



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:51 AM GMT

PDB ID : 1I2D
Title : CRYSTAL STRUCTURE OF ATP SULFURYLASE FROM PENICILLIUM
CHRYSOGENUM
Authors : MacRae, I.J.; Segel, I.H.; Fisher, A.J.
Deposited on : 2001-02-07
Resolution : 2.81 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

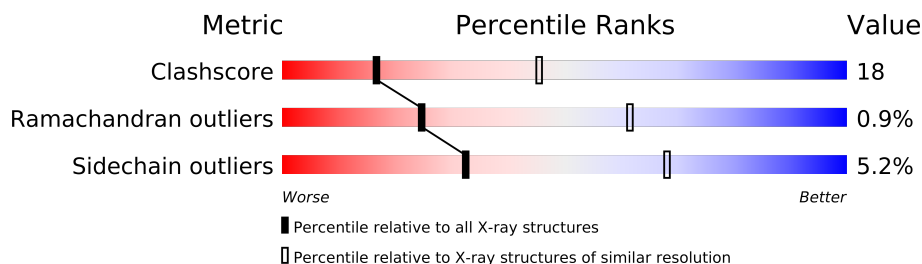
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.81 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	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)

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. 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	573	
1	B	573	
1	C	573	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 13851 atoms, of which 3 are hydrogens 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.

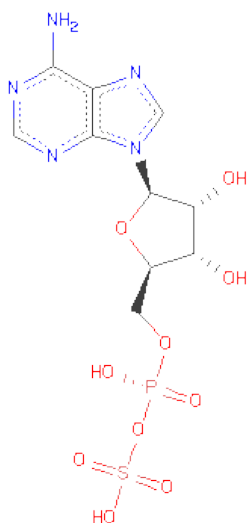
- Molecule 1 is a protein called ATP SULFURYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	572	Total	C	H	N	O	S	7	0	0
			4469	2812	1	813	831	12			
1	B	572	Total	C	H	N	O	S	0	0	0
			4469	2812	1	813	831	12			
1	C	572	Total	C	H	N	O	S	7	0	0
			4469	2812	1	813	831	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	ALA	SEE REMARK 999	UNP Q12650
B	100	GLY	ALA	SEE REMARK 999	UNP Q12650
C	100	GLY	ALA	SEE REMARK 999	UNP Q12650

- Molecule 2 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: $C_{10}H_{14}N_5O_{10}PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 1	S 1	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 1	S 1	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 1	S 1	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 1	S 1	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 1	S 1	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 1	S 1	0	0

- Molecule 3 is water.

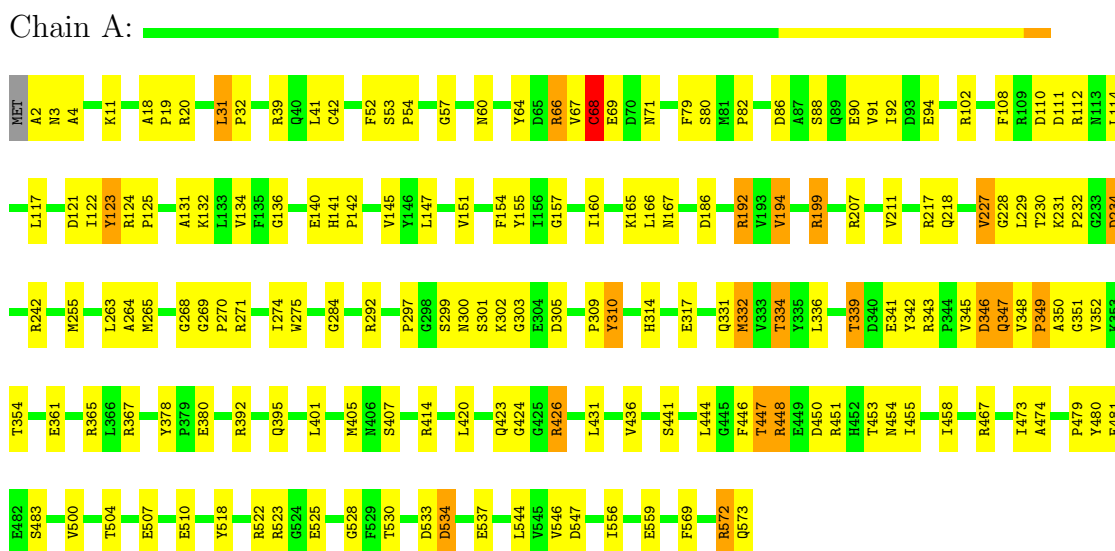
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		
3	B	87	Total	O	0	0
			87	87		
3	C	17	Total	O	0	0
			17	17		

3 Residue-property plots

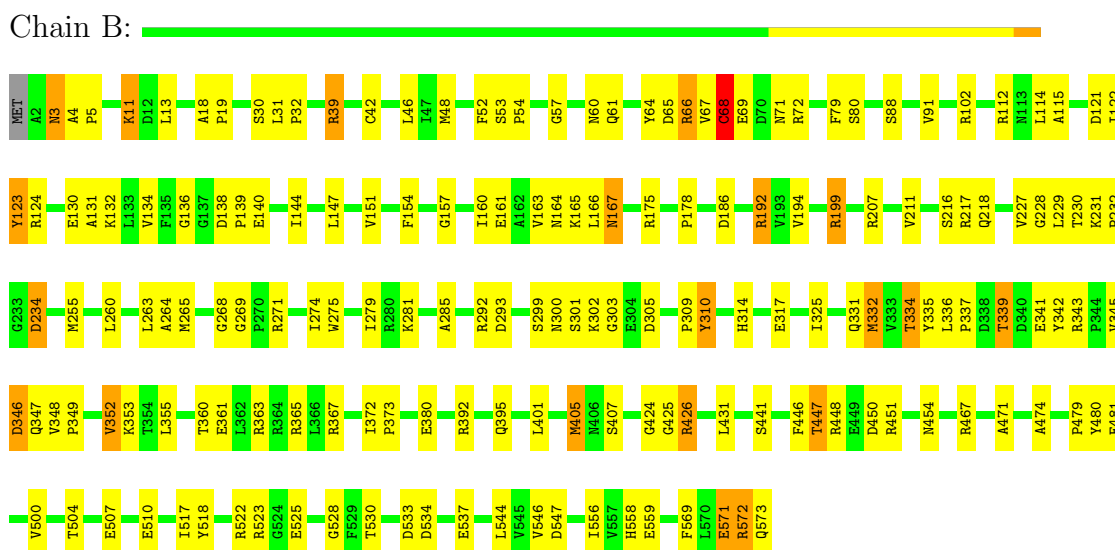
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ATP SULFURYLASE



• Molecule 1: ATP SULFURYLASE



• Molecule 1: ATP SULFURYLASE

Chain C:



MET	A2	N3	A4	P5	K11	A18	P19	L31	P32	R39	Q40	L41	C42	M48	F52	S53	P54	G57	N60	Q61	Y64	D65	R66	V67	C68	E69	D70	N71	S80	M81	P82	D86	A87	S88	Q89	E90	V91	I92	D93	E94	R102	F108	R112	M113	L114		
A115	I122	Y123	R124	K127	A131	K132	L133	V134	F135	G136	D138	P139	E140	I144	L147	V151	E153	F154	Y155	I156	G157	I160	E161	M164	K165	L166	M167	P178	A179	E180	L181	R182	V183	D186	R192	V193	V194	R199	R207	E208	L209	T210	V211				
R215	S216	R217	Q218	V227	G228	L229	T230	K231	P232	G233	D234	N253	G254	N255	L263	A264	N265	R266	M267	G268	G269	E270	R271	I274	I275	I279	R292	S299	N300	S301	K302	G303	D305	P309	Y310	H314	E317	K318	Y319	Q331	M332	V333	T334	Y335	L336	P337	D338
T339	D340	E341	Y342	R343	V348	P349	A350	G351	V352	K353	T354	L355	E361	R365	L366	R367	I372	P373	E380	I384	R392	Q395	L401	M405	N406	S407	R414	G424	G425	R426	L431	R437	S441	L444	G445	F446	T447	R448	E449	D450	R451	H452	T453				
N454	I455	A474	A475	P476	P479	Y480	E481	E482	S483	R484	V500	T504	E507	E510	Y518	R522	R523	G524	E525	G528	F529	T530	D533	D534	E537	T538	P539	L544	V545	V546	D547	F548	S549	K550	I556	V557	H558	E559	F569	R572	Q573						

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	135.67Å 162.09Å 273.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.08 – 2.81	Depositor
% Data completeness (in resolution range)	97.5 (29.08-2.81)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13851	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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: ADX

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	0.84	2/4563 (0.0%)	0.95	4/6191 (0.1%)
1	B	0.79	2/4563 (0.0%)	0.91	6/6191 (0.1%)
1	C	0.58	1/4563 (0.0%)	0.81	3/6191 (0.0%)
All	All	0.75	5/13689 (0.0%)	0.89	13/18573 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	CYS	CB-SG	13.60	2.05	1.82
1	B	68	CYS	CB-SG	11.76	2.02	1.82
1	C	68	CYS	CB-SG	6.77	1.93	1.82
1	B	481	GLU	CG-CD	5.90	1.60	1.51
1	A	481	GLU	CG-CD	5.35	1.59	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	CYS	CA-CB-SG	7.96	128.33	114.00
1	B	68	CYS	CA-CB-SG	7.49	127.48	114.00
1	B	424	GLY	N-CA-C	6.69	129.82	113.10
1	A	424	GLY	N-CA-C	6.63	129.69	113.10
1	C	424	GLY	N-CA-C	6.45	129.23	113.10

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	4468	1	4393	154	0
1	B	4468	1	4393	161	0
1	C	4468	1	4393	164	0
2	A	54	0	25	3	0
2	B	54	0	25	4	0
2	C	54	0	26	5	0
3	A	178	0	0	7	0
3	B	87	0	0	9	0
3	C	17	0	0	3	0
All	All	13848	3	13255	480	0

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 18.

The worst 5 of 480 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:68:CYS:CB	1:B:68:CYS:SG	2.02	1.46
1:A:68:CYS:CB	1:A:68:CYS:SG	2.05	1.45
1:C:134:VAL:HA	1:C:271:ARG:HH11	1.22	1.02
1:B:134:VAL:HA	1:B:271:ARG:HH11	1.23	1.00
1:A:134:VAL:HA	1:A:271:ARG:HH11	1.23	1.00

There are no symmetry-related clashes.

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	570/573 (100%)	530 (93%)	33 (6%)	7 (1%)	19	53
1	B	570/573 (100%)	519 (91%)	46 (8%)	5 (1%)	25	61
1	C	570/573 (100%)	525 (92%)	41 (7%)	4 (1%)	30	68
All	All	1710/1719 (100%)	1574 (92%)	120 (7%)	16 (1%)	25	61

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ALA
1	C	350	ALA
1	A	68	CYS
1	A	310	TYR
1	A	349	PRO

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	464/474 (98%)	440 (95%)	24 (5%)	32	68
1	B	464/474 (98%)	438 (94%)	26 (6%)	30	64
1	C	464/474 (98%)	441 (95%)	23 (5%)	34	70
All	All	1392/1422 (98%)	1319 (95%)	73 (5%)	32	68

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	186	ASP
1	B	293	ASP
1	C	426	ARG
1	B	216	SER
1	B	334	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	347	GLN
1	B	454	ASN
1	C	454	ASN
1	B	167	ASN
1	C	501	HIS

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 ⓘ

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	$\# Z > 2$
2	ADX	A	574	-	29,29,29	1.55	6 (20%)	44,45,45	1.55	8 (18%)
2	ADX	A	575	-	29,29,29	1.07	1 (3%)	44,45,45	1.57	9 (20%)
2	ADX	B	576	-	29,29,29	1.37	4 (13%)	44,45,45	1.39	5 (11%)
2	ADX	B	577	-	29,29,29	1.24	2 (6%)	44,45,45	1.44	7 (15%)
2	ADX	C	578	-	29,29,29	1.65	6 (20%)	44,45,45	1.58	7 (15%)
2	ADX	C	579	-	29,29,29	1.68	5 (17%)	44,45,45	1.49	8 (18%)

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
2	ADX	A	574	-	-	0/12/32/32	0/1/3/3
2	ADX	A	575	-	-	0/12/32/32	0/1/3/3
2	ADX	B	576	-	-	0/12/32/32	0/1/3/3
2	ADX	B	577	-	-	0/12/32/32	0/1/3/3
2	ADX	C	578	-	-	0/12/32/32	0/1/3/3
2	ADX	C	579	-	-	0/12/32/32	0/1/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	574	ADX	O4'-C1'	5.14	1.49	1.41
2	C	578	ADX	O4'-C1'	4.88	1.48	1.41
2	C	579	ADX	O4'-C1'	4.83	1.48	1.41
2	B	577	ADX	O4'-C1'	3.83	1.47	1.41
2	B	576	ADX	O4'-C1'	3.51	1.46	1.41

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	579	ADX	C8-N9-C4	-4.90	103.16	106.90
2	B	577	ADX	C8-N9-C4	-4.48	103.48	106.90
2	A	574	ADX	O4'-C1'-N9	-3.96	104.75	108.44
2	A	575	ADX	C8-N9-C4	-3.92	103.91	106.90
2	C	578	ADX	C8-N9-C4	-3.81	103.99	106.90

There are no chirality outliers.

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.