



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:23 AM UTC

PDB ID : 5MVN / pdb_00005mvn
Title : X-ray structure of the M205W mutant of GLIC in complex with propofol
Authors : Fourati, Z.; Delarue, M.
Deposited on : 2017-01-16
Resolution : 3.49 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

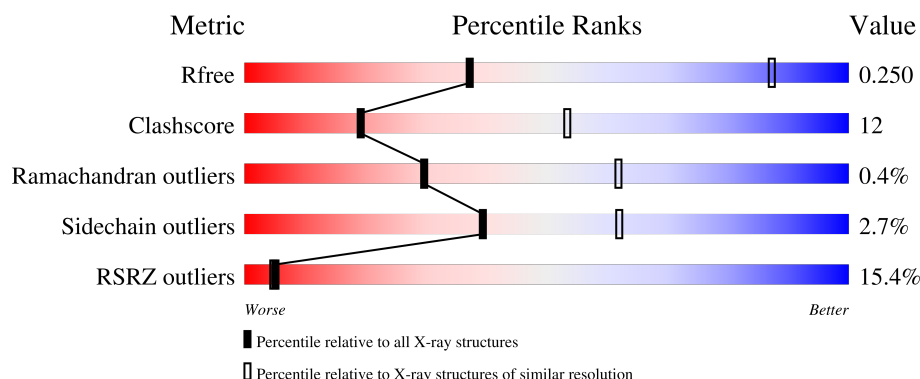
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	12% 85% 12% ..
1	B	317	10% 81% 17% .
1	C	317	18% 82% 16% ..
1	D	317	21% 86% 12% .
1	E	317	15% 81% 15% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLC	A	403	-	-	-	X
3	PLC	B	404	-	-	-	X
3	PLC	D	404	-	-	-	X
5	NA	A	409	-	-	-	X
7	PFL	B	410	-	-	X	-
7	PFL	C	407	-	-	X	-
7	PFL	D	410	-	-	X	-
7	PFL	E	408	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13210 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
1	A	311	Total	C	N	O	S	0	0	0
			2531	1670	405	453	3			
1	B	311	Total	C	N	O	S	0	0	0
			2531	1670	405	453	3			
1	C	311	Total	C	N	O	S	0	0	0
			2531	1670	405	453	3			
1	D	311	Total	C	N	O	S	0	0	0
			2531	1670	405	453	3			
1	E	311	Total	C	N	O	S	0	0	0
			2531	1670	405	453	3			

There are 5 discrepancies between the modelled and reference sequences:

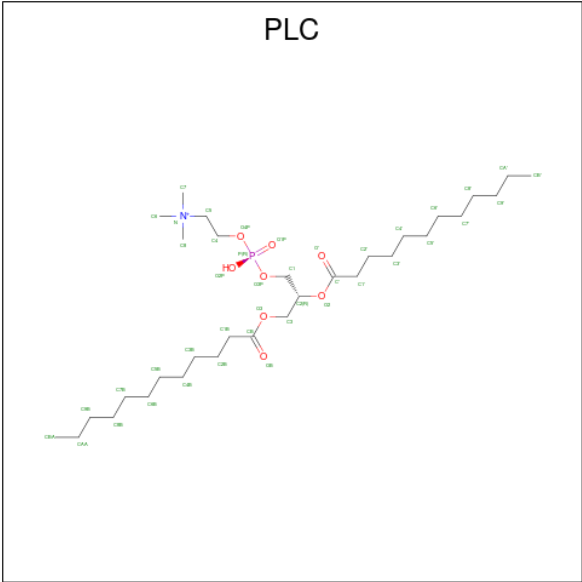
Chain	Residue	Modelled	Actual	Comment	Reference
A	205	TRP	MET	engineered mutation	UNP Q7NDN8
B	205	TRP	MET	engineered mutation	UNP Q7NDN8
C	205	TRP	MET	engineered mutation	UNP Q7NDN8
D	205	TRP	MET	engineered mutation	UNP Q7NDN8
E	205	TRP	MET	engineered mutation	UNP Q7NDN8

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



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

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

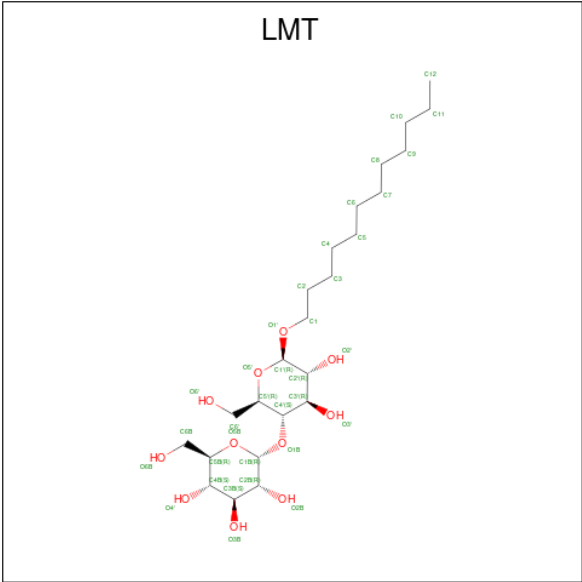
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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 (CCD ID: NA) (formula: Na).

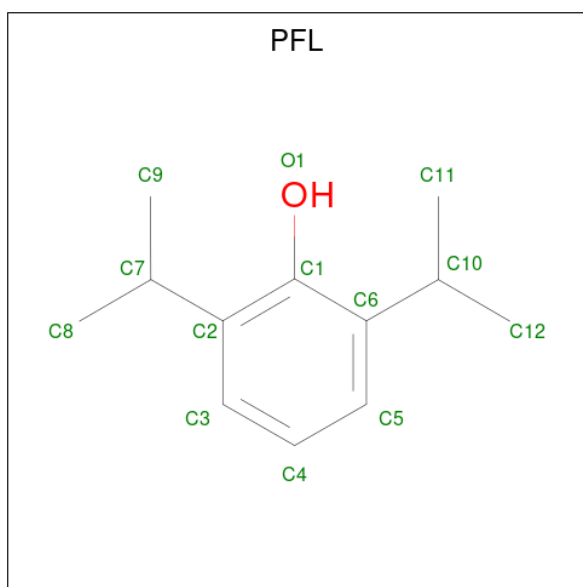
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0

- Molecule 6 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 7 is 2,6-BIS(1-METHYLETHYL)PHENOL (CCD ID: PFL) (formula: C₁₂H₁₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	12	1		
7	C	1	Total	C	O	0	0
			13	12	1		
7	D	1	Total	C	O	0	0
			13	12	1		
7	E	1	Total	C	O	0	0
			13	12	1		

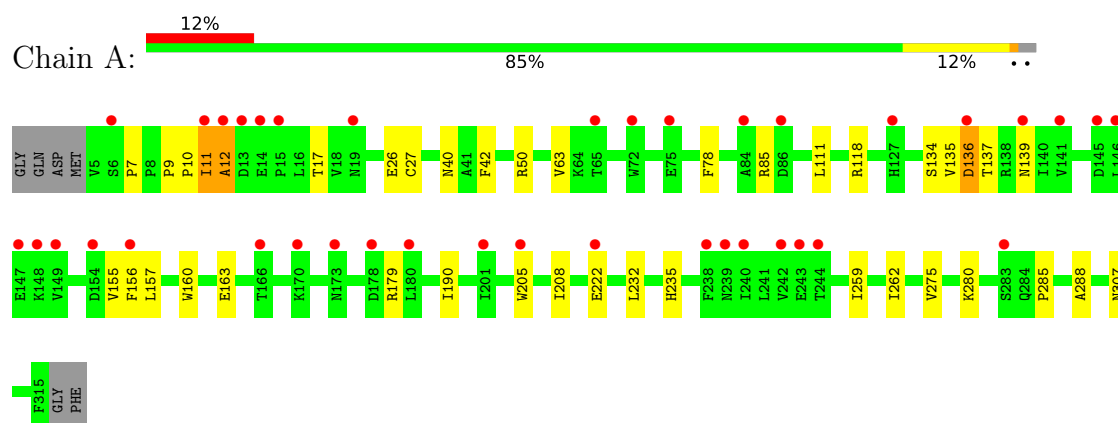
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	O	0	0
			5	5		
8	B	5	Total	O	0	0
			5	5		
8	C	6	Total	O	0	0
			6	6		
8	D	5	Total	O	0	0
			5	5		
8	E	7	Total	O	0	0
			7	7		

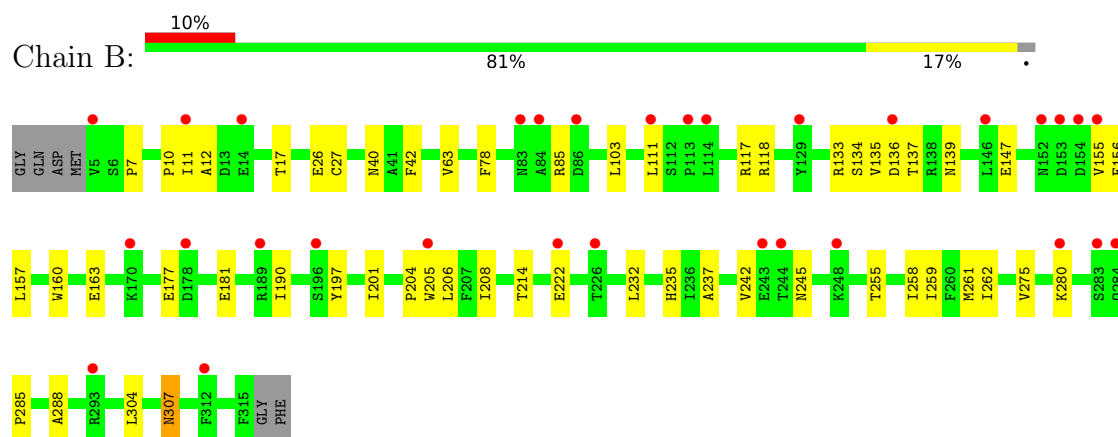
3 Residue-property plots [i](#)

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.

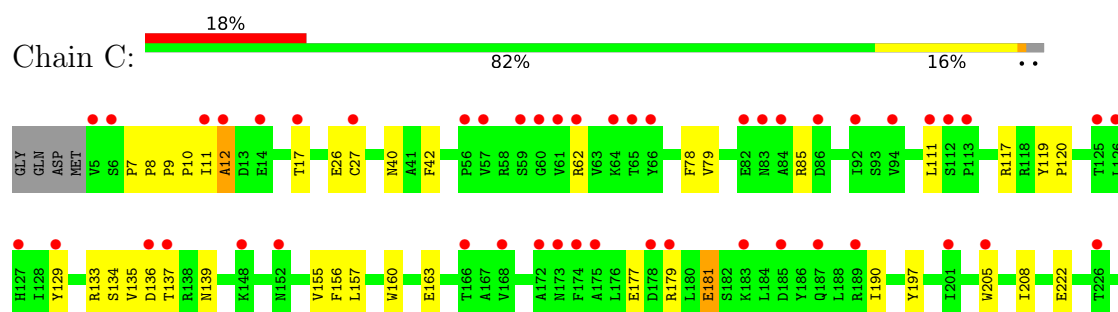
• Molecule 1: Proton-gated ion channel



• Molecule 1: Proton-gated ion channel

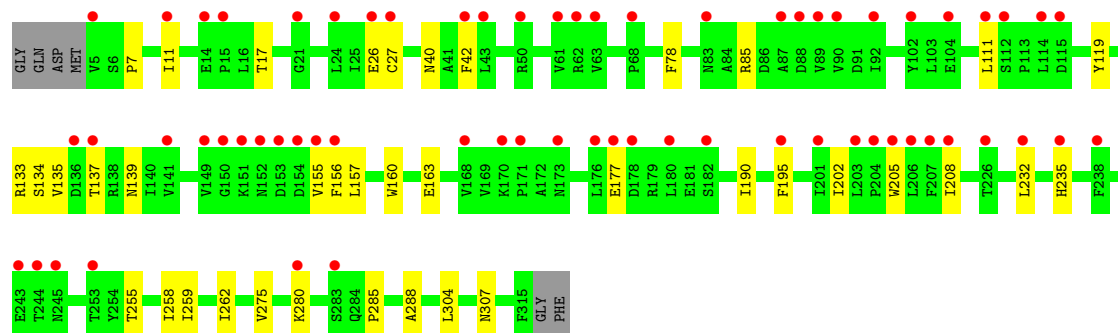
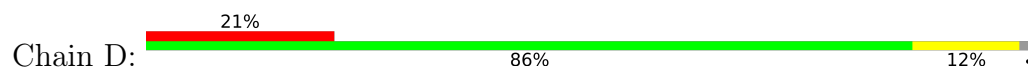


• Molecule 1: Proton-gated ion channel

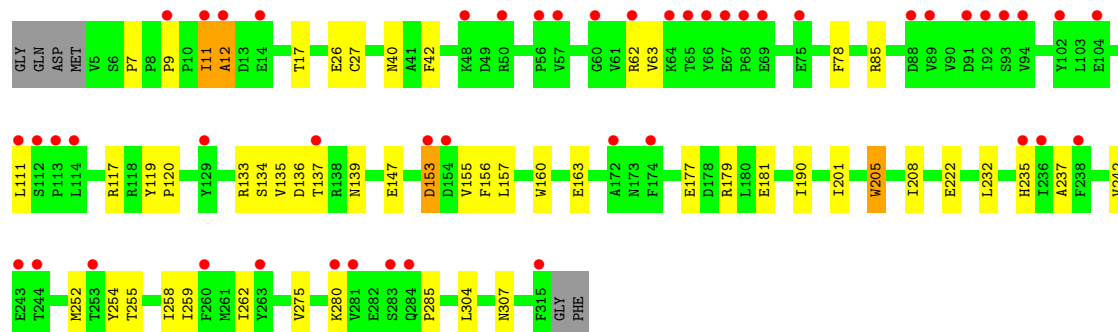
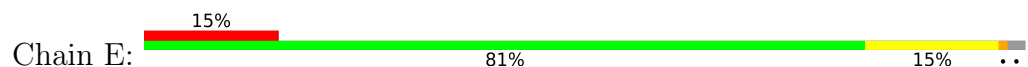




- Molecule 1: Proton-gated ion channel



- Molecule 1: Proton-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.23Å 132.47Å 159.76Å 90.00° 102.50° 90.00°	Depositor
Resolution (Å)	49.28 – 3.49 49.28 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.28-3.49) 99.1 (49.28-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.218 , 0.232 0.229 , 0.250	Depositor DCC
R_{free} test set	2365 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13210	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.77	0/2601	1.21	2/3558 (0.1%)
1	B	0.75	0/2601	1.24	3/3558 (0.1%)
1	C	0.78	0/2601	1.21	1/3558 (0.0%)
1	D	0.77	0/2601	1.21	2/3558 (0.1%)
1	E	0.76	0/2601	1.22	3/3558 (0.1%)
All	All	0.76	0/13005	1.22	11/17790 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	ILE	N-CA-C	-14.19	90.93	109.80
1	B	206	LEU	N-CA-C	-11.33	99.28	113.55
1	B	204	PRO	CA-C-N	-10.18	108.01	123.17
1	B	204	PRO	C-N-CA	-10.18	108.01	123.17
1	E	11	ILE	N-CA-C	-9.36	97.35	109.80
1	A	12	ALA	N-CA-C	-6.59	99.37	109.65
1	A	136	ASP	CA-CB-CG	-5.89	106.71	112.60
1	D	11	ILE	CB-CA-C	-5.61	103.53	111.28
1	E	153	ASP	N-CA-CB	-5.39	101.92	110.28
1	E	9	PRO	O-C-N	5.31	123.75	121.31
1	C	12	ALA	N-CA-C	-5.22	100.93	109.80

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	2531	0	2546	50	0
1	B	2531	0	2546	70	0
1	C	2531	0	2546	71	2
1	D	2531	0	2546	50	0
1	E	2531	0	2546	69	2
2	A	8	0	6	0	0
2	B	12	0	9	0	0
2	C	4	0	3	0	0
2	D	8	0	6	0	0
2	E	8	0	6	0	0
3	A	94	0	157	5	0
3	B	70	0	111	17	0
3	C	46	0	65	8	0
3	D	94	0	157	12	0
3	E	46	0	65	0	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	0	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	24	0	46	2	0
6	B	12	0	23	2	0
6	C	12	0	23	1	0
6	D	12	0	23	0	0
6	E	12	0	23	2	0
7	B	13	0	17	33	0
7	C	13	0	17	25	0
7	D	13	0	18	23	0
7	E	13	0	17	27	0
8	A	5	0	0	0	0
8	B	5	0	0	1	0
8	C	6	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	5	0	0	0	0
8	E	7	0	0	0	0
All	All	13210	0	13522	312	2

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 12.

All (312) 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)
3:B:402:PLC:H6A2	7:B:410:PFL:C11	1.41	1.49
1:D:258:ILE:HD13	7:D:410:PFL:C12	1.46	1.45
1:A:11:ILE:CG2	1:A:50:ARG:NH1	1.83	1.39
1:D:258:ILE:CD1	7:D:410:PFL:H122	1.55	1.37
1:C:258:ILE:HD12	7:C:407:PFL:C9	1.53	1.36
1:C:258:ILE:CD1	7:C:407:PFL:C9	2.05	1.34
1:B:258:ILE:CD1	7:B:410:PFL:C12	2.06	1.33
1:A:11:ILE:HG21	1:A:50:ARG:NH1	1.00	1.30
1:B:258:ILE:CD1	7:B:410:PFL:H123	1.66	1.23
3:B:402:PLC:C6B	7:B:410:PFL:C11	2.21	1.18
3:B:402:PLC:C6B	7:B:410:PFL:H112	1.71	1.18
1:B:258:ILE:HD13	7:B:410:PFL:H123	1.18	1.13
1:B:26:GLU:HG3	8:C:502:HOH:O	1.49	1.12
3:D:403:PLC:H6A2	7:D:410:PFL:C11	1.81	1.10
1:B:258:ILE:HD12	7:B:410:PFL:C12	1.77	1.10
1:C:258:ILE:CD1	7:C:407:PFL:H91	1.78	1.08
1:C:280:LYS:HE2	1:C:288:ALA:HB3	1.33	1.07
1:B:258:ILE:HD13	7:B:410:PFL:C12	1.78	1.05
1:C:197:TYR:HD1	7:C:407:PFL:H121	1.18	1.05
1:C:258:ILE:CD1	7:C:407:PFL:H93	1.78	1.04
1:C:120:PRO:HD3	7:C:407:PFL:O1	1.59	1.02
3:B:402:PLC:C4B	7:B:410:PFL:H111	1.88	1.02
1:B:26:GLU:CG	8:C:502:HOH:O	2.06	1.01
1:D:280:LYS:HE2	1:D:288:ALA:HB3	1.41	1.00
1:E:242:VAL:CG1	7:E:408:PFL:H82	1.92	1.00
1:C:280:LYS:HE2	1:C:288:ALA:CB	1.91	0.99
1:C:258:ILE:HD13	7:C:407:PFL:H93	1.43	0.97
1:D:258:ILE:HD13	7:D:410:PFL:H122	0.98	0.96
1:E:201:ILE:HD13	7:E:408:PFL:H91	1.47	0.96
1:A:11:ILE:HG21	1:A:50:ARG:CZ	1.95	0.96
3:D:403:PLC:H6A2	7:D:410:PFL:H112	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ARG:HH21	1:C:179:ARG:CZ	1.78	0.94
1:B:258:ILE:CD1	7:B:410:PFL:H121	1.97	0.94
1:C:258:ILE:HD12	7:C:407:PFL:H92	1.48	0.94
1:C:133:ARG:HH21	1:C:179:ARG:NE	1.68	0.92
3:B:402:PLC:H6A2	7:B:410:PFL:H112	0.93	0.90
3:B:402:PLC:C6B	7:B:410:PFL:H111	2.02	0.90
1:E:120:PRO:HG3	7:E:408:PFL:O1	1.72	0.89
3:D:403:PLC:H6A2	7:D:410:PFL:H111	1.55	0.88
1:B:133:ARG:HA	1:B:181:GLU:OE2	1.73	0.88
3:B:402:PLC:H6A2	7:B:410:PFL:H111	1.56	0.87
3:D:403:PLC:H4A2	7:D:410:PFL:H111	1.58	0.86
1:E:242:VAL:HG13	7:E:408:PFL:H82	1.57	0.86
1:E:201:ILE:HG21	7:E:408:PFL:H93	1.54	0.86
1:E:254:TYR:CD1	7:E:408:PFL:H121	2.11	0.86
1:C:197:TYR:CD1	7:C:407:PFL:H121	2.09	0.85
1:A:280:LYS:HE2	1:A:288:ALA:CB	2.07	0.85
1:C:258:ILE:HD13	7:C:407:PFL:C9	1.94	0.84
1:E:242:VAL:HG11	7:E:408:PFL:H82	1.60	0.84
1:B:258:ILE:HD12	7:B:410:PFL:H122	1.60	0.84
1:E:280:LYS:HE3	1:E:285:PRO:HB3	1.60	0.84
1:B:280:LYS:HZ2	1:B:285:PRO:HB3	1.42	0.83
1:C:258:ILE:HD12	7:C:407:PFL:H93	1.48	0.82
1:D:258:ILE:CD1	7:D:410:PFL:C12	2.32	0.82
3:C:401:PLC:H6A2	7:C:407:PFL:H82	1.60	0.81
1:E:201:ILE:HD13	7:E:408:PFL:C9	2.10	0.81
3:B:402:PLC:H4A2	7:B:410:PFL:H111	1.61	0.80
1:C:133:ARG:HD3	1:C:179:ARG:HE	1.45	0.80
1:E:242:VAL:HG13	7:E:408:PFL:C8	2.12	0.79
1:E:133:ARG:HA	1:E:181:GLU:OE1	1.83	0.79
1:A:11:ILE:CG2	1:A:50:ARG:HH11	1.91	0.79
1:B:156:PHE:CE1	1:C:111:LEU:HD21	2.19	0.78
3:C:401:PLC:C6B	7:C:407:PFL:H82	2.14	0.78
1:C:133:ARG:NH2	1:C:179:ARG:CZ	2.46	0.77
1:D:258:ILE:HD12	7:D:410:PFL:H122	1.62	0.77
1:A:111:LEU:HD21	1:E:156:PHE:CE1	2.19	0.77
1:B:201:ILE:HG21	7:B:410:PFL:H93	1.67	0.77
1:C:197:TYR:HD1	7:C:407:PFL:C12	1.97	0.76
1:D:280:LYS:CE	1:D:288:ALA:HB3	2.15	0.76
1:D:255:THR:HG21	7:D:410:PFL:H82	1.68	0.76
1:E:201:ILE:HG21	7:E:408:PFL:C9	2.16	0.75
1:A:280:LYS:HE2	1:A:288:ALA:HB1	1.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:403:PLC:C4B	7:D:410:PFL:H111	2.16	0.74
1:D:133:ARG:HH12	1:D:177:GLU:HB2	1.52	0.73
1:C:156:PHE:CE1	1:D:111:LEU:HD21	2.24	0.73
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.54	0.72
1:E:119:TYR:HE1	7:E:408:PFL:H83	1.54	0.72
1:B:78:PHE:HE2	1:B:85:ARG:HD3	1.55	0.72
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.55	0.71
1:A:156:PHE:CE1	1:B:111:LEU:HD21	2.25	0.71
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.57	0.70
1:A:11:ILE:CG2	1:A:50:ARG:HH12	1.75	0.70
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.56	0.70
1:E:254:TYR:CE1	7:E:408:PFL:H121	2.27	0.69
1:A:280:LYS:HE2	1:A:288:ALA:HB3	1.75	0.69
1:B:205:TRP:CH2	1:B:259:ILE:HD13	2.29	0.68
1:B:258:ILE:HD12	7:B:410:PFL:H123	1.53	0.67
1:B:280:LYS:NZ	1:B:285:PRO:HB3	2.09	0.67
1:D:156:PHE:CE1	1:E:111:LEU:HD21	2.29	0.67
1:B:133:ARG:CA	1:B:181:GLU:OE2	2.42	0.67
1:D:119:TYR:CE1	7:D:410:PFL:H81	2.30	0.67
1:A:11:ILE:HG21	1:A:50:ARG:HH12	0.84	0.67
1:B:133:ARG:HH12	1:B:177:GLU:HB2	1.59	0.66
1:E:242:VAL:CG1	7:E:408:PFL:C8	2.72	0.66
3:D:403:PLC:C6B	7:D:410:PFL:H111	2.25	0.66
1:C:133:ARG:HH12	1:C:177:GLU:HB2	1.61	0.66
3:B:402:PLC:H4A1	7:B:410:PFL:H111	1.75	0.65
3:C:401:PLC:H6A2	7:C:407:PFL:C8	2.26	0.65
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.32	0.65
1:B:242:VAL:HG11	7:B:410:PFL:H82	1.78	0.65
1:C:133:ARG:NH2	1:C:179:ARG:NH1	2.45	0.65
1:B:205:TRP:CZ2	1:B:259:ILE:HD13	2.33	0.64
1:C:133:ARG:HH21	1:C:179:ARG:NH1	1.95	0.64
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.33	0.64
1:B:237:ALA:HA	6:B:408:LMT:H92	1.79	0.64
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.33	0.63
1:B:10:PRO:HB2	1:B:12:ALA:O	1.97	0.63
1:B:63:VAL:HG11	1:C:136:ASP:OD2	1.99	0.63
1:B:242:VAL:CG1	7:B:410:PFL:H82	2.28	0.63
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.34	0.63
1:A:10:PRO:HB2	1:A:12:ALA:O	1.99	0.63
1:C:10:PRO:HB2	1:C:12:ALA:O	1.97	0.63
1:D:258:ILE:HD13	7:D:410:PFL:H123	1.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.33	0.62
1:E:119:TYR:CE1	7:E:408:PFL:H83	2.35	0.62
1:A:111:LEU:CD2	1:E:156:PHE:HE1	2.13	0.61
1:B:156:PHE:HE1	1:C:111:LEU:CD2	2.13	0.61
1:A:11:ILE:HD13	1:A:50:ARG:HH22	1.65	0.60
1:D:280:LYS:CE	1:D:288:ALA:CB	2.79	0.60
3:C:401:PLC:C6B	7:C:407:PFL:C8	2.78	0.60
1:E:237:ALA:HA	6:E:407:LMT:H92	1.83	0.60
3:B:402:PLC:C5B	7:B:410:PFL:H111	2.32	0.60
1:C:237:ALA:HA	6:C:406:LMT:H92	1.84	0.59
3:D:403:PLC:C6B	7:D:410:PFL:C11	2.70	0.59
1:B:280:LYS:HE2	1:B:288:ALA:CB	2.32	0.59
1:D:280:LYS:HE2	1:D:288:ALA:CB	2.25	0.58
3:D:403:PLC:H6A1	7:D:410:PFL:H121	1.85	0.58
1:E:205:TRP:CH2	1:E:259:ILE:HD11	2.38	0.58
1:E:258:ILE:HD12	7:E:408:PFL:H123	1.84	0.58
1:C:156:PHE:HE1	1:D:111:LEU:CD2	2.17	0.58
1:D:134:SER:HB3	1:D:139:ASN:HA	1.85	0.58
1:B:201:ILE:CG2	7:B:410:PFL:H93	2.32	0.57
1:C:156:PHE:HE1	1:D:111:LEU:HD21	1.70	0.57
1:B:280:LYS:HE2	1:B:288:ALA:HB3	1.86	0.57
3:D:403:PLC:H6A1	7:D:410:PFL:C12	2.35	0.57
1:E:120:PRO:HD3	7:E:408:PFL:H10	1.86	0.57
1:D:205:TRP:CH2	1:D:259:ILE:CD1	2.87	0.57
1:C:120:PRO:CD	7:C:407:PFL:O1	2.44	0.57
1:E:119:TYR:HE1	7:E:408:PFL:C8	2.17	0.57
1:A:280:LYS:CE	1:A:288:ALA:CB	2.80	0.56
1:B:156:PHE:CE1	1:C:111:LEU:CD2	2.85	0.56
1:A:134:SER:HB3	1:A:139:ASN:HA	1.86	0.56
1:B:255:THR:HG21	7:B:410:PFL:H83	1.87	0.56
1:C:205:TRP:O	1:C:208:ILE:HG13	2.05	0.56
1:C:280:LYS:HE2	1:C:288:ALA:HB1	1.81	0.56
1:B:103:LEU:HD22	1:C:179:ARG:NH1	2.21	0.56
1:A:280:LYS:CD	1:A:288:ALA:CB	2.84	0.56
1:B:156:PHE:HE1	1:C:111:LEU:HD21	1.71	0.56
1:D:205:TRP:CH2	1:D:259:ILE:HD11	2.41	0.56
1:E:133:ARG:CA	1:E:181:GLU:OE1	2.51	0.56
1:D:202:ILE:HG12	7:D:410:PFL:H113	1.86	0.56
1:A:111:LEU:HD21	1:E:156:PHE:HE1	1.68	0.56
1:A:11:ILE:CG2	1:A:50:ARG:CZ	2.71	0.56
1:A:280:LYS:CE	1:A:288:ALA:HB3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:HE1	1:B:111:LEU:CD2	2.19	0.55
1:D:205:TRP:O	1:D:208:ILE:HG13	2.06	0.55
1:C:134:SER:HB3	1:C:139:ASN:HA	1.87	0.55
1:A:136:ASP:OD1	1:A:179:ARG:CZ	2.54	0.55
1:A:205:TRP:CH2	1:A:259:ILE:CD1	2.90	0.55
1:A:205:TRP:O	1:A:208:ILE:HG13	2.07	0.55
1:C:205:TRP:CH2	1:C:259:ILE:CD1	2.90	0.55
1:B:134:SER:HB3	1:B:139:ASN:HA	1.89	0.55
1:B:235:HIS:HE1	1:B:262:ILE:HB	1.72	0.55
1:B:118:ARG:HH12	3:B:402:PLC:H72	1.72	0.55
1:A:136:ASP:OD2	1:E:63:VAL:HG11	2.07	0.54
1:C:258:ILE:HD11	7:C:407:PFL:H91	1.80	0.54
1:E:133:ARG:HH12	1:E:177:GLU:HB2	1.72	0.54
1:E:136:ASP:OD1	1:E:179:ARG:NH2	2.41	0.54
1:E:205:TRP:O	1:E:208:ILE:HG13	2.07	0.54
1:E:134:SER:HB3	1:E:139:ASN:HA	1.89	0.54
1:C:235:HIS:HE1	1:C:262:ILE:HB	1.73	0.54
1:E:120:PRO:CG	7:E:408:PFL:O1	2.51	0.54
1:C:255:THR:HA	7:C:407:PFL:H92	1.90	0.53
1:A:156:PHE:CE1	1:B:111:LEU:CD2	2.91	0.53
1:A:111:LEU:CD2	1:E:156:PHE:CE1	2.87	0.53
1:C:133:ARG:NH2	1:C:179:ARG:NE	2.49	0.53
1:E:120:PRO:CD	7:E:408:PFL:H10	2.38	0.53
1:C:276:GLN:O	1:C:280:LYS:HG2	2.09	0.53
1:D:119:TYR:HE1	7:D:410:PFL:H81	1.72	0.53
1:D:235:HIS:HE1	1:D:262:ILE:HB	1.74	0.53
1:E:62:ARG:HD2	1:E:63:VAL:HG23	1.90	0.53
1:E:133:ARG:CB	1:E:181:GLU:OE1	2.57	0.52
1:E:201:ILE:CD1	7:E:408:PFL:C9	2.85	0.52
1:C:26:GLU:HB2	1:C:40:ASN:HB3	1.92	0.52
1:E:205:TRP:CH2	1:E:259:ILE:CD1	2.92	0.52
1:A:26:GLU:HB2	1:A:40:ASN:HB3	1.92	0.52
1:B:133:ARG:CB	1:B:181:GLU:OE2	2.57	0.52
1:D:26:GLU:HB2	1:D:40:ASN:HB3	1.91	0.52
1:A:136:ASP:OD1	1:A:179:ARG:NH2	2.43	0.51
1:A:235:HIS:HE1	1:A:262:ILE:HB	1.75	0.51
1:C:119:TYR:CE1	7:C:407:PFL:H113	2.46	0.51
1:E:26:GLU:HB2	1:E:40:ASN:HB3	1.91	0.51
1:E:136:ASP:OD1	1:E:179:ARG:CZ	2.59	0.51
1:B:26:GLU:OE1	1:C:111:LEU:HD22	2.10	0.51
1:B:242:VAL:CG1	7:B:410:PFL:C8	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:THR:HG23	7:D:410:PFL:C3	2.41	0.50
1:B:26:GLU:HB2	1:B:40:ASN:HB3	1.93	0.50
1:B:258:ILE:HD11	7:B:410:PFL:H121	1.88	0.50
1:E:235:HIS:CD2	1:E:235:HIS:C	2.90	0.50
1:D:156:PHE:HE1	1:E:111:LEU:CD2	2.25	0.50
1:E:235:HIS:HE1	1:E:262:ILE:HB	1.76	0.49
3:B:403:PLC:HT'2	1:C:275:VAL:HG22	1.95	0.49
3:B:402:PLC:H4A2	7:B:410:PFL:C11	2.35	0.49
1:E:11:ILE:O	1:E:12:ALA:C	2.55	0.49
1:A:232:LEU:HD21	1:E:208:ILE:HG22	1.95	0.49
1:C:120:PRO:HG3	7:C:407:PFL:H10	1.95	0.49
1:A:235:HIS:C	1:A:235:HIS:CD2	2.92	0.48
1:B:235:HIS:C	1:B:235:HIS:CD2	2.91	0.48
1:B:201:ILE:O	1:B:205:TRP:HD1	1.96	0.48
1:B:205:TRP:HH2	1:B:259:ILE:HD13	1.77	0.48
1:C:119:TYR:HE1	7:C:407:PFL:H113	1.77	0.48
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.95	0.48
1:C:235:HIS:C	1:C:235:HIS:CD2	2.92	0.48
1:B:242:VAL:HG11	7:B:410:PFL:C8	2.43	0.48
1:E:205:TRP:HZ3	7:E:408:PFL:HC3	1.79	0.48
1:A:280:LYS:CD	1:A:288:ALA:HB3	2.44	0.48
1:C:280:LYS:CE	1:C:288:ALA:CB	2.79	0.48
3:C:401:PLC:H6A1	7:C:407:PFL:H82	1.91	0.48
1:C:133:ARG:HD3	1:C:179:ARG:NE	2.24	0.48
1:D:235:HIS:C	1:D:235:HIS:CD2	2.91	0.47
1:C:26:GLU:OE1	1:D:111:LEU:HD22	2.14	0.47
1:E:258:ILE:CD1	7:E:408:PFL:H123	2.44	0.47
3:C:401:PLC:H6A1	7:C:407:PFL:C8	2.44	0.47
1:E:201:ILE:HB	7:E:408:PFL:H92	1.96	0.47
1:B:205:TRP:CZ2	1:B:259:ILE:CD1	2.97	0.47
1:D:280:LYS:HE3	1:D:288:ALA:CB	2.45	0.47
3:C:401:PLC:H1'1	3:C:402:PLC:H8'2	1.96	0.47
1:D:7:PRO:HG3	1:D:135:VAL:HG21	1.95	0.47
3:A:402:PLC:H4A2	3:A:402:PLC:H5'1	1.97	0.47
1:C:7:PRO:HG3	1:C:135:VAL:HG21	1.96	0.47
1:A:7:PRO:HG3	1:A:135:VAL:HG21	1.97	0.46
1:A:63:VAL:HG21	1:B:136:ASP:CG	2.40	0.46
1:B:258:ILE:HD13	7:B:410:PFL:H121	1.75	0.46
3:B:402:PLC:H6A1	7:B:410:PFL:C11	2.35	0.46
1:A:111:LEU:HD22	1:E:26:GLU:OE1	2.15	0.46
3:A:402:PLC:H6'2	3:A:404:PLC:H2'2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:402:PLC:C4B	7:B:410:PFL:C11	2.78	0.46
1:C:7:PRO:CG	1:C:137:THR:OG1	2.64	0.46
1:B:27:CYS:SG	1:B:157:LEU:HD13	2.56	0.46
1:B:208:ILE:HG22	1:C:232:LEU:HD21	1.98	0.46
1:E:7:PRO:CG	1:E:137:THR:OG1	2.64	0.45
1:A:208:ILE:HG22	1:B:232:LEU:HD21	1.98	0.45
1:B:103:LEU:HD22	1:C:179:ARG:HH11	1.80	0.45
1:E:7:PRO:HG3	1:E:135:VAL:HG21	1.98	0.45
1:A:7:PRO:CG	1:A:137:THR:OG1	2.64	0.45
3:D:404:PLC:HT'2	1:E:275:VAL:HG22	1.98	0.45
1:C:133:ARG:NE	1:C:181:GLU:OE1	2.49	0.45
1:C:208:ILE:HG22	1:D:232:LEU:HD21	1.97	0.45
1:C:235:HIS:CE1	1:C:262:ILE:HB	2.52	0.45
1:B:7:PRO:CG	1:B:137:THR:OG1	2.65	0.44
1:D:7:PRO:CG	1:D:137:THR:OG1	2.66	0.44
1:C:156:PHE:CE1	1:D:111:LEU:CD2	2.92	0.44
1:E:235:HIS:CE1	1:E:262:ILE:HB	2.53	0.44
1:B:197:TYR:HD1	7:B:410:PFL:H91	1.83	0.44
1:D:195:PHE:CZ	1:E:252:MET:HG2	2.53	0.44
6:A:411:LMT:H61	6:E:407:LMT:H81	1.98	0.44
1:D:156:PHE:CE1	1:E:111:LEU:CD2	2.96	0.44
1:D:275:VAL:HG22	3:D:401:PLC:HT'2	1.98	0.44
1:A:27:CYS:SG	1:A:157:LEU:HD13	2.58	0.44
1:C:7:PRO:HG3	1:C:137:THR:OG1	2.18	0.44
1:D:280:LYS:HE3	1:D:288:ALA:HB1	1.98	0.44
1:A:205:TRP:CH2	1:A:259:ILE:HD11	2.53	0.43
1:B:205:TRP:HZ2	1:B:259:ILE:CD1	2.32	0.43
1:D:235:HIS:CE1	1:D:262:ILE:HB	2.54	0.43
1:C:27:CYS:SG	1:C:157:LEU:HD13	2.58	0.43
1:E:7:PRO:HG3	1:E:137:THR:OG1	2.18	0.43
1:D:27:CYS:SG	1:D:157:LEU:HD13	2.58	0.43
1:E:27:CYS:SG	1:E:157:LEU:HD13	2.58	0.43
1:E:201:ILE:CB	7:E:408:PFL:H92	2.49	0.43
1:A:275:VAL:HG22	3:A:413:PLC:HT'2	2.01	0.43
1:D:258:ILE:HD13	7:D:410:PFL:H121	1.74	0.43
3:D:403:PLC:C6B	7:D:410:PFL:C12	2.97	0.43
1:C:280:LYS:CE	1:C:288:ALA:HB3	2.25	0.43
1:D:208:ILE:HG22	1:E:232:LEU:HD21	2.00	0.43
1:A:118:ARG:HH12	3:A:402:PLC:H72	1.84	0.42
6:A:411:LMT:H102	6:B:408:LMT:H121	2.00	0.42
1:E:133:ARG:HB2	1:E:181:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HG13	7:B:410:PFL:C8	2.49	0.42
1:E:255:THR:HG23	7:E:408:PFL:C4	2.49	0.42
1:C:205:TRP:CH2	1:C:259:ILE:HD11	2.55	0.42
1:D:202:ILE:HG23	7:D:410:PFL:H112	2.01	0.42
1:A:280:LYS:HD2	1:A:285:PRO:HA	2.00	0.42
1:B:214:THR:HG22	3:B:403:PLC:H3'1	2.00	0.42
1:B:245:ASN:ND2	8:B:501:HOH:O	2.51	0.42
1:A:26:GLU:OE1	1:B:111:LEU:HD22	2.19	0.42
1:B:160:TRP:CE3	1:B:190:ILE:HD12	2.55	0.42
1:B:7:PRO:HG3	1:B:137:THR:OG1	2.19	0.42
1:B:280:LYS:HE2	1:B:288:ALA:HB1	2.01	0.42
3:A:403:PLC:HT'2	1:B:275:VAL:HG22	2.02	0.41
1:C:258:ILE:O	1:C:262:ILE:HG13	2.20	0.41
1:D:160:TRP:CE3	1:D:190:ILE:HD12	2.55	0.41
1:E:160:TRP:CE3	1:E:190:ILE:HD12	2.55	0.41
1:E:201:ILE:CG2	7:E:408:PFL:C9	2.95	0.41
1:E:205:TRP:HH2	1:E:259:ILE:HD11	1.82	0.41
1:D:195:PHE:HZ	1:E:252:MET:HG2	1.85	0.41
3:B:402:PLC:H6A1	7:B:410:PFL:H112	1.86	0.41
3:C:401:PLC:H6'2	3:C:402:PLC:H4'2	2.02	0.41
1:D:7:PRO:HG3	1:D:137:THR:OG1	2.20	0.41
1:A:7:PRO:HG2	1:A:137:THR:OG1	2.21	0.41
1:A:7:PRO:HG3	1:A:137:THR:OG1	2.20	0.41
1:D:280:LYS:HE2	1:D:285:PRO:HA	2.02	0.41
1:C:160:TRP:CE3	1:C:190:ILE:HD12	2.55	0.41
1:E:258:ILE:O	1:E:262:ILE:HG13	2.21	0.41
1:A:160:TRP:CE3	1:A:190:ILE:HD12	2.55	0.40
1:B:258:ILE:O	1:B:262:ILE:HG13	2.20	0.40
1:A:9:PRO:HA	1:A:10:PRO:HD3	1.96	0.40
1:B:261:MET:HE1	1:B:307:ASN:OD1	2.21	0.40
1:C:79:VAL:HB	1:C:129:TYR:HB2	2.03	0.40
1:E:254:TYR:CD1	7:E:408:PFL:C12	2.94	0.40
1:D:258:ILE:O	1:D:262:ILE:HG13	2.20	0.40
1:C:8:PRO:HA	1:C:9:PRO:HD3	1.99	0.40
1:C:119:TYR:HE1	7:C:407:PFL:C11	2.34	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ARG:NH1	1:E:153:ASP:CB[4_545]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ARG:NH1	1:E:153:ASP:CG[4_545]	2.17	0.03

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	309/317 (98%)	296 (96%)	12 (4%)	1 (0%)	36	67
1	B	309/317 (98%)	295 (96%)	13 (4%)	1 (0%)	36	67
1	C	309/317 (98%)	294 (95%)	14 (4%)	1 (0%)	36	67
1	D	309/317 (98%)	296 (96%)	12 (4%)	1 (0%)	36	67
1	E	309/317 (98%)	295 (96%)	12 (4%)	2 (1%)	21	54
All	All	1545/1585 (98%)	1476 (96%)	63 (4%)	6 (0%)	30	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	12	ALA
1	E	155	VAL
1	B	155	VAL
1	C	155	VAL
1	D	155	VAL
1	A	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	280/284 (99%)	274 (98%)	6 (2%)	47	66
1	B	280/284 (99%)	271 (97%)	9 (3%)	34	59
1	C	280/284 (99%)	271 (97%)	9 (3%)	34	59
1	D	280/284 (99%)	275 (98%)	5 (2%)	51	69
1	E	280/284 (99%)	271 (97%)	9 (3%)	34	59
All	All	1400/1420 (99%)	1362 (97%)	38 (3%)	39	62

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	17	THR
1	A	42	PHE
1	A	163	GLU
1	A	222	GLU
1	A	307	ASN
1	B	11	ILE
1	B	17	THR
1	B	42	PHE
1	B	117	ARG
1	B	147	GLU
1	B	163	GLU
1	B	222	GLU
1	B	304	LEU
1	B	307	ASN
1	C	11	ILE
1	C	17	THR
1	C	42	PHE
1	C	117	ARG
1	C	163	GLU
1	C	181	GLU
1	C	222	GLU
1	C	304	LEU
1	C	307	ASN
1	D	17	THR
1	D	42	PHE
1	D	163	GLU
1	D	304	LEU
1	D	307	ASN
1	E	17	THR
1	E	42	PHE

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Mol	Chain	Res	Type
1	E	117	ARG
1	E	147	GLU
1	E	163	GLU
1	E	205	TRP
1	E	222	GLU
1	E	304	LEU
1	E	307	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	HIS
1	A	239	ASN
1	A	284	GLN
1	B	235	HIS
1	B	239	ASN
1	B	284	GLN
1	C	235	HIS
1	C	239	ASN
1	C	284	GLN
1	D	235	HIS
1	D	239	ASN
1	D	284	GLN
1	E	235	HIS
1	E	239	ASN
1	E	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 13 are monoatomic - leaving 35 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	D	401	-	22,22,41	0.51	0	20,20,49	0.54	0
3	PLC	C	401	-	33,33,41	1.08	2 (6%)	39,41,49	0.99	2 (5%)
3	PLC	B	404	-	11,11,41	0.38	0	10,10,49	0.67	0
6	LMT	D	409	-	11,11,36	0.38	0	10,10,47	0.86	0
2	ACT	B	407	-	3,3,3	1.32	0	3,3,3	0.68	0
6	LMT	A	411	-	11,11,36	0.59	0	10,10,47	0.67	0
7	PFL	E	408	-	13,13,13	0.35	0	18,18,18	1.01	2 (11%)
6	LMT	C	406	-	11,11,36	0.44	0	10,10,47	0.83	0
2	ACT	D	402	-	3,3,3	1.20	0	3,3,3	0.77	0
3	PLC	A	404	-	11,11,41	0.41	0	10,10,49	0.63	0
2	ACT	A	410	-	3,3,3	1.25	0	3,3,3	0.94	0
2	ACT	D	408	-	3,3,3	1.38	0	3,3,3	0.71	0
3	PLC	B	403	-	22,22,41	0.48	0	20,20,49	0.55	0
7	PFL	C	407	-	13,13,13	0.67	0	18,18,18	0.99	1 (5%)
7	PFL	D	410	-	13,13,13	0.37	0	18,18,18	0.87	0
3	PLC	E	403	-	11,11,41	0.40	0	10,10,49	0.64	0
6	LMT	E	407	-	11,11,36	0.44	0	10,10,47	0.85	0
6	LMT	B	408	-	11,11,36	0.46	0	10,10,47	0.78	0
3	PLC	A	403	-	22,22,41	0.47	0	20,20,49	0.58	0
3	PLC	B	402	-	33,33,41	1.12	3 (9%)	39,41,49	0.99	2 (5%)
7	PFL	B	410	-	13,13,13	0.53	0	18,18,18	1.18	3 (16%)
3	PLC	C	402	-	11,11,41	0.42	0	10,10,49	0.63	0
2	ACT	B	401	-	3,3,3	1.26	0	3,3,3	0.78	0
3	PLC	D	405	-	11,11,41	0.39	0	10,10,49	0.68	0
2	ACT	A	401	-	3,3,3	1.25	0	3,3,3	0.77	0
2	ACT	E	401	-	3,3,3	1.25	0	3,3,3	0.77	0
3	PLC	D	404	-	22,22,41	0.50	0	20,20,49	0.56	0
3	PLC	A	413	-	22,22,41	0.45	0	20,20,49	0.61	0
2	ACT	E	406	-	3,3,3	1.14	0	3,3,3	0.88	0
6	LMT	A	412	-	11,11,36	0.44	0	10,10,47	0.77	0
2	ACT	C	405	-	3,3,3	1.16	0	3,3,3	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	B	409	-	3,3,3	1.26	0	3,3,3	0.79	0
3	PLC	A	402	-	33,33,41	1.05	2 (6%)	39,41,49	0.98	2 (5%)
3	PLC	E	402	-	33,33,41	1.09	3 (9%)	39,41,49	0.99	2 (5%)
3	PLC	D	403	-	33,33,41	1.09	2 (6%)	39,41,49	1.01	2 (5%)

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	D	401	-	-	5/18/18/45	-
3	PLC	C	401	-	-	12/37/37/45	-
3	PLC	B	404	-	-	0/9/9/45	-
6	LMT	D	409	-	-	0/9/9/61	-
6	LMT	A	411	-	-	0/9/9/61	-
7	PFL	E	408	-	-	0/8/8/8	0/1/1/1
6	LMT	C	406	-	-	0/9/9/61	-
3	PLC	A	404	-	-	0/9/9/45	-
3	PLC	B	403	-	-	4/18/18/45	-
7	PFL	C	407	-	-	0/8/8/8	0/1/1/1
7	PFL	D	410	-	-	0/8/8/8	0/1/1/1
3	PLC	E	403	-	-	0/9/9/45	-
6	LMT	E	407	-	-	0/9/9/61	-
6	LMT	B	408	-	-	0/9/9/61	-
3	PLC	B	402	-	-	13/37/37/45	-
3	PLC	A	403	-	-	3/18/18/45	-
7	PFL	B	410	-	-	0/8/8/8	0/1/1/1
3	PLC	C	402	-	-	1/9/9/45	-
3	PLC	D	405	-	-	0/9/9/45	-
3	PLC	D	404	-	-	3/18/18/45	-
3	PLC	A	413	-	-	5/18/18/45	-
6	LMT	A	412	-	-	1/9/9/61	-
3	PLC	A	402	-	-	11/37/37/45	-
3	PLC	E	402	-	-	13/37/37/45	-
3	PLC	D	403	-	-	13/37/37/45	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	PLC	O2-C'	2.79	1.42	1.34
3	C	401	PLC	O2-C'	2.66	1.41	1.34
3	E	402	PLC	O2-C'	2.62	1.41	1.34
3	D	403	PLC	O2-C'	2.61	1.41	1.34
3	A	402	PLC	O2-C'	2.41	1.41	1.34
3	D	403	PLC	C5-N	2.17	1.58	1.51
3	B	402	PLC	O3-CB	2.17	1.39	1.33
3	E	402	PLC	O3-CB	2.16	1.39	1.33
3	C	401	PLC	C5-N	2.16	1.58	1.51
3	B	402	PLC	C5-N	2.11	1.57	1.51
3	A	402	PLC	C5-N	2.06	1.57	1.51
3	E	402	PLC	C5-N	2.06	1.57	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	PLC	C3-C2-C1	3.35	119.59	111.78
3	B	402	PLC	C3-C2-C1	3.26	119.39	111.78
3	D	403	PLC	C2-O2-C'	3.20	125.46	117.80
3	E	402	PLC	C3-C2-C1	3.17	119.17	111.78
3	D	403	PLC	C3-C2-C1	3.17	119.17	111.78
3	C	401	PLC	C2-O2-C'	3.11	125.24	117.80
3	B	402	PLC	C2-O2-C'	3.08	125.17	117.80
3	E	402	PLC	C2-O2-C'	2.96	124.89	117.80
3	A	402	PLC	C2-O2-C'	2.91	124.76	117.80
3	A	402	PLC	C3-C2-C1	2.87	118.47	111.78
7	E	408	PFL	O1-C1-C2	-2.49	113.73	120.59
7	C	407	PFL	C3-C2-C7	2.43	123.32	119.83
7	E	408	PFL	C3-C2-C7	2.09	122.83	119.83
7	B	410	PFL	O1-C1-C6	-2.07	114.89	120.59
7	B	410	PFL	C3-C2-C7	2.02	122.74	119.83
7	B	410	PFL	C11-C10-C6	-2.02	108.23	111.71

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PLC	O4P-C4-C5-N
3	A	402	PLC	C1'-C'-O2-C2
3	A	402	PLC	O'-C'-O2-C2
3	A	402	PLC	C4-O4P-P-O3P
3	B	402	PLC	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
3	B	402	PLC	C1'-C'-O2-C2
3	B	402	PLC	C1-O3P-P-O1P
3	B	402	PLC	C1-O3P-P-O4P
3	B	402	PLC	C4-O4P-P-O1P
3	B	402	PLC	C4-O4P-P-O3P
3	C	401	PLC	O4P-C4-C5-N
3	C	401	PLC	C1'-C'-O2-C2
3	C	401	PLC	C1-O3P-P-O1P
3	C	401	PLC	C1-O3P-P-O4P
3	D	403	PLC	O4P-C4-C5-N
3	D	403	PLC	C1'-C'-O2-C2
3	D	403	PLC	C4-O4P-P-O1P
3	D	403	PLC	C4-O4P-P-O3P
3	E	402	PLC	C1'-C'-O2-C2
3	E	402	PLC	C4-O4P-P-O1P
3	E	402	PLC	C4-O4P-P-O2P
3	E	402	PLC	C4-O4P-P-O3P
3	B	402	PLC	O'-C'-O2-C2
3	C	401	PLC	O'-C'-O2-C2
3	D	403	PLC	O'-C'-O2-C2
3	E	402	PLC	O'-C'-O2-C2
3	E	402	PLC	CB-C1B-C2B-C3B
3	D	403	PLC	C'-C1'-C2'-C3'
3	B	402	PLC	CB-C1B-C2B-C3B
3	D	403	PLC	CB-C1B-C2B-C3B
3	A	402	PLC	CB-C1B-C2B-C3B
3	C	401	PLC	CB-C1B-C2B-C3B
3	E	402	PLC	C4-C5-N-C6
3	E	402	PLC	C4-C5-N-C7
3	E	402	PLC	C4-C5-N-C8
3	B	402	PLC	C'-C1'-C2'-C3'
3	D	401	PLC	C1'-C2'-C3'-C4'
3	D	401	PLC	C4'-C5'-C6'-C7'
3	C	401	PLC	C'-C1'-C2'-C3'
3	D	401	PLC	C6'-C7'-C8'-C9'
3	B	403	PLC	C1'-C2'-C3'-C4'
3	A	402	PLC	C1'-C2'-C3'-C4'
3	D	404	PLC	C6'-C7'-C8'-C9'
3	A	413	PLC	C6'-C7'-C8'-C9'
3	B	403	PLC	C4'-C5'-C6'-C7'
3	A	403	PLC	C6'-C7'-C8'-C9'
3	A	413	PLC	C4'-C5'-C6'-C7'

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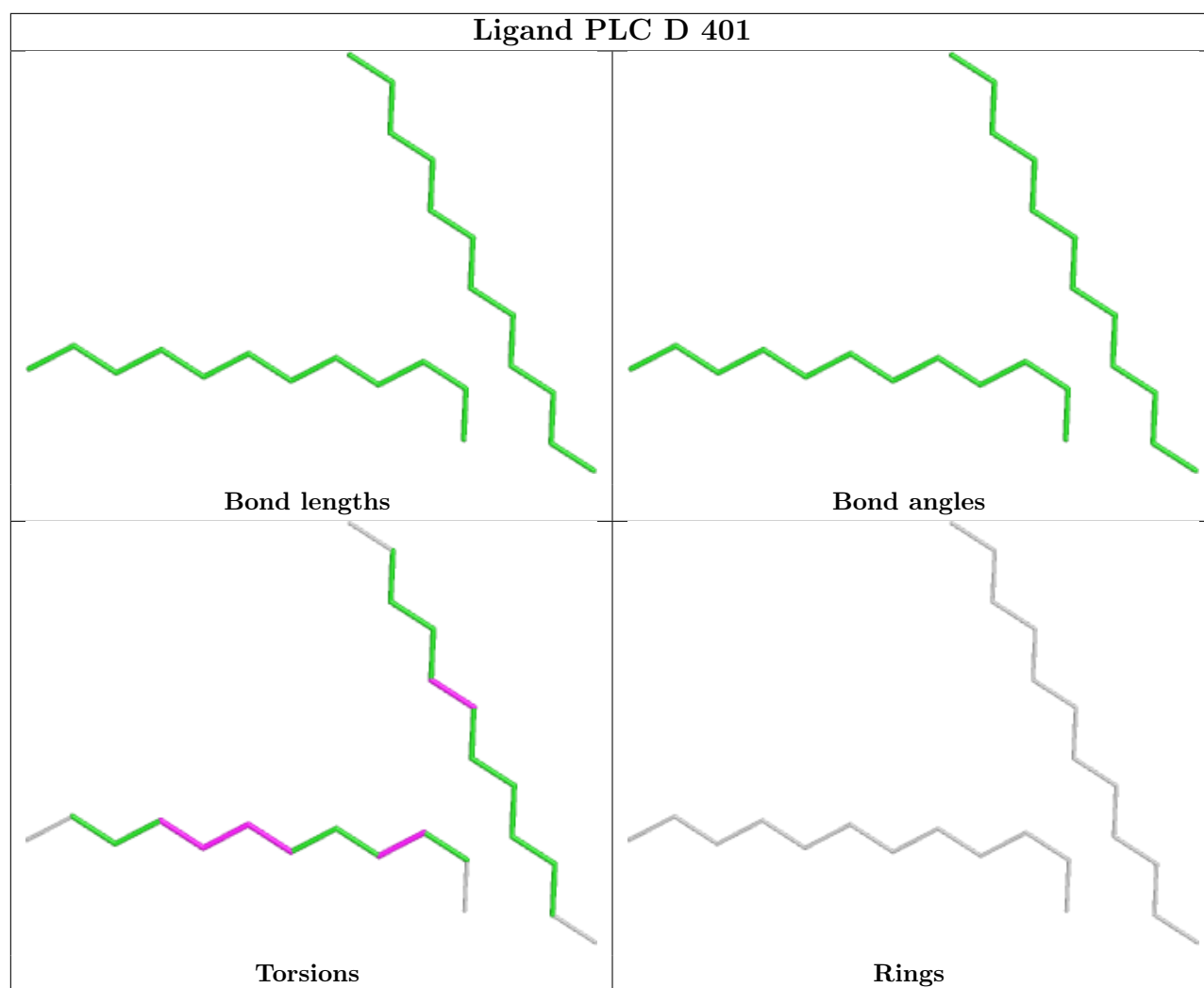
Mol	Chain	Res	Type	Atoms
3	B	403	PLC	C6'-C7'-C8'-C9'
3	A	413	PLC	C5'-C6'-C7'-C8'
3	A	402	PLC	C3-C2-O2-C'
3	B	403	PLC	C5'-C6'-C7'-C8'
3	A	402	PLC	C1B-C2B-C3B-C4B
3	D	401	PLC	C5'-C6'-C7'-C8'
3	D	401	PLC	C5B-C6B-C7B-C8B
3	D	404	PLC	C4'-C5'-C6'-C7'
3	A	403	PLC	C4'-C5'-C6'-C7'
3	A	402	PLC	C3B-C4B-C5B-C6B
3	D	404	PLC	C5'-C6'-C7'-C8'
3	A	403	PLC	C5'-C6'-C7'-C8'
6	A	412	LMT	C1-C2-C3-C4
3	E	402	PLC	C'-C1'-C2'-C3'
3	C	401	PLC	O3P-C1-C2-O2
3	C	402	PLC	C1'-C2'-C3'-C4'
3	E	402	PLC	O4P-C4-C5-N
3	D	403	PLC	C1'-C2'-C3'-C4'
3	A	402	PLC	C1-O3P-P-O1P
3	A	402	PLC	C4-O4P-P-O1P
3	E	402	PLC	C3-C2-O2-C'
3	B	402	PLC	C1B-C2B-C3B-C4B
3	B	402	PLC	C1'-C2'-C3'-C4'
3	C	401	PLC	C1'-C2'-C3'-C4'
3	E	402	PLC	C1B-C2B-C3B-C4B
3	A	413	PLC	C5B-C6B-C7B-C8B
3	D	403	PLC	C4-C5-N-C8
3	D	403	PLC	C2B-C1B-CB-O3
3	C	401	PLC	O2-C'-C1'-C2'
3	B	402	PLC	O2-C'-C1'-C2'
3	C	401	PLC	C3-C2-O2-C'
3	D	403	PLC	C4-C5-N-C6
3	D	403	PLC	C2B-C1B-CB-OB
3	D	403	PLC	C4-C5-N-C7
3	A	413	PLC	C1'-C2'-C3'-C4'
3	C	401	PLC	O'-C'-C1'-C2'
3	B	402	PLC	O'-C'-C1'-C2'

There are no ring outliers.

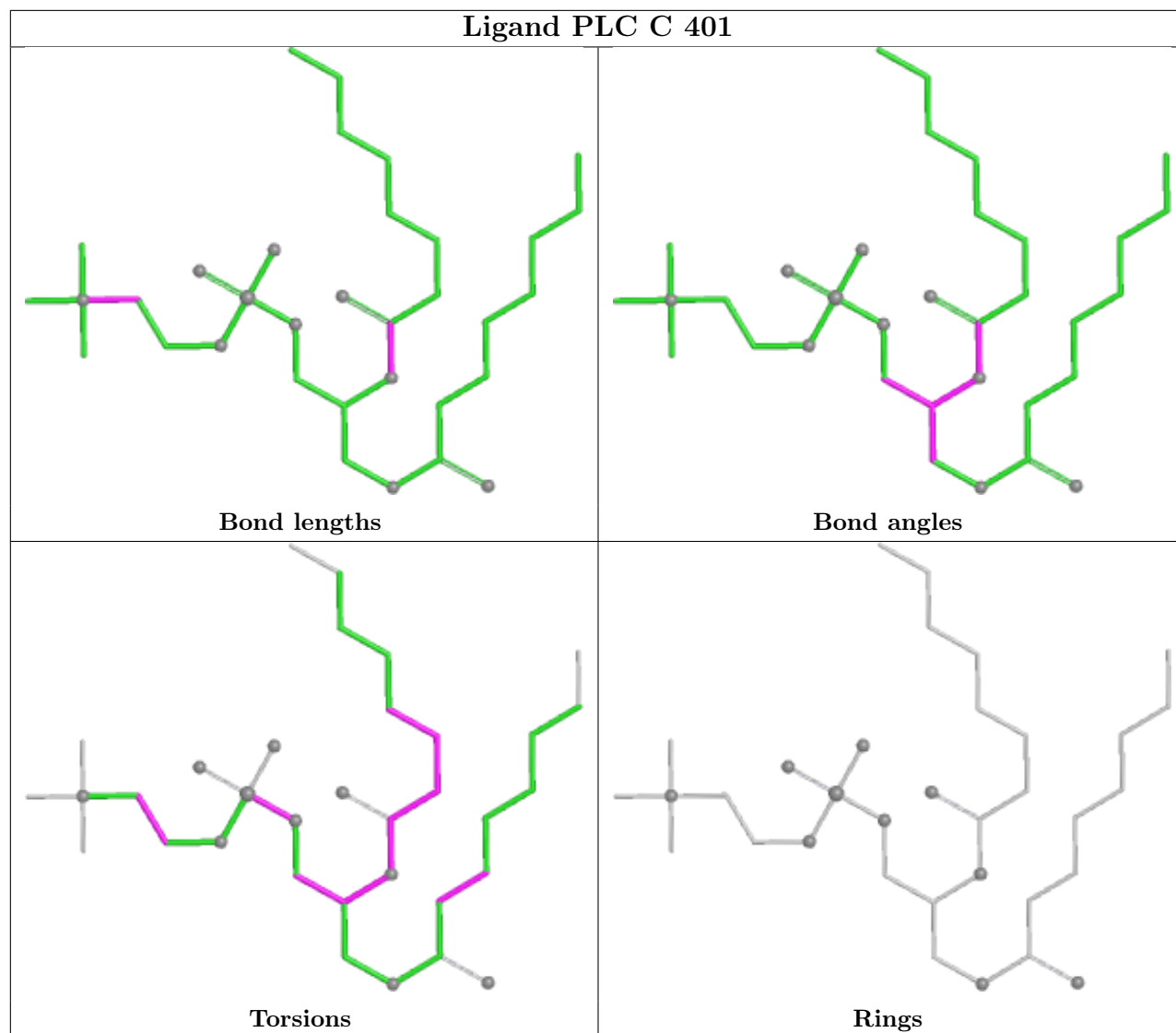
19 monomers are involved in 125 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	PLC	1	0
3	C	401	PLC	8	0
6	A	411	LMT	2	0
7	E	408	PFL	27	0
6	C	406	LMT	1	0
3	A	404	PLC	1	0
3	B	403	PLC	2	0
7	C	407	PFL	25	0
7	D	410	PFL	23	0
6	E	407	LMT	2	0
6	B	408	LMT	2	0
3	A	403	PLC	1	0
3	B	402	PLC	15	0
7	B	410	PFL	33	0
3	C	402	PLC	2	0
3	D	404	PLC	1	0
3	A	413	PLC	1	0
3	A	402	PLC	3	0
3	D	403	PLC	10	0

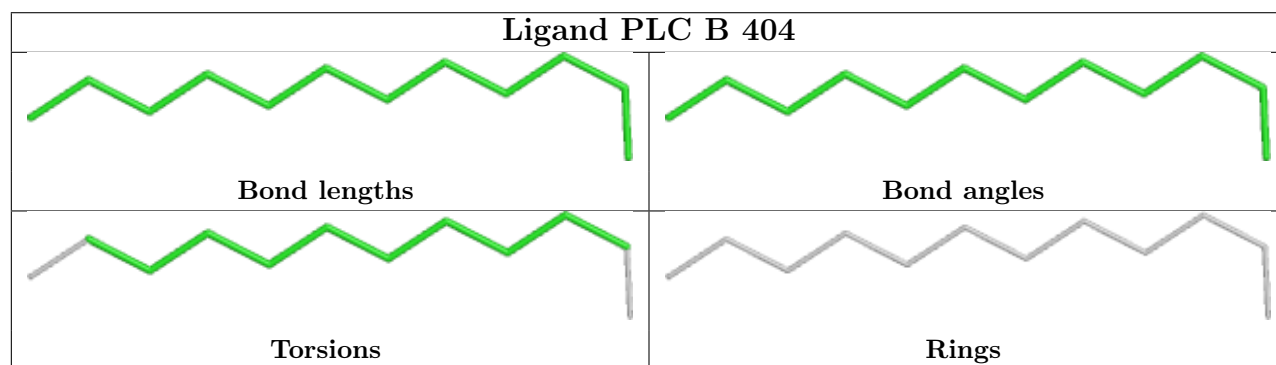
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

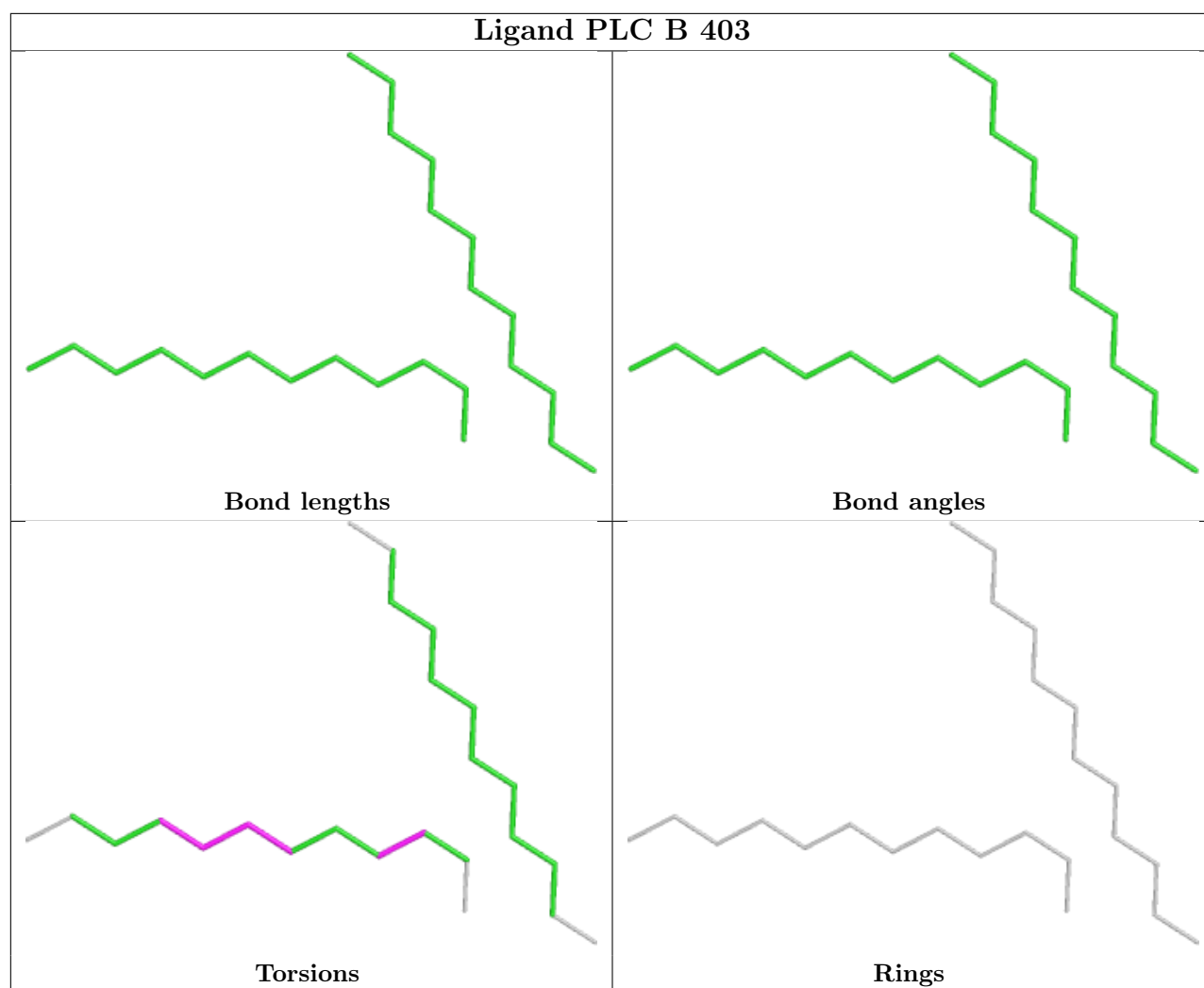


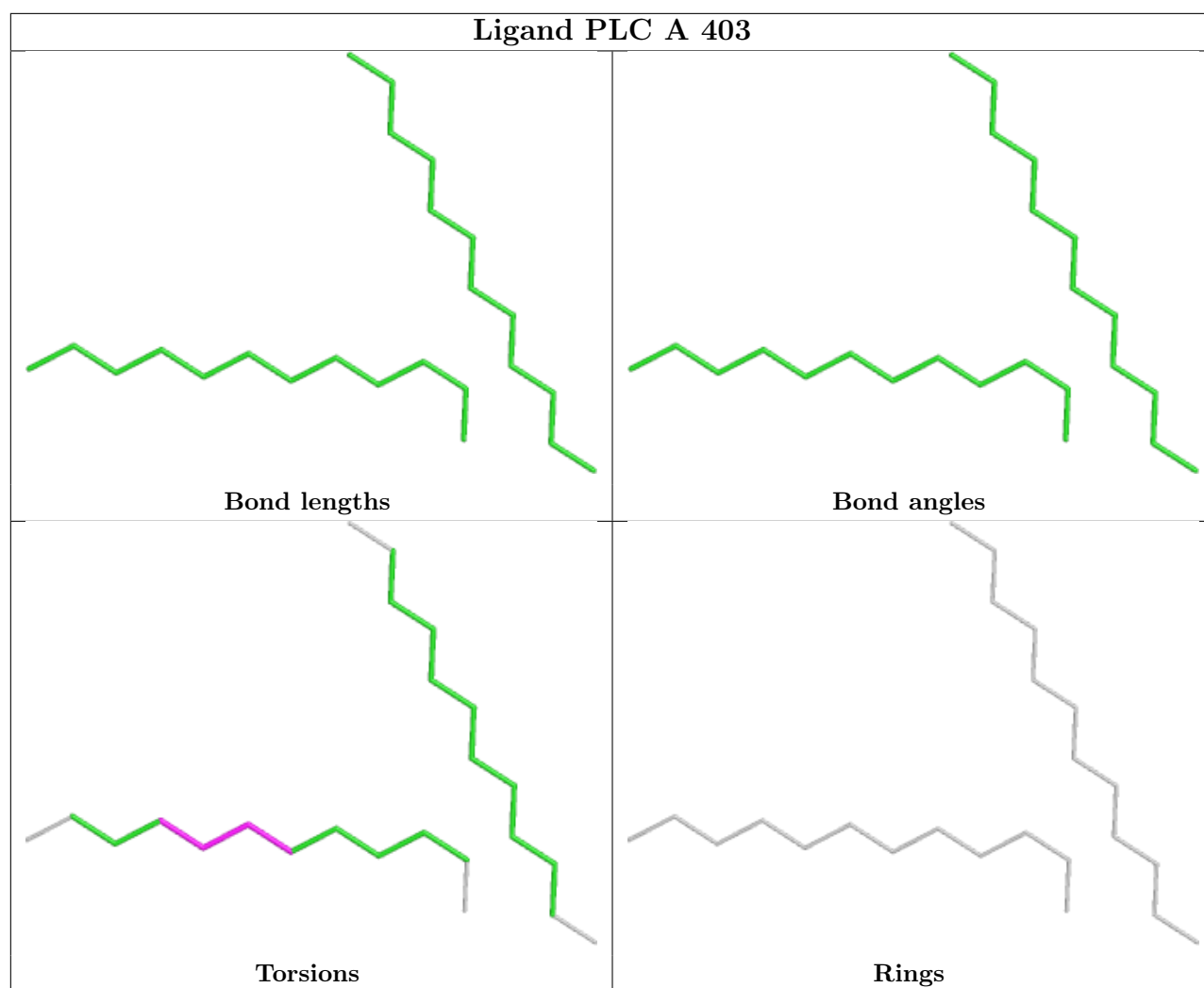
Ligand PLC C 401



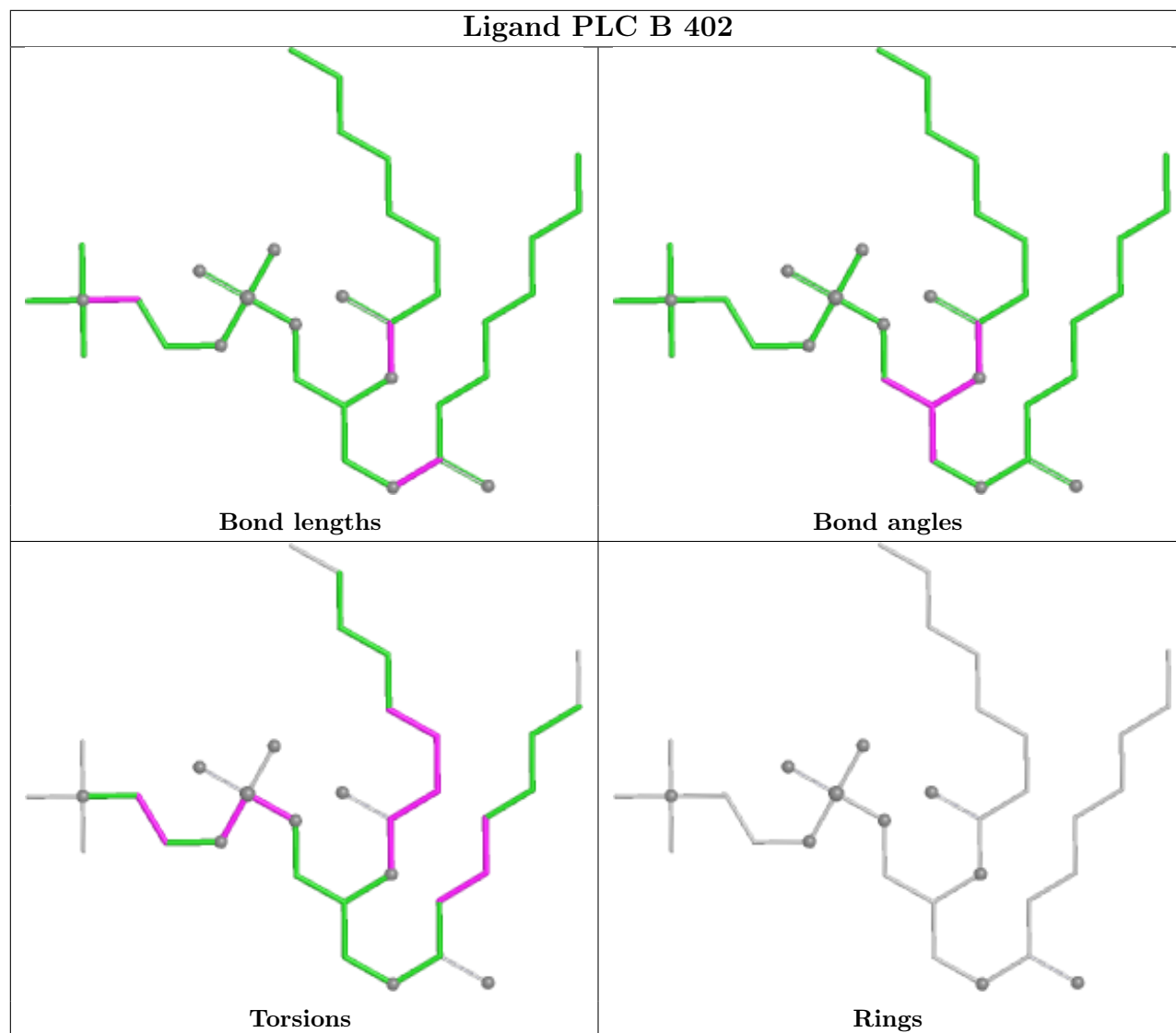
Ligand PLC B 404



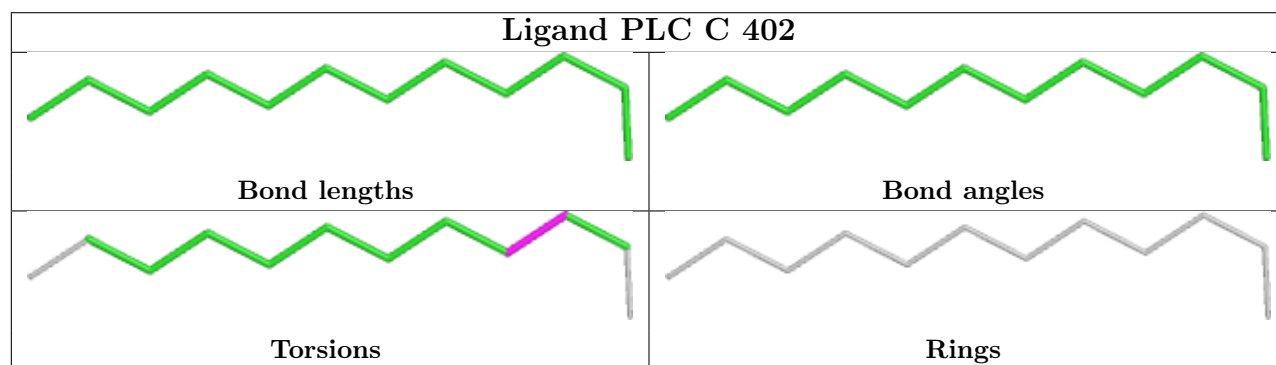


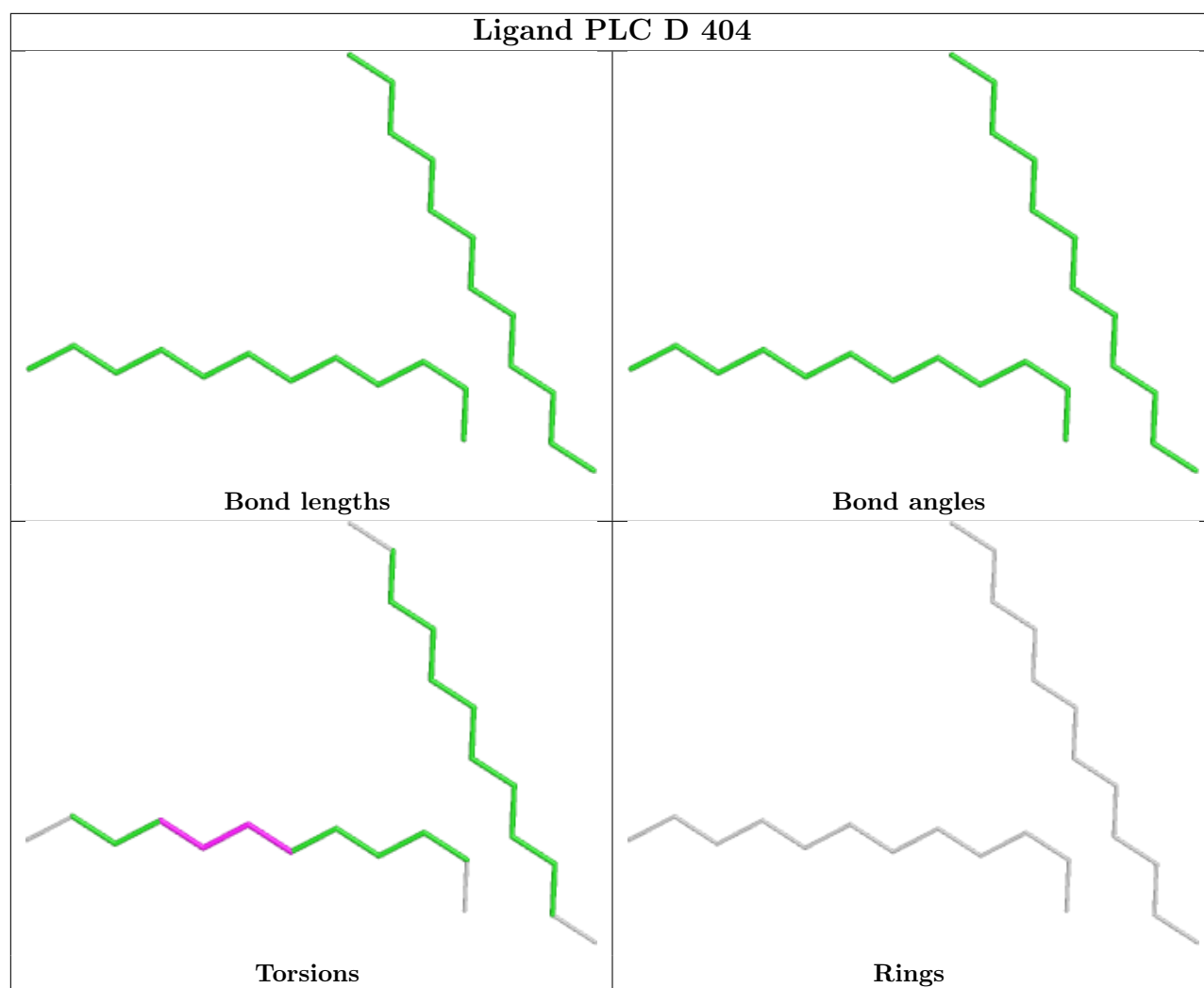


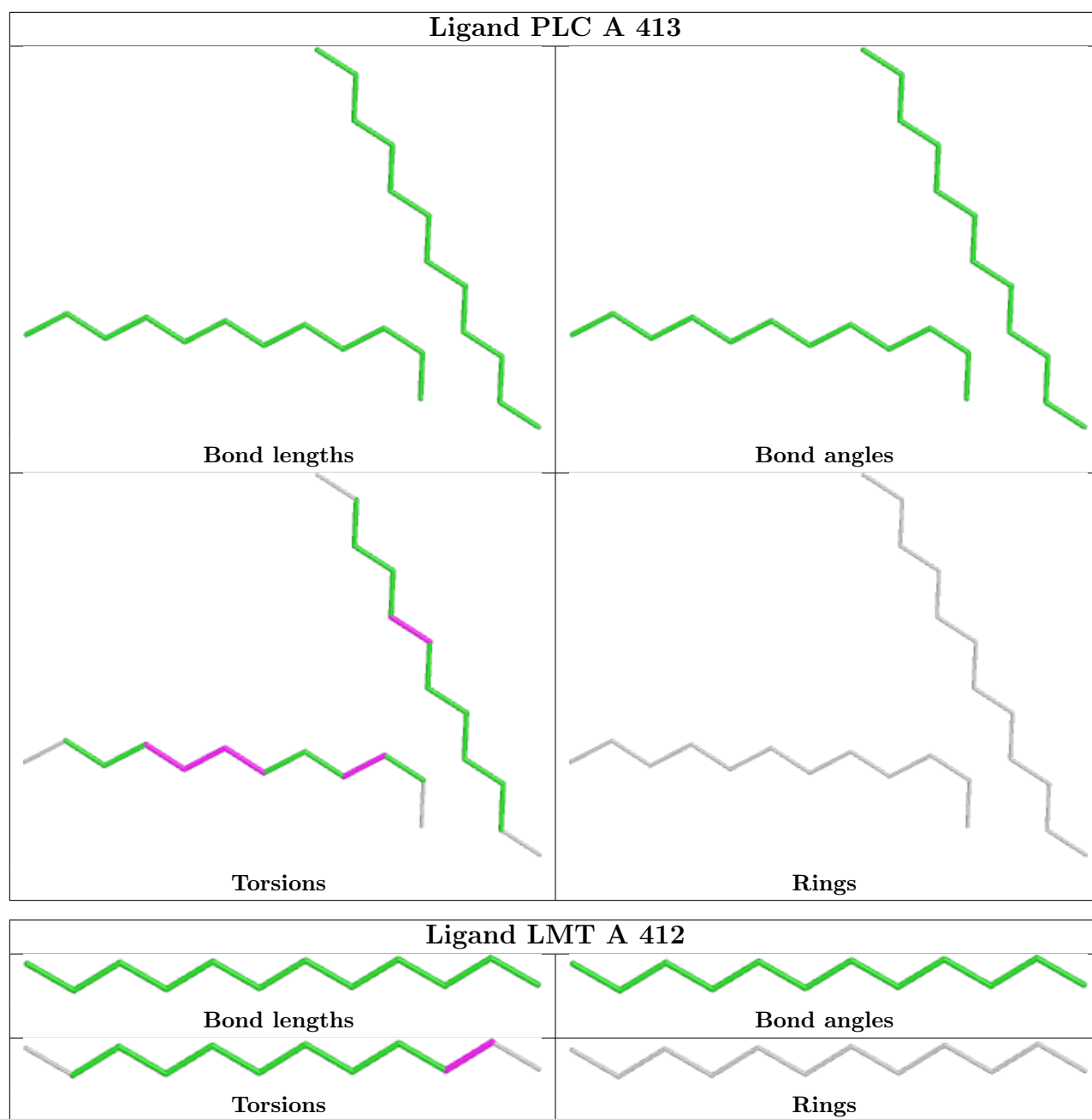
Ligand PLC B 402



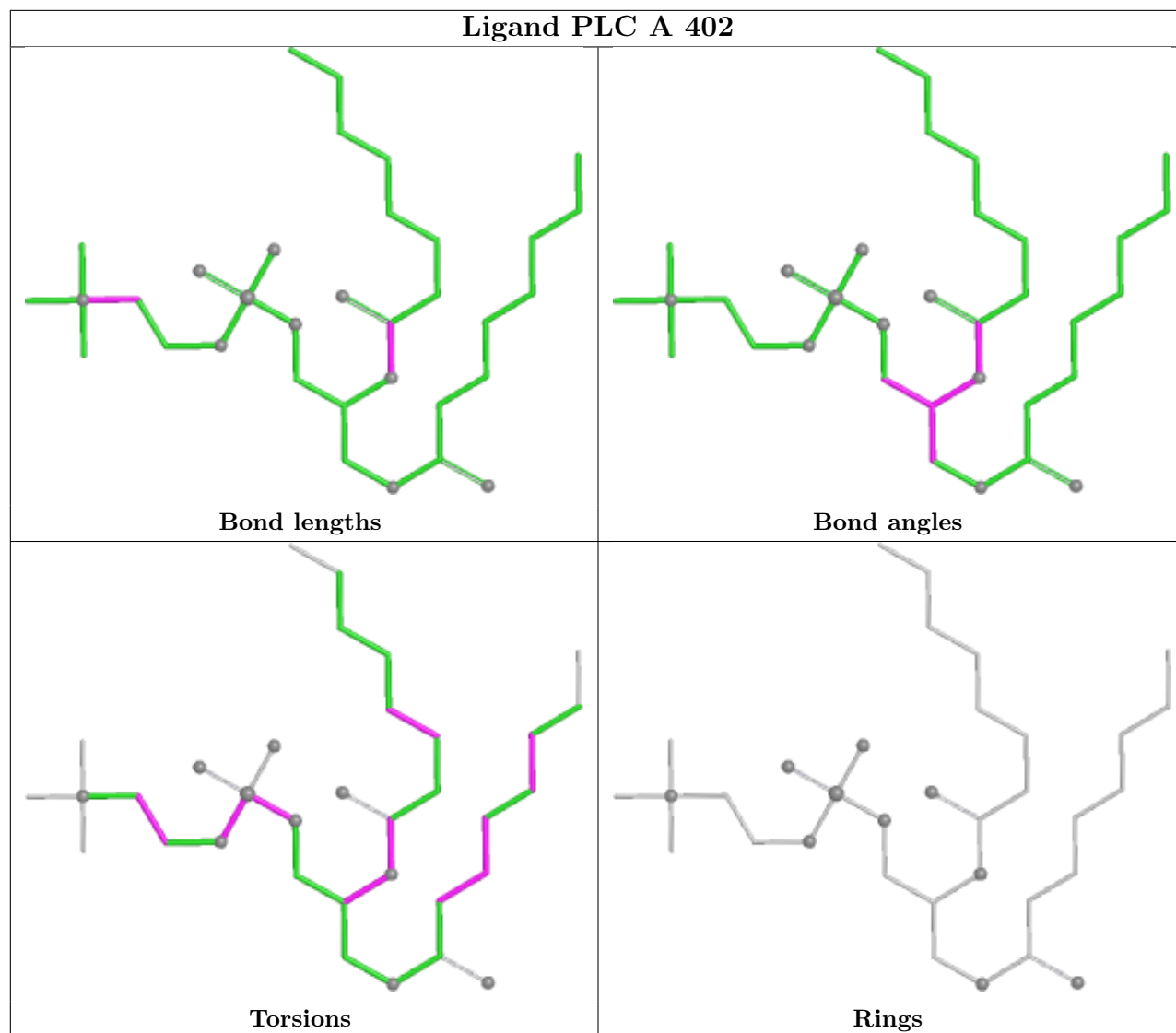
Ligand PLC C 402



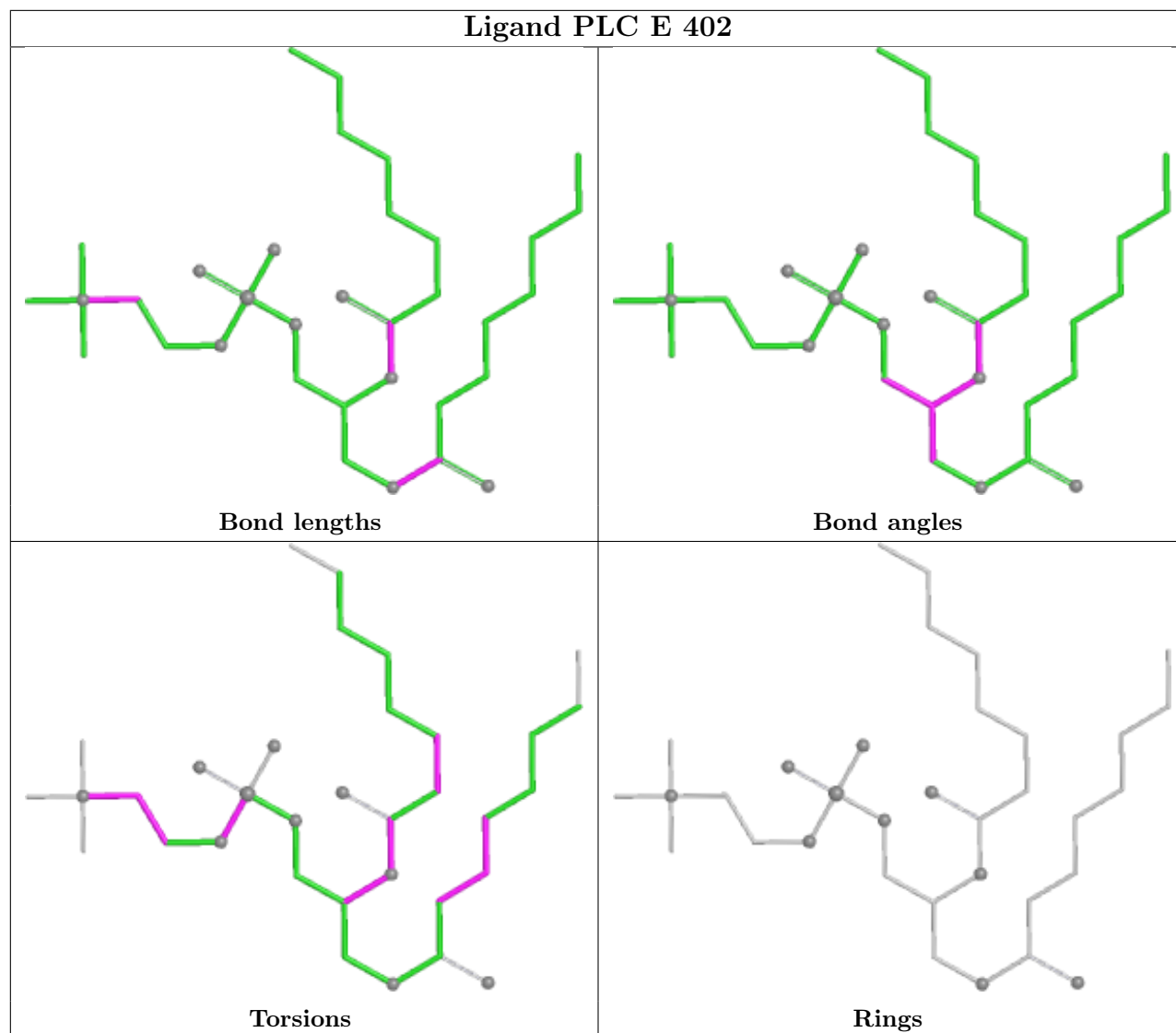


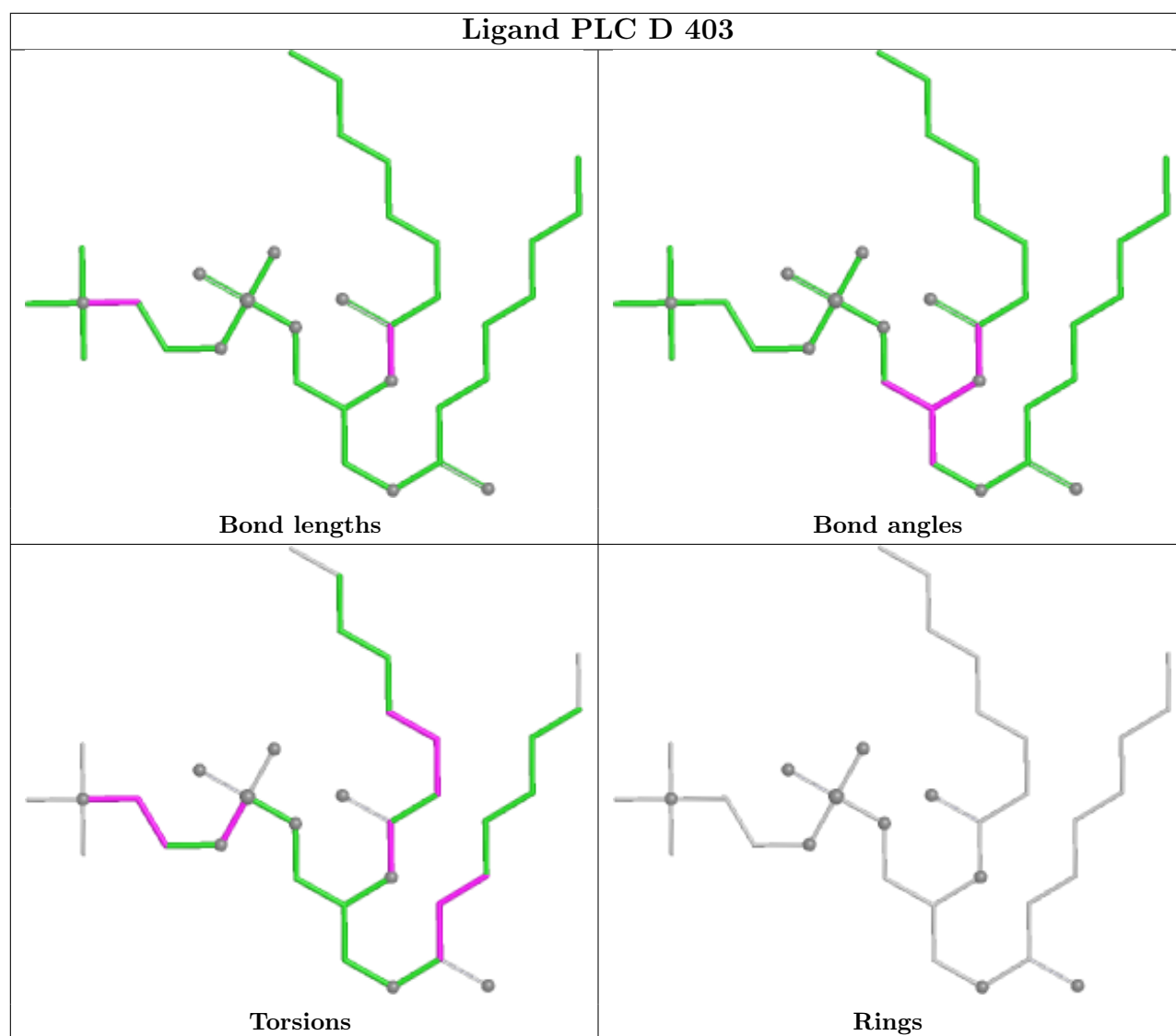


Ligand PLC A 402



Ligand PLC E 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	0.83	38 (12%) 8 6	31, 86, 131, 168	1 (0%)
1	B	311/317 (98%)	0.70	31 (9%) 12 8	58, 83, 119, 143	0
1	C	311/317 (98%)	0.99	58 (18%) 3 4	60, 86, 136, 180	0
1	D	311/317 (98%)	1.13	65 (20%) 2 3	61, 88, 133, 182	0
1	E	311/317 (98%)	0.96	48 (15%) 5 5	65, 89, 131, 160	0
All	All	1555/1585 (98%)	0.92	240 (15%) 5 5	31, 86, 131, 182	1 (0%)

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	283	SER	11.2
1	A	147	GLU	10.5
1	B	154	ASP	9.2
1	C	283	SER	8.0
1	D	154	ASP	7.0
1	E	11	ILE	6.8
1	D	244	THR	6.4
1	D	153	ASP	6.2
1	E	69	GLU	6.2
1	A	145	ASP	5.9
1	A	146	LEU	5.8
1	B	312	PHE	5.6
1	E	244	THR	5.6
1	A	14	GLU	5.4
1	E	68	PRO	5.3
1	C	129	TYR	5.3
1	A	12	ALA	5.2
1	A	13	ASP	5.2
1	E	12	ALA	5.0
1	E	89	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	60	GLY	5.0
1	A	15	PRO	5.0
1	C	64	LYS	4.9
1	C	127	HIS	4.9
1	C	57	VAL	4.8
1	C	66	TYR	4.7
1	E	92	ILE	4.7
1	D	204	PRO	4.6
1	D	178	ASP	4.6
1	C	172	ALA	4.6
1	D	180	LEU	4.5
1	D	207	PHE	4.5
1	D	136	ASP	4.5
1	B	153	ASP	4.4
1	B	283	SER	4.4
1	A	242	VAL	4.3
1	A	178	ASP	4.3
1	D	170	LYS	4.3
1	C	11	ILE	4.3
1	E	66	TYR	4.3
1	D	152	ASN	4.3
1	D	173	ASN	4.3
1	D	11	ILE	4.2
1	E	64	LYS	4.2
1	B	83	ASN	4.2
1	C	187	GLN	4.2
1	B	5	VAL	4.2
1	E	62	ARG	4.2
1	E	102	TYR	4.2
1	D	61	VAL	4.1
1	D	89	VAL	4.1
1	D	206	LEU	4.1
1	E	14	GLU	4.0
1	B	113	PRO	4.0
1	D	88	ASP	4.0
1	B	280	LYS	4.0
1	D	205	TRP	3.9
1	C	242	VAL	3.9
1	D	208	ILE	3.9
1	B	178	ASP	3.8
1	A	243	GLU	3.8
1	A	244	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	283	SER	3.8
1	C	113	PRO	3.8
1	C	14	GLU	3.7
1	D	151	LYS	3.7
1	D	141	VAL	3.7
1	C	65	THR	3.7
1	C	281	VAL	3.7
1	D	201	ILE	3.6
1	C	248	LYS	3.6
1	E	67	GLU	3.6
1	A	283	SER	3.6
1	D	21	GLY	3.5
1	B	152	ASN	3.5
1	A	166	THR	3.5
1	E	50	ARG	3.5
1	C	174	PHE	3.5
1	D	238	PHE	3.5
1	B	84	ALA	3.5
1	D	245	ASN	3.5
1	A	180	LEU	3.4
1	C	61	VAL	3.4
1	D	63	VAL	3.4
1	A	239	ASN	3.3
1	E	154	ASP	3.3
1	D	15	PRO	3.3
1	C	83	ASN	3.3
1	A	205	TRP	3.3
1	A	154	ASP	3.3
1	C	178	ASP	3.3
1	D	90	VAL	3.3
1	C	280	LYS	3.3
1	E	112	SER	3.2
1	C	125	THR	3.2
1	A	86	ASP	3.2
1	D	203	LEU	3.2
1	C	166	THR	3.2
1	C	226	THR	3.2
1	D	104	GLU	3.2
1	C	82	GLU	3.1
1	E	243	GLU	3.1
1	A	238	PHE	3.1
1	B	244	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	280	LYS	3.1
1	C	5	VAL	3.1
1	C	148	LYS	3.1
1	B	170	LYS	3.0
1	B	136	ASP	3.0
1	B	293	ARG	3.0
1	D	14	GLU	3.0
1	D	102	TYR	2.9
1	A	11	ILE	2.9
1	E	111	LEU	2.9
1	C	12	ALA	2.9
1	E	263	TYR	2.9
1	C	112	SER	2.9
1	B	205	TRP	2.9
1	A	148	LYS	2.9
1	A	170	LYS	2.9
1	C	284	GLN	2.9
1	C	173	ASN	2.9
1	D	42	PHE	2.9
1	E	60	GLY	2.9
1	D	43	LEU	2.8
1	E	153	ASP	2.8
1	C	62	ARG	2.8
1	D	149	VAL	2.8
1	E	94	VAL	2.8
1	C	238	PHE	2.8
1	D	235	HIS	2.7
1	B	11	ILE	2.7
1	C	201	ILE	2.7
1	E	88	ASP	2.7
1	E	235	HIS	2.7
1	A	149	VAL	2.7
1	B	189	ARG	2.7
1	E	48	LYS	2.7
1	C	152	ASN	2.7
1	C	244	THR	2.7
1	D	87	ALA	2.6
1	E	114	LEU	2.6
1	A	139	ASN	2.6
1	C	276	GLN	2.6
1	D	150	GLY	2.6
1	C	94	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	243	GLU	2.6
1	D	111	LEU	2.6
1	C	189	ARG	2.6
1	A	156	PHE	2.6
1	E	9	PRO	2.6
1	C	282	GLU	2.6
1	D	177	GLU	2.6
1	C	84	ALA	2.6
1	C	27	CYS	2.5
1	A	6	SER	2.5
1	C	59	SER	2.5
1	B	248	LYS	2.5
1	E	137	THR	2.5
1	D	27	CYS	2.5
1	A	240	ILE	2.5
1	A	65	THR	2.5
1	A	222	GLU	2.5
1	A	173	ASN	2.5
1	B	284	GLN	2.5
1	B	14	GLU	2.4
1	C	183	LYS	2.4
1	D	92	ILE	2.4
1	A	136	ASP	2.4
1	C	179	ARG	2.4
1	E	174	PHE	2.4
1	D	68	PRO	2.4
1	C	86	ASP	2.4
1	A	127	HIS	2.4
1	B	114	LEU	2.4
1	D	114	LEU	2.4
1	D	26	GLU	2.4
1	D	137	THR	2.3
1	B	86	ASP	2.3
1	A	72	TRP	2.3
1	E	93	SER	2.3
1	D	253	THR	2.3
1	A	19	ASN	2.3
1	E	260	PHE	2.3
1	E	236	ILE	2.3
1	C	175	ALA	2.3
1	D	226	THR	2.3
1	B	146	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	111	LEU	2.3
1	D	24	LEU	2.3
1	C	92	ILE	2.3
1	E	129	TYR	2.3
1	D	156	PHE	2.3
1	E	315	PHE	2.3
1	C	168	VAL	2.3
1	E	65	THR	2.3
1	C	136	ASP	2.3
1	B	111	LEU	2.2
1	A	84	ALA	2.2
1	C	6	SER	2.2
1	B	155	VAL	2.2
1	E	57	VAL	2.2
1	D	83	ASN	2.2
1	D	280	LYS	2.2
1	D	155	VAL	2.2
1	C	126	LEU	2.2
1	E	56	PRO	2.2
1	E	91	ASP	2.2
1	D	5	VAL	2.2
1	A	201	ILE	2.2
1	B	196	SER	2.2
1	C	56	PRO	2.2
1	E	113	PRO	2.2
1	C	185	ASP	2.2
1	C	205	TRP	2.2
1	D	62	ARG	2.1
1	E	104	GLU	2.1
1	D	232	LEU	2.1
1	D	112	SER	2.1
1	A	75	GLU	2.1
1	B	222	GLU	2.1
1	B	129	TYR	2.1
1	B	226	THR	2.1
1	C	137	THR	2.1
1	E	75	GLU	2.1
1	D	50	ARG	2.1
1	D	115	ASP	2.1
1	E	172	ALA	2.1
1	B	243	GLU	2.1
1	D	195	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	238	PHE	2.1
1	A	141	VAL	2.0
1	D	182	SER	2.0
1	C	17	THR	2.0
1	E	284	GLN	2.0
1	D	171	PRO	2.0
1	D	168	VAL	2.0
1	E	281	VAL	2.0
1	D	176	LEU	2.0
1	E	253	THR	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 oligosaccharides 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
5	NA	B	406	1/1	0.62	0.33	94,94,94,94	0
3	PLC	A	404	12/42	0.65	0.39	109,113,118,119	0
3	PLC	D	404	24/42	0.73	0.48	107,115,120,121	0
3	PLC	B	404	12/42	0.73	0.42	141,145,146,146	0
2	ACT	B	407	4/4	0.74	0.23	66,66,67,67	0
3	PLC	C	402	12/42	0.74	0.38	106,109,118,119	0
3	PLC	C	401	34/42	0.75	0.31	115,138,164,165	0
3	PLC	D	401	24/42	0.77	0.33	74,86,107,108	0
3	PLC	D	403	34/42	0.77	0.28	112,138,165,167	0
3	PLC	B	402	34/42	0.77	0.31	118,152,179,181	0
5	NA	A	409	1/1	0.77	0.98	89,89,89,89	0
3	PLC	A	413	24/42	0.77	0.38	93,98,105,106	0
3	PLC	A	403	24/42	0.79	0.42	110,112,124,124	0

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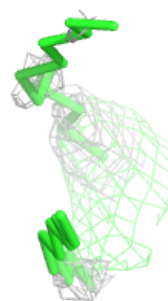
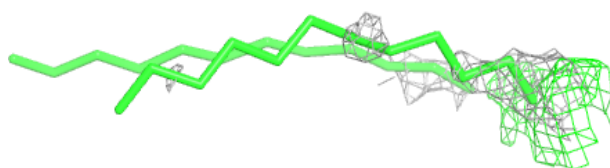
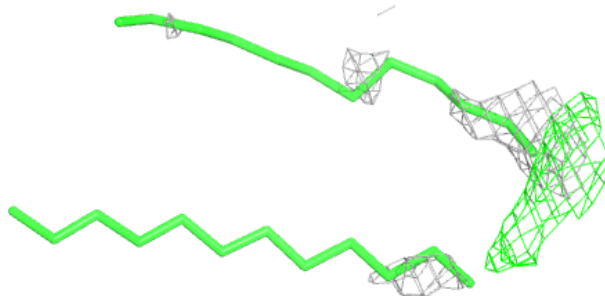
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PFL	E	408	13/13	0.79	0.26	101,104,107,107	0
3	PLC	E	403	12/42	0.80	0.30	112,116,126,127	0
3	PLC	A	402	34/42	0.81	0.28	125,150,180,181	0
5	NA	E	405	1/1	0.81	0.20	95,95,95,95	0
3	PLC	B	403	24/42	0.81	0.40	96,104,109,111	0
3	PLC	E	402	34/42	0.83	0.26	121,145,170,173	0
3	PLC	D	405	12/42	0.83	0.27	89,94,101,102	0
4	CL	A	407	1/1	0.84	0.28	147,147,147,147	0
5	NA	D	407	1/1	0.84	0.18	103,103,103,103	0
7	PFL	B	410	13/13	0.86	0.20	79,87,92,94	0
7	PFL	D	410	13/13	0.86	0.23	102,104,108,109	0
6	LMT	A	412	12/35	0.86	0.32	85,91,102,104	0
7	PFL	C	407	13/13	0.87	0.19	93,99,107,109	0
6	LMT	B	408	12/35	0.90	0.30	68,76,85,88	0
6	LMT	C	406	12/35	0.90	0.26	78,81,90,91	0
4	CL	A	406	1/1	0.90	0.30	142,142,142,142	0
5	NA	A	408	1/1	0.91	0.13	116,116,116,116	0
2	ACT	B	401	4/4	0.91	0.20	118,118,119,121	0
2	ACT	B	409	4/4	0.92	0.17	97,98,98,99	0
6	LMT	D	409	12/35	0.92	0.25	80,85,98,99	0
6	LMT	A	411	12/35	0.92	0.22	28,36,57,59	0
2	ACT	E	406	4/4	0.93	0.14	82,82,83,83	0
4	CL	A	405	1/1	0.94	0.17	82,82,82,82	0
4	CL	E	404	1/1	0.94	0.13	79,79,79,79	0
2	ACT	A	410	4/4	0.94	0.12	68,69,70,71	0
6	LMT	E	407	12/35	0.94	0.26	70,72,89,92	0
4	CL	B	405	1/1	0.95	0.15	85,85,85,85	0
4	CL	D	406	1/1	0.95	0.07	74,74,74,74	0
2	ACT	D	408	4/4	0.95	0.24	67,69,69,71	0
5	NA	C	404	1/1	0.95	0.07	58,58,58,58	0
2	ACT	E	401	4/4	0.96	0.22	99,101,102,102	0
2	ACT	C	405	4/4	0.96	0.10	70,74,74,76	0
2	ACT	A	401	4/4	0.96	0.14	99,99,99,100	0
2	ACT	D	402	4/4	0.98	0.10	84,84,84,85	0
4	CL	C	403	1/1	0.98	0.06	74,74,74,74	0

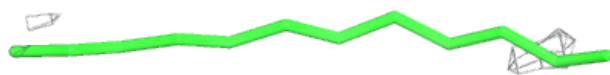
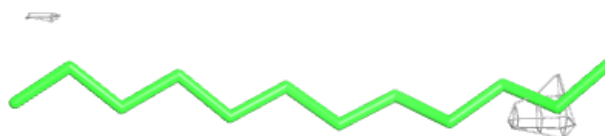
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLC 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)

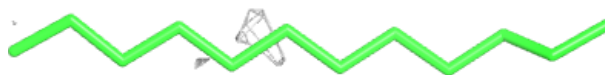
**Electron density around PLC B 404:**

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

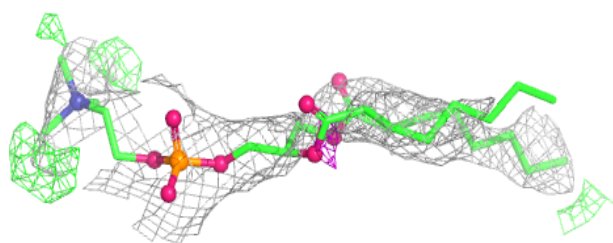
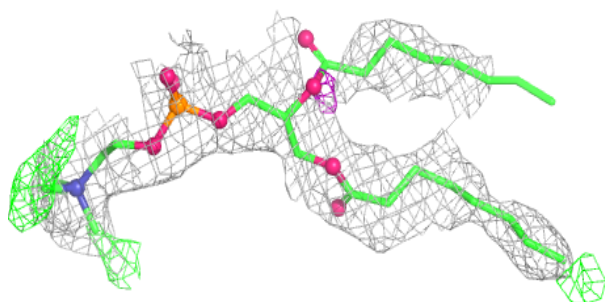


Electron density around PLC C 402:

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

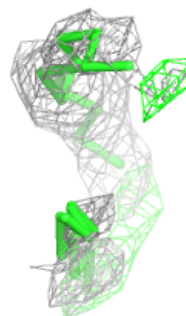
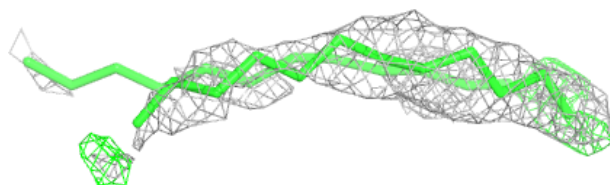
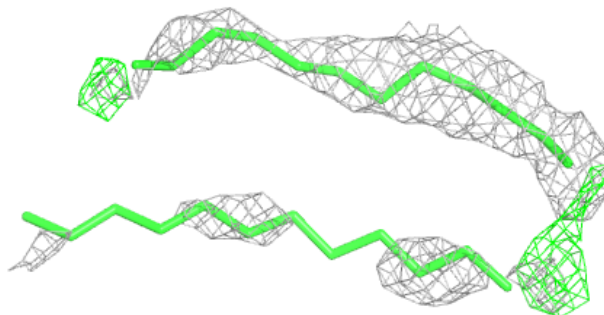
**Electron density around PLC C 401:**

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

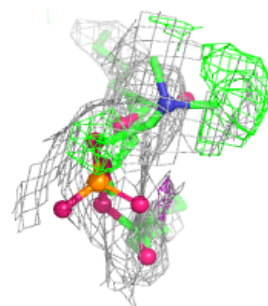
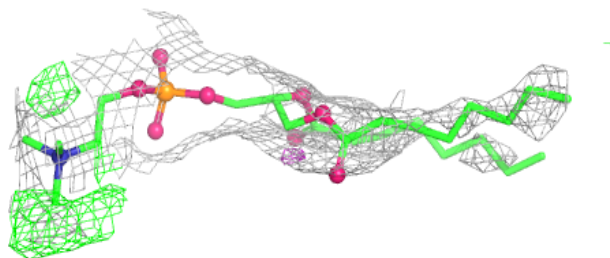
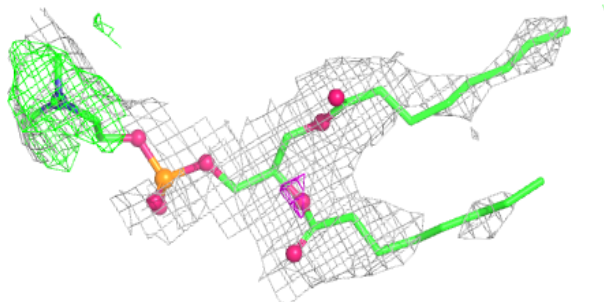


Electron density around PLC D 401:

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

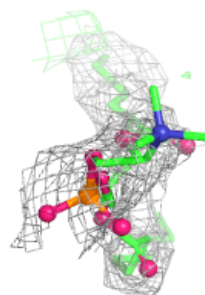
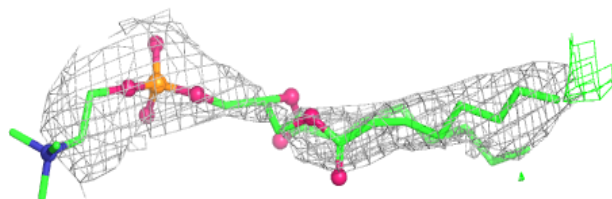
**Electron density around PLC D 403:**

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

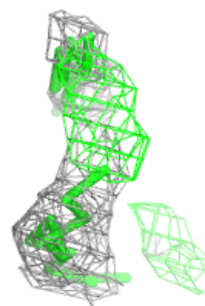
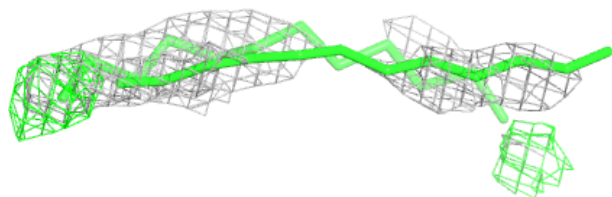
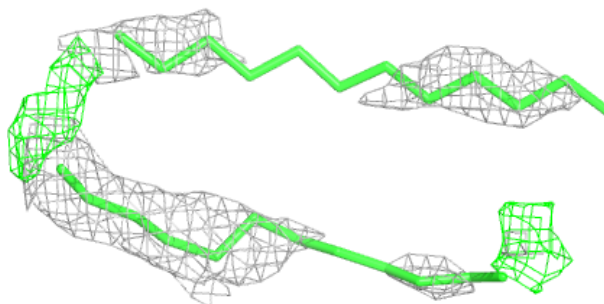


Electron density around PLC B 402:

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

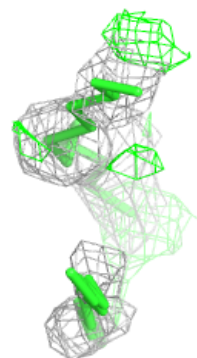
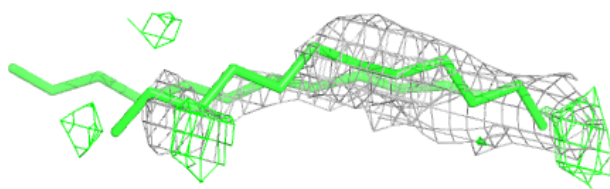
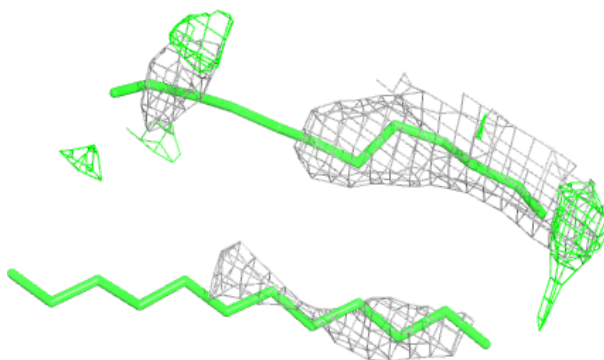
**Electron density around PLC A 413:**

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

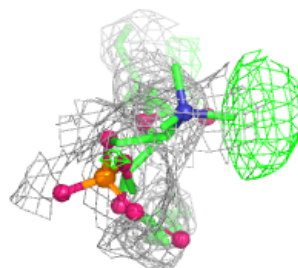
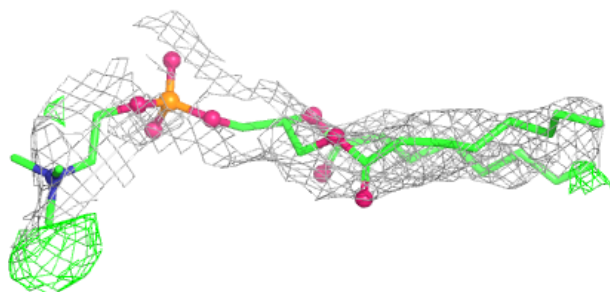
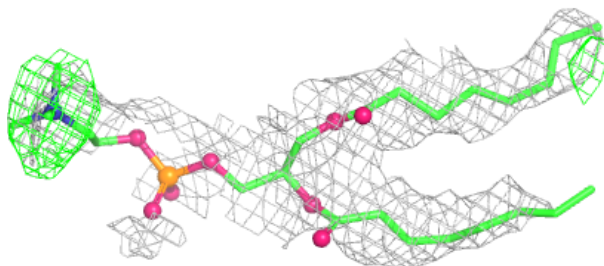


Electron density around PLC A 403:

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

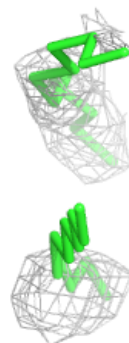
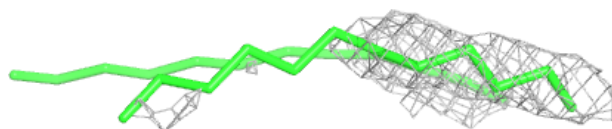
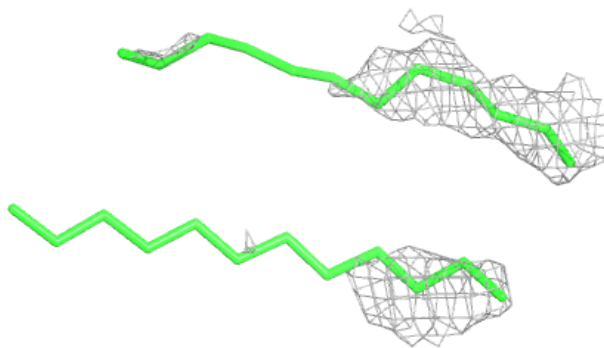
**Electron density around PLC A 402:**

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

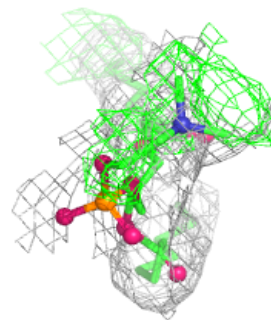
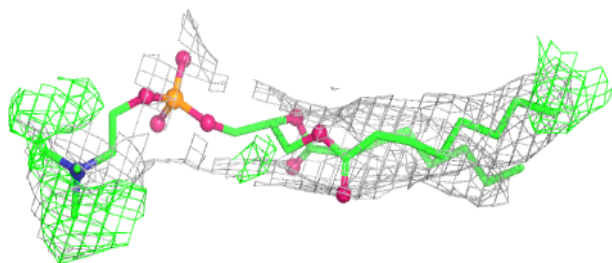
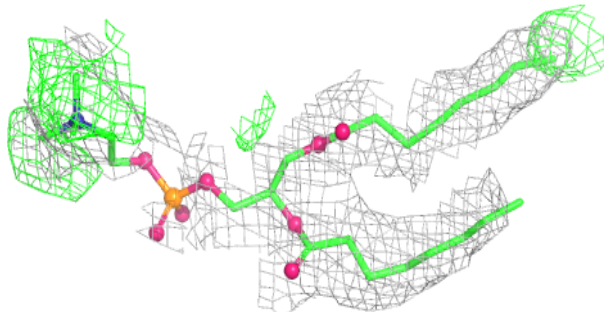


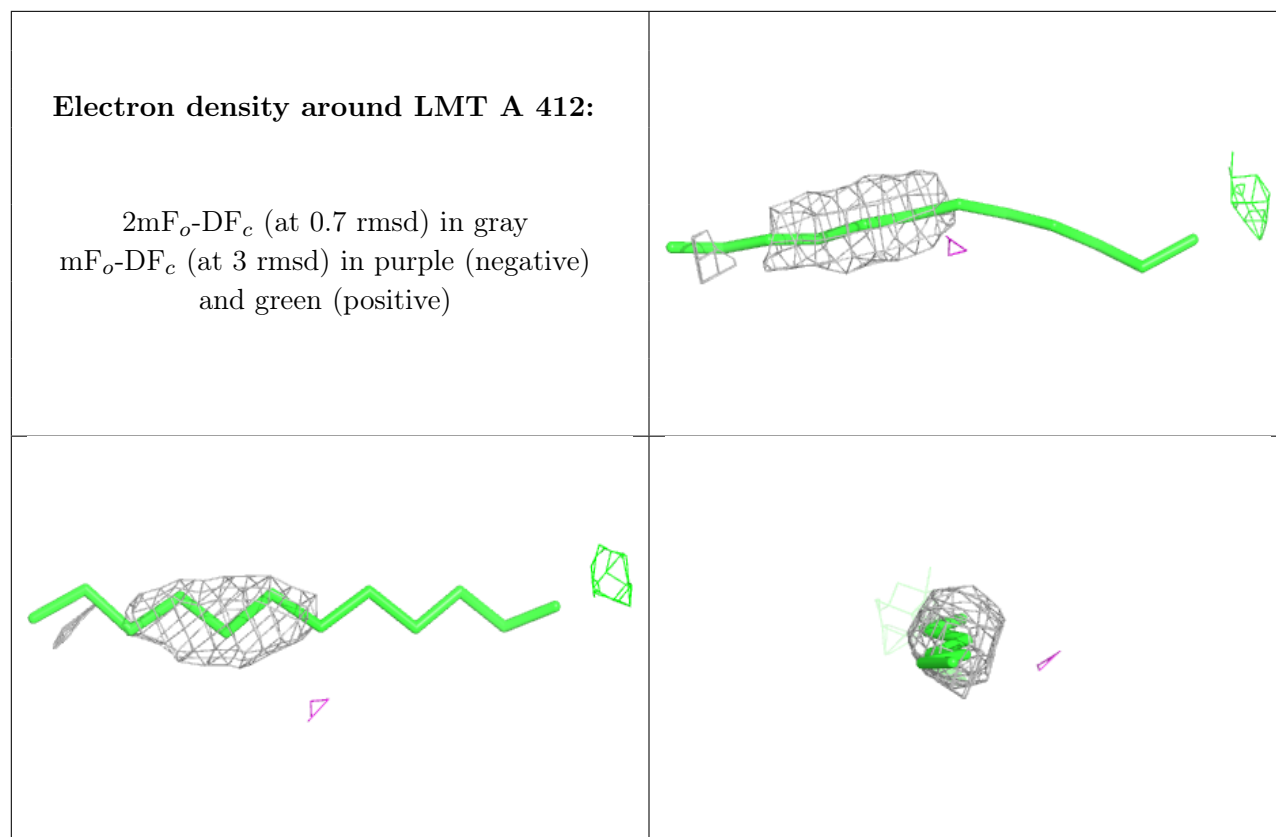
Electron density around PLC B 403:

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

**Electron density around PLC E 402:**

$2mF_o-DF_c$ (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.