



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:32 AM GMT

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 : 2013-04-29
Resolution : 1.06 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

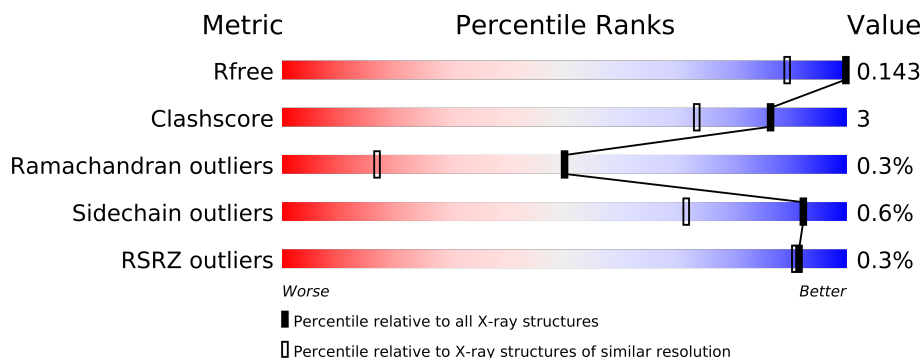
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.06 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}	66092	1012 (1.14-0.98)
Clashscore	79885	1122 (1.14-0.98)
Ramachandran outliers	78287	1057 (1.14-0.98)
Sidechain outliers	78261	1055 (1.14-0.98)
RSRZ outliers	66119	1012 (1.14-0.98)

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. 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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	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	706	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	B	707	-	X
6	GOL	B	708	-	X

2 Entry composition i

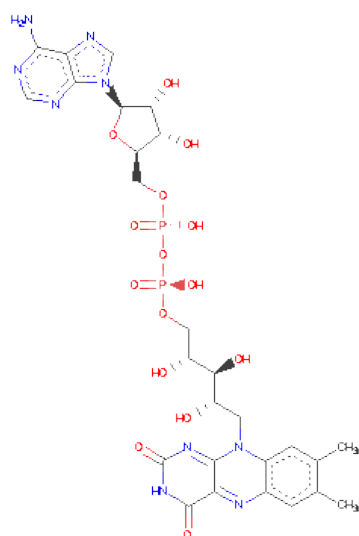
There are 8 unique types of molecules in this entry. The entry contains 11890 atoms, of which 0 are hydrogen and 0 are deuterium.

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	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: $C_{27}H_{33}N_9O_{15}P_2$).

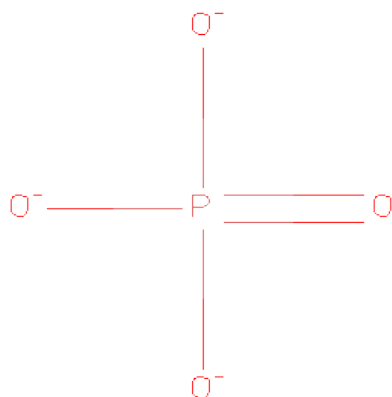


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

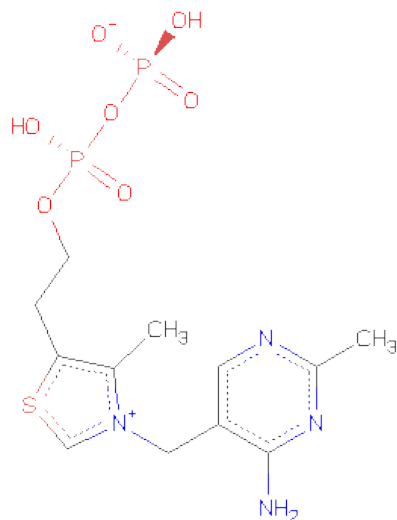
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- 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	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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		

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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.

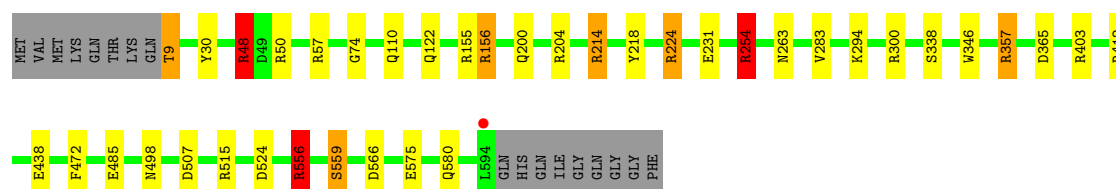
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	945	Total	O	0	106
			945	945		
8	B	954	Total	O	0	94
			954	954		

3 Residue-property plots

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.

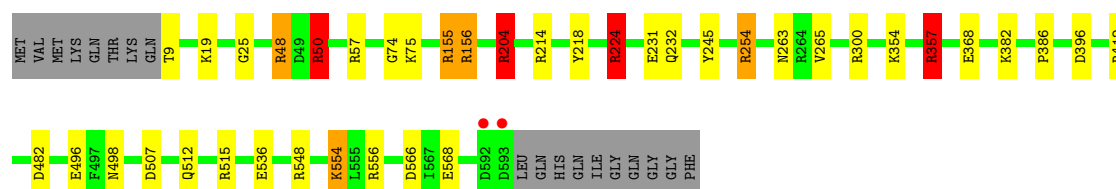
• Molecule 1: Pyruvate oxidase

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.06Å)	Xtriage
Refinement program	SHELXL-12	Depositor
R, R_{free}	0.127 , 0.150 0.125 , 0.143	Depositor DCC
R_{free} test set	18027 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	6.7	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 75.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 645341 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11890	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities 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: 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

The worst 5 of 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ARG	NE-CZ-NH2	15.46	128.03	120.30

There are no chirality outliers.

5 of 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	9	THR	Peptide

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	4863	0	0	12	0
1	B	4903	0	0	14	0
2	A	53	0	0	0	0
2	B	53	0	0	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	0	0	0
5	B	26	0	0	0	0
6	A	24	0	0	0	0
6	B	30	0	0	0	0
7	A	1	0	0	0	0
8	A	945	0	0	12	1
8	B	954	0	0	13	1
All	All	11890	0	0	26	2

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 3.

The worst 5 of 26 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:354[B]:LYS:NZ	8:B:1732:HOH:O	2.32	0.62
1:B:204[B]:ARG:NH1	8:B:1143:HOH:O	2.40	0.55
1:B:498[B]:ASN:ND2	8:B:1119[B]:HOH:O	2.43	0.51
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

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	Distance(Å)	Clash(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

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	625/603 (104%)	609 (97%)	14 (2%)	2 (0%)	50	17
1	B	628/603 (104%)	610 (97%)	17 (3%)	1 (0%)	56	19
All	All	1253/1206 (104%)	1219 (97%)	31 (2%)	3 (0%)	50	19

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 ⓘ

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%)	89	64
1	B	515/485 (106%)	513 (100%)	2 (0%)	95	78
All	All	1027/970 (106%)	1021 (99%)	6 (1%)	92	71

5 of 6 residues with a non-rotameric sidechain are listed below:

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

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 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 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	-	58,58,58	1.15	4 (6%)	85,89,89	1.25	8 (9%)
4	PO4	A	703	-	4,4,4	1.20	1 (25%)	6,6,6	0.37	0
5	TDP	A	704	3	27,27,27	1.56	5 (18%)	40,40,40	1.51	9 (22%)
6	GOL	A	705	-	5,5,5	0.62	0	5,5,5	1.11	0
6	GOL	A	706	-	5,5,5	1.01	0	5,5,5	0.87	0
6	GOL	A	707	-	5,5,5	0.20	0	5,5,5	1.09	0
6	GOL	A	708	-	5,5,5	0.68	0	5,5,5	1.52	1 (20%)
2	FAD	B	701	-	58,58,58	1.10	4 (6%)	85,89,89	1.15	7 (8%)
5	TDP	B	703	3	27,27,27	1.83	9 (33%)	40,40,40	1.60	5 (12%)
4	PO4	B	704	-	4,4,4	1.31	0	6,6,6	0.41	0
6	GOL	B	705	-	5,5,5	0.72	0	5,5,5	0.88	0
6	GOL	B	706	-	5,5,5	0.52	0	5,5,5	1.08	0
6	GOL	B	707	-	5,5,5	0.83	0	5,5,5	0.70	0
6	GOL	B	708	-	5,5,5	0.68	0	5,5,5	1.33	0
6	GOL	B	709	-	5,5,5	0.74	0	5,5,5	0.61	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	-	-	0/34/50/50	0/1/6/6
4	PO4	A	703	-	-	0/0/0/0	0/0/0/0
5	TDP	A	704	3	-	0/17/17/17	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	-	-	0/34/50/50	0/1/6/6
5	TDP	B	703	3	-	0/17/17/17	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

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	TDP	C5-S1	4.36	1.77	1.73
5	B	703	TDP	C6'-N1'	4.32	1.44	1.34
5	B	703	TDP	C4'-N3'	4.20	1.41	1.35
2	B	701	FAD	C1'-C2'	3.25	1.54	1.51
5	A	704	TDP	C6'-N1'	3.13	1.41	1.34

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	703	TDP	C4-C5-S1	6.37	115.13	109.93
2	A	701	FAD	C9A-N10-C10	-4.33	117.51	121.77
2	A	701	FAD	C1'-N10-C9A	4.31	123.06	118.87
5	A	704	TDP	C4-C5-S1	4.10	113.27	109.93
2	A	701	FAD	C4X-C10-N10	-3.83	118.60	120.51

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, 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	586/603 (97%)	-0.57	1 (0%) 93 91	4, 8, 22, 81	0
1	B	585/603 (97%)	-0.65	2 (0%) 91 91	4, 7, 17, 72	0
All	All	1171/1206 (97%)	-0.61	3 (0%) 91 91	4, 7, 20, 81	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	LEU	7.3
1	B	593	ASP	3.9
1	B	592	ASP	2.3

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	B	708	6/6	0.19	22.22	45,47,53,53	0
6	GOL	A	708	6/6	0.10	11.23	14,20,40,63	0
6	GOL	A	706	6/6	0.15	6.35	16,21,26,28	0
6	GOL	B	705	6/6	0.17	3.93	17,26,33,40	0
6	GOL	B	706	6/6	0.11	3.70	36,46,52,63	0
6	GOL	A	707	6/6	0.14	3.57	25,33,35,39	0
6	GOL	A	705	6/6	0.07	2.74	8,14,20,25	0
6	GOL	B	707	6/6	0.08	2.02	17,20,27,28	0
6	GOL	B	709	6/6	0.09	1.78	18,28,30,43	0
7	K	A	709	1/1	0.07	0.65	7,7,7,7	1
4	PO4	A	703	5/5	0.05	0.04	10,10,16,17	5
5	TDP	B	703	26/26	0.04	-0.41	4,5,6,7	0
2	FAD	A	701	53/53	0.04	-0.91	4,5,7,8	0
4	PO4	B	704	5/5	0.04	-0.97	9,10,14,16	5
5	TDP	A	704	26/26	0.04	-1.03	5,5,7,7	0
2	FAD	B	701	53/53	0.03	-1.05	4,5,6,6	0
3	MG	A	702	1/1	0.02	-2.17	5,5,5,5	0
3	MG	B	702	1/1	0.01	-4.04	5,5,5,5	0

6.5 Other polymers ⓘ

There are no such residues in this entry.