



Full wwPDB X-ray Structure Validation Report i

Jun 7, 2023 – 06:16 PM JST

PDB ID : 8IAT
Title : Crystal structure of Streptococcus pneumoniae pyruvate kinase in complex with oxalate
Authors : Nakashima, R.; Taguchi, A.
Deposited on : 2023-02-09
Resolution : 1.80 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

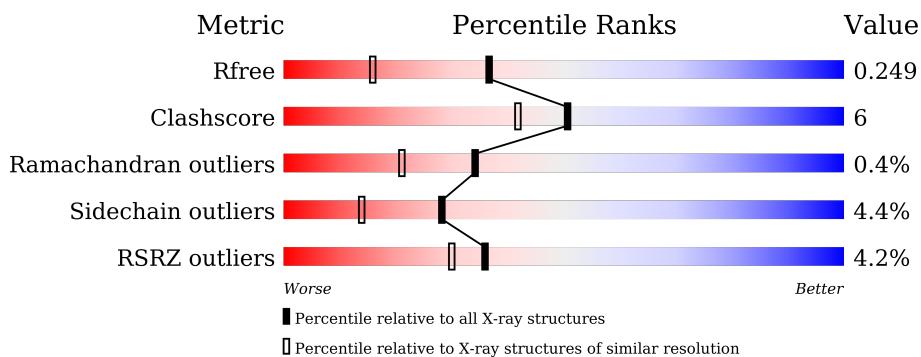
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

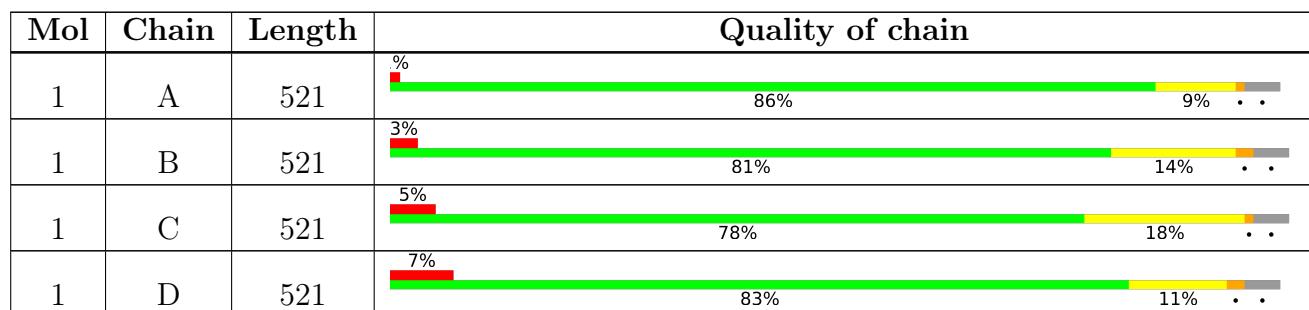
The reported resolution of this entry is 1.80 Å.

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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.



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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OXL	B	602	-	X	-	-
2	OXL	D	602	-	X	-	-
7	GOL	A	607	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16483 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	1	0
			3851	2408	665	761	17			
1	B	501	Total	C	N	O	S	0	1	0
			3851	2408	665	761	17			
1	C	501	Total	C	N	O	S	0	0	0
			3839	2399	664	759	17			
1	D	500	Total	C	N	O	S	0	0	0
			3828	2393	660	758	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8DQ84
A	-18	GLY	-	expression tag	UNP Q8DQ84
A	-17	SER	-	expression tag	UNP Q8DQ84
A	-16	SER	-	expression tag	UNP Q8DQ84
A	-15	HIS	-	expression tag	UNP Q8DQ84
A	-14	HIS	-	expression tag	UNP Q8DQ84
A	-13	HIS	-	expression tag	UNP Q8DQ84
A	-12	HIS	-	expression tag	UNP Q8DQ84
A	-11	HIS	-	expression tag	UNP Q8DQ84
A	-10	HIS	-	expression tag	UNP Q8DQ84
A	-9	SER	-	expression tag	UNP Q8DQ84
A	-8	SER	-	expression tag	UNP Q8DQ84
A	-7	GLY	-	expression tag	UNP Q8DQ84
A	-6	LEU	-	expression tag	UNP Q8DQ84
A	-5	VAL	-	expression tag	UNP Q8DQ84
A	-4	PRO	-	expression tag	UNP Q8DQ84
A	-3	ARG	-	expression tag	UNP Q8DQ84
A	-2	GLY	-	expression tag	UNP Q8DQ84
A	-1	SER	-	expression tag	UNP Q8DQ84
A	0	HIS	-	expression tag	UNP Q8DQ84
B	-19	MET	-	initiating methionine	UNP Q8DQ84

Continued on next page...

Continued from previous page...

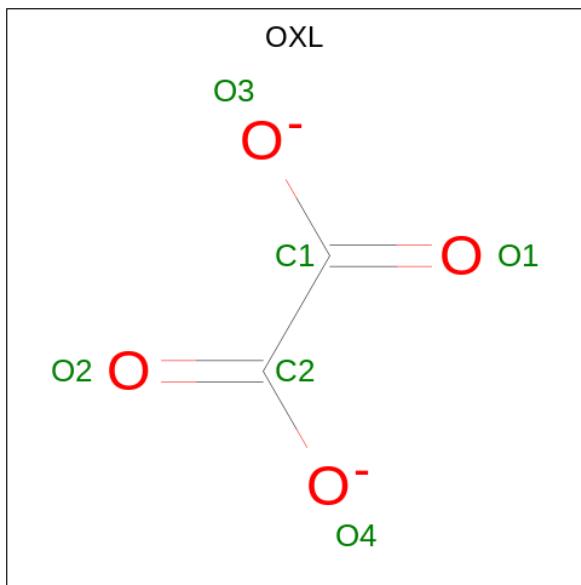
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q8DQ84
B	-17	SER	-	expression tag	UNP Q8DQ84
B	-16	SER	-	expression tag	UNP Q8DQ84
B	-15	HIS	-	expression tag	UNP Q8DQ84
B	-14	HIS	-	expression tag	UNP Q8DQ84
B	-13	HIS	-	expression tag	UNP Q8DQ84
B	-12	HIS	-	expression tag	UNP Q8DQ84
B	-11	HIS	-	expression tag	UNP Q8DQ84
B	-10	HIS	-	expression tag	UNP Q8DQ84
B	-9	SER	-	expression tag	UNP Q8DQ84
B	-8	SER	-	expression tag	UNP Q8DQ84
B	-7	GLY	-	expression tag	UNP Q8DQ84
B	-6	LEU	-	expression tag	UNP Q8DQ84
B	-5	VAL	-	expression tag	UNP Q8DQ84
B	-4	PRO	-	expression tag	UNP Q8DQ84
B	-3	ARG	-	expression tag	UNP Q8DQ84
B	-2	GLY	-	expression tag	UNP Q8DQ84
B	-1	SER	-	expression tag	UNP Q8DQ84
B	0	HIS	-	expression tag	UNP Q8DQ84
C	-19	MET	-	initiating methionine	UNP Q8DQ84
C	-18	GLY	-	expression tag	UNP Q8DQ84
C	-17	SER	-	expression tag	UNP Q8DQ84
C	-16	SER	-	expression tag	UNP Q8DQ84
C	-15	HIS	-	expression tag	UNP Q8DQ84
C	-14	HIS	-	expression tag	UNP Q8DQ84
C	-13	HIS	-	expression tag	UNP Q8DQ84
C	-12	HIS	-	expression tag	UNP Q8DQ84
C	-11	HIS	-	expression tag	UNP Q8DQ84
C	-10	HIS	-	expression tag	UNP Q8DQ84
C	-9	SER	-	expression tag	UNP Q8DQ84
C	-8	SER	-	expression tag	UNP Q8DQ84
C	-7	GLY	-	expression tag	UNP Q8DQ84
C	-6	LEU	-	expression tag	UNP Q8DQ84
C	-5	VAL	-	expression tag	UNP Q8DQ84
C	-4	PRO	-	expression tag	UNP Q8DQ84
C	-3	ARG	-	expression tag	UNP Q8DQ84
C	-2	GLY	-	expression tag	UNP Q8DQ84
C	-1	SER	-	expression tag	UNP Q8DQ84
C	0	HIS	-	expression tag	UNP Q8DQ84
D	-19	MET	-	initiating methionine	UNP Q8DQ84
D	-18	GLY	-	expression tag	UNP Q8DQ84
D	-17	SER	-	expression tag	UNP Q8DQ84

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q8DQ84
D	-15	HIS	-	expression tag	UNP Q8DQ84
D	-14	HIS	-	expression tag	UNP Q8DQ84
D	-13	HIS	-	expression tag	UNP Q8DQ84
D	-12	HIS	-	expression tag	UNP Q8DQ84
D	-11	HIS	-	expression tag	UNP Q8DQ84
D	-10	HIS	-	expression tag	UNP Q8DQ84
D	-9	SER	-	expression tag	UNP Q8DQ84
D	-8	SER	-	expression tag	UNP Q8DQ84
D	-7	GLY	-	expression tag	UNP Q8DQ84
D	-6	LEU	-	expression tag	UNP Q8DQ84
D	-5	VAL	-	expression tag	UNP Q8DQ84
D	-4	PRO	-	expression tag	UNP Q8DQ84
D	-3	ARG	-	expression tag	UNP Q8DQ84
D	-2	GLY	-	expression tag	UNP Q8DQ84
D	-1	SER	-	expression tag	UNP Q8DQ84
D	0	HIS	-	expression tag	UNP Q8DQ84

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).



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

Continued on next page...

Continued from previous page...

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

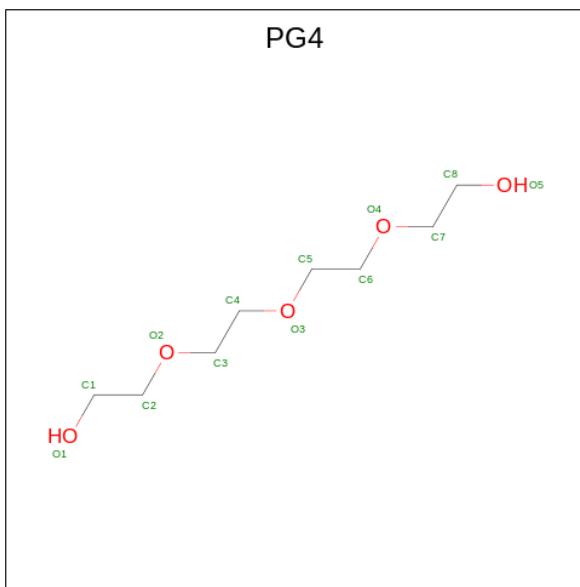
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

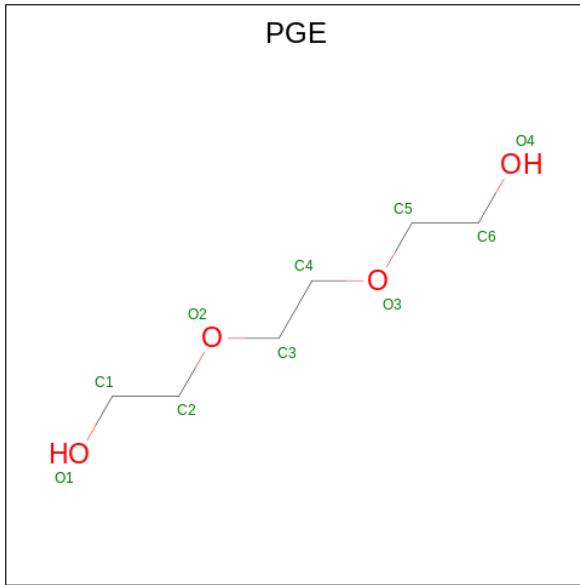
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



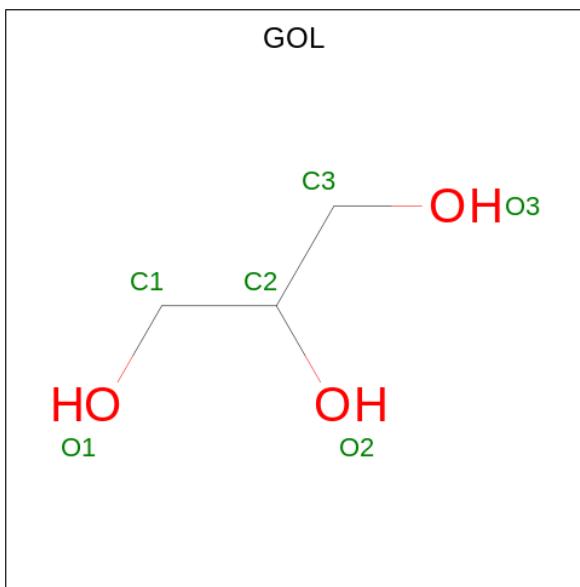
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	13	8	5	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	10	6	4	0	0
6	C	1	10	6	4	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

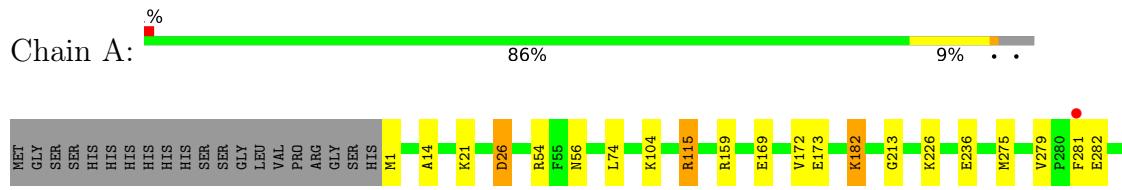
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	325	Total O 325 325	0	0
8	B	322	Total O 322 322	0	0
8	C	195	Total O 195 195	0	0
8	D	177	Total O 177 177	0	0

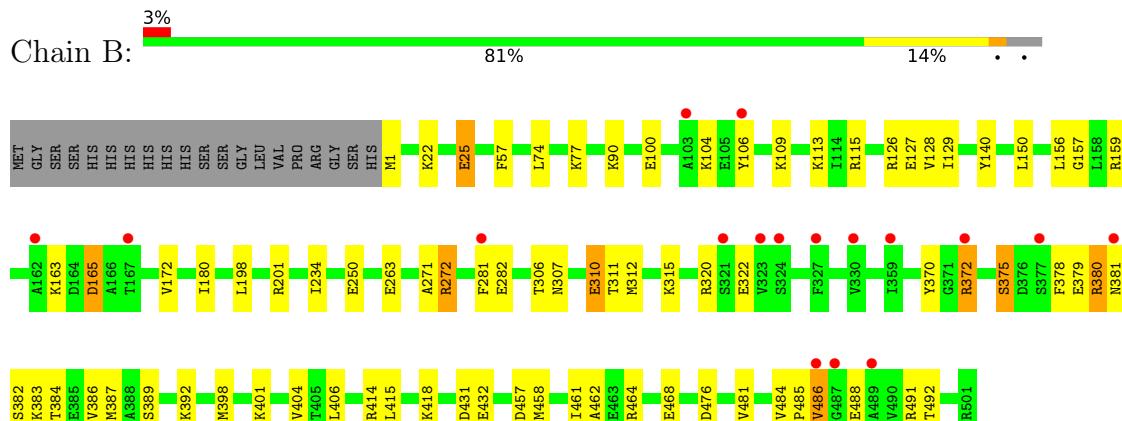
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

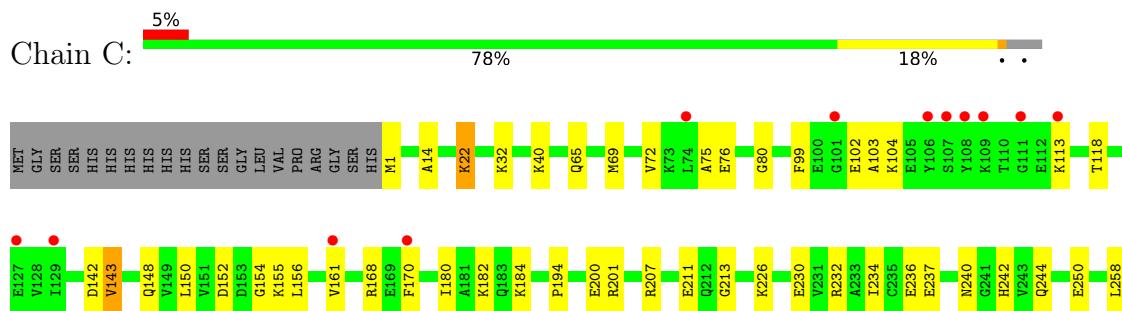
- Molecule 1: Pyruvate kinase

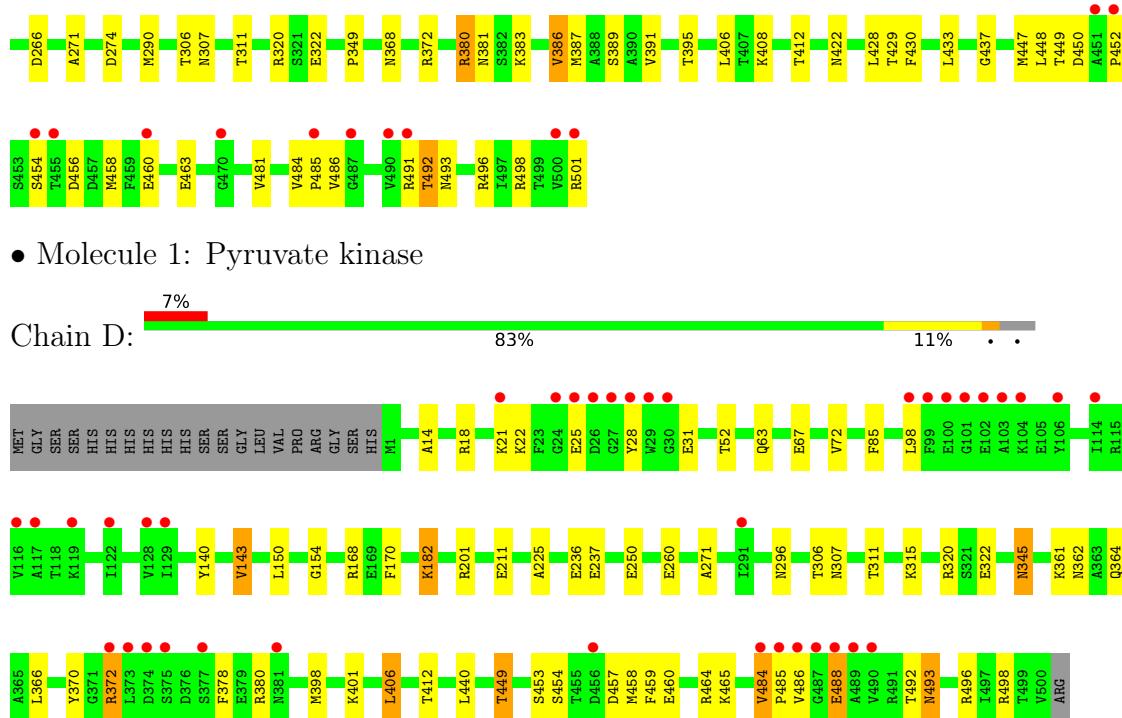


- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase





4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.05 Å 118.35 Å 99.82 Å 90.00° 108.93° 90.00°	Depositor
Resolution (Å)	48.30 – 1.80 48.30 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.30-1.80) 99.7 (48.30-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.57 (at 1.79 Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R , R_{free}	0.199 , 0.246 0.205 , 0.249	Depositor DCC
R_{free} test set	10764 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16483	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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: K, PG4, PGE, MG, OXL, GOL

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	0.74	0/3897	0.86	1/5254 (0.0%)
1	B	0.75	0/3897	0.86	3/5254 (0.1%)
1	C	0.75	0/3884	0.87	0/5238
1	D	0.71	0/3873	0.80	0/5224
All	All	0.74	0/15551	0.85	4/20970 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	272	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	115	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	414	ARG	CG-CD-NE	-5.48	100.30	111.80
1	B	414	ARG	NE-CZ-NH1	-5.42	117.59	120.30

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	3851	0	3895	41	0
1	B	3851	0	3895	48	0
1	C	3839	0	3887	61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3828	0	3874	44	0
2	A	12	0	0	0	0
2	B	12	0	0	1	0
2	C	12	0	0	2	0
2	D	12	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	13	0	18	0	0
6	A	10	0	14	1	0
6	C	10	0	14	1	0
7	A	6	0	8	6	0
8	A	325	0	0	2	0
8	B	322	0	0	3	0
8	C	195	0	0	8	0
8	D	177	0	0	3	0
All	All	16483	0	15605	177	0

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 6.

All (177) 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:D:296:ASN:HB2	8:D:840:HOH:O	1.47	1.14
1:A:54:ARG:HH12	7:A:607:GOL:H11	1.27	0.95
1:C:237:GLU:HG3	8:C:707:HOH:O	1.77	0.82
1:A:54:ARG:HH12	7:A:607:GOL:C1	1.92	0.82
1:A:320:ARG:HD2	1:D:307:ASN:HD22	1.46	0.78
1:C:236:GLU:HB2	8:C:707:HOH:O	1.86	0.75
1:B:380:ARG:NH2	1:B:389:SER:OG	2.20	0.75
1:C:22:LYS:HD2	1:C:22:LYS:N	2.03	0.73
1:A:282:GLU:HG3	1:D:362:ASN:ND2	2.04	0.73
1:A:282:GLU:HG3	1:D:362:ASN:HD22	1.52	0.72
1:A:54:ARG:NH1	7:A:607:GOL:H11	2.04	0.71
1:C:148:GLN:HE22	6:C:605:PGE:H3	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ARG:HD3	8:C:822:HOH:O	1.91	0.69
1:C:142:ASP:OD2	1:C:194:PRO:CD	2.42	0.67
1:D:459:PHE:CD2	1:D:496:ARG:NH1	2.63	0.67
1:D:143:VAL:HG22	1:D:170:PHE:CE1	2.30	0.66
1:B:281[B]:PHE:CD1	1:B:282:GLU:N	2.64	0.66
1:C:492:THR:HG21	1:D:498:ARG:NH2	2.10	0.66
1:C:387:MET:SD	1:C:493:ASN:OD1	2.55	0.65
1:A:307:ASN:HD22	1:D:320:ARG:HD2	1.61	0.64
1:D:484:VAL:HA	1:D:485:PRO:C	2.18	0.64
1:C:492:THR:HG21	1:D:498:ARG:HH21	1.63	0.64
1:B:77:LYS:NZ	8:B:701:HOH:O	2.32	0.63
1:C:498:ARG:NH1	1:C:501:ARG:HG3	2.15	0.61
1:A:455:THR:O	1:A:458:MET:HB3	2.00	0.61
1:A:391:VAL:O	1:A:395:THR:HG23	2.01	0.60
1:B:320:ARG:HD2	1:C:307:ASN:HD22	1.66	0.60
1:A:340:SER:HB3	7:A:607:GOL:H12	1.83	0.60
1:D:21:LYS:HD2	1:D:31:GLU:HG3	1.83	0.59
1:D:406:LEU:HD13	1:D:458:MET:HG2	1.85	0.59
1:B:115:ARG:HB2	1:B:128:VAL:HG22	1.85	0.58
1:C:142:ASP:OD2	1:C:194:PRO:HD2	2.03	0.58
1:B:281[B]:PHE:CE1	1:B:282:GLU:HB3	2.38	0.58
1:C:412:THR:HG23	2:C:602:OXL:O2	2.03	0.57
1:A:372:ARG:HH21	1:D:372:ARG:NH1	2.03	0.56
1:B:106:TYR:CG	1:B:126:ARG:HG3	2.41	0.56
1:D:493:ASN:C	1:D:493:ASN:HD22	2.09	0.56
1:C:463:GLU:OE2	1:C:498:ARG:NE	2.32	0.56
1:D:458:MET:HB2	1:D:486:VAL:HG21	1.88	0.56
1:B:406:LEU:HD13	1:B:458:MET:HB3	1.87	0.56
1:A:14:ALA:HB2	1:A:345:ASN:HA	1.88	0.55
1:B:281[B]:PHE:CG	1:B:282:GLU:N	2.74	0.55
1:B:384:THR:HG22	1:B:415:LEU:HD12	1.88	0.55
1:D:492:THR:HG21	8:D:743:HOH:O	2.07	0.55
1:B:198:LEU:HD21	1:B:234:ILE:HD11	1.88	0.54
1:B:464:ARG:O	1:B:468:GLU:HG3	2.07	0.54
1:A:380:ARG:HB3	1:A:386:VAL:HG12	1.90	0.54
1:D:63:GLN:NE2	1:D:67:GLU:OE1	2.41	0.54
1:C:460:GLU:HG3	8:C:701:HOH:O	2.07	0.54
1:A:490:VAL:HG23	8:A:873:HOH:O	2.07	0.54
1:C:491:ARG:C	1:C:492:THR:HG23	2.28	0.54
1:C:429:THR:O	1:C:448:LEU:HD12	2.07	0.54
1:B:401:LYS:HE2	1:B:476:ASP:OD2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:LYS:HA	1:C:386:VAL:CG1	2.38	0.53
1:C:452:PRO:HG3	1:C:486:VAL:HG21	1.90	0.53
1:D:361:LYS:O	1:D:364:GLN:HG2	2.08	0.53
1:A:387:MET:CE	1:A:493:ASN:OD1	2.56	0.53
1:D:449:THR:OG1	1:D:465:LYS:HE3	2.08	0.53
1:D:412:THR:HG21	1:D:492:THR:HG21	1.91	0.52
1:C:118:THR:OG1	1:C:168:ARG:O	2.22	0.52
1:C:65:GLN:O	1:C:69:MET:HG3	2.09	0.52
1:A:21:LYS:HE3	1:A:26:ASP:O	2.09	0.52
1:B:22:LYS:O	1:B:25:GLU:HB2	2.09	0.52
1:D:311:THR:HG23	1:D:322:GLU:OE1	2.09	0.52
1:B:404:VAL:HG11	1:B:462:ALA:HB1	1.92	0.52
1:C:240:ASN:C	1:C:242:HIS:HD2	2.13	0.52
1:B:150:LEU:HD23	1:B:157:GLY:HA2	1.92	0.51
1:D:366:LEU:HD23	1:D:370:TYR:CD2	2.45	0.51
1:B:156:LEU:HD23	1:B:157:GLY:N	2.26	0.51
1:C:240:ASN:HA	1:C:242:HIS:CD2	2.45	0.51
1:C:406:LEU:HD22	1:C:458:MET:HG2	1.91	0.51
1:A:380:ARG:NH2	1:A:389:SER:OG	2.45	0.50
1:A:452:PRO:HB3	1:A:461:ILE:HD12	1.92	0.50
1:B:481:VAL:HG13	1:B:492:THR:HG21	1.93	0.50
1:A:405:THR:HA	1:A:481:VAL:O	2.12	0.50
1:B:379:GLU:CD	1:B:381:ASN:HD21	2.15	0.50
1:C:456:ASP:O	8:C:701:HOH:O	2.20	0.50
1:D:225:ALA:HB2	1:D:260:GLU:HG3	1.93	0.50
1:A:391:VAL:HG21	1:A:481:VAL:HG21	1.94	0.49
1:A:452:PRO:HB3	1:A:461:ILE:CD1	2.42	0.49
1:B:307:ASN:HD22	1:C:320:ARG:HD2	1.77	0.49
1:D:22:LYS:O	1:D:28:TYR:CD2	2.65	0.49
1:D:449:THR:OG1	1:D:465:LYS:CE	2.60	0.49
1:C:240:ASN:O	1:C:242:HIS:CD2	2.65	0.49
1:D:14:ALA:HB2	1:D:345:ASN:HA	1.94	0.49
1:A:387:MET:HE2	1:A:493:ASN:OD1	2.13	0.49
1:C:22:LYS:N	1:C:22:LYS:CD	2.75	0.49
1:C:386:VAL:HG11	1:D:398:MET:SD	2.53	0.49
1:C:311:THR:HG23	1:C:322:GLU:OE1	2.13	0.48
1:A:104:LYS:HD2	1:A:182:LYS:HE3	1.94	0.48
1:A:387:MET:SD	1:A:495:MET:HB2	2.53	0.48
1:B:372:ARG:HH12	1:C:372:ARG:HG2	1.77	0.48
1:C:391:VAL:HG21	1:C:481:VAL:HG21	1.96	0.48
1:B:250:GLU:HG2	1:B:271:ALA:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:TYR:O	1:B:372:ARG:NH1	2.45	0.48
1:C:496:ARG:HA	1:D:493:ASN:O	2.14	0.48
1:C:213:GLY:HA2	8:C:796:HOH:O	2.13	0.47
1:B:375:SER:OG	1:B:392:LYS:NZ	2.46	0.47
1:B:271:ALA:HB1	2:B:601:OXL:C1	2.44	0.47
1:C:242:HIS:CE1	1:C:433:LEU:HD22	2.49	0.47
1:D:492:THR:CG2	8:D:743:HOH:O	2.62	0.47
1:C:258:LEU:HD23	1:C:290:MET:HE1	1.95	0.47
1:C:207:ARG:O	1:C:211:GLU:HG3	2.15	0.47
1:C:230:GLU:O	1:C:234:ILE:HD13	2.14	0.47
1:C:428:LEU:HD23	1:C:447:MET:HB3	1.97	0.47
1:B:156:LEU:HD23	1:B:156:LEU:C	2.35	0.46
1:B:457:ASP:O	1:B:461:ILE:HG13	2.15	0.46
1:A:372:ARG:HG2	1:D:372:ARG:HH12	1.79	0.46
1:D:296:ASN:HD21	1:D:378:PHE:HZ	1.62	0.46
1:B:159:ARG:O	1:B:172:VAL:HA	2.16	0.46
1:B:312:MET:HA	1:B:315:LYS:O	2.16	0.46
1:B:129:ILE:HD12	1:B:180:ILE:HG21	1.98	0.46
1:C:244:GLN:NE2	1:C:437:GLY:O	2.48	0.46
1:C:152:ASP:O	1:C:155:LYS:HG2	2.15	0.46
1:A:56:ASN:HD22	7:A:607:GOL:H31	1.81	0.45
1:C:76:GLU:O	1:C:80:GLY:N	2.46	0.45
1:D:406:LEU:HD13	1:D:458:MET:CG	2.46	0.45
1:B:140:TYR:OH	1:B:163:LYS:HB3	2.16	0.45
1:B:165:ASP:OD2	1:B:165:ASP:N	2.49	0.45
1:B:90:LYS:HD3	1:B:201:ARG:HD2	1.98	0.45
1:C:391:VAL:O	1:C:395:THR:HG23	2.16	0.45
1:C:150:LEU:HB3	1:C:154:GLY:HA2	1.99	0.45
1:A:497:ILE:HG13	1:B:387:MET:HE1	1.99	0.44
1:B:310:GLU:HG3	8:B:752:HOH:O	2.17	0.44
1:D:140:TYR:CE2	1:D:168:ARG:HA	2.52	0.44
1:B:281[B]:PHE:CD1	1:B:281[B]:PHE:C	2.91	0.44
1:C:258:LEU:CD2	1:C:290:MET:HE1	2.48	0.44
1:D:250:GLU:HB3	1:D:271:ALA:HB3	1.99	0.44
1:C:368:ASN:HD21	1:C:422:ASN:ND2	2.15	0.44
1:B:382:SER:O	1:B:386:VAL:HG13	2.17	0.44
1:B:57:PHE:O	1:B:201:ARG:NH2	2.50	0.44
1:A:386:VAL:HG11	1:B:398:MET:HG3	1.99	0.43
1:B:90:LYS:HD3	1:B:201:ARG:CD	2.48	0.43
1:D:98:LEU:HD23	1:D:182:LYS:HG3	2.00	0.43
1:A:461:ILE:O	1:A:465:LYS:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:O	1:A:172:VAL:HA	2.19	0.43
1:A:173:GLU:HG2	8:A:876:HOH:O	2.18	0.43
1:A:496:ARG:NH2	1:B:484:VAL:HG11	2.33	0.43
1:C:184:LYS:NZ	8:C:716:HOH:O	2.52	0.43
1:B:310:GLU:CG	8:B:752:HOH:O	2.67	0.43
1:B:485:PRO:HB2	1:B:486:VAL:HG22	1.99	0.43
1:D:18:ARG:HB3	1:D:31:GLU:HB2	2.01	0.43
1:C:430:PHE:HZ	1:C:486:VAL:HG11	1.83	0.43
1:D:22:LYS:O	1:D:28:TYR:HD2	1.99	0.43
1:B:311:THR:HG23	1:B:322:GLU:OE1	2.19	0.43
1:C:143:VAL:HG13	1:C:170:PHE:CZ	2.54	0.42
1:C:240:ASN:C	1:C:242:HIS:CD2	2.92	0.42
1:D:143:VAL:CG2	1:D:170:PHE:CE1	3.01	0.42
1:B:106:TYR:CD1	1:B:126:ARG:HG3	2.54	0.42
1:C:156:LEU:HD23	1:C:180:ILE:CG1	2.49	0.42
1:A:275:MET:O	1:A:279:VAL:HG22	2.20	0.42
1:C:142:ASP:OD2	1:C:194:PRO:HD3	2.17	0.42
1:C:484:VAL:HA	1:C:485:PRO:HA	1.94	0.42
1:C:99:PHE:HB2	1:C:103:ALA:O	2.18	0.42
1:C:380:ARG:NH2	1:C:389:SER:OG	2.52	0.42
1:D:52:THR:HB	1:D:440:LEU:HD21	2.01	0.42
1:D:72:VAL:HG12	1:D:85:PHE:CZ	2.55	0.42
1:C:250:GLU:HB3	1:C:274:ASP:HB2	2.02	0.41
1:A:368:ASN:OD1	1:A:422:ASN:ND2	2.53	0.41
1:C:14:ALA:HB1	1:C:349:PRO:HG3	2.02	0.41
1:C:72:VAL:O	1:C:75:ALA:HB3	2.20	0.41
1:C:271:ALA:HB1	2:C:601:OXL:C2	2.50	0.41
1:D:150:LEU:HB3	1:D:154:GLY:HA2	2.01	0.41
1:D:271:ALA:HB1	2:D:601:OXL:C1	2.50	0.41
1:B:384:THR:CG2	1:B:415:LEU:HD12	2.51	0.41
1:C:236:GLU:CB	8:C:707:HOH:O	2.58	0.41
1:A:56:ASN:HD22	7:A:607:GOL:C3	2.33	0.41
1:A:213:GLY:C	6:A:606:PGE:H3	2.41	0.41
1:A:104:LYS:HD2	1:A:182:LYS:CE	2.50	0.41
1:A:115:ARG:HD3	1:A:169:GLU:OE2	2.20	0.41
1:D:454:SER:H	1:D:457:ASP:HB3	1.86	0.41
1:C:244:GLN:HA	1:C:266:ASP:OD2	2.21	0.41
1:A:387:MET:HE3	1:A:493:ASN:OD1	2.20	0.41
1:B:378:PHE:CE2	1:B:418:LYS:HG2	2.55	0.41
1:B:415:LEU:HD23	1:B:415:LEU:HA	1.89	0.40
1:A:282:GLU:CG	1:D:362:ASN:ND2	2.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:HG21	1:A:319:THR:CG2	2.52	0.40

There are no symmetry-related clashes.

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	500/521 (96%)	491 (98%)	8 (2%)	1 (0%)	47 33
1	B	500/521 (96%)	480 (96%)	18 (4%)	2 (0%)	34 21
1	C	499/521 (96%)	481 (96%)	15 (3%)	3 (1%)	25 12
1	D	498/521 (96%)	480 (96%)	16 (3%)	2 (0%)	34 21
All	All	1997/2084 (96%)	1932 (97%)	57 (3%)	8 (0%)	34 21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	488	GLU
1	C	306	THR
1	D	306	THR
1	A	306	THR
1	B	306	THR
1	C	492	THR
1	D	488	GLU
1	C	381	ASN

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	412/428 (96%)	398 (97%)	14 (3%)	37	22
1	B	412/428 (96%)	392 (95%)	20 (5%)	25	11
1	C	411/428 (96%)	392 (95%)	19 (5%)	27	13
1	D	410/428 (96%)	390 (95%)	20 (5%)	25	11
All	All	1645/1712 (96%)	1572 (96%)	73 (4%)	28	14

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	ASP
1	A	74	LEU
1	A	182	LYS
1	A	226	LYS
1	A	236	GLU
1	A	281[A]	PHE
1	A	281[B]	PHE
1	A	345	ASN
1	A	380	ARG
1	A	386	VAL
1	A	460	GLU
1	A	488	GLU
1	A	501	ARG
1	B	1	MET
1	B	25	GLU
1	B	74	LEU
1	B	100	GLU
1	B	104	LYS
1	B	109	LYS
1	B	113	LYS
1	B	127	GLU
1	B	165	ASP
1	B	263	GLU
1	B	272	ARG
1	B	310	GLU
1	B	372	ARG
1	B	375	SER
1	B	380	ARG
1	B	383	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	431	ASP
1	B	432	GLU
1	B	486	VAL
1	B	491	ARG
1	C	1	MET
1	C	22	LYS
1	C	32	LYS
1	C	40	LYS
1	C	102	GLU
1	C	104	LYS
1	C	113	LYS
1	C	143	VAL
1	C	161	VAL
1	C	182	LYS
1	C	200	GLU
1	C	201	ARG
1	C	226	LYS
1	C	380	ARG
1	C	386	VAL
1	C	408	LYS
1	C	449	THR
1	C	450	ASP
1	C	454	SER
1	D	25	GLU
1	D	143	VAL
1	D	182	LYS
1	D	201	ARG
1	D	211	GLU
1	D	236	GLU
1	D	237	GLU
1	D	315	LYS
1	D	345	ASN
1	D	372	ARG
1	D	380	ARG
1	D	401	LYS
1	D	406	LEU
1	D	449	THR
1	D	453	SER
1	D	460	GLU
1	D	464	ARG
1	D	484	VAL
1	D	488	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	493	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	GLN
1	A	307	ASN
1	A	345	ASN
1	A	381	ASN
1	B	242	HIS
1	B	296	ASN
1	B	307	ASN
1	B	345	ASN
1	B	362	ASN
1	B	381	ASN
1	C	148	GLN
1	C	212	GLN
1	C	242	HIS
1	C	307	ASN
1	C	368	ASN
1	D	63	GLN
1	D	296	ASN
1	D	307	ASN
1	D	345	ASN
1	D	362	ASN
1	D	493	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	OXL	C	602	-	5,5,5	1.26	1 (20%)	6,6,6	1.39	0
6	PGE	A	606	-	9,9,9	0.20	0	8,8,8	0.26	0
2	OXL	B	602	-	5,5,5	1.54	2 (40%)	6,6,6	1.12	0
6	PGE	C	605	-	9,9,9	0.29	0	8,8,8	0.19	0
2	OXL	C	601	3	5,5,5	0.97	0	6,6,6	1.19	0
2	OXL	B	601	3	5,5,5	1.68	2 (40%)	6,6,6	1.38	0
2	OXL	D	602	-	5,5,5	1.43	2 (40%)	6,6,6	1.17	0
2	OXL	A	602	-	5,5,5	1.44	1 (20%)	6,6,6	1.39	0
2	OXL	D	601	3	5,5,5	1.22	1 (20%)	6,6,6	1.70	2 (33%)
7	GOL	A	607	-	5,5,5	0.21	0	5,5,5	0.51	0
2	OXL	A	601	3	5,5,5	1.79	2 (40%)	6,6,6	1.03	0
5	PG4	A	605	-	12,12,12	0.32	0	11,11,11	0.14	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	OXL	C	602	-	-	4/4/4/4	-
6	PGE	A	606	-	-	6/7/7/7	-
2	OXL	B	602	-	-	4/4/4/4	-
6	PGE	C	605	-	-	2/7/7/7	-
2	OXL	C	601	3	-	1/4/4/4	-
2	OXL	B	601	3	-	0/4/4/4	-
2	OXL	D	602	-	-	4/4/4/4	-
2	OXL	A	602	-	-	4/4/4/4	-
2	OXL	D	601	3	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	607	-	-	4/4/4/4	-
2	OXL	A	601	3	-	0/4/4/4	-
5	PG4	A	605	-	-	5/10/10/10	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	OXL	O4-C2	-2.93	1.22	1.30
2	B	602	OXL	O3-C1	-2.51	1.23	1.30
2	B	601	OXL	O2-C2	2.41	1.29	1.22
2	D	602	OXL	O4-C2	-2.40	1.23	1.30
2	B	601	OXL	O3-C1	-2.38	1.23	1.30
2	B	602	OXL	O4-C2	-2.27	1.24	1.30
2	A	601	OXL	O2-C2	2.20	1.28	1.22
2	D	601	OXL	O3-C1	-2.20	1.24	1.30
2	C	602	OXL	O3-C1	-2.18	1.24	1.30
2	A	602	OXL	O4-C2	-2.14	1.24	1.30
2	D	602	OXL	O3-C1	-2.03	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	OXL	O4-C2-C1	2.20	119.69	113.16
2	D	601	OXL	O3-C1-C2	2.06	119.29	113.16

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	602	OXL	O1-C1-C2-O2
2	B	602	OXL	O1-C1-C2-O4
2	B	602	OXL	O3-C1-C2-O2
2	B	602	OXL	O3-C1-C2-O4
7	A	607	GOL	O1-C1-C2-O2
7	A	607	GOL	O1-C1-C2-C3
7	A	607	GOL	C1-C2-C3-O3
6	A	606	PGE	O2-C3-C4-O3
6	C	605	PGE	C3-C4-O3-C5
6	C	605	PGE	O2-C3-C4-O3
2	D	602	OXL	O1-C1-C2-O4
2	D	602	OXL	O3-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	606	PGE	O3-C5-C6-O4
2	A	602	OXL	O1-C1-C2-O2
2	D	602	OXL	O1-C1-C2-O2
2	A	602	OXL	O3-C1-C2-O4
2	D	602	OXL	O3-C1-C2-O4
6	A	606	PGE	O1-C1-C2-O2
7	A	607	GOL	O2-C2-C3-O3
5	A	605	PG4	O1-C1-C2-O2
2	A	602	OXL	O1-C1-C2-O4
5	A	605	PG4	O3-C5-C6-O4
2	A	602	OXL	O3-C1-C2-O2
2	C	602	OXL	O3-C1-C2-O4
5	A	605	PG4	C8-C7-O4-C6
6	A	606	PGE	C6-C5-O3-C4
2	C	602	OXL	O3-C1-C2-O2
2	C	602	OXL	O1-C1-C2-O2
6	A	606	PGE	C3-C4-O3-C5
6	A	606	PGE	C1-C2-O2-C3
2	C	602	OXL	O1-C1-C2-O4
5	A	605	PG4	O2-C3-C4-O3
5	A	605	PG4	C1-C2-O2-C3
2	C	601	OXL	O3-C1-C2-O4
2	D	601	OXL	O3-C1-C2-O4

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	OXL	1	0
6	A	606	PGE	1	0
6	C	605	PGE	1	0
2	C	601	OXL	1	0
2	B	601	OXL	1	0
2	D	601	OXL	1	0
7	A	607	GOL	6	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, 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	501/521 (96%)	-0.27	5 (0%) 82 80	26, 38, 63, 98	0
1	B	501/521 (96%)	0.13	17 (3%) 45 39	24, 39, 70, 123	0
1	C	501/521 (96%)	0.34	24 (4%) 30 25	29, 51, 75, 111	0
1	D	500/521 (95%)	0.34	38 (7%) 13 10	32, 52, 85, 120	0
All	All	2003/2084 (96%)	0.14	84 (4%) 36 30	24, 45, 74, 123	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	VAL	9.8
1	D	30	GLY	7.7
1	B	487	GLY	7.4
1	D	489	ALA	6.5
1	C	491	ARG	6.2
1	D	487	GLY	5.4
1	D	106	TYR	4.5
1	B	372	ARG	4.3
1	C	490	VAL	4.3
1	B	281[A]	PHE	4.1
1	B	489	ALA	4.1
1	A	281[A]	PHE	4.1
1	D	486	VAL	4.1
1	A	456	ASP	4.0
1	D	29	TRP	3.9
1	D	488	GLU	3.8
1	D	26	ASP	3.5
1	D	128	VAL	3.5
1	D	490	VAL	3.4
1	D	21	LYS	3.4
1	D	103	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	161	VAL	3.3
1	D	99	PHE	3.3
1	C	487	GLY	3.3
1	C	500	VAL	3.2
1	D	129	ILE	3.2
1	D	100	GLU	3.2
1	A	381	ASN	3.2
1	C	106	TYR	3.1
1	D	24	GLY	3.1
1	D	372	ARG	3.1
1	C	501	ARG	3.1
1	D	102	GLU	3.0
1	C	452	PRO	3.0
1	D	375	SER	3.0
1	D	101	GLY	2.9
1	D	104	LYS	2.9
1	D	484	VAL	2.9
1	D	381	ASN	2.8
1	D	98	LEU	2.8
1	C	460	GLU	2.8
1	B	323	VAL	2.8
1	C	109	LYS	2.7
1	C	127	GLU	2.7
1	C	111	GLY	2.7
1	C	113	LYS	2.7
1	D	28	TYR	2.6
1	C	485	PRO	2.6
1	D	377	SER	2.5
1	B	381	ASN	2.5
1	D	122	ILE	2.5
1	D	117	ALA	2.5
1	D	27	GLY	2.4
1	B	377	SER	2.4
1	C	454	SER	2.4
1	D	485	PRO	2.4
1	C	101	GLY	2.4
1	D	374	ASP	2.4
1	D	456	ASP	2.4
1	B	327	PHE	2.4
1	C	170	PHE	2.4
1	C	129	ILE	2.4
1	D	25	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	116	VAL	2.3
1	C	74	LEU	2.3
1	C	470	GLY	2.2
1	B	324	SER	2.2
1	A	501	ARG	2.1
1	B	162	ALA	2.1
1	B	330	VAL	2.1
1	D	373	LEU	2.1
1	C	107	SER	2.1
1	D	119	LYS	2.1
1	B	106	TYR	2.1
1	C	108	TYR	2.1
1	B	321	SER	2.1
1	C	455	THR	2.1
1	B	103	ALA	2.1
1	C	451	ALA	2.1
1	B	359	ILE	2.1
1	D	114	ILE	2.1
1	D	291	ILE	2.1
1	A	454	SER	2.0
1	B	167	THR	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 monosaccharides 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
5	PG4	A	605	13/13	0.73	0.21	56,69,79,79	0
6	PGE	C	605	10/10	0.77	0.16	65,75,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OXL	C	602	6/6	0.84	0.19	60,67,69,74	0
7	GOL	A	607	6/6	0.87	0.19	42,54,58,61	0
4	K	C	604	1/1	0.90	0.08	50,50,50,50	0
6	PGE	A	606	10/10	0.92	0.09	52,55,60,66	0
2	OXL	D	601	6/6	0.92	0.08	37,45,48,52	0
3	MG	C	603	1/1	0.92	0.04	37,37,37,37	0
2	OXL	C	601	6/6	0.93	0.07	34,41,44,46	0
2	OXL	A	602	6/6	0.94	0.16	42,49,52,55	0
2	OXL	D	602	6/6	0.94	0.14	58,72,83,85	0
2	OXL	B	601	6/6	0.95	0.10	28,35,39,39	0
2	OXL	B	602	6/6	0.95	0.17	44,56,79,82	0
2	OXL	A	601	6/6	0.95	0.07	32,36,43,44	0
3	MG	A	603	1/1	0.96	0.04	32,32,32,32	0
4	K	D	604	1/1	0.98	0.04	48,48,48,48	0
4	K	A	604	1/1	0.99	0.07	37,37,37,37	0
4	K	B	604	1/1	0.99	0.05	48,48,48,48	0
3	MG	B	603	1/1	0.99	0.05	30,30,30,30	0
3	MG	D	603	1/1	0.99	0.08	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.