



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:58 PM GMT

PDB ID : 4GTD  
Title : T. Maritima FDTS (E144R mutant) with FAD and dUMP  
Authors : Mathews, I.I.; Lesley, S.A.; Kohen, A.; Prabhakar, A.  
Deposited on : 2012-08-28  
Resolution : 1.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

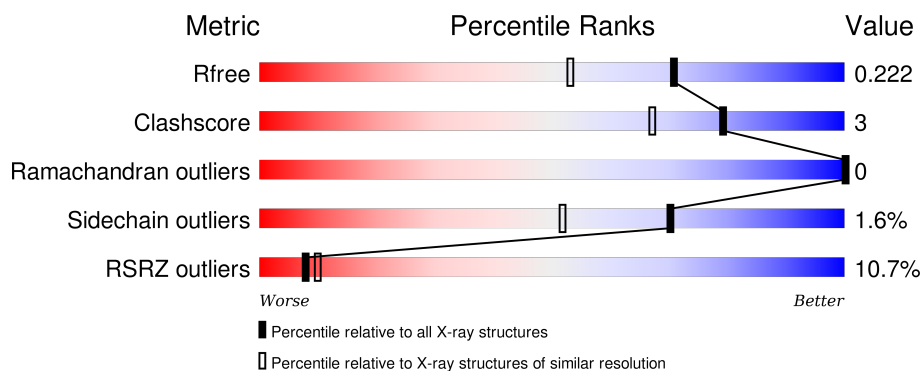
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	232	<div> <div>8%</div> <div>83% 7% 9%</div> </div>
1	B	232	<div> <div>12%</div> <div>78% 13% 8%</div> </div>
1	C	232	<div> <div>10%</div> <div>88% 6% 7%</div> </div>
1	D	232	<div> <div>10%</div> <div>85% 6% 9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FAD	B	302	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7841 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 Thymidylate synthase thyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	1	0
			1773	1154	306	307	6			
1	B	214	Total	C	N	O	S	0	0	0
			1801	1172	311	313	5			
1	C	216	Total	C	N	O	S	0	1	0
			1815	1181	311	317	6			
1	D	211	Total	C	N	O	S	0	2	0
			1785	1165	306	309	5			

There are 52 discrepancies between the modelled and reference sequences:

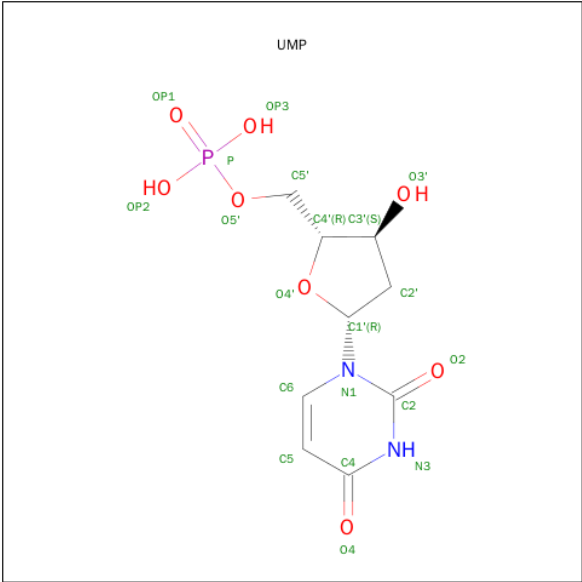
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q9WYT0
A	-10	GLY	-	EXPRESSION TAG	UNP Q9WYT0
A	-9	SER	-	EXPRESSION TAG	UNP Q9WYT0
A	-8	ASP	-	EXPRESSION TAG	UNP Q9WYT0
A	-7	LYS	-	EXPRESSION TAG	UNP Q9WYT0
A	-6	ILE	-	EXPRESSION TAG	UNP Q9WYT0
A	-5	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	-4	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	-3	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	144	ARG	GLU	ENGINEERED MUTATION	UNP Q9WYT0
B	-11	MET	-	EXPRESSION TAG	UNP Q9WYT0
B	-10	GLY	-	EXPRESSION TAG	UNP Q9WYT0
B	-9	SER	-	EXPRESSION TAG	UNP Q9WYT0
B	-8	ASP	-	EXPRESSION TAG	UNP Q9WYT0
B	-7	LYS	-	EXPRESSION TAG	UNP Q9WYT0
B	-6	ILE	-	EXPRESSION TAG	UNP Q9WYT0
B	-5	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	-4	HIS	-	EXPRESSION TAG	UNP Q9WYT0

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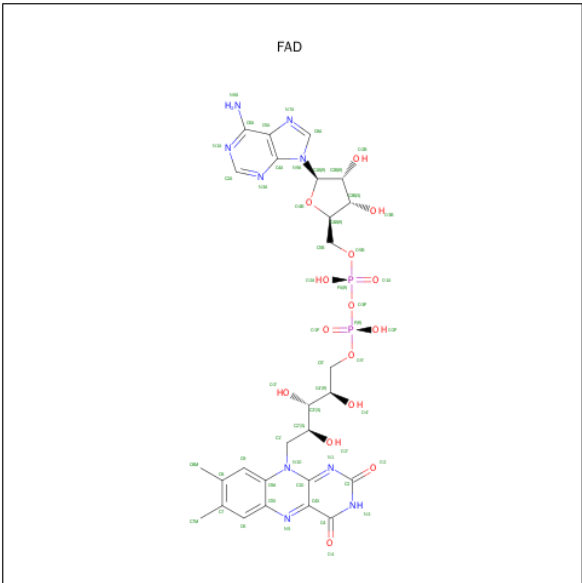
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	144	ARG	GLU	ENGINEERED MUTATION	UNP Q9WYT0
C	-11	MET	-	EXPRESSION TAG	UNP Q9WYT0
C	-10	GLY	-	EXPRESSION TAG	UNP Q9WYT0
C	-9	SER	-	EXPRESSION TAG	UNP Q9WYT0
C	-8	ASP	-	EXPRESSION TAG	UNP Q9WYT0
C	-7	LYS	-	EXPRESSION TAG	UNP Q9WYT0
C	-6	ILE	-	EXPRESSION TAG	UNP Q9WYT0
C	-5	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	-4	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	-3	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	144	ARG	GLU	ENGINEERED MUTATION	UNP Q9WYT0
D	-11	MET	-	EXPRESSION TAG	UNP Q9WYT0
D	-10	GLY	-	EXPRESSION TAG	UNP Q9WYT0
D	-9	SER	-	EXPRESSION TAG	UNP Q9WYT0
D	-8	ASP	-	EXPRESSION TAG	UNP Q9WYT0
D	-7	LYS	-	EXPRESSION TAG	UNP Q9WYT0
D	-6	ILE	-	EXPRESSION TAG	UNP Q9WYT0
D	-5	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	-4	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	-3	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	144	ARG	GLU	ENGINEERED MUTATION	UNP Q9WYT0

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula:  $C_9H_{13}N_2O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

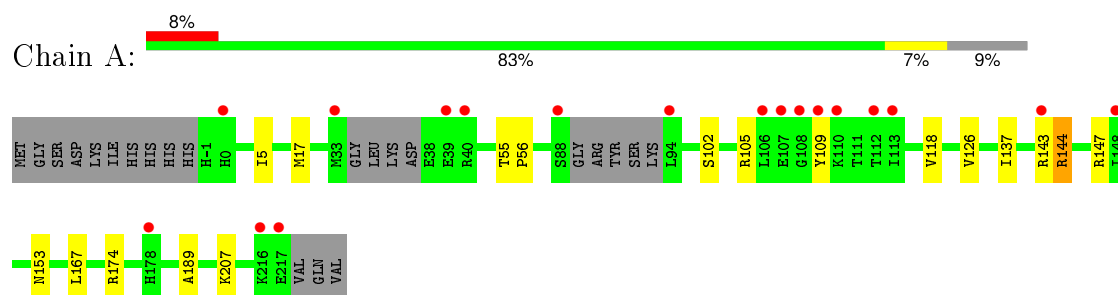
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	1
			101	101		
4	B	87	Total	O	0	0
			87	87		
4	C	105	Total	O	0	1
			106	106		
4	D	81	Total	O	0	0
			81	81		

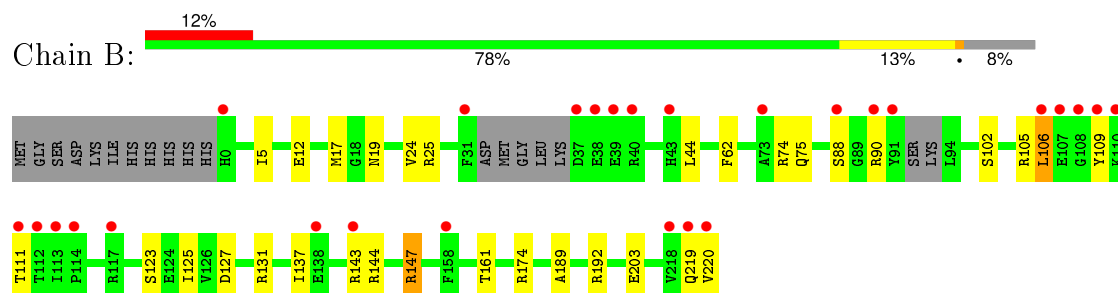
### 3 Residue-property plots [i](#)

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.

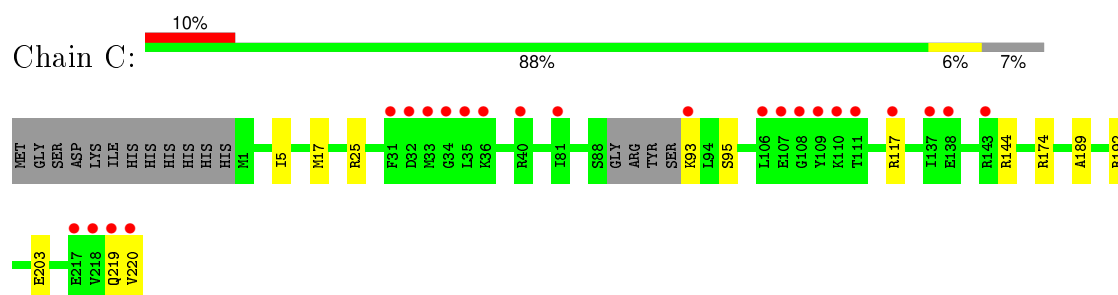
- Molecule 1: Thymidylate synthase thyX



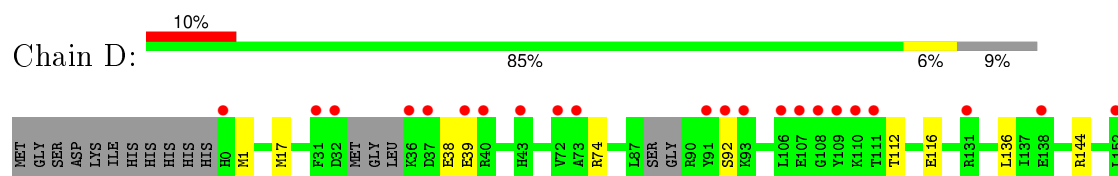
- Molecule 1: Thymidylate synthase thyX



- Molecule 1: Thymidylate synthase thyX



- Molecule 1: Thymidylate synthase thyX





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.59Å 117.39Å 142.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 1.76 29.35 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.35-1.76) 99.8 (29.35-1.76)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.179 , 0.215 0.189 , 0.222	Depositor DCC
$R_{free}$ test set	4590 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 91412 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7841	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UMP, 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	0.78	0/1825	0.81	1/2466 (0.0%)
1	B	0.78	1/1849 (0.1%)	0.78	1/2498 (0.0%)
1	C	0.84	0/1865	0.85	0/2519
1	D	0.76	1/1840 (0.1%)	0.76	0/2487
All	All	0.79	2/7379 (0.0%)	0.80	2/9970 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	GLU	CB-CG	-5.47	1.41	1.52
1	D	116	GLU	CD-OE1	5.19	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	192	ARG	NE-CZ-NH1	5.36	122.98	120.30

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	1773	0	1762	15	0
1	B	1801	0	1793	19	0
1	C	1815	0	1821	10	0
1	D	1785	0	1779	8	0
2	A	20	0	11	1	0
2	B	20	0	11	1	0
2	C	20	0	11	1	0
2	D	20	0	11	1	0
3	A	53	0	31	3	0
3	B	53	0	31	1	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	101	0	0	6	0
4	B	87	0	0	5	0
4	C	106	0	0	2	0
4	D	81	0	0	1	0
All	All	7841	0	7323	51	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.

All (51) 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)
2:B:301:UMP:HN3	1:C:174:ARG:HH12	1.10	0.97
1:B:174:ARG:HH12	2:C:302:UMP:HN3	1.18	0.88
2:A:301:UMP:HN3	1:D:174:ARG:HH12	1.23	0.86
1:C:219:GLN:O	1:C:220:VAL:HG22	1.79	0.82
1:A:174:ARG:HH12	2:D:302:UMP:HN3	1.24	0.82
1:A:17:MET:HB2	1:B:17:MET:HB2	1.60	0.81
3:A:302:FAD:HM82	4:A:484:HOH:O	1.83	0.76
1:C:17:MET:HB2	1:D:17:MET:HB2	1.70	0.71
1:B:74:ARG:NH1	4:B:426:HOH:O	2.23	0.71
1:D:167[B]:LEU:HD11	1:D:190:ILE:CG2	2.22	0.70
1:A:137:ILE:HD12	1:A:143:ARG:HG2	1.78	0.66
3:B:302:FAD:H5'1	4:B:474:HOH:O	1.96	0.65
1:B:147:ARG:NH1	4:B:470:HOH:O	2.29	0.63
1:B:219:GLN:O	1:B:220:VAL:HG22	1.98	0.63
3:A:302:FAD:H51A	4:A:485:HOH:O	2.03	0.58
1:C:203:GLU:HG2	4:C:490:HOH:O	2.05	0.57
1:A:207:LYS:HE2	4:A:466:HOH:O	2.06	0.54
1:B:105:ARG:HG3	1:B:106:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.89	0.54
1:C:192:ARG:NH2	1:C:220:VAL:HG23	2.23	0.53
1:D:1:MET:HE1	1:D:196:GLU:HG2	1.89	0.53
1:B:203:GLU:CD	4:B:431:HOH:O	2.47	0.53
1:D:167[B]:LEU:HD11	1:D:190:ILE:HG21	1.89	0.53
1:A:126:VAL:HG21	1:A:153:ASN:HD21	1.75	0.51
1:C:219:GLN:O	1:C:220:VAL:CG2	2.56	0.49
1:A:167:LEU:HD23	1:A:167:LEU:C	2.33	0.49
1:B:88:SER:OG	1:B:90:ARG:NH2	2.47	0.48
1:A:144:ARG:HG2	4:A:420:HOH:O	2.12	0.48
1:C:25:ARG:HD2	4:C:440:HOH:O	2.13	0.47
1:B:127:ASP:O	1:B:131:ARG:HG3	2.15	0.47
1:A:102:SER:O	1:A:105:ARG:HB3	2.15	0.46
1:A:137:ILE:HD11	1:A:143:ARG:HA	1.98	0.45
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.98	0.45
3:A:302:FAD:C5B	4:A:485:HOH:O	2.63	0.44
1:A:137:ILE:CD1	1:A:143:ARG:HG2	2.46	0.44
1:B:137:ILE:HD12	1:B:143:ARG:HG3	2.00	0.44
1:C:219:GLN:C	1:C:220:VAL:HG22	2.36	0.44
1:B:24:VAL:HG13	1:B:44:LEU:HD23	2.00	0.44
1:B:75:GLN:NE2	1:C:144:ARG:NH2	2.66	0.43
1:B:109:TYR:O	1:B:111:THR:HG23	2.19	0.43
1:B:62:PHE:O	1:B:161:THR:HA	2.19	0.43
1:A:118:VAL:HG13	1:D:136:LEU:HD22	2.00	0.42
1:A:207:LYS:CE	4:A:466:HOH:O	2.67	0.42
1:D:74:ARG:NH1	4:D:443:HOH:O	2.52	0.41
1:A:109:TYR:OH	1:D:144:ARG:NH2	2.53	0.41
1:B:125:ILE:HA	1:B:125:ILE:HD12	1.89	0.41
1:B:144:ARG:HA	1:B:147:ARG:CG	2.51	0.41
1:C:5:ILE:HD11	1:C:189:ALA:HB2	2.02	0.41
1:A:55:THR:OG1	1:A:56:PRO:HD3	2.21	0.41
1:B:19:ASN:HB2	4:B:409:HOH:O	2.21	0.40
1:B:102:SER:O	1:B:106:LEU:HD22	2.21	0.40

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	205/232 (88%)	199 (97%)	6 (3%)	0	100	100
1	B	208/232 (90%)	200 (96%)	8 (4%)	0	100	100
1	C	213/232 (92%)	207 (97%)	6 (3%)	0	100	100
1	D	207/232 (89%)	202 (98%)	5 (2%)	0	100	100
All	All	833/928 (90%)	808 (97%)	25 (3%)	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	189/207 (91%)	188 (100%)	1 (0%)	92	87
1	B	191/207 (92%)	187 (98%)	4 (2%)	61	37
1	C	194/207 (94%)	191 (98%)	3 (2%)	72	55
1	D	190/207 (92%)	186 (98%)	4 (2%)	61	37
All	All	764/828 (92%)	752 (98%)	12 (2%)	70	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	B	25	ARG

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Mol	Chain	Res	Type
1	B	106	LEU
1	B	123	SER
1	B	147	ARG
1	C	93	LYS
1	C	95	SER
1	C	117	ARG
1	D	38	GLU
1	D	39	GLU
1	D	92	SER
1	D	112	THR

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 ⓘ

8 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	UMP	A	301	-	16,21,21	0.72	0	23,31,31	2.12	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	A	302	-	48,58,58	2.80	13 (27%)	54,89,89	2.47	13 (24%)
2	UMP	B	301	-	16,21,21	0.95	0	23,31,31	2.81	5 (21%)
3	FAD	B	302	-	48,58,58	2.82	14 (29%)	54,89,89	2.53	12 (22%)
3	FAD	C	301	-	48,58,58	2.72	15 (31%)	54,89,89	2.34	12 (22%)
2	UMP	C	302	-	16,21,21	0.81	0	23,31,31	2.26	3 (13%)
3	FAD	D	301	-	48,58,58	2.81	14 (29%)	54,89,89	2.45	13 (24%)
2	UMP	D	302	-	16,21,21	0.67	0	23,31,31	2.00	4 (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	UMP	A	301	-	-	0/6/22/22	0/2/2/2
3	FAD	A	302	-	-	0/30/50/50	0/6/6/6
2	UMP	B	301	-	-	0/6/22/22	0/2/2/2
3	FAD	B	302	-	-	0/30/50/50	0/6/6/6
3	FAD	C	301	-	-	0/30/50/50	0/6/6/6
2	UMP	C	302	-	-	0/6/22/22	0/2/2/2
3	FAD	D	301	-	-	0/30/50/50	0/6/6/6
2	UMP	D	302	-	-	0/6/22/22	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	FAD	C9A-N10	-6.16	1.30	1.38
3	A	302	FAD	C9A-N10	-5.78	1.30	1.38
3	D	301	FAD	C9A-N10	-5.51	1.31	1.38
3	B	302	FAD	C9A-N10	-5.35	1.31	1.38
3	C	301	FAD	C1'-N10	-2.64	1.45	1.48
3	B	302	FAD	C4A-N3A	2.13	1.38	1.35
3	D	301	FAD	O4B-C1B	2.22	1.44	1.41
3	C	301	FAD	O4B-C1B	2.77	1.44	1.41
3	C	301	FAD	C4-C4X	3.00	1.47	1.41
3	A	302	FAD	C4-C4X	3.13	1.47	1.41
3	B	302	FAD	C5A-C4A	3.23	1.47	1.40
3	A	302	FAD	C5A-C4A	3.26	1.47	1.40
3	C	301	FAD	C9-C9A	3.32	1.48	1.40
3	A	302	FAD	C8-C7	3.35	1.50	1.41
3	C	301	FAD	C8-C7	3.48	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	FAD	C4-C4X	3.49	1.48	1.41
3	B	302	FAD	C8-C7	3.66	1.50	1.41
3	A	302	FAD	C9-C9A	3.73	1.48	1.40
3	C	301	FAD	C5A-C4A	3.77	1.49	1.40
3	D	301	FAD	C5A-C4A	3.79	1.49	1.40
3	B	302	FAD	C9-C9A	3.87	1.49	1.40
3	D	301	FAD	C8-C7	3.99	1.51	1.41
3	C	301	FAD	C9A-C5X	4.02	1.50	1.42
3	D	301	FAD	C4-C4X	4.05	1.49	1.41
3	D	301	FAD	C9-C9A	4.18	1.49	1.40
3	C	301	FAD	C4X-C10	4.45	1.49	1.41
3	A	302	FAD	C9A-C5X	4.47	1.51	1.42
3	A	302	FAD	C4X-C10	4.55	1.49	1.41
3	B	302	FAD	C9A-C5X	4.89	1.52	1.42
3	A	302	FAD	C6-C7	4.91	1.51	1.37
3	B	302	FAD	C6-C7	4.95	1.51	1.37
3	D	301	FAD	C9A-C5X	4.96	1.52	1.42
3	B	302	FAD	C4X-C10	5.02	1.50	1.41
3	D	301	FAD	C6-C7	5.03	1.51	1.37
3	C	301	FAD	C4X-N5	5.14	1.41	1.33
3	C	301	FAD	C6-C7	5.16	1.52	1.37
3	A	302	FAD	C10-N1	5.21	1.44	1.35
3	C	301	FAD	C10-N10	5.26	1.45	1.39
3	C	301	FAD	C5X-N5	5.40	1.44	1.35
3	D	301	FAD	C10-N10	5.40	1.45	1.39
3	D	301	FAD	C4X-C10	5.44	1.51	1.41
3	D	301	FAD	C5X-N5	5.52	1.44	1.35
3	B	302	FAD	C10-N10	5.55	1.45	1.39
3	D	301	FAD	C10-N1	5.60	1.44	1.35
3	B	302	FAD	C5X-N5	5.74	1.44	1.35
3	A	302	FAD	C10-N10	6.30	1.46	1.39
3	B	302	FAD	C10-N1	6.33	1.46	1.35
3	D	301	FAD	C6-C5X	6.50	1.51	1.41
3	A	302	FAD	C5X-N5	6.53	1.45	1.35
3	D	301	FAD	C4X-N5	6.61	1.43	1.33
3	A	302	FAD	C4X-N5	6.62	1.43	1.33
3	C	301	FAD	C10-N1	6.66	1.46	1.35
3	C	301	FAD	C6-C5X	6.71	1.51	1.41
3	B	302	FAD	C4X-N5	6.87	1.44	1.33
3	B	302	FAD	C6-C5X	7.14	1.52	1.41
3	A	302	FAD	C6-C5X	7.48	1.53	1.41

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	FAD	N3A-C2A-N1A	-10.91	120.54	128.89
3	A	302	FAD	N3A-C2A-N1A	-10.83	120.60	128.89
3	C	301	FAD	N3A-C2A-N1A	-7.64	123.05	128.89
3	D	301	FAD	N3A-C2A-N1A	-7.58	123.09	128.89
3	D	301	FAD	C4-C4X-C10	-5.95	116.13	119.94
3	A	302	FAD	C4-C4X-C10	-4.80	116.87	119.94
3	B	302	FAD	C4-C4X-C10	-4.57	117.02	119.94
3	D	301	FAD	C4X-C4-N3	-3.96	118.18	123.59
3	B	302	FAD	C1B-N9A-C4A	-3.92	121.03	126.94
3	C	301	FAD	C4X-C4-N3	-3.91	118.24	123.59
3	B	302	FAD	C4X-C4-N3	-3.65	118.60	123.59
3	C	301	FAD	C4-C4X-C10	-3.63	117.62	119.94
2	B	301	UMP	C2'-C1'-N1	-3.26	106.23	114.16
2	C	302	UMP	O5'-P-OP1	-3.07	99.33	107.14
3	A	302	FAD	C4X-C4-N3	-3.02	119.46	123.59
3	A	302	FAD	P-O3P-PA	-2.98	124.35	132.73
3	A	302	FAD	C4A-C5A-N7A	-2.92	106.79	109.48
2	A	301	UMP	C2'-C1'-N1	-2.79	107.37	114.16
2	B	301	UMP	C5-C4-N3	-2.79	115.97	123.12
3	B	302	FAD	C7-C6-C5X	-2.75	116.42	120.92
3	D	301	FAD	C6-C5X-N5	-2.66	115.55	118.96
2	D	302	UMP	C2'-C1'-N1	-2.46	108.17	114.16
3	D	301	FAD	C7-C6-C5X	-2.28	117.20	120.92
3	C	301	FAD	C4X-C10-N10	-2.27	119.18	120.52
3	C	301	FAD	C4A-C5A-N7A	-2.26	107.40	109.48
3	A	302	FAD	C1B-N9A-C4A	-2.23	123.58	126.94
2	D	302	UMP	OP3-P-O5'	-2.10	100.51	106.56
2	A	301	UMP	OP2-P-O5'	-2.04	100.70	106.56
3	D	301	FAD	C9-C9A-C5X	-2.02	116.04	119.62
3	B	302	FAD	C6-C5X-N5	-2.01	116.37	118.96
2	A	301	UMP	C2'-C3'-C4'	2.12	107.16	102.77
3	D	301	FAD	O2A-PA-O1A	2.23	124.64	112.53
3	C	301	FAD	C4-C4X-N5	2.25	121.45	118.72
3	D	301	FAD	C6-C5X-C9A	2.29	121.99	118.98
2	A	301	UMP	OP3-P-OP2	2.38	116.45	107.38
3	A	302	FAD	C2B-C1B-N9A	2.41	117.98	114.29
2	B	301	UMP	OP3-P-OP2	2.49	116.88	107.38
2	D	302	UMP	OP3-P-OP1	2.51	118.66	110.58
3	B	302	FAD	O2A-PA-O1A	2.52	126.20	112.53
3	C	301	FAD	O2A-PA-O1A	2.59	126.57	112.53
3	D	301	FAD	C2A-N1A-C6A	2.61	123.43	118.77
3	C	301	FAD	C2A-N1A-C6A	2.63	123.46	118.77
2	C	302	UMP	OP3-P-OP1	2.68	119.20	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	FAD	O2A-PA-O1A	2.84	127.93	112.53
3	C	301	FAD	C2B-C1B-N9A	2.94	118.78	114.29
3	B	302	FAD	C2A-N1A-C6A	3.10	124.31	118.77
3	A	302	FAD	C2A-N1A-C6A	3.17	124.43	118.77
3	B	302	FAD	C4-C4X-N5	3.46	122.92	118.72
2	B	301	UMP	OP3-P-OP1	3.48	121.79	110.58
3	A	302	FAD	C4-C4X-N5	3.79	123.32	118.72
3	A	302	FAD	C5X-C9A-N10	3.92	120.59	117.62
3	B	302	FAD	C5X-C9A-N10	3.98	120.64	117.62
3	C	301	FAD	C1'-N10-C9A	4.12	123.48	118.86
3	B	302	FAD	C1'-N10-C9A	4.12	123.49	118.86
3	D	301	FAD	C4-C4X-N5	4.25	123.88	118.72
3	D	301	FAD	C5X-C9A-N10	4.40	120.97	117.62
3	C	301	FAD	C5X-C9A-N10	4.52	121.05	117.62
3	A	302	FAD	C1'-N10-C9A	4.79	124.24	118.86
3	D	301	FAD	C1'-N10-C9A	5.70	125.26	118.86
3	A	302	FAD	C4-N3-C2	7.18	121.45	115.25
2	D	302	UMP	C4-N3-C2	8.08	122.14	114.14
2	A	301	UMP	C4-N3-C2	8.42	122.48	114.14
3	B	302	FAD	C4-N3-C2	8.77	122.83	115.25
3	D	301	FAD	C4-N3-C2	8.94	122.98	115.25
2	C	302	UMP	C4-N3-C2	8.97	123.03	114.14
3	C	301	FAD	C4-N3-C2	9.72	123.64	115.25
2	B	301	UMP	C4-N3-C2	10.93	124.97	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	UMP	1	0
3	A	302	FAD	3	0
2	B	301	UMP	1	0
3	B	302	FAD	1	0
2	C	302	UMP	1	0
2	D	302	UMP	1	0

## 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	210/232 (90%)	0.46	18 (8%) 13 16	20, 33, 65, 93	0
1	B	214/232 (92%)	0.69	27 (12%) 5 7	22, 37, 75, 101	0
1	C	216/232 (93%)	0.57	23 (10%) 8 10	21, 33, 71, 101	0
1	D	211/232 (90%)	0.65	23 (10%) 7 9	22, 38, 71, 97	0
All	All	851/928 (91%)	0.59	91 (10%) 8 10	20, 36, 72, 101	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	TYR	8.2
1	C	35	LEU	8.1
1	C	33	MET	7.5
1	A	33	MET	7.2
1	A	110	LYS	6.8
1	D	0	HIS	5.9
1	B	109	TYR	5.6
1	B	110	LYS	5.5
1	A	108	GLY	5.4
1	D	36	LYS	5.4
1	C	108	GLY	5.3
1	C	109	TYR	5.3
1	B	112	THR	5.0
1	D	108	GLY	4.6
1	C	138	GLU	4.5
1	B	91	TYR	4.5
1	D	40	ARG	4.4
1	B	108	GLY	4.4
1	C	31	PHE	4.4
1	A	94	LEU	4.3
1	B	31	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	217	GLU	4.2
1	A	109	TYR	4.1
1	B	38	GLU	4.1
1	D	107	GLU	4.1
1	C	106	LEU	4.0
1	A	112	THR	3.9
1	C	220	VAL	3.8
1	D	39	GLU	3.8
1	C	34	GLY	3.7
1	C	219	GLN	3.7
1	C	218	VAL	3.5
1	B	143	ARG	3.5
1	D	92	SER	3.5
1	B	90	ARG	3.5
1	B	107	GLU	3.3
1	D	32	ASP	3.3
1	B	40	ARG	3.3
1	D	106	LEU	3.2
1	A	40	ARG	3.2
1	B	220	VAL	3.1
1	D	93	LYS	3.1
1	B	0	HIS	3.1
1	A	88	SER	3.1
1	A	143	ARG	3.1
1	A	106	LEU	3.0
1	B	114	PRO	3.0
1	C	107	GLU	3.0
1	A	107	GLU	2.9
1	B	111	THR	2.9
1	C	40	ARG	2.9
1	B	117	ARG	2.9
1	C	137	ILE	2.9
1	B	219	GLN	2.8
1	D	111	THR	2.8
1	B	158	PHE	2.7
1	A	39	GLU	2.7
1	D	110	LYS	2.7
1	A	216	LYS	2.7
1	C	111	THR	2.6
1	D	138	GLU	2.6
1	D	43	HIS	2.6
1	C	93	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	106	LEU	2.5
1	B	37	ASP	2.4
1	C	36	LYS	2.4
1	A	148	ILE	2.4
1	B	218	VAL	2.4
1	B	138	GLU	2.3
1	C	110	LYS	2.3
1	D	31	PHE	2.3
1	B	88	SER	2.3
1	C	143	ARG	2.3
1	D	73	ALA	2.2
1	D	154	LEU	2.2
1	D	91	TYR	2.2
1	B	39	GLU	2.2
1	C	217	GLU	2.2
1	D	152	LEU	2.2
1	B	113	ILE	2.2
1	A	0	HIS	2.2
1	C	117	ARG	2.2
1	A	113	ILE	2.2
1	B	43	HIS	2.2
1	B	73	ALA	2.2
1	A	178	HIS	2.2
1	D	37	ASP	2.1
1	C	81	ILE	2.1
1	C	32	ASP	2.1
1	D	72	VAL	2.1
1	D	131	ARG	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	FAD	B	302	53/53	0.90	0.16	2.45	28,38,42,46	0
2	UMP	C	302	20/20	0.91	0.18	1.54	33,38,43,44	0
2	UMP	D	302	20/20	0.89	0.17	1.36	37,41,45,46	0
3	FAD	D	301	53/53	0.90	0.16	1.18	26,40,46,48	0
3	FAD	A	302	53/53	0.89	0.16	0.92	27,40,46,48	0
2	UMP	A	301	20/20	0.92	0.15	0.33	36,38,40,40	0
2	UMP	B	301	20/20	0.92	0.13	-0.28	30,35,40,40	0
3	FAD	C	301	53/53	0.92	0.12	-0.32	25,35,40,42	0

## 6.5 Other polymers

There are no such residues in this entry.