



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:38 PM UTC

PDB ID : 6HJA / pdb_00006hja
Title : Xray structure of GLIC in complex with glutarate
Authors : Fourati, Z.; Delarue, M.
Deposited on : 2018-09-03
Resolution : 2.70 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

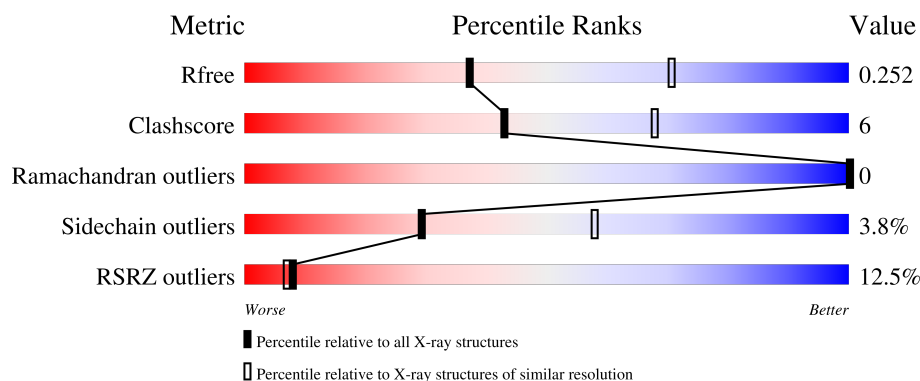
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	9% 75% 11% • 13%
1	B	359	12% 72% 12% • 13%
1	C	359	12% 73% 13% • 13%
1	D	359	11% 72% 14% • 13%
1	E	359	10% 72% 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
2	PLC	B	402	-	-	-	X
4	D12	B	406	-	-	X	-
5	GUA	B	408	-	X	-	-
5	GUA	D	406	-	X	-	-
5	GUA	D	407	-	X	-	-
6	NA	C	401	-	-	-	X

2 Entry composition [i](#)

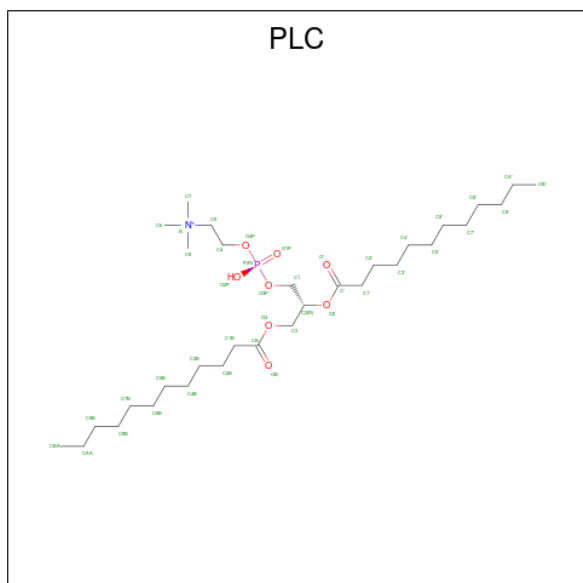
There are 7 unique types of molecules in this entry. The entry contains 13245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			2534	1669	405	456	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	2	0
			2543	1674	406	459	4			
1	E	311	Total	C	N	O	S	0	1	0
			2534	1669	405	456	4			

- Molecule 2 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



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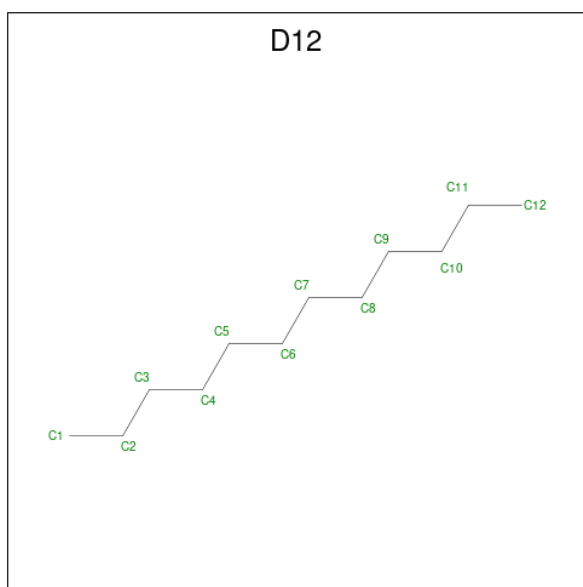
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 24 24	0	0
2	A	1	Total C 12 12	0	0
2	B	1	Total C N O P 34 24 1 8 1	0	0
2	B	1	Total C 24 24	0	0
2	B	1	Total C 12 12	0	0
2	C	1	Total C N O P 34 24 1 8 1	0	0
2	C	1	Total C 24 24	0	0
2	C	1	Total C 12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

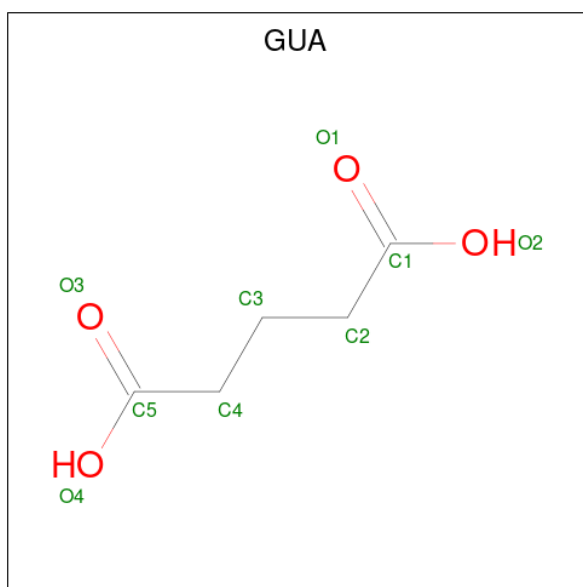
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	2	Total Cl 2 2	0	0
3	C	2	Total Cl 2 2	0	0
3	D	2	Total Cl 2 2	0	0
3	E	2	Total Cl 2 2	0	0

- Molecule 4 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



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

- Molecule 5 is GLUTARIC ACID (CCD ID: GUA) (formula: C₅H₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	5	4		
5	B	1	Total	C	O	0	0
			9	5	4		
5	D	1	Total	C	O	0	0
			9	5	4		
5	D	1	Total	C	O	0	0
			9	5	4		
5	E	1	Total	C	O	0	0
			9	5	4		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		
6	C	2	Total	Na	0	0
			2	2		
6	E	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	19	Total	O	0	0
			19	19		

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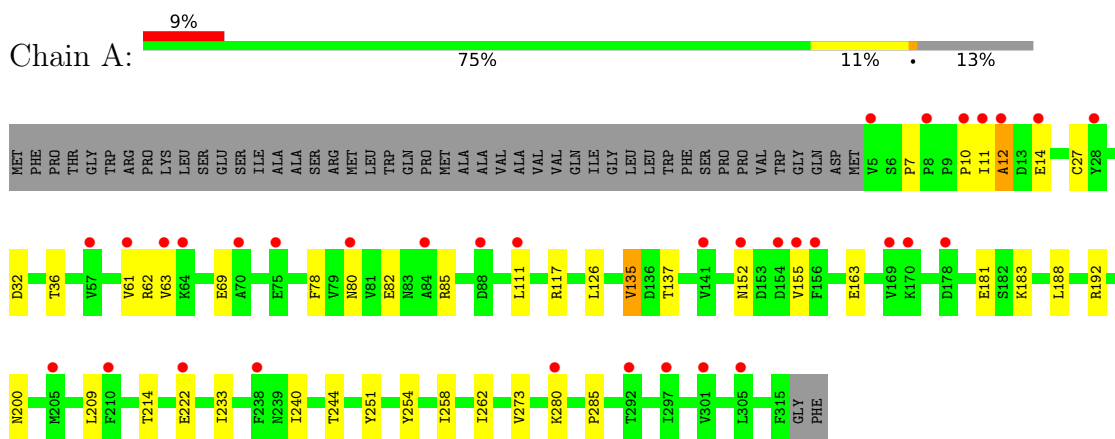
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	30	Total 30	O 30	0	0
7	C	24	Total 24	O 24	0	0
7	D	21	Total 21	O 21	0	0
7	E	23	Total 23	O 23	0	0

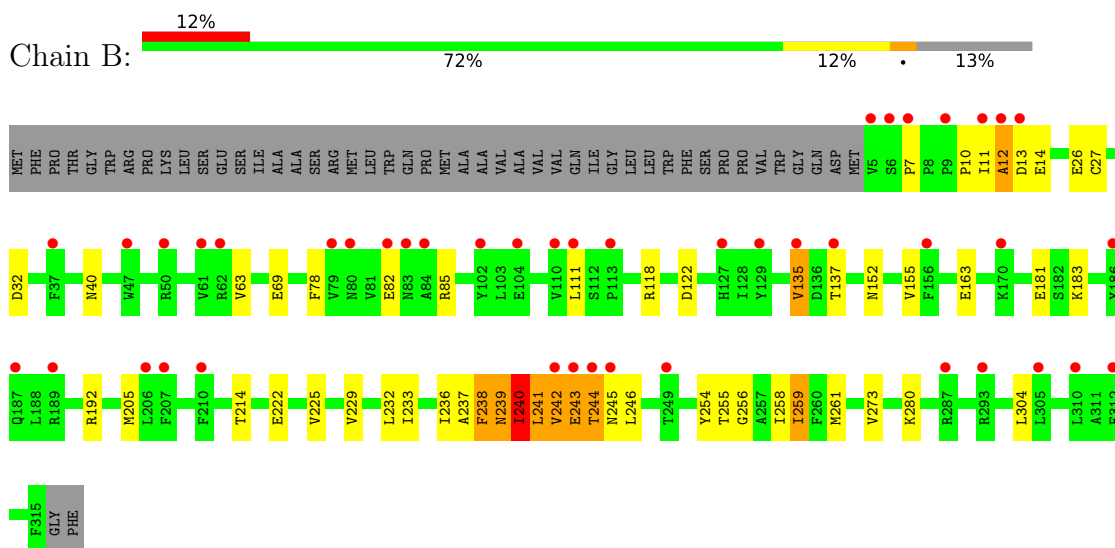
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

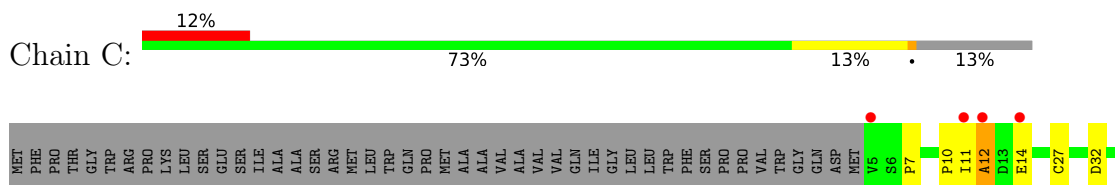
- Molecule 1: Proton-gated ion channel

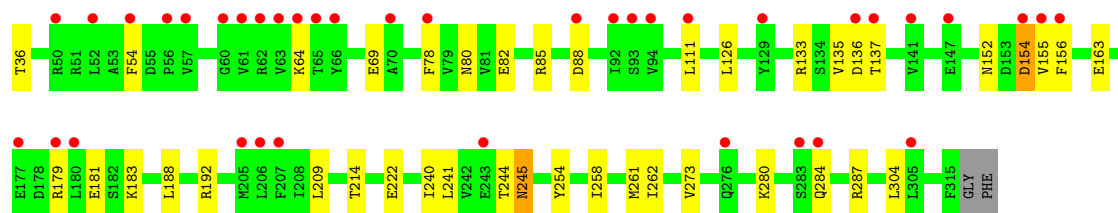


- Molecule 1: Proton-gated ion channel

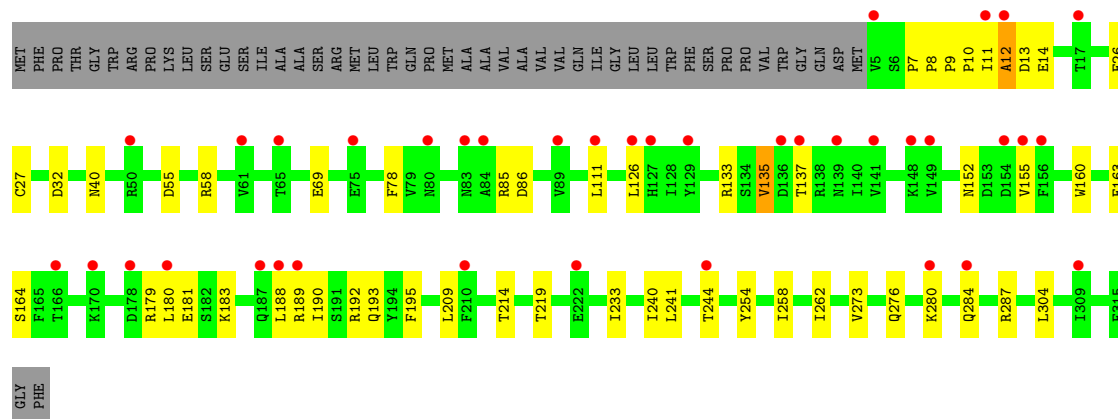
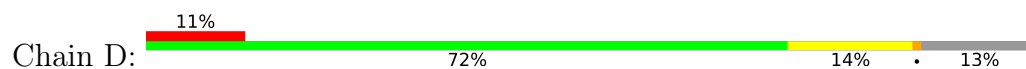


- Molecule 1: Proton-gated ion channel

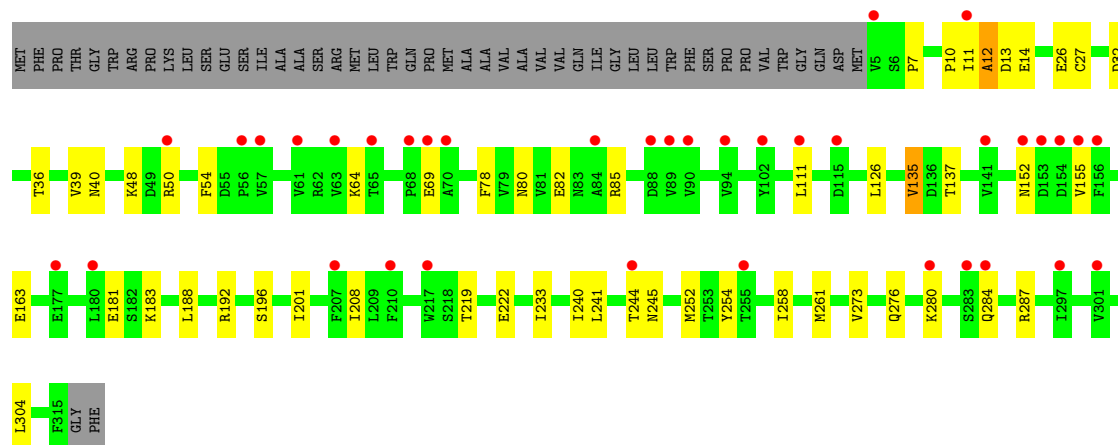
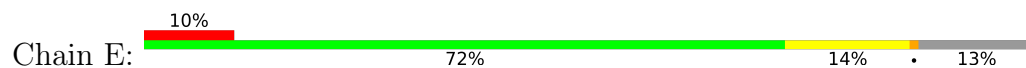




• Molecule 1: Proton-gated ion channel



• 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	180.87Å 134.41Å 160.31Å 90.00° 102.20° 90.00°	Depositor
Resolution (Å)	44.00 – 2.70 44.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.00-2.70) 99.6 (44.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.197 , 0.219 0.222 , 0.252	Depositor DCC
R_{free} test set	5409 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13245	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: PLC, CL, NA, GUA, D12

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	0.76	0/2602	1.21	5/3557 (0.1%)
1	B	1.21	15/2602 (0.6%)	1.35	24/3557 (0.7%)
1	C	0.75	0/2593	1.22	6/3545 (0.2%)
1	D	0.74	0/2611	1.22	6/3569 (0.2%)
1	E	0.75	0/2602	1.23	7/3557 (0.2%)
All	All	0.86	15/13010 (0.1%)	1.25	48/17785 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	GLU	C-N	19.37	1.57	1.33
1	B	241	LEU	C-N	17.24	1.55	1.33
1	B	244	THR	CA-CB	16.96	1.80	1.53
1	B	241	LEU	CA-C	-15.76	1.31	1.52
1	B	239	ASN	C-O	12.48	1.38	1.24
1	B	240	ILE	N-CA	11.10	1.60	1.46
1	B	239	ASN	C-N	10.96	1.48	1.33
1	B	243	GLU	N-CA	8.99	1.57	1.46
1	B	244	THR	CB-OG1	8.36	1.57	1.43
1	B	244	THR	CB-CG2	-7.13	1.29	1.52
1	B	242	VAL	CA-CB	6.22	1.61	1.54
1	B	238	PHE	CA-C	-6.21	1.44	1.52
1	B	240	ILE	CB-CG2	6.19	1.73	1.52
1	B	240	ILE	C-O	5.77	1.30	1.24
1	B	239	ASN	CA-C	5.63	1.60	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	GLU	CA-C-O	-9.35	111.00	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	VAL	CA-C-N	-8.64	109.20	120.44
1	B	242	VAL	C-N-CA	-8.64	109.20	120.44
1	B	244	THR	N-CA-C	-8.56	97.33	111.37
1	B	245	ASN	N-CA-C	7.75	121.83	112.38
1	B	242	VAL	N-CA-C	-7.72	102.25	110.36
1	B	12	ALA	N-CA-C	-7.42	98.08	109.65
1	E	245	ASN	CA-CB-CG	6.90	119.50	112.60
1	B	244	THR	N-CA-CB	6.74	121.19	109.72
1	B	242	VAL	N-CA-CB	6.66	117.91	110.51
1	E	135	VAL	CA-C-N	6.54	129.37	120.54
1	E	135	VAL	C-N-CA	6.54	129.37	120.54
1	B	135	VAL	CA-C-N	6.25	128.97	120.54
1	B	135	VAL	C-N-CA	6.25	128.97	120.54
1	A	135	VAL	CA-C-N	6.19	128.89	120.54
1	A	135	VAL	C-N-CA	6.19	128.89	120.54
1	B	236	ILE	N-CA-C	-6.18	105.11	110.74
1	D	135	VAL	CA-C-N	6.05	128.71	120.54
1	D	135	VAL	C-N-CA	6.05	128.71	120.54
1	B	240	ILE	CA-C-O	5.97	128.24	120.78
1	B	241	LEU	O-C-N	5.68	130.14	122.59
1	E	12	ALA	N-CA-C	-5.47	99.14	110.80
1	D	12	ALA	N-CA-C	-5.47	99.16	110.80
1	C	245	ASN	CA-CB-CG	5.46	118.06	112.60
1	C	154	ASP	CA-CB-CG	5.35	117.95	112.60
1	C	273	VAL	CA-C-N	5.31	127.34	120.44
1	C	273	VAL	C-N-CA	5.31	127.34	120.44
1	B	256	GLY	CA-C-N	5.30	127.34	120.44
1	B	256	GLY	C-N-CA	5.30	127.34	120.44
1	B	246	LEU	N-CA-C	5.30	118.73	109.82
1	C	12	ALA	N-CA-C	-5.28	99.55	110.80
1	E	13	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	12	ALA	N-CA-C	-5.24	99.63	110.80
1	B	273	VAL	CA-C-N	5.24	127.57	120.44
1	B	273	VAL	C-N-CA	5.24	127.57	120.44
1	D	13	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	244	THR	CA-C-N	5.22	128.96	120.60
1	B	244	THR	C-N-CA	5.22	128.96	120.60
1	B	243	GLU	CA-C-N	5.20	129.45	121.19
1	B	243	GLU	C-N-CA	5.20	129.45	121.19
1	C	88	ASP	CA-CB-CG	5.18	117.78	112.60
1	E	273	VAL	CA-C-N	5.12	127.40	120.44
1	E	273	VAL	C-N-CA	5.12	127.40	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	VAL	CA-C-N	5.10	127.37	120.44
1	A	273	VAL	C-N-CA	5.10	127.37	120.44
1	B	13	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	273	VAL	CA-C-N	5.08	127.34	120.44
1	D	273	VAL	C-N-CA	5.08	127.34	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2534	0	2550	26	0
1	B	2534	0	2550	45	0
1	C	2525	0	2545	29	0
1	D	2543	0	2555	39	0
1	E	2534	0	2550	40	0
2	A	70	0	111	1	0
2	B	70	0	111	2	0
2	C	70	0	111	1	0
2	D	70	0	111	1	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	24	0	52	2	0
4	B	12	0	26	8	0
4	C	12	0	26	0	0
4	D	12	0	26	0	0
4	E	12	0	26	0	0
5	A	9	0	0	0	0
5	B	9	0	0	0	0
5	D	18	0	0	0	0
5	E	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	0	0
7	A	19	0	0	1	0
7	B	30	0	0	0	0
7	C	24	0	0	1	0
7	D	21	0	0	3	0
7	E	23	0	0	0	0
All	All	13245	0	13415	164	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 6.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:THR:CA	1:B:244:THR:CB	1.80	1.57
1:A:200:ASN:HB3	1:B:243:GLU:OE2	1.37	1.24
1:B:82:GLU:HG2	1:B:111:LEU:HD11	1.36	1.06
1:B:244:THR:HG21	4:B:406:D12:C2	1.83	1.06
1:B:240:ILE:O	1:B:244:THR:N	1.90	1.04
1:B:244:THR:HG21	4:B:406:D12:H21	1.10	1.04
1:B:82:GLU:HG2	1:B:111:LEU:CD1	1.91	1.01
1:A:200:ASN:CB	1:B:243:GLU:OE2	2.11	0.98
1:B:244:THR:CG2	4:B:406:D12:H21	1.93	0.97
1:B:26[B]:GLU:OE2	1:C:111:LEU:HD12	1.71	0.89
1:D:133:ARG:NH2	1:D:179:ARG:HD2	1.87	0.89
1:B:239:ASN:O	1:B:243:GLU:N	2.06	0.88
1:B:63:VAL:HB	1:C:136:ASP:OD2	1.74	0.86
1:D:26[B]:GLU:OE2	1:E:111:LEU:HD12	1.77	0.85
1:D:284:GLN:HE21	1:D:287:ARG:HD3	1.41	0.84
1:E:284:GLN:HE21	1:E:287:ARG:HD3	1.43	0.84
1:B:244:THR:CA	1:B:244:THR:CG2	2.55	0.83
1:D:180:LEU:HD23	7:D:505:HOH:O	1.81	0.80
1:E:48:LYS:NZ	1:E:50:ARG:HH12	1.80	0.78
1:C:133:ARG:NH2	1:C:179:ARG:HD2	2.01	0.75
1:B:10:PRO:HB2	1:B:12:ALA:O	1.86	0.75
1:D:11:ILE:HG13	1:D:14:GLU:OE2	1.87	0.74
1:E:11:ILE:HG13	1:E:14:GLU:OE2	1.88	0.74
1:A:11:ILE:HG13	1:A:14:GLU:OE2	1.88	0.74
1:B:240:ILE:HG21	4:B:406:D12:H61	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ILE:HG13	1:C:14:GLU:OE2	1.88	0.73
1:E:48:LYS:HZ1	1:E:50:ARG:HH12	1.37	0.73
1:B:11:ILE:HG13	1:B:14:GLU:OE2	1.89	0.72
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.55	0.72
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.55	0.71
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.55	0.71
1:E:48:LYS:CE	1:E:50:ARG:HH12	2.03	0.71
1:A:111:LEU:HD12	1:E:26[B]:GLU:OE2	1.90	0.71
1:B:78:PHE:HE2	1:B:85:ARG:HD3	1.56	0.71
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.56	0.70
1:E:276:GLN:HG2	1:E:280:LYS:HE3	1.73	0.70
1:D:276:GLN:HG2	1:D:280:LYS:HE3	1.74	0.70
1:A:200:ASN:CG	1:B:243:GLU:OE2	2.35	0.69
1:E:48:LYS:CE	1:E:50:ARG:NH1	2.55	0.69
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.29	0.68
1:E:284:GLN:HE22	1:E:287:ARG:HH11	1.41	0.67
1:E:284:GLN:NE2	1:E:287:ARG:HH11	1.92	0.67
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.29	0.67
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.29	0.67
1:D:284:GLN:NE2	1:D:287:ARG:HH11	1.92	0.67
1:D:284:GLN:HE22	1:D:287:ARG:HH11	1.43	0.67
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.29	0.67
1:C:36:THR:HG22	1:C:111:LEU:HD23	1.77	0.66
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.30	0.66
1:A:36:THR:HG22	1:A:111:LEU:HD23	1.78	0.65
1:E:36:THR:HG22	1:E:111:LEU:HD23	1.78	0.65
1:B:237:ALA:HA	4:B:406:D12:H92	1.77	0.65
1:B:244:THR:CB	1:B:244:THR:HA	2.15	0.65
1:D:284:GLN:NE2	1:D:287:ARG:HD3	2.12	0.65
1:A:61:VAL:HG12	1:A:63:VAL:H	1.62	0.64
1:C:12:ALA:HB3	1:C:14:GLU:OE1	1.99	0.62
1:E:48:LYS:NZ	1:E:50:ARG:NH1	2.48	0.62
1:E:12:ALA:HB3	1:E:14:GLU:OE1	1.99	0.62
1:E:10:PRO:HB2	1:E:12:ALA:O	2.01	0.61
1:A:12:ALA:HB3	1:A:14:GLU:OE1	1.99	0.61
1:B:82:GLU:HG2	1:B:111:LEU:HD12	1.82	0.61
1:D:12:ALA:HB3	1:D:14:GLU:OE1	2.00	0.61
1:B:240:ILE:HG21	4:B:406:D12:H81	1.84	0.60
1:D:10:PRO:HB2	1:D:12:ALA:O	2.01	0.60
1:A:80:ASN:HA	1:E:26[B]:GLU:OE2	2.02	0.59
1:B:12:ALA:HB3	1:B:14:GLU:OE1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LYS:HE3	1:E:50:ARG:NH1	2.16	0.59
4:A:406:D12:H41	4:A:407:D12:H62	1.83	0.59
1:C:284:GLN:HE21	1:C:287:ARG:HD3	1.68	0.58
1:D:193:GLN:O	7:D:501:HOH:O	2.16	0.58
1:E:284:GLN:NE2	1:E:287:ARG:HD3	2.14	0.57
1:B:239:ASN:HB2	1:B:259:ILE:HG21	1.86	0.57
1:C:10:PRO:HB2	1:C:12:ALA:O	2.05	0.56
1:A:10:PRO:HB2	1:A:12:ALA:O	2.05	0.56
1:B:244:THR:CB	1:B:244:THR:C	2.73	0.56
1:E:48:LYS:HE3	1:E:50:ARG:HH12	1.69	0.56
1:C:156:PHE:CZ	1:D:111:LEU:HD21	2.43	0.54
1:C:156:PHE:CE1	1:D:111:LEU:HD21	2.43	0.54
1:B:238:PHE:O	1:B:241:LEU:HB2	2.08	0.54
1:D:276:GLN:NE2	1:D:280:LYS:HZ1	2.06	0.53
1:D:241:LEU:HD22	1:E:240:ILE:HG12	1.90	0.53
1:D:219:THR:HA	1:D:280:LYS:NZ	2.24	0.53
1:C:245:ASN:ND2	7:C:502:HOH:O	2.41	0.52
1:E:219:THR:HA	1:E:280:LYS:NZ	2.25	0.52
1:C:240:ILE:O	1:C:244:THR:HG23	2.09	0.51
1:D:276:GLN:O	1:D:280:LYS:HG3	2.11	0.51
1:B:244:THR:HG21	4:B:406:D12:C1	2.39	0.50
1:A:61:VAL:CG1	1:A:63:VAL:O	2.60	0.50
1:D:240:ILE:O	1:D:244:THR:HG23	2.11	0.50
1:E:219:THR:HA	1:E:280:LYS:HZ1	1.76	0.49
1:D:55:ASP:HB3	1:D:58:ARG:HG2	1.93	0.49
1:E:276:GLN:O	1:E:280:LYS:HG3	2.12	0.49
1:E:254:TYR:CZ	1:E:258:ILE:HD11	2.47	0.49
1:B:32:ASP:CG	1:B:192:ARG:HH22	2.20	0.49
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.94	0.48
1:E:276:GLN:CG	1:E:280:LYS:HE3	2.43	0.48
1:A:61:VAL:HG12	1:A:63:VAL:O	2.14	0.48
1:C:254:TYR:CZ	1:C:258:ILE:HD11	2.49	0.47
1:A:240:ILE:O	1:A:244:THR:HG23	2.13	0.47
1:D:7:PRO:HG3	1:D:135:VAL:HG21	1.97	0.47
1:A:117:ARG:HG3	1:A:251:TYR:CD2	2.50	0.46
1:D:276:GLN:CG	1:D:280:LYS:HE3	2.43	0.46
1:E:82:GLU:OE2	1:E:111:LEU:HD21	2.16	0.46
1:E:240:ILE:O	1:E:244:THR:HG23	2.16	0.46
1:C:7:PRO:HG3	1:C:135:VAL:HG21	1.98	0.46
1:C:82:GLU:OE2	1:C:111:LEU:HD21	2.16	0.46
1:B:241:LEU:O	1:B:244:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASN:HB3	1:A:155:VAL:HG23	1.99	0.45
1:B:214:THR:HG22	2:B:402:PLC:H3'2	1.97	0.45
1:B:261:MET:HE2	1:B:261:MET:HB3	1.91	0.45
1:C:152:ASN:HB3	1:C:155:VAL:HG23	1.99	0.45
1:A:7:PRO:HG3	1:A:135:VAL:HG21	1.98	0.45
1:A:280:LYS:HE3	1:A:285:PRO:HB3	1.99	0.45
1:B:26[B]:GLU:OE2	1:C:80:ASN:HA	2.16	0.45
1:C:241:LEU:HD22	1:D:240:ILE:HG12	1.99	0.45
1:C:284:GLN:NE2	1:C:287:ARG:HD3	2.29	0.45
1:C:209:LEU:HD13	1:C:262:ILE:HG23	1.99	0.45
1:E:152:ASN:HB3	1:E:155:VAL:HG23	1.98	0.44
1:B:225:VAL:O	1:B:229:VAL:HB	2.17	0.44
1:B:152:ASN:HB3	1:B:155:VAL:HG23	1.99	0.44
1:E:7:PRO:HG3	1:E:135:VAL:HG21	2.00	0.44
1:D:86:ASP:HB2	7:D:512:HOH:O	2.18	0.43
1:E:261:MET:HE2	1:E:261:MET:HB3	1.92	0.43
1:B:118:ARG:HH12	2:B:401:PLC:H72	1.83	0.43
1:B:122:ASP:OD1	1:B:192:ARG:HD2	2.17	0.43
1:A:214:THR:HG22	2:A:402:PLC:H3'2	2.00	0.43
1:C:284:GLN:HE22	1:C:287:ARG:HH11	1.67	0.43
1:D:152:ASN:HB3	1:D:155:VAL:HG23	1.99	0.43
1:D:219:THR:HA	1:D:280:LYS:HZ1	1.82	0.43
1:C:32:ASP:CG	1:C:192:ARG:HH22	2.27	0.43
1:B:63:VAL:HB	1:C:136:ASP:CG	2.43	0.43
1:B:238:PHE:O	1:B:241:LEU:CB	2.67	0.43
1:E:126:LEU:HD12	1:E:188:LEU:HD23	2.00	0.43
7:A:512:HOH:O	1:E:196:SER:HB3	2.19	0.42
1:A:82:GLU:OE2	1:A:111:LEU:HD21	2.19	0.42
1:D:32:ASP:CG	1:D:192:ARG:HH22	2.27	0.42
1:A:209:LEU:HD13	1:A:262:ILE:HG23	2.01	0.42
1:D:126:LEU:HD12	1:D:188:LEU:HD23	2.01	0.42
1:D:8:PRO:HA	1:D:9:PRO:HD3	1.97	0.42
1:D:26[B]:GLU:OE2	1:E:80:ASN:HA	2.19	0.42
1:D:209:LEU:HD13	1:D:262:ILE:HG23	2.01	0.42
1:B:238:PHE:O	1:B:241:LEU:N	2.46	0.42
1:D:214:THR:HG22	2:D:402:PLC:H3'2	2.01	0.42
1:A:32:ASP:CG	1:A:192:ARG:HH22	2.27	0.42
1:A:126:LEU:HD12	1:A:188:LEU:HD23	2.01	0.42
1:B:26[B]:GLU:HB2	1:B:40:ASN:HB3	2.02	0.42
1:D:195:PHE:HZ	1:E:252:MET:HG2	1.84	0.42
1:E:32:ASP:CG	1:E:192:ARG:HH22	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:SER:OG	1:D:189:ARG:CZ	2.68	0.42
1:C:214:THR:HG22	2:C:403:PLC:H3'2	2.02	0.41
1:D:26[B]:GLU:HB2	1:D:40:ASN:HB3	2.03	0.41
1:A:240:ILE:HG12	1:E:241:LEU:HD22	2.02	0.41
1:E:26[B]:GLU:HB2	1:E:40:ASN:HB3	2.02	0.41
1:A:254:TYR:CZ	1:A:258:ILE:HD11	2.56	0.41
1:B:205:MET:HE2	1:B:238:PHE:HB3	2.01	0.41
1:C:126:LEU:HD12	1:C:188:LEU:HD23	2.01	0.41
1:D:254:TYR:CZ	1:D:258:ILE:HD11	2.56	0.41
1:B:254:TYR:CZ	1:B:258:ILE:HD11	2.55	0.41
1:C:54:PHE:CD2	1:C:64:LYS:HD2	2.56	0.41
1:E:54:PHE:CD2	1:E:64:LYS:HD2	2.56	0.41
4:A:406:D12:H12	4:B:406:D12:H42	2.02	0.41
1:B:232:LEU:HD12	1:B:232:LEU:O	2.21	0.41
1:C:261:MET:HE2	1:C:261:MET:HB3	1.92	0.40
1:D:160:TRP:CE3	1:D:190:ILE:HD12	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/359 (86%)	298 (96%)	12 (4%)	0	100	100
1	B	310/359 (86%)	290 (94%)	20 (6%)	0	100	100
1	C	309/359 (86%)	297 (96%)	12 (4%)	0	100	100
1	D	311/359 (87%)	300 (96%)	11 (4%)	0	100	100
1	E	310/359 (86%)	299 (96%)	11 (4%)	0	100	100
All	All	1550/1795 (86%)	1484 (96%)	66 (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%)	272 (97%)	9 (3%)	34	64
1	B	281/319 (88%)	267 (95%)	14 (5%)	22	48
1	C	280/319 (88%)	270 (96%)	10 (4%)	31	60
1	D	282/319 (88%)	274 (97%)	8 (3%)	38	68
1	E	281/319 (88%)	269 (96%)	12 (4%)	26	54
All	All	1405/1595 (88%)	1352 (96%)	53 (4%)	29	58

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	A	62	ARG
1	A	69	GLU
1	A	137	THR
1	A	163	GLU
1	A	181	GLU
1	A	183	LYS
1	A	222	GLU
1	A	233	ILE
1	B	27	CYS
1	B	69	GLU
1	B	137	THR
1	B	163	GLU
1	B	181	GLU
1	B	183	LYS
1	B	222	GLU
1	B	233	ILE
1	B	240	ILE
1	B	242	VAL
1	B	255	THR
1	B	259	ILE
1	B	280	LYS
1	B	304	LEU

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Mol	Chain	Res	Type
1	C	27	CYS
1	C	69	GLU
1	C	137	THR
1	C	154	ASP
1	C	163	GLU
1	C	181	GLU
1	C	183	LYS
1	C	222	GLU
1	C	280	LYS
1	C	304	LEU
1	D	27	CYS
1	D	69	GLU
1	D	137	THR
1	D	163	GLU
1	D	181	GLU
1	D	183	LYS
1	D	233	ILE
1	D	304	LEU
1	E	27	CYS
1	E	39	VAL
1	E	69	GLU
1	E	137	THR
1	E	163	GLU
1	E	181	GLU
1	E	183	LYS
1	E	201	ILE
1	E	208	ILE
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	187	GLN
1	A	193	GLN
1	A	200	ASN
1	A	239	ASN
1	A	277	HIS
1	B	193	GLN
1	B	200	ASN

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Mol	Chain	Res	Type
1	B	277	HIS
1	C	193	GLN
1	C	200	ASN
1	C	239	ASN
1	C	277	HIS
1	C	284	GLN
1	D	187	GLN
1	D	193	GLN
1	D	239	ASN
1	D	276	GLN
1	D	277	HIS
1	D	284	GLN
1	E	19	ASN
1	E	83	ASN
1	E	187	GLN
1	E	193	GLN
1	E	200	ASN
1	E	239	ASN
1	E	276	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 40 ligands modelled in this entry, 15 are monoatomic - leaving 25 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
4	D12	D	405	-	11,11,11	0.96	0	10,10,10	0.42	0
4	D12	C	407	-	11,11,11	0.86	0	10,10,10	0.52	0
2	PLC	A	402	-	22,22,41	0.46	0	20,20,49	0.63	0
2	PLC	C	404	-	11,11,41	0.51	0	10,10,49	0.61	0
2	PLC	C	402	-	33,33,41	1.06	2 (6%)	39,41,49	0.95	2 (5%)
4	D12	E	405	-	11,11,11	0.66	0	10,10,10	0.56	0
5	GUA	D	406	-	8,8,8	1.82	2 (25%)	9,9,9	2.24	2 (22%)
4	D12	B	406	-	11,11,11	1.39	1 (9%)	10,10,10	1.11	1 (10%)
2	PLC	E	401	-	33,33,41	1.10	3 (9%)	39,41,49	1.08	2 (5%)
2	PLC	B	401	-	33,33,41	1.11	2 (6%)	39,41,49	0.97	2 (5%)
2	PLC	D	403	-	11,11,41	0.44	0	10,10,49	0.62	0
5	GUA	D	407	-	8,8,8	2.58	4 (50%)	9,9,9	3.06	5 (55%)
5	GUA	B	408	-	8,8,8	1.93	2 (25%)	9,9,9	2.23	3 (33%)
5	GUA	E	406	-	8,8,8	1.78	2 (25%)	9,9,9	2.55	3 (33%)
2	PLC	B	402	-	22,22,41	0.49	0	20,20,49	0.58	0
2	PLC	B	403	-	11,11,41	0.43	0	10,10,49	0.65	0
2	PLC	A	401	-	33,33,41	1.08	2 (6%)	39,41,49	0.97	2 (5%)
2	PLC	D	401	-	33,33,41	1.12	4 (12%)	39,41,49	1.08	3 (7%)
4	D12	A	406	-	11,11,11	0.81	0	10,10,10	0.50	0
5	GUA	A	409	-	8,8,8	1.87	2 (25%)	9,9,9	2.46	3 (33%)
2	PLC	A	403	-	11,11,41	0.44	0	10,10,49	0.64	0
2	PLC	C	403	-	22,22,41	0.49	0	20,20,49	0.60	0
2	PLC	D	402	-	22,22,41	0.49	0	20,20,49	0.60	0
4	D12	A	407	-	11,11,11	0.62	0	10,10,10	0.56	0
2	PLC	E	402	-	11,11,41	0.42	0	10,10,49	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	D12	D	405	-	-	1/9/9/9	-
4	D12	C	407	-	-	2/9/9/9	-
2	PLC	A	402	-	-	2/18/18/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLC	C	404	-	-	0/9/9/45	-
2	PLC	C	402	-	-	9/37/37/45	-
4	D12	E	405	-	-	0/9/9/9	-
5	GUA	D	406	-	-	6/6/6/6	-
4	D12	B	406	-	-	2/9/9/9	-
2	PLC	E	401	-	-	18/37/37/45	-
2	PLC	B	401	-	-	17/37/37/45	-
2	PLC	D	403	-	-	0/9/9/45	-
5	GUA	D	407	-	-	2/6/6/6	-
5	GUA	B	408	-	-	6/6/6/6	-
5	GUA	E	406	-	-	2/6/6/6	-
2	PLC	B	402	-	-	2/18/18/45	-
2	PLC	B	403	-	-	0/9/9/45	-
2	PLC	A	401	-	-	18/37/37/45	-
2	PLC	D	401	-	-	18/37/37/45	-
4	D12	A	406	-	-	0/9/9/9	-
5	GUA	A	409	-	-	3/6/6/6	-
2	PLC	A	403	-	-	0/9/9/45	-
2	PLC	C	403	-	-	2/18/18/45	-
2	PLC	D	402	-	-	2/18/18/45	-
4	D12	A	407	-	-	4/9/9/9	-
2	PLC	E	402	-	-	0/9/9/45	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	407	GUA	O1-C1	4.50	1.36	1.22
5	D	407	GUA	O3-C5	4.48	1.36	1.22
5	B	408	GUA	O1-C1	4.45	1.36	1.22
5	A	409	GUA	O3-C5	4.34	1.36	1.22
5	D	406	GUA	O3-C5	4.26	1.36	1.22
5	E	406	GUA	O1-C1	4.07	1.35	1.22
2	B	401	PLC	O2-C'	2.89	1.42	1.34
2	D	401	PLC	O2-C'	2.82	1.42	1.34
2	E	401	PLC	O2-C'	2.76	1.42	1.34
2	A	401	PLC	O2-C'	2.73	1.42	1.34
4	B	406	D12	C1-C2	2.59	1.68	1.50
5	D	407	GUA	O4-C5	-2.52	1.22	1.30
5	B	408	GUA	O2-C1	-2.49	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	409	GUA	O4-C5	-2.45	1.22	1.30
5	E	406	GUA	O2-C1	-2.44	1.22	1.30
5	D	406	GUA	O4-C5	-2.42	1.22	1.30
5	D	407	GUA	O2-C1	-2.41	1.22	1.30
2	E	401	PLC	C5-N	2.34	1.58	1.51
2	D	401	PLC	C5-N	2.27	1.58	1.51
2	C	402	PLC	C5-N	2.24	1.58	1.51
2	B	401	PLC	C5-N	2.18	1.58	1.51
2	D	401	PLC	P-O4P	2.17	1.67	1.59
2	C	402	PLC	O2-C'	2.15	1.40	1.34
2	D	401	PLC	C5-C4	2.08	1.57	1.51
2	A	401	PLC	C5-N	2.07	1.57	1.51
2	E	401	PLC	P-O4P	2.05	1.67	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	406	GUA	O2-C1-C2	5.25	130.59	114.00
5	D	407	GUA	O2-C1-C2	5.15	130.27	114.00
5	A	409	GUA	O4-C5-C4	5.09	130.10	114.00
5	D	406	GUA	O4-C5-C4	4.55	128.39	114.00
5	B	408	GUA	O2-C1-C2	4.43	127.98	114.00
5	D	407	GUA	O4-C5-C4	4.37	127.82	114.00
2	D	401	PLC	C2-O2-C'	3.91	127.14	117.80
2	E	401	PLC	C2-O2-C'	3.77	126.83	117.80
5	E	406	GUA	O1-C1-C2	-3.75	111.20	123.09
5	D	407	GUA	O1-C1-C2	-3.74	111.23	123.09
5	A	409	GUA	O3-C5-C4	-3.56	111.79	123.09
5	D	407	GUA	O3-C5-C4	-3.34	112.51	123.09
2	B	401	PLC	C2-O2-C'	3.29	125.68	117.80
5	B	408	GUA	O1-C1-C2	-3.19	112.98	123.09
5	D	406	GUA	O3-C5-C4	-3.14	113.13	123.09
2	A	401	PLC	C2-O2-C'	3.11	125.25	117.80
2	A	401	PLC	C3-C2-C1	2.74	118.18	111.78
2	C	402	PLC	C3-C2-C1	2.61	117.87	111.78
2	E	401	PLC	C3-C2-C1	2.50	117.62	111.78
2	D	401	PLC	C3-C2-C1	2.48	117.56	111.78
5	D	407	GUA	C4-C3-C2	-2.39	107.20	112.20
2	B	401	PLC	C3-C2-C1	2.36	117.28	111.78
5	E	406	GUA	C4-C3-C2	-2.34	107.31	112.20
4	B	406	D12	C5-C4-C3	-2.24	103.05	114.37
2	C	402	PLC	O2-C'-O'	-2.09	118.82	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	409	GUA	O4-C5-O3	-2.04	118.09	123.33
2	D	401	PLC	C4-C5-N	2.04	122.36	115.82
5	B	408	GUA	C4-C3-C2	-2.03	107.95	112.20

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PLC	O4P-C4-C5-N
2	A	401	PLC	C1'-C'-O2-C2
2	A	401	PLC	C1-O3P-P-O1P
2	A	401	PLC	C4-O4P-P-O1P
2	A	401	PLC	C4-O4P-P-O3P
2	B	401	PLC	O4P-C4-C5-N
2	B	401	PLC	C1'-C'-O2-C2
2	B	401	PLC	C1-O3P-P-O1P
2	B	401	PLC	C4-O4P-P-O1P
2	B	401	PLC	C4-O4P-P-O3P
2	C	402	PLC	O4P-C4-C5-N
2	C	402	PLC	C1'-C'-O2-C2
2	D	401	PLC	C1'-C'-O2-C2
2	D	401	PLC	C4-O4P-P-O3P
2	E	401	PLC	O4P-C4-C5-N
2	E	401	PLC	C1'-C'-O2-C2
2	E	401	PLC	C4-O4P-P-O1P
2	E	401	PLC	C4-O4P-P-O3P
2	A	401	PLC	O'-C'-O2-C2
2	B	401	PLC	O'-C'-O2-C2
2	C	402	PLC	O'-C'-O2-C2
2	D	401	PLC	O'-C'-O2-C2
2	E	401	PLC	O'-C'-O2-C2
2	E	401	PLC	C4-C5-N-C8
2	D	401	PLC	C4-C5-N-C8
2	B	401	PLC	C'-C1'-C2'-C3'
2	C	402	PLC	CB-C1B-C2B-C3B
5	D	406	GUA	C1-C2-C3-C4
2	A	401	PLC	CB-C1B-C2B-C3B
2	E	401	PLC	CB-C1B-C2B-C3B
2	A	401	PLC	C'-C1'-C2'-C3'
2	D	401	PLC	CB-C1B-C2B-C3B
5	D	406	GUA	C2-C3-C4-C5
2	D	401	PLC	C'-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	E	401	PLC	C'-C1'-C2'-C3'
5	B	408	GUA	C1-C2-C3-C4
5	B	408	GUA	C2-C3-C4-C5
2	D	401	PLC	C4-C5-N-C7
2	B	401	PLC	CB-C1B-C2B-C3B
2	E	401	PLC	C4-C5-N-C7
2	E	401	PLC	C4-C5-N-C6
2	A	401	PLC	C3B-C4B-C5B-C6B
2	A	401	PLC	C1B-C2B-C3B-C4B
2	D	401	PLC	C1'-C2'-C3'-C4'
2	E	401	PLC	C1'-C2'-C3'-C4'
4	B	406	D12	C7-C8-C9-C10
2	D	401	PLC	C4-C5-N-C6
2	B	401	PLC	C1'-C2'-C3'-C4'
2	E	401	PLC	C3B-C4B-C5B-C6B
2	D	401	PLC	C3B-C4B-C5B-C6B
2	A	401	PLC	C1'-C2'-C3'-C4'
2	C	402	PLC	C3B-C4B-C5B-C6B
5	A	409	GUA	C2-C3-C4-C5
2	A	402	PLC	C8'-C9'-CA'-CB'
4	C	407	D12	C4-C5-C6-C7
2	D	402	PLC	C8'-C9'-CA'-CB'
2	A	401	PLC	C4B-C5B-C6B-C7B
2	B	402	PLC	C8'-C9'-CA'-CB'
2	C	403	PLC	C8'-C9'-CA'-CB'
4	B	406	D12	C11-C10-C9-C8
4	D	405	D12	C1-C2-C3-C4
2	C	402	PLC	O3P-C1-C2-O2
2	D	401	PLC	O4P-C4-C5-N
2	A	401	PLC	C4-C5-N-C8
2	C	402	PLC	O3P-C1-C2-C3
4	A	407	D12	C1-C2-C3-C4
2	B	401	PLC	C3B-C4B-C5B-C6B
2	B	401	PLC	C1-O3P-P-O4P
2	C	402	PLC	C4-O4P-P-O1P
2	D	401	PLC	C1-O3P-P-O1P
2	D	401	PLC	C4-O4P-P-O1P
2	E	401	PLC	C1-O3P-P-O1P
2	B	402	PLC	C1'-C2'-C3'-C4'
4	A	407	D12	C4-C5-C6-C7
2	A	401	PLC	C4-C5-N-C6
4	C	407	D12	C5-C6-C7-C8

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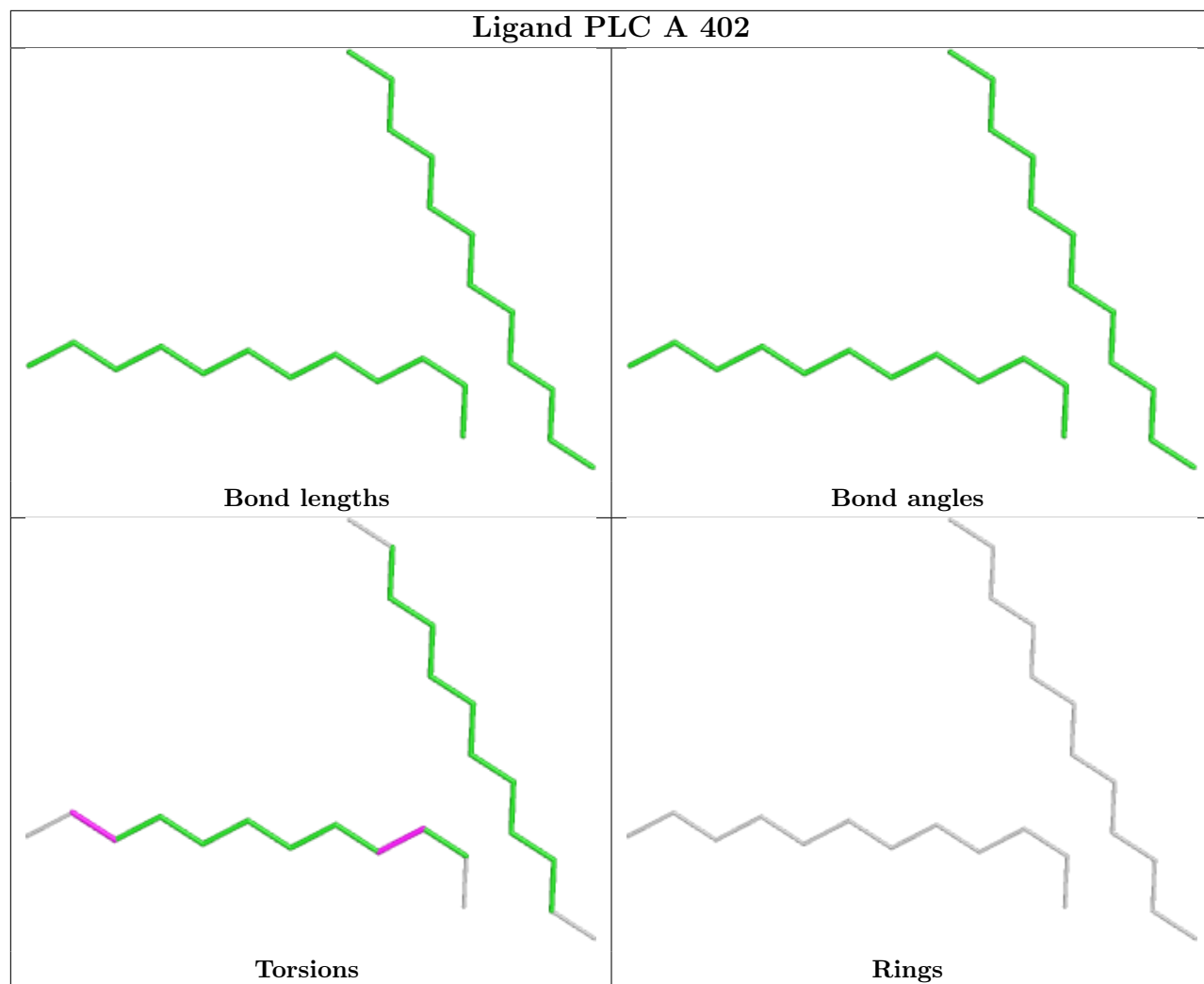
Mol	Chain	Res	Type	Atoms
5	B	408	GUA	O2-C1-C2-C3
5	A	409	GUA	O2-C1-C2-C3
2	D	402	PLC	C1'-C2'-C3'-C4'
5	B	408	GUA	O1-C1-C2-C3
2	C	403	PLC	C1'-C2'-C3'-C4'
5	A	409	GUA	O1-C1-C2-C3
5	D	407	GUA	C3-C4-C5-O3
5	E	406	GUA	C3-C4-C5-O3
2	A	401	PLC	C1-C2-O2-C'
2	D	401	PLC	C1-C2-O2-C'
2	E	401	PLC	C1-C2-O2-C'
2	A	402	PLC	C1'-C2'-C3'-C4'
5	D	406	GUA	C3-C4-C5-O3
2	A	401	PLC	C4-C5-N-C7
5	D	406	GUA	C3-C4-C5-O4
4	A	407	D12	C5-C6-C7-C8
5	E	406	GUA	C3-C4-C5-O4
5	D	407	GUA	C3-C4-C5-O4
4	A	407	D12	C6-C7-C8-C9
5	B	408	GUA	C3-C4-C5-O4
5	B	408	GUA	C3-C4-C5-O3
5	D	406	GUA	O2-C1-C2-C3
5	D	406	GUA	O1-C1-C2-C3
2	E	401	PLC	C1B-C2B-C3B-C4B
2	A	401	PLC	O2-C'-C1'-C2'
2	D	401	PLC	C1B-C2B-C3B-C4B
2	E	401	PLC	C2B-C1B-CB-O3
2	B	401	PLC	C2B-C3B-C4B-C5B
2	D	401	PLC	C2B-C1B-CB-O3
2	B	401	PLC	O2-C'-C1'-C2'
2	B	401	PLC	C1-C2-O2-C'
2	C	402	PLC	C4-C5-N-C8
2	E	401	PLC	O2-C'-C1'-C2'
2	A	401	PLC	O'-C'-C1'-C2'
2	D	401	PLC	O2-C'-C1'-C2'
2	B	401	PLC	C4-C5-N-C8
2	B	401	PLC	O'-C'-C1'-C2'
2	E	401	PLC	C2B-C1B-CB-OB
2	D	401	PLC	C2B-C1B-CB-OB
2	B	401	PLC	C2B-C1B-CB-O3

There are no ring outliers.

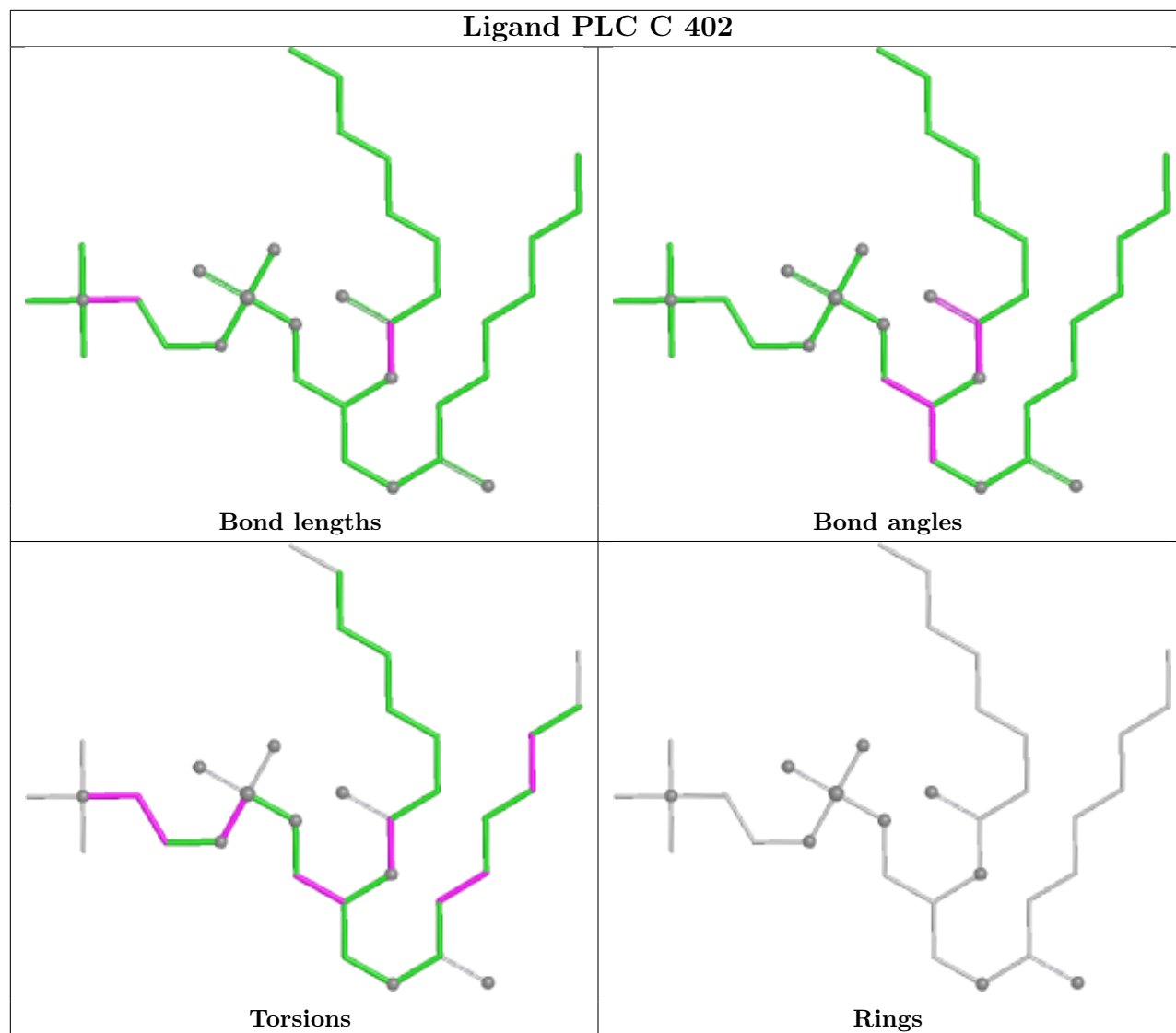
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	PLC	1	0
4	B	406	D12	8	0
2	B	401	PLC	1	0
2	B	402	PLC	1	0
4	A	406	D12	2	0
2	C	403	PLC	1	0
2	D	402	PLC	1	0
4	A	407	D12	1	0

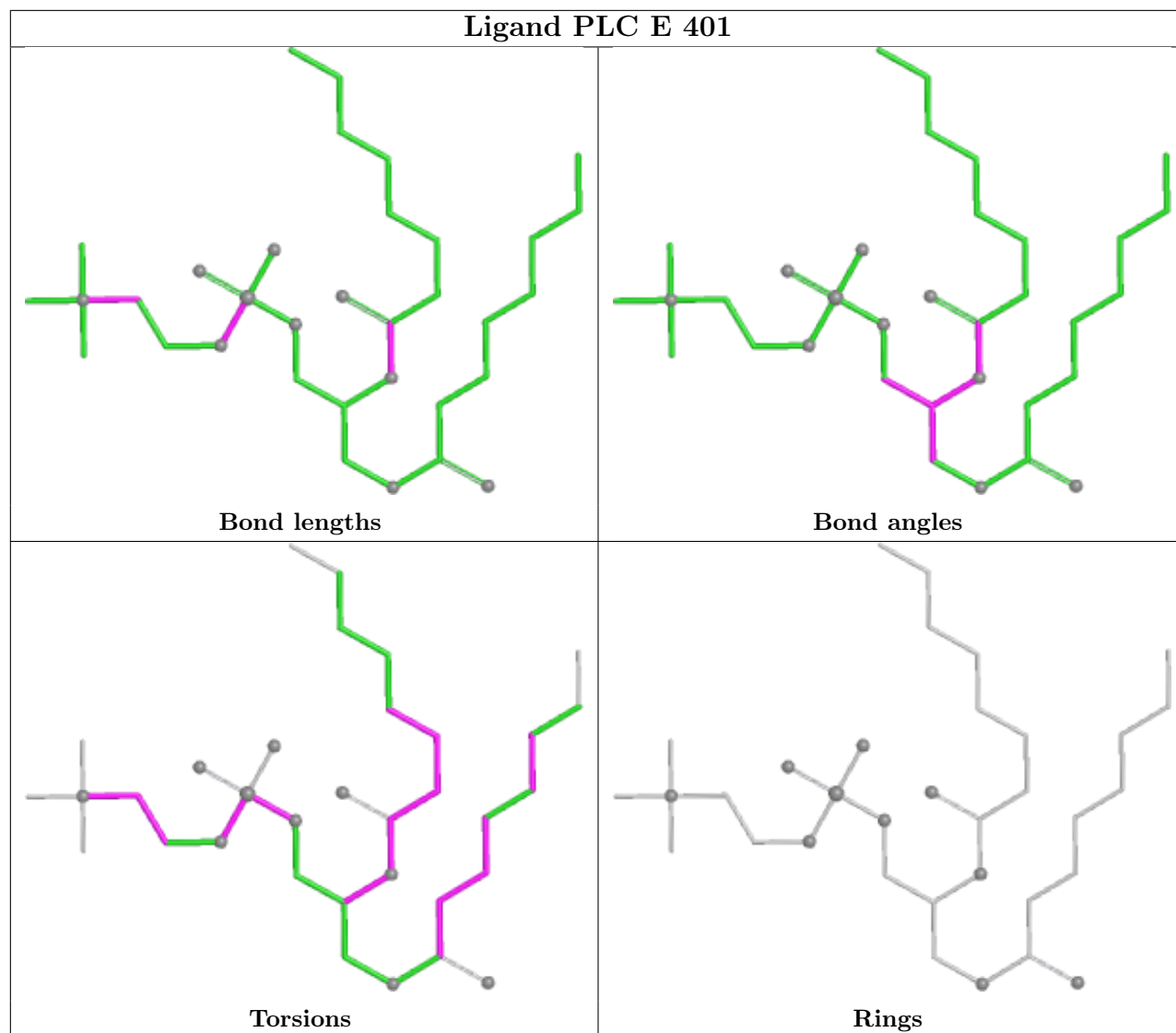
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



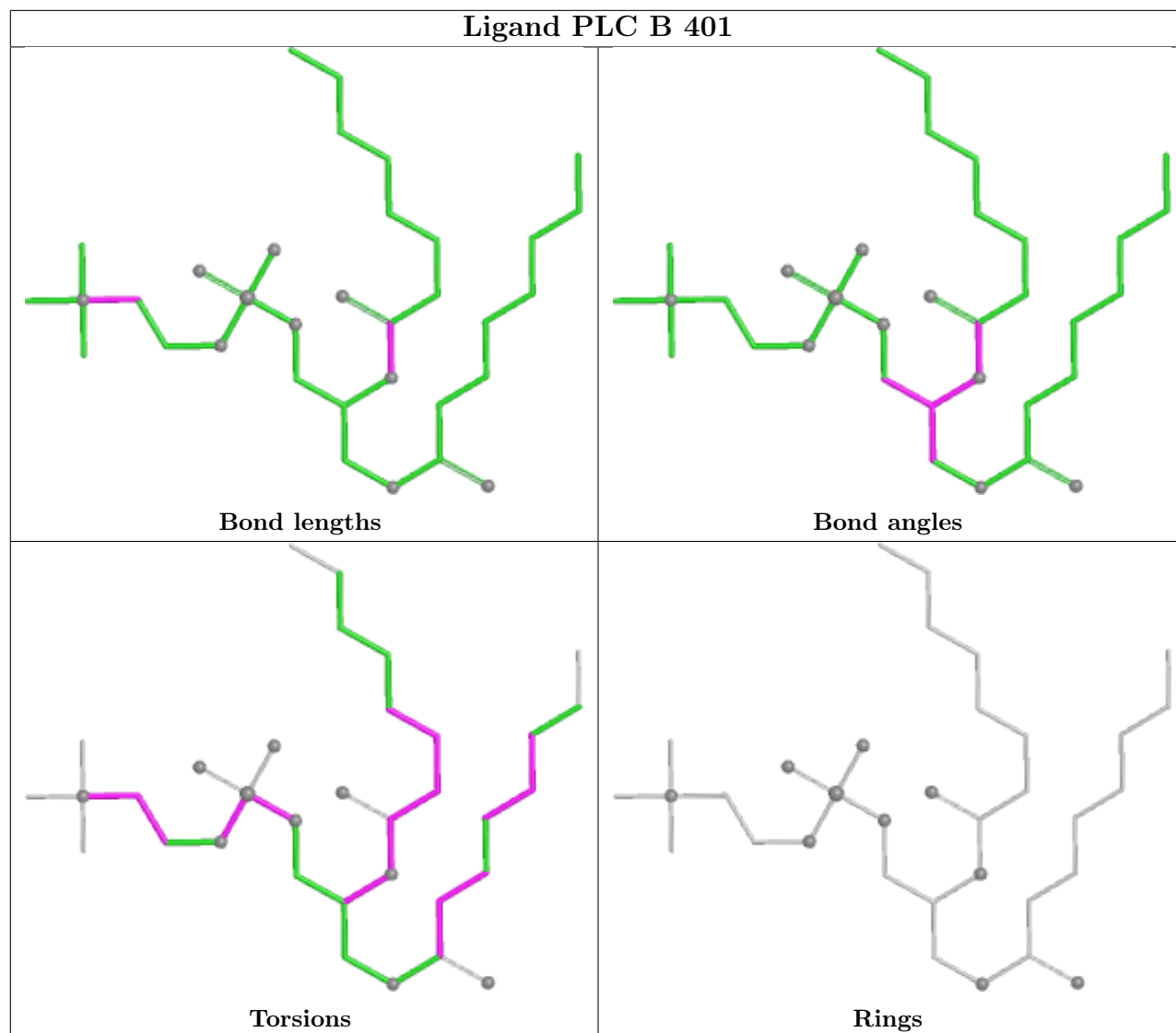
Ligand PLC C 402

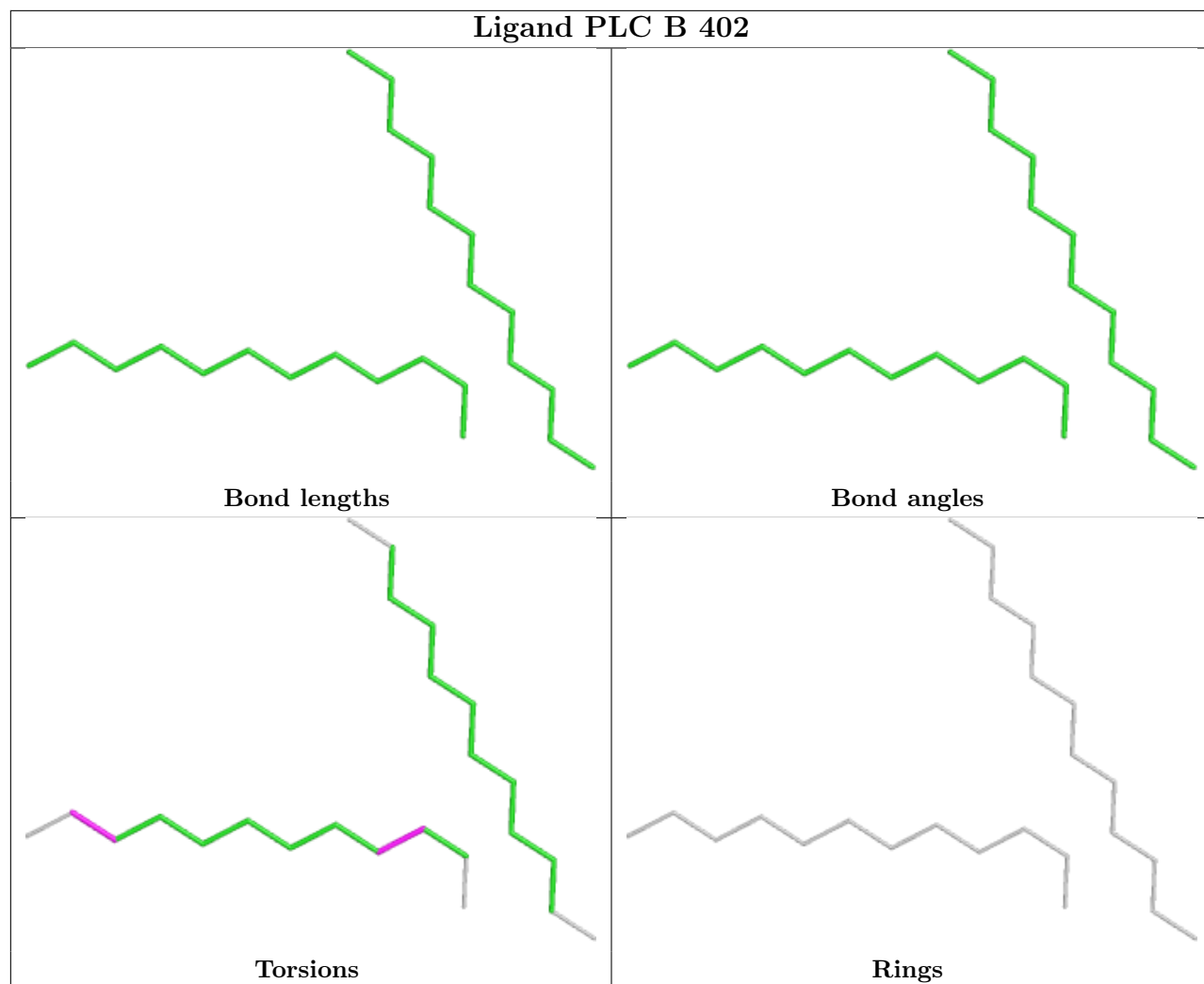


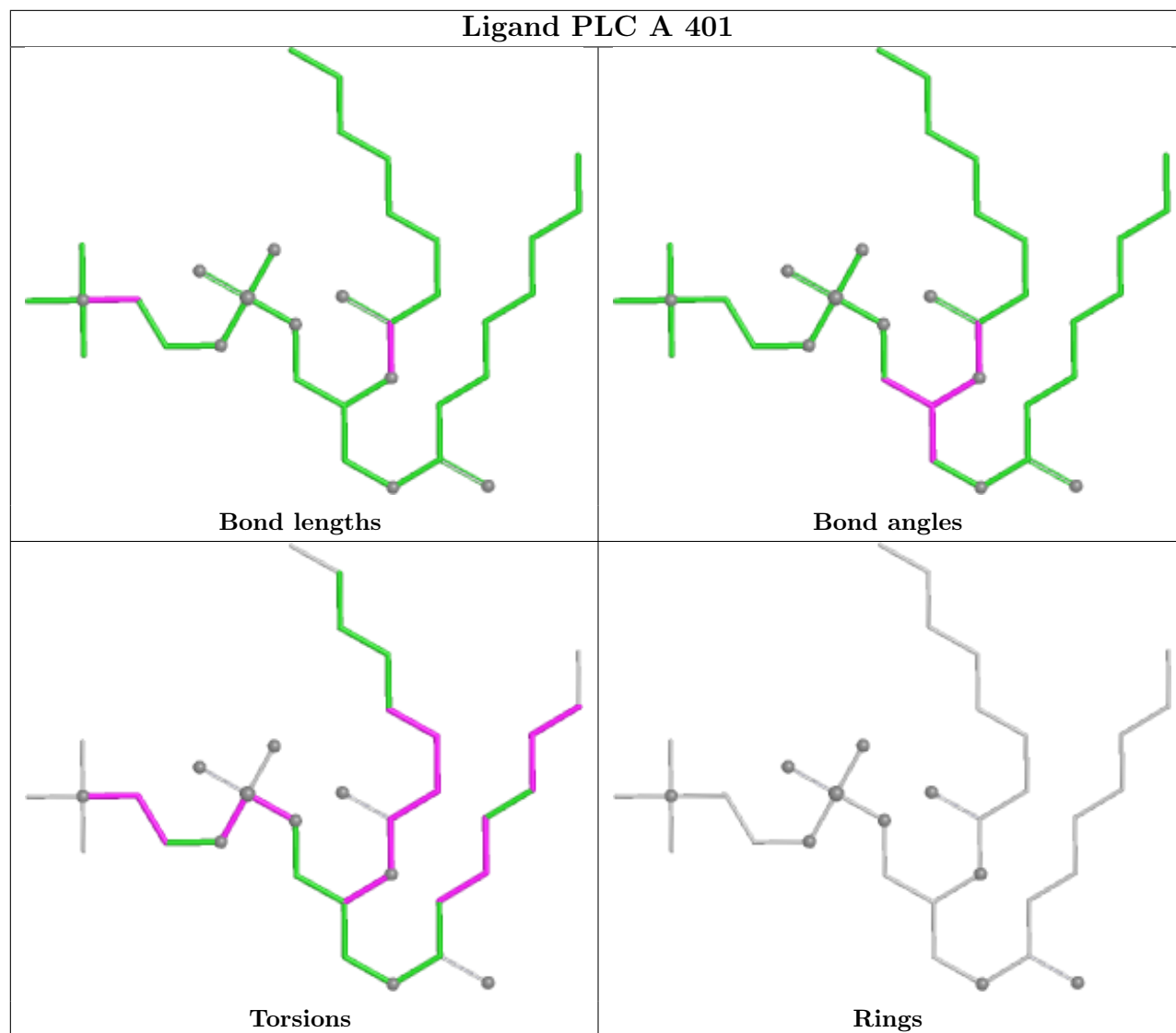
Ligand PLC E 401

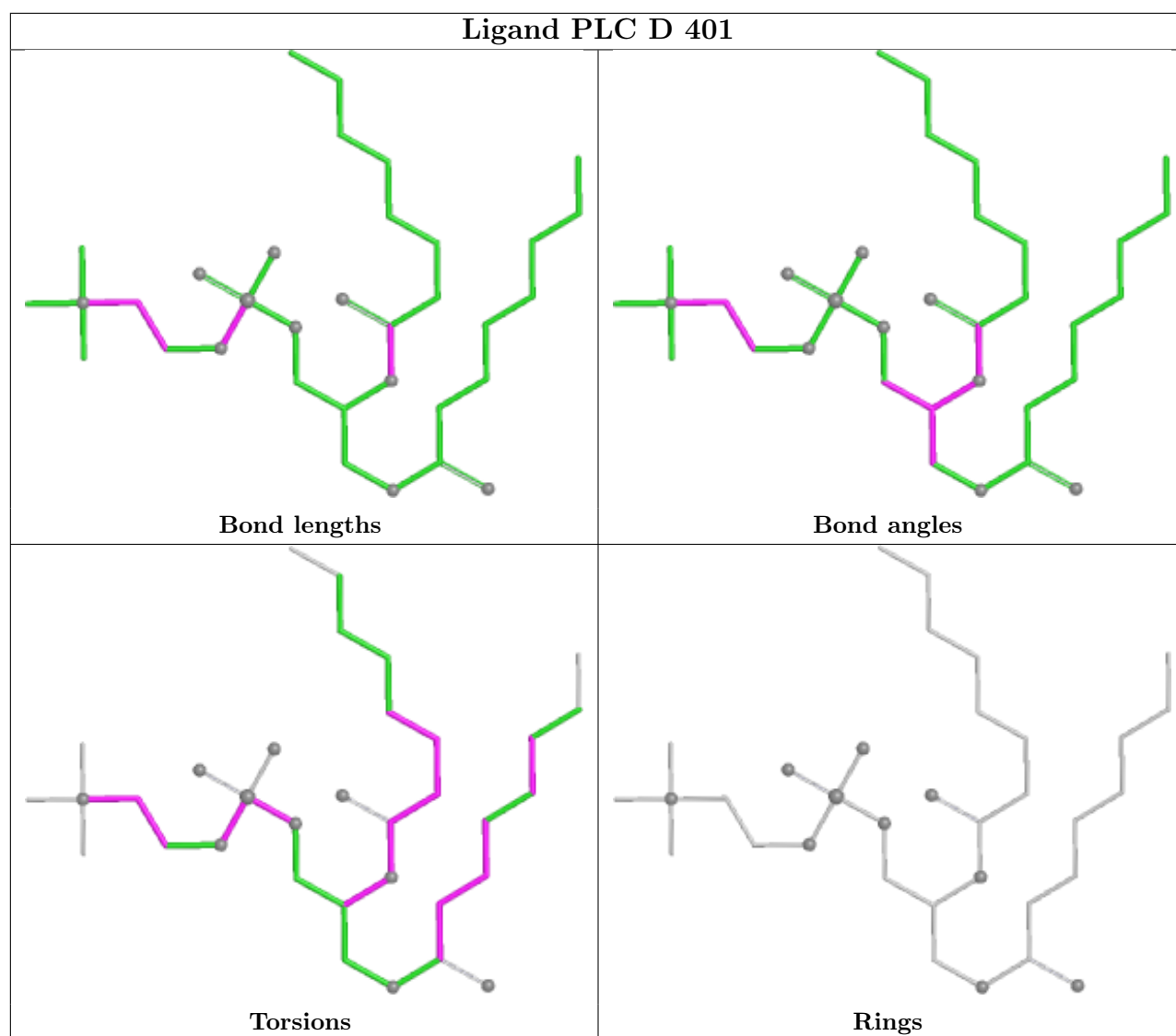


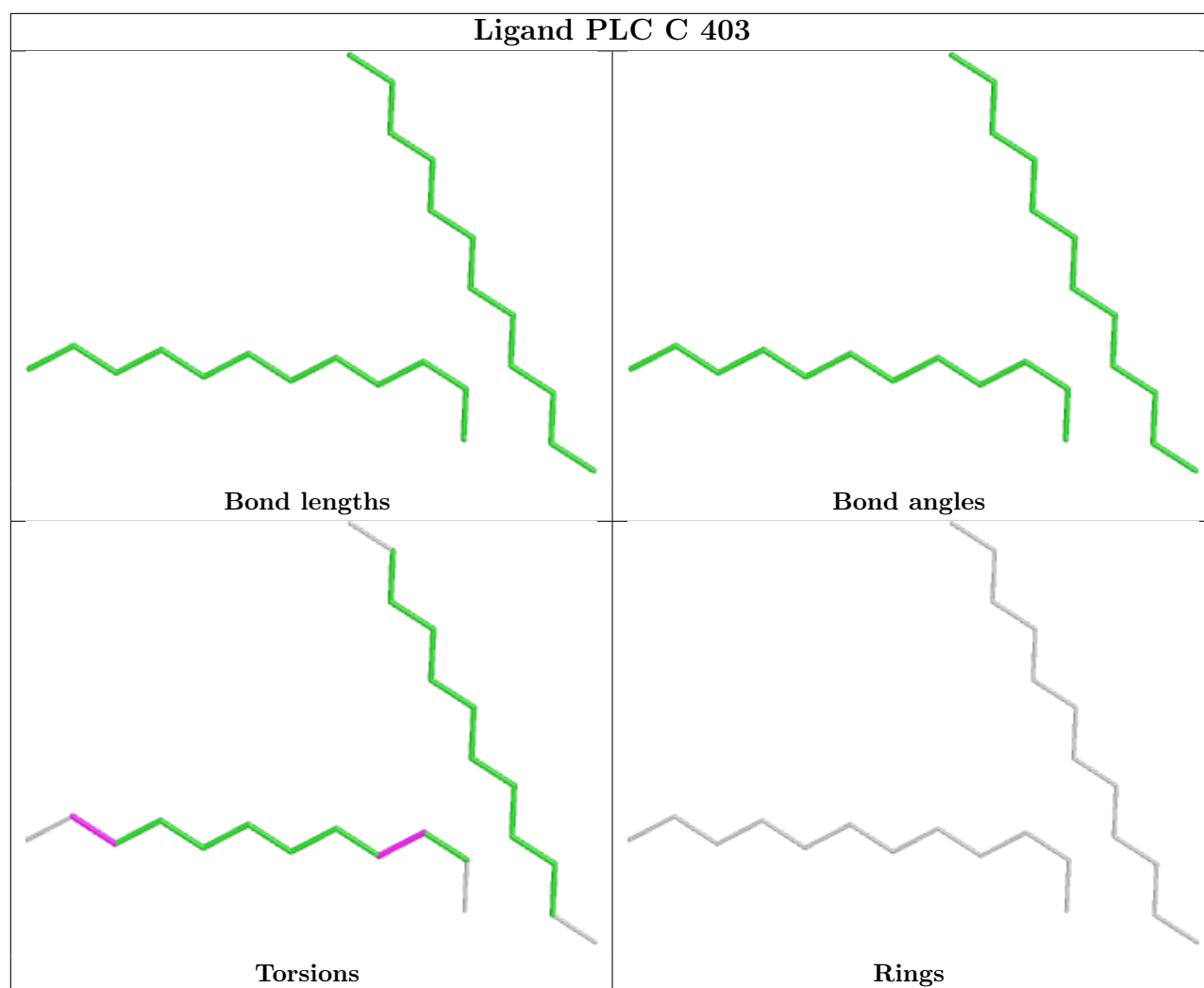
Ligand PLC B 401

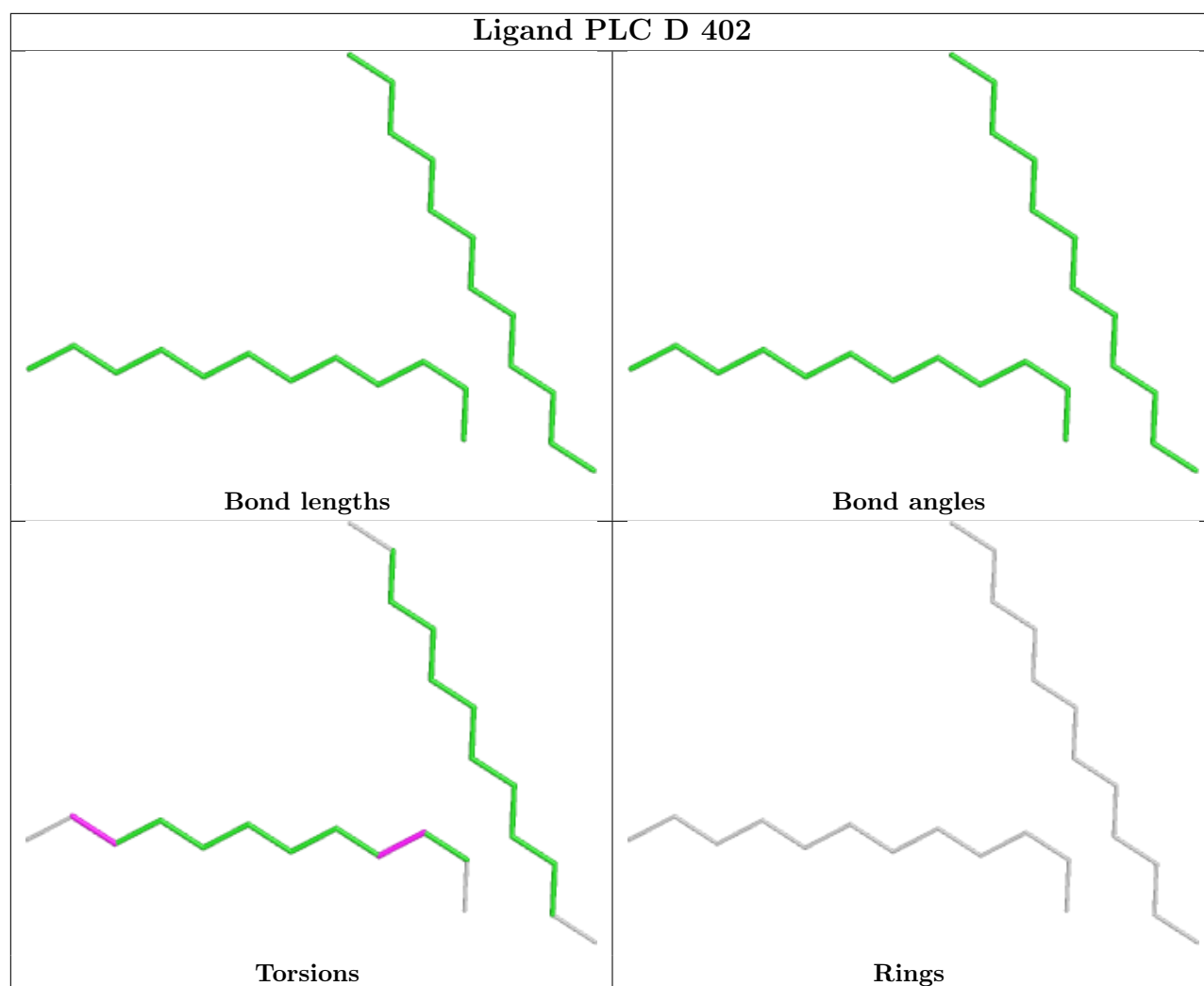












5.7 Other polymers [i](#)

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%)	0.79	34 (10%)	10 9	50, 102, 154, 218	1 (0%)
1	B	311/359 (86%)	1.03	44 (14%)	6 5	32, 99, 151, 194	1 (0%)
1	C	311/359 (86%)	0.83	42 (13%)	7 6	78, 98, 159, 218	0
1	D	311/359 (86%)	0.79	38 (12%)	8 7	41, 101, 157, 216	2 (0%)
1	E	311/359 (86%)	0.86	37 (11%)	9 7	49, 101, 146, 203	1 (0%)
All	All	1555/1795 (86%)	0.86	195 (12%)	8 7	32, 100, 155, 218	5 (0%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	57	VAL	7.0
1	D	5	VAL	6.4
1	E	57	VAL	6.2
1	B	5	VAL	5.8
1	A	154	ASP	5.3
1	C	65	THR	5.3
1	B	83	ASN	5.2
1	A	11	ILE	5.0
1	C	61	VAL	5.0
1	E	154	ASP	5.0
1	A	156	PHE	5.0
1	C	66	TYR	4.8
1	E	11	ILE	4.8
1	E	284	GLN	4.8
1	B	111	LEU	4.7
1	C	94	VAL	4.7
1	D	141	VAL	4.6
1	D	170	LYS	4.5
1	A	75	GLU	4.5
1	B	11	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	93	SER	4.5
1	A	297	ILE	4.4
1	D	189	ARG	4.3
1	E	180	LEU	4.2
1	D	178	ASP	4.2
1	A	61	VAL	4.2
1	C	154	ASP	4.1
1	E	283	SER	4.1
1	B	129	TYR	4.1
1	D	156	PHE	4.0
1	D	154	ASP	3.9
1	C	92	ILE	3.9
1	B	207	PHE	3.8
1	C	64	LYS	3.7
1	C	63	VAL	3.7
1	A	111	LEU	3.7
1	E	297	ILE	3.7
1	C	5	VAL	3.6
1	B	245	ASN	3.6
1	B	102	TYR	3.5
1	B	80	ASN	3.5
1	E	61	VAL	3.5
1	B	170	LYS	3.5
1	D	11	ILE	3.5
1	D	111	LEU	3.5
1	B	244	THR	3.4
1	C	207	PHE	3.4
1	C	179	ARG	3.3
1	D	180	LEU	3.3
1	B	84	ALA	3.3
1	A	170	LYS	3.3
1	C	62	ARG	3.2
1	D	155	VAL	3.2
1	C	111	LEU	3.2
1	C	56	PRO	3.2
1	D	84	ALA	3.2
1	C	136	ASP	3.2
1	C	11	ILE	3.2
1	A	178	ASP	3.1
1	D	280	LYS	3.1
1	D	244	THR	3.1
1	B	210	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	113	PRO	3.1
1	A	63	VAL	3.1
1	B	242	VAL	3.1
1	B	6	SER	3.0
1	B	206	LEU	3.0
1	E	115	ASP	3.0
1	C	156	PHE	3.0
1	E	280	LYS	3.0
1	A	12	ALA	3.0
1	C	141	VAL	3.0
1	A	80	ASN	3.0
1	D	136	ASP	3.0
1	E	89	VAL	2.9
1	D	65	THR	2.9
1	B	61	VAL	2.9
1	E	156	PHE	2.9
1	D	127	HIS	2.9
1	B	79	VAL	2.9
1	E	207	PHE	2.9
1	E	50	ARG	2.8
1	E	5	VAL	2.8
1	C	283	SER	2.8
1	D	80	ASN	2.8
1	B	127	HIS	2.8
1	B	249	THR	2.8
1	A	301	VAL	2.8
1	D	12	ALA	2.8
1	D	17	THR	2.8
1	E	102	TYR	2.8
1	A	5	VAL	2.7
1	C	205	MET	2.7
1	B	104	GLU	2.7
1	E	88	ASP	2.7
1	C	276	GLN	2.7
1	B	186	TYR	2.7
1	B	287	ARG	2.7
1	E	217	TRP	2.7
1	B	187	GLN	2.6
1	A	84	ALA	2.6
1	D	126	LEU	2.6
1	E	111	LEU	2.6
1	E	301	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	129	TYR	2.6
1	D	137	THR	2.6
1	D	309	ILE	2.6
1	B	47	TRP	2.5
1	B	13	ASP	2.5
1	C	88	ASP	2.5
1	D	61	VAL	2.5
1	B	12	ALA	2.5
1	B	312	PHE	2.5
1	A	10	PRO	2.5
1	D	148	LYS	2.5
1	B	243	GLU	2.5
1	A	155	VAL	2.5
1	D	210	PHE	2.5
1	A	64	LYS	2.5
1	D	83	ASN	2.4
1	A	222	GLU	2.4
1	B	82	GLU	2.4
1	E	155	VAL	2.4
1	C	54	PHE	2.4
1	E	84	ALA	2.4
1	A	292	THR	2.4
1	A	57	VAL	2.4
1	A	169	VAL	2.4
1	B	110	VAL	2.4
1	B	305	LEU	2.4
1	E	65	THR	2.4
1	A	14	GLU	2.4
1	E	177	GLU	2.4
1	B	9	PRO	2.4
1	A	141	VAL	2.4
1	B	50	ARG	2.4
1	A	305	LEU	2.3
1	E	69	GLU	2.3
1	E	94	VAL	2.3
1	B	37	PHE	2.3
1	B	137	THR	2.3
1	A	280	LYS	2.3
1	E	63	VAL	2.3
1	A	70	ALA	2.3
1	E	56	PRO	2.3
1	A	210	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	238	PHE	2.3
1	B	156	PHE	2.3
1	C	12	ALA	2.3
1	B	62	ARG	2.3
1	C	147	GLU	2.2
1	C	243	GLU	2.2
1	C	284	GLN	2.2
1	B	189	ARG	2.2
1	C	180	LEU	2.2
1	C	155	VAL	2.2
1	A	205	MET	2.2
1	C	78	PHE	2.2
1	D	222	GLU	2.2
1	D	50	ARG	2.2
1	A	152	ASN	2.2
1	E	68	PRO	2.2
1	E	90	VAL	2.2
1	E	244	THR	2.2
1	C	50	ARG	2.2
1	C	206	LEU	2.2
1	B	135	VAL	2.2
1	C	177	GLU	2.1
1	C	137	THR	2.1
1	E	152	ASN	2.1
1	C	129	TYR	2.1
1	A	88	ASP	2.1
1	C	70	ALA	2.1
1	D	75	GLU	2.1
1	B	293	ARG	2.1
1	D	187	GLN	2.1
1	A	28	TYR	2.1
1	C	60	GLY	2.1
1	D	89	VAL	2.1
1	E	141	VAL	2.1
1	B	7	PRO	2.1
1	D	284	GLN	2.1
1	D	139	ASN	2.1
1	E	70	ALA	2.0
1	D	166	THR	2.0
1	B	310	LEU	2.0
1	C	52	LEU	2.0
1	D	188	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	14	GLU	2.0
1	E	210	PHE	2.0
1	E	153	ASP	2.0
1	A	8	PRO	2.0
1	E	255	THR	2.0
1	C	305	LEU	2.0
1	D	149	VAL	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
6	NA	C	401	1/1	0.00	0.86	144,144,144,144	0
6	NA	B	405	1/1	0.55	0.32	115,115,115,115	0
6	NA	E	404	1/1	0.68	0.30	125,125,125,125	0
2	PLC	D	401	34/42	0.74	0.29	110,133,164,168	0
2	PLC	B	402	24/42	0.75	0.47	100,120,145,152	0
2	PLC	C	404	12/42	0.75	0.32	115,117,120,121	0
2	PLC	B	401	34/42	0.75	0.31	104,141,182,184	0
2	PLC	C	402	34/42	0.76	0.27	104,136,169,170	0
2	PLC	D	402	24/42	0.77	0.36	99,107,127,130	0
2	PLC	A	403	12/42	0.77	0.31	118,122,132,132	0
2	PLC	E	402	12/42	0.78	0.34	125,127,131,132	0
2	PLC	D	403	12/42	0.78	0.33	117,118,125,126	0
2	PLC	C	403	24/42	0.79	0.33	93,104,107,109	0
2	PLC	E	401	34/42	0.79	0.27	117,148,182,184	0
2	PLC	A	401	34/42	0.79	0.29	112,150,181,183	0
3	CL	A	405	1/1	0.81	0.27	163,163,163,163	0

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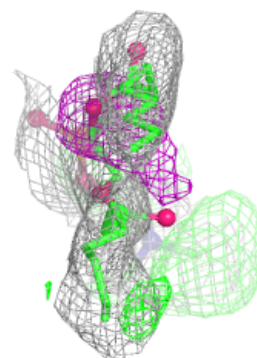
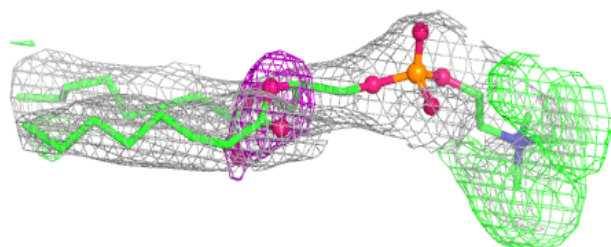
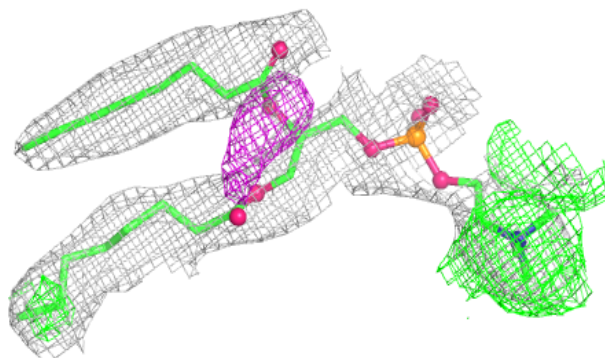
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLC	A	402	24/42	0.81	0.33	92,101,116,122	0
4	D12	C	407	12/12	0.83	0.22	51,60,68,69	0
4	D12	E	405	12/12	0.84	0.26	75,77,85,86	0
2	PLC	B	403	12/42	0.85	0.29	123,125,128,130	0
4	D12	D	405	12/12	0.85	0.25	66,78,87,87	0
4	D12	A	407	12/12	0.86	0.24	71,74,79,79	0
4	D12	B	406	12/12	0.86	0.23	23,32,82,84	0
4	D12	A	406	12/12	0.87	0.22	72,78,85,87	0
3	CL	D	404	1/1	0.91	0.16	106,106,106,106	0
3	CL	A	408	1/1	0.91	0.12	119,119,119,119	0
3	CL	E	403	1/1	0.92	0.13	115,115,115,115	0
5	GUA	A	409	9/9	0.92	0.21	122,124,130,132	0
6	NA	C	406	1/1	0.92	0.14	107,107,107,107	0
5	GUA	B	408	9/9	0.92	0.18	113,114,119,121	0
5	GUA	E	406	9/9	0.93	0.19	114,115,126,126	0
3	CL	C	408	1/1	0.93	0.13	120,120,120,120	0
3	CL	C	405	1/1	0.93	0.18	107,107,107,107	0
3	CL	D	408	1/1	0.93	0.12	118,118,118,118	0
5	GUA	D	407	9/9	0.93	0.17	115,117,119,121	0
3	CL	B	404	1/1	0.94	0.13	120,120,120,120	0
3	CL	E	407	1/1	0.95	0.12	117,117,117,117	0
5	GUA	D	406	9/9	0.95	0.18	119,122,129,132	0
3	CL	B	407	1/1	0.96	0.11	113,113,113,113	0
3	CL	A	404	1/1	0.96	0.10	101,101,101,101	0

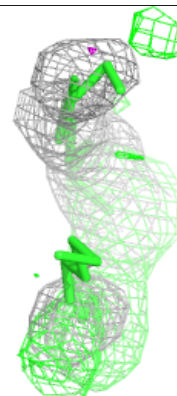
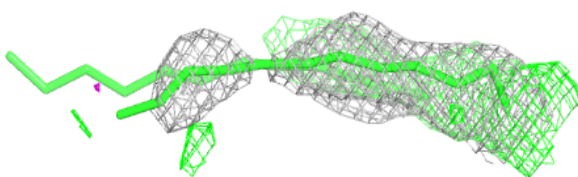
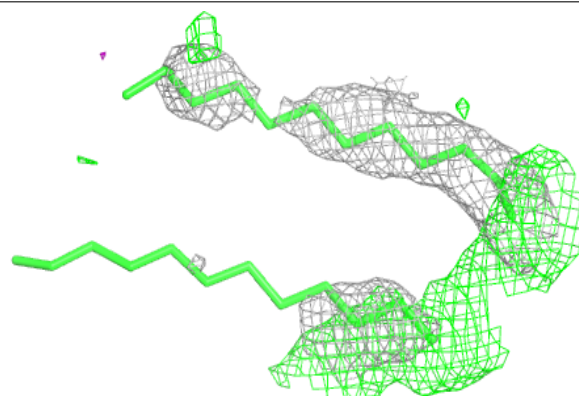
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

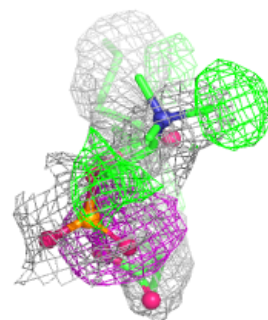
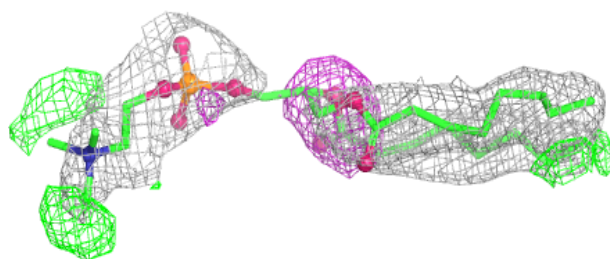
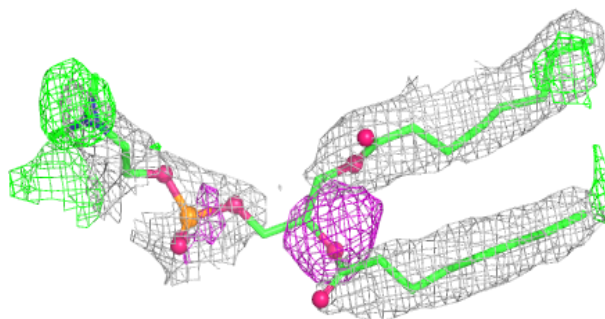
**Electron density around PLC B 402:**

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

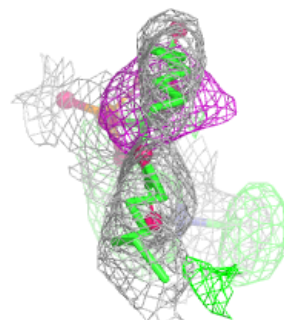
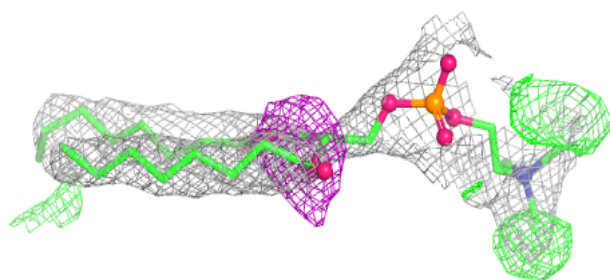
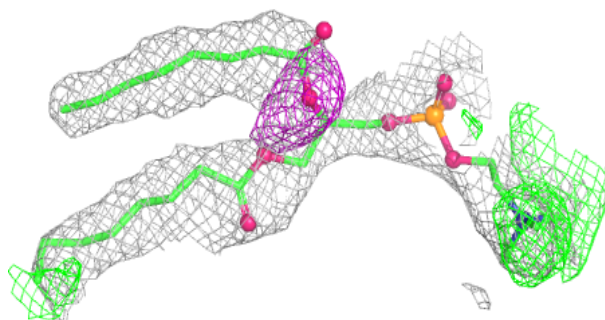


Electron density around PLC B 401:

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

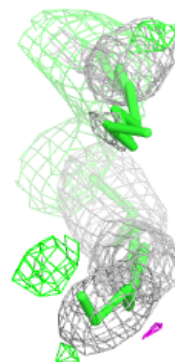
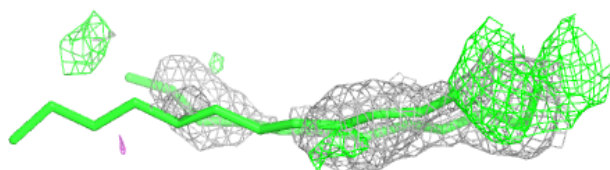
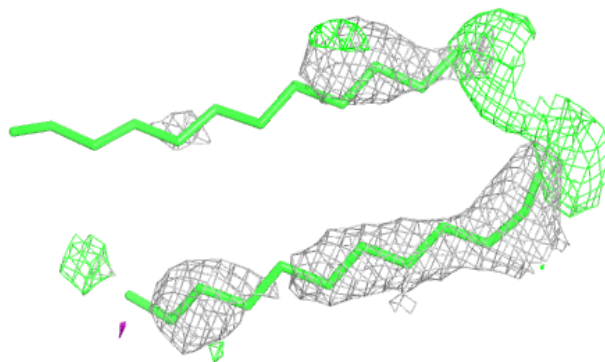
**Electron density around PLC C 402:**

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

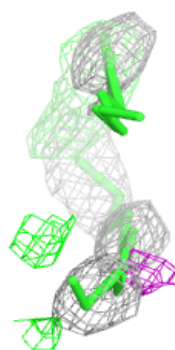
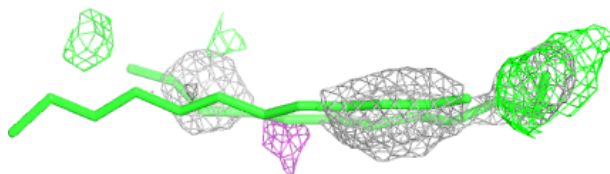
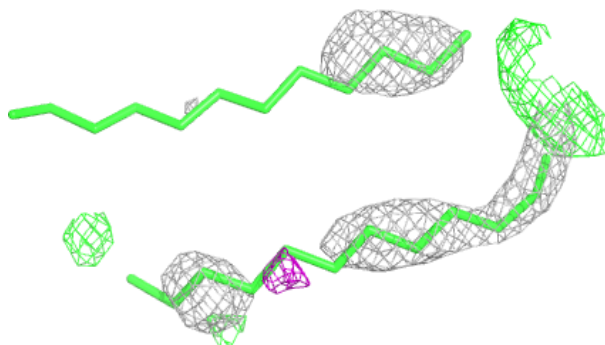


Electron density around PLC D 402:

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

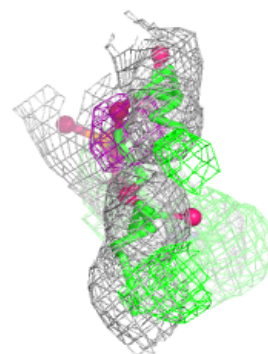
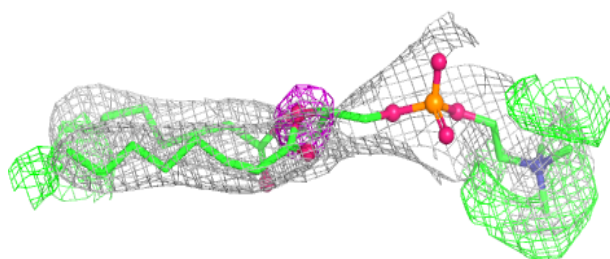
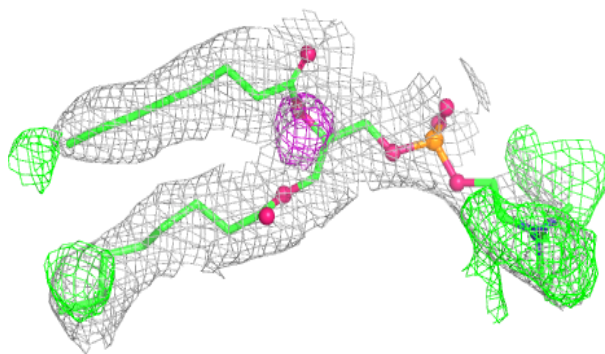
**Electron density around PLC C 403:**

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

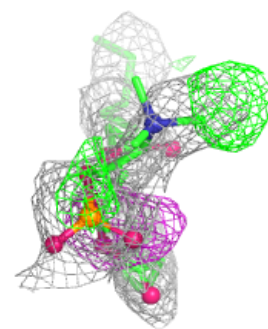
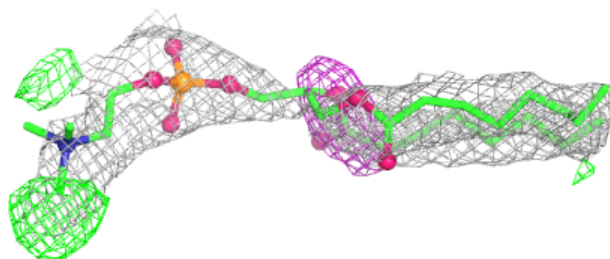
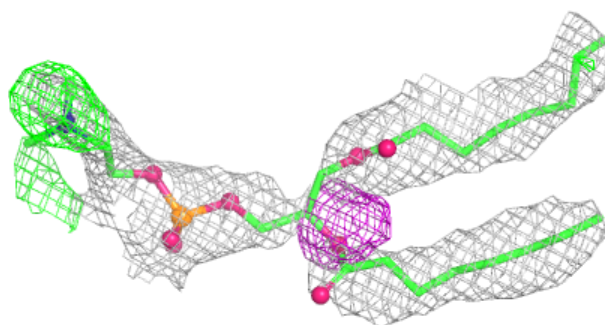


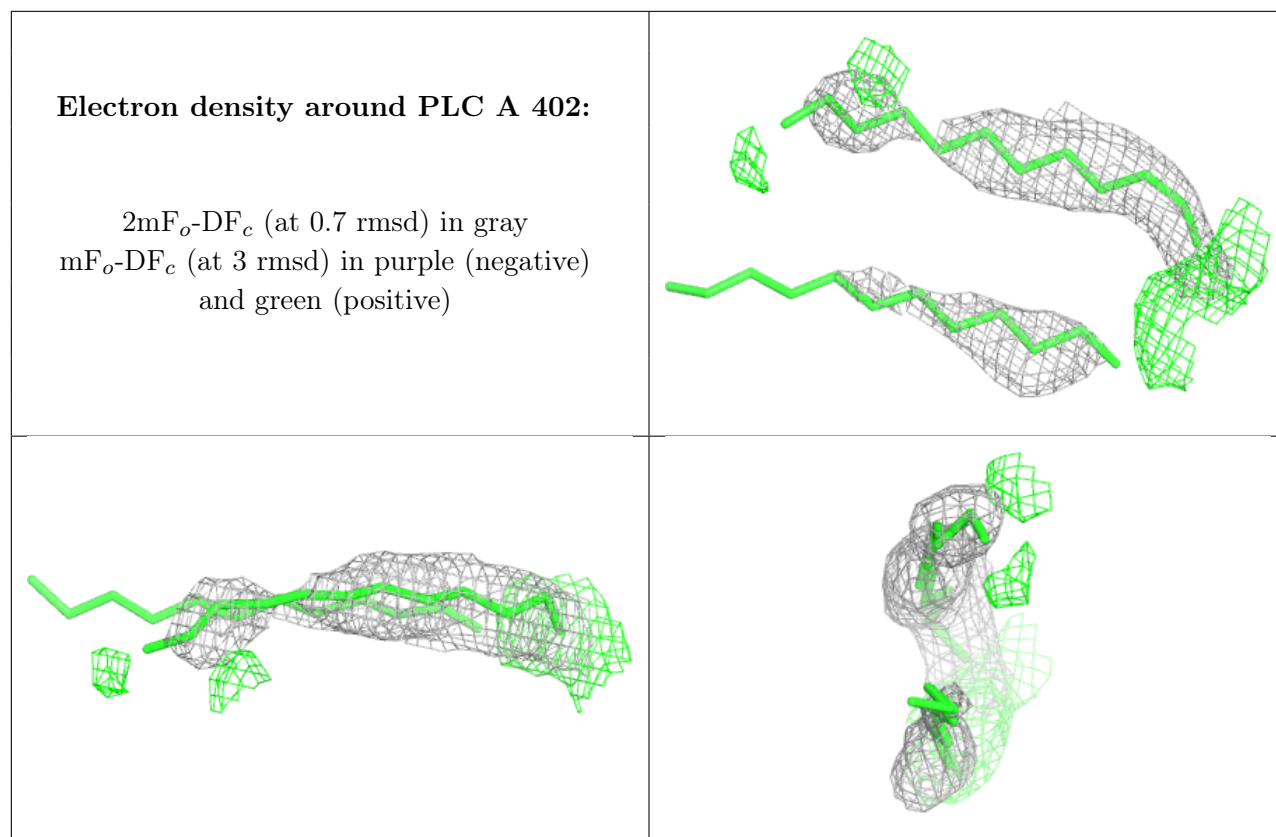
Electron density around PLC E 401:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.