



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:02 PM GMT

PDB ID : 1WAM
Title : Structure of UDP-galactopyranose mutase from Klebsiella Pneumoniae with FADH-
Authors : Beis, K.; Srikannathasan, V.; Naismith, J.H.
Deposited on : 2004-10-27
Resolution : 2.35 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

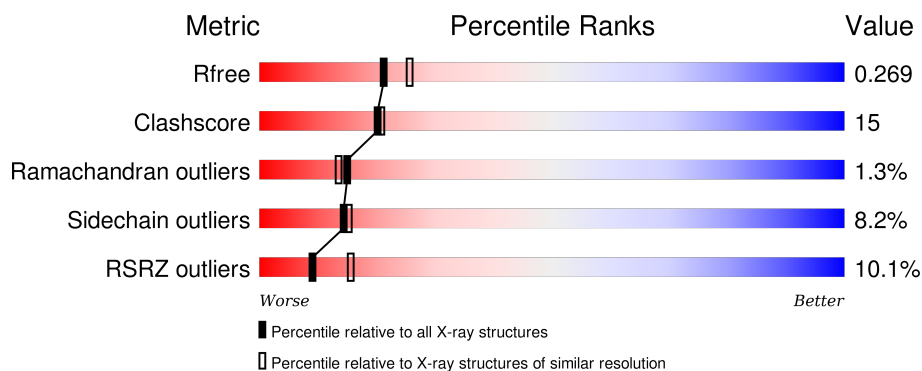
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	384	<div> <div>10%</div> <div>73%</div> <div>19%</div> <div>5% ..</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3246 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.

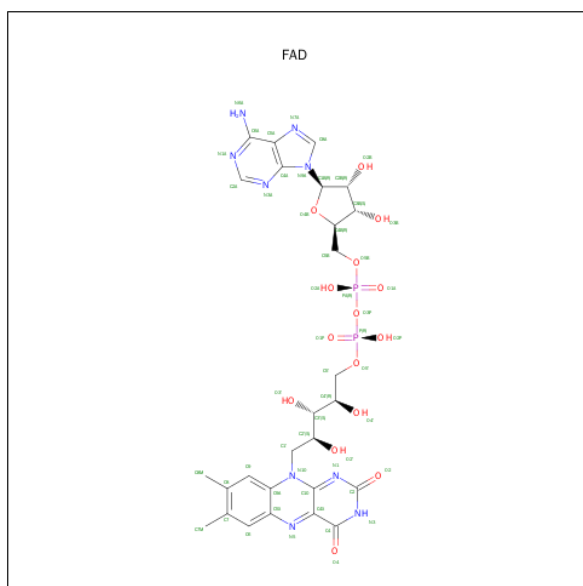
- Molecule 1 is a protein called UDP-GALACTOPYRANOSE MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	377	3077	1968	518	574	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLU	GLN	CONFLICT	UNP Q48485
A	262	GLN	ASP	CONFLICT	UNP Q48485

- 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
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total 116	O 116	0	0

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 ($\text{RSRZ} > 2$). 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.

Chain A:

10% 73% 19% 5% 3%

Label	Value
R361	10%
T362	73%
V365	19%
Y366	5%
L367	3%
N368	10%
T371	73%
E372	19%
N373	5%
Q374	3%
F375	10%
M376	73%
T380	19%
V381	5%
S382	3%
V383	10%
ARG	73%
P132	10%
Q133	73%
T134	19%
F135	5%
E136	3%
A139	10%
L140	73%
R141	19%
F142	5%
I143	3%
G144	10%
L147	73%
Y155	19%
K158	5%
Q159	3%
W160	10%
Q163	73%
P164	19%
S165	5%
E166	3%
L167	10%
S170	73%
L171	19%
L172	5%
K173	3%
R174	10%
L175	73%
P176	19%
V177	5%
F186	3%
M187	10%
H188	73%
M193	19%
M201	5%
I202	3%
L205	10%
E209	73%
R217	19%
E218	5%
F219	3%
I220	10%
F221	73%
V221	19%
E222	5%
E223	3%
R224	10%
V230	73%
E231	19%
G342	5%
R343	3%
I344	10%
G345	73%
T346	19%
Y347	5%
R348	3%
D351	10%

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.00Å 86.00Å 100.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.12 – 2.35 27.11 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.12-2.35) 99.5 (27.11-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.200 , 0.268 0.199 , 0.269	Depositor DCC
R_{free} test set	914 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.8	EDS
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 18319 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3246	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.71	0/3159	0.78	2/4277 (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	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	193	MET	CG-SD-CE	-5.79	90.94	100.20
1	A	351	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Peptide
1	A	373	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3077	0	2949	90	0
2	A	53	0	31	1	0
3	A	116	0	0	11	0
All	All	3246	0	2980	90	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 15.

All (90) 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:A:366:TYR:HA	1:A:376:MET:CE	1.85	1.06
1:A:366:TYR:HA	1:A:376:MET:HE3	1.37	1.03
1:A:143:ILE:HD12	1:A:147:LEU:HB3	1.48	0.93
1:A:141:ARG:HG3	1:A:144:GLY:HA2	1.60	0.82
1:A:308:GLU:O	1:A:309:ASN:HB2	1.78	0.81
1:A:73:VAL:HG12	1:A:201:MET:HE1	1.62	0.81
1:A:73:VAL:HG12	1:A:201:MET:CE	2.13	0.79
1:A:44:ASP:HB2	1:A:53:MET:HE2	1.66	0.76
1:A:47:ASP:HB3	1:A:50:THR:HG22	1.70	0.73
1:A:45:ALA:N	1:A:53:MET:HE1	2.05	0.71
1:A:134:THR:HG23	1:A:139:ALA:CB	2.22	0.70
1:A:134:THR:HG23	1:A:139:ALA:HB3	1.75	0.69
1:A:45:ALA:C	1:A:53:MET:HE3	2.13	0.68
1:A:362:THR:OG1	1:A:380:THR:HG21	1.94	0.68
1:A:279:THR:HG21	3:A:2090:HOH:O	1.93	0.67
1:A:186:PHE:HB3	1:A:188:HIS:HD2	1.59	0.67
1:A:366:TYR:HA	1:A:376:MET:HE1	1.72	0.66
1:A:126:ASP:H	1:A:141:ARG:HB3	1.60	0.66
1:A:87:LYS:HE2	3:A:2025:HOH:O	1.95	0.65
1:A:110:LYS:NZ	1:A:111:THR:HG22	2.11	0.65
1:A:329:LEU:O	1:A:333:GLU:HG3	1.96	0.65
1:A:373:ASN:H	1:A:374:GLN:HG3	1.61	0.65
1:A:45:ALA:O	1:A:53:MET:HE3	1.98	0.63
1:A:50:THR:HG23	1:A:52:VAL:H	1.62	0.63
1:A:44:ASP:C	1:A:53:MET:HE1	2.18	0.63
1:A:201:MET:HE2	1:A:205:ILE:HD11	1.82	0.62
1:A:47:ASP:O	1:A:50:THR:O	2.18	0.61
1:A:50:THR:HG21	1:A:297:VAL:HG23	1.81	0.61
1:A:365:VAL:HG12	1:A:376:MET:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:N	1:A:53:MET:CE	2.64	0.61
1:A:366:TYR:CA	1:A:376:MET:CE	2.71	0.60
1:A:110:LYS:HZ1	1:A:111:THR:HG22	1.66	0.60
1:A:44:ASP:HB2	1:A:53:MET:CE	2.31	0.59
1:A:159:GLN:O	1:A:250:ARG:HD2	2.03	0.58
1:A:88:ALA:HB2	1:A:97:LEU:HD22	1.86	0.58
1:A:160:TRP:HA	1:A:250:ARG:HD2	1.87	0.57
1:A:246:ARG:NH2	1:A:308:GLU:HA	2.18	0.57
1:A:141:ARG:HG3	1:A:144:GLY:CA	2.31	0.57
1:A:376:MET:HA	1:A:376:MET:HE2	1.86	0.56
1:A:61:ILE:HD11	1:A:287:PHE:CE2	2.41	0.56
1:A:125:GLY:O	3:A:2036:HOH:O	2.17	0.56
1:A:142:PHE:HB3	1:A:175:LEU:HD23	1.86	0.56
1:A:383:VAL:HG13	3:A:2093:HOH:O	2.06	0.55
1:A:325:LEU:HD21	1:A:383:VAL:HG11	1.89	0.53
1:A:217:ARG:NH2	1:A:223:GLU:OE2	2.37	0.53
1:A:163:GLN:HB2	1:A:166:GLU:HG3	1.91	0.52
1:A:365:VAL:C	1:A:376:MET:HE1	2.29	0.52
1:A:136:GLU:OE2	1:A:139:ALA:HB2	2.10	0.51
1:A:61:ILE:CD1	1:A:287:PHE:CE2	2.94	0.51
1:A:134:THR:HG21	1:A:140:LEU:HG	1.92	0.51
1:A:366:TYR:CA	1:A:376:MET:HE1	2.38	0.51
1:A:47:ASP:CB	1:A:50:THR:HG22	2.39	0.51
1:A:366:TYR:N	1:A:376:MET:HE1	2.26	0.51
1:A:325:LEU:HD21	1:A:383:VAL:CG1	2.41	0.50
1:A:73:VAL:HG12	1:A:201:MET:HE3	1.92	0.50
1:A:240:TYR:OH	1:A:335:GLU:OE1	2.22	0.50
1:A:135:PHE:N	1:A:135:PHE:CD2	2.75	0.50
1:A:170:SER:O	1:A:171:ILE:HG12	2.11	0.50
1:A:126:ASP:N	1:A:141:ARG:HB3	2.27	0.49
1:A:55:HIS:H	1:A:284:HIS:CD2	2.31	0.48
1:A:175:LEU:HD22	1:A:177:VAL:HG13	1.96	0.47
1:A:131:ASP:N	1:A:132:PRO:CD	2.78	0.47
1:A:47:ASP:OD2	1:A:50:THR:HG22	2.14	0.47
1:A:136:GLU:HB3	1:A:165:SER:HA	1.97	0.47
1:A:135:PHE:HD2	1:A:135:PHE:H	1.59	0.46
1:A:272:CYS:SG	3:A:2074:HOH:O	2.06	0.46
1:A:134:THR:HG23	1:A:139:ALA:HB1	1.97	0.46
1:A:163:GLN:HB3	3:A:2041:HOH:O	2.17	0.45
1:A:342:GLY:O	1:A:346:THR:OG1	2.30	0.43
1:A:108:PHE:HB3	3:A:2030:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASP:HB3	1:A:141:ARG:CB	2.48	0.43
1:A:170:SER:O	1:A:171:ILE:CG1	2.67	0.43
1:A:348:ARG:NH2	1:A:381:VAL:HG11	2.34	0.43
1:A:37:HIS:CD2	3:A:2008:HOH:O	2.71	0.43
1:A:224:ARG:CG	1:A:230:VAL:HG21	2.49	0.43
1:A:87:LYS:HE3	3:A:2024:HOH:O	2.19	0.42
1:A:141:ARG:HD3	1:A:141:ARG:HA	1.83	0.42
1:A:267:ALA:O	1:A:282:THR:HA	2.20	0.41
1:A:50:THR:HG23	1:A:52:VAL:HG23	2.03	0.41
1:A:219:PHE:HD2	3:A:2068:HOH:O	2.04	0.41
1:A:120:LEU:O	1:A:124:LYS:HB2	2.21	0.41
1:A:60:HIS:O	1:A:193:MET:HE1	2.20	0.41
1:A:159:GLN:O	1:A:250:ARG:CD	2.68	0.41
1:A:50:THR:HG23	1:A:52:VAL:N	2.34	0.41
1:A:133:GLN:HG3	3:A:2039:HOH:O	2.20	0.41
1:A:158:LYS:HD2	1:A:274:VAL:HA	2.03	0.41
1:A:40:GLY:HA2	2:A:1384:FAD:O3B	2.20	0.41
1:A:142:PHE:HD1	1:A:172:LEU:CD1	2.35	0.40
1:A:365:VAL:HG12	1:A:376:MET:CE	2.48	0.40
1:A:155:TYR:HD1	1:A:272:CYS:HA	1.87	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	373/384 (97%)	354 (95%)	14 (4%)	5 (1%)	15 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PRO

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Mol	Chain	Res	Type
1	A	171	ILE
1	A	170	SER
1	A	309	ASN
1	A	372	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	331/338 (98%)	304 (92%)	27 (8%)	14 15

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	8	ILE
1	A	50	THR
1	A	97	LEU
1	A	110	LYS
1	A	124	LYS
1	A	131	ASP
1	A	135	PHE
1	A	136	GLU
1	A	141	ARG
1	A	147	LEU
1	A	167	LEU
1	A	171	ILE
1	A	172	LEU
1	A	174	ARG
1	A	175	LEU
1	A	177	VAL
1	A	209	GLU
1	A	221	VAL
1	A	255	LYS
1	A	274	VAL
1	A	279	THR

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Mol	Chain	Res	Type
1	A	304	ARG
1	A	324	LEU
1	A	329	LEU
1	A	335	GLU
1	A	380	THR

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	55	HIS
1	A	188	HIS
1	A	284	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	1384	-	48,58,58	1.61	6 (12%)	54,89,89	2.27	9 (16%)

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	1384	-	-	0/30/50/50	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1384	FAD	C8M-C8	2.08	1.55	1.51
2	A	1384	FAD	PA-O1A	3.33	1.63	1.51
2	A	1384	FAD	C10-N1	3.42	1.41	1.35
2	A	1384	FAD	C4-N3	4.45	1.41	1.33
2	A	1384	FAD	C5X-N5	4.56	1.42	1.35
2	A	1384	FAD	C4X-N5	5.41	1.41	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1384	FAD	N3A-C2A-N1A	-12.41	119.39	128.89
2	A	1384	FAD	C4-C4X-C10	-3.81	117.50	119.94
2	A	1384	FAD	P-O3P-PA	-2.70	125.14	132.73
2	A	1384	FAD	C4B-O4B-C1B	-2.01	107.51	109.72
2	A	1384	FAD	C2A-N1A-C6A	2.05	122.44	118.77
2	A	1384	FAD	O2A-PA-O3P	2.74	117.50	105.09
2	A	1384	FAD	C4-C4X-N5	2.84	122.16	118.72
2	A	1384	FAD	C1'-N10-C9A	2.91	122.12	118.86
2	A	1384	FAD	C4-N3-C2	5.46	119.97	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1384	FAD	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, 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	377/384 (98%)	0.39	38 (10%) 9 15	31, 42, 56, 67	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	ASN	6.0
1	A	135	PHE	5.6
1	A	371	THR	4.3
1	A	15	GLY	4.3
1	A	323	ALA	4.1
1	A	13	PHE	4.1
1	A	341	VAL	4.0
1	A	319	MET	3.8
1	A	171	ILE	3.6
1	A	132	PRO	3.3
1	A	233	SER	3.2
1	A	16	ALA	3.1
1	A	308	GLU	3.0
1	A	11	ALA	2.9
1	A	17	VAL	2.9
1	A	241	GLY	2.8
1	A	373	ASN	2.8
1	A	330	SER	2.8
1	A	361	LYS	2.8
1	A	42	SER	2.8
1	A	368	ASN	2.8
1	A	14	SER	2.8
1	A	10	GLY	2.7
1	A	307	GLU	2.7
1	A	8	ILE	2.7
1	A	202	ILE	2.7
1	A	342	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	292	GLN	2.5
1	A	170	SER	2.3
1	A	374	GLN	2.3
1	A	232	TYR	2.2
1	A	344	LEU	2.2
1	A	51	ASN	2.2
1	A	131	ASP	2.1
1	A	345	GLY	2.1
1	A	375	PRO	2.1
1	A	140	LEU	2.1
1	A	136	GLU	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	A	1384	53/53	0.96	0.14	-0.70	24,33,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.