-8.61	121.36	128.86
3	A	1000	SFD	N3A-C2A-N1A	-8.47	121.48	128.86
3	A	1000	SFD	C7R-C8R-C9R	-5.40	92.10	102.62
3	C	3000	SFD	C7R-C8R-C9R	-5.31	92.27	102.62
3	A	1000	SFD	O3-S-O1	-5.15	106.41	118.74

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1000	SFD	C5F
3	C	3000	SFD	C5F

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

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	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2182:ASP	C	2183:LYS	N	1.05
1	A	182:ASP	C	183:LYS	N	1.04

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.