



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:50 PM GMT

PDB ID : 3APY
Title : Properties and crystal structure of methylenetetrahydrofolatereductase from
Thermus thermophilus HB8
Authors : Yamada, K.
Deposited on : 2010-10-21
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

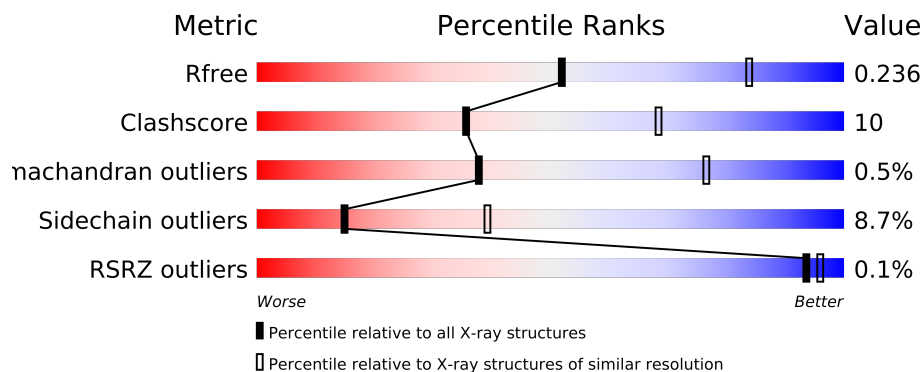
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	310	
1	B	310	
1	C	310	
1	D	310	
1	E	310	
1	F	310	
1	G	310	
1	H	310	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	H	312	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19755 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Methylenetetrahydrofolatereductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	B	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	C	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	D	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	E	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	F	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	G	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			
1	H	291	Total	C	N	O	S	0	0	0
			2302	1469	422	406	5			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
A	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
A	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
A	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
A	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
A	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
A	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
A	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
A	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
A	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
A	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
A	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
A	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
B	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
B	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
B	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
B	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
B	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
B	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
B	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
B	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
B	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
C	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
C	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
C	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
C	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
C	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
C	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
C	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
C	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
C	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
D	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
D	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
D	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
D	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
D	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
D	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
D	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
D	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
D	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6

Continued on next page...

Continued from previous page...

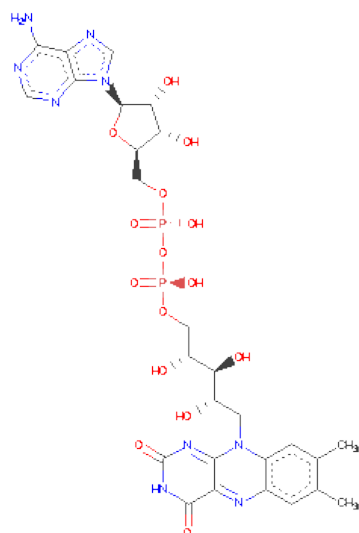
Chain	Residue	Modelled	Actual	Comment	Reference
D	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
E	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
E	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
E	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
E	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
E	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
E	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
E	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
E	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
E	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
F	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
F	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
F	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
F	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
F	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
F	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
F	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
F	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
F	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
G	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
G	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
G	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
G	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
G	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
G	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
G	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
G	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
G	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	297	ALA	-	EXPRESSION TAG	UNP Q5SLG6
H	298	LYS	-	EXPRESSION TAG	UNP Q5SLG6
H	299	LEU	-	EXPRESSION TAG	UNP Q5SLG6
H	300	ALA	-	EXPRESSION TAG	UNP Q5SLG6
H	301	ALA	-	EXPRESSION TAG	UNP Q5SLG6
H	302	ALA	-	EXPRESSION TAG	UNP Q5SLG6
H	303	LEU	-	EXPRESSION TAG	UNP Q5SLG6
H	304	GLU	-	EXPRESSION TAG	UNP Q5SLG6
H	305	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	306	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	307	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	308	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	309	HIS	-	EXPRESSION TAG	UNP Q5SLG6
H	310	HIS	-	EXPRESSION TAG	UNP Q5SLG6

- 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
			53	27	9	15	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

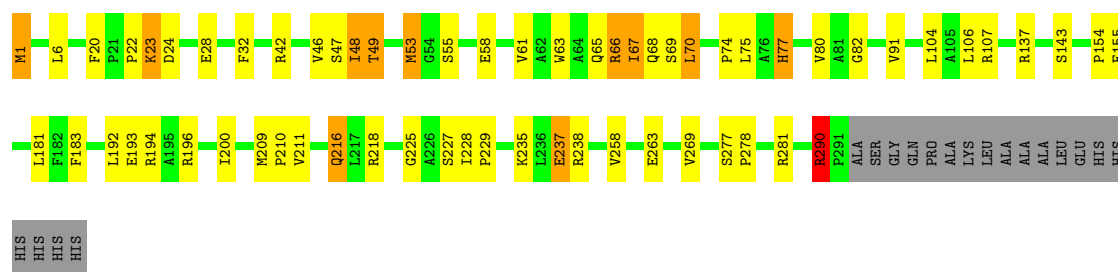
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	111	Total	O	0	0
			111	111		
4	C	117	Total	O	0	0
			117	117		
4	D	97	Total	O	0	0
			97	97		
4	E	127	Total	O	0	0
			127	127		
4	F	119	Total	O	0	0
			119	119		

Continued on next page...

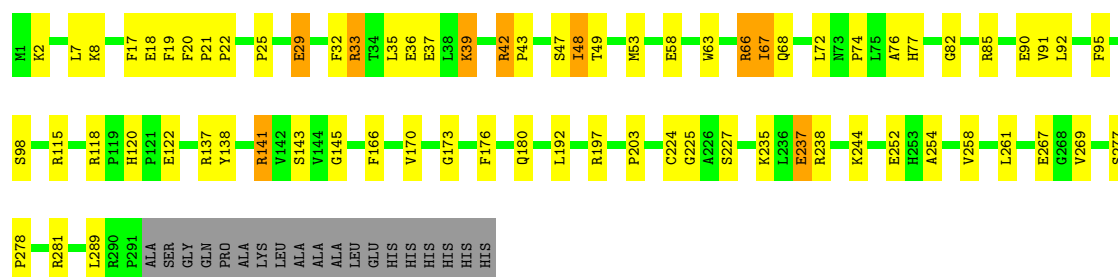
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	111	Total 111	O 111	0	0
4	H	115	Total 115	O 115	0	0



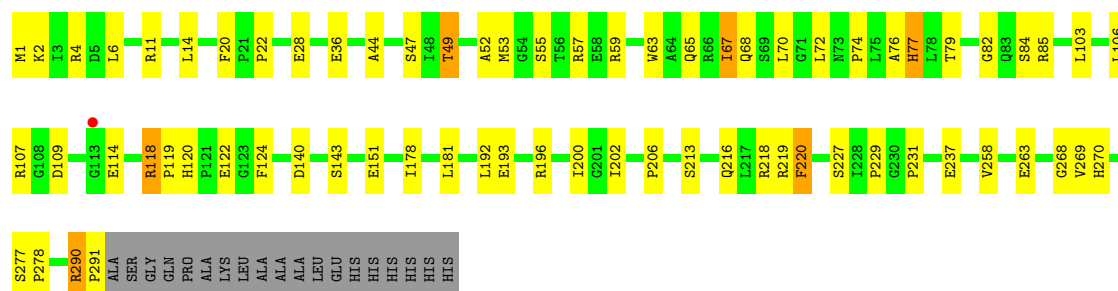
• Molecule 1: Methylene tetrahydrofolate reductase

Chain E:



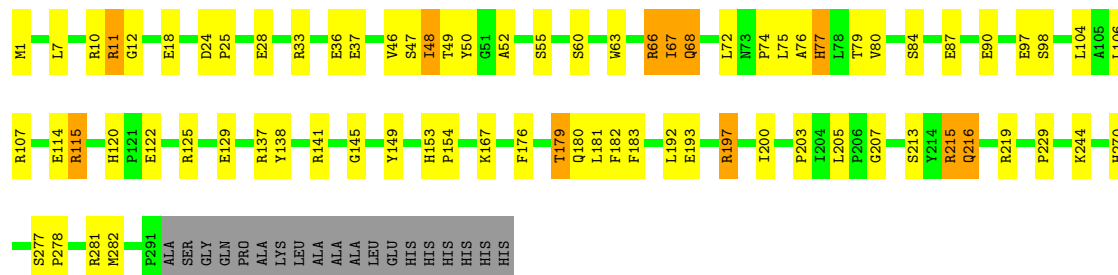
• Molecule 1: Methylene tetrahydrofolate reductase

Chain F:



• Molecule 1: Methylene tetrahydrofolate reductase

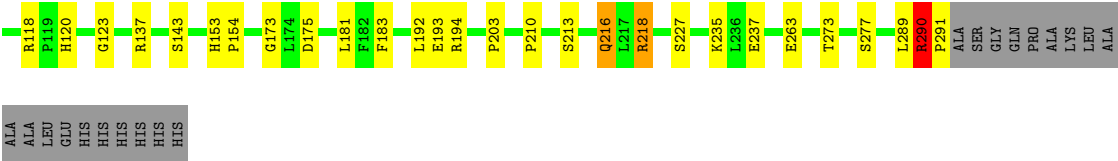
Chain G:



• Molecule 1: Methylene tetrahydrofolate reductase

Chain H:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.59Å 90.93Å 125.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.96-2.80) 93.8 (19.96-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.64 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.204 , 0.306 0.189 , 0.236	Depositor DCC
R_{free} test set	3050 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 3.9	EDS
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	13 of 60581 reflections (0.021%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19755	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 55.73 % 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 3.0318e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.70	0/2357	0.78	1/3185 (0.0%)
1	B	0.67	0/2357	0.73	0/3185
1	C	0.71	0/2357	0.77	1/3185 (0.0%)
1	D	0.68	0/2357	0.75	0/3185
1	E	0.70	0/2357	0.74	1/3185 (0.0%)
1	F	0.69	0/2357	0.73	0/3185
1	G	0.71	0/2357	0.75	0/3185
1	H	0.65	0/2357	0.72	0/3185
All	All	0.69	0/18856	0.75	3/25480 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	GLY	N-CA-C	-7.63	94.02	113.10
1	C	52	ALA	N-CA-C	-6.78	92.70	111.00
1	E	33	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	290	ARG	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2302	0	2319	71	0
1	B	2302	0	2319	46	0
1	C	2302	0	2319	47	0
1	D	2302	0	2319	46	0
1	E	2302	0	2319	55	0
1	F	2302	0	2319	45	0
1	G	2302	0	2319	66	0
1	H	2302	0	2319	39	0
2	A	53	0	31	5	0
2	B	53	0	31	2	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
2	E	53	0	31	0	0
2	F	53	0	31	2	0
2	G	53	0	31	3	0
2	H	53	0	31	1	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	1	0
3	H	1	0	0	0	0
4	A	112	0	0	6	0
4	B	111	0	0	5	0
4	C	117	0	0	7	0
4	D	97	0	0	4	0
4	E	127	0	0	7	0
4	F	119	0	0	5	0
4	G	111	0	0	3	0
4	H	115	0	0	7	0
All	All	19755	0	18800	395	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 395 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:67:ILE:HD11	1:D:74:PRO:HB3	1.36	1.04
1:A:290:ARG:HH11	1:A:290:ARG:HG2	1.24	0.99
1:H:290:ARG:O	1:H:290:ARG:HD3	1.61	0.99
1:A:52:ALA:HB2	1:A:56:THR:HG23	1.46	0.98
1:A:237:GLU:HG3	1:B:218:ARG:HH12	1.27	0.98

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	289/310 (93%)	280 (97%)	8 (3%)	1 (0%)	50	84
1	B	289/310 (93%)	278 (96%)	8 (3%)	3 (1%)	22	60
1	C	289/310 (93%)	275 (95%)	13 (4%)	1 (0%)	50	84
1	D	289/310 (93%)	274 (95%)	13 (4%)	2 (1%)	30	69
1	E	289/310 (93%)	277 (96%)	11 (4%)	1 (0%)	50	84
1	F	289/310 (93%)	275 (95%)	12 (4%)	2 (1%)	30	69
1	G	289/310 (93%)	272 (94%)	17 (6%)	0	100	100
1	H	289/310 (93%)	279 (96%)	8 (3%)	2 (1%)	30	69
All	All	2312/2480 (93%)	2210 (96%)	90 (4%)	12 (0%)	38	76

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	290	ARG
1	C	52	ALA
1	D	290	ARG
1	H	290	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	114	GLU

5.3.2 Protein sidechains ⓘ

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	236/249 (95%)	215 (91%)	21 (9%)	14	38
1	B	236/249 (95%)	219 (93%)	17 (7%)	21	50
1	C	236/249 (95%)	220 (93%)	16 (7%)	22	54
1	D	236/249 (95%)	211 (89%)	25 (11%)	10	27
1	E	236/249 (95%)	213 (90%)	23 (10%)	12	32
1	F	236/249 (95%)	216 (92%)	20 (8%)	15	41
1	G	236/249 (95%)	218 (92%)	18 (8%)	19	46
1	H	236/249 (95%)	211 (89%)	25 (11%)	10	27
All	All	1888/1992 (95%)	1723 (91%)	165 (9%)	15	39

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	228	ILE
1	E	118	ARG
1	H	114	GLU
1	D	237	GLU
1	E	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	68	GLN
1	E	68	GLN
1	H	68	GLN
1	D	77	HIS
1	D	83	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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	311	-	58,58,58	1.12	4 (6%)	85,89,89	1.77	15 (17%)
2	FAD	B	311	-	58,58,58	1.09	4 (6%)	85,89,89	1.97	13 (15%)
2	FAD	C	311	-	58,58,58	0.94	4 (6%)	85,89,89	2.04	15 (17%)
2	FAD	D	311	-	58,58,58	1.00	3 (5%)	85,89,89	1.89	15 (17%)
2	FAD	E	311	-	58,58,58	1.04	3 (5%)	85,89,89	1.87	13 (15%)
2	FAD	F	311	-	58,58,58	1.17	5 (8%)	85,89,89	1.89	18 (21%)
2	FAD	G	311	-	58,58,58	1.13	5 (8%)	85,89,89	2.08	17 (20%)
2	FAD	H	311	-	58,58,58	1.06	3 (5%)	85,89,89	1.86	10 (11%)

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	311	-	-	0/34/50/50	0/1/6/6
2	FAD	B	311	-	-	0/34/50/50	0/1/6/6
2	FAD	C	311	-	-	0/34/50/50	0/1/6/6
2	FAD	D	311	-	-	0/34/50/50	0/1/6/6
2	FAD	E	311	-	-	0/34/50/50	0/1/6/6
2	FAD	F	311	-	-	0/34/50/50	0/1/6/6
2	FAD	G	311	-	-	0/34/50/50	0/1/6/6
2	FAD	H	311	-	-	0/34/50/50	0/1/6/6

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	311	FAD	C1'-N10	3.80	1.52	1.48
2	A	311	FAD	C2A-N3A	3.64	1.39	1.32
2	F	311	FAD	C2A-N3A	3.64	1.39	1.32
2	F	311	FAD	C6-C5X	-3.29	1.37	1.41
2	A	311	FAD	C5X-N5	3.25	1.40	1.35

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	311	FAD	N3A-C2A-N1A	-12.51	118.25	128.71
2	H	311	FAD	N3A-C2A-N1A	-11.62	118.99	128.71
2	G	311	FAD	N3A-C2A-N1A	-11.01	119.50	128.71
2	C	311	FAD	N3A-C2A-N1A	-10.64	119.82	128.71
2	D	311	FAD	N3A-C2A-N1A	-9.95	120.39	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	291/310 (93%)	-0.72	0 100 100	6, 17, 33, 45	1 (0%)
1	B	291/310 (93%)	-0.65	1 (0%) 91 93	5, 18, 34, 46	1 (0%)
1	C	291/310 (93%)	-0.69	0 100 100	5, 18, 34, 56	1 (0%)
1	D	291/310 (93%)	-0.64	0 100 100	5, 18, 33, 46	1 (0%)
1	E	291/310 (93%)	-0.70	0 100 100	7, 18, 36, 52	1 (0%)
1	F	291/310 (93%)	-0.67	1 (0%) 91 93	7, 18, 35, 47	1 (0%)
1	G	291/310 (93%)	-0.68	0 100 100	6, 17, 33, 50	1 (0%)
1	H	291/310 (93%)	-0.64	0 100 100	5, 18, 35, 47	1 (0%)
All	All	2328/2480 (93%)	-0.67	2 (0%) 93 96	5, 18, 34, 56	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	GLY	3.8
1	F	113	GLY	2.1

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CL	H	312	1/1	0.22	17.30	31,31,31,31	0
2	FAD	A	311	53/53	0.12	-0.04	9,11,14,14	0
2	FAD	C	311	53/53	0.12	-0.08	5,10,15,15	0
3	CL	E	312	1/1	0.17	-0.13	37,37,37,37	0
2	FAD	B	311	53/53	0.12	-0.18	6,14,18,19	0
2	FAD	F	311	53/53	0.12	-0.28	2,16,19,22	0
2	FAD	H	311	53/53	0.12	-0.37	11,15,18,19	0
2	FAD	E	311	53/53	0.11	-0.43	6,9,13,14	0
2	FAD	D	311	53/53	0.13	-0.45	7,12,18,19	0
2	FAD	G	311	53/53	0.11	-0.67	4,9,13,13	0
3	CL	D	312	1/1	0.15	-0.71	40,40,40,40	0
3	CL	A	312	1/1	0.09	-1.39	31,31,31,31	0
3	CL	F	312	1/1	0.10	-3.02	41,41,41,41	0
3	CL	G	312	1/1	0.08	-25.14	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.