



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 07:01 AM GMT

PDB ID : 3CR8  
Title : Hexameric APS kinase from Thiobacillus denitrificans  
Authors : Gay, S.C.; Segel, I.H.; Fisher, A.J.  
Deposited on : 2008-04-04  
Resolution : 2.95 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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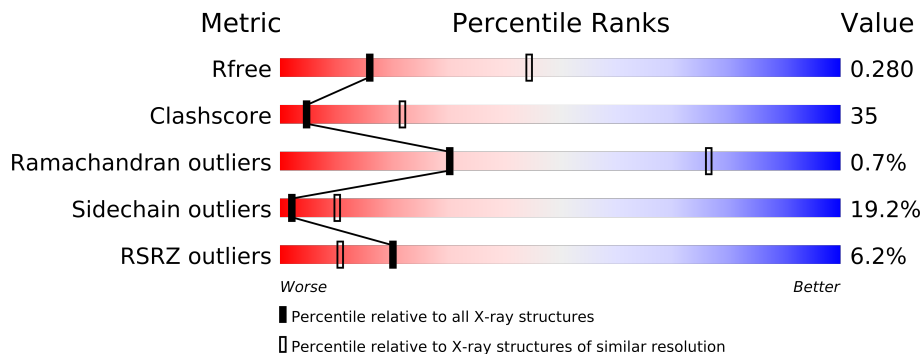
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.95 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))
$R_{free}$	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

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.

Mol	Chain	Length	Quality of chain
1	A	552	
1	B	552	
1	C	552	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11339 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 Sulfate adenylyltransferase, adenylylsulfate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3761	2390	676	679	16			
1	B	493	Total	C	N	O	S	0	0	0
			3744	2378	671	679	16			
1	C	493	Total	C	N	O	S	0	0	0
			3748	2380	670	682	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	LEU	-	EXPRESSION TAG	UNP Q3SM86
A	546	GLU	-	EXPRESSION TAG	UNP Q3SM86
A	547	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	548	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	549	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	550	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	551	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	552	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	545	LEU	-	EXPRESSION TAG	UNP Q3SM86
B	546	GLU	-	EXPRESSION TAG	UNP Q3SM86
B	547	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	548	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	549	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	550	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	551	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	552	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	545	LEU	-	EXPRESSION TAG	UNP Q3SM86
C	546	GLU	-	EXPRESSION TAG	UNP Q3SM86
C	547	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	548	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	549	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	550	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	551	HIS	-	EXPRESSION TAG	UNP Q3SM86

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Chain	Residue	Modelled	Actual	Comment	Reference
C	552	HIS	-	EXPRESSION TAG	UNP Q3SM86

- Molecule 2 is water.

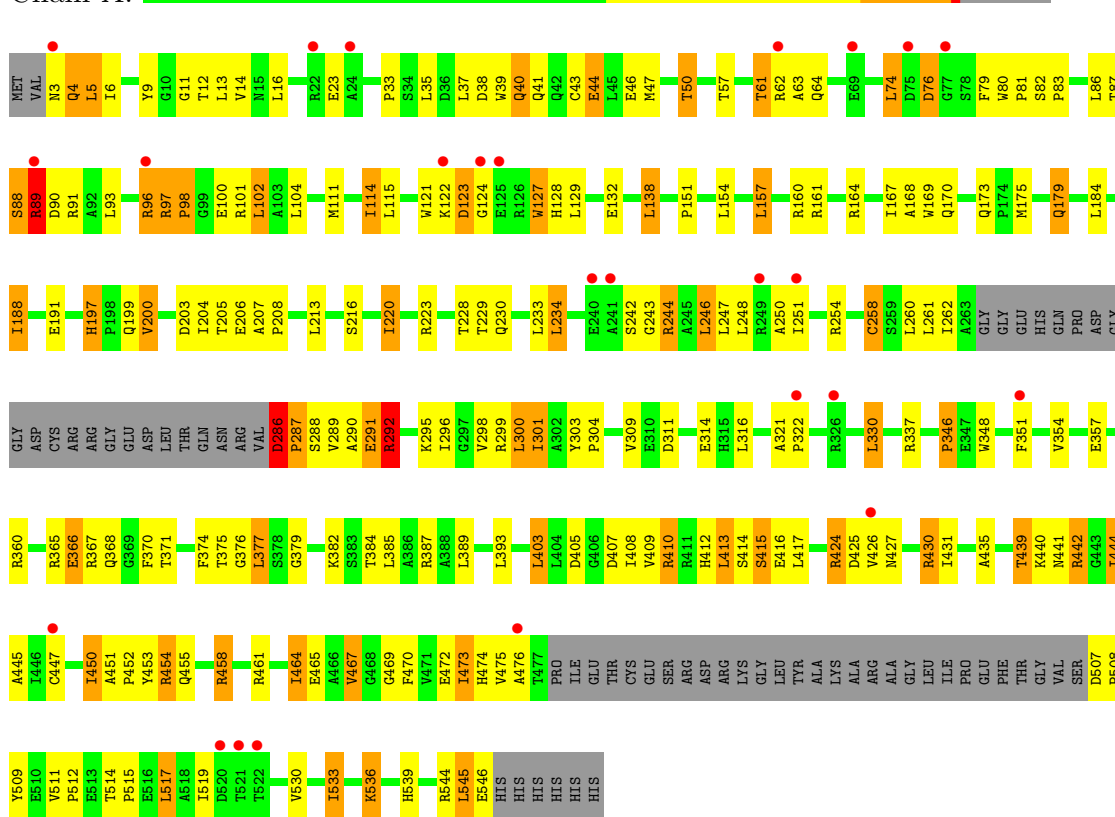
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total 31	O 31	0	0
2	B	22	Total 22	O 22	0	0
2	C	33	Total 33	O 33	0	0

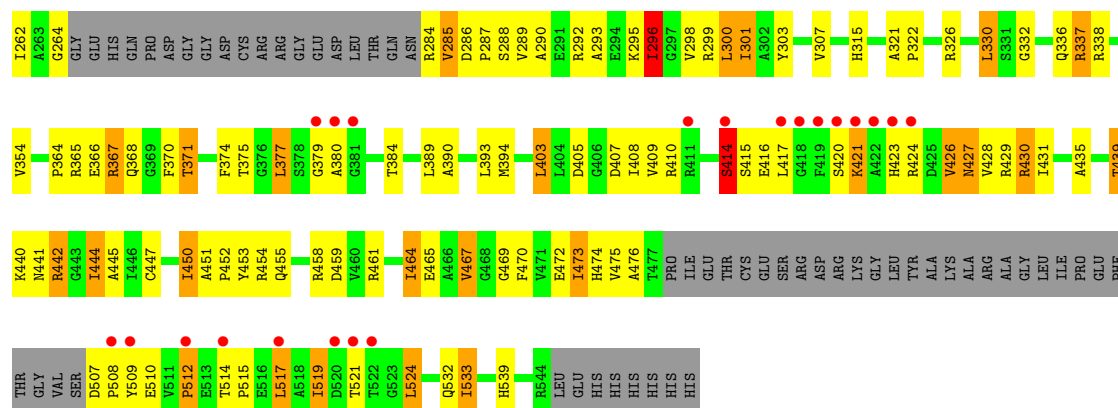
### 3 Residue-property plots

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.

- Molecule 1: Sulfate adenylyltransferase, adenylylsulfate kinase

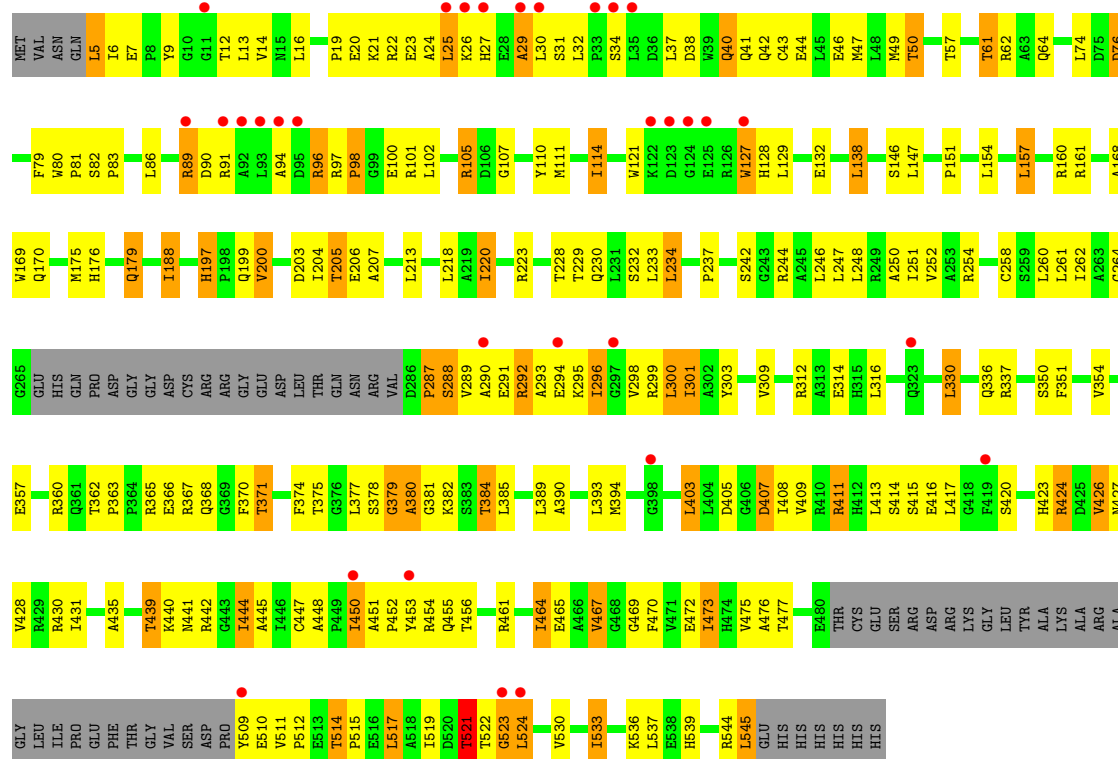
Chain A:





● Molecule 1: Sulfate adenylyltransferase, adenylylsulfate kinase

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.07Å 227.21Å 106.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.03 – 2.95 35.03 – 2.95	Depositor EDS
% Data completeness (in resolution range)	92.1 (35.03-2.95) 92.1 (35.03-2.95)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.243 , 0.282 0.238 , 0.280	Depositor DCC
$R_{free}$ test set	1888 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 38323 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.67	2/3843 (0.1%)	0.87	15/5227 (0.3%)
1	B	0.68	0/3825	0.83	8/5205 (0.2%)
1	C	0.65	0/3829	0.88	12/5209 (0.2%)
All	All	0.66	2/11497 (0.0%)	0.86	35/15641 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	CYS	CB-SG	-5.88	1.72	1.81
1	A	447	CYS	CB-SG	-5.42	1.73	1.81

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	SER	CB-CA-C	11.04	131.07	110.10
1	C	522	THR	N-CA-CB	-10.76	89.85	110.30
1	C	521	THR	CB-CA-C	-10.58	83.03	111.60
1	B	416	GLU	N-CA-CB	-9.50	93.50	110.60
1	C	29	ALA	CB-CA-C	-9.35	96.08	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	286	ASP	Peptide
1	C	380	ALA	Peptide

## 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	3761	0	3716	267	0
1	B	3744	0	3685	289	1
1	C	3748	0	3684	235	0
2	A	31	0	0	2	0
2	B	22	0	0	0	0
2	C	33	0	0	4	0
All	All	11339	0	11085	773	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 35.

The worst 5 of 773 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:SER:HB2	1:A:417:LEU:CD1	1.57	1.35
1:B:4:GLN:NE2	1:B:5:LEU:HB2	1.42	1.34
1:C:288:SER:O	1:C:291:GLU:HB2	1.32	1.28
1:A:244:ARG:N	1:A:244:ARG:HD2	1.40	1.22
1:C:287:PRO:O	1:C:291:GLU:HG2	1.32	1.22

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:B:430:ARG:NH2	1:B:430:ARG:NH2[3.455]	1.87	0.33

## 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	487/552 (88%)	441 (91%)	44 (9%)	2 (0%)	43	85
1	B	487/552 (88%)	440 (90%)	42 (9%)	5 (1%)	22	68
1	C	487/552 (88%)	438 (90%)	46 (9%)	3 (1%)	33	79
All	All	1461/1656 (88%)	1319 (90%)	132 (9%)	10 (1%)	30	76

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	GLU
1	C	366	GLU
1	A	98	PRO
1	B	69	GLU
1	B	366	GLU

### 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	376/449 (84%)	311 (83%)	65 (17%)	3	13
1	B	373/449 (83%)	295 (79%)	78 (21%)	1	7
1	C	373/449 (83%)	301 (81%)	72 (19%)	2	10
All	All	1122/1347 (83%)	907 (81%)	215 (19%)	2	10

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	HIS

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Mol	Chain	Res	Type
1	B	371	THR
1	C	407	ASP
1	B	205	THR
1	B	248	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	HIS
1	B	173	GLN
1	C	230	GLN
1	A	539	HIS
1	B	4	GLN

### 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 ⓘ

There are no ligands in this entry.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	493/552 (89%)	0.26	25 (5%)	27 13	30, 55, 94, 118	11 (2%)
1	B	493/552 (89%)	0.20	36 (7%)	15 8	26, 57, 93, 129	6 (1%)
1	C	493/552 (89%)	0.24	31 (6%)	19 10	26, 57, 94, 114	7 (1%)
All	All	1479/1656 (89%)	0.23	92 (6%)	20 11	26, 56, 94, 129	24 (1%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	422	ALA	6.2
1	B	418	GLY	5.5
1	C	124	GLY	5.4
1	B	379	GLY	5.2
1	B	380	ALA	4.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.