



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:37 am BST

PDB ID : 6U01
Title : Dihydropicolinate synthase (DHDPS) from C.jejuni, N84D mutant with pyruvate bound in the active site
Authors : Saran, S.; Majdi Yazdi, M.; Lehnert, L.; Palmer, D.R.J.; Sanders, D.A.R.
Deposited on : 2019-08-13
Resolution : 1.87 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 : 2.11
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) : 2.11

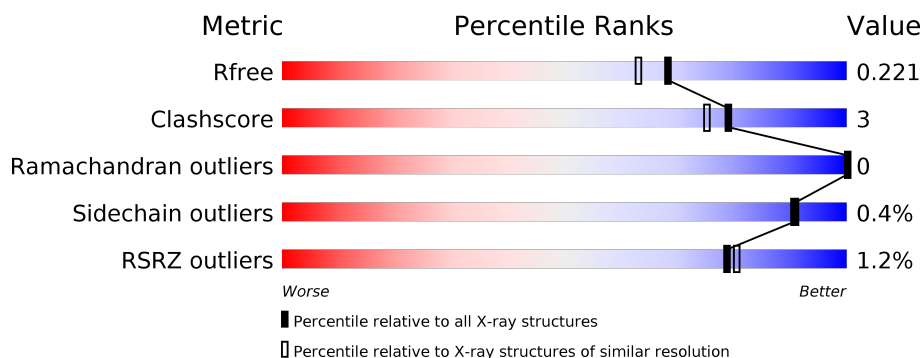
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 on 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	<div> <div>92%</div> <div>5%</div> </div>
1	B	310	<div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	C	310	<div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	D	310	<div> <div>87%</div> <div>9%</div> <div>5%</div> </div>
1	E	310	<div> <div>89%</div> <div>7%</div> <div>5%</div> </div>
1	F	310	<div> <div>88%</div> <div>7%</div> <div>5%</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14829 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	2	0
			2280	1451	379	437	13			
1	B	296	Total	C	N	O	S	0	1	0
			2282	1451	379	439	13			
1	C	296	Total	C	N	O	S	0	2	0
			2285	1453	380	439	13			
1	D	296	Total	C	N	O	S	0	1	0
			2280	1450	379	438	13			
1	E	296	Total	C	N	O	S	0	3	0
			2291	1456	381	440	14			
1	F	297	Total	C	N	O	S	0	0	0
			2284	1452	378	441	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP A0A2U0QMK8
A	-10	ARG	-	expression tag	UNP A0A2U0QMK8
A	-9	GLY	-	expression tag	UNP A0A2U0QMK8
A	-8	SER	-	expression tag	UNP A0A2U0QMK8
A	-7	HIS	-	expression tag	UNP A0A2U0QMK8
A	-6	HIS	-	expression tag	UNP A0A2U0QMK8
A	-5	HIS	-	expression tag	UNP A0A2U0QMK8
A	-4	HIS	-	expression tag	UNP A0A2U0QMK8
A	-3	HIS	-	expression tag	UNP A0A2U0QMK8
A	-2	HIS	-	expression tag	UNP A0A2U0QMK8
A	-1	GLY	-	expression tag	UNP A0A2U0QMK8
A	0	SER	-	expression tag	UNP A0A2U0QMK8
A	84	ASP	ASN	engineered mutation	UNP A0A2U0QMK8
B	-11	MET	-	expression tag	UNP A0A2U0QMK8
B	-10	ARG	-	expression tag	UNP A0A2U0QMK8
B	-9	GLY	-	expression tag	UNP A0A2U0QMK8
B	-8	SER	-	expression tag	UNP A0A2U0QMK8

Continued on next page...

Continued from previous page...

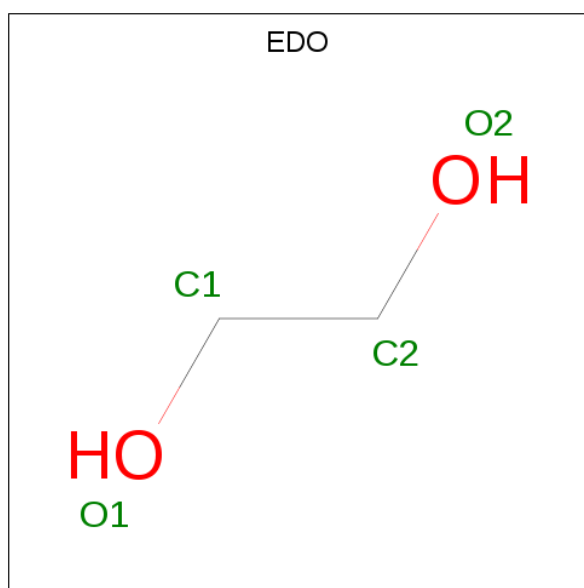
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP A0A2U0QMK8
B	-6	HIS	-	expression tag	UNP A0A2U0QMK8
B	-5	HIS	-	expression tag	UNP A0A2U0QMK8
B	-4	HIS	-	expression tag	UNP A0A2U0QMK8
B	-3	HIS	-	expression tag	UNP A0A2U0QMK8
B	-2	HIS	-	expression tag	UNP A0A2U0QMK8
B	-1	GLY	-	expression tag	UNP A0A2U0QMK8
B	0	SER	-	expression tag	UNP A0A2U0QMK8
B	84	ASP	ASN	engineered mutation	UNP A0A2U0QMK8
C	-11	MET	-	expression tag	UNP A0A2U0QMK8
C	-10	ARG	-	expression tag	UNP A0A2U0QMK8
C	-9	GLY	-	expression tag	UNP A0A2U0QMK8
C	-8	SER	-	expression tag	UNP A0A2U0QMK8
C	-7	HIS	-	expression tag	UNP A0A2U0QMK8
C	-6	HIS	-	expression tag	UNP A0A2U0QMK8
C	-5	HIS	-	expression tag	UNP A0A2U0QMK8
C	-4	HIS	-	expression tag	UNP A0A2U0QMK8
C	-3	HIS	-	expression tag	UNP A0A2U0QMK8
C	-2	HIS	-	expression tag	UNP A0A2U0QMK8
C	-1	GLY	-	expression tag	UNP A0A2U0QMK8
C	0	SER	-	expression tag	UNP A0A2U0QMK8
C	84	ASP	ASN	engineered mutation	UNP A0A2U0QMK8
D	-11	MET	-	expression tag	UNP A0A2U0QMK8
D	-10	ARG	-	expression tag	UNP A0A2U0QMK8
D	-9	GLY	-	expression tag	UNP A0A2U0QMK8
D	-8	SER	-	expression tag	UNP A0A2U0QMK8
D	-7	HIS	-	expression tag	UNP A0A2U0QMK8
D	-6	HIS	-	expression tag	UNP A0A2U0QMK8
D	-5	HIS	-	expression tag	UNP A0A2U0QMK8
D	-4	HIS	-	expression tag	UNP A0A2U0QMK8
D	-3	HIS	-	expression tag	UNP A0A2U0QMK8
D	-2	HIS	-	expression tag	UNP A0A2U0QMK8
D	-1	GLY	-	expression tag	UNP A0A2U0QMK8
D	0	SER	-	expression tag	UNP A0A2U0QMK8
D	84	ASP	ASN	engineered mutation	UNP A0A2U0QMK8
E	-11	MET	-	expression tag	UNP A0A2U0QMK8
E	-10	ARG	-	expression tag	UNP A0A2U0QMK8
E	-9	GLY	-	expression tag	UNP A0A2U0QMK8
E	-8	SER	-	expression tag	UNP A0A2U0QMK8
E	-7	HIS	-	expression tag	UNP A0A2U0QMK8
E	-6	HIS	-	expression tag	UNP A0A2U0QMK8
E	-5	HIS	-	expression tag	UNP A0A2U0QMK8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP A0A2U0QMK8
E	-3	HIS	-	expression tag	UNP A0A2U0QMK8
E	-2	HIS	-	expression tag	UNP A0A2U0QMK8
E	-1	GLY	-	expression tag	UNP A0A2U0QMK8
E	0	SER	-	expression tag	UNP A0A2U0QMK8
E	84	ASP	ASN	engineered mutation	UNP A0A2U0QMK8
F	-11	MET	-	expression tag	UNP A0A2U0QMK8
F	-10	ARG	-	expression tag	UNP A0A2U0QMK8
F	-9	GLY	-	expression tag	UNP A0A2U0QMK8
F	-8	SER	-	expression tag	UNP A0A2U0QMK8
F	-7	HIS	-	expression tag	UNP A0A2U0QMK8
F	-6	HIS	-	expression tag	UNP A0A2U0QMK8
F	-5	HIS	-	expression tag	UNP A0A2U0QMK8
F	-4	HIS	-	expression tag	UNP A0A2U0QMK8
F	-3	HIS	-	expression tag	UNP A0A2U0QMK8
F	-2	HIS	-	expression tag	UNP A0A2U0QMK8
F	-1	GLY	-	expression tag	UNP A0A2U0QMK8
F	0	SER	-	expression tag	UNP A0A2U0QMK8
F	84	ASP	ASN	engineered mutation	UNP A0A2U0QMK8

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



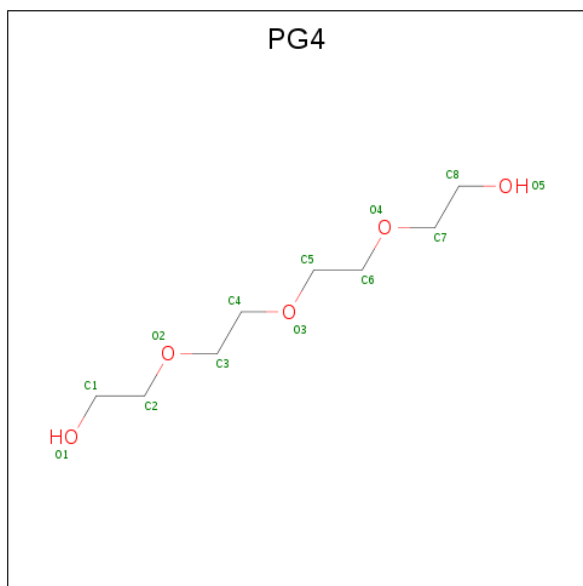
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	E	1	Total	C	O	0	0
			4	2	2		
2	E	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 TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

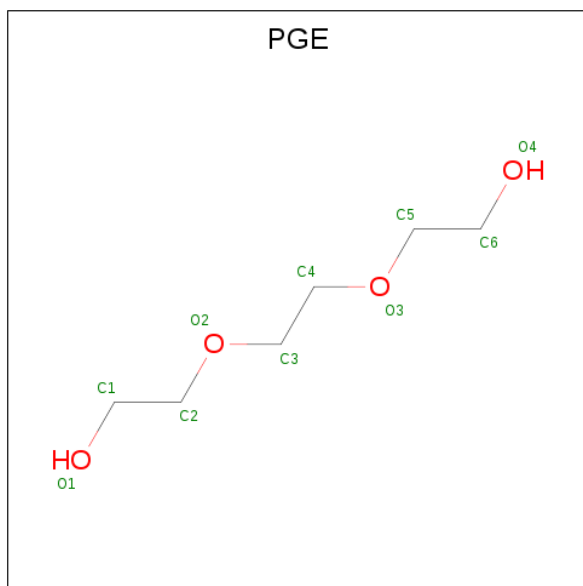


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		
4	C	1	Total	Mg	0	0
			1	1		
4	F	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



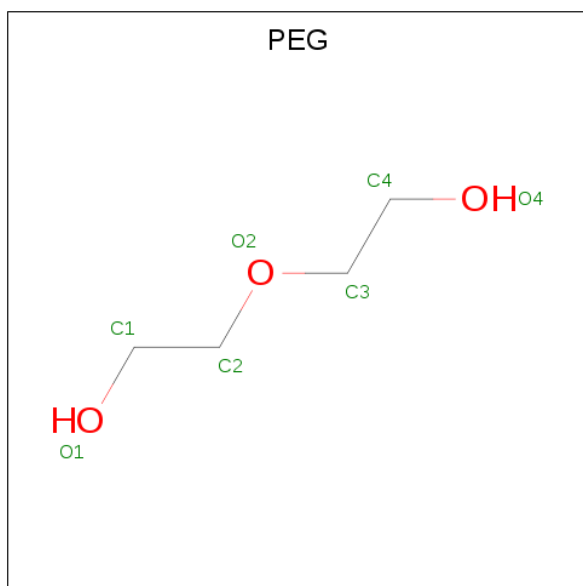
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	182	Total 182	O 182	0	0
9	B	164	Total 164	O 164	0	0
9	C	155	Total 155	O 155	0	0
9	D	151	Total 151	O 151	0	0
9	E	164	Total 164	O 164	0	0
9	F	171	Total 171	O 171	0	0

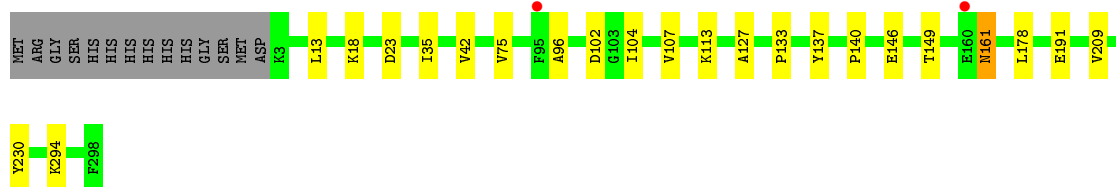
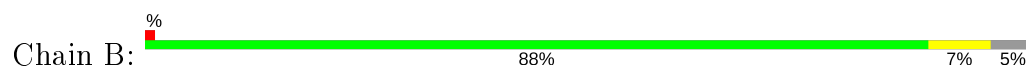
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

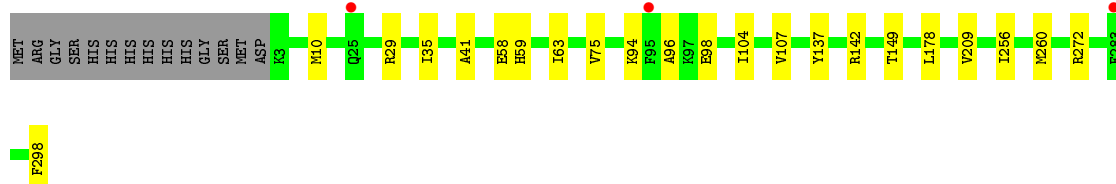
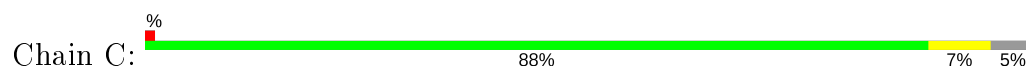
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



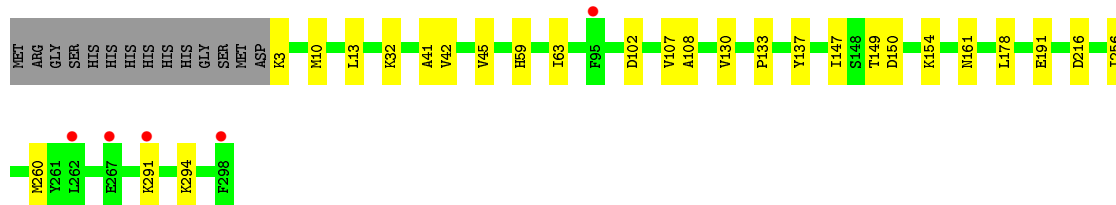
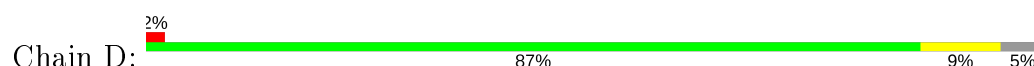
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



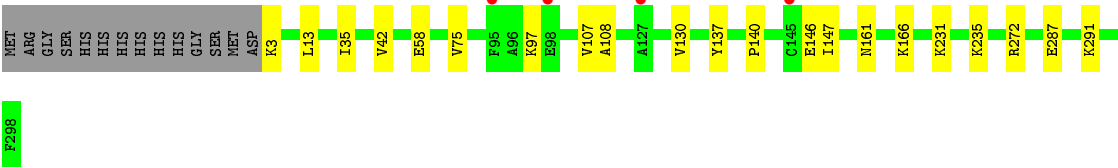
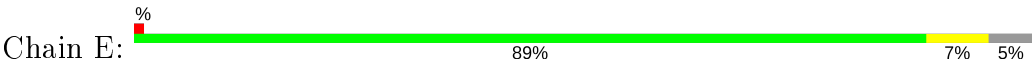
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



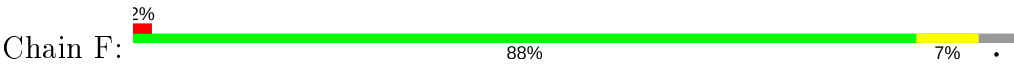
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



● 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, α , β , γ	84.99Å 231.42Å 200.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 1.87 43.76 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.44-1.87) 99.2 (43.76-1.87)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.87Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.189 , 0.221 0.189 , 0.221	Depositor DCC
R_{free} test set	8064 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14829	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/2314	0.49	0/3128
1	B	0.28	0/2311	0.49	0/3124
1	C	0.27	0/2320	0.49	0/3136
1	D	0.31	0/2310	0.50	0/3124
1	E	0.29	0/2326	0.49	0/3144
1	F	0.29	0/2308	0.49	0/3121
All	All	0.29	0/13889	0.49	0/18777

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	166	KPI	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2280	0	2313	9	0
1	B	2282	0	2318	14	0
1	C	2285	0	2320	12	0
1	D	2280	0	2309	16	0
1	E	2291	0	2324	15	0
1	F	2284	0	2312	14	0
2	A	4	0	6	1	0
2	B	12	0	17	2	0
2	C	4	0	6	1	0
2	E	8	0	12	0	0
2	F	16	0	24	0	0
3	A	13	0	18	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	F	2	0	0	0	0
5	B	10	0	14	0	0
5	C	10	0	14	0	0
5	D	10	0	14	2	0
5	E	10	0	14	0	0
6	B	4	0	3	0	0
6	C	12	0	9	0	0
6	D	4	0	3	0	0
6	E	4	0	3	0	0
7	E	6	0	8	3	0
8	F	7	0	10	1	0
9	A	182	0	0	1	0
9	B	164	0	0	0	0
9	C	155	0	0	0	0
9	D	151	0	0	3	0
9	E	164	0	0	3	0
9	F	171	0	0	2	0
All	All	14829	0	14071	78	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.

The worst 5 of 78 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:142:ARG:HE	2:A:301:EDO:H21	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:GLU:HG3	7:E:304:GOL:H2	1.68	0.74
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.75	0.67
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.76	0.67
1:E:58:GLU:OE2	1:E:272:ARG:NH2	2.26	0.66

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	295/310 (95%)	290 (98%)	5 (2%)	0	100	100
1	B	294/310 (95%)	289 (98%)	5 (2%)	0	100	100
1	C	295/310 (95%)	290 (98%)	5 (2%)	0	100	100
1	D	294/310 (95%)	289 (98%)	5 (2%)	0	100	100
1	E	296/310 (96%)	291 (98%)	5 (2%)	0	100	100
1	F	294/310 (95%)	289 (98%)	5 (2%)	0	100	100
All	All	1768/1860 (95%)	1738 (98%)	30 (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	248/260 (95%)	246 (99%)	2 (1%)	81	80
1	B	249/260 (96%)	247 (99%)	2 (1%)	81	80
1	C	250/260 (96%)	250 (100%)	0	100	100
1	D	248/260 (95%)	246 (99%)	2 (1%)	81	80
1	E	251/260 (96%)	251 (100%)	0	100	100
1	F	248/260 (95%)	247 (100%)	1 (0%)	91	90
All	All	1494/1560 (96%)	1487 (100%)	7 (0%)	91	88

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	294	LYS
1	F	2	ASP
1	D	191	GLU
1	A	161[B]	ASN
1	D	291	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	B	166	1	10,13,14	0.60	0	6,15,17	3.27	3 (50%)
1	KPI	A	166	1	10,13,14	0.67	0	6,15,17	3.24	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KPI	D	166	1	10,13,14	0.65	0	6,15,17	3.45	3 (50%)
1	KPI	C	166	1	10,13,14	1.41	1 (10%)	6,15,17	3.74	3 (50%)
1	KPI	F	166	1	10,13,14	1.39	1 (10%)	6,15,17	3.25	2 (33%)
1	KPI	E	166	1	10,13,14	1.39	1 (10%)	6,15,17	3.44	2 (33%)

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	B	166	1	-	0/9/14/16	-
1	KPI	A	166	1	-	0/9/14/16	-
1	KPI	D	166	1	-	1/9/14/16	-
1	KPI	C	166	1	-	1/9/14/16	-
1	KPI	F	166	1	-	1/9/14/16	-
1	KPI	E	166	1	-	2/9/14/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	KPI	O-C	4.05	1.36	1.19
1	E	166	KPI	O-C	4.01	1.35	1.19
1	C	166	KPI	O-C	3.98	1.35	1.19

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	KPI	C1-CX1-CX2	-8.04	109.01	117.92
1	D	166	KPI	C1-CX1-CX2	-7.25	109.89	117.92
1	E	166	KPI	C1-CX1-CX2	-7.23	109.91	117.92
1	B	166	KPI	C1-CX1-CX2	-6.77	110.42	117.92
1	F	166	KPI	C1-CX1-CX2	-6.75	110.44	117.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	C1-CX1-NZ-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	F	166	KPI	C1-CX1-NZ-CE
1	E	166	KPI	C-CA-CB-CG
1	E	166	KPI	C1-CX1-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 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	$\# Z > 2$
5	PGE	D	301	-	9,9,9	0.30	0	8,8,8	0.31	0
6	ACT	C	305	-	1,3,3	1.32	0	0,3,3	0.00	-
6	ACT	E	305	-	1,3,3	1.33	0	0,3,3	0.00	-
3	PG4	A	302	-	12,12,12	0.52	0	11,11,11	0.17	0
6	ACT	B	308	-	1,3,3	1.18	0	0,3,3	0.00	-
5	PGE	C	303	-	9,9,9	0.30	0	8,8,8	0.25	0
2	EDO	C	302	-	3,3,3	0.37	0	2,2,2	0.33	0
2	EDO	F	303	-	3,3,3	0.45	0	2,2,2	0.25	0
2	EDO	B	305	4	3,3,3	0.42	0	2,2,2	0.34	0
6	ACT	D	302	-	1,3,3	1.46	0	0,3,3	0.00	-
2	EDO	F	306	-	3,3,3	0.44	0	2,2,2	0.42	0
5	PGE	B	307	-	9,9,9	0.30	0	8,8,8	0.32	0
7	GOL	E	304	-	5,5,5	0.43	0	5,5,5	0.47	0
2	EDO	A	301	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	B	304	-	3,3,3	0.45	0	2,2,2	0.34	0
2	EDO	F	304	-	3,3,3	0.44	0	2,2,2	0.42	0
2	EDO	F	305	-	3,3,3	0.45	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	306	-	3,3,3	0.47	0	2,2,2	0.36	0
2	EDO	E	302	-	3,3,3	0.41	0	2,2,2	0.42	0
6	ACT	C	306	-	1,3,3	1.46	0	0,3,3	0.00	-
6	ACT	C	304	-	1,3,3	1.25	0	0,3,3	0.00	-
2	EDO	E	301	-	3,3,3	0.49	0	2,2,2	0.28	0
5	PGE	E	303	-	9,9,9	0.31	0	8,8,8	0.33	0
8	PEG	F	307	-	6,6,6	0.49	0	5,5,5	0.28	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	301	PGE	O2-C3-C4-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	E	304	GOL	O1-C1-C2-C3
8	F	307	PEG	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
5	D	301	PGE	O3-C5-C6-O4

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	301	PGE	2	0
2	C	302	EDO	1	0
2	B	305	EDO	2	0
7	E	304	GOL	3	0
2	A	301	EDO	1	0
8	F	307	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/310 (95%)	0.12	2 (0%) 87 88	18, 25, 39, 48	0
1	B	295/310 (95%)	0.13	2 (0%) 87 88	18, 25, 39, 48	0
1	C	295/310 (95%)	0.26	3 (1%) 82 83	20, 27, 40, 52	0
1	D	295/310 (95%)	0.22	5 (1%) 70 72	20, 27, 41, 48	0
1	E	295/310 (95%)	0.09	4 (1%) 75 77	19, 26, 39, 49	0
1	F	296/310 (95%)	0.17	6 (2%) 65 67	18, 26, 41, 51	0
All	All	1771/1860 (95%)	0.17	22 (1%) 79 80	18, 26, 40, 52	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	95	PHE	4.4
1	E	127	ALA	2.7
1	F	267	GLU	2.6
1	D	298	PHE	2.5
1	F	266	ILE	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	A	166	14/15	0.93	0.13	17,22,29,30	0
1	KPI	E	166	14/15	0.93	0.11	18,24,28,32	0
1	KPI	C	166	14/15	0.94	0.15	17,23,29,31	0
1	KPI	D	166	14/15	0.95	0.12	20,25,30,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	KPI	F	166	14/15	0.96	0.13	19,23,30,34	0
1	KPI	B	166	14/15	0.96	0.10	15,20,30,30	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
6	ACT	C	306	4/4	0.75	0.20	39,43,45,51	0
2	EDO	F	305	4/4	0.78	0.35	37,45,46,51	0
6	ACT	B	308	4/4	0.78	0.19	45,50,52,62	0
2	EDO	C	302	4/4	0.82	0.29	28,29,34,40	0
6	ACT	D	302	4/4	0.82	0.18	35,39,43,45	0
2	EDO	F	306	4/4	0.83	0.18	29,31,34,35	0
6	ACT	E	305	4/4	0.87	0.21	29,39,40,46	0
6	ACT	C	304	4/4	0.87	0.26	35,39,39,53	0
2	EDO	E	302	4/4	0.87	0.20	32,37,37,39	0
8	PEG	F	307	7/7	0.88	0.12	39,41,44,51	0
2	EDO	B	306	4/4	0.89	0.12	40,41,44,44	0
2	EDO	A	301	4/4	0.89	0.10	39,40,46,50	0
5	PGE	C	303	10/10	0.89	0.16	35,42,49,52	0
4	MG	F	301	1/1	0.90	0.24	54,54,54,54	0
6	ACT	C	305	4/4	0.91	0.14	47,47,49,52	0
7	GOL	E	304	6/6	0.91	0.26	32,37,38,39	0
5	PGE	D	301	10/10	0.91	0.14	32,36,45,54	0
5	PGE	E	303	10/10	0.91	0.17	34,38,47,51	0
5	PGE	B	307	10/10	0.91	0.16	31,39,42,50	0
3	PG4	A	302	13/13	0.92	0.14	28,34,47,50	0
2	EDO	B	304	4/4	0.92	0.13	30,35,36,43	0
2	EDO	F	304	4/4	0.92	0.23	38,42,42,44	0
4	MG	F	302	1/1	0.92	0.07	34,34,34,34	0
2	EDO	B	305	4/4	0.92	0.21	25,29,29,38	0
2	EDO	E	301	4/4	0.95	0.11	24,28,31,35	0
4	MG	B	302	1/1	0.96	0.10	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	C	301	1/1	0.96	0.18	48,48,48,48	0
2	EDO	F	303	4/4	0.97	0.12	21,24,27,27	0
4	MG	B	303	1/1	0.98	0.12	33,33,33,33	0
4	MG	B	301	1/1	0.98	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.