wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 05:49 AM EDT

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 (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 (1)) were used in the production of this report:

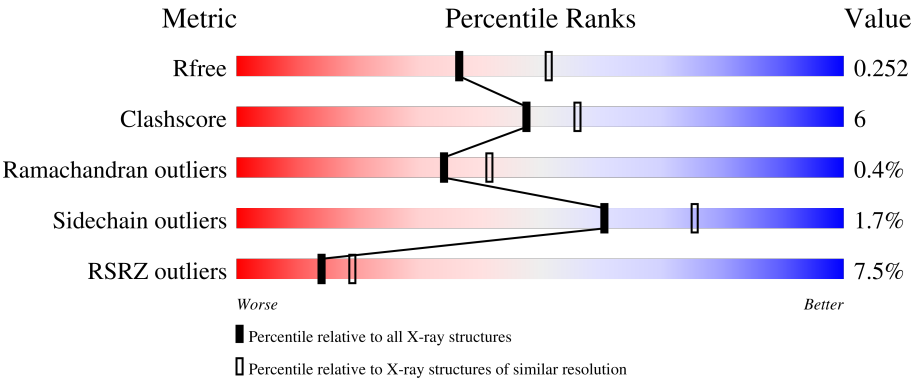
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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 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.

Mol	Chain	Length	Quality of chain
1	A	542	6% 85% 10% 5%
1	B	542	4% 70% 6% 24%
1	C	542	% 84% 11% 5%
1	D	542	10% 75% 13% • 12%
1	E	542	% 85% 10% •

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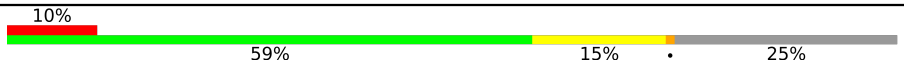
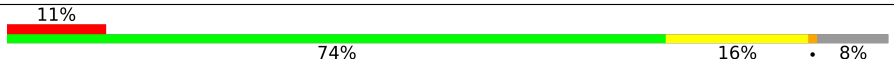
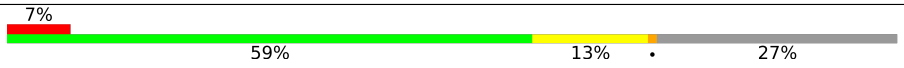
Mol	Chain	Length	Quality of chain
1	F	542	
1	G	542	
1	H	542	

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	-
4	FLC	C	601	-	X	-	-

2 Entry composition (i)

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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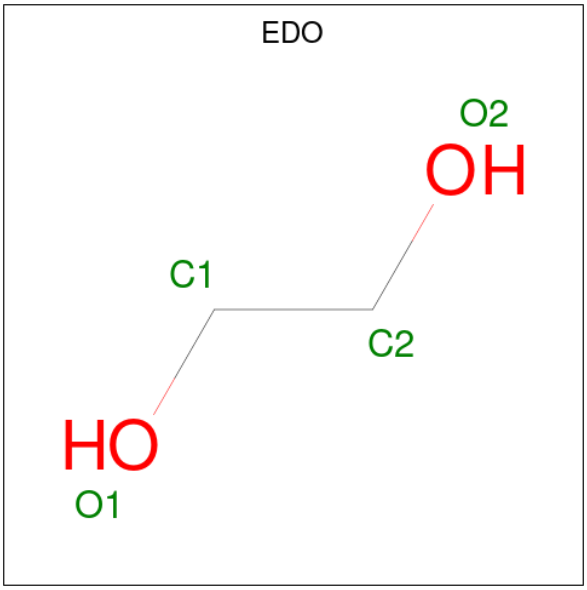
Chain	Residue	Modelled	Actual	Comment	Reference
E	2	GLU	-	expression tag	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	531	GLY	SER	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	531	GLY	SER	engineered mutation	UNP P30613
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: $C_2H_6O_2$).



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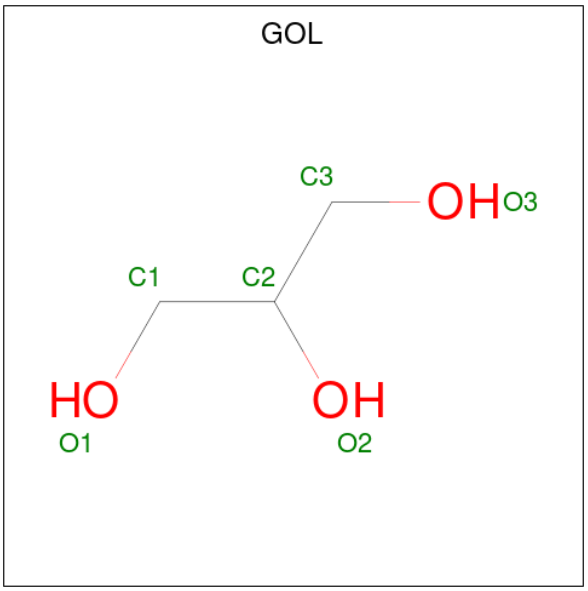
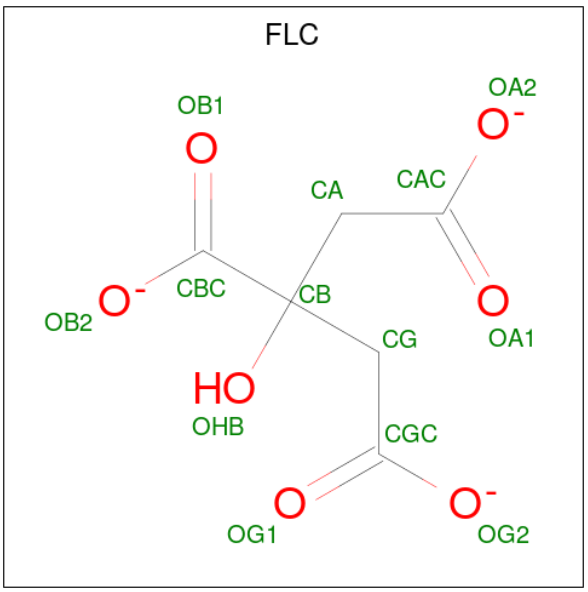
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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 18 6 5 7	0	0
4	D	1	Total C H O 18 6 5 7	0	0

- Molecule 5 is water.

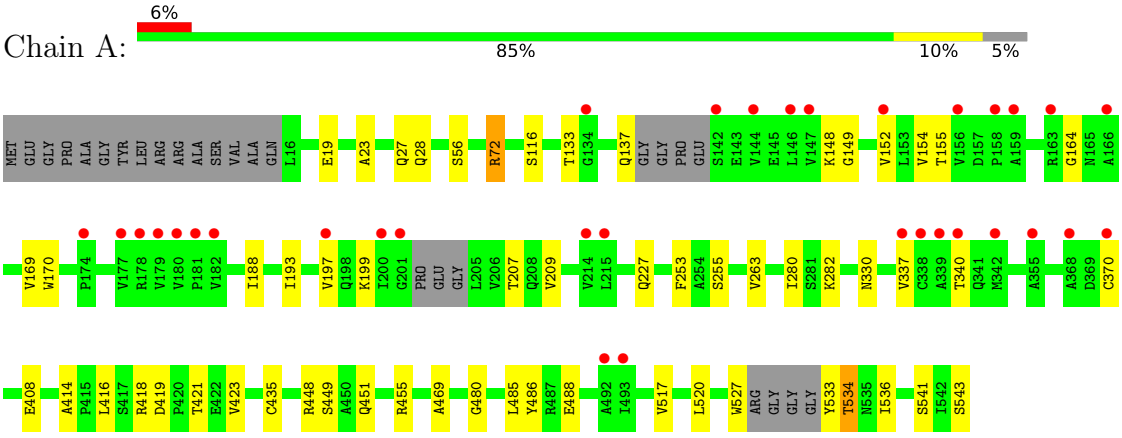
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	87	Total O 87 87	0	0
5	B	63	Total O 63 63	0	0
5	C	67	Total O 67 67	0	0
5	E	64	Total O 64 64	0	0
5	D	73	Total O 73 73	0	0
5	F	15	Total O 15 15	0	0
5	G	11	Total O 11 11	0	0
5	H	2	Total O 2 2	0	0

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.

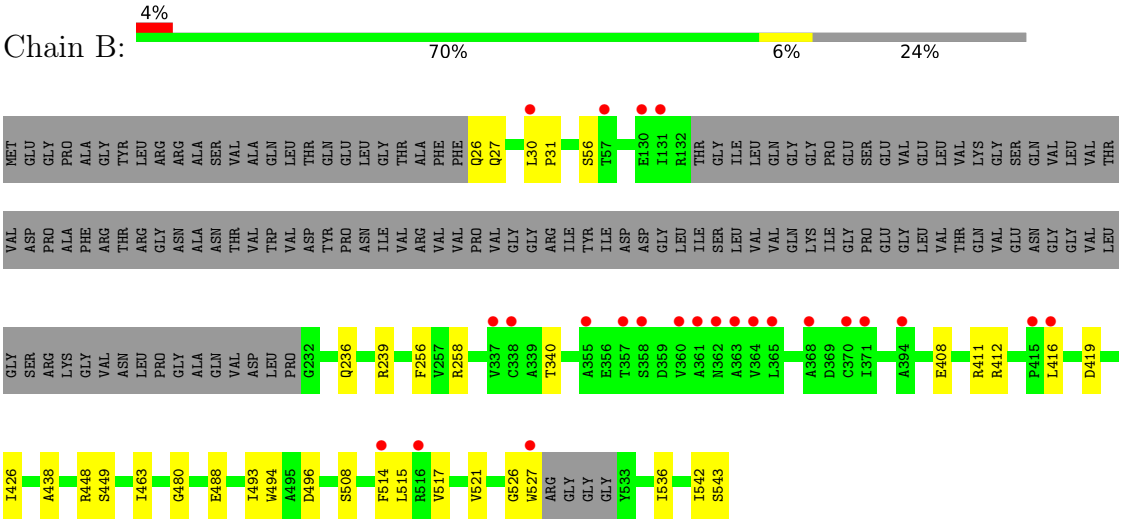
• Molecule 1: Pyruvate kinase PKLR

Chain A:



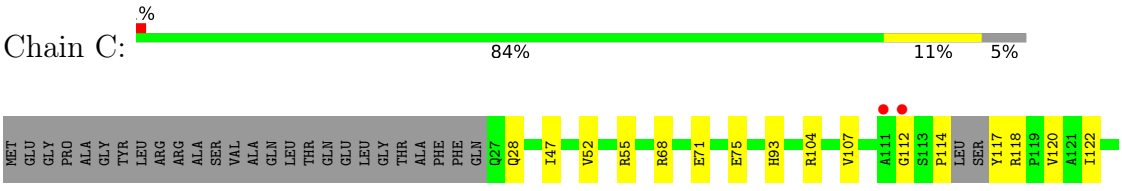
• Molecule 1: Pyruvate kinase PKLR

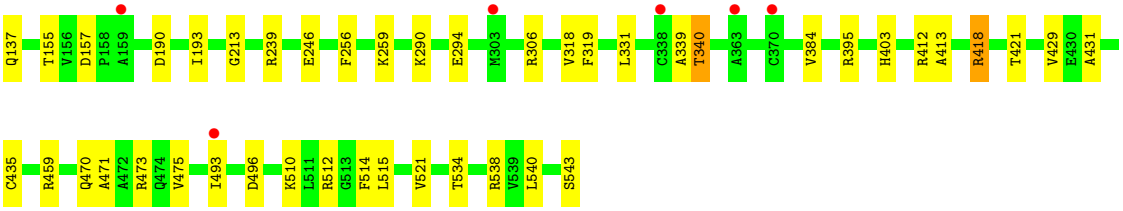
Chain B:



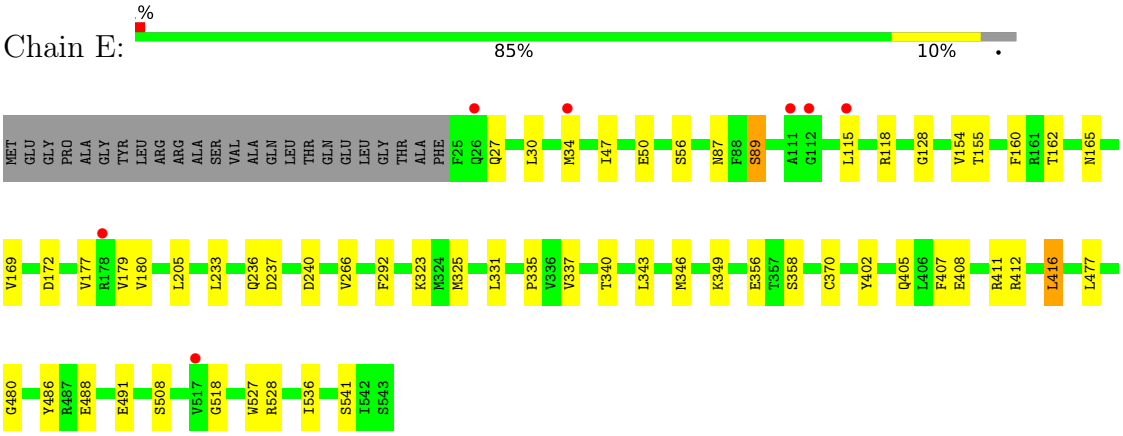
• Molecule 1: Pyruvate kinase PKLR

Chain C:

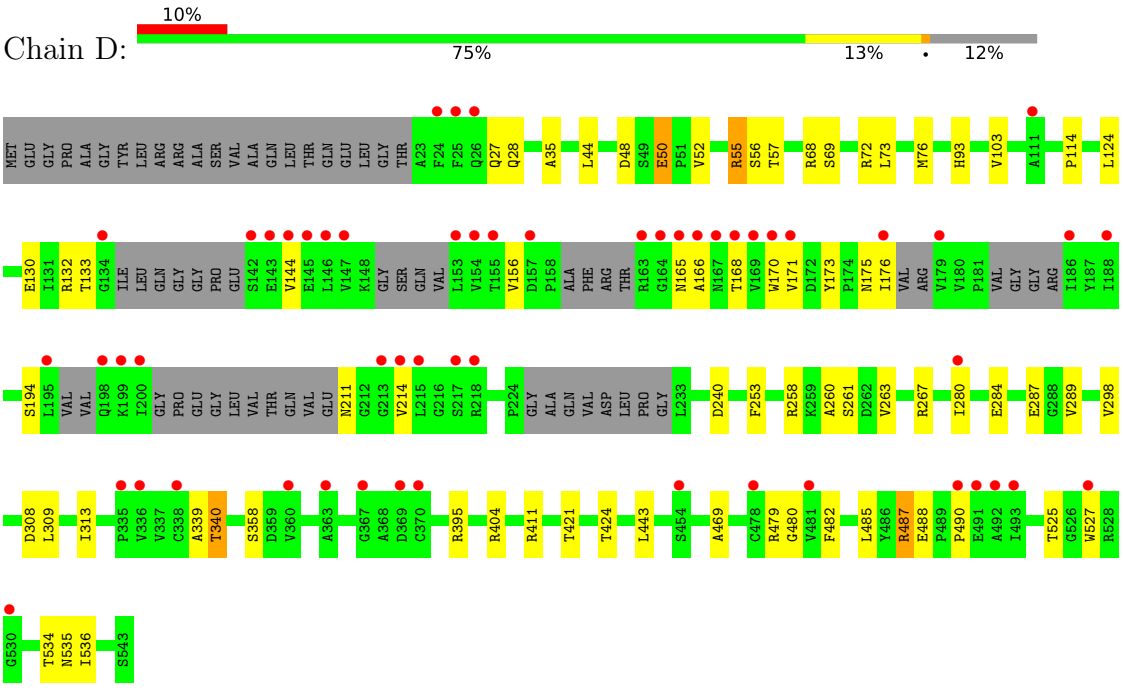




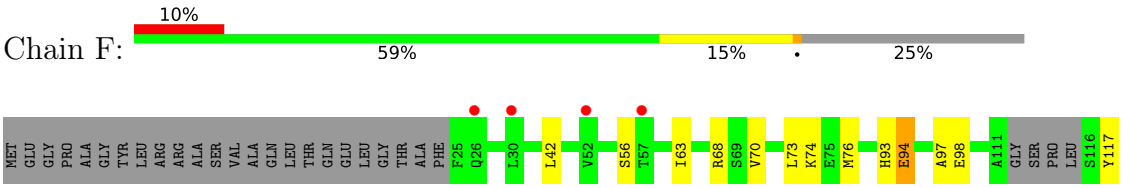
• Molecule 1: Pyruvate kinase PKLR

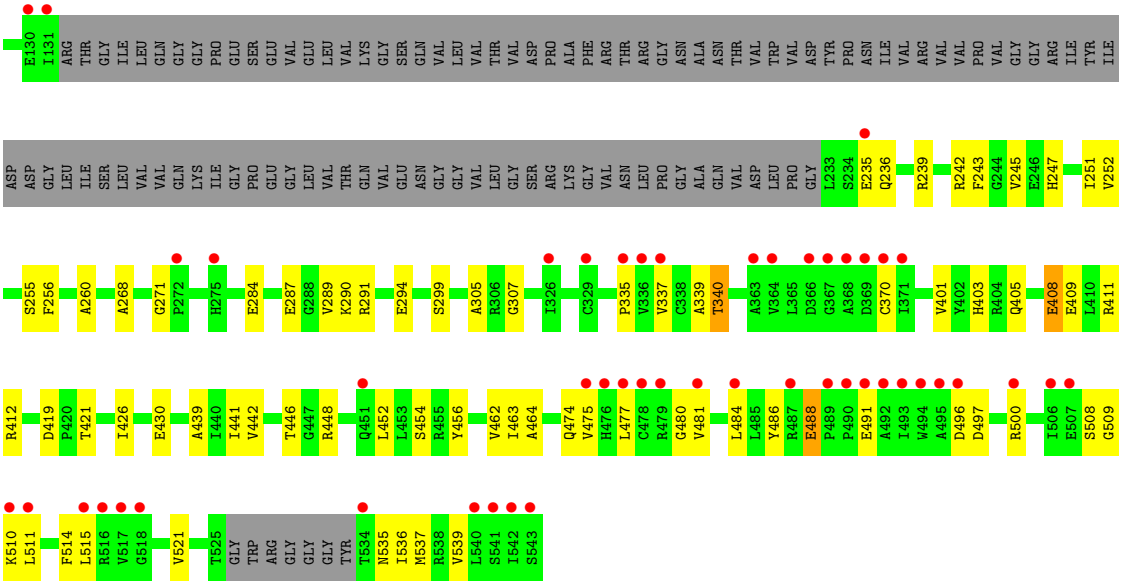


• Molecule 1: Pyruvate kinase PKLR



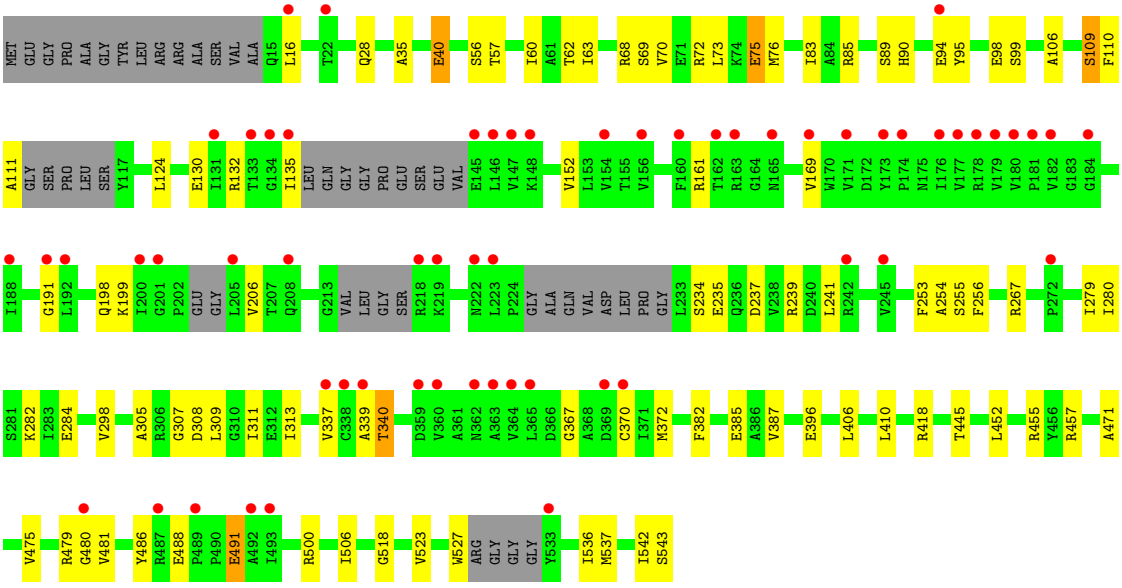
• Molecule 1: Pyruvate kinase PKLR





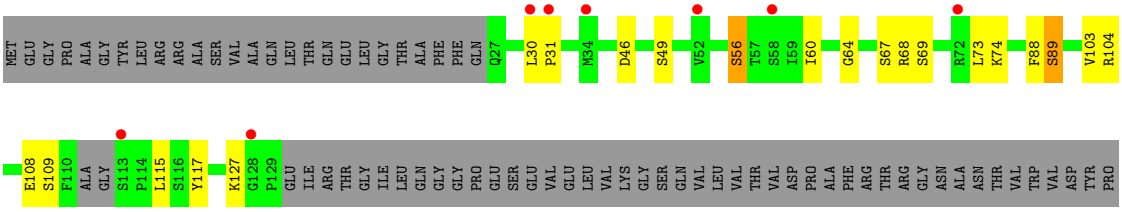
• Molecule 1: Pyruvate kinase PKLR

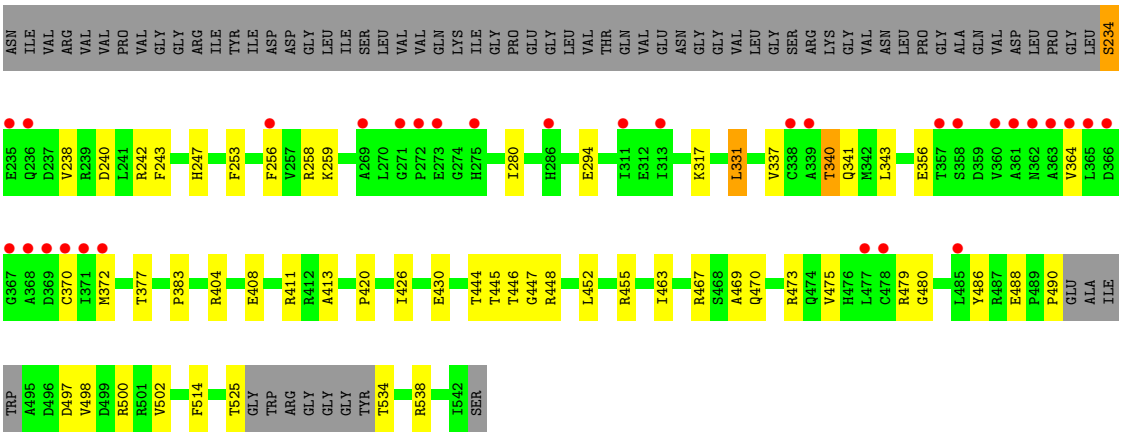
Chain G:



• Molecule 1: Pyruvate kinase PKLR

Chain H:




ASN ILE VAL ARG VAL VAL PRO VAL GLY GLY ARG ILE TYR ILE ASP ASP GLY LEU ILE SER LEU VAL VAL GLN LYS ILE GLY PRO GLU GLY LEU VAL THR GLN VAL GLU ASN GLY GLY VAL LEU GLY SER ARG LYS GLY VAL ASN LEU PRO GLY ALA GLN VAL ASP LEU PRO GLY LEU S234
E235 Q236 D237 V238 R239 D240 L241 R242 F243 H247 F253 F256 V257 R258 K259 A269 L270 G271 P272 E273 G274 H275 I280 H286 E294 I311 E312 I313 K317 L331 V337 C338 A339 T340 Q341 M342 L343 E356 T357 S358 D359 V360 A361 N362 A363 V364 L365 D366
G367 A368 D369 C370 I371 M372 T377 P383 R404 E408 R411 R412 A413 P420 I426 E430 T444 T445 T446 G447 R448 L452 R455 I463 R467 S468 A469 Q470 R473 Q474 V475 H476 L477 C478 R479 G480 L485 Y486 R487 E488 P489 P490 GLU ALA ILE
TRP A495 D496 D497 V498 D499 R500 R501 V502 F514 T525 GLY TRP ARG GLY GLY GLY TYR T534 R538 I542 SER

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, GOL, 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(^{o})	Ideal(^{o})
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 (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	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 (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	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	F	117	TYR

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Mol	Chain	Res	Type
1	G	40	GLU
1	H	470	GLN
1	F	255	SER
1	F	408	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	$\#\|Z\| > 2$
3	GOL	F	602	-	5,5,5	0.50	0	5,5,5	0.66	0
3	GOL	F	603	-	5,5,5	0.65	0	5,5,5	0.80	0
2	EDO	C	604	-	3,3,3	0.49	0	2,2,2	0.30	0
4	FLC	C	601	-	12,12,12	2.11	1 (8%)	17,17,17	3.25	10 (58%)
2	EDO	B	602	-	3,3,3	0.62	0	2,2,2	0.18	0
3	GOL	B	604	-	5,5,5	0.60	0	5,5,5	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	603	-	5,5,5	0.69	0	5,5,5	0.76	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
2	EDO	C	608	-	3,3,3	0.42	0	2,2,2	0.40	0
3	GOL	E	604	-	5,5,5	0.88	0	5,5,5	1.45	1 (20%)
2	EDO	G	601	-	3,3,3	0.48	0	2,2,2	0.40	0
2	EDO	E	601	-	3,3,3	0.51	0	2,2,2	0.40	0
2	EDO	C	606	-	3,3,3	0.65	0	2,2,2	0.31	0
3	GOL	G	603	-	5,5,5	0.66	0	5,5,5	1.41	1 (20%)
3	GOL	C	609	-	5,5,5	0.91	0	5,5,5	1.22	0
2	EDO	B	601	-	3,3,3	0.54	0	2,2,2	0.72	0
4	FLC	D	601	-	12,12,12	1.47	1 (8%)	17,17,17	1.59	2 (11%)
2	EDO	C	605	-	3,3,3	0.58	0	2,2,2	0.29	0
2	EDO	C	602	-	3,3,3	0.50	0	2,2,2	0.32	0
2	EDO	E	602	-	3,3,3	0.44	0	2,2,2	0.58	0
2	EDO	A	601	-	3,3,3	0.44	0	2,2,2	0.66	0
3	GOL	H	601	-	5,5,5	0.38	0	5,5,5	0.34	0
2	EDO	A	602	-	3,3,3	0.45	0	2,2,2	0.71	0
2	EDO	C	603	-	3,3,3	0.53	0	2,2,2	0.30	0
2	EDO	D	602	-	3,3,3	0.58	0	2,2,2	0.56	0
2	EDO	F	601	-	3,3,3	0.49	0	2,2,2	0.86	0
3	GOL	A	604	-	5,5,5	0.50	0	5,5,5	1.39	1 (20%)
3	GOL	H	602	-	5,5,5	0.52	0	5,5,5	0.52	0
3	GOL	A	603	-	5,5,5	0.63	0	5,5,5	1.03	0
2	EDO	C	607	-	3,3,3	0.49	0	2,2,2	0.33	0
3	GOL	D	603	-	5,5,5	0.48	0	5,5,5	1.04	0
3	GOL	E	603	-	5,5,5	0.45	0	5,5,5	0.55	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
3	GOL	F	602	-	-	2/4/4/4	-
3	GOL	F	603	-	-	2/4/4/4	-
2	EDO	C	604	-	-	0/1/1/1	-
4	FLC	C	601	-	-	8/16/16/16	-
2	EDO	B	602	-	-	0/1/1/1	-
3	GOL	B	604	-	-	4/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	605	-	-	2/4/4/4	-
2	EDO	G	602	-	-	1/1/1/1	-
2	EDO	C	608	-	-	0/1/1/1	-
3	GOL	E	604	-	-	2/4/4/4	-
2	EDO	G	601	-	-	1/1/1/1	-
2	EDO	E	601	-	-	1/1/1/1	-
2	EDO	C	606	-	-	0/1/1/1	-
3	GOL	G	603	-	-	3/4/4/4	-
3	GOL	C	609	-	-	2/4/4/4	-
2	EDO	B	601	-	-	1/1/1/1	-
4	FLC	D	601	-	-	9/16/16/16	-
2	EDO	C	605	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-
2	EDO	E	602	-	-	0/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
3	GOL	H	601	-	-	2/4/4/4	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	C	603	-	-	0/1/1/1	-
2	EDO	D	602	-	-	1/1/1/1	-
2	EDO	F	601	-	-	1/1/1/1	-
3	GOL	A	604	-	-	4/4/4/4	-
3	GOL	H	602	-	-	4/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
2	EDO	C	607	-	-	0/1/1/1	-
3	GOL	D	603	-	-	3/4/4/4	-
3	GOL	E	603	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	FLC	CB-CBC	5.90	1.59	1.53
4	D	601	FLC	CB-CBC	2.67	1.56	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	601	FLC	OB2-CBC-CB	5.98	123.44	113.05
4	C	601	FLC	CA-CB-CBC	5.43	121.76	110.11
4	C	601	FLC	OB2-CBC-OB1	-5.17	107.38	123.82
4	C	601	FLC	OB1-CBC-CB	4.78	129.02	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	601	FLC	OB2-CBC-CB	4.26	120.46	113.05

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-C3
3	A	604	GOL	C1-C2-C3-O3
3	B	603	GOL	O1-C1-C2-C3
3	C	609	GOL	C1-C2-C3-O3
3	C	609	GOL	O2-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	603	GOL	1	0
4	C	601	FLC	1	0
3	B	603	GOL	1	0
2	E	601	EDO	2	0
2	C	606	EDO	1	0
3	G	603	GOL	1	0
4	D	601	FLC	2	0
2	C	605	EDO	5	0
2	A	602	EDO	2	0
2	C	603	EDO	4	0
2	D	602	EDO	3	0
2	F	601	EDO	2	0
3	H	602	GOL	1	0
2	C	607	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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 (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, 95^{th} 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
3	GOL	F	602	6/6	0.84	0.17	43,63,75,80	0
2	EDO	B	602	4/4	0.84	0.16	40,48,53,53	0
3	GOL	A	603	6/6	0.85	0.20	49,64,74,79	0
3	GOL	D	603	6/6	0.86	0.24	47,58,70,70	0
3	GOL	G	603	6/6	0.86	0.17	44,56,78,82	0
2	EDO	G	602	4/4	0.88	0.23	42,50,55,56	0
3	GOL	B	604	6/6	0.89	0.19	36,50,70,70	0
3	GOL	H	601	6/6	0.89	0.18	51,64,76,76	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
4	FLC	D	601	13/13	0.90	0.12	44,59,72,72	0
3	GOL	E	605	6/6	0.91	0.28	32,49,59,71	0
2	EDO	E	601	4/4	0.91	0.29	27,44,53,59	0
2	EDO	B	601	4/4	0.91	0.20	38,45,48,55	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
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	A	602	4/4	0.91	0.17	43,55,66,66	0
3	GOL	A	604	6/6	0.92	0.31	27,44,61,64	0
3	GOL	H	602	6/6	0.92	0.09	52,64,75,77	0
3	GOL	C	609	6/6	0.92	0.33	28,43,55,55	0
2	EDO	C	602	4/4	0.92	0.13	50,60,69,71	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	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	A	601	4/4	0.95	0.22	29,38,49,58	0
2	EDO	C	605	4/4	0.96	0.19	29,45,54,58	0
2	EDO	C	607	4/4	0.96	0.24	43,54,59,68	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.