



## Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2021 – 02:10 PM EST

PDB ID : 7KZ2  
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, Y110F mutant with pyruvate bound in the active site and L-lysine bound at the allosteric site in C2221 space group  
Authors : Saran, S.; Sanders, D.A.R.  
Deposited on : 2020-12-09  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.24  
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) : 2.24

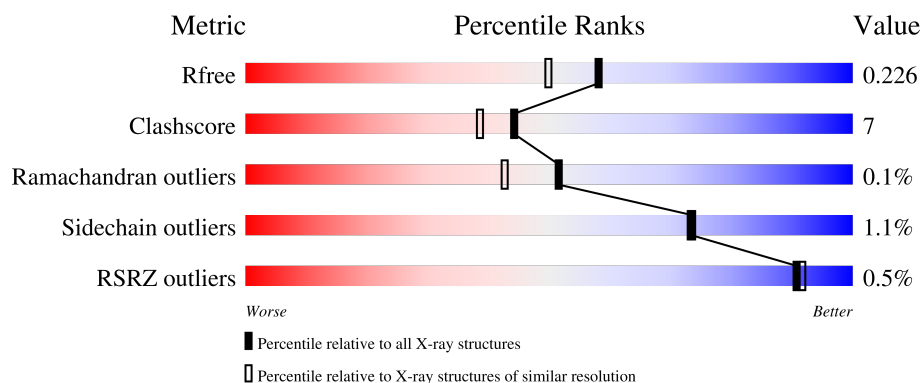
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	310	<div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	C	310	<div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	D	310	<div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	E	310	<div> <div>%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	310	<div> <div></div> <div>%</div> <div>89%</div> <div>6% • 5%</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
3	PEG	A	302	-	-	X	X
3	PEG	A	303	-	-	-	X
3	PEG	A	304	-	-	X	X
3	PEG	A	305	-	-	X	-
3	PEG	A	307	-	-	X	-
3	PEG	E	303	-	-	X	-
3	PEG	F	302	-	-	X	X
3	PEG	F	303	-	-	-	X
4	EDO	A	311	-	-	-	X
4	EDO	A	312	-	-	X	-
4	EDO	B	305	-	-	X	X
4	EDO	C	305	-	-	X	-
4	EDO	D	302	-	-	X	X
5	ACT	A	313	-	-	X	-
5	ACT	A	314	-	-	-	X
5	ACT	B	309	-	-	X	X
5	ACT	F	305	-	-	-	X
6	PGE	C	310	-	-	X	-
6	PGE	E	305	-	-	X	-
6	PGE	F	306	-	-	X	-
6	PGE	F	307	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15048 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	296	Total	C	N	O	S	0	0	0
			2273	1446	378	436	13			
1	B	296	Total	C	N	O	S	0	0	0
			2273	1446	378	436	13			
1	C	296	Total	C	N	O	S	0	0	0
			2271	1445	377	436	13			
1	D	296	Total	C	N	O	S	0	0	0
			2272	1446	377	436	13			
1	E	296	Total	C	N	O	S	0	0	0
			2277	1449	379	436	13			
1	F	296	Total	C	N	O	S	0	0	0
			2275	1448	378	436	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	110	PHE	TYR	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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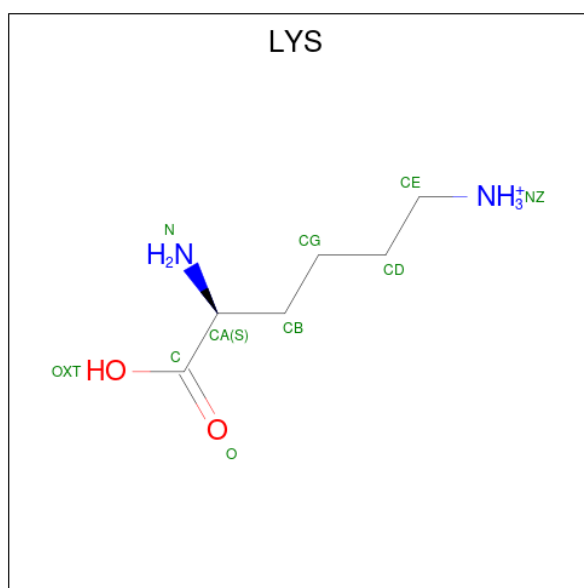
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	110	PHE	TYR	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	110	PHE	TYR	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	110	PHE	TYR	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	110	PHE	TYR	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	110	PHE	TYR	engineered mutation	UNP Q9PPB4

- Molecule 2 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



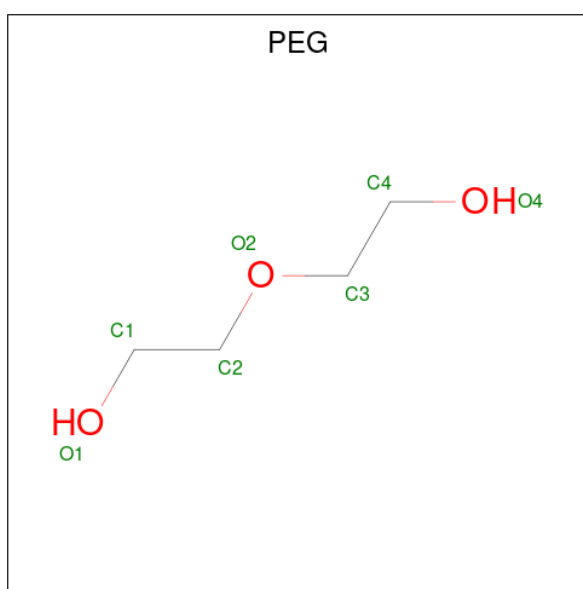
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



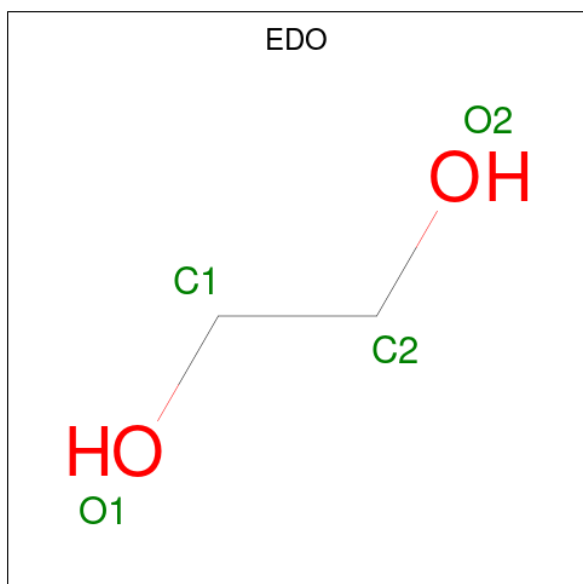
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

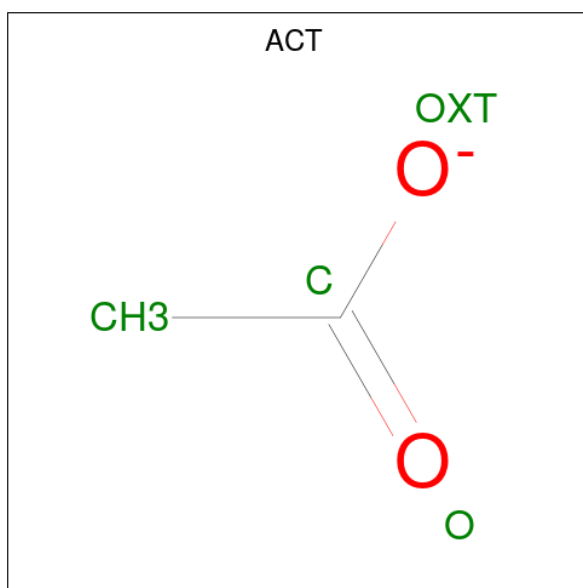
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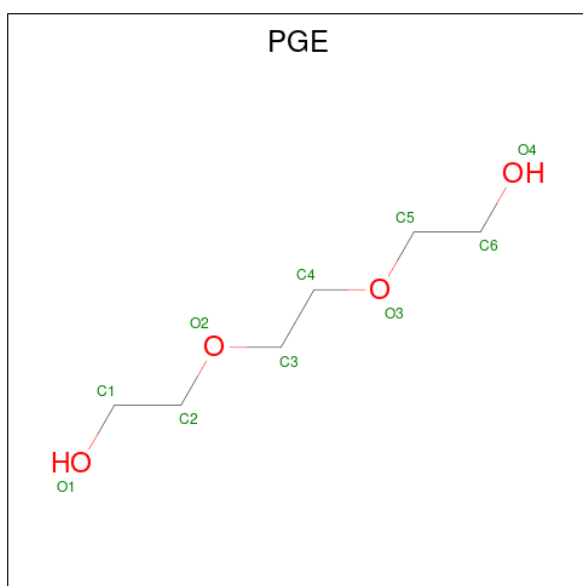
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	Mg 2	0	0
7	C	1	Total 1	Mg 1	0	0

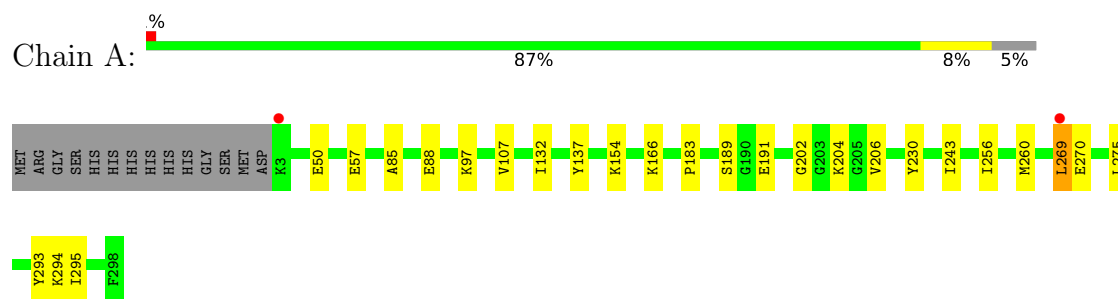
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	190	Total 190	O 190	0	0
8	B	198	Total 198	O 198	0	0
8	C	176	Total 176	O 176	0	0
8	D	193	Total 193	O 193	0	0
8	E	164	Total 164	O 164	0	0
8	F	178	Total 178	O 178	0	0

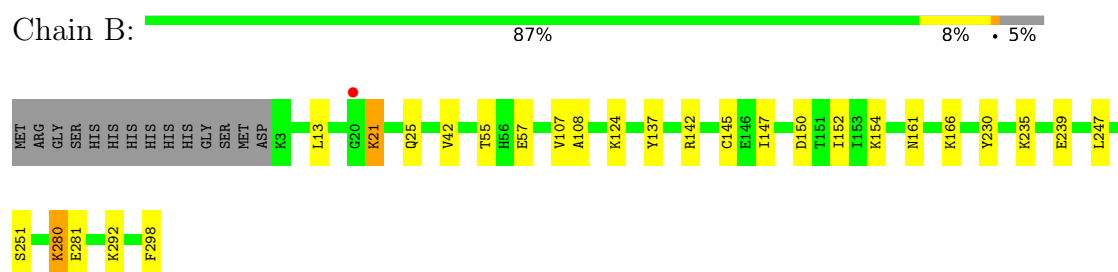
### 3 Residue-property plots [i](#)

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.

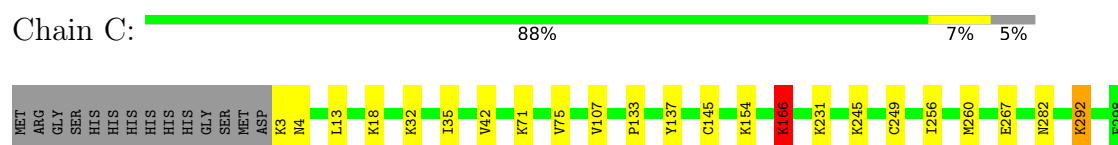
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



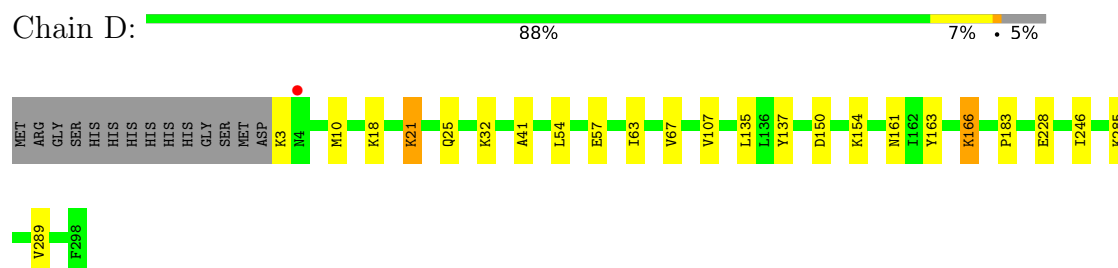
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



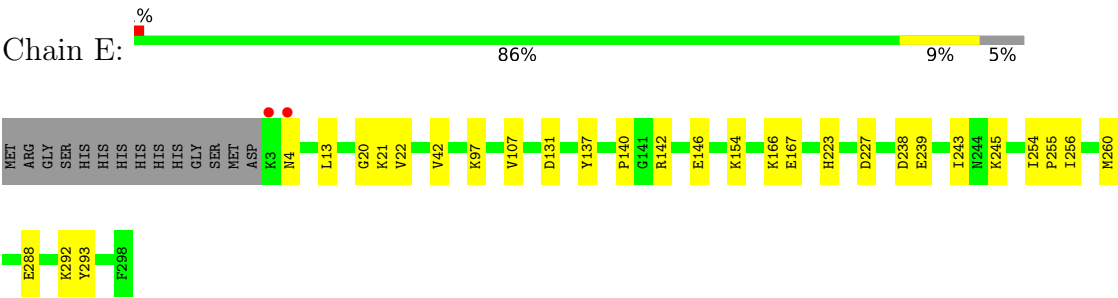
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



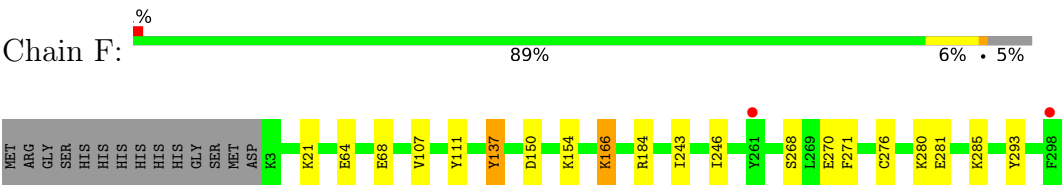
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



● 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, $\alpha$ , $\beta$ , $\gamma$	85.58Å 231.80Å 200.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 1.90 46.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.03-1.90) 88.0 (46.03-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.56 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.186 , 0.218 0.197 , 0.226	Depositor DCC
$R_{free}$ test set	7812 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGE, EDO, ACT, MG, PEG, KPI

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	0/2295	0.62	0/3103
1	B	0.50	0/2295	0.55	0/3103
1	C	0.42	0/2293	0.53	0/3101
1	D	0.48	0/2294	0.54	0/3102
1	E	0.47	1/2299 (0.0%)	0.57	0/3107
1	F	0.49	0/2297	0.58	0/3105
All	All	0.48	1/13773 (0.0%)	0.57	0/18621

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	167	GLU	CD-OE2	-5.38	1.19	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	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	2273	0	2305	40	0
1	B	2273	0	2306	28	0
1	C	2271	0	2298	34	0
1	D	2272	0	2301	19	0
1	E	2277	0	2316	25	0
1	F	2275	0	2310	20	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
2	C	10	0	12	0	0
2	D	10	0	12	1	0
2	E	10	0	12	0	0
2	F	10	0	12	0	0
3	A	42	0	60	23	0
3	B	7	0	10	1	0
3	C	14	0	20	0	0
3	E	14	0	20	6	0
3	F	14	0	20	8	0
4	A	20	0	30	7	0
4	B	16	0	24	10	0
4	C	20	0	30	12	0
4	D	4	0	6	4	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
5	A	8	0	6	3	0
5	B	4	0	3	3	0
5	F	4	0	3	0	0
6	A	10	0	14	5	0
6	B	10	0	14	3	0
6	C	10	0	14	11	0
6	D	10	0	14	2	0
6	E	10	0	14	8	0
6	F	20	0	28	8	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	A	190	0	0	4	0
8	B	198	0	0	4	0
8	C	176	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	193	0	0	5	0
8	E	164	0	0	5	0
8	F	178	0	0	4	0
All	All	15048	0	14250	185	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.

All (185) 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)
4:A:311:EDO:H22	8:A:512:HOH:O	1.33	1.24
1:A:294:LYS:HZ2	3:A:304:PEG:H31	1.05	1.16
1:B:55:THR:OG1	4:B:305:EDO:H22	1.47	1.14
1:A:154:LYS:HZ2	6:A:315:PGE:H62	0.98	1.11
1:F:154:LYS:HE3	6:F:306:PGE:H2	1.30	1.10
1:A:294:LYS:NZ	3:A:304:PEG:H31	1.67	1.09
1:B:57:GLU:HB2	4:B:305:EDO:H21	1.34	1.08
1:A:191:GLU:OE2	5:A:313:ACT:H3	1.53	1.08
3:F:302:PEG:H12	3:F:302:PEG:H41	1.40	1.01
1:E:154:LYS:NZ	6:E:305:PGE:H6	1.77	1.00
1:F:154:LYS:CE	6:F:306:PGE:H2	1.94	0.98
4:C:307:EDO:H21	8:C:555:HOH:O	1.64	0.96
1:B:57:GLU:HB2	4:B:305:EDO:C2	1.96	0.95
1:C:154:LYS:HD3	6:C:310:PGE:H62	1.49	0.92
1:A:154:LYS:NZ	6:A:315:PGE:H62	1.87	0.88
1:A:204:LYS:NZ	3:A:307:PEG:H21	1.90	0.87
1:D:183:PRO:O	4:D:302:EDO:H12	1.74	0.87
1:A:295:ILE:HD12	3:A:305:PEG:H22	1.57	0.86
1:F:150:ASP:HB3	6:F:306:PGE:H22	1.58	0.86
1:C:71:LYS:NZ	4:C:305:EDO:C2	2.39	0.85
1:C:154:LYS:CD	6:C:310:PGE:H62	2.07	0.84
1:C:71:LYS:HZ3	4:C:305:EDO:C2	1.92	0.83
1:A:204:LYS:NZ	3:A:307:PEG:C2	2.42	0.83
1:A:294:LYS:HE3	3:A:302:PEG:O4	1.80	0.82
1:F:276:CYS:HA	3:F:302:PEG:H11	1.62	0.81
1:E:154:LYS:HZ2	6:E:305:PGE:H6	1.45	0.81
1:A:294:LYS:HZ1	3:A:302:PEG:H12	1.48	0.79
4:A:312:EDO:H21	8:A:556:HOH:O	1.84	0.78
1:C:75:VAL:O	4:C:308:EDO:C1	2.32	0.78
1:B:298:PHE:O	4:B:306:EDO:H11	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LYS:NZ	4:C:305:EDO:H22	1.99	0.77
1:E:154:LYS:HZ3	6:E:305:PGE:H6	1.46	0.76
1:A:294:LYS:HG2	3:A:304:PEG:H32	1.67	0.76
1:A:191:GLU:CD	5:A:313:ACT:H3	2.04	0.76
3:A:305:PEG:C2	8:A:456:HOH:O	2.33	0.76
1:A:294:LYS:HD3	3:A:304:PEG:H12	1.67	0.76
3:A:305:PEG:H21	8:A:456:HOH:O	1.84	0.75
1:B:280:LYS:HB2	1:B:280:LYS:NZ	2.02	0.75
1:C:75:VAL:O	4:C:308:EDO:H11	1.87	0.75
1:A:294:LYS:NZ	3:A:302:PEG:H12	2.02	0.74
1:F:271:PHE:H	3:F:302:PEG:H22	1.53	0.73
8:E:429:HOH:O	3:F:302:PEG:H12	1.88	0.73
1:B:124:LYS:NZ	8:B:401:HOH:O	2.23	0.71
1:A:204:LYS:HZ1	3:A:307:PEG:H21	1.55	0.70
1:E:154:LYS:HZ2	6:E:305:PGE:C6	2.05	0.70
1:D:3:LYS:N	8:D:404:HOH:O	2.24	0.70
1:A:154:LYS:HZ2	6:A:315:PGE:C6	1.91	0.69
1:E:154:LYS:NZ	6:E:305:PGE:C6	2.54	0.69
1:B:57:GLU:HG2	4:B:305:EDO:O1	1.93	0.69
1:B:280:LYS:HB2	1:B:280:LYS:HZ2	1.56	0.69
1:C:154:LYS:CD	6:C:310:PGE:C6	2.71	0.69
1:A:204:LYS:HZ3	3:A:307:PEG:H21	1.58	0.69
1:D:150:ASP:HB3	6:D:303:PGE:H62	1.75	0.68
1:B:55:THR:OG1	4:B:305:EDO:C2	2.36	0.68
1:A:132:ILE:HG22	4:A:309:EDO:H12	1.76	0.67
1:E:154:LYS:CE	6:E:305:PGE:O1	2.41	0.67
1:B:150:ASP:HB3	6:B:310:PGE:H2	1.75	0.67
1:A:204:LYS:HZ1	3:A:307:PEG:C2	2.06	0.67
1:E:154:LYS:HE3	6:E:305:PGE:O1	1.95	0.67
1:F:154:LYS:NZ	6:F:306:PGE:H6	2.11	0.66
3:A:303:PEG:H12	3:A:303:PEG:H41	1.76	0.66
1:B:235:LYS:O	1:B:239:GLU:HG3	1.95	0.66
6:C:310:PGE:H52	6:C:310:PGE:O2	1.96	0.65
4:C:307:EDO:C2	8:C:555:HOH:O	2.30	0.65
1:D:154:LYS:NZ	6:D:303:PGE:H6	2.12	0.64
1:C:18:LYS:HE3	1:C:267:GLU:OE2	1.98	0.64
1:A:204:LYS:NZ	3:A:307:PEG:H22	2.11	0.64
1:C:75:VAL:O	4:C:308:EDO:H12	1.97	0.63
1:D:137:TYR:CE1	1:D:166:KPI:HEA	2.33	0.63
4:B:303:EDO:H21	8:B:407:HOH:O	1.99	0.62
1:A:294:LYS:CE	3:A:302:PEG:O4	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LYS:HZ2	4:C:305:EDO:C2	2.11	0.62
1:B:154:LYS:HD3	6:B:310:PGE:H4	1.81	0.62
1:C:71:LYS:NZ	4:C:305:EDO:H21	2.16	0.61
1:C:71:LYS:HZ2	4:C:305:EDO:H22	1.64	0.61
8:E:429:HOH:O	3:F:302:PEG:H41	2.01	0.61
1:C:4:ASN:HB2	1:C:133:PRO:HG3	1.84	0.60
1:A:294:LYS:HG2	3:A:304:PEG:C3	2.32	0.59
1:E:223:HIS:O	1:E:227:ASP:HB2	2.01	0.59
1:A:204:LYS:HZ3	3:A:307:PEG:C2	2.11	0.59
1:C:154:LYS:HD2	6:C:310:PGE:C6	2.32	0.58
3:E:303:PEG:H12	8:F:477:HOH:O	2.02	0.58
1:F:137:TYR:CE1	1:F:166:KPI:HEA	2.38	0.58
1:E:97:LYS:NZ	1:E:131:ASP:OD1	2.30	0.58
1:B:25:GLN:H	5:B:309:ACT:H1	1.68	0.58
1:C:137:TYR:CE1	1:C:166:KPI:HEA	2.39	0.58
1:D:183:PRO:O	4:D:302:EDO:C1	2.49	0.58
1:F:137:TYR:CZ	1:F:166:KPI:HEA	2.40	0.57
1:A:295:ILE:HD12	3:A:305:PEG:C2	2.34	0.56
3:F:302:PEG:H41	3:F:302:PEG:C1	2.23	0.56
1:F:154:LYS:HE3	6:F:306:PGE:C2	2.20	0.56
4:D:302:EDO:H21	8:D:553:HOH:O	2.07	0.55
1:A:57:GLU:HG3	4:A:310:EDO:O1	2.06	0.55
1:B:25:GLN:H	5:B:309:ACT:CH3	2.20	0.55
1:C:137:TYR:CZ	1:C:166:KPI:HEA	2.41	0.55
3:F:302:PEG:H12	3:F:302:PEG:C4	2.24	0.55
1:E:140:PRO:HG3	1:E:146:GLU:OE1	2.08	0.54
1:E:238:ASP:O	3:E:302:PEG:H42	2.08	0.54
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.90	0.54
1:C:154:LYS:HD2	6:C:310:PGE:H62	1.88	0.54
1:A:294:LYS:NZ	3:A:304:PEG:C3	2.58	0.53
1:C:154:LYS:HE2	6:C:310:PGE:H12	1.90	0.53
1:E:20:GLY:HA2	8:E:458:HOH:O	2.07	0.53
3:E:303:PEG:C1	8:F:477:HOH:O	2.55	0.53
1:B:298:PHE:HD1	4:B:306:EDO:H12	1.74	0.53
4:A:312:EDO:H12	8:B:507:HOH:O	2.08	0.52
1:C:35:ILE:HG12	1:C:75:VAL:HG21	1.92	0.52
1:B:57:GLU:CB	4:B:305:EDO:H21	2.24	0.52
1:F:154:LYS:NZ	6:F:306:PGE:H2	2.25	0.51
1:F:154:LYS:HZ2	6:F:306:PGE:H6	1.75	0.51
1:C:154:LYS:HD3	6:C:310:PGE:C6	2.29	0.51
1:B:154:LYS:CD	6:B:310:PGE:H4	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.93	0.51
3:E:303:PEG:C2	8:F:477:HOH:O	2.59	0.51
1:A:154:LYS:NZ	6:A:315:PGE:H12	2.26	0.50
1:D:57:GLU:HG2	8:D:490:HOH:O	2.11	0.50
1:E:288:GLU:OE2	1:E:292:LYS:NZ	2.44	0.50
1:E:21:LYS:HZ2	1:E:22:VAL:HB	1.76	0.50
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.92	0.50
1:D:137:TYR:CZ	1:D:166:KPI:HEA	2.47	0.50
1:C:154:LYS:HZ3	6:C:310:PGE:H52	1.76	0.50
1:C:3:LYS:N	8:C:403:HOH:O	2.46	0.49
1:F:243:ILE:HB	1:F:293:TYR:CE2	2.47	0.49
1:F:281:GLU:O	1:F:285:LYS:HG3	2.13	0.49
1:B:25:GLN:HG3	5:B:309:ACT:H1	1.95	0.49
1:C:13:LEU:HD11	1:C:42:VAL:HB	1.94	0.48
1:C:154:LYS:HD2	6:C:310:PGE:H6	1.95	0.48
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.94	0.48
1:B:13:LEU:HD11	1:B:42:VAL:HB	1.95	0.48
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.94	0.48
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.95	0.48
1:E:239:GLU:O	3:E:302:PEG:H12	2.13	0.48
1:A:189:SER:HB3	1:A:206:VAL:HG12	1.96	0.48
1:A:202:GLY:HA3	4:A:312:EDO:H22	1.95	0.47
1:C:231:LYS:HG2	8:C:489:HOH:O	2.13	0.47
1:E:292:LYS:HD3	8:E:513:HOH:O	2.14	0.47
1:D:18:LYS:O	1:D:21:LYS:HE2	2.15	0.47
4:D:302:EDO:O2	8:D:401:HOH:O	2.20	0.46
1:F:64:GLU:O	1:F:68:GLU:HG2	2.15	0.46
1:E:256:ILE:O	1:E:260:MET:HG2	2.16	0.46
1:A:183:PRO:O	4:A:312:EDO:O1	2.32	0.46
1:F:268:SER:OG	1:F:270:GLU:HG3	2.15	0.46
1:B:292:LYS:NZ	8:B:406:HOH:O	2.47	0.46
1:A:294:LYS:HZ1	3:A:302:PEG:C1	2.25	0.45
1:C:292:LYS:N	1:C:292:LYS:HD2	2.31	0.45
1:D:246:ILE:HD12	1:D:246:ILE:HA	1.89	0.45
3:F:302:PEG:C1	3:F:302:PEG:C4	2.90	0.45
1:B:108:ALA:HB2	1:B:147:ILE:HD11	1.99	0.45
1:B:55:THR:HG1	4:B:305:EDO:H22	1.73	0.44
1:D:54:LEU:O	2:D:301:LYS:HE3	2.16	0.44
1:A:85:ALA:HB3	1:A:88:GLU:HB2	1.99	0.44
1:D:161:ASN:OD1	1:D:161:ASN:N	2.38	0.44
1:E:21:LYS:HD2	1:E:21:LYS:HA	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:ILE:HB	1:E:293:TYR:CE2	2.53	0.44
3:E:303:PEG:H22	8:F:477:HOH:O	2.16	0.44
1:E:13:LEU:HD11	1:E:42:VAL:HB	1.98	0.44
1:A:243:ILE:HB	1:A:293:TYR:CE1	2.54	0.43
1:E:254:ILE:HB	1:E:255:PRO:HD3	2.00	0.43
1:A:269:LEU:HA	1:A:269:LEU:HD23	1.83	0.43
1:B:107:VAL:HA	1:B:137:TYR:HB3	2.00	0.43
1:B:147:ILE:HG22	1:B:152:ILE:HG13	2.01	0.43
1:C:71:LYS:HD2	4:C:305:EDO:H22	1.99	0.43
1:B:142:ARG:NH2	1:B:251:SER:HB3	2.33	0.43
1:F:154:LYS:HZ1	6:F:306:PGE:H6	1.80	0.43
1:A:154:LYS:HZ3	6:A:315:PGE:H12	1.85	0.42
1:C:256:ILE:O	1:C:260:MET:HG2	2.20	0.42
1:D:135:LEU:HD13	1:D:163:TYR:CZ	2.55	0.42
1:A:230:TYR:HD2	1:B:230:TYR:CD2	2.38	0.42
1:A:256:ILE:O	1:A:260:MET:HG2	2.20	0.42
1:C:245:LYS:HD2	1:C:245:LYS:HA	1.84	0.42
1:D:285:LYS:O	1:D:289:VAL:HG23	2.20	0.42
1:C:231:LYS:HD2	1:D:228:GLU:OE2	2.20	0.42
1:F:21:LYS:HB2	1:F:21:LYS:HE2	1.75	0.42
1:E:142:ARG:HD2	1:F:111:TYR:O	2.21	0.41
1:F:246:ILE:HD12	1:F:246:ILE:HA	1.92	0.41
1:C:249:CYS:SG	1:C:282:ASN:HB3	2.60	0.41
1:E:21:LYS:NZ	8:E:406:HOH:O	2.49	0.41
1:A:50:GLU:HG2	1:A:275:LEU:HD12	2.02	0.41
1:A:191:GLU:CD	5:A:313:ACT:CH3	2.83	0.41
1:D:25:GLN:HG3	8:D:530:HOH:O	2.21	0.41
1:B:21:LYS:HE3	3:B:302:PEG:H11	2.03	0.41
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.87	0.41
1:C:154:LYS:CE	6:C:310:PGE:H12	2.51	0.41
1:E:154:LYS:HE3	6:E:305:PGE:C2	2.51	0.40
1:D:63:ILE:O	1:D:67:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	293/310 (94%)	286 (98%)	5 (2%)	2 (1%)	22	12
1	B	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	C	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	D	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	E	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	F	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
All	All	1758/1860 (94%)	1724 (98%)	32 (2%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	GLU
1	A	269	LEU

### 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	246/260 (95%)	245 (100%)	1 (0%)	91	91
1	B	246/260 (95%)	241 (98%)	5 (2%)	55	51
1	C	245/260 (94%)	242 (99%)	3 (1%)	71	70
1	D	245/260 (94%)	243 (99%)	2 (1%)	81	82
1	E	247/260 (95%)	245 (99%)	2 (1%)	81	82
1	F	246/260 (95%)	243 (99%)	3 (1%)	71	70
All	All	1475/1560 (95%)	1459 (99%)	16 (1%)	73	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	B	21	LYS
1	B	145	CYS
1	B	161	ASN
1	B	280	LYS
1	B	281	GLU
1	C	32	LYS
1	C	145	CYS
1	C	292	LYS
1	D	21	LYS
1	D	32	LYS
1	E	4	ASN
1	E	245	LYS
1	F	137	TYR
1	F	184	ARG
1	F	280	LYS

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

Mol	Chain	Res	Type
1	B	4	ASN
1	E	4	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	F	166	1	10,13,14	1.42	1 (10%)	6,15,17	4.77	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KPI	C	166	1	10,13,14	1.45	1 (10%)	6,15,17	4.99	2 (33%)
1	KPI	E	166	1	10,13,14	0.81	0	6,15,17	2.95	3 (50%)
1	KPI	B	166	1	10,13,14	0.80	0	6,15,17	3.53	3 (50%)
1	KPI	D	166	1	10,13,14	0.71	0	6,15,17	4.79	2 (33%)
1	KPI	A	166	1	10,13,14	0.77	0	6,15,17	2.09	1 (16%)

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	F	166	1	-	3/9/14/16	-
1	KPI	C	166	1	-	4/9/14/16	-
1	KPI	E	166	1	-	0/9/14/16	-
1	KPI	B	166	1	-	5/9/14/16	-
1	KPI	D	166	1	-	3/9/14/16	-
1	KPI	A	166	1	-	0/9/14/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	KPI	O-C	4.15	1.36	1.19
1	C	166	KPI	O-C	4.04	1.36	1.19

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	KPI	C1-CX1-CX2	-9.99	106.85	117.92
1	D	166	KPI	C1-CX1-CX2	-9.88	106.98	117.92
1	F	166	KPI	C1-CX1-CX2	-9.77	107.10	117.92
1	C	166	KPI	CD-CE-NZ	6.78	123.00	110.66
1	B	166	KPI	C1-CX1-CX2	-6.60	110.61	117.92
1	F	166	KPI	CD-CE-NZ	5.81	121.23	110.66
1	D	166	KPI	CD-CE-NZ	5.74	121.10	110.66
1	E	166	KPI	C1-CX1-CX2	5.01	123.47	117.92
1	A	166	KPI	CE-NZ-CX1	4.89	134.91	121.77
1	E	166	KPI	CE-NZ-CX1	4.37	133.53	121.77
1	B	166	KPI	CE-NZ-CX1	3.80	131.98	121.77
1	B	166	KPI	CD-CE-NZ	3.61	117.23	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	166	KPI	C1-CX1-NZ	-2.13	117.81	123.12

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	166	KPI	C-CA-CB-CG
1	B	166	KPI	C1-CX1-NZ-CE
1	B	166	KPI	CX2-CX1-NZ-CE
1	C	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	CX2-CX1-NZ-CE
1	D	166	KPI	C1-CX1-NZ-CE
1	D	166	KPI	CX2-CX1-NZ-CE
1	F	166	KPI	C1-CX1-NZ-CE
1	F	166	KPI	CX2-CX1-NZ-CE
1	B	166	KPI	CG-CD-CE-NZ
1	C	166	KPI	CG-CD-CE-NZ
1	D	166	KPI	CG-CD-CE-NZ
1	F	166	KPI	CG-CD-CE-NZ
1	B	166	KPI	N-CA-CB-CG
1	C	166	KPI	CE-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 3 are monoatomic - leaving 47 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	$\# Z  > 2$
6	PGE	E	305	-	9,9,9	0.37	0	8,8,8	0.56	0
4	EDO	C	306	-	3,3,3	0.38	0	2,2,2	0.60	0
4	EDO	B	306	-	3,3,3	0.48	0	2,2,2	0.40	0
4	EDO	C	307	-	3,3,3	0.31	0	2,2,2	0.25	0
3	PEG	C	302	-	6,6,6	0.32	0	5,5,5	0.61	0
3	PEG	A	303	-	6,6,6	0.40	0	5,5,5	0.42	0
3	PEG	C	303	-	6,6,6	0.40	0	5,5,5	0.91	0
2	LYS	E	301	-	5,9,9	0.33	0	4,10,10	0.43	0
4	EDO	D	302	-	3,3,3	0.33	0	2,2,2	0.55	0
6	PGE	B	310	-	9,9,9	0.38	0	8,8,8	0.91	0
3	PEG	E	303	-	6,6,6	0.48	0	5,5,5	0.51	0
4	EDO	B	304	-	3,3,3	0.26	0	2,2,2	0.19	0
4	EDO	B	305	-	3,3,3	0.68	0	2,2,2	0.59	0
6	PGE	A	315	-	9,9,9	0.43	0	8,8,8	0.43	0
3	PEG	A	307	-	6,6,6	0.35	0	5,5,5	0.51	0
2	LYS	B	301	-	5,9,9	0.31	0	4,10,10	0.38	0
4	EDO	A	311	-	3,3,3	0.32	0	2,2,2	0.16	0
3	PEG	F	302	-	6,6,6	0.63	0	5,5,5	0.92	0
6	PGE	F	306	-	9,9,9	0.39	0	8,8,8	0.27	0
3	PEG	E	302	-	6,6,6	0.62	0	5,5,5	1.46	1 (20%)
2	LYS	C	301	-	5,9,9	0.43	0	4,10,10	0.54	0
3	PEG	A	304	-	6,6,6	0.36	0	5,5,5	0.49	0
4	EDO	F	304	-	3,3,3	0.43	0	2,2,2	0.32	0
6	PGE	F	307	-	9,9,9	0.39	0	8,8,8	0.68	0
4	EDO	E	304	-	3,3,3	0.23	0	2,2,2	0.48	0
2	LYS	F	301	-	5,9,9	0.44	0	4,10,10	0.46	0
4	EDO	A	312	-	3,3,3	0.58	0	2,2,2	0.36	0
4	EDO	A	308	-	3,3,3	0.49	0	2,2,2	0.23	0
2	LYS	A	301	-	5,9,9	0.40	0	4,10,10	0.50	0
5	ACT	F	305	-	1,3,3	0.95	0	0,3,3	-	-
5	ACT	B	309	-	1,3,3	1.89	0	0,3,3	-	-
3	PEG	A	302	-	6,6,6	0.32	0	5,5,5	0.62	0
4	EDO	C	305	-	3,3,3	0.26	0	2,2,2	0.41	0
4	EDO	C	304	-	3,3,3	0.39	0	2,2,2	0.29	0
3	PEG	A	305	-	6,6,6	0.41	0	5,5,5	0.96	0
4	EDO	C	308	-	3,3,3	0.43	0	2,2,2	0.21	0
3	PEG	A	306	-	6,6,6	0.29	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	303	-	3,3,3	0.30	0	2,2,2	0.81	0
3	PEG	B	302	-	6,6,6	0.33	0	5,5,5	0.62	0
4	EDO	A	309	-	3,3,3	0.41	0	2,2,2	0.57	0
6	PGE	C	310	-	9,9,9	0.50	0	8,8,8	0.46	0
5	ACT	A	313	-	1,3,3	1.02	0	0,3,3	-	-
5	ACT	A	314	-	1,3,3	1.33	0	0,3,3	-	-
3	PEG	F	303	-	6,6,6	0.46	0	5,5,5	0.41	0
2	LYS	D	301	-	5,9,9	0.51	0	4,10,10	0.65	0
6	PGE	D	303	-	9,9,9	0.52	0	8,8,8	0.46	0
4	EDO	A	310	-	3,3,3	0.30	0	2,2,2	0.37	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
6	PGE	E	305	-	-	6/7/7/7	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	B	306	-	-	1/1/1/1	-
4	EDO	C	307	-	-	1/1/1/1	-
3	PEG	C	302	-	-	3/4/4/4	-
3	PEG	A	303	-	-	3/4/4/4	-
3	PEG	C	303	-	-	1/4/4/4	-
2	LYS	E	301	-	-	0/5/9/9	-
4	EDO	D	302	-	-	0/1/1/1	-
6	PGE	B	310	-	-	6/7/7/7	-
3	PEG	E	303	-	-	1/4/4/4	-
4	EDO	B	304	-	-	0/1/1/1	-
4	EDO	B	305	-	-	1/1/1/1	-
6	PGE	A	315	-	-	3/7/7/7	-
3	PEG	A	307	-	-	0/4/4/4	-
2	LYS	B	301	-	-	1/5/9/9	-
4	EDO	A	311	-	-	0/1/1/1	-
3	PEG	F	302	-	-	3/4/4/4	-
6	PGE	F	306	-	-	4/7/7/7	-
3	PEG	E	302	-	-	2/4/4/4	-
2	LYS	C	301	-	-	2/5/9/9	-
3	PEG	A	304	-	-	1/4/4/4	-
4	EDO	F	304	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	F	307	-	-	5/7/7/7	-
4	EDO	E	304	-	-	1/1/1/1	-
2	LYS	F	301	-	-	1/5/9/9	-
4	EDO	A	312	-	-	1/1/1/1	-
4	EDO	A	308	-	-	1/1/1/1	-
2	LYS	A	301	-	-	2/5/9/9	-
3	PEG	A	302	-	-	1/4/4/4	-
4	EDO	C	305	-	-	1/1/1/1	-
4	EDO	C	304	-	-	0/1/1/1	-
3	PEG	A	305	-	-	4/4/4/4	-
4	EDO	C	308	-	-	1/1/1/1	-
3	PEG	A	306	-	-	2/4/4/4	-
4	EDO	B	303	-	-	0/1/1/1	-
3	PEG	B	302	-	-	3/4/4/4	-
4	EDO	A	309	-	-	1/1/1/1	-
6	PGE	C	310	-	-	2/7/7/7	-
3	PEG	F	303	-	-	3/4/4/4	-
2	LYS	D	301	-	-	0/5/9/9	-
6	PGE	D	303	-	-	3/7/7/7	-
4	EDO	A	310	-	-	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(°)	Ideal(°)
3	E	302	PEG	C3-O2-C2	-2.45	102.68	113.29

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	302	PEG	C1-C2-O2-C3
3	B	302	PEG	C4-C3-O2-C2
6	B	310	PGE	O2-C3-C4-O3
6	F	307	PGE	O2-C3-C4-O3
6	F	306	PGE	O2-C3-C4-O3
3	A	303	PEG	O1-C1-C2-O2
6	A	315	PGE	O3-C5-C6-O4
6	B	310	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
6	F	307	PGE	O1-C1-C2-O2
4	A	309	EDO	O1-C1-C2-O2
3	A	305	PEG	O2-C3-C4-O4
3	A	306	PEG	O1-C1-C2-O2
6	F	306	PGE	O3-C5-C6-O4
3	F	303	PEG	O2-C3-C4-O4
6	B	310	PGE	O1-C1-C2-O2
3	A	303	PEG	O2-C3-C4-O4
3	A	305	PEG	O1-C1-C2-O2
4	C	307	EDO	O1-C1-C2-O2
4	E	304	EDO	O1-C1-C2-O2
6	F	306	PGE	O1-C1-C2-O2
6	D	303	PGE	O3-C5-C6-O4
6	E	305	PGE	O3-C5-C6-O4
4	C	306	EDO	O1-C1-C2-O2
6	E	305	PGE	O2-C3-C4-O3
3	C	303	PEG	O2-C3-C4-O4
3	C	302	PEG	O1-C1-C2-O2
6	A	315	PGE	O2-C3-C4-O3
3	B	302	PEG	O1-C1-C2-O2
3	C	302	PEG	O2-C3-C4-O4
6	F	307	PGE	O3-C5-C6-O4
6	F	307	PGE	C3-C4-O3-C5
3	A	302	PEG	C1-C2-O2-C3
3	E	303	PEG	C1-C2-O2-C3
6	C	310	PGE	C1-C2-O2-C3
3	A	305	PEG	C4-C3-O2-C2
3	E	302	PEG	O1-C1-C2-O2
6	F	307	PGE	C6-C5-O3-C4
3	E	302	PEG	C1-C2-O2-C3
3	F	303	PEG	O1-C1-C2-O2
4	B	305	EDO	O1-C1-C2-O2
3	F	303	PEG	C4-C3-O2-C2
3	F	302	PEG	O2-C3-C4-O4
2	C	301	LYS	C-CA-CB-CG
3	C	302	PEG	C1-C2-O2-C3
3	F	302	PEG	O1-C1-C2-O2
2	A	301	LYS	CG-CD-CE-NZ
4	A	308	EDO	O1-C1-C2-O2
4	B	306	EDO	O1-C1-C2-O2
4	F	304	EDO	O1-C1-C2-O2
6	E	305	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	F	306	PGE	C4-C3-O2-C2
6	A	315	PGE	C1-C2-O2-C3
6	B	310	PGE	C1-C2-O2-C3
6	B	310	PGE	C3-C4-O3-C5
3	B	302	PEG	C1-C2-O2-C3
3	A	303	PEG	C4-C3-O2-C2
6	B	310	PGE	C6-C5-O3-C4
6	E	305	PGE	C3-C4-O3-C5
2	A	301	LYS	CE-CD-CG-CB
3	A	304	PEG	C1-C2-O2-C3
2	B	301	LYS	CG-CD-CE-NZ
4	A	312	EDO	O1-C1-C2-O2
4	C	305	EDO	O1-C1-C2-O2
6	E	305	PGE	O1-C1-C2-O2
6	E	305	PGE	C6-C5-O3-C4
6	D	303	PGE	C4-C3-O2-C2
4	C	308	EDO	O1-C1-C2-O2
3	A	306	PEG	C1-C2-O2-C3
2	C	301	LYS	CE-CD-CG-CB
6	C	310	PGE	O1-C1-C2-O2
2	F	301	LYS	CG-CD-CE-NZ
3	A	305	PEG	C1-C2-O2-C3
6	D	303	PGE	C6-C5-O3-C4

There are no ring outliers.

29 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	305	PGE	8	0
4	B	306	EDO	2	0
4	C	307	EDO	2	0
3	A	303	PEG	1	0
4	D	302	EDO	4	0
6	B	310	PGE	3	0
3	E	303	PEG	4	0
4	B	305	EDO	7	0
6	A	315	PGE	5	0
3	A	307	PEG	7	0
4	A	311	EDO	1	0
3	F	302	PEG	8	0
6	F	306	PGE	8	0
3	E	302	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	PEG	6	0
4	A	312	EDO	4	0
5	B	309	ACT	3	0
3	A	302	PEG	5	0
4	C	305	EDO	7	0
3	A	305	PEG	4	0
4	C	308	EDO	3	0
4	B	303	EDO	1	0
3	B	302	PEG	1	0
4	A	309	EDO	1	0
6	C	310	PGE	11	0
5	A	313	ACT	3	0
2	D	301	LYS	1	0
6	D	303	PGE	2	0
4	A	310	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	295/310 (95%)	-0.06	2 (0%) 87 88	23, 29, 51, 63	0
1	B	295/310 (95%)	-0.16	1 (0%) 94 94	23, 29, 49, 61	0
1	C	295/310 (95%)	-0.13	0 100 100	23, 30, 46, 57	0
1	D	295/310 (95%)	-0.10	1 (0%) 94 94	22, 31, 50, 67	0
1	E	295/310 (95%)	-0.13	2 (0%) 87 88	25, 32, 50, 75	0
1	F	295/310 (95%)	-0.08	2 (0%) 87 88	21, 31, 51, 68	0
All	All	1770/1860 (95%)	-0.11	8 (0%) 91 92	21, 31, 50, 75	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	LYS	3.4
1	E	4	ASN	2.4
1	F	298	PHE	2.3
1	A	269	LEU	2.2
1	B	20	GLY	2.1
1	A	3	LYS	2.0
1	F	261	TYR	2.0
1	D	4	ASN	2.0

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KPI	B	166	14/15	0.79	0.19	22,28,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	A	166	14/15	0.85	0.20	22,29,46,48	0
1	KPI	D	166	14/15	0.85	0.18	26,32,45,48	0
1	KPI	E	166	14/15	0.85	0.16	24,29,46,46	0
1	KPI	C	166	14/15	0.86	0.17	21,26,43,49	0
1	KPI	F	166	14/15	0.88	0.16	22,29,45,46	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	PEG	F	303	7/7	0.58	0.48	20,20,20,20	0
5	ACT	A	314	4/4	0.66	0.52	20,20,20,20	0
5	ACT	F	305	4/4	0.67	0.49	20,20,20,20	0
3	PEG	A	303	7/7	0.68	0.48	20,20,20,20	0
4	EDO	B	305	4/4	0.69	0.48	20,20,20,20	0
3	PEG	A	306	7/7	0.71	0.37	20,20,20,20	0
3	PEG	B	302	7/7	0.71	0.37	20,20,20,20	0
6	PGE	F	307	10/10	0.71	0.52	20,20,20,20	0
5	ACT	B	309	4/4	0.74	0.53	20,20,20,20	0
4	EDO	A	311	4/4	0.76	0.47	20,20,20,20	0
3	PEG	F	302	7/7	0.76	0.61	20,20,20,20	0
4	EDO	D	302	4/4	0.77	0.61	20,20,20,20	0
3	PEG	A	304	7/7	0.79	0.41	20,20,20,20	0
3	PEG	A	305	7/7	0.80	0.67	20,20,20,20	0
4	EDO	A	308	4/4	0.80	0.28	20,20,20,20	0
3	PEG	C	303	7/7	0.80	0.59	20,20,20,20	0
3	PEG	A	302	7/7	0.80	0.51	20,20,20,20	0
4	EDO	C	306	4/4	0.80	0.42	20,20,20,20	0
3	PEG	E	303	7/7	0.81	0.52	20,20,20,20	0
4	EDO	B	303	4/4	0.81	0.71	20,20,20,20	0
6	PGE	B	310	10/10	0.81	0.31	20,20,20,20	0
4	EDO	A	310	4/4	0.81	0.48	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PGE	E	305	10/10	0.82	0.34	20,20,20,20	0
3	PEG	E	302	7/7	0.82	0.36	20,20,20,20	0
4	EDO	C	305	4/4	0.83	0.49	20,20,20,20	0
6	PGE	A	315	10/10	0.84	0.32	20,20,20,20	0
3	PEG	C	302	7/7	0.84	0.47	20,20,20,20	0
5	ACT	A	313	4/4	0.85	0.36	20,20,20,20	0
4	EDO	C	307	4/4	0.85	0.38	20,20,20,20	0
7	MG	B	307	1/1	0.85	0.11	30,30,30,30	0
6	PGE	F	306	10/10	0.86	0.35	20,20,20,20	0
4	EDO	A	312	4/4	0.87	0.57	20,20,20,20	0
4	EDO	E	304	4/4	0.87	0.65	20,20,20,20	0
3	PEG	A	307	7/7	0.87	0.39	20,20,20,20	0
6	PGE	D	303	10/10	0.88	0.30	20,20,20,20	0
6	PGE	C	310	10/10	0.89	0.32	20,20,20,20	0
4	EDO	C	304	4/4	0.89	0.40	20,20,20,20	0
4	EDO	F	304	4/4	0.89	0.57	20,20,20,20	0
4	EDO	B	304	4/4	0.90	0.45	20,20,20,20	0
4	EDO	B	306	4/4	0.90	0.58	20,20,20,20	0
4	EDO	C	308	4/4	0.90	0.65	20,20,20,20	0
2	LYS	A	301	10/10	0.91	0.15	28,34,35,36	0
2	LYS	D	301	10/10	0.91	0.12	30,32,39,39	0
4	EDO	A	309	4/4	0.91	0.41	20,20,20,20	0
2	LYS	C	301	10/10	0.93	0.12	25,29,31,31	0
2	LYS	F	301	10/10	0.93	0.11	28,31,37,38	0
2	LYS	E	301	10/10	0.94	0.10	26,34,41,41	0
2	LYS	B	301	10/10	0.95	0.11	25,30,37,38	0
7	MG	B	308	1/1	0.96	0.04	30,30,30,30	0
7	MG	C	309	1/1	0.99	0.25	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.