Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 03:53 PM JST

PDB ID	:	5AZB
Title	:	Crystal structure of Escherichia coli Lgt in complex with phosphatidylglycerol and the inhibitor palmitic acid
Authors	:	Zhang, X.C.; Mao, G.; Zhao, Y.
Deposited on	:	2015-09-30
Resolution	:	1.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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.

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

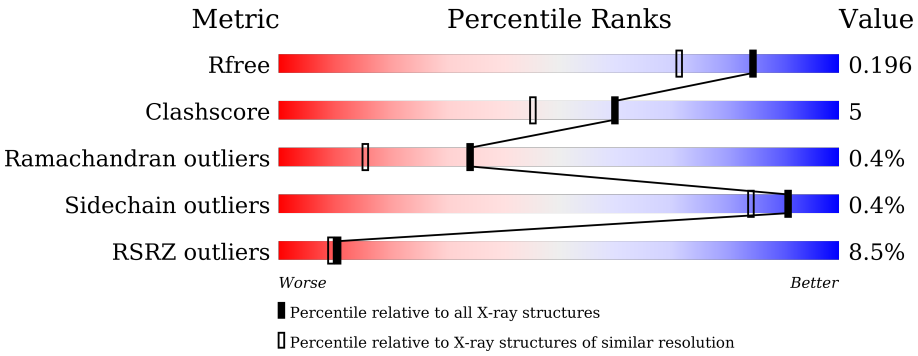
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	300	8%, 86%, 9%, 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2711 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.

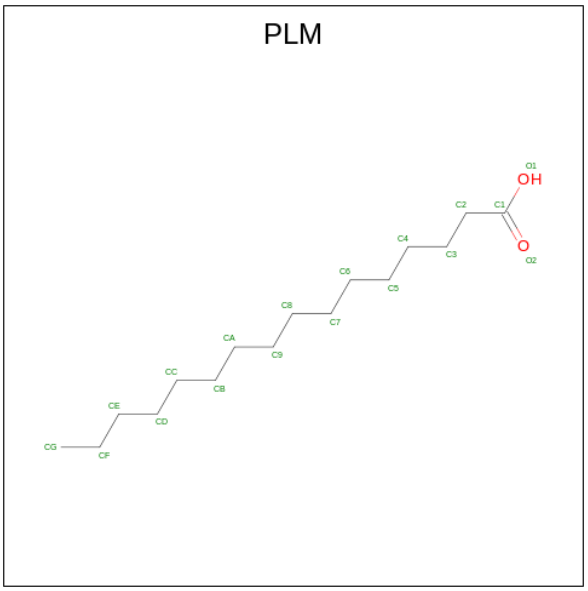
- Molecule 1 is a protein called Prolipoprotein diacylglyceryl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2371	1598	386	374	13	0	15	0

There are 10 discrepancies between the modelled and reference sequences:

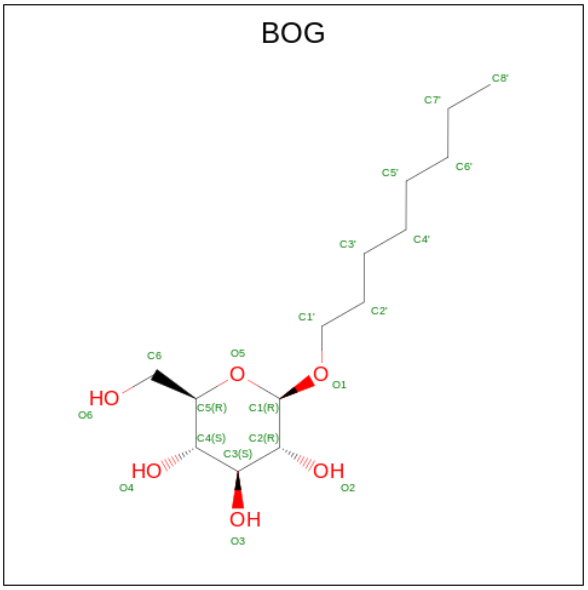
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P60955
A	1	VAL	-	expression tag	UNP P60955
A	292	LEU	-	expression tag	UNP P60955
A	293	GLU	-	expression tag	UNP P60955
A	294	HIS	-	expression tag	UNP P60955
A	295	HIS	-	expression tag	UNP P60955
A	296	HIS	-	expression tag	UNP P60955
A	297	HIS	-	expression tag	UNP P60955
A	298	HIS	-	expression tag	UNP P60955
A	299	HIS	-	expression tag	UNP P60955

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 9 2	0	0
2	A	1	Total C O 18 16 2	0	0

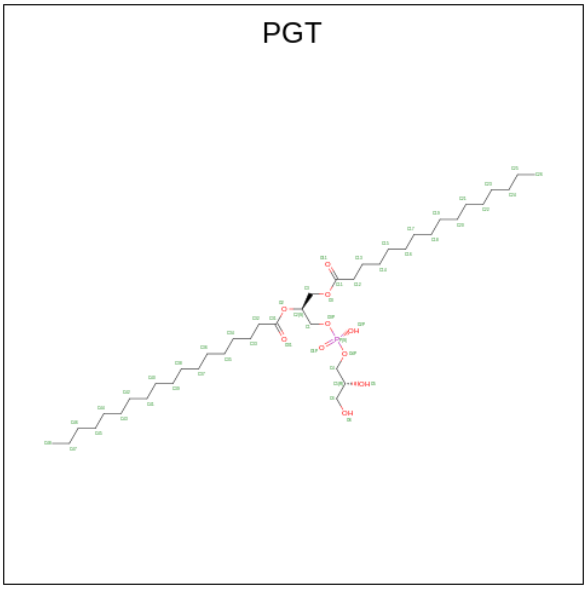
- Molecule 3 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 14 6	0	0

- Molecule 4 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPH

ORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 40 29 10 1	0	0
4	A	1	Total C O P 51 40 10 1	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 18 18	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 18 18	0	0
4	A	1	Total C 13 13	0	0
4	A	1	Total C 18 18	0	0
4	A	1	Total C 9 9	0	0

- Molecule 5 is water.

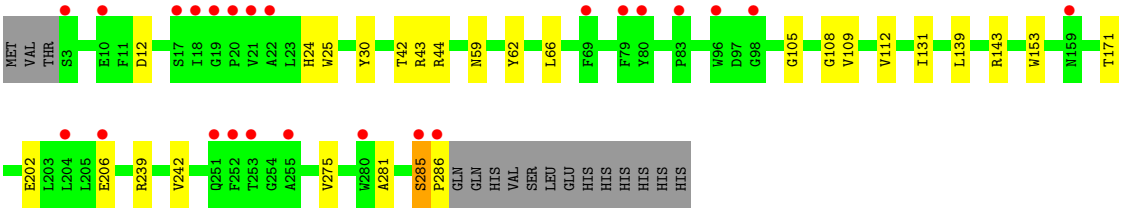
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	103	Total O 103 103	0	0

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: Prolipoprotein diacylglyceryl transferase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.41Å 60.97Å 117.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.43 – 1.60 38.29 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.43-1.60) 99.4 (38.29-1.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.59Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1634)	Depositor
R, R_{free}	0.179 , 0.222 0.186 , 0.196	Depositor DCC
R_{free} test set	2470 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2711	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PLM, BOG, PGT

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	0.35	0/2492	0.51	0/3387

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	2371	0	2434	24	0
2	A	29	0	45	0	0
3	A	20	0	28	1	0
4	A	188	0	306	13	0
5	A	103	0	0	4	0
All	All	2711	0	2813	25	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 5.

All (25) 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:206:GLU:OE2	1:A:239[B]:ARG:HD2	1.52	1.09
1:A:206:GLU:OE2	1:A:239[B]:ARG:CD	2.08	1.00
1:A:206:GLU:OE1	5:A:401:HOH:O	1.78	0.99
1:A:275:VAL:HG22	4:A:307:PGT:H402	1.86	0.56
1:A:131[A]:ILE:HG23	4:A:305:PGT:H241	1.88	0.56
1:A:281:ALA:O	1:A:285:SER:HB3	2.06	0.55
1:A:206:GLU:OE2	1:A:239[B]:ARG:HD3	2.03	0.54
1:A:66:LEU:HD11	4:A:305:PGT:H442	1.89	0.54
1:A:43:ARG:HH21	4:A:310:PGT:H422	1.72	0.53
1:A:44[B]:ARG:NH2	5:A:404:HOH:O	2.27	0.52
1:A:62:TYR:HB3	4:A:305:PGT:H441	1.91	0.51
1:A:202:GLU:HG2	1:A:242:VAL:HG21	1.93	0.51
1:A:42[A]:THR:HG21	5:A:417:HOH:O	2.12	0.49
1:A:59:ASN:HD22	4:A:309:PGT:H483	1.78	0.48
1:A:105:GLY:O	1:A:109[B]:VAL:HG23	2.14	0.48
1:A:24:HIS:CE1	4:A:305:PGT:H5	2.50	0.46
1:A:12:ASP:H	4:A:312:PGT:H321	1.81	0.45
1:A:25:TRP:CE2	4:A:312:PGT:H351	2.52	0.45
1:A:171[B]:THR:HG22	5:A:445:HOH:O	2.17	0.45
1:A:139:LEU:O	1:A:143:ARG:HG2	2.17	0.44
1:A:112:VAL:HG22	4:A:309:PGT:H391	1.99	0.44
3:A:303:BOG:H5'2	4:A:305:PGT:H131	2.00	0.43
1:A:108:GLY:HA2	4:A:309:PGT:H332	2.02	0.42
1:A:30:TYR:HB3	4:A:305:PGT:H331	2.01	0.42
1:A:285:SER:HB2	1:A:286:PRO:HD2	2.03	0.40

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	297/300 (99%)	288 (97%)	8 (3%)	1 (0%)	41 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	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	252/253 (100%)	251 (100%)	1 (0%)	91 84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	TRP

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	59	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	PGT	A	306	-	15,15,50	0.31	0	14,14,56	0.61	0
3	BOG	A	303	-	20,20,20	1.11	3 (15%)	25,25,25	1.12	2 (8%)
2	PLM	A	301	-	10,10,17	0.66	0	10,10,17	1.11	1 (10%)
4	PGT	A	309	-	17,17,50	0.27	0	16,16,56	0.69	0
4	PGT	A	310	-	12,12,50	0.29	0	11,11,56	0.59	0
4	PGT	A	307	-	17,17,50	0.23	0	16,16,56	0.77	0
2	PLM	A	302	-	17,17,17	0.60	0	17,17,17	0.87	0
4	PGT	A	311	-	17,17,50	0.29	0	16,16,56	0.64	0
4	PGT	A	304	-	39,39,50	0.94	2 (5%)	42,45,56	1.49	5 (11%)
4	PGT	A	312	-	8,8,50	0.21	0	7,7,56	0.64	0
4	PGT	A	305	-	50,50,50	0.88	2 (4%)	53,56,56	1.34	4 (7%)
4	PGT	A	308	-	4,4,50	0.14	0	3,3,56	0.57	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	PGT	A	306	-	-	5/13/13/55	-
3	BOG	A	303	-	-	4/11/31/31	0/1/1/1
2	PLM	A	301	-	-	4/8/8/15	-
4	PGT	A	309	-	-	5/15/15/55	-
4	PGT	A	310	-	-	7/10/10/55	-
4	PGT	A	307	-	-	4/15/15/55	-
2	PLM	A	302	-	-	5/15/15/15	-
4	PGT	A	311	-	-	9/15/15/55	-
4	PGT	A	304	-	-	17/44/44/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGT	A	312	-	-	3/6/6/55	-
4	PGT	A	305	-	-	23/55/55/55	-
4	PGT	A	308	-	-	1/2/2/55	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	305	PGT	O2-C2	-3.29	1.38	1.46
4	A	304	PGT	O2-C2	-2.87	1.39	1.46
4	A	305	PGT	O3-C3	-2.85	1.38	1.45
4	A	304	PGT	O3-C3	-2.69	1.39	1.45
3	A	303	BOG	O5-C1	2.38	1.47	1.41
3	A	303	BOG	C3-C2	-2.21	1.46	1.52
3	A	303	BOG	C4-C3	-2.10	1.47	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	305	PGT	C15-C14-C13	5.90	144.37	114.42
4	A	304	PGT	O3-C3-C2	4.20	120.65	108.43
4	A	304	PGT	C15-C14-C13	4.06	144.25	113.42
4	A	305	PGT	O2-C31-C32	3.76	119.61	111.50
4	A	304	PGT	O2-C31-C32	3.32	118.67	111.50
4	A	304	PGT	C2-O2-C31	3.24	125.76	117.79
3	A	303	BOG	C1'-O1-C1	3.00	118.82	113.84
4	A	305	PGT	O3-C3-C2	2.97	117.09	108.43
4	A	304	PGT	O3-C11-C12	2.85	120.85	111.91
4	A	305	PGT	O3-C11-C12	2.53	119.85	111.91
3	A	303	BOG	O1-C1'-C2'	2.22	117.35	109.56
2	A	301	PLM	O1-C1-C2	2.10	120.78	114.03

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	BOG	C2'-C1'-O1-C1
4	A	304	PGT	C4-C5-C6-O6
4	A	305	PGT	C1-O3P-P-O1P
4	A	305	PGT	O11-C11-O3-C3
4	A	305	PGT	C12-C11-O3-C3
4	A	305	PGT	O4P-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
4	A	305	PGT	C32-C33-C34-C35
4	A	305	PGT	C18-C19-C20-C21
4	A	305	PGT	O4P-C4-C5-C6
4	A	305	PGT	C31-C32-C33-C34
4	A	304	PGT	C1-O3P-P-O4P
4	A	304	PGT	C4-O4P-P-O3P
4	A	306	PGT	C34-C35-C36-C37
4	A	310	PGT	C34-C35-C36-C37
4	A	311	PGT	C42-C43-C44-C45
4	A	305	PGT	C43-C44-C45-C46
4	A	306	PGT	C38-C39-C40-C41
4	A	304	PGT	C36-C37-C38-C39
4	A	309	PGT	C42-C43-C44-C45
4	A	304	PGT	C32-C33-C34-C35
4	A	305	PGT	C16-C17-C18-C19
4	A	311	PGT	C33-C34-C35-C36
4	A	307	PGT	C33-C34-C35-C36
4	A	310	PGT	C35-C36-C37-C38
2	A	301	PLM	C4-C5-C6-C7
4	A	311	PGT	C34-C35-C36-C37
4	A	304	PGT	O5-C5-C6-O6
4	A	305	PGT	C13-C14-C15-C16
4	A	311	PGT	C40-C41-C42-C43
4	A	312	PGT	C33-C34-C35-C36
4	A	304	PGT	C33-C34-C35-C36
2	A	302	PLM	C3-C4-C5-C6
4	A	305	PGT	C45-C46-C47-C48
4	A	307	PGT	C36-C37-C38-C39
4	A	304	PGT	O31-C31-O2-C2
4	A	304	PGT	O3P-C1-C2-C3
4	A	305	PGT	C36-C37-C38-C39
4	A	312	PGT	C31-C32-C33-C34
3	A	303	BOG	C3'-C4'-C5'-C6'
4	A	311	PGT	C45-C46-C47-C48
4	A	304	PGT	C34-C35-C36-C37
4	A	309	PGT	C34-C35-C36-C37
4	A	306	PGT	C37-C38-C39-C40
4	A	306	PGT	C43-C44-C45-C46
4	A	311	PGT	C43-C44-C45-C46
4	A	307	PGT	C31-C32-C33-C34
4	A	310	PGT	C37-C38-C39-C40
2	A	302	PLM	C2-C3-C4-C5

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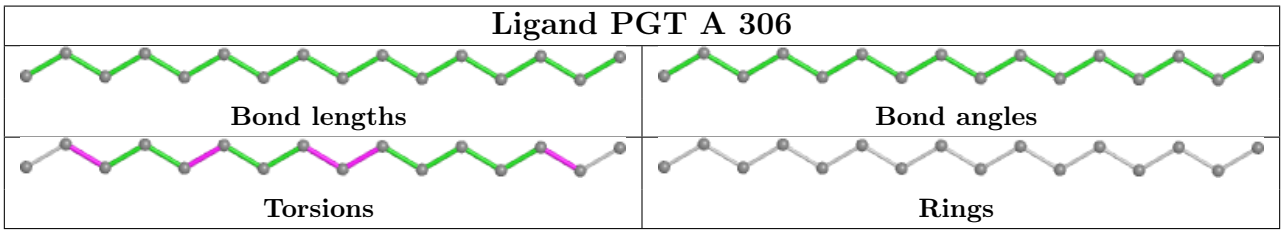
Mol	Chain	Res	Type	Atoms
4	A	305	PGT	C1-C2-C3-O3
4	A	304	PGT	O3P-C1-C2-O2
4	A	304	PGT	C12-C13-C14-C15
4	A	309	PGT	C31-C32-C33-C34
4	A	304	PGT	C5-C4-O4P-P
4	A	305	PGT	C34-C35-C36-C37
4	A	304	PGT	C11-C12-C13-C14
4	A	305	PGT	C19-C20-C21-C22
4	A	308	PGT	C32-C33-C34-C35
4	A	304	PGT	C3-C2-O2-C31
3	A	303	BOG	C4'-C5'-C6'-C7'
4	A	310	PGT	C36-C37-C38-C39
4	A	305	PGT	C1-O3P-P-O4P
4	A	305	PGT	C12-C13-C14-C15
4	A	304	PGT	C1-O3P-P-O2P
4	A	304	PGT	C4-O4P-P-O2P
4	A	305	PGT	C4-O4P-P-O2P
4	A	311	PGT	C32-C33-C34-C35
4	A	305	PGT	O2-C2-C3-O3
4	A	311	PGT	C37-C38-C39-C40
4	A	309	PGT	C35-C36-C37-C38
4	A	305	PGT	C37-C38-C39-C40
4	A	305	PGT	C42-C43-C44-C45
2	A	302	PLM	CA-CB-CC-CD
4	A	306	PGT	C31-C32-C33-C34
2	A	301	PLM	O2-C1-C2-C3
2	A	301	PLM	O1-C1-C2-C3
3	A	303	BOG	C1'-C2'-C3'-C4'
4	A	311	PGT	C31-C32-C33-C34
2	A	302	PLM	O1-C1-C2-C3
4	A	307	PGT	C34-C35-C36-C37
4	A	310	PGT	C40-C41-C42-C43
4	A	309	PGT	C43-C44-C45-C46
2	A	302	PLM	O2-C1-C2-C3
4	A	305	PGT	C23-C24-C25-C26
4	A	312	PGT	C36-C37-C38-C39
4	A	310	PGT	C33-C34-C35-C36
4	A	310	PGT	C31-C32-C33-C34
2	A	301	PLM	C2-C3-C4-C5

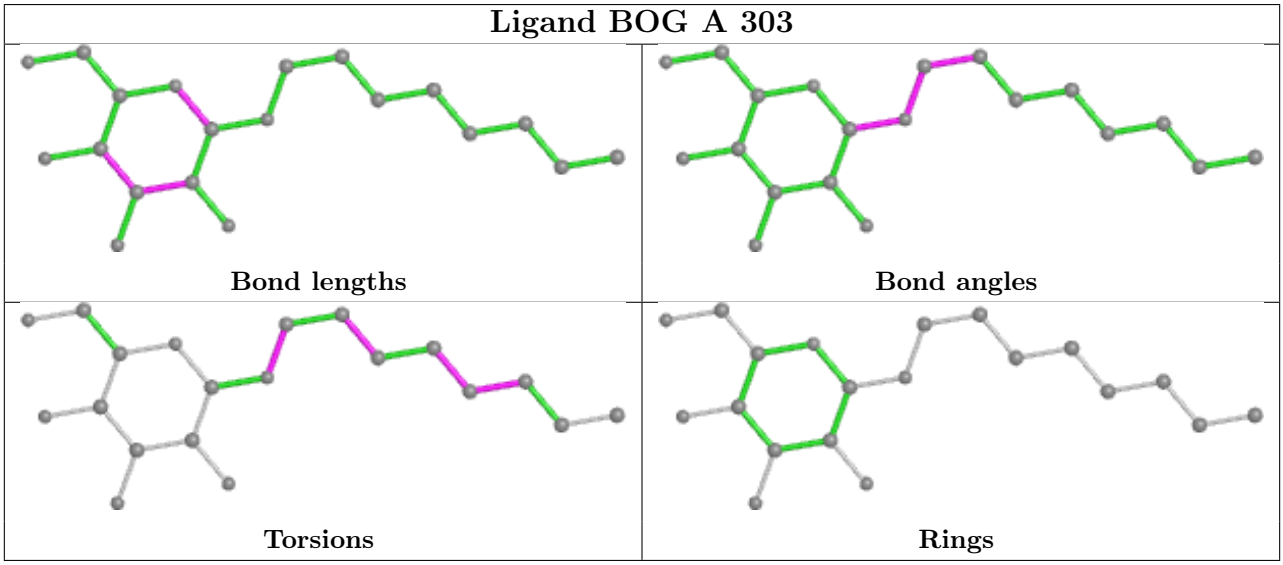
There are no ring outliers.

6 monomers are involved in 13 short contacts:

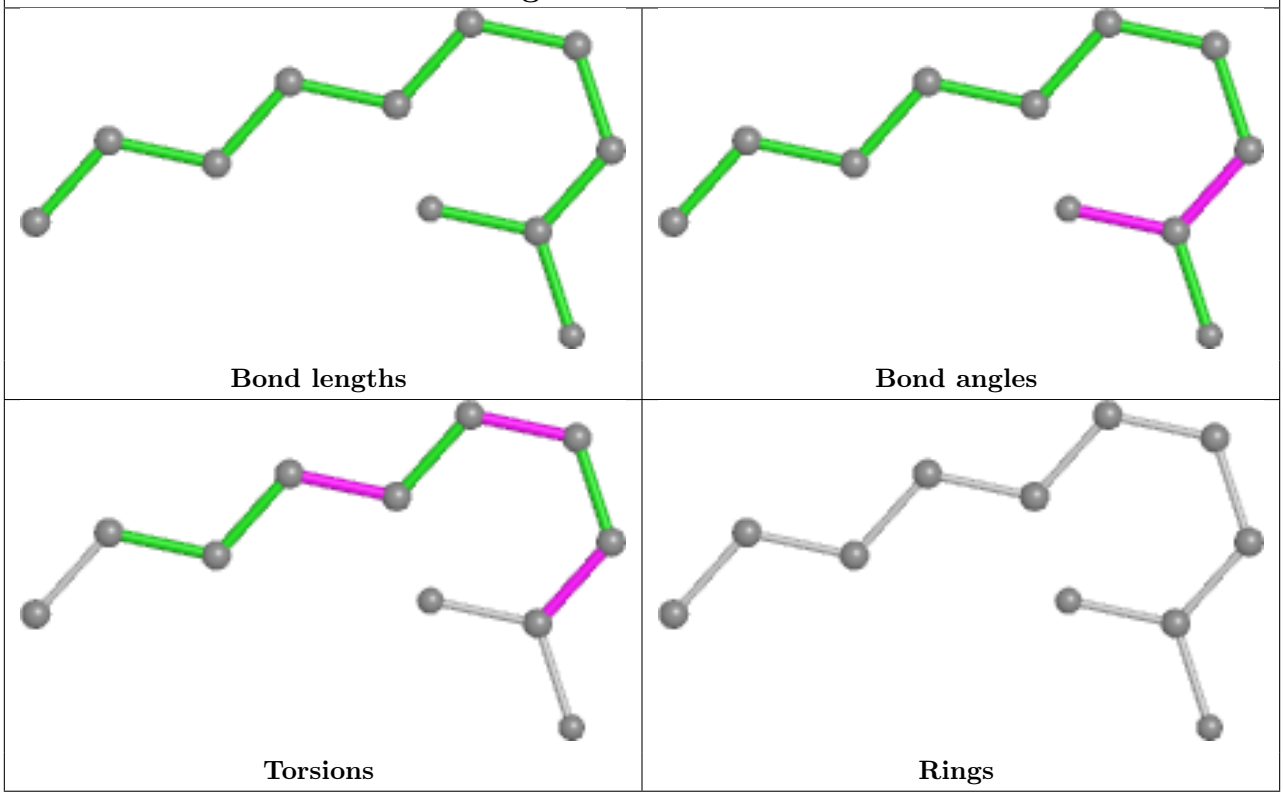
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	BOG	1	0
4	A	309	PGT	3	0
4	A	310	PGT	1	0
4	A	307	PGT	1	0
4	A	312	PGT	2	0
4	A	305	PGT	6	0

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.

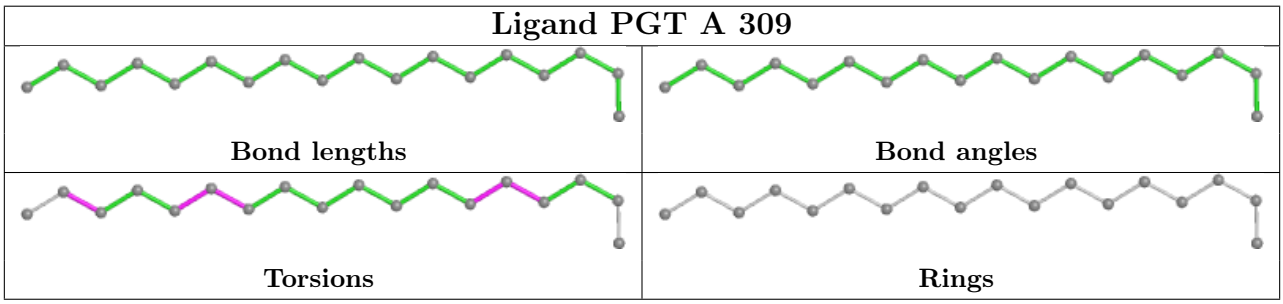




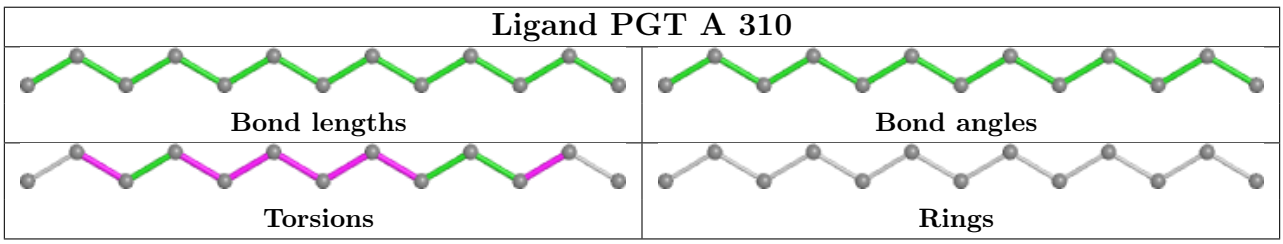
Ligand PLM A 301



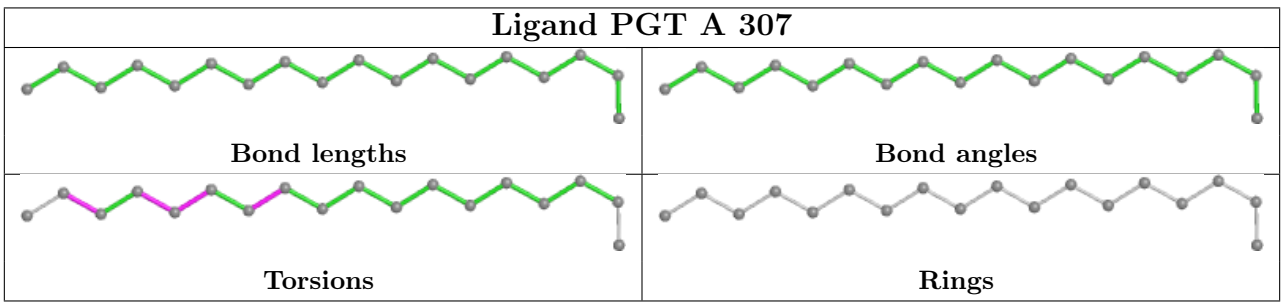
Ligand PGT A 309



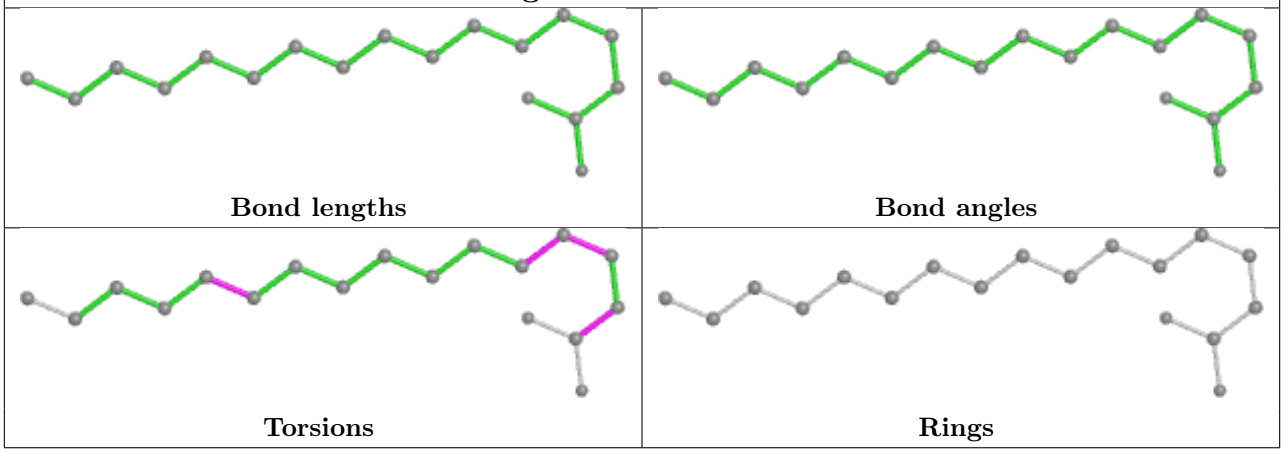
Ligand PGT A 310



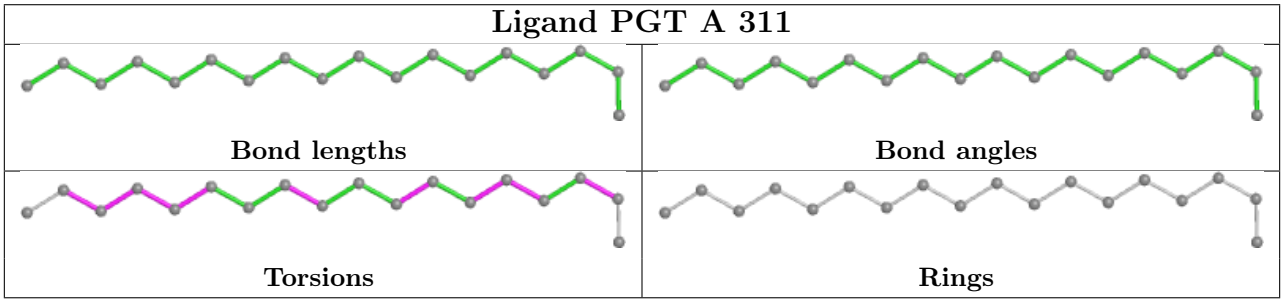
Ligand PGT A 307



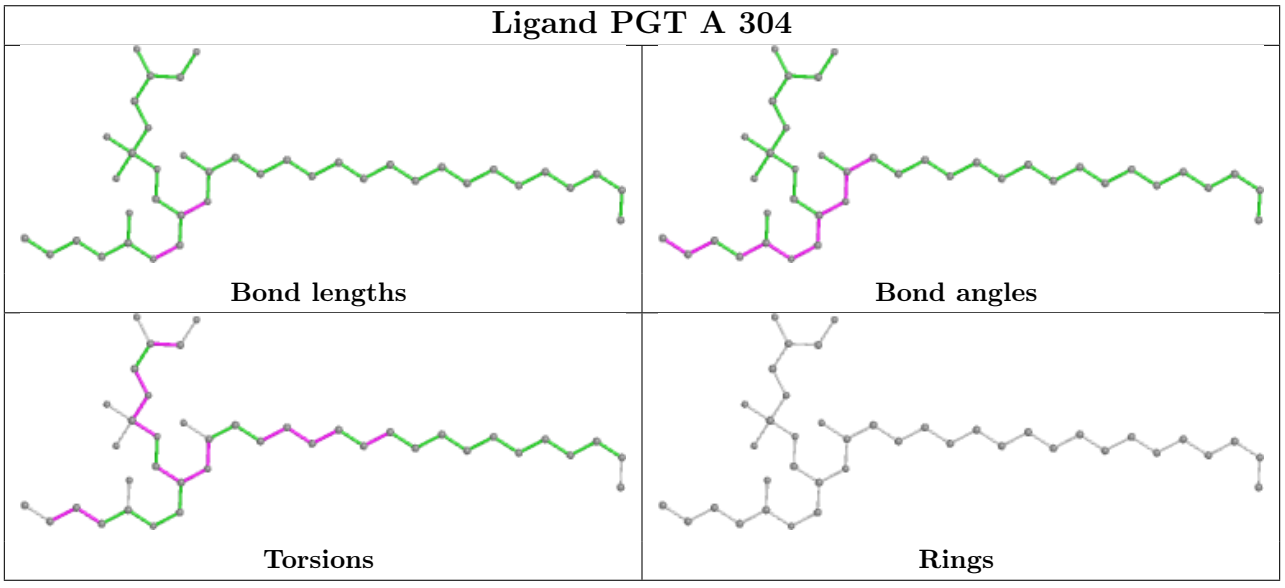
Ligand PLM A 302



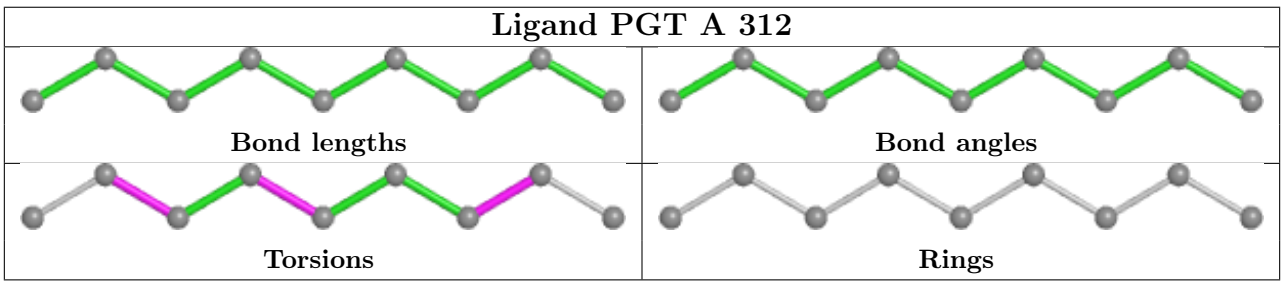
Ligand PGT A 311

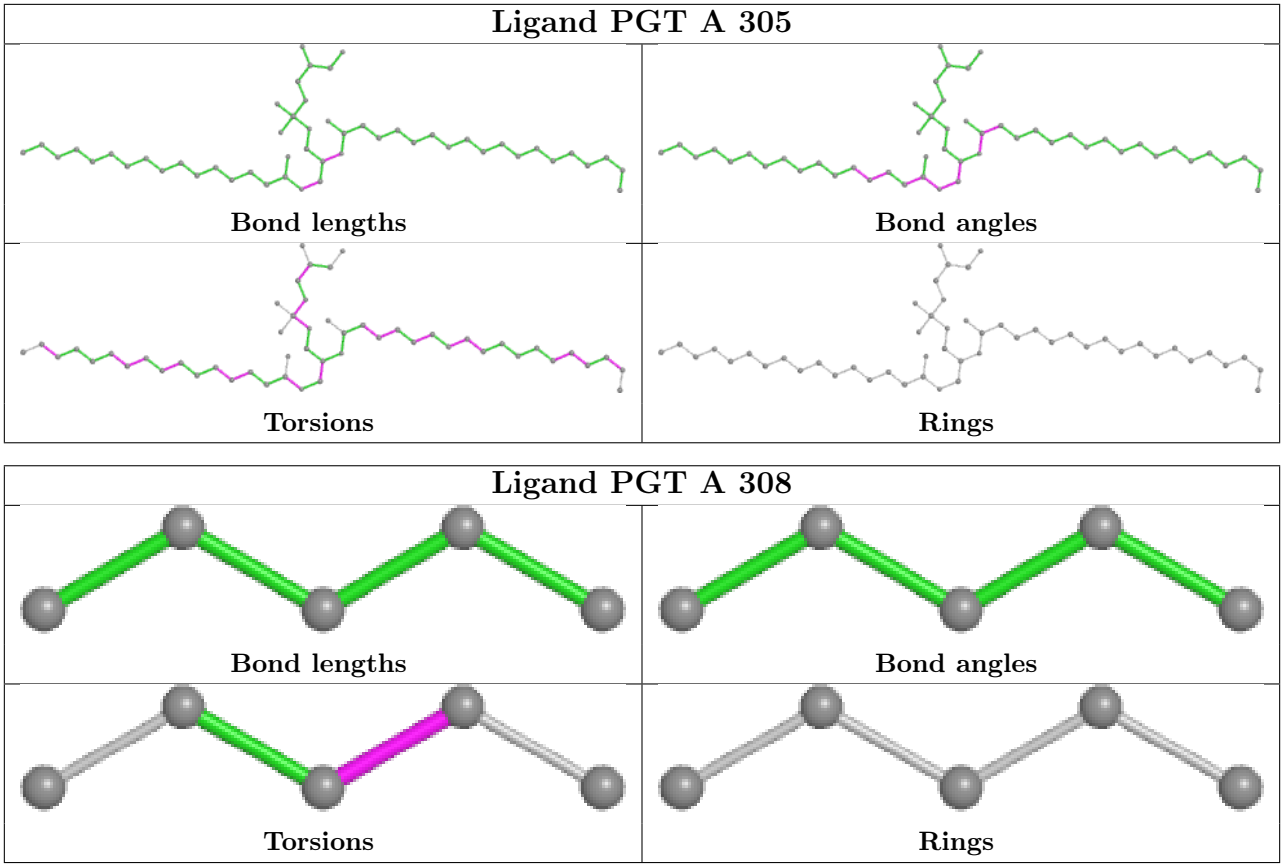


Ligand PGT A 304



Ligand PGT A 312





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	284/300 (94%)	0.30	24 (8%)	10	9	18, 27, 53, 80	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	PRO	6.8
1	A	285	SER	6.6
1	A	20	PRO	6.1
1	A	18	ILE	5.3
1	A	79	PHE	4.8
1	A	98	GLY	4.1
1	A	19	GLY	3.8
1	A	251	GLN	3.5
1	A	10	GLU	3.2
1	A	22	ALA	3.2
1	A	3	SER	3.1
1	A	96	TRP	3.1
1	A	253	THR	3.0
1	A	21	VAL	3.0
1	A	255	ALA	2.9
1	A	252	PHE	2.9
1	A	280	TRP	2.7
1	A	80	TYR	2.7
1	A	83	PRO	2.6
1	A	206	GLU	2.6
1	A	17	SER	2.6
1	A	69	PHE	2.3
1	A	159	ASN	2.1
1	A	204[A]	LEU	2.0

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)

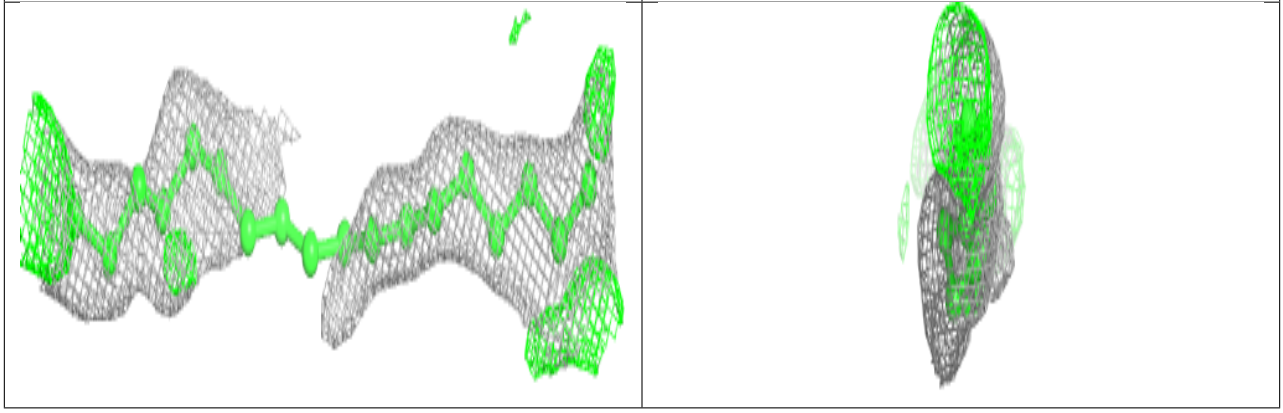
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGT	A	309	18/51	0.68	0.20	48,55,108,115	0
4	PGT	A	311	18/51	0.75	0.18	47,62,87,89	0
4	PGT	A	304	40/51	0.77	0.20	38,61,147,161	0
4	PGT	A	307	18/51	0.77	0.22	38,56,79,91	0
4	PGT	A	310	13/51	0.78	0.18	40,49,70,74	0
4	PGT	A	305	51/51	0.79	0.22	33,68,130,160	0
3	BOG	A	303	20/20	0.83	0.13	35,55,100,101	0
2	PLM	A	301	11/18	0.84	0.15	37,41,60,81	0
4	PGT	A	306	16/51	0.84	0.26	30,49,66,66	0
4	PGT	A	308	5/51	0.85	0.10	40,44,54,54	0
4	PGT	A	312	9/51	0.87	0.12	42,53,69,89	0
2	PLM	A	302	18/18	0.91	0.12	24,42,70,101	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.

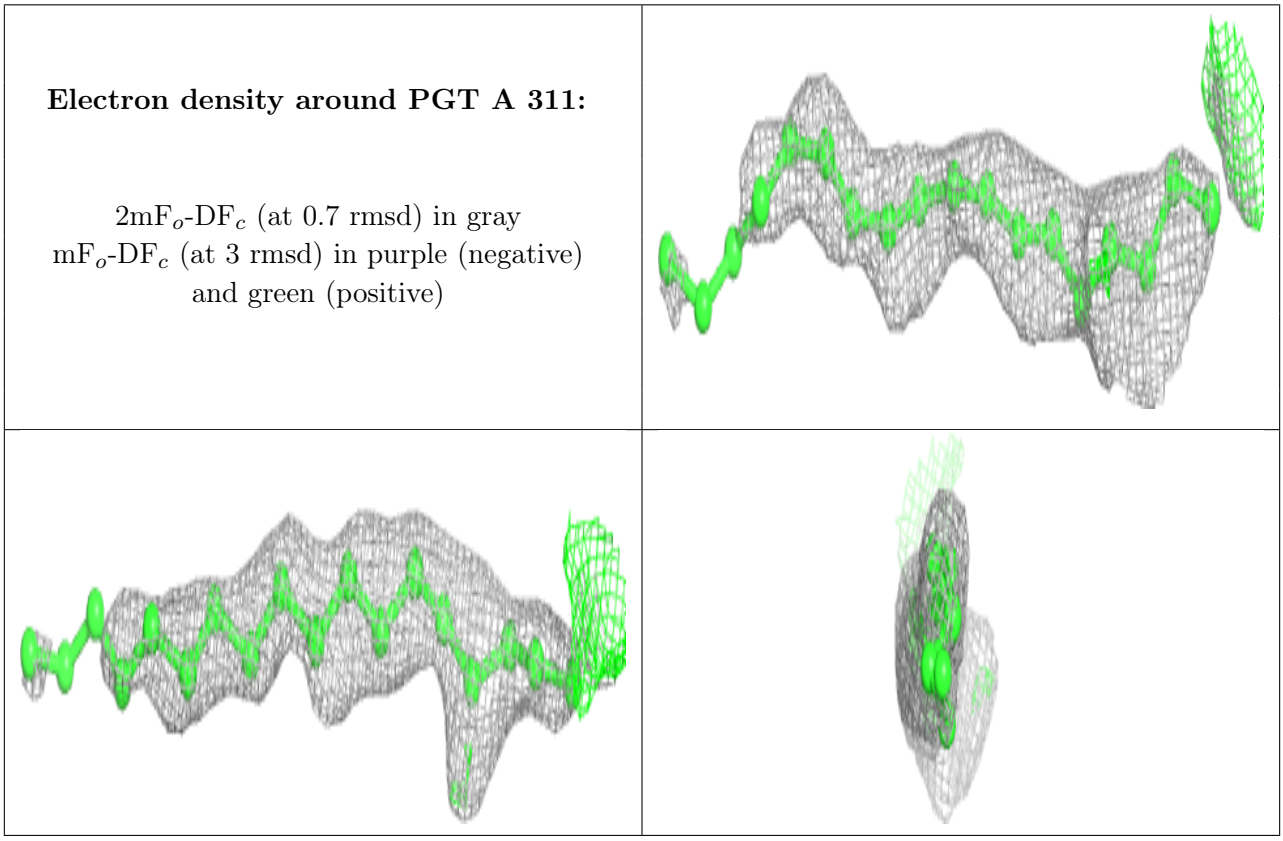
Electron density around PGT A 309:

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



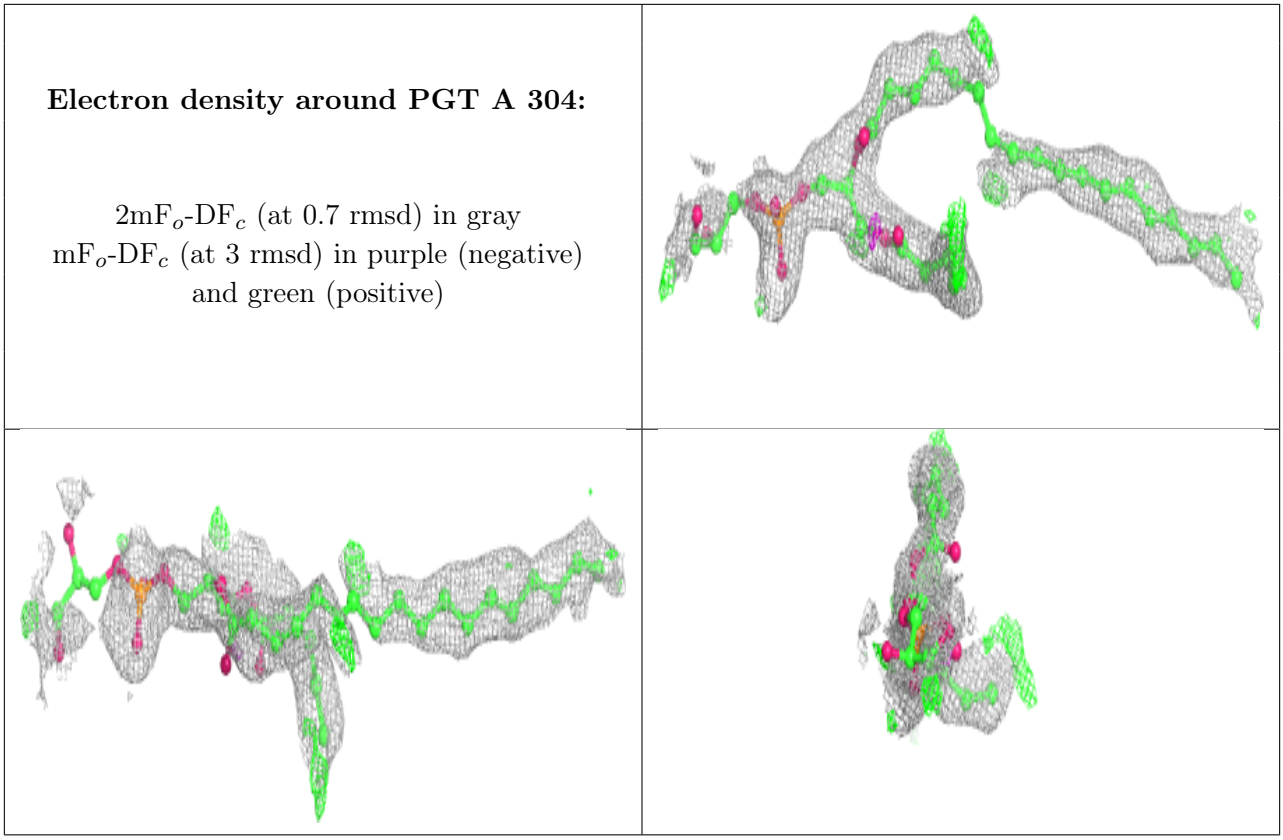
Electron density around PGT A 311:

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



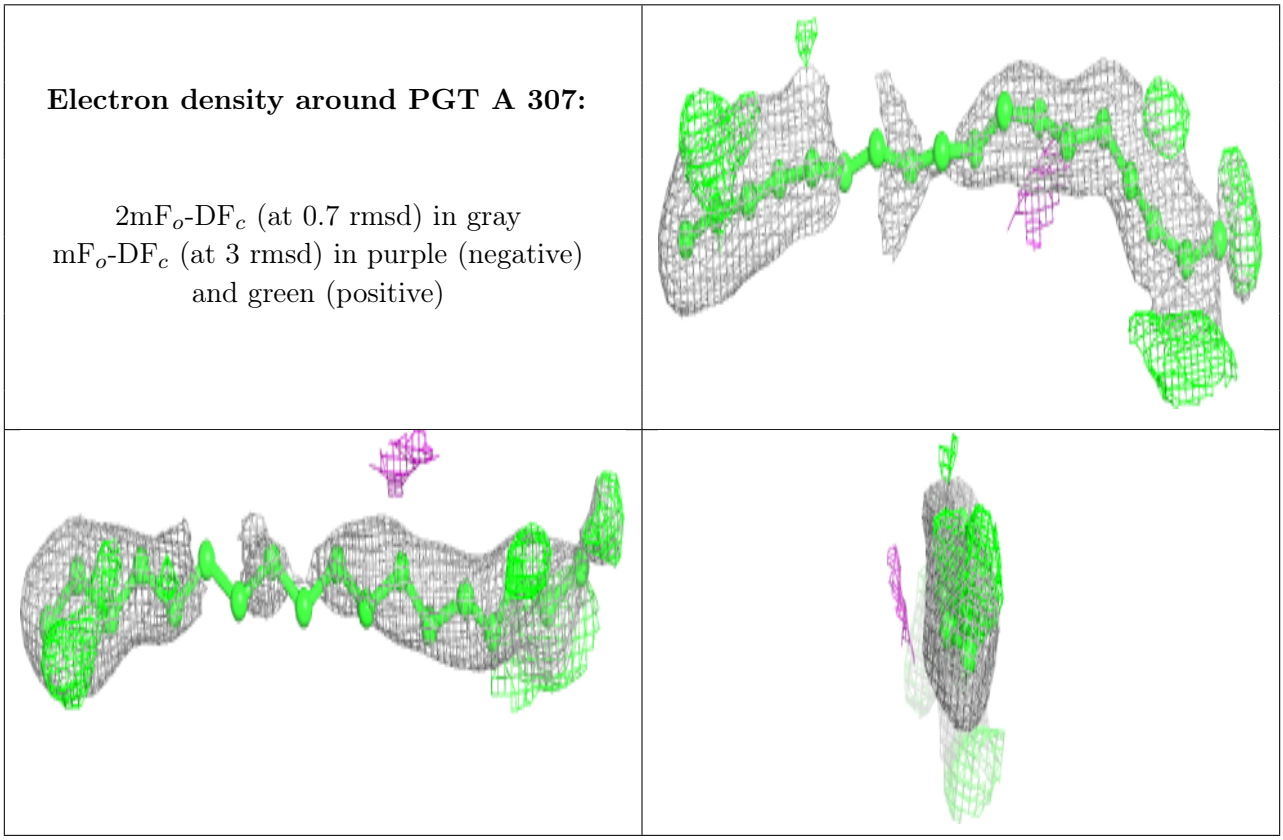
Electron density around PGT A 304:

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



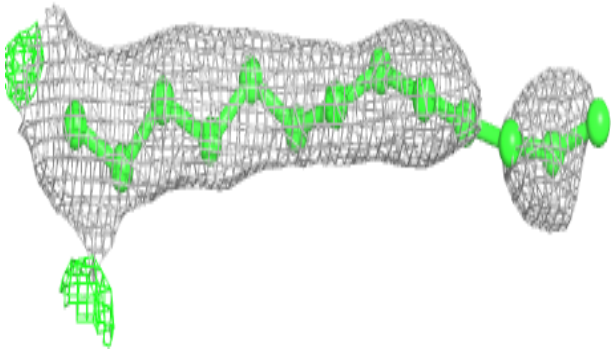
Electron density around PGT A 307:

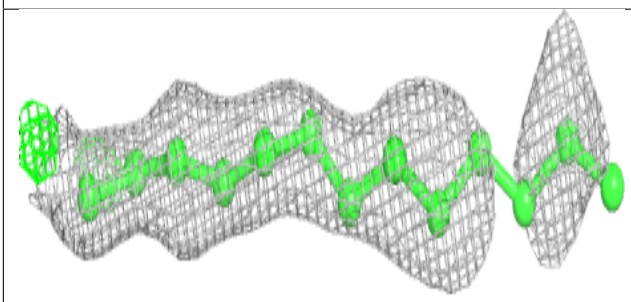
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

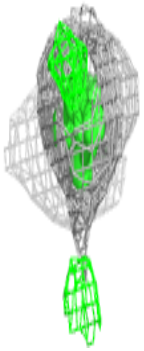


Electron density around PGT A 310:

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

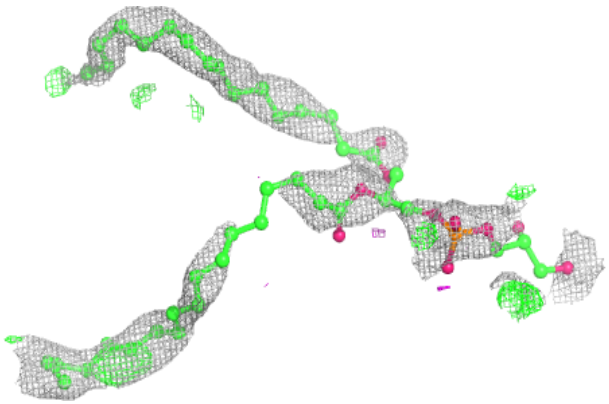


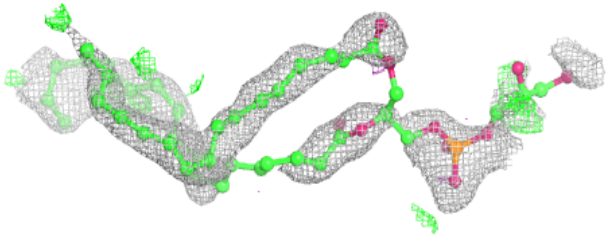


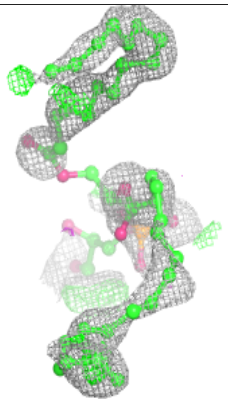


Electron density around PGT A 305:

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

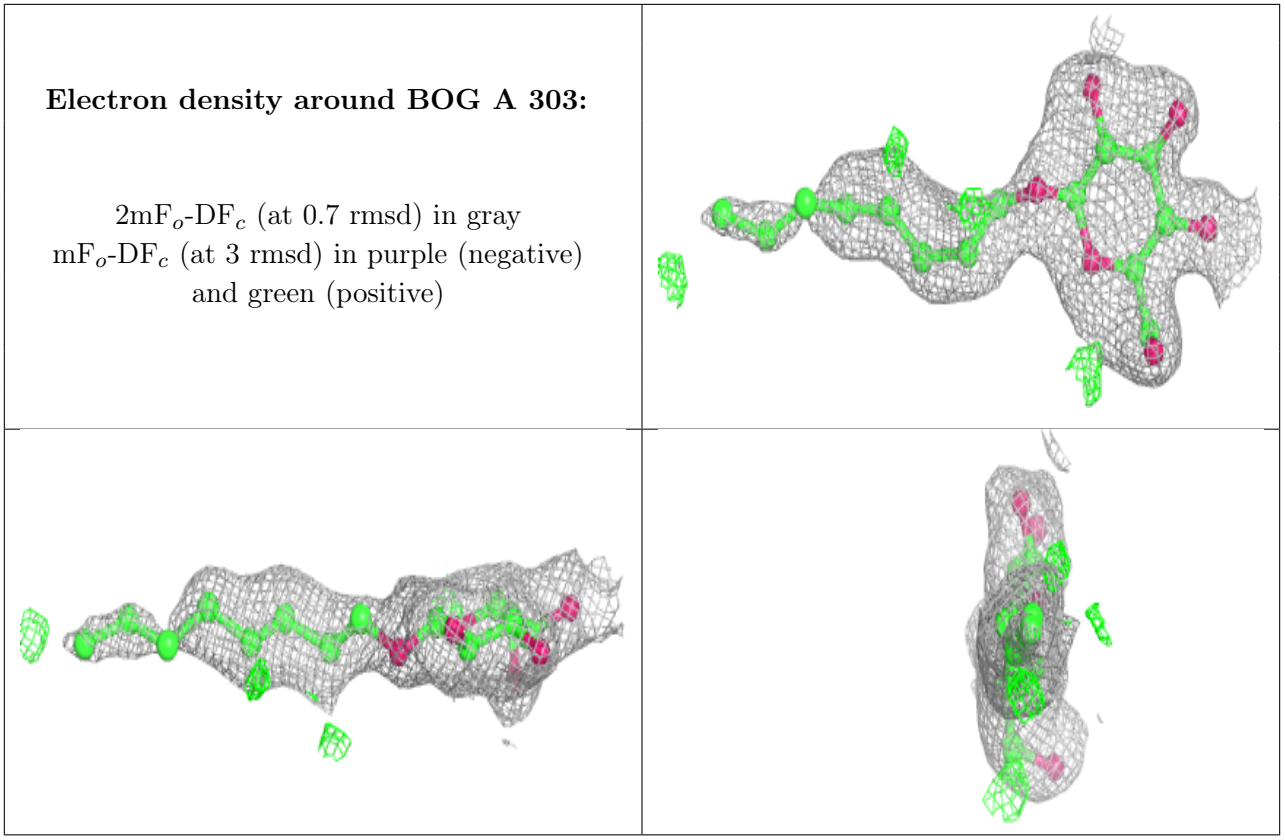






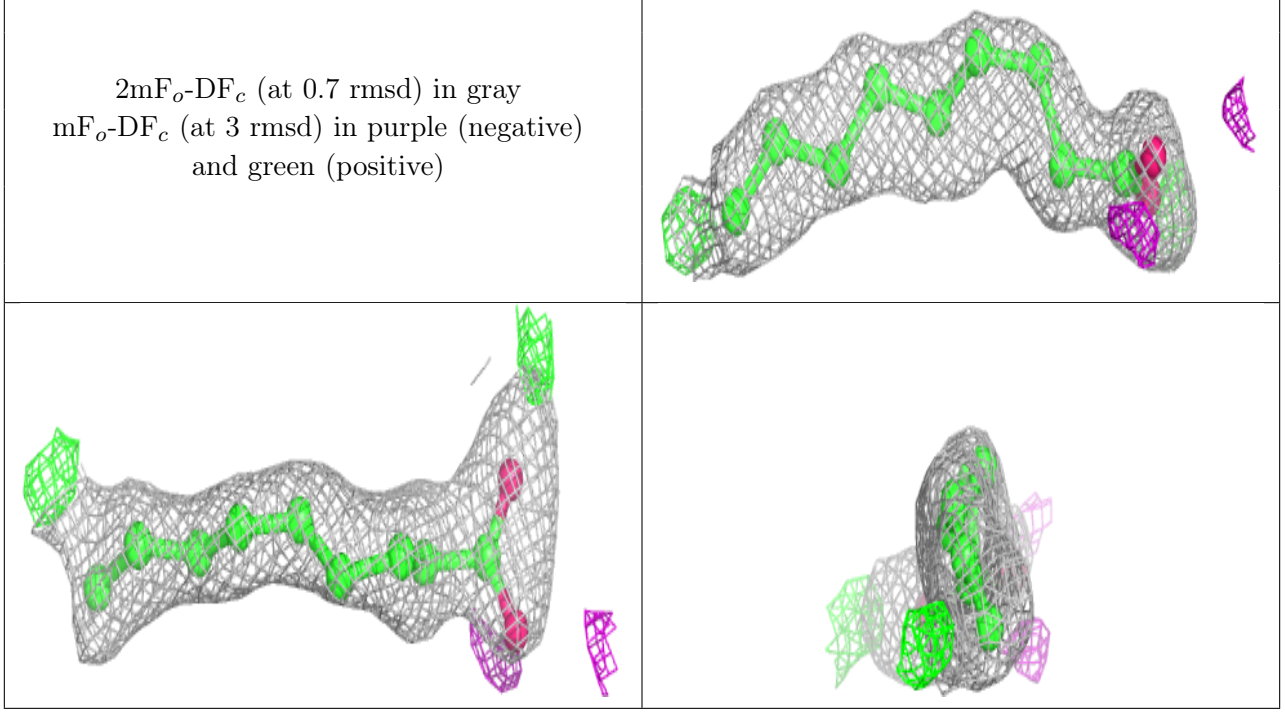
Electron density around BOG A 303:

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



Electron density around PLM A 301:

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



Electron density around PGT A 306:

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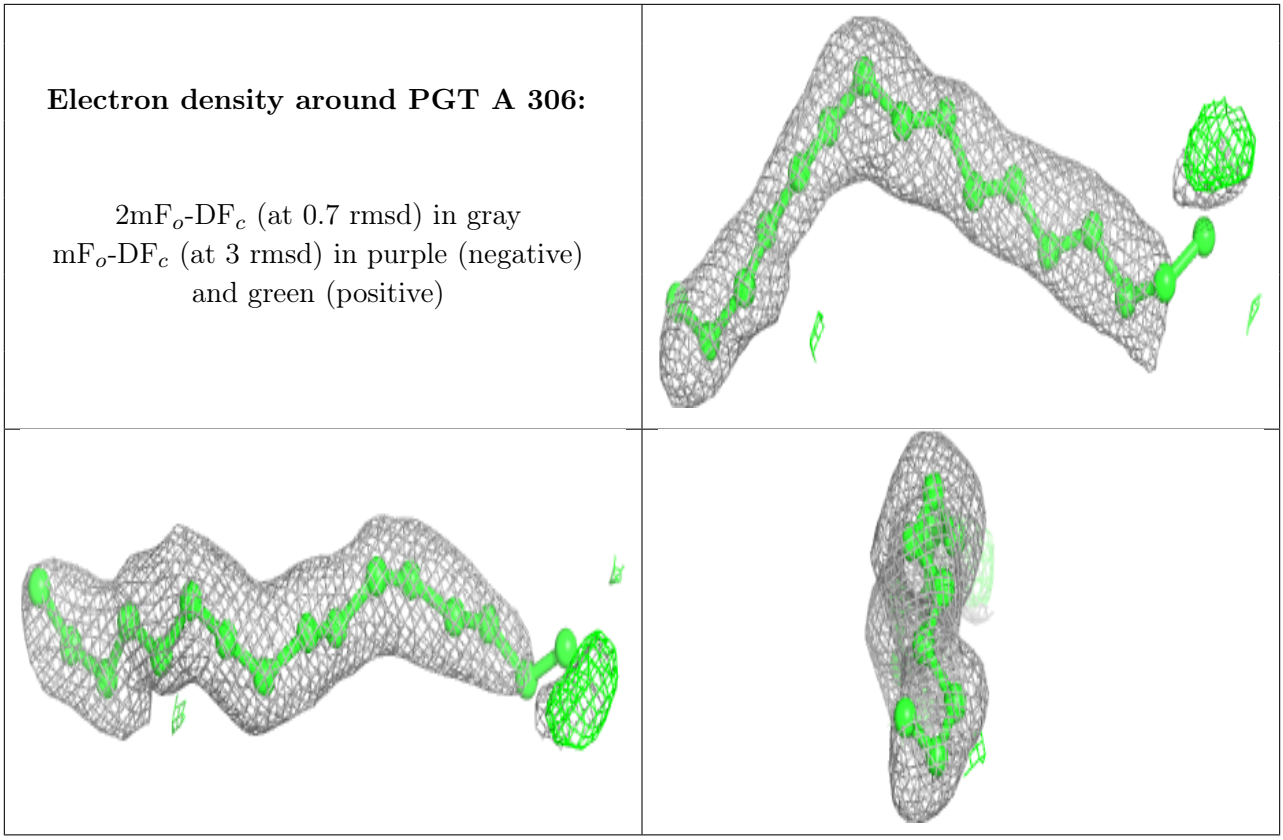
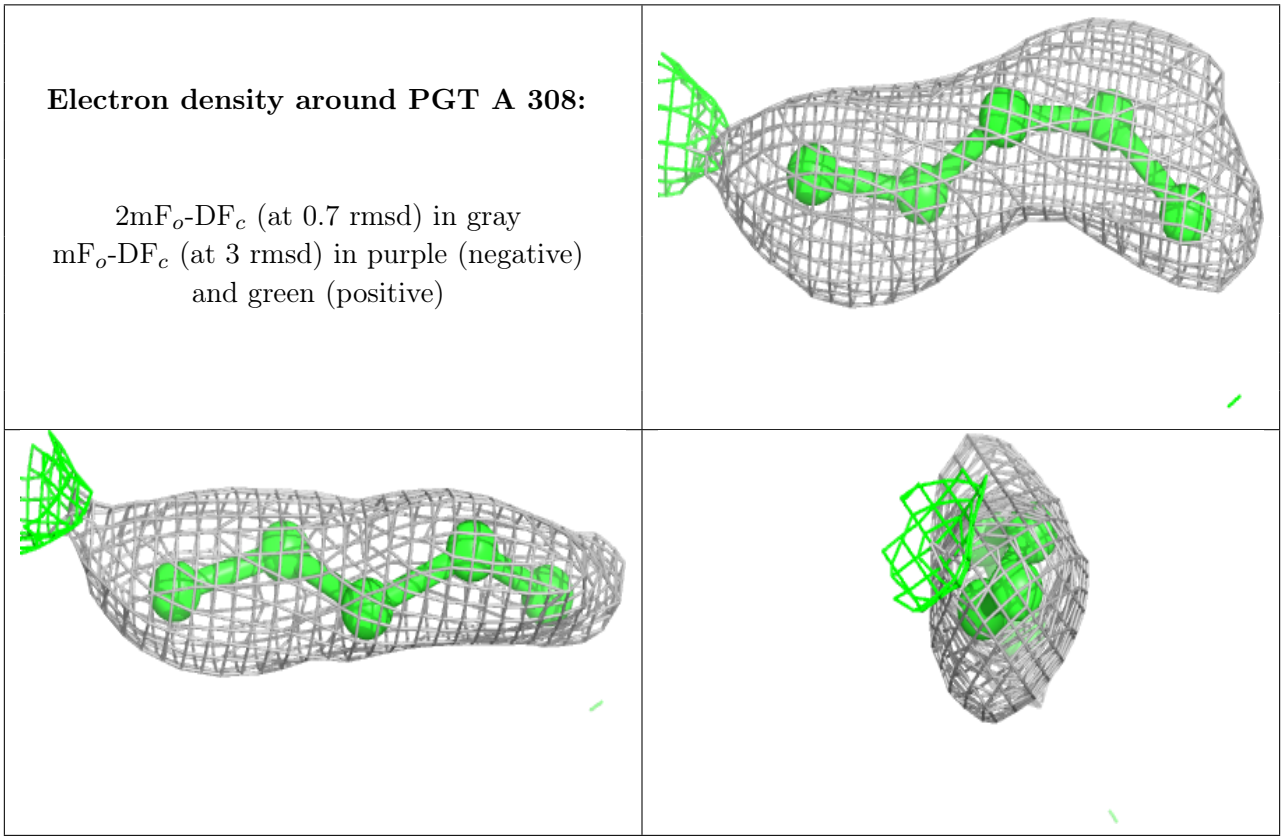
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



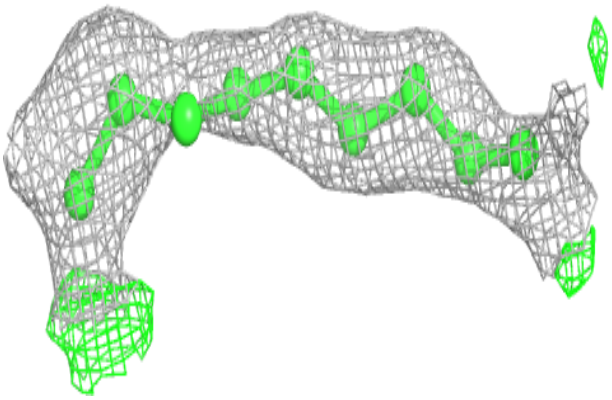
Electron density around PGT A 308:

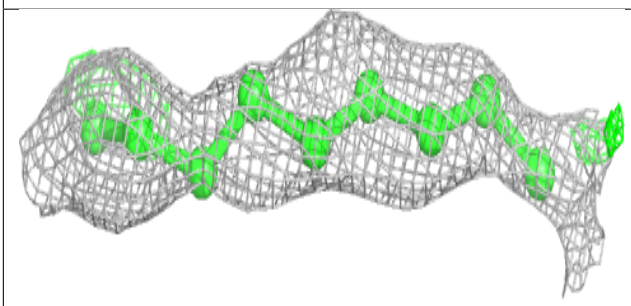
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

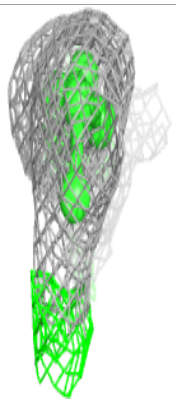


Electron density around PGT A 312:

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

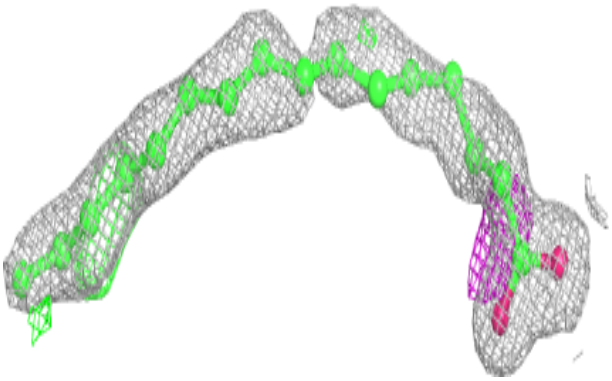


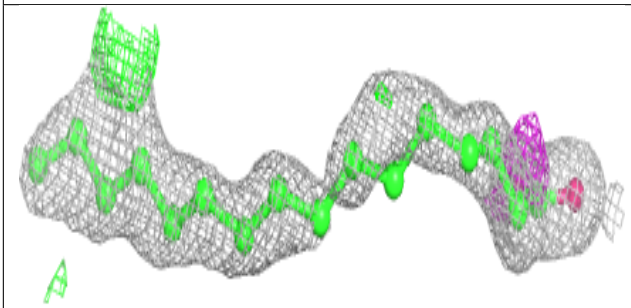


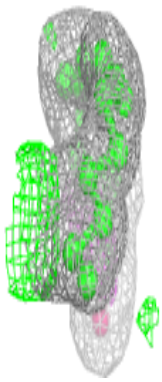


Electron density around PLM A 302:

$2mF_o$-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.