



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:18 PM GMT

PDB ID : 2FJB  
Title : Adenosine-5'-phosphosulfatereductase 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 validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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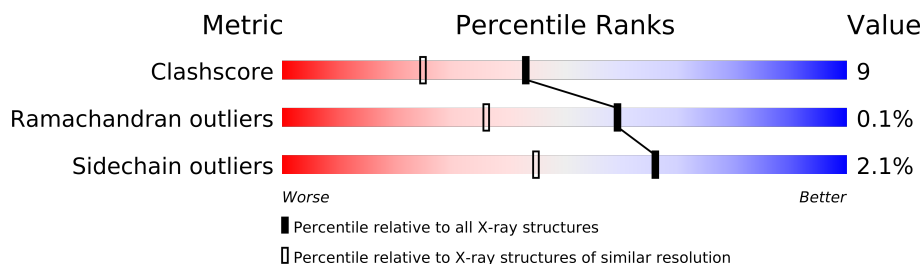
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14529 atoms, of which 0 are hydrogen and 0 are deuterium.

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	6	0
			5187	3358	851	948	30			
1	C	642	Total	C	N	O	S	0	6	0
			5184	3355	851	949	29			

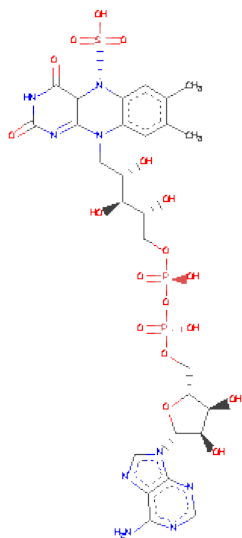
- Molecule 2 is a protein called adenylylsulfate reductase, subunit B.

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	2	0
			1180	750	193	220	17			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

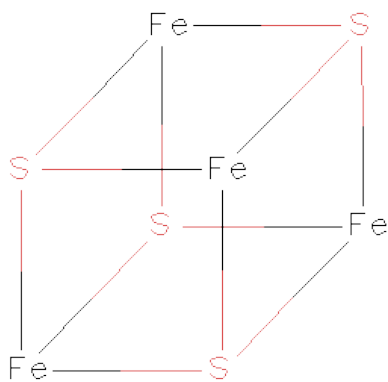
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 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<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>18</sub>P<sub>2</sub>S).



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

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



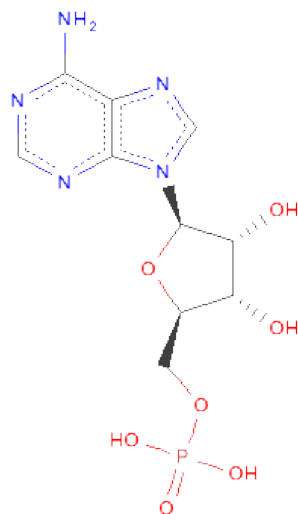
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	579	Total	O	0	0
			579	579		
7	B	169	Total	O	0	0
			169	169		
7	C	635	Total	O	0	0
			635	635		
7	D	204	Total	O	0	0
			204	204		

### 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 errors 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.

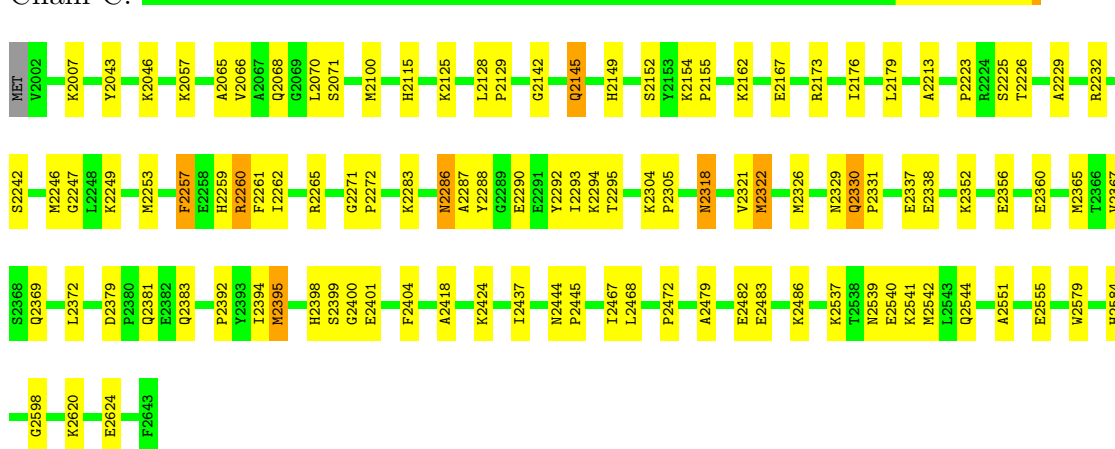
- Molecule 1: adenylylsulfate reductase, subunit A

Chain A:



- Molecule 1: adenylylsulfate reductase, subunit A

Chain C:



- Molecule 2: adenylylsulfate reductase, subunit B

Chain B:



- Molecule 2: adenylylsulfate reductase, subunit B

Chain D:

MET	P2702	S2703	F2704	K2714	A2715	L2716	E2717	R2718	T2719	A2720	C2725	P2726	K2734	E2735	K2736	M2737	C2750	Y2767	V2768	D2769	M2787	K2796	V2797	L2798	F2802	L2826	E2834	P2835	E2836	A2850
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	18.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SF4, SFD, AMP

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	C	1	0	0	0	0
4	A	57	0	31	4	0
4	C	57	0	31	5	0
5	B	16	0	0	1	0
5	D	16	0	0	1	0
6	A	46	0	22	7	0
6	C	23	0	11	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 225 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1000:SFD:S	4:A:1000:SFD:N5F	1.97	1.35
4:C:3000:SFD:S	4: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	Distance(Å)	Clash(Å)
1:A:182:ASP:OD1	2:D:2836:GLU:OE2[2_655]	2.11	0.09

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	30	10
2	D	149/150 (99%)	147 (99%)	2 (1%)	0	100	100
All	All	1589/1586 (100%)	1542 (97%)	46 (3%)	1 (0%)	59	36

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	531/526 (101%)	517 (97%)	14 (3%)	59	35
1	C	531/526 (101%)	520 (98%)	11 (2%)	66	45
2	B	130/130 (100%)	127 (98%)	3 (2%)	63	41
2	D	131/130 (101%)	130 (99%)	1 (1%)	89	81
All	All	1323/1312 (101%)	1294 (98%)	29 (2%)	66	43

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

Mol	Chain	Res	Type
1	A	539	ASN
1	C	2257	PHE
2	B	769	ASP
1	C	2007	LYS
1	C	2260	ARG

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

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Mol	Chain	Res	Type
1	C	2259	HIS
1	C	2584	HIS
1	C	2115	HIS
1	A	318	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	$\# Z  > 2$
4	SFD	A	1000	-	62,62,62	4.82	38 (61%)	95,97,97	2.55	36 (37%)
6	AMP	A	1302	-	25,25,25	3.16	12 (48%)	38,38,38	4.63	19 (50%)
6	AMP	A	1303	-	25,25,25	3.07	13 (52%)	38,38,38	4.37	21 (55%)
5	SF4	B	1100	2	12,12,12	11.25	10 (83%)	0,24,24	0.00	-
5	SF4	B	1110	2	12,12,12	14.96	11 (91%)	0,24,24	0.00	-
6	AMP	C	1301	3	25,25,25	3.18	12 (48%)	38,38,38	4.73	20 (52%)
4	SFD	C	3000	-	62,62,62	4.87	38 (61%)	95,97,97	2.80	35 (36%)
5	SF4	D	3100	2	12,12,12	12.51	11 (91%)	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SF4	D	3110	2	12,12,12	13.34	12 (100%)	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
4	SFD	A	1000	-	1/1/16/17	0/38/88/88	0/1/6/6
6	AMP	A	1302	-	1/1/5/5	0/10/26/26	0/1/3/3
6	AMP	A	1303	-	1/1/5/5	0/10/26/26	0/1/3/3
5	SF4	B	1100	2	-	0/0/48/48	0/0/5/5
5	SF4	B	1110	2	-	0/0/48/48	0/0/5/5
6	AMP	C	1301	3	1/1/5/5	0/10/26/26	0/1/3/3
4	SFD	C	3000	-	1/1/16/17	0/38/88/88	0/1/6/6
5	SF4	D	3100	2	-	0/0/48/48	0/0/5/5
5	SF4	D	3110	2	-	0/0/48/48	0/0/5/5

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1110	SF4	S2-FE4	-29.27	2.13	2.33
5	D	3100	SF4	S2-FE4	-24.16	2.17	2.33
5	D	3110	SF4	S2-FE4	-23.32	2.17	2.33
5	D	3110	SF4	S2-FE3	-22.86	2.17	2.33
5	B	1110	SF4	S2-FE3	-21.49	2.18	2.33

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1301	AMP	O4'-C1'-N9	19.16	126.26	108.44
6	A	1302	AMP	O4'-C1'-N9	18.26	125.43	108.44
6	A	1303	AMP	O4'-C1'-N9	14.72	122.13	108.44
6	A	1302	AMP	N3-C2-N1	-12.23	118.49	128.71
4	C	3000	SFD	C5F-N5F-S	-12.21	97.23	117.39

All (5) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
6	A	1302	AMP	C1'
4	A	1000	SFD	C5F

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.