Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2017 – 03:54 AM EDT

PDB ID	:	3CLS
Title	:	Crystal structure of the R236C mutant of ETF from Methylophilus methylotrophus
Authors	:	Katona, G.; Leys, D.
Deposited on	:	unknown
Resolution	:	1.65 Å(reported)

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

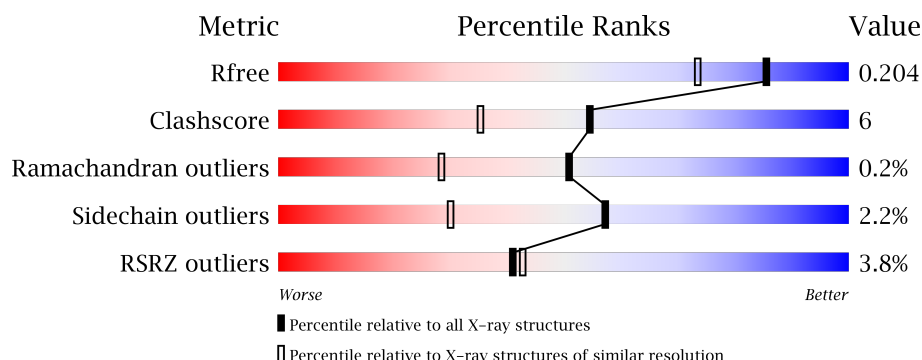|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 1.65 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	Percentile Ranks	Value
Rfree		0.204
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		2.2%
RSRZ outliers		3.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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	C	264	5% / 86% / 7% · ·
2	D	321	3% / 90% / 9% ··

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5053 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 Electron transfer flavoprotein subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	254	Total	C	N	O	S	0	4	0
			1950	1222	327	387	14			

- Molecule 2 is a protein called Electron transfer flavoprotein subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	318	Total	C	N	O	S	0	3	0
			2334	1468	392	466	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	236	CYS	ARG	ENGINEERED	UNP P53571

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).
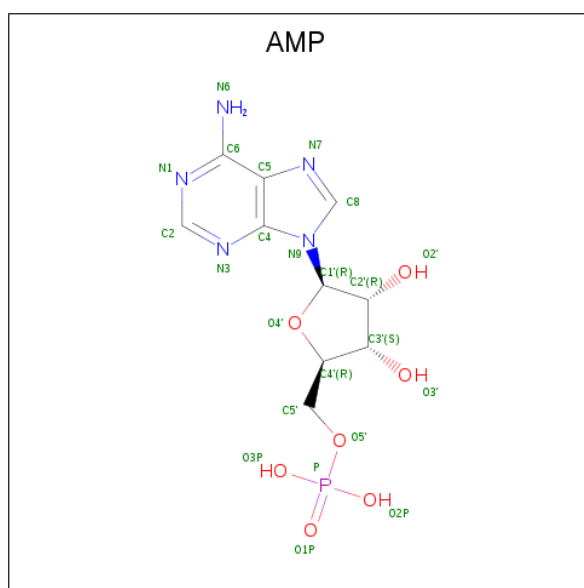
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	C	1	23	10	5	7	1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
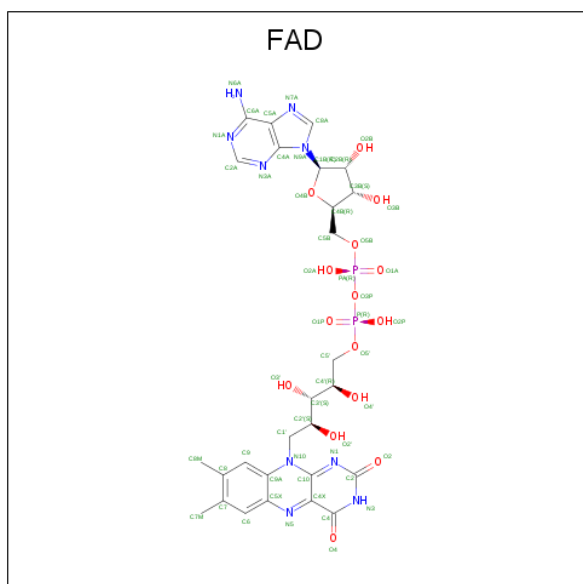
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	D	1	53	27	9	15	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	307	307	307	0	0
5	D	386	386	386	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 d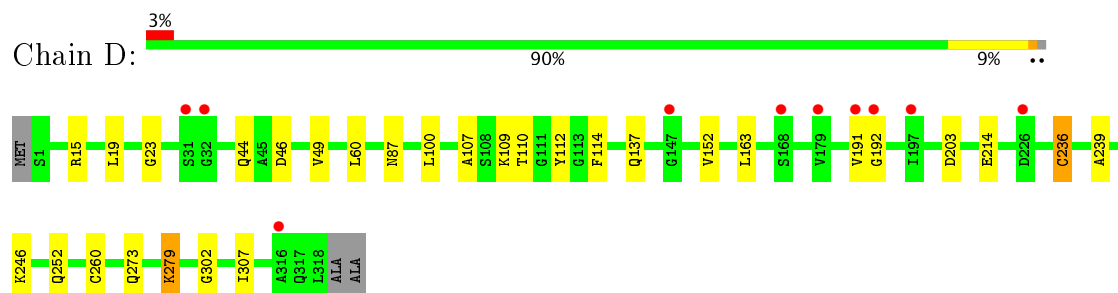ot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Electron transfer flavoprotein subunit beta
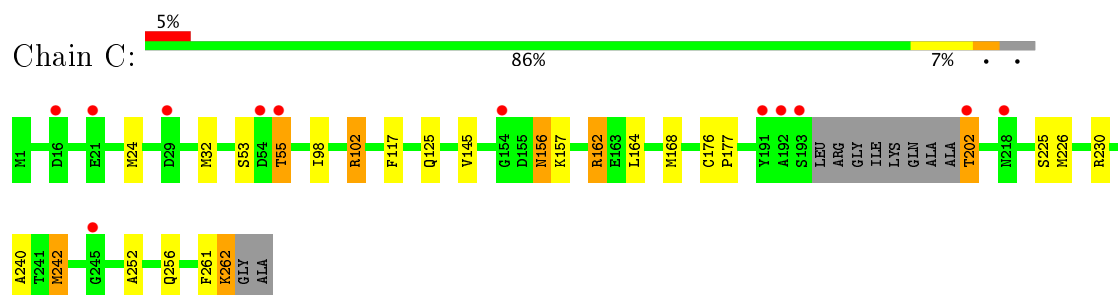
- Molecule 2: Electron transfer flavoprotein subunit alpha

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	117.53Å 117.53Å 84.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.65 19.68 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-1.65) 95.6 (19.68-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$<I/\sigma(I)>$ [1]	1.63 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.163 , 0.191 0.175 , 0.204	Depositor DCC
R_{free} test set	3836 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.1	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5053	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, 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	C	0.88	2/1974 (0.1%)	0.93	2/2671 (0.1%)
2	D	0.88	4/2372 (0.2%)	0.92	3/3232 (0.1%)
All	All	0.88	6/4346 (0.1%)	0.92	5/5903 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	214	GLU	CB-CG	7.54	1.66	1.52
2	D	214	GLU	CG-CD	7.05	1.62	1.51
1	C	125	GLN	CG-CD	6.30	1.65	1.51
1	C	162	ARG	CB-CG	-5.98	1.36	1.52
2	D	279	LYS	CD-CE	5.80	1.65	1.51
2	D	279	LYS	CE-NZ	5.28	1.62	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	279	LYS	CD-CE-NZ	7.36	128.62	111.70
1	C	242	MET	CG-SD-CE	-5.98	90.64	100.20
2	D	15	ARG	NE-CZ-NH2	5.50	123.05	120.30
2	D	100	LEU	CB-CG-CD2	5.44	120.24	111.00
1	C	117	PHE	CB-CG-CD2	-5.14	117.20	120.80

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	C	1950	0	1916	33	0
2	D	2334	0	2293	26	0
3	C	23	0	12	0	0
4	D	53	0	31	3	0
5	C	307	0	0	11	0
5	D	386	0	0	6	0
All	All	5053	0	4252	52	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 6.

All (52) 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:98:ILE:HG13	1:C:226[B]:MET:CE	1.87	1.05
2:D:137[A]:GLN:NE2	5:D:1493:HOH:O	2.04	0.91
1:C:98:ILE:HG13	1:C:226[B]:MET:HE1	1.54	0.86
1:C:98:ILE:HG13	1:C:226[B]:MET:HE2	1.55	0.86
1:C:240:ALA:HB3	1:C:242:MET:CE	2.06	0.85
1:C:240:ALA:HB3	1:C:242:MET:HE1	1.66	0.77
1:C:24:MET:CE	5:C:1560:HOH:O	2.34	0.74
1:C:226[A]:MET:HE3	2:D:112:TYR:O	1.87	0.73
1:C:32:MET:HG2	5:C:1525:HOH:O	1.87	0.73
1:C:261:PHE:O	1:C:262:LYS:HB2	1.86	0.73
2:D:23:GLY:HA2	2:D:163:LEU:CD2	2.22	0.70
2:D:252:GLN:NE2	5:D:1701:HOH:O	2.26	0.67
1:C:226[B]:MET:HE3	2:D:114:PHE:CB	2.26	0.65
2:D:87[B]:ASN:OD1	5:D:1442:HOH:O	2.15	0.65
2:D:23:GLY:HA2	2:D:163:LEU:HD21	1.81	0.62
1:C:24:MET:HE2	5:C:1560:HOH:O	1.97	0.61
1:C:98:ILE:CG1	1:C:226[B]:MET:HE2	2.32	0.59
1:C:226[A]:MET:CE	2:D:112:TYR:O	2.51	0.57
1:C:102:ARG:HG3	5:C:1562:HOH:O	2.05	0.57
2:D:44:GLN:NE2	5:D:1392:HOH:O	2.33	0.56
1:C:156:ASN:HD22	1:C:156:ASN:C	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ALA:HB3	1:C:242:MET:HE3	1.87	0.54
1:C:240:ALA:CB	1:C:242:MET:CE	2.84	0.53
1:C:102:ARG:CZ	5:C:1566:HOH:O	2.56	0.53
1:C:53:SER:OG	1:C:55:THR:HG23	2.10	0.52
1:C:164:LEU:HD12	1:C:168:MET:HG3	1.93	0.51
1:C:226[B]:MET:HE3	2:D:114:PHE:HB3	1.92	0.51
2:D:307:ILE:HG23	4:D:1319:FAD:C2A	2.41	0.51
1:C:98:ILE:HG12	5:C:1390:HOH:O	2.10	0.50
2:D:239:ALA:HB1	2:D:246:LYS:HD3	1.92	0.50
2:D:163:LEU:HD22	2:D:163:LEU:N	2.26	0.49
2:D:46:ASP:O	2:D:49:VAL:HG13	2.12	0.49
1:C:102:ARG:NE	5:C:1566:HOH:O	2.45	0.49
2:D:307:ILE:HG23	4:D:1319:FAD:H2A	1.95	0.48
5:C:1416:HOH:O	2:D:109:LYS:HE3	2.15	0.47
2:D:114:PHE:HA	2:D:152:VAL:O	2.15	0.47
2:D:203:ASP:HA	2:D:260:CYS:HA	1.97	0.47
2:D:236:CYS:SG	4:D:1319:FAD:H1'2	2.55	0.47
2:D:273:GLN:HG3	5:D:1701:HOH:O	2.14	0.45
1:C:225:SER:HA	5:C:1505:HOH:O	2.16	0.45
1:C:226[B]:MET:HE3	2:D:114:PHE:HB2	1.97	0.45
1:C:102:ARG:NH2	5:C:1566:HOH:O	2.49	0.44
1:C:176:CYS:HA	1:C:177:PRO:C	2.36	0.44
1:C:252:ALA:O	1:C:256:GLN:HG3	2.18	0.43
1:C:156:ASN:HD22	1:C:157:LYS:N	2.16	0.43
2:D:110:THR:HG23	5:D:1459:HOH:O	2.18	0.42
1:C:24:MET:HE1	1:C:230:ARG:O	2.19	0.42
1:C:226[B]:MET:CE	2:D:107:ALA:HB1	2.49	0.42
1:C:202:THR:N	5:C:1271:HOH:O	2.53	0.42
1:C:242:MET:CE	2:D:302:GLY:HA3	2.50	0.42
2:D:163:LEU:N	2:D:163:LEU:CD2	2.83	0.41
2:D:191:VAL:HG23	2:D:192:GLY:O	2.21	0.41

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	C	254/264 (96%)	249 (98%)	4 (2%)	1 (0%)	38	17
2	D	319/321 (99%)	312 (98%)	7 (2%)	0	100	100
All	All	573/585 (98%)	561 (98%)	11 (2%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	VAL

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	C	204/216 (94%)	198 (97%)	6 (3%)	48	18
2	D	252/259 (97%)	248 (98%)	4 (2%)	68	45
All	All	456/475 (96%)	446 (98%)	10 (2%)	57	30

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	55	THR
1	C	102	ARG
1	C	156	ASN
1	C	162	ARG
1	C	202	THR
1	C	262	LYS
2	D	19	LEU
2	D	60	LEU
2	D	236	CYS
2	D	279	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	121	GLN
1	C	156	ASN
1	C	175	ASN
1	C	256	GLN
2	D	12	ASN

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 ⓘ

2 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	$\#|Z| > 2$
3	AMP	C	1262	-	22,25,25	1.47	5 (22%)	24,38,38	2.13	7 (29%)
4	FAD	D	1319	-	51,58,58	1.52	8 (15%)	54,89,89	2.24	7 (12%)

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
3	AMP	C	1262	-	-	0/6/26/26	0/3/3/3
4	FAD	D	1319	-	-	0/28/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1319	FAD	C2B-C1B	-3.85	1.47	1.53
3	C	1262	AMP	O4'-C1'	-2.89	1.37	1.41
3	C	1262	AMP	P-O3P	-2.70	1.43	1.54
3	C	1262	AMP	C5-N7	-2.14	1.32	1.39
4	D	1319	FAD	C4-N3	2.12	1.36	1.33
3	C	1262	AMP	C2-N1	2.31	1.38	1.33
4	D	1319	FAD	C2A-N1A	2.32	1.38	1.33
3	C	1262	AMP	C5-C4	2.53	1.46	1.40
4	D	1319	FAD	C5X-N5	2.85	1.39	1.35
4	D	1319	FAD	C2A-N3A	3.03	1.37	1.32
4	D	1319	FAD	C4X-N5	3.40	1.38	1.33
4	D	1319	FAD	C1'-N10	3.81	1.52	1.48
4	D	1319	FAD	C10-N1	4.10	1.39	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1319	FAD	N3A-C2A-N1A	-10.25	119.93	128.86
3	C	1262	AMP	N3-C2-N1	-7.01	122.75	128.86
4	D	1319	FAD	C4X-C4-N3	-4.17	117.54	123.48
3	C	1262	AMP	C1'-N9-C4	-3.35	120.84	126.64
4	D	1319	FAD	C4B-O4B-C1B	-3.15	106.42	109.77
3	C	1262	AMP	C5'-C4'-C3'	-2.46	105.89	115.29
4	D	1319	FAD	C4A-C5A-N7A	-2.39	107.10	109.41
3	C	1262	AMP	C5-C6-N6	-2.22	115.95	120.47
3	C	1262	AMP	O5'-P-O1P	-2.19	100.34	106.47
4	D	1319	FAD	O4'-C4'-C3'	2.33	114.86	109.09
3	C	1262	AMP	P-O5'-C5'	2.44	125.01	118.30
4	D	1319	FAD	C1'-N10-C9A	2.62	120.75	118.35
3	C	1262	AMP	N6-C6-N1	3.11	124.94	118.77
4	D	1319	FAD	C4-N3-C2	9.07	123.09	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1319	FAD	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	C	254/264 (96%)	-0.10	12 (4%)	32	31	0, 10, 30, 48	0
2	D	318/321 (99%)	-0.13	10 (3%)	49	52	2, 12, 33, 48	0
All	All	572/585 (97%)	-0.12	22 (3%)	41	43	0, 11, 31, 48	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	192	GLY	5.9
1	C	191	TYR	5.3
2	D	32	GLY	5.0
2	D	191	VAL	4.3
1	C	193	SER	4.0
1	C	21	GLU	3.5
1	C	202	THR	3.2
2	D	31	SER	3.1
2	D	197	ILE	3.0
2	D	226	ASP	2.9
1	C	55	THR	2.9
2	D	179	VAL	2.5
2	D	316	ALA	2.3
1	C	16	ASP	2.2
2	D	168	SER	2.2
1	C	218	ASN	2.2
2	D	147	GLY	2.2
1	C	192	ALA	2.2
1	C	154	GLY	2.1
1	C	245	GLY	2.1
1	C	29	ASP	2.1
1	C	54	ASP	2.0

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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	FAD	D	1319	53/53	0.95	0.07	-0.01	3,5,9,10	0
3	AMP	C	1262	23/23	0.98	0.05	-1.15	2,3,4,6	0

6.5 Other polymers ⓘ

There are no such residues in this entry.