



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:30 PM EDT

PDB ID : 6WP3 / pdb_00006wp3
Title : Pyruvate Kinase M2 Mutant-K433Q
Authors : Nandi, S.; Razzaghi, M.; Srivastava, D.; Dey, M.
Deposited on : 2020-04-26
Resolution : 1.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

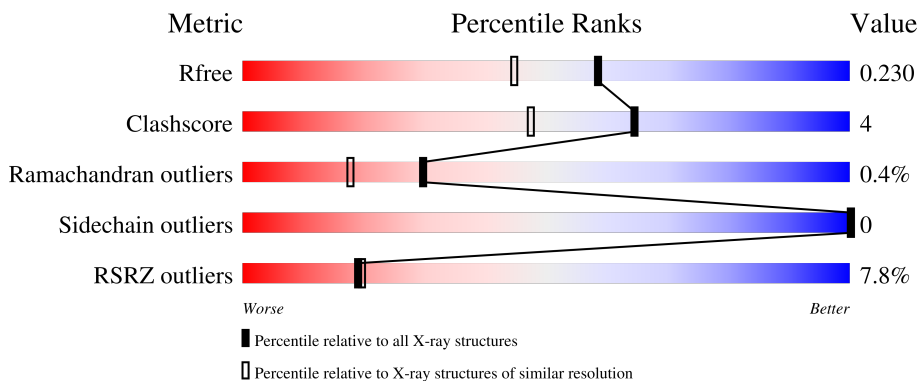
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	550	
1	B	550	

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	OXL	A	605	-	X	-	-
3	OXL	B	604	-	X	-	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 7444 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 kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	510	3793	2389	666	713	25	0	0	0
1	B	428	3200	2008	572	598	22	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

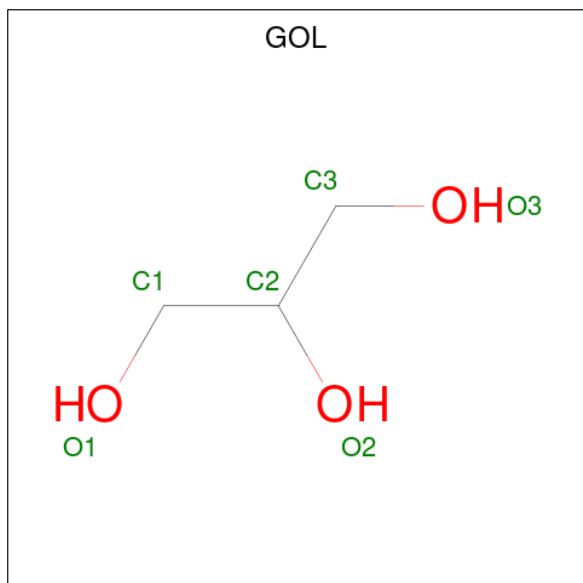
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
A	433	GLN	LYS	engineered mutation	UNP P14618
B	-18	MET	-	initiating methionine	UNP P14618
B	-17	GLY	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
B	433	GLN	LYS	engineered mutation	UNP P14618

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



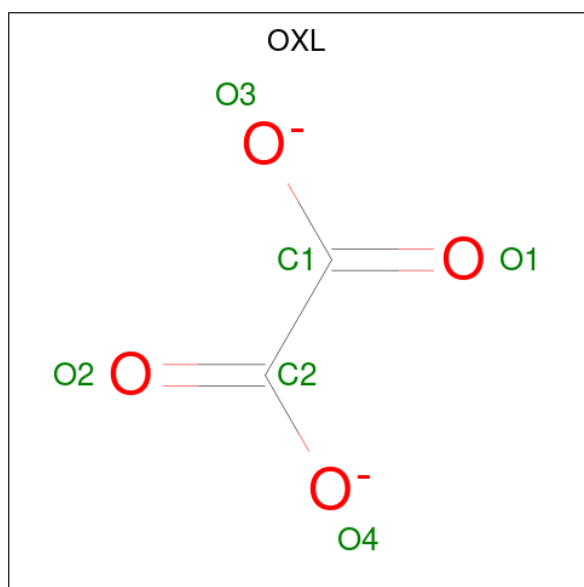
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).

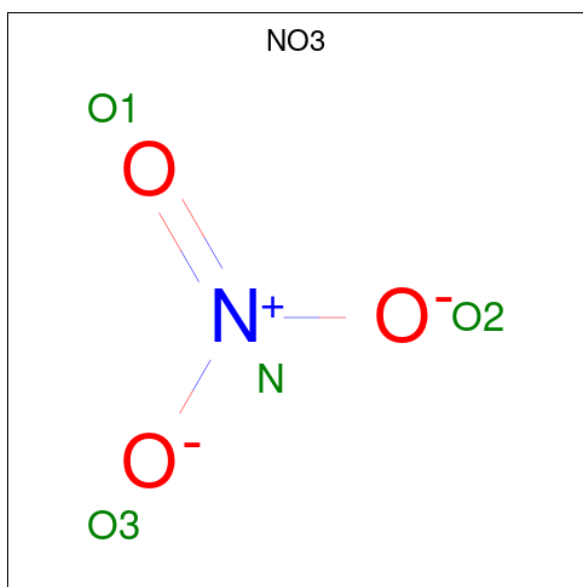


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N O 4 1 3	0	0
5	B	1	Total N O 4 1 3	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cl 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	213	Total O 213 213	0	0
8	B	172	Total O 172 172	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.38Å 94.23Å 109.64Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	47.11 – 1.84 47.11 – 1.84	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.11-1.84) 97.6 (47.11-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.84Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.203 , 0.230 0.204 , 0.230	Depositor DCC
R_{free} test set	4815 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7444	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, OXL, K, CL, NO3, MG

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	0.34	0/3850	0.55	0/5213
1	B	0.34	0/3250	0.55	2/4398 (0.0%)
All	All	0.34	0/7100	0.55	2/9611 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	486	VAL	CA-C-N	-5.54	111.25	120.68
1	B	486	VAL	C-N-CA	-5.54	111.25	120.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3793	0	3747	34	1
1	B	3200	0	3186	23	1
2	A	24	0	31	4	0
2	B	18	0	24	2	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	A	213	0	0	4	0
8	B	172	0	0	1	0
All	All	7444	0	6988	55	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 (55) 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:B:410:GLU:HG3	1:B:440:GLN:HE21	1.30	0.94
1:A:83:TYR:HE1	2:A:604:GOL:H2	1.50	0.75
1:B:407:ASP:OD2	1:B:436:ARG:NH2	2.21	0.74
1:A:494:MET:CE	1:A:531:PRO:HD2	2.18	0.73
1:B:410:GLU:HG3	1:B:440:GLN:NE2	2.04	0.73
1:A:83:TYR:CE1	2:A:604:GOL:H2	2.25	0.71
1:A:494:MET:HE2	1:A:531:PRO:HD2	1.74	0.69
1:B:16:GLN:HB2	1:B:18:LEU:HD13	1.75	0.67
1:A:479:GLN:C	1:A:481:ALA:HB3	2.21	0.66
1:A:87:THR:HG21	2:A:604:GOL:H11	1.81	0.62
1:B:436:ARG:HB3	2:B:603:GOL:H11	1.80	0.62
1:B:244:PHE:HD1	1:B:273:ASN:HD22	1.50	0.60
1:A:39:PRO:O	8:A:701:HOH:O	2.16	0.59
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.85	0.59
1:A:339:ARG:NH2	8:A:707:HOH:O	2.34	0.59
1:A:127:SER:O	8:A:702:HOH:O	2.17	0.57
1:A:395:PHE:CZ	1:A:399:ARG:HD2	2.39	0.57
1:A:494:MET:HE1	1:A:530:VAL:HA	1.87	0.57
1:B:272:GLU:HB3	1:B:293:ALA:HB3	1.86	0.56
1:A:395:PHE:CE2	1:A:399:ARG:HD2	2.40	0.56
1:A:132:VAL:HG21	1:A:153:ASP:HA	1.89	0.55
1:A:272:GLU:HB3	1:A:293:ALA:HB3	1.90	0.54
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.89	0.53
1:A:327:ALA:HB1	1:A:360:MET:HE2	1.91	0.52
1:A:16:GLN:NE2	1:A:447:ARG:HD3	2.24	0.52
1:A:331:LEU:O	1:A:334:MET:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MET:HG3	1:A:150:GLU:HG3	1.92	0.52
1:B:39:PRO:O	8:B:701:HOH:O	2.18	0.51
1:A:494:MET:HE1	1:A:531:PRO:HD2	1.93	0.49
1:A:40:ILE:O	8:A:703:HOH:O	2.20	0.49
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.48	0.49
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.95	0.48
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.94	0.48
1:A:27:LEU:HD23	1:B:401:LEU:HD12	1.96	0.47
1:B:505:LYS:HE2	1:B:531:PRO:OXT	2.14	0.46
1:A:494:MET:HB3	1:A:494:MET:HE3	1.71	0.46
1:A:505:LYS:HA	1:A:530:VAL:HG12	1.97	0.46
1:A:437:SER:HB3	1:A:522:THR:HG21	1.99	0.45
1:A:514:GLY:HA2	1:A:522:THR:HA	1.98	0.44
1:B:216:VAL:HB	2:B:602:GOL:H31	2.00	0.44
1:A:397:GLU:CD	1:B:25:THR:HB	2.42	0.44
1:B:393:GLN:O	1:B:397:GLU:HG3	2.17	0.43
1:B:40:ILE:O	1:B:383:ARG:NH2	2.49	0.43
1:A:244:PHE:CZ	2:A:603:GOL:H11	2.54	0.43
1:B:224:LYS:NZ	1:B:228:ASP:OD2	2.48	0.43
1:A:163:ASN:ND2	1:A:217:ASP:OD2	2.53	0.42
1:A:164:ILE:O	1:A:168:VAL:HG22	2.20	0.42
1:B:55:SER:HA	1:B:60:THR:HG21	2.03	0.41
1:B:18:LEU:O	1:B:22:MET:HG2	2.20	0.41
1:B:288:ASP:O	1:B:323:PRO:HD2	2.21	0.40
1:B:15:THR:HG22	1:B:38:PRO:HG2	2.02	0.40
1:B:331:LEU:HD23	1:B:344:GLU:HB3	2.03	0.40
1:B:453:VAL:HG21	1:B:493:ALA:HB2	2.03	0.40
1:A:121:THR:HB	1:A:157:LEU:HD11	2.03	0.40
1:B:103:ILE:HD13	1:B:492:PHE:CE1	2.57	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:A:434:SER:OG	1:B:223:GLU:OE1[3_455]	2.13	0.07

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	500/550 (91%)	487 (97%)	10 (2%)	3 (1%)	21	9
1	B	420/550 (76%)	414 (99%)	5 (1%)	1 (0%)	43	34
All	All	920/1100 (84%)	901 (98%)	15 (2%)	4 (0%)	30	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	517	PRO
1	A	328	THR
1	B	328	THR

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	387/452 (86%)	387 (100%)	0	100	100
1	B	331/452 (73%)	331 (100%)	0	100	100
All	All	718/904 (79%)	718 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	210	ASN
1	A	227	GLN
1	A	393	GLN
1	A	440	GLN
1	B	44	ASN
1	B	391	HIS
1	B	393	GLN
1	B	433	GLN
1	B	440	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	GOL	A	604	-	5,5,5	1.50	1 (20%)	5,5,5	1.40	0
2	GOL	A	603	-	5,5,5	0.65	0	5,5,5	1.33	1 (20%)
5	NO3	A	607	-	1,3,3	0.36	0	0,3,3	-	-
2	GOL	B	603	-	5,5,5	1.04	0	5,5,5	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	602	-	5,5,5	0.80	0	5,5,5	1.20	1 (20%)
2	GOL	A	601	-	5,5,5	0.91	0	5,5,5	0.96	0
5	NO3	B	606	-	1,3,3	0.53	0	0,3,3	-	-
3	OXL	B	604	4	5,5,5	1.37	0	6,6,6	2.22	2 (33%)
2	GOL	B	601	-	5,5,5	0.75	0	5,5,5	1.35	1 (20%)
2	GOL	B	602	-	5,5,5	0.75	0	5,5,5	1.07	0
3	OXL	A	605	4	5,5,5	1.53	0	6,6,6	1.80	2 (33%)

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	GOL	A	604	-	-	4/4/4/4	-
2	GOL	A	603	-	-	2/4/4/4	-
2	GOL	B	603	-	-	0/4/4/4	-
2	GOL	A	602	-	-	0/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
3	OXL	B	604	4	-	4/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-
2	GOL	B	602	-	-	3/4/4/4	-
3	OXL	A	605	4	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	GOL	O2-C2	-2.11	1.37	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	OXL	O4-C2-C1	3.56	119.74	112.83
3	B	604	OXL	O3-C1-C2	3.49	119.59	112.83
3	A	605	OXL	O4-C2-C1	3.10	118.85	112.83
3	A	605	OXL	O3-C1-C2	2.69	118.05	112.83
2	A	602	GOL	C3-C2-C1	-2.36	103.15	111.80
2	B	601	GOL	C3-C2-C1	-2.23	103.62	111.80
2	A	603	GOL	C3-C2-C1	-2.11	104.07	111.80

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	GOL	C1-C2-C3-O3
2	A	604	GOL	O1-C1-C2-O2
2	A	604	GOL	O1-C1-C2-C3
2	A	604	GOL	C1-C2-C3-O3
2	B	602	GOL	O1-C1-C2-C3
2	B	602	GOL	C1-C2-C3-O3
2	A	603	GOL	O2-C2-C3-O3
2	A	604	GOL	O2-C2-C3-O3
3	A	605	OXL	O1-C1-C2-O2
3	A	605	OXL	O3-C1-C2-O4
2	B	602	GOL	O2-C2-C3-O3
3	A	605	OXL	O3-C1-C2-O2
3	B	604	OXL	O3-C1-C2-O4
3	B	604	OXL	O1-C1-C2-O2
3	A	605	OXL	O1-C1-C2-O4
3	B	604	OXL	O1-C1-C2-O4
3	B	604	OXL	O3-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	GOL	3	0
2	A	603	GOL	1	0
2	B	603	GOL	1	0
2	B	602	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

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	510/550 (92%)	0.41	48 (9%) 14 15	17, 28, 49, 61	0
1	B	428/550 (77%)	0.37	25 (5%) 29 30	17, 29, 46, 56	0
All	All	938/1100 (85%)	0.40	73 (7%) 19 20	17, 29, 48, 61	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	PRO	5.0
1	A	190	ALA	4.8
1	A	401	LEU	4.8
1	A	516	ARG	4.5
1	B	13	ILE	4.3
1	A	518	GLY	4.3
1	A	402	ALA	4.0
1	A	482	TRP	4.0
1	B	120	ARG	3.9
1	B	520	GLY	3.9
1	A	481	ALA	3.5
1	A	186	LYS	3.3
1	B	221	VAL	3.3
1	A	131	GLU	3.2
1	B	482	TRP	3.2
1	A	407	ASP	3.2
1	A	192	PHE	3.2
1	B	259	GLY	3.1
1	A	41	THR	3.1
1	A	170	VAL	3.1
1	B	214	ALA	3.1
1	A	132	VAL	2.9
1	B	487	ASP	2.9
1	A	127	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	2.9
1	A	187	GLN	2.8
1	A	513	THR	2.7
1	A	470	PHE	2.7
1	A	191	ASP	2.7
1	A	512	LEU	2.7
1	B	14	GLN	2.6
1	A	156	ILE	2.6
1	A	199	ASN	2.6
1	A	137	GLY	2.6
1	B	402	ALA	2.6
1	A	519	SER	2.6
1	B	83	TYR	2.5
1	A	514	GLY	2.5
1	B	207	LYS	2.5
1	B	481	ALA	2.5
1	A	154	GLU	2.5
1	A	197	VAL	2.5
1	B	491	ASN	2.5
1	B	480	GLU	2.4
1	B	121	THR	2.4
1	A	478	VAL	2.4
1	B	226	ILE	2.4
1	A	126	GLY	2.3
1	A	400	ARG	2.3
1	B	231	PHE	2.3
1	A	406	SER	2.3
1	A	531	PRO	2.3
1	A	195	THR	2.2
1	A	200	GLY	2.2
1	A	184	GLN	2.2
1	B	222	SER	2.2
1	A	100	SER	2.2
1	A	135	LYS	2.2
1	A	148	TYR	2.1
1	A	168	VAL	2.1
1	B	254	VAL	2.1
1	A	181	ILE	2.1
1	A	139	THR	2.1
1	A	136	LYS	2.1
1	A	188	LYS	2.1
1	B	261	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	185	VAL	2.1
1	A	40	ILE	2.0
1	A	124	ILE	2.0
1	B	521	PHE	2.0
1	B	40	ILE	2.0
1	B	119	ILE	2.0
1	B	514	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	K	B	607	1/1	0.82	0.17	50,50,50,50	0
2	GOL	B	603	6/6	0.83	0.15	31,40,43,54	0
2	GOL	B	602	6/6	0.84	0.14	34,39,46,52	0
2	GOL	A	603	6/6	0.85	0.16	27,29,32,35	0
7	CL	B	608	1/1	0.85	0.12	59,59,59,59	0
2	GOL	A	602	6/6	0.86	0.12	27,35,36,41	0
2	GOL	A	604	6/6	0.86	0.19	26,29,34,38	0
2	GOL	A	601	6/6	0.93	0.08	23,25,28,30	0
2	GOL	B	601	6/6	0.93	0.07	25,28,30,30	0
5	NO3	A	607	4/4	0.95	0.17	32,33,36,36	0
5	NO3	B	606	4/4	0.95	0.13	31,32,32,35	0
3	OXL	B	604	6/6	0.96	0.07	25,28,30,31	0
3	OXL	A	605	6/6	0.97	0.05	19,20,22,23	0
4	MG	B	605	1/1	0.97	0.04	26,26,26,26	0
4	MG	A	606	1/1	0.99	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.