



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 25, 2021 – 12:15 PM EDT

PDB ID : 7KKT  
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, N84D 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 : 2020-10-28  
Resolution : 1.71 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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

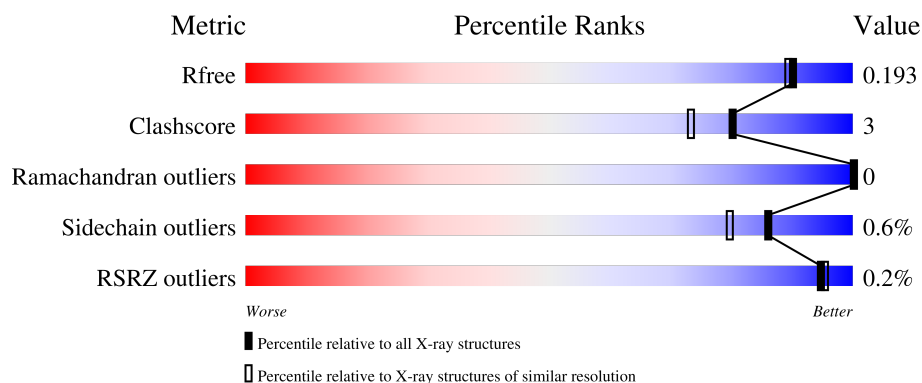
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


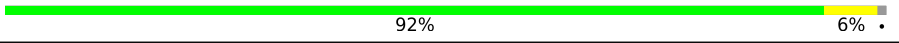
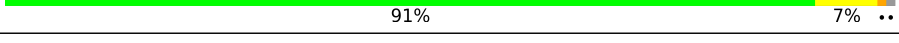
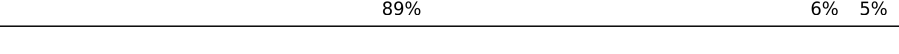

The reported resolution of this entry is 1.71 Å.

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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	 88% 7% 5%
1	B	310	 92% 6% .
1	C	310	 91% 7% ..
1	D	310	 89% 6% 5%
1	E	310	 90% 5% .

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Mol	Chain	Length	Quality of chain
1	F	310	<div><div></div><div>90%</div><div>5%5%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15621 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
			2284	1451	379	441	13			
1	B	306	Total	C	N	O	S	0	4	0
			2372	1501	400	456	15			
1	C	306	Total	C	N	O	S	0	3	0
			2372	1502	401	455	14			
1	D	296	Total	C	N	O	S	0	2	0
			2282	1450	378	441	13			
1	E	297	Total	C	N	O	S	0	0	0
			2280	1449	378	440	13			
1	F	296	Total	C	N	O	S	0	2	0
			2284	1451	379	441	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	84	ASP	ASN	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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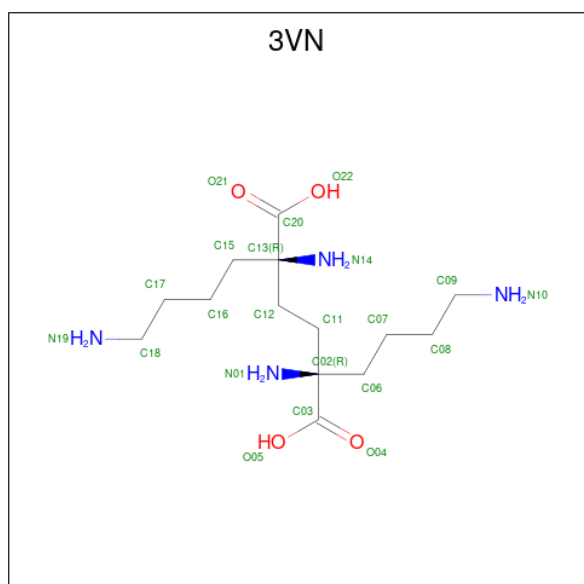
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	84	ASP	ASN	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	84	ASP	ASN	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	84	ASP	ASN	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	84	ASP	ASN	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	84	ASP	ASN	engineered mutation	UNP Q9PPB4

- Molecule 2 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (three-letter code: 3VN) (formula: C<sub>14</sub>H<sub>30</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	O	0
			22	14	4	4	

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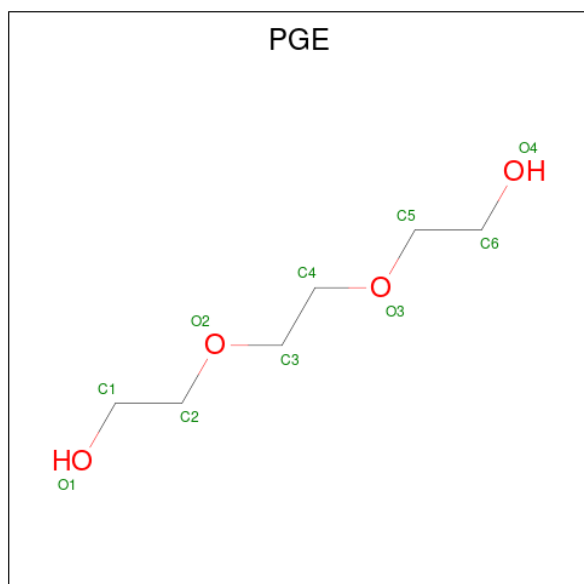
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			22	14	4	4		
2	C	1	Total	C	N	O	0	0
			22	14	4	4		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	6	Total	Mg	0	0
			6	6		
3	F	2	Total	Mg	0	0
			2	2		

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



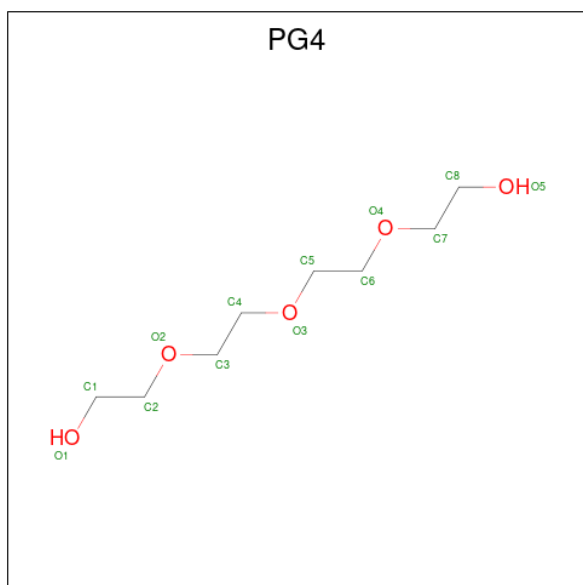
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

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

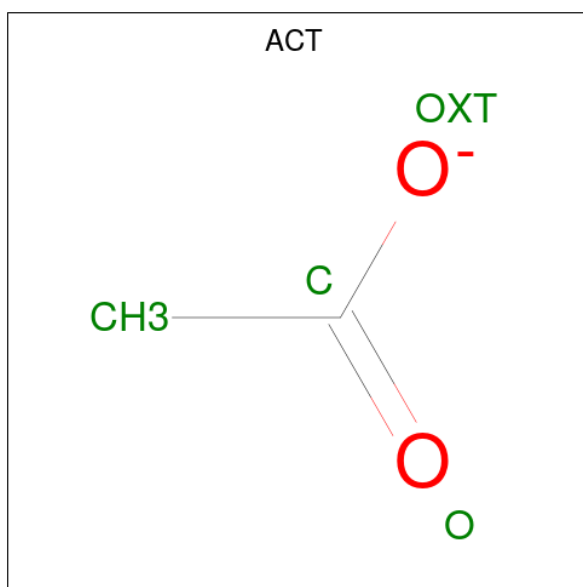
- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).





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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



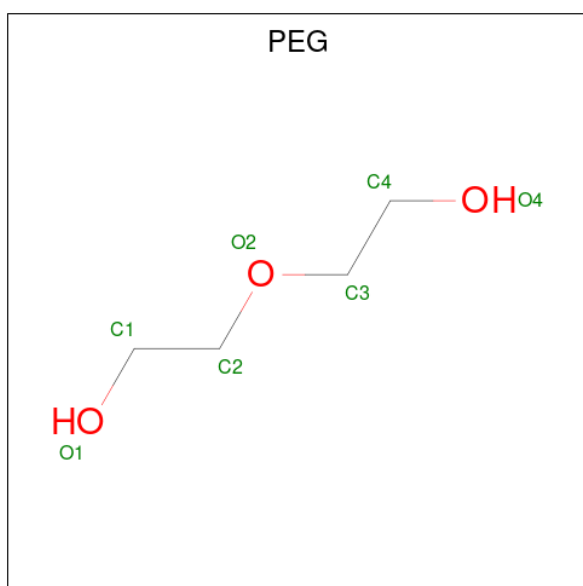
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total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

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

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



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			6	3	3		


- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	250	Total	O	0	0
			250	250		
10	B	266	Total	O	0	0
			266	266		
10	C	250	Total	O	0	0
			250	250		
10	D	231	Total	O	0	0
			231	231		
10	E	255	Total	O	0	0
			255	255		
10	F	228	Total	O	0	0
			228	228		

### 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

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: 



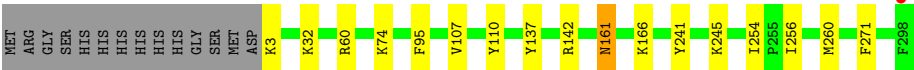
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F: 

90%

5%

5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.02Å 225.47Å 200.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 1.71 49.13 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.13-1.71) 98.3 (49.13-1.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 1.71Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, $R_{free}$	0.164 , 0.195 0.163 , 0.193	Depositor DCC
$R_{free}$ test set	10161 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, KPI, EDO, PG4, 3VN, GOL, ACT, MG, 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	0.49	0/2318	0.61	0/3132
1	B	0.43	0/2423	0.58	0/3273
1	C	0.46	0/2416	0.60	0/3264
1	D	0.42	0/2316	0.57	0/3129
1	E	0.45	0/2304	0.60	0/3115
1	F	0.42	0/2318	0.61	0/3132
All	All	0.44	0/14095	0.60	0/19045

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

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	C	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	2284	0	2319	12	0
1	B	2372	0	2384	14	0
1	C	2372	0	2386	22	0
1	D	2282	0	2319	13	0
1	E	2280	0	2306	10	0
1	F	2284	0	2320	9	0
2	A	22	0	28	0	0
2	B	22	0	28	0	0
2	C	22	0	28	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	6	0	0	0	0
3	F	2	0	0	0	0
4	A	10	0	14	0	0
4	C	10	0	14	4	0
4	F	10	0	14	0	0
5	B	13	0	18	2	0
5	D	13	0	18	2	0
6	B	8	0	6	1	0
6	C	8	0	6	0	0
6	D	4	0	3	0	0
6	E	4	0	3	0	0
7	B	8	0	12	0	0
7	C	16	0	24	3	0
7	D	20	0	30	1	0
7	E	16	0	24	1	0
7	F	16	0	24	0	0
8	C	7	0	10	0	0
8	E	14	0	20	0	0
9	D	6	0	8	0	0
10	A	250	0	0	1	0
10	B	266	0	0	1	0
10	C	250	0	0	1	0
10	D	231	0	0	1	0
10	E	255	0	0	2	0
10	F	228	0	0	2	0
All	All	15621	0	14366	77	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 77 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:E:161:ASN:ND2	7:E:313:EDO:H11	2.09	0.67
1:B:142:ARG:HE	6:B:307:ACT:H2	1.63	0.63
1:C:150:ASP:HB3	4:C:304:PGE:H22	1.81	0.62
1:B:128:GLN:NE2	10:B:403:HOH:O	2.25	0.62
1:B:150:ASP:HB3	5:B:302:PG4:H32	1.81	0.62

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	307/310 (99%)	302 (98%)	5 (2%)	0	100	100
1	C	306/310 (99%)	300 (98%)	6 (2%)	0	100	100
1	D	295/310 (95%)	290 (98%)	5 (2%)	0	100	100
1	E	294/310 (95%)	290 (99%)	4 (1%)	0	100	100
1	F	295/310 (95%)	291 (99%)	4 (1%)	0	100	100
All	All	1792/1860 (96%)	1763 (98%)	29 (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	250/260 (96%)	249 (100%)	1 (0%)	91	86
1	B	261/260 (100%)	259 (99%)	2 (1%)	81	73
1	C	260/260 (100%)	259 (100%)	1 (0%)	91	86
1	D	250/260 (96%)	249 (100%)	1 (0%)	91	86
1	E	247/260 (95%)	246 (100%)	1 (0%)	91	86
1	F	250/260 (96%)	246 (98%)	4 (2%)	62	47
All	All	1518/1560 (97%)	1508 (99%)	10 (1%)	86	76

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	110	TYR
1	F	161[A]	ASN
1	F	161[B]	ASN
1	C	280	LYS
1	D	137	TYR

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

Mol	Chain	Res	Type
1	A	223	HIS

### 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	0.62	0	6,15,17	1.96	2 (33%)
1	KPI	C	166	1	10,13,14	1.59	2 (20%)	6,15,17	3.20	2 (33%)
1	KPI	F	166	1	10,13,14	1.18	1 (10%)	6,15,17	3.19	2 (33%)
1	KPI	A	166	1	10,13,14	1.39	1 (10%)	6,15,17	2.34	2 (33%)
1	KPI	E	166	1	10,13,14	0.44	0	6,15,17	2.15	2 (33%)
1	KPI	D	166	1	10,13,14	0.69	0	6,15,17	2.15	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	-	1/9/14/16	-
1	KPI	C	166	1	-	1/9/14/16	-
1	KPI	F	166	1	-	1/9/14/16	-
1	KPI	A	166	1	-	0/9/14/16	-
1	KPI	E	166	1	-	1/9/14/16	-
1	KPI	D	166	1	-	1/9/14/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	O-C	4.14	1.36	1.19
1	A	166	KPI	O-C	3.78	1.35	1.19
1	F	166	KPI	O-C	3.25	1.32	1.19
1	C	166	KPI	CB-CA	2.20	1.56	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	KPI	C1-CX1-CX2	-7.00	110.16	117.92
1	F	166	KPI	C1-CX1-CX2	-6.99	110.18	117.92
1	A	166	KPI	C1-CX1-CX2	-4.78	112.62	117.92
1	D	166	KPI	C1-CX1-CX2	-4.38	113.06	117.92
1	E	166	KPI	C1-CX1-CX2	-4.36	113.10	117.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 18 are monoatomic - leaving 37 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	$\# Z  > 2$
2	3VN	B	301	3	15,21,21	0.46	0	12,28,28	0.90	0
6	ACT	D	304	-	1,3,3	1.52	0	0,3,3	-	-
7	EDO	D	306	-	3,3,3	0.40	0	2,2,2	0.63	0
7	EDO	D	308	-	3,3,3	0.43	0	2,2,2	0.59	0
7	EDO	E	313	-	3,3,3	0.64	0	2,2,2	0.65	0
6	ACT	B	306	-	1,3,3	1.32	0	0,3,3	-	-
7	EDO	B	309	-	3,3,3	0.53	0	2,2,2	0.08	0
8	PEG	E	308	-	6,6,6	0.47	0	5,5,5	0.26	0
2	3VN	A	301	-	15,21,21	0.49	0	12,28,28	1.03	1 (8%)
4	PGE	F	303	-	9,9,9	0.29	0	8,8,8	0.34	0
6	ACT	C	307	-	1,3,3	1.68	0	0,3,3	-	-
6	ACT	B	307	-	1,3,3	1.00	0	0,3,3	-	-
8	PEG	E	307	-	6,6,6	0.49	0	5,5,5	0.27	0
7	EDO	F	307	-	3,3,3	0.45	0	2,2,2	0.43	0
7	EDO	D	309	-	3,3,3	0.38	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	F	306	-	3,3,3	0.53	0	2,2,2	0.13	0
4	PGE	C	304	-	9,9,9	0.27	0	8,8,8	0.33	0
5	PG4	B	302	-	12,12,12	0.51	0	11,11,11	0.30	0
7	EDO	D	307	-	3,3,3	0.43	0	2,2,2	0.49	0
7	EDO	E	310	-	3,3,3	0.41	0	2,2,2	0.55	0
4	PGE	A	305	-	9,9,9	0.33	0	8,8,8	0.19	0
7	EDO	D	305	-	3,3,3	0.40	0	2,2,2	0.51	0
7	EDO	E	312	-	3,3,3	0.56	0	2,2,2	0.22	0
7	EDO	F	304	-	3,3,3	0.47	0	2,2,2	0.41	0
6	ACT	C	306	-	1,3,3	1.50	0	0,3,3	-	-
7	EDO	C	309	-	3,3,3	0.57	0	2,2,2	0.19	0
7	EDO	C	311	-	3,3,3	0.54	0	2,2,2	0.07	0
7	EDO	C	310	-	3,3,3	0.54	0	2,2,2	0.13	0
7	EDO	E	311	-	3,3,3	0.52	0	2,2,2	0.30	0
9	GOL	D	310	-	5,5,5	0.32	0	5,5,5	0.79	0
6	ACT	E	309	-	1,3,3	1.37	0	0,3,3	-	-
8	PEG	C	305	-	6,6,6	0.45	0	5,5,5	0.50	0
7	EDO	F	305	-	3,3,3	0.46	0	2,2,2	0.46	0
7	EDO	B	308	-	3,3,3	0.37	0	2,2,2	0.65	0
7	EDO	C	308	-	3,3,3	0.47	0	2,2,2	0.41	0
5	PG4	D	301	-	12,12,12	0.52	0	11,11,11	0.31	0
2	3VN	C	301	-	15,21,21	0.51	0	12,28,28	0.89	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	3VN	B	301	3	-	0/19/31/31	-
7	EDO	D	306	-	-	1/1/1/1	-
7	EDO	D	308	-	-	0/1/1/1	-
7	EDO	E	313	-	-	0/1/1/1	-
7	EDO	B	309	-	-	0/1/1/1	-
8	PEG	E	308	-	-	0/4/4/4	-
2	3VN	A	301	-	-	0/19/31/31	-
4	PGE	F	303	-	-	1/7/7/7	-
8	PEG	E	307	-	-	2/4/4/4	-
7	EDO	F	307	-	-	0/1/1/1	-
7	EDO	D	309	-	-	1/1/1/1	-
7	EDO	F	306	-	-	0/1/1/1	-
4	PGE	C	304	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	B	302	-	-	1/10/10/10	-
7	EDO	D	307	-	-	0/1/1/1	-
7	EDO	E	310	-	-	1/1/1/1	-
4	PGE	A	305	-	-	0/7/7/7	-
7	EDO	D	305	-	-	0/1/1/1	-
7	EDO	E	312	-	-	0/1/1/1	-
7	EDO	F	304	-	-	1/1/1/1	-
7	EDO	C	309	-	-	0/1/1/1	-
7	EDO	C	311	-	-	1/1/1/1	-
7	EDO	C	310	-	-	1/1/1/1	-
7	EDO	E	311	-	-	0/1/1/1	-
9	GOL	D	310	-	-	2/4/4/4	-
8	PEG	C	305	-	-	2/4/4/4	-
7	EDO	F	305	-	-	0/1/1/1	-
7	EDO	B	308	-	-	1/1/1/1	-
7	EDO	C	308	-	-	0/1/1/1	-
5	PG4	D	301	-	-	3/10/10/10	-
2	3VN	C	301	-	-	0/19/31/31	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	3VN	C16-C15-C13	-2.09	111.49	115.20

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	310	GOL	O1-C1-C2-C3
5	D	301	PG4	O2-C3-C4-O3
5	D	301	PG4	O4-C7-C8-O5
7	C	310	EDO	O1-C1-C2-O2
9	D	310	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 14 short contacts:

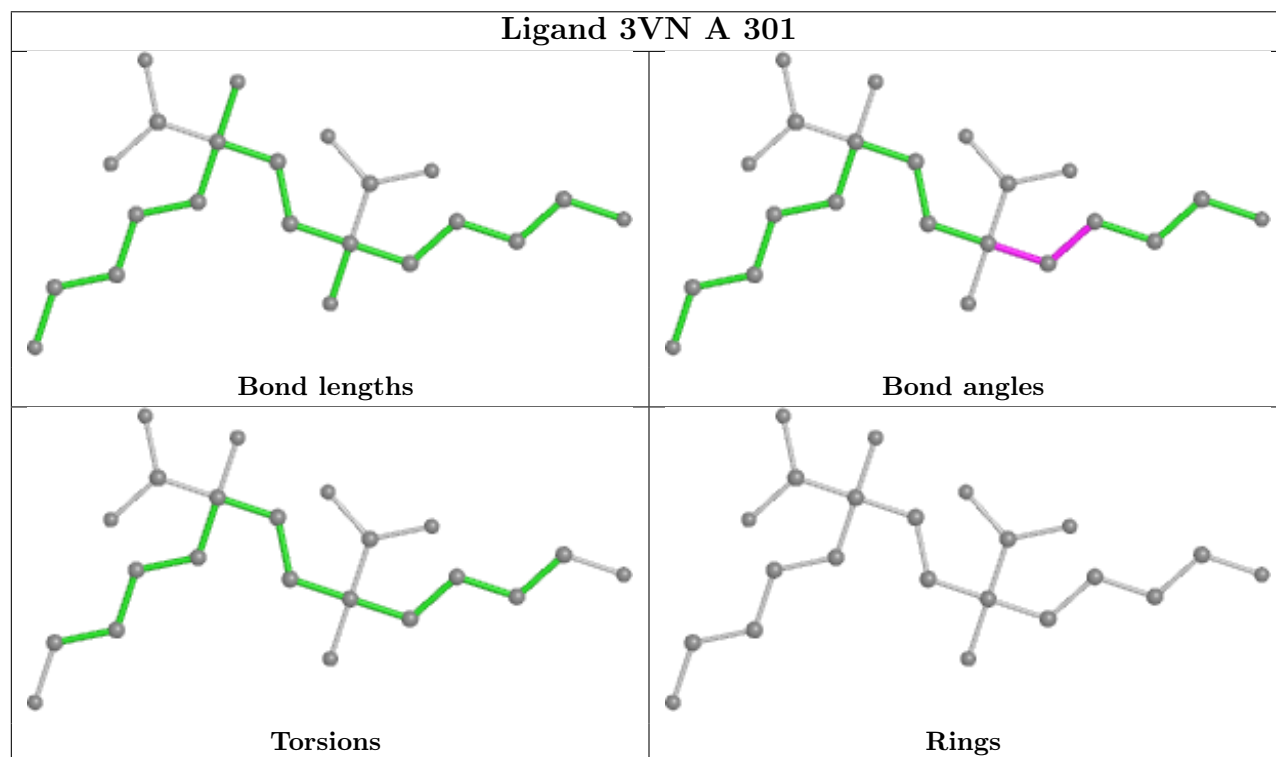
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	313	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	307	ACT	1	0
4	C	304	PGE	4	0
5	B	302	PG4	2	0
7	D	307	EDO	1	0
7	C	311	EDO	1	0
7	C	310	EDO	1	0
7	C	308	EDO	1	0
5	D	301	PG4	2	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	295/310 (95%)	-0.40	0	100   100	13, 18, 30, 41	0
1	B	305/310 (98%)	-0.44	1 (0%)	94   95	14, 19, 34, 47	0
1	C	305/310 (98%)	-0.42	1 (0%)	94   95	13, 18, 32, 50	0
1	D	295/310 (95%)	-0.35	0	100   100	15, 19, 33, 41	0
1	E	296/310 (95%)	-0.45	1 (0%)	94   95	13, 18, 30, 52	0
1	F	295/310 (95%)	-0.27	1 (0%)	94   95	15, 20, 36, 46	0
All	All	1791/1860 (96%)	-0.39	4 (0%)	95   95	13, 19, 33, 52	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-6	HIS	2.8
1	F	298	PHE	2.5
1	E	2	ASP	2.1
1	B	-7	HIS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	KPI	B	166	14/15	0.94	0.10	12,17,23,26	0
1	KPI	A	166	14/15	0.95	0.11	10,15,23,24	0
1	KPI	D	166	14/15	0.95	0.10	13,15,24,24	0
1	KPI	F	166	14/15	0.95	0.10	14,18,22,26	0
1	KPI	E	166	14/15	0.96	0.08	11,16,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	C	166	14/15	0.96	0.07	12,18,22,24	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

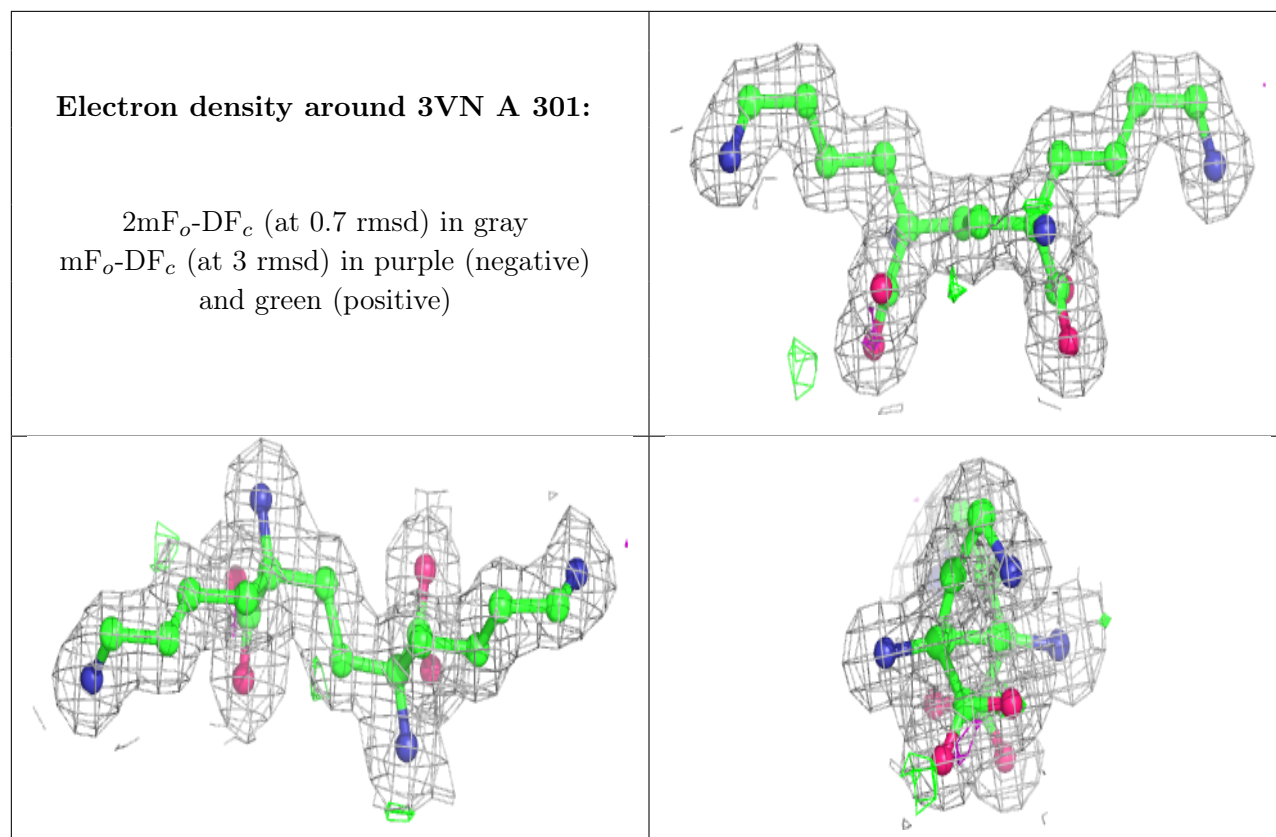
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	D	302	1/1	0.46	0.10	47,47,47,47	0
9	GOL	D	310	6/6	0.53	0.31	40,46,56,57	0
6	ACT	D	304	4/4	0.61	0.29	33,37,45,55	0
7	EDO	E	313	4/4	0.67	0.25	28,33,35,43	0
8	PEG	C	305	7/7	0.77	0.23	34,40,47,50	0
3	MG	E	305	1/1	0.80	0.23	53,53,53,53	0
3	MG	A	303	1/1	0.80	0.14	44,44,44,44	0
6	ACT	E	309	4/4	0.80	0.26	34,36,47,48	0
8	PEG	E	308	7/7	0.82	0.18	35,44,52,53	0
7	EDO	C	308	4/4	0.82	0.12	33,38,45,52	0
8	PEG	E	307	7/7	0.83	0.12	32,34,46,49	0
6	ACT	B	306	4/4	0.83	0.14	38,45,53,58	0
7	EDO	C	309	4/4	0.83	0.28	35,41,43,50	0
7	EDO	E	310	4/4	0.85	0.30	33,42,42,50	0
7	EDO	D	305	4/4	0.85	0.38	34,38,48,48	0
6	ACT	C	307	4/4	0.87	0.15	38,50,51,52	0
7	EDO	F	307	4/4	0.87	0.17	42,49,50,51	0
7	EDO	B	308	4/4	0.87	0.45	32,34,42,48	0
7	EDO	D	306	4/4	0.87	0.22	24,35,36,41	0
7	EDO	D	307	4/4	0.87	0.20	31,37,43,51	0
3	MG	B	304	1/1	0.87	0.17	42,42,42,42	0
5	PG4	D	301	13/13	0.88	0.18	26,40,56,62	0
3	MG	B	303	1/1	0.89	0.12	42,42,42,42	0
4	PGE	C	304	10/10	0.89	0.12	25,36,44,56	0
4	PGE	A	305	10/10	0.90	0.10	33,41,45,50	0
7	EDO	C	310	4/4	0.91	0.18	28,33,35,47	0
5	PG4	B	302	13/13	0.91	0.12	29,36,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	F	305	4/4	0.91	0.28	40,40,47,51	0
7	EDO	D	309	4/4	0.91	0.12	35,37,42,51	0
6	ACT	B	307	4/4	0.92	0.09	30,32,40,51	0
7	EDO	E	311	4/4	0.92	0.11	29,40,44,45	0
7	EDO	D	308	4/4	0.92	0.12	31,37,42,44	0
7	EDO	F	304	4/4	0.92	0.09	37,41,46,46	0
4	PGE	F	303	10/10	0.92	0.12	29,34,40,50	0
6	ACT	C	306	4/4	0.93	0.10	26,35,44,45	0
3	MG	E	306	1/1	0.93	0.10	47,47,47,47	0
7	EDO	C	311	4/4	0.93	0.27	24,34,38,46	0
7	EDO	F	306	4/4	0.94	0.12	21,26,30,39	0
2	3VN	B	301	22/22	0.94	0.08	12,19,22,23	0
3	MG	E	303	1/1	0.95	0.23	38,38,38,38	0
2	3VN	A	301	22/22	0.95	0.08	15,19,21,22	0
2	3VN	C	301	22/22	0.95	0.08	14,17,20,23	0
7	EDO	B	309	4/4	0.95	0.18	17,26,38,38	0
7	EDO	E	312	4/4	0.97	0.06	19,23,24,26	0
3	MG	C	303	1/1	0.98	0.05	19,19,19,19	0
3	MG	F	301	1/1	0.98	0.19	29,29,29,29	0
3	MG	A	302	1/1	0.98	0.05	20,20,20,20	0
3	MG	D	303	1/1	0.99	0.13	17,17,17,17	0
3	MG	F	302	1/1	0.99	0.16	19,19,19,19	0
3	MG	E	301	1/1	0.99	0.10	29,29,29,29	0
3	MG	E	302	1/1	0.99	0.04	30,30,30,30	0
3	MG	C	302	1/1	1.00	0.13	17,17,17,17	0
3	MG	E	304	1/1	1.00	0.14	17,17,17,17	0
3	MG	A	304	1/1	1.00	0.11	16,16,16,16	0
3	MG	B	305	1/1	1.00	0.10	16,16,16,16	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.