wwPDB X-ray Structure Validation Summary Report (i)

Dec 6, 2016 – 01:03 AM EST

PDB ID	:	5MGY
Title	:	Crystal structure of Pseudomonas stutzeri flavinyl transferase ApbE, apo form
Authors	:	Zhang, L.; Trncik, C.; Andrade, S.L.A.; Einsle, O.
Deposited on	:	2016-11-22
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

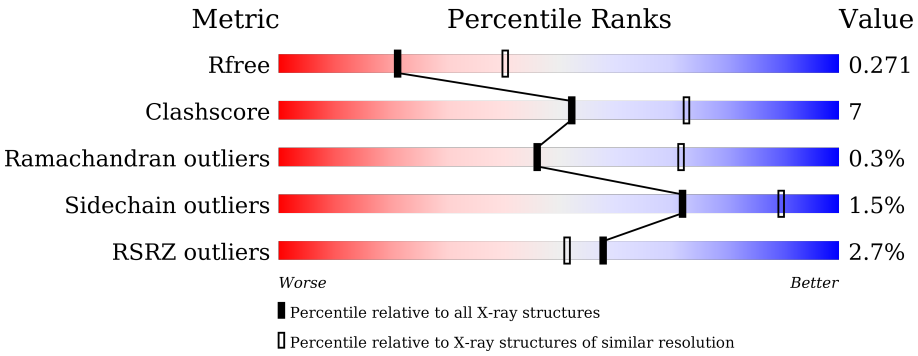
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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 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))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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. 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	332	3% 80% 11% • 8%
1	B	332	2% 79% 11% • 9%
1	C	332	2% 83% 10% • 7%
1	D	332	% 80% 11% • 7%
1	E	332	2% 83% 11% • 5%
1	F	332	2% 79% 15% • 5%

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Mol	Chain	Length	Quality of chain
1	G	332	5% 72% 16% 10%
1	H	332	3% 83% 12% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18725 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 FAD:protein FMN transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	316	Total	C	N	O	S	0	0	0
			2388	1495	415	470	8			
1	B	303	Total	C	N	O	S	0	0	0
			2288	1431	392	457	8			
1	G	299	Total	C	N	O	S	0	0	0
			2261	1422	385	446	8			
1	A	305	Total	C	N	O	S	0	0	0
			2306	1444	395	459	8			
1	C	310	Total	C	N	O	S	0	0	0
			2334	1466	400	460	8			
1	D	309	Total	C	N	O	S	0	0	0
			2330	1464	399	459	8			
1	E	316	Total	C	N	O	S	0	0	0
			2388	1495	415	470	8			
1	F	315	Total	C	N	O	S	0	0	0
			2377	1489	411	469	8			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	27	MET	-	initiating methionine	UNP H7EX88
H	28	ALA	-	expression tag	UNP H7EX88
H	29	MET	-	expression tag	UNP H7EX88
H	30	ASP	-	expression tag	UNP H7EX88
H	31	LEU	-	expression tag	UNP H7EX88
H	32	PHE	-	expression tag	UNP H7EX88
H	33	GLN	-	expression tag	UNP H7EX88
H	34	ASP	-	expression tag	UNP H7EX88
H	35	LYS	-	expression tag	UNP H7EX88
H	36	VAL	-	expression tag	UNP H7EX88
H	37	GLU	-	expression tag	UNP H7EX88
H	38	ALA	-	expression tag	UNP H7EX88
H	39	PHE	-	expression tag	UNP H7EX88

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Chain	Residue	Modelled	Actual	Comment	Reference
H	40	THR	-	expression tag	UNP H7EX88
H	41	GLY	-	expression tag	UNP H7EX88
H	42	PRO	-	expression tag	UNP H7EX88
H	43	THR	-	expression tag	UNP H7EX88
H	351	VAL	-	expression tag	UNP H7EX88
H	352	GLU	-	expression tag	UNP H7EX88
H	353	HIS	-	expression tag	UNP H7EX88
H	354	HIS	-	expression tag	UNP H7EX88
H	355	HIS	-	expression tag	UNP H7EX88
H	356	HIS	-	expression tag	UNP H7EX88
H	357	HIS	-	expression tag	UNP H7EX88
H	358	HIS	-	expression tag	UNP H7EX88
B	27	MET	-	initiating methionine	UNP H7EX88
B	28	ALA	-	expression tag	UNP H7EX88
B	29	MET	-	expression tag	UNP H7EX88
B	30	ASP	-	expression tag	UNP H7EX88
B	31	LEU	-	expression tag	UNP H7EX88
B	32	PHE	-	expression tag	UNP H7EX88
B	33	GLN	-	expression tag	UNP H7EX88
B	34	ASP	-	expression tag	UNP H7EX88
B	35	LYS	-	expression tag	UNP H7EX88
B	36	VAL	-	expression tag	UNP H7EX88
B	37	GLU	-	expression tag	UNP H7EX88
B	38	ALA	-	expression tag	UNP H7EX88
B	39	PHE	-	expression tag	UNP H7EX88
B	40	THR	-	expression tag	UNP H7EX88
B	41	GLY	-	expression tag	UNP H7EX88
B	42	PRO	-	expression tag	UNP H7EX88
B	43	THR	-	expression tag	UNP H7EX88
B	351	VAL	-	expression tag	UNP H7EX88
B	352	GLU	-	expression tag	UNP H7EX88
B	353	HIS	-	expression tag	UNP H7EX88
B	354	HIS	-	expression tag	UNP H7EX88
B	355	HIS	-	expression tag	UNP H7EX88
B	356	HIS	-	expression tag	UNP H7EX88
B	357	HIS	-	expression tag	UNP H7EX88
B	358	HIS	-	expression tag	UNP H7EX88
G	27	MET	-	initiating methionine	UNP H7EX88
G	28	ALA	-	expression tag	UNP H7EX88
G	29	MET	-	expression tag	UNP H7EX88
G	30	ASP	-	expression tag	UNP H7EX88
G	31	LEU	-	expression tag	UNP H7EX88

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Chain	Residue	Modelled	Actual	Comment	Reference
G	32	PHE	-	expression tag	UNP H7EX88
G	33	GLN	-	expression tag	UNP H7EX88
G	34	ASP	-	expression tag	UNP H7EX88
G	35	LYS	-	expression tag	UNP H7EX88
G	36	VAL	-	expression tag	UNP H7EX88
G	37	GLU	-	expression tag	UNP H7EX88
G	38	ALA	-	expression tag	UNP H7EX88
G	39	PHE	-	expression tag	UNP H7EX88
G	40	THR	-	expression tag	UNP H7EX88
G	41	GLY	-	expression tag	UNP H7EX88
G	42	PRO	-	expression tag	UNP H7EX88
G	43	THR	-	expression tag	UNP H7EX88
G	351	VAL	-	expression tag	UNP H7EX88
G	352	GLU	-	expression tag	UNP H7EX88
G	353	HIS	-	expression tag	UNP H7EX88
G	354	HIS	-	expression tag	UNP H7EX88
G	355	HIS	-	expression tag	UNP H7EX88
G	356	HIS	-	expression tag	UNP H7EX88
G	357	HIS	-	expression tag	UNP H7EX88
G	358	HIS	-	expression tag	UNP H7EX88
A	27	MET	-	initiating methionine	UNP H7EX88
A	28	ALA	-	expression tag	UNP H7EX88
A	29	MET	-	expression tag	UNP H7EX88
A	30	ASP	-	expression tag	UNP H7EX88
A	31	LEU	-	expression tag	UNP H7EX88
A	32	PHE	-	expression tag	UNP H7EX88
A	33	GLN	-	expression tag	UNP H7EX88
A	34	ASP	-	expression tag	UNP H7EX88
A	35	LYS	-	expression tag	UNP H7EX88
A	36	VAL	-	expression tag	UNP H7EX88
A	37	GLU	-	expression tag	UNP H7EX88
A	38	ALA	-	expression tag	UNP H7EX88
A	39	PHE	-	expression tag	UNP H7EX88
A	40	THR	-	expression tag	UNP H7EX88
A	41	GLY	-	expression tag	UNP H7EX88
A	42	PRO	-	expression tag	UNP H7EX88
A	43	THR	-	expression tag	UNP H7EX88
A	351	VAL	-	expression tag	UNP H7EX88
A	352	GLU	-	expression tag	UNP H7EX88
A	353	HIS	-	expression tag	UNP H7EX88
A	354	HIS	-	expression tag	UNP H7EX88
A	355	HIS	-	expression tag	UNP H7EX88

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Chain	Residue	Modelled	Actual	Comment	Reference
A	356	HIS	-	expression tag	UNP H7EX88
A	357	HIS	-	expression tag	UNP H7EX88
A	358	HIS	-	expression tag	UNP H7EX88
C	27	MET	-	initiating methionine	UNP H7EX88
C	28	ALA	-	expression tag	UNP H7EX88
C	29	MET	-	expression tag	UNP H7EX88
C	30	ASP	-	expression tag	UNP H7EX88
C	31	LEU	-	expression tag	UNP H7EX88
C	32	PHE	-	expression tag	UNP H7EX88
C	33	GLN	-	expression tag	UNP H7EX88
C	34	ASP	-	expression tag	UNP H7EX88
C	35	LYS	-	expression tag	UNP H7EX88
C	36	VAL	-	expression tag	UNP H7EX88
C	37	GLU	-	expression tag	UNP H7EX88
C	38	ALA	-	expression tag	UNP H7EX88
C	39	PHE	-	expression tag	UNP H7EX88
C	40	THR	-	expression tag	UNP H7EX88
C	41	GLY	-	expression tag	UNP H7EX88
C	42	PRO	-	expression tag	UNP H7EX88
C	43	THR	-	expression tag	UNP H7EX88
C	351	VAL	-	expression tag	UNP H7EX88
C	352	GLU	-	expression tag	UNP H7EX88
C	353	HIS	-	expression tag	UNP H7EX88
C	354	HIS	-	expression tag	UNP H7EX88
C	355	HIS	-	expression tag	UNP H7EX88
C	356	HIS	-	expression tag	UNP H7EX88
C	357	HIS	-	expression tag	UNP H7EX88
C	358	HIS	-	expression tag	UNP H7EX88
D	27	MET	-	initiating methionine	UNP H7EX88
D	28	ALA	-	expression tag	UNP H7EX88
D	29	MET	-	expression tag	UNP H7EX88
D	30	ASP	-	expression tag	UNP H7EX88
D	31	LEU	-	expression tag	UNP H7EX88
D	32	PHE	-	expression tag	UNP H7EX88
D	33	GLN	-	expression tag	UNP H7EX88
D	34	ASP	-	expression tag	UNP H7EX88
D	35	LYS	-	expression tag	UNP H7EX88
D	36	VAL	-	expression tag	UNP H7EX88
D	37	GLU	-	expression tag	UNP H7EX88
D	38	ALA	-	expression tag	UNP H7EX88
D	39	PHE	-	expression tag	UNP H7EX88
D	40	THR	-	expression tag	UNP H7EX88

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Chain	Residue	Modelled	Actual	Comment	Reference
D	41	GLY	-	expression tag	UNP H7EX88
D	42	PRO	-	expression tag	UNP H7EX88
D	43	THR	-	expression tag	UNP H7EX88
D	351	VAL	-	expression tag	UNP H7EX88
D	352	GLU	-	expression tag	UNP H7EX88
D	353	HIS	-	expression tag	UNP H7EX88
D	354	HIS	-	expression tag	UNP H7EX88
D	355	HIS	-	expression tag	UNP H7EX88
D	356	HIS	-	expression tag	UNP H7EX88
D	357	HIS	-	expression tag	UNP H7EX88
D	358	HIS	-	expression tag	UNP H7EX88
E	27	MET	-	initiating methionine	UNP H7EX88
E	28	ALA	-	expression tag	UNP H7EX88
E	29	MET	-	expression tag	UNP H7EX88
E	30	ASP	-	expression tag	UNP H7EX88
E	31	LEU	-	expression tag	UNP H7EX88
E	32	PHE	-	expression tag	UNP H7EX88
E	33	GLN	-	expression tag	UNP H7EX88
E	34	ASP	-	expression tag	UNP H7EX88
E	35	LYS	-	expression tag	UNP H7EX88
E	36	VAL	-	expression tag	UNP H7EX88
E	37	GLU	-	expression tag	UNP H7EX88
E	38	ALA	-	expression tag	UNP H7EX88
E	39	PHE	-	expression tag	UNP H7EX88
E	40	THR	-	expression tag	UNP H7EX88
E	41	GLY	-	expression tag	UNP H7EX88
E	42	PRO	-	expression tag	UNP H7EX88
E	43	THR	-	expression tag	UNP H7EX88
E	351	VAL	-	expression tag	UNP H7EX88
E	352	GLU	-	expression tag	UNP H7EX88
E	353	HIS	-	expression tag	UNP H7EX88
E	354	HIS	-	expression tag	UNP H7EX88
E	355	HIS	-	expression tag	UNP H7EX88
E	356	HIS	-	expression tag	UNP H7EX88
E	357	HIS	-	expression tag	UNP H7EX88
E	358	HIS	-	expression tag	UNP H7EX88
F	27	MET	-	initiating methionine	UNP H7EX88
F	28	ALA	-	expression tag	UNP H7EX88
F	29	MET	-	expression tag	UNP H7EX88
F	30	ASP	-	expression tag	UNP H7EX88
F	31	LEU	-	expression tag	UNP H7EX88
F	32	PHE	-	expression tag	UNP H7EX88

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Chain	Residue	Modelled	Actual	Comment	Reference
F	33	GLN	-	expression tag	UNP H7EX88
F	34	ASP	-	expression tag	UNP H7EX88
F	35	LYS	-	expression tag	UNP H7EX88
F	36	VAL	-	expression tag	UNP H7EX88
F	37	GLU	-	expression tag	UNP H7EX88
F	38	ALA	-	expression tag	UNP H7EX88
F	39	PHE	-	expression tag	UNP H7EX88
F	40	THR	-	expression tag	UNP H7EX88
F	41	GLY	-	expression tag	UNP H7EX88
F	42	PRO	-	expression tag	UNP H7EX88
F	43	THR	-	expression tag	UNP H7EX88
F	351	VAL	-	expression tag	UNP H7EX88
F	352	GLU	-	expression tag	UNP H7EX88
F	353	HIS	-	expression tag	UNP H7EX88
F	354	HIS	-	expression tag	UNP H7EX88
F	355	HIS	-	expression tag	UNP H7EX88
F	356	HIS	-	expression tag	UNP H7EX88
F	357	HIS	-	expression tag	UNP H7EX88
F	358	HIS	-	expression tag	UNP H7EX88

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is water.

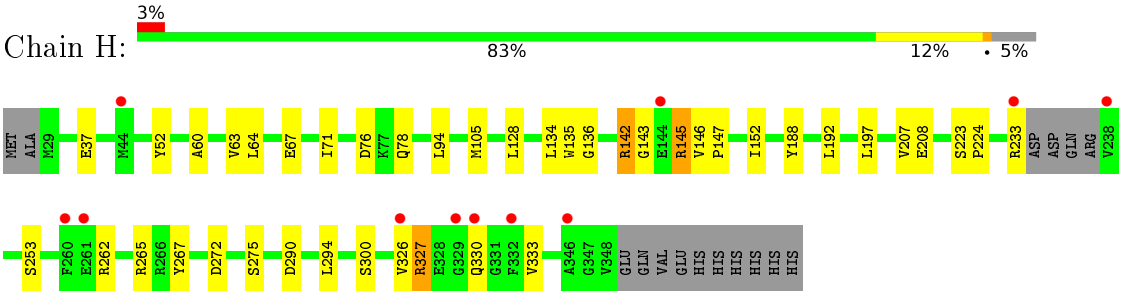
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	6	Total O 6 6	0	0
3	B	9	Total O 9 9	0	0
3	G	3	Total O 3 3	0	0
3	A	12	Total O 12 12	0	0
3	C	3	Total O 3 3	0	0
3	D	5	Total O 5 5	0	0
3	E	5	Total O 5 5	0	0
3	F	2	Total O 2 2	0	0

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.

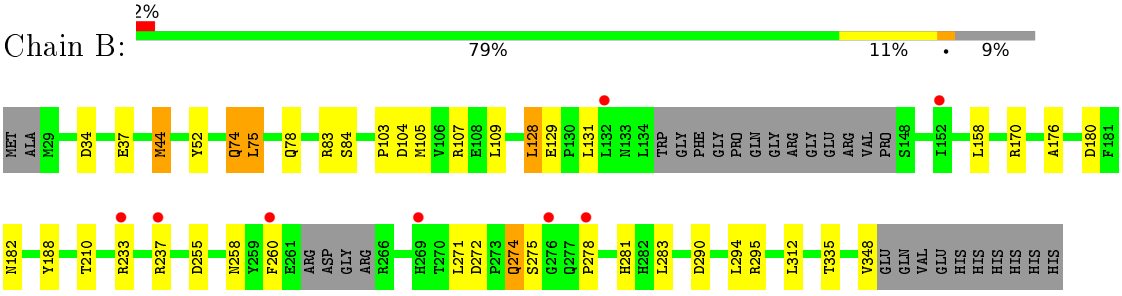
- Molecule 1: FAD:protein FMN transferase

Chain H:



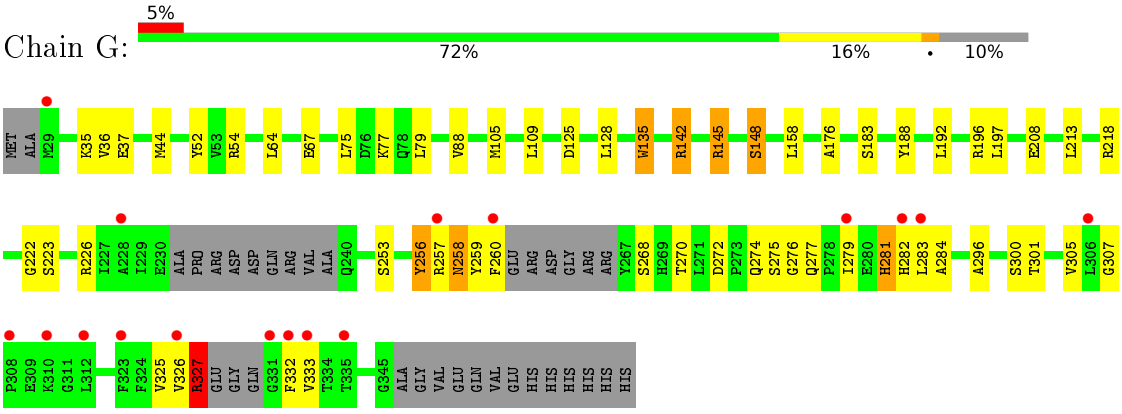
- Molecule 1: FAD:protein FMN transferase

Chain B:



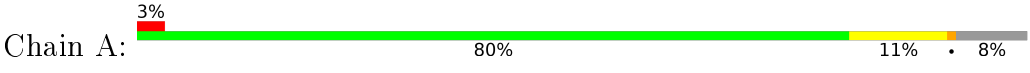
- Molecule 1: FAD:protein FMN transferase

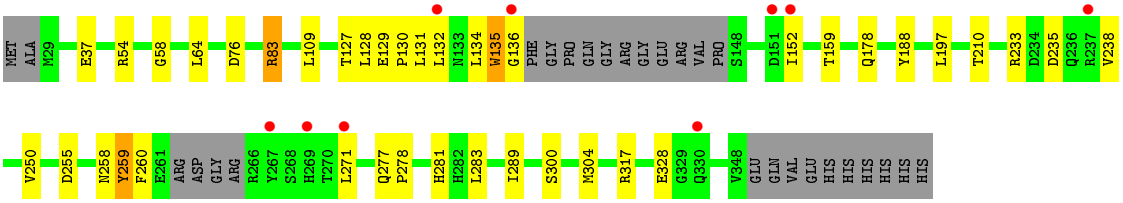
Chain G:



- Molecule 1: FAD:protein FMN transferase

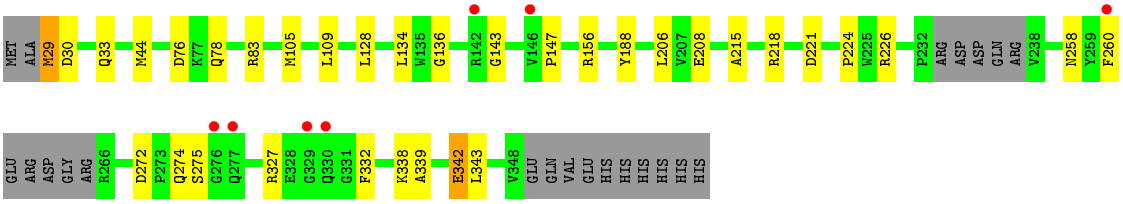
Chain A:





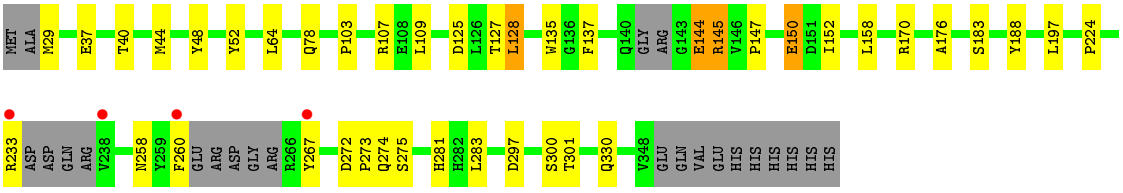
• Molecule 1: FAD:protein FMN transferase

Chain C:



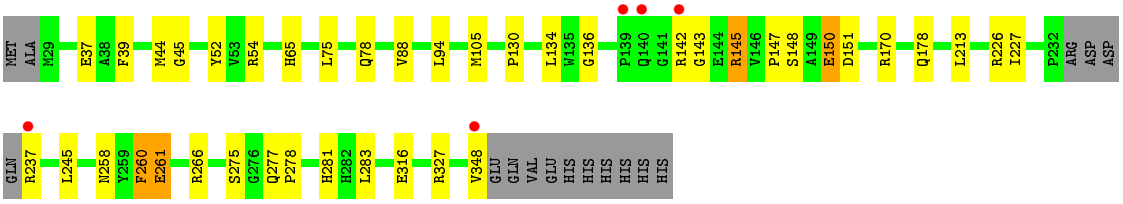
• Molecule 1: FAD:protein FMN transferase

Chain D:



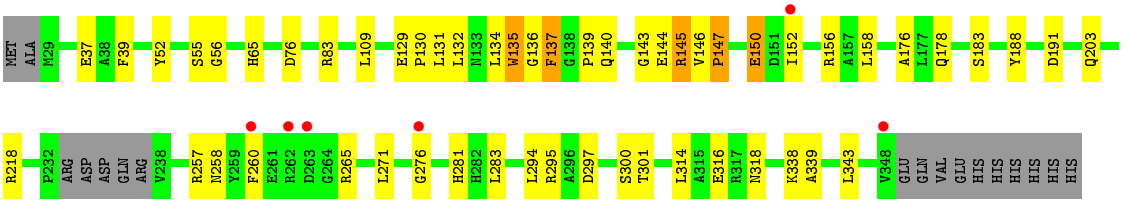
• Molecule 1: FAD:protein FMN transferase

Chain E:



• Molecule 1: FAD:protein FMN transferase

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	135.66Å 91.98Å 138.06Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	138.06 – 2.60 138.06 – 2.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (138.06-2.60) 100.0 (138.06-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.232 , 0.274 0.233 , 0.271	Depositor DCC
R_{free} test set	5134 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 21.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.000 for h,-k,-l 0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18725	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.34 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.7302e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.04	3/2343 (0.1%)	1.05	6/3171 (0.2%)
1	B	0.95	1/2323 (0.0%)	1.06	12/3143 (0.4%)
1	C	0.88	1/2374 (0.0%)	0.97	5/3214 (0.2%)
1	D	0.91	3/2369 (0.1%)	1.02	8/3206 (0.2%)
1	E	0.87	0/2429	1.04	10/3287 (0.3%)
1	F	0.92	2/2418 (0.1%)	1.10	10/3273 (0.3%)
1	G	1.04	3/2299 (0.1%)	1.08	11/3110 (0.4%)
1	H	0.92	1/2429 (0.0%)	1.05	11/3287 (0.3%)
All	All	0.94	14/18984 (0.1%)	1.05	73/25691 (0.3%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	281	HIS	C-N	24.09	1.89	1.34
1	A	259	TYR	C-N	18.56	1.76	1.34
1	D	150	GLU	CG-CD	8.63	1.64	1.51
1	C	342	GLU	CD-OE2	-7.88	1.17	1.25
1	B	74	GLN	CG-CD	-7.76	1.33	1.51

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	145	ARG	NE-CZ-NH2	-17.41	111.60	120.30
1	G	145	ARG	NE-CZ-NH1	-13.63	113.48	120.30
1	D	145	ARG	NE-CZ-NH2	11.78	126.19	120.30
1	F	146	VAL	C-N-CD	-10.91	96.59	120.60
1	H	76	ASP	CB-CG-OD2	10.39	127.65	118.30

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	2306	0	2261	31	1
1	B	2288	0	2250	26	1
1	C	2334	0	2295	19	0
1	D	2330	0	2292	21	0
1	E	2388	0	2349	30	0
1	F	2377	0	2336	53	0
1	G	2261	0	2220	61	0
1	H	2388	0	2349	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	0	1	0
3	B	9	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	6	0	0	0	0
All	All	18725	0	18352	248	1

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 7.

The worst 5 of 248 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:F:134:LEU:HD11	1:F:147:PRO:CB	1.27	1.54
1:A:259:TYR:C	1:A:260:PHE:N	1.76	1.38
1:F:134:LEU:CD1	1:F:147:PRO:CB	2.02	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:HIS:C	1:G:282:HIS:N	1.89	1.24
1:F:134:LEU:CD1	1:F:147:PRO:CG	2.20	1.18

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:SER:OG	1:A:328:GLU:OE1[2_646]	2.18	0.02

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	299/332 (90%)	283 (95%)	14 (5%)	2 (1%)	26	51
1	B	297/332 (90%)	279 (94%)	18 (6%)	0	100	100
1	C	304/332 (92%)	289 (95%)	14 (5%)	1 (0%)	46	72
1	D	301/332 (91%)	291 (97%)	9 (3%)	1 (0%)	46	72
1	E	312/332 (94%)	297 (95%)	15 (5%)	0	100	100
1	F	311/332 (94%)	298 (96%)	11 (4%)	2 (1%)	30	56
1	G	291/332 (88%)	275 (94%)	15 (5%)	1 (0%)	46	72
1	H	312/332 (94%)	301 (96%)	11 (4%)	0	100	100
All	All	2427/2656 (91%)	2313 (95%)	107 (4%)	7 (0%)	46	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	G	148	SER
1	F	276	GLY

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Mol	Chain	Res	Type
1	C	221	ASP
1	D	330	GLN

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	243/265 (92%)	241 (99%)	2 (1%)	86	95
1	B	242/265 (91%)	238 (98%)	4 (2%)	68	88
1	C	245/265 (92%)	243 (99%)	2 (1%)	86	95
1	D	245/265 (92%)	243 (99%)	2 (1%)	86	95
1	E	250/265 (94%)	243 (97%)	7 (3%)	51	78
1	F	249/265 (94%)	245 (98%)	4 (2%)	70	89
1	G	239/265 (90%)	235 (98%)	4 (2%)	68	88
1	H	250/265 (94%)	245 (98%)	5 (2%)	63	85
All	All	1963/2120 (93%)	1933 (98%)	30 (2%)	72	90

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	C	128	LEU
1	F	144	GLU
1	C	29	MET
1	D	128	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	HIS
1	D	65	HIS
1	F	281	HIS

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Mol	Chain	Res	Type
1	C	240	GLN
1	C	281	HIS

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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	281:HIS	C	282:HIS	N	1.89
1	A	259:TYR	C	260:PHE	N	1.76

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	305/332 (91%)	-0.19	9 (2%)	54	47	26, 48, 106, 146	0
1	B	303/332 (91%)	-0.21	8 (2%)	59	53	25, 44, 109, 143	0
1	C	310/332 (93%)	-0.21	7 (2%)	64	57	29, 54, 106, 141	0
1	D	309/332 (93%)	-0.22	4 (1%)	79	75	28, 49, 106, 144	0
1	E	316/332 (95%)	-0.17	5 (1%)	74	69	31, 53, 113, 145	0
1	F	315/332 (94%)	-0.17	6 (1%)	70	64	27, 52, 131, 170	0
1	G	299/332 (90%)	0.11	17 (5%)	27	20	29, 69, 116, 154	0
1	H	316/332 (95%)	-0.20	11 (3%)	48	40	26, 50, 107, 154	0
All	All	2473/2656 (93%)	-0.16	67 (2%)	58	51	25, 51, 113, 170	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	331	GLY	9.4
1	G	282	HIS	8.6
1	G	326	VAL	5.2
1	D	260	PHE	4.8
1	E	140	GLN	4.8

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 carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	MG	D	401	1/1	0.95	0.13	0.55	51,51,51,51	0
2	MG	F	401	1/1	0.82	0.07	-1.30	46,46,46,46	0
2	MG	H	401	1/1	0.83	0.11	-1.53	51,51,51,51	0
2	MG	B	401	1/1	0.92	0.11	-2.09	45,45,45,45	0
2	MG	G	401	1/1	0.94	0.08	-2.72	61,61,61,61	0
2	MG	A	401	1/1	0.97	0.08	-2.97	40,40,40,40	0
2	MG	E	401	1/1	0.95	0.11	-3.49	51,51,51,51	0
2	MG	C	401	1/1	0.99	0.05	-4.13	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.