



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:26 PM GMT

PDB ID : 1JJC
Title : Crystal structure at 2.6Å resolution of phenylalanyl-tRNA synthetase complexed with phenylalanyl-adenylate in the presence of manganese
Authors : Safro, M.G.; Fishman, R.; Moor, N.; Ankilova, V.
Deposited on : 2001-07-04
Resolution : 2.60 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>

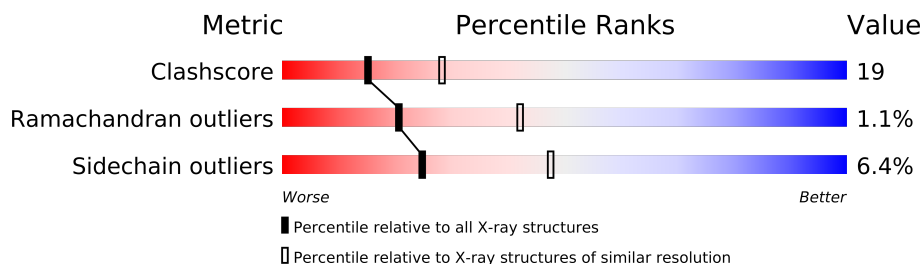
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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	350	
2	B	785	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	B	902	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8579 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 PHENYLALANYL-TRNA SYNTHETASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2123	1388	363	365	7			

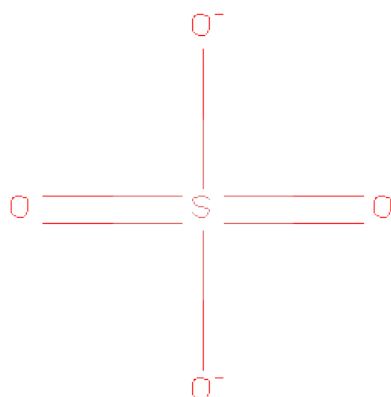
- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	785	Total	C	N	O	S	0	0	0
			6127	3925	1091	1101	10			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

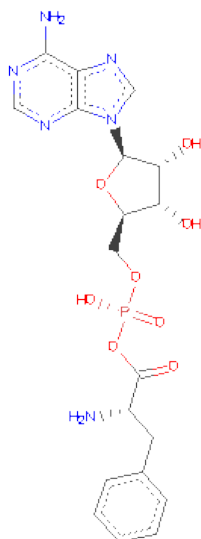
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is ADENOSINE-5'-[PHENYLALANINYL-PHOSPHATE] (three-letter code: FA5) (formula: C₁₉H₂₃N₆O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			34	19	6	8	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		
6	B	224	Total	O	0	0
			224	224		

F728	D729	Q732	G733	P734	P735	L736	P737	H740	H741	S742	L743	A744	F745	H746	L747	R748	T755	L756	D757	D758	E759	E760	V761	E762	E763	A764	V765	S766	R767	V768	A769	L772	R773	A774	R775	G776	F777	G778	L779	T784	P785
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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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.40Å 173.40Å 138.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	95.7 (50.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8579	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: MN, SO4, FA5

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	0.45	0/2191	0.75	3/2971 (0.1%)
2	B	0.46	2/6280 (0.0%)	0.67	9/8536 (0.1%)
All	All	0.45	2/8471 (0.0%)	0.69	12/11507 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	408	PRO	N-CD	-18.08	1.22	1.47
2	B	38	VAL	C-O	5.72	1.34	1.23

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	A	263	PRO	CA-N-CD	-6.94	101.78	111.50
2	B	324	VAL	N-CA-C	-6.90	92.36	111.00
1	A	262	GLU	CA-C-N	6.80	136.13	117.10
2	B	324	VAL	N-CA-CB	6.72	126.29	111.50

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	2123	0	2075	106	6
2	B	6127	0	6180	229	0
3	B	1	0	0	0	0
4	B	5	0	0	2	0
5	A	34	0	22	0	0
6	A	65	0	0	1	1
6	B	224	0	0	11	9
All	All	8579	0	8277	313	9

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 19.

The worst 5 of 313 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:239:MET:HE3	2:B:250:ASN:HB3	1.40	1.04
2:B:467:GLN:HE21	2:B:467:GLN:HA	1.21	1.03
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.25	0.99
1:A:348:GLY:O	1:A:350:LEU:HD12	1.63	0.98
2:B:408:PRO:HD2	6:B:944:HOH:O	1.63	0.96

The worst 5 of 9 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)
6:B:1045:HOH:O	6:B:1110:HOH:O[2_664]	0.20	2.00
6:A:1043:HOH:O	6:B:950:HOH:O[5_665]	0.22	1.98
6:B:1018:HOH:O	6:B:1078:HOH:O[3_565]	0.59	1.61
1:A:350:LEU:O	6:B:1071:HOH:O[4_555]	1.46	0.74
1:A:350:LEU:N	6:B:1071:HOH:O[4_555]	1.63	0.57

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	264/350 (75%)	252 (96%)	10 (4%)	2 (1%)	27	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	783/785 (100%)	737 (94%)	37 (5%)	9 (1%)	21	42
All	All	1047/1135 (92%)	989 (94%)	47 (4%)	11 (1%)	21	42

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	VAL
2	B	244	ASN
2	B	323	GLU
2	B	439	GLY
2	B	725	LEU

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	214/277 (77%)	202 (94%)	12 (6%)	30	55
2	B	630/630 (100%)	588 (93%)	42 (7%)	23	44
All	All	844/907 (93%)	790 (94%)	54 (6%)	25	47

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	191	LEU
2	B	325	ARG
2	B	670	LEU
2	B	276	ARG
2	B	283	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	212	HIS
2	B	258	GLN
2	B	669	HIS

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Mol	Chain	Res	Type
2	B	231	GLN
2	B	244	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
5	FA5	A	999	-	37,37,37	2.86	7 (18%)	54,54,54	2.20	4 (7%)
4	SO4	B	902	-	4,4,4	2.39	2 (50%)	6,6,6	2.55	3 (50%)

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
5	FA5	A	999	-	-	0/21/39/39	0/2/4/4
4	SO4	B	902	-	-	0/0/0/0	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	FA5	C2-N1	10.95	1.55	1.33
5	A	999	FA5	OP3-C	8.24	1.48	1.37
5	A	999	FA5	C8-N9	-6.84	1.26	1.36
5	A	999	FA5	C8-N7	3.50	1.41	1.34
5	A	999	FA5	O4'-C1'	3.35	1.46	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	FA5	N3-C2-N1	-12.95	117.88	128.71
5	A	999	FA5	OP3-C-O	5.05	126.11	122.11
5	A	999	FA5	P-OP3-C	-4.46	108.86	121.39
4	B	902	SO4	O2-S-O1	-3.87	96.74	109.53
4	B	902	SO4	O4-S-O1	3.64	143.18	110.12

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.