

Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 11:06 pm BST

PDB ID : 5L9O

Title : Crystal structure of Agrobacterium tumefaciens C58 strain PBP SocA in com-

plex with glucopine

Authors : Marty, L.; Morera, S.

 $Deposited \ on \quad : \quad 2016\text{-}06\text{-}10$

Resolution : 1.84 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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

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)

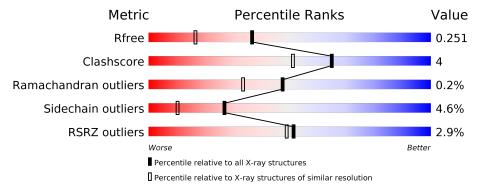
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.84 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 <=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	268	82%	8%	10%
1	В	268	78%	12%	• 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	В	304	_	_	X	_



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3944 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 Deoxyfructosyl-amino Acid Transporter Periplasmic Binding Protein.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	241	Total	С	N	О	S	0	0	0
1	1 A	<u> </u>	1817	1163	303	347	4	U	0	0
1	D	242	Total	С	N	О	S	0	0	0
1	$\begin{vmatrix} 1 & \begin{vmatrix} B & \end{vmatrix} \end{vmatrix}$	B 243	1830	1171	305	349	5	U	U	U

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	expression tag	UNP Q7D447
A	17	SER	-	expression tag	UNP Q7D447
A	18	SER	-	expression tag	UNP Q7D447
A	19	HIS	-	expression tag	UNP Q7D447
A	20	HIS	-	expression tag	UNP Q7D447
A	21	HIS	-	expression tag	UNP Q7D447
A	22	HIS	-	expression tag	UNP Q7D447
A	23	HIS	-	expression tag	UNP Q7D447
A	24	HIS	-	expression tag	UNP Q7D447
A	25	SER	-	expression tag	UNP Q7D447
A	26	SER	-	expression tag	UNP Q7D447
A	27	GLY	-	expression tag	UNP Q7D447
A	28	LEU	-	expression tag	UNP Q7D447
A	29	VAL	_	expression tag	UNP Q7D447
A	30	PRO	-	expression tag	UNP Q7D447
A	31	ARG	_	expression tag	UNP Q7D447
A	32	GLY	-	expression tag	UNP Q7D447
A	33	SER	-	expression tag	UNP Q7D447
A	34	HIS	-	expression tag	UNP Q7D447
A	35	MET	-	expression tag	UNP Q7D447
A	278	HIS	=	expression tag	UNP Q7D447
A	279	HIS	-	expression tag	UNP Q7D447
A	280	HIS	-	expression tag	UNP Q7D447
A	281	HIS	-	expression tag	UNP Q7D447

Continued on next page...

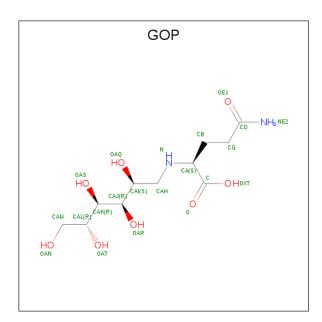


 $Continued\ from\ previous\ page...$

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	HIS	-	expression tag	UNP Q7D447
A	283	HIS	-	expression tag	UNP Q7D447
В	16	GLY	-	expression tag	UNP Q7D447
В	17	SER	-	expression tag	UNP Q7D447
В	18	SER	-	expression tag	UNP Q7D447
В	19	HIS	-	expression tag	UNP Q7D447
В	20	HIS	-	expression tag	UNP Q7D447
В	21	HIS	-	expression tag	UNP Q7D447
В	22	HIS	-	expression tag	UNP Q7D447
В	23	HIS	_	expression tag	UNP Q7D447
В	24	HIS	-	expression tag	UNP Q7D447
В	25	SER	-	expression tag	UNP Q7D447
В	26	SER	-	expression tag	UNP Q7D447
В	27	GLY	-	expression tag	UNP Q7D447
В	28	LEU	-	expression tag	UNP Q7D447
В	29	VAL	-	expression tag	UNP Q7D447
В	30	PRO	_	expression tag	UNP Q7D447
В	31	ARG	-	expression tag	UNP Q7D447
В	32	GLY	-	expression tag	UNP Q7D447
В	33	SER	-	expression tag	UNP Q7D447
В	34	HIS	-	expression tag	UNP Q7D447
В	35	MET	-	expression tag	UNP Q7D447
В	278	HIS	-	expression tag	UNP Q7D447
В	279	HIS		expression tag	UNP Q7D447
В	280	HIS	-	expression tag	UNP Q7D447
В	281	HIS	-	expression tag	UNP Q7D447
В	282	HIS		expression tag	UNP Q7D447
В	283	HIS		expression tag	UNP Q7D447

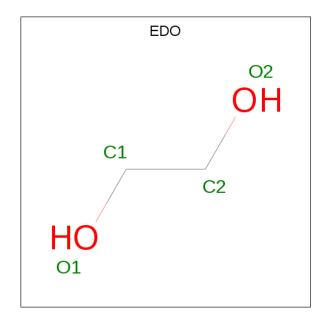
 \bullet Molecule 2 is Glucopine (three-letter code: GOP) (formula: $\rm C_{11}H_{22}N_2O_8).$





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
9	Λ.	1	Total	С	N	О	0	0	
	A	1	21	11	2	8	U		
9	D	1	Total	С	N	О	0	0	
2	Б	1	21	11	2	8	U	U	

 \bullet Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



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

Continued on next page...



Continued from previous page...

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

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0

• Molecule 5 is water.

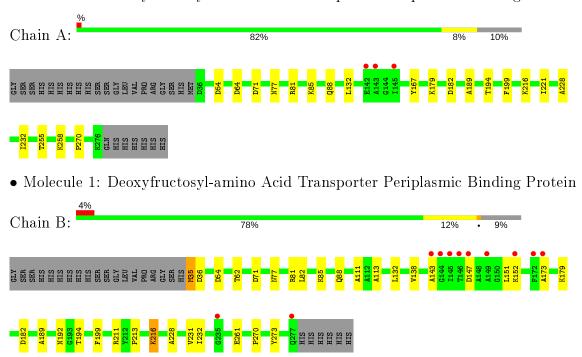
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	A	126	Total O 126 126	0	0
5	В	87	Total O 87 87	0	0



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: Deoxyfructosyl-amino Acid Transporter Periplasmic Binding Protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	$39.60 ext{Å}$ $62.29 ext{Å}$ $84.23 ext{Å}$	Depositor
a, b, c, α , β , γ	90.00° 101.40° 90.00°	Depositor
Resolution (Å)	33.83 - 1.84	Depositor
Resolution (A)	41.28 - 1.84	EDS
% Data completeness	96.5 (33.83-1.84)	Depositor
(in resolution range)	96.3 (41.28-1.84)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	0.98 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
υ .	0.218 , 0.252	Depositor
R, R_{free}	0.221 , 0.251	DCC
R_{free} test set	1688 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35 \; , 44.7$	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3944	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 77.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3045e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



¹Intensities estimated from amplitudes.

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: CA, EDO, GOP

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		
Moi Chain		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.45	0/1857	0.61	0/2517	
1	В	0.43	0/1870	0.60	0/2534	
All	All	0.44	0/3727	0.61	0/5051	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1817	0	1795	13	0
1	В	1830	0	1806	19	0
2	A	21	0	0	1	0
2	В	21	0	0	1	0
3	A	24	0	36	3	0
3	В	16	0	24	6	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
5	A	126	0	0	0	0
5	В	87	0	0	0	0
All	All	3944	0	3661	30	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 4.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$ m overlap~(\AA)$
1:B:270:PRO:HD3	3:B:304:EDO:H21	1.53	0.91
1:A:132:LEU:HD12	3:A:306:EDO:H12	1.64	0.78
1:B:143:ALA:HB2	1:B:216:LYS:HE2	1.68	0.74
1:A:77:ASN:HD21	1:A:81:ARG:HH21	1.45	0.65
1:B:77:ASN:HD21	1:B:81:ARG:HH21	1.45	0.64
1:B:35:MET:N	3:B:305:EDO:HO2	1.98	0.60
1:B:211:ARG:O	1:B:213:PRO:HD3	2.02	0.59
1:A:77:ASN:ND2	1:A:81:ARG:HE	2.04	0.56
1:B:132:LEU:HD12	3:B:304:EDO:H11	1.87	0.56
1:B:77:ASN:ND2	1:B:81:ARG:HE	2.05	0.54
1:A:270:PRO:HD3	3:A:306:EDO:H22	1.89	0.53
1:B:261:GLU:HA	3:B:302:EDO:H21	1.92	0.52
1:A:228:ALA:HB2	2:A:301:GOP:OAN	2.10	0.52
1:B:270:PRO:CD	3:B:304:EDO:H21	2.35	0.52
1:A:270:PRO:HD3	3:A:306:EDO:C2	2.40	0.51
1:A:189:ALA:HB1	1:A:194:THR:HB	1.93	0.50
1:A:258:LYS:HG2	1:B:152:LYS:HE2	1.93	0.50
1:B:228:ALA:HB2	2:B:301:GOP:OAN	2.13	0.49
1:B:85:LYS:H	1:B:88:GLN:HE21	1.62	0.48
1:B:111:ALA:HB3	1:B:231:VAL:HB	1.97	0.47
1:A:85:LYS:H	1:A:88:GLN:HE21	1.63	0.46
1:B:273:TYR:HE2	3:B:304:EDO:HO1	1.62	0.46
1:A:255:THR:HG23	1:B:173:ALA:HB2	1.96	0.46
1:A:85:LYS:H	1:A:88:GLN:NE2	2.15	0.45
1:B:85:LYS:H	1:B:88:GLN:NE2	2.14	0.45
1:B:138:VAL:HG11	1:B:151:LEU:HD21	1.98	0.44
1:B:54:ASP:OD2	1:B:182:ASP:HB2	2.18	0.44
1:A:54:ASP:OD2	1:A:182:ASP:HB2	2.18	0.43
1:A:167:TYR:CZ	1:A:221:ILE:HG21	2.54	0.43
1:B:189:ALA:HB1	1:B:194:THR:HB	2.01	0.42

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	${f Analysed}$	Favoured	Allowed	Outliers	Perce	ntiles
1	A	239/268~(89%)	235 (98%)	4 (2%)	0	100	100
1	В	$241/268 \ (90\%)$	234 (97%)	6 (2%)	1 (0%)	34	20
All	All	$480/536 \ (90\%)$	469 (98%)	10 (2%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	113	ALA

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	llysed Rotameric Outliers		Percentiles		
1	A	185/209~(88%)	179 (97%)	6 (3%)	39 21		
1	В	186/209~(89%)	175 (94%)	11 (6%)	19 5		
All	All	371/418 (89%)	354 (95%)	17 (5%)	27 10		

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	A	71	ASP
1	A	179	LYS
1	A	199	PHE
1	A	216	LYS

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	A	232	ILE
1	В	35	MET
1	В	36	ASP
1	В	62	THR
1	В	71	ASP
1	В	82	LEU
1	В	147	ASP
1	В	179	LYS
1	В	192	ASN
1	В	199	PHE
1	В	216	LYS
1	В	232	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	88	GLN
1	A	94	GLN
1	A	183	ASN
1	A	220	ASN
1	В	77	ASN
1	В	88	GLN
1	В	94	GLN
1	В	183	ASN
1	В	192	ASN
1	В	220	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	Trens	Chain	Res	Link	Вс	nd leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	$\mid \# Z > 2 \mid$
3	EDO	A	306	_	3,3,3	0.53	0	2,2,2	0.23	0
2	GOP	A	301	_	17,20,20	0.70	0	19,26,26	2.01	3 (15%)
3	EDO	A	303	_	3,3,3	0.57	0	2,2,2	0.35	0
3	EDO	В	305	_	3,3,3	0.58	0	2,2,2	0.26	0
3	EDO	A	307	_	3,3,3	0.62	0	2,2,2	0.22	0
3	EDO	A	304	_	3,3,3	0.57	0	2,2,2	0.34	0
3	EDO	В	304	_	3,3,3	0.47	0	2,2,2	0.41	0
2	GOP	В	301	-	17,20,20	0.69	0	19,26,26	1.81	2 (10%)
3	EDO	A	305	_	3,3,3	0.60	0	2,2,2	0.30	0
3	EDO	В	303	_	3,3,3	0.60	0	2,2,2	0.28	0
3	EDO	В	302	_	3,3,3	0.42	0	2,2,2	0.48	0
3	EDO	A	302	_	3,3,3	0.58	0	2,2,2	0.27	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
3	EDO	A	306	_	-	1/1/1/1	_
2	GOP	A	301	_	-	3/24/28/28	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	В	305	_	-	0/1/1/1	-
3	EDO	A	307	_	-	0/1/1/1	-
3	EDO	A	304	_	-	1/1/1/1	-
3	EDO	В	304	_	-	1/1/1/1	-
2	GOP	В	301	_	-	2/24/28/28	-
3	EDO	A	305	-	-	0/1/1/1	-
3	EDO	В	303	_	_	0/1/1/1	_
3	EDO	В	302	-	-	1/1/1/1	-
3	EDO	A	302	_	_	0/1/1/1	_



There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	A	301	GOP	CAL-CAK-CAJ	6.74	123.01	112.47
2	В	301	GOP	CAL-CAK-CAJ	6.34	122.39	112.47
2	A	301	GOP	CAM-CAL-CAK	3.08	119.09	112.41
2	В	301	GOP	CAM-CAL-CAK	3.01	118.94	112.41
2	A	301	GOP	OAN-CAM-CAL	2.92	117.44	111.07

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	302	EDO	O1-C1-C2-O2
2	A	301	GOP	CAK-CAL-CAM-OAN
3	A	304	EDO	O1-C1-C2-O2
2	В	301	GOP	NE2-CD-CG-CB
2	В	301	GOP	OE1-CD-CG-CB
3	В	304	EDO	O1-C1-C2-O2
3	A	306	EDO	O1-C1-C2-O2
2	A	301	GOP	NE2-CD-CG-CB
2	A	301	GOP	OE1-CD-CG-CB

There are no ring outliers.

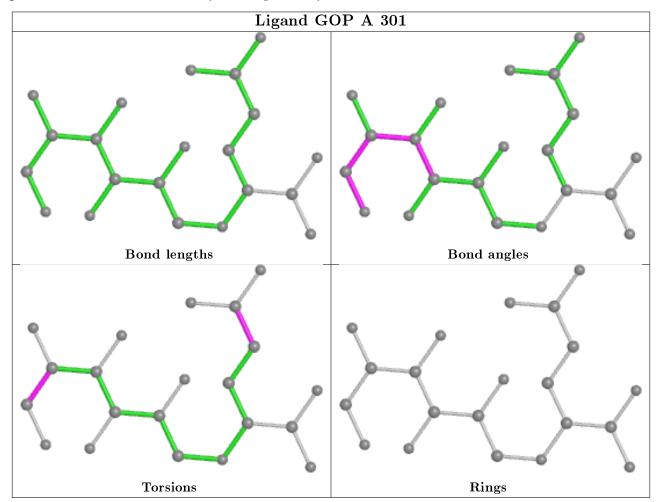
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	306	EDO	3	0
2	A	301	GOP	1	0
3	В	305	EDO	1	0
3	В	304	EDO	4	0
2	В	301	GOP	1	0
3	В	302	EDO	1	0

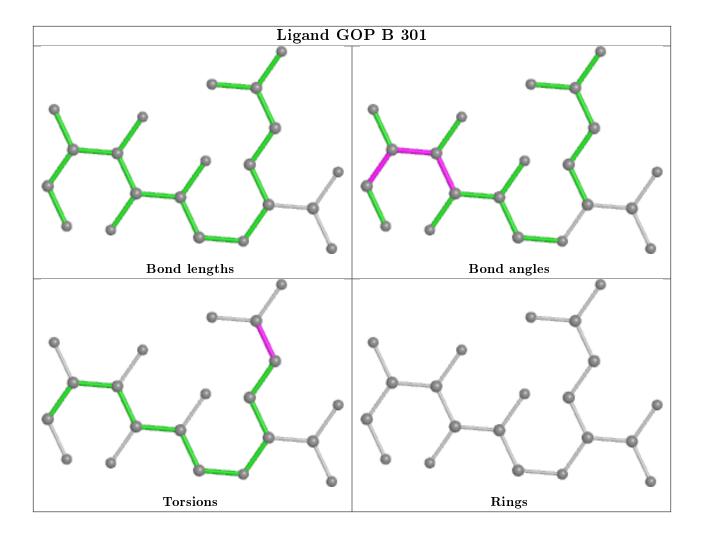
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	241/268 (89%)	-0.05	3 (1%) 79 79	20, 36, 58, 77	0
1	В	243/268 (90%)	0.29	11 (4%) 33 30	23, 45, 77, 109	0
All	All	484/536 (90%)	0.12	14 (2%) 51 49	20, 40, 71, 109	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	143	ALA	9.8
1	В	144	GLY	7.0
1	A	145	ILE	3.9
1	В	277	GLN	3.9
1	В	146	THR	3.6
1	В	235	GLY	3.1
1	В	172	PHE	2.9
1	В	147	ASP	2.8
1	В	152	LYS	2.7
1	A	143	ALA	2.6
1	В	149	ALA	2.5
1	В	173	ALA	2.5
1	A	142	GLU	2.4
1	В	145	ILE	2.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

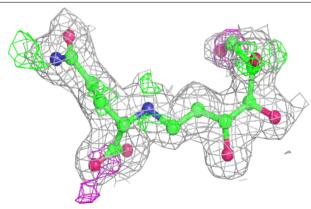
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	CA	A	308	1/1	0.63	0.12	99,99,99,99	0
3	EDO	В	305	4/4	0.64	0.24	67,67,69,70	0
3	EDO	A	303	4/4	0.64	0.28	70,71,72,72	0
3	EDO	A	302	4/4	0.64	0.36	66,67,67,68	0
3	EDO	A	305	4/4	0.69	0.22	54,55,56,57	0
3	EDO	A	307	4/4	0.75	0.14	67,67,68,68	0
3	EDO	В	303	4/4	0.82	0.16	65,66,66,66	0
3	EDO	A	304	4/4	0.86	0.17	49,51,51,52	0
2	GOP	A	301	21/21	0.88	0.12	18,23,30,31	0
3	EDO	В	302	4/4	0.91	0.41	36,38,39,41	0
3	EDO	В	304	4/4	0.93	0.25	32,37,37,37	0
2	GOP	В	301	21/21	0.93	0.10	23,31,33,34	0
4	CA	В	306	1/1	0.94	0.12	59,59,59,59	0
3	EDO	A	306	4/4	0.94	0.24	25,29,31,31	0

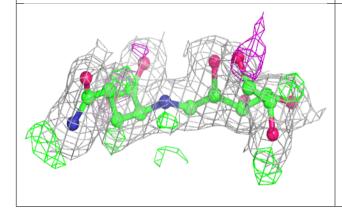
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

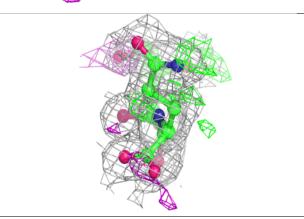


Electron density around GOP A 301:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

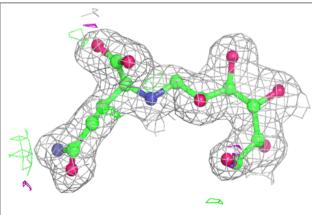


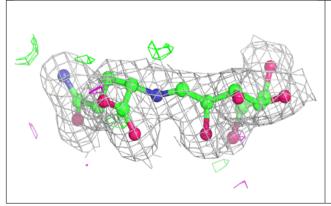


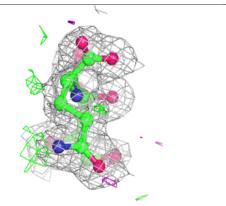


Electron density around GOP B 301:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

