wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 02:24 AM JST

PDB ID	:	6KH2
Title	:	Crystal structure of Nicotinic acid mononucleotide adenylyltransferase mutant P22K/Y84V/Y118D/C132L/W176Y from Escherichia coli
Authors	:	Feng, Y.; Xue, S.; Zhao, Z.; Wang, X.
Deposited on	:	2019-07-12
Resolution	:	3.04 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

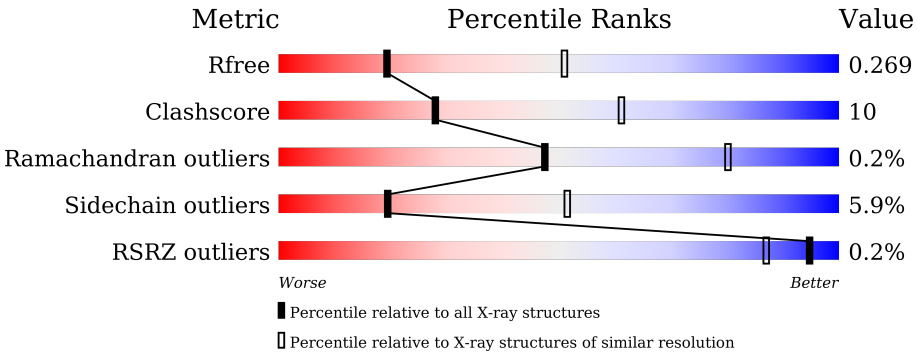
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	213	76% 23%
1	B	213	% 71% 26%
1	C	213	69% 29%
1	D	213	75% 19%
1	E	213	72% 22%
1	F	213	71% 23%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10189 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 Probable nicotinate-nucleotide adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1727	1104	298	321	4			
1	B	213	Total	C	N	O	S	0	0	0
			1727	1104	298	321	4			
1	C	213	Total	C	N	O	S	0	0	0
			1727	1104	298	321	4			
1	D	206	Total	C	N	O	S	0	0	0
			1664	1062	290	308	4			
1	E	207	Total	C	N	O	S	0	0	0
			1673	1067	291	311	4			
1	F	207	Total	C	N	O	S	0	0	0
			1671	1066	291	310	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	LYS	PRO	engineered mutation	UNP A0A222QGJ8
A	84	VAL	TYR	engineered mutation	UNP A0A222QGJ8
A	118	ASP	TYR	engineered mutation	UNP A0A222QGJ8
A	132	LEU	CYS	engineered mutation	UNP A0A222QGJ8
A	176	TYR	TRP	engineered mutation	UNP A0A222QGJ8
B	22	LYS	PRO	engineered mutation	UNP A0A222QGJ8
B	84	VAL	TYR	engineered mutation	UNP A0A222QGJ8
B	118	ASP	TYR	engineered mutation	UNP A0A222QGJ8
B	132	LEU	CYS	engineered mutation	UNP A0A222QGJ8
B	176	TYR	TRP	engineered mutation	UNP A0A222QGJ8
C	22	LYS	PRO	engineered mutation	UNP A0A222QGJ8
C	84	VAL	TYR	engineered mutation	UNP A0A222QGJ8
C	118	ASP	TYR	engineered mutation	UNP A0A222QGJ8
C	132	LEU	CYS	engineered mutation	UNP A0A222QGJ8
C	176	TYR	TRP	engineered mutation	UNP A0A222QGJ8
D	22	LYS	PRO	engineered mutation	UNP A0A222QGJ8
D	84	VAL	TYR	engineered mutation	UNP A0A222QGJ8

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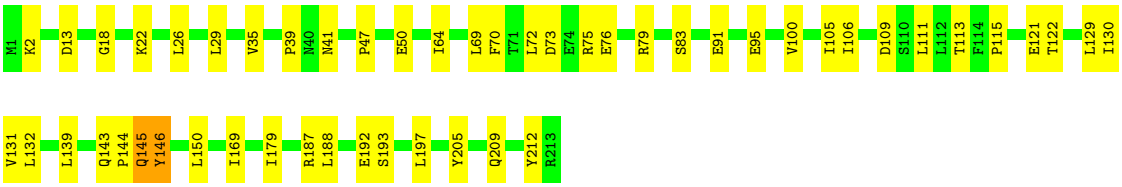
Chain	Residue	Modelled	Actual	Comment	Reference
D	118	ASP	TYR	engineered mutation	UNP A0A222QGJ8
D	132	LEU	CYS	engineered mutation	UNP A0A222QGJ8
D	176	TYR	TRP	engineered mutation	UNP A0A222QGJ8
E	22	LYS	PRO	engineered mutation	UNP A0A222QGJ8
E	84	VAL	TYR	engineered mutation	UNP A0A222QGJ8
E	118	ASP	TYR	engineered mutation	UNP A0A222QGJ8
E	132	LEU	CYS	engineered mutation	UNP A0A222QGJ8
E	176	TYR	TRP	engineered mutation	UNP A0A222QGJ8
F	22	LYS	PRO	engineered mutation	UNP A0A222QGJ8
F	84	VAL	TYR	engineered mutation	UNP A0A222QGJ8
F	118	ASP	TYR	engineered mutation	UNP A0A222QGJ8
F	132	LEU	CYS	engineered mutation	UNP A0A222QGJ8
F	176	TYR	TRP	engineered mutation	UNP A0A222QGJ8

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

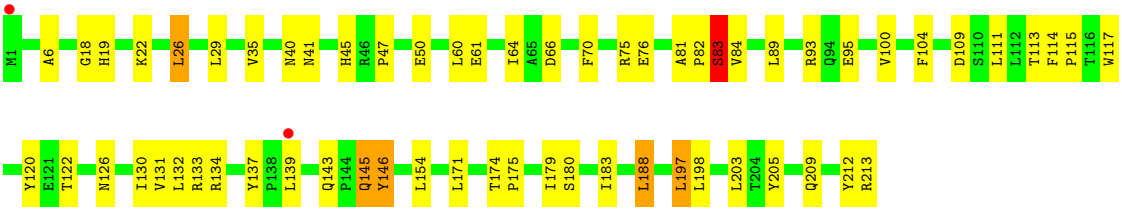
• Molecule 1: Probable nicotinate-nucleotide adenylyltransferase

Chain A:



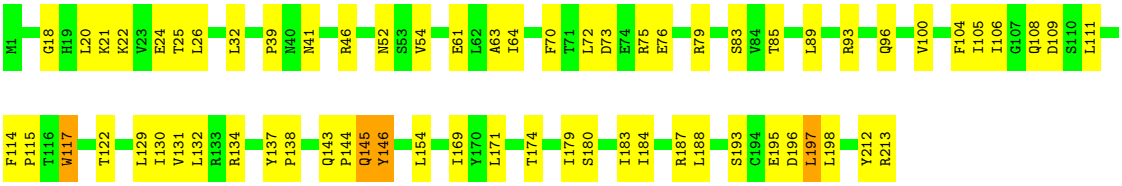
• Molecule 1: Probable nicotinate-nucleotide adenylyltransferase

Chain B:



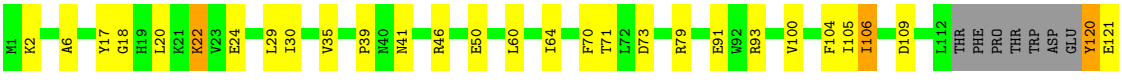
• Molecule 1: Probable nicotinate-nucleotide adenylyltransferase

Chain C:



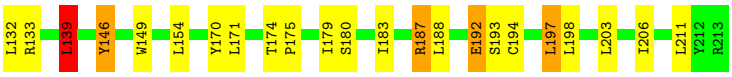
• Molecule 1: Probable nicotinate-nucleotide adenylyltransferase

Chain D:



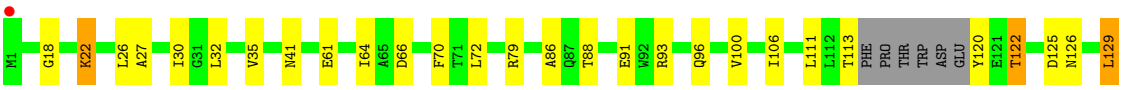
• Molecule 1: Probable nicotinate-nucleotide adenylyltransferase

Chain E:



• Molecule 1: Probable nicotinate-nucleotide adenylyltransferase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.69Å 130.21Å 106.74Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	48.70 – 3.04 48.70 – 3.04	Depositor EDS
% Data completeness (in resolution range)	63.4 (48.70-3.04) 63.4 (48.70-3.04)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.232 , 0.268 0.234 , 0.269	Depositor DCC
R_{free} test set	1359 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10189	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.26	0/1773	0.47	0/2419
1	B	0.27	0/1773	0.47	0/2419
1	C	0.26	0/1773	0.48	0/2419
1	D	0.26	0/1705	0.51	1/2322 (0.0%)
1	E	0.26	0/1714	0.50	1/2334 (0.0%)
1	F	0.26	0/1712	0.49	1/2332 (0.0%)
All	All	0.26	0/10450	0.49	3/14245 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	139	LEU	CA-CB-CG	7.70	133.02	115.30
1	D	139	LEU	CA-CB-CG	5.78	128.59	115.30
1	F	139	LEU	CA-CB-CG	5.42	127.76	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1727	0	1714	30	0
1	B	1727	0	1714	38	0
1	C	1727	0	1714	40	0
1	D	1664	0	1663	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1673	0	1669	32	0
1	F	1671	0	1670	34	0
All	All	10189	0	10144	201	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 10.

The worst 5 of 201 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:29:LEU:HA	1:B:175:PRO:HB3	1.58	0.84
1:B:29:LEU:HA	1:E:175:PRO:HB3	1.66	0.77
1:B:64:ILE:HG13	1:B:70:PHE:HB2	1.67	0.75
1:D:22:LYS:HD2	1:D:132:LEU:HD13	1.67	0.75
1:F:64:ILE:HG13	1:F:70:PHE:HB2	1.69	0.74

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	29 65
1	B	211/213 (99%)	200 (95%)	10 (5%)	1 (0%)	29 65
1	C	211/213 (99%)	205 (97%)	5 (2%)	1 (0%)	29 65
1	D	202/213 (95%)	194 (96%)	8 (4%)	0	100 100
1	E	203/213 (95%)	192 (95%)	11 (5%)	0	100 100
1	F	203/213 (95%)	197 (97%)	6 (3%)	0	100 100
All	All	1241/1278 (97%)	1190 (96%)	48 (4%)	3 (0%)	47 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	83	SER
1	A	144	PRO
1	C	144	PRO

5.3.2 Protein sidechains (i)

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	190/190 (100%)	182 (96%)	8 (4%)	30	64
1	B	190/190 (100%)	176 (93%)	14 (7%)	13	42
1	C	190/190 (100%)	182 (96%)	8 (4%)	30	64
1	D	183/190 (96%)	170 (93%)	13 (7%)	14	44
1	E	184/190 (97%)	173 (94%)	11 (6%)	19	51
1	F	184/190 (97%)	172 (94%)	12 (6%)	17	47
All	All	1121/1140 (98%)	1055 (94%)	66 (6%)	19	51

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	88	THR
1	F	122	THR
1	F	197	LEU
1	C	117	TRP
1	C	109	ASP

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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^{th} 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^2)	Q<0.9
1	A	213/213 (100%)	-0.36	0 100 100	39, 60, 86, 94	0
1	B	213/213 (100%)	-0.32	2 (0%) 84 62	37, 59, 82, 97	0
1	C	213/213 (100%)	-0.37	0 100 100	40, 60, 88, 105	0
1	D	206/213 (96%)	-0.32	0 100 100	37, 55, 89, 115	0
1	E	207/213 (97%)	-0.34	0 100 100	42, 58, 89, 105	0
1	F	207/213 (97%)	-0.38	1 (0%) 91 75	37, 56, 84, 110	0
All	All	1259/1278 (98%)	-0.35	3 (0%) 95 87	37, 58, 86, 115	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.6
1	F	1	MET	2.6
1	B	139	LEU	2.6

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.