Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 04:54 PM EDT

PDB ID	:	7KG5
Title	:	Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H56W mutant with pyruvate bound in the active site
Authors	:	Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.
Deposited on	:	2020-10-15
Resolution	:	1.95 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*
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:

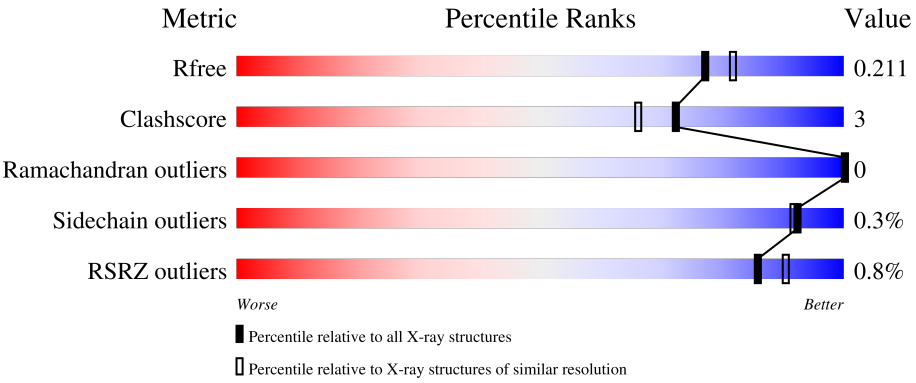
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	87% 9% ·
1	B	310	93% · 5%
1	C	310	89% 6% 5%
1	D	310	89% 6% 5%
1	E	310	89% 6% 5%

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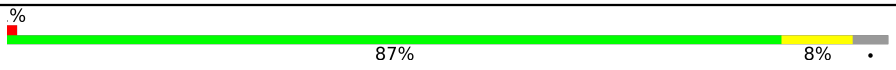
Mol	Chain	Length	Quality of chain
1	F	310	

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	EDO	C	304	-	-	X	-
4	PEG	A	310	-	-	X	-
4	PEG	F	305	-	-	X	-
5	ACT	D	307	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 15020 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	297	Total	C	N	O	S	0	2	0
			2306	1469	381	443	13			
1	B	296	Total	C	N	O	S	0	1	0
			2298	1466	380	439	13			
1	C	296	Total	C	N	O	S	0	1	0
			2298	1466	380	439	13			
1	D	296	Total	C	N	O	S	0	2	0
			2286	1455	378	440	13			
1	E	296	Total	C	N	O	S	0	1	0
			2285	1455	378	439	13			
1	F	297	Total	C	N	O	S	0	3	0
			2296	1460	379	444	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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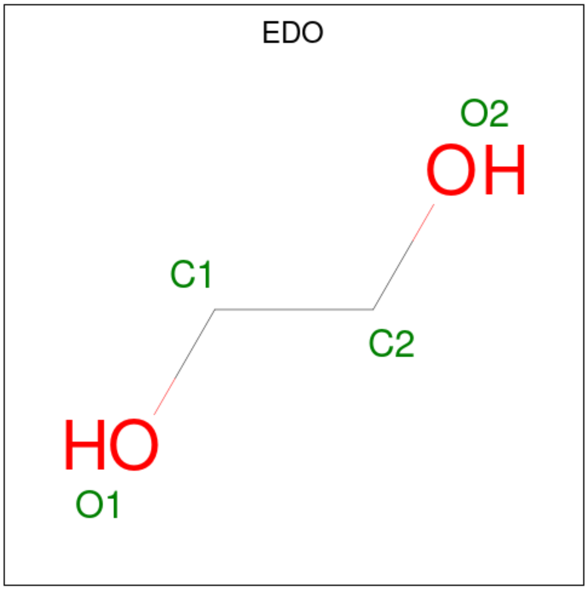
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	56	TRP	HIS	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	3	Total Mg 3 3	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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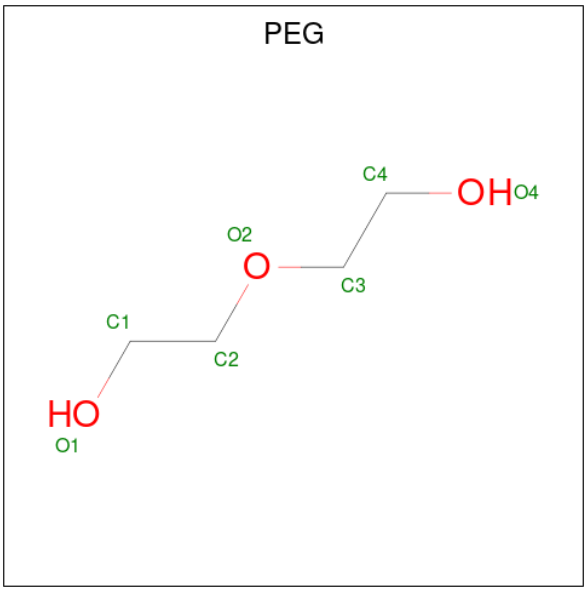
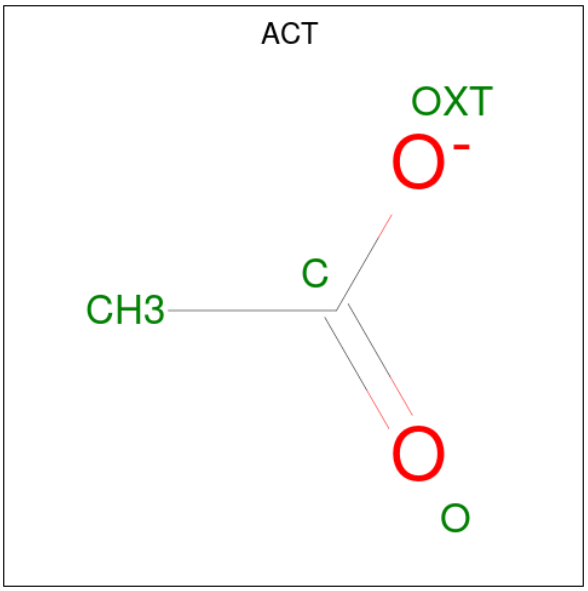
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0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

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



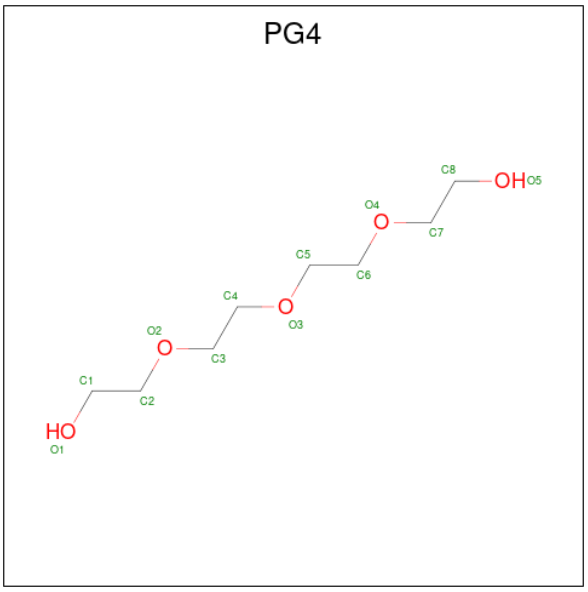
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0

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



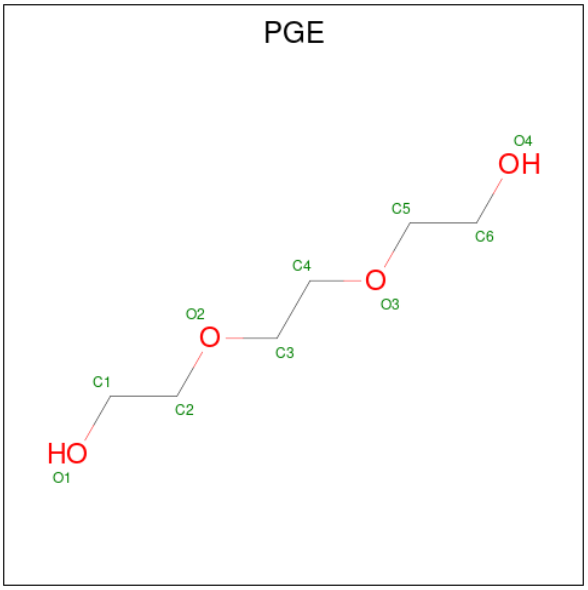
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0
6	D	1	Total C O 13 8 5	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

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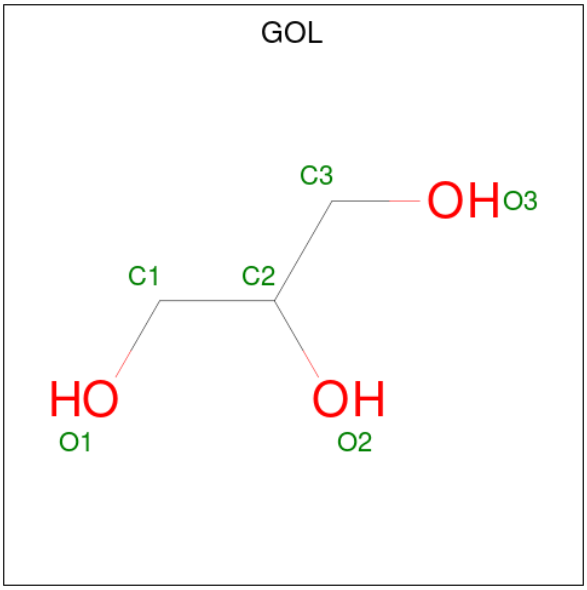
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 10 6 4	0	0
7	E	1	Total C O 10 6 4	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	E	1	Total C O 6 3 3	0	0
8	E	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	161	Total O 161 161	0	0
9	B	159	Total O 159 159	0	0
9	C	155	Total O 155 155	0	0

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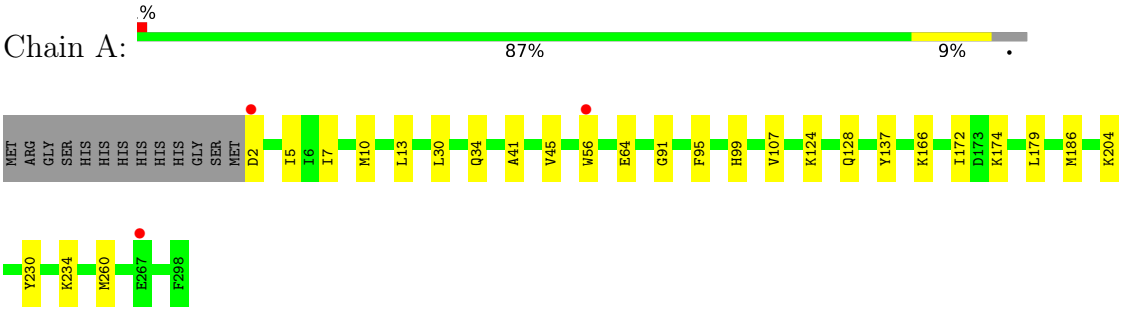
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	153	Total O 153 153	0	0
9	E	153	Total O 153 153	0	0
9	F	160	Total O 160 160	0	0

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.

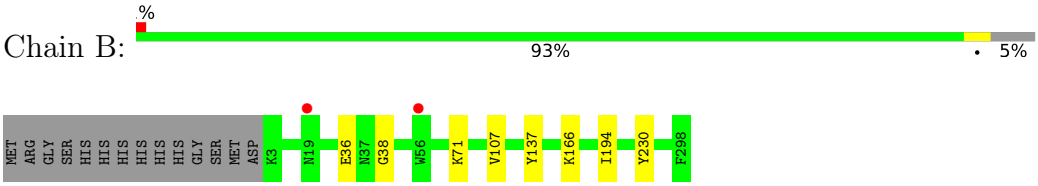
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A:



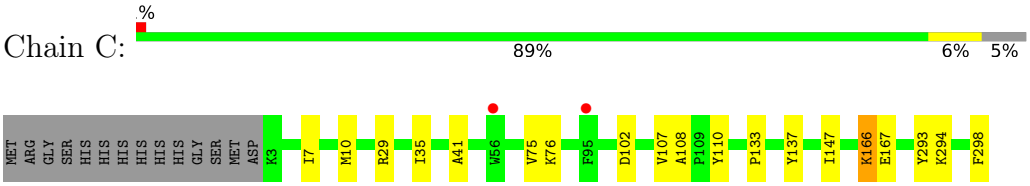
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:



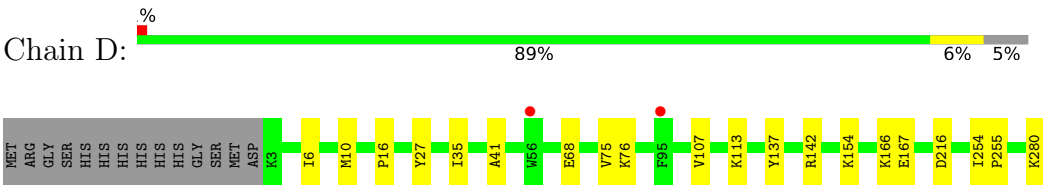
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C:



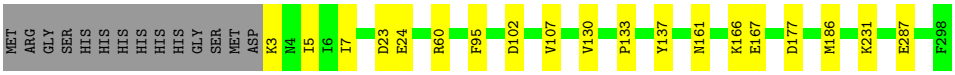
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D:



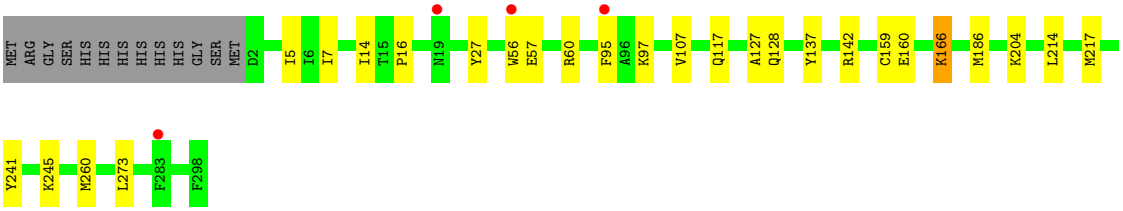
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:



• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	85.13Å 231.25Å 202.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.30 – 1.95 46.30 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.30-1.95) 98.1 (46.30-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.95Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.174 , 0.210 0.176 , 0.211	Depositor DCC
R_{free} test set	7105 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15020	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.41	0/2339	0.52	0/3163
1	B	0.39	0/2325	0.53	0/3144
1	C	0.38	1/2325 (0.0%)	0.52	0/3144
1	D	0.40	2/2321 (0.1%)	0.53	0/3137
1	E	0.37	1/2315 (0.0%)	0.52	0/3129
1	F	0.36	0/2336	0.53	0/3159
All	All	0.38	4/13961 (0.0%)	0.53	0/18876

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	167	GLU	CD-OE2	-5.18	1.20	1.25
1	D	167	GLU	CD-OE1	-5.13	1.20	1.25
1	D	167	GLU	CD-OE2	-5.13	1.20	1.25
1	E	167	GLU	CD-OE1	-5.11	1.20	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2306	0	2336	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2298	0	2326	6	0
1	C	2298	0	2330	14	0
1	D	2286	0	2323	11	0
1	E	2285	0	2322	14	0
1	F	2296	0	2327	23	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	24	0	36	6	0
3	B	28	0	42	3	0
3	C	20	0	30	4	0
3	D	8	0	12	0	0
3	E	20	0	30	7	0
3	F	8	0	12	1	0
4	A	14	0	20	9	0
4	C	21	0	30	1	0
4	D	14	0	20	0	0
4	F	14	0	20	6	0
5	A	4	0	3	1	0
5	C	8	0	6	0	0
5	D	8	0	6	2	0
5	E	4	0	3	0	0
5	F	12	0	9	1	0
6	A	13	0	18	0	0
6	D	13	0	18	1	0
7	B	20	0	28	1	0
7	C	10	0	14	0	0
7	E	10	0	14	0	0
8	B	6	0	8	0	0
8	C	6	0	8	0	0
8	E	12	0	16	1	0
9	A	161	0	0	0	0
9	B	159	0	0	1	0
9	C	155	0	0	2	0
9	D	153	0	0	1	0
9	E	153	0	0	1	0
9	F	160	0	0	3	0
All	All	15020	0	14367	97	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 3.

All (97) 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:F:159:CYS:HA	4:F:305:PEG:H21	1.36	1.07
1:C:166:KPI:H1A	9:C:460:HOH:O	1.58	1.04
1:A:30:LEU:HB3	4:A:310:PEG:H31	1.60	0.84
1:A:7:ILE:HG21	1:A:186:MET:HE3	1.58	0.83
1:E:5:ILE:HD12	1:E:186:MET:HE2	1.68	0.75
1:C:76:LYS:HD2	3:C:304:EDO:H22	1.70	0.73
1:F:166:KPI:H1A	9:F:428:HOH:O	1.90	0.72
1:A:7:ILE:HG21	1:A:186:MET:CE	2.19	0.71
1:F:5:ILE:HD12	1:F:186:MET:HE2	1.71	0.71
1:A:64:GLU:HG2	3:A:308:EDO:H12	1.73	0.70
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.76	0.68
1:A:34:GLN:HG2	4:A:310:PEG:H11	1.75	0.68
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.76	0.66
1:D:142:ARG:HE	5:D:307:ACT:H2	1.59	0.65
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.79	0.65
1:F:142:ARG:HE	5:F:308:ACT:H2	1.61	0.65
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.78	0.64
1:A:5:ILE:HD12	1:A:186:MET:HE2	1.80	0.64
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.79	0.63
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.79	0.63
1:D:154:LYS:HD3	6:D:309:PG4:H12	1.81	0.63
1:F:7:ILE:HG21	1:F:186:MET:CE	2.28	0.63
1:A:30:LEU:HB3	4:A:310:PEG:H12	1.80	0.62
1:A:13:LEU:HD22	4:A:310:PEG:H42	1.84	0.60
1:E:7:ILE:HG21	1:E:186:MET:CE	2.33	0.59
1:E:7:ILE:HG21	1:E:186:MET:HE3	1.84	0.59
1:C:35:ILE:HG12	1:C:75:VAL:HG21	1.84	0.58
1:C:7:ILE:H	3:C:304:EDO:H21	1.69	0.57
1:C:7:ILE:HG13	3:E:304:EDO:H11	1.86	0.57
1:A:45:VAL:O	3:A:303:EDO:O1	2.25	0.55
1:F:7:ILE:HG21	1:F:186:MET:HE2	1.88	0.54
1:A:260:MET:CE	4:A:310:PEG:H21	2.38	0.53
1:B:38:GLY:HA2	3:B:307:EDO:H11	1.91	0.53
1:E:24:GLU:HB2	3:E:306:EDO:H22	1.90	0.52
1:A:230:TYR:HD2	1:B:230:TYR:HD2	1.58	0.52
1:F:128:GLN:HG2	4:F:305:PEG:H32	1.92	0.51
1:A:174:LYS:HA	3:A:305:EDO:H11	1.91	0.51
1:F:7:ILE:HG21	1:F:186:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TYR:HD2	1:B:230:TYR:CD2	2.28	0.51
3:E:305:EDO:H21	1:F:273:LEU:HD21	1.93	0.51
1:F:214:LEU:HB3	1:F:217:MET:HE3	1.94	0.50
1:F:56:TRP:CE3	1:F:57:GLU:HG2	2.46	0.49
3:B:307:EDO:H22	9:B:401:HOH:O	2.12	0.49
1:E:23:ASP:HA	3:E:306:EDO:H11	1.95	0.49
1:E:3:LYS:N	9:E:406:HOH:O	2.46	0.48
1:A:260:MET:HE1	4:A:310:PEG:H21	1.95	0.48
1:D:113:LYS:NZ	9:D:405:HOH:O	2.41	0.48
1:F:56:TRP:CZ2	1:F:95:PHE:CE1	3.01	0.48
1:C:7:ILE:N	3:C:304:EDO:H21	2.28	0.47
1:F:56:TRP:HE3	1:F:57:GLU:HG2	1.78	0.47
1:A:186:MET:HE1	1:A:204:LYS:HG3	1.97	0.47
1:C:10:MET:HG2	1:C:41:ALA:HB3	1.97	0.47
1:C:166:KPI:C1	9:C:460:HOH:O	2.38	0.47
1:D:6:ILE:HG12	1:D:76:LYS:HD3	1.96	0.47
1:F:127:ALA:O	4:F:306:PEG:H32	2.15	0.46
1:A:230:TYR:HE2	5:A:311:ACT:H1	1.81	0.46
1:F:60:ARG:HB2	1:F:95:PHE:HZ	1.81	0.46
1:A:99:HIS:O	3:A:308:EDO:H11	2.16	0.45
1:F:117:GLN:HB2	3:F:304:EDO:H11	1.98	0.45
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.97	0.45
3:C:304:EDO:H12	3:E:304:EDO:O1	2.16	0.45
1:E:287:GLU:HG3	3:E:307:EDO:H11	1.97	0.45
4:F:306:PEG:H41	9:F:441:HOH:O	2.17	0.45
1:E:24:GLU:H	3:E:306:EDO:H11	1.82	0.44
1:C:108:ALA:HB2	1:C:147:ILE:HD11	2.00	0.44
1:B:36:GLU:O	7:B:302:PGE:H62	2.18	0.44
1:A:234:LYS:HD3	3:B:311:EDO:H11	2.00	0.43
1:F:97:LYS:NZ	9:F:408:HOH:O	2.44	0.43
1:A:172:ILE:HG23	1:B:194:ILE:HG21	2.01	0.43
1:C:102:ASP:O	1:C:133:PRO:HD2	2.19	0.43
1:A:91:GLY:HA3	4:A:309:PEG:H31	2.00	0.43
1:E:177:ASP:OD1	8:E:310:GOL:H32	2.19	0.42
1:A:174:LYS:CA	3:A:305:EDO:H11	2.49	0.42
4:F:305:PEG:H41	4:F:305:PEG:H22	1.50	0.42
1:E:102:ASP:O	1:E:133:PRO:HD2	2.19	0.42
1:A:179:LEU:HD22	3:A:307:EDO:H21	2.00	0.42
1:F:241:TYR:CE2	1:F:245:LYS:HG3	2.53	0.42
1:D:35:ILE:HG12	1:D:75:VAL:HG21	2.01	0.42
1:C:293:TYR:C	1:C:294:LYS:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:LYS:HD3	1:E:231:LYS:HA	1.72	0.41
1:C:29:ARG:HG2	1:C:298:PHE:CE1	2.56	0.41
1:C:110:TYR:CZ	4:C:309:PEG:H42	2.55	0.41
1:A:124:LYS:HE2	1:A:128:GLN:NE2	2.35	0.41
1:D:142:ARG:NE	5:D:307:ACT:H2	2.32	0.41
1:E:60:ARG:HG3	1:E:95:PHE:CZ	2.56	0.41
1:A:10:MET:HG2	1:A:41:ALA:HB3	2.03	0.41
1:F:160:GLU:H	4:F:305:PEG:C1	2.34	0.41
1:E:130:VAL:O	1:E:161:ASN:ND2	2.53	0.41
1:F:16:PRO:HD2	1:F:27:TYR:HD1	1.85	0.40
1:A:260:MET:HE2	4:A:310:PEG:H21	2.02	0.40
1:F:14:ILE:HD13	1:F:260:MET:HG3	2.04	0.40
1:D:16:PRO:HD2	1:D:27:TYR:HD1	1.86	0.40
1:A:56[B]:TRP:CH2	1:A:95:PHE:HB3	2.56	0.40
1:D:254:ILE:HB	1:D:255:PRO:HD3	2.03	0.40
1:A:34:GLN:HE21	4:A:310:PEG:C1	2.34	0.40
1:D:216:ASP:OD1	1:D:216:ASP:N	2.54	0.40
1:F:186:MET:HE3	1:F:204:LYS:CB	2.51	0.40

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	296/310 (96%)	290 (98%)	6 (2%)	0	100	100
1	B	294/310 (95%)	289 (98%)	5 (2%)	0	100	100
1	C	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	D	295/310 (95%)	289 (98%)	6 (2%)	0	100	100
1	E	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	F	297/310 (96%)	292 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1770/1860 (95%)	1736 (98%)	34 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	251/260 (96%)	250 (100%)	1 (0%)	91 90
1	B	249/260 (96%)	248 (100%)	1 (0%)	91 90
1	C	249/260 (96%)	249 (100%)	0	100 100
1	D	250/260 (96%)	248 (99%)	2 (1%)	81 80
1	E	249/260 (96%)	249 (100%)	0	100 100
1	F	252/260 (97%)	252 (100%)	0	100 100
All	All	1500/1560 (96%)	1496 (100%)	4 (0%)	92 92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	B	71	LYS
1	D	68	GLU
1	D	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	11,13,14	1.23	1 (9%)	10,15,17	2.58	6 (60%)
1	KPI	C	166	1	11,13,14	1.14	2 (18%)	10,15,17	2.75	5 (50%)
1	KPI	F	166	1	11,13,14	1.01	0	10,15,17	2.50	4 (40%)
1	KPI	B	166	1	11,13,14	1.72	3 (27%)	10,15,17	2.58	3 (30%)
1	KPI	E	166	1	11,13,14	0.99	0	10,15,17	2.37	4 (40%)
1	KPI	D	166	1	11,13,14	1.09	1 (9%)	10,15,17	2.21	4 (40%)

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	-	0/13/14/16	-
1	KPI	C	166	1	-	0/13/14/16	-
1	KPI	F	166	1	-	0/13/14/16	-
1	KPI	B	166	1	-	4/13/14/16	-
1	KPI	E	166	1	-	1/13/14/16	-
1	KPI	D	166	1	-	0/13/14/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	KPI	C1-CX1	3.51	1.56	1.49
1	A	166	KPI	CX2-CX1	3.33	1.53	1.49
1	C	166	KPI	CX2-CX1	2.48	1.52	1.49
1	D	166	KPI	CX2-CX1	2.29	1.52	1.49
1	B	166	KPI	O2-CX2	2.28	1.28	1.22
1	B	166	KPI	CX2-CX1	2.20	1.52	1.49
1	C	166	KPI	CA-N	-2.09	1.41	1.48

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	166	KPI	CE-NZ-CX1	5.77	137.42	121.70
1	F	166	KPI	CE-NZ-CX1	5.46	136.57	121.70
1	D	166	KPI	CE-NZ-CX1	5.17	135.79	121.70
1	A	166	KPI	CE-NZ-CX1	5.09	135.56	121.70
1	C	166	KPI	CE-NZ-CX1	5.03	135.40	121.70
1	B	166	KPI	CE-NZ-CX1	4.86	134.95	121.70
1	C	166	KPI	O2-CX2-CX1	-4.56	115.55	121.38
1	B	166	KPI	C1-CX1-CX2	4.54	122.57	118.17
1	B	166	KPI	O2-CX2-CX1	3.70	126.10	121.38
1	F	166	KPI	O2-CX2-CX1	-3.51	116.90	121.38
1	A	166	KPI	CX2-CX1-NZ	3.47	123.42	114.98
1	C	166	KPI	O1-CX2-CX1	3.31	123.54	116.35
1	F	166	KPI	CX2-CX1-NZ	3.00	122.29	114.98
1	D	166	KPI	CX2-CX1-NZ	2.79	121.78	114.98
1	F	166	KPI	C1-CX1-CX2	-2.74	115.51	118.17
1	A	166	KPI	C1-CX1-NZ	-2.66	116.16	123.11
1	A	166	KPI	O2-CX2-CX1	-2.65	118.00	121.38
1	C	166	KPI	CX2-CX1-NZ	2.53	121.13	114.98
1	E	166	KPI	CX2-CX1-NZ	2.40	120.83	114.98
1	C	166	KPI	C1-CX1-CX2	2.36	120.46	118.17
1	E	166	KPI	O2-CX2-CX1	-2.34	118.39	121.38
1	A	166	KPI	C1-CX1-CX2	2.31	120.41	118.17
1	A	166	KPI	O1-CX2-CX1	2.28	121.30	116.35
1	E	166	KPI	O1-CX2-CX1	2.18	121.08	116.35
1	D	166	KPI	O1-CX2-CX1	2.11	120.94	116.35
1	D	166	KPI	O2-CX2-CX1	-2.05	118.77	121.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	166	KPI	NZ-CX1-CX2-O1
1	B	166	KPI	NZ-CX1-CX2-O2
1	B	166	KPI	C1-CX1-CX2-O1
1	B	166	KPI	C1-CX1-CX2-O2
1	E	166	KPI	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 13 are monoatomic - leaving 55 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	A	309	-	6,6,6	0.48	0	5,5,5	0.31	0
8	GOL	B	313	-	5,5,5	0.29	0	5,5,5	0.35	0
4	PEG	D	305	-	6,6,6	0.48	0	5,5,5	0.29	0
3	EDO	F	303	-	3,3,3	0.54	0	2,2,2	0.21	0
5	ACT	D	308	-	3,3,3	0.78	0	3,3,3	1.33	0
3	EDO	E	305	-	3,3,3	0.51	0	2,2,2	0.11	0
7	PGE	E	301	-	9,9,9	0.33	0	8,8,8	0.19	0
8	GOL	E	310	-	5,5,5	0.33	0	5,5,5	0.31	0
3	EDO	A	306	-	3,3,3	0.57	0	2,2,2	0.14	0
3	EDO	C	304	-	3,3,3	0.34	0	2,2,2	0.47	0
3	EDO	D	304	-	3,3,3	0.48	0	2,2,2	0.31	0
4	PEG	F	306	-	6,6,6	0.48	0	5,5,5	0.65	0
3	EDO	C	308	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	B	308	-	3,3,3	0.45	0	2,2,2	0.43	0
5	ACT	D	307	-	3,3,3	0.76	0	3,3,3	1.27	0
4	PEG	C	311	-	6,6,6	0.49	0	5,5,5	0.42	0
6	PG4	D	309	-	12,12,12	0.52	0	11,11,11	0.27	0
7	PGE	B	302	-	9,9,9	0.30	0	8,8,8	0.32	0
5	ACT	F	307	-	3,3,3	0.76	0	3,3,3	1.33	0
3	EDO	C	305	-	3,3,3	0.50	0	2,2,2	0.28	0
4	PEG	A	310	-	6,6,6	0.69	0	5,5,5	0.51	0
3	EDO	D	303	-	3,3,3	0.39	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	B	309	-	3,3,3	0.48	0	2,2,2	0.25	0
3	EDO	B	306	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	E	304	-	3,3,3	0.47	0	2,2,2	0.42	0
5	ACT	F	309	-	3,3,3	0.76	0	3,3,3	1.35	0
8	GOL	C	314	-	5,5,5	0.31	0	5,5,5	0.34	0
5	ACT	C	312	-	3,3,3	0.75	0	3,3,3	1.27	0
3	EDO	B	307	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	C	306	-	3,3,3	0.53	0	2,2,2	0.22	0
4	PEG	D	306	-	6,6,6	0.48	0	5,5,5	0.22	0
8	GOL	E	311	-	5,5,5	0.36	0	5,5,5	0.35	0
7	PGE	B	301	-	9,9,9	0.30	0	8,8,8	0.32	0
7	PGE	C	301	-	9,9,9	0.32	0	8,8,8	0.29	0
3	EDO	E	307	-	3,3,3	0.51	0	2,2,2	0.30	0
3	EDO	A	304	-	3,3,3	0.41	0	2,2,2	0.52	0
6	PG4	A	312	-	12,12,12	0.51	0	11,11,11	0.19	0
5	ACT	A	311	-	3,3,3	0.79	0	3,3,3	1.31	0
3	EDO	A	308	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	C	307	-	3,3,3	0.53	0	2,2,2	0.26	0
3	EDO	E	306	-	3,3,3	0.42	0	2,2,2	0.41	0
3	EDO	B	312	-	3,3,3	0.45	0	2,2,2	0.38	0
5	ACT	F	308	-	3,3,3	0.72	0	3,3,3	1.38	0
4	PEG	C	310	-	6,6,6	0.48	0	5,5,5	0.19	0
3	EDO	A	305	-	3,3,3	0.40	0	2,2,2	0.40	0
4	PEG	F	305	-	6,6,6	0.59	0	5,5,5	0.57	0
3	EDO	A	307	-	3,3,3	0.38	0	2,2,2	0.67	0
3	EDO	B	310	-	3,3,3	0.60	0	2,2,2	0.18	0
3	EDO	B	311	-	3,3,3	0.47	0	2,2,2	0.36	0
4	PEG	C	309	2	6,6,6	0.52	0	5,5,5	0.27	0
3	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.48	0
3	EDO	E	308	-	3,3,3	0.46	0	2,2,2	0.38	0
5	ACT	C	313	-	3,3,3	0.81	0	3,3,3	1.51	0
3	EDO	F	304	-	3,3,3	0.38	0	2,2,2	0.43	0
5	ACT	E	309	-	3,3,3	0.77	0	3,3,3	1.42	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
4	PEG	A	309	-	-	1/4/4/4	-
8	GOL	B	313	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	D	305	-	-	0/4/4/4	-
3	EDO	F	303	-	-	0/1/1/1	-
3	EDO	E	305	-	-	0/1/1/1	-
7	PGE	E	301	-	-	0/7/7/7	-
8	GOL	E	310	-	-	2/4/4/4	-
3	EDO	A	306	-	-	1/1/1/1	-
3	EDO	C	304	-	-	1/1/1/1	-
3	EDO	D	304	-	-	1/1/1/1	-
4	PEG	F	306	-	-	3/4/4/4	-
3	EDO	C	308	-	-	1/1/1/1	-
3	EDO	B	308	-	-	0/1/1/1	-
4	PEG	C	311	-	-	4/4/4/4	-
6	PG4	D	309	-	-	2/10/10/10	-
7	PGE	B	302	-	-	6/7/7/7	-
3	EDO	C	305	-	-	0/1/1/1	-
4	PEG	A	310	-	-	0/4/4/4	-
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	B	309	-	-	0/1/1/1	-
3	EDO	B	306	-	-	0/1/1/1	-
3	EDO	E	304	-	-	1/1/1/1	-
8	GOL	C	314	-	-	4/4/4/4	-
3	EDO	B	307	-	-	1/1/1/1	-
3	EDO	C	306	-	-	1/1/1/1	-
4	PEG	D	306	-	-	1/4/4/4	-
8	GOL	E	311	-	-	2/4/4/4	-
7	PGE	C	301	-	-	1/7/7/7	-
3	EDO	E	307	-	-	1/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
6	PG4	A	312	-	-	0/10/10/10	-
3	EDO	A	308	-	-	1/1/1/1	-
3	EDO	C	307	-	-	1/1/1/1	-
3	EDO	E	306	-	-	1/1/1/1	-
3	EDO	B	312	-	-	1/1/1/1	-
4	PEG	C	310	-	-	1/4/4/4	-
3	EDO	A	305	-	-	0/1/1/1	-
4	PEG	F	305	-	-	2/4/4/4	-
3	EDO	A	307	-	-	1/1/1/1	-
3	EDO	B	310	-	-	0/1/1/1	-
3	EDO	B	311	-	-	0/1/1/1	-
4	PEG	C	309	2	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	E	308	-	-	1/1/1/1	-
7	PGE	B	301	-	-	1/7/7/7	-
3	EDO	F	304	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	313	GOL	O1-C1-C2-C3
8	E	310	GOL	O1-C1-C2-C3
8	E	311	GOL	O1-C1-C2-C3
4	F	306	PEG	C4-C3-O2-C2
4	C	309	PEG	O2-C3-C4-O4
4	F	306	PEG	O2-C3-C4-O4
4	C	311	PEG	O2-C3-C4-O4
8	C	314	GOL	O1-C1-C2-C3
8	C	314	GOL	C1-C2-C3-O3
4	C	311	PEG	O1-C1-C2-O2
4	F	305	PEG	C4-C3-O2-C2
8	B	313	GOL	O1-C1-C2-O2
4	C	310	PEG	O2-C3-C4-O4
4	F	306	PEG	O1-C1-C2-O2
7	B	302	PGE	O3-C5-C6-O4
3	A	306	EDO	O1-C1-C2-O2
4	C	309	PEG	C1-C2-O2-C3
7	B	302	PGE	O2-C3-C4-O3
8	E	311	GOL	O1-C1-C2-O2
4	A	309	PEG	O2-C3-C4-O4
3	E	308	EDO	O1-C1-C2-O2
7	B	302	PGE	C4-C3-O2-C2
7	B	302	PGE	C6-C5-O3-C4
6	D	309	PG4	C3-C4-O3-C5
8	C	314	GOL	O1-C1-C2-O2
8	C	314	GOL	O2-C2-C3-O3
8	E	310	GOL	O1-C1-C2-O2
4	C	311	PEG	C1-C2-O2-C3
7	B	302	PGE	C1-C2-O2-C3
7	C	301	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	F	305	PEG	O1-C1-C2-O2
3	C	304	EDO	O1-C1-C2-O2
3	D	304	EDO	O1-C1-C2-O2
3	B	312	EDO	O1-C1-C2-O2
7	B	301	PGE	O1-C1-C2-O2
3	C	308	EDO	O1-C1-C2-O2
3	E	304	EDO	O1-C1-C2-O2
4	D	306	PEG	O1-C1-C2-O2
4	C	311	PEG	C4-C3-O2-C2
3	A	307	EDO	O1-C1-C2-O2
3	A	308	EDO	O1-C1-C2-O2
3	B	307	EDO	O1-C1-C2-O2
3	C	307	EDO	O1-C1-C2-O2
3	E	306	EDO	O1-C1-C2-O2
6	D	309	PG4	C1-C2-O2-C3
7	B	302	PGE	O1-C1-C2-O2
3	C	306	EDO	O1-C1-C2-O2
3	E	307	EDO	O1-C1-C2-O2

There are no ring outliers.

23 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	309	PEG	1	0
3	E	305	EDO	1	0
8	E	310	GOL	1	0
3	C	304	EDO	4	0
4	F	306	PEG	2	0
5	D	307	ACT	2	0
6	D	309	PG4	1	0
7	B	302	PGE	1	0
4	A	310	PEG	8	0
3	E	304	EDO	2	0
3	B	307	EDO	2	0
3	E	307	EDO	1	0
5	A	311	ACT	1	0
3	A	308	EDO	2	0
3	E	306	EDO	3	0
5	F	308	ACT	1	0
3	A	305	EDO	2	0
4	F	305	PEG	4	0
3	A	307	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	311	EDO	1	0
4	C	309	PEG	1	0
3	A	303	EDO	1	0
3	F	304	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	296/310 (95%)	-0.08	3 (1%) 82 87	21, 27, 41, 59	0
1	B	295/310 (95%)	-0.14	2 (0%) 87 92	21, 27, 41, 54	0
1	C	295/310 (95%)	-0.04	2 (0%) 87 92	22, 28, 42, 53	0
1	D	295/310 (95%)	-0.07	3 (1%) 82 87	21, 28, 44, 56	1 (0%)
1	E	295/310 (95%)	-0.15	0 100 100	21, 29, 42, 54	0
1	F	296/310 (95%)	0.01	4 (1%) 75 82	21, 29, 44, 58	1 (0%)
All	All	1772/1860 (95%)	-0.08	14 (0%) 86 90	21, 28, 43, 59	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56[A]	TRP	4.1
1	D	56	TRP	3.3
1	C	56[A]	TRP	2.8
1	F	283	PHE	2.6
1	B	56[A]	TRP	2.5
1	D	95	PHE	2.5
1	B	19	ASN	2.4
1	F	95	PHE	2.3
1	F	56	TRP	2.2
1	A	2	ASP	2.1
1	C	95	PHE	2.1
1	F	19	ASN	2.1
1	D	298	PHE	2.0
1	A	267	GLU	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	B	166	14/15	0.72	0.19	20,20,20,20	0
1	KPI	E	166	14/15	0.75	0.19	20,20,20,20	0
1	KPI	D	166	14/15	0.76	0.20	20,20,20,20	0
1	KPI	A	166	14/15	0.76	0.20	20,20,20,20	0
1	KPI	F	166	14/15	0.78	0.19	20,20,20,20	0
1	KPI	C	166	14/15	0.81	0.20	20,20,20,20	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	C	311	7/7	0.73	0.33	42,47,52,61	0
8	GOL	B	313	6/6	0.73	0.21	42,52,60,76	0
5	ACT	F	309	4/4	0.76	0.16	40,47,50,53	0
3	EDO	F	303	4/4	0.77	0.16	39,40,44,47	0
4	PEG	F	306	7/7	0.77	0.25	32,40,45,45	0
5	ACT	C	313	4/4	0.78	0.29	37,48,49,50	0
3	EDO	C	305	4/4	0.79	0.19	40,41,47,61	0
8	GOL	C	314	6/6	0.79	0.22	40,49,50,53	0
8	GOL	E	310	6/6	0.80	0.17	48,50,58,58	0
2	MG	D	301	1/1	0.81	0.15	58,58,58,58	0
3	EDO	C	308	4/4	0.81	0.23	46,52,54,57	0
2	MG	C	302	1/1	0.83	0.16	56,56,56,56	0
5	ACT	D	307	4/4	0.83	0.19	39,41,48,58	0
3	EDO	E	304	4/4	0.84	0.12	33,36,43,47	0
2	MG	F	302	1/1	0.84	0.12	55,55,55,55	0
8	GOL	E	311	6/6	0.84	0.23	51,54,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	E	305	4/4	0.85	0.31	31,31,44,50	0
3	EDO	A	306	4/4	0.85	0.18	34,39,41,47	0
4	PEG	C	309	7/7	0.85	0.16	38,42,56,57	0
4	PEG	C	310	7/7	0.86	0.18	35,44,56,62	0
5	ACT	A	311	4/4	0.86	0.19	42,44,47,53	0
3	EDO	C	307	4/4	0.86	0.14	43,44,44,53	0
4	PEG	A	309	7/7	0.87	0.13	38,45,55,56	0
3	EDO	B	306	4/4	0.87	0.20	35,36,37,56	0
3	EDO	B	312	4/4	0.87	0.28	41,42,44,56	0
7	PGE	C	301	10/10	0.87	0.13	34,39,47,50	0
5	ACT	F	307	4/4	0.88	0.14	47,54,55,65	0
7	PGE	E	301	10/10	0.88	0.13	41,45,49,50	0
3	EDO	A	308	4/4	0.89	0.34	36,39,46,56	0
4	PEG	D	306	7/7	0.89	0.21	42,49,53,55	0
7	PGE	B	302	10/10	0.89	0.20	39,44,52,62	0
7	PGE	B	301	10/10	0.90	0.14	32,43,47,47	0
3	EDO	B	308	4/4	0.90	0.26	38,44,45,49	0
4	PEG	D	305	7/7	0.90	0.20	42,45,49,52	0
3	EDO	B	310	4/4	0.90	0.14	28,33,36,41	0
6	PG4	D	309	13/13	0.91	0.16	36,43,59,62	0
3	EDO	D	304	4/4	0.91	0.15	38,39,41,47	0
2	MG	E	303	1/1	0.91	0.11	44,44,44,44	0
3	EDO	C	306	4/4	0.92	0.12	30,31,37,42	0
3	EDO	A	307	4/4	0.92	0.28	29,38,38,40	0
3	EDO	E	308	4/4	0.92	0.15	36,37,38,44	0
3	EDO	B	307	4/4	0.92	0.16	32,37,43,49	0
2	MG	C	303	1/1	0.92	0.15	51,51,51,51	0
2	MG	D	302	1/1	0.93	0.07	36,36,36,36	0
3	EDO	E	306	4/4	0.93	0.27	33,44,48,48	0
4	PEG	F	305	7/7	0.93	0.16	25,29,31,33	0
5	ACT	F	308	4/4	0.94	0.16	33,42,44,52	0
3	EDO	A	305	4/4	0.94	0.21	27,33,41,43	0
6	PG4	A	312	13/13	0.94	0.14	30,35,46,47	0
3	EDO	C	304	4/4	0.94	0.23	35,36,37,38	0
5	ACT	D	308	4/4	0.94	0.16	31,41,43,51	0
3	EDO	B	311	4/4	0.94	0.10	36,40,42,42	0
2	MG	A	302	1/1	0.95	0.10	46,46,46,46	0
5	ACT	C	312	4/4	0.95	0.13	39,46,47,48	0
2	MG	B	303	1/1	0.95	0.04	31,31,31,31	0
2	MG	B	304	1/1	0.95	0.31	48,48,48,48	0
3	EDO	A	303	4/4	0.95	0.16	34,36,37,38	0
3	EDO	E	307	4/4	0.95	0.14	31,33,34,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	304	4/4	0.95	0.15	37,38,41,42	0
3	EDO	D	303	4/4	0.95	0.17	29,36,50,54	0
3	EDO	F	304	4/4	0.95	0.26	27,38,41,48	0
4	PEG	A	310	7/7	0.96	0.23	23,30,34,34	0
3	EDO	B	309	4/4	0.96	0.11	33,35,38,43	0
2	MG	A	301	1/1	0.97	0.03	30,30,30,30	0
5	ACT	E	309	4/4	0.97	0.07	30,33,34,35	0
2	MG	E	302	1/1	0.97	0.09	42,42,42,42	0
2	MG	B	305	1/1	0.98	0.09	39,39,39,39	0
2	MG	F	301	1/1	0.99	0.16	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.