Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 10:52 am GMT

PDB ID	:	5L9L
Title	:	Crystal structure of the PBP MotA from A. tumefaciens B6 in complex with glucopine
Authors	:	Marty, L.; Morera, S.
Deposited on	:	2016-06-10
Resolution	:	1.80 Å(reported)

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

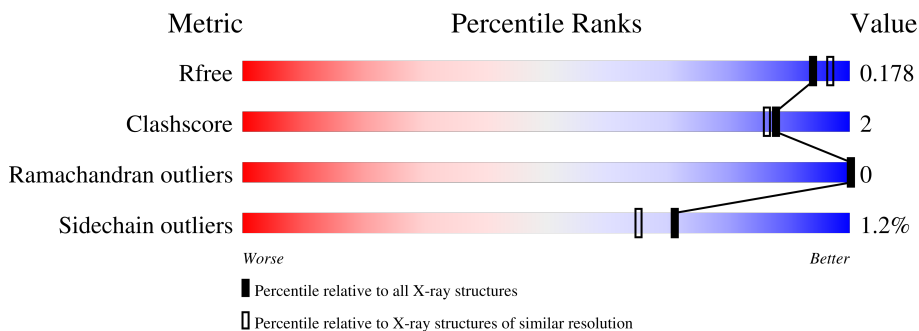|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	Percentile Ranks	Value
Rfree		0.178
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.2%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

❙ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	351	86% 6% 8%
1	B	351	86% 6% 8%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5495 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 periplasmic binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total 2482	C 1579	N 416	O 478	S 9	0	0	0
1	B	322	Total 2479	C 1577	N 415	O 477	S 10	0	1	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP A0A109C781
A	11	GLY	-	expression tag	UNP A0A109C781
A	12	SER	-	expression tag	UNP A0A109C781
A	13	SER	-	expression tag	UNP A0A109C781
A	14	HIS	-	expression tag	UNP A0A109C781
A	15	HIS	-	expression tag	UNP A0A109C781
A	16	HIS	-	expression tag	UNP A0A109C781
A	17	HIS	-	expression tag	UNP A0A109C781
A	18	HIS	-	expression tag	UNP A0A109C781
A	19	HIS	-	expression tag	UNP A0A109C781
A	20	SER	-	expression tag	UNP A0A109C781
A	21	SER	-	expression tag	UNP A0A109C781
A	22	GLY	-	expression tag	UNP A0A109C781
A	23	LEU	-	expression tag	UNP A0A109C781
A	24	VAL	-	expression tag	UNP A0A109C781
A	25	PRO	-	expression tag	UNP A0A109C781
A	26	ARG	-	expression tag	UNP A0A109C781
A	27	GLY	-	expression tag	UNP A0A109C781
A	28	SER	-	expression tag	UNP A0A109C781
A	29	HIS	-	expression tag	UNP A0A109C781
A	30	MET	-	expression tag	UNP A0A109C781
A	355	HIS	-	expression tag	UNP A0A109C781
A	356	HIS	-	expression tag	UNP A0A109C781
A	357	HIS	-	expression tag	UNP A0A109C781
A	358	HIS	-	expression tag	UNP A0A109C781

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Chain	Residue	Modelled	Actual	Comment	Reference
A	359	HIS	-	expression tag	UNP A0A109C781
A	360	HIS	-	expression tag	UNP A0A109C781
B	10	MET	-	initiating methionine	UNP A0A109C781
B	11	GLY	-	expression tag	UNP A0A109C781
B	12	SER	-	expression tag	UNP A0A109C781
B	13	SER	-	expression tag	UNP A0A109C781
B	14	HIS	-	expression tag	UNP A0A109C781
B	15	HIS	-	expression tag	UNP A0A109C781
B	16	HIS	-	expression tag	UNP A0A109C781
B	17	HIS	-	expression tag	UNP A0A109C781
B	18	HIS	-	expression tag	UNP A0A109C781
B	19	HIS	-	expression tag	UNP A0A109C781
B	20	SER	-	expression tag	UNP A0A109C781
B	21	SER	-	expression tag	UNP A0A109C781
B	22	GLY	-	expression tag	UNP A0A109C781
B	23	LEU	-	expression tag	UNP A0A109C781
B	24	VAL	-	expression tag	UNP A0A109C781
B	25	PRO	-	expression tag	UNP A0A109C781
B	26	ARG	-	expression tag	UNP A0A109C781
B	27	GLY	-	expression tag	UNP A0A109C781
B	28	SER	-	expression tag	UNP A0A109C781
B	29	HIS	-	expression tag	UNP A0A109C781
B	30	MET	-	expression tag	UNP A0A109C781
B	355	HIS	-	expression tag	UNP A0A109C781
B	356	HIS	-	expression tag	UNP A0A109C781
B	357	HIS	-	expression tag	UNP A0A109C781
B	358	HIS	-	expression tag	UNP A0A109C781
B	359	HIS	-	expression tag	UNP A0A109C781
B	360	HIS	-	expression tag	UNP A0A109C781

- Molecule 2 is Glucopine (three-letter code: GOP) (formula: $C_{11}H_{22}N_2O_8$).
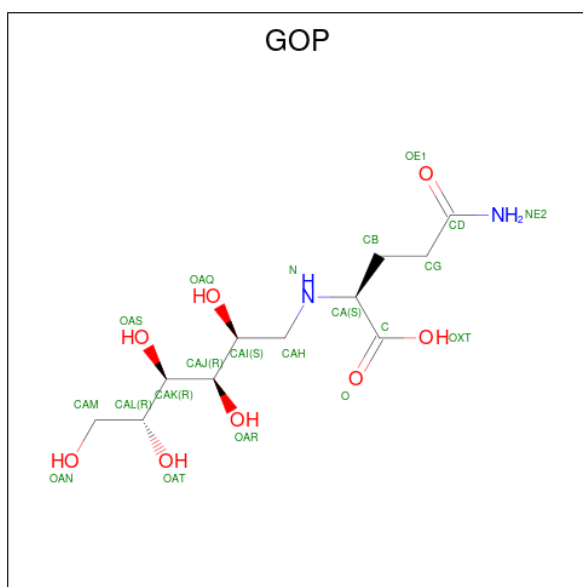
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 21	C 11	N 2	O 8	0	0
2	B	1	Total 21	C 11	N 2	O 8	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	Ca 4	0	0
3	B	3	Total 3	Ca 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	221	Total 221	O 221	0	0
5	B	208	Total 208	O 208	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.
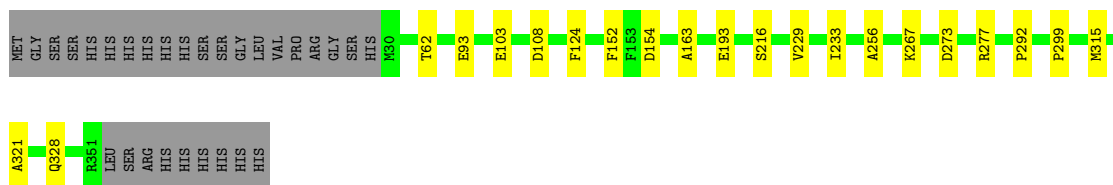
• Molecule 1: periplasmic binding protein

Chain A:
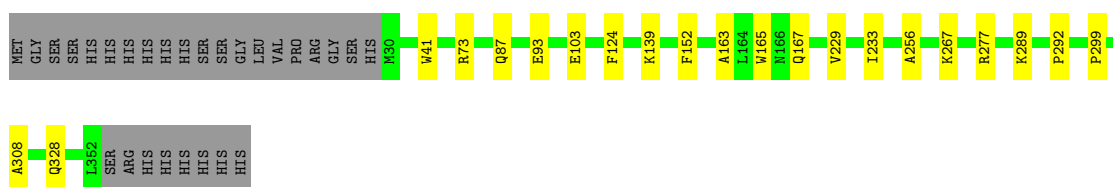
• Molecule 1: periplasmic binding protein

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	70.82Å 70.82Å 133.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.14 – 1.80 48.52 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (18.14-1.80) 99.3 (48.52-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 1.79Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.205 , 0.241 0.160 , 0.178	Depositor DCC
R_{free} test set	3031 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.1	EDS
L-test for twinning[2]	$< |L| > = 0.38, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.340 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5495	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CA, 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	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.50	0/2544	0.63	0/3460
1	B	0.50	0/2544	0.63	0/3459
All	All	0.50	0/5088	0.63	0/6919

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 ⓘ

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	2482	0	2402	10	0
1	B	2479	0	2401	11	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
4	A	16	0	24	0	0
4	B	40	0	60	3	0
5	A	221	0	0	0	0
5	B	208	0	0	0	0
All	All	5495	0	4887	20	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 2.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:HZ1	1:B:62:THR:HG23	1.57	0.69
1:B:292:PRO:HG3	1:B:299:PRO:HD3	1.83	0.60
1:A:292:PRO:HG3	1:A:299:PRO:HD3	1.84	0.59
1:B:216:SER:HB2	4:B:406:EDO:H21	1.92	0.52
1:A:163:ALA:HB2	1:A:229:VAL:HG11	1.91	0.51
1:B:163:ALA:HB2	1:B:229:VAL:HG11	1.93	0.51
1:A:103:GLU:HG2	1:A:267:LYS:HA	1.94	0.48
1:B:103:GLU:HG2	1:B:267:LYS:HA	1.95	0.48
1:A:289:LYS:HB2	1:A:308:ALA:HB2	1.97	0.47
1:B:216:SER:HB2	4:B:406:EDO:C2	2.44	0.47
1:B:93:GLU:HG3	1:B:124:PHE:HB2	1.97	0.46
1:A:93:GLU:HG3	1:A:124:PHE:HB2	1.98	0.45
1:B:256:ALA:HB3	1:B:328:GLN:HG2	2.00	0.44
1:A:256:ALA:HB3	1:A:328:GLN:HG2	2.00	0.44
1:B:152:PHE:CE2	1:B:233:ILE:HG13	2.54	0.43
1:B:315:MET:O	1:B:321:ALA:HB2	2.19	0.42
1:B:154:ASP:HA	4:B:408:EDO:H21	2.01	0.42
1:A:152:PHE:CE2	1:A:233:ILE:HG13	2.55	0.41
1:A:41:TRP:HE1	1:A:87:GLN:NE2	2.18	0.41
1:A:165:TRP:CE2	1:A:167:GLN:HB2	2.56	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	321/351 (92%)	310 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	321/351 (92%)	313 (98%)	8 (2%)	0	100	100
All	All	642/702 (92%)	623 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	249/274 (91%)	247 (99%)	2 (1%)	81	78
1	B	249/274 (91%)	245 (98%)	4 (2%)	62	54
All	All	498/548 (91%)	492 (99%)	6 (1%)	71	65

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ARG
1	A	277	ARG
1	B	108	ASP
1	B	193	GLU
1	B	273	ASP
1	B	277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	167	GLN
1	A	240	GLN
1	A	244	ASN
1	A	334	ASN
1	B	87	GLN
1	B	167	GLN

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Mol	Chain	Res	Type
1	B	240	GLN
1	B	244	ASN
1	B	334	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	EDO	A	409	-	3,3,3	0.50	0	2,2,2	0.11	0
4	EDO	A	406	-	3,3,3	0.42	0	2,2,2	0.24	0
4	EDO	B	406	-	3,3,3	0.49	0	2,2,2	0.22	0
4	EDO	B	413	-	3,3,3	0.51	0	2,2,2	0.27	0
2	GOP	A	401	-	20,20,20	2.24	7 (35%)	23,26,26	1.97	7 (30%)
4	EDO	A	407	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	B	407	-	3,3,3	0.54	0	2,2,2	0.25	0
4	EDO	B	410	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	B	412	-	3,3,3	0.47	0	2,2,2	0.24	0
4	EDO	B	414	-	3,3,3	0.52	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	GOP	B	401	-	20,20,20	2.10	7 (35%)	23,26,26	1.52	6 (26%)
4	EDO	B	408	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	A	408	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	B	409	-	3,3,3	0.51	0	2,2,2	0.17	0
4	EDO	B	411	-	3,3,3	0.46	0	2,2,2	0.37	0
4	EDO	B	405	-	3,3,3	0.48	0	2,2,2	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	409	-	-	0/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	B	413	-	-	1/1/1/1	-
2	GOP	A	401	-	-	5/28/28/28	-
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	B	410	-	-	0/1/1/1	-
4	EDO	B	412	-	-	1/1/1/1	-
4	EDO	B	414	-	-	0/1/1/1	-
2	GOP	B	401	-	-	4/28/28/28	-
4	EDO	B	408	-	-	1/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
4	EDO	B	409	-	-	1/1/1/1	-
4	EDO	B	411	-	-	1/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GOP	OAQ-CAI	-5.20	1.32	1.43
2	B	401	GOP	OAQ-CAI	-4.51	1.33	1.43
2	A	401	GOP	OAR-CAJ	-4.32	1.32	1.43
2	B	401	GOP	OAS-CAK	-3.77	1.34	1.43
2	A	401	GOP	OAT-CAL	-3.32	1.36	1.43
2	A	401	GOP	CD-NE2	3.30	1.43	1.32
2	B	401	GOP	OAR-CAJ	-3.26	1.35	1.43
2	B	401	GOP	OAT-CAL	-3.12	1.36	1.43
2	A	401	GOP	OAS-CAK	-2.98	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GOP	CD-NE2	2.85	1.42	1.32
2	B	401	GOP	OXT-C	-2.41	1.22	1.30
2	A	401	GOP	OE1-CD	-2.32	1.17	1.24
2	A	401	GOP	OXT-C	-2.27	1.23	1.30
2	B	401	GOP	CAH-CAI	2.11	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GOP	CAL-CAK-CAJ	4.93	120.18	112.47
2	A	401	GOP	OAT-CAL-CAK	3.32	117.17	109.10
2	A	401	GOP	OAN-CAM-CAL	-3.09	104.33	111.07
2	B	401	GOP	OXT-C-O	-3.02	117.22	124.09
2	B	401	GOP	CAI-CAJ-CAK	2.86	116.94	112.47
2	A	401	GOP	CAM-CAL-CAK	-2.54	106.90	112.41
2	B	401	GOP	OXT-C-CA	2.37	121.29	113.40
2	A	401	GOP	OXT-C-CA	2.35	121.22	113.40
2	A	401	GOP	CAH-CAI-CAJ	2.35	118.38	110.93
2	B	401	GOP	OAQ-CAI-CAH	2.34	114.40	109.69
2	A	401	GOP	OAS-CAK-CAL	2.07	113.82	108.81
2	B	401	GOP	CB-CA-C	2.06	115.31	110.35
2	B	401	GOP	CAL-CAK-CAJ	2.04	115.65	112.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOP	OAT-CAL-CAM-OAN
2	B	401	GOP	CB-CA-N-CAH
2	A	401	GOP	CAK-CAL-CAM-OAN
2	A	401	GOP	CAI-CAJ-CAK-CAL
2	B	401	GOP	N-CA-CB-CG
2	A	401	GOP	N-CAH-CAI-CAJ
4	B	406	EDO	O1-C1-C2-O2
4	B	411	EDO	O1-C1-C2-O2
4	B	412	EDO	O1-C1-C2-O2
2	B	401	GOP	N-CAH-CAI-CAJ
2	B	401	GOP	C-CA-CB-CG
4	B	405	EDO	O1-C1-C2-O2
4	B	413	EDO	O1-C1-C2-O2
2	A	401	GOP	CB-CA-N-CAH
4	A	406	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	408	EDO	O1-C1-C2-O2
4	B	409	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	406	EDO	2	0
4	B	408	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.

Ligand GOP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand GOP B 401

Bond lengths

Bond angles

Torsions

Rings
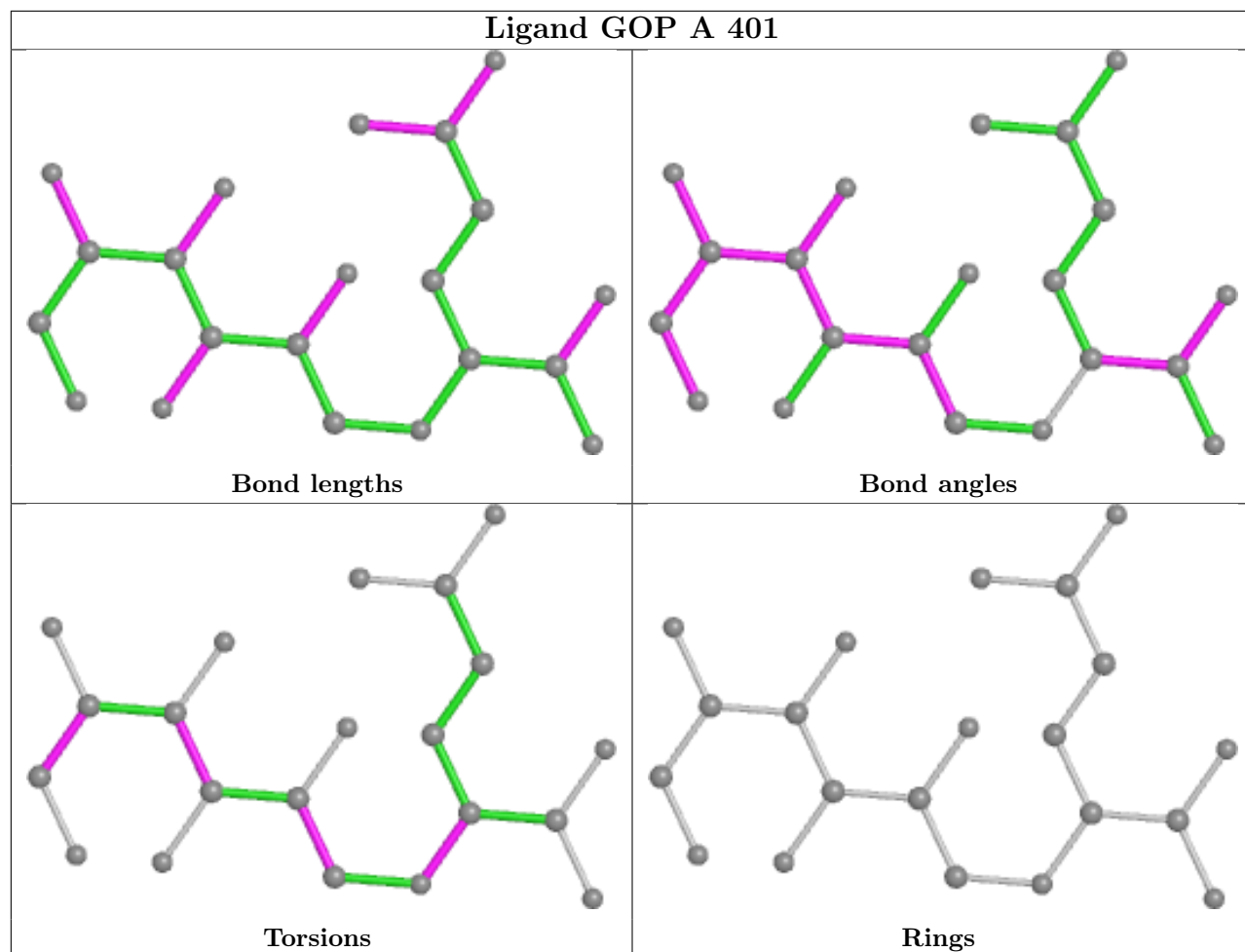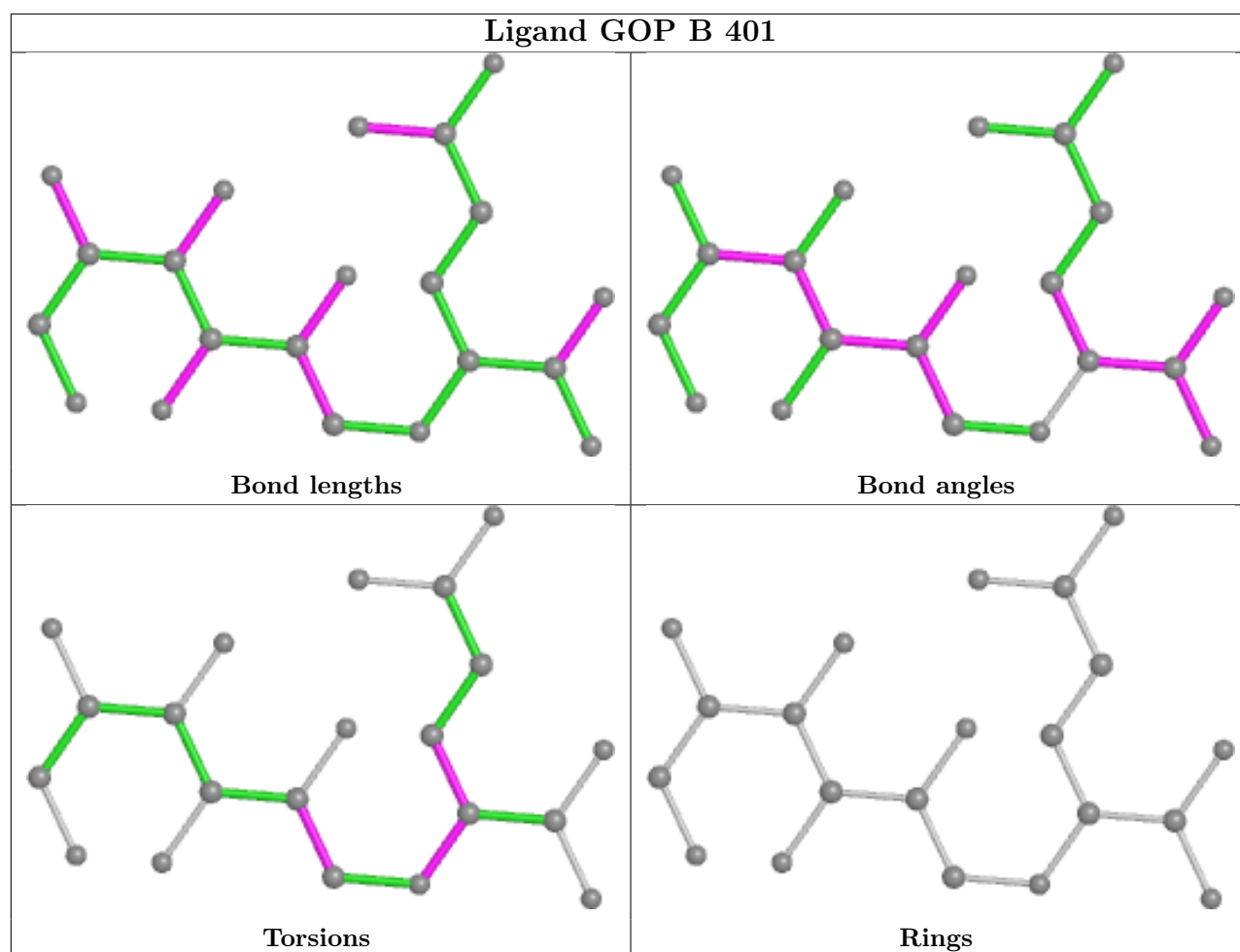
5.7 Other polymers (i)

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

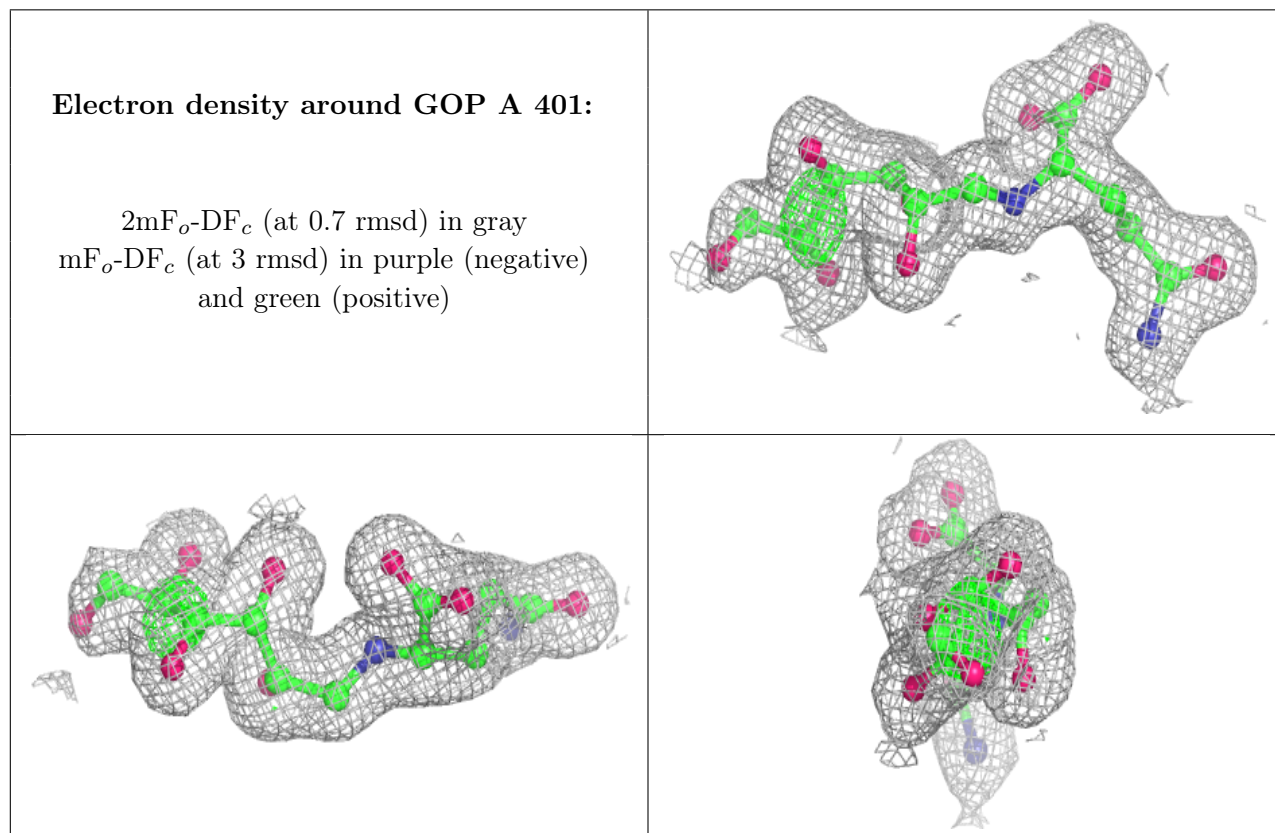Unable to reproduce the depositors R factor - this section is therefore empty.
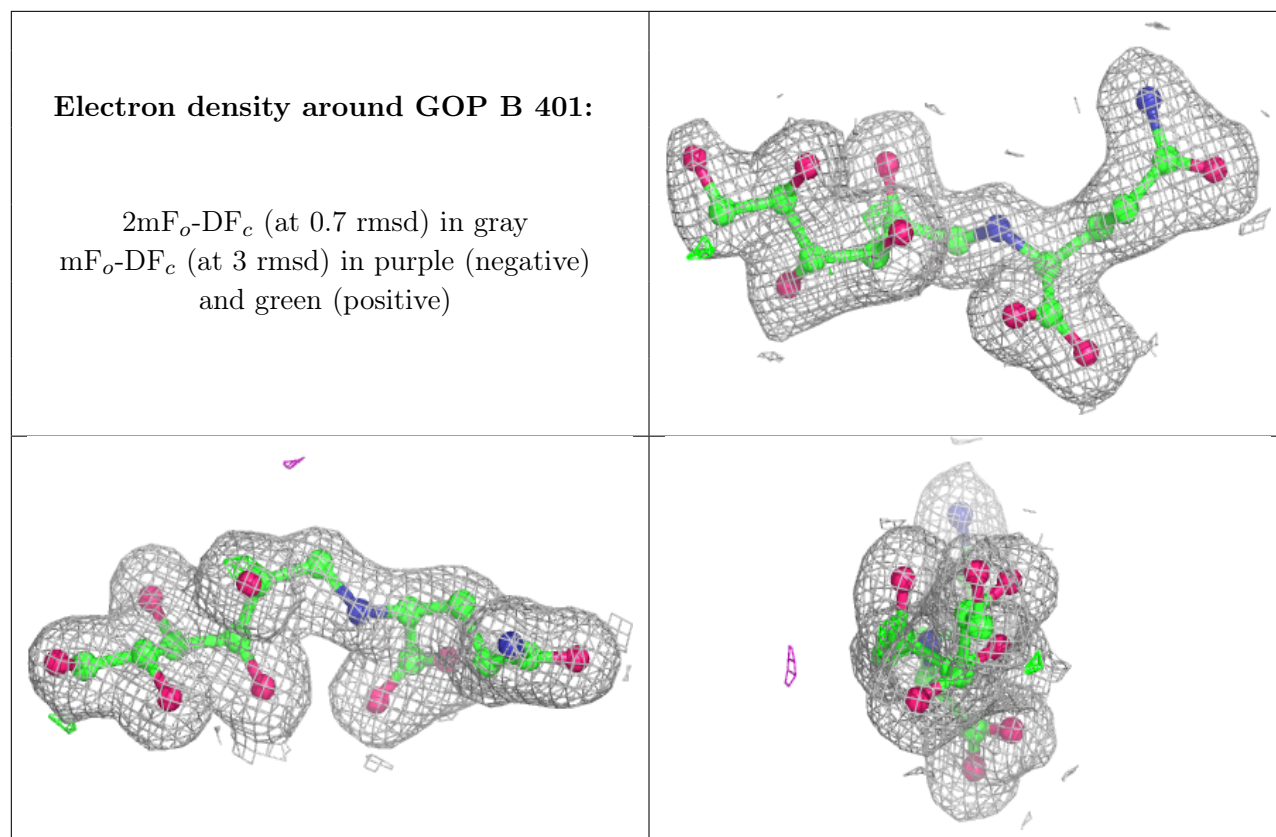
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 401:

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

Electron density around GOP B 401:

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

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.