



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2017 – 03:04 AM EST

PDB ID : 4KGD  
Title : High-resolution crystal structure of pyruvate oxidase from *L. plantarum* in complex with phosphate  
Authors : Neumann, P.; Tittmann, K.  
Deposited on : unknown  
Resolution : 1.06 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 : 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

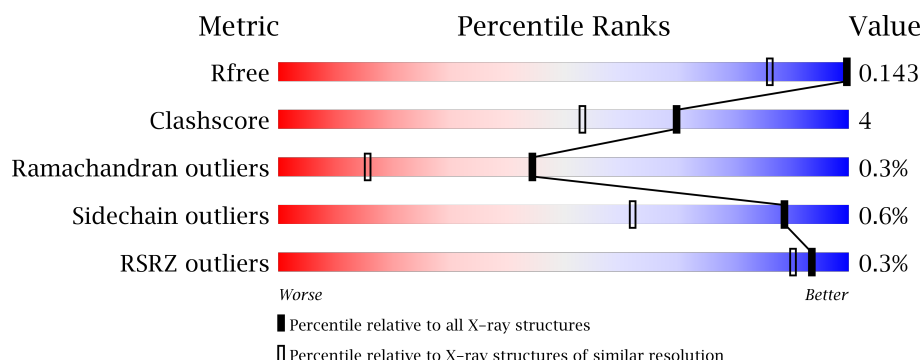
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.06 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	1262 (1.12-1.00)
Clashscore	112137	1336 (1.12-1.00)
Ramachandran outliers	110173	1269 (1.12-1.00)
Sidechain outliers	110143	1267 (1.12-1.00)
RSRZ outliers	101464	1268 (1.12-1.00)

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	
1	B	603	

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
6	GOL	A	705	-	-	-	X
6	GOL	A	706	-	-	-	X
6	GOL	A	707	-	-	-	X
6	GOL	A	708	-	-	-	X
6	GOL	B	705	-	-	-	X
6	GOL	B	707	-	-	-	X
6	GOL	B	708	-	-	-	X
6	GOL	B	709	-	-	-	X
7	K	A	709	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11890 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
			4863	3078	844	923	18			
1	B	585	Total	C	N	O	S	0	44	0
			4903	3101	858	925	19			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



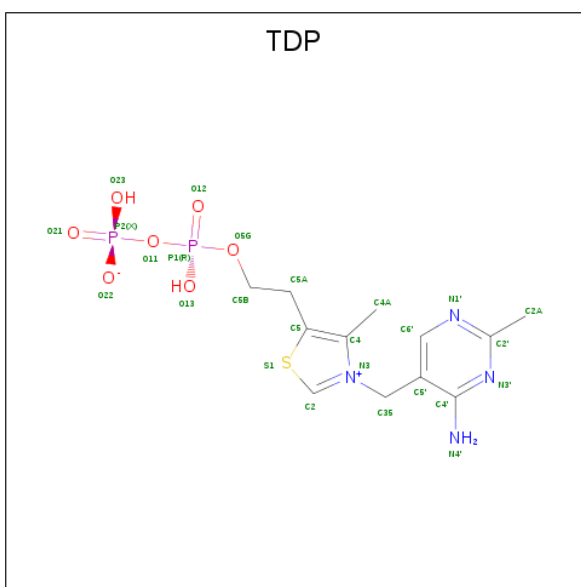
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



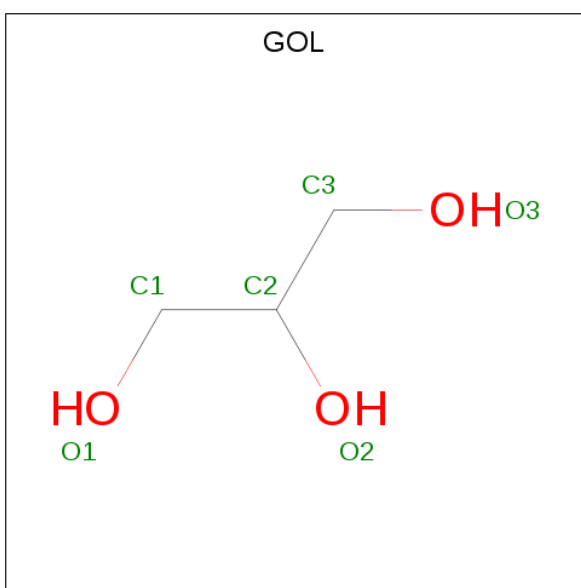
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula:  $C_{12}H_{18}N_4O_7P_2S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
5	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



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

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		

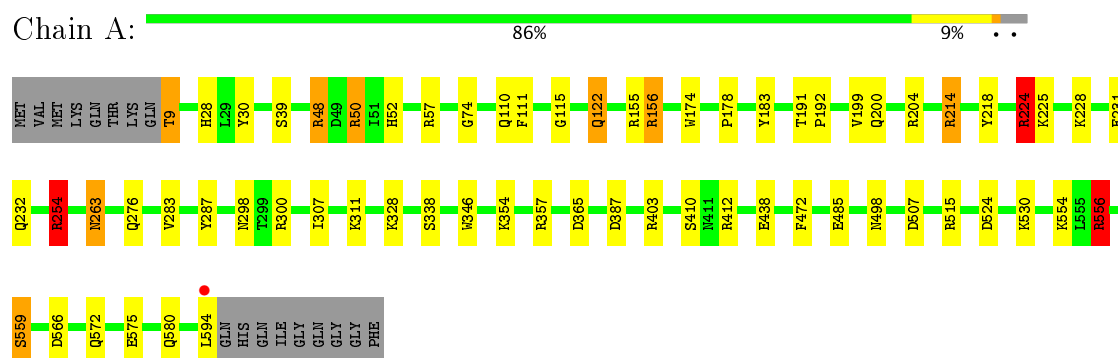
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	945	Total	O	0	106
			945	945		
8	B	954	Total	O	0	94
			954	954		

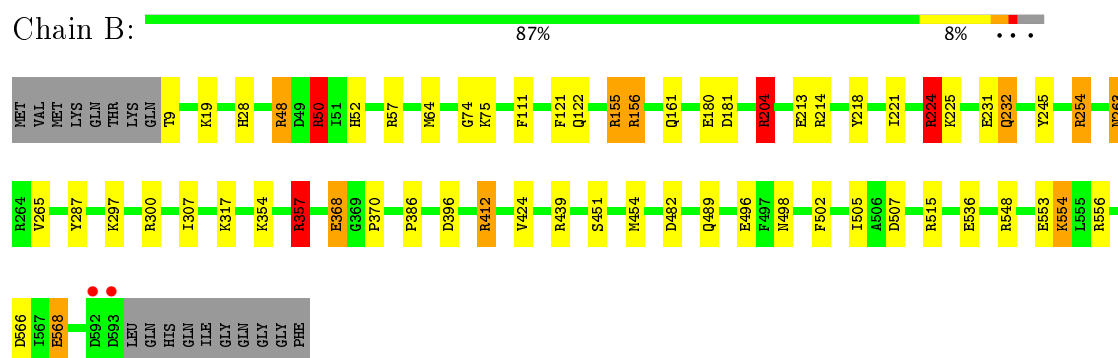
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	119.28Å 154.16Å 165.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.06 47.62 – 1.06	Depositor EDS
% Data completeness (in resolution range)	91.6 (30.00-1.06) 88.3 (47.62-1.06)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 1.06Å)	Xtriage
Refinement program	SHELX, SHELXL	Depositor
R, $R_{free}$	0.127 , 0.150 0.125 , 0.143	Depositor DCC
$R_{free}$ test set	19361 reflections (3.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.7	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 78.7	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	11890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, PO4, TDP, K, 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	0.77	3/4977 (0.1%)	1.32	59/6764 (0.9%)
1	B	0.77	6/5014 (0.1%)	1.34	56/6806 (0.8%)
All	All	0.77	9/9991 (0.1%)	1.33	115/13570 (0.8%)

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	6
1	B	0	9
All	All	0	15

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	VAL	CB-CG2	-7.19	1.37	1.52
1	B	204[A]	ARG	CZ-NH2	6.02	1.40	1.33
1	B	204[B]	ARG	CZ-NH2	6.02	1.40	1.33
1	B	496	GLU	CD-OE2	-5.89	1.19	1.25
1	B	568[A]	GLU	CD-OE2	5.82	1.32	1.25
1	B	568[B]	GLU	CD-OE2	5.82	1.32	1.25
1	B	231	GLU	CD-OE1	-5.61	1.19	1.25
1	A	485	GLU	CD-OE1	-5.58	1.19	1.25
1	A	575	GLU	CD-OE2	5.57	1.31	1.25

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48[A]	ARG	NE-CZ-NH1	26.04	133.32	120.30
1	A	48[B]	ARG	NE-CZ-NH1	26.04	133.32	120.30
1	B	204[A]	ARG	NE-CZ-NH2	23.88	132.24	120.30
1	B	204[B]	ARG	NE-CZ-NH2	23.88	132.24	120.30
1	B	155	ARG	NE-CZ-NH2	15.46	128.03	120.30
1	A	357	ARG	NE-CZ-NH2	-15.45	112.58	120.30
1	B	204[A]	ARG	CD-NE-CZ	14.35	143.69	123.60
1	B	204[B]	ARG	CD-NE-CZ	14.35	143.69	123.60
1	B	357[A]	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	B	357[C]	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	B	204[A]	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	B	204[B]	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	A	48[A]	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	A	48[B]	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	B	155	ARG	NE-CZ-NH1	-10.77	114.92	120.30
1	A	412	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	A	357	ARG	NH1-CZ-NH2	10.56	131.02	119.40
1	A	214[A]	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	214[B]	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	57[A]	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	A	57[B]	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	B	265	VAL	CG1-CB-CG2	9.55	126.17	110.90
1	A	155	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	B	57[A]	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	B	57[B]	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	B	515	ARG	NE-CZ-NH1	-9.31	115.64	120.30
1	A	155	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	A	224	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	B	568[A]	GLU	OE1-CD-OE2	-8.50	113.10	123.30
1	B	568[B]	GLU	OE1-CD-OE2	-8.50	113.10	123.30
1	B	57[A]	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	B	57[B]	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	B	548	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	50	ARG	CG-CD-NE	8.39	129.42	111.80
1	B	300	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	A	300	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	403	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	B	50	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	155	ARG	CD-NE-CZ	7.98	134.78	123.60
1	B	48	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	B	515	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	B	218	TYR	CB-CG-CD1	7.84	125.70	121.00
1	A	357	ARG	NE-CZ-NH1	-7.83	116.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	ASP	CB-CG-OD1	7.76	125.28	118.30
1	B	496	GLU	OE1-CD-OE2	-7.68	114.09	123.30
1	B	566	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	412	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	265	VAL	CB-CA-C	7.46	125.58	111.40
1	A	50	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	224[A]	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	224[B]	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	156[A]	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	156[B]	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	554[A]	LYS	CD-CE-NZ	7.17	128.20	111.70
1	B	554[B]	LYS	CD-CE-NZ	7.17	128.20	111.70
1	B	396	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	50	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	A	365	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	254	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	231	GLU	OE1-CD-OE2	-6.76	115.18	123.30
1	A	48[A]	ARG	NH1-CZ-NH2	-6.74	111.99	119.40
1	A	48[B]	ARG	NH1-CZ-NH2	-6.74	111.99	119.40
1	A	155	ARG	CD-NE-CZ	6.69	132.97	123.60
1	A	156[A]	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	156[B]	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	74	GLY	O-C-N	-6.64	112.07	122.70
1	A	204	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	50	ARG	NH1-CZ-NH2	-6.51	112.24	119.40
1	A	283	VAL	CA-CB-CG1	-6.50	101.16	110.90
1	A	254	ARG	CD-NE-CZ	6.47	132.66	123.60
1	A	283	VAL	CG1-CB-CG2	6.35	121.06	110.90
1	A	204	ARG	CD-NE-CZ	6.34	132.47	123.60
1	A	200	GLN	CB-CG-CD	6.30	127.99	111.60
1	B	231	GLU	OE1-CD-OE2	-6.29	115.76	123.30
1	A	403	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	57[A]	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	57[B]	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	524[A]	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	A	524[B]	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	A	472	PHE	CB-CG-CD1	5.93	124.95	120.80
1	A	556[A]	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	556[B]	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	232[A]	GLN	OE1-CD-NE2	-5.73	108.73	121.90
1	B	232[B]	GLN	OE1-CD-NE2	-5.73	108.73	121.90
1	B	566	ASP	CB-CG-OD1	5.68	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	283	VAL	CA-CB-CG2	5.65	119.37	110.90
1	B	357[A]	ARG	NH1-CZ-NH2	5.60	125.56	119.40
1	B	357[C]	ARG	NH1-CZ-NH2	5.60	125.56	119.40
1	A	515	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	218	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	A	346	TRP	CA-CB-CG	5.44	124.03	113.70
1	B	536	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	B	507	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	482	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	9	THR	CA-CB-CG2	-5.36	104.90	112.40
1	A	30	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	A	412	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	A	438	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	A	575	GLU	CG-CD-OE2	5.27	128.84	118.30
1	A	122	GLN	CB-CG-CD	-5.24	97.99	111.60
1	B	265	VAL	N-CA-CB	5.20	122.93	111.50
1	A	507	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	204[A]	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	B	204[B]	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	B	232[A]	GLN	CG-CD-NE2	5.17	129.09	116.70
1	B	232[B]	GLN	CG-CD-NE2	5.17	129.09	116.70
1	A	30	TYR	CB-CG-CD2	5.16	124.10	121.00
1	A	218	TYR	CB-CG-CD1	5.15	124.09	121.00
1	B	74	GLY	O-C-N	-5.12	114.51	122.70
1	B	214[A]	ARG	CD-NE-CZ	5.12	130.77	123.60
1	B	214[B]	ARG	CD-NE-CZ	5.12	130.77	123.60
1	A	74	GLY	C-N-CA	5.06	134.35	121.70
1	B	245	TYR	CB-CG-CD1	5.02	124.01	121.00
1	A	575	GLU	CG-CD-OE1	-5.01	108.29	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156[A]	ARG	Sidechain
1	A	224	ARG	Sidechain
1	A	254	ARG	Sidechain
1	A	48[A]	ARG	Sidechain
1	A	556[A]	ARG	Sidechain
1	A	9	THR	Peptide
1	B	155	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	156[A]	ARG	Sidechain
1	B	204[A]	ARG	Sidechain
1	B	224[A]	ARG	Sidechain
1	B	254	ARG	Sidechain
1	B	357[A]	ARG	Sidechain
1	B	48	ARG	Sidechain
1	B	50	ARG	Sidechain
1	B	556[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	4863	0	4808	38	0
1	B	4903	0	4852	43	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	26	0	16	1	0
5	B	26	0	16	1	0
6	A	24	0	32	0	0
6	B	30	0	40	3	0
7	A	1	0	0	0	0
8	A	945	0	0	28	1
8	B	954	0	0	28	1
All	All	11890	0	9826	83	2

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 (83) 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)
5:A:704:TDP:C2	5:A:704:TDP:H2	0.97	1.50
5:B:703:TDP:C2	5:B:703:TDP:H2	0.97	1.49
1:A:328:LYS:HE3	8:A:1570[A]:HOH:O	1.82	0.79
1:B:225:LYS:HD3	8:B:971[B]:HOH:O	1.85	0.77
1:B:568[B]:GLU:HG2	8:B:1334:HOH:O	1.85	0.76
1:B:439:ARG:HH12	6:B:708:GOL:H12	1.51	0.76
1:B:213[A]:GLU:HG2	8:B:1585:HOH:O	1.86	0.76
1:B:370[B]:PRO:HG2	8:B:1531:HOH:O	1.84	0.76
1:A:225:LYS:HD3	8:A:1707[B]:HOH:O	1.86	0.74
1:B:122[B]:GLN:HA	8:B:1458:HOH:O	1.86	0.74
1:A:328:LYS:HE3	8:A:1571[B]:HOH:O	1.90	0.72
8:A:946:HOH:O	1:B:317[B]:LYS:HE3	1.92	0.69
1:A:224:ARG:HD2	8:A:1470:HOH:O	1.93	0.66
1:A:554:LYS:HE2	8:A:1276[A]:HOH:O	1.96	0.65
1:A:572[A]:GLN:HG2	8:A:1573:HOH:O	1.97	0.65
1:A:354[B]:LYS:HE2	8:A:1280:HOH:O	1.95	0.65
1:B:232[A]:GLN:HG2	8:B:1523:HOH:O	1.98	0.64
1:B:354[B]:LYS:NZ	8:B:1732:HOH:O	2.32	0.62
1:B:122[A]:GLN:HA	8:B:1458:HOH:O	1.99	0.62
1:A:178:PRO:HD2	8:A:1188[B]:HOH:O	1.98	0.62
1:B:75[B]:LYS:HG2	8:B:1497:HOH:O	1.98	0.61
1:B:297:LYS:HE2	8:B:1350:HOH:O	2.01	0.60
1:A:498[B]:ASN:HB3	8:A:1273:HOH:O	2.02	0.59
1:B:489[B]:GLN:HG2	8:B:1345:HOH:O	2.02	0.58
1:B:121:PHE:CD2	1:B:122[B]:GLN:HG2	2.39	0.57
1:A:298[B]:ASN:HB2	8:A:1181:HOH:O	2.04	0.57
1:A:199[A]:VAL:HG21	8:A:1658:HOH:O	2.04	0.56
1:A:232[B]:GLN:HG3	8:A:1116:HOH:O	2.07	0.53
1:A:530[A]:LYS:HE3	8:A:1675:HOH:O	2.09	0.53
1:B:204[B]:ARG:NH1	8:B:1143:HOH:O	2.40	0.53
1:B:498[A]:ASN:HB2	8:B:1394:HOH:O	2.08	0.53
1:B:64[A]:MET:SD	1:B:424[A]:VAL:HG12	2.50	0.52
1:A:498[A]:ASN:HB2	8:A:1273:HOH:O	2.10	0.52
1:A:50:ARG:HG3	8:A:1568:HOH:O	2.09	0.52
1:B:498[B]:ASN:HB3	8:B:1394:HOH:O	2.10	0.51
1:B:368:GLU:HG3	8:B:1681:HOH:O	2.09	0.51
1:B:498[B]:ASN:ND2	8:B:1119[B]:HOH:O	2.43	0.51
1:A:572[A]:GLN:HG3	8:A:1574:HOH:O	2.09	0.51
1:A:276:GLN:OE1	1:A:594:LEU:HG	2.11	0.51
1:B:307[B]:ILE:HD11	8:B:1569:HOH:O	2.10	0.50
1:B:454[B]:MET:HE3	1:B:502:PHE:CE1	2.47	0.49
6:B:709:GOL:H31	8:B:939:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75[B]:LYS:HD3	8:B:1497:HOH:O	2.12	0.49
1:A:110:GLN:NE2	8:A:902[B]:HOH:O	2.46	0.49
1:A:498[B]:ASN:ND2	8:A:1150[B]:HOH:O	2.45	0.49
1:A:228[B]:LYS:HE3	8:A:1684:HOH:O	2.13	0.49
1:B:232[B]:GLN:HG3	8:B:1113:HOH:O	2.12	0.49
1:B:75[B]:LYS:HD3	8:B:1593:HOH:O	2.12	0.49
1:B:553:GLU:OE2	1:B:554[A]:LYS:HE2	2.12	0.47
1:A:191[B]:THR:HG22	1:A:192:PRO:HD2	1.97	0.47
1:A:183:TYR:CD2	1:B:317[B]:LYS:HD2	2.49	0.46
1:A:192:PRO:HG3	8:A:1329:HOH:O	2.14	0.46
1:B:224[B]:ARG:NH2	8:B:1498:HOH:O	2.48	0.46
1:B:50:ARG:NH2	8:B:1060:HOH:O	2.48	0.46
1:B:19[B]:LYS:NZ	8:B:1629[B]:HOH:O	2.50	0.45
1:B:554[B]:LYS:HE2	8:B:1640[B]:HOH:O	2.15	0.45
1:B:111[B]:PHE:CE2	1:B:122[B]:GLN:HG3	2.52	0.45
1:A:387:ASP:HA	1:A:410[B]:SER:O	2.17	0.45
1:B:554[A]:LYS:NZ	8:B:1367[A]:HOH:O	2.49	0.45
1:B:111[B]:PHE:CZ	1:B:122[B]:GLN:HG3	2.52	0.45
1:A:122:GLN:HA	8:A:1607:HOH:O	2.17	0.45
1:B:412:ARG:HG2	6:B:708:GOL:H32	1.99	0.44
1:A:556[B]:ARG:NH1	8:A:1277[B]:HOH:O	2.49	0.44
1:A:254:ARG:NH2	8:A:1583:HOH:O	2.50	0.44
1:A:307[B]:ILE:HG12	2:A:701:FAD:C4A	2.47	0.44
1:B:28:HIS:HA	1:B:52[B]:HIS:O	2.17	0.44
1:B:161:GLN:HG3	8:B:1288:HOH:O	2.17	0.44
1:B:454[B]:MET:HE2	1:B:505:ILE:HG21	2.00	0.44
1:B:357[A]:ARG:NH2	8:B:1099:HOH:O	2.51	0.44
1:A:111[A]:PHE:CE2	1:A:115:GLY:HA3	2.53	0.43
1:A:580:GLN:NE2	8:A:1192:HOH:O	2.47	0.43
1:A:199[A]:VAL:HG13	8:A:1286:HOH:O	2.18	0.43
1:A:214[A]:ARG:CZ	1:A:594:LEU:HD11	2.50	0.42
1:B:451[B]:SER:O	1:B:454[B]:MET:HG2	2.19	0.42
1:B:221:ILE:HD12	1:B:224[A]:ARG:NH2	2.35	0.42
1:A:28:HIS:HA	1:A:52:HIS:O	2.20	0.42
1:A:307[B]:ILE:HG23	2:A:701:FAD:N1A	2.35	0.42
1:A:192:PRO:HD3	8:A:1329:HOH:O	2.20	0.41
1:B:180[A]:GLU:HG2	1:B:181:ASP:OD1	2.20	0.41
1:A:263:ASN:HB2	1:A:287:TYR:OH	2.21	0.41
1:B:263:ASN:HB2	1:B:287:TYR:OH	2.21	0.41
1:A:311[B]:LYS:HE3	8:A:1009:HOH:O	2.21	0.40
1:A:39:SER:HB3	1:A:174:TRP:CD2	2.56	0.40



All (2) 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)
8:A:1048:HOH:O	8:A:1048:HOH:O[4_565]	2.16	0.04
8:B:1109:HOH:O	8:B:1109:HOH:O[4_565]	2.18	0.02

## 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	625/603 (104%)	609 (97%)	14 (2%)	2 (0%)	44	16
1	B	628/603 (104%)	610 (97%)	17 (3%)	1 (0%)	51	18
All	All	1253/1206 (104%)	1219 (97%)	31 (2%)	3 (0%)	44	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	B	263	ASN
1	A	559	SER

### 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	A	512/485 (106%)	508 (99%)	4 (1%)	85	54
1	B	515/485 (106%)	513 (100%)	2 (0%)	93	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1027/970 (106%)	1021 (99%)	6 (1%)	89	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	254	ARG
1	A	338	SER
1	A	559	SER
1	B	368	GLU
1	B	386	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	GLN

### 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 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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	1.26	5 (9%)	54,89,89	2.14	8 (14%)
4	PO4	A	703	-	4,4,4	1.68	1 (25%)	6,6,6	1.38	1 (16%)
5	TDP	A	704	3	21,27,27	1.35	3 (14%)	25,40,40	1.40	5 (20%)
6	GOL	A	705	-	5,5,5	0.69	0	5,5,5	1.17	0
6	GOL	A	706	-	5,5,5	1.09	0	5,5,5	0.98	0
6	GOL	A	707	-	5,5,5	0.23	0	5,5,5	1.13	1 (20%)
6	GOL	A	708	-	5,5,5	0.75	0	5,5,5	1.53	1 (20%)
2	FAD	B	701	-	51,58,58	1.27	5 (9%)	54,89,89	1.76	3 (5%)
5	TDP	B	703	3	21,27,27	2.02	6 (28%)	25,40,40	1.16	2 (8%)
4	PO4	B	704	-	4,4,4	1.95	2 (50%)	6,6,6	1.81	1 (16%)
6	GOL	B	705	-	5,5,5	0.76	0	5,5,5	0.87	0
6	GOL	B	706	-	5,5,5	0.55	0	5,5,5	1.05	0
6	GOL	B	707	-	5,5,5	0.89	0	5,5,5	0.70	0
6	GOL	B	708	-	5,5,5	0.71	0	5,5,5	1.25	0
6	GOL	B	709	-	5,5,5	0.80	0	5,5,5	0.69	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
4	PO4	A	703	-	-	0/0/0/0	0/0/0/0
5	TDP	A	704	3	-	0/16/17/17	0/2/2/2
6	GOL	A	705	-	-	0/4/4/4	0/0/0/0
6	GOL	A	706	-	-	0/4/4/4	0/0/0/0
6	GOL	A	707	-	-	0/4/4/4	0/0/0/0
6	GOL	A	708	-	-	0/4/4/4	0/0/0/0
2	FAD	B	701	-	-	0/28/50/50	0/6/6/6
5	TDP	B	703	3	-	0/16/17/17	0/2/2/2
4	PO4	B	704	-	-	0/0/0/0	0/0/0/0
6	GOL	B	705	-	-	0/4/4/4	0/0/0/0
6	GOL	B	706	-	-	0/4/4/4	0/0/0/0
6	GOL	B	707	-	-	0/4/4/4	0/0/0/0
6	GOL	B	708	-	-	0/4/4/4	0/0/0/0
6	GOL	B	709	-	-	0/4/4/4	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAD	C1'-N10	-3.25	1.45	1.48
4	A	703	PO4	P-O4	-2.98	1.43	1.54
4	B	704	PO4	P-O1	-2.59	1.44	1.50
4	B	704	PO4	P-O4	-2.54	1.45	1.54
5	B	703	TDP	C35-N3	-2.41	1.44	1.48
2	B	701	FAD	C6-C5X	-2.18	1.38	1.41
5	B	703	TDP	C6'-C5'	-2.08	1.33	1.37
2	A	701	FAD	C4-N3	2.09	1.36	1.33
2	A	701	FAD	C5X-N5	2.37	1.38	1.35
2	A	701	FAD	C10-N1	2.40	1.36	1.33
2	B	701	FAD	C5X-N5	2.40	1.39	1.35
5	A	704	TDP	C4'-N3'	2.55	1.38	1.35
2	B	701	FAD	C4-N3	2.70	1.37	1.33
5	B	703	TDP	C4-N3	2.73	1.42	1.39
2	A	701	FAD	C4X-N5	3.00	1.37	1.33
5	A	704	TDP	P2-O11	3.01	1.64	1.60
5	A	704	TDP	C6'-N1'	3.29	1.41	1.34
2	B	701	FAD	C9A-N10	3.33	1.43	1.38
5	B	703	TDP	P2-O11	4.15	1.66	1.60
2	B	701	FAD	C4X-N5	4.39	1.39	1.33
5	B	703	TDP	C4'-N3'	4.48	1.41	1.35
5	B	703	TDP	C6'-N1'	4.54	1.44	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FAD	C4X-C4-N3	-5.38	115.82	123.48
2	B	701	FAD	C4X-C4-N3	-5.30	115.93	123.48
5	A	704	TDP	C5'-C6'-N1'	-3.23	118.40	123.87
6	A	708	GOL	O2-C2-C3	-3.05	94.41	108.84
2	A	701	FAD	N3A-C2A-N1A	-2.90	126.33	128.86
2	A	701	FAD	C4X-C10-N10	-2.77	118.60	120.52
2	A	701	FAD	C4-C4X-C10	-2.28	118.12	119.96
5	A	704	TDP	N1'-C2'-N3'	-2.15	121.87	125.59
6	A	707	GOL	C3-C2-C1	-2.04	103.42	111.52
5	A	704	TDP	C5-C4-N3	2.15	111.87	107.57
5	B	703	TDP	O23-P2-O22	2.19	116.46	107.61
2	A	701	FAD	C1'-C2'-C3'	2.26	116.29	109.82
5	A	704	TDP	C6'-C5'-C4'	2.46	118.96	115.68
4	A	703	PO4	O4-P-O3	2.62	117.52	107.90
2	A	701	FAD	C5A-C6A-N6A	2.62	125.82	120.47
5	B	703	TDP	C6'-C5'-C4'	2.72	119.30	115.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	TDP	C6'-N1'-C2'	2.89	120.88	115.88
2	B	701	FAD	C1'-N10-C9A	3.31	121.38	118.35
4	B	704	PO4	O4-P-O3	3.45	120.57	107.90
2	A	701	FAD	C1'-N10-C9A	5.15	123.06	118.35
2	B	701	FAD	C4-N3-C2	8.92	122.96	115.16
2	A	701	FAD	C4-N3-C2	11.09	124.86	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	2	0
5	A	704	TDP	1	0
5	B	703	TDP	1	0
6	B	708	GOL	2	0
6	B	709	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%)	-0.59	1 (0%) 94 90	4, 8, 22, 81	0
1	B	585/603 (97%)	-0.64	2 (0%) 93 90	4, 7, 17, 72	0
All	All	1171/1206 (97%)	-0.61	3 (0%) 93 90	4, 7, 20, 81	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	LEU	6.5
1	B	593	ASP	4.0
1	B	592	ASP	2.5

### 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( $\text{\AA}^2$ )	Q<0.9
6	GOL	B	708	6/6	0.50	0.22	25.61	45,47,53,53	0
6	GOL	A	708	6/6	0.97	0.12	15.50	14,20,40,63	0
6	GOL	A	706	6/6	0.95	0.13	5.52	16,21,26,28	0
6	GOL	A	707	6/6	0.85	0.14	4.03	25,33,35,39	0
6	GOL	B	705	6/6	0.94	0.18	3.20	17,26,33,40	0
6	GOL	A	705	6/6	0.96	0.08	2.89	8,14,20,25	0
6	GOL	B	709	6/6	0.91	0.11	2.85	18,28,30,43	0
7	K	A	709	1/1	1.00	0.08	2.44	7,7,7,7	1
6	GOL	B	707	6/6	0.96	0.08	2.23	17,20,27,28	0
4	PO4	A	703	5/5	0.99	0.06	0.06	10,10,16,17	5
5	TDP	B	703	26/26	1.00	0.05	-0.37	4,5,6,7	0
4	PO4	B	704	5/5	0.99	0.04	-0.88	9,10,14,16	5
5	TDP	A	704	26/26	1.00	0.04	-0.99	5,5,7,7	0
2	FAD	A	701	53/53	1.00	0.04	-1.11	4,5,7,8	0
2	FAD	B	701	53/53	1.00	0.03	-1.12	4,5,6,6	0
3	MG	A	702	1/1	1.00	0.02	-2.58	5,5,5,5	0
3	MG	B	702	1/1	1.00	0.01	-4.81	5,5,5,5	0
6	GOL	B	706	6/6	0.86	0.11	-	36,46,52,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.