



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:58 PM GMT

PDB ID : 4GTC
Title : T. Maritima FDTS (E144R mutant) plus FAD
Authors : Mathews, I.I.; Lesley, S.A.; Kohen, A.; Prabhakar, A.
Deposited on : 2012-08-28
Resolution : 1.97 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
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 (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

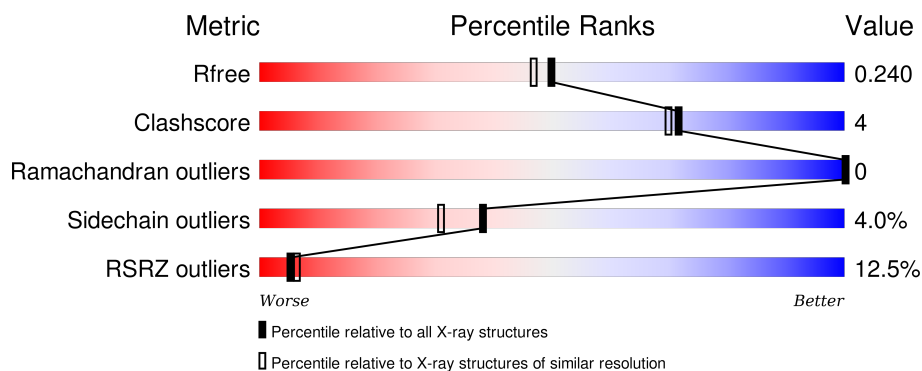
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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 $\leq 5\%$. 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>11%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	232	<div> <div>12%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>9%</div> </div> </div>
1	C	232	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
1	D	232	<div> <div>13%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </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
2	FAD	B	301	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7721 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	218	Total	C	N	O	S	0	0	0
			1832	1189	319	318	6			
1	B	212	Total	C	N	O	S	0	0	0
			1778	1156	306	311	5			
1	C	219	Total	C	N	O	S	0	0	0
			1840	1197	318	320	5			
1	D	216	Total	C	N	O	S	0	0	0
			1811	1178	312	316	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 FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

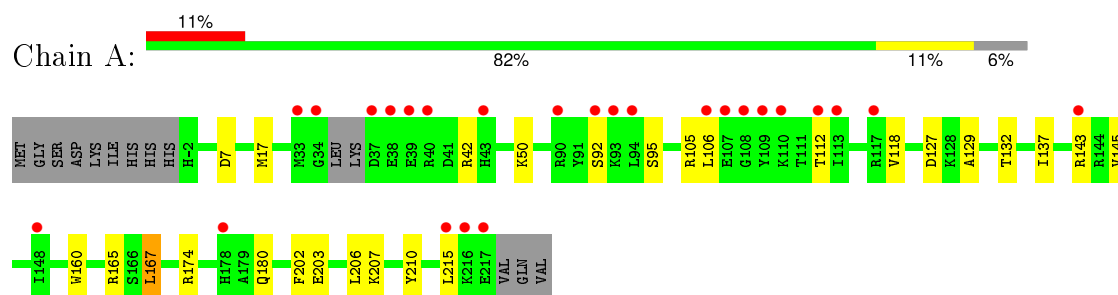
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total	O	0	0
			80	80		
3	B	58	Total	O	0	0
			58	58		
3	C	72	Total	O	0	1
			73	73		
3	D	55	Total	O	0	0
			55	55		

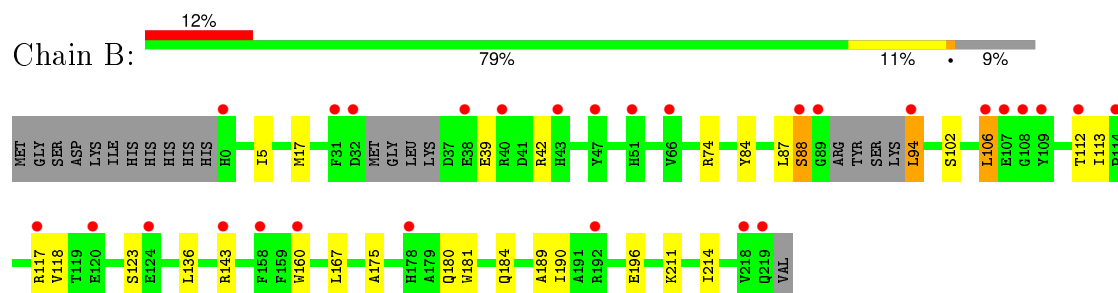
3 Residue-property plots [i](#)

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.

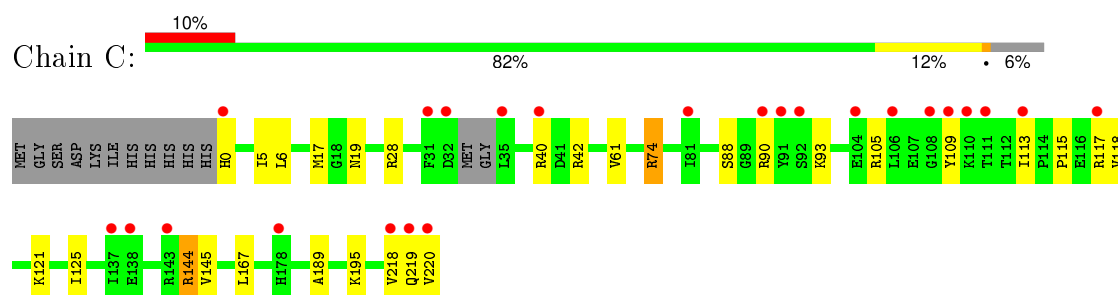
- Molecule 1: Thymidylate synthase thyX



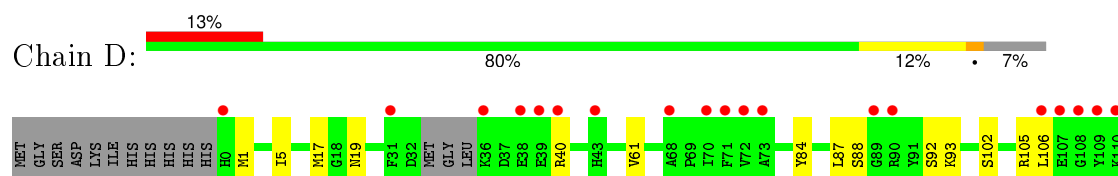
- Molecule 1: Thymidylate synthase thyX

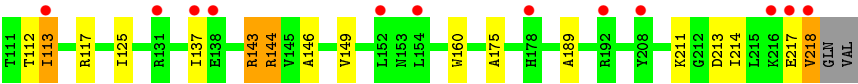


- Molecule 1: Thymidylate synthase thyX



- 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, α , β , γ	54.13Å 117.06Å 142.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.26 – 1.97 29.26 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.26-1.97) 98.7 (29.26-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.193 , 0.236 0.198 , 0.240	Depositor DCC
R_{free} test set	3279 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 63875 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7721	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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, 0.375 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: 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	0.81	1/1883 (0.1%)	0.82	2/2544 (0.1%)
1	B	0.74	0/1825	0.79	0/2467
1	C	0.79	0/1889	0.82	2/2553 (0.1%)
1	D	0.78	0/1859	0.77	0/2512
All	All	0.78	1/7456 (0.0%)	0.80	4/10076 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TRP	CB-CG	-5.29	1.40	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	C	74	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	7	ASP	CB-CG-OD1	5.55	123.30	118.30
1	C	74	ARG	NE-CZ-NH1	5.34	122.97	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	1832	0	1816	15	0
1	B	1778	0	1766	21	0
1	C	1840	0	1840	23	0
1	D	1811	0	1807	17	0
2	A	35	0	20	2	0
2	B	53	0	31	0	0
2	C	53	0	31	2	0
2	D	53	0	31	0	0
3	A	80	0	0	2	0
3	B	58	0	0	1	0
3	C	73	0	0	3	0
3	D	55	0	0	1	0
All	All	7721	0	7342	64	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 4.

All (64) 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:C:17:MET:HB2	1:D:17:MET:HB2	1.64	0.80
1:C:113:ILE:HD13	1:C:121:LYS:HZ1	1.53	0.71
1:C:113:ILE:HD13	1:C:121:LYS:NZ	2.06	0.70
1:C:219:GLN:O	1:C:220:VAL:HG22	1.98	0.64
1:C:113:ILE:CD1	1:C:121:LYS:HZ1	2.12	0.63
2:A:301:FAD:H51A	3:A:471:HOH:O	1.99	0.63
1:C:5:ILE:HD11	1:C:189:ALA:HB2	1.84	0.59
1:B:87:LEU:HD23	1:B:94:LEU:HD12	1.84	0.59
1:C:195:LYS:NZ	3:C:471:HOH:O	2.35	0.57
1:B:180:GLN:HG3	1:C:144:ARG:HH11	1.70	0.56
1:C:74:ARG:HD3	3:C:408:HOH:O	2.05	0.56
1:D:102:SER:O	1:D:105:ARG:HB3	2.06	0.56
1:C:167:LEU:HD23	1:C:167:LEU:C	2.26	0.55
1:B:102:SER:O	1:B:106:LEU:HD22	2.06	0.54
1:A:202:PHE:CE2	1:A:206:LEU:HD11	2.44	0.53
1:C:218:VAL:O	1:C:218:VAL:HG12	2.08	0.53
1:A:17:MET:HB2	1:B:17:MET:HB2	1.93	0.51
1:C:19:ASN:HB2	3:C:427:HOH:O	2.09	0.51
1:A:137:ILE:HD11	1:A:143:ARG:HA	1.93	0.51
1:C:167:LEU:O	1:C:167:LEU:HD23	2.10	0.51
1:B:143:ARG:HB2	1:B:143:ARG:CZ	2.42	0.50
1:A:129:ALA:HA	1:D:125:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ASN:HB2	3:D:427:HOH:O	2.11	0.49
1:D:137:ILE:HD11	1:D:143:ARG:HA	1.94	0.49
1:B:180:GLN:HG3	1:C:144:ARG:HD3	1.94	0.48
1:D:87:LEU:HD11	1:D:92:SER:OG	2.13	0.48
1:A:180:GLN:HG3	1:D:144:ARG:HE	1.79	0.48
1:A:132:THR:OG1	1:D:125:ILE:HD11	2.14	0.47
1:B:84:TYR:CE2	1:B:160:TRP:CD1	3.02	0.47
1:B:88:SER:HB2	2:C:301:FAD:O4	2.14	0.47
1:D:5:ILE:HD11	1:D:189:ALA:HB2	1.96	0.47
1:B:87:LEU:CD2	1:B:94:LEU:HD12	2.44	0.47
1:B:5:ILE:HD11	1:B:189:ALA:CB	2.44	0.47
1:A:50:LYS:NZ	3:A:476:HOH:O	2.48	0.47
1:A:165:ARG:NH2	2:C:301:FAD:O3B	2.47	0.47
1:A:203:GLU:O	1:A:207:LYS:HG3	2.13	0.47
1:D:217:GLU:O	1:D:218:VAL:C	2.54	0.46
1:B:167:LEU:HD11	1:B:190:ILE:CG2	2.45	0.46
1:A:174:ARG:NH2	2:A:301:FAD:O3'	2.49	0.45
1:C:5:ILE:HG22	1:C:6:LEU:HG	1.98	0.45
1:D:113:ILE:HG23	1:D:117:ARG:HB3	1.98	0.45
1:A:145:VAL:HG11	1:D:106:LEU:HD11	1.99	0.45
1:B:112:THR:HG22	1:B:112:THR:O	2.17	0.45
1:A:112:THR:HG22	1:A:112:THR:O	2.16	0.45
1:A:167:LEU:HD23	1:A:167:LEU:C	2.38	0.45
1:B:175:ALA:HA	1:B:214:ILE:HD11	1.99	0.44
1:A:106:LEU:HD13	1:A:118:VAL:CG1	2.48	0.44
1:D:175:ALA:HA	1:D:214:ILE:HD11	2.01	0.43
1:D:146:ALA:O	1:D:149:VAL:HG22	2.18	0.43
1:B:181:TRP:H	1:C:144:ARG:HH12	1.66	0.43
1:B:167:LEU:HD11	1:B:190:ILE:HG21	2.00	0.43
1:B:74:ARG:CD	1:C:74:ARG:HG2	2.49	0.42
1:B:42:ARG:NH2	3:B:458:HOH:O	2.52	0.42
1:D:112:THR:HG22	1:D:112:THR:O	2.20	0.42
1:C:28:ARG:NH2	1:C:40:ARG:HD3	2.35	0.42
1:C:125:ILE:HD12	1:C:125:ILE:HA	1.92	0.41
1:B:106:LEU:HD11	1:C:145:VAL:HG11	2.02	0.41
1:C:105:ARG:NH1	1:C:109:TYR:OH	2.46	0.41
1:B:181:TRP:O	1:B:184:GLN:HB2	2.21	0.41
1:B:113:ILE:CD1	1:B:118:VAL:HG23	2.51	0.41
1:C:61:VAL:HG11	1:D:61:VAL:HG21	2.03	0.41
1:A:210:TYR:CE1	1:A:215:LEU:HD12	2.55	0.41
1:D:84:TYR:CE2	1:D:160:TRP:CD1	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HD22	1:C:118:VAL:HG13	2.04	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	214/232 (92%)	204 (95%)	10 (5%)	0	100	100
1	B	206/232 (89%)	198 (96%)	8 (4%)	0	100	100
1	C	215/232 (93%)	209 (97%)	6 (3%)	0	100	100
1	D	212/232 (91%)	203 (96%)	9 (4%)	0	100	100
All	All	847/928 (91%)	814 (96%)	33 (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	194/207 (94%)	189 (97%)	5 (3%)	54	51
1	B	189/207 (91%)	181 (96%)	8 (4%)	36	29
1	C	196/207 (95%)	188 (96%)	8 (4%)	37	30
1	D	192/207 (93%)	182 (95%)	10 (5%)	29	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	771/828 (93%)	740 (96%)	31 (4%)	38 31

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	92	SER
1	A	95	SER
1	A	105	ARG
1	A	127	ASP
1	B	39	GLU
1	B	88	SER
1	B	94	LEU
1	B	106	LEU
1	B	117	ARG
1	B	123	SER
1	B	196	GLU
1	B	211	LYS
1	C	0	HIS
1	C	42	ARG
1	C	88	SER
1	C	90	ARG
1	C	93	LYS
1	C	115	PRO
1	C	117	ARG
1	C	144	ARG
1	D	1	MET
1	D	40	ARG
1	D	88	SER
1	D	93	LYS
1	D	113	ILE
1	D	143	ARG
1	D	144	ARG
1	D	211	LYS
1	D	213	ASP
1	D	218	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS

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Mol	Chain	Res	Type
1	C	169	ASN
1	D	185	GLN

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 ⓘ

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	FAD	A	301	-	29,37,58	1.03	2 (6%)	32,56,89	2.83	7 (21%)
2	FAD	B	301	-	48,58,58	3.13	13 (27%)	54,89,89	2.86	14 (25%)
2	FAD	C	301	-	48,58,58	3.10	16 (33%)	54,89,89	2.54	14 (25%)
2	FAD	D	300	-	48,58,58	2.96	15 (31%)	54,89,89	2.84	12 (22%)

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	FAD	A	301	-	-	0/26/46/50	0/3/3/6
2	FAD	B	301	-	-	0/30/50/50	0/6/6/6
2	FAD	C	301	-	-	0/30/50/50	0/6/6/6
2	FAD	D	300	-	-	0/30/50/50	0/6/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	FAD	C9A-N10	-6.54	1.29	1.38
2	C	301	FAD	C9A-N10	-6.31	1.30	1.38
2	B	301	FAD	C9A-N10	-5.35	1.31	1.38
2	C	301	FAD	PA-O1A	2.13	1.59	1.51
2	C	301	FAD	O4B-C1B	2.15	1.43	1.41
2	A	301	FAD	C2A-N3A	2.17	1.36	1.32
2	D	300	FAD	C2A-N3A	2.35	1.36	1.32
2	D	300	FAD	C4-N3	2.41	1.37	1.33
2	C	301	FAD	C2A-N3A	2.54	1.36	1.32
2	D	300	FAD	C5A-C4A	3.20	1.47	1.40
2	D	300	FAD	C9-C9A	3.49	1.48	1.40
2	A	301	FAD	C5A-C4A	3.49	1.48	1.40
2	B	301	FAD	C5A-C4A	3.62	1.48	1.40
2	D	300	FAD	C4-C4X	3.63	1.48	1.41
2	B	301	FAD	C9-C9A	3.65	1.48	1.40
2	D	300	FAD	C8-C7	3.80	1.51	1.41
2	C	301	FAD	C5A-C4A	3.84	1.49	1.40
2	C	301	FAD	C4-C4X	3.98	1.49	1.41
2	B	301	FAD	C8-C7	4.04	1.51	1.41
2	C	301	FAD	C9-C9A	4.15	1.49	1.40
2	C	301	FAD	C8-C7	4.18	1.52	1.41
2	B	301	FAD	C4-C4X	4.47	1.50	1.41
2	C	301	FAD	C9A-C5X	4.87	1.52	1.42
2	C	301	FAD	C4X-C10	5.12	1.50	1.41
2	B	301	FAD	C9A-C5X	5.16	1.53	1.42
2	D	300	FAD	C9A-C5X	5.17	1.53	1.42
2	B	301	FAD	C6-C7	5.19	1.52	1.37
2	C	301	FAD	C6-C7	5.20	1.52	1.37
2	D	300	FAD	C6-C7	5.25	1.52	1.37
2	D	300	FAD	C4X-C10	5.28	1.50	1.41
2	B	301	FAD	C4X-C10	5.74	1.51	1.41
2	D	300	FAD	C5X-N5	5.76	1.44	1.35
2	D	300	FAD	C10-N10	5.81	1.45	1.39
2	C	301	FAD	C5X-N5	6.52	1.45	1.35
2	B	301	FAD	C5X-N5	6.56	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	FAD	C10-N1	6.60	1.46	1.35
2	D	300	FAD	C10-N1	6.76	1.46	1.35
2	D	300	FAD	C6-C5X	6.80	1.52	1.41
2	C	301	FAD	C4X-N5	6.88	1.44	1.33
2	B	301	FAD	C10-N1	6.94	1.47	1.35
2	C	301	FAD	C6-C5X	7.24	1.52	1.41
2	B	301	FAD	C10-N10	7.64	1.48	1.39
2	C	301	FAD	C10-N10	7.64	1.48	1.39
2	B	301	FAD	C4X-N5	7.65	1.45	1.33
2	D	300	FAD	C4X-N5	7.76	1.45	1.33
2	B	301	FAD	C6-C5X	7.90	1.53	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FAD	N3A-C2A-N1A	-11.78	119.87	128.89
2	B	301	FAD	N3A-C2A-N1A	-10.85	120.59	128.89
2	C	301	FAD	N3A-C2A-N1A	-10.20	121.09	128.89
2	D	300	FAD	N3A-C2A-N1A	-8.00	122.77	128.89
2	D	300	FAD	C4-C4X-C10	-7.30	115.27	119.94
2	B	301	FAD	C4-C4X-C10	-6.68	115.67	119.94
2	C	301	FAD	C4-C4X-C10	-5.80	116.23	119.94
2	A	301	FAD	P-O3P-PA	-4.68	119.59	132.73
2	A	301	FAD	C4'-C3'-C2'	-4.58	105.00	112.47
2	D	300	FAD	C4X-C4-N3	-4.26	117.76	123.59
2	B	301	FAD	C4X-C4-N3	-3.57	118.71	123.59
2	D	300	FAD	O4'-C4'-C5'	-3.32	102.96	110.19
2	C	301	FAD	C1B-N9A-C4A	-3.27	122.01	126.94
2	D	300	FAD	C7-C6-C5X	-3.15	115.77	120.92
2	C	301	FAD	C4A-C5A-N7A	-3.11	106.61	109.48
2	D	300	FAD	C4A-C5A-N7A	-3.07	106.66	109.48
2	D	300	FAD	C1B-N9A-C4A	-2.83	122.67	126.94
2	C	301	FAD	C4X-C4-N3	-2.71	119.88	123.59
2	C	301	FAD	P-O3P-PA	-2.55	125.57	132.73
2	B	301	FAD	C4A-C5A-N7A	-2.40	107.27	109.48
2	A	301	FAD	C1B-N9A-C4A	-2.31	123.46	126.94
2	B	301	FAD	C1B-N9A-C4A	-2.22	123.60	126.94
2	C	301	FAD	O3P-PA-O5B	-2.18	97.15	102.94
2	B	301	FAD	C7-C6-C5X	-2.08	117.53	120.92
2	D	300	FAD	O2P-P-O1P	2.08	123.80	112.53
2	B	301	FAD	O2A-PA-O1A	2.18	124.37	112.53
2	C	301	FAD	O2A-PA-O1A	2.38	125.44	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FAD	C2A-N1A-C6A	2.52	123.27	118.77
2	C	301	FAD	O4B-C1B-N9A	2.68	113.71	108.10
2	B	301	FAD	C2A-N1A-C6A	2.91	123.96	118.77
2	A	301	FAD	C2A-N1A-C6A	3.50	125.02	118.77
2	C	301	FAD	C1'-N10-C9A	3.57	122.87	118.86
2	A	301	FAD	O2A-PA-O1A	3.57	131.89	112.53
2	B	301	FAD	C4B-O4B-C1B	3.76	113.85	109.72
2	A	301	FAD	C2B-C1B-N9A	3.89	120.24	114.29
2	B	301	FAD	C1'-N10-C9A	3.98	123.33	118.86
2	C	301	FAD	C4-C4X-N5	4.44	124.11	118.72
2	C	301	FAD	C5X-C9A-N10	4.45	121.00	117.62
2	B	301	FAD	C2B-C1B-N9A	4.82	121.66	114.29
2	D	300	FAD	C5X-C9A-N10	4.82	121.28	117.62
2	B	301	FAD	C4-C4X-N5	4.95	124.73	118.72
2	D	300	FAD	C1'-N10-C9A	5.07	124.55	118.86
2	D	300	FAD	C4-C4X-N5	5.09	124.90	118.72
2	B	301	FAD	C5X-C9A-N10	5.51	121.81	117.62
2	C	301	FAD	C4-N3-C2	8.28	122.40	115.25
2	B	301	FAD	C4-N3-C2	9.85	123.76	115.25
2	D	300	FAD	C4-N3-C2	11.63	125.30	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FAD	2	0
2	C	301	FAD	2	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

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, 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	218/232 (93%)	0.89	25 (11%) 6 8	24, 37, 64, 77	0
1	B	212/232 (91%)	0.94	28 (13%) 4 5	25, 40, 69, 93	0
1	C	219/232 (94%)	0.91	24 (10%) 7 9	24, 36, 68, 89	0
1	D	216/232 (93%)	1.07	31 (14%) 3 4	25, 39, 65, 79	0
All	All	865/928 (93%)	0.95	108 (12%) 5 6	24, 38, 66, 93	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	35	LEU	6.8
1	D	218	VAL	6.5
1	B	106	LEU	6.4
1	B	109	TYR	6.1
1	A	34	GLY	5.6
1	C	0	HIS	5.5
1	C	109	TYR	5.1
1	D	40	ARG	5.1
1	D	109	TYR	5.0
1	C	106	LEU	4.6
1	C	218	VAL	4.5
1	A	37	ASP	4.4
1	A	216	LYS	4.2
1	A	112	THR	4.2
1	D	36	LYS	4.1
1	C	31	PHE	4.1
1	A	33	MET	4.1
1	C	220	VAL	4.0
1	A	217	GLU	4.0
1	A	40	ARG	3.8
1	C	90	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	107	GLU	3.8
1	C	219	GLN	3.7
1	A	94	LEU	3.7
1	D	39	GLU	3.6
1	C	138	GLU	3.5
1	A	90	ARG	3.5
1	B	218	VAL	3.5
1	D	113	ILE	3.4
1	D	217	GLU	3.4
1	A	113	ILE	3.4
1	B	108	GLY	3.4
1	C	110	LYS	3.4
1	C	91	TYR	3.3
1	A	93	LYS	3.3
1	D	178	HIS	3.3
1	D	38	GLU	3.3
1	C	143	ARG	3.2
1	D	138	GLU	3.2
1	D	216	LYS	3.2
1	C	111	THR	3.2
1	A	108	GLY	3.2
1	D	108	GLY	3.1
1	D	0	HIS	3.1
1	B	32	ASP	3.0
1	B	107	GLU	3.0
1	D	90	ARG	3.0
1	C	92	SER	3.0
1	C	137	ILE	2.9
1	D	192	ARG	2.9
1	B	40	ARG	2.9
1	C	108	GLY	2.9
1	A	109	TYR	2.8
1	B	158	PHE	2.8
1	B	160	TRP	2.8
1	B	66	VAL	2.7
1	B	143	ARG	2.7
1	B	112	THR	2.7
1	B	31	PHE	2.7
1	A	110	LYS	2.7
1	B	88	SER	2.7
1	B	43	HIS	2.7
1	A	178	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	110	LYS	2.6
1	D	152	LEU	2.6
1	B	117	ARG	2.6
1	D	131	ARG	2.6
1	D	31	PHE	2.6
1	B	178	HIS	2.6
1	D	208	TYR	2.5
1	D	70	ILE	2.5
1	B	192	ARG	2.5
1	B	114	PRO	2.5
1	B	120	GLU	2.4
1	D	106	LEU	2.4
1	A	106	LEU	2.4
1	C	40	ARG	2.4
1	B	219	GLN	2.4
1	D	73	ALA	2.4
1	B	38	GLU	2.4
1	D	154	LEU	2.4
1	B	124	GLU	2.3
1	B	0	HIS	2.3
1	C	178	HIS	2.3
1	A	39	GLU	2.2
1	D	137	ILE	2.2
1	B	47	TYR	2.2
1	A	92	SER	2.2
1	B	51	HIS	2.2
1	D	68	ALA	2.2
1	D	71	PHE	2.2
1	C	81	ILE	2.2
1	A	117	ARG	2.2
1	C	32	ASP	2.1
1	B	89	GLY	2.1
1	D	89	GLY	2.1
1	D	43	HIS	2.1
1	A	148	ILE	2.1
1	A	215	LEU	2.1
1	A	143	ARG	2.1
1	D	72	VAL	2.1
1	A	107	GLU	2.0
1	C	117	ARG	2.0
1	B	94	LEU	2.0
1	C	104	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	38	GLU	2.0
1	A	43	HIS	2.0
1	C	113	ILE	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, 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
2	FAD	B	301	53/53	0.78	0.26	2.54	33,50,63,65	0
2	FAD	C	301	53/53	0.83	0.22	1.71	34,48,55,57	0
2	FAD	A	301	35/53	0.86	0.20	1.11	31,47,56,61	0
2	FAD	D	300	53/53	0.89	0.15	0.02	33,44,50,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.