Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 08:39 PM EDT

PDB ID	:	6HZ0
Title	:	THE GLIC PENTAMERIC LIGAND-GATED ION CHANNEL MUTANT K248A
Authors	:	Hu, H.D.; Delarue, M.
Deposited on	:	2018-10-22
Resolution	:	2.75 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

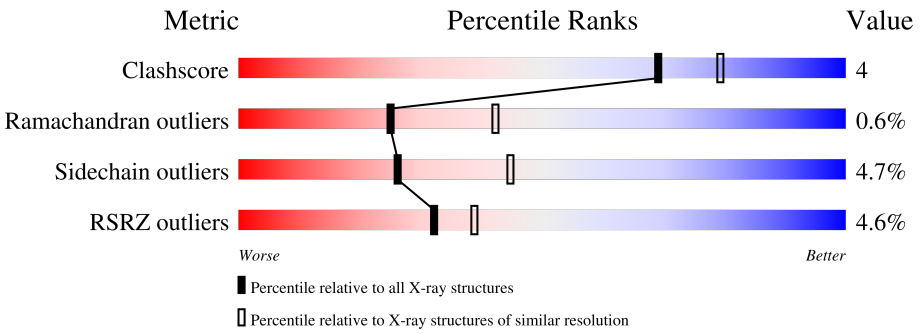
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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))
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	317	4% 82% 14% • • •
1	B	317	4% 85% 12% • •
1	C	317	5% 85% 12% • •
1	D	317	4% 85% 12% • •
1	E	317	5% 86% 11% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLC	A	403	-	-	-	X
6	LMT	E	409	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13490 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.

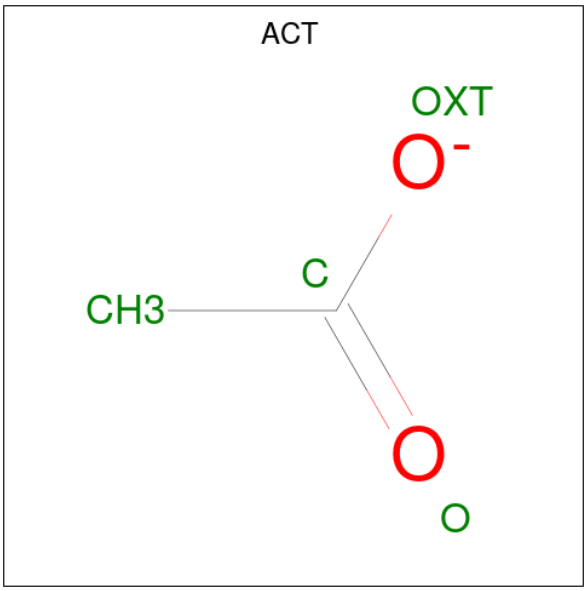
- Molecule 1 is a protein called Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	2541	1674	405	458	4	0	3	0
1	B	311	2538	1673	404	457	4	0	3	0
1	C	311	2533	1670	404	455	4	0	2	0
1	D	311	2544	1677	404	459	4	0	4	0
1	E	311	2539	1675	405	455	4	0	3	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	ALA	LYS	engineered mutation	UNP Q7NDN8
B	248	ALA	LYS	engineered mutation	UNP Q7NDN8
C	248	ALA	LYS	engineered mutation	UNP Q7NDN8
D	248	ALA	LYS	engineered mutation	UNP Q7NDN8
E	248	ALA	LYS	engineered mutation	UNP Q7NDN8

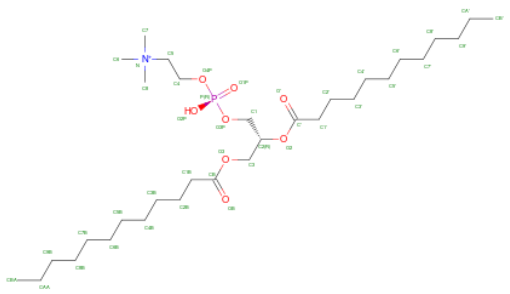
- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).

PLC



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 34 24 1 8 1	0	0
3	A	1	Total C 12 12	0	0
3	B	1	Total C 24 24	0	0
3	B	1	Total C N O P 34 24 1 8 1	0	0
3	B	1	Total C 24 24	0	0
3	B	1	Total C 12 12	0	0
3	C	1	Total C N O P 34 24 1 8 1	0	0
3	C	1	Total C 24 24	0	0
3	C	1	Total C 12 12	0	0
3	D	1	Total C N O P 34 24 1 8 1	0	0
3	D	1	Total C 24 24	0	0
3	D	1	Total C 12 12	0	0
3	E	1	Total C N O P 34 24 1 8 1	0	0
3	E	1	Total C 24 24	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 12 12	0	0

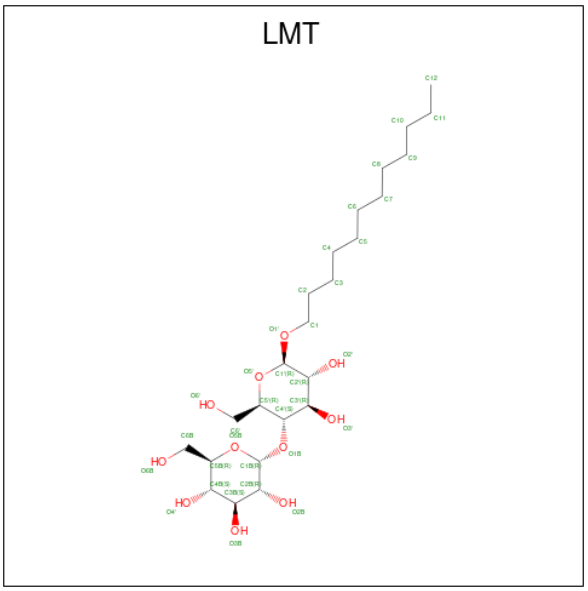
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0

- Molecule 6 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 12 12	0	0
6	B	1	Total C 12 12	0	0
6	C	1	Total C 12 12	0	0
6	D	1	Total C 12 12	0	0
6	E	1	Total C 12 12	0	0
6	E	1	Total C 12 12	0	0

- Molecule 7 is water.

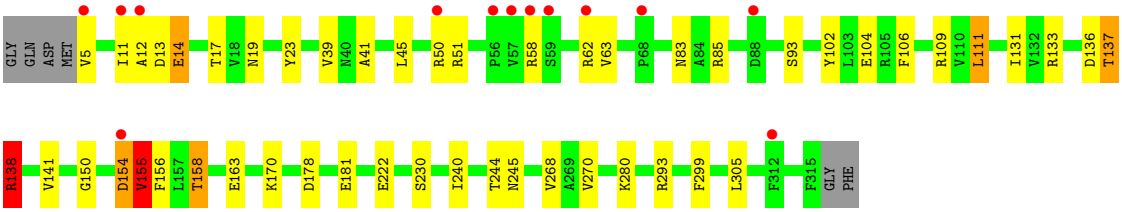
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	65	Total O 65 65	0	0
7	B	67	Total O 67 67	0	0
7	C	65	Total O 65 65	0	0
7	D	65	Total O 65 65	0	0
7	E	58	Total O 58 58	0	0

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.

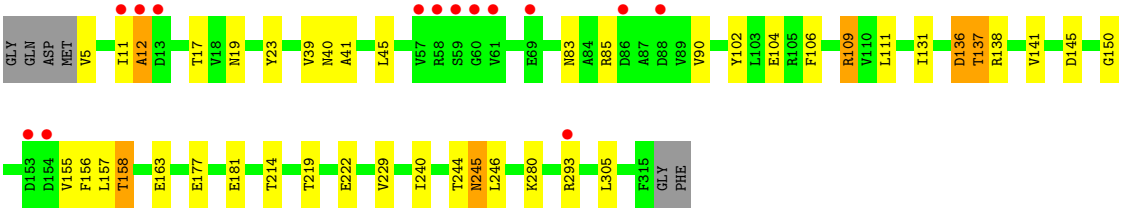
• Molecule 1: Proton-gated ion channel

Chain A:



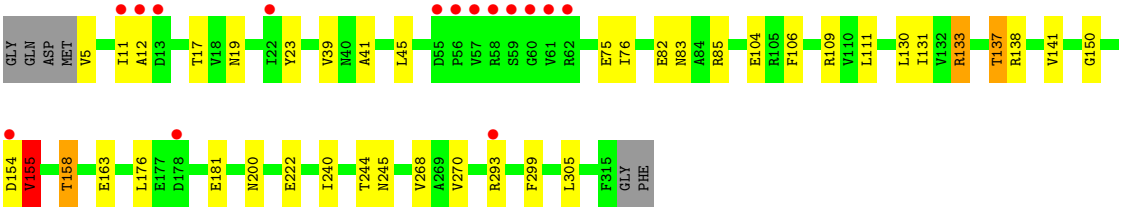
• Molecule 1: Proton-gated ion channel

Chain B:



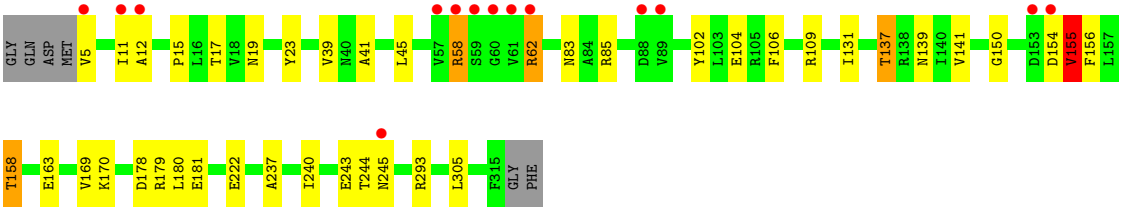
• Molecule 1: Proton-gated ion channel

Chain C:



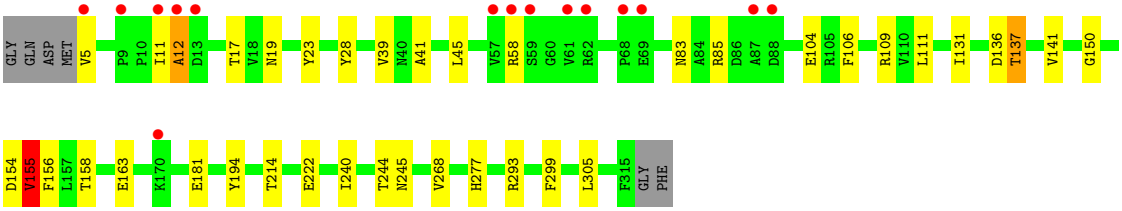
• Molecule 1: Proton-gated ion channel

Chain D:



- Molecule 1: Proton-gated ion channel

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	180.87Å 132.68Å 159.33Å 90.00° 101.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.75) 99.2 (20.00-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.210 , 0.238 (Not available) , (Not available)	Depositor DCC
R_{free} test set	4801 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13490	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ACT, CL, PLC, LMT

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	0.71	2/2615 (0.1%)	0.90	7/3575 (0.2%)
1	B	0.71	1/2615 (0.0%)	1.00	8/3575 (0.2%)
1	C	0.68	1/2607 (0.0%)	0.89	6/3564 (0.2%)
1	D	0.71	1/2624 (0.0%)	0.90	7/3587 (0.2%)
1	E	0.68	1/2616 (0.0%)	0.88	5/3575 (0.1%)
All	All	0.70	6/13077 (0.0%)	0.91	33/17876 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	GLU	CG-CD	6.77	1.62	1.51
1	A	154	ASP	C-N	6.48	1.49	1.34
1	D	222	GLU	CG-CD	6.41	1.61	1.51
1	C	222	GLU	CG-CD	6.23	1.61	1.51
1	B	222	GLU	CG-CD	6.19	1.61	1.51
1	E	222	GLU	CG-CD	5.57	1.60	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109	ARG	NE-CZ-NH2	19.59	130.10	120.30
1	B	109	ARG	NE-CZ-NH1	-15.92	112.34	120.30
1	C	133	ARG	CG-CD-NE	-8.05	94.89	111.80
1	E	136	ASP	CB-CG-OD1	7.27	124.85	118.30
1	D	222	GLU	OE1-CD-OE2	-6.35	115.69	123.30
1	C	155	VAL	CB-CA-C	6.33	123.44	111.40
1	D	155	VAL	CB-CA-C	6.33	123.43	111.40
1	E	155	VAL	CB-CA-C	6.31	123.39	111.40
1	A	155	VAL	CB-CA-C	6.30	123.38	111.40
1	C	109	ARG	NE-CZ-NH2	-6.11	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	109	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	138	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	E	109	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	293	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	109	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	109	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	51	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	12	ALA	N-CA-C	5.40	125.59	111.00
1	D	62	ARG	CA-CB-CG	5.39	125.27	113.40
1	E	12	ALA	N-CA-C	5.39	125.56	111.00
1	A	133	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	C	138	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	293	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	145	ASP	CB-CG-OD1	5.28	123.06	118.30
1	C	222	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	293	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	58	ARG	CB-CG-CD	5.10	124.87	111.60
1	B	138	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	D	109	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	222	GLU	OE1-CD-OE2	-5.06	117.22	123.30
1	B	246	LEU	CB-CA-C	-5.05	100.60	110.20
1	E	293	ARG	NE-CZ-NH1	5.03	122.82	120.30

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)	H(added)	Clashes	Symm-Clashes
1	A	2541	0	2559	27	0
1	B	2538	0	2560	28	0
1	C	2533	0	2556	20	0
1	D	2544	0	2566	20	0
1	E	2539	0	2569	16	0
2	A	8	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	6	1	0
2	C	8	0	6	1	0
2	D	8	0	6	1	0
2	E	8	0	6	0	0
3	A	46	0	65	0	0
3	B	94	0	157	0	0
3	C	70	0	111	0	0
3	D	70	0	111	0	0
3	E	70	0	111	1	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
4	E	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	12	0	23	0	0
6	B	12	0	23	0	0
6	C	12	0	23	0	0
6	D	12	0	23	1	0
6	E	24	0	46	0	0
7	A	65	0	0	5	0
7	B	67	0	0	3	0
7	C	65	0	0	2	0
7	D	65	0	0	6	0
7	E	58	0	0	1	0
All	All	13490	0	13533	98	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 (98) 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:C:133:ARG:NH1	1:C:176:LEU:O	2.02	0.92
1:D:158:THR:HG22	7:D:559:HOH:O	1.82	0.78
1:B:158:THR:HG22	7:B:561:HOH:O	1.87	0.75
1:C:158:THR:HG22	7:C:557:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:VAL:HG22	7:D:531:HOH:O	1.93	0.67
4:D:405:CL:CL	7:D:550:HOH:O	2.50	0.67
1:A:158:THR:HG22	7:A:551:HOH:O	1.97	0.65
1:A:158:THR:CG2	7:A:551:HOH:O	2.45	0.65
1:D:154:ASP:O	1:D:155:VAL:C	2.37	0.63
1:A:14:GLU:O	1:A:138:ARG:NH1	2.31	0.63
1:E:154:ASP:O	1:E:155:VAL:C	2.37	0.63
1:A:11:ILE:HG23	1:A:50:ARG:NH2	2.14	0.63
1:C:158:THR:CG2	7:C:557:HOH:O	2.46	0.63
1:C:154:ASP:O	1:C:155:VAL:C	2.38	0.61
1:C:200:ASN:OD1	1:D:243[B]:GLU:HG3	2.01	0.59
1:A:156:PHE:CZ	1:B:111:LEU:HD12	2.40	0.57
1:D:237:ALA:HA	6:D:408:LMT:H101	1.87	0.56
1:B:158:THR:CG2	7:B:561:HOH:O	2.46	0.55
1:B:131:ILE:HD13	2:B:402:ACT:H2	1.89	0.54
1:A:111:LEU:HD21	1:E:28:TYR:HB3	1.91	0.52
1:B:155:VAL:O	1:B:155:VAL:HG13	2.08	0.52
1:B:90:VAL:O	1:C:75:GLU:OE1	2.28	0.52
1:A:93:SER:OG	1:B:136:ASP:OD1	2.29	0.51
1:A:136:ASP:HB2	7:A:518:HOH:O	2.10	0.51
1:C:131:ILE:HD13	2:C:401:ACT:H2	1.93	0.50
1:E:277:HIS:HE1	7:E:533:HOH:O	1.95	0.50
1:D:243[B]:GLU:OE1	7:D:501:HOH:O	2.19	0.49
1:B:11:ILE:HD12	1:B:12:ALA:HB2	1.95	0.49
1:D:11:ILE:HD12	1:D:12:ALA:HB2	1.94	0.49
1:E:11:ILE:HD12	1:E:12:ALA:HB2	1.95	0.49
1:C:11:ILE:HD12	1:C:12:ALA:HB2	1.94	0.48
1:D:156:PHE:CZ	1:E:111:LEU:HD12	2.48	0.48
1:A:63:VAL:HG21	1:B:136:ASP:HB2	1.95	0.47
1:A:85:ARG:NE	1:A:104:GLU:OE2	2.46	0.47
1:B:214:THR:HG21	1:C:270:VAL:HG12	1.97	0.47
1:D:85:ARG:NE	1:D:104:GLU:OE2	2.46	0.47
1:A:131:ILE:HD11	1:A:181:GLU:HG2	1.97	0.47
1:A:136:ASP:CB	7:A:518:HOH:O	2.62	0.47
1:D:131:ILE:HD11	1:D:181:GLU:HG2	1.98	0.46
1:B:41:ALA:HB3	1:B:106:PHE:CE2	2.51	0.46
1:C:85:ARG:NE	1:C:104:GLU:OE2	2.47	0.46
1:A:41:ALA:HB3	1:A:106:PHE:CE2	2.51	0.46
1:B:85:ARG:NE	1:B:104:GLU:OE2	2.47	0.46
1:C:41:ALA:HB3	1:C:106:PHE:CE2	2.51	0.46
1:A:111:LEU:HD23	1:E:156:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:HD11	1:B:181:GLU:HG2	1.98	0.46
1:D:41:ALA:HB3	1:D:106:PHE:CE2	2.51	0.46
1:E:41:ALA:HB3	1:E:106:PHE:CE2	2.51	0.45
1:D:15:PRO:HB3	1:D:139:ASN:ND2	2.31	0.45
1:A:154:ASP:O	1:A:155:VAL:C	2.55	0.45
1:B:156:PHE:O	1:B:156:PHE:CD2	2.70	0.45
1:D:181:GLU:OE2	2:D:401:ACT:O	2.35	0.45
1:E:131:ILE:HD11	1:E:181:GLU:HG2	1.99	0.44
1:E:85:ARG:NE	1:E:104:GLU:OE2	2.47	0.44
1:B:19:ASN:O	1:B:45:LEU:HA	2.18	0.43
1:D:158:THR:CG2	7:D:559:HOH:O	2.51	0.43
1:D:11:ILE:HD12	1:D:12:ALA:CB	2.49	0.43
1:D:179:ARG:NH1	7:D:506:HOH:O	2.51	0.43
1:A:12:ALA:O	1:A:14:GLU:N	2.51	0.43
1:B:40:ASN:ND2	1:C:82:GLU:O	2.51	0.43
1:A:270:VAL:HG12	1:E:214:THR:HG21	2.00	0.43
1:D:19:ASN:O	1:D:45:LEU:HA	2.19	0.43
1:B:11:ILE:HD12	1:B:12:ALA:CB	2.48	0.43
1:A:19:ASN:O	1:A:45:LEU:HA	2.19	0.43
1:B:156:PHE:CZ	1:C:111:LEU:HD12	2.54	0.42
1:E:23:TYR:HA	1:E:150:GLY:O	2.19	0.42
1:C:131:ILE:HD11	1:C:181:GLU:HG2	2.01	0.42
1:E:194:TYR:CZ	3:E:403:PLC:O'	2.72	0.42
1:A:181:GLU:OE2	2:A:401:ACT:O	2.37	0.42
1:B:156:PHE:CD2	1:B:156:PHE:C	2.92	0.42
1:C:11:ILE:HD12	1:C:12:ALA:CB	2.48	0.42
1:C:23:TYR:HA	1:C:150:GLY:O	2.20	0.42
1:E:11:ILE:HD12	1:E:12:ALA:CB	2.49	0.42
1:A:230:SER:HB2	1:B:229:VAL:HG11	2.02	0.42
1:E:19:ASN:O	1:E:45:LEU:HA	2.19	0.42
1:C:19:ASN:O	1:C:45:LEU:HA	2.20	0.42
1:D:45:LEU:HB2	1:D:102:TYR:HB3	2.02	0.42
1:D:240:ILE:O	1:D:244:THR:HG23	2.19	0.42
7:A:554:HOH:O	1:B:177:GLU:HG2	2.20	0.41
1:A:156:PHE:HZ	1:B:111:LEU:HD12	1.83	0.41
1:B:240:ILE:O	1:B:244:THR:HG23	2.20	0.41
1:D:23:TYR:HA	1:D:150:GLY:O	2.20	0.41
1:A:45:LEU:HB2	1:A:102:TYR:HB3	2.03	0.41
1:B:45:LEU:HB2	1:B:102:TYR:HB3	2.00	0.41
1:A:23:TYR:HA	1:A:150:GLY:O	2.19	0.41
1:C:240:ILE:O	1:C:244:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:O	1:A:244:THR:HG23	2.20	0.41
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.73	0.41
1:B:219:THR:HG22	1:B:280[A]:LYS:HE3	2.02	0.41
1:B:245:ASN:HB2	7:B:520:HOH:O	2.21	0.41
1:A:11:ILE:HD12	1:A:12:ALA:N	2.36	0.41
1:A:268:VAL:HG12	1:A:299:PHE:HZ	1.86	0.41
1:B:23:TYR:HA	1:B:150:GLY:O	2.20	0.41
1:E:268:VAL:HG12	1:E:299:PHE:HZ	1.85	0.41
1:C:268:VAL:HG12	1:C:299:PHE:HZ	1.85	0.41
1:E:240:ILE:O	1:E:244:THR:HG23	2.21	0.41
1:C:76:ILE:CG2	1:C:130:LEU:HD22	2.52	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	312/317 (98%)	299 (96%)	10 (3%)	3 (1%)	15	27
1	B	312/317 (98%)	298 (96%)	13 (4%)	1 (0%)	41	60
1	C	311/317 (98%)	297 (96%)	12 (4%)	2 (1%)	25	42
1	D	313/317 (99%)	298 (95%)	13 (4%)	2 (1%)	25	42
1	E	312/317 (98%)	298 (96%)	12 (4%)	2 (1%)	25	42
All	All	1560/1585 (98%)	1490 (96%)	60 (4%)	10 (1%)	25	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	137	THR
1	B	137	THR
1	C	137	THR

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Mol	Chain	Res	Type
1	E	137	THR
1	A	137	THR
1	D	155	VAL
1	A	13	ASP
1	A	155	VAL
1	E	155	VAL
1	C	155	VAL

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	282/283 (100%)	265 (94%)	17 (6%)	19	33
1	B	282/283 (100%)	270 (96%)	12 (4%)	29	48
1	C	281/283 (99%)	271 (96%)	10 (4%)	35	55
1	D	283/283 (100%)	268 (95%)	15 (5%)	22	38
1	E	282/283 (100%)	271 (96%)	11 (4%)	32	52
All	All	1410/1415 (100%)	1345 (95%)	65 (5%)	26	46

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	14	GLU
1	A	17	THR
1	A	39	VAL
1	A	58	ARG
1	A	62	ARG
1	A	83	ASN
1	A	111	LEU
1	A	137	THR
1	A	138	ARG
1	A	141	VAL
1	A	158	THR

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Mol	Chain	Res	Type
1	A	163	GLU
1	A	170	LYS
1	A	178	ASP
1	A	245	ASN
1	A	305	LEU
1	B	5	VAL
1	B	17	THR
1	B	39	VAL
1	B	83	ASN
1	B	109	ARG
1	B	136	ASP
1	B	137	THR
1	B	141	VAL
1	B	158	THR
1	B	163	GLU
1	B	245	ASN
1	B	305	LEU
1	C	5	VAL
1	C	17	THR
1	C	39	VAL
1	C	83	ASN
1	C	137	THR
1	C	141	VAL
1	C	158	THR
1	C	163	GLU
1	C	245	ASN
1	C	305	LEU
1	D	5	VAL
1	D	17	THR
1	D	39	VAL
1	D	58	ARG
1	D	62	ARG
1	D	83	ASN
1	D	137	THR
1	D	141	VAL
1	D	158	THR
1	D	163	GLU
1	D	170	LYS
1	D	178	ASP
1	D	180	LEU
1	D	245	ASN
1	D	305	LEU

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Mol	Chain	Res	Type
1	E	5	VAL
1	E	17	THR
1	E	39	VAL
1	E	58	ARG
1	E	83	ASN
1	E	137	THR
1	E	141	VAL
1	E	158	THR
1	E	163	GLU
1	E	245	ASN
1	E	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	245	ASN
1	A	284	GLN
1	B	19	ASN
1	B	245	ASN
1	C	19	ASN
1	C	245	ASN
1	D	19	ASN
1	D	245	ASN
1	D	284	GLN
1	E	19	ASN
1	E	245	ASN
1	E	284	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)

Of 44 ligands modelled in this entry, 13 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
3	PLC	B	405	-	11,11,41	0.81	0	10,10,49	0.53	0
6	LMT	D	408	-	11,11,36	1.24	1 (9%)	10,10,47	1.08	0
3	PLC	E	405	-	11,11,41	1.28	0	10,10,49	0.97	0
3	PLC	B	403	-	33,33,41	1.62	2 (6%)	39,41,49	1.46	6 (15%)
3	PLC	B	404	-	22,22,41	1.05	0	20,20,49	0.77	0
3	PLC	C	402	-	33,33,41	1.73	5 (15%)	39,41,49	1.81	8 (20%)
2	ACT	D	401	-	3,3,3	0.87	0	3,3,3	1.25	0
3	PLC	E	403	-	33,33,41	1.56	3 (9%)	39,41,49	1.47	4 (10%)
6	LMT	E	401	-	11,11,36	1.13	0	10,10,47	0.90	0
2	ACT	E	402	-	3,3,3	0.78	0	3,3,3	1.13	0
3	PLC	D	402	-	33,33,41	1.60	2 (6%)	39,41,49	1.55	5 (12%)
2	ACT	C	407	-	3,3,3	0.88	0	3,3,3	1.05	0
6	LMT	A	410	-	11,11,36	1.24	0	10,10,47	0.98	0
6	LMT	E	409	-	11,11,36	1.10	0	10,10,47	0.82	0
3	PLC	A	403	-	11,11,41	0.70	0	10,10,49	0.19	0
2	ACT	C	401	-	3,3,3	0.89	0	3,3,3	0.78	0
2	ACT	B	408	-	3,3,3	1.14	0	3,3,3	0.72	0
6	LMT	B	409	-	11,11,36	1.24	1 (9%)	10,10,47	1.04	0
2	ACT	A	401	-	3,3,3	0.79	0	3,3,3	1.20	0
2	ACT	D	407	-	3,3,3	1.02	0	3,3,3	0.25	0
3	PLC	B	401	-	22,22,41	1.13	0	20,20,49	0.94	0
2	ACT	A	409	-	3,3,3	0.84	0	3,3,3	1.51	1 (33%)
2	ACT	E	408	-	3,3,3	0.93	0	3,3,3	1.09	0
3	PLC	C	403	-	22,22,41	1.34	0	20,20,49	1.12	1 (5%)
3	PLC	D	403	-	22,22,41	1.09	0	20,20,49	0.81	0
3	PLC	E	404	-	22,22,41	1.07	0	20,20,49	0.88	0
3	PLC	D	404	-	11,11,41	0.82	0	10,10,49	0.38	0
6	LMT	C	408	-	11,11,36	1.10	0	10,10,47	0.70	0
3	PLC	A	402	-	33,33,41	1.65	2 (6%)	39,41,49	1.66	6 (15%)
3	PLC	C	404	-	11,11,41	0.94	0	10,10,49	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	B	402	-	3,3,3	1.06	0	3,3,3	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLC	B	405	-	-	4/9/9/45	-
6	LMT	D	408	-	-	1/9/9/61	-
3	PLC	E	405	-	-	0/9/9/45	-
3	PLC	B	403	-	-	15/37/37/45	-
3	PLC	B	404	-	-	6/18/18/45	-
3	PLC	C	402	-	-	18/37/37/45	-
3	PLC	E	403	-	-	19/37/37/45	-
6	LMT	E	401	-	-	0/9/9/61	-
3	PLC	D	402	-	-	18/37/37/45	-
6	LMT	A	410	-	-	3/9/9/61	-
6	LMT	E	409	-	-	1/9/9/61	-
3	PLC	A	403	-	-	2/9/9/45	-
6	LMT	B	409	-	-	2/9/9/61	-
3	PLC	B	401	-	-	5/18/18/45	-
3	PLC	C	403	-	-	5/18/18/45	-
3	PLC	D	403	-	-	8/18/18/45	-
3	PLC	E	404	-	-	5/18/18/45	-
3	PLC	D	404	-	-	3/9/9/45	-
6	LMT	C	408	-	-	0/9/9/61	-
3	PLC	A	402	-	-	17/37/37/45	-
3	PLC	C	404	-	-	4/9/9/45	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	PLC	O2-C'	5.89	1.50	1.34
3	D	402	PLC	O2-C'	5.88	1.50	1.34
3	B	403	PLC	O2-C'	5.63	1.50	1.34
3	A	402	PLC	O3-CB	5.60	1.49	1.33
3	C	402	PLC	O2-C'	5.58	1.50	1.34
3	D	402	PLC	O3-CB	5.54	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	PLC	O3-CB	5.39	1.49	1.33
3	B	403	PLC	O3-CB	5.37	1.49	1.33
3	E	403	PLC	O2-C'	5.31	1.49	1.34
3	E	403	PLC	O3-CB	5.13	1.48	1.33
3	C	402	PLC	C1-C2	2.49	1.58	1.50
3	E	403	PLC	C1-C2	2.22	1.57	1.50
6	B	409	LMT	C4-C3	2.11	1.62	1.51
6	D	408	LMT	C4-C3	2.10	1.62	1.51
3	C	402	PLC	C1'-C'	2.10	1.56	1.50
3	C	402	PLC	P-O3P	2.06	1.67	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	PLC	O2-C'-C1'	6.24	124.97	111.48
3	E	403	PLC	O2-C'-C1'	5.46	123.30	111.48
3	A	402	PLC	O2-C'-C1'	5.34	123.04	111.48
3	D	402	PLC	O2-C'-C1'	5.03	122.35	111.48
3	A	402	PLC	C2-O2-C'	4.75	129.17	117.80
3	B	403	PLC	O2-C'-C1'	4.56	121.36	111.48
3	B	403	PLC	C2-O2-C'	4.29	128.06	117.80
3	D	402	PLC	C2-O2-C'	4.23	127.92	117.80
3	C	402	PLC	C2-O2-C'	4.19	127.83	117.80
3	C	402	PLC	O2-C'-O'	-3.88	114.63	123.70
3	A	402	PLC	O3-CB-C1B	3.27	121.81	111.83
3	D	402	PLC	O3-CB-C1B	3.19	121.56	111.83
3	E	403	PLC	O3-CB-C1B	3.03	121.09	111.83
3	A	402	PLC	O2-C2-C3	3.01	119.15	108.34
3	B	403	PLC	O3-CB-C1B	2.99	120.95	111.83
3	E	403	PLC	O2-C'-O'	-2.98	116.75	123.70
3	C	402	PLC	C3-O3-CB	2.88	127.64	117.12
3	C	402	PLC	O3-CB-C1B	2.70	120.06	111.83
3	A	402	PLC	O3-C3-C2	2.67	116.10	108.40
3	E	403	PLC	C3-O3-CB	2.59	126.59	117.12
3	D	402	PLC	C3-O3-CB	2.57	126.51	117.12
3	B	403	PLC	C3-O3-CB	2.43	126.00	117.12
3	C	403	PLC	C4B-C3B-C2B	2.35	126.27	114.37
3	C	402	PLC	O2-C2-C1	2.29	116.56	108.34
3	C	402	PLC	C2'-C1'-C'	2.24	121.91	113.69
3	A	402	PLC	O2-C'-O'	-2.21	118.53	123.70
3	D	402	PLC	O2-C'-O'	-2.19	118.58	123.70
3	B	403	PLC	O2-C2-C1	2.17	116.13	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	PLC	O2-C'-O'	-2.14	118.69	123.70
3	C	402	PLC	O3-CB-OB	-2.13	118.30	123.63
2	A	409	ACT	OXT-C-CH3	2.06	123.70	115.05

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PLC	O4P-C4-C5-N
3	A	402	PLC	C1-O3P-P-O1P
3	A	402	PLC	C1-O3P-P-O2P
3	A	402	PLC	C1-O3P-P-O4P
3	A	402	PLC	C4-O4P-P-O1P
3	A	402	PLC	C4-O4P-P-O2P
3	A	402	PLC	C4-O4P-P-O3P
3	B	403	PLC	O4P-C4-C5-N
3	B	403	PLC	C1-O3P-P-O1P
3	B	403	PLC	C1-O3P-P-O2P
3	B	403	PLC	C1-O3P-P-O4P
3	B	403	PLC	C4-O4P-P-O1P
3	C	402	PLC	O4P-C4-C5-N
3	C	402	PLC	C1'-C'-O2-C2
3	C	402	PLC	C1-O3P-P-O4P
3	D	402	PLC	O4P-C4-C5-N
3	D	402	PLC	C1'-C'-O2-C2
3	D	402	PLC	C4-O4P-P-O1P
3	D	402	PLC	C4-O4P-P-O2P
3	D	402	PLC	C4-O4P-P-O3P
3	E	403	PLC	C1'-C'-O2-C2
3	E	403	PLC	C1-O3P-P-O1P
3	E	403	PLC	C1-O3P-P-O4P
3	E	403	PLC	C4-O4P-P-O3P
3	A	402	PLC	O'-C'-O2-C2
3	C	402	PLC	O'-C'-O2-C2
3	D	402	PLC	O'-C'-O2-C2
3	E	403	PLC	O'-C'-O2-C2
3	A	402	PLC	C1'-C'-O2-C2
3	B	403	PLC	C1'-C'-O2-C2
3	C	402	PLC	OB-CB-O3-C3
3	C	402	PLC	C1B-CB-O3-C3
3	A	402	PLC	C1B-CB-O3-C3
3	B	403	PLC	CB-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
3	B	403	PLC	O'-C'-O2-C2
3	C	402	PLC	C'-C1'-C2'-C3'
3	E	403	PLC	C'-C1'-C2'-C3'
3	E	403	PLC	CB-C1B-C2B-C3B
3	A	402	PLC	OB-CB-O3-C3
3	D	402	PLC	CB-C1B-C2B-C3B
3	A	402	PLC	C'-C1'-C2'-C3'
3	D	402	PLC	C'-C1'-C2'-C3'
3	A	402	PLC	C3-C2-O2-C'
3	D	403	PLC	C6B-C7B-C8B-C9B
3	C	402	PLC	C3B-C4B-C5B-C6B
3	D	403	PLC	C2'-C3'-C4'-C5'
3	C	404	PLC	C1'-C2'-C3'-C4'
3	E	404	PLC	C4B-C5B-C6B-C7B
3	B	403	PLC	C'-C1'-C2'-C3'
3	D	402	PLC	C3B-C4B-C5B-C6B
3	E	403	PLC	C1B-C2B-C3B-C4B
3	B	404	PLC	C2'-C3'-C4'-C5'
3	C	403	PLC	C2'-C3'-C4'-C5'
3	E	403	PLC	C3B-C4B-C5B-C6B
3	B	404	PLC	C1'-C2'-C3'-C4'
3	C	402	PLC	C1B-C2B-C3B-C4B
3	D	402	PLC	C1B-C2B-C3B-C4B
3	D	403	PLC	C1'-C2'-C3'-C4'
3	A	402	PLC	C1'-C2'-C3'-C4'
3	B	401	PLC	C2'-C3'-C4'-C5'
3	C	403	PLC	C1'-C2'-C3'-C4'
3	B	403	PLC	C3B-C4B-C5B-C6B
3	D	402	PLC	C3'-C4'-C5'-C6'
3	E	404	PLC	C2'-C3'-C4'-C5'
3	C	402	PLC	C2B-C3B-C4B-C5B
3	B	403	PLC	C3'-C4'-C5'-C6'
3	A	402	PLC	C1-C2-C3-O3
3	E	404	PLC	C1'-C2'-C3'-C4'
3	B	403	PLC	C1B-C2B-C3B-C4B
3	B	404	PLC	C5B-C6B-C7B-C8B
3	D	404	PLC	C2'-C3'-C4'-C5'
3	D	404	PLC	C1'-C2'-C3'-C4'
3	B	403	PLC	C1-C2-O2-C'
3	C	404	PLC	C'-C1'-C2'-C3'
3	E	403	PLC	C2B-C3B-C4B-C5B
6	A	410	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	E	403	PLC	C4B-C5B-C6B-C7B
3	E	403	PLC	C1-C2-C3-O3
3	A	402	PLC	C2B-C3B-C4B-C5B
3	C	403	PLC	C3B-C4B-C5B-C6B
3	B	405	PLC	C2'-C3'-C4'-C5'
3	D	403	PLC	C3B-C4B-C5B-C6B
3	C	402	PLC	C4B-C5B-C6B-C7B
3	D	402	PLC	C4B-C5B-C6B-C7B
3	D	402	PLC	C1'-C2'-C3'-C4'
3	E	403	PLC	O3P-C1-C2-O2
3	C	402	PLC	C1-C2-C3-O3
3	B	404	PLC	C8B-C9B-CAA-CBA
3	D	403	PLC	C4'-C5'-C6'-C7'
3	A	402	PLC	O2-C2-C3-O3
3	D	403	PLC	C2B-C3B-C4B-C5B
3	B	401	PLC	CB-C1B-C2B-C3B
3	E	403	PLC	O4P-C4-C5-N
3	C	404	PLC	C2'-C3'-C4'-C5'
3	B	404	PLC	C6'-C7'-C8'-C9'
3	E	403	PLC	O3P-C1-C2-C3
3	E	403	PLC	C4'-C5'-C6'-C7'
3	B	401	PLC	C2B-C3B-C4B-C5B
3	D	403	PLC	C8'-C9'-CA'-CB'
3	B	405	PLC	C1'-C2'-C3'-C4'
3	C	403	PLC	C8'-C9'-CA'-CB'
3	E	404	PLC	C1B-C2B-C3B-C4B
3	C	402	PLC	C1-O3P-P-O1P
3	D	402	PLC	C1-O3P-P-O1P
3	B	405	PLC	C'-C1'-C2'-C3'
3	B	404	PLC	C8'-C9'-CA'-CB'
3	A	403	PLC	C3'-C4'-C5'-C6'
3	C	402	PLC	CB-C1B-C2B-C3B
3	E	404	PLC	C8'-C9'-CA'-CB'
3	D	402	PLC	C3-C2-O2-C'
3	D	404	PLC	C8'-C9'-CA'-CB'
6	D	408	LMT	C2-C3-C4-C5
3	B	401	PLC	C4'-C5'-C6'-C7'
6	A	410	LMT	C3-C4-C5-C6
6	E	409	LMT	C3-C4-C5-C6
3	D	402	PLC	C2'-C3'-C4'-C5'
3	D	403	PLC	C5B-C6B-C7B-C8B
3	C	402	PLC	C1-C2-O2-C'

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Mol	Chain	Res	Type	Atoms
3	B	405	PLC	C3'-C4'-C5'-C6'
3	A	403	PLC	C'-C1'-C2'-C3'
3	C	404	PLC	C6'-C7'-C8'-C9'
3	C	403	PLC	C2B-C3B-C4B-C5B
3	E	403	PLC	O2-C2-C3-O3
3	D	402	PLC	C2B-C3B-C4B-C5B
3	B	403	PLC	C2'-C3'-C4'-C5'
3	C	402	PLC	O2-C'-C1'-C2'
3	B	401	PLC	C8B-C9B-CAA-CBA
6	A	410	LMT	C1-C2-C3-C4
3	C	402	PLC	C3'-C4'-C5'-C6'
6	B	409	LMT	C3-C4-C5-C6
3	B	403	PLC	C4B-C5B-C6B-C7B
3	E	403	PLC	C2B-C1B-CB-O3
3	C	402	PLC	O'-C'-C1'-C2'
3	D	402	PLC	C4'-C5'-C6'-C7'
3	E	403	PLC	C2B-C1B-CB-OB
6	B	409	LMT	C5-C6-C7-C8

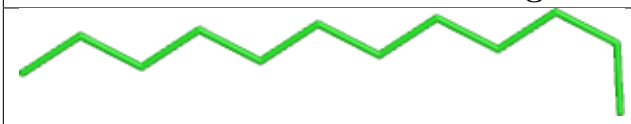
There are no ring outliers.

6 monomers are involved in 6 short contacts:

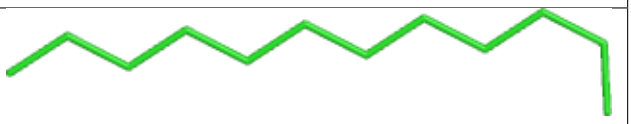
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	408	LMT	1	0
2	D	401	ACT	1	0
3	E	403	PLC	1	0
2	C	401	ACT	1	0
2	A	401	ACT	1	0
2	B	402	ACT	1	0

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.

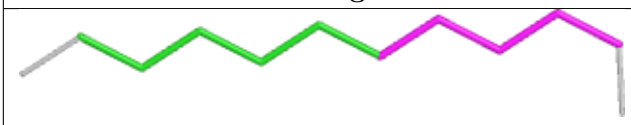
Ligand PLC B 405



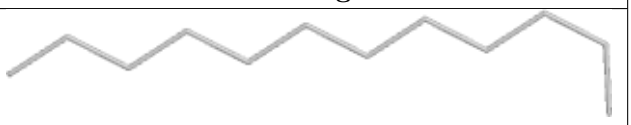
Bond lengths



Bond angles



Torsions



Rings

Ligand LMT D 408

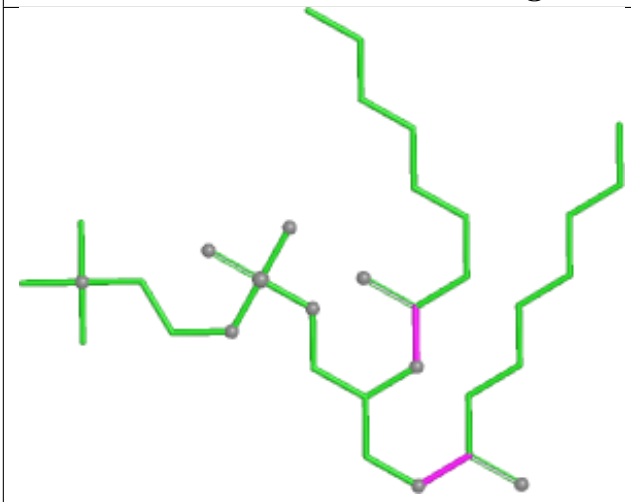
Bond lengths

Bond angles

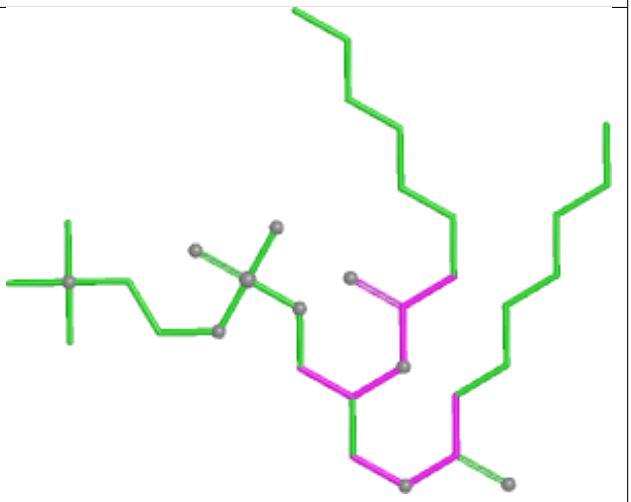
Torsions

Rings

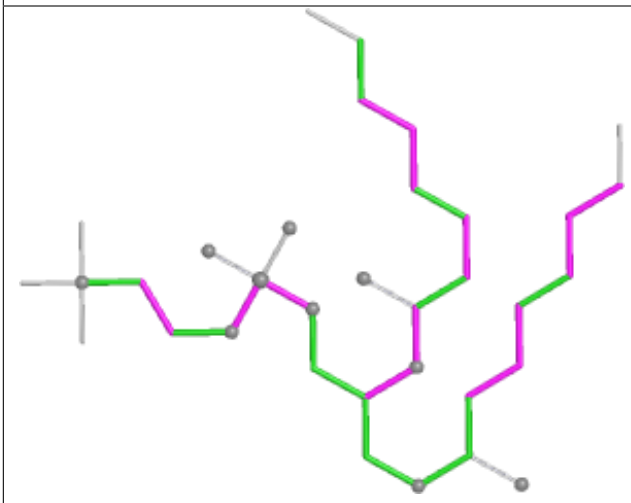
Ligand PLC B 403



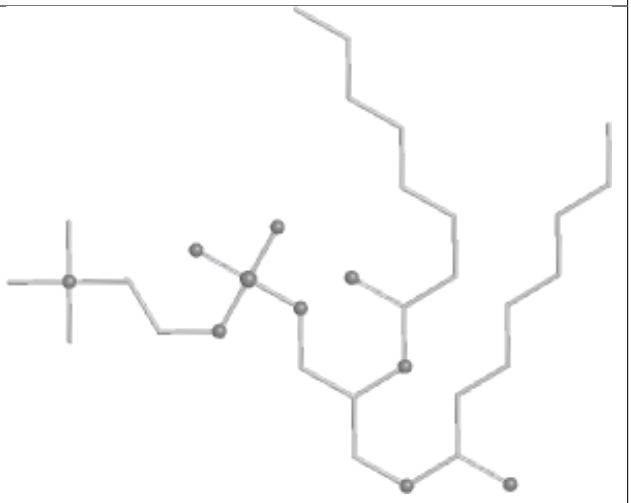
Bond lengths



Bond angles

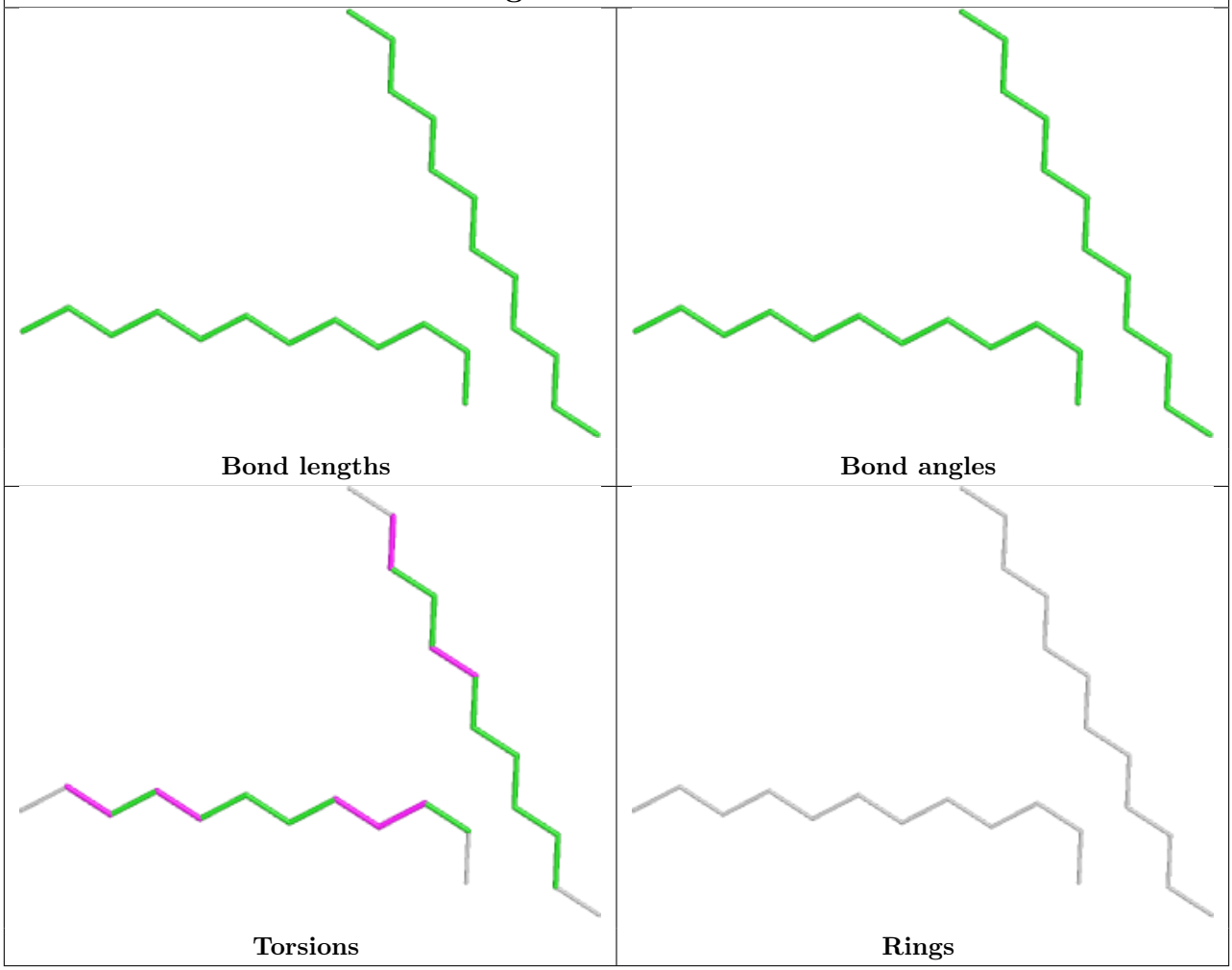


Torsions

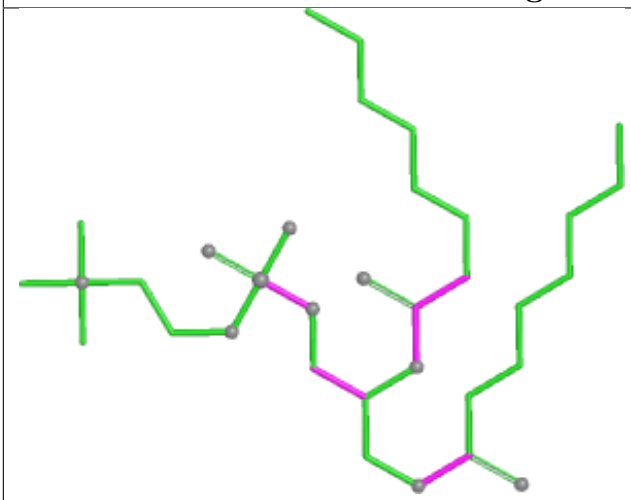


Rings

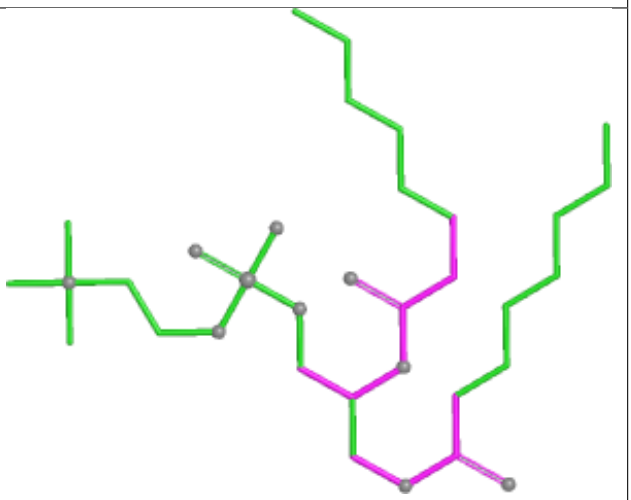
Ligand PLC B 404



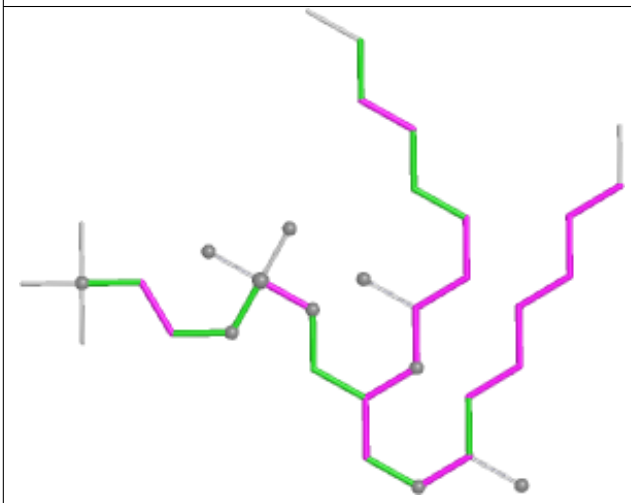
Ligand PLC C 402



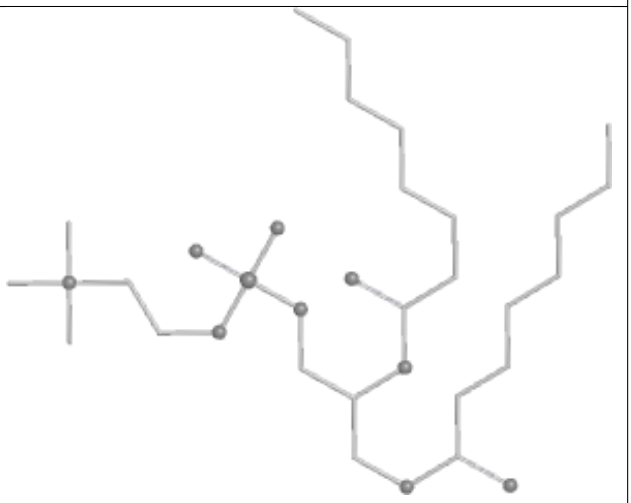
Bond lengths



Bond angles

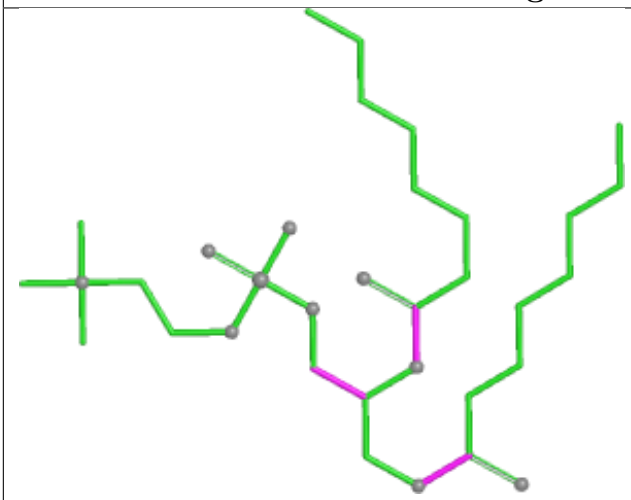


Torsions

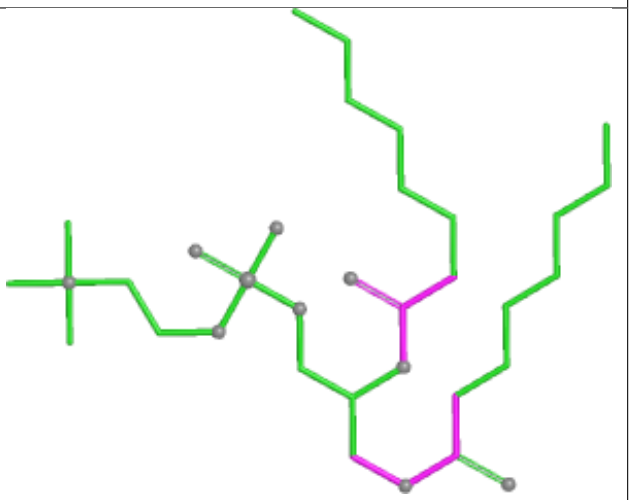


Rings

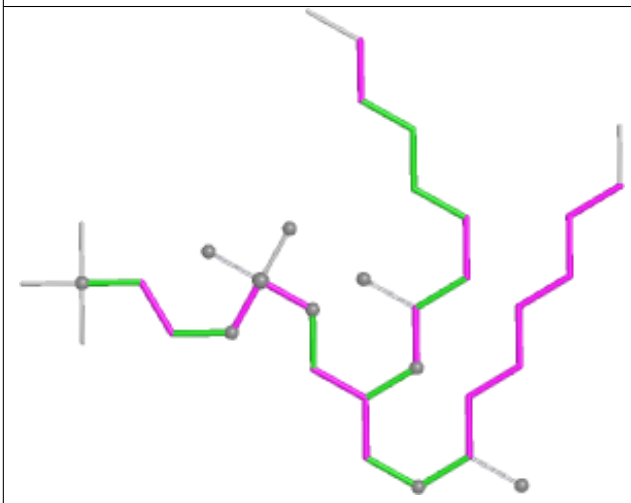
Ligand PLC E 403



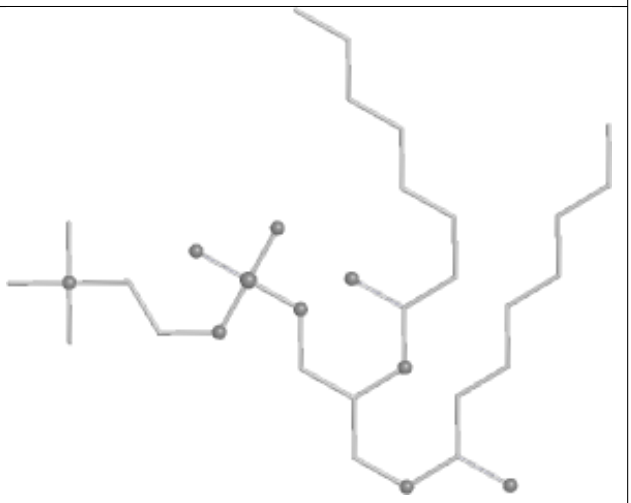
Bond lengths



Bond angles

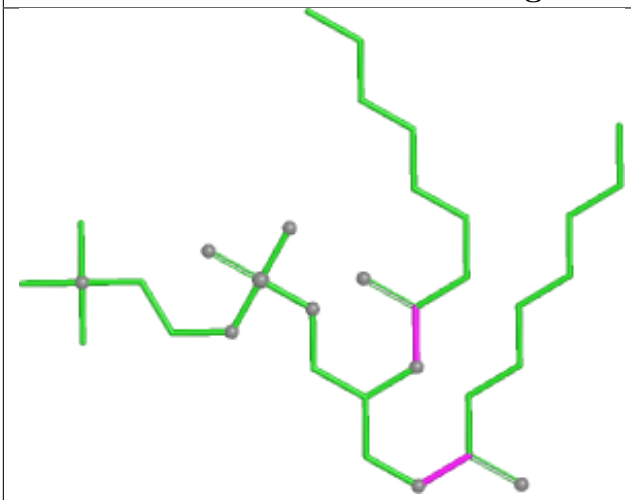


Torsions

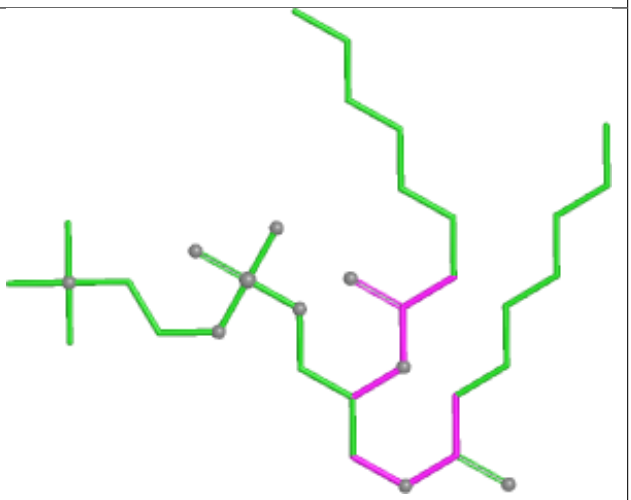


Rings

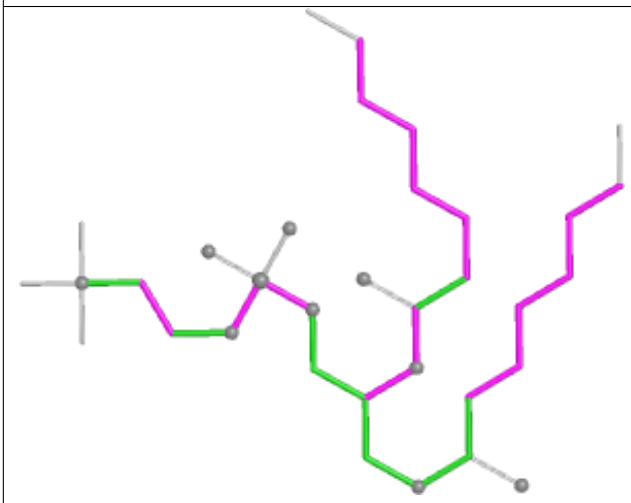
Ligand PLC D 402



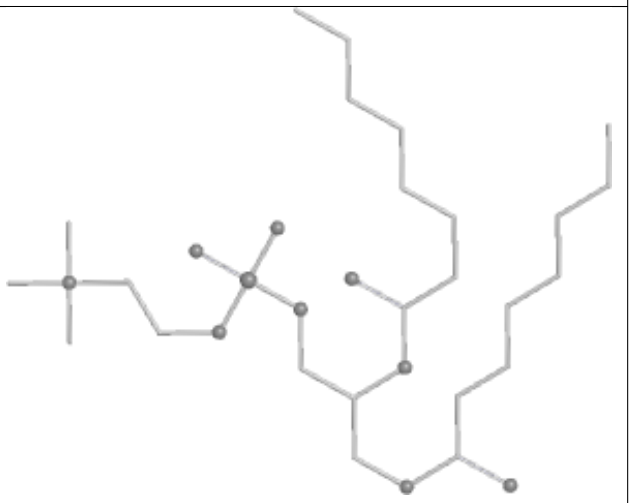
Bond lengths



Bond angles



Torsions



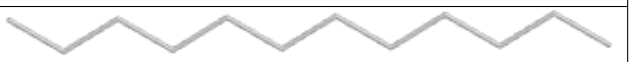
Rings

Ligand LMT A 410

Bond lengths

Bond angles

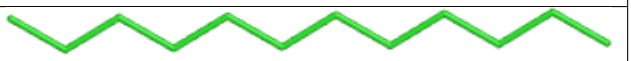
Torsions



Rings

Ligand LMT E 409

Bond lengths

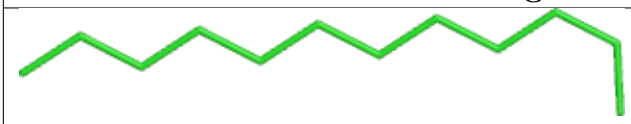


Bond angles

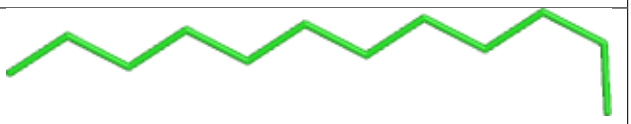
Torsions

Rings

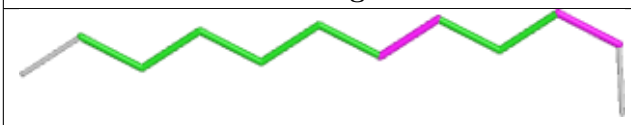
Ligand PLC A 403



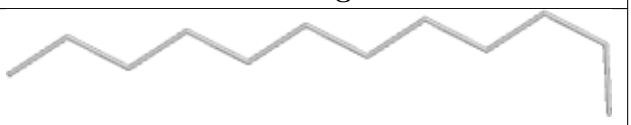
Bond lengths



Bond angles



Torsions



Rings

Ligand LMT B 409

Bond lengths

Bond angles

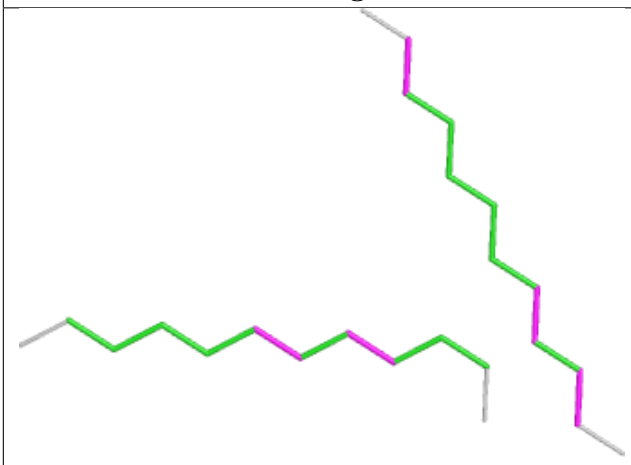
Torsions

Rings

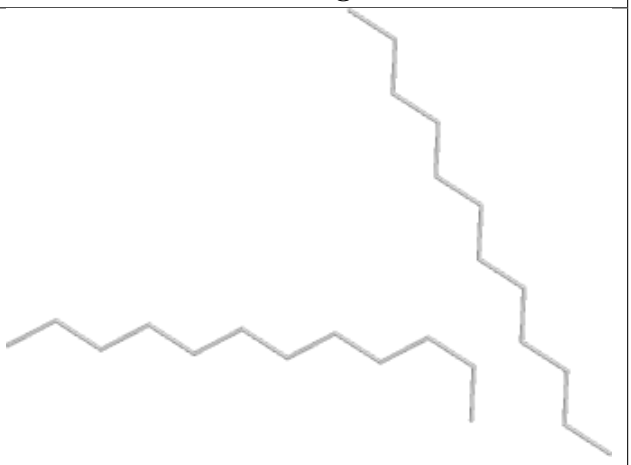
Ligand PLC B 401

Bond lengths

Bond angles

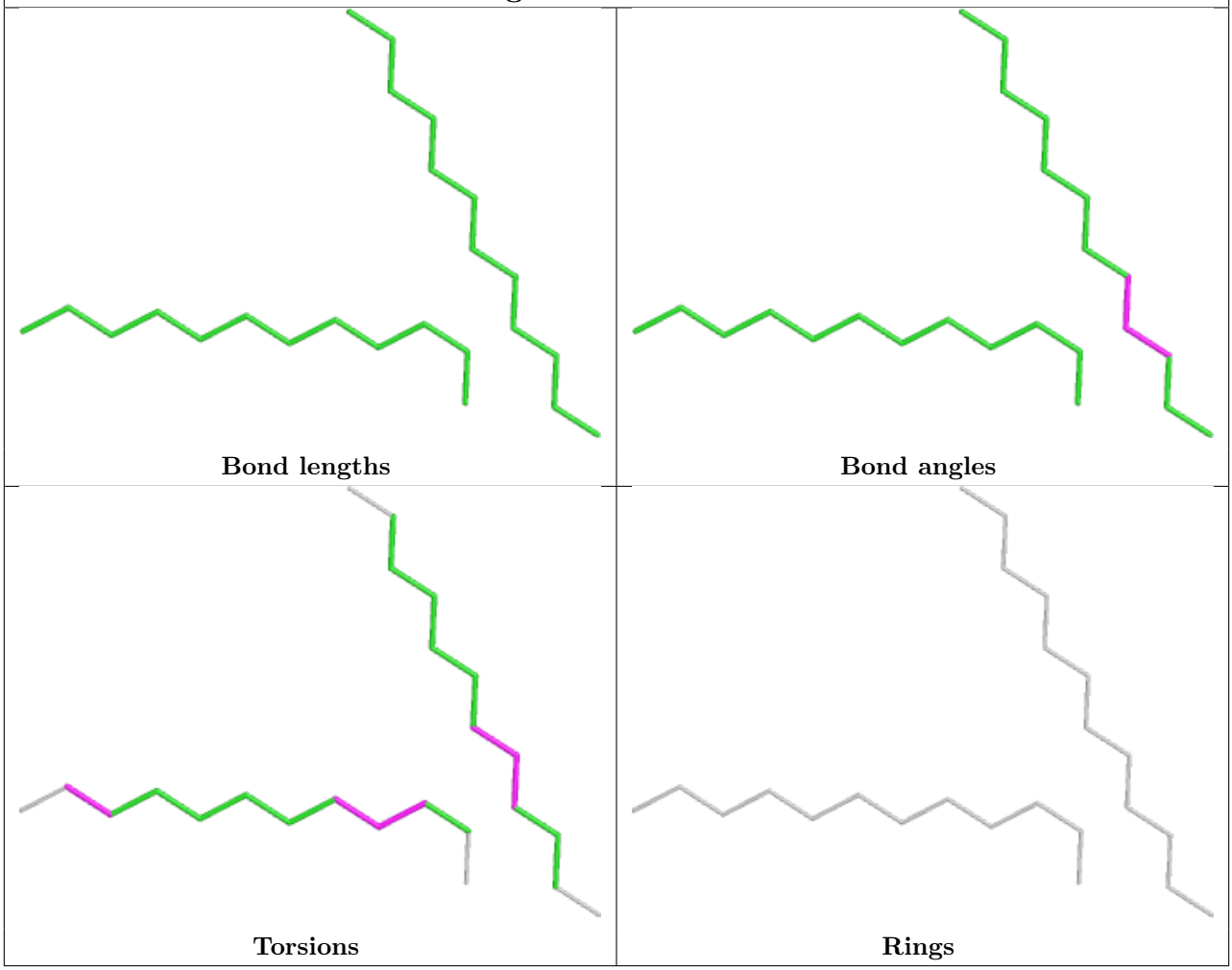


Torsions

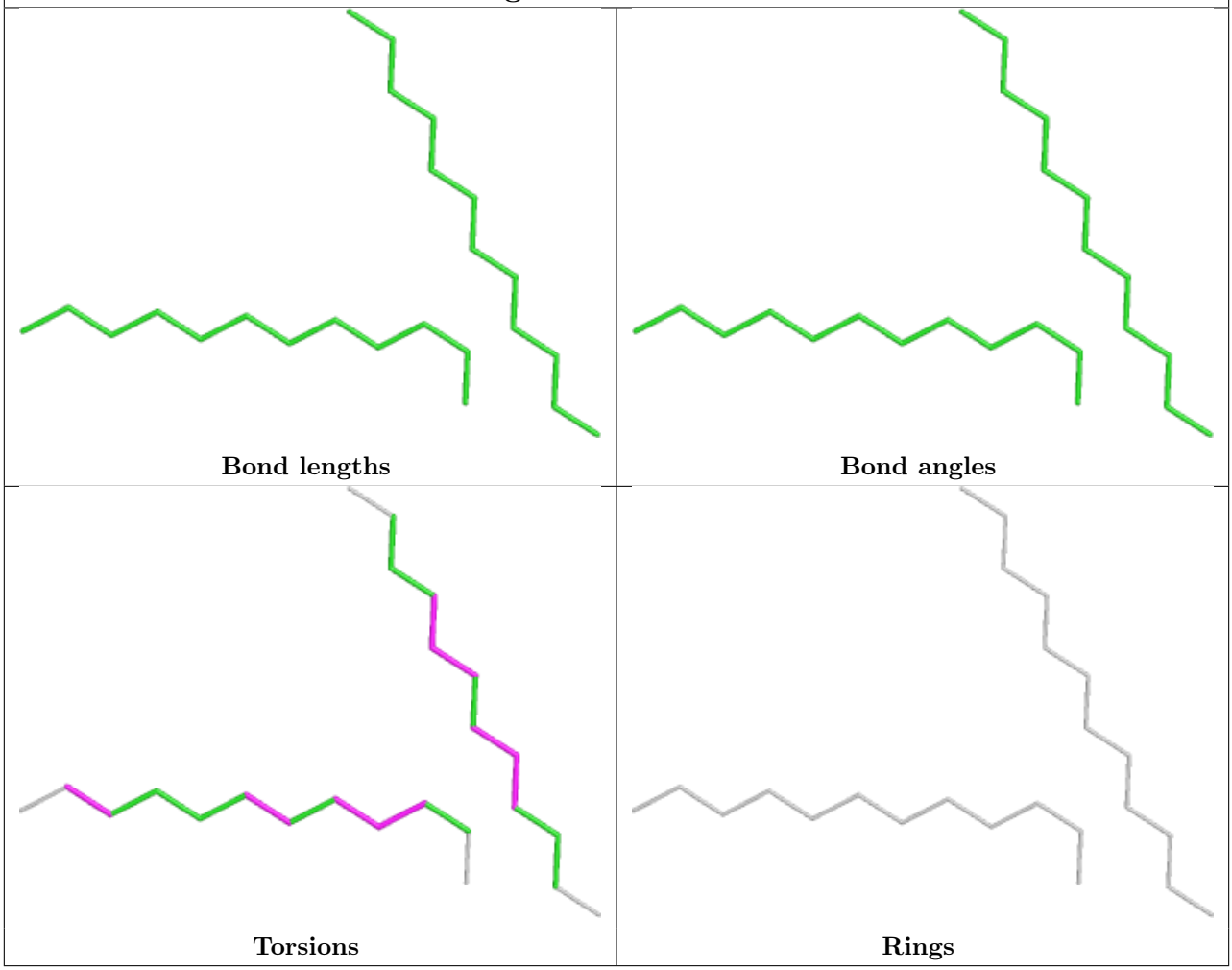


Rings

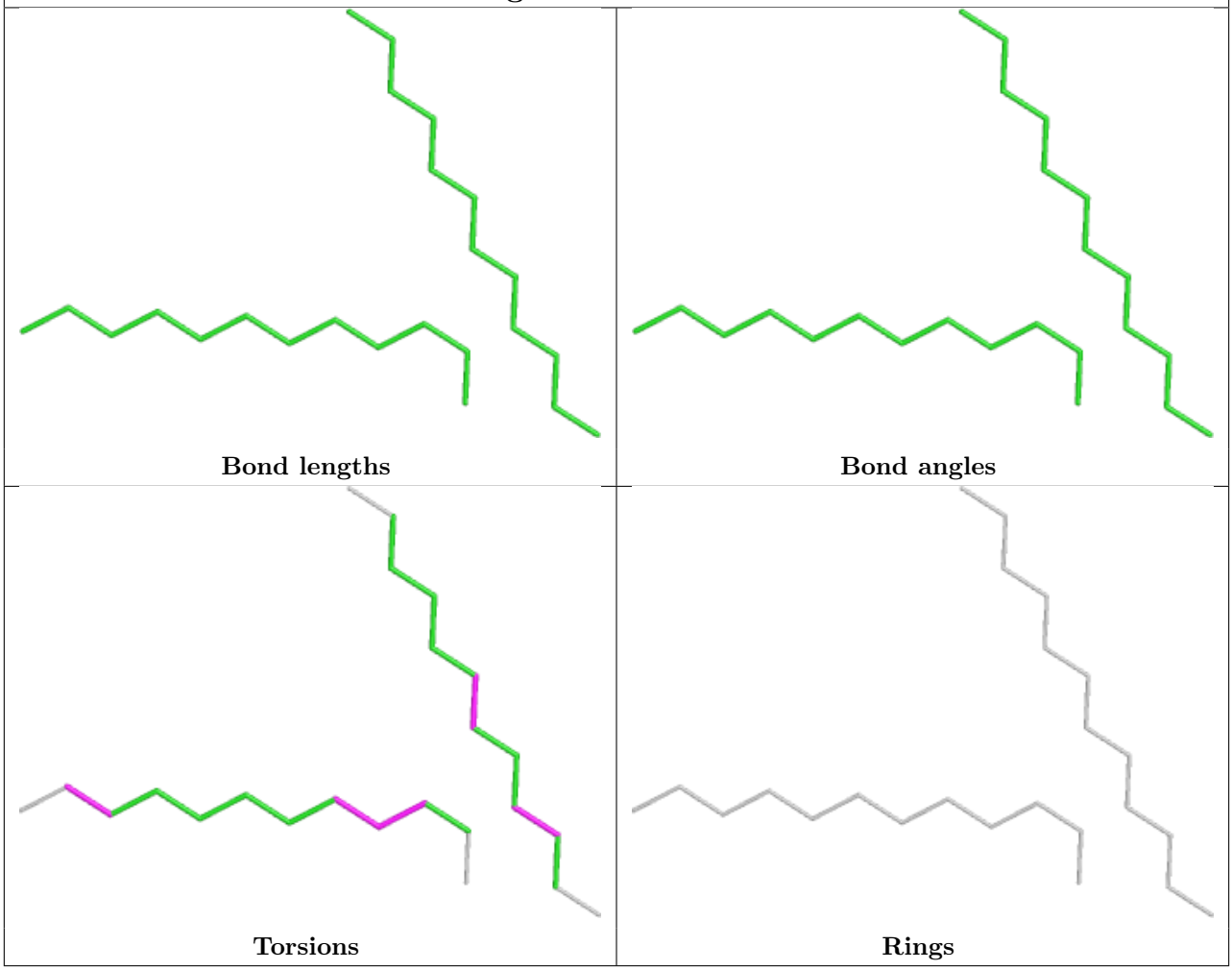
Ligand PLC C 403



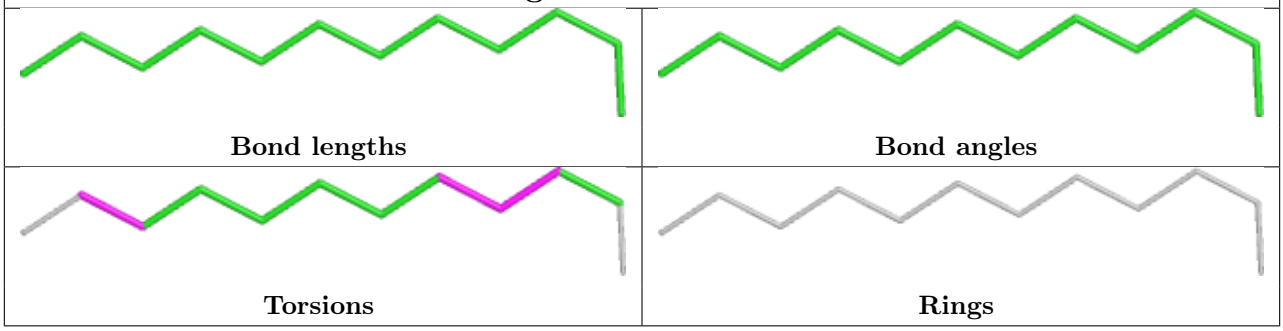
Ligand PLC D 403



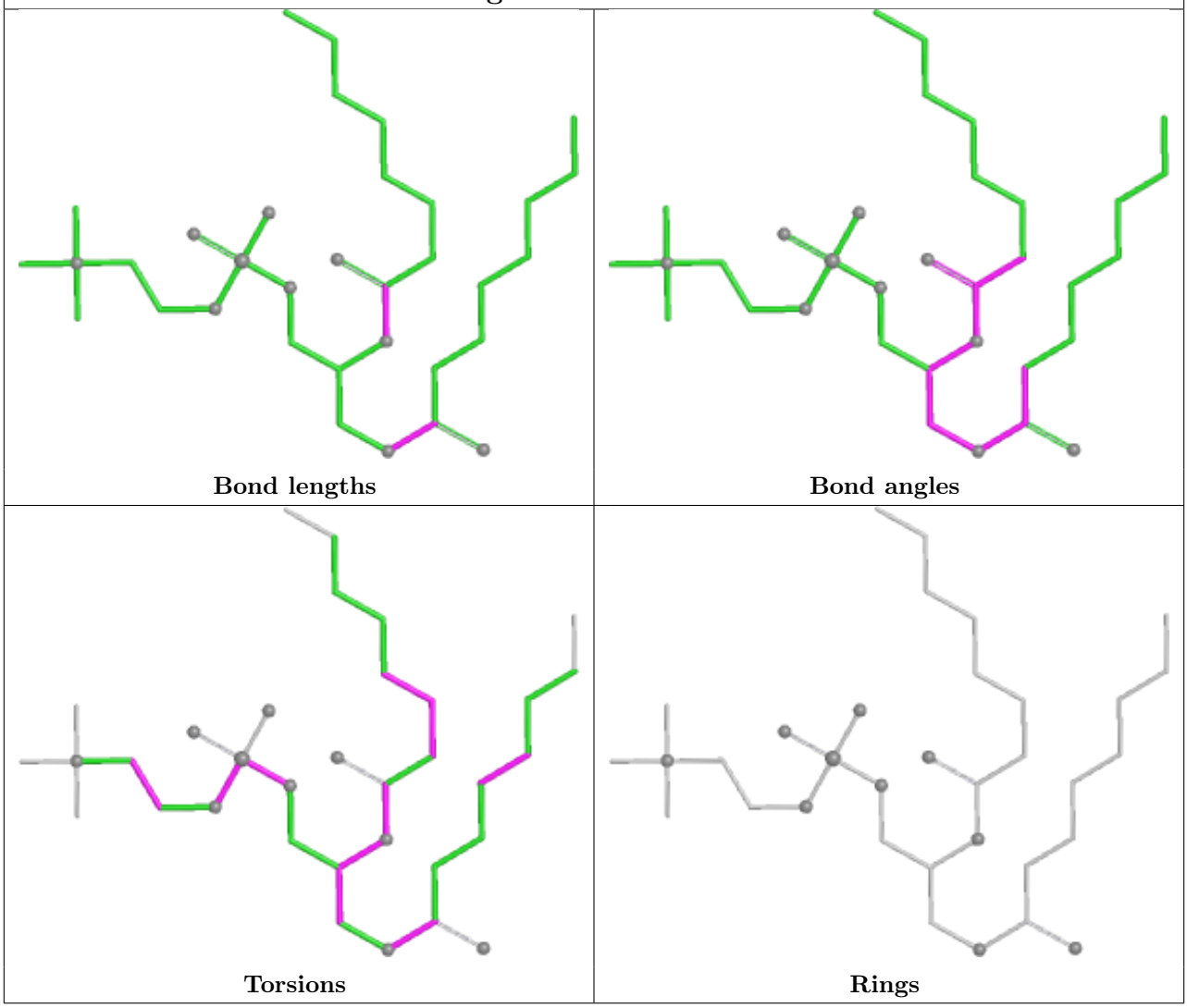
Ligand PLC E 404



Ligand PLC D 404



Ligand PLC A 402



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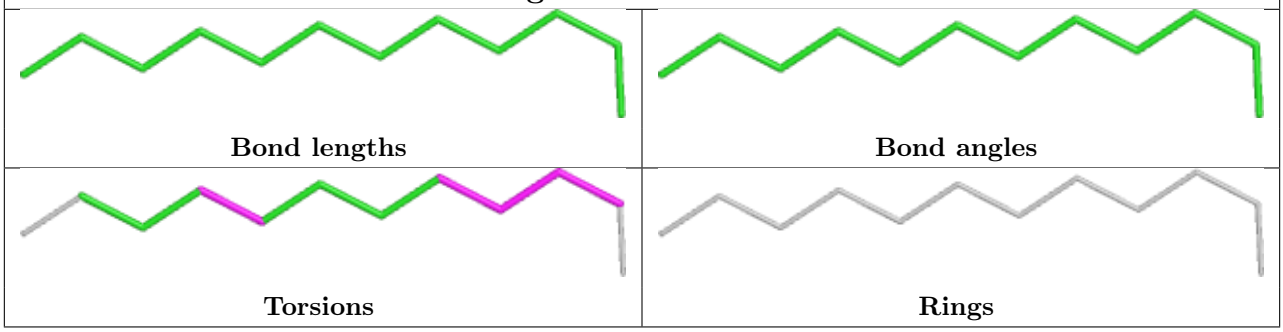

5.7 Other polymers (i)

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, 95th 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	311/317 (98%)	-0.22	13 (4%)	36	43	42, 66, 112, 144	0
1	B	311/317 (98%)	-0.25	14 (4%)	33	39	40, 65, 103, 129	0
1	C	311/317 (98%)	-0.18	15 (4%)	30	36	39, 65, 110, 150	0
1	D	311/317 (98%)	-0.23	14 (4%)	33	39	39, 64, 113, 145	0
1	E	311/317 (98%)	-0.14	15 (4%)	30	36	42, 66, 109, 137	0
All	All	1555/1585 (98%)	-0.21	71 (4%)	32	39	39, 65, 111, 150	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	ARG	5.7
1	A	57	VAL	5.6
1	D	57	VAL	5.6
1	E	58	ARG	5.5
1	A	11	ILE	4.9
1	E	62	ARG	4.7
1	C	13	ASP	4.5
1	C	11	ILE	3.9
1	D	61	VAL	3.9
1	B	12	ALA	3.8
1	E	11	ILE	3.8
1	C	12	ALA	3.5
1	D	59	SER	3.4
1	D	58	ARG	3.3
1	E	61	VAL	3.3
1	A	58	ARG	3.3
1	D	12	ALA	3.1
1	C	61	VAL	3.0
1	C	60	GLY	3.0
1	C	59	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	68	PRO	2.9
1	B	86	ASP	2.9
1	C	178	ASP	2.8
1	D	11	ILE	2.8
1	B	293	ARG	2.8
1	C	62	ARG	2.8
1	C	57	VAL	2.7
1	C	154	ASP	2.7
1	B	11	ILE	2.7
1	A	88[A]	ASP	2.7
1	E	57	VAL	2.7
1	B	13	ASP	2.7
1	B	154	ASP	2.7
1	E	13	ASP	2.6
1	A	59	SER	2.6
1	B	59	SER	2.6
1	B	69	GLU	2.6
1	E	5	VAL	2.5
1	B	58	ARG	2.5
1	C	56	PRO	2.5
1	B	88[A]	ASP	2.5
1	D	153	ASP	2.5
1	B	60	GLY	2.4
1	E	12	ALA	2.4
1	E	59	SER	2.4
1	B	57	VAL	2.4
1	D	154	ASP	2.4
1	E	170	LYS	2.4
1	E	88	ASP	2.4
1	E	87	ALA	2.3
1	D	89	VAL	2.3
1	E	69	GLU	2.3
1	C	293	ARG	2.3
1	D	88[A]	ASP	2.3
1	A	154	ASP	2.3
1	D	60	GLY	2.2
1	D	62	ARG	2.2
1	B	153	ASP	2.2
1	B	61	VAL	2.1
1	C	55	ASP	2.1
1	D	5	VAL	2.1
1	D	245	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	5	VAL	2.1
1	A	12	ALA	2.1
1	A	312	PHE	2.1
1	A	50	ARG	2.1
1	E	9	PRO	2.0
1	A	62	ARG	2.0
1	A	56	PRO	2.0
1	C	22	ILE	2.0
1	A	68	PRO	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, 95th 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
3	PLC	C	402	34/42	0.54	0.39	59,113,167,195	0
5	NA	A	407	1/1	0.56	0.23	79,79,79,79	0
3	PLC	C	404	12/42	0.57	0.38	76,93,105,108	0
6	LMT	D	408	12/35	0.58	0.39	52,57,71,77	0
5	NA	E	407	1/1	0.63	0.34	86,86,86,86	0
3	PLC	A	402	34/42	0.63	0.38	68,122,163,181	0
3	PLC	E	403	34/42	0.64	0.35	62,119,156,160	0
3	PLC	A	403	12/42	0.68	0.43	76,97,106,111	0
6	LMT	A	410	12/35	0.69	0.39	41,50,84,89	0
6	LMT	C	408	12/35	0.69	0.32	42,54,74,75	0
3	PLC	E	405	12/42	0.69	0.33	65,82,106,112	0
3	PLC	D	402	34/42	0.70	0.32	71,112,148,177	0
6	LMT	B	409	12/35	0.70	0.37	49,52,75,81	0
6	LMT	E	409	12/35	0.70	0.40	48,65,90,95	0

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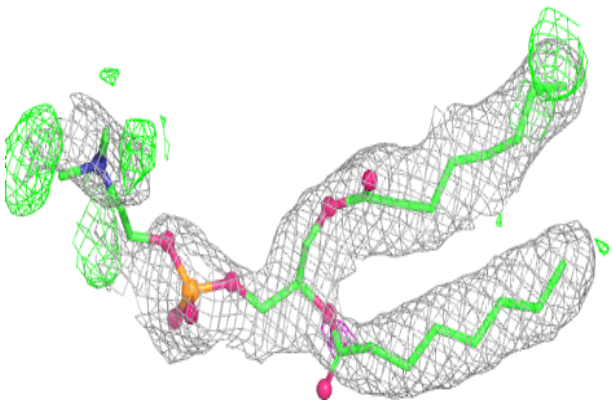
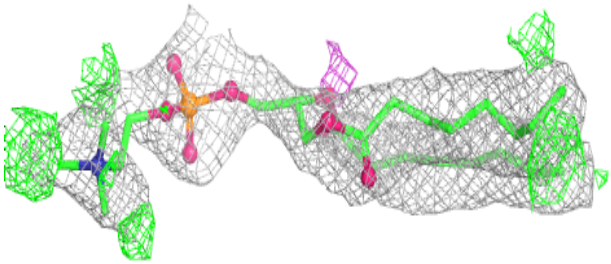
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PLC	B	405	12/42	0.71	0.35	73,90,100,103	0
3	PLC	B	403	34/42	0.72	0.38	68,122,150,165	0
3	PLC	B	401	24/42	0.73	0.29	52,78,104,109	0
5	NA	B	407	1/1	0.75	0.12	65,65,65,65	0
3	PLC	B	404	24/42	0.76	0.28	55,75,97,104	0
3	PLC	E	404	24/42	0.77	0.29	56,74,101,106	0
3	PLC	C	403	24/42	0.77	0.27	55,71,92,96	0
5	NA	D	406	1/1	0.77	0.19	80,80,80,80	0
3	PLC	D	403	24/42	0.80	0.27	51,76,106,110	0
5	NA	C	406	1/1	0.82	0.14	79,79,79,79	0
3	PLC	D	404	12/42	0.82	0.32	74,81,101,108	0
2	ACT	B	402	4/4	0.86	0.29	90,92,101,106	0
6	LMT	E	401	12/35	0.88	0.32	45,54,70,73	0
4	CL	A	406	1/1	0.88	0.29	93,93,93,93	0
5	NA	A	408	1/1	0.93	0.30	58,58,58,58	0
4	CL	A	405	1/1	0.94	0.17	78,78,78,78	0
2	ACT	E	402	4/4	0.95	0.19	87,89,95,95	0
2	ACT	E	408	4/4	0.96	0.11	60,60,60,65	0
2	ACT	C	401	4/4	0.96	0.16	85,88,104,112	0
2	ACT	C	407	4/4	0.96	0.14	75,77,78,80	0
2	ACT	D	401	4/4	0.96	0.15	67,78,78,78	0
2	ACT	D	407	4/4	0.96	0.11	63,63,65,67	0
2	ACT	A	401	4/4	0.96	0.18	81,82,84,84	0
4	CL	C	405	1/1	0.97	0.06	74,74,74,74	0
4	CL	D	405	1/1	0.97	0.07	73,73,73,73	0
4	CL	E	406	1/1	0.97	0.07	78,78,78,78	0
2	ACT	B	408	4/4	0.97	0.10	67,70,70,70	0
2	ACT	A	409	4/4	0.97	0.11	61,62,62,63	0
4	CL	B	406	1/1	0.98	0.07	73,73,73,73	0
4	CL	A	404	1/1	0.98	0.09	73,73,73,73	0

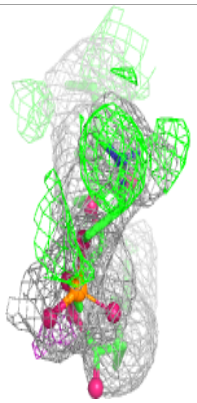
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLC C 402:

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

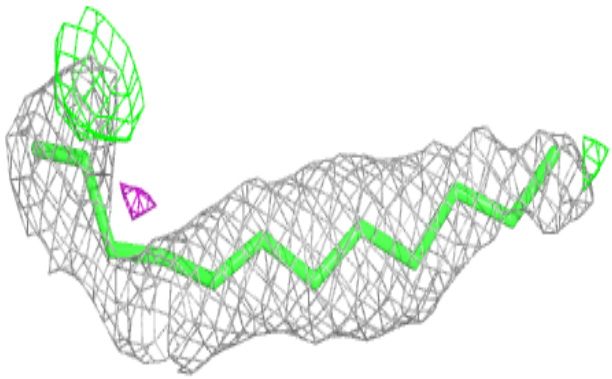


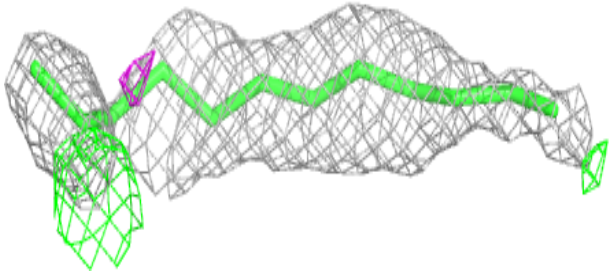




Electron density around PLC C 404:

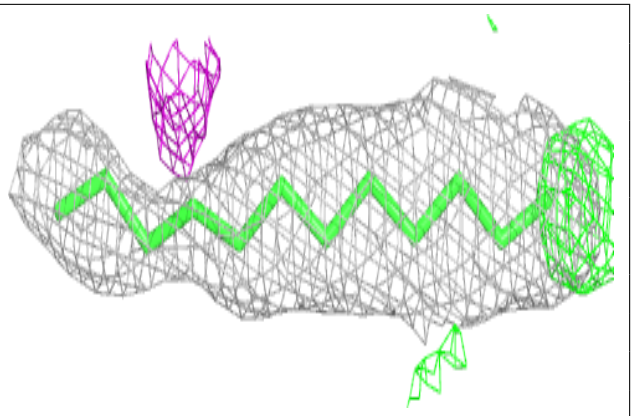
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

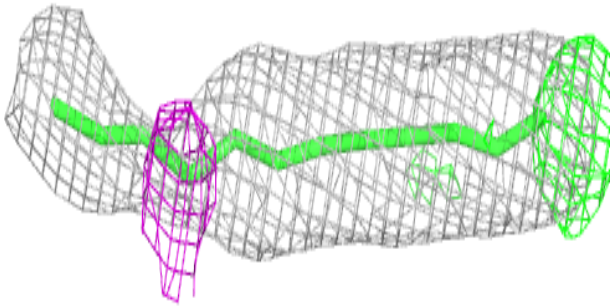


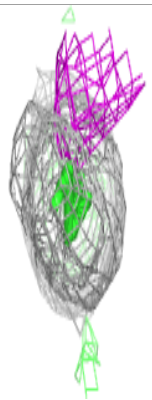


Electron density around LMT D 408:

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

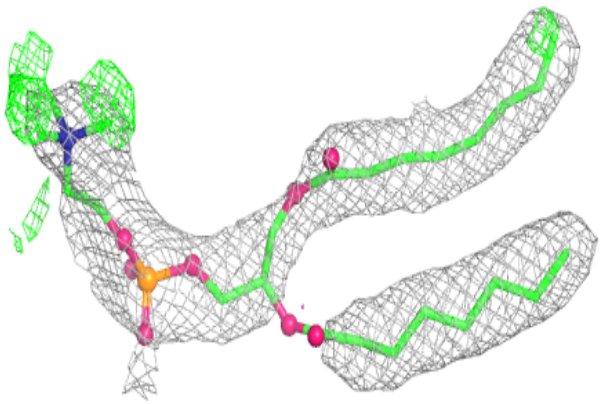


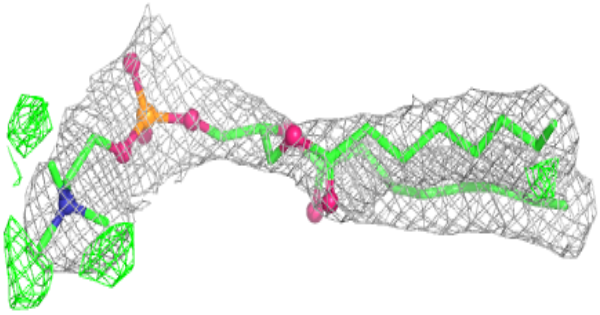


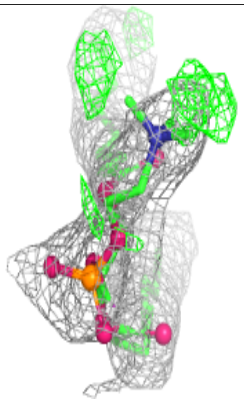


Electron density around PLC A 402:

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

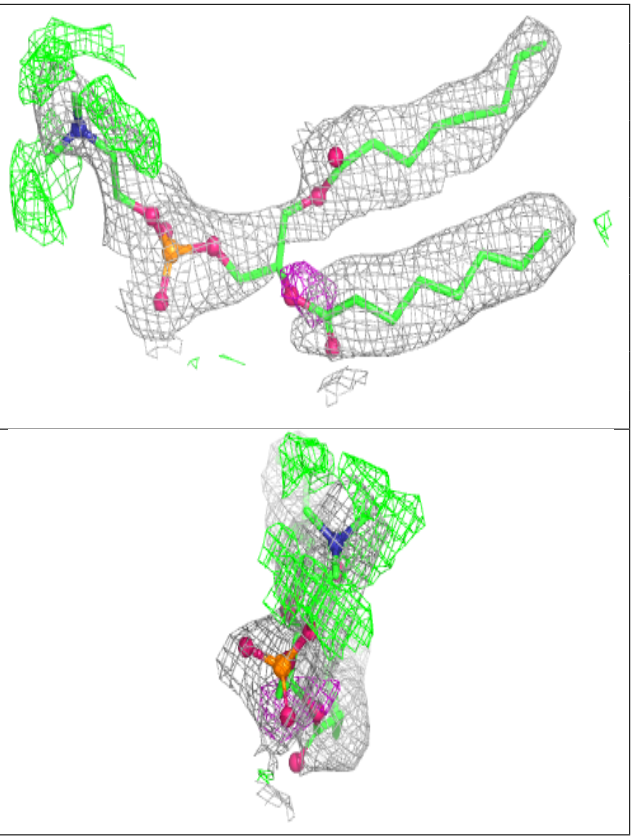


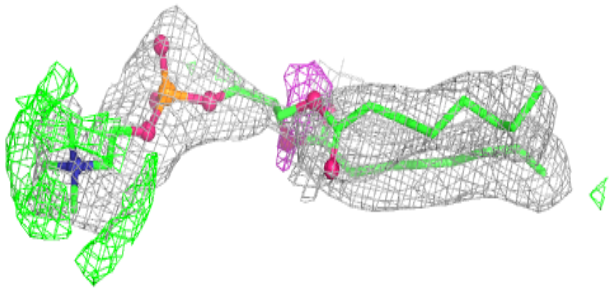




Electron density around PLC E 403:

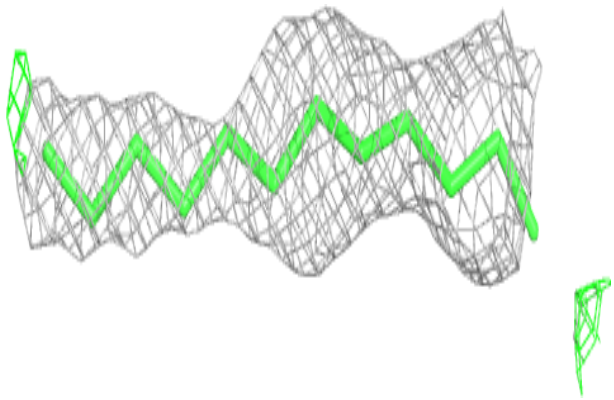
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

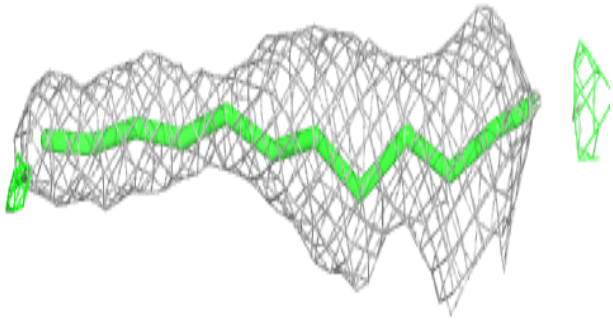


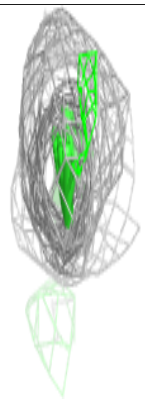


Electron density around PLC A 403:

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

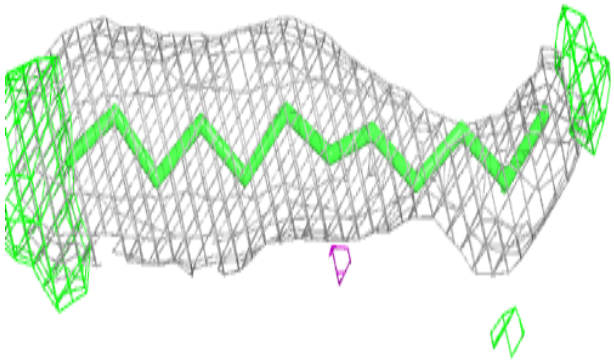


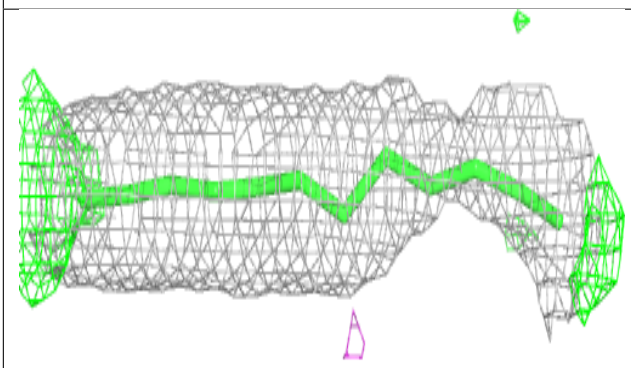


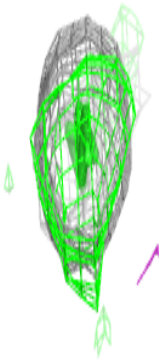


Electron density around LMT A 410:

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

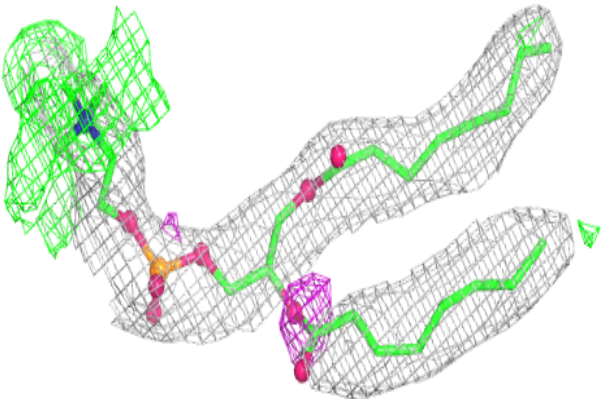


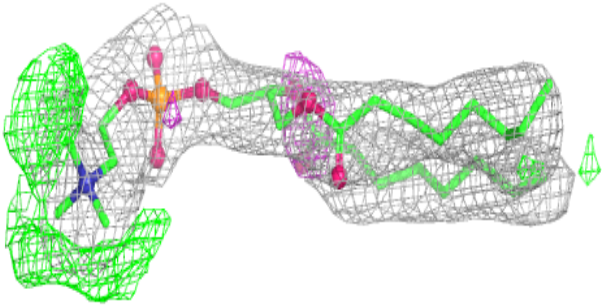


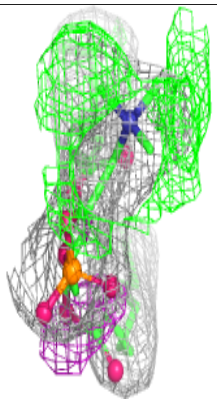


Electron density around PLC D 402:

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

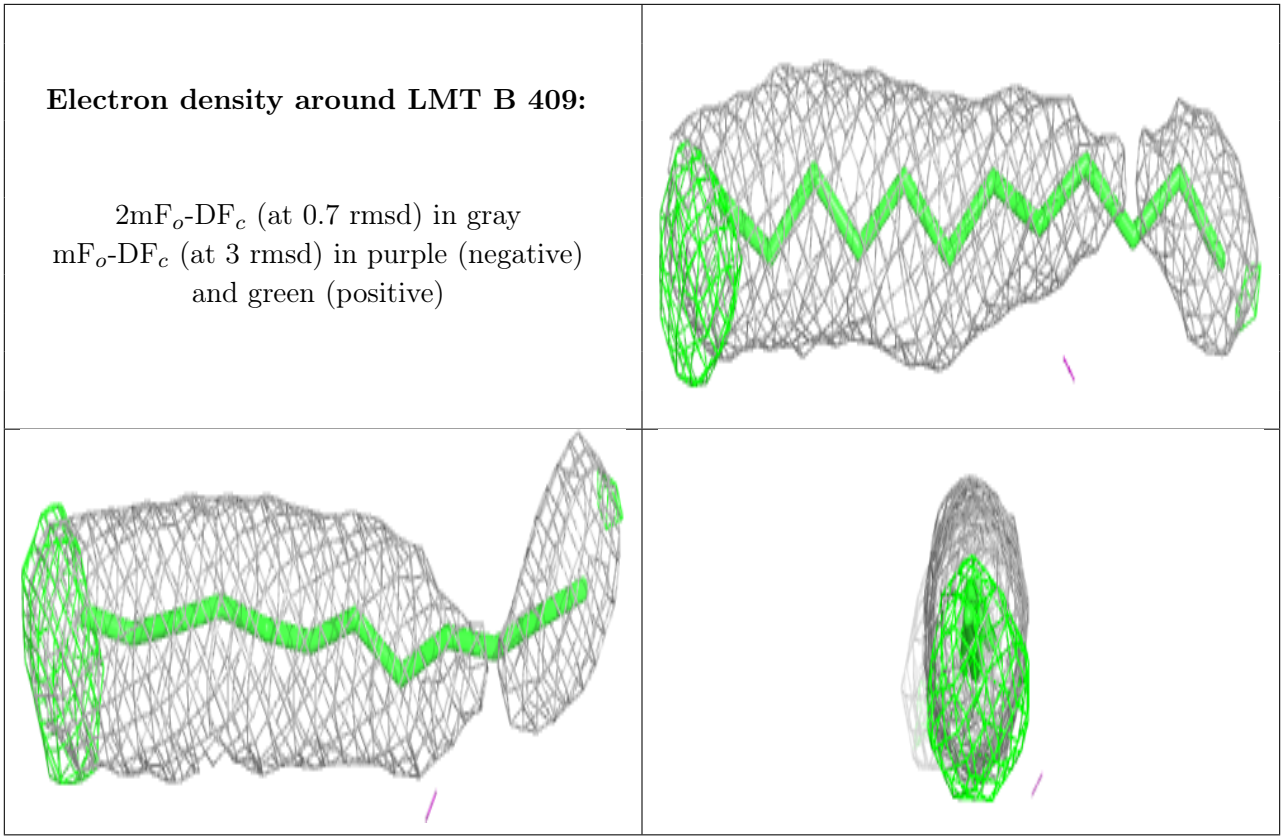






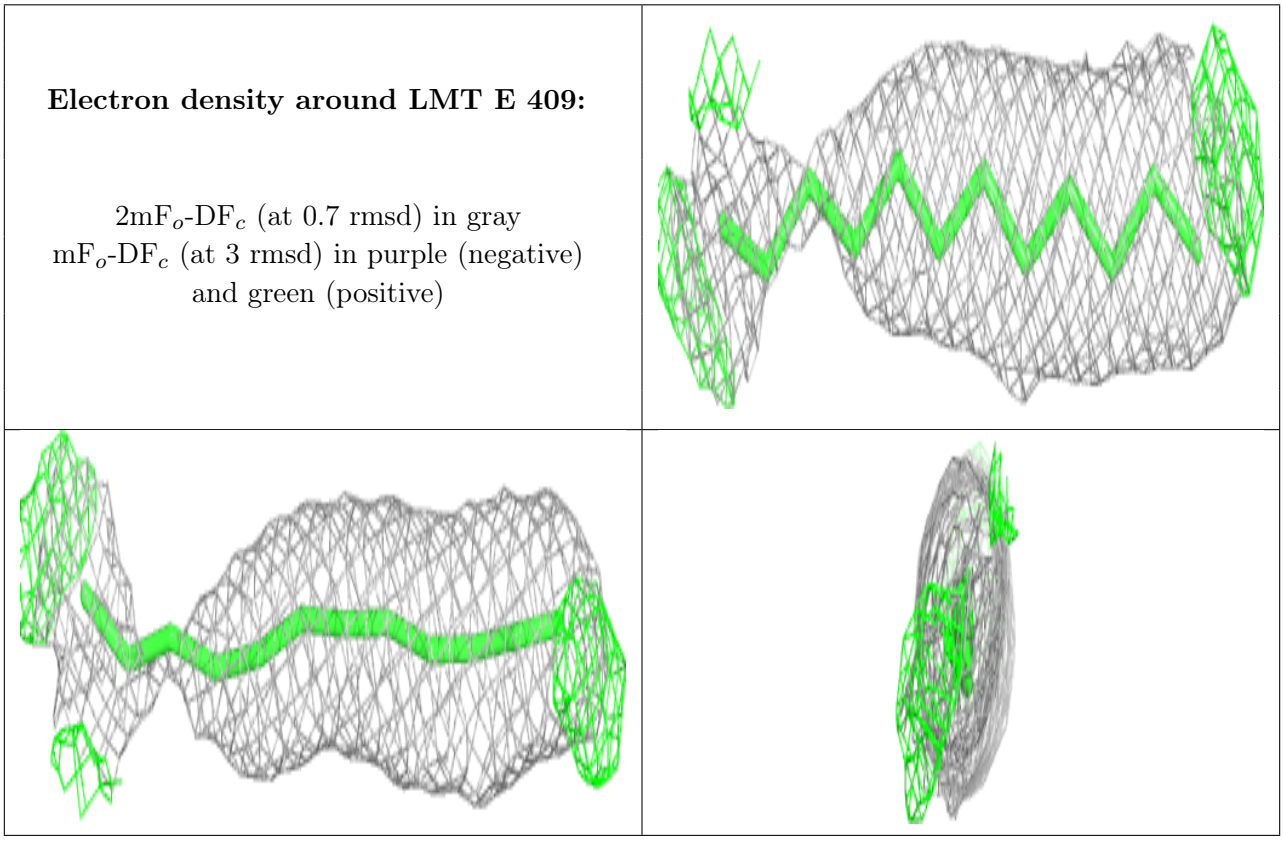
Electron density around LMT B 409:

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



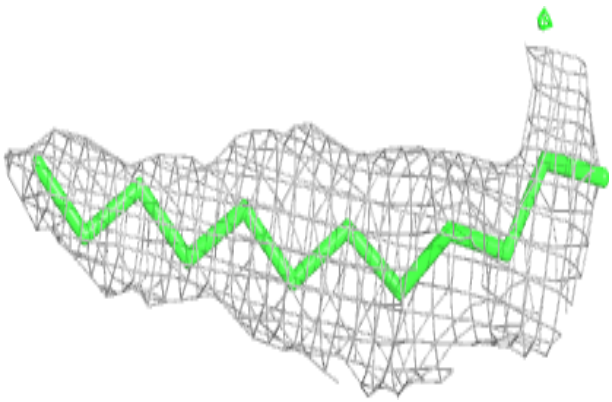
Electron density around LMT E 409:

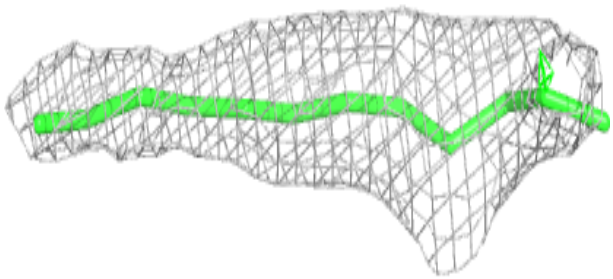
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLC B 405:

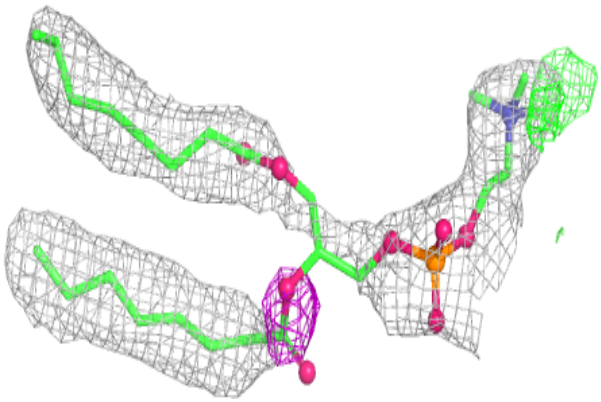
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

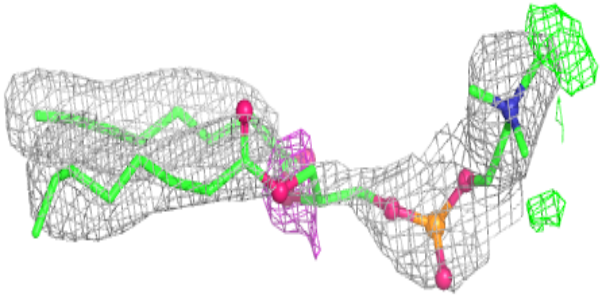


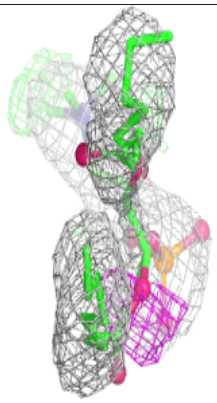


Electron density around PLC B 403:

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

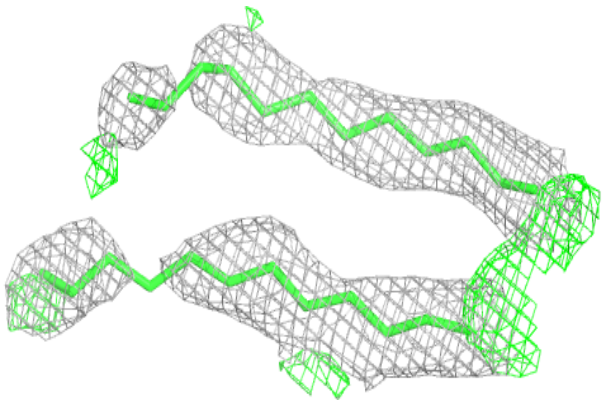


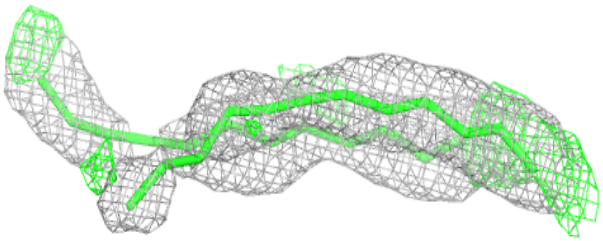


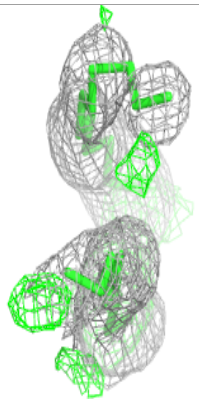


Electron density around PLC B 401:

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

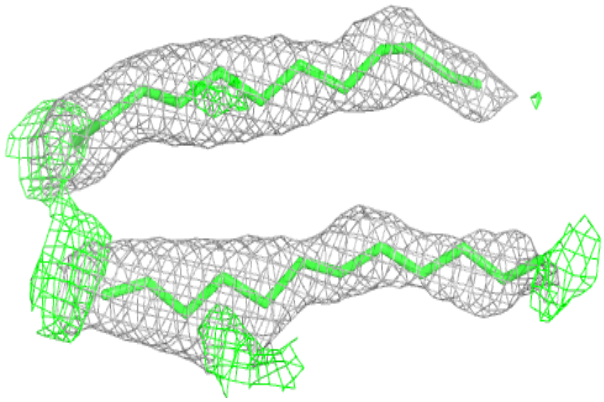


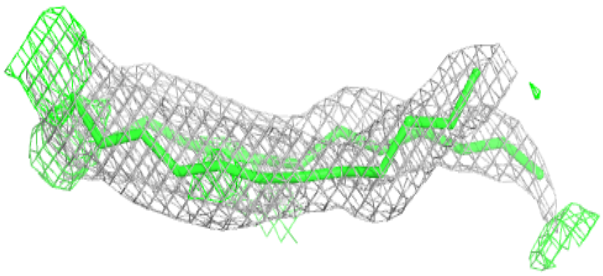


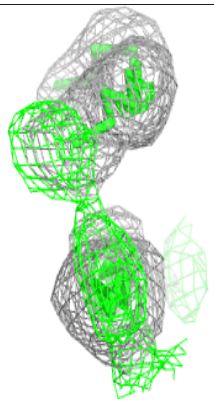


Electron density around PLC B 404:

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

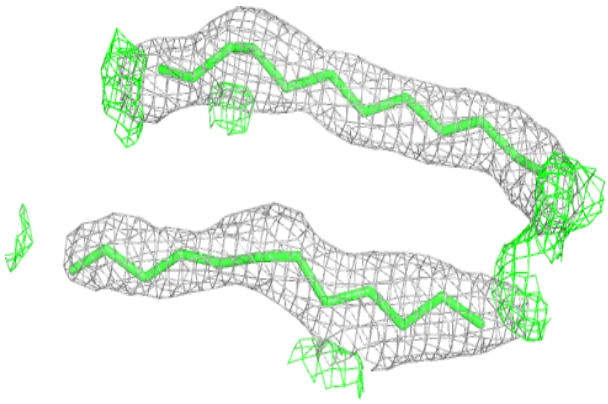


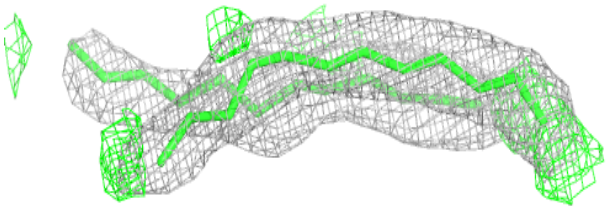


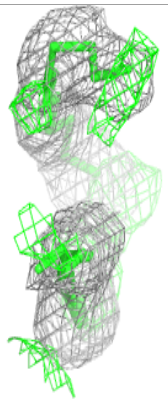


Electron density around PLC E 404:

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

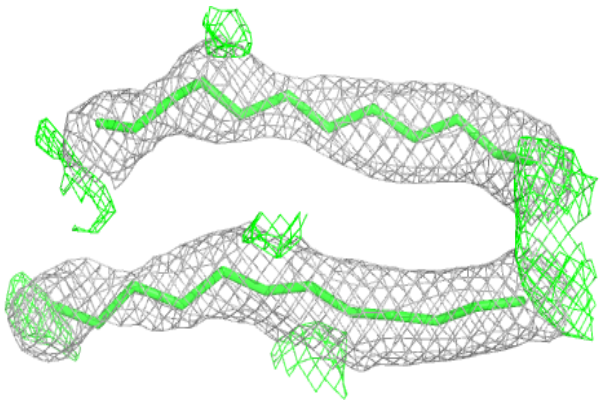


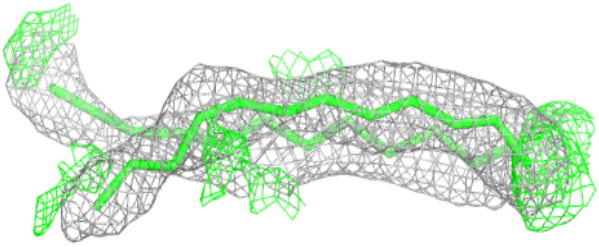


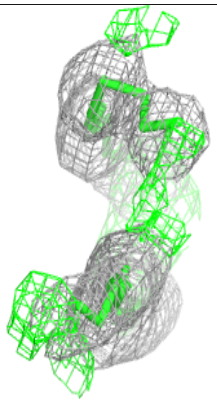


Electron density around PLC C 403:

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

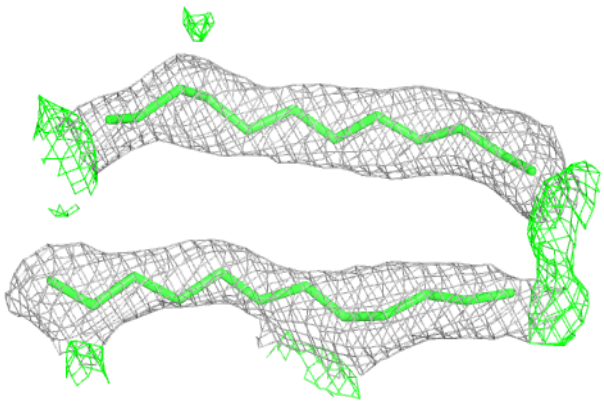


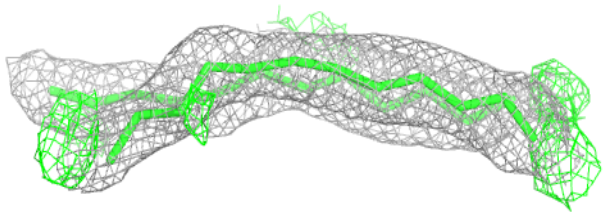


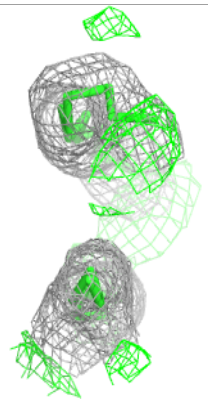


Electron density around PLC D 403:

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

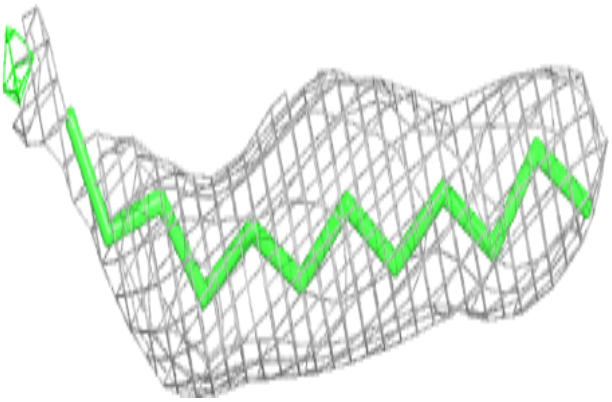


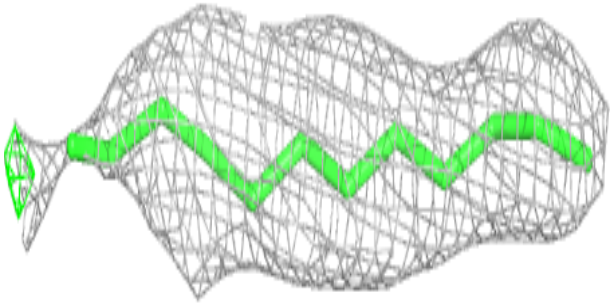


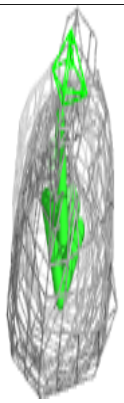


Electron density around PLC D 404:

$2mF_o$-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.