



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:54 PM UTC

PDB ID : 4MLR / pdb_00004mlr
Title : dihydrodipicolinate synthase from *C. jejuni*, Y110F mutation with pyruvate and Lysine
Authors : Conly, C.J.T.
Deposited on : 2013-09-06
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

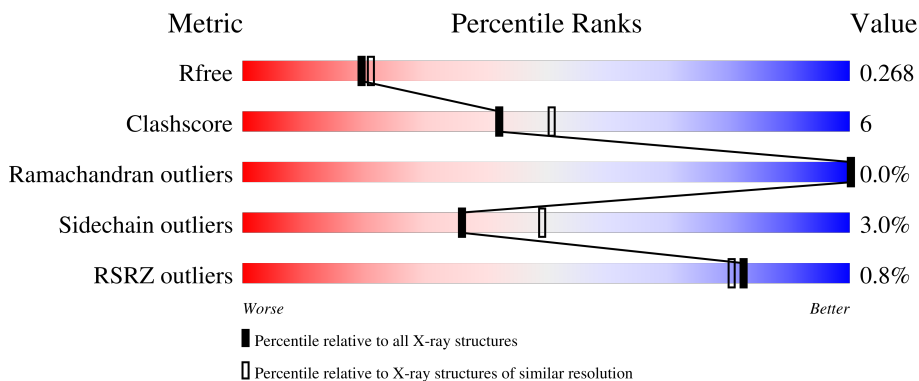
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	306	 83% 13% ..
1	B	306	 2% 80% 15% ..
1	C	306	 81% 14% ..
1	D	306	 % 76% 18% ..
1	E	306	 82% 13% .

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Mol	Chain	Length	Quality of chain
1	F	306	 80% 15% . .
1	G	306	 % 74% 22% . .
1	H	306	 2% 78% 17% . .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 18601 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 dihydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2282	1454	379	436	13	0	1	0
1	B	296	2278	1450	379	436	13	1	0	0
1	C	295	2269	1444	377	435	13	0	0	0
1	D	295	2278	1447	382	436	13	0	1	0
1	E	294	2261	1440	375	433	13	0	0	0
1	F	296	2278	1450	379	436	13	1	0	0
1	G	296	2278	1450	379	436	13	0	0	0
1	H	295	2269	1444	377	435	13	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	ALA	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	110	PHE	TYR	engineered mutation	UNP Q9PPB4
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4

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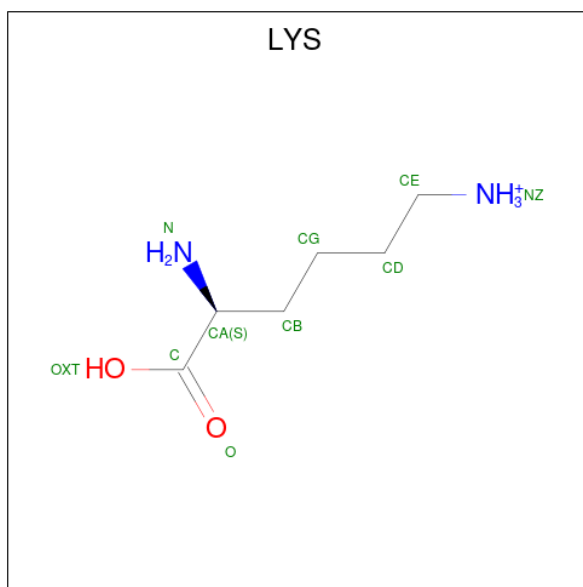
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	ALA	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	110	PHE	TYR	engineered mutation	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	ALA	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	110	PHE	TYR	engineered mutation	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	ALA	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	110	PHE	TYR	engineered mutation	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	ALA	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	110	PHE	TYR	engineered mutation	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	ALA	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	110	PHE	TYR	engineered mutation	UNP Q9PPB4
G	-7	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	HIS	-	expression tag	UNP Q9PPB4
G	-5	HIS	-	expression tag	UNP Q9PPB4
G	-4	HIS	-	expression tag	UNP Q9PPB4
G	-3	HIS	-	expression tag	UNP Q9PPB4
G	-2	HIS	-	expression tag	UNP Q9PPB4
G	-1	ALA	-	expression tag	UNP Q9PPB4
G	0	SER	-	expression tag	UNP Q9PPB4
G	110	PHE	TYR	engineered mutation	UNP Q9PPB4
H	-7	HIS	-	expression tag	UNP Q9PPB4
H	-6	HIS	-	expression tag	UNP Q9PPB4
H	-5	HIS	-	expression tag	UNP Q9PPB4
H	-4	HIS	-	expression tag	UNP Q9PPB4
H	-3	HIS	-	expression tag	UNP Q9PPB4
H	-2	HIS	-	expression tag	UNP Q9PPB4
H	-1	ALA	-	expression tag	UNP Q9PPB4
H	0	SER	-	expression tag	UNP Q9PPB4
H	110	PHE	TYR	engineered mutation	UNP Q9PPB4

- Molecule 2 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



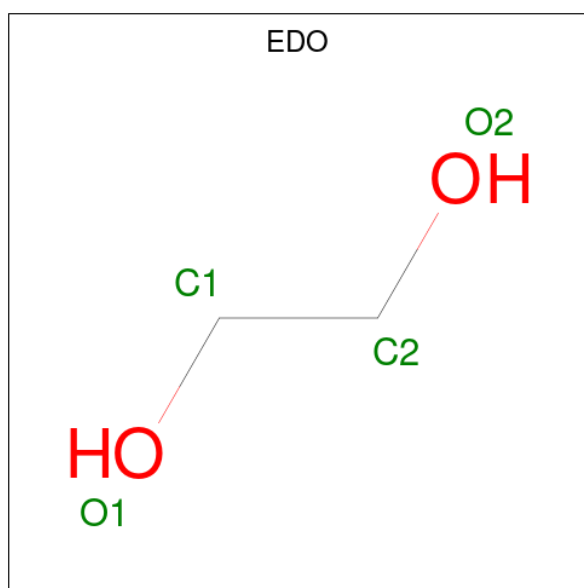
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



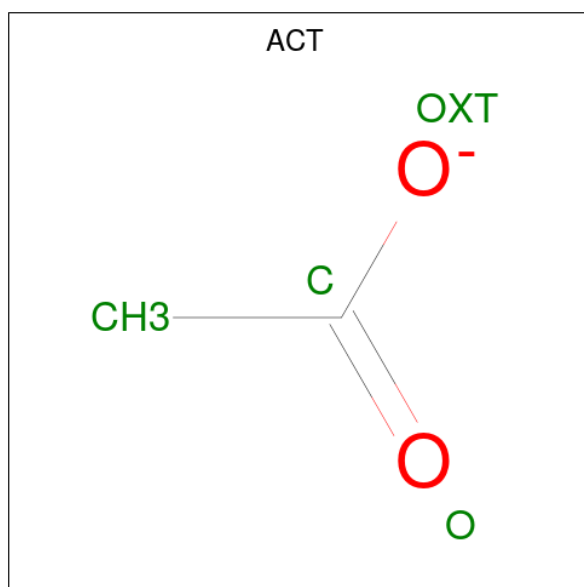
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

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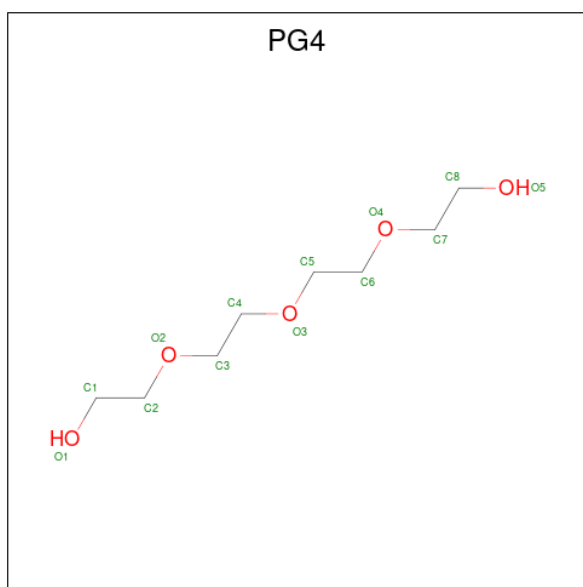
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



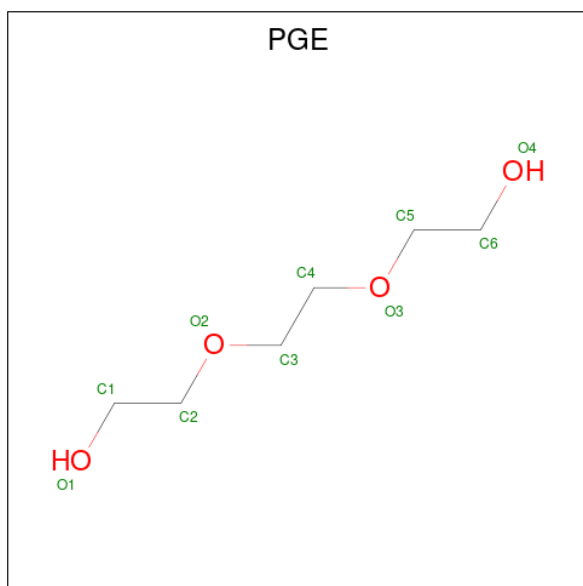
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



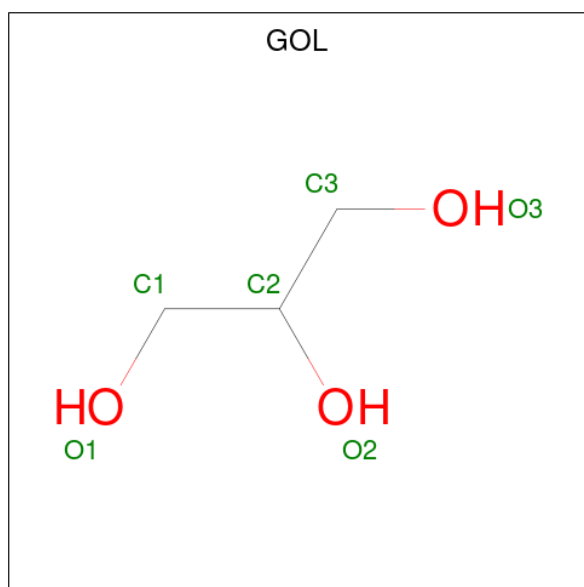
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	42	Total	O	0	0
			42	42		
8	B	29	Total	O	0	0
			29	29		
8	C	23	Total	O	0	0
			23	23		
8	D	23	Total	O	0	0
			23	23		
8	E	32	Total	O	0	0
			32	32		

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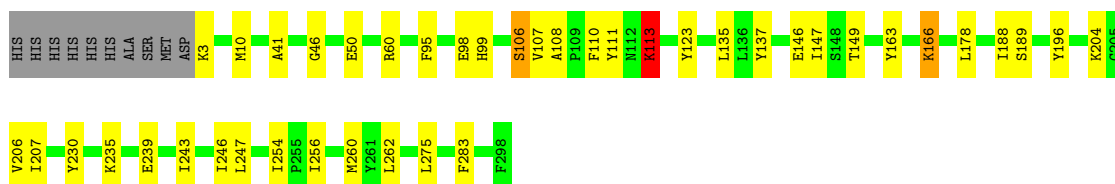
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	23	Total O 23 23	0	0
8	G	17	Total O 17 17	0	0
8	H	13	Total O 13 13	0	0

3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

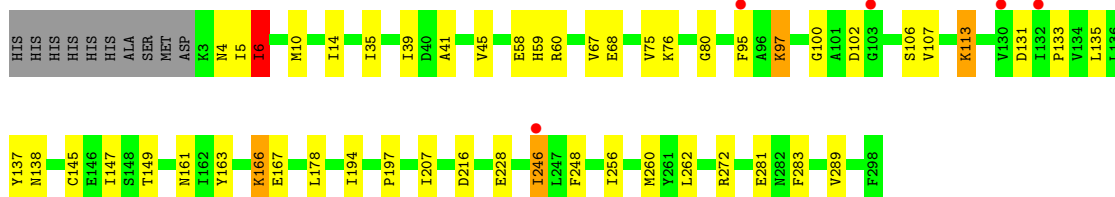
- Molecule 1: dihydrodipicolinate synthase

Chain A: 




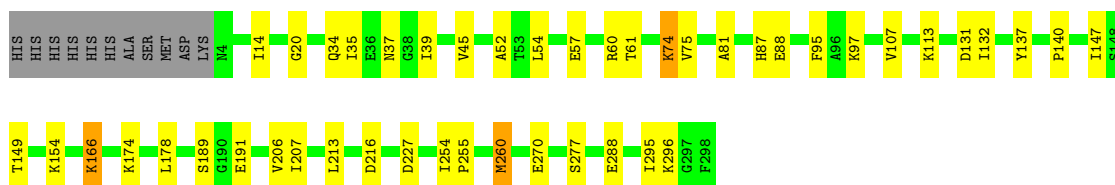
- Molecule 1: dihydrodipicolinate synthase

Chain B: 




- Molecule 1: dihydrodipicolinate synthase

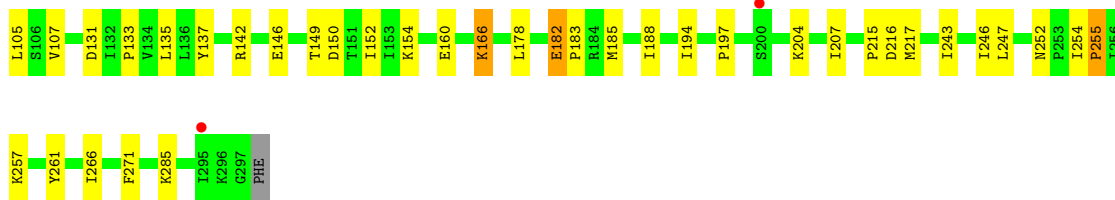
Chain C: 



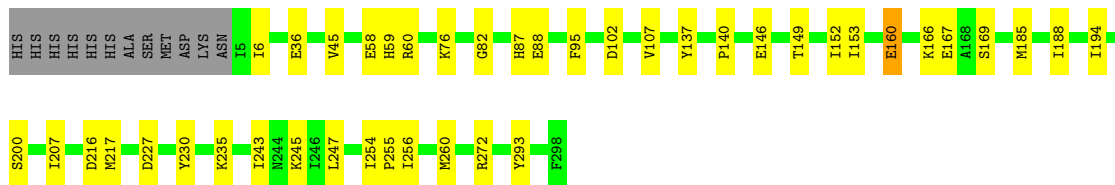
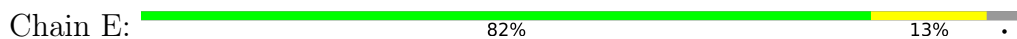
- Molecule 1: dihydrodipicolinate synthase

Chain D: 

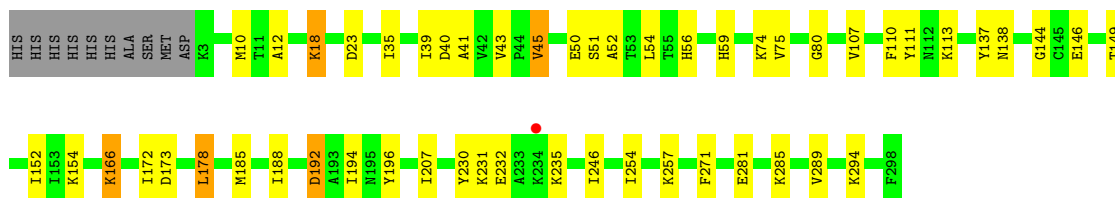
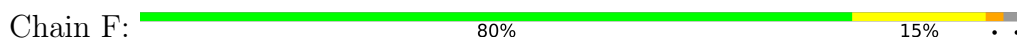




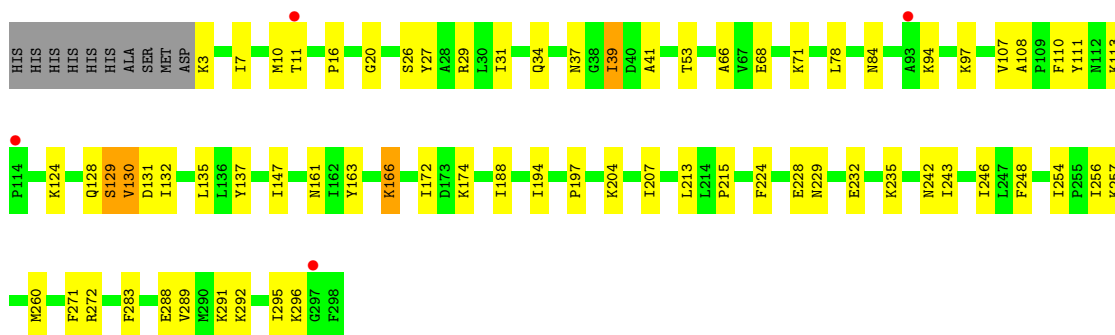
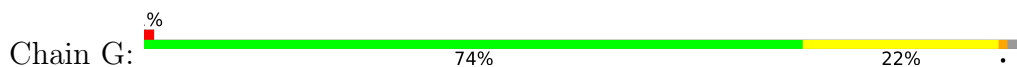
• Molecule 1: dihydrodipicolinate synthase



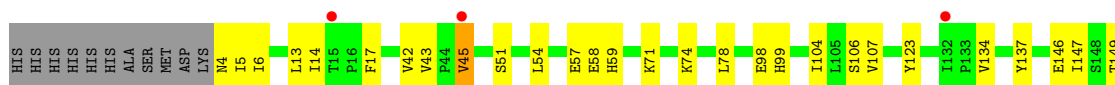
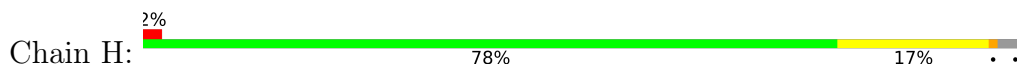
• Molecule 1: dihydrodipicolinate synthase

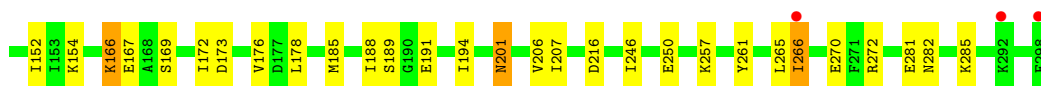


• Molecule 1: dihydrodipicolinate synthase



• Molecule 1: dihydrodipicolinate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.98Å 97.61Å 131.40Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	43.45 – 2.20 43.45 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.45-2.20) 99.8 (43.45-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.20Å)	Xtrriage
Refinement program	PHENIX dev_1356	Depositor
R, R_{free}	0.214 , 0.269 0.217 , 0.268	Depositor DCC
R_{free} test set	5833 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtrriage
Anisotropy	0.070	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18601	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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, PGE, PG4, EDO, KPI, ACT

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	0.53	2/2309 (0.1%)	0.79	1/3121 (0.0%)
1	B	0.58	3/2302 (0.1%)	0.77	0/3111
1	C	0.56	2/2293 (0.1%)	0.77	0/3100
1	D	0.69	2/2301 (0.1%)	0.79	0/3109
1	E	0.49	0/2285	0.78	0/3089
1	F	0.42	0/2302	0.76	0/3111
1	G	0.57	1/2302 (0.0%)	0.77	2/3111 (0.1%)
1	H	0.47	0/2293	0.75	0/3100
All	All	0.54	10/18387 (0.1%)	0.77	3/24852 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	LYS	C-O	-10.61	1.19	1.23
1	A	113	LYS	C-O	-9.85	1.19	1.23
1	B	113	LYS	C-O	-9.29	1.19	1.23
1	B	80	GLY	C-O	-7.38	1.17	1.24
1	C	81	ALA	C-O	-6.95	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	113	LYS	CB-CA-C	-9.80	104.24	111.20
1	A	46	GLY	N-CA-C	-5.94	104.11	112.60
1	G	224	PHE	N-CA-C	-5.33	105.64	111.82

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	2282	0	2328	24	0
1	B	2278	0	2319	28	0
1	C	2269	0	2306	23	0
1	D	2278	0	2322	37	0
1	E	2261	0	2300	25	0
1	F	2278	0	2319	30	0
1	G	2278	0	2319	41	0
1	H	2269	0	2306	31	0
2	A	20	0	24	1	0
2	B	10	0	12	0	0
2	C	10	0	12	1	0
2	E	10	0	12	0	0
2	F	10	0	12	2	0
2	G	10	0	12	0	0
2	H	10	0	12	2	0
3	A	12	0	18	1	0
3	D	4	0	6	0	0
3	E	8	0	12	0	0
3	G	12	0	18	0	0
4	A	4	0	3	0	0
4	F	4	0	3	1	0
5	B	13	0	18	0	0
5	C	13	0	18	1	0
6	B	10	0	14	0	0
6	C	10	0	14	0	0
6	E	10	0	14	0	0
6	F	10	0	14	1	0
6	H	10	0	14	1	0
7	C	6	0	8	1	0
8	A	42	0	0	0	0
8	B	29	0	0	0	0
8	C	23	0	0	0	0
8	D	23	0	0	0	0
8	E	32	0	0	0	0
8	F	23	0	0	0	0
8	G	17	0	0	0	0
8	H	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18601	0	18789	234	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 234 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:G:246:ILE:HG13	1:G:289:VAL:HG21	1.52	0.89
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.60	0.83
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.64	0.79
1:D:254:ILE:HB	1:D:255:PRO:HD3	1.65	0.78
1:G:107:VAL:HA	1:G:137:TYR:HB3	1.68	0.75

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	294/306 (96%)	287 (98%)	7 (2%)	0	100	100
1	B	293/306 (96%)	286 (98%)	7 (2%)	0	100	100
1	C	292/306 (95%)	284 (97%)	8 (3%)	0	100	100
1	D	293/306 (96%)	285 (97%)	8 (3%)	0	100	100
1	E	291/306 (95%)	284 (98%)	7 (2%)	0	100	100
1	F	293/306 (96%)	284 (97%)	9 (3%)	0	100	100
1	G	293/306 (96%)	285 (97%)	7 (2%)	1 (0%)	36	42
1	H	292/306 (95%)	280 (96%)	12 (4%)	0	100	100
All	All	2341/2448 (96%)	2275 (97%)	65 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	129	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	249/257 (97%)	246 (99%)	3 (1%)	63 78
1	B	248/257 (96%)	239 (96%)	9 (4%)	31 42
1	C	247/257 (96%)	241 (98%)	6 (2%)	43 58
1	D	248/257 (96%)	239 (96%)	9 (4%)	31 42
1	E	246/257 (96%)	242 (98%)	4 (2%)	55 71
1	F	248/257 (96%)	239 (96%)	9 (4%)	31 42
1	G	248/257 (96%)	241 (97%)	7 (3%)	38 52
1	H	247/257 (96%)	234 (95%)	13 (5%)	20 26
All	All	1981/2056 (96%)	1921 (97%)	60 (3%)	36 49

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	160	GLU
1	H	147	ILE
1	F	178	LEU
1	H	146	GLU
1	H	266	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	99	HIS
1	F	99	HIS
1	H	4	ASN
1	G	34	GLN

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Mol	Chain	Res	Type
1	D	242	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 non-standard protein/DNA/RNA residues 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
1	KPI	C	166	1	11,13,14	2.07	2 (18%)	9,15,17	2.36	2 (22%)
1	KPI	F	166	1	11,13,14	2.06	2 (18%)	9,15,17	2.53	2 (22%)
1	KPI	B	166	1	11,13,14	2.10	2 (18%)	9,15,17	2.30	2 (22%)
1	KPI	A	166	1	11,13,14	2.08	2 (18%)	9,15,17	2.05	3 (33%)
1	KPI	G	166	1	11,13,14	2.08	2 (18%)	9,15,17	2.55	2 (22%)
1	KPI	H	166	1	11,13,14	2.08	2 (18%)	9,15,17	2.49	2 (22%)
1	KPI	E	166	1	11,13,14	2.12	2 (18%)	9,15,17	2.45	3 (33%)
1	KPI	D	166	1	11,13,14	2.06	2 (18%)	9,15,17	2.41	2 (22%)

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
1	KPI	C	166	1	-	2/13/14/16	-
1	KPI	F	166	1	-	3/13/14/16	-
1	KPI	B	166	1	-	0/13/14/16	-
1	KPI	A	166	1	-	1/13/14/16	-
1	KPI	G	166	1	-	1/13/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	H	166	1	-	0/13/14/16	-
1	KPI	E	166	1	-	0/13/14/16	-
1	KPI	D	166	1	-	1/13/14/16	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	KPI	C1-CX1	-5.29	1.39	1.49
1	G	166	KPI	C1-CX1	-5.27	1.39	1.49
1	H	166	KPI	C1-CX1	-5.27	1.39	1.49
1	B	166	KPI	C1-CX1	-5.26	1.39	1.49
1	F	166	KPI	C1-CX1	-5.25	1.39	1.49

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	KPI	C1-CX1-CX2	-5.91	112.54	118.11
1	G	166	KPI	C1-CX1-CX2	-5.71	112.73	118.11
1	H	166	KPI	C1-CX1-CX2	-5.53	112.90	118.11
1	E	166	KPI	C1-CX1-CX2	-5.36	113.06	118.11
1	C	166	KPI	C1-CX1-CX2	-5.34	113.08	118.11

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	166	KPI	CG-CD-CE-NZ
1	F	166	KPI	C1-CX1-NZ-CE
1	F	166	KPI	CX2-CX1-NZ-CE
1	C	166	KPI	CG-CD-CE-NZ
1	A	166	KPI	CG-CD-CE-NZ

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	166	KPI	1	0
1	F	166	KPI	1	0
1	B	166	KPI	2	0
1	A	166	KPI	1	0
1	G	166	KPI	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	166	KPI	2	0
1	D	166	KPI	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 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	EDO	G	302	-	3,3,3	0.61	0	2,2,2	0.38	0
2	LYS	A	301	-	8,9,9	0.85	1 (12%)	7,10,10	1.08	1 (14%)
2	LYS	H	301	-	8,9,9	0.84	1 (12%)	7,10,10	1.10	1 (14%)
5	PG4	C	302	-	12,12,12	0.72	0	11,11,11	0.73	0
3	EDO	A	306	-	3,3,3	0.59	0	2,2,2	0.38	0
6	PGE	F	302	-	9,9,9	0.69	0	8,8,8	0.72	0
5	PG4	B	302	-	12,12,12	0.68	0	11,11,11	0.74	0
4	ACT	F	303	-	3,3,3	0.81	0	3,3,3	1.35	0
2	LYS	E	301	-	8,9,9	0.83	1 (12%)	7,10,10	1.08	1 (14%)
3	EDO	A	303	-	3,3,3	0.59	0	2,2,2	0.34	0
2	LYS	G	301	-	8,9,9	0.85	1 (12%)	7,10,10	1.13	1 (14%)
3	EDO	D	301	-	3,3,3	0.59	0	2,2,2	0.38	0
3	EDO	E	303	-	3,3,3	0.58	0	2,2,2	0.36	0
6	PGE	C	303	-	9,9,9	0.68	0	8,8,8	0.72	0
6	PGE	H	302	-	9,9,9	0.67	0	8,8,8	0.78	0
6	PGE	B	303	-	9,9,9	0.69	0	8,8,8	0.74	0
3	EDO	G	303	-	3,3,3	0.59	0	2,2,2	0.38	0
7	GOL	C	304	-	5,5,5	0.38	0	5,5,5	0.28	0
2	LYS	F	301	-	8,9,9	0.86	1 (12%)	7,10,10	1.06	1 (14%)
3	EDO	E	304	-	3,3,3	0.58	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	G	304	-	3,3,3	0.58	0	2,2,2	0.36	0
6	PGE	E	302	-	9,9,9	0.69	0	8,8,8	0.70	0
3	EDO	A	305	-	3,3,3	0.57	0	2,2,2	0.33	0
2	LYS	C	301	-	8,9,9	0.85	1 (12%)	7,10,10	1.07	1 (14%)
2	LYS	A	302	-	8,9,9	0.86	1 (12%)	7,10,10	1.13	1 (14%)
2	LYS	B	301	-	8,9,9	0.83	1 (12%)	7,10,10	1.06	1 (14%)
4	ACT	A	304	-	3,3,3	0.81	0	3,3,3	1.33	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	EDO	G	302	-	-	1/1/1/1	-
2	LYS	A	301	-	-	0/9/9/9	-
2	LYS	H	301	-	-	1/9/9/9	-
5	PG4	C	302	-	-	3/10/10/10	-
3	EDO	A	306	-	-	0/1/1/1	-
6	PGE	F	302	-	-	3/7/7/7	-
5	PG4	B	302	-	-	1/10/10/10	-
2	LYS	E	301	-	-	1/9/9/9	-
3	EDO	A	303	-	-	0/1/1/1	-
2	LYS	G	301	-	-	0/9/9/9	-
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	E	303	-	-	1/1/1/1	-
6	PGE	C	303	-	-	3/7/7/7	-
6	PGE	H	302	-	-	3/7/7/7	-
6	PGE	B	303	-	-	2/7/7/7	-
3	EDO	G	303	-	-	0/1/1/1	-
7	GOL	C	304	-	-	2/4/4/4	-
2	LYS	F	301	-	-	0/9/9/9	-
3	EDO	E	304	-	-	1/1/1/1	-
3	EDO	G	304	-	-	0/1/1/1	-
6	PGE	E	302	-	-	4/7/7/7	-
3	EDO	A	305	-	-	1/1/1/1	-
2	LYS	C	301	-	-	0/9/9/9	-
2	LYS	A	302	-	-	0/9/9/9	-
2	LYS	B	301	-	-	2/9/9/9	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	LYS	OXT-C	-2.29	1.23	1.30
2	F	301	LYS	OXT-C	-2.28	1.23	1.30
2	G	301	LYS	OXT-C	-2.28	1.23	1.30
2	A	301	LYS	OXT-C	-2.27	1.23	1.30
2	C	301	LYS	OXT-C	-2.26	1.23	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	LYS	OXT-C-O	-2.88	117.55	124.08
2	A	302	LYS	OXT-C-O	-2.86	117.59	124.08
2	H	301	LYS	OXT-C-O	-2.79	117.75	124.08
2	A	301	LYS	OXT-C-O	-2.73	117.88	124.08
2	E	301	LYS	OXT-C-O	-2.72	117.92	124.08

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	LYS	C-CA-CB-CG
7	C	304	GOL	O1-C1-C2-C3
6	H	302	PGE	O2-C3-C4-O3
5	C	302	PG4	O3-C5-C6-O4
6	C	303	PGE	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	LYS	2	0
5	C	302	PG4	1	0
6	F	302	PGE	1	0
4	F	303	ACT	1	0
6	H	302	PGE	1	0
7	C	304	GOL	1	0
2	F	301	LYS	2	0
3	A	305	EDO	1	0
2	C	301	LYS	1	0
2	A	302	LYS	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	295/306 (96%)	0.14	0 100 100	25, 40, 57, 73	1 (0%)
1	B	295/306 (96%)	0.34	5 (1%) 69 66	32, 45, 67, 88	1 (0%)
1	C	294/306 (96%)	0.25	0 100 100	32, 45, 67, 85	0
1	D	294/306 (96%)	0.47	3 (1%) 79 77	18, 51, 73, 84	1 (0%)
1	E	293/306 (95%)	0.29	0 100 100	33, 46, 64, 77	1 (0%)
1	F	295/306 (96%)	0.31	1 (0%) 90 88	34, 47, 64, 72	1 (0%)
1	G	295/306 (96%)	0.51	4 (1%) 73 71	37, 52, 71, 85	0
1	H	294/306 (96%)	0.63	6 (2%) 65 62	40, 57, 79, 92	1 (0%)
All	All	2355/2448 (96%)	0.37	19 (0%) 82 80	18, 48, 70, 92	6 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	298	PHE	3.5
1	B	95	PHE	3.1
1	H	15	THR	3.1
1	G	114	PRO	2.7
1	B	130	VAL	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KPI	A	166	14/15	0.87	0.12	26,37,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	KPI	G	166	14/15	0.87	0.12	45,55,70,72	0
1	KPI	H	166	14/15	0.87	0.15	35,45,78,89	0
1	KPI	F	166	14/15	0.88	0.12	29,42,55,55	0
1	KPI	D	166	14/15	0.89	0.15	32,46,63,67	0
1	KPI	B	166	14/15	0.91	0.10	30,38,57,57	0
1	KPI	E	166	14/15	0.92	0.15	29,44,74,82	0
1	KPI	C	166	14/15	0.93	0.11	26,44,61,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(\AA^2)	Q<0.9
4	ACT	A	304	4/4	0.51	0.23	71,72,73,75	0
3	EDO	A	305	4/4	0.71	0.18	57,64,66,67	0
6	PGE	B	303	10/10	0.76	0.17	60,78,83,84	0
6	PGE	E	302	10/10	0.76	0.15	70,72,72,72	0
6	PGE	C	303	10/10	0.78	0.15	60,65,74,74	0
3	EDO	E	303	4/4	0.79	0.18	64,68,72,74	0
4	ACT	F	303	4/4	0.80	0.18	56,57,62,64	0
3	EDO	G	304	4/4	0.80	0.12	60,61,62,63	0
7	GOL	C	304	6/6	0.80	0.13	58,66,66,70	0
3	EDO	G	302	4/4	0.82	0.15	46,48,55,57	0
3	EDO	D	301	4/4	0.83	0.14	57,61,68,73	0
2	LYS	A	301	10/10	0.83	0.14	35,47,59,61	0
2	LYS	H	301	10/10	0.84	0.12	48,55,69,69	0
2	LYS	B	301	10/10	0.84	0.13	49,59,73,83	0
6	PGE	H	302	10/10	0.84	0.12	53,72,80,80	0
2	LYS	C	301	10/10	0.84	0.14	51,60,67,75	0
2	LYS	A	302	10/10	0.86	0.12	38,56,59,61	0
3	EDO	G	303	4/4	0.86	0.11	58,59,60,62	0
5	PG4	B	302	13/13	0.86	0.12	53,60,68,71	0
2	LYS	G	301	10/10	0.86	0.12	40,49,75,81	0
3	EDO	A	303	4/4	0.88	0.11	47,49,53,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LYS	E	301	10/10	0.88	0.10	41,47,64,68	0
3	EDO	A	306	4/4	0.88	0.12	57,60,61,62	0
2	LYS	F	301	10/10	0.88	0.10	36,48,55,59	0
3	EDO	E	304	4/4	0.89	0.12	54,57,59,59	0
6	PGE	F	302	10/10	0.89	0.11	60,64,74,74	0
5	PG4	C	302	13/13	0.90	0.10	44,60,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.