



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 08:52 pm BST

PDB ID : 3N25
Title : The structure of muscle pyruvate kinase in complex with proline, pyruvate, and Mn²⁺
Authors : Fenton, A.W.; Johnson, T.A.; Holyoak, T.
Deposited on : 2010-05-17
Resolution : 2.41 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

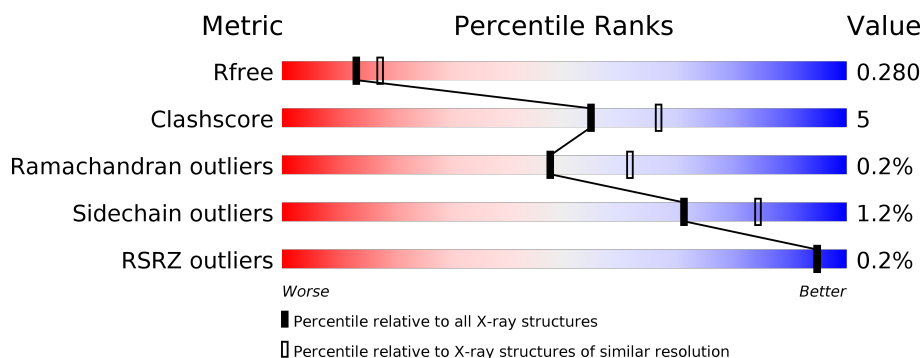
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 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	531	<div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	B	531	<div> <div>81%</div> <div>15%</div> <div>.</div> </div>
1	C	531	<div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	D	531	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	E	531	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	F	531	<div> <div>85%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	531	<div><div></div><div>86%</div><div>10%</div><div></div></div>
1	H	531	<div><div></div><div>83%</div><div>15%</div><div></div></div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 33971 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 isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	14	0
			4061	2559	719	753	30			
1	B	508	Total	C	N	O	S	0	11	0
			3981	2508	709	736	28			
1	C	512	Total	C	N	O	S	0	14	0
			4033	2543	712	749	29			
1	D	521	Total	C	N	O	S	0	9	0
			4050	2547	718	756	29			
1	E	521	Total	C	N	O	S	0	8	0
			4049	2545	718	756	30			
1	F	515	Total	C	N	O	S	0	8	0
			4015	2525	711	750	29			
1	G	510	Total	C	N	O	S	0	6	0
			3961	2495	700	738	28			
1	H	519	Total	C	N	O	S	0	14	0
			4080	2570	722	759	29			

There are 24 discrepancies between the modelled and reference sequences:

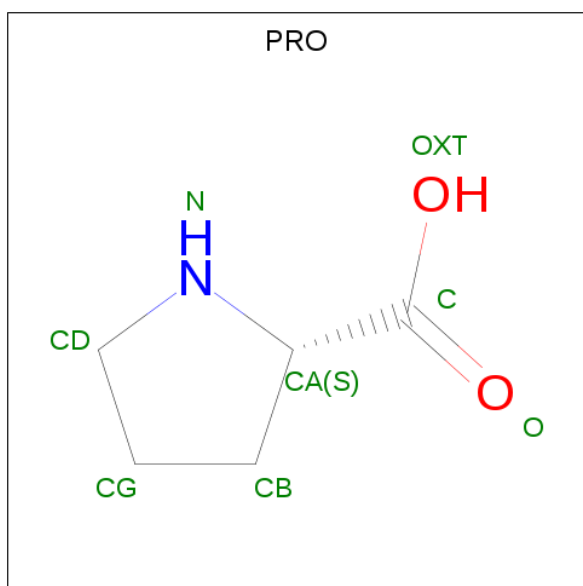
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LYS	MET	SEE REMARK 999	UNP P11974
A	400	ALA	SER	SEE REMARK 999	UNP P11974
A	403	GLN	HIS	SEE REMARK 999	UNP P11974
B	29	LYS	MET	SEE REMARK 999	UNP P11974
B	400	ALA	SER	SEE REMARK 999	UNP P11974
B	403	GLN	HIS	SEE REMARK 999	UNP P11974
C	29	LYS	MET	SEE REMARK 999	UNP P11974
C	400	ALA	SER	SEE REMARK 999	UNP P11974
C	403	GLN	HIS	SEE REMARK 999	UNP P11974
D	29	LYS	MET	SEE REMARK 999	UNP P11974
D	400	ALA	SER	SEE REMARK 999	UNP P11974
D	403	GLN	HIS	SEE REMARK 999	UNP P11974
E	29	LYS	MET	SEE REMARK 999	UNP P11974

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Chain	Residue	Modelled	Actual	Comment	Reference
E	400	ALA	SER	SEE REMARK 999	UNP P11974
E	403	GLN	HIS	SEE REMARK 999	UNP P11974
F	29	LYS	MET	SEE REMARK 999	UNP P11974
F	400	ALA	SER	SEE REMARK 999	UNP P11974
F	403	GLN	HIS	SEE REMARK 999	UNP P11974
G	29	LYS	MET	SEE REMARK 999	UNP P11974
G	400	ALA	SER	SEE REMARK 999	UNP P11974
G	403	GLN	HIS	SEE REMARK 999	UNP P11974
H	29	LYS	MET	SEE REMARK 999	UNP P11974
H	400	ALA	SER	SEE REMARK 999	UNP P11974
H	403	GLN	HIS	SEE REMARK 999	UNP P11974

- Molecule 2 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	5	1	2		
2	B	1	Total	C	N	O	0	0
			8	5	1	2		
2	C	1	Total	C	N	O	0	0
			8	5	1	2		
2	D	1	Total	C	N	O	0	0
			8	5	1	2		
2	E	1	Total	C	N	O	0	0
			8	5	1	2		
2	F	1	Total	C	N	O	0	0
			8	5	1	2		

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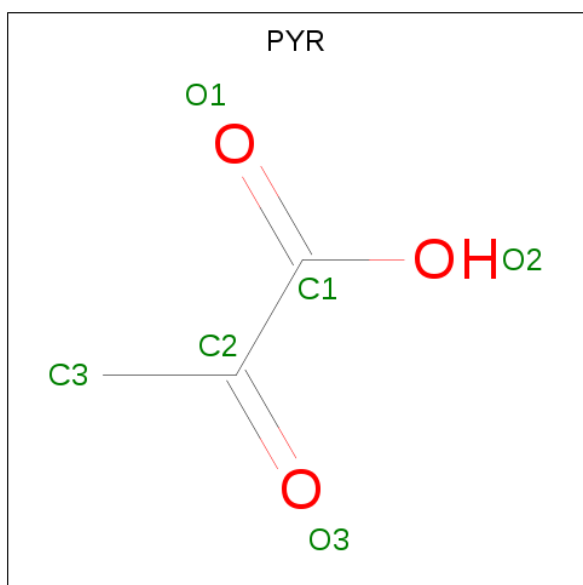
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			8	5	1	2		
2	H	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: C₃H₄O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	E	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	A	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

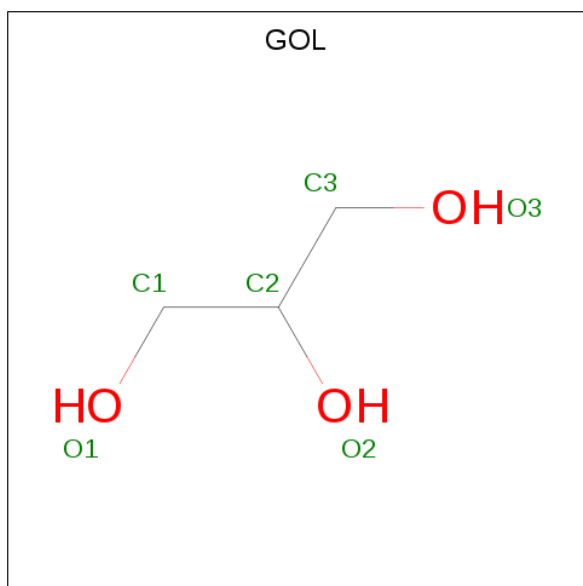
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Na 1 1	0	0
6	D	2	Total Na 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	2	Total	Na	0	0
			2	2		
6	H	2	Total	Na	0	0
			2	2		
6	B	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		
6	A	2	Total	Na	0	0
			2	2		
6	F	1	Total	Na	0	0
			1	1		

- 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	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			4	2	2		

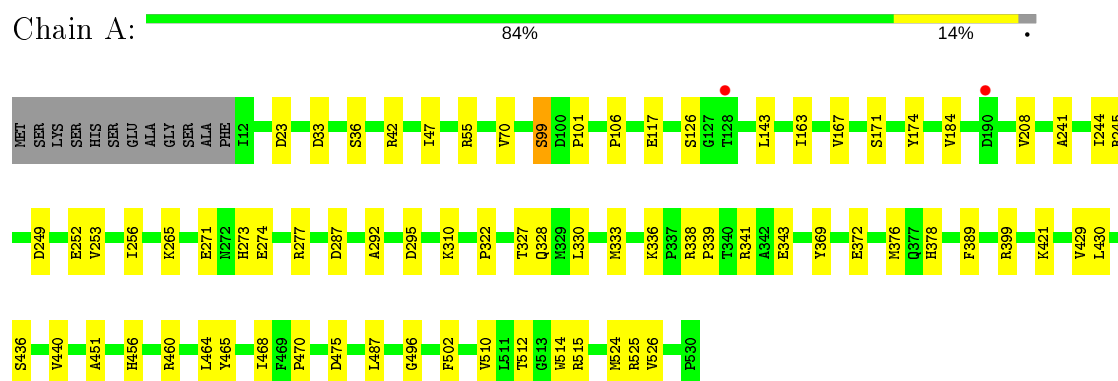
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	193	Total	O	0	0
			193	193		
9	B	147	Total	O	0	0
			147	147		
9	C	199	Total	O	0	0
			199	199		
9	D	192	Total	O	0	0
			192	192		
9	E	190	Total	O	0	0
			190	190		
9	F	186	Total	O	0	0
			186	186		
9	G	126	Total	O	0	0
			126	126		
9	H	194	Total	O	0	0
			194	194		

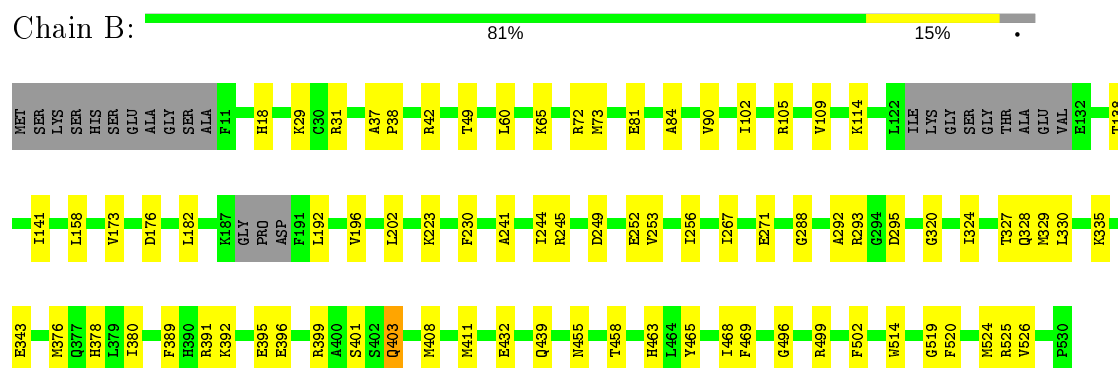
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

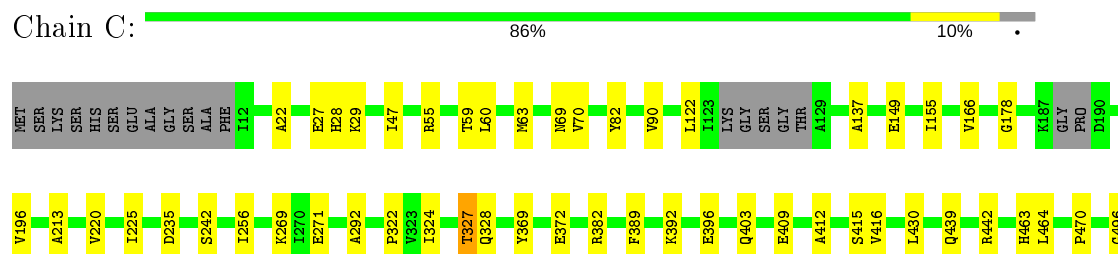
- Molecule 1: Pyruvate kinase isozymes M1/M2



- Molecule 1: Pyruvate kinase isozymes M1/M2



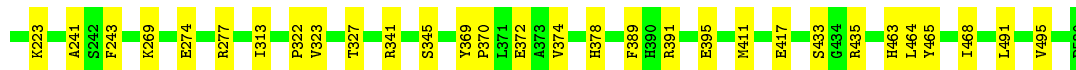
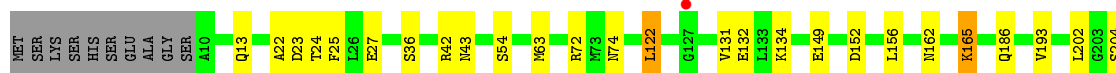
- Molecule 1: Pyruvate kinase isozymes M1/M2





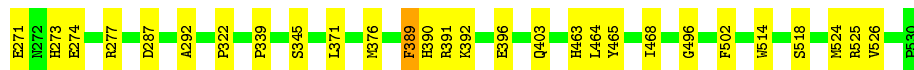
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain D: 88% 10%



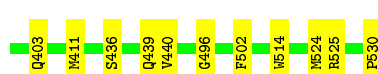
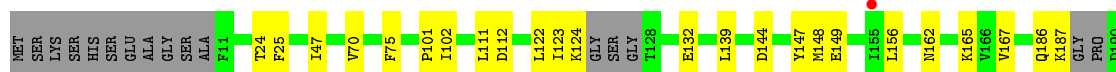
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain E: 88% 10%



- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain F: 85% 12%



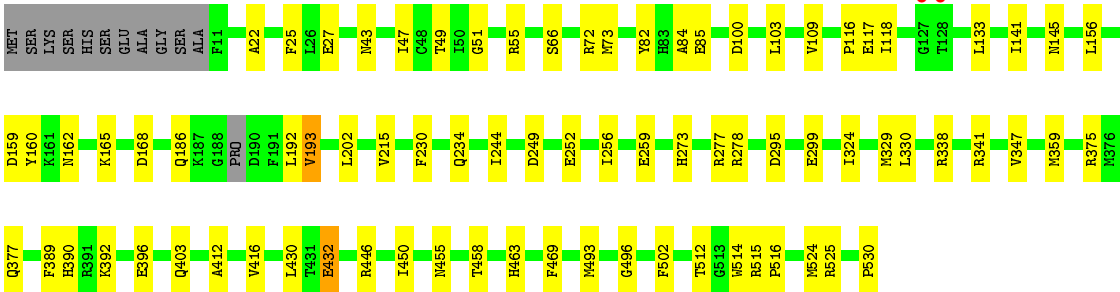
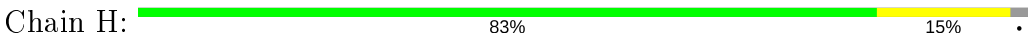
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain G: 86% 10%





- Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.37Å 108.75Å 144.26Å 95.18° 93.38° 112.23°	Depositor
Resolution (Å)	36.59 – 2.41 36.59 – 2.41	Depositor EDS
% Data completeness (in resolution range)	83.0 (36.59-2.41) 82.9 (36.59-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.42Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.268 0.219 , 0.280	Depositor DCC
R_{free} test set	7394 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , -3.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	33971	wwPDB-VP
Average B, all atoms (Å ²)	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.98% 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, NA, K, MN, EDO, PYR

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	0.44	0/4165	0.56	0/5614
1	B	0.42	0/4071	0.56	0/5484
1	C	0.45	0/4125	0.58	0/5561
1	D	0.44	0/4132	0.57	0/5572
1	E	0.45	0/4127	0.58	0/5563
1	F	0.45	0/4090	0.57	0/5511
1	G	0.41	0/4037	0.55	0/5440
1	H	0.44	0/4172	0.56	0/5618
All	All	0.44	0/32919	0.57	0/44363

There are no bond length outliers.

There are no bond angle outliers.

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	4061	0	4191	63	0
1	B	3981	0	4092	67	0
1	C	4033	0	4127	40	0
1	D	4050	0	4138	33	0
1	E	4049	0	4138	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4015	0	4104	47	0
1	G	3961	0	4047	39	0
1	H	4080	0	4185	66	0
2	A	8	0	7	0	0
2	B	8	0	7	1	0
2	C	8	0	7	3	0
2	D	8	0	7	2	0
2	E	8	0	7	1	0
2	F	8	0	7	0	0
2	G	8	0	7	1	0
2	H	8	0	7	2	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	0	3	1	0
4	B	6	0	3	1	0
4	C	6	0	3	0	0
4	D	6	0	3	1	0
4	E	6	0	3	0	0
4	F	6	0	3	2	0
4	G	6	0	3	2	0
4	H	6	0	3	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	2	0	0	0	0
7	A	18	0	24	2	0
7	B	18	0	24	2	0
7	C	12	0	16	0	0
7	D	18	0	24	2	0
7	E	12	0	16	0	0
7	F	18	0	24	3	0
7	G	12	0	16	1	0
7	H	6	0	8	2	0
8	A	12	0	18	0	0
8	B	8	0	12	1	0
8	C	4	0	6	0	0
8	D	12	0	18	2	0
8	E	16	0	24	0	0
8	F	4	0	6	0	0
8	H	4	0	6	0	0
9	A	193	0	0	4	0
9	B	147	0	0	5	0
9	C	199	0	0	6	0
9	D	192	0	0	2	0
9	E	190	0	0	5	0
9	F	186	0	0	10	0
9	G	126	0	0	6	0
9	H	194	0	0	7	0
All	All	33971	0	33344	345	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 5.

The worst 5 of 345 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524[B]:MET:HE2	1:B:524[B]:MET:CE	1.89	1.02
1:A:524[B]:MET:HE2	1:B:524[B]:MET:HE2	1.36	1.01
1:F:274:GLU:HG3	1:F:277:ARG:NH2	1.88	0.88
1:A:524[B]:MET:HE2	1:B:524[B]:MET:HB3	1.56	0.86
1:A:524[B]:MET:CE	1:B:524[B]:MET:CE	2.54	0.86

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	531/531 (100%)	518 (98%)	13 (2%)	0	100	100
1	B	513/531 (97%)	497 (97%)	14 (3%)	2 (0%)	34	47
1	C	520/531 (98%)	502 (96%)	17 (3%)	1 (0%)	47	61
1	D	528/531 (99%)	516 (98%)	11 (2%)	1 (0%)	47	61
1	E	527/531 (99%)	510 (97%)	15 (3%)	2 (0%)	34	47
1	F	517/531 (97%)	497 (96%)	20 (4%)	0	100	100
1	G	510/531 (96%)	494 (97%)	14 (3%)	2 (0%)	34	47
1	H	529/531 (100%)	510 (96%)	19 (4%)	0	100	100
All	All	4175/4248 (98%)	4044 (97%)	123 (3%)	8 (0%)	47	61

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	177	ASP
1	D	327	THR
1	B	327	THR
1	C	327	THR
1	G	327	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	439/434 (101%)	434 (99%)	5 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	429/434 (99%)	422 (98%)	7 (2%)	62	78
1	C	435/434 (100%)	433 (100%)	2 (0%)	88	95
1	D	435/434 (100%)	430 (99%)	5 (1%)	73	86
1	E	434/434 (100%)	431 (99%)	3 (1%)	84	92
1	F	432/434 (100%)	425 (98%)	7 (2%)	62	78
1	G	426/434 (98%)	420 (99%)	6 (1%)	67	81
1	H	439/434 (101%)	431 (98%)	8 (2%)	59	75
All	All	3469/3472 (100%)	3426 (99%)	43 (1%)	71	84

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	162	ASN
1	F	167	VAL
1	H	259[B]	GLU
1	E	345	SER
1	E	389	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	390	HIS
1	F	390	HIS
1	H	145	ASN
1	B	378	HIS
1	G	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 28 are monoatomic - leaving 50 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
4	PYR	B	1500	3	2,5,5	1.93	1 (50%)	2,6,6	0.27	0
7	GOL	D	6304	-	5,5,5	0.33	0	5,5,5	0.51	0
8	EDO	E	6046	-	3,3,3	0.48	0	2,2,2	0.38	0
7	GOL	D	6204	-	5,5,5	0.34	0	5,5,5	0.37	0
7	GOL	F	6306	-	5,5,5	0.33	0	5,5,5	0.46	0
7	GOL	D	6056	-	5,5,5	0.42	0	5,5,5	0.28	0
8	EDO	C	6014	-	3,3,3	0.46	0	2,2,2	0.37	0
8	EDO	D	6017	-	3,3,3	0.51	0	2,2,2	0.28	0
8	EDO	E	6015	-	3,3,3	0.53	0	2,2,2	0.31	0
8	EDO	E	6049	-	3,3,3	0.56	0	2,2,2	0.25	0
4	PYR	G	1500	3	2,5,5	1.93	1 (50%)	2,6,6	0.73	0
7	GOL	A	6002	-	5,5,5	0.34	0	5,5,5	0.56	0
4	PYR	E	1500	3	2,5,5	1.94	1 (50%)	2,6,6	0.26	0
8	EDO	F	6012	-	3,3,3	0.48	0	2,2,2	0.42	0
8	EDO	H	6037	-	3,3,3	0.58	0	2,2,2	0.22	0
7	GOL	F	6010	-	5,5,5	0.34	0	5,5,5	0.35	0
7	GOL	C	6055	-	5,5,5	0.36	0	5,5,5	0.18	0
7	GOL	F	6206	-	5,5,5	0.44	0	5,5,5	0.44	0
8	EDO	E	6039	-	3,3,3	0.53	0	2,2,2	0.21	0
8	EDO	A	6043	-	3,3,3	0.51	0	2,2,2	0.29	0
4	PYR	F	1500	3	2,5,5	2.03	1 (50%)	2,6,6	0.85	0
7	GOL	A	6201	-	5,5,5	0.31	0	5,5,5	0.51	0
7	GOL	A	6301	-	5,5,5	0.37	0	5,5,5	0.30	0
8	EDO	D	6011	-	3,3,3	0.47	0	2,2,2	0.45	0
4	PYR	H	1500	3	2,5,5	1.94	1 (50%)	2,6,6	0.55	0
4	PYR	A	1000	3	2,5,5	2.20	1 (50%)	2,6,6	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	H	6308	-	5,5,5	0.33	0	5,5,5	0.48	0
8	EDO	D	6033	-	3,3,3	0.50	0	2,2,2	0.22	0
8	EDO	A	6051	-	3,3,3	0.42	0	2,2,2	0.48	0
8	EDO	B	6013	-	3,3,3	0.45	0	2,2,2	0.38	0
7	GOL	C	6303	-	5,5,5	0.39	0	5,5,5	0.30	0
7	GOL	B	6007	-	5,5,5	0.29	0	5,5,5	0.37	0
8	EDO	B	6048	-	3,3,3	0.47	0	2,2,2	0.28	0
4	PYR	C	1500	3	2,5,5	1.85	1 (50%)	2,6,6	0.71	0
7	GOL	E	6205	-	5,5,5	0.37	0	5,5,5	0.35	0
7	GOL	E	6305	-	5,5,5	0.28	0	5,5,5	0.67	0
8	EDO	A	6050	-	3,3,3	0.47	0	2,2,2	0.43	0
7	GOL	B	6302	-	5,5,5	0.37	0	5,5,5	0.50	0
7	GOL	G	6207	-	5,5,5	0.35	0	5,5,5	0.34	0
7	GOL	G	6307	-	5,5,5	0.35	0	5,5,5	0.23	0
7	GOL	B	6202	-	5,5,5	0.31	0	5,5,5	0.39	0
4	PYR	D	1500	3	2,5,5	1.73	1 (50%)	2,6,6	1.04	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
4	PYR	B	1500	3	-	0/0/4/4	-
7	GOL	D	6304	-	-	4/4/4/4	-
8	EDO	E	6046	-	-	0/1/1/1	-
7	GOL	D	6204	-	-	2/4/4/4	-
7	GOL	F	6306	-	-	2/4/4/4	-
7	GOL	D	6056	-	-	0/4/4/4	-
8	EDO	C	6014	-	-	1/1/1/1	-
8	EDO	D	6017	-	-	0/1/1/1	-
8	EDO	E	6015	-	-	1/1/1/1	-
8	EDO	E	6049	-	-	1/1/1/1	-
4	PYR	G	1500	3	-	0/0/4/4	-
7	GOL	A	6002	-	-	2/4/4/4	-
4	PYR	E	1500	3	-	0/0/4/4	-
8	EDO	F	6012	-	-	1/1/1/1	-
8	EDO	H	6037	-	-	1/1/1/1	-
7	GOL	F	6010	-	-	2/4/4/4	-
7	GOL	C	6055	-	-	0/4/4/4	-
7	GOL	F	6206	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	E	6039	-	-	1/1/1/1	-
8	EDO	A	6043	-	-	1/1/1/1	-
4	PYR	F	1500	3	-	0/0/4/4	-
7	GOL	A	6201	-	-	2/4/4/4	-
7	GOL	A	6301	-	-	0/4/4/4	-
8	EDO	D	6011	-	-	1/1/1/1	-
4	PYR	H	1500	3	-	0/0/4/4	-
4	PYR	A	1000	3	-	0/0/4/4	-
7	GOL	H	6308	-	-	0/4/4/4	-
8	EDO	D	6033	-	-	1/1/1/1	-
8	EDO	A	6051	-	-	1/1/1/1	-
8	EDO	B	6013	-	-	0/1/1/1	-
7	GOL	C	6303	-	-	1/4/4/4	-
7	GOL	B	6007	-	-	2/4/4/4	-
8	EDO	B	6048	-	-	1/1/1/1	-
4	PYR	C	1500	3	-	0/0/4/4	-
7	GOL	E	6205	-	-	2/4/4/4	-
7	GOL	E	6305	-	-	4/4/4/4	-
8	EDO	A	6050	-	-	0/1/1/1	-
7	GOL	B	6302	-	-	0/4/4/4	-
7	GOL	G	6207	-	-	0/4/4/4	-
7	GOL	G	6307	-	-	2/4/4/4	-
7	GOL	B	6202	-	-	2/4/4/4	-
4	PYR	D	1500	3	-	0/0/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	PYR	O3-C2	3.10	1.32	1.22
4	F	1500	PYR	O3-C2	2.85	1.31	1.22
4	E	1500	PYR	O3-C2	2.75	1.31	1.22
4	H	1500	PYR	O3-C2	2.74	1.31	1.22
4	B	1500	PYR	O3-C2	2.72	1.31	1.22

There are no bond angle outliers.

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	6204	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	F	6010	GOL	O1-C1-C2-O2
7	F	6010	GOL	O1-C1-C2-C3
7	G	6307	GOL	O1-C1-C2-C3
7	F	6206	GOL	O1-C1-C2-C3

There are no ring outliers.

15 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1500	PYR	1	0
7	D	6304	GOL	2	0
7	F	6306	GOL	1	0
8	D	6017	EDO	2	0
4	G	1500	PYR	2	0
7	F	6010	GOL	2	0
4	F	1500	PYR	2	0
7	A	6301	GOL	2	0
4	A	1000	PYR	1	0
7	H	6308	GOL	2	0
8	B	6048	EDO	1	0
7	B	6302	GOL	1	0
7	G	6207	GOL	1	0
7	B	6202	GOL	1	0
4	D	1500	PYR	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	519/531 (97%)	-0.73	2 (0%) 92 91	2, 5, 11, 18	1 (0%)
1	B	508/531 (95%)	-0.49	0 100 100	2, 5, 10, 16	0
1	C	512/531 (96%)	-0.77	0 100 100	2, 4, 9, 18	0
1	D	521/531 (98%)	-0.74	1 (0%) 95 95	2, 5, 11, 16	0
1	E	521/531 (98%)	-0.77	0 100 100	2, 4, 11, 18	0
1	F	515/531 (96%)	-0.71	2 (0%) 92 91	2, 3, 8, 19	0
1	G	510/531 (96%)	-0.51	2 (0%) 92 91	2, 3, 9, 13	0
1	H	519/531 (97%)	-0.70	2 (0%) 92 91	2, 4, 9, 14	0
All	All	4125/4248 (97%)	-0.68	9 (0%) 95 95	2, 4, 10, 19	1 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	155	ILE	3.4
1	H	128	THR	2.7
1	A	128	THR	2.7
1	G	201	PHE	2.3
1	D	127	GLY	2.2

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. 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
7	GOL	A	6301	6/6	0.79	0.19	46,47,48,49	0
8	EDO	D	6017	4/4	0.82	0.40	48,49,50,50	0
8	EDO	A	6051	4/4	0.85	0.16	49,50,50,51	0
7	GOL	C	6055	6/6	0.87	0.21	53,54,54,54	0
8	EDO	A	6043	4/4	0.88	0.19	64,65,66,66	0
8	EDO	H	6037	4/4	0.88	0.12	40,41,41,41	0
7	GOL	B	6302	6/6	0.89	0.17	34,36,37,37	0
7	GOL	F	6010	6/6	0.89	0.14	53,53,53,53	0
8	EDO	E	6049	4/4	0.89	0.16	38,40,41,42	0
7	GOL	G	6307	6/6	0.90	0.17	44,45,45,46	0
7	GOL	F	6306	6/6	0.90	0.16	38,39,40,40	0
7	GOL	B	6202	6/6	0.90	0.16	62,63,63,64	0
7	GOL	B	6007	6/6	0.91	0.18	48,48,49,49	0
6	NA	G	2000	1/1	0.91	0.08	41,41,41,41	0
8	EDO	B	6013	4/4	0.92	0.18	54,54,55,55	0
7	GOL	G	6207	6/6	0.92	0.12	39,40,40,40	0
8	EDO	C	6014	4/4	0.92	0.11	37,37,38,38	0
8	EDO	F	6012	4/4	0.93	0.11	33,33,33,34	0
8	EDO	E	6046	4/4	0.93	0.20	27,30,31,33	0
7	GOL	E	6205	6/6	0.93	0.09	28,29,31,31	0
6	NA	A	1300	1/1	0.93	0.08	40,40,40,40	0
7	GOL	C	6303	6/6	0.93	0.15	28,30,31,31	0
8	EDO	D	6011	4/4	0.93	0.13	46,46,46,46	0
7	GOL	D	6204	6/6	0.94	0.13	36,36,36,37	0
8	EDO	A	6050	4/4	0.94	0.12	43,44,44,44	0
7	GOL	A	6201	6/6	0.94	0.12	29,30,30,32	0
6	NA	D	2000	1/1	0.94	0.06	35,35,35,35	0
7	GOL	H	6308	6/6	0.94	0.14	22,22,24,26	0
7	GOL	D	6056	6/6	0.94	0.11	35,37,38,39	0
2	PRO	A	1200	8/8	0.94	0.11	21,21,22,23	0
6	NA	F	2000	1/1	0.95	0.12	27,27,27,27	0
2	PRO	D	1600	8/8	0.95	0.11	23,23,24,24	0
6	NA	H	2000	1/1	0.95	0.08	40,40,40,40	0
8	EDO	D	6033	4/4	0.95	0.11	33,34,35,36	0
6	NA	B	2000	1/1	0.95	0.10	48,48,48,48	0
7	GOL	F	6206	6/6	0.96	0.15	34,36,36,36	0
6	NA	H	2100	1/1	0.96	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PRO	G	1600	8/8	0.96	0.09	38,38,38,38	0
2	PRO	E	1600	8/8	0.96	0.10	24,24,24,24	0
8	EDO	E	6015	4/4	0.96	0.11	35,36,36,36	0
7	GOL	A	6002	6/6	0.96	0.13	28,30,31,32	0
5	K	B	1700	1/1	0.96	0.05	38,38,38,38	0
2	PRO	B	1600	8/8	0.97	0.10	26,26,26,27	0
7	GOL	E	6305	6/6	0.97	0.09	21,21,21,22	0
2	PRO	H	1600	8/8	0.97	0.10	17,18,18,18	0
2	PRO	C	1600	8/8	0.97	0.12	20,20,21,21	0
6	NA	E	2000	1/1	0.97	0.10	31,31,31,31	0
2	PRO	F	1600	8/8	0.97	0.11	17,18,18,19	0
8	EDO	B	6048	4/4	0.97	0.10	28,28,28,28	0
4	PYR	A	1000	6/6	0.97	0.11	22,24,25,27	0
4	PYR	B	1500	6/6	0.97	0.10	32,33,33,34	0
4	PYR	D	1500	6/6	0.97	0.11	13,15,17,20	0
6	NA	D	2100	1/1	0.98	0.08	21,21,21,21	0
5	K	H	1700	1/1	0.98	0.10	26,26,26,26	0
6	NA	A	2100	1/1	0.98	0.13	29,29,29,29	0
8	EDO	E	6039	4/4	0.98	0.07	33,34,34,34	0
4	PYR	G	1500	6/6	0.98	0.08	21,22,24,25	0
7	GOL	D	6304	6/6	0.98	0.11	29,30,31,33	0
6	NA	E	2100	1/1	0.98	0.10	13,13,13,13	0
4	PYR	H	1500	6/6	0.98	0.09	17,18,18,19	0
6	NA	C	2000	1/1	0.98	0.07	22,22,22,22	0
4	PYR	F	1500	6/6	0.98	0.08	6,7,7,9	0
3	MN	C	640	1/1	0.99	0.07	15,15,15,15	0
3	MN	G	640	1/1	0.99	0.04	26,26,26,26	0
5	K	F	1700	1/1	0.99	0.07	17,17,17,17	0
4	PYR	C	1500	6/6	0.99	0.09	11,12,12,13	0
4	PYR	E	1500	6/6	0.99	0.08	10,12,14,14	0
5	K	G	1700	1/1	0.99	0.07	42,42,42,42	0
5	K	D	1700	1/1	0.99	0.05	22,22,22,22	0
5	K	A	1100	1/1	0.99	0.09	23,23,23,23	0
3	MN	H	640	1/1	0.99	0.08	16,16,16,16	0
3	MN	E	640	1/1	0.99	0.10	21,21,21,21	0
5	K	E	1700	1/1	0.99	0.10	25,25,25,25	0
3	MN	B	640	1/1	0.99	0.05	33,33,33,33	0
3	MN	F	640	1/1	1.00	0.05	18,18,18,18	0
3	MN	D	640	1/1	1.00	0.09	20,20,20,20	0
3	MN	A	640	1/1	1.00	0.07	17,17,17,17	0
5	K	C	1700	1/1	1.00	0.08	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.