



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 12:19 AM EDT

PDB ID : 6I35  
Title : Crystal structure of human glycine decarboxylase (P-protein) bound with pyridoxyl-glycine-5'-monophosphate  
Authors : Van Laer, B.; Kapp, U.; Leonard, G.; Mueller-Dieckmann, C.  
Deposited on : 2018-11-05  
Resolution : 2.00 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

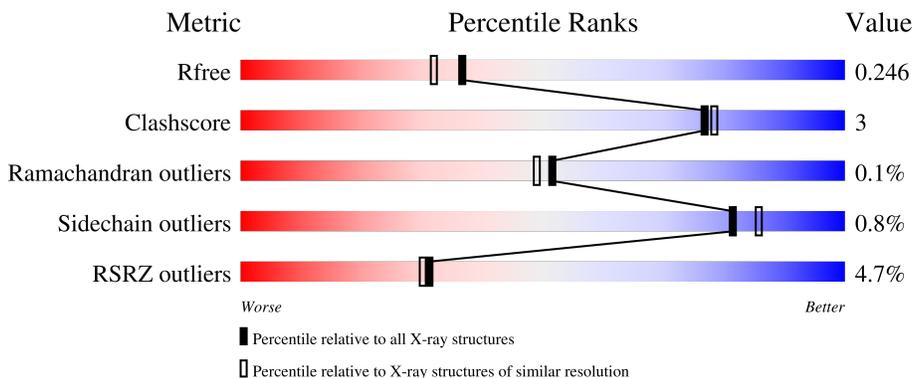
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	984	
1	B	984	
1	C	984	
1	D	984	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 30932 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 Glycine dehydrogenase (decarboxylating), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	953	7433	4684	1317	1378	54	0	0	0
1	B	954	7442	4688	1318	1382	54	0	0	0
1	C	953	7433	4684	1317	1378	54	0	0	0
1	D	954	7442	4688	1318	1382	54	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

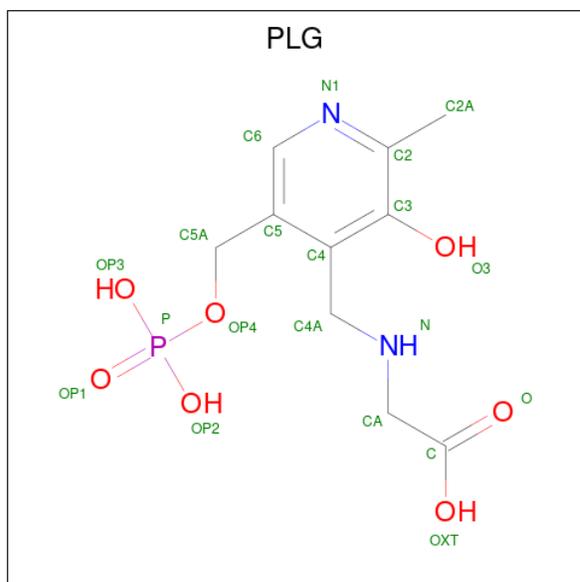
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP P23378
A	1021	GLY	-	expression tag	UNP P23378
A	1022	HIS	-	expression tag	UNP P23378
A	1023	HIS	-	expression tag	UNP P23378
A	1024	HIS	-	expression tag	UNP P23378
A	1025	HIS	-	expression tag	UNP P23378
A	1026	HIS	-	expression tag	UNP P23378
A	1027	HIS	-	expression tag	UNP P23378
B	44	MET	-	initiating methionine	UNP P23378
B	1021	GLY	-	expression tag	UNP P23378
B	1022	HIS	-	expression tag	UNP P23378
B	1023	HIS	-	expression tag	UNP P23378
B	1024	HIS	-	expression tag	UNP P23378
B	1025	HIS	-	expression tag	UNP P23378
B	1026	HIS	-	expression tag	UNP P23378
B	1027	HIS	-	expression tag	UNP P23378
C	44	MET	-	initiating methionine	UNP P23378
C	1021	GLY	-	expression tag	UNP P23378
C	1022	HIS	-	expression tag	UNP P23378
C	1023	HIS	-	expression tag	UNP P23378
C	1024	HIS	-	expression tag	UNP P23378

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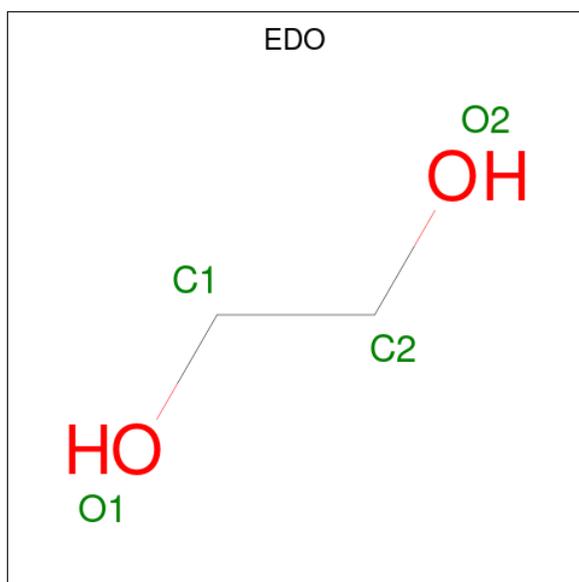
Chain	Residue	Modelled	Actual	Comment	Reference
C	1025	HIS	-	expression tag	UNP P23378
C	1026	HIS	-	expression tag	UNP P23378
C	1027	HIS	-	expression tag	UNP P23378
D	44	MET	-	initiating methionine	UNP P23378
D	1021	GLY	-	expression tag	UNP P23378
D	1022	HIS	-	expression tag	UNP P23378
D	1023	HIS	-	expression tag	UNP P23378
D	1024	HIS	-	expression tag	UNP P23378
D	1025	HIS	-	expression tag	UNP P23378
D	1026	HIS	-	expression tag	UNP P23378
D	1027	HIS	-	expression tag	UNP P23378

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



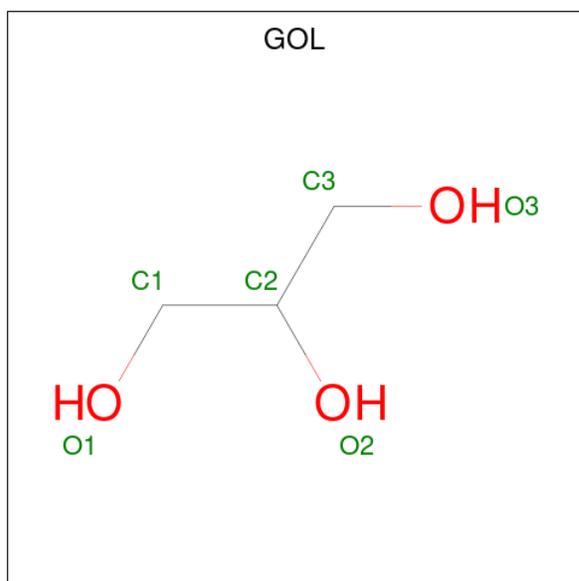
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



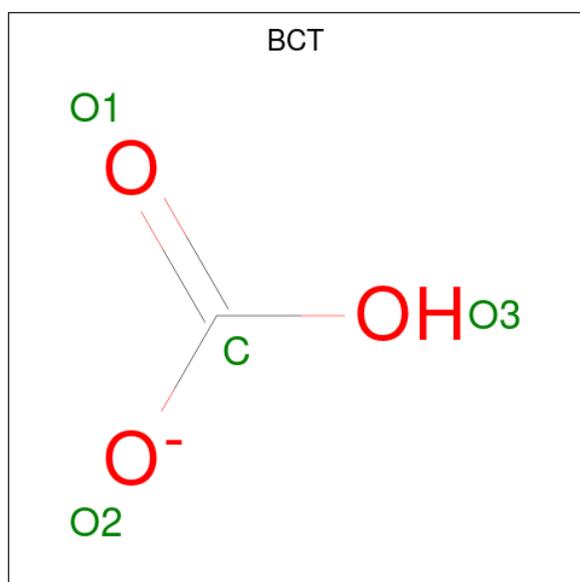
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			4	2 2		
3	B	1	Total	C O	0	0
			4	2 2		
3	C	1	Total	C O	0	0
			4	2 2		
3	D	1	Total	C O	0	0
			4	2 2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



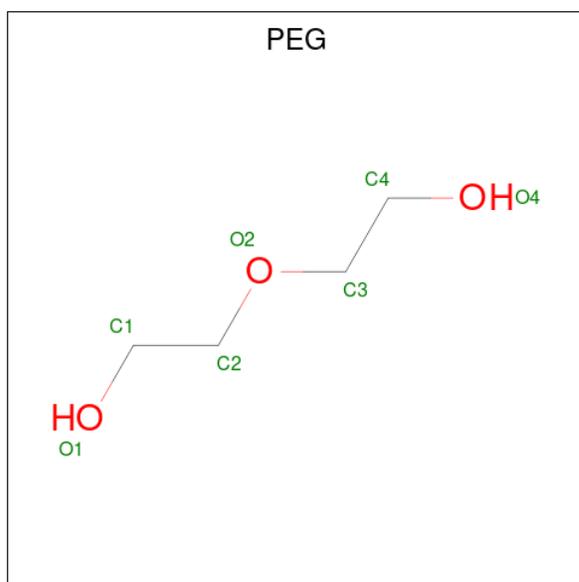
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $\text{C}_4\text{H}_{10}\text{O}_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0

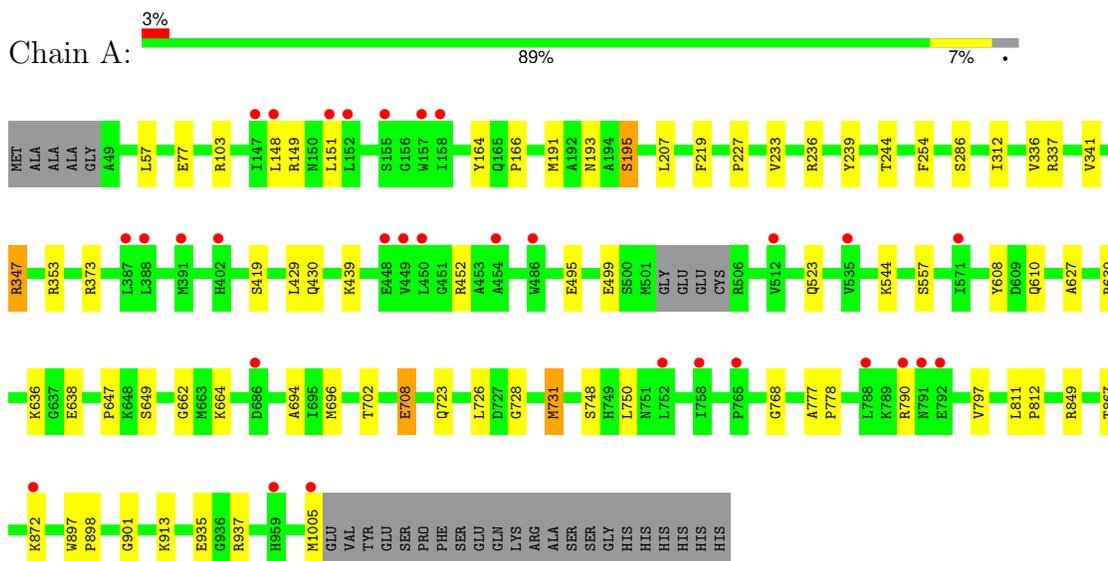
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	318	Total O 318 318	0	0
7	B	192	Total O 192 192	0	0
7	C	314	Total O 314 314	0	0
7	D	200	Total O 200 200	0	0

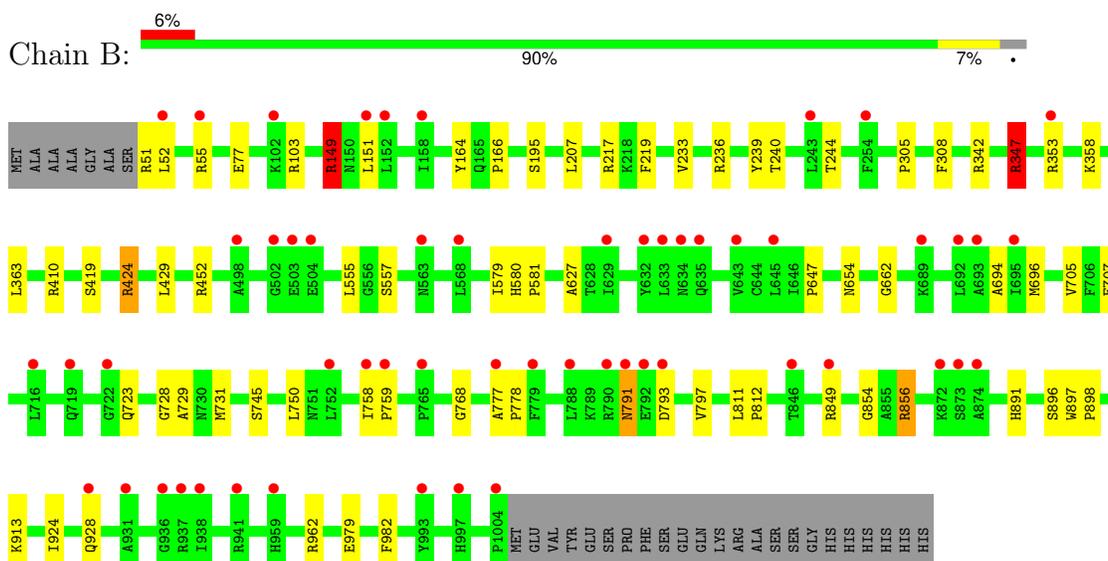
### 3 Residue-property plots [i](#)

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.

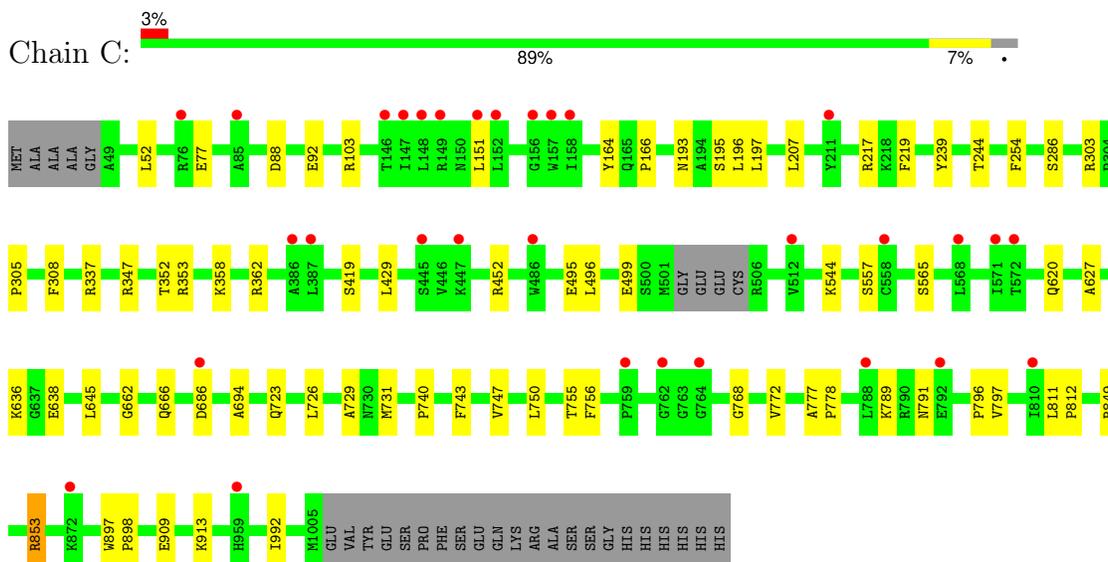
- Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial



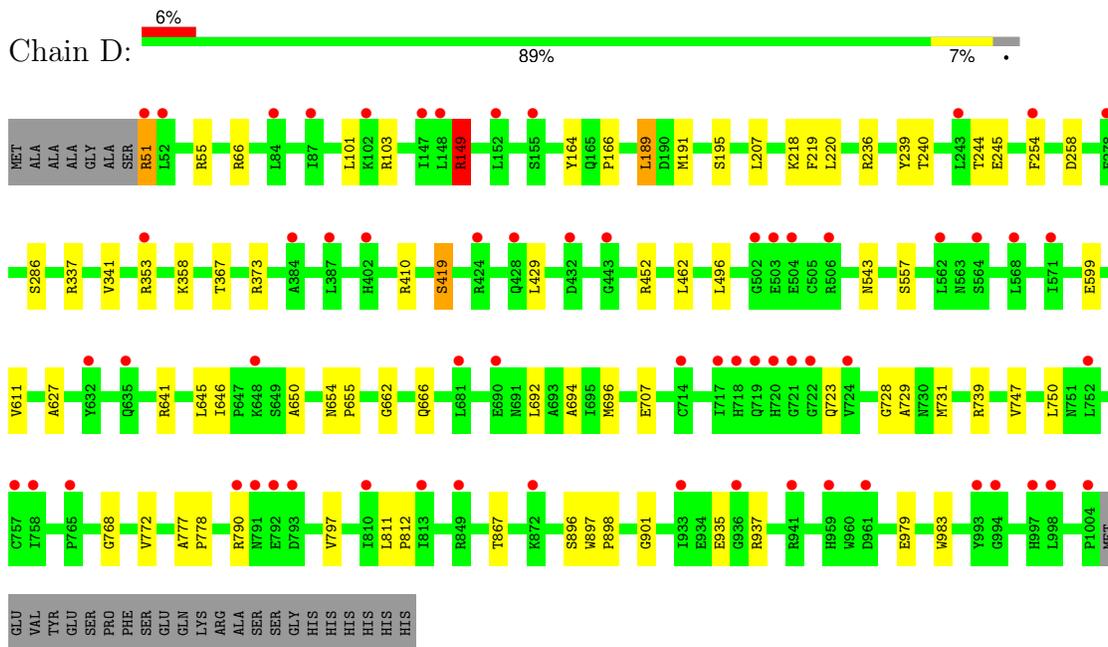
- Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial



- Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial



• Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.66Å 123.44Å 197.67Å 90.00° 97.93° 90.00°	Depositor
Resolution (Å)	49.33 – 2.00 49.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.33-2.00) 99.0 (49.33-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.215 , 0.240 0.222 , 0.246	Depositor DCC
$R_{free}$ test set	13576 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtrriage
Anisotropy	0.358	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	30932	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.09 % 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 5.1082e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, EDO, GOL, PLG, BCT

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	0.61	0/7599	0.69	3/10291 (0.0%)
1	B	0.57	0/7609	0.66	2/10306 (0.0%)
1	C	0.62	1/7599 (0.0%)	0.69	2/10291 (0.0%)
1	D	0.58	0/7609	0.66	2/10306 (0.0%)
All	All	0.59	1/30416 (0.0%)	0.67	9/41194 (0.0%)

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	A	0	8
1	B	0	8
1	C	0	5
1	D	0	6
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	909	GLU	CD-OE2	-5.41	1.19	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	B	149	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	731	MET	CG-SD-CE	5.77	109.43	100.20
1	A	347	ARG	NE-CZ-NH1	-5.66	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	ARG	NE-CZ-NH2	-5.64	117.48	120.30

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	337	ARG	Sidechain
1	A	373	ARG	Sidechain

## 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	7433	0	7371	42	0
1	B	7442	0	7373	47	0
1	C	7433	0	7371	38	1
1	D	7442	0	7373	58	0
2	A	20	0	11	0	0
2	B	20	0	11	2	0
2	C	20	0	11	1	0
2	D	20	0	11	1	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
4	C	12	0	16	0	0
5	A	4	0	0	0	0
6	B	7	0	10	1	0
6	C	14	0	20	3	0
6	D	7	0	10	2	0
7	A	318	0	0	2	0
7	B	192	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	314	0	0	0	0
7	D	200	0	0	2	0
All	All	30932	0	29636	178	1

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 178 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:B:856:ARG:HH11	1:B:856:ARG:HG3	1.13	1.06
1:B:580:HIS:ND1	1:B:581:PRO:HD2	1.94	0.82
1:A:191:MET:SD	1:A:341:VAL:HG21	2.20	0.81
1:C:495:GLU:OE2	1:D:51:ARG:HD2	1.81	0.81
1:D:191:MET:SD	1:D:341:VAL:HG21	2.23	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:GLU:OE2	1:C:853:ARG:NH1[1_455]	1.99	0.21

## 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	949/984 (96%)	922 (97%)	26 (3%)	1 (0%)	51 49
1	B	952/984 (97%)	922 (97%)	29 (3%)	1 (0%)	51 49
1	C	949/984 (96%)	923 (97%)	25 (3%)	1 (0%)	51 49
1	D	952/984 (97%)	920 (97%)	31 (3%)	1 (0%)	51 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3802/3936 (97%)	3687 (97%)	111 (3%)	4 (0%)	51	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	C	195	SER
1	D	195	SER
1	B	195	SER

### 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	805/829 (97%)	801 (100%)	4 (0%)	88	92
1	B	806/829 (97%)	796 (99%)	10 (1%)	71	76
1	C	805/829 (97%)	800 (99%)	5 (1%)	86	90
1	D	806/829 (97%)	799 (99%)	7 (1%)	78	83
All	All	3222/3316 (97%)	3196 (99%)	26 (1%)	81	86

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	LEU
1	C	686	ASP
1	D	707	GLU
1	C	557	SER
1	C	791	ASN

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	610	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

18 ligands 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
4	GOL	C	1103	-	5,5,5	0.64	0	5,5,5	0.74	0
3	EDO	A	1102	-	3,3,3	0.70	0	2,2,2	0.27	0
4	GOL	A	1103	-	5,5,5	0.45	0	5,5,5	0.59	0
6	PEG	C	1106	-	6,6,6	0.71	0	5,5,5	0.37	0
3	EDO	D	1102	-	3,3,3	0.43	0	2,2,2	1.11	0
3	EDO	C	1102	-	3,3,3	0.45	0	2,2,2	0.30	0
3	EDO	B	3001	-	3,3,3	0.40	0	2,2,2	0.45	0
4	GOL	C	1105	-	5,5,5	0.58	0	5,5,5	0.20	0
4	GOL	B	3004	-	5,5,5	0.26	0	5,5,5	0.31	0
2	PLG	B	3003	-	20,20,20	2.76	3 (15%)	26,28,28	2.21	8 (30%)
5	BCT	A	1105	-	3,3,3	1.62	1 (33%)	2,3,3	0.38	0
6	PEG	C	1104	-	6,6,6	0.64	0	5,5,5	0.62	0
6	PEG	D	1103	-	6,6,6	0.54	0	5,5,5	0.68	0
4	GOL	A	1104	-	5,5,5	0.55	0	5,5,5	1.18	0
2	PLG	A	1101	-	20,20,20	2.06	3 (15%)	26,28,28	2.42	13 (50%)
6	PEG	B	3002	-	6,6,6	0.60	0	5,5,5	0.67	0
2	PLG	D	1101	-	20,20,20	2.51	6 (30%)	26,28,28	2.40	9 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLG	C	1101	-	20,20,20	2.15	9 (45%)	26,28,28	2.03	9 (34%)

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	GOL	C	1103	-	-	4/4/4/4	-
3	EDO	A	1102	-	-	1/1/1/1	-
4	GOL	A	1103	-	-	2/4/4/4	-
6	PEG	C	1106	-	-	2/4/4/4	-
3	EDO	D	1102	-	-	1/1/1/1	-
3	EDO	C	1102	-	-	0/1/1/1	-
3	EDO	B	3001	-	-	1/1/1/1	-
4	GOL	C	1105	-	-	2/4/4/4	-
4	GOL	B	3004	-	-	3/4/4/4	-
2	PLG	B	3003	-	-	3/12/12/12	0/1/1/1
6	PEG	C	1104	-	-	3/4/4/4	-
6	PEG	D	1103	-	-	3/4/4/4	-
4	GOL	A	1104	-	-	3/4/4/4	-
2	PLG	A	1101	-	-	3/12/12/12	0/1/1/1
6	PEG	B	3002	-	-	3/4/4/4	-
2	PLG	D	1101	-	-	3/12/12/12	0/1/1/1
2	PLG	C	1101	-	-	2/12/12/12	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3003	PLG	C3-C2	7.66	1.48	1.41
2	B	3003	PLG	C5-C4	6.83	1.50	1.40
2	A	1101	PLG	C3-C2	6.36	1.47	1.41
2	D	1101	PLG	C3-C2	6.03	1.47	1.41
2	B	3003	PLG	C3-C4	6.03	1.48	1.40

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	PLG	C4A-N-CA	7.76	121.76	112.72

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3003	PLG	C4A-N-CA	6.75	120.58	112.72
2	A	1101	PLG	OP3-P-OP4	-4.57	94.75	106.67
2	A	1101	PLG	OP4-P-OP1	4.47	118.52	106.44
2	D	1101	PLG	C4A-C4-C5	4.47	124.61	119.75

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

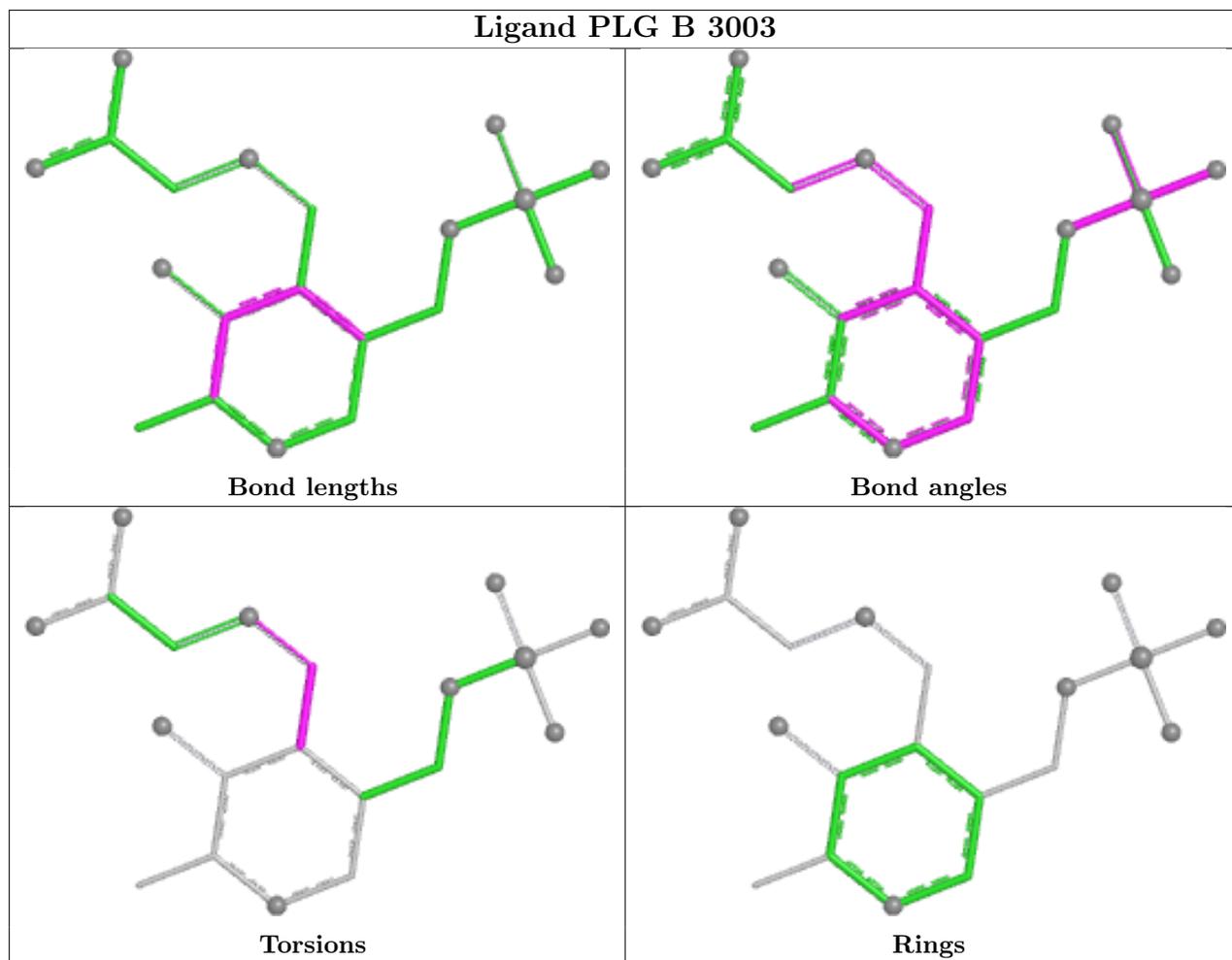
Mol	Chain	Res	Type	Atoms
2	A	1101	PLG	C3-C4-C4A-N
2	A	1101	PLG	C5-C4-C4A-N
2	B	3003	PLG	C5-C4-C4A-N
2	C	1101	PLG	C3-C4-C4A-N
2	C	1101	PLG	C5-C4-C4A-N

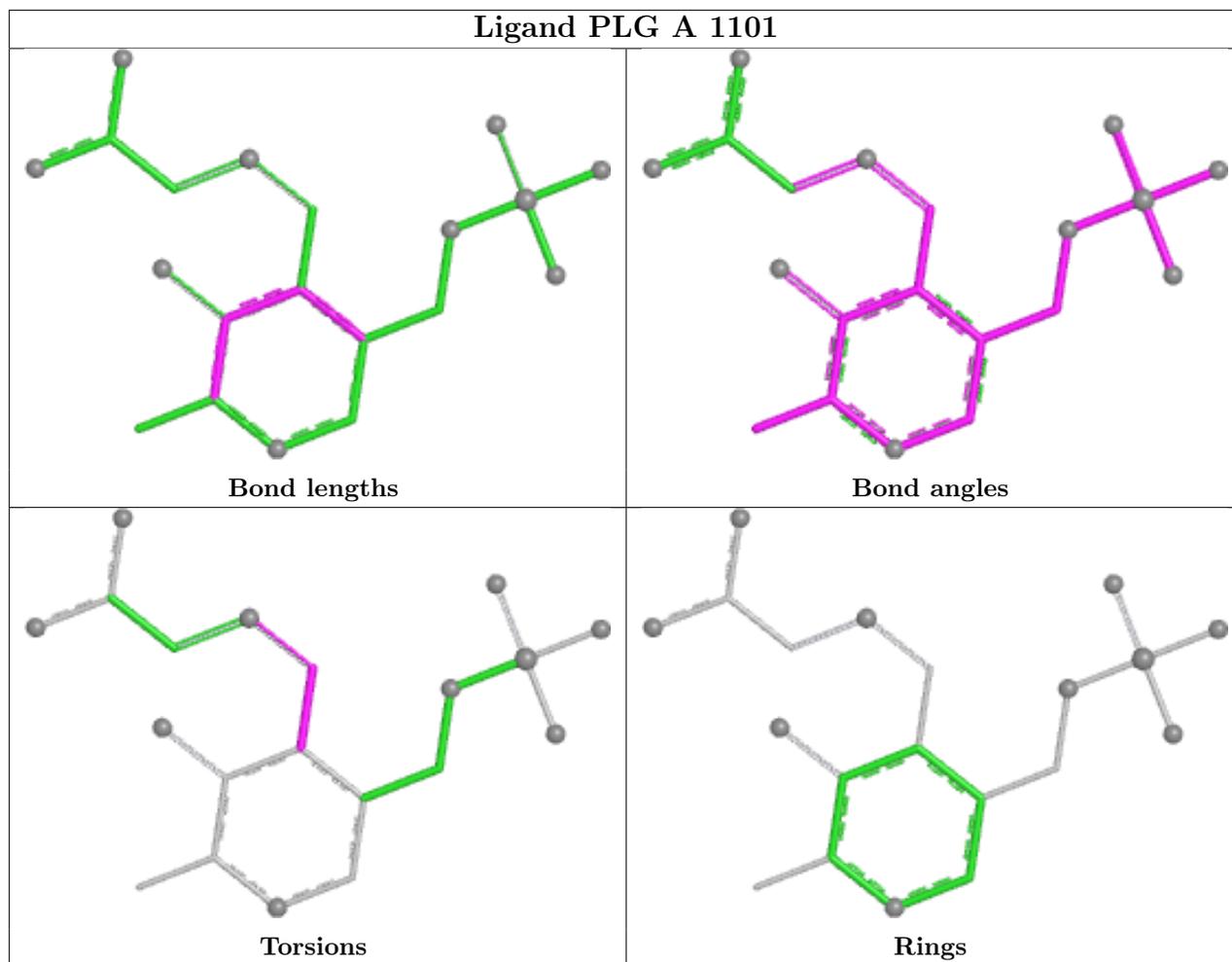
There are no ring outliers.

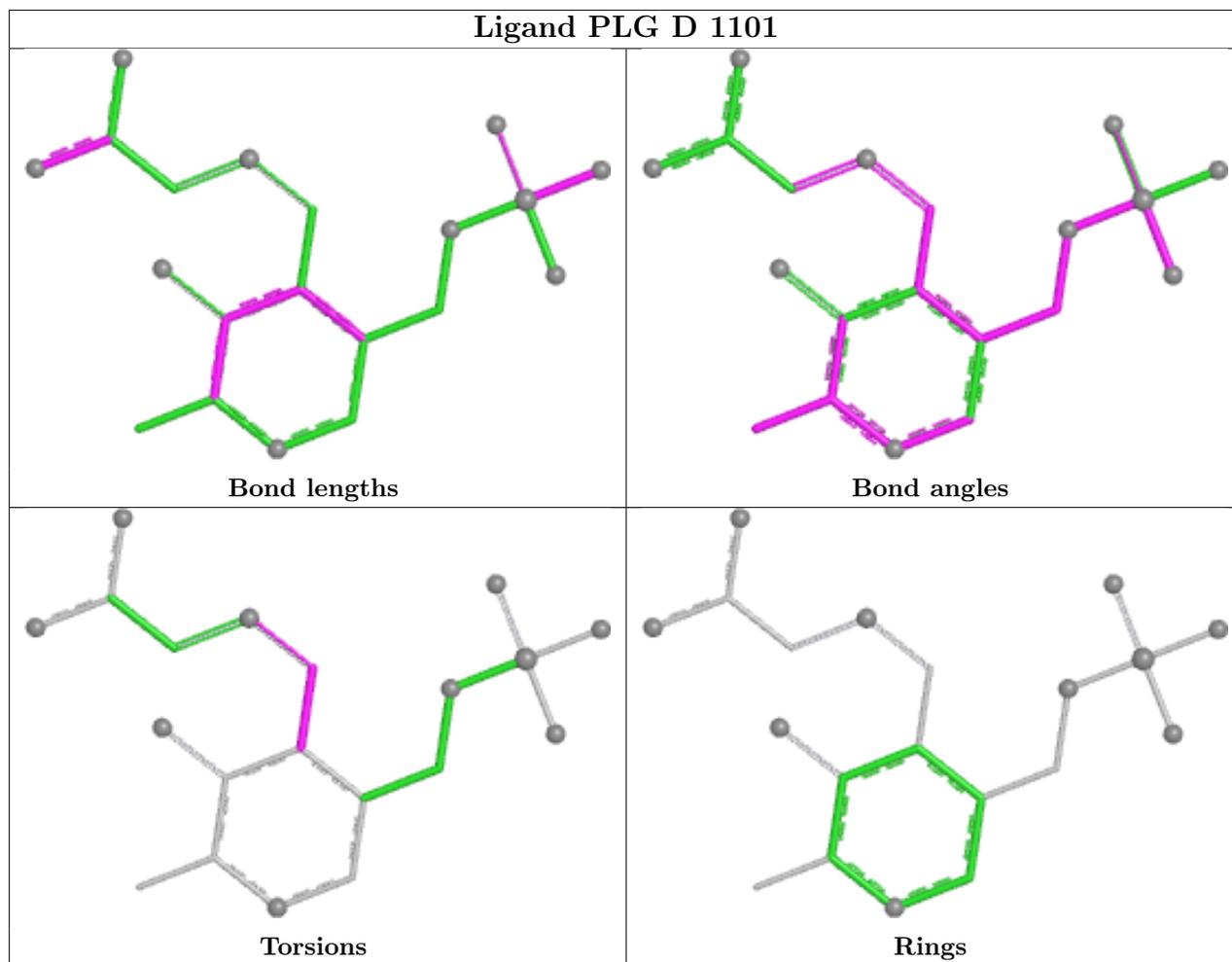
6 monomers are involved in 9 short contacts:

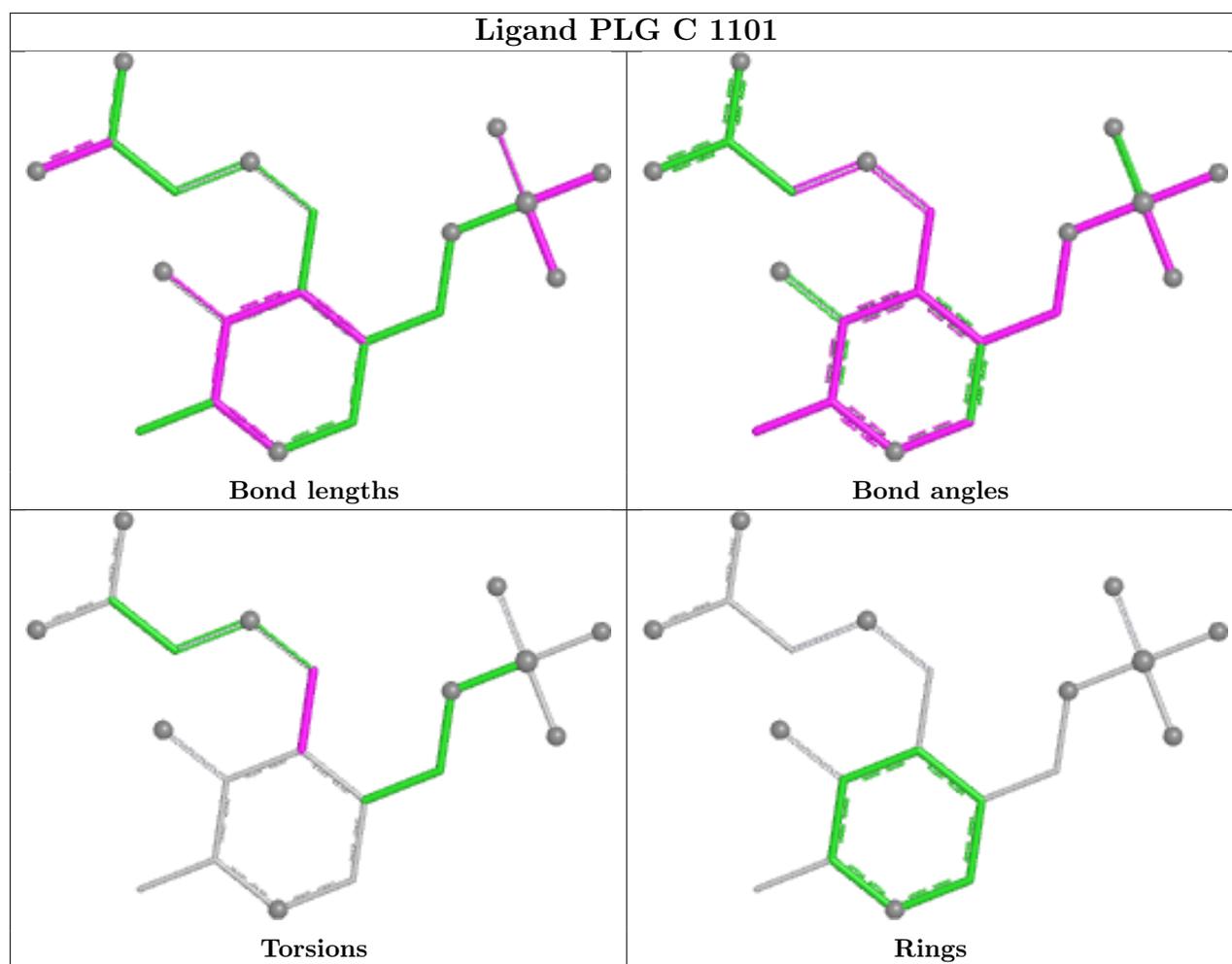
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1106	PEG	3	0
2	B	3003	PLG	2	0
6	D	1103	PEG	2	0
6	B	3002	PEG	1	0
2	D	1101	PLG	1	0
2	C	1101	PLG	1	0

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 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	953/984 (96%)	0.09	30 (3%) 49 48	28, 41, 62, 99	0
1	B	954/984 (96%)	0.33	55 (5%) 23 22	32, 54, 80, 99	0
1	C	953/984 (96%)	0.10	31 (3%) 46 45	26, 40, 61, 92	0
1	D	954/984 (96%)	0.28	63 (6%) 18 17	31, 52, 80, 99	0
All	All	3814/3936 (96%)	0.20	179 (4%) 31 30	26, 46, 76, 99	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	792	GLU	6.5
1	C	959	HIS	4.9
1	B	629	ILE	4.9
1	D	722	GLY	4.8
1	B	52	LEU	4.7

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

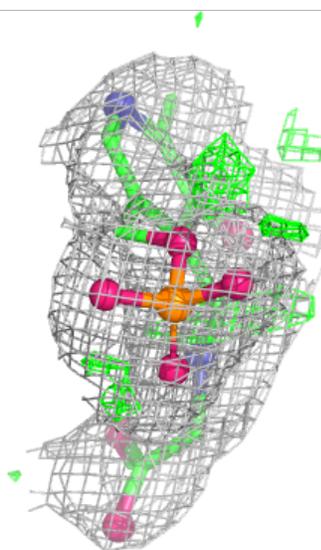
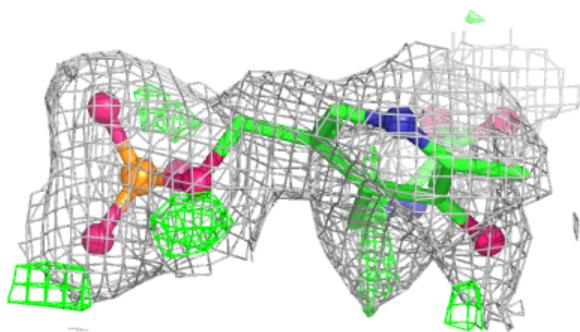
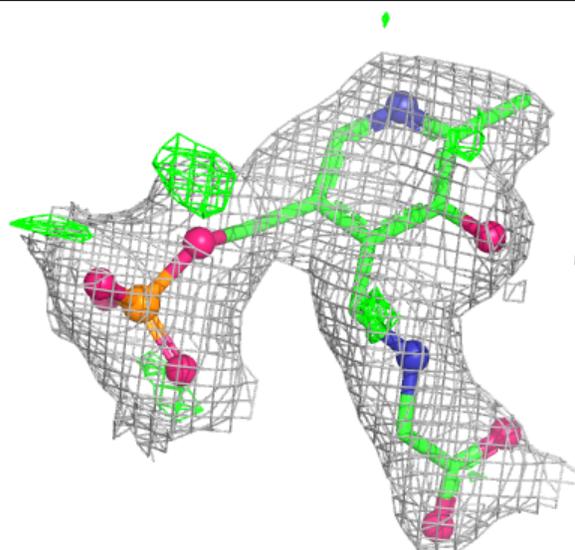
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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
6	PEG	C	1106	7/7	0.53	0.30	63,65,68,69	0
3	EDO	A	1102	4/4	0.57	0.34	59,59,61,62	0
6	PEG	B	3002	7/7	0.76	0.28	54,57,67,70	0
3	EDO	B	3001	4/4	0.78	0.16	63,63,63,64	0
6	PEG	C	1104	7/7	0.80	0.14	46,58,68,70	0
5	BCT	A	1105	4/4	0.81	0.14	53,56,62,64	0
6	PEG	D	1103	7/7	0.81	0.22	52,64,65,71	0
4	GOL	C	1103	6/6	0.82	0.24	45,58,58,62	0
4	GOL	C	1105	6/6	0.84	0.22	39,44,45,50	0
3	EDO	D	1102	4/4	0.85	0.36	40,41,45,47	0
3	EDO	C	1102	4/4	0.85	0.12	57,60,60,61	0
4	GOL	A	1103	6/6	0.87	0.22	55,62,65,67	0
4	GOL	A	1104	6/6	0.90	0.16	49,53,56,63	0
4	GOL	B	3004	6/6	0.94	0.22	48,50,53,59	0
2	PLG	D	1101	20/20	0.94	0.17	42,60,71,73	0
2	PLG	A	1101	20/20	0.97	0.20	26,33,49,54	0
2	PLG	B	3003	20/20	0.97	0.16	44,58,65,66	0
2	PLG	C	1101	20/20	0.97	0.18	25,32,49,52	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.

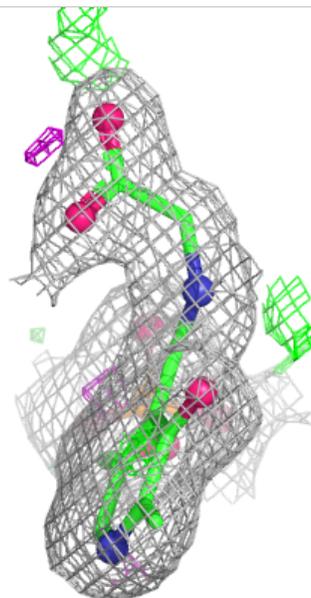
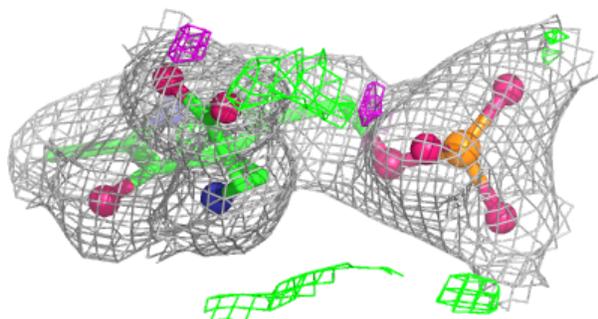
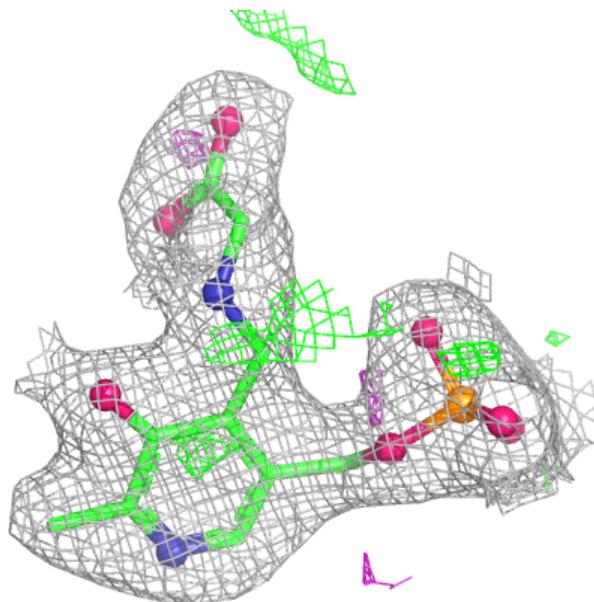
**Electron density around PLG D 1101:**

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



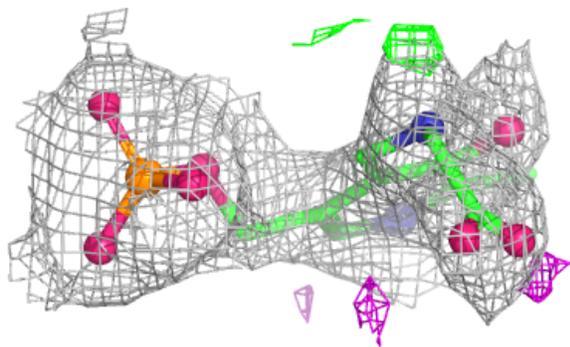
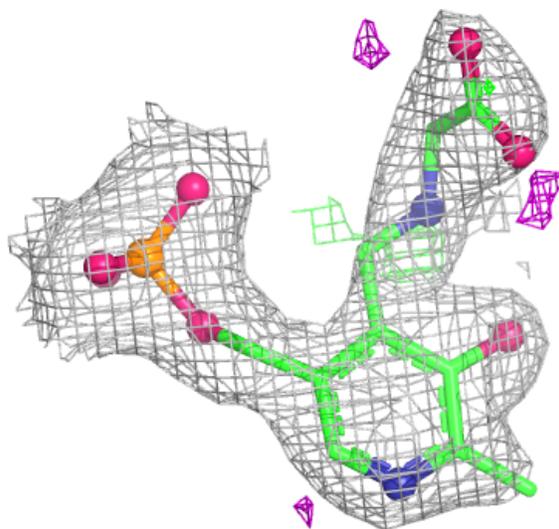
**Electron density around PLG A 1101:**

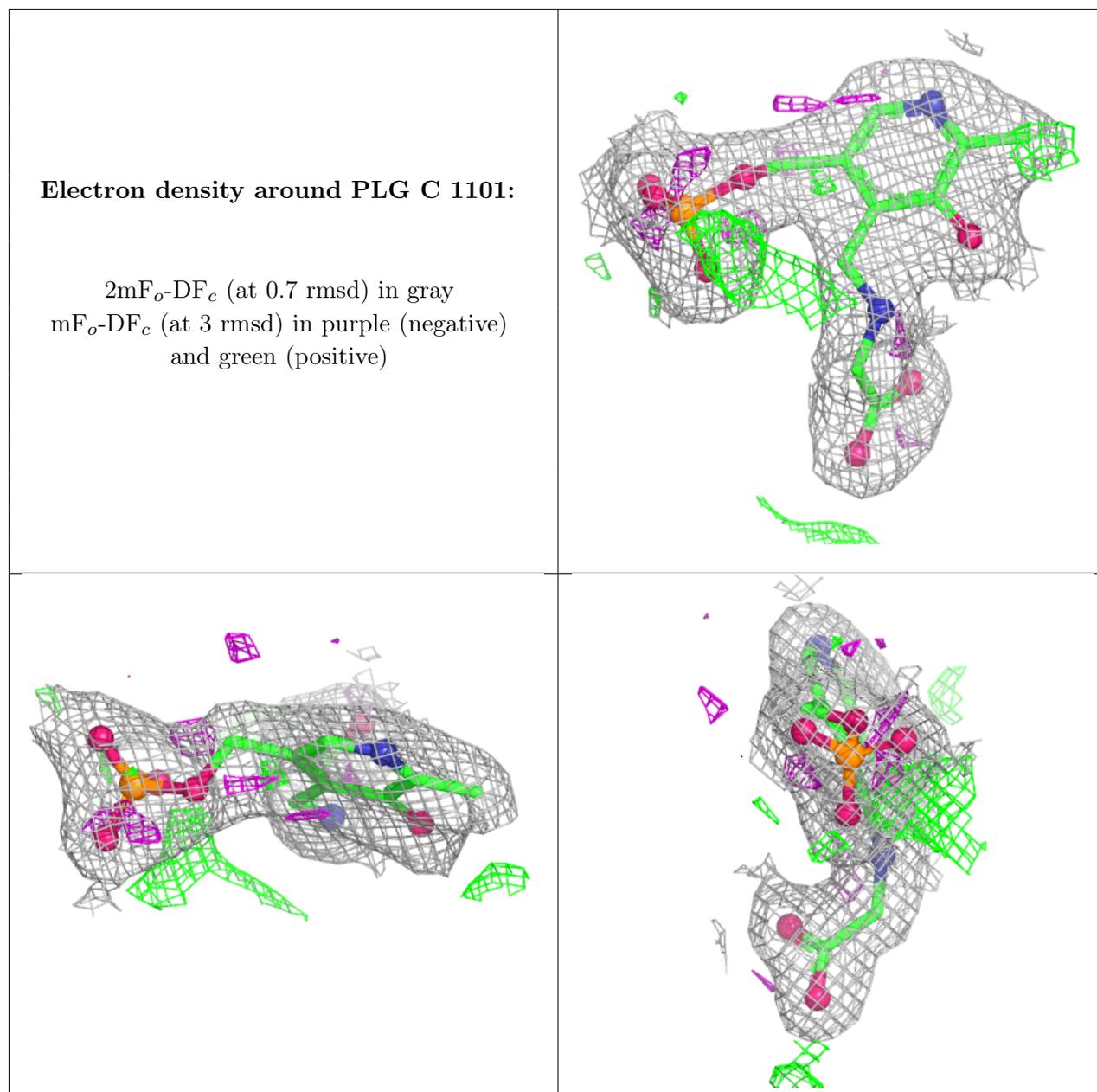
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PLG B 3003:**

$2mF_o-DF_c$  (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.