



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:15 pm GMT

PDB ID : 1V5G
Title : Crystal Structure of the Reaction Intermediate between Pyruvate oxidase containing FAD and TPP, and Substrate Pyruvate
Authors : Hossain, M.T.; Suzuki, K.; Yamamoto, T.; Imamura, S.; Sekiguchi, T.; Takenaka, A.
Deposited on : 2003-11-22
Resolution : 1.96 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

<https://www.wwpdb.org/validation/2017/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	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

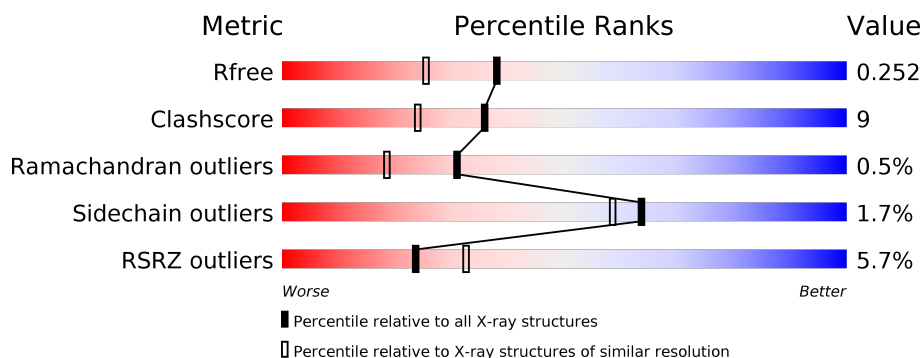
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	111664	2220 (1.96-1.96)
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (1.96-1.96)

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	589	<div> <div>6%</div> <div>83%</div> <div>16%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5362 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.

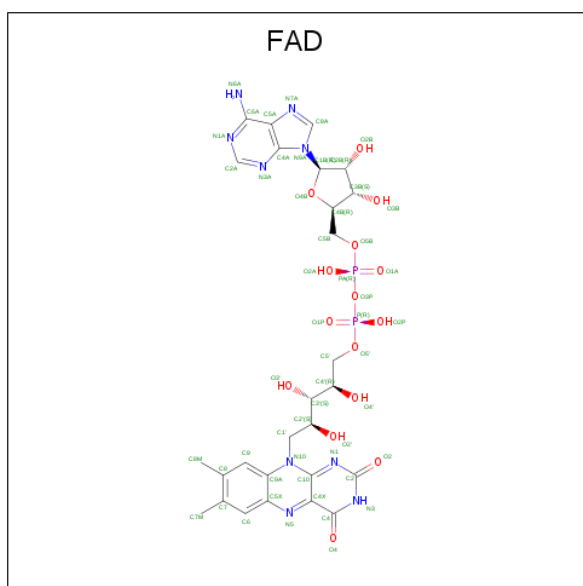
- Molecule 1 is a protein called Pyruvate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	72	0	0
			4590	2908	774	888	20			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

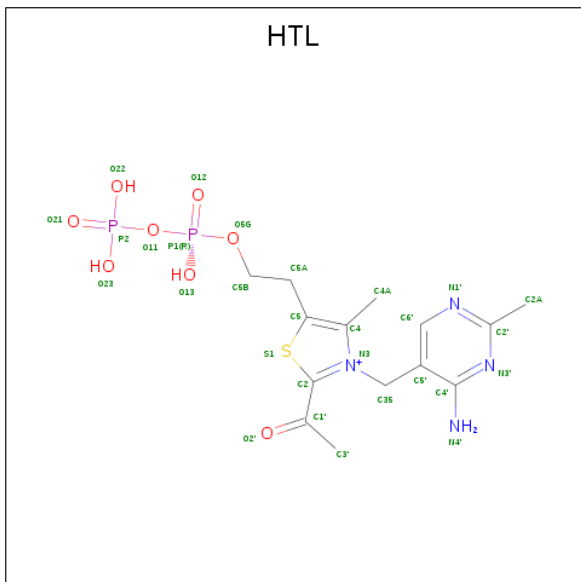
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	29	14	4	8	2	0	0

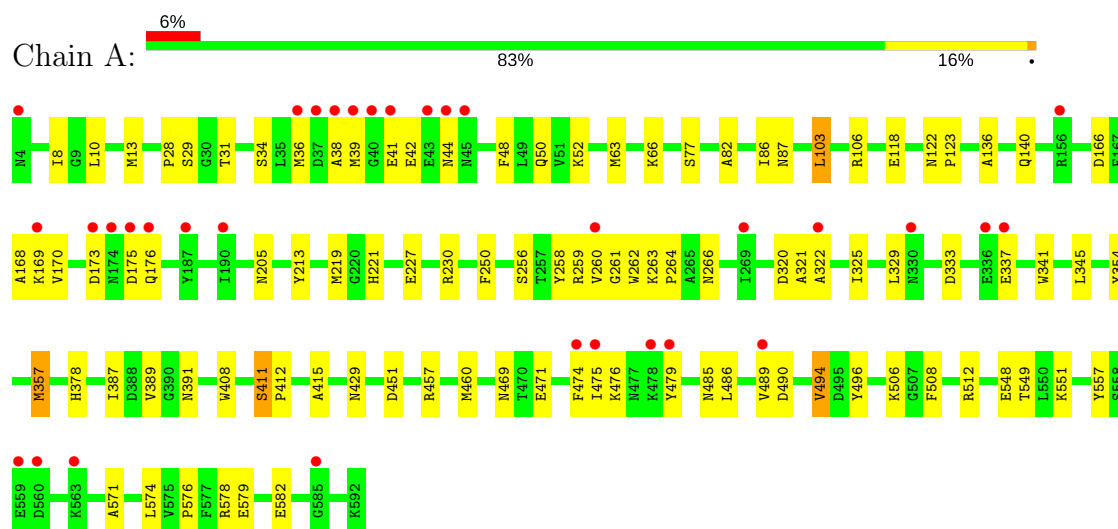
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	689	Total	O	0	0
			689	689		

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 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 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: Pyruvate oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.01Å 105.50Å 155.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.96 38.96 – 1.92	Depositor EDS
% Data completeness (in resolution range)	94.4 (10.00-1.96) 96.5 (38.96-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.01 (at 1.92Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.244 0.203 , 0.252	Depositor DCC
R_{free} test set	4804 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5362	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 0.333 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: MG, HTL, 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	0.31	0/4686	0.60	1/6362 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	SER	N-CA-C	-5.39	96.45	111.00

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	A	4590	0	4489	77	0
2	A	1	0	0	0	0
3	A	53	0	31	5	0
4	A	29	0	18	4	0
5	A	689	0	0	8	0
All	All	5362	0	4538	79	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 9.

All (79) 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:221:HIS:CE1	1:A:322:ALA:HB2	2.05	0.92
1:A:258:TYR:H	1:A:266:ASN:HD21	1.19	0.87
1:A:166:ASP:O	1:A:169:LYS:HG2	1.80	0.82
1:A:166:ASP:HB2	1:A:169:LYS:HE3	1.64	0.79
1:A:221:HIS:NE2	1:A:322:ALA:HB2	1.96	0.79
1:A:10:LEU:HD13	1:A:41:GLU:HB2	1.67	0.77
1:A:34:SER:HB3	1:A:168:ALA:HB3	1.66	0.77
1:A:205:ASN:HD21	1:A:333:ASP:H	1.36	0.72
1:A:36:MET:HG2	1:A:39:MET:HE2	1.72	0.71
1:A:258:TYR:H	1:A:266:ASN:ND2	1.88	0.71
1:A:320:ASP:OD2	1:A:322:ALA:HB3	1.92	0.69
1:A:258:TYR:N	1:A:266:ASN:HD21	1.92	0.64
1:A:469:ASN:O	1:A:471:GLU:HG3	1.98	0.63
1:A:34:SER:CB	1:A:168:ALA:HB3	2.29	0.63
1:A:411:SER:O	1:A:415:ALA:HA	1.99	0.61
1:A:221:HIS:CD2	1:A:322:ALA:HB2	2.36	0.60
1:A:50:GLN:HE21	1:A:52:LYS:NZ	2.01	0.59
1:A:576:PRO:HG2	1:A:579:GLU:HG3	1.85	0.59
1:A:136:ALA:H	1:A:140:GLN:NE2	2.02	0.58
1:A:494:VAL:HG22	1:A:496:TYR:CE2	2.39	0.57
1:A:13:MET:HB3	1:A:44:ASN:ND2	2.19	0.57
1:A:136:ALA:H	1:A:140:GLN:HE21	1.53	0.56
4:A:1602:HTL:H4'2	4:A:1602:HTL:C1'	2.18	0.55
1:A:38:ALA:HB2	5:A:1825:HOH:O	2.06	0.55
1:A:429:ASN:HB2	1:A:460:MET:HE1	1.88	0.54
1:A:387:ILE:HG13	1:A:408:TRP:CE2	2.44	0.53
1:A:256:SER:OG	1:A:261:GLY:HA2	2.09	0.53
1:A:475:ILE:HD11	4:A:1602:HTL:H4A3	1.90	0.53
1:A:8:ILE:HD12	1:A:170:VAL:HB	1.90	0.53
1:A:571:ALA:HB1	1:A:574:LEU:HD12	1.90	0.52
1:A:260:VAL:HB	3:A:1601:FAD:C4X	2.39	0.52
1:A:387:ILE:HG13	1:A:408:TRP:NE1	2.26	0.51
1:A:476:LYS:O	1:A:479:TYR:HB2	2.11	0.51
1:A:28:PRO:HA	1:A:36:MET:CE	2.41	0.51
1:A:82:ALA:HB1	1:A:103:LEU:HG	1.92	0.50
3:A:1601:FAD:N1	3:A:1601:FAD:H2'	2.27	0.50
1:A:230:ARG:HE	1:A:250:PHE:HE1	1.58	0.50
1:A:221:HIS:HE1	5:A:1619:HOH:O	1.93	0.50
1:A:221:HIS:CD2	1:A:322:ALA:CB	2.95	0.49
1:A:354:TYR:O	1:A:357:MET:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG21	5:A:2291:HOH:O	2.12	0.49
1:A:512:ARG:HD3	5:A:2114:HOH:O	2.10	0.49
1:A:391:ASN:HD22	1:A:474:PHE:HD1	1.60	0.49
1:A:551:LYS:HG2	1:A:557:TYR:CE2	2.48	0.49
1:A:260:VAL:O	1:A:260:VAL:HG12	2.13	0.48
1:A:258:TYR:CG	1:A:259:ARG:N	2.79	0.48
1:A:63:MET:SD	1:A:66:LYS:HD2	2.53	0.48
1:A:176:GLN:HG3	5:A:1869:HOH:O	2.12	0.48
1:A:39:MET:HE1	1:A:48:PHE:HB2	1.95	0.48
1:A:260:VAL:HB	3:A:1601:FAD:N5	2.28	0.48
1:A:173:ASP:HB3	1:A:175:ASP:OD1	2.13	0.48
1:A:321:ALA:O	1:A:325:ILE:HG12	2.14	0.47
1:A:506:LYS:HG3	1:A:508:PHE:CE1	2.49	0.47
1:A:389:VAL:HG13	3:A:1601:FAD:HM71	1.96	0.46
1:A:322:ALA:HB3	5:A:1824:HOH:O	2.14	0.46
1:A:263:LYS:HB3	1:A:264:PRO:HD3	1.96	0.46
1:A:29:SER:HB2	1:A:77:SER:HB3	1.98	0.46
1:A:106:ARG:HG3	1:A:118:GLU:HB2	1.98	0.46
1:A:29:SER:CB	1:A:77:SER:HB3	2.46	0.45
1:A:176:GLN:NE2	1:A:176:GLN:HA	2.32	0.45
1:A:391:ASN:HB2	4:A:1602:HTL:O22	2.17	0.45
1:A:548:GLU:HG2	1:A:549:THR:HG23	1.99	0.45
1:A:221:HIS:NE2	1:A:322:ALA:CB	2.74	0.44
1:A:322:ALA:HB1	5:A:1775:HOH:O	2.17	0.43
1:A:378:HIS:HD2	5:A:1847:HOH:O	2.01	0.43
1:A:489:VAL:HG23	1:A:490:ASP:OD1	2.18	0.43
1:A:38:ALA:O	1:A:41:GLU:HG2	2.18	0.43
1:A:50:GLN:HE21	1:A:52:LYS:HZ1	1.66	0.43
1:A:412:PRO:HA	3:A:1601:FAD:HM81	1.99	0.43
1:A:578:ARG:O	1:A:582:GLU:HG3	2.19	0.43
1:A:86:ILE:HG23	1:A:87:ASN:N	2.34	0.42
1:A:122:ASN:N	1:A:123:PRO:CD	2.83	0.42
1:A:13:MET:HB3	1:A:44:ASN:HD21	1.83	0.42
1:A:341:TRP:NE1	1:A:345:LEU:HD11	2.35	0.42
1:A:227:GLU:HG2	1:A:329:LEU:HD11	2.02	0.41
1:A:475:ILE:CD1	4:A:1602:HTL:H4A3	2.50	0.41
1:A:50:GLN:HE21	1:A:52:LYS:HZ3	1.67	0.41
1:A:262:TRP:HB3	1:A:264:PRO:HD2	2.02	0.40
1:A:476:LYS:HG3	1:A:489:VAL:HG21	2.04	0.40

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	587/589 (100%)	558 (95%)	26 (4%)	3 (0%)	31 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	486	LEU
1	A	485	ASN

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	482/482 (100%)	474 (98%)	8 (2%)	63 58

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	A	213	TYR
1	A	219	MET
1	A	337	GLU
1	A	357	MET
1	A	451	ASP
1	A	457	ARG
1	A	494	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	50	GLN
1	A	64	GLN
1	A	96	ASN
1	A	140	GLN
1	A	176	GLN
1	A	195	GLN
1	A	205	ASN
1	A	206	ASN
1	A	221	HIS
1	A	266	ASN
1	A	312	HIS
1	A	378	HIS
1	A	391	ASN
1	A	394	GLN
1	A	429	ASN

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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
3	FAD	A	1601	-	51,58,58	1.11	4 (7%)	57,89,89	1.97	5 (8%)
4	HTL	A	1602	2	24,30,30	1.00	2 (8%)	28,45,45	2.07	4 (14%)

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	FAD	A	1601	-	-	0/28/50/50	0/6/6/6
4	HTL	A	1602	2	-	0/16/21/21	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1602	HTL	C4'-N3'	2.30	1.38	1.35
4	A	1602	HTL	C5'-C4'	2.35	1.46	1.42
3	A	1601	FAD	C9A-N10	2.47	1.41	1.38
3	A	1601	FAD	C4-N3	2.53	1.37	1.33
3	A	1601	FAD	C10-N1	2.60	1.36	1.33
3	A	1601	FAD	C4X-N5	3.76	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1601	FAD	C4X-C4-N3	-4.64	116.88	123.47
4	A	1602	HTL	C35-C5'-C6'	-2.14	116.60	120.69
4	A	1602	HTL	C2A-C2'-N3'	2.07	120.67	117.20
3	A	1601	FAD	C5X-C9A-N10	2.13	119.34	117.71
4	A	1602	HTL	C6'-N1'-C2'	2.31	119.98	115.95
3	A	1601	FAD	C4X-N5-C5X	3.48	120.41	116.76
3	A	1601	FAD	C1'-N10-C9A	4.98	122.73	118.31
4	A	1602	HTL	C4-N3-C2	8.94	113.61	108.64
3	A	1601	FAD	C4-N3-C2	10.56	124.13	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1601	FAD	5	0
4	A	1602	HTL	4	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	580/589 (98%)	0.42	33 (5%) 24 32	15, 21, 38, 70	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	GLU	5.3
1	A	479	TYR	5.0
1	A	40	GLY	4.3
1	A	4	ASN	4.0
1	A	38	ALA	4.0
1	A	44	ASN	3.5
1	A	187	TYR	3.3
1	A	336	GLU	3.3
1	A	43	GLU	3.3
1	A	260	VAL	3.3
1	A	37	ASP	3.3
1	A	330	ASN	3.2
1	A	190	ILE	3.0
1	A	45	ASN	3.0
1	A	174	ASN	2.9
1	A	560	ASP	2.8
1	A	175	ASP	2.8
1	A	36	MET	2.8
1	A	173	ASP	2.6
1	A	322	ALA	2.6
1	A	169	LYS	2.5
1	A	269	ILE	2.4
1	A	39	MET	2.4
1	A	337	GLU	2.4
1	A	559	GLU	2.3
1	A	156	ARG	2.2
1	A	475	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	585	GLY	2.2
1	A	563	LYS	2.2
1	A	176	GLN	2.1
1	A	489	VAL	2.0
1	A	474	PHE	2.0
1	A	478	LYS	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. 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	B-factors(Å ²)	Q<0.9
3	FAD	A	1601	53/53	0.90	0.17	16,20,23,26	0
4	HTL	A	1602	29/29	0.96	0.12	11,19,23,30	0
2	MG	A	1603	1/1	0.97	0.12	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.