



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:52 PM GMT

PDB ID : 2EZ8  
Title : Pyruvate oxidase variant F479W in complex with reaction intermediate 2-lactyl-thiamin diphosphate  
Authors : Wille, G.; Meyer, D.; Steinmetz, A.; Hinze, E.; Golbik, R.; Tittmann, K.  
Deposited on : 2005-11-10  
Resolution : 1.96 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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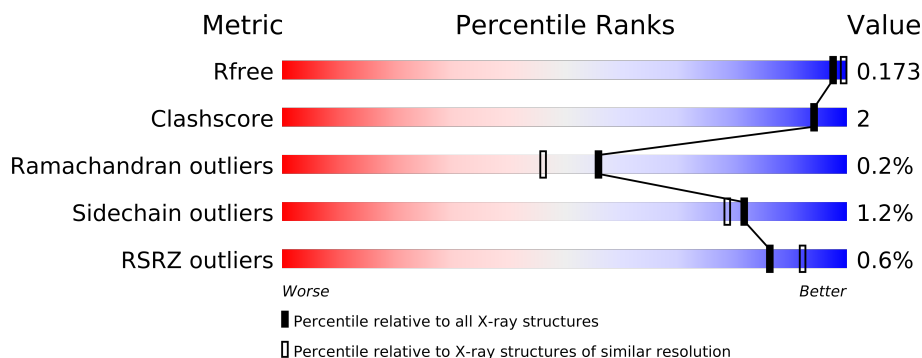
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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  $\geq 3$ , 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	603	
1	B	603	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10225 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 Pyruvate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4523	2868	780	861	14			
1	B	585	Total	C	N	O	S	0	0	0
			4523	2868	780	861	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	479	TRP	PHE	ENGINEERED	UNP P37063
A	561	MET	THR	see remark 999	UNP P37063
B	479	TRP	PHE	ENGINEERED	UNP P37063
B	561	MET	THR	see remark 999	UNP P37063

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

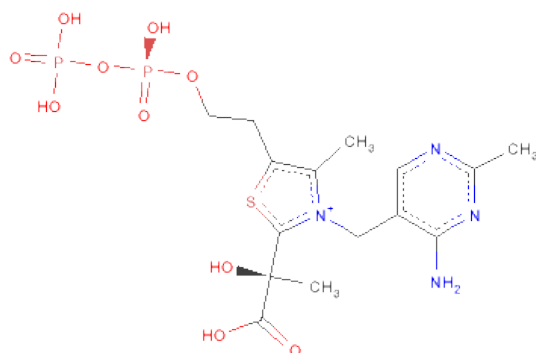
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

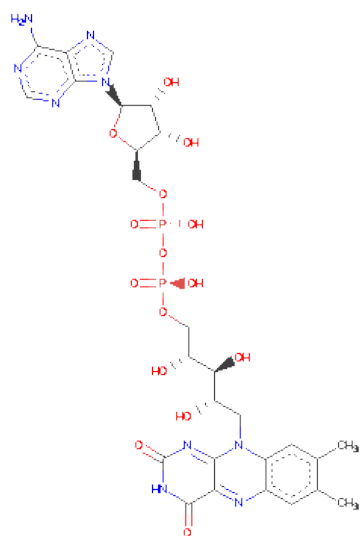
- Molecule 4 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-CARBOXY-1-HYDROXYETHYL)-5-(2-{[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDL) (formula:

$C_{15}H_{23}N_4O_{10}P_2S$ ).



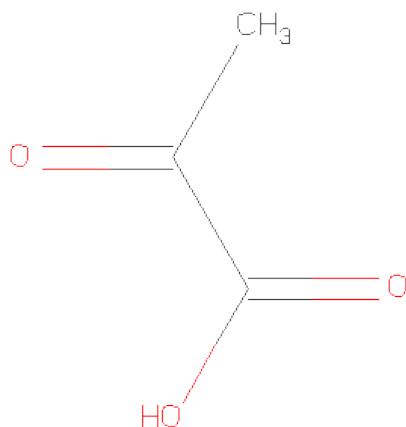
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	32	15	4	10	2	1	0	0
4	B	1	32	15	4	10	2	1	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

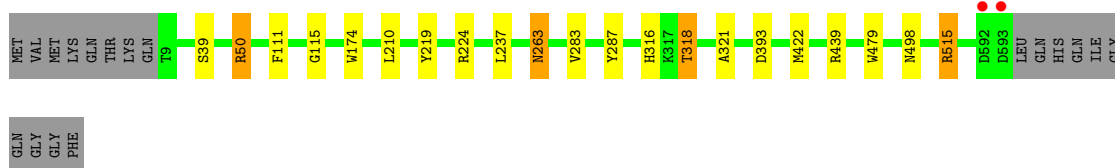
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	504	Total	O	0	0
			504	504		
7	B	489	Total	O	0	0
			489	489		

### 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.

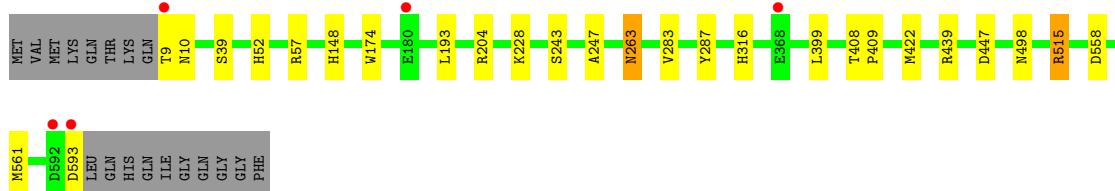
- Molecule 1: Pyruvate oxidase

Chain A: 



- Molecule 1: Pyruvate oxidase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.13Å 154.46Å 165.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 1.96 24.96 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.0 (24.96-1.96) 98.0 (24.96-1.96)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.94 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.149 , 0.172 0.151 , 0.173	Depositor DCC
$R_{free}$ test set	2105 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 32.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 105590 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: NA, MG, PYR, FAD, TDL

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	0.64	0/4619	0.65	3/6291 (0.0%)
1	B	0.68	0/4619	0.66	4/6291 (0.1%)
All	All	0.66	0/9238	0.65	7/12582 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	439	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	439	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	515	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	515	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	515	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	447	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4523	0	4468	13	0
1	B	4523	0	4468	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	19	2	0
4	B	32	0	19	1	0
5	A	53	0	31	0	0
5	B	53	0	31	0	0
6	A	6	0	3	0	0
6	B	6	0	3	0	0
7	A	504	0	0	6	0
7	B	489	0	0	4	0
All	All	10225	0	9042	28	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 2.

All (28) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:318:THR:HG23	7:A:2114:HOH:O	1.76	0.84
1:A:318:THR:HG21	1:A:321:ALA:HB2	1.76	0.68
1:B:57:ARG:HD2	7:B:1859:HOH:O	1.95	0.66
1:A:318:THR:CG2	7:A:2114:HOH:O	2.41	0.62
1:A:422:MET:SD	4:A:1611:TDL:HM43	2.45	0.56
1:B:422:MET:SD	4:B:1616:TDL:HM43	2.47	0.55
1:A:316:HIS:HE1	7:A:2055:HOH:O	1.91	0.53
1:B:204:ARG:HG2	1:B:204:ARG:HH11	1.73	0.53
1:B:9:THR:HG23	1:B:10:ASN:H	1.74	0.52
7:A:1774:HOH:O	1:B:148:HIS:HE1	1.93	0.51
1:B:39:SER:HB3	1:B:174:TRP:CD2	2.46	0.50
1:B:316:HIS:HE1	7:B:1855:HOH:O	1.94	0.50
1:A:111:PHE:CE1	1:A:115:GLY:HA3	2.47	0.49
1:A:263:ASN:HB2	1:A:287:TYR:OH	2.13	0.48
1:B:399:LEU:HD23	1:B:399:LEU:C	2.33	0.48
1:A:39:SER:HB3	1:A:174:TRP:CD2	2.50	0.46
1:B:263:ASN:HB2	1:B:287:TYR:OH	2.16	0.45
1:A:316:HIS:HD2	7:A:1677:HOH:O	2.00	0.44
1:A:50:ARG:NH1	7:A:1892:HOH:O	2.50	0.44
1:B:243:SER:HB2	1:B:247:ALA:HB3	2.00	0.43
1:B:408:THR:HB	1:B:409:PRO:HD2	2.01	0.43
1:A:219:TYR:HB3	1:A:283:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:228:LYS:HE3	1:B:228:LYS:HB2	1.89	0.42
1:B:316:HIS:HD2	7:B:1723:HOH:O	2.02	0.42
1:A:210:LEU:HD21	1:A:237:LEU:HD22	2.01	0.42
1:B:52:HIS:HE1	7:B:1886:HOH:O	2.02	0.42
1:B:558:ASP:HB3	1:B:561:MET:HE3	2.02	0.41
1:A:479:TRP:CD1	4:A:1611:TDL:HLB3	2.56	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	A	583/603 (97%)	570 (98%)	12 (2%)	1 (0%)	56	46
1	B	583/603 (97%)	571 (98%)	11 (2%)	1 (0%)	56	46
All	All	1166/1206 (97%)	1141 (98%)	23 (2%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	B	263	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	470/485 (97%)	464 (99%)	6 (1%)	80	76
1	B	470/485 (97%)	465 (99%)	5 (1%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	940/970 (97%)	929 (99%)	11 (1%)	82	79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	224	ARG
1	A	318	THR
1	A	393	ASP
1	A	498	ASN
1	A	515	ARG
1	B	193	LEU
1	B	283	VAL
1	B	498	ASN
1	B	515	ARG
1	B	593	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	148	HIS
1	A	176	GLN
1	A	316	HIS
1	A	464	HIS
1	A	476	GLN
1	B	10	ASN
1	B	52	HIS
1	B	148	HIS
1	B	276	GLN
1	B	316	HIS
1	B	464	HIS
1	B	476	GLN
1	B	572	GLN
1	B	588	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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$
4	TDL	A	1611	2	33,33,33	1.48	6 (18%)	48,51,51	2.05	14 (29%)
5	FAD	A	1614	-	58,58,58	1.24	2 (3%)	85,89,89	2.20	18 (21%)
6	PYR	A	1615	-	5,5,5	3.34	3 (60%)	6,6,6	1.42	2 (33%)
4	TDL	B	1616	2	33,33,33	1.44	5 (15%)	48,51,51	2.14	14 (29%)
5	FAD	B	1617	-	58,58,58	1.12	2 (3%)	85,89,89	2.22	17 (20%)
6	PYR	B	1618	-	5,5,5	3.43	3 (60%)	6,6,6	1.66	1 (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
4	TDL	A	1611	2	-	0/23/29/29	0/2/2/2
5	FAD	A	1614	-	-	0/34/50/50	0/1/6/6
6	PYR	A	1615	-	-	0/4/4/4	0/0/0/0
4	TDL	B	1616	2	-	0/23/29/29	0/2/2/2
5	FAD	B	1617	-	-	0/34/50/50	0/1/6/6
6	PYR	B	1618	-	-	0/4/4/4	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1614	FAD	C1'-C2'	6.74	1.58	1.51
6	B	1618	PYR	C2-C1	-6.11	1.39	1.53
5	B	1617	FAD	C1'-C2'	6.02	1.57	1.51
6	A	1615	PYR	C2-C1	-5.46	1.40	1.53
6	A	1615	PYR	O3-C2	4.34	1.32	1.23
4	B	1616	TDL	C5-C4	4.32	1.41	1.36
4	A	1611	TDL	C5-C4	4.31	1.41	1.36
6	B	1618	PYR	O3-C2	3.81	1.31	1.23
4	A	1611	TDL	CLA-CLC	2.72	1.58	1.54
4	B	1616	TDL	CLA-CLC	2.64	1.58	1.54
4	A	1611	TDL	PB-O3A	2.60	1.64	1.60
6	A	1615	PYR	O1-C1	2.59	1.30	1.22
6	B	1618	PYR	O1-C1	2.48	1.30	1.22
4	B	1616	TDL	C2-S1	2.47	1.76	1.73
4	B	1616	TDL	PB-O3A	2.46	1.64	1.60
5	A	1614	FAD	C4A-N9A	-2.44	1.34	1.37
4	A	1611	TDL	C7'-C5'	2.43	1.56	1.51
5	B	1617	FAD	C4A-N9A	-2.42	1.34	1.37
4	A	1611	TDL	C2-S1	2.13	1.76	1.73
4	B	1616	TDL	C7'-C5'	2.12	1.55	1.51
4	A	1611	TDL	OL3-CLC	2.03	1.29	1.22

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1617	FAD	C2'-C1'-N10	-11.34	97.41	112.45
5	A	1614	FAD	C2'-C1'-N10	-10.95	97.92	112.45
5	B	1617	FAD	N3A-C2A-N1A	-9.76	120.55	128.71
5	A	1614	FAD	N3A-C2A-N1A	-8.77	121.38	128.71
4	A	1611	TDL	C6-C5-C4	6.28	132.01	127.44
4	B	1616	TDL	OL2-CLC-CLA	6.11	123.35	113.29
5	A	1614	FAD	C2-N1-C10	5.99	121.02	114.98
4	B	1616	TDL	C6-C5-C4	5.80	131.66	127.44
4	A	1611	TDL	OL2-CLC-CLA	5.25	121.94	113.29
5	B	1617	FAD	C2-N1-C10	5.18	120.20	114.98
5	A	1614	FAD	C4X-C10-N10	-5.07	117.98	120.51
5	B	1617	FAD	C9A-N10-C10	-4.85	117.00	121.77
4	B	1616	TDL	OL1-CLA-C2	4.26	117.48	107.98
4	B	1616	TDL	C2-CLA-CLC	-4.07	103.87	113.34
4	A	1611	TDL	CM2-C2'-N1'	3.87	121.63	117.02
5	B	1617	FAD	N3A-C4A-N9A	3.79	132.27	125.43
5	A	1614	FAD	N3A-C4A-N9A	3.65	132.02	125.43
4	A	1611	TDL	C5-C4-N3	3.62	115.22	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1617	FAD	C4X-C10-N10	-3.59	118.72	120.51
4	A	1611	TDL	CM4-C4-C5	-3.55	120.23	129.10
5	A	1614	FAD	C9A-N10-C10	-3.43	118.40	121.77
4	B	1616	TDL	C5-C4-N3	3.28	114.51	107.66
4	B	1616	TDL	C5'-C7'-N3	-3.28	107.70	113.26
6	B	1618	PYR	O2-C1-C2	3.28	121.59	114.37
4	B	1616	TDL	N1'-C2'-N3'	-3.27	119.75	125.65
5	B	1617	FAD	C1'-N10-C9A	3.13	121.92	118.87
4	A	1611	TDL	C2-CLA-CLC	-3.10	106.14	113.34
4	B	1616	TDL	C2-N3-C4	2.98	112.36	109.76
5	A	1614	FAD	C9A-C5X-N5	-2.96	117.82	122.37
4	B	1616	TDL	CM2-C2'-N1'	2.96	120.54	117.02
4	A	1611	TDL	N1'-C2'-N3'	-2.95	120.33	125.65
5	B	1617	FAD	C4X-C10-N1	-2.87	119.86	122.73
5	A	1614	FAD	C1'-N10-C9A	2.84	121.63	118.87
4	B	1616	TDL	CM4-C4-C5	-2.83	122.03	129.10
4	A	1611	TDL	C5'-C7'-N3	-2.82	108.48	113.26
5	A	1614	FAD	C8A-N9A-C4A	2.80	109.04	106.90
4	A	1611	TDL	OL1-CLA-C2	2.78	114.18	107.98
5	A	1614	FAD	C1B-N9A-C4A	-2.75	121.88	126.64
5	A	1614	FAD	C1'-N10-C10	-2.71	115.32	119.17
4	B	1616	TDL	OL2-CLC-OL3	-2.69	115.30	123.76
4	A	1611	TDL	OL2-CLC-OL3	-2.65	115.41	123.76
4	B	1616	TDL	C6'-N1'-C2'	2.61	120.27	115.68
5	B	1617	FAD	C8A-N9A-C4A	2.61	108.89	106.90
4	A	1611	TDL	C6'-N1'-C2'	2.54	120.14	115.68
5	A	1614	FAD	C4X-C10-N1	-2.52	120.21	122.73
5	A	1614	FAD	C1'-C2'-C3'	2.49	116.93	109.82
4	B	1616	TDL	C7-C6-C5	2.48	119.16	112.48
6	A	1615	PYR	O2-C1-C2	2.46	119.79	114.37
5	B	1617	FAD	C1'-C2'-C3'	2.46	116.85	109.82
4	A	1611	TDL	C7-C6-C5	2.45	119.07	112.48
5	B	1617	FAD	C5A-C4A-N3A	-2.31	120.67	125.70
4	A	1611	TDL	C6-C5-S1	-2.26	117.74	120.74
5	A	1614	FAD	N1-C10-N10	2.22	121.81	115.97
5	B	1617	FAD	C5X-C9A-N10	2.21	118.98	116.80
5	B	1617	FAD	O2P-P-O1P	2.19	124.42	112.21
5	B	1617	FAD	C4-N3-C2	-2.17	120.93	125.39
5	A	1614	FAD	C5A-C4A-N3A	-2.17	120.98	125.70
5	B	1617	FAD	C1B-N9A-C4A	-2.17	122.89	126.64
5	B	1617	FAD	C9A-C5X-N5	-2.11	119.14	122.37
5	A	1614	FAD	C6-C5X-N5	2.07	121.39	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1617	FAD	N1-C10-N10	2.07	121.42	115.97
4	B	1616	TDL	C2'-N3'-C4'	2.06	122.08	118.18
5	A	1614	FAD	O2P-P-O1P	2.05	123.64	112.21
5	A	1614	FAD	O2'-C2'-C1'	2.04	114.78	109.71
4	A	1611	TDL	O3B-PB-O2B	2.03	115.52	107.61
6	A	1615	PYR	O2-C1-O1	-2.00	118.89	123.62

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	585/603 (97%)	-0.48	2 (0%) 91 95	6, 11, 22, 46	0
1	B	585/603 (97%)	-0.47	5 (0%) 81 88	6, 10, 21, 48	0
All	All	1170/1206 (97%)	-0.47	7 (0%) 86 92	6, 10, 21, 48	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	592	ASP	4.7
1	A	592	ASP	4.6
1	B	593	ASP	3.8
1	A	593	ASP	3.3
1	B	9	THR	2.2
1	B	368	GLU	2.1
1	B	180	GLU	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NA	B	1511	1/1	0.09	1.55	5,5,5,5	1
6	PYR	A	1615	6/6	0.16	1.38	20,22,23,24	0
4	TDL	A	1611	32/32	0.08	1.30	7,11,23,25	0
3	NA	A	1513	1/1	0.09	1.21	5,5,5,5	1
4	TDL	B	1616	32/32	0.08	1.03	5,10,23,25	0
6	PYR	B	1618	6/6	0.14	1.01	17,20,21,26	0
5	FAD	A	1614	53/53	0.06	-0.38	6,8,10,10	0
5	FAD	B	1617	53/53	0.06	-0.66	5,7,9,9	0
2	MG	B	1512	1/1	0.04	-1.56	9,9,9,9	0
2	MG	A	1510	1/1	0.04	-2.15	9,9,9,9	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.