wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 05:50 AM EDT

PDB ID	:	6NN8
Title	:	The structure of human liver pyruvate kinase, hLPYK-S531E
Authors	:	McFarlane, J.S.; Ronnebaum, T.A.; Meneely, K.M.; Fenton, A.W.; Lamb, A.L.
Deposited on	:	2019-01-14
Resolution	:	2.42 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 (i)) were used in the production of this report:

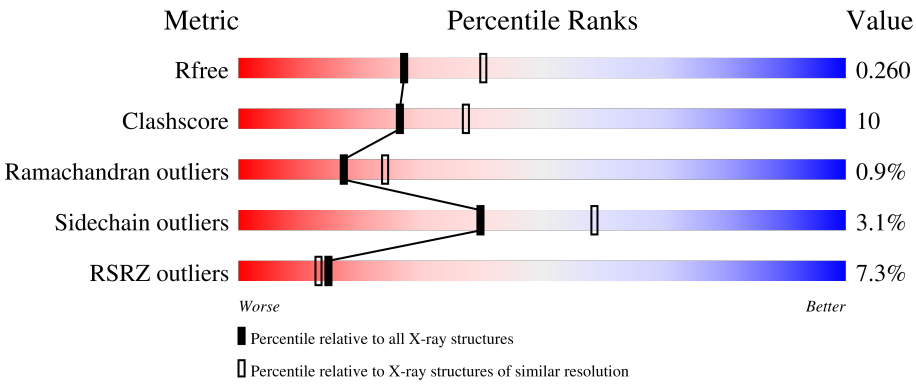
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.42 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 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	543	4%, 76%, 16%, • 7%
1	B	543	4%, 76%, 18%, • 5%
1	C	543	4%, 76%, 15%, 8%
1	D	543	6%, 59%, 17%, • 22%
1	E	543	6%, 74%, 19%, • 6%

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Mol	Chain	Length	Quality of chain
1	F	543	7% 54% 22% 23%
1	G	543	9% 51% 20% 27%
1	H	543	9% 50% 23% 25%

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	A	604	-	-	X	-
2	EDO	G	601	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 57131 atoms, of which 28756 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
			Total	C	H	N	O	S			
1	A	505	7738	2410	3909	690	711	18	0	0	0
1	B	518	7937	2473	4006	710	730	18	0	0	0
1	C	499	7675	2390	3880	683	704	18	0	0	0
1	D	421	6468	2018	3259	580	592	19	0	1	0
1	E	509	7828	2438	3957	701	714	18	0	0	0
1	F	417	6429	2006	3239	577	589	18	0	0	0
1	G	395	6086	1895	3076	542	555	18	0	0	0
1	H	407	6310	1965	3184	568	575	18	0	0	0

There are 24 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	531	GLU	SER	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	531	GLU	SER	engineered mutation	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	531	GLU	SER	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	531	GLU	SER	engineered mutation	UNP P30613
E	1	MET	-	expression tag	UNP P30613

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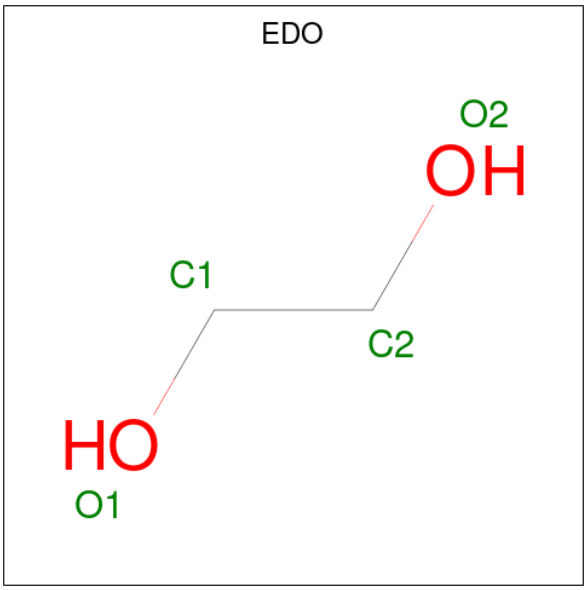
Chain	Residue	Modelled	Actual	Comment	Reference
E	2	GLU	-	expression tag	UNP P30613
E	531	GLU	SER	engineered mutation	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	531	GLU	SER	engineered mutation	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	531	GLU	SER	engineered mutation	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	531	GLU	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
			Total	C	H	O		
2	A	1	10	2	6	2	0	0
			Total	C	H	O		
2	A	1	10	2	6	2	0	0
			Total	C	H	O		
2	A	1	10	2	6	2	0	0
			Total	C	H	O		
2	A	1	10	2	6	2	0	0
			Total	C	H	O		
2	A	1	10	2	6	2	0	0
			Total	C	H	O		
2	A	1	10	2	6	2	0	0

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	71	71	71	0	0
3	B	58	58	58	0	0
3	C	54	54	54	0	0
3	D	16	16	16	0	0
3	E	34	34	34	0	0

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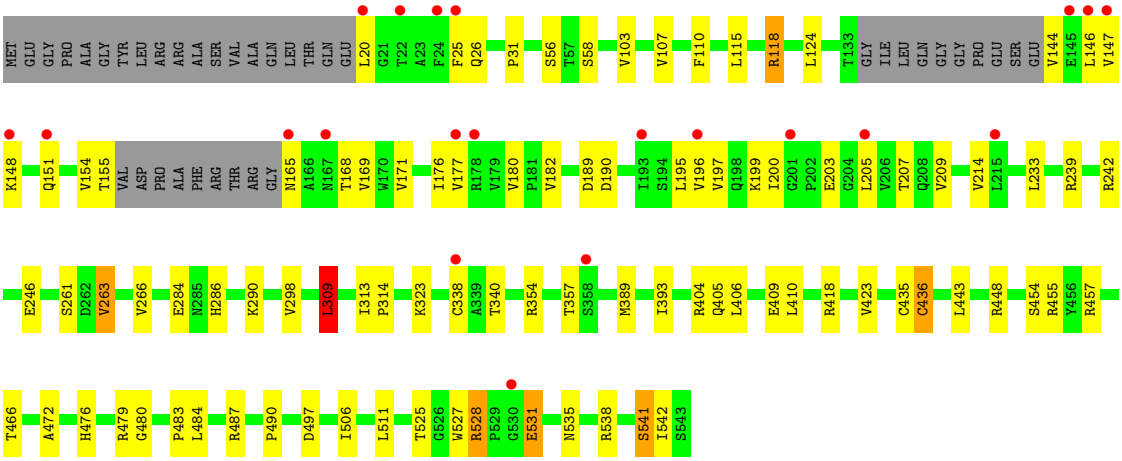
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	F	6	6	6	0	0
			Total	O		
3	G	10	10	10	0	0
			Total	O		
3	H	1	1	1	0	0

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.

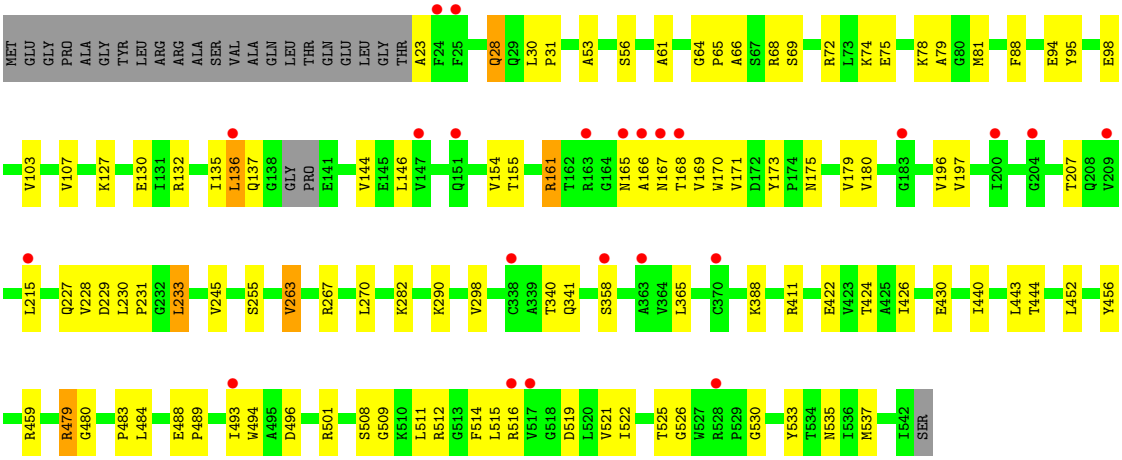
• Molecule 1: Pyruvate kinase PKLR

Chain A:



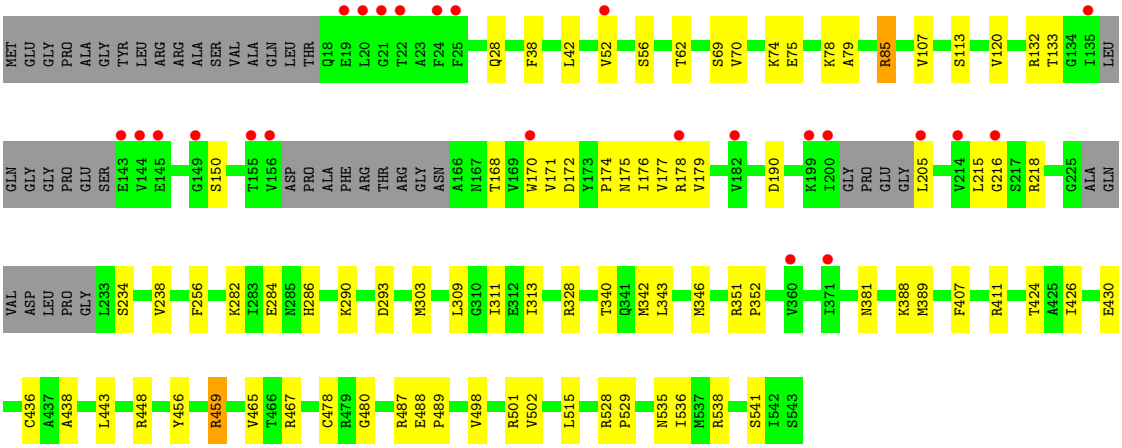
• Molecule 1: Pyruvate kinase PKLR

Chain B:



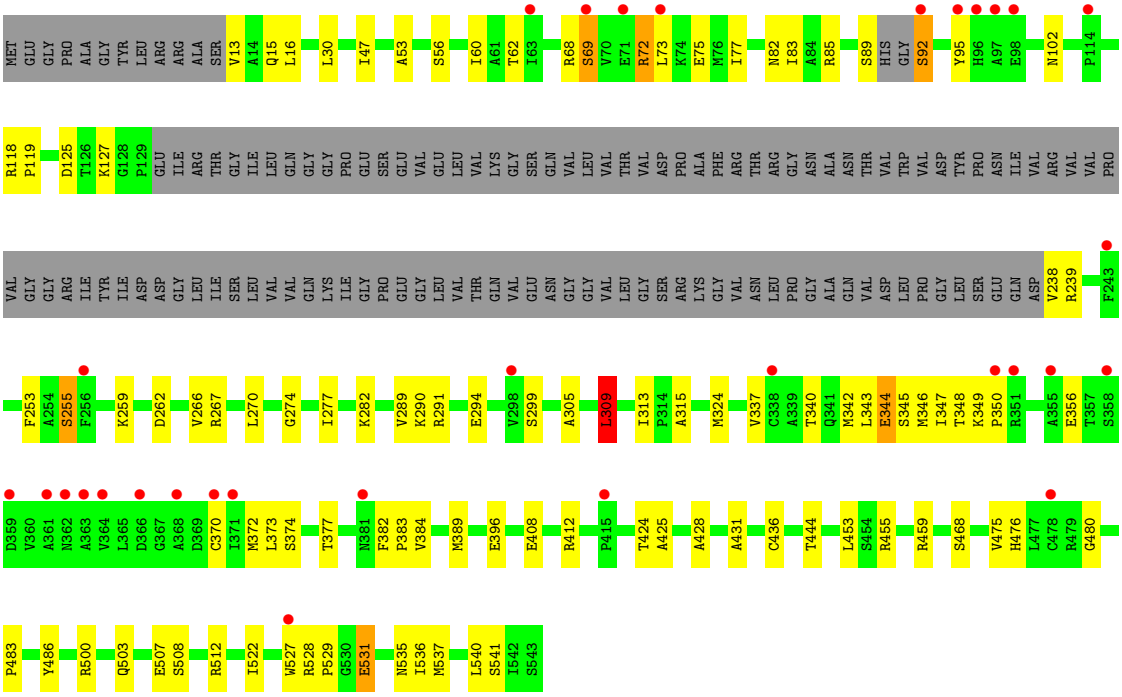
• Molecule 1: Pyruvate kinase PKLR

Chain C:



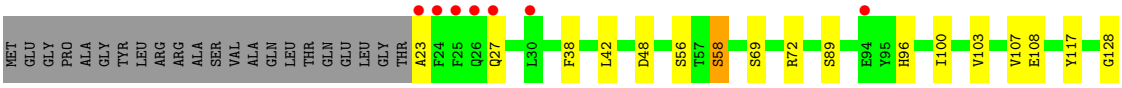
• Molecule 1: Pyruvate kinase PKLR

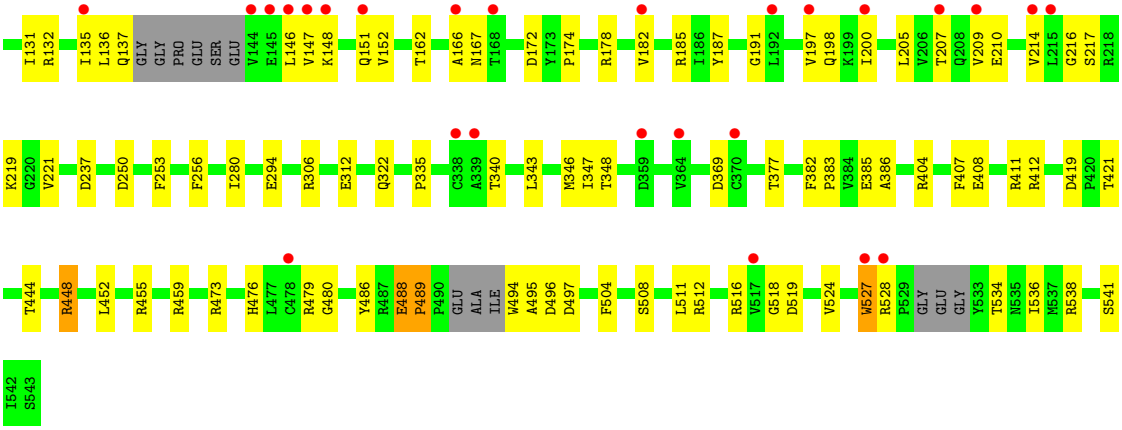
Chain D:



• Molecule 1: Pyruvate kinase PKLR

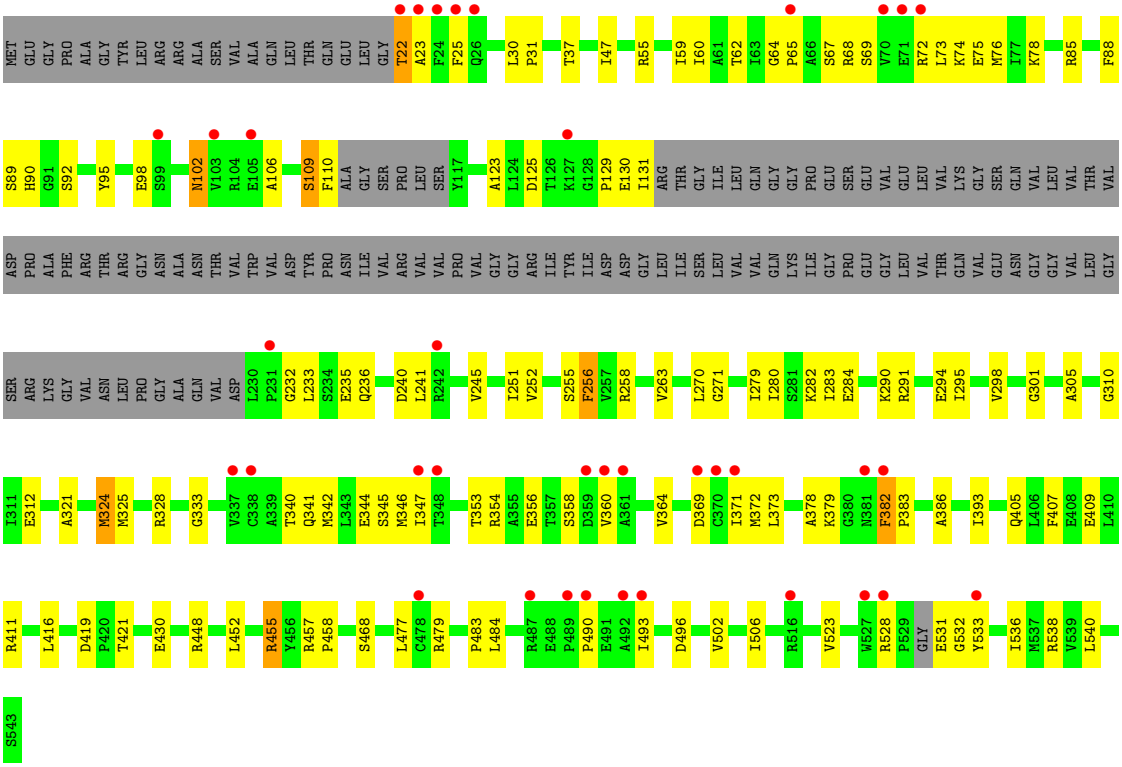
Chain E:





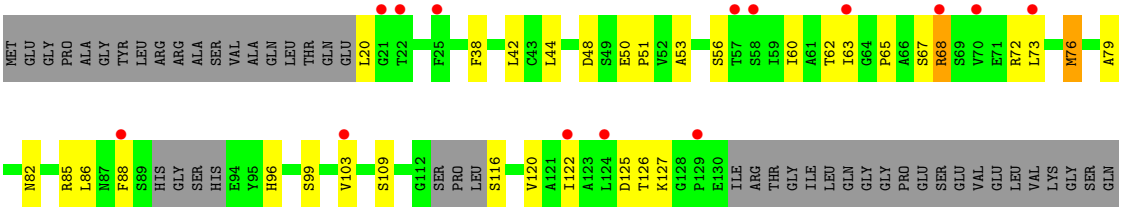
• Molecule 1: Pyruvate kinase PKLR

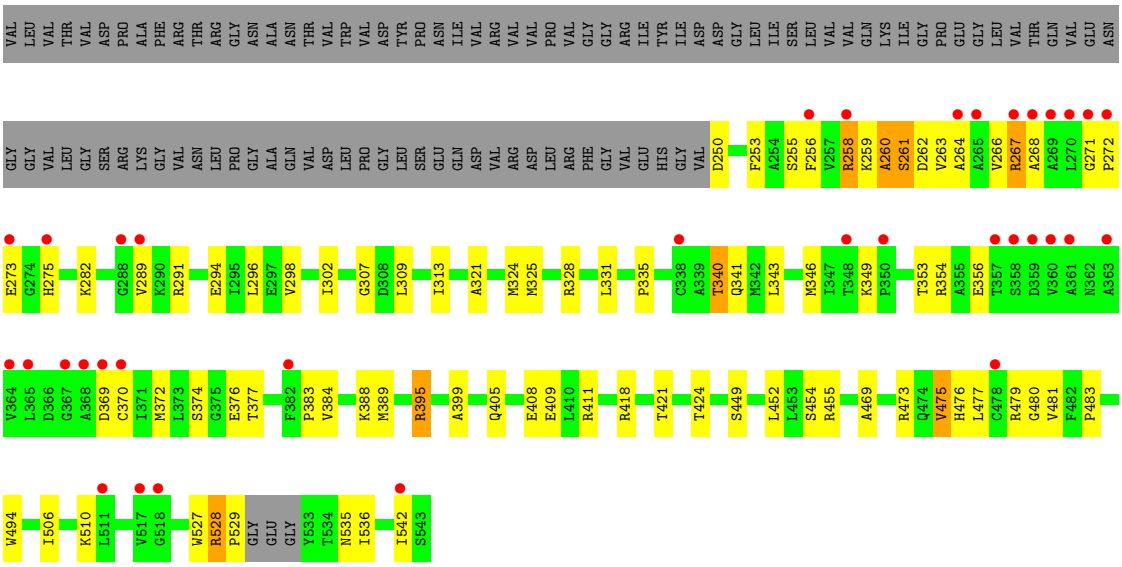
Chain F:



• Molecule 1: Pyruvate kinase PKLR

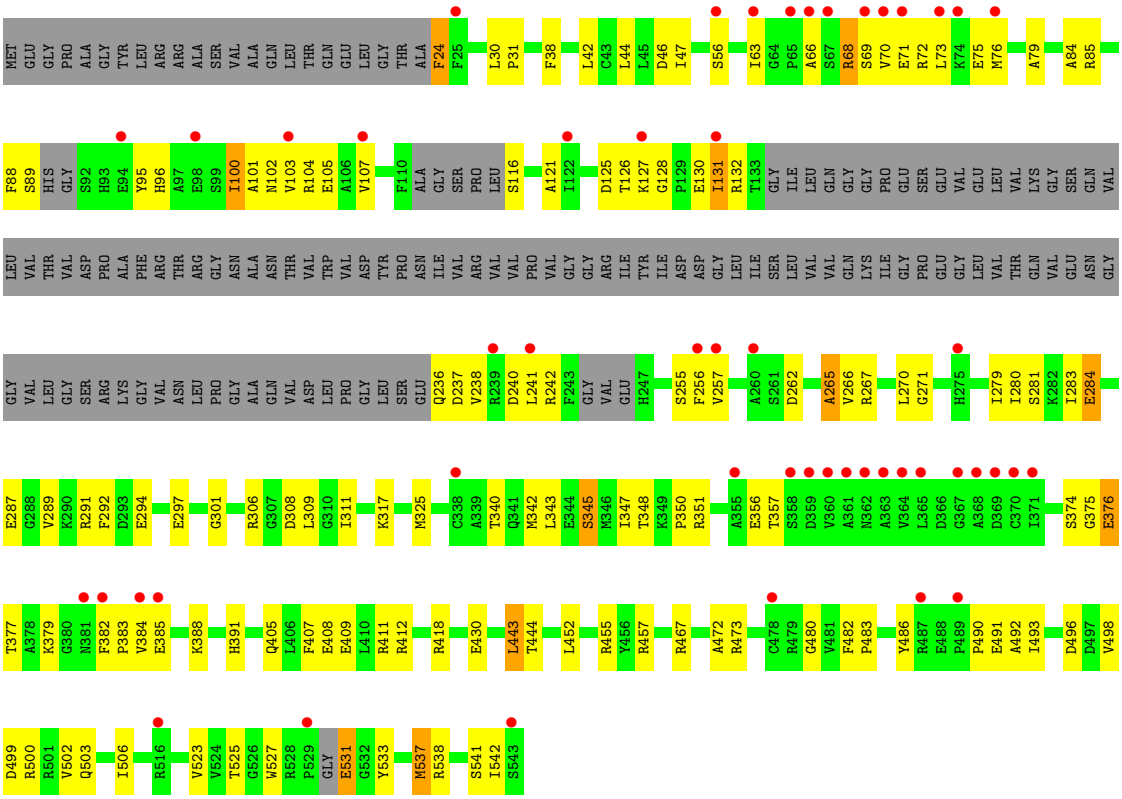
Chain G:





- Molecule 1: Pyruvate kinase PKLR

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.91Å 139.41Å 181.29Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	39.54 – 2.42 39.54 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.54-2.42) 98.7 (39.54-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.208 , 0.260 0.208 , 0.260	Depositor DCC
R_{free} test set	2006 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	57131	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.74	2/3890 (0.1%)	0.85	5/5269 (0.1%)
1	B	0.67	0/3995	0.81	2/5413 (0.0%)
1	C	0.66	2/3852 (0.1%)	0.80	5/5212 (0.1%)
1	D	0.63	0/3263	0.75	2/4412 (0.0%)
1	E	0.64	0/3933	0.82	4/5326 (0.1%)
1	F	0.57	0/3241	0.74	0/4380
1	G	0.58	0/3055	0.73	1/4127 (0.0%)
1	H	0.59	0/3173	0.75	2/4283 (0.0%)
All	All	0.64	4/28402 (0.0%)	0.79	21/38422 (0.1%)

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	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	VAL	CB-CG2	-5.78	1.40	1.52
1	C	436	CYS	CB-SG	-5.43	1.73	1.81
1	C	478	CYS	CB-SG	-5.38	1.73	1.81
1	A	338	CYS	CB-SG	5.03	1.90	1.82

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	479	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	B	459	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	D	459	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	448	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	459	ARG	NE-CZ-NH1	5.99	123.30	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	531	GLU	Peptide
1	B	533	TYR	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	3829	3909	3907	77	0
1	B	3931	4006	4005	66	0
1	C	3795	3880	3876	54	0
1	D	3209	3259	3270	74	0
1	E	3871	3957	3954	72	0
1	F	3190	3239	3239	90	0
1	G	3010	3076	3072	96	0
1	H	3126	3184	3179	93	0
2	A	40	60	60	12	0
2	B	28	42	42	5	0
2	C	24	36	36	3	0
2	D	16	24	24	2	0
2	E	28	42	42	6	0
2	F	8	12	12	0	0
2	G	8	12	12	9	0
2	H	12	18	18	3	0
3	A	71	0	0	0	0
3	B	58	0	0	1	0
3	C	54	0	0	1	0
3	D	16	0	0	1	0
3	E	34	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	6	0	0	0	0
3	G	10	0	0	2	0
3	H	1	0	0	0	0
All	All	28375	28756	28748	588	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 10.

The worst 5 of 588 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:146:LEU:HD21	1:A:214:VAL:HG22	1.26	1.13
1:E:185:ARG:NH1	1:E:210:GLU:OE2	2.03	0.92
1:F:483:PRO:O	1:F:484:LEU:HD23	1.70	0.91
1:G:53:ALA:HB3	2:G:601:EDO:H12	1.50	0.91
1:D:266:VAL:O	1:D:270:LEU:HD12	1.70	0.91

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	499/543 (92%)	484 (97%)	12 (2%)	3 (1%)	25 35
1	B	514/543 (95%)	495 (96%)	14 (3%)	5 (1%)	15 22
1	C	489/543 (90%)	471 (96%)	17 (4%)	1 (0%)	47 61
1	D	416/543 (77%)	405 (97%)	10 (2%)	1 (0%)	47 61
1	E	501/543 (92%)	481 (96%)	13 (3%)	7 (1%)	11 14
1	F	409/543 (75%)	378 (92%)	26 (6%)	5 (1%)	13 17
1	G	385/543 (71%)	355 (92%)	27 (7%)	3 (1%)	19 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	395/543 (73%)	366 (93%)	22 (6%)	7 (2%)	8 10
All	All	3608/4344 (83%)	3435 (95%)	141 (4%)	32 (1%)	17 24

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	151	GLN
1	E	495	ALA
1	B	137	GLN
1	E	166	ALA
1	F	532	GLY

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	405/433 (94%)	398 (98%)	7 (2%)	60 77
1	B	415/433 (96%)	406 (98%)	9 (2%)	52 69
1	C	402/433 (93%)	397 (99%)	5 (1%)	71 84
1	D	336/433 (78%)	321 (96%)	15 (4%)	27 42
1	E	410/433 (95%)	401 (98%)	9 (2%)	52 69
1	F	334/433 (77%)	322 (96%)	12 (4%)	35 52
1	G	314/433 (72%)	299 (95%)	15 (5%)	25 40
1	H	328/433 (76%)	309 (94%)	19 (6%)	20 31
All	All	2944/3464 (85%)	2853 (97%)	91 (3%)	40 58

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	20	LEU
1	G	528	ARG
1	G	76	MET
1	G	370	CYS

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Mol	Chain	Res	Type
1	H	89	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	403	HIS
1	H	403	HIS

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)

41 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	604	-	3,3,3	0.44	0	2,2,2	0.75	0
2	EDO	F	601	-	3,3,3	0.53	0	2,2,2	0.20	0
2	EDO	G	601	-	3,3,3	0.43	0	2,2,2	0.63	0
2	EDO	F	602	-	3,3,3	0.49	0	2,2,2	0.20	0
2	EDO	B	603	-	3,3,3	1.05	0	2,2,2	1.13	0
2	EDO	C	603	-	3,3,3	0.36	0	2,2,2	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	E	601	-	3,3,3	0.60	0	2,2,2	1.06	0
2	EDO	H	602	-	3,3,3	0.47	0	2,2,2	0.58	0
2	EDO	E	602	-	3,3,3	0.68	0	2,2,2	0.36	0
2	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.42	0
2	EDO	B	604	-	3,3,3	0.64	0	2,2,2	1.30	0
2	EDO	H	601	-	3,3,3	0.68	0	2,2,2	0.55	0
2	EDO	E	603	-	3,3,3	0.61	0	2,2,2	0.36	0
2	EDO	A	602	-	3,3,3	0.45	0	2,2,2	0.39	0
2	EDO	C	602	-	3,3,3	0.73	0	2,2,2	0.32	0
2	EDO	A	601	-	3,3,3	0.59	0	2,2,2	1.57	1 (50%)
2	EDO	E	606	-	3,3,3	0.43	0	2,2,2	0.70	0
2	EDO	A	603	-	3,3,3	0.55	0	2,2,2	0.12	0
2	EDO	B	607	-	3,3,3	0.44	0	2,2,2	0.63	0
2	EDO	A	607	-	3,3,3	0.57	0	2,2,2	0.14	0
2	EDO	D	602	-	3,3,3	0.59	0	2,2,2	0.50	0
2	EDO	A	604	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	D	601	-	3,3,3	0.52	0	2,2,2	0.05	0
2	EDO	H	603	-	3,3,3	0.45	0	2,2,2	0.51	0
2	EDO	B	605	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	A	605	-	3,3,3	0.81	0	2,2,2	0.49	0
2	EDO	E	605	-	3,3,3	0.46	0	2,2,2	0.03	0
2	EDO	D	604	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	C	606	-	3,3,3	0.57	0	2,2,2	0.14	0
2	EDO	C	601	-	3,3,3	0.79	0	2,2,2	0.54	0
2	EDO	A	609	-	3,3,3	0.46	0	2,2,2	0.55	0
2	EDO	E	604	-	3,3,3	0.62	0	2,2,2	0.84	0
2	EDO	B	602	-	3,3,3	0.43	0	2,2,2	0.51	0
2	EDO	G	602	-	3,3,3	0.52	0	2,2,2	0.12	0
2	EDO	B	601	-	3,3,3	0.57	0	2,2,2	0.45	0
2	EDO	B	606	-	3,3,3	0.41	0	2,2,2	0.39	0
2	EDO	A	606	-	3,3,3	0.52	0	2,2,2	0.15	0
2	EDO	A	608	-	3,3,3	0.95	0	2,2,2	0.62	0
2	EDO	E	607	-	3,3,3	0.57	0	2,2,2	0.69	0
2	EDO	D	603	-	3,3,3	0.46	0	2,2,2	0.48	0
2	EDO	C	605	-	3,3,3	0.44	0	2,2,2	0.40	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	604	-	-	1/1/1/1	-
2	EDO	F	601	-	-	1/1/1/1	-
2	EDO	G	601	-	-	0/1/1/1	-
2	EDO	F	602	-	-	1/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	E	601	-	-	0/1/1/1	-
2	EDO	H	602	-	-	1/1/1/1	-
2	EDO	E	602	-	-	1/1/1/1	-
2	EDO	A	610	-	-	0/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-
2	EDO	H	601	-	-	0/1/1/1	-
2	EDO	E	603	-	-	1/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	E	606	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	607	-	-	1/1/1/1	-
2	EDO	A	607	-	-	1/1/1/1	-
2	EDO	D	602	-	-	0/1/1/1	-
2	EDO	A	604	-	-	1/1/1/1	-
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	H	603	-	-	1/1/1/1	-
2	EDO	B	605	-	-	0/1/1/1	-
2	EDO	A	605	-	-	1/1/1/1	-
2	EDO	E	605	-	-	1/1/1/1	-
2	EDO	D	604	-	-	1/1/1/1	-
2	EDO	C	606	-	-	1/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	A	609	-	-	1/1/1/1	-
2	EDO	E	604	-	-	0/1/1/1	-
2	EDO	B	602	-	-	1/1/1/1	-
2	EDO	G	602	-	-	0/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	B	606	-	-	1/1/1/1	-
2	EDO	A	606	-	-	1/1/1/1	-
2	EDO	A	608	-	-	1/1/1/1	-
2	EDO	E	607	-	-	0/1/1/1	-
2	EDO	D	603	-	-	1/1/1/1	-
2	EDO	C	605	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	EDO	O1-C1-C2	-2.22	95.90	111.91

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	EDO	O1-C1-C2-O2
2	A	605	EDO	O1-C1-C2-O2
2	B	606	EDO	O1-C1-C2-O2
2	E	602	EDO	O1-C1-C2-O2
2	F	602	EDO	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	601	EDO	9	0
2	H	602	EDO	2	0
2	E	602	EDO	2	0
2	B	604	EDO	3	0
2	H	601	EDO	1	0
2	E	603	EDO	3	0
2	A	601	EDO	3	0
2	D	602	EDO	1	0
2	A	604	EDO	5	0
2	B	605	EDO	2	0
2	C	606	EDO	1	0
2	C	601	EDO	2	0
2	A	609	EDO	1	0
2	A	608	EDO	3	0
2	E	607	EDO	1	0
2	D	603	EDO	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 (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	505/543 (93%)	0.14	21 (4%)	36	34	26, 41, 73, 88	0
1	B	518/543 (95%)	0.27	23 (4%)	34	32	26, 45, 75, 88	0
1	C	499/543 (91%)	0.26	24 (4%)	30	28	30, 45, 72, 92	0
1	D	421/543 (77%)	0.48	31 (7%)	14	13	30, 58, 82, 91	0
1	E	509/543 (93%)	0.30	33 (6%)	18	17	28, 48, 77, 92	0
1	F	417/543 (76%)	0.54	37 (8%)	9	8	39, 63, 85, 94	0
1	G	395/543 (72%)	0.66	49 (12%)	4	3	38, 62, 85, 95	0
1	H	407/543 (74%)	0.69	50 (12%)	4	3	41, 64, 85, 93	0
All	All	3671/4344 (84%)	0.40	268 (7%)	15	13	26, 53, 82, 95	0

The worst 5 of 268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	272	PRO	7.5
1	E	25	PHE	6.6
1	E	146	LEU	6.6
1	G	270	LEU	5.5
1	A	215	LEU	5.3

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
2	EDO	H	601	4/4	0.72	0.39	61,73,86,86	0
2	EDO	H	603	4/4	0.73	0.21	65,78,84,87	0
2	EDO	E	607	4/4	0.76	0.24	46,68,82,93	0
2	EDO	F	601	4/4	0.76	0.20	58,74,88,89	0
2	EDO	A	603	4/4	0.77	0.26	62,74,82,82	0
2	EDO	C	606	4/4	0.77	0.21	51,62,64,69	0
2	EDO	E	604	4/4	0.80	0.55	54,65,73,77	0
2	EDO	G	602	4/4	0.80	0.22	56,72,86,86	0
2	EDO	B	603	4/4	0.81	0.40	43,56,73,73	0
2	EDO	B	604	4/4	0.82	0.29	45,63,72,76	0
2	EDO	A	602	4/4	0.83	0.16	65,78,89,89	0
2	EDO	A	610	4/4	0.85	0.15	56,68,83,83	0
2	EDO	A	608	4/4	0.85	0.28	36,45,54,54	0
2	EDO	D	602	4/4	0.85	0.17	54,65,74,78	0
2	EDO	C	602	4/4	0.86	0.42	41,57,70,81	0
2	EDO	A	604	4/4	0.86	0.28	44,55,65,79	0
2	EDO	F	602	4/4	0.86	0.25	67,80,89,91	0
2	EDO	B	607	4/4	0.87	0.19	62,74,90,90	0
2	EDO	D	603	4/4	0.87	0.20	49,59,70,71	0
2	EDO	D	601	4/4	0.87	0.35	57,73,87,87	0
2	EDO	A	601	4/4	0.88	0.27	46,56,58,58	0
2	EDO	A	609	4/4	0.88	0.24	49,59,70,72	0
2	EDO	A	605	4/4	0.89	0.39	35,56,65,71	0
2	EDO	A	607	4/4	0.89	0.28	41,56,59,71	0
2	EDO	D	604	4/4	0.90	0.28	61,74,76,85	0
2	EDO	H	602	4/4	0.90	0.31	45,59,71,72	0
2	EDO	C	603	4/4	0.90	0.26	45,55,66,70	0
2	EDO	B	601	4/4	0.91	0.23	43,54,58,65	0
2	EDO	B	605	4/4	0.91	0.24	49,59,60,63	0
2	EDO	B	602	4/4	0.92	0.13	50,60,69,82	0
2	EDO	C	601	4/4	0.93	0.19	41,49,53,58	0
2	EDO	G	601	4/4	0.94	0.17	49,59,74,74	0
2	EDO	E	606	4/4	0.94	0.13	54,65,74,89	0
2	EDO	E	602	4/4	0.94	0.24	40,55,66,66	0
2	EDO	C	604	4/4	0.94	0.11	52,63,73,73	0
2	EDO	E	605	4/4	0.94	0.22	50,64,68,82	0
2	EDO	A	606	4/4	0.95	0.13	42,50,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	E	601	4/4	0.95	0.22	44,53,65,69	0
2	EDO	E	603	4/4	0.96	0.17	42,51,67,80	0
2	EDO	C	605	4/4	0.96	0.20	43,58,69,79	0
2	EDO	B	606	4/4	0.96	0.27	47,58,64,70	0

6.5 Other polymers (i)

There are no such residues in this entry.