



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 12:14 PM EDT

PDB ID : 7KG9
Title : Dihydropicolinate synthase (DHDPS) from *C.jejuni*, H56W mutant with pyruvate bound in the active site and L-lysine bound at the allosteric site
Authors : Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.
Deposited on : 2020-10-16
Resolution : 2.06 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	:	2.23.2
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)	:	2.23.2

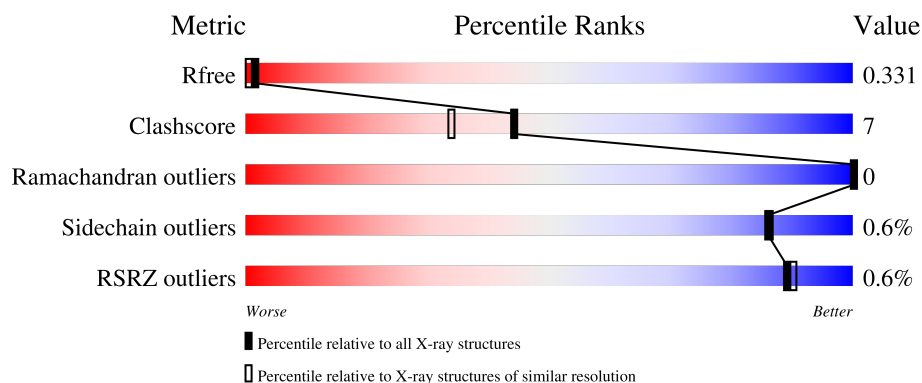
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


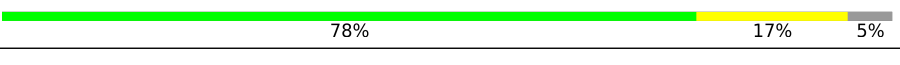
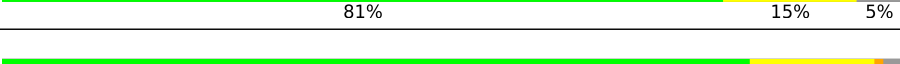
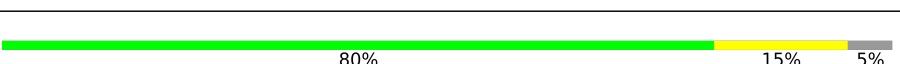

The reported resolution of this entry is 2.06 Å.

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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	310	 2% 80% 15% 5%
1	B	310	 78% 17% 5%
1	C	310	 81% 15% 5%
1	D	310	 84% 14% 2%
1	E	310	 80% 15% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	<div><div><div>%</div><div><div></div><div>82%</div><div>13%</div><div></div></div><div></div></div></div>

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	F	303	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14779 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 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	1	0	0
			2274	1449	376	436	13			
1	B	296	Total	C	N	O	S	0	0	0
			2283	1455	378	437	13			
1	C	296	Total	C	N	O	S	0	0	0
			2283	1455	378	437	13			
1	D	304	Total	C	N	O	S	1	0	0
			2349	1493	394	448	14			
1	E	296	Total	C	N	O	S	0	0	0
			2283	1455	378	437	13			
1	F	297	Total	C	N	O	S	0	0	0
			2290	1459	379	439	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
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	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	56	TRP	HIS	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

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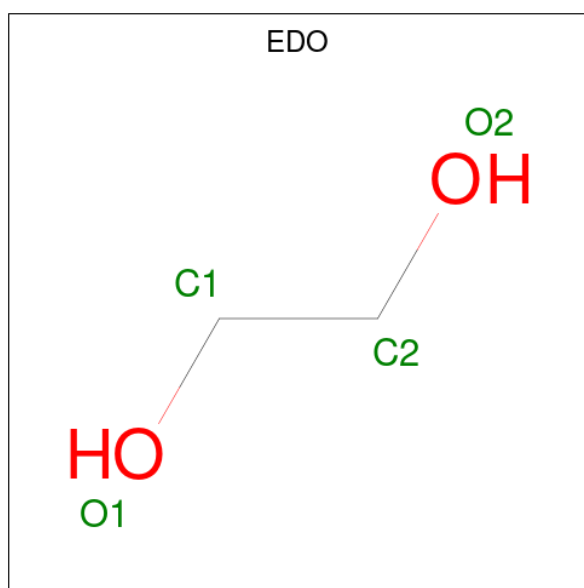
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	56	TRP	HIS	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	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	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	56	TRP	HIS	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	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	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	56	TRP	HIS	engineered mutation	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	56	TRP	HIS	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	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	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	56	TRP	HIS	engineered mutation	UNP Q9PPB4

- 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	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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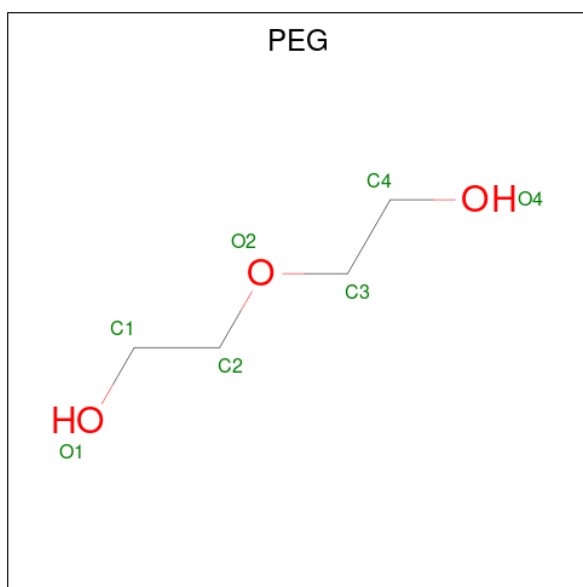
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



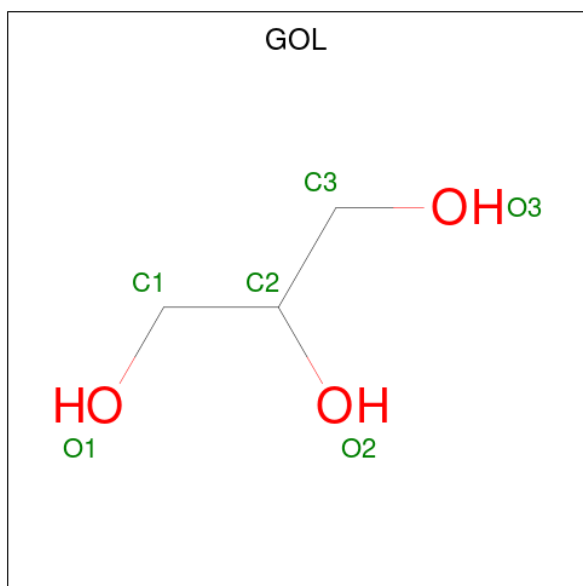
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

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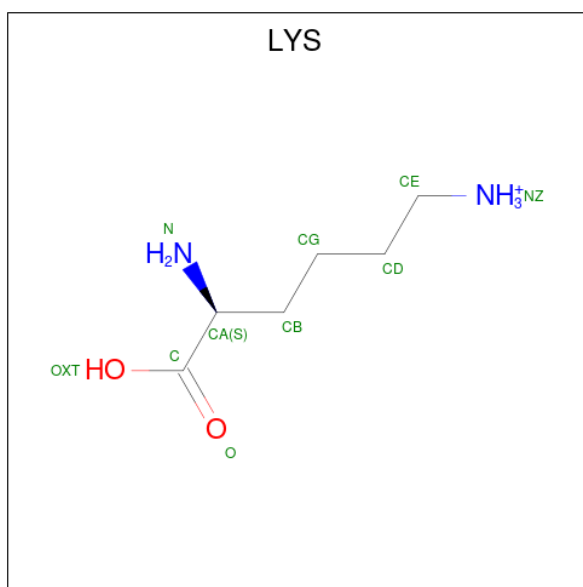
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



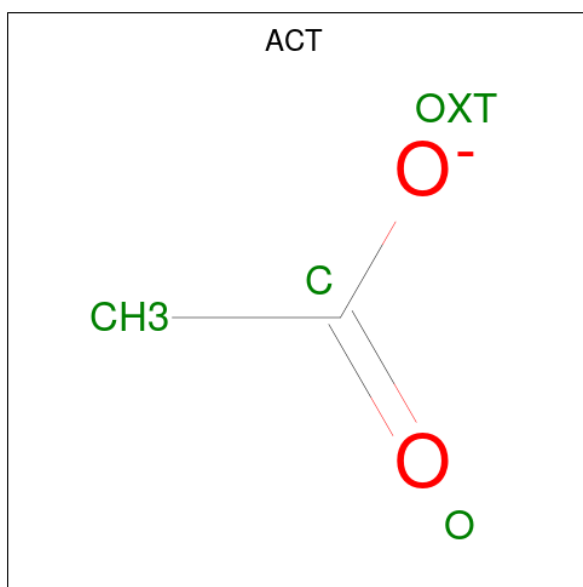
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

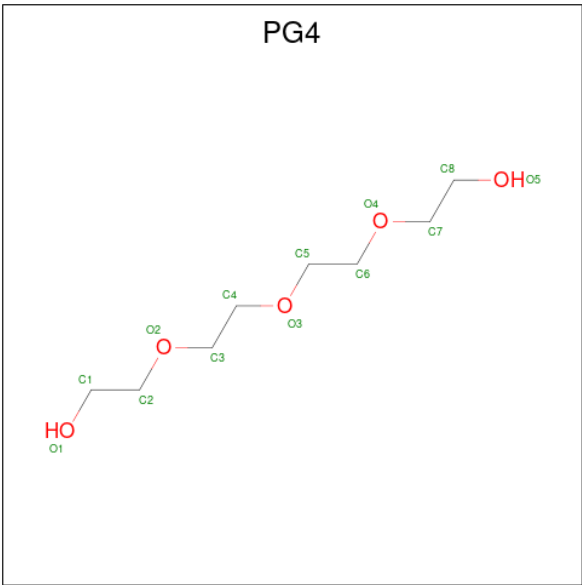


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Mg	0	0
			2	2		
8	C	1	Total	Mg	0	0
			1	1		
8	D	2	Total	Mg	0	0
			2	2		
8	F	2	Total	Mg	0	0
			2	2		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

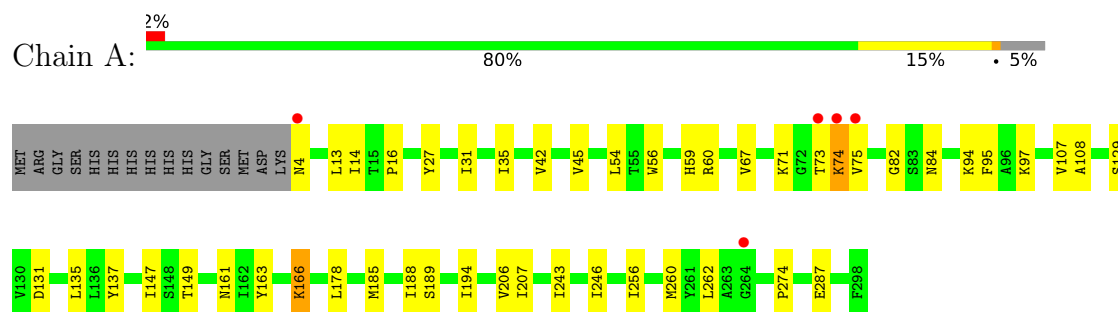
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	132	Total	O	0	0
			132	132		
10	B	112	Total	O	0	0
			112	112		
10	C	121	Total	O	0	0
			121	121		
10	D	142	Total	O	0	0
			142	142		
10	E	138	Total	O	0	0
			138	138		
10	F	119	Total	O	0	0
			119	119		

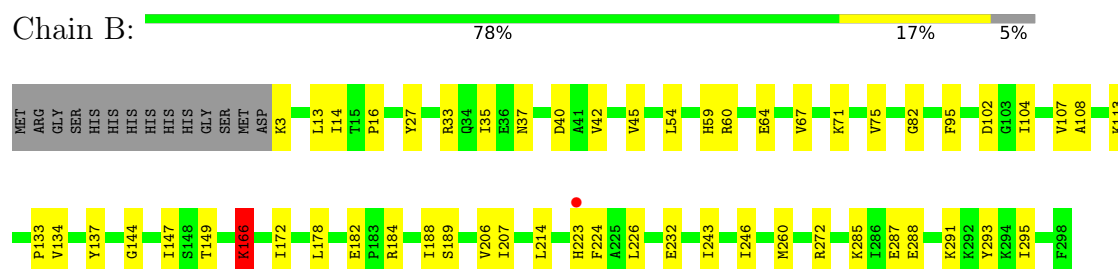
3 Residue-property plots [i](#)

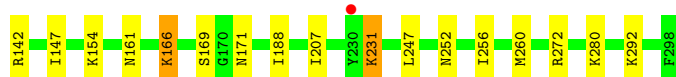
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-hydroxy-tetrahydronicotinate synthase

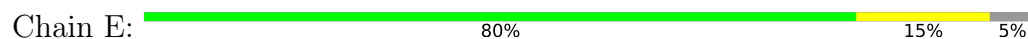


- Molecule 1: 4-hydroxy-tetrahydronicotinate synthase

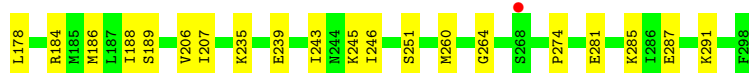
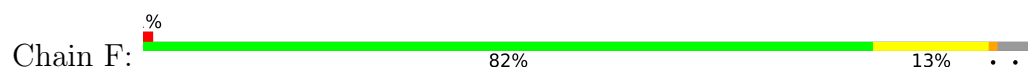




- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.83Å 225.17Å 200.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.06 49.10 – 2.06	Depositor EDS
% Data completeness (in resolution range)	92.0 (49.04-2.06) 92.0 (49.10-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.07Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.275 , 0.331 0.275 , 0.331	Depositor DCC
R_{free} test set	5453 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14779	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PGE, PG4, GOL, ACT, KPI, PEG, MG

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	0.26	0/2299	0.50	3/3110 (0.1%)
1	B	0.25	0/2308	0.47	0/3121
1	C	0.24	0/2308	0.44	0/3121
1	D	0.24	0/2378	0.44	0/3215
1	E	0.25	0/2308	0.44	0/3121
1	F	0.25	0/2315	0.44	0/3130
All	All	0.25	0/13916	0.46	3/18818 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LYS	CB-CG-CD	-8.20	90.28	111.60
1	A	74	LYS	CD-CE-NZ	-6.91	95.81	111.70
1	A	74	LYS	CG-CD-CE	5.35	127.95	111.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	KPI	Mainchain
1	C	166	KPI	Mainchain
1	D	166	KPI	Mainchain

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	2274	0	2308	34	0
1	B	2283	0	2321	39	0
1	C	2283	0	2321	30	0
1	D	2349	0	2373	29	0
1	E	2283	0	2321	29	0
1	F	2290	0	2325	29	0
2	A	12	0	18	0	0
2	B	16	0	24	0	0
2	C	16	0	24	3	0
2	D	12	0	18	3	0
2	F	12	0	18	0	0
3	A	10	0	14	0	0
3	F	20	0	28	4	0
4	A	7	0	10	2	0
4	B	7	0	10	0	0
4	C	7	0	10	0	0
4	D	7	0	10	0	0
4	F	14	0	20	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	10	0	12	0	0
6	B	10	0	12	1	0
6	C	10	0	12	1	0
6	D	10	0	12	2	0
6	E	10	0	12	1	0
6	F	10	0	12	0	0
7	A	4	0	3	0	0
7	B	4	0	3	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
8	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	2	0	0	0	0
9	B	13	0	18	0	0
9	D	13	0	18	2	0
10	A	132	0	0	3	0
10	B	112	0	0	2	0
10	C	121	0	0	1	0
10	D	142	0	0	2	0
10	E	138	0	0	2	0
10	F	119	0	0	3	0
All	All	14779	0	14303	186	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 7.

The worst 5 of 186 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:74:LYS:HD2	1:A:74:LYS:N	1.82	0.95
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.68	0.75
1:A:35:ILE:HG12	1:A:75:VAL:HG21	1.65	0.75
1:D:169:SER:H	2:D:301:EDO:H12	1.51	0.74
1:B:287:GLU:O	1:B:291:LYS:NZ	2.20	0.74

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	292/310 (94%)	285 (98%)	7 (2%)	0	100	100
1	B	293/310 (94%)	287 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	D	301/310 (97%)	294 (98%)	7 (2%)	0	100	100
1	E	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	F	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
All	All	1766/1860 (95%)	1728 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	247/260 (95%)	246 (100%)	1 (0%)	91	91
1	B	248/260 (95%)	247 (100%)	1 (0%)	91	91
1	C	248/260 (95%)	248 (100%)	0	100	100
1	D	255/260 (98%)	252 (99%)	3 (1%)	71	69
1	E	248/260 (95%)	246 (99%)	2 (1%)	81	81
1	F	249/260 (96%)	248 (100%)	1 (0%)	91	91
All	All	1495/1560 (96%)	1487 (100%)	8 (0%)	86	89

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	138	ASN
1	E	74	LYS
1	D	292	LYS
1	D	231	LYS
1	E	36	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	223	HIS
1	C	25	GLN
1	E	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	A	166	1	10,13,14	0.61	0	6,15,17	3.06	2 (33%)
1	KPI	D	166	1	10,13,14	1.41	1 (10%)	6,15,17	3.11	3 (50%)
1	KPI	E	166	1	10,13,14	0.64	0	6,15,17	3.26	3 (50%)
1	KPI	C	166	1	10,13,14	1.41	1 (10%)	6,15,17	3.13	2 (33%)
1	KPI	B	166	1	10,13,14	1.42	1 (10%)	6,15,17	3.01	2 (33%)
1	KPI	F	166	1	10,13,14	0.65	0	6,15,17	3.42	3 (50%)

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	A	166	1	-	2/9/14/16	-
1	KPI	D	166	1	-	4/9/14/16	-
1	KPI	E	166	1	-	2/9/14/16	-
1	KPI	C	166	1	-	4/9/14/16	-
1	KPI	B	166	1	-	2/9/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	F	166	1	-	0/9/14/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	KPI	O-C	4.17	1.36	1.19
1	D	166	KPI	O-C	4.14	1.36	1.19
1	C	166	KPI	O-C	4.11	1.36	1.19

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	KPI	C1-CX1-CX2	-6.97	110.20	117.92
1	E	166	KPI	C1-CX1-CX2	-6.62	110.58	117.92
1	C	166	KPI	C1-CX1-CX2	-6.44	110.79	117.92
1	A	166	KPI	C1-CX1-CX2	-6.37	110.87	117.92
1	D	166	KPI	C1-CX1-CX2	-6.32	110.92	117.92

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	KPI	C1-CX1-NZ-CE
1	B	166	KPI	C-CA-CB-CG
1	B	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	C-CA-CB-CG
1	C	166	KPI	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 7 are monoatomic - leaving 38 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	C	306	-	6,6,6	0.49	0	5,5,5	0.30	0
2	EDO	F	302	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	D	302	-	3,3,3	0.43	0	2,2,2	0.32	0
4	PEG	F	309	-	6,6,6	0.49	0	5,5,5	0.30	0
2	EDO	D	303	-	3,3,3	0.44	0	2,2,2	0.36	0
6	LYS	C	307	-	5,9,9	0.27	0	4,10,10	0.43	0
4	PEG	D	306	-	6,6,6	0.49	0	5,5,5	0.24	0
2	EDO	C	302	-	3,3,3	0.44	0	2,2,2	0.35	0
5	GOL	B	308	-	5,5,5	0.35	0	5,5,5	0.36	0
9	PG4	D	307	-	12,12,12	0.52	0	11,11,11	0.21	0
3	PGE	F	304	-	9,9,9	0.33	0	8,8,8	0.22	0
2	EDO	B	304	-	3,3,3	0.45	0	2,2,2	0.34	0
4	PEG	B	307	-	6,6,6	0.49	0	5,5,5	0.24	0
4	PEG	A	305	-	6,6,6	0.50	0	5,5,5	0.27	0
3	PGE	A	304	-	9,9,9	0.30	0	8,8,8	0.33	0
6	LYS	F	310	-	5,9,9	0.30	0	4,10,10	0.42	0
2	EDO	C	304	-	3,3,3	0.43	0	2,2,2	0.46	0
9	PG4	B	309	-	12,12,12	0.53	0	11,11,11	0.21	0
2	EDO	B	301	-	3,3,3	0.48	0	2,2,2	0.29	0
2	EDO	A	301	-	3,3,3	0.43	0	2,2,2	0.39	0
6	LYS	A	307	-	5,9,9	0.28	0	4,10,10	0.50	0
3	PGE	F	305	-	9,9,9	0.32	0	8,8,8	0.31	0
6	LYS	B	310	-	5,9,9	0.25	0	4,10,10	0.62	0
2	EDO	F	301	-	3,3,3	0.46	0	2,2,2	0.26	0
2	EDO	D	301	-	3,3,3	0.46	0	2,2,2	0.28	0
6	LYS	D	308	-	5,9,9	0.26	0	4,10,10	0.43	0
6	LYS	E	301	-	5,9,9	0.26	0	4,10,10	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	301	-	3,3,3	0.46	0	2,2,2	0.36	0
5	GOL	A	306	-	5,5,5	0.37	0	5,5,5	0.29	0
7	ACT	A	308	-	1,3,3	1.31	0	0,3,3	-	-
2	EDO	A	302	-	3,3,3	0.45	0	2,2,2	0.33	0
2	EDO	B	303	-	3,3,3	0.46	0	2,2,2	0.35	0
4	PEG	F	308	-	6,6,6	0.48	0	5,5,5	0.18	0
2	EDO	B	302	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	F	303	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	C	303	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.35	0
7	ACT	B	311	-	1,3,3	1.44	0	0,3,3	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	C	306	-	-	1/4/4/4	-
2	EDO	F	302	-	-	0/1/1/1	-
2	EDO	D	302	-	-	0/1/1/1	-
4	PEG	F	309	-	-	2/4/4/4	-
2	EDO	D	303	-	-	0/1/1/1	-
6	LYS	C	307	-	-	1/5/9/9	-
4	PEG	D	306	-	-	1/4/4/4	-
2	EDO	C	302	-	-	0/1/1/1	-
5	GOL	B	308	-	-	2/4/4/4	-
9	PG4	D	307	-	-	7/10/10/10	-
3	PGE	F	304	-	-	3/7/7/7	-
2	EDO	B	304	-	-	0/1/1/1	-
4	PEG	B	307	-	-	1/4/4/4	-
4	PEG	A	305	-	-	2/4/4/4	-
3	PGE	A	304	-	-	3/7/7/7	-
6	LYS	F	310	-	-	0/5/9/9	-
2	EDO	C	304	-	-	0/1/1/1	-
9	PG4	B	309	-	-	7/10/10/10	-
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
6	LYS	A	307	-	-	0/5/9/9	-
3	PGE	F	305	-	-	4/7/7/7	-
6	LYS	B	310	-	-	1/5/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	F	301	-	-	0/1/1/1	-
2	EDO	D	301	-	-	0/1/1/1	-
6	LYS	D	308	-	-	1/5/9/9	-
6	LYS	E	301	-	-	0/5/9/9	-
2	EDO	C	301	-	-	0/1/1/1	-
5	GOL	A	306	-	-	2/4/4/4	-
2	EDO	A	302	-	-	0/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
4	PEG	F	308	-	-	2/4/4/4	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	F	303	-	-	0/1/1/1	-
2	EDO	C	303	-	-	0/1/1/1	-
2	EDO	A	303	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	306	GOL	O1-C1-C2-C3
4	F	309	PEG	O1-C1-C2-O2
9	D	307	PG4	O3-C5-C6-O4
3	F	305	PGE	O2-C3-C4-O3
9	B	309	PG4	O3-C5-C6-O4

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	303	EDO	1	0
6	C	307	LYS	1	0
2	C	302	EDO	3	0
9	D	307	PG4	2	0
3	F	304	PGE	3	0
4	A	305	PEG	2	0
3	F	305	PGE	1	0
6	B	310	LYS	1	0
2	D	301	EDO	2	0
6	D	308	LYS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	301	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	294/310 (94%)	0.22	5 (1%) 70 71	17, 22, 30, 37	0
1	B	295/310 (95%)	0.19	1 (0%) 94 94	17, 23, 33, 41	0
1	C	295/310 (95%)	0.23	0 100 100	16, 23, 32, 39	0
1	D	303/310 (97%)	0.19	1 (0%) 94 94	18, 23, 32, 38	0
1	E	295/310 (95%)	0.29	1 (0%) 94 94	17, 23, 32, 44	0
1	F	296/310 (95%)	0.21	2 (0%) 87 88	17, 22, 32, 37	0
All	All	1778/1860 (95%)	0.22	10 (0%) 89 90	16, 23, 32, 44	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	VAL	3.7
1	A	74	LYS	3.5
1	A	4	ASN	3.3
1	F	56	TRP	2.9
1	E	267	GLU	2.5

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	F	166	14/15	0.75	0.19	19,23,29,29	14
1	KPI	C	166	14/15	0.85	0.20	17,21,25,25	3
1	KPI	B	166	14/15	0.86	0.16	15,21,27,28	0
1	KPI	E	166	14/15	0.88	0.16	17,20,25,26	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	KPI	A	166	14/15	0.88	0.19	16,22,25,26	2
1	KPI	D	166	14/15	0.89	0.18	19,22,25,28	2

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(\AA^2)	Q<0.9
7	ACT	B	311	4/4	0.43	0.40	42,42,44,46	0
4	PEG	F	308	7/7	0.71	0.27	30,31,41,42	0
2	EDO	A	301	4/4	0.73	0.28	25,26,31,32	0
4	PEG	D	306	7/7	0.76	0.22	28,30,39,40	0
3	PGE	F	304	10/10	0.79	0.26	26,32,36,40	0
2	EDO	F	303	4/4	0.79	0.43	40,40,41,49	0
2	EDO	C	303	4/4	0.80	0.23	22,26,28,28	0
4	PEG	A	305	7/7	0.81	0.26	30,33,38,46	0
2	EDO	D	301	4/4	0.81	0.19	20,20,22,23	0
9	PG4	B	309	13/13	0.81	0.14	21,27,34,35	0
8	MG	B	306	1/1	0.82	0.08	26,26,26,26	0
7	ACT	A	308	4/4	0.82	0.16	29,29,29,31	0
8	MG	F	306	1/1	0.83	0.15	31,31,31,31	0
2	EDO	C	304	4/4	0.83	0.27	26,27,28,28	0
4	PEG	F	309	7/7	0.84	0.14	17,23,25,28	0
2	EDO	B	304	4/4	0.84	0.25	24,29,30,34	0
2	EDO	C	301	4/4	0.85	0.14	26,31,31,33	0
2	EDO	D	303	4/4	0.85	0.28	25,27,27,30	0
6	LYS	B	310	10/10	0.85	0.14	20,26,29,29	0
2	EDO	C	302	4/4	0.85	0.37	29,33,33,33	0
6	LYS	C	307	10/10	0.87	0.16	19,24,25,26	0
8	MG	C	305	1/1	0.87	0.10	32,32,32,32	0
8	MG	D	305	1/1	0.87	0.09	39,39,39,39	0
5	GOL	A	306	6/6	0.87	0.17	28,30,37,40	0
2	EDO	A	302	4/4	0.87	0.15	28,32,34,38	0
5	GOL	B	308	6/6	0.88	0.14	21,24,28,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PGE	F	305	10/10	0.88	0.14	20,23,26,27	0
3	PGE	A	304	10/10	0.89	0.14	19,27,31,32	0
6	LYS	E	301	10/10	0.89	0.14	18,22,25,25	0
2	EDO	B	301	4/4	0.89	0.24	23,27,28,34	0
6	LYS	A	307	10/10	0.90	0.17	21,24,25,27	0
9	PG4	D	307	13/13	0.90	0.18	21,27,36,36	0
6	LYS	D	308	10/10	0.91	0.12	19,22,24,25	0
2	EDO	D	302	4/4	0.91	0.16	24,25,26,27	0
2	EDO	B	302	4/4	0.92	0.23	26,26,27,27	0
6	LYS	F	310	10/10	0.92	0.15	18,22,26,26	0
2	EDO	B	303	4/4	0.92	0.12	29,30,31,32	0
8	MG	F	307	1/1	0.92	0.10	29,29,29,29	0
4	PEG	C	306	7/7	0.92	0.09	24,25,27,32	0
2	EDO	F	301	4/4	0.92	0.13	19,23,26,27	0
2	EDO	F	302	4/4	0.94	0.10	20,20,21,22	0
8	MG	B	305	1/1	0.95	0.09	20,20,20,20	0
2	EDO	A	303	4/4	0.95	0.12	29,32,35,37	0
4	PEG	B	307	7/7	0.96	0.08	20,22,25,25	0
8	MG	D	304	1/1	0.97	0.11	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.