



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2021 – 11:24 AM EST

PDB ID : 7KM0  
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H59A mutant with pyruvate bound in the active site and R,R-bislysine bound at the allosteric site  
Authors : Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.  
Deposited on : 2020-11-02  
Resolution : 2.60 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.

---

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

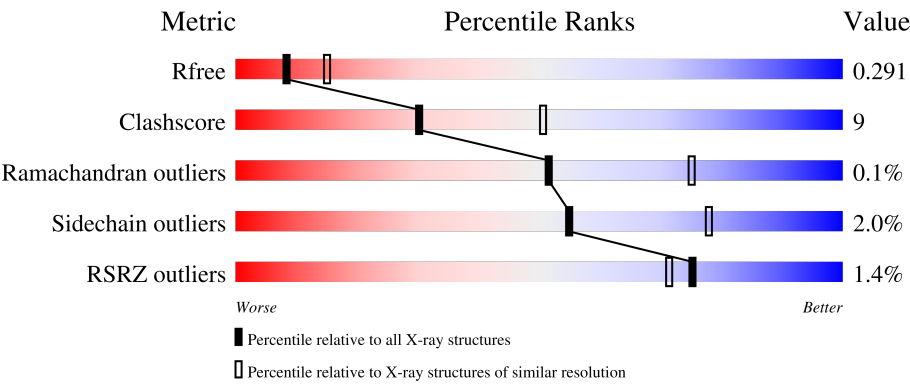
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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>2%</div><div>73%22%5%</div></div>
1	B	310	<div><div>2%</div><div>75%19%5%</div></div>
1	C	310	<div><div>2%</div><div>72%23%5%</div></div>
1	D	310	<div><div>2%</div><div>76%19%5%</div></div>
1	E	310	<div><div>2%</div><div>74%21%5%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	310	<div> <div>%</div> <div> </div> <div>72% 23% 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
5	EDO	A	305	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14108 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
			2262	1438	374	437	13			
1	B	296	Total	C	N	O	S	0	0	0
			2266	1441	375	437	13			
1	C	296	Total	C	N	O	S	0	0	0
			2259	1437	372	437	13			
1	D	296	Total	C	N	O	S	0	0	0
			2246	1428	371	434	13			
1	E	296	Total	C	N	O	S	0	0	0
			2258	1433	375	437	13			
1	F	296	Total	C	N	O	S	0	0	0
			2274	1447	377	437	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	59	ALA	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

*Continued on next page...*

*Continued from previous page...*

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	59	ALA	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	59	ALA	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	59	ALA	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

*Continued on next page...*

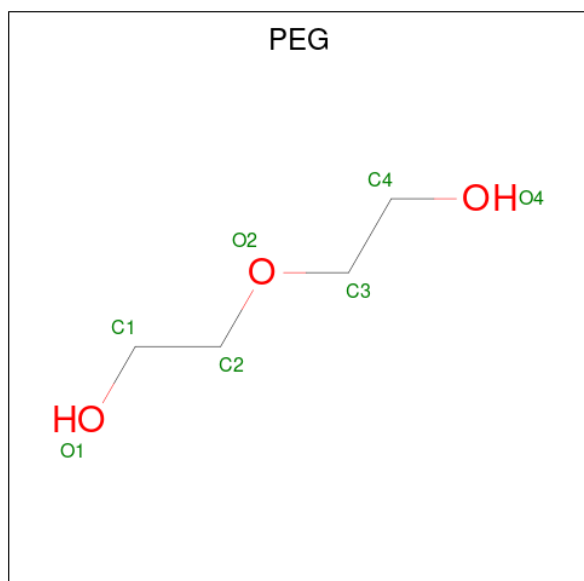
Continued from previous page...

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	59	ALA	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	59	ALA	HIS	engineered mutation	UNP Q9PPB4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

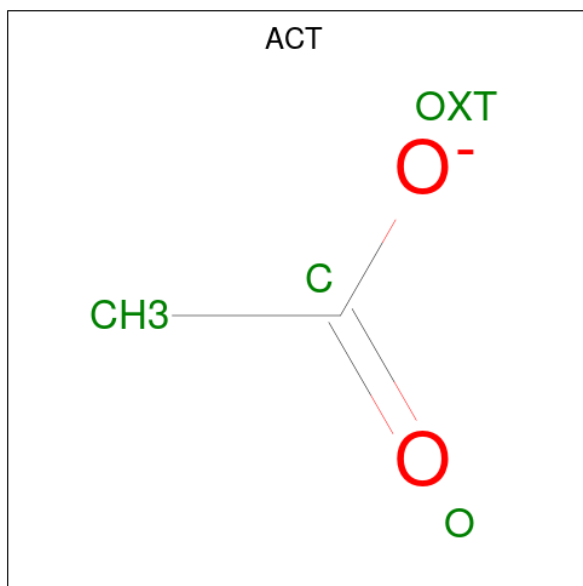
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

- 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	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

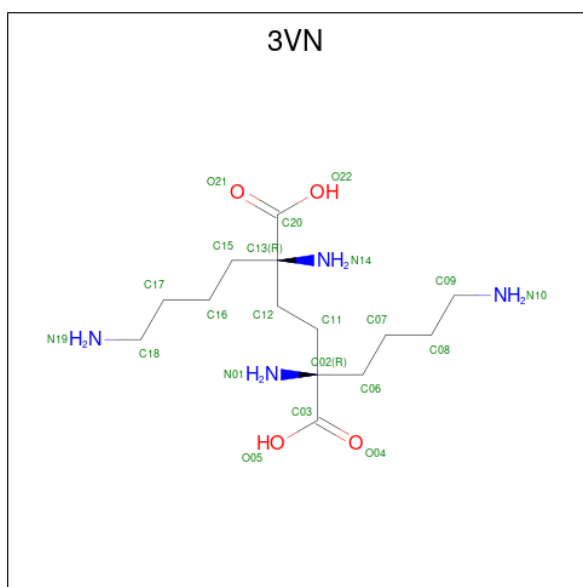
- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

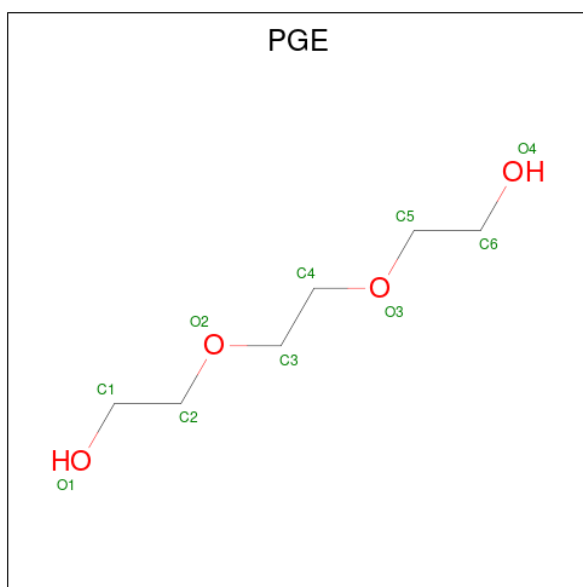
- Molecule 6 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (three-letter code: 3VN) (formula:  $C_{14}H_{30}N_4O_4$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			22	14	4	4		
6	D	1	Total	C	N	O	0	0
			22	14	4	4		
6	E	1	Total	C	N	O	0	0
			22	14	4	4		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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

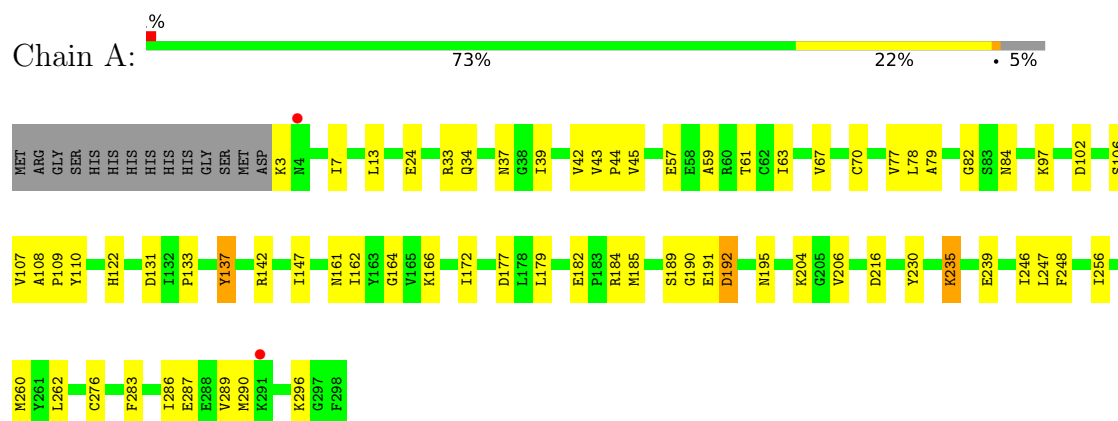
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	78	Total 78	O 78	0	0
8	B	68	Total 68	O 68	0	0
8	C	67	Total 67	O 67	0	0
8	D	60	Total 60	O 60	0	0
8	E	75	Total 75	O 75	0	0
8	F	73	Total 73	O 73	0	0

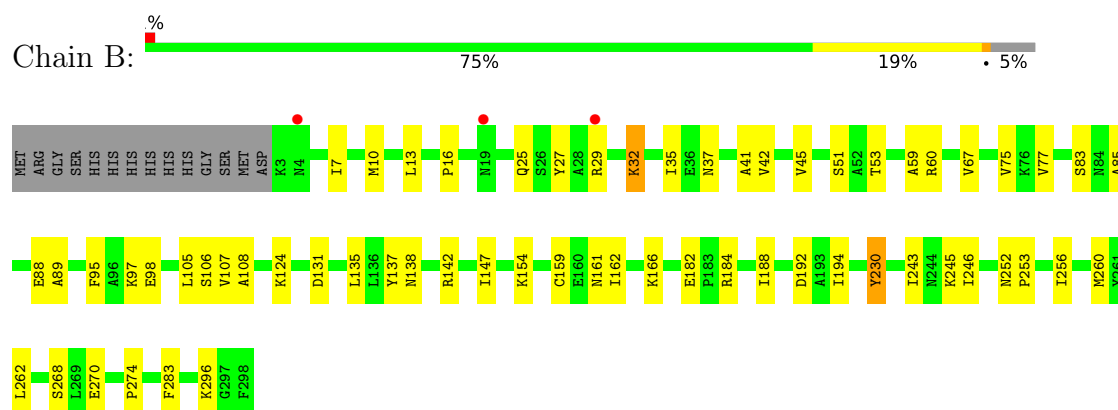
### 3 Residue-property plots [i](#)

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.

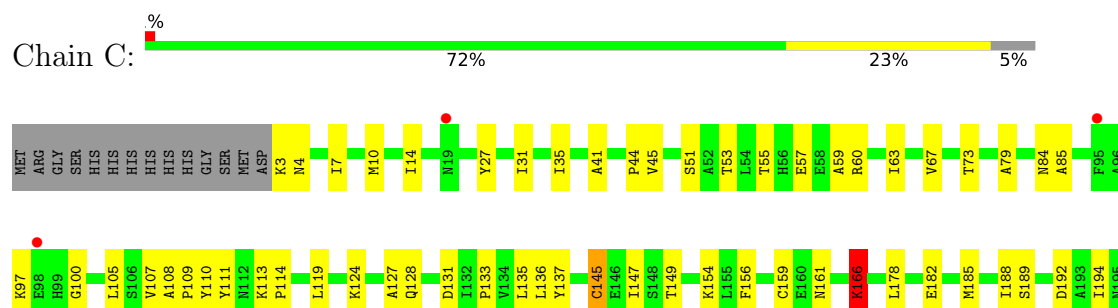
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

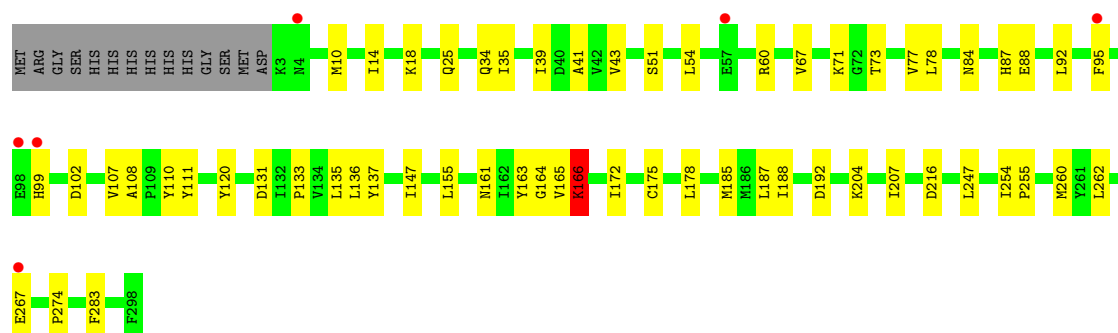
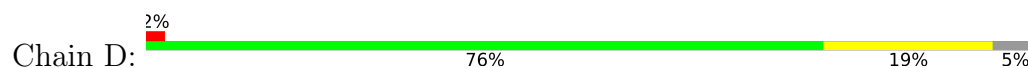


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

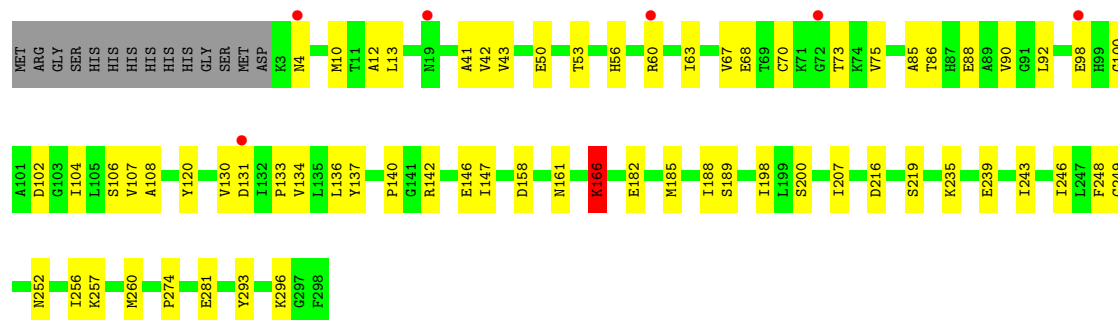
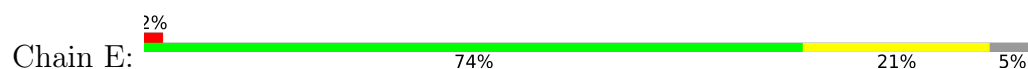




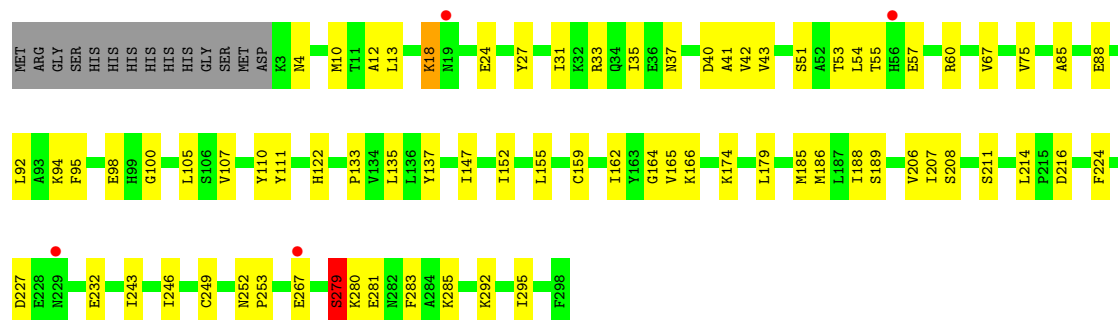
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- 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, $\alpha$ , $\beta$ , $\gamma$	84.90Å 230.40Å 201.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.30 – 2.60 21.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (21.30-2.60) 98.8 (21.30-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.95 (at 2.60Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.235 , 0.293 0.234 , 0.291	Depositor DCC
$R_{free}$ test set	3046 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtriage
Anisotropy	1.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	14108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: MG, PEG, ACT, 3VN, KPI, EDO, PGE

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	0.39	1/2285 (0.0%)	0.51	0/3093
1	B	0.55	1/2289 (0.0%)	0.53	0/3097
1	C	0.40	0/2282	0.55	0/3089
1	D	0.49	0/2269	0.58	0/3075
1	E	0.52	0/2280	0.57	0/3084
1	F	0.35	0/2297	0.54	0/3105
All	All	0.45	2/13702 (0.0%)	0.55	0/18543

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
1	D	0	1
1	E	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	CYS	CB-SG	-5.56	1.72	1.81
1	B	230	TYR	CE2-CZ	-5.28	1.31	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	166	KPI	Mainchain
1	D	166	KPI	Mainchain
1	E	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	2262	0	2284	45	0
1	B	2266	0	2295	41	0
1	C	2259	0	2278	50	0
1	D	2246	0	2247	43	0
1	E	2258	0	2286	39	0
1	F	2274	0	2318	50	0
2	A	1	0	0	0	0
3	A	7	0	10	3	0
3	C	7	0	10	1	0
3	D	7	0	10	0	0
4	A	4	0	3	1	0
5	A	8	0	12	5	0
5	B	4	0	6	0	0
5	D	8	0	12	0	0
6	B	22	0	28	6	0
6	D	22	0	28	3	0
6	E	22	0	28	3	0
7	B	10	0	14	1	0
8	A	78	0	0	1	0
8	B	68	0	0	4	0
8	C	67	0	0	1	0
8	D	60	0	0	0	0
8	E	75	0	0	2	0
8	F	73	0	0	1	0
All	All	14108	0	13869	256	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 9.

All (256) 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:C:97:LYS:HE2	1:C:131:ASP:OD1	1.67	0.95
6:E:301:3VN:H23	1:F:51:SER:O	1.71	0.90
1:A:246:ILE:HG21	1:A:289:VAL:HG11	1.52	0.88
6:E:301:3VN:C18	1:F:51:SER:O	2.26	0.83
1:F:246:ILE:HD11	1:F:285:LYS:HG2	1.61	0.82
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.68	0.74
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.67	0.74
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.69	0.74
1:E:4:ASN:HB2	1:E:133:PRO:HG3	1.71	0.72
1:C:97:LYS:CE	1:C:131:ASP:OD1	2.38	0.72
6:B:301:3VN:N19	1:C:51:SER:O	2.23	0.71
1:F:55:THR:HG22	1:F:57:GLU:H	1.56	0.71
1:C:45:VAL:HG11	1:C:59:ALA:HA	1.72	0.71
1:E:131:ASP:HA	1:E:161:ASN:HD21	1.56	0.71
1:F:12:ALA:HA	1:F:43:VAL:HB	1.73	0.70
1:B:25:GLN:NE2	8:B:401:HOH:O	2.25	0.70
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.74	0.69
1:E:130:VAL:O	1:E:161:ASN:ND2	2.27	0.67
1:B:13:LEU:HD11	1:B:42:VAL:HB	1.78	0.66
1:D:60:ARG:HE	1:D:99:HIS:HE1	1.42	0.66
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.79	0.65
1:B:45:VAL:HG11	1:B:59:ALA:HA	1.79	0.65
1:B:51:SER:O	6:B:301:3VN:N10	2.32	0.62
1:B:10:MET:HG2	1:B:41:ALA:HB3	1.81	0.62
1:B:154:LYS:HD2	7:B:303:PGE:H2	1.82	0.61
1:B:51:SER:HB2	6:B:301:3VN:H12	1.65	0.61
1:E:235:LYS:O	1:E:239:GLU:HG3	1.99	0.61
1:D:108:ALA:HB2	1:D:147:ILE:HD11	1.83	0.61
1:E:12:ALA:HA	1:E:43:VAL:HB	1.83	0.61
1:C:127:ALA:O	1:C:161:ASN:ND2	2.34	0.60
1:D:178:LEU:HD22	1:D:185:MET:HE1	1.83	0.60
1:C:10:MET:HG2	1:C:41:ALA:HB3	1.83	0.60
1:D:175:CYS:HB3	1:D:187:LEU:HD21	1.84	0.60
1:C:288:GLU:HA	1:C:291:LYS:HE2	1.85	0.59
1:E:73:THR:HG23	1:E:75:VAL:H	1.67	0.59
1:C:119:LEU:HD11	1:C:145:CYS:SG	2.43	0.59
1:A:33:ARG:O	1:A:37:ASN:ND2	2.32	0.58
1:D:18:LYS:HD3	1:D:267:GLU:OE1	2.02	0.58
1:C:108:ALA:HB2	1:C:147:ILE:HD11	1.85	0.58
1:A:33:ARG:NH2	1:A:296:LYS:O	2.21	0.58
1:D:95:PHE:O	1:D:99:HIS:HD2	1.87	0.58
1:D:25:GLN:N	1:D:25:GLN:OE1	2.35	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:LEU:HD11	1:F:42:VAL:HB	1.85	0.57
1:E:243:ILE:HA	1:E:246:ILE:HG22	1.85	0.57
1:E:142:ARG:NH1	1:F:111:TYR:O	2.36	0.57
1:F:10:MET:HG2	1:F:41:ALA:HB3	1.85	0.57
1:C:243:ILE:HA	1:C:246:ILE:HG22	1.86	0.57
1:A:13:LEU:HD11	1:A:42:VAL:HB	1.86	0.56
1:F:216:ASP:OD1	1:F:216:ASP:N	2.38	0.56
1:C:166:KPI:HDA	1:C:207:ILE:HD12	1.86	0.56
1:F:18:LYS:HE3	1:F:267:GLU:OE1	2.06	0.55
6:E:301:3VN:N19	1:F:51:SER:O	2.39	0.55
1:A:191:GLU:HA	5:A:305:EDO:H22	1.88	0.55
1:C:3:LYS:NZ	1:C:159:CYS:O	2.40	0.55
1:C:4:ASN:HB3	1:C:133:PRO:HG3	1.89	0.55
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.88	0.55
1:D:131:ASP:OD1	1:D:131:ASP:N	2.35	0.55
1:E:281:GLU:N	1:E:281:GLU:OE1	2.38	0.54
1:F:147:ILE:O	1:F:174:LYS:NZ	2.36	0.53
1:E:13:LEU:HD11	1:E:42:VAL:HB	1.89	0.53
1:C:14:ILE:HD13	1:C:260:MET:HG3	1.89	0.53
1:A:216:ASP:OD1	1:A:216:ASP:N	2.42	0.53
1:E:104:ILE:HD11	1:E:134:VAL:HG22	1.91	0.53
1:D:35:ILE:HG21	1:D:73:THR:HG21	1.91	0.53
1:D:137:TYR:CE1	1:D:166:KPI:HEA	2.44	0.53
1:F:60:ARG:HB2	1:F:95:PHE:CZ	2.44	0.53
1:C:149:THR:HG23	1:C:178:LEU:HD23	1.90	0.53
1:D:120:TYR:HA	1:D:155:LEU:HD21	1.91	0.52
1:C:124:LYS:HE3	1:C:128:GLN:NE2	2.24	0.52
1:C:189:SER:HB3	1:C:206:VAL:HG12	1.91	0.52
1:D:60:ARG:CG	1:D:99:HIS:CE1	2.92	0.52
1:B:85:ALA:HA	1:C:53:THR:HG22	1.90	0.52
1:A:7:ILE:HB	1:A:204:LYS:O	2.09	0.52
1:C:44:PRO:HD2	1:C:79:ALA:HA	1.90	0.52
1:E:102:ASP:O	1:E:133:PRO:HD2	2.09	0.52
1:F:31:ILE:O	1:F:35:ILE:HG12	2.10	0.52
1:F:188:ILE:HG21	1:F:207:ILE:HG13	1.91	0.52
1:F:67:VAL:HG11	1:F:100:GLY:HA3	1.92	0.52
1:C:256:ILE:O	1:C:260:MET:HG2	2.10	0.51
1:C:35:ILE:HG21	1:C:73:THR:HG21	1.92	0.51
1:B:7:ILE:HG22	1:B:188:ILE:HD11	1.91	0.51
1:C:214:LEU:HD11	1:C:243:ILE:HD13	1.93	0.51
1:D:188:ILE:HG21	1:D:207:ILE:HG13	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ARG:HG3	1:D:99:HIS:CE1	2.46	0.49
1:D:67:VAL:HA	1:D:77:VAL:HG21	1.94	0.49
1:C:97:LYS:O	1:C:97:LYS:HG2	2.13	0.49
1:A:172:ILE:HG23	1:B:194:ILE:HG21	1.93	0.49
1:A:287:GLU:HA	1:A:290:MET:HE3	1.95	0.49
1:F:246:ILE:HD12	1:F:249:CYS:HB3	1.94	0.49
1:A:59:ALA:O	1:A:63:ILE:HG13	2.13	0.48
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.96	0.48
1:A:3:LYS:HE2	1:A:162:ILE:O	2.13	0.48
1:F:51:SER:HA	1:F:54:LEU:HD12	1.95	0.48
1:F:24:GLU:N	8:F:312:HOH:O	2.44	0.48
1:A:190:GLY:O	5:A:305:EDO:H11	2.13	0.48
1:F:27:TYR:O	1:F:31:ILE:HG13	2.12	0.48
1:E:10:MET:HG2	1:E:41:ALA:HB3	1.94	0.48
1:E:88:GLU:O	1:E:92:LEU:HG	2.14	0.48
1:E:67:VAL:HG11	1:E:100:GLY:HA3	1.95	0.48
1:D:84:ASN:ND2	6:D:301:3VN:O05	2.47	0.48
1:B:83:SER:HB3	1:B:89:ALA:HB2	1.94	0.47
1:A:235:LYS:O	1:A:239:GLU:HG3	2.14	0.47
1:E:85:ALA:HA	1:F:53:THR:HG22	1.95	0.47
1:F:155:LEU:HB3	1:F:162:ILE:HD13	1.95	0.47
1:A:142:ARG:HG2	1:D:111:TYR:O	2.13	0.47
1:B:83:SER:OG	1:B:88:GLU:HG3	2.14	0.47
1:D:14:ILE:HD13	1:D:260:MET:HG3	1.97	0.47
3:A:302:PEG:H11	6:D:301:3VN:H3	1.97	0.47
1:C:216:ASP:N	1:C:216:ASP:OD1	2.48	0.47
1:A:67:VAL:HA	1:A:77:VAL:HG21	1.97	0.47
1:A:97:LYS:HE2	1:A:131:ASP:HB2	1.97	0.47
1:A:182:GLU:OE2	1:A:184:ARG:HD3	2.14	0.47
1:F:4:ASN:HB3	1:F:133:PRO:HG3	1.95	0.47
1:A:177:ASP:OD2	4:A:303:ACT:H1	2.15	0.47
1:A:195:ASN:ND2	8:A:406:HOH:O	2.40	0.47
3:A:302:PEG:O2	6:D:301:3VN:H7	2.15	0.47
1:C:55:THR:OG1	1:C:57:GLU:HG2	2.15	0.46
1:C:10:MET:HA	1:C:41:ALA:O	2.15	0.46
1:B:252:ASN:ND2	8:B:405:HOH:O	2.31	0.46
1:E:189:SER:HB2	1:E:198:ILE:HG21	1.96	0.46
1:F:292:LYS:HD3	1:F:292:LYS:N	2.30	0.46
1:B:243:ILE:HA	1:B:246:ILE:HG22	1.96	0.46
1:C:67:VAL:HG11	1:C:100:GLY:HA3	1.97	0.46
1:B:16:PRO:HD2	1:B:27:TYR:HD1	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ASP:O	1:D:133:PRO:HD2	2.16	0.46
1:A:276:CYS:HA	5:A:304:EDO:H11	1.97	0.46
1:E:108:ALA:HB2	1:E:147:ILE:HD11	1.98	0.46
1:E:248:PHE:CE2	1:E:252:ASN:HB2	2.51	0.46
1:D:135:LEU:HD13	1:D:163:TYR:CZ	2.51	0.46
1:D:166:KPI:HDA	1:D:207:ILE:HD12	1.98	0.46
1:A:45:VAL:HG11	1:A:59:ALA:HA	1.97	0.46
1:A:37:ASN:OD1	1:A:296:LYS:HD3	2.16	0.46
1:B:98:GLU:HB2	8:B:436:HOH:O	2.15	0.45
1:F:94:LYS:O	1:F:98:GLU:HG2	2.16	0.45
1:A:189:SER:HB3	1:A:206:VAL:HG12	1.97	0.45
1:A:230:TYR:HD2	1:B:230:TYR:HD2	1.63	0.45
1:B:105:LEU:HD13	1:B:135:LEU:HD23	1.97	0.45
1:B:142:ARG:O	1:C:111:TYR:HA	2.16	0.45
1:F:208:SER:HB3	1:F:211:SER:OG	2.17	0.45
1:B:274:PRO:HB2	1:C:114:PRO:HB3	1.99	0.45
1:D:92:LEU:HA	1:D:95:PHE:HD2	1.81	0.45
1:E:188:ILE:HG21	1:E:207:ILE:HG13	1.98	0.45
1:E:274:PRO:HB3	1:F:122:HIS:HB2	1.99	0.45
1:B:159:CYS:HB2	1:B:162:ILE:HD12	1.97	0.45
1:E:246:ILE:HD12	1:E:249:CYS:HB3	1.99	0.45
1:F:164:GLY:HA3	1:F:186:MET:O	2.17	0.45
1:D:164:GLY:HA2	1:D:185:MET:HG2	1.97	0.45
1:E:140:PRO:HG3	1:E:146:GLU:OE2	2.16	0.45
1:C:3:LYS:NZ	1:C:156:PHE:O	2.32	0.45
1:D:216:ASP:OD1	1:D:216:ASP:N	2.50	0.45
1:A:248:PHE:CZ	5:A:305:EDO:H12	2.52	0.45
1:A:34:GLN:OE1	1:A:39:ILE:HG13	2.17	0.45
1:D:262:LEU:HD21	1:D:283:PHE:CE2	2.52	0.44
1:E:50:GLU:OE2	1:E:257:LYS:NZ	2.31	0.44
1:E:98:GLU:HG3	1:E:98:GLU:O	2.17	0.44
1:F:164:GLY:HA2	1:F:185:MET:CG	2.47	0.44
1:A:84:ASN:HA	1:A:109:PRO:HB3	1.98	0.44
1:A:108:ALA:HB2	1:A:147:ILE:HD11	1.99	0.44
1:C:63:ILE:O	1:C:67:VAL:HG23	2.18	0.44
1:C:84:ASN:HA	1:C:109:PRO:HB3	1.99	0.44
1:E:86:THR:O	1:E:90:VAL:HG23	2.17	0.44
1:F:246:ILE:HD12	1:F:246:ILE:HA	1.58	0.44
1:B:35:ILE:HG12	1:B:75:VAL:HG21	1.98	0.44
1:D:43:VAL:HG22	1:D:78:LEU:HB3	2.00	0.44
1:B:182:GLU:OE2	1:B:184:ARG:NH2	2.46	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:O	1:D:165:VAL:HA	2.18	0.44
1:F:55:THR:HG22	1:F:57:GLU:N	2.27	0.44
1:B:262:LEU:HD21	1:B:283:PHE:CE1	2.53	0.44
1:F:60:ARG:HB2	1:F:95:PHE:CE2	2.53	0.44
1:A:286:ILE:HG22	1:A:290:MET:HE2	1.99	0.44
1:C:7:ILE:HB	1:C:204:LYS:O	2.17	0.44
1:C:243:ILE:HB	1:C:293:TYR:CE2	2.53	0.44
1:F:214:LEU:HD21	1:F:295:ILE:HG12	2.00	0.44
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.80	0.43
1:D:51:SER:HA	1:D:54:LEU:HD12	2.00	0.43
1:D:254:ILE:HB	1:D:255:PRO:HD3	2.00	0.43
1:C:105:LEU:HD13	1:C:135:LEU:HD23	2.00	0.43
1:A:192:ASP:H	5:A:305:EDO:H22	1.83	0.43
1:D:71:LYS:HD2	1:D:71:LYS:HA	1.82	0.43
1:E:182:GLU:HB3	1:E:185:MET:HE3	2.00	0.43
1:C:154:LYS:NZ	3:C:301:PEG:H22	2.33	0.43
1:F:88:GLU:O	1:F:92:LEU:HG	2.18	0.43
1:A:102:ASP:O	1:A:133:PRO:HD2	2.18	0.43
1:B:252:ASN:ND2	1:B:253:PRO:HA	2.33	0.43
1:A:44:PRO:HD2	1:A:79:ALA:HA	1.99	0.43
1:B:97:LYS:HE3	1:B:131:ASP:HB2	2.00	0.43
1:B:138:ASN:HB2	1:B:147:ILE:HD12	2.01	0.43
1:E:120:TYR:OH	1:E:158:ASP:OD2	2.25	0.43
1:A:230:TYR:CD2	1:B:230:TYR:HD2	2.37	0.43
1:C:27:TYR:O	1:C:31:ILE:HG13	2.19	0.43
1:D:161:ASN:OD1	1:D:161:ASN:N	2.43	0.43
1:E:239:GLU:HA	8:E:460:HOH:O	2.18	0.43
1:F:185:MET:HG2	1:F:186:MET:N	2.32	0.43
1:A:262:LEU:HD21	1:A:283:PHE:CZ	2.54	0.43
1:C:124:LYS:HE3	1:C:128:GLN:HE22	1.83	0.43
1:E:53:THR:HG22	1:F:85:ALA:HA	1.99	0.43
1:C:247:LEU:HD13	1:C:256:ILE:HD13	2.00	0.43
1:A:142:ARG:HB3	1:D:111:TYR:CD1	2.54	0.42
1:B:37:ASN:OD1	1:B:296:LYS:HE2	2.19	0.42
1:C:194:ILE:HG21	1:D:172:ILE:HG23	2.01	0.42
1:E:56:HIS:O	1:E:60:ARG:HG3	2.19	0.42
6:B:301:3VN:H11	6:B:301:3VN:H6	1.68	0.42
1:B:268:SER:OG	1:B:270:GLU:HG3	2.20	0.42
1:E:256:ILE:O	1:E:260:MET:HG2	2.19	0.42
1:F:35:ILE:HG23	1:F:75:VAL:HG21	2.01	0.42
1:B:245:LYS:HA	1:B:245:LYS:HD2	1.91	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:ILE:HD13	1:F:165:VAL:HG11	2.01	0.42
6:B:301:3VN:O21	6:B:301:3VN:H13	2.19	0.42
1:C:292:LYS:NZ	8:C:411:HOH:O	2.50	0.42
1:A:24:GLU:OE2	1:A:61:THR:HG21	2.19	0.42
1:E:296:LYS:NZ	8:E:406:HOH:O	2.39	0.42
1:F:224:PHE:CD2	1:F:232:GLU:HB3	2.55	0.41
1:A:164:GLY:HA2	1:A:185:MET:HG3	2.01	0.41
1:B:108:ALA:HB2	1:B:147:ILE:HD11	2.02	0.41
1:E:136:LEU:O	1:E:166:KPI:N	2.53	0.41
1:F:164:GLY:HA2	1:F:185:MET:HG3	2.01	0.41
1:C:136:LEU:O	1:C:166:KPI:N	2.53	0.41
1:D:175:CYS:HB3	1:D:187:LEU:CD2	2.49	0.41
1:F:243:ILE:HA	1:F:246:ILE:HG22	2.01	0.41
1:B:67:VAL:HA	1:B:77:VAL:HG21	2.01	0.41
1:D:87:HIS:CD2	1:D:88:GLU:HG3	2.56	0.41
1:E:243:ILE:HB	1:E:293:TYR:CE1	2.55	0.41
1:F:33:ARG:O	1:F:37:ASN:ND2	2.54	0.41
1:F:246:ILE:HD13	1:F:285:LYS:HE2	2.01	0.41
1:A:43:VAL:HA	1:A:78:LEU:O	2.20	0.41
1:C:60:ARG:HA	1:C:60:ARG:HD3	1.92	0.41
1:D:43:VAL:HA	1:D:78:LEU:O	2.21	0.41
1:D:67:VAL:HG21	1:D:99:HIS:O	2.21	0.41
1:E:70:CYS:O	1:E:73:THR:HG22	2.21	0.41
1:F:179:LEU:HA	1:F:179:LEU:HD23	1.83	0.41
1:A:122:HIS:HB2	1:D:274:PRO:HB3	2.03	0.41
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.89	0.41
1:B:29:ARG:HA	1:B:32:LYS:HG2	2.03	0.41
1:C:182:GLU:HB3	1:C:185:MET:HE3	2.02	0.41
1:C:188:ILE:HG21	1:C:207:ILE:HG13	2.02	0.41
1:A:256:ILE:O	1:A:260:MET:HG2	2.21	0.41
1:B:60:ARG:HG2	1:B:95:PHE:CE1	2.56	0.41
1:B:142:ARG:NE	1:C:111:TYR:O	2.54	0.41
1:D:34:GLN:OE1	1:D:39:ILE:HG13	2.21	0.41
1:B:124:LYS:HE2	8:B:454:HOH:O	2.20	0.40
1:C:196:TYR:HE1	1:C:230:TYR:HD1	1.69	0.40
1:B:51:SER:O	6:B:301:3VN:C09	2.69	0.40
1:B:53:THR:HG22	1:C:85:ALA:HA	2.03	0.40
1:C:247:LEU:HD23	1:C:247:LEU:HA	1.83	0.40
1:F:189:SER:HB3	1:F:206:VAL:HG12	2.04	0.40
1:F:252:ASN:ND2	1:F:253:PRO:HA	2.37	0.40
1:A:82:GLY:O	3:A:302:PEG:H22	2.20	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:HG21	1:A:289:VAL:CG1	2.38	0.40
1:B:256:ILE:O	1:B:260:MET:HG2	2.22	0.40
1:E:63:ILE:O	1:E:67:VAL:HG23	2.20	0.40
1:F:105:LEU:HD13	1:F:135:LEU:HD23	2.03	0.40
1:F:159:CYS:HB2	1:F:162:ILE:HD12	2.04	0.40
1:F:279:SER:O	1:F:283:PHE:HB2	2.21	0.40
1:D:204:LYS:HD3	1:D:204:LYS:HA	1.82	0.40
1:D:247:LEU:HD23	1:D:247:LEU:HA	1.90	0.40
1:E:216:ASP:N	1:E:216:ASP:OD1	2.55	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%)	7 (2%)	0	100	100
1	B	293/310 (94%)	284 (97%)	9 (3%)	0	100	100
1	C	293/310 (94%)	283 (97%)	10 (3%)	0	100	100
1	D	293/310 (94%)	282 (96%)	11 (4%)	0	100	100
1	E	293/310 (94%)	281 (96%)	12 (4%)	0	100	100
1	F	293/310 (94%)	283 (97%)	9 (3%)	1 (0%)	41	64
All	All	1758/1860 (94%)	1699 (97%)	58 (3%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	279	SER

### 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	244/259 (94%)	237 (97%)	7 (3%)	42	68
1	B	245/259 (95%)	241 (98%)	4 (2%)	62	82
1	C	243/259 (94%)	238 (98%)	5 (2%)	53	77
1	D	239/259 (92%)	237 (99%)	2 (1%)	81	92
1	E	244/259 (94%)	240 (98%)	4 (2%)	62	82
1	F	247/259 (95%)	240 (97%)	7 (3%)	43	69
All	All	1462/1554 (94%)	1433 (98%)	29 (2%)	55	78

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	106	SER
1	A	110	TYR
1	A	137	TYR
1	A	161	ASN
1	A	192	ASP
1	A	235	LYS
1	B	32	LYS
1	B	106	SER
1	B	161	ASN
1	B	192	ASP
1	C	110	TYR
1	C	113	LYS
1	C	145	CYS
1	C	192	ASP
1	C	219	SER
1	D	110	TYR
1	D	192	ASP
1	E	68	GLU
1	E	106	SER
1	E	200	SER
1	E	219	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	18	LYS
1	F	40	ASP
1	F	110	TYR
1	F	227	ASP
1	F	279	SER
1	F	280	LYS
1	F	281	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	99	HIS
1	B	99	HIS
1	C	128	GLN
1	C	201	ASN
1	D	99	HIS
1	E	161	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KPI	A	166	1	10,13,14	0.65	0	6,15,17	3.11	3 (50%)
1	KPI	D	166	1	10,13,14	1.42	1 (10%)	6,15,17	3.05	3 (50%)
1	KPI	C	166	1	10,13,14	1.36	1 (10%)	6,15,17	3.23	3 (50%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KPI	E	166	1	10,13,14	1.42	1 (10%)	6,15,17	2.96	4 (66%)
1	KPI	B	166	1	10,13,14	0.71	0	6,15,17	2.99	3 (50%)
1	KPI	F	166	1	10,13,14	0.58	0	6,15,17	2.66	3 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	A	166	1	-	4/9/14/16	-
1	KPI	D	166	1	-	4/9/14/16	-
1	KPI	C	166	1	-	1/9/14/16	-
1	KPI	E	166	1	-	2/9/14/16	-
1	KPI	B	166	1	-	2/9/14/16	-
1	KPI	F	166	1	-	1/9/14/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	KPI	O-C	4.12	1.36	1.19
1	E	166	KPI	O-C	4.09	1.36	1.19
1	C	166	KPI	O-C	4.05	1.36	1.19

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	KPI	C1-CX1-CX2	-6.64	110.57	117.92
1	B	166	KPI	C1-CX1-CX2	-6.01	111.26	117.92
1	E	166	KPI	C1-CX1-CX2	-5.98	111.30	117.92
1	A	166	KPI	C1-CX1-CX2	-5.87	111.42	117.92
1	D	166	KPI	C1-CX1-CX2	-5.68	111.63	117.92
1	F	166	KPI	C1-CX1-CX2	-5.32	112.03	117.92
1	A	166	KPI	CE-NZ-CX1	3.43	130.99	121.77
1	D	166	KPI	CD-CE-NZ	3.29	116.65	110.66
1	A	166	KPI	C1-CX1-NZ	3.20	131.10	123.12
1	D	166	KPI	C1-CX1-NZ	2.93	130.43	123.12
1	C	166	KPI	C1-CX1-NZ	2.76	129.99	123.12
1	B	166	KPI	CD-CE-NZ	2.69	115.56	110.66
1	E	166	KPI	C1-CX1-NZ	2.63	129.68	123.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	KPI	CD-CE-NZ	2.53	115.26	110.66
1	C	166	KPI	CE-NZ-CX1	2.52	128.55	121.77
1	B	166	KPI	C1-CX1-NZ	2.48	129.31	123.12
1	E	166	KPI	CD-CE-NZ	2.24	114.74	110.66
1	F	166	KPI	C1-CX1-NZ	2.06	128.25	123.12
1	E	166	KPI	CE-NZ-CX1	2.03	127.24	121.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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
7	PGE	B	303	-	9,9,9	0.33	0	8,8,8	0.28	0
3	PEG	C	301	-	6,6,6	0.47	0	5,5,5	0.39	0
6	3VN	E	301	-	15,21,21	0.87	0	12,28,28	2.02	4 (33%)
5	EDO	A	304	-	3,3,3	0.46	0	2,2,2	0.26	0
6	3VN	B	301	-	15,21,21	0.87	0	12,28,28	2.02	4 (33%)
3	PEG	D	302	-	6,6,6	0.49	0	5,5,5	0.16	0
5	EDO	B	302	-	3,3,3	0.53	0	2,2,2	0.20	0
5	EDO	D	303	-	3,3,3	0.47	0	2,2,2	0.31	0
5	EDO	D	304	-	3,3,3	0.45	0	2,2,2	0.50	0
3	PEG	A	302	-	6,6,6	0.48	0	5,5,5	0.25	0
5	EDO	A	305	-	3,3,3	0.53	0	2,2,2	0.12	0
4	ACT	A	303	-	1,3,3	6.63	1 (100%)	0,3,3	-	-
6	3VN	D	301	-	15,21,21	0.78	0	12,28,28	1.63	3 (25%)

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
7	PGE	B	303	-	-	1/7/7/7	-
3	PEG	C	301	-	-	1/4/4/4	-
6	3VN	E	301	-	-	7/19/31/31	-
5	EDO	A	304	-	-	0/1/1/1	-
6	3VN	B	301	-	-	3/19/31/31	-
3	PEG	D	302	-	-	3/4/4/4	-
5	EDO	B	302	-	-	0/1/1/1	-
5	EDO	D	303	-	-	0/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
3	PEG	A	302	-	-	3/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	304	-	-	0/1/1/1	-
6	3VN	D	301	-	-	6/19/31/31	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	ACT	CH3-C	6.63	1.57	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	301	3VN	C16-C15-C13	-3.45	109.07	115.20
6	B	301	3VN	C12-C11-C02	-3.26	109.44	115.19
6	B	301	3VN	C11-C12-C13	-3.25	109.45	115.19
6	E	301	3VN	C07-C06-C02	-3.24	109.44	115.20
6	E	301	3VN	C16-C15-C13	-3.24	109.45	115.20
6	E	301	3VN	C11-C12-C13	-3.24	109.47	115.19
6	E	301	3VN	C12-C11-C02	-3.23	109.48	115.19
6	B	301	3VN	C16-C15-C13	-3.22	109.48	115.20
6	B	301	3VN	C07-C06-C02	-3.22	109.49	115.20
6	D	301	3VN	C12-C11-C02	-2.52	110.75	115.19
6	D	301	3VN	C07-C06-C02	-2.13	111.43	115.20

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	301	3VN	C03-C02-C06-C07
6	D	301	3VN	C11-C02-C06-C07
3	A	302	PEG	O2-C3-C4-O4
3	D	302	PEG	O1-C1-C2-O2
3	D	302	PEG	O2-C3-C4-O4
6	D	301	3VN	C02-C06-C07-C08
6	D	301	3VN	N01-C02-C06-C07
6	E	301	3VN	N01-C02-C06-C07
3	C	301	PEG	O2-C3-C4-O4
6	B	301	3VN	C15-C16-C17-C18
6	E	301	3VN	C06-C07-C08-C09
6	D	301	3VN	C06-C07-C08-C09
6	E	301	3VN	N14-C13-C15-C16
6	E	301	3VN	C11-C02-C06-C07

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	E	301	3VN	C12-C13-C15-C16
6	B	301	3VN	C07-C08-C09-N10
6	E	301	3VN	C07-C08-C09-N10
3	D	302	PEG	C4-C3-O2-C2
3	A	302	PEG	O1-C1-C2-O2
6	E	301	3VN	C15-C16-C17-C18
7	B	303	PGE	C4-C3-O2-C2
3	A	302	PEG	C1-C2-O2-C3
6	B	301	3VN	C16-C17-C18-N19
6	D	301	3VN	C16-C17-C18-N19

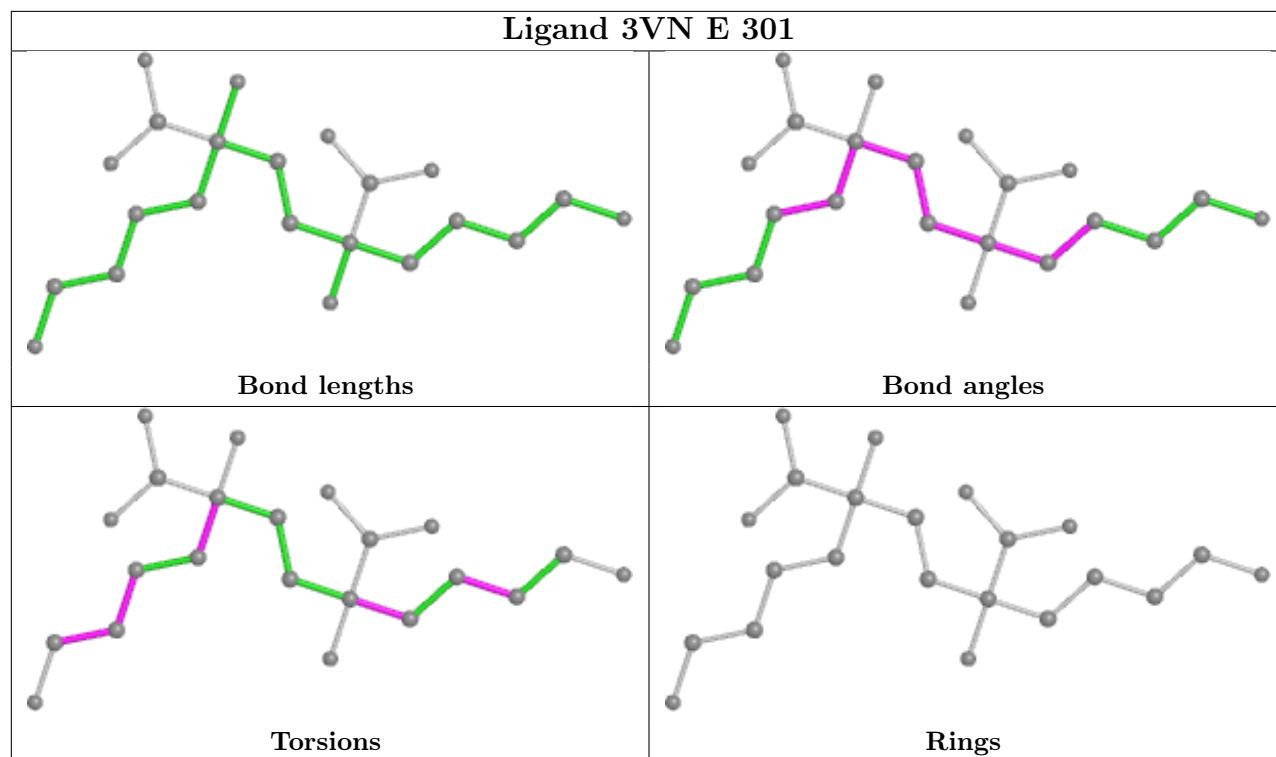
There are no ring outliers.

9 monomers are involved in 21 short contacts:

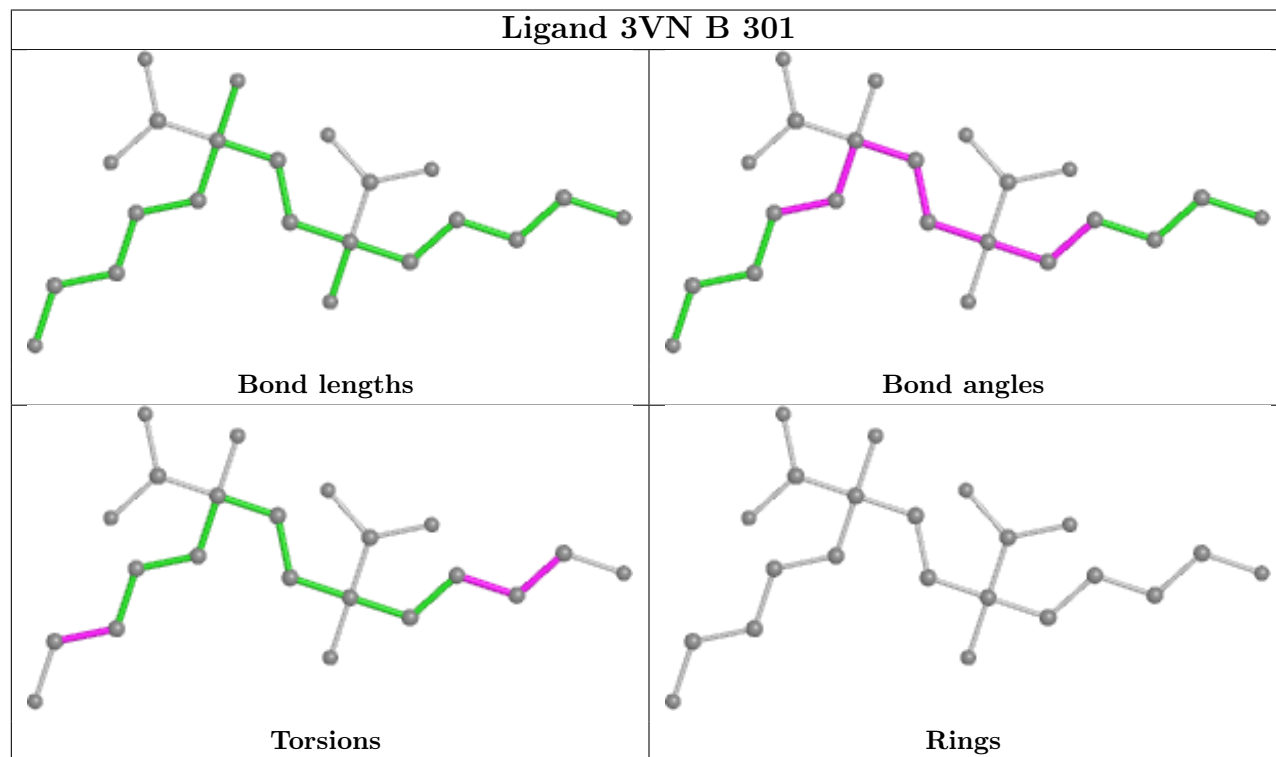
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	303	PGE	1	0
3	C	301	PEG	1	0
6	E	301	3VN	3	0
5	A	304	EDO	1	0
6	B	301	3VN	6	0
3	A	302	PEG	3	0
5	A	305	EDO	4	0
4	A	303	ACT	1	0
6	D	301	3VN	3	0

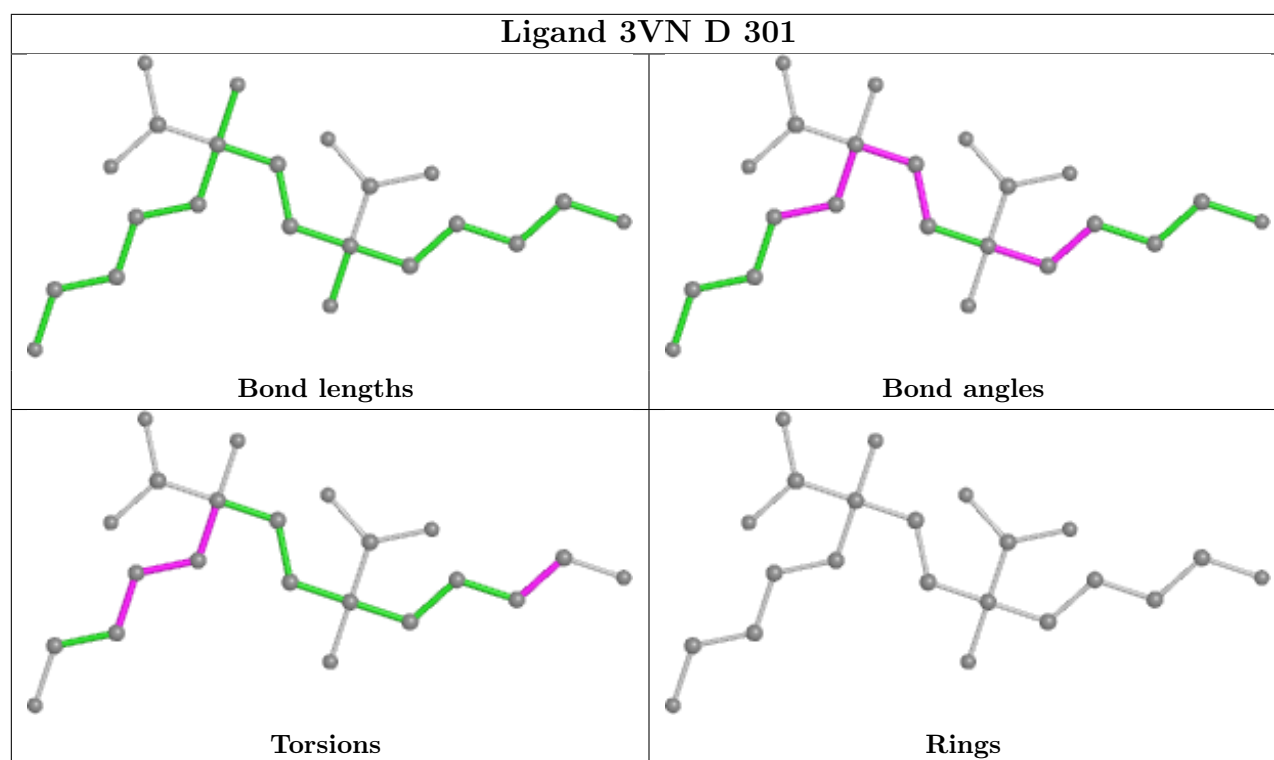
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand 3VN E 301



## Ligand 3VN B 301





## 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<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 86	9, 15, 24, 33	0
1	B	295/310 (95%)	0.07	3 (1%) 82 80	8, 14, 22, 37	0
1	C	295/310 (95%)	0.07	4 (1%) 75 71	9, 14, 24, 37	0
1	D	295/310 (95%)	0.11	6 (2%) 65 60	10, 16, 28, 38	0
1	E	295/310 (95%)	0.10	6 (2%) 65 60	11, 17, 29, 39	0
1	F	295/310 (95%)	0.16	4 (1%) 75 71	12, 18, 27, 38	0
All	All	1770/1860 (95%)	0.09	25 (1%) 75 71	8, 16, 26, 39	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ASN	4.8
1	D	98	GLU	4.1
1	D	95	PHE	3.4
1	E	131	ASP	3.3
1	B	4	ASN	3.2
1	F	267	GLU	3.2
1	D	4	ASN	3.0
1	F	56	HIS	3.0
1	C	95	PHE	2.9
1	C	98	GLU	2.9
1	E	19	ASN	2.6
1	D	57	GLU	2.6
1	E	4	ASN	2.6
1	B	29	ARG	2.4
1	F	19	ASN	2.4
1	A	291	LYS	2.4
1	C	19	ASN	2.4
1	E	98	GLU	2.4
1	D	267	GLU	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	267	GLU	2.2
1	E	72	GLY	2.2
1	B	19	ASN	2.1
1	D	99	HIS	2.1
1	E	60	ARG	2.0
1	F	229	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	F	166	14/15	0.83	0.20	12,14,19,20	0
1	KPI	D	166	14/15	0.84	0.20	12,14,16,17	0
1	KPI	E	166	14/15	0.85	0.22	13,15,18,18	0
1	KPI	B	166	14/15	0.86	0.21	9,11,16,16	0
1	KPI	A	166	14/15	0.86	0.21	11,12,16,16	0
1	KPI	C	166	14/15	0.88	0.21	9,10,13,14	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(Å <sup>2</sup> )	Q<0.9
6	3VN	E	301	22/22	0.80	0.30	15,18,24,25	0
6	3VN	B	301	22/22	0.81	0.28	12,15,20,21	0
5	EDO	A	304	4/4	0.81	0.28	16,17,17,17	0
5	EDO	D	304	4/4	0.85	0.17	12,15,15,16	0
3	PEG	D	302	7/7	0.87	0.20	15,15,17,17	0
5	EDO	A	305	4/4	0.88	0.28	11,12,12,13	0

*Continued on next page...*

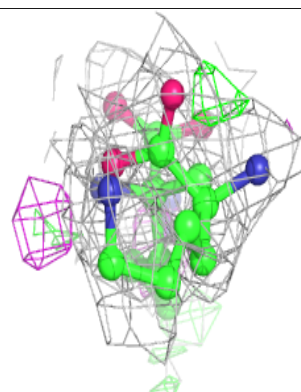
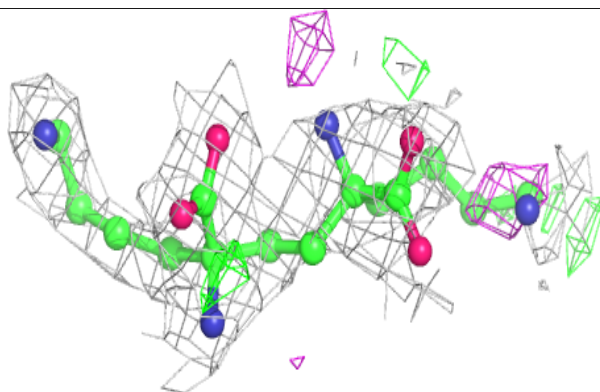
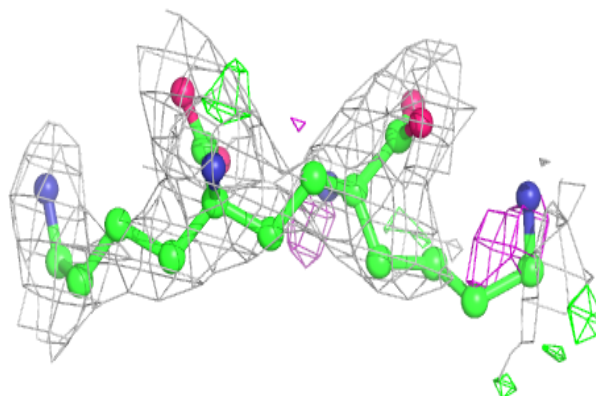
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	C	301	7/7	0.89	0.17	11,12,13,14	0
5	EDO	D	303	4/4	0.90	0.37	14,15,16,17	0
6	3VN	D	301	22/22	0.90	0.22	15,17,19,22	0
2	MG	A	301	1/1	0.90	0.08	12,12,12,12	0
5	EDO	B	302	4/4	0.91	0.24	11,11,12,13	0
4	ACT	A	303	4/4	0.91	0.18	10,13,13,14	0
7	PGE	B	303	10/10	0.91	0.17	11,12,15,16	0
3	PEG	A	302	7/7	0.92	0.21	17,17,18,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

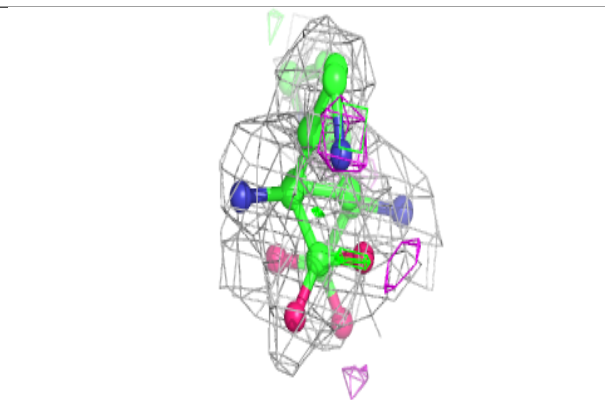
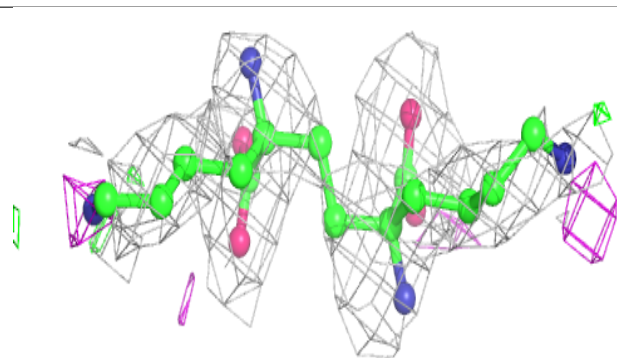
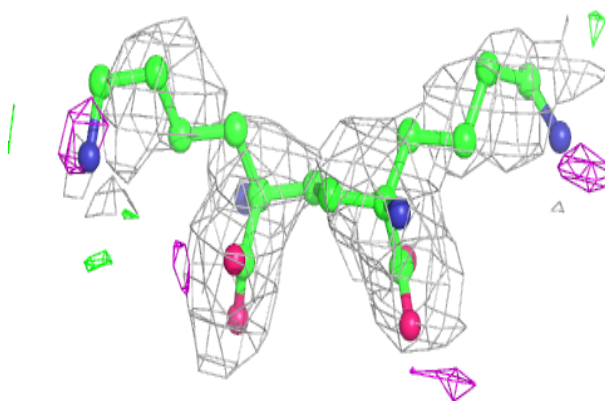
**Electron density around 3VN E 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

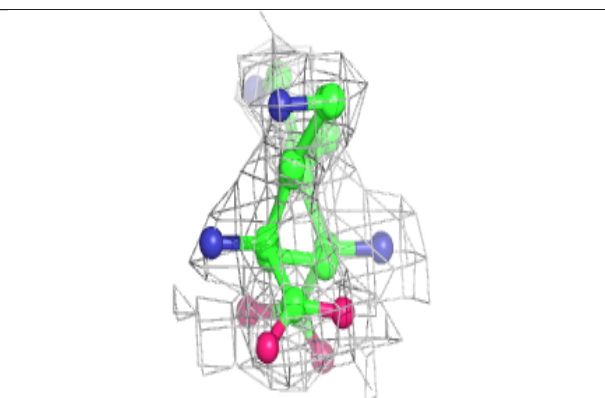
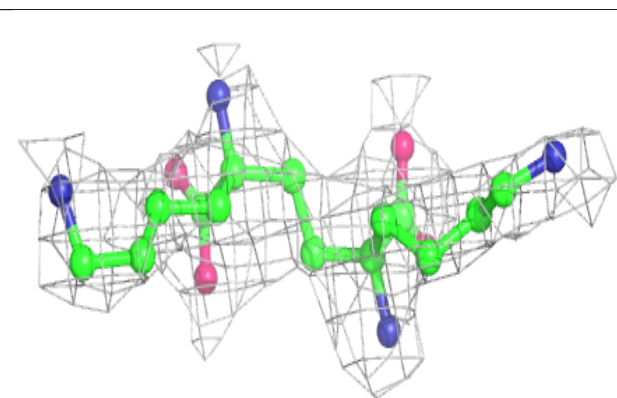
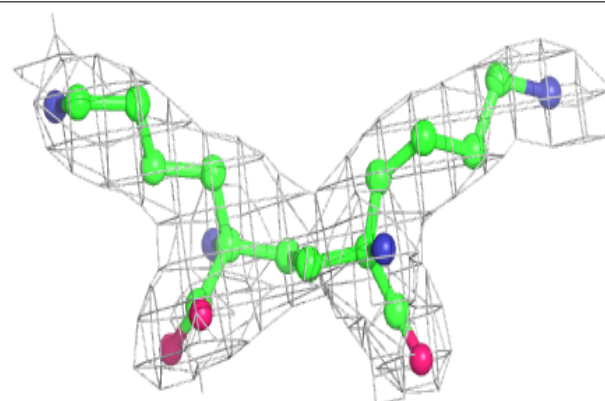


**Electron density around 3VN B 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 3VN D 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.