



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:17 pm GMT

PDB ID : 4FEE  
Title : High-resolution structure of pyruvate oxidase in complex with reaction intermediate 2-hydroxyethyl-thiamin diphosphate carbanion-enamine, crystal B  
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Deposited on : 2012-05-30  
Resolution : 1.13 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](mailto: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.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

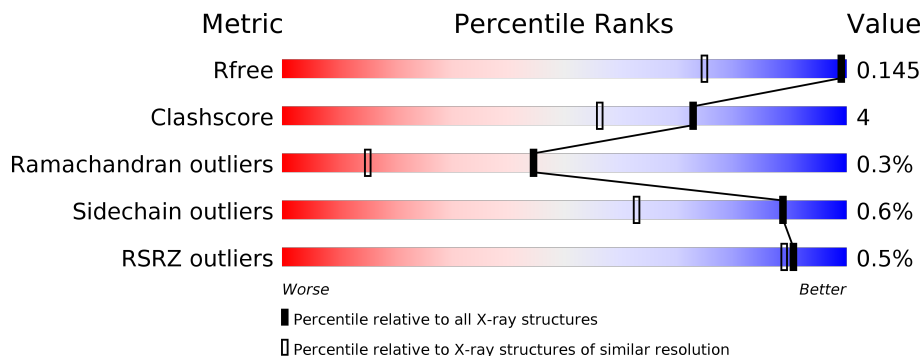
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.13 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))
$R_{free}$	100719	1062 (1.16-1.08)
Clashscore	112137	1107 (1.16-1.08)
Ramachandran outliers	110173	1065 (1.16-1.08)
Sidechain outliers	110143	1062 (1.16-1.08)
RSRZ outliers	101464	1067 (1.16-1.08)

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. 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	603	<div> <div></div> <div>89%</div> <div>7%</div> <div>...</div> </div>
1	B	603	<div> <div></div> <div>87%</div> <div>9%</div> <div>...</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	702	-	-	-	X
3	GOL	A	705	-	-	-	X
3	GOL	A	706	-	-	-	X
3	GOL	A	709	-	-	-	X
3	GOL	B	706	-	-	-	X
3	GOL	B	707	-	-	-	X
4	PYR	A	703	-	-	X	-
4	PYR	A	704	-	-	-	X
4	PYR	B	703	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11714 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	586	Total	C	N	O	S	0	41	0
			4890	3095	853	923	19			
1	B	583	Total	C	N	O	S	0	44	0
			4884	3093	847	923	21			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



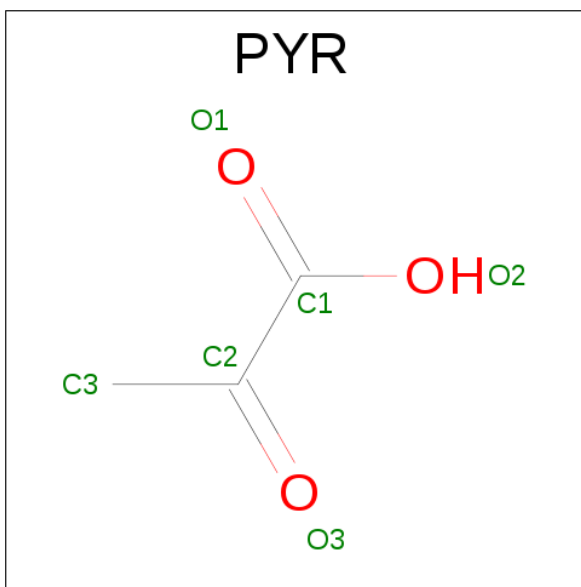
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



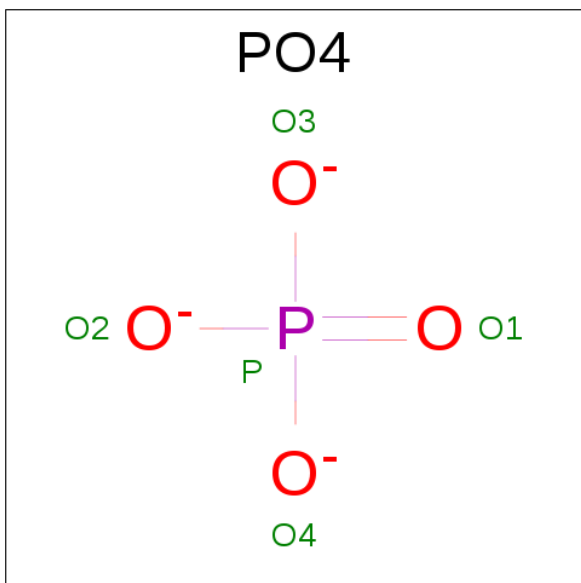
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



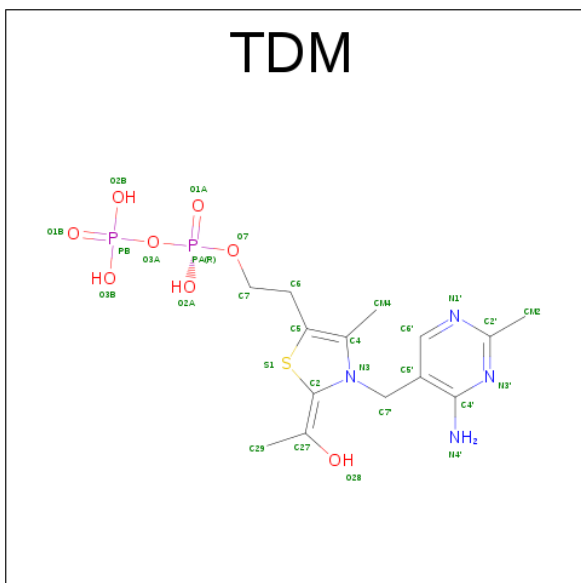
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0
5	B	1	Total 5	O 4	P 1	0	0

- Molecule 6 is 2-[(2E)-3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-HYDROXYETHYLIDENE)-4-METHYL-2,3-DIHYDRO-1,3-THIAZOL-5-YL]ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TDM) (formula:  $C_{14}H_{22}N_4O_8P_2S$ ).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is water.

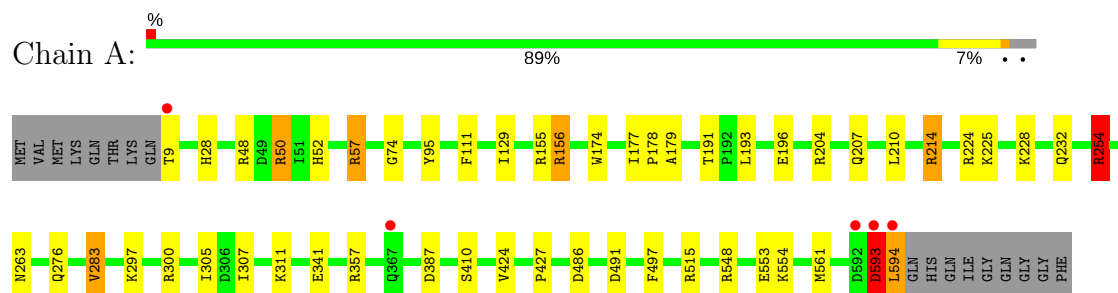
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	827	Total 843	O 843	0	16
8	B	844	Total 861	O 861	0	15



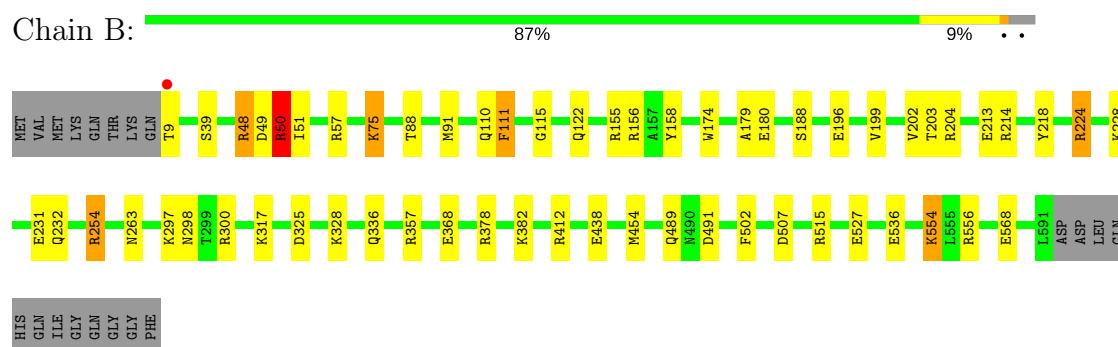
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Pyruvate oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.07Å 154.46Å 165.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.13 47.69 – 1.13	Depositor EDS
% Data completeness (in resolution range)	95.1 (20.00-1.13) 92.5 (47.69-1.13)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 1.13Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.122 , 0.149 0.125 , 0.145	Depositor DCC
$R_{free}$ test set	10989 reflections (2.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.4	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 66.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	11714	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, TDM, PO4, PYR, 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	0.68	0/4998	1.29	45/6789 (0.7%)
1	B	0.69	0/4990	1.24	40/6775 (0.6%)
All	All	0.68	0/9988	1.26	85/13564 (0.6%)

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	4
1	B	0	4
All	All	0	8

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ARG	NE-CZ-NH2	22.83	131.71	120.30
1	A	357	ARG	NE-CZ-NH1	-20.63	109.98	120.30
1	A	48[A]	ARG	NE-CZ-NH1	19.24	129.92	120.30
1	A	48[B]	ARG	NE-CZ-NH1	19.24	129.92	120.30
1	B	155	ARG	NE-CZ-NH1	-18.08	111.26	120.30
1	B	357[A]	ARG	NE-CZ-NH2	-15.34	112.63	120.30
1	B	357[C]	ARG	NE-CZ-NH2	-15.34	112.63	120.30
1	A	155	ARG	NE-CZ-NH2	14.79	127.69	120.30
1	A	155	ARG	NE-CZ-NH1	-13.03	113.78	120.30
1	A	57	ARG	NE-CZ-NH2	-12.87	113.87	120.30
1	A	357	ARG	NH1-CZ-NH2	12.71	133.38	119.40
1	B	156	ARG	NE-CZ-NH2	-12.53	114.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ARG	NE-CZ-NH1	12.29	126.45	120.30
1	A	515	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	A	57	ARG	NE-CZ-NH1	11.91	126.26	120.30
1	A	196	GLU	OE1-CD-OE2	11.66	137.29	123.30
1	A	300	ARG	NE-CZ-NH2	-11.51	114.55	120.30
1	B	155	ARG	CD-NE-CZ	11.19	139.27	123.60
1	B	515	ARG	NE-CZ-NH2	11.08	125.84	120.30
1	B	556	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	B	57	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	B	156	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	B	515	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	B	556	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	A	50[A]	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	A	50[B]	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	B	57	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	B	48	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	50[A]	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	50[B]	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	95[A]	TYR	CB-CG-CD2	8.37	126.02	121.00
1	A	95[B]	TYR	CB-CG-CD2	8.37	126.02	121.00
1	B	412	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	155	ARG	CD-NE-CZ	7.78	134.49	123.60
1	A	196	GLU	CA-CB-CG	-7.54	96.82	113.40
1	A	357	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	548	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	B	536	GLU	OE1-CD-OE2	-7.51	114.28	123.30
1	A	74	GLY	O-C-N	-7.18	111.21	122.70
1	B	180	GLU	OE1-CD-OE2	-7.18	114.69	123.30
1	A	283	VAL	CG1-CB-CG2	7.12	122.28	110.90
1	B	568	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	A	48[A]	ARG	NH1-CZ-NH2	-6.99	111.71	119.40
1	A	48[B]	ARG	NH1-CZ-NH2	-6.99	111.71	119.40
1	A	491	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	593	ASP	CB-CG-OD1	-6.85	112.14	118.30
1	A	111[A]	PHE	CD1-CE1-CZ	6.85	128.31	120.10
1	A	111[B]	PHE	CD1-CE1-CZ	6.85	128.31	120.10
1	A	95[A]	TYR	CB-CG-CD1	-6.78	116.93	121.00
1	A	95[B]	TYR	CB-CG-CD1	-6.78	116.93	121.00
1	B	357[A]	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	357[C]	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	111[A]	PHE	CD1-CE1-CZ	6.54	127.94	120.10
1	B	111[B]	PHE	CD1-CE1-CZ	6.54	127.94	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214[A]	ARG	CD-NE-CZ	6.48	132.67	123.60
1	B	214[B]	ARG	CD-NE-CZ	6.48	132.67	123.60
1	B	254	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	B	300	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	A	214[A]	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	214[B]	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	218	TYR	CB-CG-CD1	6.14	124.69	121.00
1	A	548	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	180	GLU	CG-CD-OE1	5.72	129.73	118.30
1	A	254[A]	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	254[B]	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	49	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	A	74	GLY	C-N-CA	5.63	135.78	121.70
1	B	507	ASP	CB-CG-OD1	5.63	123.36	118.30
1	B	50[A]	ARG	CD-NE-CZ	5.56	131.38	123.60
1	B	50[B]	ARG	CD-NE-CZ	5.56	131.38	123.60
1	A	497	PHE	CB-CG-CD2	-5.55	116.91	120.80
1	B	158	TYR	CB-CG-CD2	5.52	124.31	121.00
1	A	111[A]	PHE	CG-CD1-CE1	-5.50	114.75	120.80
1	A	111[B]	PHE	CG-CD1-CE1	-5.50	114.75	120.80
1	A	491	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	180	GLU	CB-CG-CD	5.40	128.77	114.20
1	B	491	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	75[A]	LYS	N-CA-CB	5.32	120.18	110.60
1	B	75[B]	LYS	N-CA-CB	5.32	120.18	110.60
1	A	497	PHE	CB-CG-CD1	5.23	124.46	120.80
1	B	48	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
1	A	156[A]	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	156[B]	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	231	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	B	568	GLU	CG-CD-OE1	5.02	128.33	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156[A]	ARG	Sidechain
1	A	204[A]	ARG	Sidechain
1	A	254[A]	ARG	Sidechain
1	A	50[A]	ARG	Sidechain
1	B	224	ARG	Sidechain
1	B	254	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	48	ARG	Sidechain
1	B	50[A]	ARG	Sidechain

## 5.2 Too-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 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	4890	0	4836	34	0
1	B	4884	0	4849	39	1
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	24	0	32	2	0
3	B	12	0	16	1	0
4	A	12	0	6	4	0
4	B	12	0	6	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	29	0	19	0	0
6	B	29	0	19	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	843	0	0	21	0
8	B	861	0	0	28	1
All	All	11714	0	9845	77	1

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 4.

All (77) 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:177:ILE:HB	8:A:8725:HOH:O	1.84	0.77
1:B:202[B]:VAL:HB	8:B:1497:HOH:O	1.85	0.75
1:B:382[A]:LYS:HD2	8:B:1596:HOH:O	1.87	0.74
1:A:178:PRO:HD2	8:A:8725:HOH:O	1.90	0.72
1:A:553:GLU:OE2	1:A:554[A]:LYS:HE2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:THR:O	1:B:91[C]:MET:HG2	1.90	0.71
1:A:276:GLN:OE1	1:A:594:LEU:HB2	1.91	0.71
4:A:703:PYR:H31	8:A:8159:HOH:O	2.01	0.61
1:B:213[A]:GLU:HG2	8:B:1379:HOH:O	2.01	0.60
1:A:486:ASP:OD2	1:A:554[A]:LYS:HE3	2.02	0.60
1:A:341[A]:GLU:HG3	8:A:8820:HOH:O	2.03	0.58
1:B:75[B]:LYS:HG2	8:B:1221:HOH:O	2.03	0.58
1:B:199[B]:VAL:HA	8:B:1497:HOH:O	2.04	0.57
1:B:232[B]:GLN:HG3	8:B:1115:HOH:O	2.05	0.57
1:A:191[B]:THR:HG22	8:A:8647:HOH:O	2.04	0.56
1:B:75[B]:LYS:HD3	8:B:1221:HOH:O	2.06	0.55
1:B:378:ARG:O	1:B:382[C]:LYS:HG2	2.06	0.55
1:B:328[B]:LYS:HD3	8:B:1623:HOH:O	2.06	0.55
4:A:703:PYR:H33	8:A:8608:HOH:O	2.06	0.54
1:B:122[A]:GLN:HA	8:B:1557:HOH:O	2.06	0.54
1:A:214[A]:ARG:NH1	1:A:594:LEU:HG	2.23	0.54
1:A:232[B]:GLN:HG3	8:A:8344:HOH:O	2.07	0.54
1:A:193:LEU:HD12	8:B:1489:HOH:O	2.07	0.54
1:B:202[B]:VAL:HG21	8:B:1319:HOH:O	2.08	0.53
1:B:204:ARG:NE	8:B:1178:HOH:O	2.42	0.53
1:B:382[B]:LYS:HD3	8:B:1387:HOH:O	2.08	0.53
3:A:709:GOL:H12	8:A:8127:HOH:O	2.07	0.52
1:B:382[A]:LYS:HE3	8:B:1387:HOH:O	2.09	0.52
1:A:174:TRP:CE3	3:A:706:GOL:H11	2.46	0.50
1:B:454[B]:MET:HE3	1:B:502:PHE:CE1	2.47	0.50
1:A:214[A]:ARG:CZ	1:A:594:LEU:HG	2.42	0.49
1:A:561:MET:CE	4:A:703:PYR:H32	2.43	0.49
1:B:75[B]:LYS:HG2	8:B:1393:HOH:O	2.12	0.48
1:A:387:ASP:HA	1:A:410[B]:SER:O	2.14	0.48
1:B:554[A]:LYS:HD2	8:B:1519:HOH:O	2.12	0.48
1:A:207:GLN:HG2	8:A:8774:HOH:O	2.14	0.48
1:A:224:ARG:HD2	8:A:8704:HOH:O	2.12	0.48
1:B:110:GLN:NE2	8:B:1228[B]:HOH:O	2.46	0.48
1:A:311[B]:LYS:HE3	8:A:8434:HOH:O	2.13	0.47
1:B:224:ARG:NE	8:B:1288:HOH:O	2.47	0.47
8:A:8809:HOH:O	1:B:317:LYS:HE3	2.14	0.47
1:A:225:LYS:NZ	8:A:8192:HOH:O	2.47	0.46
1:B:50[B]:ARG:NE	8:B:1494:HOH:O	2.49	0.46
1:B:204:ARG:HD3	8:B:1178:HOH:O	2.16	0.45
1:B:202[B]:VAL:HG12	1:B:336:GLN:OE1	2.16	0.45
1:A:129:ILE:HA	8:A:8805:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527[A]:GLU:HG2	8:B:977:HOH:O	2.15	0.45
1:B:382[C]:LYS:NZ	8:B:1642:HOH:O	2.49	0.45
1:A:224:ARG:NH2	8:A:8697:HOH:O	2.49	0.44
1:A:224:ARG:NE	8:A:8697:HOH:O	2.50	0.44
1:A:9:THR:HG23	1:A:179:ALA:CB	2.47	0.44
1:B:489[B]:GLN:NE2	8:B:1634:HOH:O	2.50	0.44
1:A:228[B]:LYS:O	1:A:232[B]:GLN:HG3	2.18	0.44
1:B:489[B]:GLN:HG2	8:B:1429:HOH:O	2.16	0.43
1:B:228[B]:LYS:HD2	8:B:1554:HOH:O	2.18	0.43
1:B:325:ASP:OD2	1:B:328[B]:LYS:HG3	2.18	0.43
1:B:50[A]:ARG:NH2	8:B:1066:HOH:O	2.50	0.43
1:B:438:GLU:HA	1:B:438:GLU:OE1	2.18	0.43
1:A:307[A]:ILE:HD11	8:A:8634:HOH:O	2.19	0.42
1:A:593:ASP:C	1:A:594:LEU:O	2.57	0.42
1:B:9:THR:HG23	1:B:179:ALA:HB3	2.01	0.42
1:B:199[B]:VAL:O	1:B:203:THR:OG1	2.32	0.42
1:A:254[A]:ARG:NH2	8:A:8473:HOH:O	2.53	0.42
1:A:193:LEU:N	8:A:8258[A]:HOH:O	2.48	0.42
3:B:707:GOL:H31	8:B:887:HOH:O	2.19	0.42
1:A:28:HIS:HA	1:A:52:HIS:O	2.20	0.42
1:B:297:LYS:HG3	1:B:298[B]:ASN:ND2	2.35	0.41
1:A:9:THR:HG23	1:A:179:ALA:HB3	2.03	0.41
1:A:561:MET:HE1	4:A:703:PYR:H32	2.03	0.41
1:B:50[B]:ARG:HB2	8:B:1494:HOH:O	2.21	0.41
1:A:297[A]:LYS:HD3	8:A:8489:HOH:O	2.20	0.41
1:A:283:VAL:HG13	1:A:305:ILE:HB	2.03	0.41
1:A:57:ARG:NH1	8:A:8694:HOH:O	2.54	0.40
1:A:424[B]:VAL:C	1:A:427[B]:PRO:HD2	2.42	0.40
1:B:39:SER:HB3	1:B:174:TRP:CD2	2.56	0.40
1:B:111[A]:PHE:CE2	1:B:115:GLY:HA3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:NH2	8:B:901:HOH:O[3_655]	1.93	0.27



## 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	626/603 (104%)	610 (97%)	14 (2%)	2 (0%)	44	15
1	B	628/603 (104%)	610 (97%)	17 (3%)	1 (0%)	51	17
All	All	1254/1206 (104%)	1220 (97%)	31 (2%)	3 (0%)	44	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	ASP
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	513/485 (106%)	510 (99%)	3 (1%)	89	63
1	B	514/485 (106%)	508 (99%)	6 (1%)	75	39
All	All	1027/970 (106%)	1018 (99%)	9 (1%)	89	49

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210[A]	LEU
1	A	210[B]	LEU
1	A	594	LEU

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Mol	Chain	Res	Type
1	B	188	SER
1	B	196[A]	GLU
1	B	196[B]	GLU
1	B	368	GLU
1	B	554[A]	LYS
1	B	554[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	701	-	51,58,58	1.38	8 (15%)	54,89,89	2.20	8 (14%)
3	GOL	A	702	-	5,5,5	0.37	0	5,5,5	0.53	0
4	PYR	A	703	-	2,5,5	3.44	1 (50%)	2,6,6	1.51	0
4	PYR	A	704	-	2,5,5	2.72	1 (50%)	2,6,6	1.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	705	-	5,5,5	0.76	0	5,5,5	0.77	0
3	GOL	A	706	-	5,5,5	0.28	0	5,5,5	0.65	0
5	PO4	A	707	-	4,4,4	1.55	1 (25%)	6,6,6	1.94	2 (33%)
6	TDM	A	708	7	25,30,30	2.05	7 (28%)	29,45,45	3.49	11 (37%)
3	GOL	A	709	-	5,5,5	0.47	0	5,5,5	0.90	0
2	FAD	B	701	-	51,58,58	1.41	4 (7%)	54,89,89	1.80	5 (9%)
4	PYR	B	702	-	2,5,5	1.88	1 (50%)	2,6,6	1.71	1 (50%)
4	PYR	B	703	-	2,5,5	2.54	1 (50%)	2,6,6	0.87	0
6	TDM	B	704	7	25,30,30	2.11	8 (32%)	29,45,45	3.17	8 (27%)
5	PO4	B	705	-	4,4,4	1.27	0	6,6,6	1.42	1 (16%)
3	GOL	B	706	-	5,5,5	0.95	0	5,5,5	0.49	0
3	GOL	B	707	-	5,5,5	0.62	0	5,5,5	0.85	0

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	701	-	-	0/28/50/50	0/6/6/6
3	GOL	A	702	-	-	0/4/4/4	0/0/0/0
4	PYR	A	703	-	-	0/0/4/4	0/0/0/0
4	PYR	A	704	-	-	0/0/4/4	0/0/0/0
3	GOL	A	705	-	-	0/4/4/4	0/0/0/0
3	GOL	A	706	-	-	0/4/4/4	0/0/0/0
5	PO4	A	707	-	-	0/0/0/0	0/0/0/0
6	TDM	A	708	7	-	0/16/21/21	0/2/2/2
3	GOL	A	709	-	-	0/4/4/4	0/0/0/0
2	FAD	B	701	-	-	0/28/50/50	0/6/6/6
4	PYR	B	702	-	-	0/0/4/4	0/0/0/0
4	PYR	B	703	-	-	0/0/4/4	0/0/0/0
6	TDM	B	704	7	-	0/16/21/21	0/2/2/2
5	PO4	B	705	-	-	0/0/0/0	0/0/0/0
3	GOL	B	706	-	-	0/4/4/4	0/0/0/0
3	GOL	B	707	-	-	0/4/4/4	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	PYR	C3-C2	-4.86	1.34	1.49
4	A	704	PYR	C3-C2	-3.84	1.37	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	PYR	C3-C2	-3.58	1.38	1.49
5	A	707	PO4	P-O4	-3.06	1.43	1.54
4	B	702	PYR	C3-C2	-2.65	1.41	1.49
2	A	701	FAD	C2B-C1B	-2.53	1.49	1.53
6	A	708	TDM	C2'-N1'	-2.37	1.30	1.34
2	A	701	FAD	C1'-N10	-2.22	1.46	1.48
6	B	704	TDM	C2'-N1'	-2.15	1.30	1.34
6	B	704	TDM	O7-C7	2.10	1.53	1.44
2	A	701	FAD	C2A-N3A	2.33	1.36	1.32
6	B	704	TDM	C7'-C5'	2.33	1.56	1.51
6	B	704	TDM	C4'-N3'	2.40	1.38	1.35
2	A	701	FAD	C10-N1	2.46	1.36	1.33
2	A	701	FAD	C9A-N10	2.47	1.42	1.38
2	B	701	FAD	C9A-N10	2.78	1.42	1.38
2	A	701	FAD	C5X-N5	2.83	1.39	1.35
6	A	708	TDM	PB-O3A	2.95	1.64	1.60
6	B	704	TDM	O28-C27	3.07	1.40	1.31
6	A	708	TDM	C2'-N3'	3.22	1.39	1.34
2	A	701	FAD	O4B-C1B	3.28	1.45	1.41
6	A	708	TDM	C6'-N1'	3.34	1.41	1.34
6	A	708	TDM	O28-C27	3.34	1.40	1.31
2	B	701	FAD	C4-N3	3.45	1.39	1.33
2	A	701	FAD	C4X-N5	3.64	1.38	1.33
6	A	708	TDM	C4'-N3'	3.76	1.40	1.35
6	B	704	TDM	C6'-N1'	3.77	1.42	1.34
6	B	704	TDM	PB-O3A	4.02	1.66	1.60
2	B	701	FAD	C5X-N5	4.69	1.42	1.35
6	A	708	TDM	C2-N3	4.84	1.46	1.38
2	B	701	FAD	C4X-N5	5.44	1.41	1.33
6	B	704	TDM	C2-N3	5.89	1.48	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	704	TDM	C29-C27-C2	-10.14	110.11	124.73
6	A	708	TDM	O28-C27-C2	-9.66	110.19	119.99
6	B	704	TDM	O28-C27-C2	-9.36	110.50	119.99
6	A	708	TDM	C29-C27-C2	-9.25	111.41	124.73
2	B	701	FAD	C4X-C4-N3	-5.41	115.78	123.48
2	A	701	FAD	C4X-C4-N3	-5.22	116.05	123.48
2	A	701	FAD	C4X-C10-N10	-4.23	117.58	120.52
2	A	701	FAD	N3A-C2A-N1A	-3.70	125.64	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	704	TDM	O28-C27-C29	-3.56	107.24	114.71
6	A	708	TDM	O28-C27-C29	-3.27	107.86	114.71
6	A	708	TDM	C5'-C6'-N1'	-3.11	118.60	123.87
2	A	701	FAD	C4-C4X-C10	-3.00	117.54	119.96
6	B	704	TDM	C5'-C6'-N1'	-2.75	119.22	123.87
6	A	708	TDM	CM4-C4-N3	-2.75	119.23	122.69
6	B	704	TDM	C6-C5-C4	-2.55	125.39	127.43
2	A	701	FAD	C9A-C5X-N5	-2.38	118.69	122.24
2	B	701	FAD	C9A-C5X-N5	-2.34	118.75	122.24
6	A	708	TDM	C6-C5-C4	-2.14	125.72	127.43
5	A	707	PO4	O4-P-O1	-2.13	101.91	110.97
2	B	701	FAD	C4X-C10-N10	-2.12	119.05	120.52
6	A	708	TDM	C5-C4-N3	2.05	111.95	107.66
6	B	704	TDM	N4'-C4'-N3'	2.25	120.33	117.00
6	A	708	TDM	C6'-C5'-C4'	2.37	118.83	115.68
4	B	702	PYR	O3-C2-C3	2.41	125.65	120.16
6	B	704	TDM	C6'-N1'-C2'	2.55	120.29	115.88
2	A	701	FAD	C5A-C6A-N6A	2.70	125.97	120.47
5	B	705	PO4	O4-P-O3	3.01	118.97	107.90
6	A	708	TDM	C6'-N1'-C2'	3.18	121.38	115.88
5	A	707	PO4	O4-P-O3	4.09	122.91	107.90
2	B	701	FAD	C1'-N10-C9A	4.21	122.20	118.35
6	A	708	TDM	CM2-C2'-N1'	4.60	122.25	117.06
2	A	701	FAD	C1'-N10-C9A	5.25	123.16	118.35
6	B	704	TDM	C2-N3-C4	6.08	112.02	108.64
2	B	701	FAD	C4-N3-C2	8.60	122.68	115.16
6	A	708	TDM	C2-N3-C4	9.10	113.70	108.64
2	A	701	FAD	C4-N3-C2	10.91	124.70	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	PYR	4	0
3	A	706	GOL	1	0
3	A	709	GOL	1	0
3	B	707	GOL	1	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, 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	586/603 (97%)	-0.43	5 (0%) 84 82	4, 8, 18, 48	9 (1%)
1	B	583/603 (96%)	-0.48	1 (0%) 94 92	4, 7, 16, 34	10 (1%)
All	All	1169/1206 (96%)	-0.45	6 (0%) 90 89	4, 7, 18, 48	19 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	LEU	10.3
1	A	592	ASP	4.4
1	A	593	ASP	3.4
1	A	9	THR	2.6
1	B	9	THR	2.0
1	A	367[A]	GLN	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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	709	6/6	0.81	0.24	14.73	18,26,26,31	6
3	GOL	B	707	6/6	0.80	0.17	14.66	20,24,24,36	6
3	GOL	B	706	6/6	0.95	0.11	10.17	17,19,20,22	0
4	PYR	A	704	6/6	0.95	0.09	7.86	13,14,16,18	6
3	GOL	A	706	6/6	0.83	0.16	6.83	42,47,48,49	0
3	GOL	A	705	6/6	0.91	0.15	6.59	17,23,28,36	0
4	PYR	B	703	6/6	0.95	0.10	5.37	11,13,14,17	6
3	GOL	A	702	6/6	0.95	0.10	3.99	7,15,17,21	6
4	PYR	A	703	6/6	0.96	0.07	1.34	14,15,15,23	6
5	PO4	A	707	5/5	0.98	0.08	0.80	9,11,14,21	5
4	PYR	B	702	6/6	0.97	0.09	0.78	12,12,14,18	6
5	PO4	B	705	5/5	0.99	0.06	-0.28	8,10,13,20	5
6	TDM	A	708	29/29	1.00	0.04	-0.85	5,6,8,10	0
2	FAD	A	701	53/53	0.99	0.04	-0.94	4,5,7,8	0
2	FAD	B	701	53/53	1.00	0.03	-1.27	4,4,6,6	0
6	TDM	B	704	29/29	1.00	0.04	-1.35	4,6,7,10	0
7	MG	B	708	1/1	1.00	0.02	-3.31	5,5,5,5	0
7	MG	A	710	1/1	1.00	0.02	-4.36	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.