



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 09:53 AM BST

PDB ID : 6NN7
Title : The structure of human liver pyruvate kinase, hLPYK-GGG
Authors : McFarlane, J.S.; Ronnebaum, T.A.; Meneely, K.M.; Fenton, A.W.; Lamb, A.L.
Deposited on : 2019-01-14
Resolution : 2.32 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 : 2.13.1
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) : 2.13.1

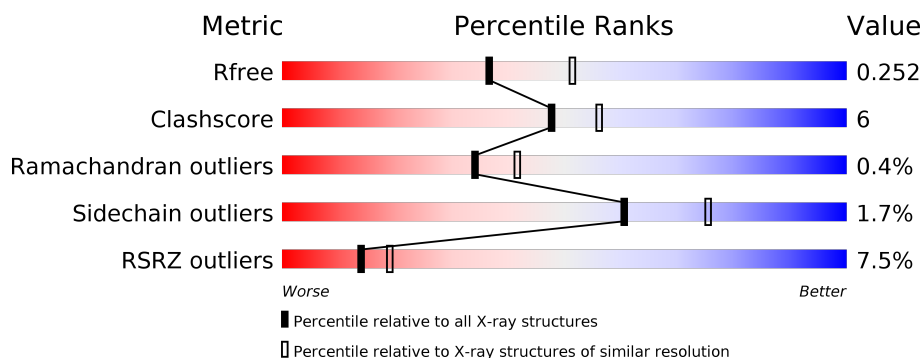
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	542	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	542	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>6%</div> <div>24%</div> </div> </div>
1	C	542	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
1	D	542	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>12%</div> </div> </div>
1	E	542	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>.</div> </div> </div>
1	F	542	<div> <div>10%</div> <div> <div></div> <div>59%</div> <div>15%</div> <div>25%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	542	
1	H	542	

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
2	EDO	C	603	-	-	X	-
2	EDO	C	605	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 58243 atoms, of which 29236 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 PKLR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	516	Total	C	H	N	O	S	0	0	0
			7927	2469	4006	706	728	18			
1	B	414	Total	C	H	N	O	S	0	0	0
			6369	1980	3212	574	585	18			
1	C	514	Total	C	H	N	O	S	0	0	0
			7851	2440	3964	705	724	18			
1	E	518	Total	C	H	N	O	S	0	0	0
			7919	2463	3998	710	730	18			
1	D	479	Total	C	H	N	O	S	0	0	0
			7361	2295	3715	658	675	18			
1	F	406	Total	C	H	N	O	S	0	0	0
			6256	1943	3158	562	575	18			
1	G	496	Total	C	H	N	O	S	0	0	0
			7660	2388	3869	685	700	18			
1	H	398	Total	C	H	N	O	S	0	0	0
			6118	1895	3092	552	561	18			

There are 32 discrepancies between the modelled and reference sequences:

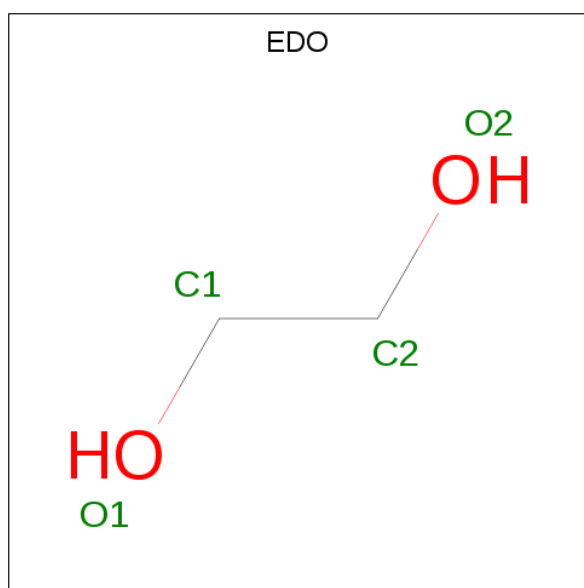
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	531	GLY	SER	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	531	GLY	SER	engineered mutation	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	531	GLY	SER	engineered mutation	UNP P30613
E	1	MET	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	GLU	-	expression tag	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	531	GLY	SER	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	531	GLY	SER	engineered mutation	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	531	GLY	SER	engineered mutation	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	531	GLY	SER	engineered mutation	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	531	GLY	SER	engineered mutation	UNP P30613

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



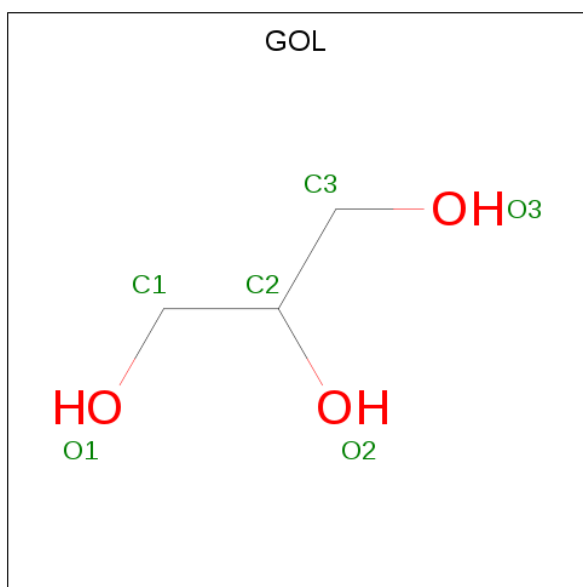
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

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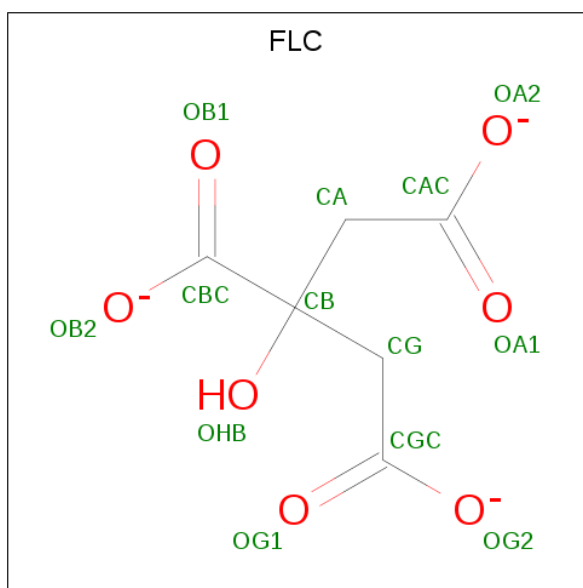
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	F	1	Total	C	H	O	0	0
			10	2	6	2		
2	G	1	Total	C	H	O	0	0
			10	2	6	2		
2	G	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			13	3	7	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	G	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			18	6	5	7		
4	D	1	Total	C	H	O	0	0
			18	6	5	7		

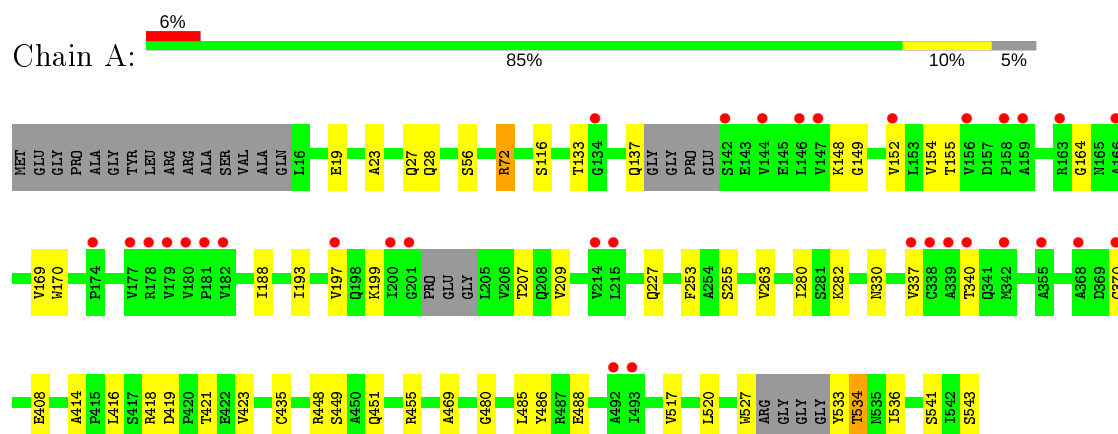
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		
5	B	63	Total	O	0	0
			63	63		
5	C	67	Total	O	0	0
			67	67		
5	E	64	Total	O	0	0
			64	64		
5	D	73	Total	O	0	0
			73	73		
5	F	15	Total	O	0	0
			15	15		
5	G	11	Total	O	0	0
			11	11		
5	H	2	Total	O	0	0
			2	2		

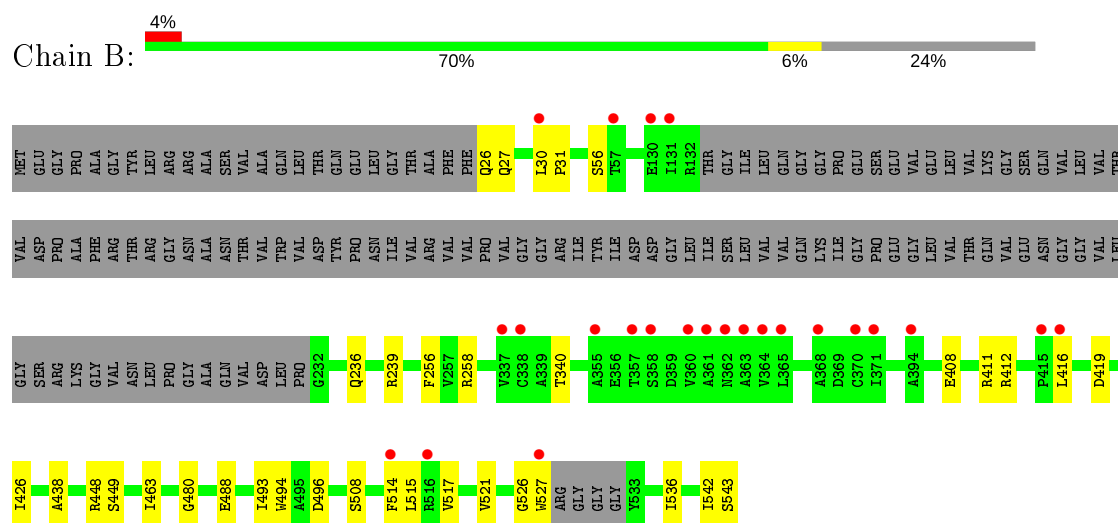
3 Residue-property plots [i](#)

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.

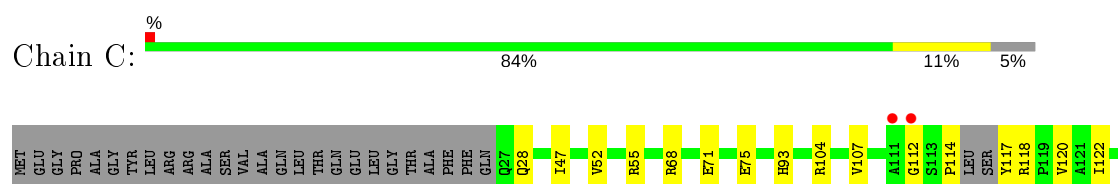
• Molecule 1: Pyruvate kinase PKLR

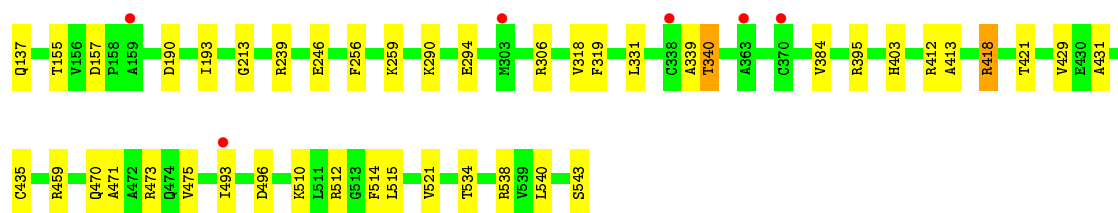


• Molecule 1: Pyruvate kinase PKLR

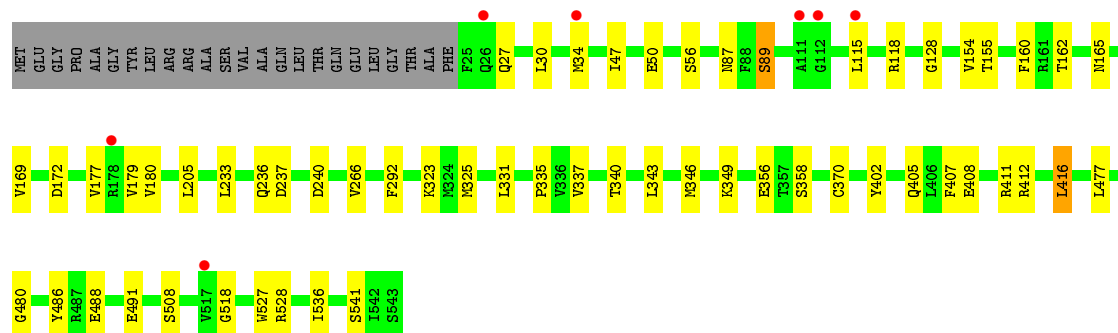
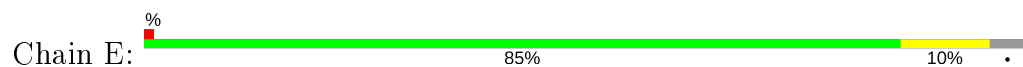


• Molecule 1: Pyruvate kinase PKLR

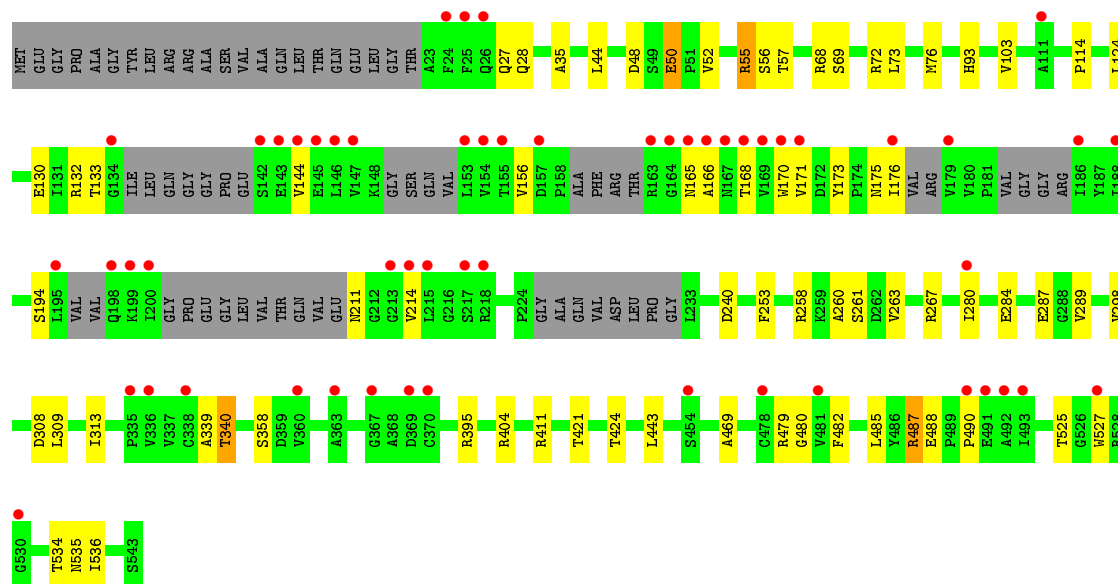




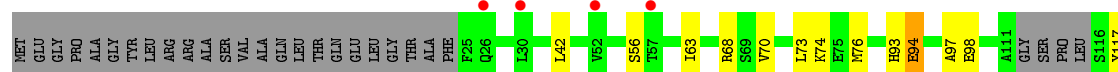
• Molecule 1: Pyruvate kinase PKLR

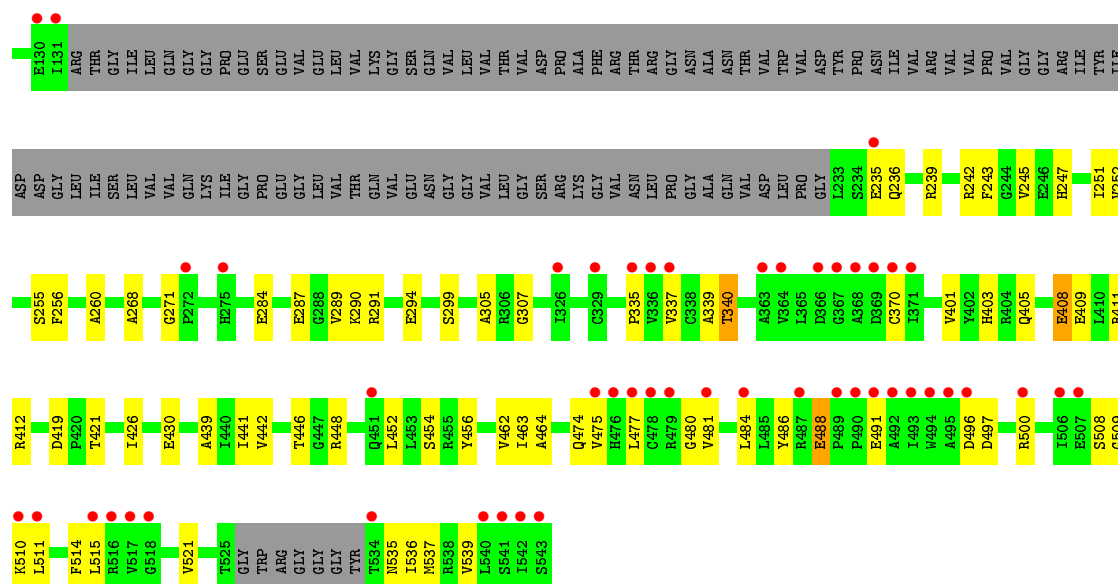


• Molecule 1: Pyruvate kinase PKLR

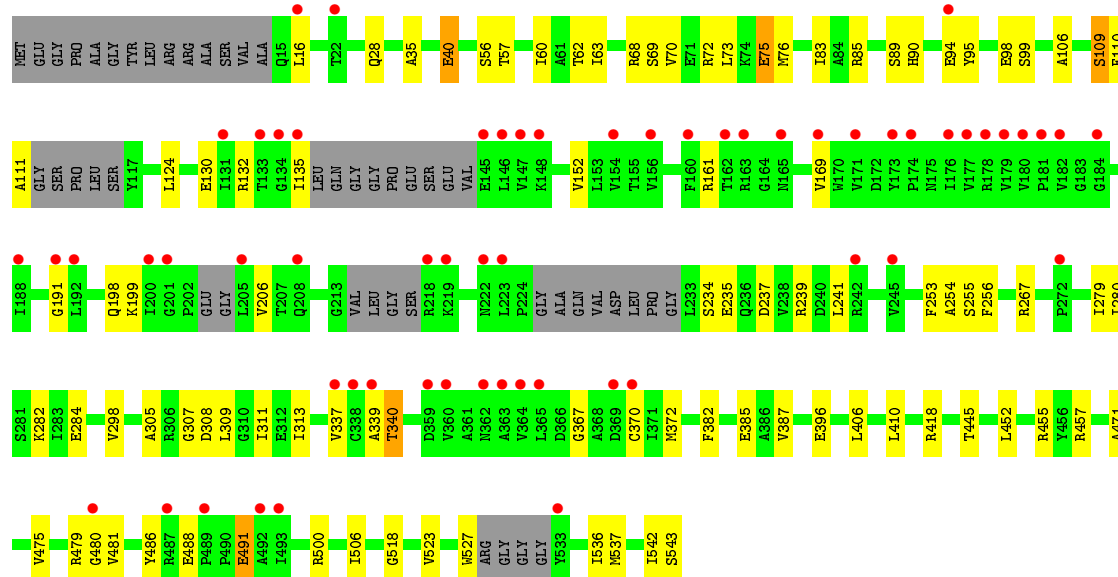
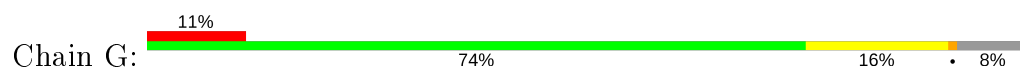


• Molecule 1: Pyruvate kinase PKLR

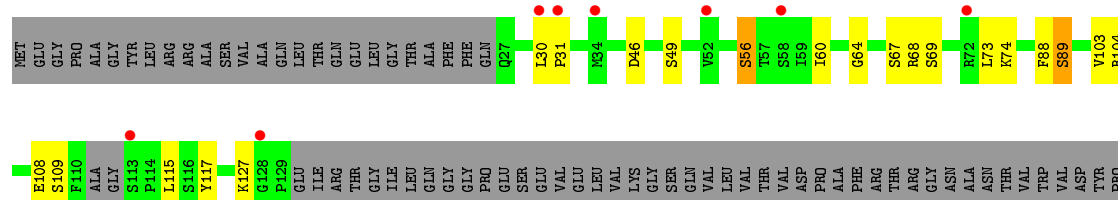




• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR



TRP	ASN	E235	G357	ASN
A495	ILE	Q236	A358	ILE
D496	VAL	D237	D359	VAL
D497	ARG	V238	C370	ARG
V498	VAL	R239	I371	VAL
D499	VAL	D240	K372	VAL
R500	PRO	L241		PRO
R501	VAL	A242	T377	VAL
V502	GLY	F243	F383	GLY
	GLY	H247		GLY
F514	ARG		R404	ARG
	ILE	F253		ILE
T525	TYR		E408	TYR
GLY	ILE	F256		ILE
TRP	ASP	V257	R411	ASP
ARG	ASP	R258	R412	ARG
GLY	GLY	K259	A413	GLY
GLY	LEU			GLY
GLY	ILE	A269	P420	ILE
TYR	SER	L270		TYR
	LEU	G271	I426	LEU
VAL	VAL	P272		VAL
	VAL	E273	E430	
GLN	GLN	G274	T444	GLN
LYS	LYS	H275	T445	LYS
ILE	ILE		T446	ILE
	GLY	I280	G447	
GLY	PRO	H286	R448	GLY
GLY	GLU			GLY
LEU	GLY	E294	I452	LEU
VAL	VAL		R455	VAL
THR	THR	I311		THR
	GLN	E312		
VAL	VAL	I313	I463	VAL
GLU	GLU			GLU
ASN	ASN	K317	R467	ASN
GLY	GLY		S468	GLY
	GLY	L331	A469	
VAL	VAL		Q470	VAL
LEU	LEU	V337		LEU
GLY	GLY	G338	R473	GLY
SER	SER	A339	Q474	SER
ARG	ARG	T340	V475	ARG
LYS	LYS	Q341	R476	LYS
	GLY	N342	I477	
VAL	VAL	L343	C478	VAL
ASN	ASN		R479	ASN
	LEU	E356	Q480	
LEU	PRO	T357		LEU
PRO	PRO	S358	L485	PRO
GLY	GLY	D359	Y486	GLY
ALA	ALA	V360	R487	ALA
GLN	GLN	A361	E488	GLN
VAL	VAL	N362	P489	VAL
ASP	ASP	A363	P490	ASP
LEU	LEU	V364	GLU	LEU
PRO	PRO	L365	ALA	PRO
GLY	GLY	D366	ILE	GLY
LEU	LEU			LEU
S234	S234			S234

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.36Å 106.20Å 151.71Å 76.44° 80.06° 71.37°	Depositor
Resolution (Å)	39.06 – 2.32 39.06 – 2.32	Depositor EDS
% Data completeness (in resolution range)	89.4 (39.06-2.32) 89.4 (39.06-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.191 , 0.251 0.191 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (1.14%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	58243	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, FLC, EDO

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	0.64	0/3981	0.76	0/5392
1	B	0.63	0/3206	0.78	0/4333
1	C	0.62	0/3949	0.76	3/5349 (0.1%)
1	D	0.60	0/3699	0.76	2/4998 (0.0%)
1	E	0.61	0/3985	0.74	1/5399 (0.0%)
1	F	0.56	0/3143	0.73	0/4245
1	G	0.54	0/3847	0.70	0/5203
1	H	0.49	0/3068	0.67	1/4143 (0.0%)
All	All	0.59	0/28878	0.74	7/39062 (0.0%)

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	C	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	418	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	D	267	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	C	418	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	306	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	H	475	VAL	CB-CA-C	-5.27	101.39	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	112	GLY	Peptide
1	G	254	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3921	4006	4004	36	0
1	B	3157	3212	3212	28	0
1	C	3887	3964	3963	51	0
1	D	3646	3715	3708	44	0
1	E	3921	3998	3997	36	0
1	F	3098	3158	3156	66	0
1	G	3791	3869	3868	67	0
1	H	3026	3092	3091	49	0
2	A	8	12	12	2	0
2	B	8	12	12	0	0
2	C	28	42	42	11	0
2	D	4	6	6	3	0
2	E	8	12	12	2	0
2	F	4	6	6	2	0
2	G	8	12	12	0	0
3	A	12	16	16	0	0
3	B	12	15	16	1	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	E	18	23	24	0	0
3	F	12	16	16	1	0
3	G	6	8	8	1	0
3	H	12	16	16	1	0
4	C	13	5	5	1	0
4	D	13	5	5	2	0
5	A	87	0	0	1	0
5	B	63	0	0	1	0
5	C	67	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	73	0	0	1	0
5	E	64	0	0	1	0
5	F	15	0	0	0	0
5	G	11	0	0	0	0
5	H	2	0	0	0	0
All	All	29007	29236	29223	355	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.

The worst 5 of 355 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:236:GLN:OE1	1:B:239:ARG:NH2	1.98	0.96
1:F:337:VAL:HG22	1:F:370:CYS:HB2	1.52	0.90
1:G:527:TRP:HB2	1:G:536:ILE:HD11	1.57	0.87
1:H:446:THR:HG22	3:H:602:GOL:H31	1.55	0.86
1:F:419:ASP:OD2	1:F:448:ARG:NH2	2.14	0.81

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	508/542 (94%)	495 (97%)	12 (2%)	1 (0%)	47	58
1	B	408/542 (75%)	392 (96%)	15 (4%)	1 (0%)	47	58
1	C	510/542 (94%)	497 (98%)	12 (2%)	1 (0%)	47	58
1	D	461/542 (85%)	447 (97%)	12 (3%)	2 (0%)	34	41
1	E	516/542 (95%)	498 (96%)	16 (3%)	2 (0%)	34	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	398/542 (73%)	378 (95%)	19 (5%)	1 (0%)	41	50
1	G	482/542 (89%)	466 (97%)	12 (2%)	4 (1%)	19	23
1	H	388/542 (72%)	375 (97%)	11 (3%)	2 (0%)	29	35
All	All	3671/4336 (85%)	3548 (97%)	109 (3%)	14 (0%)	34	41

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	117	TYR
1	C	340	THR
1	E	416	LEU
1	D	340	THR
1	G	109	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	416/431 (96%)	409 (98%)	7 (2%)	60	75
1	B	331/431 (77%)	328 (99%)	3 (1%)	78	89
1	C	410/431 (95%)	405 (99%)	5 (1%)	71	83
1	D	385/431 (89%)	379 (98%)	6 (2%)	62	77
1	E	414/431 (96%)	409 (99%)	5 (1%)	71	83
1	F	326/431 (76%)	317 (97%)	9 (3%)	43	59
1	G	401/431 (93%)	396 (99%)	5 (1%)	71	83
1	H	320/431 (74%)	310 (97%)	10 (3%)	40	55
All	All	3003/3448 (87%)	2953 (98%)	50 (2%)	60	75

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	214	VAL

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Mol	Chain	Res	Type
1	F	94	GLU
1	H	259	LYS
1	D	261	SER
1	D	488	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 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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

33 ligands are modelled in this entry.

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	EDO	C	602	-	3,3,3	0.50	0	2,2,2	0.32	0
3	GOL	E	605	-	5,5,5	0.57	0	5,5,5	1.05	0
2	EDO	G	602	-	3,3,3	0.54	0	2,2,2	0.58	0
3	GOL	F	602	-	5,5,5	0.50	0	5,5,5	0.66	0
2	EDO	G	601	-	3,3,3	0.48	0	2,2,2	0.40	0
2	EDO	B	601	-	3,3,3	0.54	0	2,2,2	0.72	0
2	EDO	A	602	-	3,3,3	0.45	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	602	-	3,3,3	0.62	0	2,2,2	0.18	0
2	EDO	D	602	-	3,3,3	0.58	0	2,2,2	0.56	0
2	EDO	C	606	-	3,3,3	0.65	0	2,2,2	0.31	0
3	GOL	C	609	-	5,5,5	0.91	0	5,5,5	1.22	0
4	FLC	C	601	-	3,12,12	1.71	1 (33%)	3,17,17	2.03	1 (33%)
2	EDO	C	603	-	3,3,3	0.53	0	2,2,2	0.30	0
2	EDO	C	607	-	3,3,3	0.49	0	2,2,2	0.33	0
3	GOL	H	601	-	5,5,5	0.38	0	5,5,5	0.34	0
2	EDO	E	602	-	3,3,3	0.44	0	2,2,2	0.58	0
2	EDO	C	608	-	3,3,3	0.42	0	2,2,2	0.40	0
2	EDO	A	601	-	3,3,3	0.44	0	2,2,2	0.66	0
2	EDO	C	605	-	3,3,3	0.58	0	2,2,2	0.29	0
3	GOL	E	604	-	5,5,5	0.88	0	5,5,5	1.45	1 (20%)
3	GOL	G	603	-	5,5,5	0.66	0	5,5,5	1.41	1 (20%)
2	EDO	C	604	-	3,3,3	0.49	0	2,2,2	0.30	0
3	GOL	F	603	-	5,5,5	0.65	0	5,5,5	0.80	0
3	GOL	A	603	-	5,5,5	0.63	0	5,5,5	1.03	0
3	GOL	B	603	-	5,5,5	0.69	0	5,5,5	0.76	0
2	EDO	F	601	-	3,3,3	0.49	0	2,2,2	0.86	0
3	GOL	H	602	-	5,5,5	0.52	0	5,5,5	0.52	0
3	GOL	A	604	-	5,5,5	0.50	0	5,5,5	1.39	1 (20%)
2	EDO	E	601	-	3,3,3	0.51	0	2,2,2	0.40	0
4	FLC	D	601	-	3,12,12	1.46	0	3,17,17	2.36	1 (33%)
3	GOL	E	603	-	5,5,5	0.45	0	5,5,5	0.55	0
3	GOL	D	603	-	5,5,5	0.48	0	5,5,5	1.04	0
3	GOL	B	604	-	5,5,5	0.60	0	5,5,5	0.78	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	EDO	C	602	-	-	1/1/1/1	-
3	GOL	E	605	-	-	2/4/4/4	-
2	EDO	G	602	-	-	1/1/1/1	-
3	GOL	F	602	-	-	2/4/4/4	-
2	EDO	G	601	-	-	1/1/1/1	-
2	EDO	B	601	-	-	1/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	602	-	-	1/1/1/1	-
2	EDO	C	606	-	-	0/1/1/1	-
3	GOL	C	609	-	-	2/4/4/4	-
4	FLC	C	601	-	-	4/6/16/16	-
2	EDO	C	603	-	-	0/1/1/1	-
2	EDO	C	607	-	-	0/1/1/1	-
3	GOL	H	601	-	-	2/4/4/4	-
2	EDO	E	602	-	-	0/1/1/1	-
2	EDO	C	608	-	-	0/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
2	EDO	C	605	-	-	1/1/1/1	-
3	GOL	E	604	-	-	2/4/4/4	-
3	GOL	G	603	-	-	3/4/4/4	-
2	EDO	C	604	-	-	0/1/1/1	-
3	GOL	F	603	-	-	2/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
2	EDO	F	601	-	-	1/1/1/1	-
3	GOL	H	602	-	-	4/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
2	EDO	E	601	-	-	1/1/1/1	-
4	FLC	D	601	-	-	3/6/16/16	-
3	GOL	E	603	-	-	4/4/4/4	-
3	GOL	D	603	-	-	3/4/4/4	-
3	GOL	B	604	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	FLC	CA-CB	-2.51	1.51	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	FLC	CB-CA-CAC	-3.67	109.11	114.98
4	C	601	FLC	CB-CA-CAC	2.71	119.32	114.98
3	G	603	GOL	O2-C2-C3	2.52	120.24	109.12
3	E	604	GOL	O1-C1-C2	2.38	121.59	110.20
3	A	604	GOL	O2-C2-C1	-2.08	99.98	109.12

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	605	GOL	O1-C1-C2-C3
3	F	602	GOL	O1-C1-C2-C3
3	C	609	GOL	C1-C2-C3-O3
3	C	609	GOL	O2-C2-C3-O3
4	C	601	FLC	CAC-CA-CB-CBC

There are no ring outliers.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	EDO	2	0
2	D	602	EDO	3	0
2	C	606	EDO	1	0
4	C	601	FLC	1	0
2	C	603	EDO	4	0
2	C	607	EDO	1	0
2	C	605	EDO	5	0
3	G	603	GOL	1	0
3	F	603	GOL	1	0
3	B	603	GOL	1	0
2	F	601	EDO	2	0
3	H	602	GOL	1	0
2	E	601	EDO	2	0
4	D	601	FLC	2	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	516/542 (95%)	0.22	33 (6%) 19 25	21, 35, 63, 87	0
1	B	414/542 (76%)	0.26	24 (5%) 23 29	23, 35, 61, 86	0
1	C	514/542 (94%)	0.10	8 (1%) 72 78	23, 36, 55, 76	0
1	D	479/542 (88%)	0.52	55 (11%) 4 7	23, 38, 72, 84	0
1	E	518/542 (95%)	0.04	7 (1%) 75 80	25, 37, 58, 78	0
1	F	406/542 (74%)	0.65	53 (13%) 3 4	31, 48, 74, 88	0
1	G	496/542 (91%)	0.58	60 (12%) 4 6	33, 52, 71, 84	0
1	H	398/542 (73%)	0.64	39 (9%) 7 10	36, 54, 73, 87	0
All	All	3741/4336 (86%)	0.36	279 (7%) 14 19	21, 42, 68, 88	0

The worst 5 of 279 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	527	TRP	7.0
1	F	511	LEU	5.8
1	D	168	THR	5.8
1	D	144	VAL	5.8
1	H	256	PHE	5.7

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 monosaccharides 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
2	EDO	G	601	4/4	0.76	0.29	52,64,77,77	0
3	GOL	F	603	6/6	0.79	0.19	52,66,81,81	0
2	EDO	B	602	4/4	0.84	0.16	40,48,53,53	0
3	GOL	F	602	6/6	0.84	0.17	43,63,75,80	0
3	GOL	A	603	6/6	0.85	0.20	49,64,74,79	0
3	GOL	G	603	6/6	0.86	0.17	44,56,78,82	0
3	GOL	D	603	6/6	0.86	0.24	47,58,70,70	0
2	EDO	G	602	4/4	0.88	0.23	42,50,55,56	0
3	GOL	H	601	6/6	0.89	0.18	51,64,76,76	0
3	GOL	B	604	6/6	0.89	0.19	36,50,70,70	0
4	FLC	D	601	13/13	0.90	0.12	44,59,72,72	0
3	GOL	E	604	6/6	0.90	0.30	36,50,60,63	0
2	EDO	E	602	4/4	0.90	0.20	36,45,55,66	0
2	EDO	A	602	4/4	0.91	0.17	43,55,66,66	0
3	GOL	B	603	6/6	0.91	0.18	35,51,67,67	0
2	EDO	F	601	4/4	0.91	0.43	48,58,65,72	0
2	EDO	E	601	4/4	0.91	0.29	27,44,53,59	0
3	GOL	E	605	6/6	0.91	0.28	32,49,59,71	0
3	GOL	E	603	6/6	0.91	0.14	50,64,75,77	0
4	FLC	C	601	13/13	0.91	0.19	31,44,54,63	0
2	EDO	B	601	4/4	0.91	0.20	38,45,48,55	0
2	EDO	C	602	4/4	0.92	0.13	50,60,69,71	0
3	GOL	H	602	6/6	0.92	0.09	52,64,75,77	0
3	GOL	A	604	6/6	0.92	0.31	27,44,61,64	0
3	GOL	C	609	6/6	0.92	0.33	28,43,55,55	0
2	EDO	C	604	4/4	0.94	0.27	41,49,55,57	0
2	EDO	C	603	4/4	0.94	0.21	38,46,56,58	0
2	EDO	A	601	4/4	0.95	0.22	29,38,49,58	0
2	EDO	C	606	4/4	0.95	0.17	39,47,54,55	0
2	EDO	D	602	4/4	0.95	0.30	37,50,54,65	0
2	EDO	C	607	4/4	0.96	0.24	43,54,59,68	0
2	EDO	C	605	4/4	0.96	0.19	29,45,54,58	0
2	EDO	C	608	4/4	0.97	0.08	48,57,66,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.