



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:43 PM UTC

PDB ID : 6HJB / pdb_00006hjb
Title : Xray structure of GLIC in complex with malonate
Authors : Fourati, Z.; Delarue, M.
Deposited on : 2018-09-03
Resolution : 3.00 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

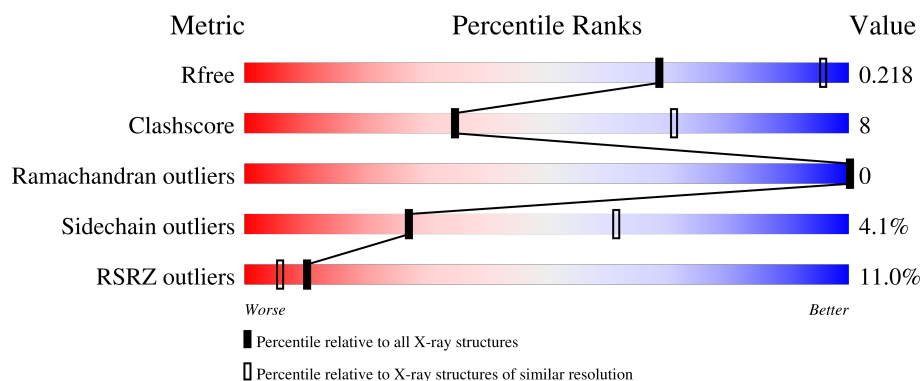
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	359	7% 71% 15% • 13%
1	B	359	8% 69% 18% • 13%
1	C	359	12% 72% 14% • 13%
1	D	359	12% 70% 16% 13%
1	E	359	9% 71% 14% • 13%

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
6	MLA	A	406	-	X	-	-
6	MLA	B	406	-	X	-	-
6	MLA	D	407	-	X	-	-
6	MLA	E	408	-	X	-	-

2 Entry composition ⓘ

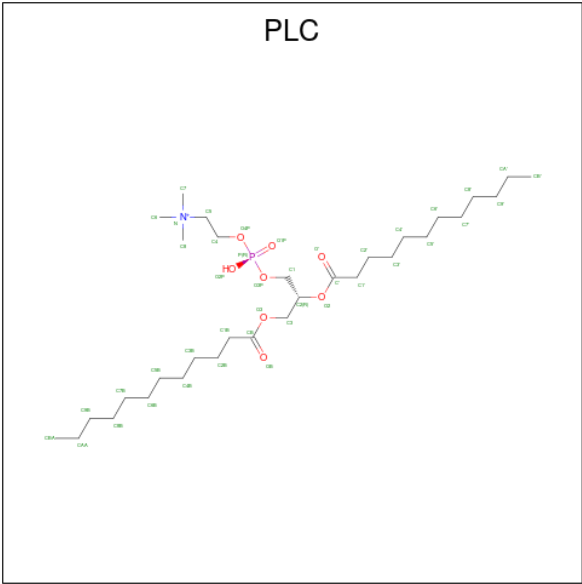
There are 7 unique types of molecules in this entry. The entry contains 13192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			2534	1669	405	456	4			
1	B	311	Total	C	N	O	S	0	2	0
			2545	1675	409	457	4			
1	C	311	Total	C	N	O	S	0	0	0
			2525	1664	404	453	4			
1	D	311	Total	C	N	O	S	0	0	0
			2525	1664	404	453	4			
1	E	311	Total	C	N	O	S	0	0	0
			2525	1664	404	453	4			

- Molecule 2 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			34	24	1	8	1		

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	2	Total Cl 2 2	0	0
3	C	2	Total Cl 2 2	0	0
3	D	2	Total Cl 2 2	0	0
3	E	2	Total Cl 2 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

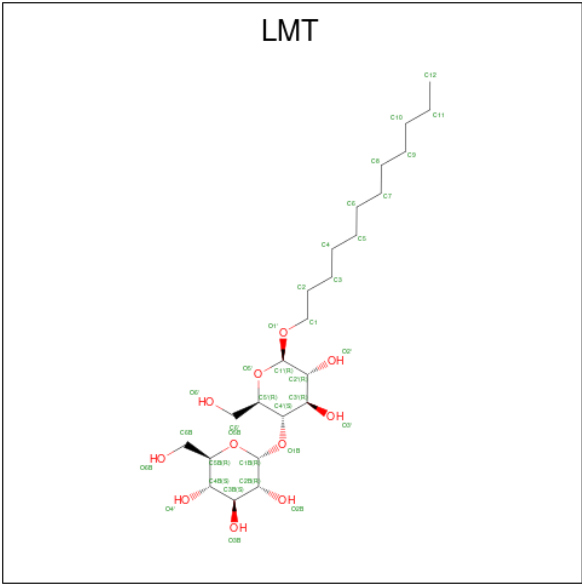
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0

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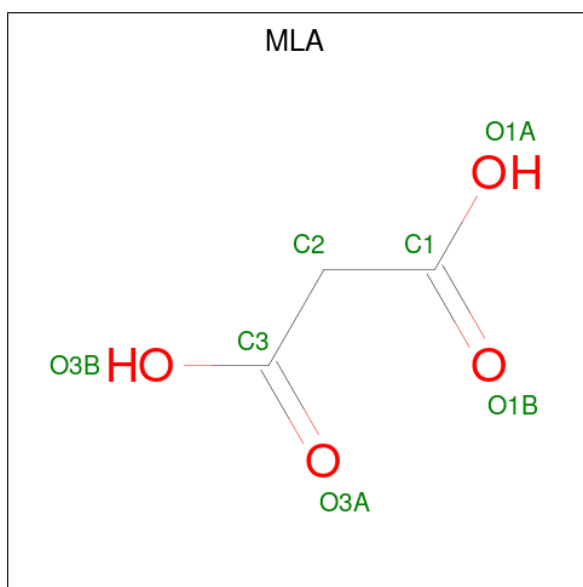
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		
4	D	2	Total	Na	0	0
			2	2		
4	E	1	Total	Na	0	0
			1	1		

- Molecule 5 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			12	12		
5	B	1	Total	C	0	0
			35	24		
				O		
				11		
5	C	1	Total	C	0	0
			12	12		
5	D	1	Total	C	0	0
			12	12		
5	E	1	Total	C	0	0
			12	12		
5	E	1	Total	C	0	0
			12	12		

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula: C₃H₄O₄).



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

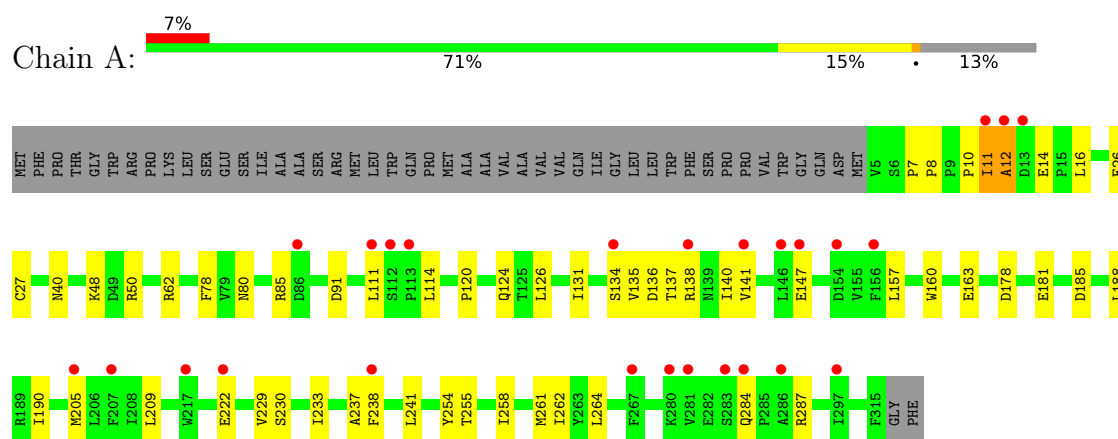
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	33	Total	O	0	0
			33	33		
7	B	36	Total	O	0	0
			36	36		
7	C	25	Total	O	0	0
			25	25		
7	D	30	Total	O	0	0
			30	30		
7	E	25	Total	O	0	0
			25	25		

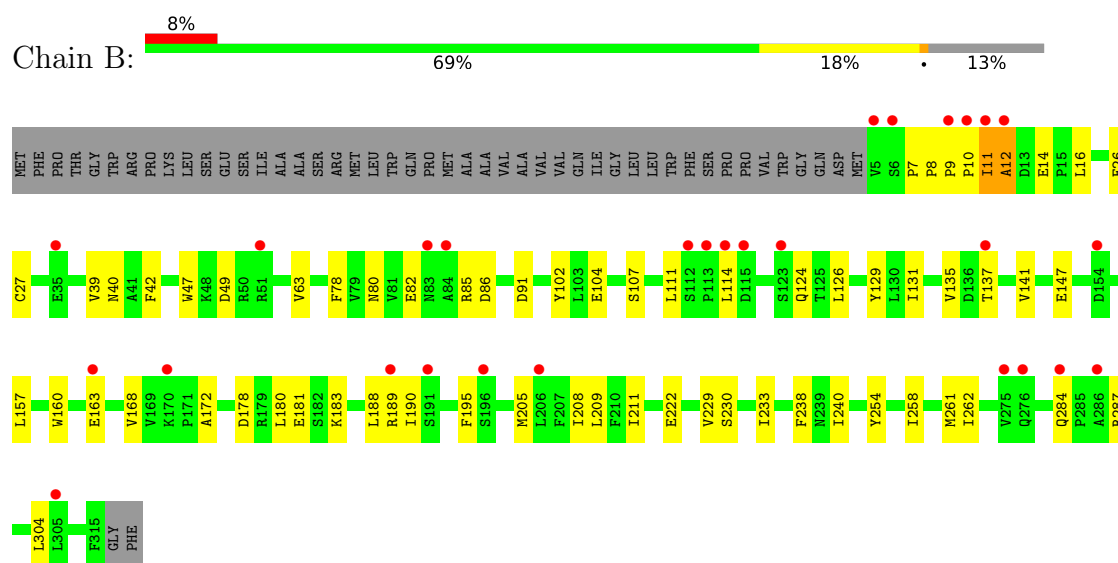
3 Residue-property plots [i](#)

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

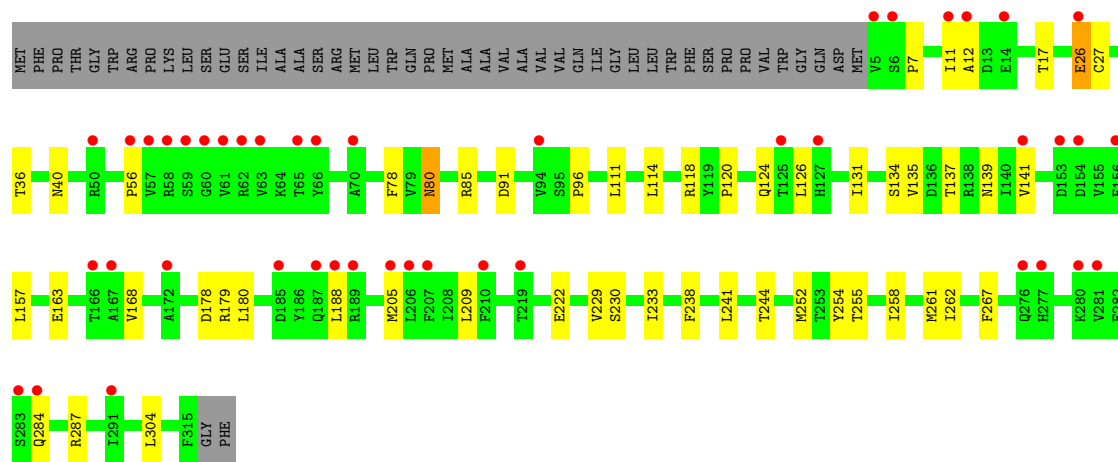


- Molecule 1: Proton-gated ion channel

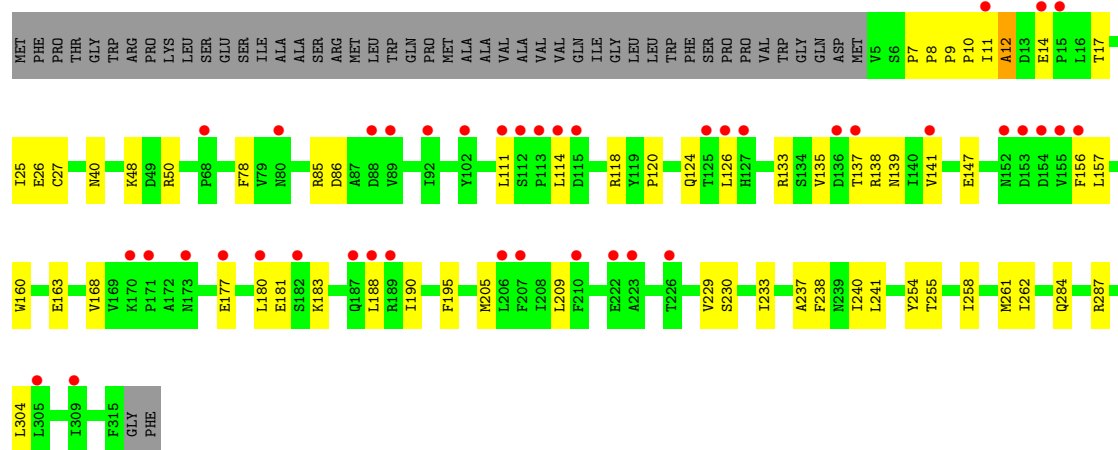


- Molecule 1: Proton-gated ion channel

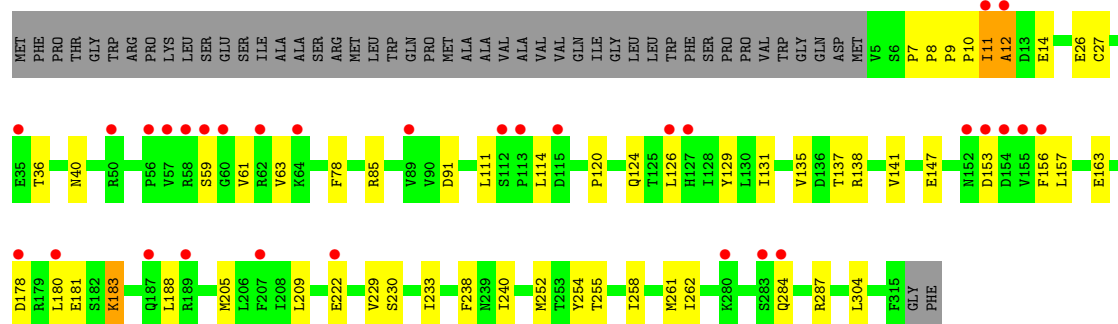
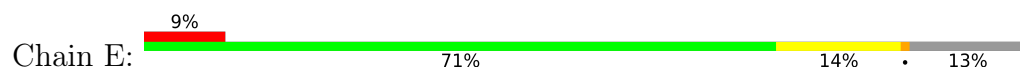




• Molecule 1: Proton-gated ion channel



• 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	180.10Å 133.37Å 158.99Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	49.00 – 3.00 49.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.00-3.00) 99.8 (49.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.182 , 0.199 0.206 , 0.218	Depositor DCC
R_{free} test set	4090 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13192	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: NA, LMT, MLA, CL, 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	0.78	0/2602	1.24	4/3557 (0.1%)
1	B	0.79	0/2613	1.23	6/3571 (0.2%)
1	C	0.77	0/2593	1.22	6/3545 (0.2%)
1	D	0.78	0/2593	1.24	9/3545 (0.3%)
1	E	0.76	0/2593	1.22	2/3545 (0.1%)
All	All	0.78	0/12994	1.23	27/17763 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	ALA	N-CA-C	-6.86	96.20	110.80
1	E	12	ALA	N-CA-C	-6.72	96.49	110.80
1	D	139	ASN	CA-CB-CG	6.61	119.21	112.60
1	A	12	ALA	N-CA-C	-6.52	96.92	110.80
1	B	12	ALA	N-CA-C	-6.33	97.31	110.80
1	D	138	ARG	N-CA-C	6.03	117.71	108.42
1	E	91	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	168	VAL	CA-C-N	5.75	128.63	120.53
1	B	168	VAL	C-N-CA	5.75	128.63	120.53
1	D	168	VAL	CA-C-N	5.70	128.57	120.53
1	D	168	VAL	C-N-CA	5.70	128.57	120.53
1	A	91	ASP	CA-CB-CG	5.63	118.23	112.60
1	D	86	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	12	ALA	N-CA-C	-5.40	99.30	110.80
1	D	138	ARG	CA-C-N	5.36	129.49	121.72
1	D	138	ARG	C-N-CA	5.36	129.49	121.72
1	C	26	GLU	CB-CG-CD	5.28	121.58	112.60
1	B	91	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	168	VAL	CA-C-N	5.20	127.86	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	VAL	C-N-CA	5.20	127.86	120.53
1	B	49	ASP	CA-C-N	5.18	127.95	120.38
1	B	49	ASP	C-N-CA	5.18	127.95	120.38
1	C	91	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	25	ILE	N-CA-C	-5.12	107.41	111.81
1	A	80	ASN	CA-CB-CG	5.11	117.71	112.60
1	C	80	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	185	ASP	CA-CB-CG	5.00	117.61	112.60

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	2534	0	2550	44	0
1	B	2545	0	2562	44	0
1	C	2525	0	2545	38	0
1	D	2525	0	2545	44	0
1	E	2525	0	2545	43	0
2	A	46	0	65	0	0
2	B	24	0	46	0	0
2	C	80	0	107	2	0
2	D	46	0	65	2	0
2	E	46	0	65	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
5	A	12	0	23	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	35	0	46	4	0
5	C	12	0	23	2	0
5	D	12	0	23	1	0
5	E	24	0	46	5	0
6	A	7	0	2	0	0
6	B	7	0	2	0	0
6	C	7	0	3	0	0
6	D	7	0	2	0	0
6	E	7	0	2	0	0
7	A	33	0	0	0	0
7	B	36	0	0	2	0
7	C	25	0	0	1	0
7	D	30	0	0	4	0
7	E	25	0	0	2	0
All	All	13192	0	13267	198	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 8.

All (198) 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:E:7:PRO:HG2	1:E:137:THR:HG21	1.27	1.14
1:D:26:GLU:OE2	1:E:111:LEU:HD12	1.49	1.10
1:C:7:PRO:HG2	1:C:137:THR:HG21	1.24	1.09
1:C:284:GLN:HE21	1:C:287:ARG:HD3	1.22	1.05
1:D:7:PRO:HG2	1:D:137:THR:HG21	1.38	1.05
1:B:284:GLN:HE21	1:B:287:ARG:HD3	1.21	1.05
1:A:284:GLN:HE21	1:A:287:ARG:HD3	1.20	1.04
1:E:284:GLN:HE21	1:E:287:ARG:HD3	1.21	1.01
1:D:284:GLN:HE21	1:D:287:ARG:HD2	1.31	0.96
1:A:48:LYS:HE3	1:A:50:ARG:HG3	1.45	0.96
1:E:7:PRO:CG	1:E:137:THR:HG21	1.96	0.95
1:A:284:GLN:HE22	1:A:287:ARG:HH11	1.16	0.94
1:C:7:PRO:CG	1:C:137:THR:HG21	1.99	0.93
1:B:284:GLN:HE22	1:B:287:ARG:HH11	1.18	0.92
1:C:284:GLN:NE2	1:C:287:ARG:HD3	1.86	0.90
1:A:284:GLN:NE2	1:A:287:ARG:HD3	1.85	0.90
1:B:284:GLN:NE2	1:B:287:ARG:HD3	1.86	0.90
1:C:284:GLN:HE22	1:C:287:ARG:HH11	1.16	0.90
1:E:284:GLN:NE2	1:E:287:ARG:HD3	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:GLN:HE22	1:E:287:ARG:HH11	1.16	0.88
1:B:82:GLU:HG2	1:B:111:LEU:HD11	1.57	0.86
1:B:7:PRO:HG2	1:B:137:THR:CG2	2.05	0.85
1:A:111:LEU:HD21	1:E:156:PHE:CE1	2.12	0.84
1:C:26:GLU:OE1	1:D:111:LEU:HD23	1.77	0.83
1:B:7:PRO:HG2	1:B:137:THR:HG21	1.58	0.82
1:E:7:PRO:HG2	1:E:137:THR:CG2	2.09	0.81
1:C:7:PRO:HG2	1:C:137:THR:CG2	2.09	0.81
1:D:284:GLN:NE2	1:D:287:ARG:HD2	1.95	0.81
1:D:7:PRO:CG	1:D:137:THR:HG21	2.11	0.80
1:E:10:PRO:HB2	1:E:12:ALA:O	1.82	0.79
1:A:8:PRO:HG2	1:A:138:ARG:NH1	1.98	0.78
1:B:82:GLU:HG2	1:B:111:LEU:CD1	2.13	0.77
1:B:10:PRO:HB2	1:B:12:ALA:O	1.83	0.77
1:A:8:PRO:HG2	1:A:138:ARG:HH11	1.50	0.77
1:D:10:PRO:HB2	1:D:12:ALA:O	1.85	0.76
1:A:136:ASP:HB2	7:E:502:HOH:O	1.84	0.76
1:A:16:LEU:HB2	1:A:138:ARG:NE	2.01	0.75
1:C:284:GLN:NE2	1:C:287:ARG:HH11	1.87	0.73
1:E:284:GLN:NE2	1:E:287:ARG:HH11	1.87	0.73
1:A:284:GLN:NE2	1:A:287:ARG:HH11	1.87	0.72
1:D:7:PRO:HG2	1:D:137:THR:CG2	2.20	0.71
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.73	0.71
1:E:147:GLU:HB2	7:E:505:HOH:O	1.89	0.70
1:D:48:LYS:HE2	1:D:50:ARG:HG3	1.72	0.70
1:E:36:THR:HG22	1:E:111:LEU:HD23	1.73	0.70
1:D:12:ALA:HB3	1:D:14:GLU:OE1	1.92	0.70
1:B:284:GLN:NE2	1:B:287:ARG:HH11	1.88	0.69
1:E:7:PRO:CG	1:E:137:THR:CG2	2.66	0.69
1:A:48:LYS:HE2	1:A:50:ARG:NH1	2.07	0.69
5:C:404:LMT:H82	5:E:401:LMT:H72	1.75	0.69
1:C:36:THR:HG22	1:C:111:LEU:HD23	1.74	0.68
1:A:16:LEU:HB2	1:A:138:ARG:CZ	2.23	0.68
1:A:10:PRO:HB2	1:A:12:ALA:O	1.93	0.68
1:D:237:ALA:HA	5:D:404:LMT:H102	1.77	0.67
1:D:284:GLN:HE22	1:D:287:ARG:NH1	1.92	0.66
1:D:133:ARG:HG3	1:D:181:GLU:OE2	1.95	0.65
7:C:501:HOH:O	1:D:133:ARG:NH2	2.30	0.65
1:C:7:PRO:CG	1:C:137:THR:CG2	2.71	0.64
1:A:111:LEU:HD21	1:E:156:PHE:HE1	1.59	0.64
1:B:7:PRO:CG	1:B:137:THR:CG2	2.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HG13	1:A:14:GLU:OE2	1.99	0.62
1:C:284:GLN:HE22	1:C:287:ARG:NH1	1.93	0.62
1:B:208:ILE:HD11	7:B:515:HOH:O	1.99	0.62
5:B:403:LMT:H72	5:E:401:LMT:H71	1.81	0.62
5:B:403:LMT:H6E	1:C:244:THR:HG22	1.82	0.61
1:B:284:GLN:HE22	1:B:287:ARG:NH1	1.95	0.61
1:E:284:GLN:HE22	1:E:287:ARG:NH1	1.94	0.60
1:D:156:PHE:CD2	7:D:518:HOH:O	2.52	0.60
1:A:111:LEU:CD2	1:E:156:PHE:HE1	2.15	0.59
1:A:26[B]:GLU:OE2	1:B:80:ASN:HA	2.01	0.59
1:B:11:ILE:HG13	1:B:14:GLU:OE2	2.03	0.58
1:A:134:SER:HA	1:A:140:ILE:HD12	1.84	0.58
1:A:48:LYS:HE3	1:A:50:ARG:CG	2.28	0.58
1:A:284:GLN:HE22	1:A:287:ARG:NH1	1.94	0.58
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.39	0.58
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.39	0.57
1:C:26:GLU:OE1	1:D:111:LEU:CD2	2.50	0.57
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.40	0.57
1:D:7:PRO:HG3	1:D:135:VAL:HG21	1.86	0.57
1:B:205:MET:HE2	1:B:238:PHE:HB3	1.86	0.57
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.40	0.57
1:B:230:SER:HB2	1:C:229:VAL:HG11	1.87	0.57
1:D:7:PRO:CG	1:D:137:THR:CG2	2.82	0.56
1:D:205:MET:HE2	1:D:238:PHE:HB3	1.88	0.56
1:E:205:MET:HE2	1:E:238:PHE:HB3	1.87	0.56
1:C:205:MET:HE2	1:C:238:PHE:HB3	1.87	0.56
1:D:230:SER:HB2	1:E:229:VAL:HG11	1.88	0.55
1:A:7:PRO:HG3	1:A:135:VAL:HG21	1.88	0.55
1:A:205:MET:HE2	1:A:238:PHE:HB3	1.87	0.55
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.41	0.55
5:C:404:LMT:H102	5:E:401:LMT:H92	1.89	0.55
1:D:26:GLU:HB2	1:D:40:ASN:HB3	1.89	0.54
1:E:7:PRO:HG3	1:E:137:THR:CG2	2.37	0.54
1:C:7:PRO:HG3	1:C:135:VAL:HG21	1.88	0.54
1:C:36:THR:CG2	1:C:111:LEU:HD23	2.38	0.53
1:D:126:LEU:HD12	1:D:188:LEU:HD23	1.91	0.53
1:D:195:PHE:HZ	1:E:252:MET:HG2	1.73	0.53
1:E:36:THR:CG2	1:E:111:LEU:HD23	2.37	0.53
1:E:126:LEU:HD12	1:E:188:LEU:HD23	1.91	0.53
1:A:16:LEU:HD13	1:A:138:ARG:NH1	2.23	0.53
1:B:129:TYR:CD1	1:B:183:LYS:HE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD12	1:A:188:LEU:HD23	1.91	0.53
1:B:160:TRP:CE3	1:B:190:ILE:HD12	2.44	0.52
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.73	0.52
1:D:133:ARG:CG	1:D:181:GLU:OE2	2.57	0.52
1:B:284:GLN:NE2	1:B:287:ARG:CD	2.69	0.51
1:E:11:ILE:HG13	1:E:14:GLU:OE2	2.09	0.51
1:A:160:TRP:CE3	1:A:190:ILE:HD12	2.45	0.51
1:B:172:ALA:HB3	1:B:183:LYS:HB3	1.93	0.51
1:C:126:LEU:HD12	1:C:188:LEU:HD23	1.91	0.51
1:E:26:GLU:HB2	1:E:40:ASN:HB3	1.93	0.51
1:B:284:GLN:NE2	1:B:287:ARG:NH1	2.58	0.50
1:A:284:GLN:NE2	1:A:287:ARG:NH1	2.57	0.50
1:B:195:PHE:HZ	1:C:252:MET:HG2	1.77	0.49
1:C:284:GLN:NE2	1:C:287:ARG:CD	2.69	0.49
1:E:7:PRO:HG3	1:E:135:VAL:HG21	1.93	0.49
1:B:208:ILE:CD1	7:B:515:HOH:O	2.57	0.49
1:C:284:GLN:NE2	1:C:287:ARG:NH1	2.57	0.49
1:A:48:LYS:HE2	1:A:50:ARG:HH11	1.76	0.48
1:B:126:LEU:HD12	1:B:188:LEU:HD23	1.95	0.48
1:B:26[B]:GLU:HB2	1:B:40:ASN:HB3	1.95	0.48
1:D:48:LYS:NZ	1:D:50:ARG:NH1	2.61	0.48
1:A:284:GLN:NE2	1:A:287:ARG:CD	2.68	0.48
1:E:284:GLN:NE2	1:E:287:ARG:CD	2.69	0.48
1:E:254:TYR:CZ	1:E:258:ILE:HD11	2.50	0.47
1:C:26:GLU:HB2	1:C:40:ASN:HB3	1.97	0.47
5:A:405:LMT:H112	5:E:401:LMT:H102	1.97	0.47
1:A:27:CYS:HB3	1:A:157:LEU:HD13	1.97	0.46
1:E:129:TYR:CD1	1:E:183:LYS:HE2	2.50	0.46
1:A:26[B]:GLU:HB2	1:A:40:ASN:HB3	1.96	0.46
1:B:254:TYR:CZ	1:B:258:ILE:HD11	2.51	0.46
1:B:39:VAL:O	1:B:107:SER:HA	2.15	0.46
1:B:12:ALA:HB3	1:B:14:GLU:OE1	2.15	0.46
1:A:254:TYR:CZ	1:A:258:ILE:HD11	2.51	0.46
1:D:254:TYR:CZ	1:D:258:ILE:HD11	2.50	0.45
1:D:241:LEU:HD22	1:E:240:ILE:HG12	1.98	0.45
1:C:254:TYR:CZ	1:C:258:ILE:HD11	2.52	0.45
1:E:27:CYS:HB3	1:E:157:LEU:HD13	1.97	0.45
1:A:229:VAL:HG11	1:E:230:SER:HB2	1.98	0.45
1:E:59:SER:C	1:E:61:VAL:H	2.25	0.45
1:B:26[A]:GLU:HB2	1:B:40:ASN:HB3	1.99	0.45
1:B:114:LEU:HD22	1:B:124:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:PRO:HG3	1:C:137:THR:CG2	2.47	0.45
1:C:56:PRO:HD3	1:C:96:PRO:HB3	1.99	0.44
1:C:261:MET:HE2	1:C:261:MET:HB3	1.94	0.44
1:E:8:PRO:HA	1:E:9:PRO:HD3	1.90	0.44
2:C:408:PLC:H1A1	2:C:408:PLC:H31	1.78	0.44
5:B:403:LMT:H91	5:E:401:LMT:H91	1.99	0.44
1:D:261:MET:HE2	1:D:261:MET:HB3	1.94	0.44
1:D:27:CYS:HB3	1:D:157:LEU:HD13	2.00	0.44
1:E:284:GLN:NE2	1:E:287:ARG:NH1	2.57	0.44
1:A:111:LEU:CD2	1:E:156:PHE:CE1	2.89	0.44
1:C:27:CYS:HB3	1:C:157:LEU:HD13	1.98	0.44
1:A:114:LEU:HD22	1:A:124:GLN:HG3	2.00	0.44
1:D:12:ALA:HB3	1:D:14:GLU:CD	2.42	0.44
1:D:114:LEU:HD22	1:D:124:GLN:HG3	2.00	0.43
1:B:27:CYS:HB3	1:B:157:LEU:HD13	2.00	0.43
1:B:211:ILE:HG13	1:C:267:PHE:HD1	1.81	0.43
1:E:135:VAL:HG23	1:E:138:ARG:H	1.83	0.43
1:D:177:GLU:OE1	7:D:501:HOH:O	2.21	0.43
1:B:16:LEU:HD11	1:B:47:TRP:HB2	1.99	0.43
1:C:134:SER:HB3	1:C:139:ASN:HA	2.00	0.43
1:B:209:LEU:HD13	1:B:262:ILE:HG23	2.01	0.43
1:E:114:LEU:HD22	1:E:124:GLN:HG3	2.01	0.43
1:C:209:LEU:HD13	1:C:262:ILE:HG23	2.01	0.43
1:C:230:SER:HB2	1:D:229:VAL:HG11	2.01	0.43
1:A:230:SER:HB2	1:B:229:VAL:HG11	2.00	0.43
1:C:241:LEU:HD22	1:D:240:ILE:HG12	2.01	0.42
1:A:241:LEU:HD22	1:B:240:ILE:HG12	2.00	0.42
1:A:48:LYS:CE	1:A:50:ARG:NH1	2.78	0.42
1:B:230:SER:CB	1:C:229:VAL:HG11	2.49	0.42
1:E:261:MET:HE2	1:E:261:MET:HB3	1.94	0.42
1:D:209:LEU:HD13	1:D:262:ILE:HG23	2.02	0.42
1:A:26[A]:GLU:HB2	1:A:40:ASN:HB3	2.01	0.42
1:D:156:PHE:CE2	7:D:518:HOH:O	2.72	0.42
2:D:401:PLC:H6'2	2:D:401:PLC:H2A1	2.01	0.41
1:D:160:TRP:CE3	1:D:190:ILE:HD12	2.55	0.41
1:E:209:LEU:HD13	1:E:262:ILE:HG23	2.02	0.41
1:D:8:PRO:HA	1:D:9:PRO:HD3	1.90	0.41
1:D:120:PRO:HD3	1:D:255:THR:OG1	2.20	0.41
1:A:261:MET:HE2	1:A:261:MET:HB3	1.94	0.41
1:E:12:ALA:HB3	1:E:14:GLU:OE1	2.20	0.41
1:C:114:LEU:HD22	1:C:124:GLN:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:MET:HA	1:A:264:LEU:HD12	2.03	0.41
1:B:102:TYR:HE1	1:B:104:GLU:HG2	1.86	0.41
1:D:118:ARG:HH12	2:D:401:PLC:H41	1.85	0.41
1:B:8:PRO:HA	1:B:9:PRO:HD3	1.96	0.41
1:B:26[B]:GLU:OE2	1:C:80:ASN:HA	2.20	0.41
1:C:120:PRO:HD3	1:C:255:THR:OG1	2.20	0.41
1:D:230:SER:CB	1:E:229:VAL:HG11	2.50	0.41
1:A:237:ALA:HB2	5:B:403:LMT:H111	2.02	0.40
1:A:120:PRO:HD3	1:A:255:THR:OG1	2.21	0.40
1:D:284:GLN:HE22	1:D:287:ARG:HH11	1.69	0.40
1:B:261:MET:HE2	1:B:261:MET:HB3	1.95	0.40
1:A:209:LEU:HD13	1:A:262:ILE:HG23	2.02	0.40
1:C:118:ARG:HH12	2:C:401:PLC:H52	1.86	0.40
1:D:156:PHE:HD2	7:D:518:HOH:O	1.96	0.40
1:E:120:PRO:HD3	1:E:255:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/359 (86%)	301 (97%)	9 (3%)	0	100	100
1	B	311/359 (87%)	299 (96%)	12 (4%)	0	100	100
1	C	309/359 (86%)	299 (97%)	10 (3%)	0	100	100
1	D	309/359 (86%)	298 (96%)	11 (4%)	0	100	100
1	E	309/359 (86%)	297 (96%)	12 (4%)	0	100	100
All	All	1548/1795 (86%)	1494 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/319 (88%)	270 (96%)	11 (4%)	28	62
1	B	282/319 (88%)	268 (95%)	14 (5%)	22	56
1	C	280/319 (88%)	269 (96%)	11 (4%)	28	62
1	D	280/319 (88%)	271 (97%)	9 (3%)	34	67
1	E	280/319 (88%)	267 (95%)	13 (5%)	24	58
All	All	1403/1595 (88%)	1345 (96%)	58 (4%)	27	61

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	62	ARG
1	A	131	ILE
1	A	137	THR
1	A	141	VAL
1	A	147	GLU
1	A	163	GLU
1	A	178	ASP
1	A	181	GLU
1	A	222	GLU
1	A	233	ILE
1	B	11	ILE
1	B	42	PHE
1	B	63	VAL
1	B	86	ASP
1	B	131	ILE
1	B	141	VAL
1	B	147	GLU
1	B	163	GLU
1	B	178	ASP
1	B	180	LEU
1	B	181	GLU
1	B	222	GLU

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Mol	Chain	Res	Type
1	B	233	ILE
1	B	304	LEU
1	C	11	ILE
1	C	17	THR
1	C	131	ILE
1	C	141	VAL
1	C	163	GLU
1	C	178	ASP
1	C	179	ARG
1	C	180	LEU
1	C	222	GLU
1	C	233	ILE
1	C	304	LEU
1	D	11	ILE
1	D	17	THR
1	D	141	VAL
1	D	147	GLU
1	D	163	GLU
1	D	180	LEU
1	D	183	LYS
1	D	233	ILE
1	D	304	LEU
1	E	11	ILE
1	E	63	VAL
1	E	131	ILE
1	E	141	VAL
1	E	153	ASP
1	E	163	GLU
1	E	178	ASP
1	E	180	LEU
1	E	181	GLU
1	E	183	LYS
1	E	222	GLU
1	E	233	ILE
1	E	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	HIS
1	A	284	GLN
1	B	277	HIS

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Mol	Chain	Res	Type
1	B	284	GLN
1	B	307	ASN
1	C	277	HIS
1	C	284	GLN
1	D	139	ASN
1	D	173	ASN
1	D	277	HIS
1	D	284	GLN
1	E	187	GLN
1	E	277	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 17 are monoatomic - leaving 22 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
6	MLA	E	408	-	6,6,6	3.00	4 (66%)	7,7,7	3.42	4 (57%)
2	PLC	D	402	-	11,11,41	0.49	0	10,10,49	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MLA	A	406	-	6,6,6	2.91	4 (66%)	7,7,7	3.41	4 (57%)
2	PLC	B	401	-	11,11,41	0.47	0	10,10,49	0.60	0
2	PLC	C	408	-	33,33,41	1.32	5 (15%)	39,41,49	1.09	3 (7%)
2	PLC	D	401	-	33,33,41	1.21	4 (12%)	39,41,49	1.14	4 (10%)
2	PLC	A	401	-	33,33,41	1.18	4 (12%)	39,41,49	1.00	2 (5%)
5	LMT	C	404	-	11,11,36	0.69	0	10,10,47	0.64	0
5	LMT	E	401	-	11,11,36	0.71	0	10,10,47	0.44	0
6	MLA	C	407	-	6,6,6	2.48	3 (50%)	7,7,7	2.52	2 (28%)
5	LMT	E	405	-	11,11,36	0.74	0	10,10,47	0.47	0
5	LMT	A	405	-	11,11,36	0.76	0	10,10,47	0.60	0
2	PLC	A	402	-	11,11,41	0.47	0	10,10,49	0.67	0
6	MLA	D	407	-	6,6,6	2.19	2 (33%)	7,7,7	2.74	3 (42%)
6	MLA	B	406	-	6,6,6	1.80	2 (33%)	7,7,7	3.09	4 (57%)
2	PLC	C	401	-	33,33,41	1.16	4 (12%)	39,41,49	1.09	3 (7%)
2	PLC	E	403	-	11,11,41	0.54	0	10,10,49	0.54	0
5	LMT	D	404	-	11,11,36	0.78	0	10,10,47	0.52	0
5	LMT	B	403	-	36,36,36	1.55	8 (22%)	47,47,47	1.59	10 (21%)
2	PLC	C	402	-	11,11,41	0.52	0	10,10,49	0.61	0
2	PLC	B	407	-	11,11,41	0.32	0	10,10,49	0.85	0
2	PLC	E	402	-	33,33,41	1.01	1 (3%)	39,41,49	1.08	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
6	MLA	E	408	-	-	0/4/4/4	-
2	PLC	D	402	-	-	0/9/9/45	-
6	MLA	A	406	-	-	2/4/4/4	-
2	PLC	B	401	-	-	1/9/9/45	-
2	PLC	C	408	-	-	18/37/37/45	-
2	PLC	D	401	-	-	13/37/37/45	-
2	PLC	A	401	-	-	12/37/37/45	-
5	LMT	C	404	-	-	0/9/9/61	-
5	LMT	E	401	-	-	0/9/9/61	-
6	MLA	C	407	-	-	0/4/4/4	-
5	LMT	E	405	-	-	0/9/9/61	-
5	LMT	A	405	-	-	0/9/9/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLC	A	402	-	-	0/9/9/45	-
6	MLA	D	407	-	-	2/4/4/4	-
6	MLA	B	406	-	-	2/4/4/4	-
2	PLC	C	401	-	-	12/37/37/45	-
2	PLC	E	403	-	-	2/9/9/45	-
5	LMT	D	404	-	-	0/9/9/61	-
5	LMT	B	403	-	-	13/21/61/61	0/2/2/2
2	PLC	C	402	-	-	0/9/9/45	-
2	PLC	B	407	-	-	1/9/9/45	-
2	PLC	E	402	-	-	19/37/37/45	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	407	MLA	O3A-C3	4.74	1.37	1.22
6	E	408	MLA	O1B-C1	4.47	1.36	1.22
6	E	408	MLA	O3A-C3	4.45	1.36	1.22
6	D	407	MLA	O1B-C1	4.25	1.36	1.22
6	A	406	MLA	O3A-C3	4.17	1.35	1.22
6	A	406	MLA	O1B-C1	3.86	1.34	1.22
5	B	403	LMT	C3'-C4'	3.74	1.62	1.52
6	B	406	MLA	O1B-C1	3.55	1.33	1.22
5	B	403	LMT	C4B-C5B	3.46	1.60	1.53
5	B	403	LMT	C4B-C3B	3.44	1.61	1.52
5	B	403	LMT	C3'-C2'	3.24	1.60	1.52
6	A	406	MLA	O3B-C3	-3.15	1.20	1.30
2	C	408	PLC	O2-C'	3.01	1.42	1.34
6	E	408	MLA	O3B-C3	-2.99	1.20	1.30
2	D	401	PLC	O2-C'	2.91	1.42	1.34
2	A	401	PLC	O2-C'	2.84	1.42	1.34
6	A	406	MLA	O1A-C1	-2.83	1.21	1.30
5	B	403	LMT	C4'-C5'	2.82	1.60	1.52
2	C	401	PLC	O2-C'	2.81	1.42	1.34
6	C	407	MLA	O3B-C3	-2.80	1.21	1.30
6	D	407	MLA	O1A-C1	-2.74	1.21	1.30
2	C	408	PLC	P-O4P	2.64	1.69	1.59
2	C	401	PLC	O3-CB	2.56	1.40	1.33
2	D	401	PLC	O3-CB	2.50	1.40	1.33
2	A	401	PLC	C5-N	2.49	1.59	1.51
2	E	402	PLC	O2-C'	2.48	1.41	1.34
6	B	406	MLA	O1A-C1	-2.39	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	PLC	P-O4P	2.29	1.68	1.59
2	A	401	PLC	P-O4P	2.28	1.68	1.59
2	A	401	PLC	O3-CB	2.27	1.40	1.33
2	C	408	PLC	C5-N	2.19	1.58	1.51
2	C	408	PLC	C5-C4	2.19	1.57	1.51
2	C	408	PLC	O3-CB	2.18	1.39	1.33
6	E	408	MLA	O1A-C1	-2.17	1.23	1.30
5	B	403	LMT	C1'-C2'	2.17	1.58	1.52
6	C	407	MLA	O1A-C1	2.16	1.38	1.30
2	C	401	PLC	P-O4P	2.16	1.67	1.59
2	C	401	PLC	C5-N	2.16	1.58	1.51
5	B	403	LMT	C3B-C2B	2.07	1.57	1.52
2	D	401	PLC	C5-N	2.04	1.57	1.51
5	B	403	LMT	C1B-C2B	2.03	1.58	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	406	MLA	O1A-C1-C2	5.54	131.68	114.51
6	E	408	MLA	O1A-C1-C2	5.07	130.23	114.51
6	D	407	MLA	O1A-C1-C2	4.96	129.88	114.51
6	A	406	MLA	O1A-C1-C2	4.95	129.86	114.51
6	C	407	MLA	O3B-C3-C2	4.79	129.34	114.51
6	A	406	MLA	O3B-C3-C2	4.71	129.12	114.51
6	E	408	MLA	O3B-C3-C2	4.65	128.92	114.51
6	B	406	MLA	O1B-C1-C2	-4.24	110.03	122.11
6	E	408	MLA	O1B-C1-C2	-4.03	110.64	122.11
6	A	406	MLA	O1B-C1-C2	-4.02	110.65	122.11
6	D	407	MLA	O1B-C1-C2	-3.90	111.01	122.11
5	B	403	LMT	O1'-C1'-C2'	-3.86	102.42	108.27
5	B	403	LMT	O5B-C5B-C4B	3.84	116.63	109.70
6	A	406	MLA	O3A-C3-C2	-3.75	111.42	122.11
6	E	408	MLA	O3A-C3-C2	-3.63	111.77	122.11
2	E	402	PLC	C3-C2-C1	3.57	120.11	111.78
6	C	407	MLA	O3A-C3-C2	-3.44	112.32	122.11
2	E	402	PLC	C2-O2-C'	3.36	125.83	117.80
2	C	408	PLC	O3-CB-OB	-3.32	115.32	123.63
5	B	403	LMT	C3B-C4B-C5B	3.24	116.11	110.23
2	A	401	PLC	C2-O2-C'	3.22	125.50	117.80
2	D	401	PLC	O3-CB-OB	-2.98	116.18	123.63
5	B	403	LMT	C1B-O5B-C5B	2.95	119.48	113.72
6	B	406	MLA	O3A-C3-C2	2.95	130.50	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	LMT	O1B-C4'-C3'	2.91	114.64	107.23
2	A	401	PLC	C3-C2-C1	2.90	118.55	111.78
2	D	401	PLC	C3-C2-C1	2.89	118.53	111.78
2	C	401	PLC	O3-CB-OB	-2.85	116.51	123.63
6	D	407	MLA	O3A-C3-C2	2.60	129.51	122.11
2	C	401	PLC	C2-O2-C'	2.57	123.96	117.80
5	B	403	LMT	C4B-C3B-C2B	2.48	115.18	110.83
2	C	408	PLC	O3-CB-C1B	2.34	118.98	111.83
2	D	401	PLC	C2-O2-C'	2.33	123.38	117.80
5	B	403	LMT	C2'-C3'-C4'	2.27	114.84	109.68
2	D	401	PLC	O3-CB-C1B	2.18	118.49	111.83
5	B	403	LMT	C1-O1'-C1'	2.17	117.39	113.68
2	C	401	PLC	C3-C2-C1	2.16	116.83	111.78
5	B	403	LMT	O3B-C3B-C4B	-2.15	105.32	110.38
6	B	406	MLA	O3B-C3-O3A	-2.11	117.90	123.33
2	C	408	PLC	C2-O2-C'	2.10	122.83	117.80
5	B	403	LMT	O4'-C4B-C5B	-2.01	104.37	109.32

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PLC	C1'-C'-O2-C2
2	A	401	PLC	C1-O3P-P-O1P
2	A	401	PLC	C1-O3P-P-O2P
2	C	401	PLC	O4P-C4-C5-N
2	C	401	PLC	C1'-C'-O2-C2
2	C	401	PLC	C1B-CB-O3-C3
2	C	401	PLC	OB-CB-O3-C3
2	C	401	PLC	C4-O4P-P-O2P
2	C	401	PLC	C4-O4P-P-O3P
2	C	408	PLC	C2-C1-O3P-P
2	C	408	PLC	C1B-CB-O3-C3
2	C	408	PLC	OB-CB-O3-C3
2	C	408	PLC	C1-O3P-P-O1P
2	C	408	PLC	C1-O3P-P-O2P
2	C	408	PLC	C1-O3P-P-O4P
2	D	401	PLC	C1'-C'-O2-C2
2	D	401	PLC	C1B-CB-O3-C3
2	D	401	PLC	OB-CB-O3-C3
2	D	401	PLC	C4-O4P-P-O3P
2	E	402	PLC	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
2	E	402	PLC	C1'-C'-O2-C2
2	E	402	PLC	C4-O4P-P-O3P
5	B	403	LMT	C3'-C4'-O1B-C1B
2	A	401	PLC	O'-C'-O2-C2
2	C	401	PLC	O'-C'-O2-C2
2	D	401	PLC	O'-C'-O2-C2
2	E	402	PLC	O'-C'-O2-C2
2	E	402	PLC	C4-C5-N-C8
2	E	402	PLC	CB-C1B-C2B-C3B
2	E	402	PLC	C4-C5-N-C7
2	A	401	PLC	CB-C1B-C2B-C3B
2	C	408	PLC	CB-C1B-C2B-C3B
2	D	401	PLC	C'-C1'-C2'-C3'
2	E	402	PLC	C'-C1'-C2'-C3'
2	C	401	PLC	C3-C2-O2-C'
5	B	403	LMT	C2-C3-C4-C5
2	A	401	PLC	C3B-C4B-C5B-C6B
2	C	408	PLC	C1-C2-C3-O3
2	E	402	PLC	C4-C5-N-C6
2	A	401	PLC	C1B-C2B-C3B-C4B
2	E	402	PLC	C1B-C2B-C3B-C4B
5	B	403	LMT	C7-C8-C9-C10
2	C	401	PLC	O2-C2-C3-O3
2	E	403	PLC	C5'-C6'-C7'-C8'
2	E	402	PLC	C3B-C4B-C5B-C6B
2	C	408	PLC	C2B-C3B-C4B-C5B
2	E	402	PLC	C3'-C4'-C5'-C6'
5	B	403	LMT	O5'-C5'-C6'-O6'
5	B	403	LMT	C3-C4-C5-C6
5	B	403	LMT	C2B-C1B-O1B-C4'
5	B	403	LMT	C5-C6-C7-C8
5	B	403	LMT	C2-C1-O1'-C1'
2	C	408	PLC	O3P-C1-C2-C3
2	C	408	PLC	C1'-C'-O2-C2
2	B	401	PLC	C3'-C4'-C5'-C6'
2	E	402	PLC	C4B-C5B-C6B-C7B
5	B	403	LMT	O1'-C1-C2-C3
2	A	401	PLC	C3-C2-O2-C'
2	D	401	PLC	C3-C2-O2-C'
2	C	408	PLC	O'-C'-O2-C2
2	C	408	PLC	O3P-C1-C2-O2
2	A	401	PLC	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
2	D	401	PLC	O4P-C4-C5-N
2	E	402	PLC	O3P-C1-C2-O2
2	E	403	PLC	C1'-C2'-C3'-C4'
2	A	401	PLC	C1-O3P-P-O4P
2	C	401	PLC	C4-O4P-P-O1P
2	D	401	PLC	C4-O4P-P-O2P
2	E	402	PLC	C1-O3P-P-O1P
2	E	402	PLC	C4-O4P-P-O1P
5	B	403	LMT	O5B-C1B-O1B-C4'
6	B	406	MLA	O1B-C1-C2-C3
6	D	407	MLA	O1B-C1-C2-C3
2	A	401	PLC	C'-C1'-C2'-C3'
5	B	403	LMT	O5'-C1'-O1'-C1
2	C	408	PLC	C1B-C2B-C3B-C4B
2	C	408	PLC	C1-C2-O2-C'
2	E	402	PLC	C3-C2-O2-C'
6	B	406	MLA	O1A-C1-C2-C3
6	D	407	MLA	O1A-C1-C2-C3
2	C	408	PLC	O2-C2-C3-O3
2	D	401	PLC	O2-C2-C3-O3
2	B	407	PLC	C2'-C3'-C4'-C5'
2	C	401	PLC	CB-C1B-C2B-C3B
5	B	403	LMT	C4-C5-C6-C7
5	B	403	LMT	C11-C10-C9-C8
2	C	408	PLC	C2B-C1B-CB-O3
2	E	402	PLC	C2B-C1B-CB-O3
2	C	401	PLC	C1-C2-C3-O3
2	D	401	PLC	CB-C1B-C2B-C3B
6	A	406	MLA	O1A-C1-C2-C3
6	A	406	MLA	O1B-C1-C2-C3
2	C	408	PLC	C2B-C1B-CB-OB
2	D	401	PLC	O2-C'-C1'-C2'
2	E	402	PLC	C2B-C1B-CB-OB
2	D	401	PLC	O'-C'-C1'-C2'
2	A	401	PLC	C4B-C5B-C6B-C7B

There are no ring outliers.

8 monomers are involved in 12 short contacts:

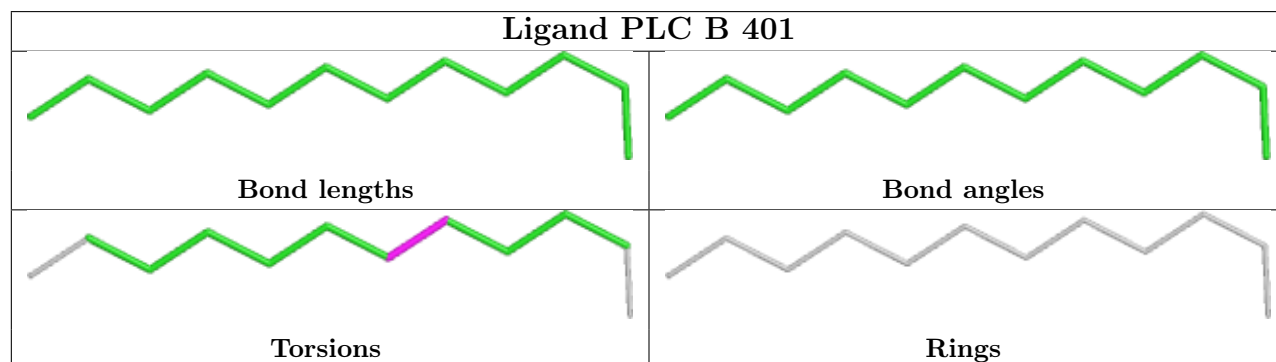
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	408	PLC	1	0
2	D	401	PLC	2	0

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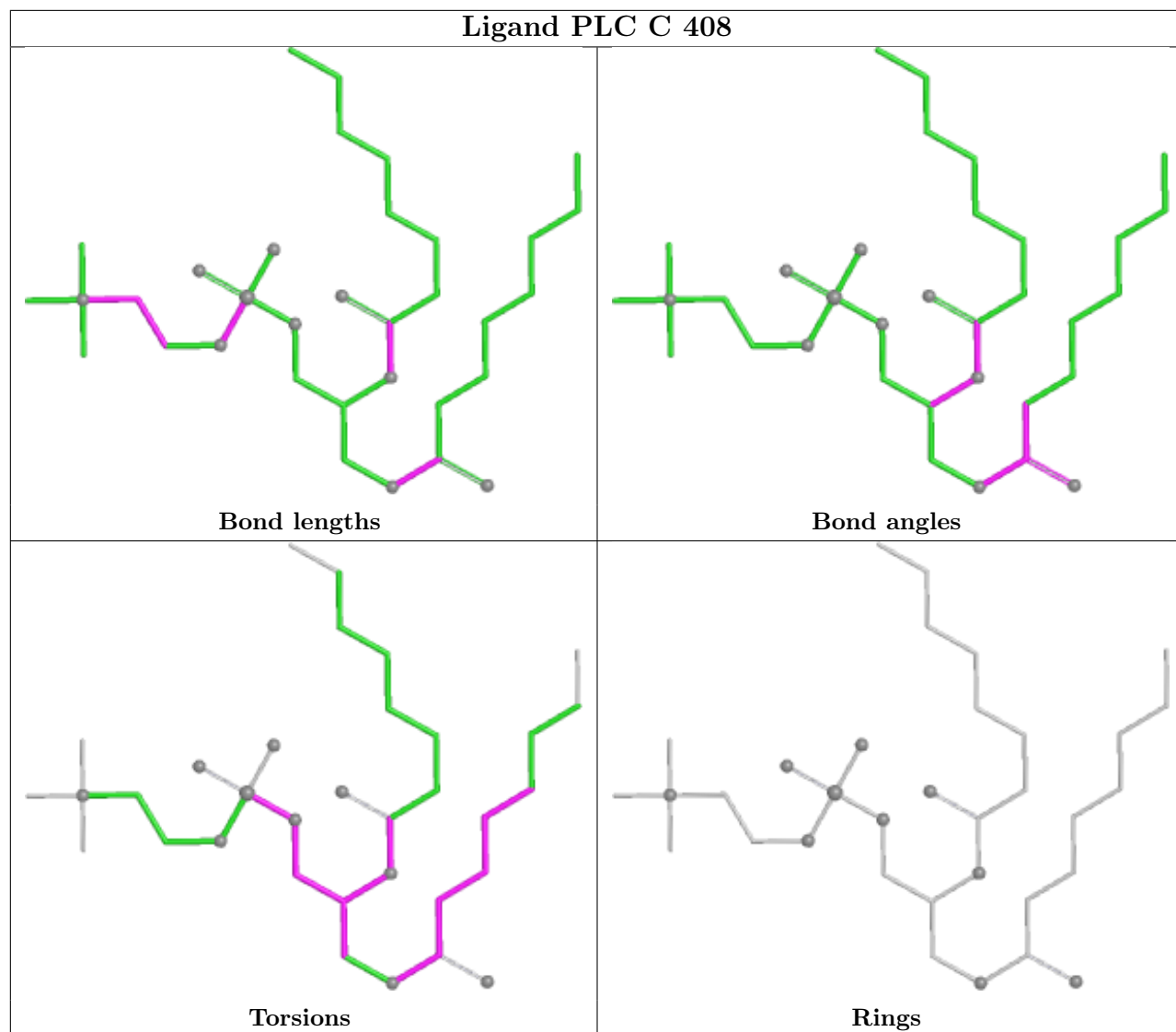
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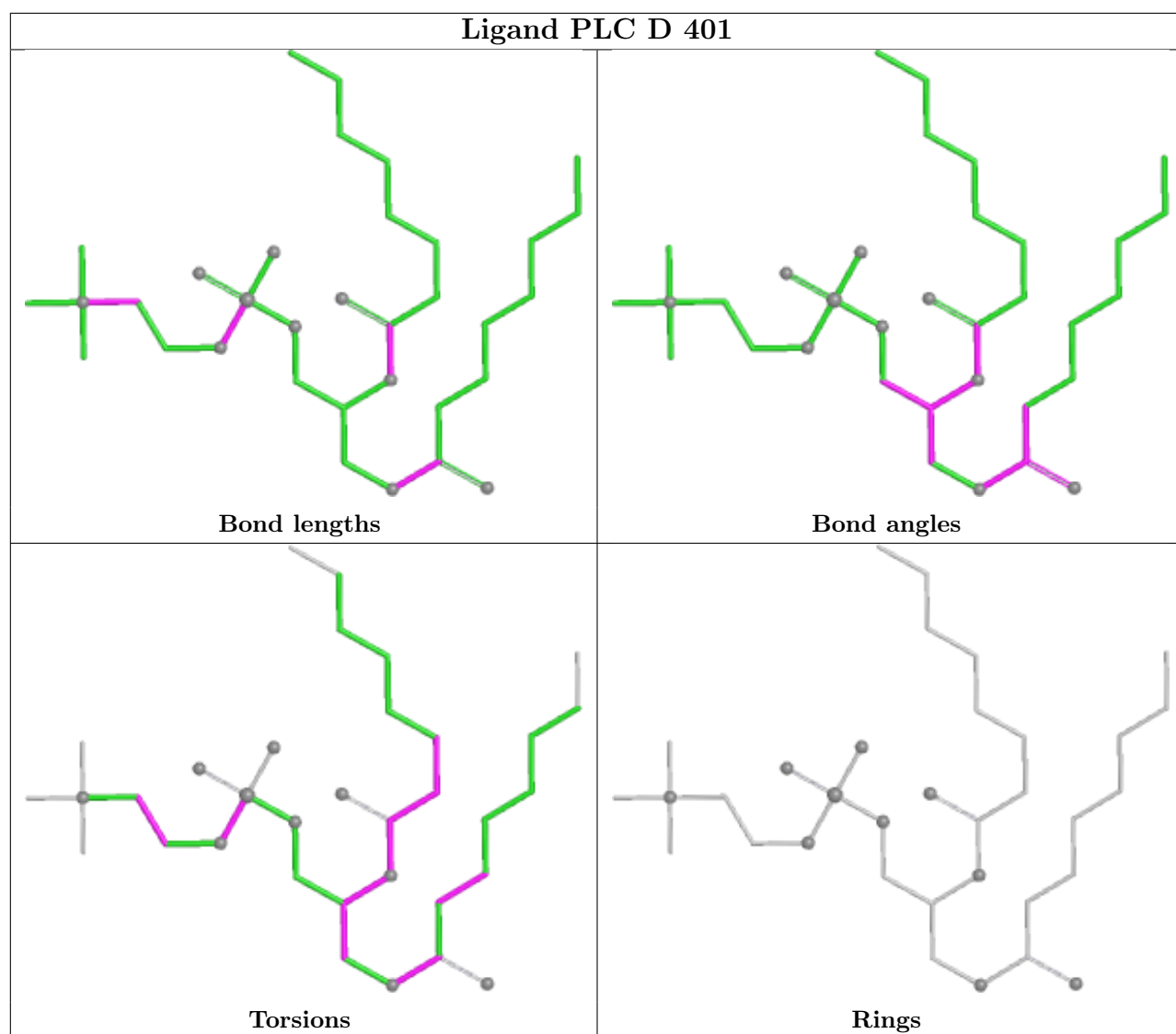
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	404	LMT	2	0
5	E	401	LMT	5	0
5	A	405	LMT	1	0
2	C	401	PLC	1	0
5	D	404	LMT	1	0
5	B	403	LMT	4	0

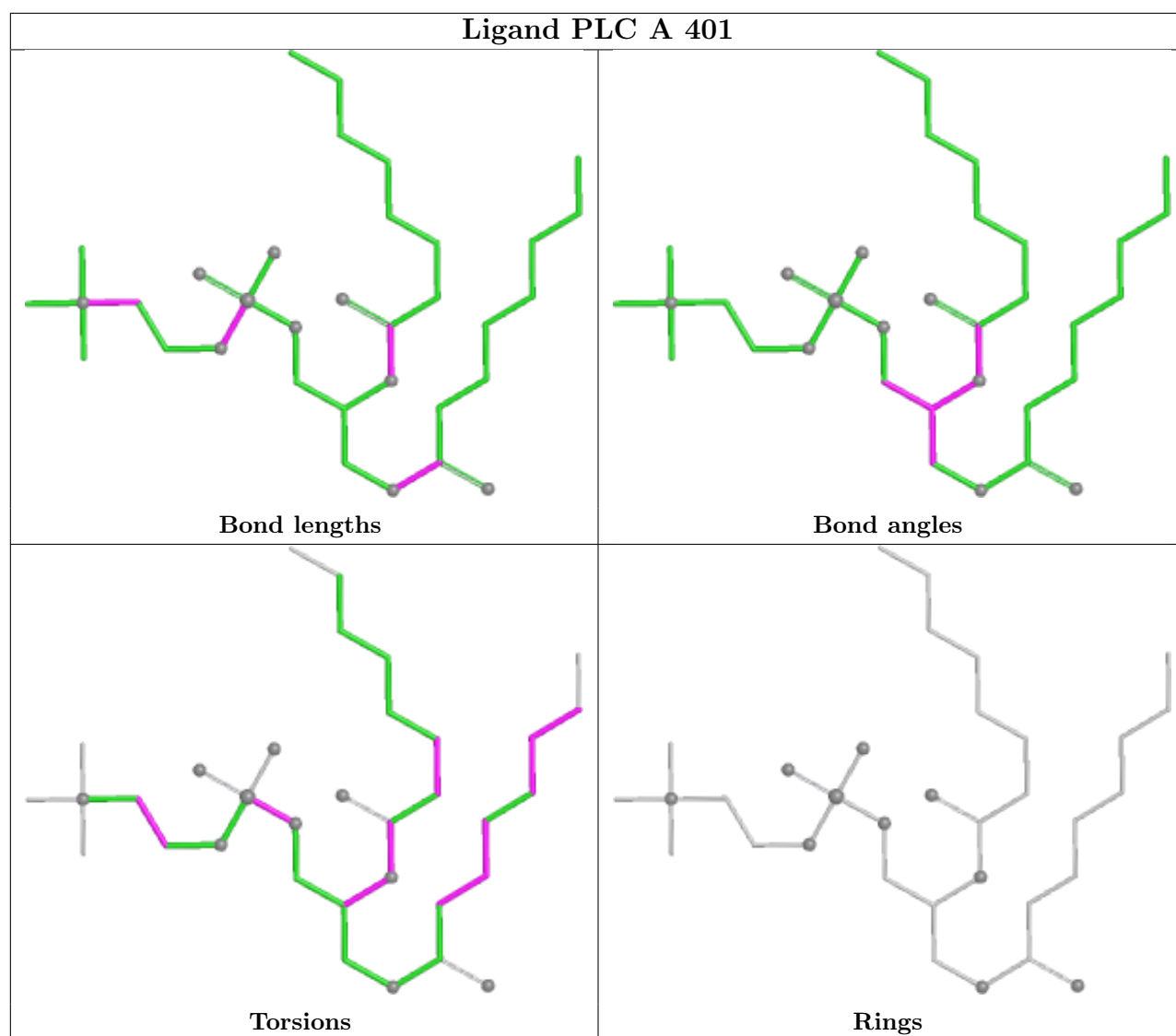
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

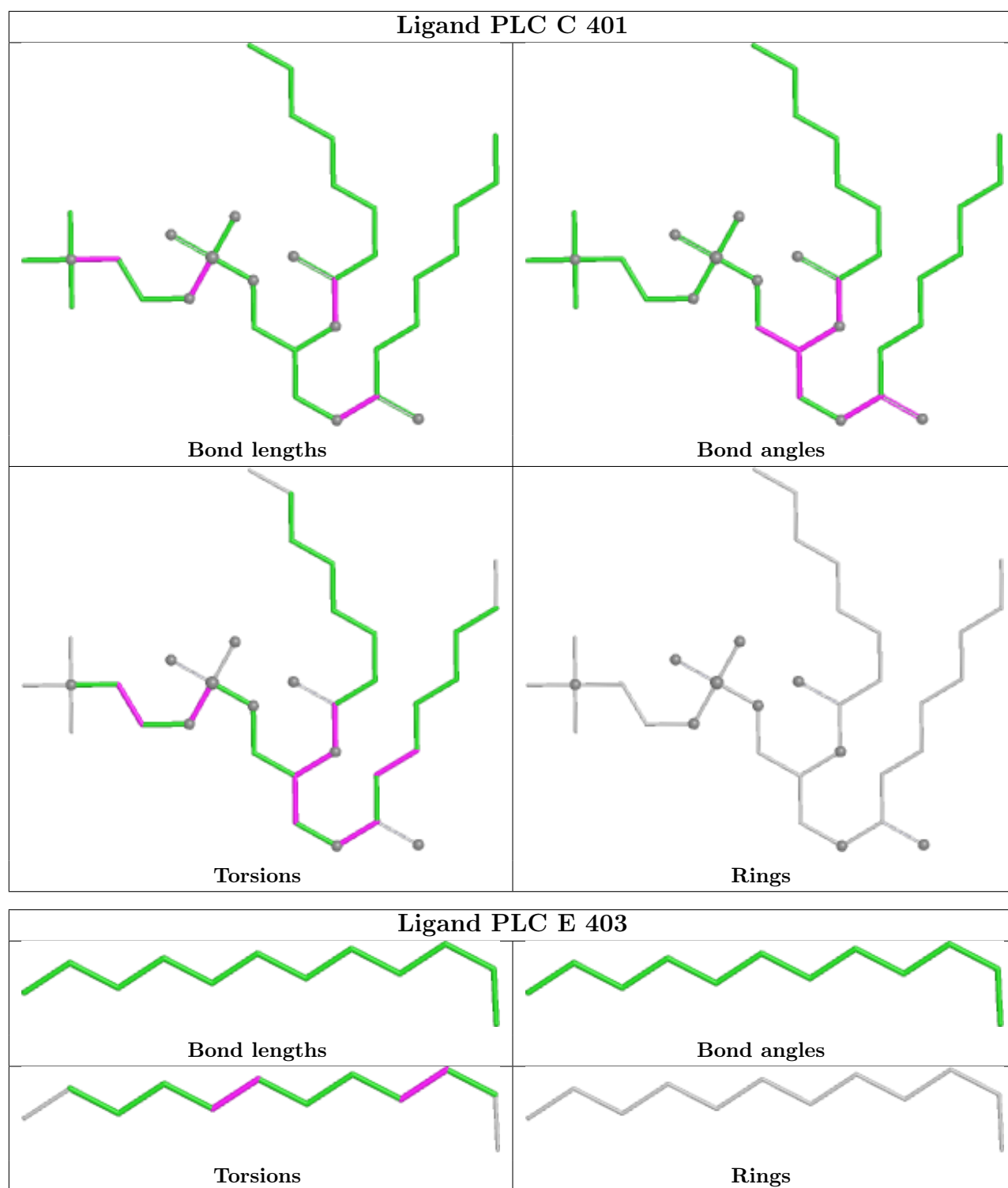


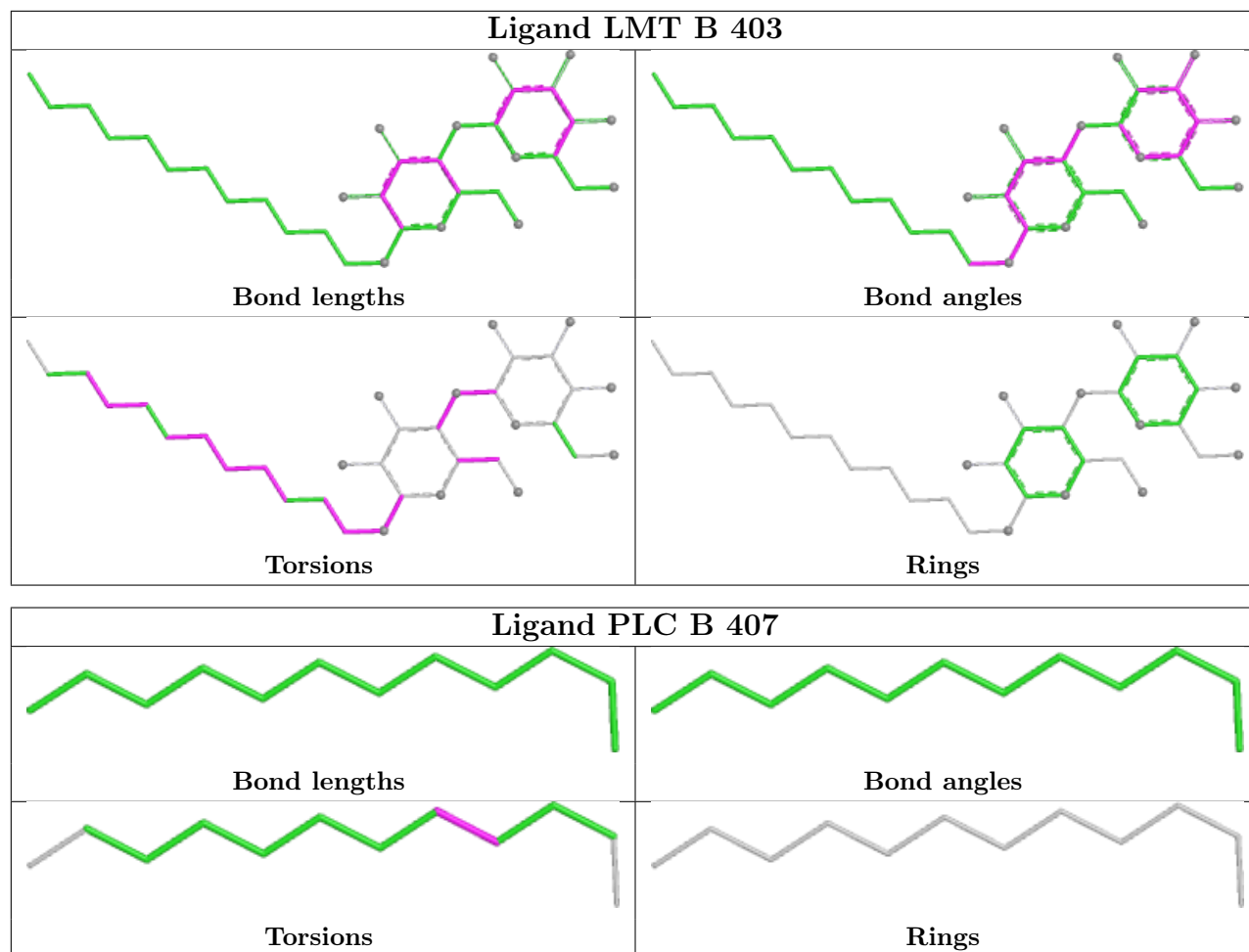
Ligand PLC C 408

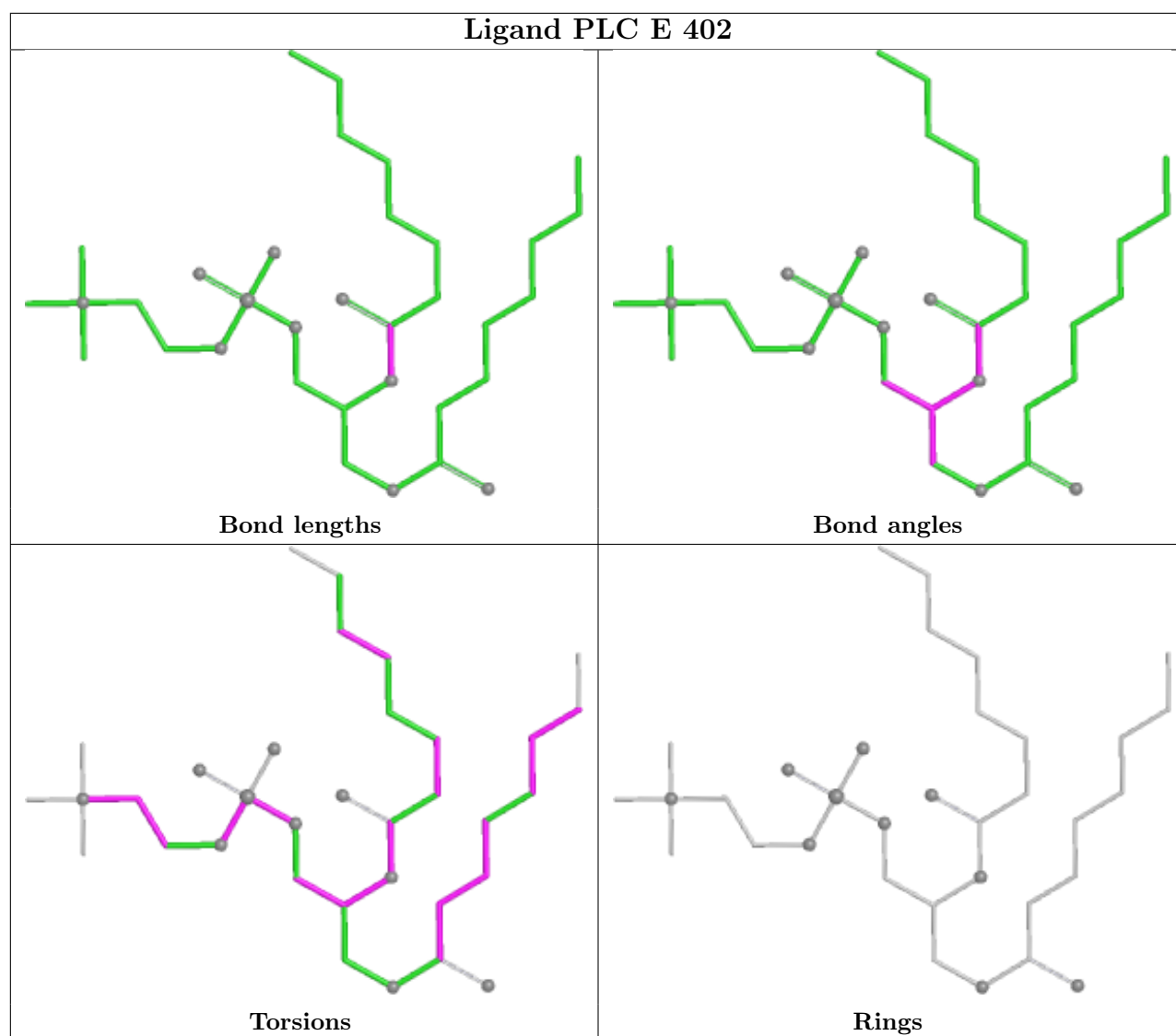












5.7 Other polymers [i](#)

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	311/359 (86%)	0.40	26 (8%)	17	9	41, 83, 127, 166	1 (0%)
1	B	311/359 (86%)	0.41	28 (9%)	15	8	38, 80, 124, 169	2 (0%)
1	C	311/359 (86%)	0.71	44 (14%)	6	4	62, 84, 133, 177	0
1	D	311/359 (86%)	0.74	42 (13%)	7	4	61, 86, 136, 182	0
1	E	311/359 (86%)	0.69	31 (9%)	12	7	60, 85, 129, 167	0
All	All	1555/1795 (86%)	0.59	171 (10%)	10	6	38, 83, 132, 182	3 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	154	ASP	13.2
1	E	283	SER	10.0
1	D	154	ASP	9.9
1	C	60	GLY	9.4
1	A	283	SER	7.6
1	A	154	ASP	7.1
1	C	283	SER	6.8
1	E	153	ASP	6.2
1	B	11	ILE	6.2
1	C	154	ASP	5.6
1	C	62	ARG	5.2
1	C	57	VAL	5.0
1	C	166	THR	5.0
1	E	156	PHE	4.7
1	A	147	GLU	4.7
1	E	152	ASN	4.6
1	B	12	ALA	4.6
1	D	153	ASP	4.4
1	B	113	PRO	4.4
1	C	56	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	156	PHE	4.3
1	E	284	GLN	4.3
1	D	127	HIS	4.3
1	E	155	VAL	4.2
1	C	187	GLN	4.2
1	E	112	SER	4.1
1	B	9	PRO	4.0
1	C	189	ARG	3.9
1	D	111	LEU	3.9
1	D	210	PHE	3.9
1	B	154	ASP	3.9
1	D	189	ARG	3.8
1	B	83	ASN	3.7
1	D	113	PRO	3.7
1	C	156	PHE	3.7
1	E	50	ARG	3.7
1	D	187	GLN	3.7
1	E	56	PRO	3.6
1	B	115	ASP	3.6
1	E	113	PRO	3.6
1	C	210	PHE	3.5
1	C	59	SER	3.5
1	D	112	SER	3.5
1	D	207	PHE	3.5
1	B	114	LEU	3.4
1	D	173	ASN	3.4
1	E	60	GLY	3.4
1	C	219	THR	3.3
1	C	276	GLN	3.3
1	C	284	GLN	3.3
1	E	11	ILE	3.3
1	B	189	ARG	3.3
1	B	6	SER	3.3
1	A	267	PHE	3.3
1	A	11	ILE	3.3
1	D	188	LEU	3.2
1	D	14	GLU	3.2
1	E	222	GLU	3.2
1	E	59	SER	3.2
1	C	26	GLU	3.2
1	D	126	LEU	3.2
1	D	155	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	187	GLN	3.1
1	D	80	ASN	3.1
1	D	226	THR	3.1
1	B	5	VAL	3.1
1	C	207	PHE	3.1
1	D	170	LYS	3.1
1	D	222	GLU	3.1
1	D	89	VAL	3.0
1	B	112	SER	3.0
1	E	58	ARG	3.0
1	C	127	HIS	3.0
1	A	156	PHE	3.0
1	D	152	ASN	3.0
1	A	286	ALA	2.9
1	C	66	TYR	2.9
1	D	88	ASP	2.9
1	B	305	LEU	2.9
1	D	125	THR	2.9
1	D	137	THR	2.9
1	C	63	VAL	2.9
1	E	127	HIS	2.9
1	A	13	ASP	2.9
1	C	153	ASP	2.9
1	C	11	ILE	2.9
1	B	284	GLN	2.9
1	E	189	ARG	2.9
1	C	280	LYS	2.9
1	C	172	ALA	2.8
1	E	89	VAL	2.8
1	C	125	THR	2.8
1	A	146	LEU	2.8
1	B	123	SER	2.8
1	E	207	PHE	2.8
1	D	180	LEU	2.7
1	D	136	ASP	2.7
1	E	62	ARG	2.7
1	A	281	VAL	2.7
1	C	61	VAL	2.7
1	D	223	ALA	2.7
1	A	141	VAL	2.7
1	B	276	GLN	2.7
1	E	35	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	92	ILE	2.7
1	D	206	LEU	2.7
1	A	111	LEU	2.6
1	D	141	VAL	2.6
1	E	115	ASP	2.6
1	D	115	ASP	2.6
1	C	14	GLU	2.5
1	C	94	VAL	2.5
1	C	58	ARG	2.5
1	B	275	VAL	2.5
1	B	137	THR	2.5
1	D	171	PRO	2.5
1	C	205	MET	2.5
1	C	188	LEU	2.5
1	E	12	ALA	2.4
1	D	11	ILE	2.4
1	B	51	ARG	2.4
1	C	50	ARG	2.4
1	B	10	PRO	2.4
1	D	309	ILE	2.4
1	A	138	ARG	2.4
1	B	170	LYS	2.4
1	D	68	PRO	2.4
1	A	12	ALA	2.4
1	A	205	MET	2.4
1	B	196	SER	2.4
1	C	281	VAL	2.4
1	C	12	ALA	2.4
1	C	291	ILE	2.4
1	C	206	LEU	2.4
1	D	114	LEU	2.4
1	E	180	LEU	2.3
1	E	280	LYS	2.3
1	B	35	GLU	2.3
1	C	65	THR	2.3
1	C	277	HIS	2.3
1	A	280	LYS	2.3
1	C	5	VAL	2.2
1	D	305	LEU	2.2
1	D	182	SER	2.2
1	D	15	PRO	2.2
1	A	222	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	206	LEU	2.2
1	A	112	SER	2.2
1	A	297	ILE	2.2
1	E	64	LYS	2.2
1	A	207	PHE	2.2
1	B	191	SER	2.1
1	A	86	ASP	2.1
1	E	126	LEU	2.1
1	C	185	ASP	2.1
1	D	177	GLU	2.1
1	C	6	SER	2.1
1	A	134	SER	2.1
1	A	217	TRP	2.1
1	D	102	TYR	2.1
1	B	84	ALA	2.1
1	C	70	ALA	2.1
1	C	167	ALA	2.1
1	A	238	PHE	2.1
1	B	163	GLU	2.1
1	B	286	ALA	2.0
1	E	178	ASP	2.0
1	C	141	VAL	2.0
1	A	113	PRO	2.0
1	A	284	GLN	2.0
1	E	57	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

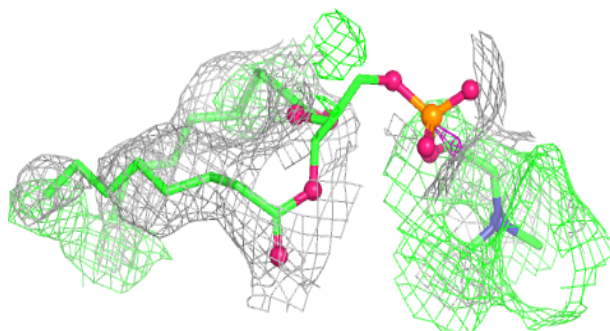
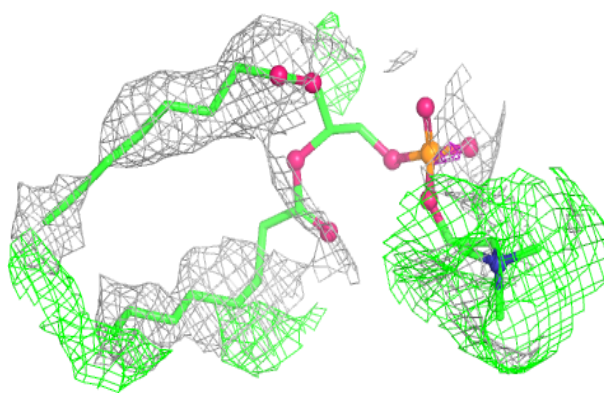
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLC	C	408	34/42	0.53	0.33	85,138,164,165	0
2	PLC	D	401	34/42	0.77	0.24	80,129,155,158	0
2	PLC	D	402	12/42	0.77	0.26	93,99,103,104	0
2	PLC	E	402	34/42	0.77	0.30	109,145,195,197	0
2	PLC	C	401	34/42	0.78	0.26	83,129,160,163	0
2	PLC	A	401	34/42	0.81	0.24	88,121,155,157	0
2	PLC	C	402	12/42	0.81	0.29	94,100,109,110	0
2	PLC	E	403	12/42	0.81	0.32	101,120,131,132	0
2	PLC	A	402	12/42	0.82	0.27	102,106,114,115	0
5	LMT	A	405	12/35	0.82	0.28	68,72,78,79	0
5	LMT	E	401	12/35	0.85	0.29	71,76,90,91	0
5	LMT	C	404	12/35	0.86	0.24	66,72,78,79	0
4	NA	E	404	1/1	0.87	0.29	101,101,101,101	0
5	LMT	D	404	12/35	0.87	0.25	63,70,82,82	0
2	PLC	B	401	12/42	0.87	0.22	95,97,101,102	0
5	LMT	E	405	12/35	0.88	0.24	70,72,74,76	0
2	PLC	B	407	12/42	0.89	0.27	92,96,107,107	0
5	LMT	B	403	35/35	0.89	0.23	84,134,152,152	0
4	NA	D	403	1/1	0.90	0.19	97,97,97,97	0
4	NA	C	403	1/1	0.90	0.21	94,94,94,94	0
4	NA	D	408	1/1	0.91	0.50	85,85,85,85	0
4	NA	B	402	1/1	0.92	0.20	92,92,92,92	0
6	MLA	D	407	7/7	0.93	0.15	88,88,89,91	0
3	CL	B	405	1/1	0.94	0.12	74,74,74,74	0
6	MLA	B	406	7/7	0.94	0.14	89,93,96,97	0
4	NA	A	404	1/1	0.94	0.10	82,82,82,82	0
3	CL	E	406	1/1	0.95	0.12	80,80,80,80	0
3	CL	C	405	1/1	0.95	0.14	82,82,82,82	0
3	CL	C	406	1/1	0.95	0.08	74,74,74,74	0
3	CL	B	404	1/1	0.96	0.12	75,75,75,75	0
3	CL	E	407	1/1	0.96	0.08	73,73,73,73	0
3	CL	D	405	1/1	0.96	0.08	84,84,84,84	0
3	CL	D	406	1/1	0.96	0.08	73,73,73,73	0
6	MLA	E	408	7/7	0.96	0.09	78,81,82,82	0
6	MLA	C	407	7/7	0.97	0.09	71,75,81,84	0
3	CL	A	407	1/1	0.97	0.13	81,81,81,81	0
3	CL	A	403	1/1	0.97	0.09	92,92,92,92	0
6	MLA	A	406	7/7	0.98	0.12	84,85,89,90	0
3	CL	A	408	1/1	0.99	0.09	67,67,67,67	0

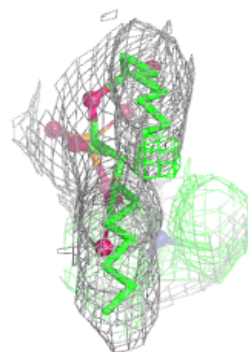
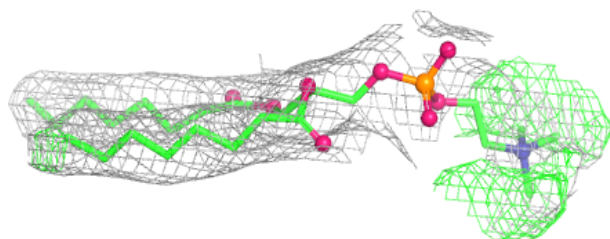
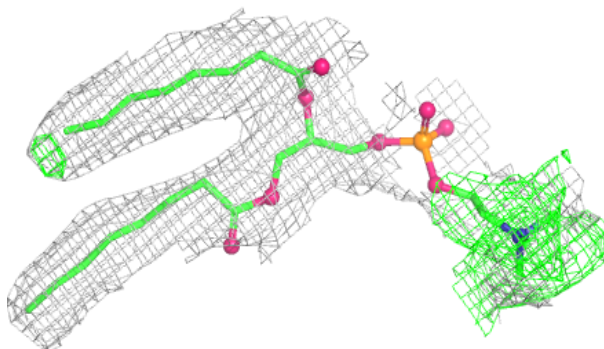
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLC C 408:

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

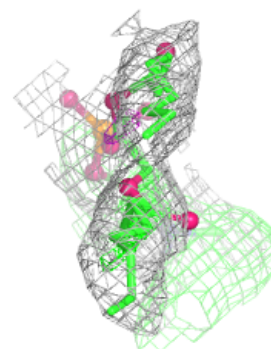
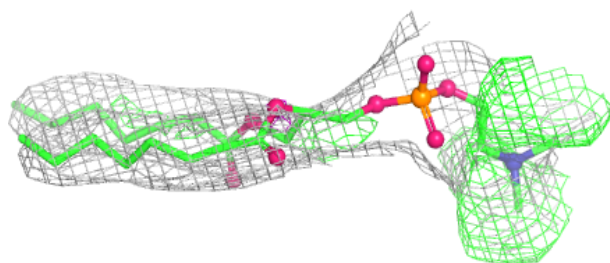
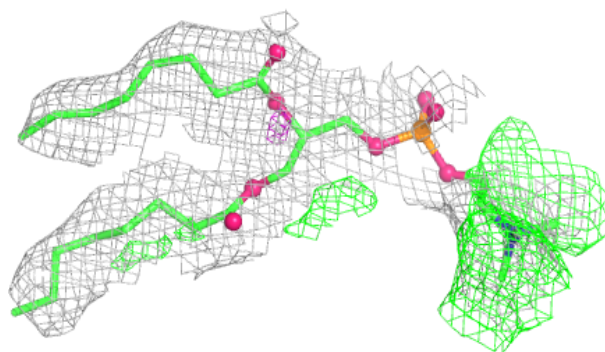
**Electron density around PLC D 401:**

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

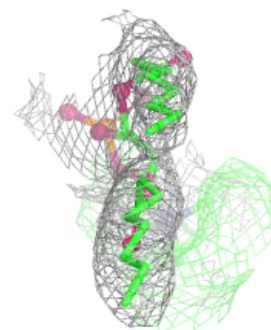
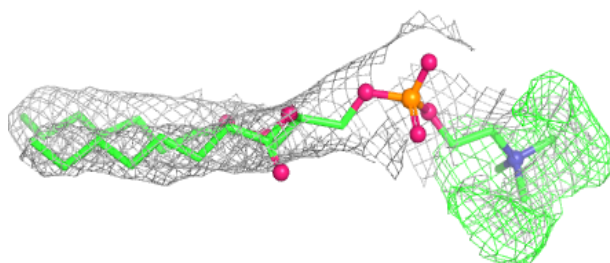
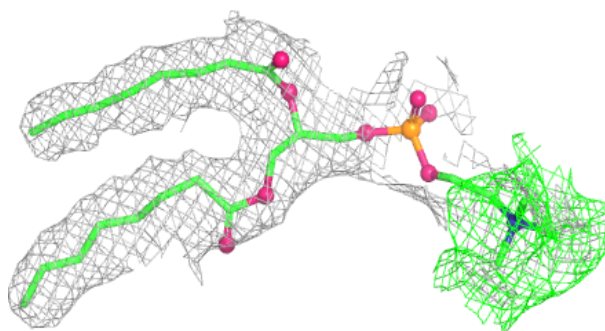


Electron density around PLC E 402:

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

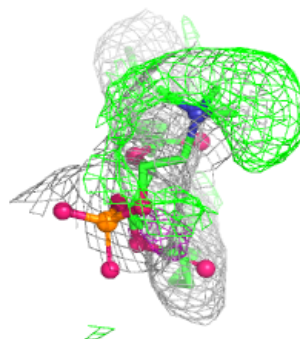
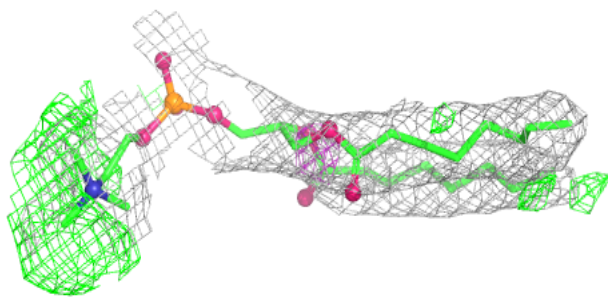
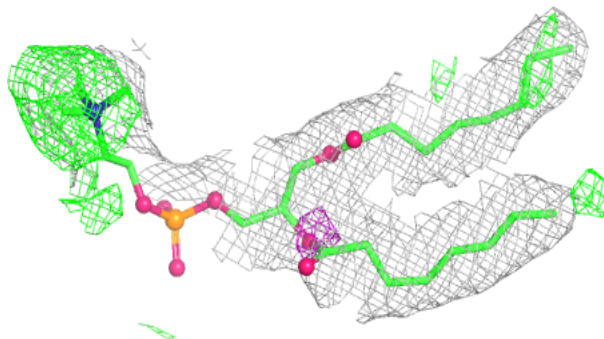
**Electron density around PLC C 401:**

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

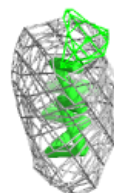
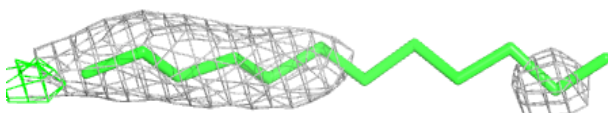
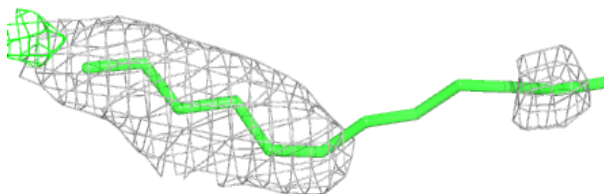


Electron density around PLC A 401:

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

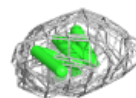
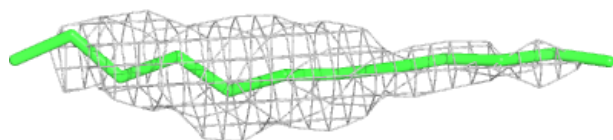
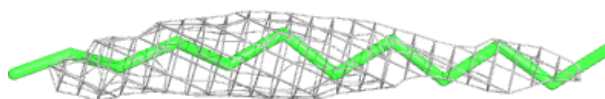
**Electron density around PLC E 403:**

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

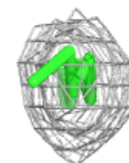
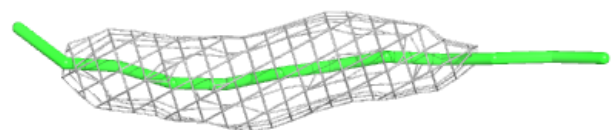
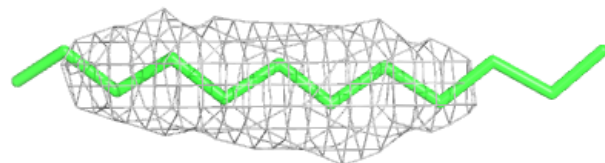


Electron density around PLC B 401:

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

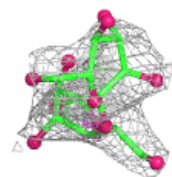
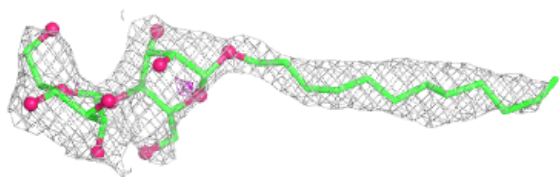
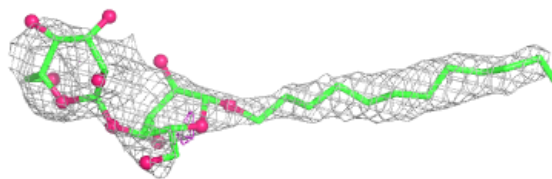
**Electron density around PLC B 407:**

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



Electron density around LMT B 403:

$2mF_o-DF_c$ (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.