



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5IPY
Title : Crystal structure of WT RnTmm
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Deposited on : 2016-03-10
Resolution : 1.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

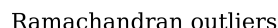
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

i

X-RAY DIFFRACTION

A.

 R_{free}

		c

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8866 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 Flavin-containing monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3580	2288	606	669	17			
1	B	445	Total	C	N	O	S	0	1	0
			3590	2294	609	670	17			

There are 16 discrepancies between the modelled and reference sequences:

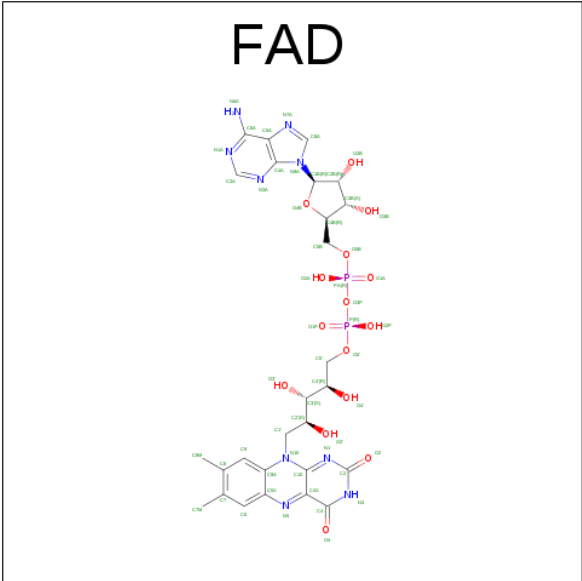
Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	GLU	engineered mutation	UNP A3SLM3
A	154	ALA	ASP	engineered mutation	UNP A3SLM3
A	448	HIS	-	expression tag	UNP A3SLM3
A	449	HIS	-	expression tag	UNP A3SLM3
A	450	HIS	-	expression tag	UNP A3SLM3
A	451	HIS	-	expression tag	UNP A3SLM3
A	452	HIS	-	expression tag	UNP A3SLM3
A	453	HIS	-	expression tag	UNP A3SLM3
B	153	ALA	GLU	engineered mutation	UNP A3SLM3
B	154	ALA	ASP	engineered mutation	UNP A3SLM3
B	448	HIS	-	expression tag	UNP A3SLM3
B	449	HIS	-	expression tag	UNP A3SLM3
B	450	HIS	-	expression tag	UNP A3SLM3
B	451	HIS	-	expression tag	UNP A3SLM3
B	452	HIS	-	expression tag	UNP A3SLM3
B	453	HIS	-	expression tag	UNP A3SLM3

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

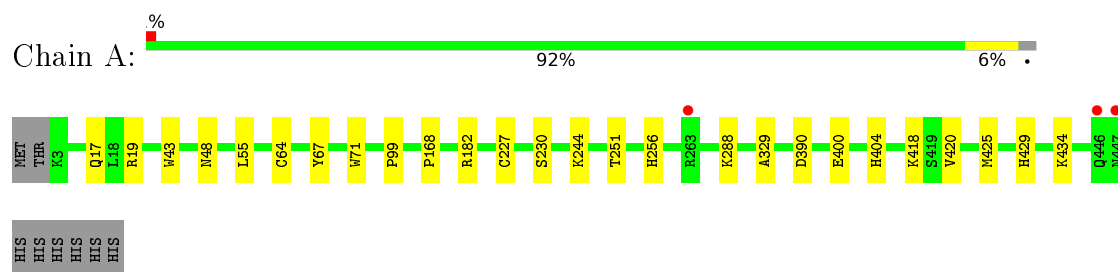
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	765	Total	O	0	0
			765	765		
4	B	729	Total	O	0	0
			729	729		

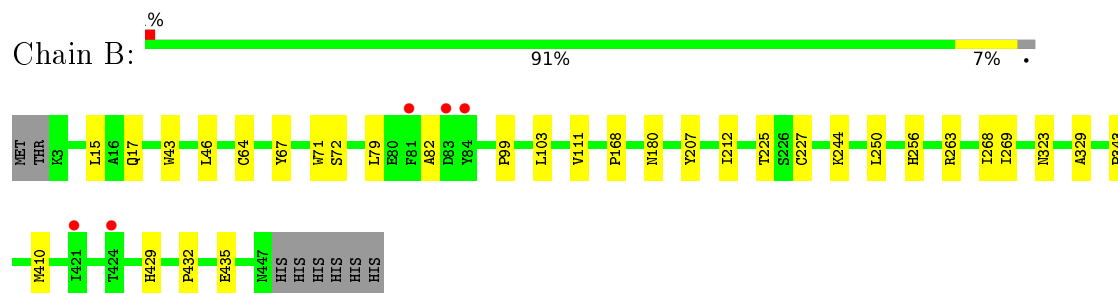
3 Residue-property plots [i](#)

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: Flavin-containing monooxygenase



- Molecule 1: Flavin-containing monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.50Å 85.39Å 79.53Å 90.00° 113.03° 90.00°	Depositor
Resolution (Å)	42.14 – 1.50 42.69 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (42.14-1.50) 98.5 (42.69-1.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.146 , 0.169 0.144 , 0.167	Depositor DCC
R_{free} test set	7143 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8866	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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: NAP, FAD

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	0.37	0/3690	0.54	0/5009
1	B	0.35	0/3701	0.52	0/5024
All	All	0.36	0/7391	0.53	0/10033

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	3580	0	3359	20	0
1	B	3590	0	3365	21	0
2	A	48	0	25	1	0
2	B	48	0	25	3	0
3	A	53	0	31	0	0
3	B	53	0	31	1	0
4	A	765	0	0	8	0
4	B	729	0	0	9	0
All	All	8866	0	6836	41	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 41 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:B:64:CYS:SG	4:B:601:HOH:O	2.46	0.72
1:A:64:CYS:SG	4:A:926:HOH:O	2.53	0.66
1:A:64:CYS:SG	4:A:651:HOH:O	2.55	0.64
1:A:64:CYS:SG	4:A:614:HOH:O	2.55	0.64
1:B:256:HIS:HD2	4:B:1170:HOH:O	1.86	0.58

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	443/453 (98%)	427 (96%)	16 (4%)	0	100	100
1	B	444/453 (98%)	429 (97%)	15 (3%)	0	100	100
All	All	887/906 (98%)	856 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	365/373 (98%)	362 (99%)	3 (1%)	86	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	366/373 (98%)	363 (99%)	3 (1%)	86	70
All	All	731/746 (98%)	725 (99%)	6 (1%)	86	70

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ARG
1	B	343	PRO
1	B	43	TRP
1	A	43	TRP
1	B	180	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	180	ASN
1	B	446	GLN
1	B	323	ASN
1	A	429	HIS
1	B	256	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	NAP	A	501	-	45,52,52	2.28	14 (31%)	55,80,80	1.95	9 (16%)
3	FAD	A	502	-	52,58,58	1.15	4 (7%)	52,89,89	2.22	14 (26%)
2	NAP	B	501	-	45,52,52	1.00	2 (4%)	55,80,80	1.55	7 (12%)
3	FAD	B	502	-	52,58,58	1.20	8 (15%)	52,89,89	2.47	9 (17%)

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	NAP	A	501	-	-	0/27/67/67	0/5/5/5
3	FAD	A	502	-	-	0/30/50/50	0/6/6/6
2	NAP	B	501	-	-	0/27/67/67	0/5/5/5
3	FAD	B	502	-	-	0/30/50/50	0/6/6/6

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAP	C3B-C2B	-5.44	1.40	1.53
2	A	501	NAP	C3N-C7N	-3.43	1.45	1.50
3	B	502	FAD	C6-C5X	-2.42	1.38	1.41
2	A	501	NAP	C2D-C1D	-2.23	1.50	1.53
2	A	501	NAP	O4B-C4B	-2.22	1.39	1.45

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAP	N3A-C2A-N1A	-8.16	122.46	128.87
3	B	502	FAD	C4-C4X-C10	-7.93	114.87	119.94
2	B	501	NAP	N3A-C2A-N1A	-7.20	123.22	128.87
3	A	502	FAD	C4-C4X-C10	-5.05	116.71	119.94
3	A	502	FAD	N3A-C2A-N1A	-5.05	124.91	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAP	1	0
2	B	501	NAP	3	0
3	B	502	FAD	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](#)

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, 95th 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	445/453 (98%)	-0.26	3 (0%) 89 91	6, 10, 21, 38	0
1	B	445/453 (98%)	-0.19	5 (1%) 82 85	6, 11, 23, 32	0
All	All	890/906 (98%)	-0.23	8 (0%) 85 87	6, 11, 23, 38	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	THR	2.9
1	B	421	ILE	2.8
1	A	447	ASN	2.7
1	B	83	ASP	2.6
1	B	81	PHE	2.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FAD	B	502	53/53	0.98	0.09	0.39	5,6,9,11	0
3	FAD	A	502	53/53	0.98	0.08	0.05	4,6,9,9	0
2	NAP	A	501	48/48	0.98	0.06	-0.56	6,8,14,17	0
2	NAP	B	501	48/48	0.98	0.06	-0.81	5,8,13,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.