



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 11:30 am GMT

PDB ID : 6C6B
Title : Co-crystal structure of adenylyl-sulfate kinase from *Cryptococcus neoformans* bound to ADP
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-01-18
Resolution : 2.00 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

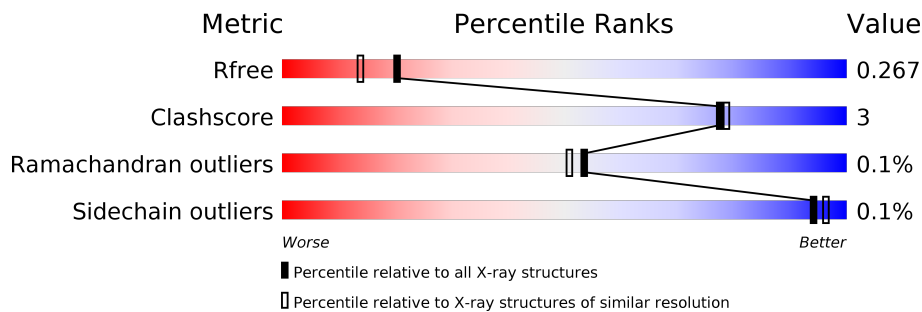
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	211	 87% 6% 7%
1	B	211	 89% 6% 6%
1	C	211	 84% 7% 9%
1	D	211	 80% 11% 9%
1	E	211	 84% 7% 9%
1	F	211	 84% 9% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9421 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 Adenylyl-sulfate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	1	0
			1508	959	258	290	1			
1	B	199	Total	C	N	O	S	0	0	0
			1519	962	263	293	1			
1	C	193	Total	C	N	O	S	0	0	0
			1467	927	255	284	1			
1	D	191	Total	C	N	O	S	0	0	0
			1444	913	250	280	1			
1	E	192	Total	C	N	O	S	0	0	0
			1409	893	242	273	1			
1	F	196	Total	C	N	O	S	0	1	0
			1497	950	257	289	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP J9VMZ3
A	-6	ALA	-	expression tag	UNP J9VMZ3
A	-5	HIS	-	expression tag	UNP J9VMZ3
A	-4	HIS	-	expression tag	UNP J9VMZ3
A	-3	HIS	-	expression tag	UNP J9VMZ3
A	-2	HIS	-	expression tag	UNP J9VMZ3
A	-1	HIS	-	expression tag	UNP J9VMZ3
A	0	HIS	-	expression tag	UNP J9VMZ3
B	-7	MET	-	expression tag	UNP J9VMZ3
B	-6	ALA	-	expression tag	UNP J9VMZ3
B	-5	HIS	-	expression tag	UNP J9VMZ3
B	-4	HIS	-	expression tag	UNP J9VMZ3
B	-3	HIS	-	expression tag	UNP J9VMZ3
B	-2	HIS	-	expression tag	UNP J9VMZ3
B	-1	HIS	-	expression tag	UNP J9VMZ3
B	0	HIS	-	expression tag	UNP J9VMZ3
C	-7	MET	-	expression tag	UNP J9VMZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ALA	-	expression tag	UNP J9VMZ3
C	-5	HIS	-	expression tag	UNP J9VMZ3
C	-4	HIS	-	expression tag	UNP J9VMZ3
C	-3	HIS	-	expression tag	UNP J9VMZ3
C	-2	HIS	-	expression tag	UNP J9VMZ3
C	-1	HIS	-	expression tag	UNP J9VMZ3
C	0	HIS	-	expression tag	UNP J9VMZ3
D	-7	MET	-	expression tag	UNP J9VMZ3
D	-6	ALA	-	expression tag	UNP J9VMZ3
D	-5	HIS	-	expression tag	UNP J9VMZ3
D	-4	HIS	-	expression tag	UNP J9VMZ3
D	-3	HIS	-	expression tag	UNP J9VMZ3
D	-2	HIS	-	expression tag	UNP J9VMZ3
D	-1	HIS	-	expression tag	UNP J9VMZ3
D	0	HIS	-	expression tag	UNP J9VMZ3
E	-7	MET	-	expression tag	UNP J9VMZ3
E	-6	ALA	-	expression tag	UNP J9VMZ3
E	-5	HIS	-	expression tag	UNP J9VMZ3
E	-4	HIS	-	expression tag	UNP J9VMZ3
E	-3	HIS	-	expression tag	UNP J9VMZ3
E	-2	HIS	-	expression tag	UNP J9VMZ3
E	-1	HIS	-	expression tag	UNP J9VMZ3
E	0	HIS	-	expression tag	UNP J9VMZ3
F	-7	MET	-	expression tag	UNP J9VMZ3
F	-6	ALA	-	expression tag	UNP J9VMZ3
F	-5	HIS	-	expression tag	UNP J9VMZ3
F	-4	HIS	-	expression tag	UNP J9VMZ3
F	-3	HIS	-	expression tag	UNP J9VMZ3
F	-2	HIS	-	expression tag	UNP J9VMZ3
F	-1	HIS	-	expression tag	UNP J9VMZ3
F	0	HIS	-	expression tag	UNP J9VMZ3

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



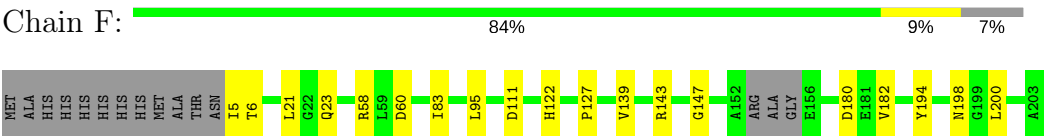
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	3
			115	115		
4	B	117	Total	O	0	2
			119	119		
4	C	51	Total	O	0	0
			51	51		
4	D	45	Total	O	0	2
			47	47		
4	E	30	Total	O	0	0
			30	30		
4	F	40	Total	O	0	1
			41	41		

- Molecule 1: Adenylyl-sulfate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	86.33Å 86.33Å 160.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.66 – 2.00 43.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.66-2.00) 99.9 (43.56-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.00Å)	Xtriage
Refinement program	PHENIX dev_2499	Depositor
R, R_{free}	0.224 , 0.267 0.224 , 0.267	Depositor DCC
R_{free} test set	1946 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l 0.297 for h,-h-k,-l 0.074 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9421	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: EDO, ADP

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	0.50	0/1540	0.61	0/2091
1	B	0.49	0/1548	0.59	0/2103
1	C	0.38	0/1496	0.54	0/2032
1	D	0.35	0/1472	0.54	0/2004
1	E	0.33	0/1436	0.52	0/1960
1	F	0.35	0/1529	0.54	0/2079
All	All	0.41	0/9021	0.56	0/12269

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	1508	0	1492	8	0
1	B	1519	0	1494	10	0
1	C	1467	0	1420	11	0
1	D	1444	0	1396	15	0
1	E	1409	0	1332	8	0
1	F	1497	0	1468	12	0
2	A	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	0	0
2	C	27	0	12	1	0
2	D	27	0	12	2	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
3	A	4	0	6	0	0
3	B	8	0	12	1	0
4	A	115	0	0	0	0
4	B	119	0	0	1	0
4	C	51	0	0	1	0
4	D	47	0	0	2	0
4	E	30	0	0	0	0
4	F	41	0	0	1	0
All	All	9421	0	8692	57	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 3.

The worst 5 of 57 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)
1:A:58:ARG:NH1	1:A:60:ASP:OD2	1.88	1.06
1:F:58:ARG:NH1	1:F:60:ASP:OD2	2.02	0.92
1:B:58:ARG:NH1	1:B:60:ASP:OD2	2.10	0.84
1:B:84:ARG:HD3	3:B:302:EDO:H21	1.62	0.80
1:C:62:ASP:OD2	4:C:401:HOH:O	2.00	0.79

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	194/211 (92%)	191 (98%)	3 (2%)	0	100	100
1	B	195/211 (92%)	190 (97%)	5 (3%)	0	100	100
1	C	189/211 (90%)	185 (98%)	4 (2%)	0	100	100
1	D	187/211 (89%)	183 (98%)	3 (2%)	1 (0%)	31	25
1	E	188/211 (89%)	184 (98%)	4 (2%)	0	100	100
1	F	193/211 (92%)	189 (98%)	4 (2%)	0	100	100
All	All	1146/1266 (90%)	1122 (98%)	23 (2%)	1 (0%)	53	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	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	160/175 (91%)	160 (100%)	0	100	100
1	B	160/175 (91%)	160 (100%)	0	100	100
1	C	152/175 (87%)	152 (100%)	0	100	100
1	D	150/175 (86%)	150 (100%)	0	100	100
1	E	140/175 (80%)	140 (100%)	0	100	100
1	F	158/175 (90%)	157 (99%)	1 (1%)	87	91
All	All	920/1050 (88%)	919 (100%)	1 (0%)	94	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	23	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

9 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	ADP	A	300	-	25,29,29	1.08	2 (8%)	25,45,45	1.63	3 (12%)
3	EDO	A	301	-	3,3,3	0.48	0	2,2,2	0.30	0
2	ADP	B	300	-	25,29,29	1.06	1 (4%)	25,45,45	1.69	4 (16%)
3	EDO	B	301	-	3,3,3	0.51	0	2,2,2	0.16	0
3	EDO	B	302	-	3,3,3	0.64	0	2,2,2	0.36	0
2	ADP	C	300	-	25,29,29	1.10	1 (4%)	25,45,45	1.62	5 (20%)
2	ADP	D	300	-	25,29,29	1.06	1 (4%)	25,45,45	1.65	2 (8%)
2	ADP	E	300	-	25,29,29	1.14	1 (4%)	25,45,45	1.71	5 (20%)
2	ADP	F	300	-	25,29,29	1.08	2 (8%)	25,45,45	1.73	4 (16%)

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	ADP	A	300	-	-	0/12/32/32	0/3/3/3
3	EDO	A	301	-	-	0/1/1/1	0/0/0/0
2	ADP	B	300	-	-	0/12/32/32	0/3/3/3
3	EDO	B	301	-	-	0/1/1/1	0/0/0/0
3	EDO	B	302	-	-	0/1/1/1	0/0/0/0
2	ADP	C	300	-	-	0/12/32/32	0/3/3/3
2	ADP	D	300	-	-	0/12/32/32	0/3/3/3
2	ADP	E	300	-	-	0/12/32/32	0/3/3/3
2	ADP	F	300	-	-	0/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	300	ADP	O4'-C1'	2.08	1.44	1.41
2	B	300	ADP	C5-C4	2.59	1.46	1.40
2	A	300	ADP	O4'-C1'	2.61	1.44	1.41
2	A	300	ADP	C5-C4	3.30	1.47	1.40
2	F	300	ADP	C5-C4	3.31	1.48	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	300	ADP	N3-C2-N1	-6.36	123.42	128.86
2	D	300	ADP	N3-C2-N1	-6.06	123.67	128.86
2	A	300	ADP	N3-C2-N1	-5.76	123.93	128.86
2	B	300	ADP	N3-C2-N1	-5.70	123.98	128.86
2	C	300	ADP	N3-C2-N1	-5.41	124.23	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	ADP	1	0
3	B	302	EDO	1	0
2	C	300	ADP	1	0
2	D	300	ADP	2	0
2	E	300	ADP	1	0
2	F	300	ADP	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.