



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:43 PM UTC

PDB ID : 8T56 / pdb_00008t56
EMDB ID : EMD-41043
Title : Structure of mechanically activated ion channel OSCA1.2 in peptidiscs
Authors : Burendei, B.; Jojoa-Cruz, S.; Lee, W.H.; Ward, A.B.
Deposited on : 2023-06-12
Resolution : 2.80 Å(reported)
Based on initial model : 6MGV

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

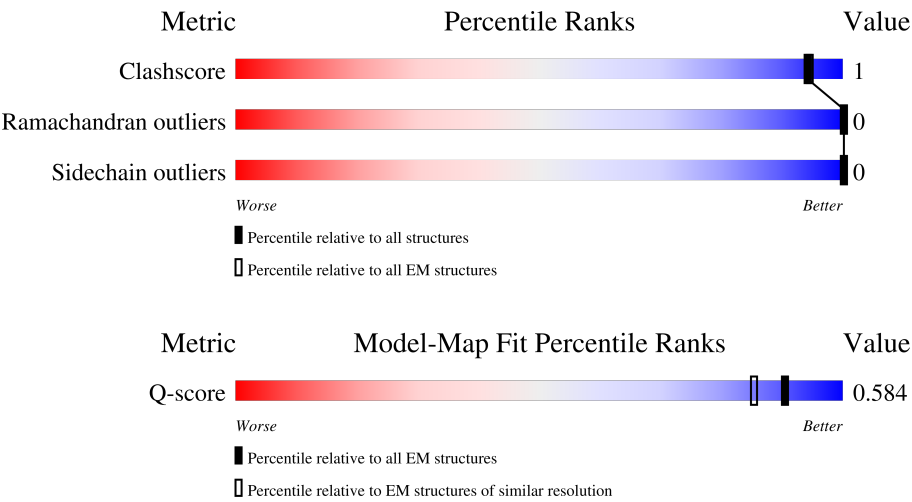
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	781	73%5%21%
1	B	781	74%5%21%
2	C	37	16% 81%14%5%
2	D	37	95%. .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	37	5% 86% 11%
2	F	37	41% 62% 5% 32%
2	G	37	16% 81% 14% 5%
2	H	37	95%
2	I	37	5% 86% 11%
2	J	37	41% 62% 5% 32%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13096 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Calcium permeable stress-gated cation channel 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	617	Total	C	N	O	S	0	0
			5005	3339	806	836	24		
1	B	617	Total	C	N	O	S	0	0
			5005	3339	806	836	24		

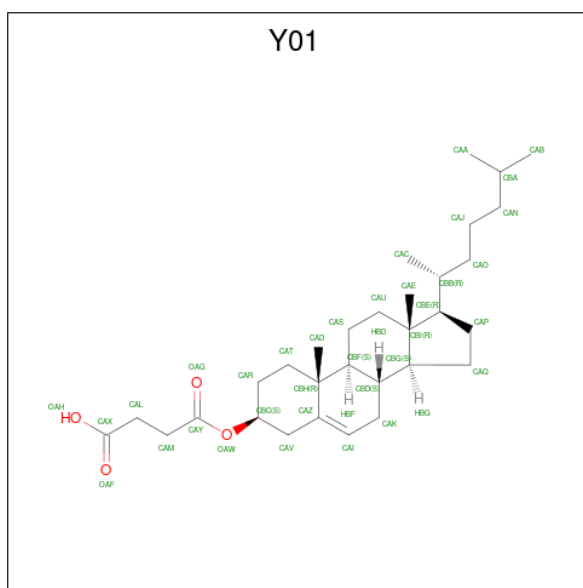
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	772	GLY	-	expression tag	UNP Q5XEZ5
A	773	THR	-	expression tag	UNP Q5XEZ5
A	774	GLY	-	expression tag	UNP Q5XEZ5
A	775	THR	-	expression tag	UNP Q5XEZ5
A	776	LEU	-	expression tag	UNP Q5XEZ5
A	777	GLU	-	expression tag	UNP Q5XEZ5
A	778	VAL	-	expression tag	UNP Q5XEZ5
A	779	LEU	-	expression tag	UNP Q5XEZ5
A	780	PHE	-	expression tag	UNP Q5XEZ5
A	781	GLN	-	expression tag	UNP Q5XEZ5
B	772	GLY	-	expression tag	UNP Q5XEZ5
B	773	THR	-	expression tag	UNP Q5XEZ5
B	774	GLY	-	expression tag	UNP Q5XEZ5
B	775	THR	-	expression tag	UNP Q5XEZ5
B	776	LEU	-	expression tag	UNP Q5XEZ5
B	777	GLU	-	expression tag	UNP Q5XEZ5
B	778	VAL	-	expression tag	UNP Q5XEZ5
B	779	LEU	-	expression tag	UNP Q5XEZ5
B	780	PHE	-	expression tag	UNP Q5XEZ5
B	781	GLN	-	expression tag	UNP Q5XEZ5

- Molecule 2 is a protein called NSPr peptide.

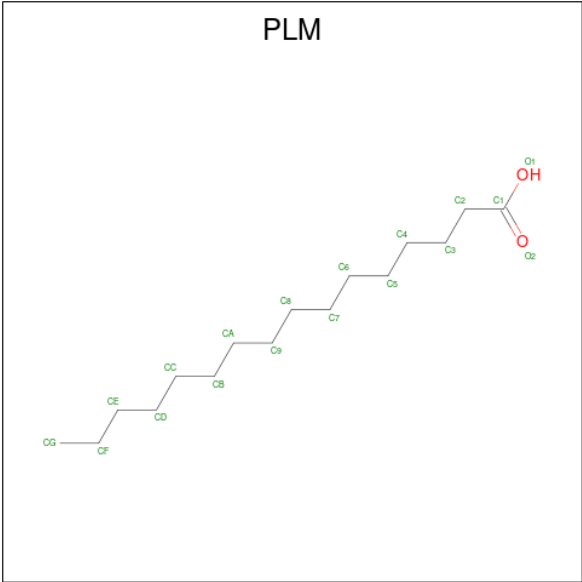
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	35	Total 300	C 204	N 45	O 51	0	0
2	D	36	Total 311	C 213	N 46	O 52	0	0
2	E	36	Total 311	C 213	N 46	O 52	0	0
2	F	25	Total 216	C 147	N 32	O 37	0	0
2	G	35	Total 300	C 204	N 45	O 51	0	0
2	H	36	Total 311	C 213	N 46	O 52	0	0
2	I	36	Total 311	C 213	N 46	O 52	0	0
2	J	25	Total 216	C 147	N 32	O 37	0	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total 35	C 31	O 4	0
3	B	1	Total 35	C 31	O 4	0

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: $\text{C}_{16}\text{H}_{32}\text{O}_2$).



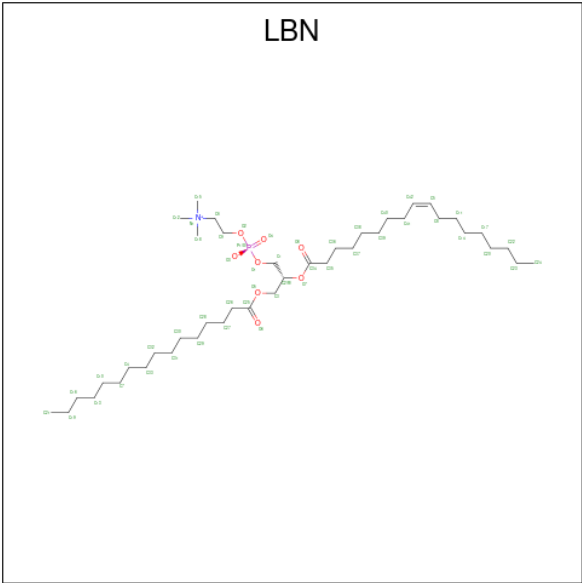
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	

Continued on next page...

Continued from previous page...

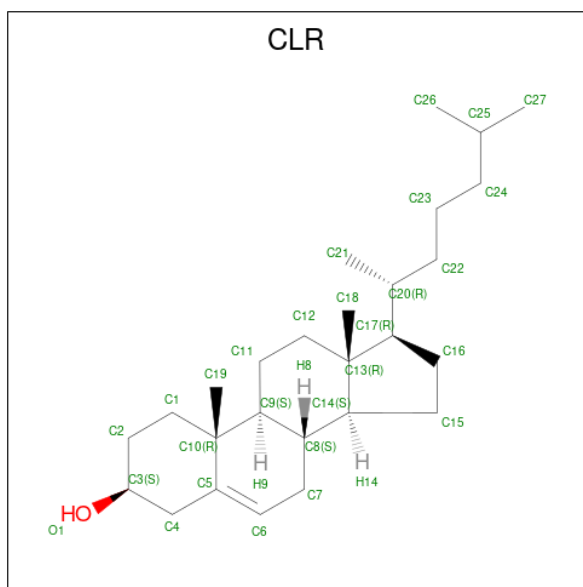
Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	D	1	Total	C	O	0
			18	16	2	
4	D	1	Total	C	O	0
			18	16	2	
4	E	1	Total	C	O	0
			18	16	2	
4	H	1	Total	C	O	0
			18	16	2	
4	H	1	Total	C	O	0
			18	16	2	
4	I	1	Total	C	O	0
			18	16	2	

- Molecule 5 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).

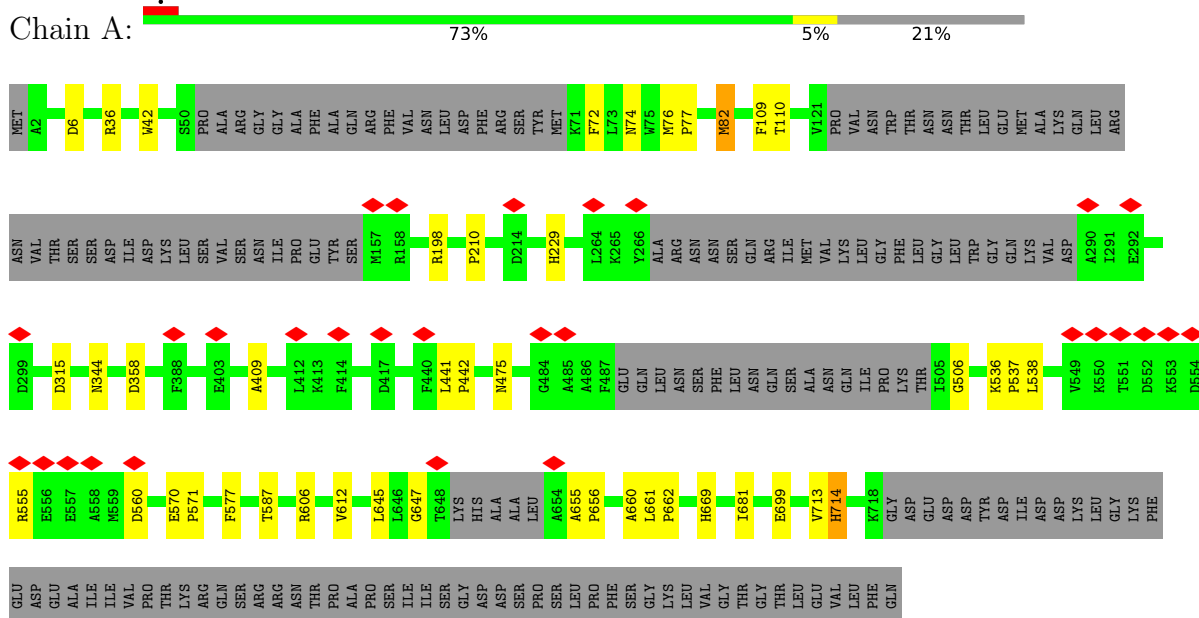


Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	
6	E	1	Total	C	O	0
			28	27	1	
6	G	1	Total	C	O	0
			28	27	1	
6	H	1	Total	C	O	0
			28	27	1	
6	I	1	Total	C	O	0
			28	27	1	

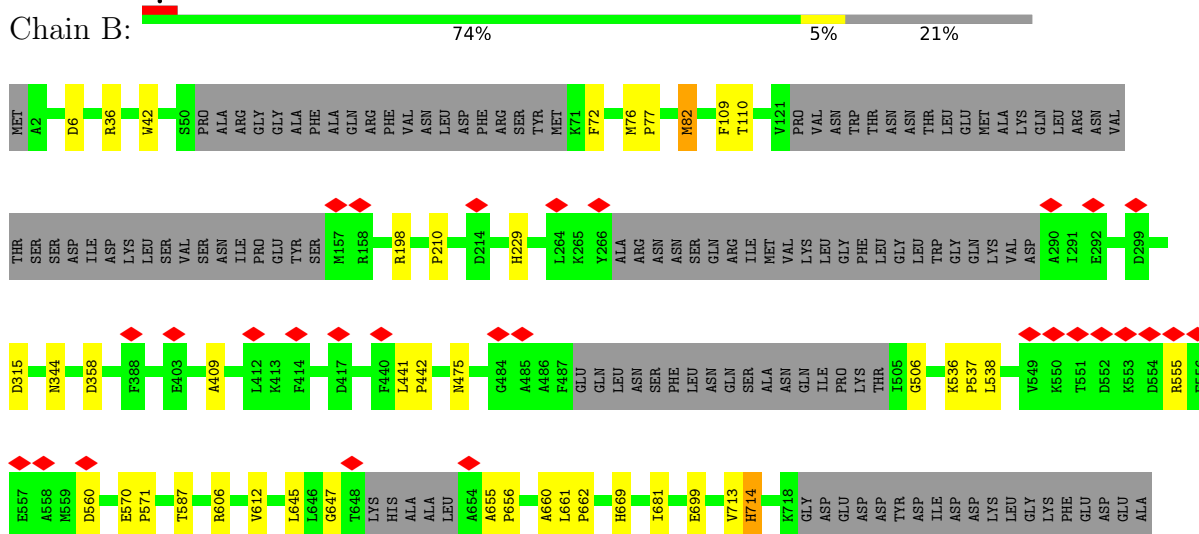
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Calcium permeable stress-gated cation channel 1



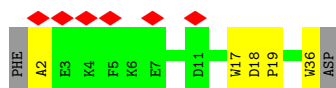
- Molecule 1: Calcium permeable stress-gated cation channel 1



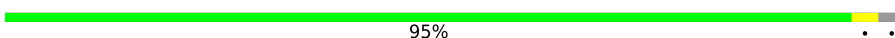
ILE ILE VAL PRO THR LYS ARG GLN SER ARG ARG ASN THR PRO ALA PRO SER ILE ILE SER GLY ASP ASP PRO SER LEU PHE SER GLY LYS VAL GLY THR THR LEU VAL LEU PHE GLN

• Molecule 2: NSPr peptide

Chain C: 



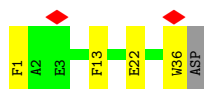
• Molecule 2: NSPr peptide

Chain D: 



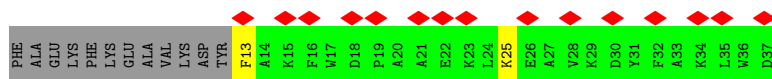
• Molecule 2: NSPr peptide

Chain E: 



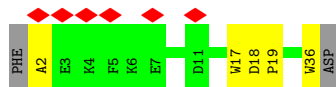
• Molecule 2: NSPr peptide

Chain F: 

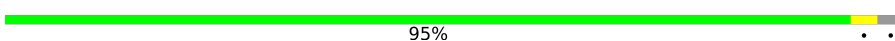


• Molecule 2: NSPr peptide

Chain G: 



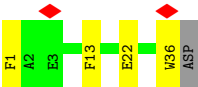
• Molecule 2: NSPr peptide

Chain H: 

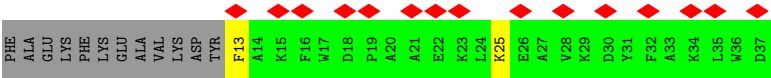
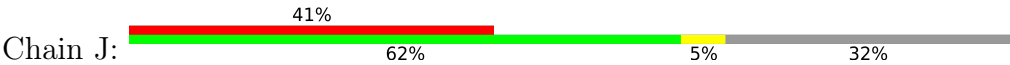


• Molecule 2: NSPr peptide

Chain I: 



● Molecule 2: NSPr peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	52250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0138	Depositor
Map size (Å)	226.59999, 226.59999, 226.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, PLM, Y01, LBN

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	1.30	5/5149 (0.1%)	1.13	32/6998 (0.5%)
1	B	1.30	5/5149 (0.1%)	1.14	31/6998 (0.4%)
2	C	1.20	2/310 (0.6%)	1.02	2/415 (0.5%)
2	D	1.35	2/322 (0.6%)	1.03	0/431
2	E	1.43	3/322 (0.9%)	1.07	3/431 (0.7%)
2	F	1.22	1/224 (0.4%)	1.01	0/300
2	G	1.20	2/310 (0.6%)	1.02	2/415 (0.5%)
2	H	1.35	2/322 (0.6%)	1.03	0/431
2	I	1.43	3/322 (0.9%)	1.07	3/431 (0.7%)
2	J	1.23	1/224 (0.4%)	1.01	0/300
All	All	1.30	26/12654 (0.2%)	1.12	73/17150 (0.4%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	36	TRP	CZ2-CH2	6.38	1.49	1.37
2	E	36	TRP	CZ2-CH2	6.37	1.49	1.37
2	D	36	TRP	CZ2-CH2	6.09	1.48	1.37
2	H	36	TRP	CZ2-CH2	6.09	1.48	1.37
2	C	36	TRP	CD2-CE3	5.82	1.49	1.40
2	G	36	TRP	CD2-CE3	5.80	1.49	1.40
2	E	1	PHE	CG-CD1	5.72	1.50	1.38
2	I	1	PHE	CG-CD1	5.72	1.50	1.38
2	I	36	TRP	CD2-CE3	5.59	1.49	1.40
2	E	36	TRP	CD2-CE3	5.58	1.49	1.40
1	A	475	ASN	CB-CG	-5.53	1.38	1.52
1	B	475	ASN	CB-CG	-5.53	1.38	1.52
1	A	210	PRO	N-CD	-5.29	1.40	1.47
1	B	210	PRO	N-CD	-5.29	1.40	1.47
2	F	13	PHE	CG-CD2	5.25	1.49	1.38
2	J	13	PHE	CG-CD2	5.25	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	TRP	NE1-CE2	-5.24	1.31	1.37
1	B	42	TRP	NE1-CE2	-5.24	1.31	1.37
2	D	36	TRP	CD2-CE3	5.18	1.48	1.40
2	H	36	TRP	CD2-CE3	5.18	1.48	1.40
2	C	36	TRP	CZ2-CH2	5.16	1.47	1.37
2	G	36	TRP	CZ2-CH2	5.16	1.47	1.37
1	A	669	HIS	CB-CG	-5.09	1.43	1.50
1	B	669	HIS	CB-CG	-5.09	1.43	1.50
1	A	538	LEU	CB-CG	-5.07	1.43	1.53
1	B	538	LEU	CB-CG	-5.07	1.43	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	VAL	N-CA-C	9.73	119.31	111.62
1	B	612	VAL	N-CA-C	9.71	119.29	111.62
1	A	229	HIS	CA-C-N	7.62	127.33	119.56
1	A	229	HIS	C-N-CA	7.62	127.33	119.56
1	B	229	HIS	CA-C-N	7.60	127.31	119.56
1	B	229	HIS	C-N-CA	7.60	127.31	119.56
1	A	409	ALA	CA-C-N	7.58	127.29	119.56
1	A	409	ALA	C-N-CA	7.58	127.29	119.56
1	A	587	THR	CA-C-N	7.57	127.28	119.56
1	A	587	THR	C-N-CA	7.57	127.28	119.56
1	B	587	THR	CA-C-N	7.57	127.28	119.56
1	B	587	THR	C-N-CA	7.57	127.28	119.56
1	B	409	ALA	CA-C-N	7.55	127.26	119.56
1	B	409	ALA	C-N-CA	7.55	127.26	119.56
1	B	681	ILE	N-CA-C	7.48	120.08	112.90
1	A	681	ILE	N-CA-C	7.45	120.05	112.90
1	A	210	PRO	CA-C-N	6.93	126.89	120.03
1	A	210	PRO	C-N-CA	6.93	126.89	120.03
1	B	210	PRO	CA-C-N	6.93	126.89	120.03
1	B	210	PRO	C-N-CA	6.93	126.89	120.03
1	B	699	GLU	CA-C-N	6.77	126.39	119.56
1	B	699	GLU	C-N-CA	6.77	126.39	119.56
1	A	699	GLU	CA-C-N	6.75	126.38	119.56
1	A	699	GLU	C-N-CA	6.75	126.38	119.56
1	B	72	PHE	N-CA-C	-6.59	103.87	114.09
1	A	72	PHE	N-CA-C	-6.59	103.87	114.09
1	A	647	GLY	CA-C-O	-6.52	117.98	122.22
1	B	647	GLY	CA-C-O	-6.48	118.01	122.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	714	HIS	CA-C-N	6.06	127.42	119.84
1	B	714	HIS	C-N-CA	6.06	127.42	119.84
1	A	714	HIS	CA-C-N	6.05	127.40	119.84
1	A	714	HIS	C-N-CA	6.05	127.40	119.84
1	B	344	ASN	CA-C-N	6.02	126.13	119.87
1	B	344	ASN	C-N-CA	6.02	126.13	119.87
1	A	344	ASN	CA-C-N	6.00	126.11	119.87
1	A	344	ASN	C-N-CA	6.00	126.11	119.87
1	A	358	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	358	ASP	CA-CB-CG	5.94	118.54	112.60
2	I	1	PHE	CA-C-N	5.76	128.00	120.28
2	I	1	PHE	C-N-CA	5.76	128.00	120.28
2	E	1	PHE	CA-C-N	5.72	127.95	120.28
2	E	1	PHE	C-N-CA	5.72	127.95	120.28
2	I	13	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	6	ASP	N-CA-C	-5.63	105.52	112.90
1	A	6	ASP	N-CA-C	-5.63	105.52	112.90
2	E	13	PHE	CA-CB-CG	5.63	119.43	113.80
1	A	82	MET	CA-C-N	5.38	125.32	119.78
1	A	82	MET	C-N-CA	5.38	125.32	119.78
1	B	82	MET	CA-C-N	5.38	125.32	119.78
1	B	82	MET	C-N-CA	5.38	125.32	119.78
1	A	475	ASN	CA-C-N	-5.19	116.45	122.63
1	A	475	ASN	C-N-CA	-5.19	116.45	122.63
1	B	475	ASN	CA-C-N	-5.17	116.47	122.63
1	B	475	ASN	C-N-CA	-5.17	116.47	122.63
1	A	560	ASP	CA-C-N	5.08	125.52	120.04
1	A	560	ASP	C-N-CA	5.08	125.52	120.04
1	B	560	ASP	CA-C-N	5.08	125.52	120.04
1	B	560	ASP	C-N-CA	5.08	125.52	120.04
2	C	2	ALA	CA-C-N	5.08	127.08	120.28
2	C	2	ALA	C-N-CA	5.08	127.08	120.28
1	A	612	VAL	CB-CA-C	-5.07	106.53	111.05
2	G	2	ALA	CA-C-N	5.06	127.06	120.28
2	G	2	ALA	C-N-CA	5.06	127.06	120.28
1	A	315	ASP	CA-C-N	5.06	124.72	119.56
1	A	315	ASP	C-N-CA	5.06	124.72	119.56
1	B	315	ASP	CA-C-N	5.04	124.70	119.56
1	B	315	ASP	C-N-CA	5.04	124.70	119.56
1	B	612	VAL	CB-CA-C	-5.03	106.57	111.05
1	B	198	ARG	CA-C-N	5.03	125.31	119.47
1	B	198	ARG	C-N-CA	5.03	125.31	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	CA-C-N	5.01	125.28	119.47
1	A	198	ARG	C-N-CA	5.01	125.28	119.47
1	A	577	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5005	0	5097	13	0
1	B	5005	0	5097	12	0
2	C	300	0	295	2	0
2	D	311	0	307	0	0
2	E	311	0	307	1	0
2	F	216	0	207	1	0
2	G	300	0	295	2	0
2	H	311	0	307	0	0
2	I	311	0	307	1	0
2	J	216	0	207	1	0
3	A	35	0	49	0	0
3	B	35	0	49	0	0
4	A	180	0	310	0	0
4	B	180	0	310	0	0
4	D	36	0	62	0	0
4	E	18	0	31	0	0
4	H	36	0	62	0	0
4	I	18	0	31	0	0
5	A	52	0	0	0	0
5	B	52	0	0	0	0
6	C	28	0	46	0	0
6	D	28	0	46	0	0
6	E	28	0	46	0	0
6	G	28	0	46	0	0
6	H	28	0	46	0	0
6	I	28	0	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13096	0	13606	31	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 1.

All (31) 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:76:MET:HB2	1:B:77:PRO:HD3	1.93	0.51
1:A:76:MET:HB2	1:A:77:PRO:HD3	1.93	0.50
1:A:661:LEU:HB2	1:A:662:PRO:HD3	1.94	0.49
1:B:36:ARG:NH1	1:B:555:ARG:HG2	2.27	0.49
1:B:661:LEU:HB2	1:B:662:PRO:HD3	1.94	0.49
1:A:36:ARG:NH1	1:A:555:ARG:HG2	2.27	0.48
1:A:506:GLY:O	1:A:645:LEU:HD13	2.15	0.47
1:B:506:GLY:O	1:B:645:LEU:HD13	2.15	0.46
1:B:536:LYS:HB3	1:B:537:PRO:HD3	1.98	0.46
1:A:536:LYS:HB3	1:A:537:PRO:HD3	1.98	0.45
1:B:713:VAL:O	1:B:714:HIS:C	2.60	0.45
1:B:441:LEU:N	1:B:442:PRO:HD2	2.33	0.44
2:C:18:ASP:HB2	2:C:19:PRO:HD3	1.99	0.44
1:A:441:LEU:N	1:A:442:PRO:HD2	2.32	0.44
2:I:22:GLU:OE2	2:J:25:LYS:NZ	2.49	0.44
2:G:18:ASP:HB2	2:G:19:PRO:HD3	1.99	0.44
2:G:17:TRP:O	2:G:18:ASP:C	2.61	0.43
1:A:713:VAL:O	1:A:714:HIS:C	2.60	0.43
1:B:82:MET:O	1:B:606:ARG:NH2	2.52	0.43
1:A:82:MET:O	1:A:606:ARG:NH2	2.52	0.43
1:B:570:GLU:N	1:B:571:PRO:CD	2.82	0.42
1:A:74:ASN:OD1	1:A:74:ASN:N	2.53	0.42
2:E:22:GLU:OE2	2:F:25:LYS:NZ	2.49	0.41
1:A:570:GLU:N	1:A:571:PRO:CD	2.82	0.41
1:A:660:ALA:O	1:A:661:LEU:C	2.62	0.41
1:B:109:PHE:O	1:B:110:THR:C	2.60	0.41
2:C:17:TRP:O	2:C:18:ASP:C	2.61	0.41
1:A:109:PHE:O	1:A:110:THR:C	2.60	0.40
1:A:655:ALA:N	1:A:656:PRO:CD	2.85	0.40
1:B:655:ALA:N	1:B:656:PRO:CD	2.85	0.40
1:B:660:ALA:O	1:B:661:LEU:C	2.62	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 PDB entries followed by that with respect to all EM entries.

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	605/781 (78%)	601 (99%)	4 (1%)	0	100	100
1	B	605/781 (78%)	601 (99%)	4 (1%)	0	100	100
2	C	33/37 (89%)	33 (100%)	0	0	100	100
2	D	34/37 (92%)	34 (100%)	0	0	100	100
2	E	34/37 (92%)	34 (100%)	0	0	100	100
2	F	23/37 (62%)	23 (100%)	0	0	100	100
2	G	33/37 (89%)	33 (100%)	0	0	100	100
2	H	34/37 (92%)	34 (100%)	0	0	100	100
2	I	34/37 (92%)	34 (100%)	0	0	100	100
2	J	23/37 (62%)	23 (100%)	0	0	100	100
All	All	1458/1858 (78%)	1450 (100%)	8 (0%)	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 PDB entries followed by that with respect to all EM entries.

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	531/674 (79%)	531 (100%)	0	100	100
1	B	531/674 (79%)	531 (100%)	0	100	100
2	C	28/30 (93%)	28 (100%)	0	100	100
2	D	29/30 (97%)	29 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	29/30 (97%)	29 (100%)	0	100	100
2	F	20/30 (67%)	20 (100%)	0	100	100
2	G	28/30 (93%)	28 (100%)	0	100	100
2	H	29/30 (97%)	29 (100%)	0	100	100
2	I	29/30 (97%)	29 (100%)	0	100	100
2	J	20/30 (67%)	20 (100%)	0	100	100
All	All	1274/1588 (80%)	1274 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	615	GLN
1	A	669	HIS
1	B	223	HIS
1	B	232	HIS
1	B	426	GLN
1	B	615	GLN
1	B	669	HIS

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](#)

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PLM	D	102	-	17,17,17	0.84	0	17,17,17	0.59	0
4	PLM	D	103	-	17,17,17	0.86	1 (5%)	17,17,17	0.62	0
4	PLM	B	804	-	17,17,17	0.89	1 (5%)	17,17,17	0.58	0
4	PLM	A	806	-	17,17,17	0.87	0	17,17,17	0.61	0
6	CLR	G	801	-	31,31,31	4.01	21 (67%)	48,48,48	2.21	16 (33%)
6	CLR	H	101	-	31,31,31	4.09	21 (67%)	48,48,48	2.29	19 (39%)
4	PLM	A	802	-	17,17,17	0.86	0	17,17,17	0.61	0
4	PLM	B	810	-	17,17,17	0.82	0	17,17,17	0.70	0
4	PLM	A	810	-	17,17,17	0.81	0	17,17,17	0.69	0
4	PLM	E	102	-	17,17,17	0.88	1 (5%)	17,17,17	0.66	1 (5%)
4	PLM	B	808	-	17,17,17	0.88	1 (5%)	17,17,17	0.47	0
4	PLM	B	807	-	17,17,17	1.06	1 (5%)	17,17,17	0.46	0
4	PLM	I	102	-	17,17,17	0.88	1 (5%)	17,17,17	0.66	1 (5%)
4	PLM	B	806	-	17,17,17	0.86	0	17,17,17	0.61	0
4	PLM	B	803	-	17,17,17	0.82	1 (5%)	17,17,17	0.72	0
4	PLM	H	103	-	17,17,17	0.86	1 (5%)	17,17,17	0.62	0
6	CLR	C	801	-	31,31,31	4.01	21 (67%)	48,48,48	2.21	16 (33%)
3	Y01	B	801	-	38,38,38	2.39	16 (42%)	57,57,57	2.08	20 (35%)
4	PLM	B	811	-	17,17,17	0.93	1 (5%)	17,17,17	0.46	0
6	CLR	I	101	-	31,31,31	3.92	20 (64%)	48,48,48	2.16	17 (35%)
6	CLR	D	101	-	31,31,31	4.09	21 (67%)	48,48,48	2.30	19 (39%)
4	PLM	A	808	-	17,17,17	0.88	1 (5%)	17,17,17	0.47	0
4	PLM	A	804	-	17,17,17	0.89	1 (5%)	17,17,17	0.58	0
4	PLM	A	809	-	17,17,17	0.86	0	17,17,17	0.62	0
4	PLM	B	802	-	17,17,17	0.86	0	17,17,17	0.61	0
5	LBN	B	812	-	51,51,51	1.81	7 (13%)	57,59,59	1.52	10 (17%)
5	LBN	A	812	-	51,51,51	1.81	7 (13%)	57,59,59	1.52	10 (17%)
3	Y01	A	801	-	38,38,38	2.39	17 (44%)	57,57,57	2.08	20 (35%)
4	PLM	B	805	-	17,17,17	0.77	0	17,17,17	0.83	1 (5%)
4	PLM	A	805	-	17,17,17	0.77	0	17,17,17	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CLR	E	101	-	31,31,31	3.92	20 (64%)	48,48,48	2.16	17 (35%)
4	PLM	H	102	-	17,17,17	0.84	0	17,17,17	0.60	0
4	PLM	A	803	-	17,17,17	0.82	1 (5%)	17,17,17	0.72	0
4	PLM	A	807	-	17,17,17	1.06	1 (5%)	17,17,17	0.46	0
4	PLM	A	811	-	17,17,17	0.93	1 (5%)	17,17,17	0.45	0
4	PLM	B	809	-	17,17,17	0.87	0	17,17,17	0.62	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	PLM	D	102	-	-	5/15/15/15	-
4	PLM	D	103	-	-	9/15/15/15	-
4	PLM	B	804	-	-	5/15/15/15	-
4	PLM	A	806	-	-	6/15/15/15	-
6	CLR	G	801	-	-	4/10/68/68	0/4/4/4
6	CLR	H	101	-	-	7/10/68/68	0/4/4/4
4	PLM	A	802	-	-	8/15/15/15	-
4	PLM	B	810	-	-	5/15/15/15	-
4	PLM	A	810	-	-	5/15/15/15	-
4	PLM	E	102	-	-	6/15/15/15	-
4	PLM	B	808	-	-	3/15/15/15	-
4	PLM	B	807	-	-	3/15/15/15	-
4	PLM	I	102	-	-	6/15/15/15	-
4	PLM	B	806	-	-	6/15/15/15	-
4	PLM	B	803	-	-	5/15/15/15	-
4	PLM	H	103	-	-	9/15/15/15	-
6	CLR	C	801	-	-	4/10/68/68	0/4/4/4
3	Y01	B	801	-	-	13/19/77/77	0/4/4/4
4	PLM	B	811	-	-	9/15/15/15	-
6	CLR	I	101	-	-	6/10/68/68	0/4/4/4
6	CLR	D	101	-	-	7/10/68/68	0/4/4/4
4	PLM	A	808	-	-	3/15/15/15	-
4	PLM	A	804	-	-	5/15/15/15	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLM	A	809	-	-	6/15/15/15	-
4	PLM	B	802	-	-	8/15/15/15	-
5	LBN	B	812	-	-	35/55/55/55	-
5	LBN	A	812	-	-	35/55/55/55	-
3	Y01	A	801	-	-	13/19/77/77	0/4/4/4
4	PLM	B	805	-	-	4/15/15/15	-
4	PLM	A	805	-	-	4/15/15/15	-
6	CLR	E	101	-	-	6/10/68/68	0/4/4/4
4	PLM	H	102	-	-	5/15/15/15	-
4	PLM	A	803	-	-	5/15/15/15	-
4	PLM	A	807	-	-	3/15/15/15	-
4	PLM	A	811	-	-	9/15/15/15	-
4	PLM	B	809	-	-	6/15/15/15	-

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	101	CLR	C10-C9	9.25	1.70	1.56
6	H	101	CLR	C10-C9	9.23	1.70	1.56
6	I	101	CLR	C10-C9	8.88	1.70	1.56
6	E	101	CLR	C10-C9	8.84	1.70	1.56
6	C	801	CLR	C10-C9	8.81	1.70	1.56
6	G	801	CLR	C10-C9	8.76	1.70	1.56
6	C	801	CLR	C8-C14	7.24	1.67	1.53
6	G	801	CLR	C8-C14	7.24	1.67	1.53
6	H	101	CLR	C8-C14	7.22	1.67	1.53
6	D	101	CLR	C8-C14	7.19	1.67	1.53
6	D	101	CLR	C4-C5	7.02	1.65	1.51
6	H	101	CLR	C4-C5	7.02	1.65	1.51
6	E	101	CLR	C4-C5	6.95	1.65	1.51
6	I	101	CLR	C4-C5	6.91	1.65	1.51
6	G	801	CLR	C4-C5	6.84	1.65	1.51
6	C	801	CLR	C4-C5	6.82	1.65	1.51
6	E	101	CLR	C8-C14	6.76	1.66	1.53
6	I	101	CLR	C8-C14	6.71	1.66	1.53
6	D	101	CLR	C13-C17	6.55	1.67	1.55
6	H	101	CLR	C13-C17	6.55	1.67	1.55
5	A	812	LBN	P1-O2	6.50	1.84	1.59
5	B	812	LBN	P1-O2	6.50	1.84	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	801	CLR	C13-C17	6.35	1.66	1.55
6	C	801	CLR	C13-C17	6.32	1.66	1.55
6	I	101	CLR	C13-C17	6.06	1.66	1.55
6	E	101	CLR	C13-C17	6.03	1.66	1.55
6	C	801	CLR	C4-C3	5.78	1.62	1.52
6	G	801	CLR	C4-C3	5.78	1.62	1.52
6	G	801	CLR	C7-C6	5.76	1.62	1.50
6	C	801	CLR	C7-C6	5.75	1.61	1.50
3	A	801	Y01	CBD-CBF	5.72	1.64	1.53
3	B	801	Y01	CBD-CBF	5.72	1.64	1.53
6	E	101	CLR	C4-C3	5.70	1.62	1.52
6	I	101	CLR	C4-C3	5.70	1.62	1.52
6	G	801	CLR	C1-C10	5.58	1.64	1.54
6	C	801	CLR	C1-C10	5.57	1.64	1.54
6	H	101	CLR	C4-C3	5.56	1.62	1.52
6	D	101	CLR	C4-C3	5.53	1.61	1.52
6	D	101	CLR	C8-C9	5.45	1.63	1.53
6	H	101	CLR	C8-C9	5.42	1.63	1.53
6	D	101	CLR	C1-C10	5.41	1.64	1.54
6	H	101	CLR	C1-C10	5.41	1.64	1.54
3	B	801	Y01	CAT-CBH	5.36	1.64	1.54
3	A	801	Y01	CAT-CBH	5.34	1.64	1.54
6	E	101	CLR	C7-C6	5.33	1.61	1.50
6	I	101	CLR	C7-C6	5.29	1.61	1.50
6	D	101	CLR	C7-C6	5.24	1.60	1.50
6	H	101	CLR	C7-C6	5.24	1.60	1.50
6	G	801	CLR	C8-C9	5.18	1.63	1.53
6	C	801	CLR	C8-C9	5.17	1.63	1.53
6	D	101	CLR	C20-C17	5.15	1.63	1.54
6	H	101	CLR	C20-C17	5.13	1.63	1.54
6	E	101	CLR	C8-C9	5.11	1.63	1.53
6	I	101	CLR	C8-C9	5.11	1.63	1.53
6	E	101	CLR	C1-C10	4.95	1.63	1.54
6	I	101	CLR	C1-C10	4.95	1.63	1.54
3	B	801	Y01	CBH-CAZ	4.75	1.61	1.52
3	A	801	Y01	CBH-CAZ	4.74	1.61	1.52
6	I	101	CLR	C11-C9	4.70	1.61	1.53
6	E	101	CLR	C11-C9	4.70	1.61	1.53
6	E	101	CLR	C20-C17	4.57	1.62	1.54
6	C	801	CLR	C20-C17	4.56	1.62	1.54
6	I	101	CLR	C20-C17	4.56	1.62	1.54
6	G	801	CLR	C20-C17	4.54	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	101	CLR	C11-C9	4.54	1.61	1.53
6	H	101	CLR	C11-C9	4.54	1.61	1.53
6	E	101	CLR	C10-C5	4.42	1.61	1.52
6	I	101	CLR	C10-C5	4.42	1.61	1.52
6	C	801	CLR	C7-C8	4.35	1.60	1.53
6	G	801	CLR	C7-C8	4.35	1.60	1.53
6	C	801	CLR	C10-C5	4.25	1.61	1.52
6	G	801	CLR	C10-C5	4.25	1.61	1.52
6	E	101	CLR	C7-C8	4.22	1.59	1.53
6	I	101	CLR	C7-C8	4.22	1.59	1.53
5	B	812	LBN	C1-C2	4.21	1.64	1.50
5	A	812	LBN	C1-C2	4.20	1.63	1.50
3	B	801	Y01	CBB-CBE	4.18	1.61	1.54
3	A	801	Y01	CBB-CBE	4.15	1.61	1.54
6	H	101	CLR	C10-C5	4.12	1.60	1.52
6	D	101	CLR	C10-C5	4.12	1.60	1.52
6	C	801	CLR	C11-C9	4.01	1.60	1.53
6	G	801	CLR	C11-C9	4.01	1.60	1.53
6	D	101	CLR	C7-C8	3.98	1.59	1.53
6	H	101	CLR	C7-C8	3.98	1.59	1.53
6	D	101	CLR	C12-C11	3.93	1.61	1.53
6	H	101	CLR	C12-C11	3.92	1.61	1.53
5	A	812	LBN	P1-O1	3.85	1.74	1.59
5	B	812	LBN	P1-O1	3.85	1.74	1.59
3	A	801	Y01	CBH-CBF	3.84	1.62	1.56
3	B	801	Y01	CBH-CBF	3.84	1.62	1.56
5	B	812	LBN	C6-N1	3.68	1.62	1.51
5	A	812	LBN	C6-N1	3.67	1.62	1.51
6	G	801	CLR	C12-C11	3.51	1.60	1.53
6	C	801	CLR	C12-C11	3.49	1.60	1.53
6	D	101	CLR	C18-C13	3.45	1.60	1.54
6	H	101	CLR	C18-C13	3.45	1.60	1.54
6	E	101	CLR	C12-C11	3.44	1.60	1.53
6	I	101	CLR	C12-C11	3.44	1.60	1.53
3	A	801	Y01	CAE-CBI	3.30	1.59	1.54
3	B	801	Y01	CAE-CBI	3.30	1.59	1.54
5	A	812	LBN	C6-C9	3.29	1.61	1.51
5	B	812	LBN	C6-C9	3.29	1.61	1.51
3	A	801	Y01	CBI-CBE	3.26	1.61	1.55
3	B	801	Y01	CBI-CBE	3.26	1.61	1.55
6	I	101	CLR	C18-C13	3.09	1.59	1.54
6	C	801	CLR	C18-C13	3.08	1.59	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	801	CLR	C18-C13	3.08	1.59	1.54
6	E	101	CLR	C18-C13	3.06	1.59	1.54
6	H	101	CLR	C12-C13	2.95	1.59	1.54
6	G	801	CLR	C22-C20	2.94	1.61	1.54
6	D	101	CLR	C12-C13	2.94	1.59	1.54
6	C	801	CLR	C22-C20	2.93	1.61	1.54
6	D	101	CLR	C22-C20	2.92	1.61	1.54
6	H	101	CLR	C22-C20	2.92	1.61	1.54
6	E	101	CLR	C22-C20	2.81	1.61	1.54
6	I	101	CLR	C22-C20	2.81	1.61	1.54
4	A	807	PLM	C2-C1	2.79	1.57	1.50
4	B	807	PLM	C2-C1	2.79	1.57	1.50
3	A	801	Y01	CAS-CBF	2.77	1.58	1.53
3	B	801	Y01	CAS-CBF	2.77	1.58	1.53
3	A	801	Y01	CAV-CBC	2.72	1.58	1.52
3	B	801	Y01	CAV-CBC	2.72	1.58	1.52
3	A	801	Y01	CAL-CAX	2.66	1.56	1.50
3	B	801	Y01	CAL-CAX	2.66	1.56	1.50
6	D	101	CLR	C1-C2	2.66	1.58	1.53
5	A	812	LBN	C3-C2	2.65	1.59	1.50
5	B	812	LBN	C3-C2	2.65	1.59	1.50
6	H	101	CLR	C1-C2	2.64	1.58	1.53
6	C	801	CLR	C1-C2	2.62	1.58	1.53
6	E	101	CLR	C12-C13	2.61	1.58	1.54
6	I	101	CLR	C12-C13	2.61	1.58	1.54
6	D	101	CLR	C15-C14	2.61	1.59	1.54
6	E	101	CLR	C1-C2	2.59	1.58	1.53
6	I	101	CLR	C1-C2	2.59	1.58	1.53
6	C	801	CLR	C13-C14	2.59	1.59	1.55
6	G	801	CLR	C13-C14	2.59	1.59	1.55
6	G	801	CLR	C1-C2	2.58	1.58	1.53
6	H	101	CLR	C15-C14	2.56	1.59	1.54
6	C	801	CLR	C6-C5	2.50	1.38	1.33
6	G	801	CLR	C6-C5	2.50	1.38	1.33
6	C	801	CLR	C12-C13	2.39	1.58	1.54
6	G	801	CLR	C12-C13	2.39	1.58	1.54
3	A	801	Y01	CAU-CBI	2.39	1.58	1.54
3	B	801	Y01	CAU-CBI	2.36	1.58	1.54
6	C	801	CLR	C15-C14	2.36	1.59	1.54
4	A	811	PLM	C2-C1	2.36	1.56	1.50
4	B	811	PLM	C2-C1	2.36	1.56	1.50
6	C	801	CLR	C19-C10	2.35	1.58	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	801	CLR	C19-C10	2.35	1.58	1.54
6	G	801	CLR	C15-C14	2.34	1.59	1.54
6	D	101	CLR	C19-C10	2.33	1.58	1.54
6	H	101	CLR	C19-C10	2.33	1.58	1.54
3	A	801	Y01	CBI-CBG	2.31	1.59	1.55
3	B	801	Y01	CBI-CBG	2.31	1.59	1.55
4	A	808	PLM	C2-C1	2.29	1.55	1.50
4	B	808	PLM	C2-C1	2.29	1.55	1.50
6	E	101	CLR	C13-C14	2.28	1.59	1.55
6	I	101	CLR	C13-C14	2.28	1.59	1.55
6	I	101	CLR	C6-C5	2.27	1.37	1.33
6	H	101	CLR	C6-C5	2.27	1.37	1.33
3	A	801	Y01	CAD-CBH	2.26	1.58	1.54
3	B	801	Y01	CAD-CBH	2.26	1.58	1.54
6	D	101	CLR	C6-C5	2.25	1.37	1.33
6	E	101	CLR	C6-C5	2.24	1.37	1.33
3	A	801	Y01	OAH-CAX	-2.24	1.23	1.30
3	B	801	Y01	OAH-CAX	-2.24	1.23	1.30
4	E	102	PLM	C2-C1	2.22	1.55	1.50
4	I	102	PLM	C2-C1	2.22	1.55	1.50
3	A	801	Y01	OAW-CAY	2.21	1.40	1.34
3	B	801	Y01	OAW-CAY	2.18	1.40	1.34
4	A	804	PLM	C2-C1	2.16	1.55	1.50
4	B	804	PLM	C2-C1	2.15	1.55	1.50
4	H	103	PLM	C2-C1	2.09	1.55	1.50
4	D	103	PLM	C2-C1	2.08	1.55	1.50
5	B	812	LBN	O7-C34	2.08	1.40	1.34
3	B	801	Y01	CAR-CBC	2.07	1.56	1.51
3	A	801	Y01	CAR-CBC	2.06	1.56	1.51
5	A	812	LBN	O7-C34	2.06	1.40	1.34
6	D	101	CLR	C13-C14	2.05	1.58	1.55
6	H	101	CLR	C13-C14	2.05	1.58	1.55
4	A	803	PLM	C2-C1	2.03	1.55	1.50
4	B	803	PLM	C2-C1	2.03	1.55	1.50
3	A	801	Y01	CBD-CBG	2.02	1.57	1.53
6	I	101	CLR	C15-C14	2.02	1.58	1.54
6	E	101	CLR	C15-C14	2.01	1.58	1.54

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	101	CLR	C3-C4-C5	5.74	121.19	112.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	101	CLR	C3-C4-C5	5.74	121.19	112.05
3	A	801	Y01	CAO-CBB-CBE	5.71	122.17	110.33
3	B	801	Y01	CAO-CBB-CBE	5.71	122.16	110.33
6	C	801	CLR	C4-C5-C10	-5.04	109.97	116.42
6	G	801	CLR	C4-C5-C10	-5.01	110.00	116.42
3	A	801	Y01	OAW-CAY-OAG	-4.89	112.28	123.70
3	B	801	Y01	OAW-CAY-OAG	-4.87	112.31	123.70
6	C	801	CLR	C4-C5-C6	4.87	127.17	120.57
6	D	101	CLR	C3-C4-C5	4.86	119.79	112.05
3	A	801	Y01	CAS-CBF-CBH	4.86	119.07	113.08
3	B	801	Y01	CAS-CBF-CBH	4.86	119.07	113.08
6	H	101	CLR	C3-C4-C5	4.85	119.77	112.05
6	G	801	CLR	C4-C5-C6	4.84	127.13	120.57
5	B	812	LBN	C2-O7-C34	4.82	129.34	117.80
5	A	812	LBN	C2-O7-C34	4.81	129.30	117.80
6	I	101	CLR	C4-C5-C6	4.58	126.77	120.57
6	C	801	CLR	C3-C4-C5	4.55	119.31	112.05
6	E	101	CLR	C4-C5-C6	4.55	126.74	120.57
6	G	801	CLR	C3-C4-C5	4.53	119.28	112.05
6	E	101	CLR	C4-C5-C10	-4.53	110.63	116.42
6	D	101	CLR	C4-C5-C6	4.52	126.69	120.57
6	I	101	CLR	C4-C5-C10	-4.51	110.64	116.42
6	H	101	CLR	C4-C5-C6	4.49	126.66	120.57
6	C	801	CLR	C18-C13-C12	-4.43	104.07	110.61
6	G	801	CLR	C18-C13-C12	-4.43	104.07	110.61
6	H	101	CLR	C22-C20-C17	4.36	119.37	110.33
6	D	101	CLR	C22-C20-C17	4.34	119.33	110.33
6	D	101	CLR	C4-C5-C10	-4.29	110.92	116.42
6	H	101	CLR	C4-C5-C10	-4.27	110.96	116.42
6	D	101	CLR	C7-C8-C14	4.25	116.95	110.93
6	H	101	CLR	C7-C8-C14	4.22	116.91	110.93
6	D	101	CLR	C18-C13-C12	-4.18	104.44	110.61
6	H	101	CLR	C18-C13-C12	-4.16	104.48	110.61
6	E	101	CLR	C18-C13-C12	-4.08	104.58	110.61
3	B	801	Y01	CAT-CAR-CBC	4.07	116.97	110.33
6	I	101	CLR	C18-C13-C12	-4.06	104.61	110.61
3	A	801	Y01	CAT-CAR-CBC	4.05	116.95	110.33
6	C	801	CLR	C7-C8-C14	4.00	116.60	110.93
6	G	801	CLR	C7-C8-C14	4.00	116.60	110.93
6	I	101	CLR	C7-C8-C14	3.86	116.40	110.93
6	E	101	CLR	C7-C8-C14	3.84	116.38	110.93
6	C	801	CLR	C22-C20-C17	3.78	118.17	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	801	CLR	C22-C20-C17	3.78	118.17	110.33
3	B	801	Y01	OAW-CAY-CAM	3.78	119.66	111.48
3	A	801	Y01	OAW-CAY-CAM	3.77	119.64	111.48
6	D	101	CLR	C1-C10-C5	3.65	115.04	108.74
6	H	101	CLR	C15-C14-C8	3.65	124.92	119.10
6	C	801	CLR	C1-C10-C5	3.64	115.03	108.74
6	H	101	CLR	C1-C10-C5	3.63	115.00	108.74
6	D	101	CLR	C15-C14-C8	3.63	124.89	119.10
6	G	801	CLR	C1-C10-C5	3.62	114.99	108.74
5	A	812	LBN	O7-C34-C35	3.57	119.21	111.48
6	G	801	CLR	C15-C14-C8	3.57	124.80	119.10
6	C	801	CLR	C15-C14-C8	3.55	124.77	119.10
5	B	812	LBN	O7-C34-C35	3.54	119.14	111.48
3	A	801	Y01	CAS-CBF-CBD	3.38	116.49	111.78
3	B	801	Y01	CAS-CBF-CBD	3.38	116.49	111.78
6	G	801	CLR	C2-C1-C10	3.36	119.94	112.78
6	C	801	CLR	C2-C1-C10	3.34	119.90	112.78
3	A	801	Y01	CAP-CBE-CBB	3.34	117.23	112.18
3	B	801	Y01	CAP-CBE-CBB	3.32	117.21	112.18
5	A	812	LBN	O3-P1-O4	3.32	127.89	112.44
5	B	812	LBN	O3-P1-O4	3.31	127.86	112.44
6	G	801	CLR	C8-C7-C6	3.30	117.33	112.76
6	E	101	CLR	C11-C9-C10	3.29	117.14	113.08
6	I	101	CLR	C11-C9-C10	3.29	117.14	113.08
6	C	801	CLR	C8-C7-C6	3.27	117.30	112.76
6	H	101	CLR	C2-C1-C10	3.23	119.66	112.78
6	D	101	CLR	C2-C1-C10	3.21	119.63	112.78
6	H	101	CLR	C19-C10-C5	-3.16	103.55	108.38
6	D	101	CLR	C19-C10-C5	-3.16	103.56	108.38
5	A	812	LBN	O7-C34-O8	-3.13	116.38	123.70
5	B	812	LBN	O7-C34-O8	-3.12	116.41	123.70
3	A	801	Y01	CBC-OAW-CAY	3.11	125.25	117.80
3	B	801	Y01	CBC-OAW-CAY	3.11	125.24	117.80
6	E	101	CLR	C22-C20-C17	3.07	116.69	110.33
6	I	101	CLR	C22-C20-C17	3.07	116.69	110.33
6	E	101	CLR	C14-C8-C9	3.05	113.08	109.09
6	I	101	CLR	C14-C8-C9	3.05	113.07	109.09
6	G	801	CLR	C11-C9-C10	2.90	116.66	113.08
6	C	801	CLR	C11-C9-C10	2.89	116.64	113.08
6	D	101	CLR	C16-C17-C20	2.84	116.48	112.18
6	D	101	CLR	C8-C7-C6	2.84	116.69	112.76
6	H	101	CLR	C8-C7-C6	2.84	116.69	112.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	101	CLR	C16-C17-C20	2.82	116.45	112.18
5	B	812	LBN	O2-P1-O4	-2.72	98.16	108.94
5	A	812	LBN	O2-P1-O4	-2.71	98.18	108.94
3	B	801	Y01	CBC-CAV-CAZ	2.71	115.45	111.45
3	A	801	Y01	CBC-CAV-CAZ	2.69	115.42	111.45
6	E	101	CLR	C2-C1-C10	2.69	118.50	112.78
6	I	101	CLR	C2-C1-C10	2.69	118.50	112.78
6	D	101	CLR	C11-C9-C10	2.66	116.36	113.08
6	H	101	CLR	C11-C9-C10	2.63	116.33	113.08
6	I	101	CLR	C8-C7-C6	2.62	116.40	112.76
6	I	101	CLR	C19-C10-C9	-2.62	108.72	111.66
6	E	101	CLR	C8-C7-C6	2.61	116.38	112.76
6	H	101	CLR	C1-C2-C3	2.61	113.93	110.48
6	D	101	CLR	C1-C2-C3	2.60	113.93	110.48
6	E	101	CLR	C19-C10-C9	-2.60	108.75	111.66
3	A	801	Y01	CAR-CBC-CAV	2.57	114.55	110.97
6	H	101	CLR	C14-C8-C9	2.56	112.43	109.09
6	D	101	CLR	C14-C8-C9	2.56	112.42	109.09
3	A	801	Y01	CAR-CAT-CBH	2.56	118.22	112.78
3	B	801	Y01	CAR-CBC-CAV	2.55	114.51	110.97
3	B	801	Y01	CAR-CAT-CBH	2.54	118.19	112.78
5	A	812	LBN	O5-C3-C2	2.52	115.66	108.40
5	B	812	LBN	O5-C3-C2	2.52	115.66	108.40
6	E	101	CLR	C1-C10-C5	2.52	113.08	108.74
6	I	101	CLR	C1-C10-C5	2.52	113.08	108.74
6	D	101	CLR	C12-C11-C9	2.51	117.41	113.14
6	H	101	CLR	C12-C11-C9	2.49	117.37	113.14
3	A	801	Y01	CAQ-CAP-CBE	2.49	110.01	105.14
3	B	801	Y01	CAQ-CAP-CBE	2.49	110.01	105.14
3	B	801	Y01	CAQ-CBG-CBD	2.49	123.07	119.10
3	A	801	Y01	CAQ-CBG-CBD	2.47	123.04	119.10
3	B	801	Y01	CBD-CAK-CAI	2.46	116.18	112.76
5	A	812	LBN	C18-N1-C12	-2.46	102.51	108.98
5	B	812	LBN	C18-N1-C12	-2.45	102.54	108.98
6	I	101	CLR	C16-C17-C13	-2.45	100.96	103.84
3	A	801	Y01	CBD-CAK-CAI	2.45	116.15	112.76
6	E	101	CLR	C16-C17-C13	-2.43	100.98	103.84
3	A	801	Y01	CAM-CAL-CAX	2.38	119.98	113.67
3	B	801	Y01	CAM-CAL-CAX	2.38	119.98	113.67
6	G	801	CLR	C16-C17-C20	2.36	115.75	112.18
6	H	101	CLR	C19-C10-C1	-2.36	105.84	109.43
6	C	801	CLR	C16-C17-C20	2.34	115.72	112.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	101	CLR	C19-C10-C1	-2.34	105.87	109.43
6	E	101	CLR	C19-C10-C5	-2.34	104.81	108.38
6	I	101	CLR	C19-C10-C5	-2.34	104.81	108.38
3	A	801	Y01	CAS-CAU-CBI	2.33	116.67	112.74
3	A	801	Y01	CAJ-CAO-CBB	2.32	121.57	115.08
3	B	801	Y01	CAS-CAU-CBI	2.32	116.66	112.74
3	B	801	Y01	CAJ-CAO-CBB	2.32	121.55	115.08
5	B	812	LBN	O5-C25-C26	2.31	118.87	111.83
5	A	812	LBN	O5-C25-C26	2.30	118.86	111.83
6	I	101	CLR	C15-C14-C8	2.30	122.77	119.10
6	E	101	CLR	C15-C14-C8	2.29	122.75	119.10
6	G	801	CLR	C19-C10-C1	-2.29	105.95	109.43
6	H	101	CLR	C16-C17-C13	-2.28	101.16	103.84
6	C	801	CLR	C19-C10-C1	-2.28	105.96	109.43
6	D	101	CLR	C16-C17-C13	-2.27	101.17	103.84
6	E	101	CLR	C12-C13-C17	2.24	119.89	116.60
6	I	101	CLR	C12-C13-C17	2.23	119.89	116.60
6	C	801	CLR	C19-C10-C5	-2.22	104.99	108.38
6	G	801	CLR	C19-C10-C5	-2.22	104.99	108.38
5	A	812	LBN	O5-C25-O6	-2.22	118.08	123.63
5	B	812	LBN	O5-C25-O6	-2.21	118.11	123.63
6	G	801	CLR	C12-C11-C9	2.20	116.87	113.14
6	C	801	CLR	C12-C11-C9	2.18	116.84	113.14
6	E	101	CLR	C12-C11-C9	2.17	116.83	113.14
4	A	805	PLM	C3-C2-C1	-2.16	108.86	114.51
4	B	805	PLM	C3-C2-C1	-2.16	108.86	114.51
6	I	101	CLR	C12-C11-C9	2.15	116.79	113.14
6	G	801	CLR	C16-C17-C13	-2.15	101.31	103.84
3	A	801	Y01	CAE-CBI-CBG	2.12	115.53	111.68
3	B	801	Y01	CAE-CBI-CBG	2.12	115.53	111.68
6	C	801	CLR	C16-C17-C13	-2.11	101.36	103.84
6	H	101	CLR	C1-C10-C9	2.07	111.47	108.74
6	D	101	CLR	C1-C10-C9	2.05	111.44	108.74
3	A	801	Y01	CAD-CBH-CAT	-2.04	106.32	109.43
3	B	801	Y01	CAD-CBH-CAT	-2.04	106.32	109.43
4	I	102	PLM	C3-C2-C1	-2.03	109.22	114.51
3	A	801	Y01	OAW-CBC-CAR	-2.03	103.58	108.37
4	E	102	PLM	C3-C2-C1	-2.02	109.23	114.51
3	B	801	Y01	OAW-CBC-CAR	-2.02	103.59	108.37
5	B	812	LBN	C37-C36-C35	2.02	120.55	113.13
5	A	812	LBN	C37-C36-C35	2.01	120.53	113.13

There are no chirality outliers.

All (278) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	812	LBN	C1-O1-P1-O2
5	A	812	LBN	C1-O1-P1-O3
5	A	812	LBN	C9-O2-P1-O1
5	A	812	LBN	C9-O2-P1-O3
5	A	812	LBN	C9-O2-P1-O4
5	A	812	LBN	O8-C34-O7-C2
5	B	812	LBN	C1-O1-P1-O2
5	B	812	LBN	C1-O1-P1-O3
5	B	812	LBN	C9-O2-P1-O1
5	B	812	LBN	C9-O2-P1-O3
5	B	812	LBN	C9-O2-P1-O4
5	B	812	LBN	O8-C34-O7-C2
5	A	812	LBN	O6-C25-O5-C3
5	B	812	LBN	O6-C25-O5-C3
3	A	801	Y01	OAG-CAY-OAW-CBC
3	B	801	Y01	OAG-CAY-OAW-CBC
5	A	812	LBN	C26-C25-O5-C3
5	B	812	LBN	C26-C25-O5-C3
3	A	801	Y01	CAM-CAY-OAW-CBC
3	B	801	Y01	CAM-CAY-OAW-CBC
5	A	812	LBN	C35-C34-O7-C2
5	B	812	LBN	C35-C34-O7-C2
6	D	101	CLR	C13-C17-C20-C22
6	H	101	CLR	C13-C17-C20-C22
4	D	102	PLM	C1-C2-C3-C4
4	H	102	PLM	C1-C2-C3-C4
5	A	812	LBN	C34-C35-C36-C37
5	B	812	LBN	C34-C35-C36-C37
6	E	101	CLR	C22-C23-C24-C25
6	I	101	CLR	C22-C23-C24-C25
4	A	811	PLM	C1-C2-C3-C4
4	B	811	PLM	C1-C2-C3-C4
3	A	801	Y01	CAO-CBB-CBE-CAP
3	B	801	Y01	CAO-CBB-CBE-CAP
3	A	801	Y01	CAO-CBB-CBE-CBI
3	B	801	Y01	CAO-CBB-CBE-CBI
6	D	101	CLR	C16-C17-C20-C22
6	H	101	CLR	C16-C17-C20-C22
6	E	101	CLR	C20-C22-C23-C24
6	I	101	CLR	C20-C22-C23-C24
5	B	812	LBN	C37-C38-C39-C40
5	A	812	LBN	C7-C10-C13-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	812	LBN	C37-C38-C39-C40
5	B	812	LBN	C7-C10-C13-C16
4	D	103	PLM	CA-CB-CC-CD
4	E	102	PLM	C5-C6-C7-C8
4	H	103	PLM	CA-CB-CC-CD
4	I	102	PLM	C5-C6-C7-C8
5	A	812	LBN	C32-C33-C4-C7
5	A	812	LBN	C36-C37-C38-C39
5	B	812	LBN	C32-C33-C4-C7
5	B	812	LBN	C36-C37-C38-C39
3	A	801	Y01	CAO-CAJ-CAN-CBA
3	B	801	Y01	CAO-CAJ-CAN-CBA
4	A	811	PLM	C6-C7-C8-C9
4	B	811	PLM	C6-C7-C8-C9
4	A	802	PLM	C4-C5-C6-C7
4	B	802	PLM	C4-C5-C6-C7
5	A	812	LBN	C27-C28-C29-C30
5	B	812	LBN	C27-C28-C29-C30
4	A	809	PLM	C7-C8-C9-CA
4	B	809	PLM	C7-C8-C9-CA
5	A	812	LBN	C26-C27-C28-C29
4	A	802	PLM	C7-C8-C9-CA
4	B	802	PLM	C7-C8-C9-CA
5	B	812	LBN	C26-C27-C28-C29
5	A	812	LBN	C17-C20-C22-C23
5	B	812	LBN	C17-C20-C22-C23
4	A	810	PLM	C9-CA-CB-CC
4	B	810	PLM	C9-CA-CB-CC
4	D	103	PLM	C6-C7-C8-C9
4	H	103	PLM	C6-C7-C8-C9
5	B	812	LBN	C10-C13-C16-C19
5	A	812	LBN	C10-C13-C16-C19
5	A	812	LBN	C35-C36-C37-C38
5	B	812	LBN	C35-C36-C37-C38
3	A	801	Y01	CAJ-CAO-CBB-CBE
3	B	801	Y01	CAJ-CAO-CBB-CBE
5	A	812	LBN	C29-C30-C31-C32
5	B	812	LBN	C29-C30-C31-C32
4	A	804	PLM	C4-C5-C6-C7
4	B	804	PLM	C4-C5-C6-C7
4	A	811	PLM	C2-C3-C4-C5
4	B	811	PLM	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	807	PLM	CC-CD-CE-CF
4	B	807	PLM	CC-CD-CE-CF
4	D	102	PLM	C8-C9-CA-CB
4	H	102	PLM	C8-C9-CA-CB
4	A	807	PLM	C2-C3-C4-C5
4	B	807	PLM	C2-C3-C4-C5
5	A	812	LBN	C14-C17-C20-C22
5	B	812	LBN	C14-C17-C20-C22
4	A	806	PLM	C9-CA-CB-CC
4	B	806	PLM	C9-CA-CB-CC
6	D	101	CLR	C16-C17-C20-C21
6	H	101	CLR	C16-C17-C20-C21
6	D	101	CLR	C13-C17-C20-C21
6	H	101	CLR	C13-C17-C20-C21
5	A	812	LBN	C39-C40-C41-C42
5	B	812	LBN	C39-C40-C41-C42
4	A	806	PLM	C2-C3-C4-C5
4	B	806	PLM	C2-C3-C4-C5
4	D	102	PLM	C9-CA-CB-CC
4	H	102	PLM	C9-CA-CB-CC
5	A	812	LBN	C30-C31-C32-C33
5	B	812	LBN	C30-C31-C32-C33
4	B	805	PLM	CD-CE-CF-CG
4	A	805	PLM	CD-CE-CF-CG
5	A	812	LBN	C33-C4-C7-C10
5	B	812	LBN	C33-C4-C7-C10
4	A	809	PLM	CA-CB-CC-CD
4	B	809	PLM	CA-CB-CC-CD
5	A	812	LBN	C1-C2-C3-O5
5	B	812	LBN	C1-C2-C3-O5
4	E	102	PLM	C3-C4-C5-C6
4	I	102	PLM	C3-C4-C5-C6
6	D	101	CLR	C22-C23-C24-C25
6	H	101	CLR	C22-C23-C24-C25
4	A	802	PLM	C3-C4-C5-C6
4	B	802	PLM	C3-C4-C5-C6
4	A	810	PLM	C2-C3-C4-C5
4	B	810	PLM	C2-C3-C4-C5
6	C	801	CLR	C23-C24-C25-C27
6	G	801	CLR	C23-C24-C25-C27
4	A	808	PLM	C9-CA-CB-CC
4	B	808	PLM	C9-CA-CB-CC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	E	101	CLR	C13-C17-C20-C22
6	I	101	CLR	C13-C17-C20-C22
4	D	103	PLM	C3-C4-C5-C6
4	D	103	PLM	CB-CC-CD-CE
4	H	103	PLM	CB-CC-CD-CE
4	H	103	PLM	C3-C4-C5-C6
4	B	804	PLM	C2-C3-C4-C5
4	A	804	PLM	C2-C3-C4-C5
5	A	812	LBN	N1-C6-C9-O2
5	B	812	LBN	N1-C6-C9-O2
4	A	807	PLM	CB-CC-CD-CE
4	B	807	PLM	CB-CC-CD-CE
6	D	101	CLR	C23-C24-C25-C27
6	H	101	CLR	C23-C24-C25-C27
4	D	103	PLM	CC-CD-CE-CF
4	H	103	PLM	CC-CD-CE-CF
4	B	809	PLM	C8-C9-CA-CB
4	A	809	PLM	C8-C9-CA-CB
4	B	811	PLM	CB-CC-CD-CE
4	A	811	PLM	CB-CC-CD-CE
6	E	101	CLR	C16-C17-C20-C22
6	I	101	CLR	C16-C17-C20-C22
4	A	806	PLM	C6-C7-C8-C9
4	B	806	PLM	C6-C7-C8-C9
5	A	812	LBN	O7-C2-C3-O5
5	B	812	LBN	O7-C2-C3-O5
4	A	811	PLM	CD-CE-CF-CG
4	B	811	PLM	CD-CE-CF-CG
4	A	802	PLM	CB-CC-CD-CE
4	A	804	PLM	C6-C7-C8-C9
4	B	804	PLM	C6-C7-C8-C9
5	B	812	LBN	C38-C39-C40-C41
5	A	812	LBN	C38-C39-C40-C41
4	B	802	PLM	CB-CC-CD-CE
4	A	811	PLM	CC-CD-CE-CF
4	B	811	PLM	CC-CD-CE-CF
3	A	801	Y01	CAC-CBB-CBE-CAP
3	B	801	Y01	CAC-CBB-CBE-CAP
5	A	812	LBN	C25-C26-C27-C28
5	B	812	LBN	C25-C26-C27-C28
6	D	101	CLR	C23-C24-C25-C26
6	H	101	CLR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	802	PLM	CD-CE-CF-CG
4	B	802	PLM	CD-CE-CF-CG
6	C	801	CLR	C23-C24-C25-C26
6	G	801	CLR	C23-C24-C25-C26
3	A	801	Y01	CAJ-CAN-CBA-CAB
3	B	801	Y01	CAJ-CAN-CBA-CAB
6	E	101	CLR	C23-C24-C25-C26
6	I	101	CLR	C23-C24-C25-C26
4	B	808	PLM	CC-CD-CE-CF
4	A	808	PLM	CC-CD-CE-CF
4	A	803	PLM	C6-C7-C8-C9
4	B	803	PLM	C6-C7-C8-C9
3	A	801	Y01	CAM-CAL-CAX-OAF
3	B	801	Y01	CAM-CAL-CAX-OAF
4	A	803	PLM	O2-C1-C2-C3
4	B	803	PLM	O2-C1-C2-C3
4	A	803	PLM	CA-CB-CC-CD
4	B	803	PLM	CA-CB-CC-CD
6	C	801	CLR	C16-C17-C20-C22
6	G	801	CLR	C16-C17-C20-C22
4	A	802	PLM	O1-C1-C2-C3
4	B	802	PLM	O1-C1-C2-C3
4	A	803	PLM	O1-C1-C2-C3
4	B	803	PLM	O1-C1-C2-C3
4	B	806	PLM	C7-C8-C9-CA
4	A	806	PLM	C7-C8-C9-CA
4	A	802	PLM	O2-C1-C2-C3
4	B	802	PLM	O2-C1-C2-C3
4	D	102	PLM	O2-C1-C2-C3
4	H	102	PLM	O2-C1-C2-C3
4	A	804	PLM	O1-C1-C2-C3
4	B	804	PLM	O1-C1-C2-C3
6	E	101	CLR	C13-C17-C20-C21
6	I	101	CLR	C13-C17-C20-C21
3	A	801	Y01	CAM-CAL-CAX-OAH
3	B	801	Y01	CAM-CAL-CAX-OAH
5	A	812	LBN	C40-C41-C42-C5
5	B	812	LBN	C40-C41-C42-C5
4	A	809	PLM	CD-CE-CF-CG
4	B	809	PLM	CD-CE-CF-CG
4	D	103	PLM	O2-C1-C2-C3
4	H	103	PLM	O2-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	102	PLM	C4-C5-C6-C7
4	I	102	PLM	C4-C5-C6-C7
4	D	103	PLM	C5-C6-C7-C8
4	H	103	PLM	C5-C6-C7-C8
4	A	804	PLM	O2-C1-C2-C3
4	B	804	PLM	O2-C1-C2-C3
4	D	103	PLM	C4-C5-C6-C7
4	H	103	PLM	C4-C5-C6-C7
4	E	102	PLM	O1-C1-C2-C3
4	E	102	PLM	O2-C1-C2-C3
4	I	102	PLM	O1-C1-C2-C3
4	I	102	PLM	O2-C1-C2-C3
4	D	103	PLM	O1-C1-C2-C3
4	H	103	PLM	O1-C1-C2-C3
4	A	805	PLM	CA-CB-CC-CD
4	B	805	PLM	CA-CB-CC-CD
4	A	805	PLM	O1-C1-C2-C3
4	B	805	PLM	O1-C1-C2-C3
4	A	810	PLM	O1-C1-C2-C3
4	A	810	PLM	O2-C1-C2-C3
4	B	810	PLM	O1-C1-C2-C3
4	B	810	PLM	O2-C1-C2-C3
4	A	809	PLM	O2-C1-C2-C3
4	B	809	PLM	O2-C1-C2-C3
4	D	102	PLM	O1-C1-C2-C3
4	H	102	PLM	O1-C1-C2-C3
4	A	809	PLM	O1-C1-C2-C3
4	B	809	PLM	O1-C1-C2-C3
5	A	812	LBN	C42-C5-C8-C11
5	B	812	LBN	C42-C5-C8-C11
4	A	805	PLM	O2-C1-C2-C3
4	B	805	PLM	O2-C1-C2-C3
5	A	812	LBN	C13-C10-C7-C4
5	B	812	LBN	C13-C10-C7-C4
4	B	806	PLM	O2-C1-C2-C3
4	A	806	PLM	O2-C1-C2-C3
4	A	808	PLM	CB-CC-CD-CE
4	B	808	PLM	CB-CC-CD-CE
4	B	811	PLM	O1-C1-C2-C3
4	A	811	PLM	O1-C1-C2-C3
4	E	102	PLM	CD-CE-CF-CG
4	A	803	PLM	C9-CA-CB-CC

Continued on next page...

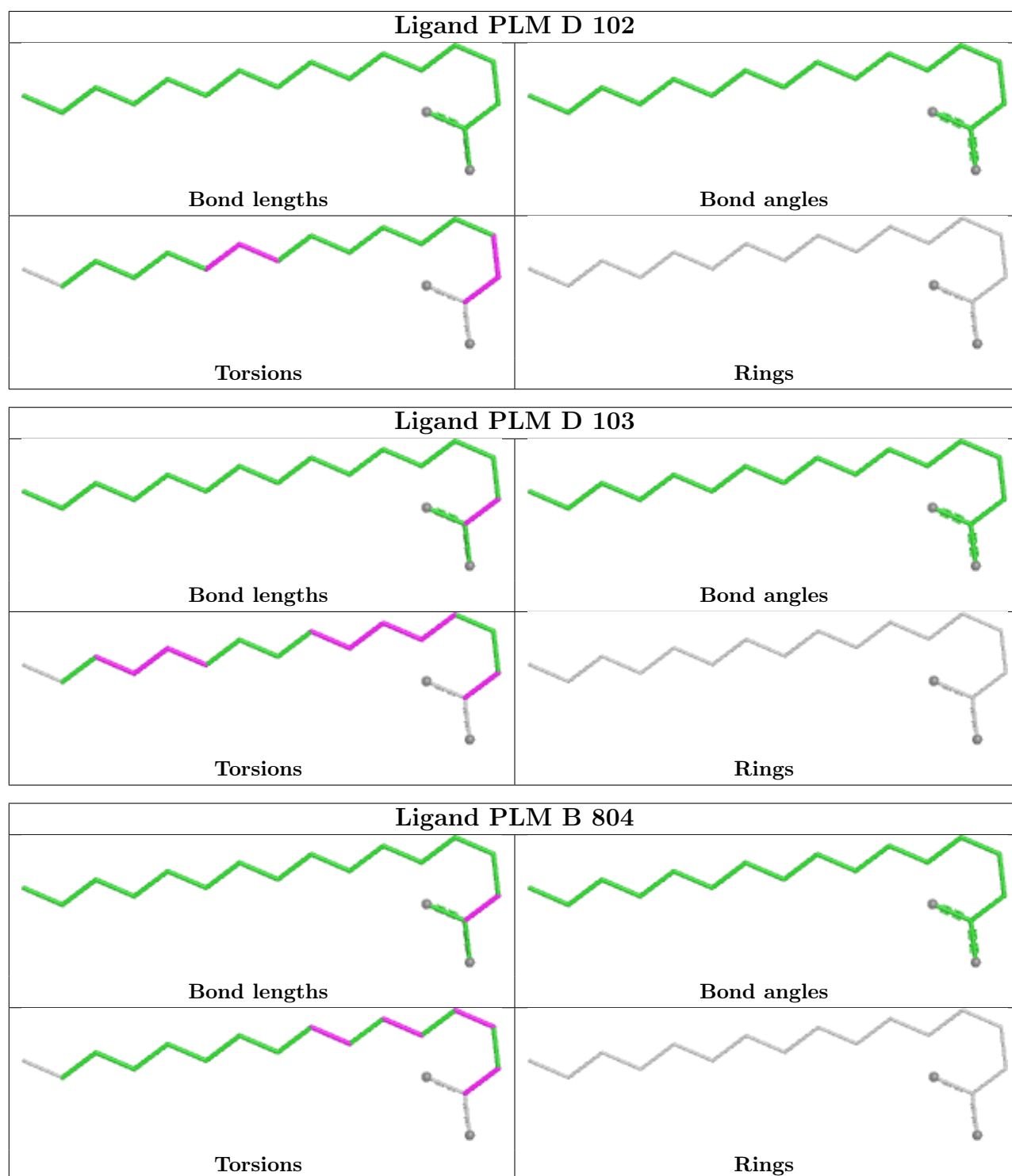
Continued from previous page...

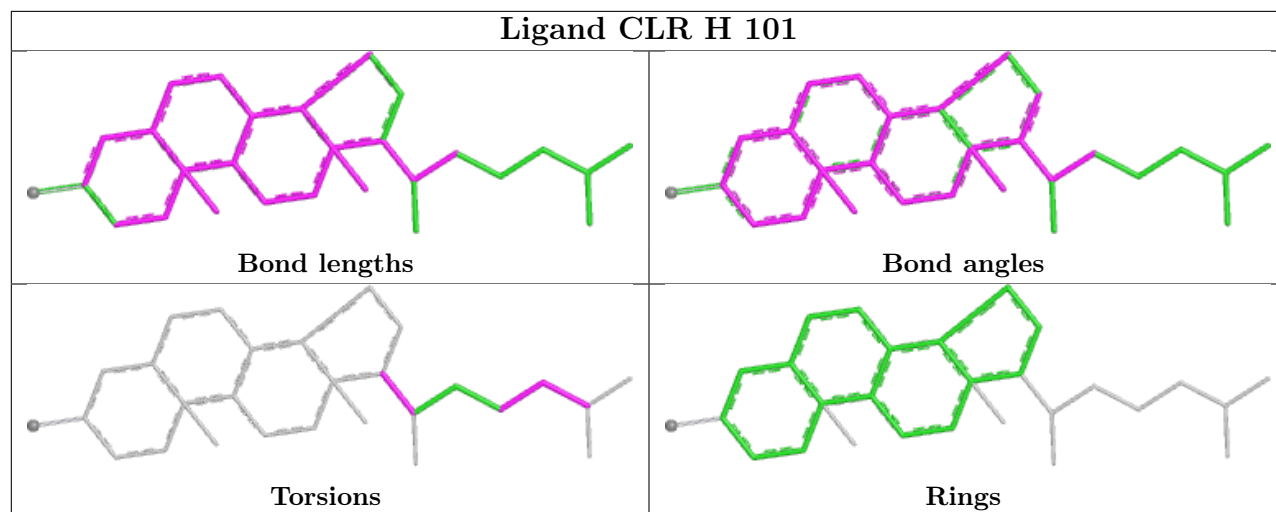
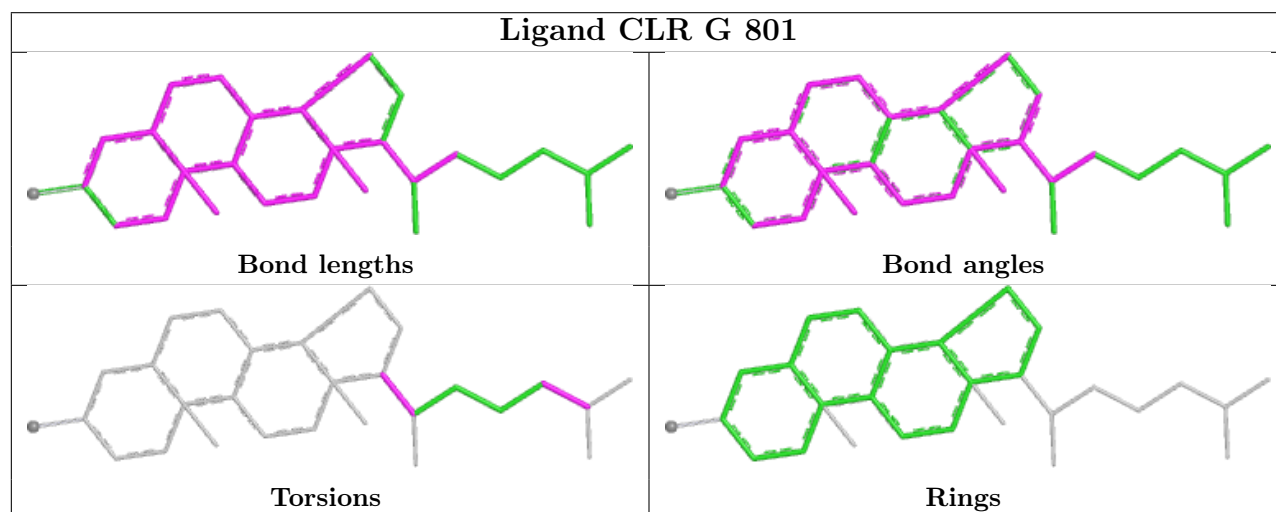
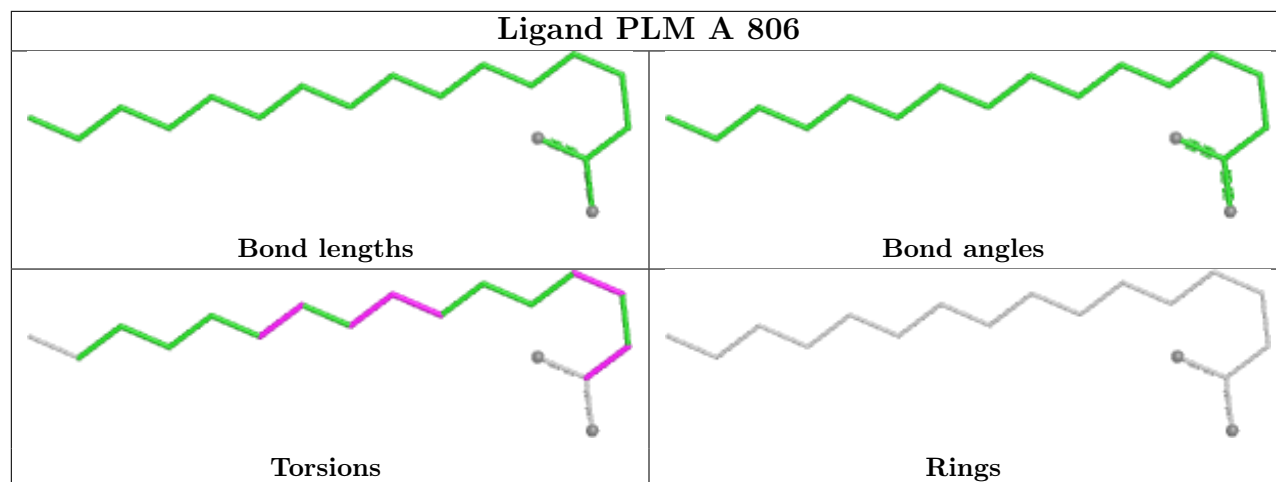
Mol	Chain	Res	Type	Atoms
4	B	803	PLM	C9-CA-CB-CC
4	I	102	PLM	CD-CE-CF-CG
4	A	802	PLM	C5-C6-C7-C8
4	B	802	PLM	C5-C6-C7-C8
4	A	806	PLM	O1-C1-C2-C3
4	B	806	PLM	O1-C1-C2-C3
4	A	811	PLM	C8-C9-CA-CB
4	B	811	PLM	C8-C9-CA-CB
6	G	801	CLR	C13-C17-C20-C22
4	A	811	PLM	O2-C1-C2-C3
4	B	811	PLM	O2-C1-C2-C3
6	C	801	CLR	C13-C17-C20-C22
5	A	812	LBN	C8-C11-C14-C17
5	B	812	LBN	C8-C11-C14-C17
5	A	812	LBN	O5-C25-C26-C27
5	B	812	LBN	O5-C25-C26-C27
3	A	801	Y01	CAL-CAM-CAY-OAW
3	B	801	Y01	CAL-CAM-CAY-OAW
4	A	810	PLM	C6-C7-C8-C9
3	A	801	Y01	CAJ-CAN-CBA-CAA
3	B	801	Y01	CAJ-CAN-CBA-CAA
4	B	810	PLM	C6-C7-C8-C9
5	A	812	LBN	O6-C25-C26-C27
5	B	812	LBN	O6-C25-C26-C27
3	A	801	Y01	CAN-CAJ-CAO-CBB
3	B	801	Y01	CAN-CAJ-CAO-CBB

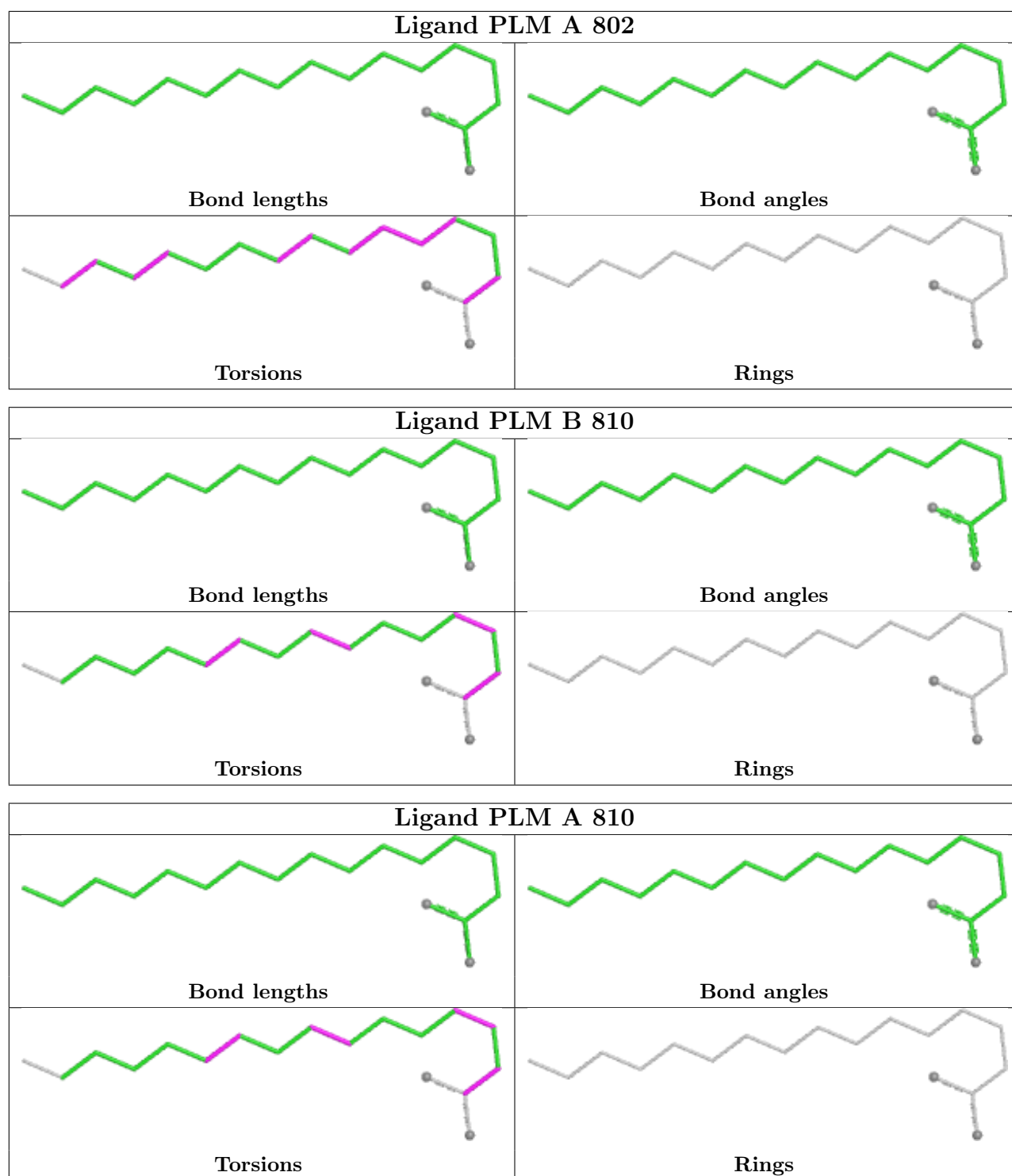
There are no ring outliers.

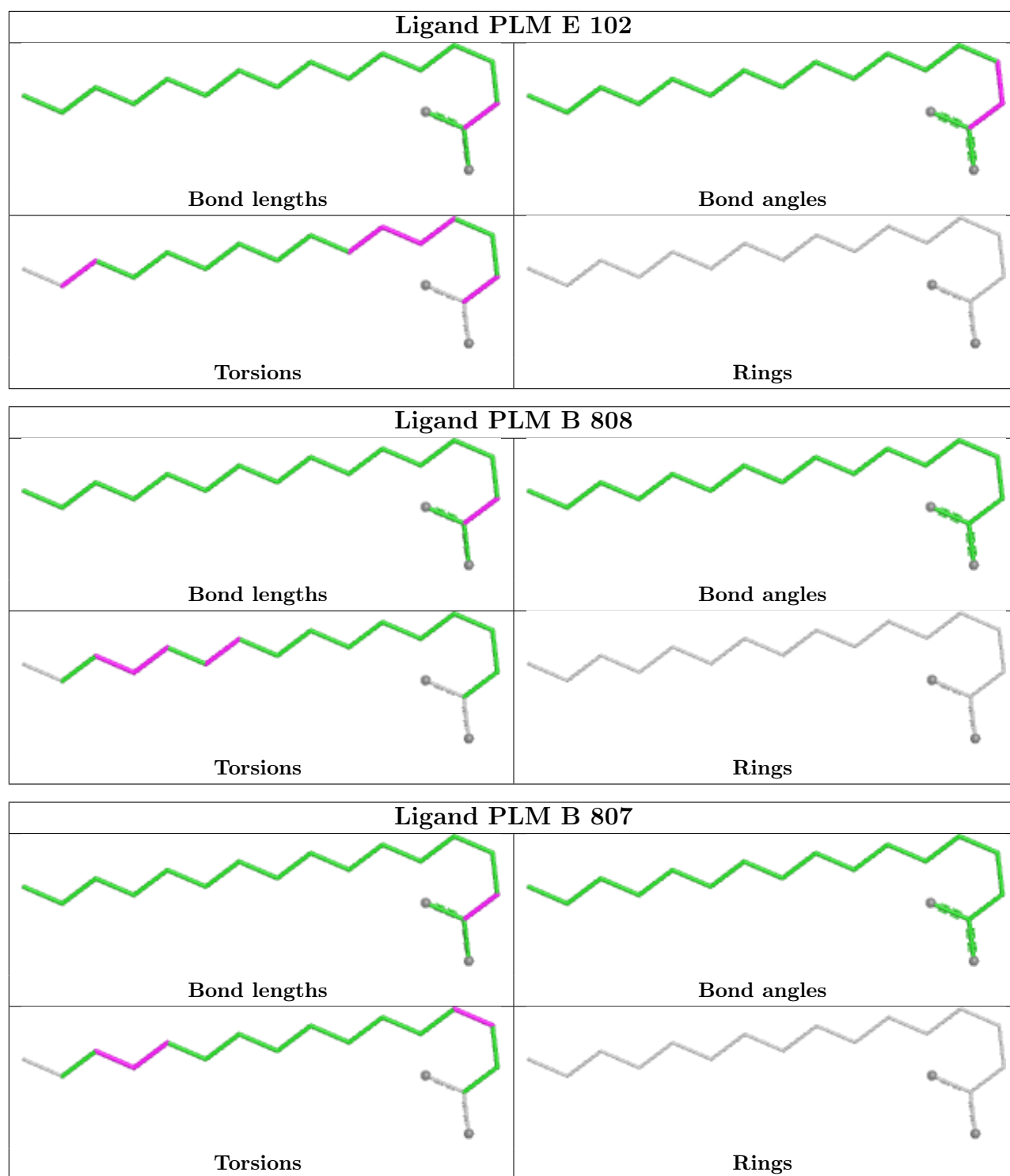
No monomer is involved in short contacts.

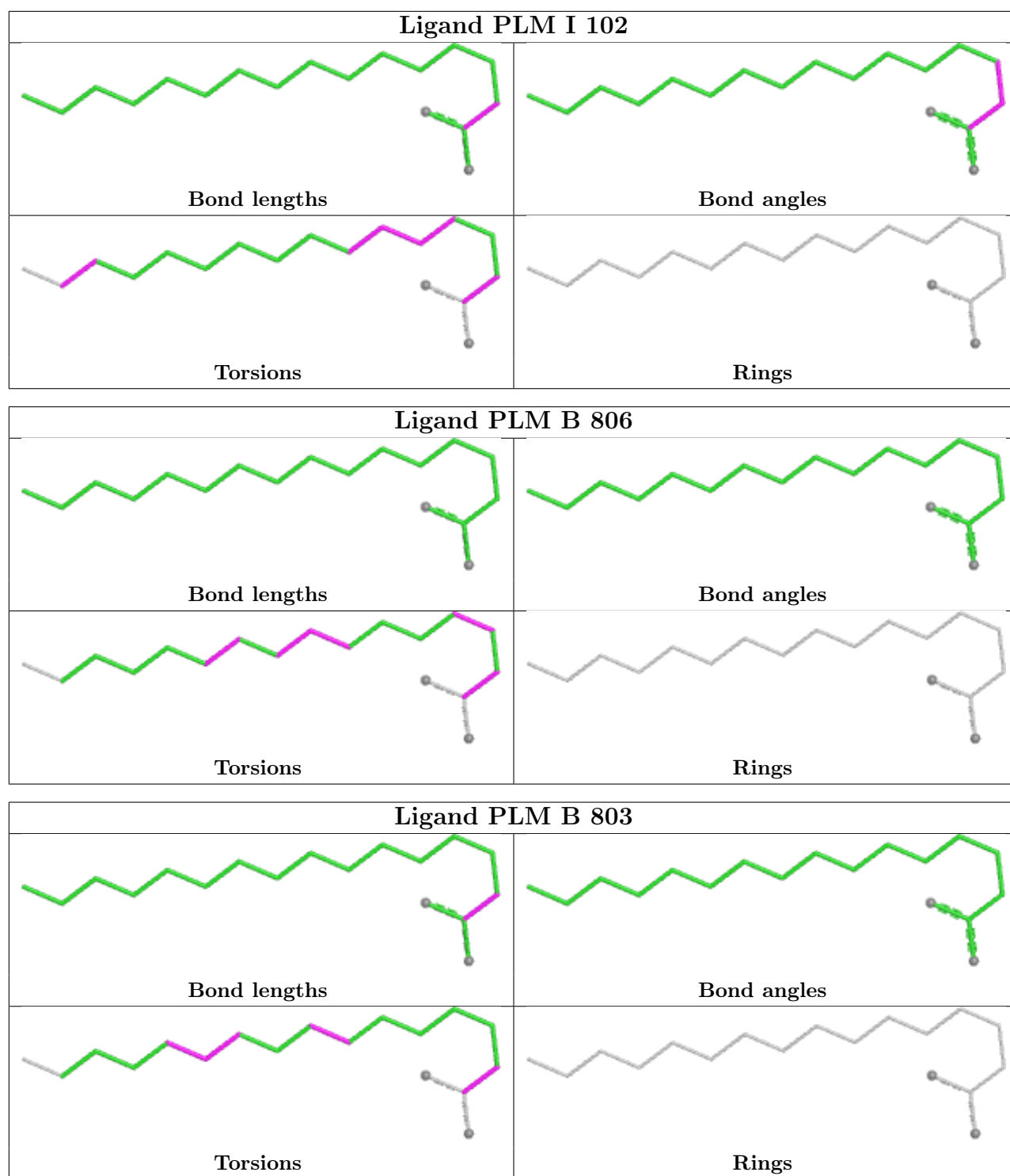
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

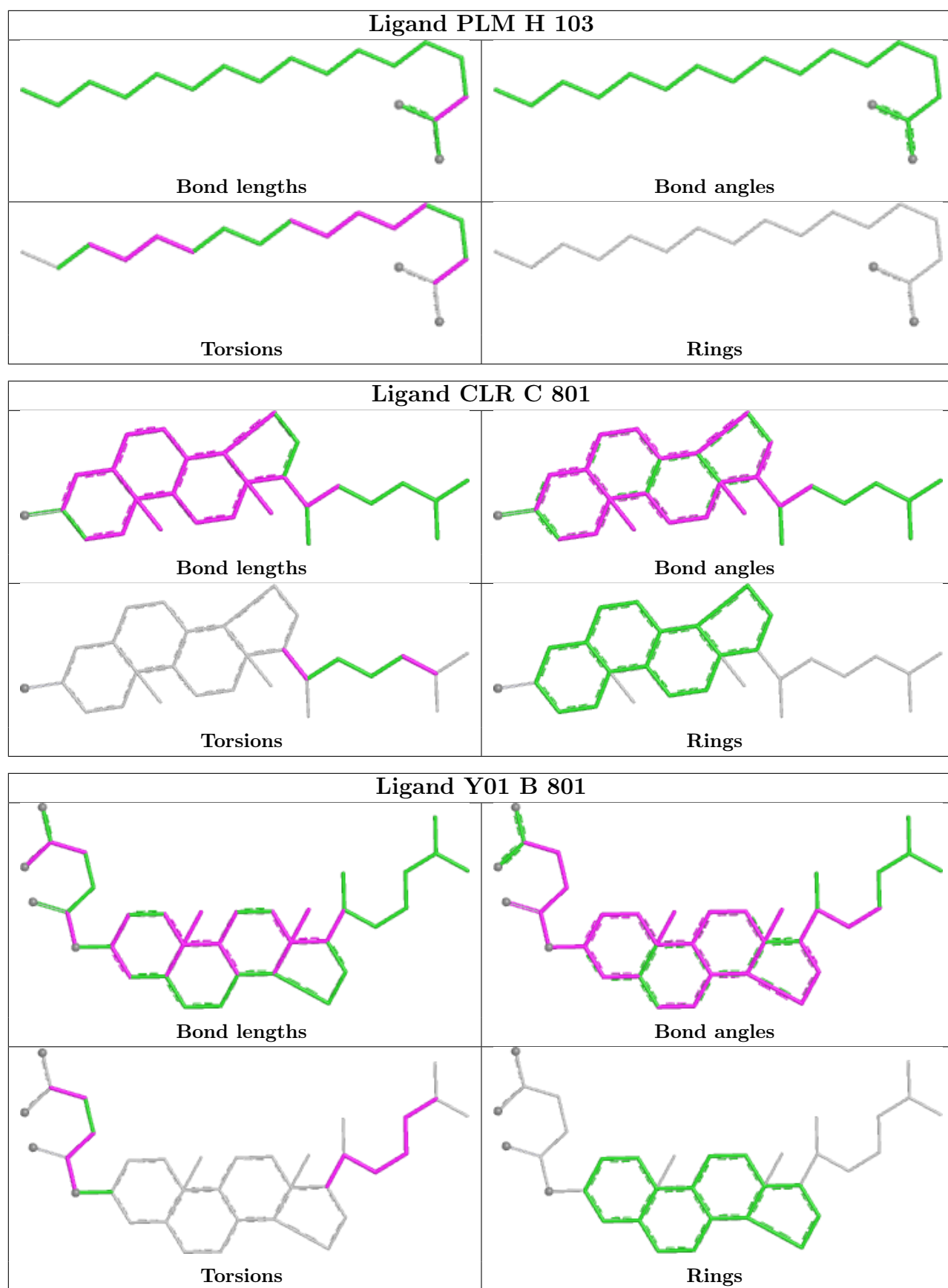


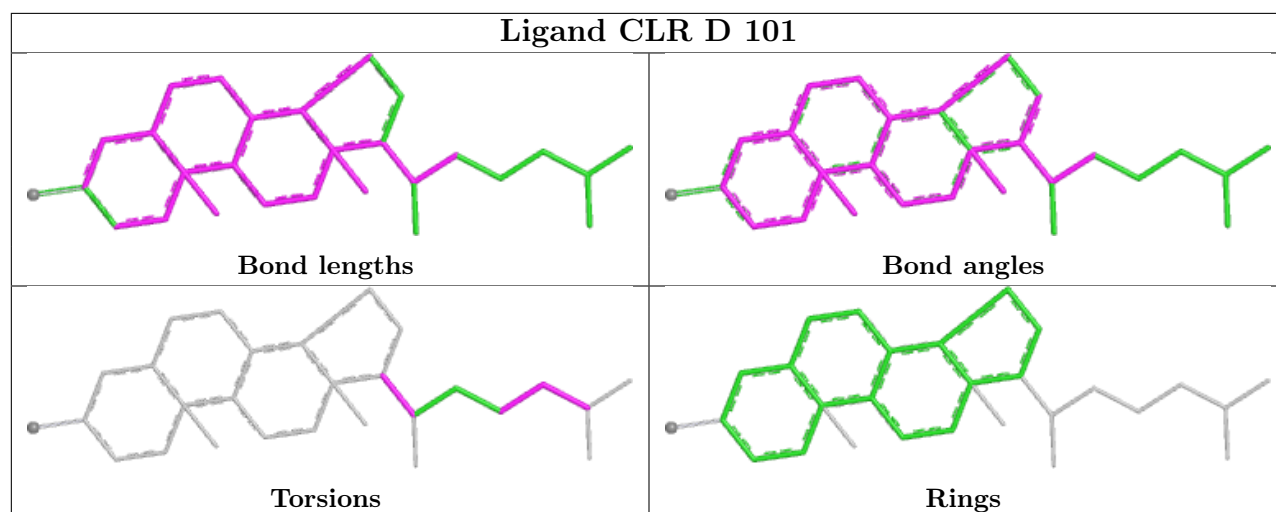
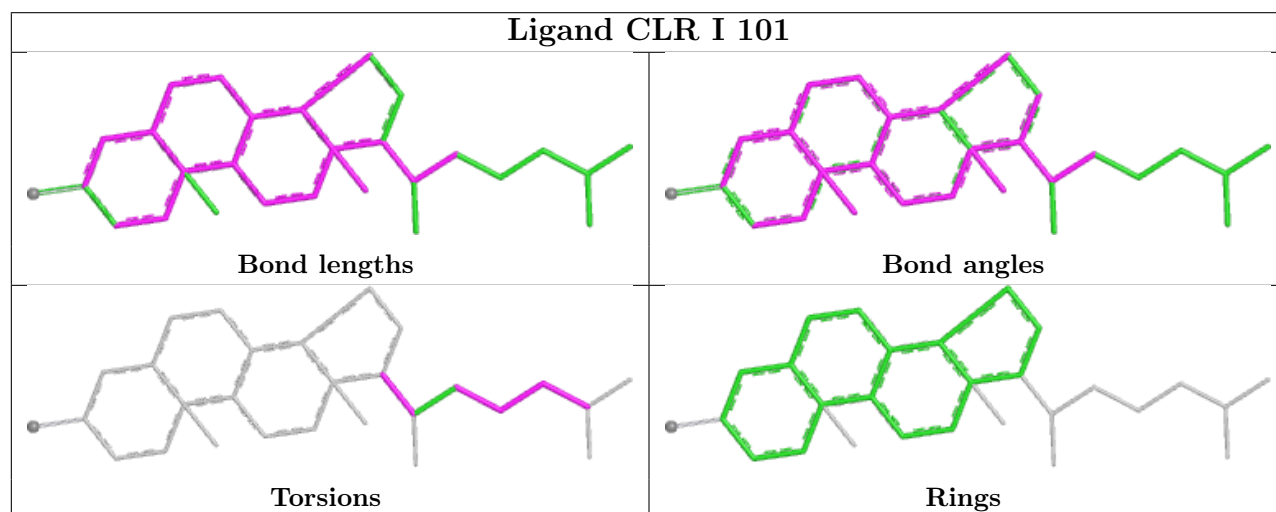
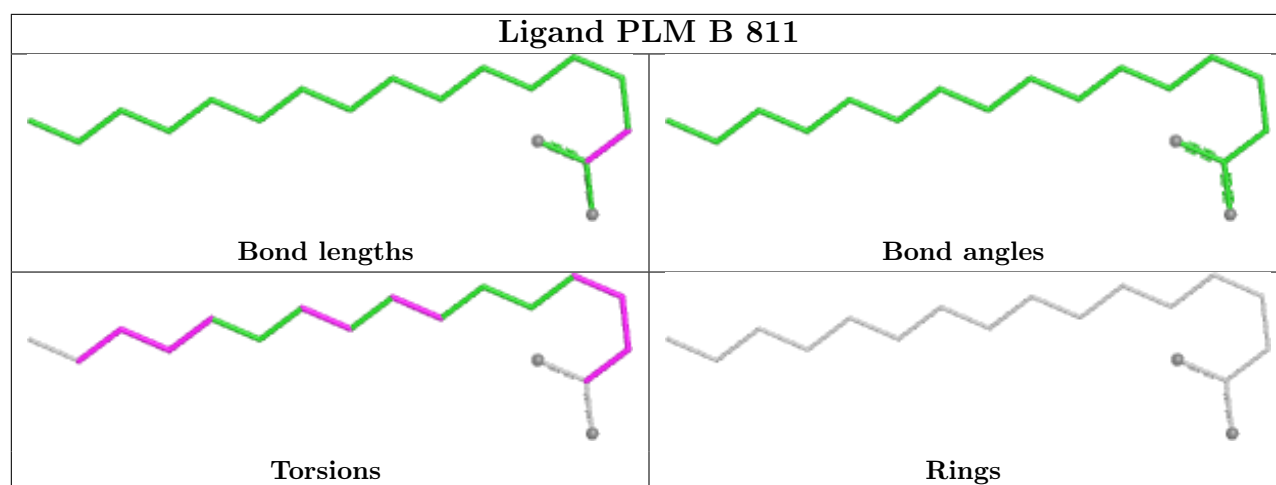


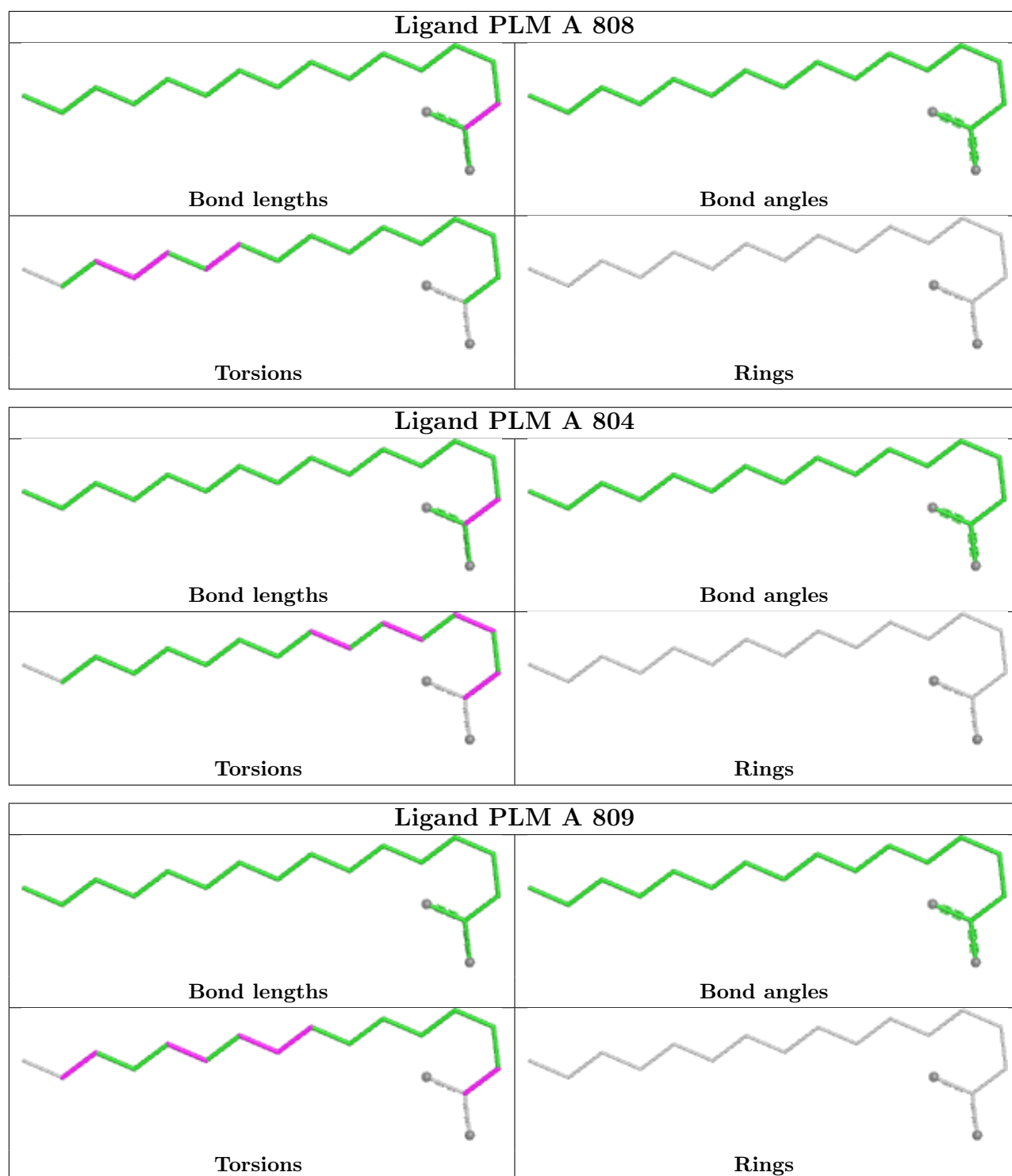


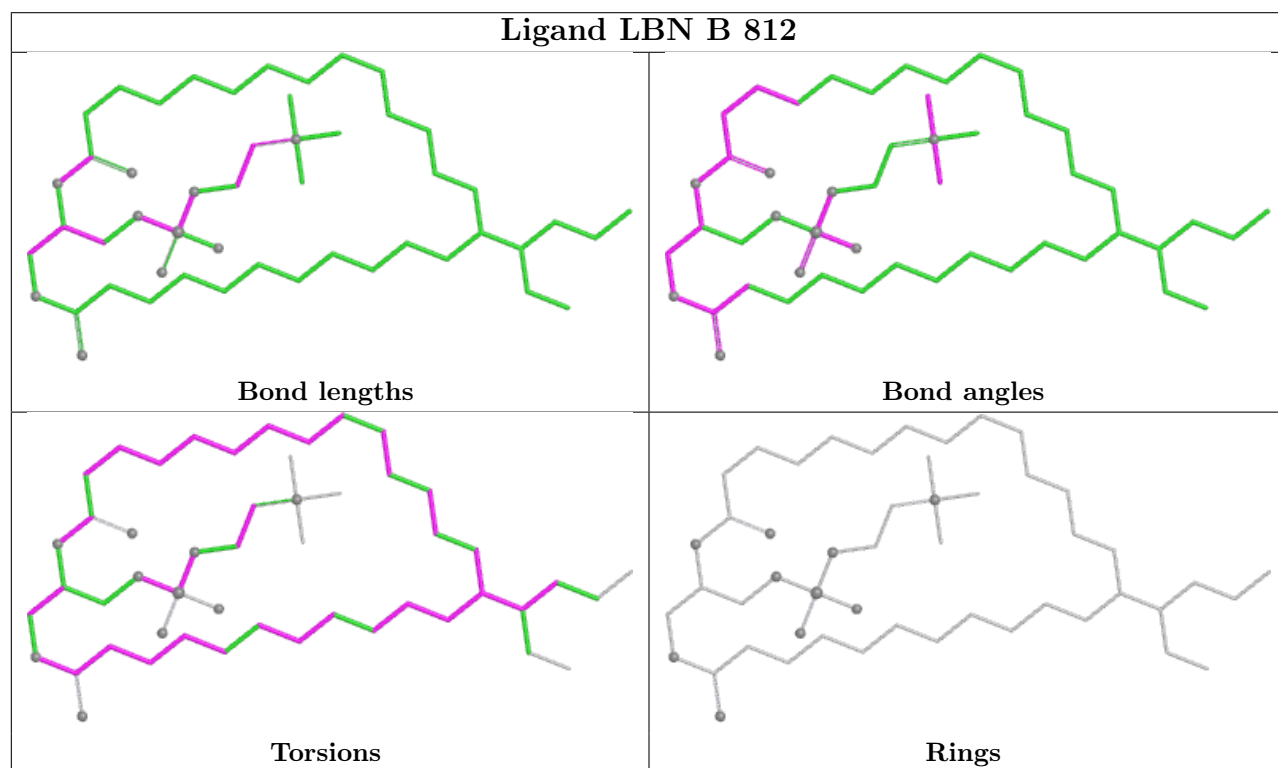
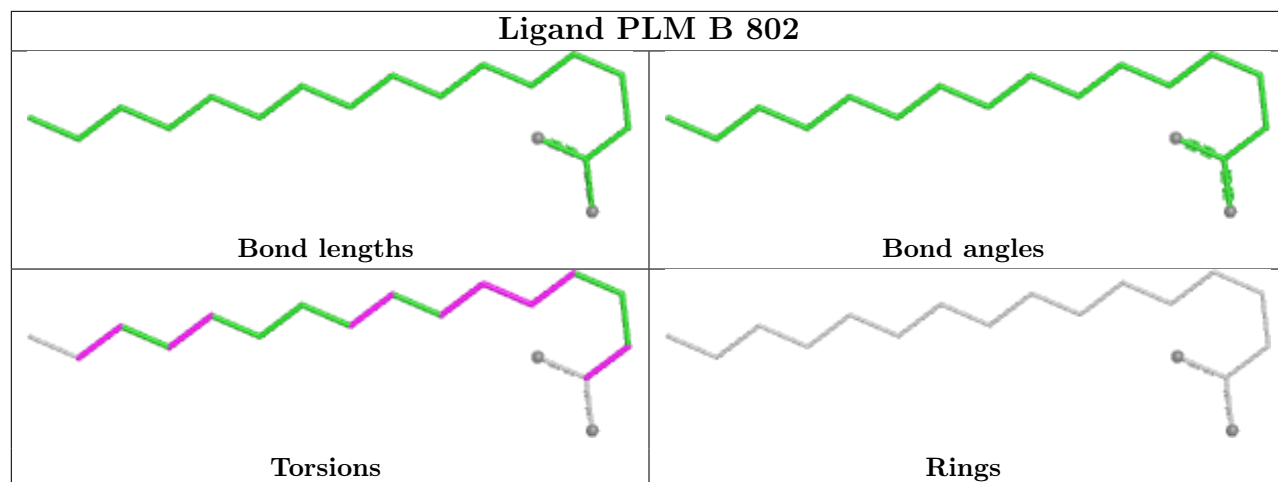


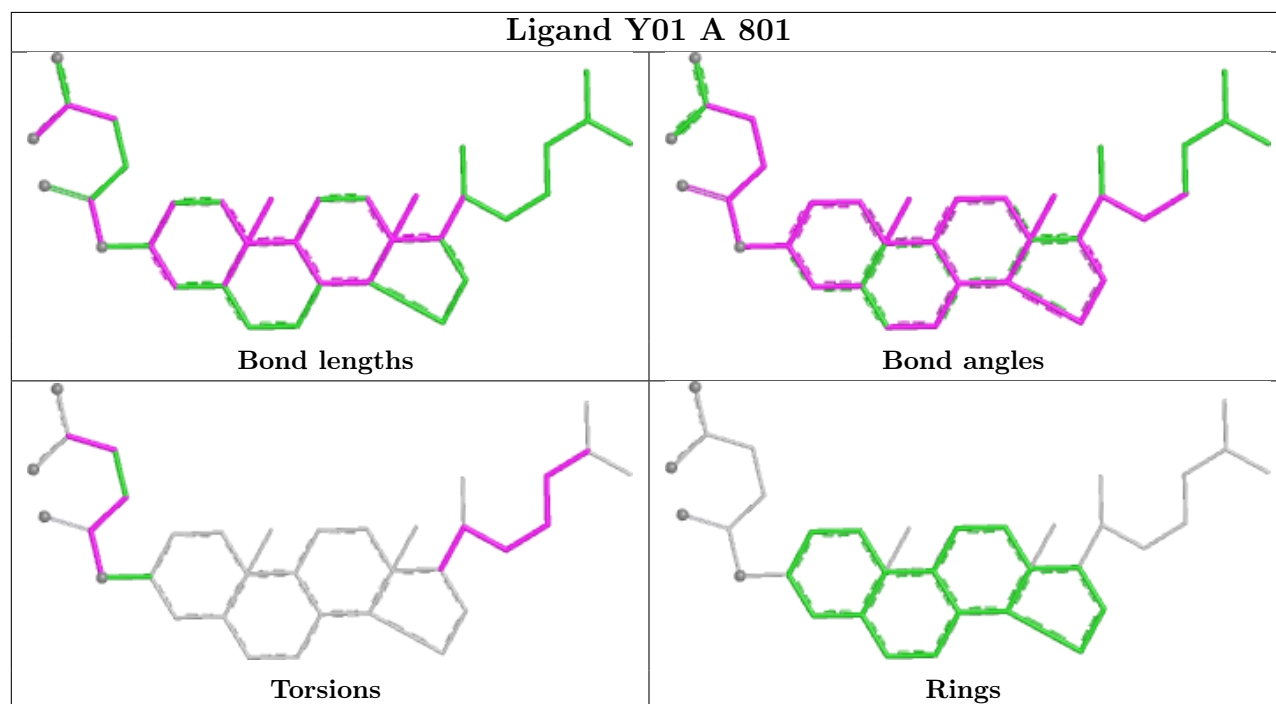
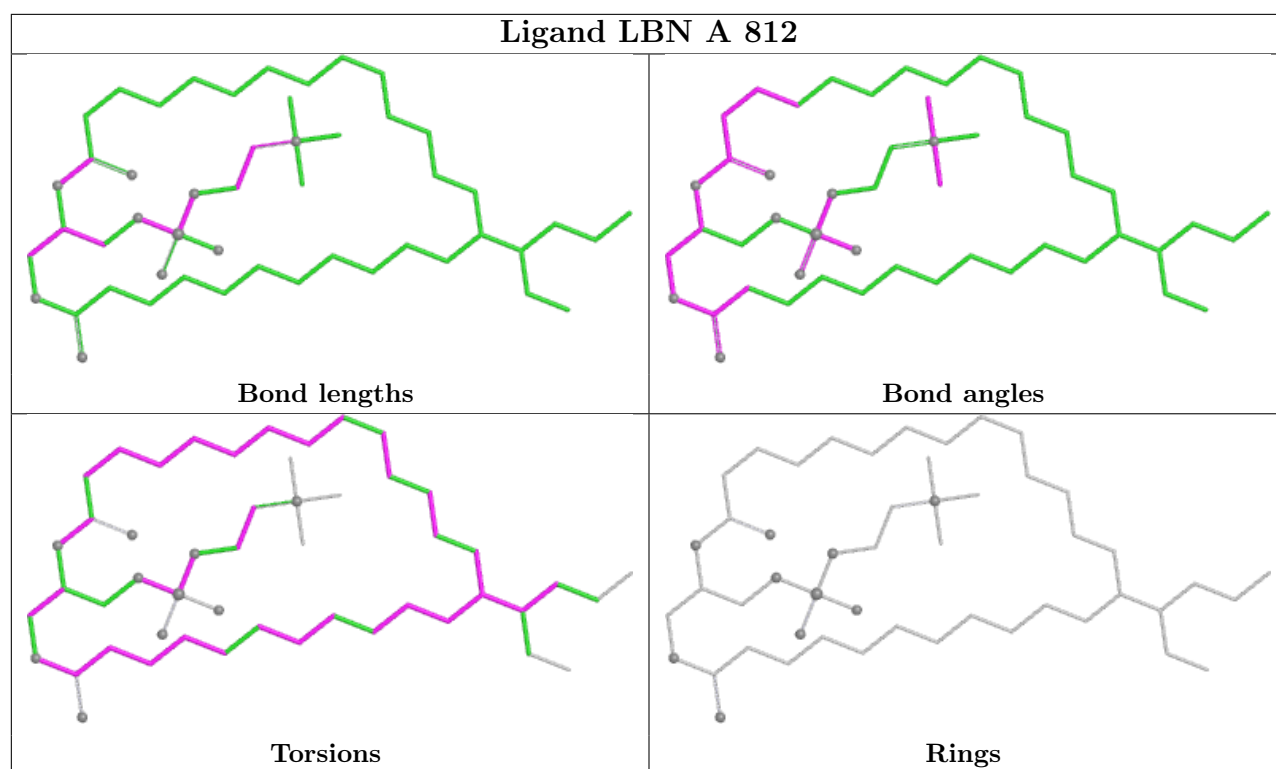


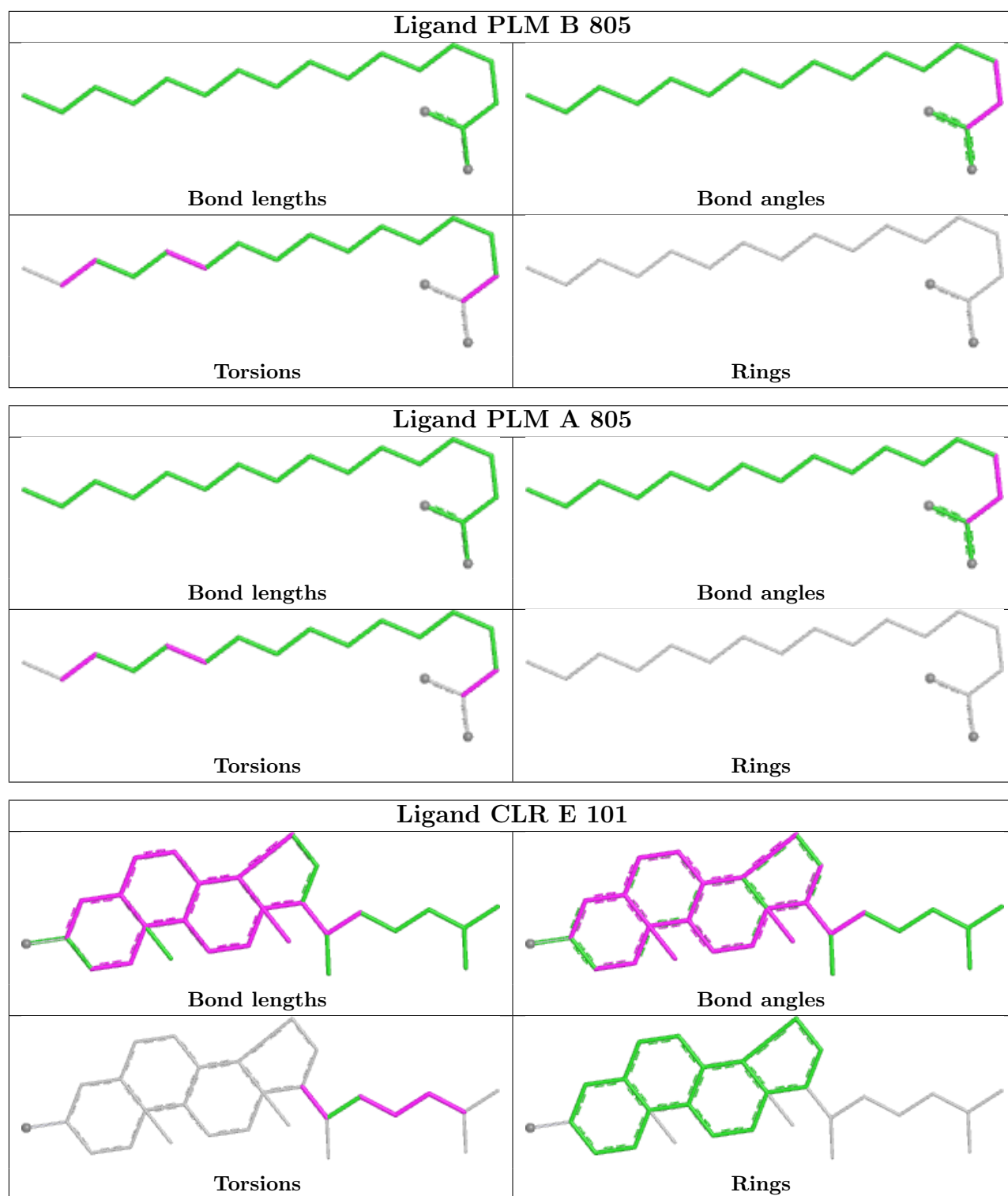


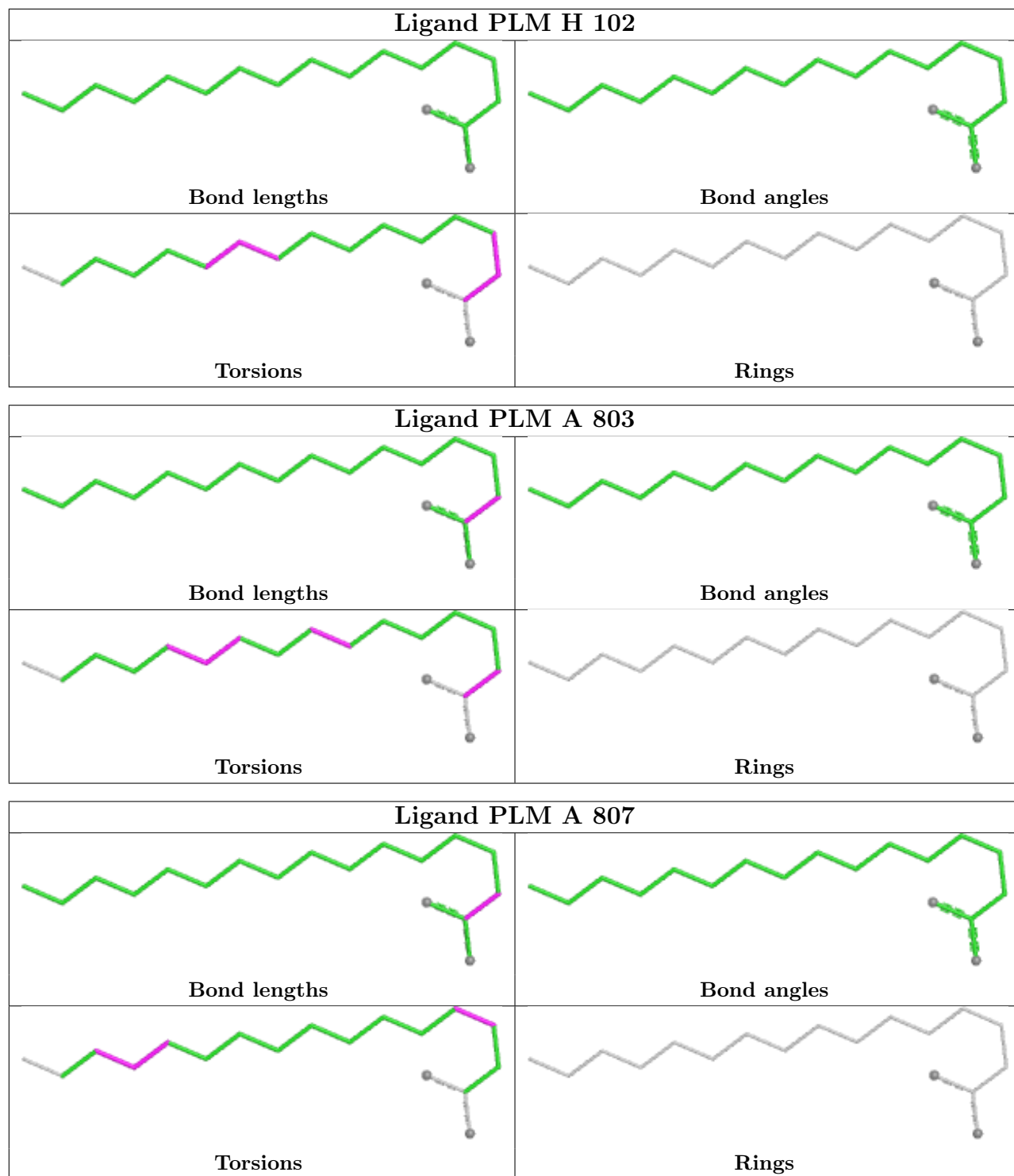


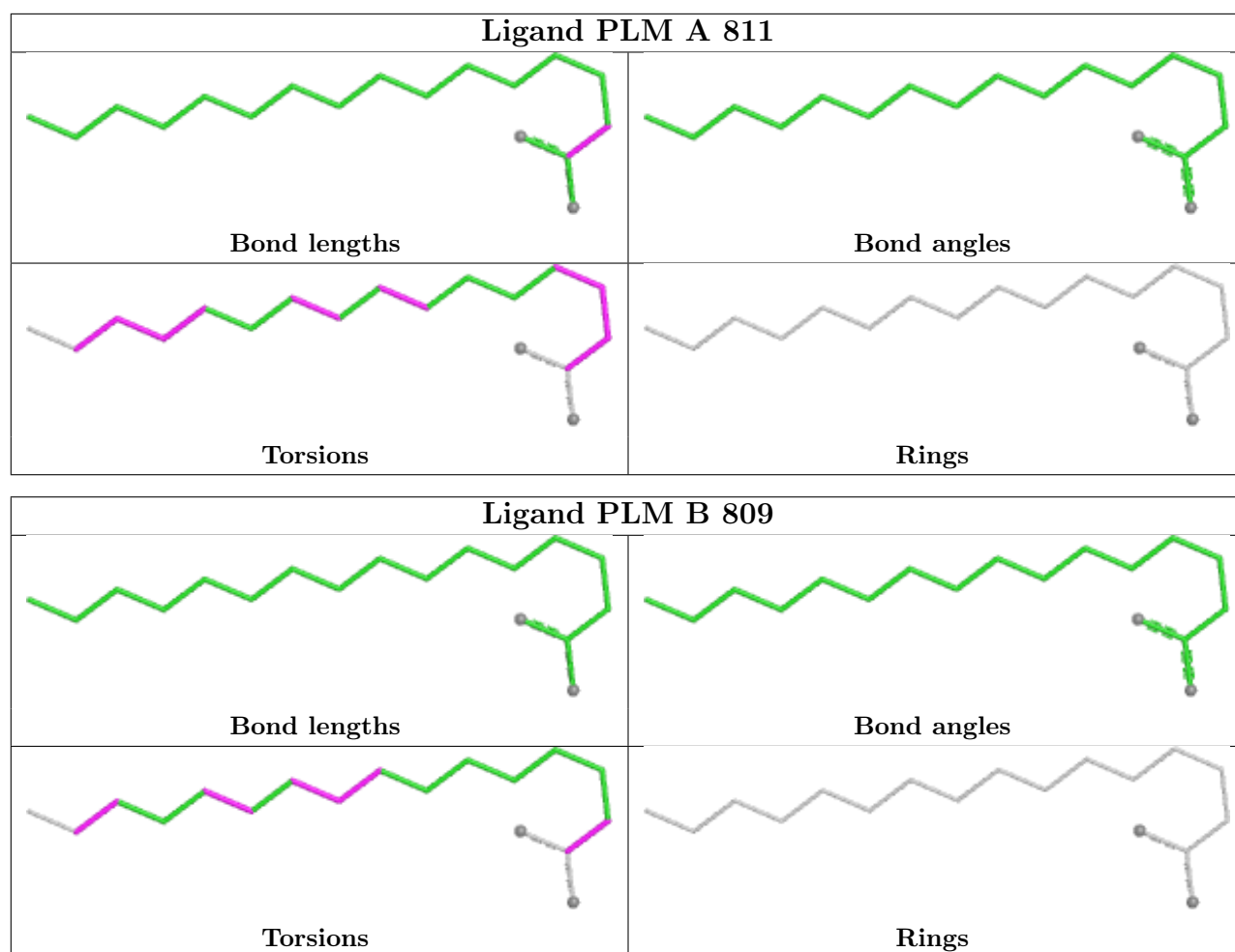












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

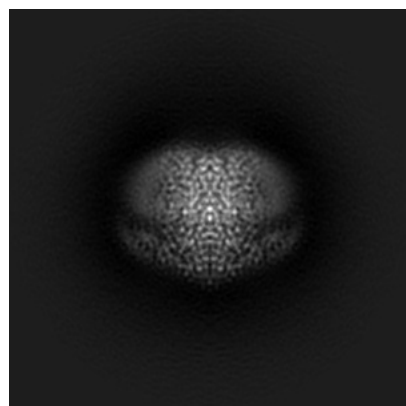
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41043. These allow visual inspection of the internal detail of the map and identification of artifacts.

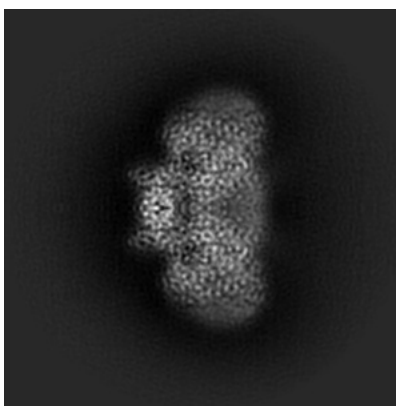
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

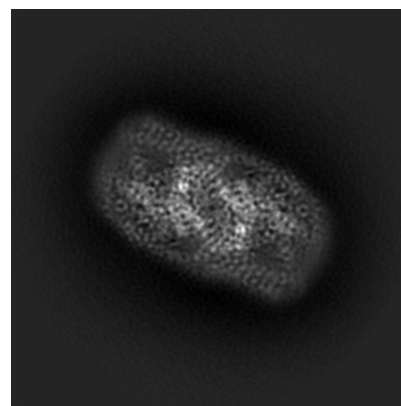
6.1.1 Primary map



X

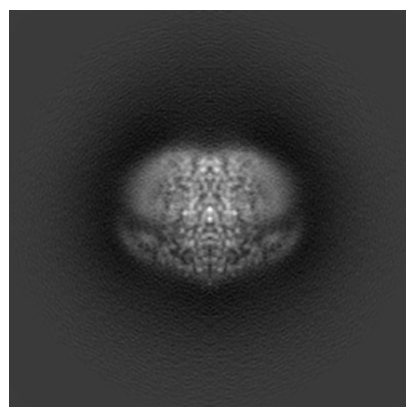


Y

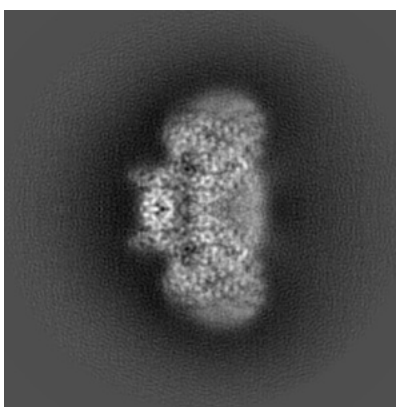


Z

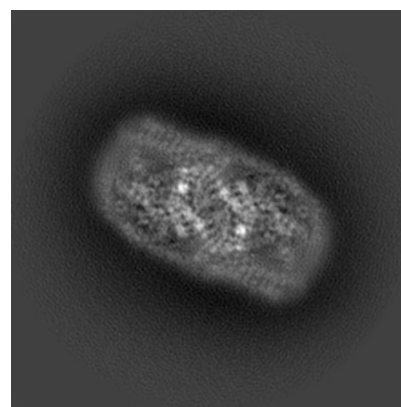
6.1.2 Raw map



X



Y

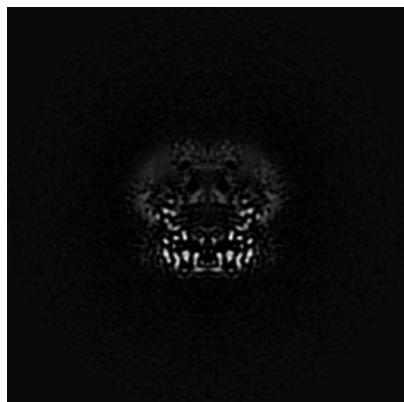


Z

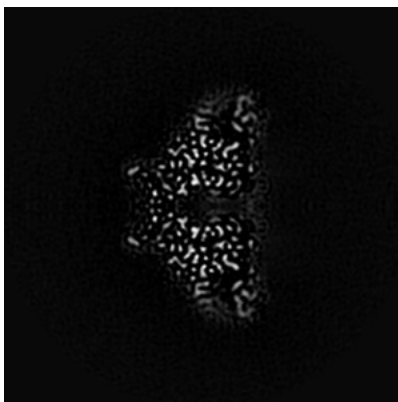
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

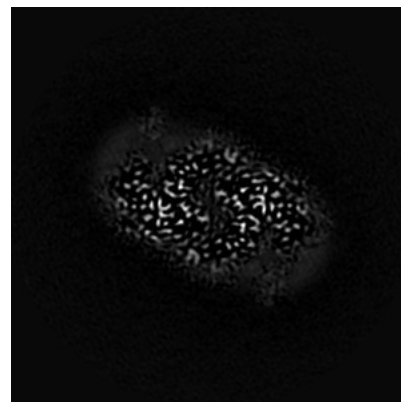
6.2.1 Primary map



X Index: 110

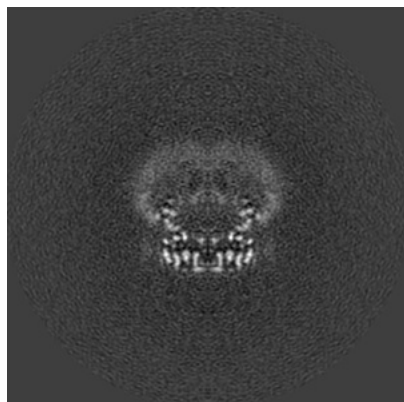


Y Index: 110

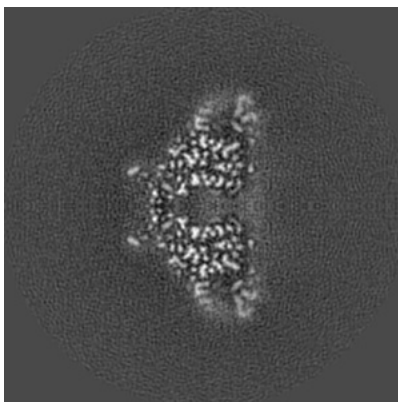


Z Index: 110

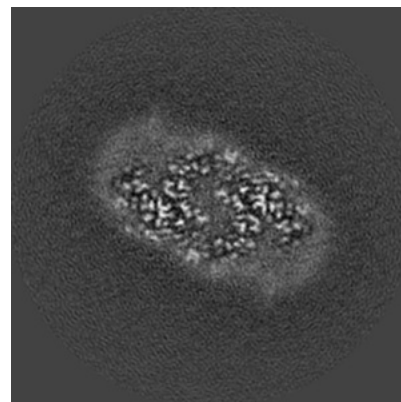
6.2.2 Raw map



X Index: 110



Y Index: 110

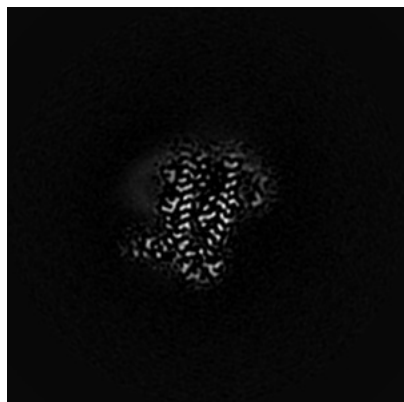


Z Index: 110

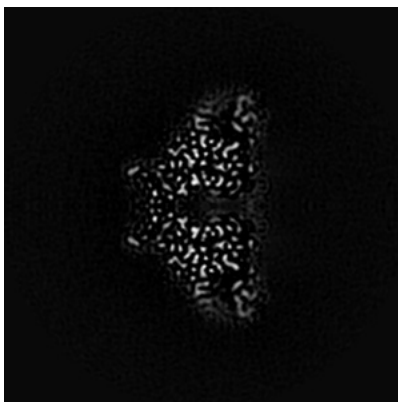
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

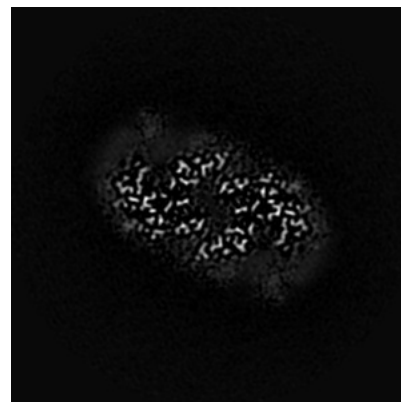
6.3.1 Primary map



X Index: 127

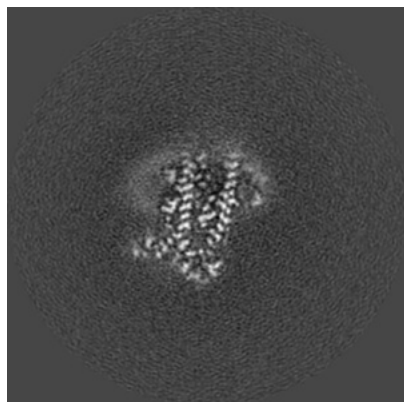


Y Index: 110

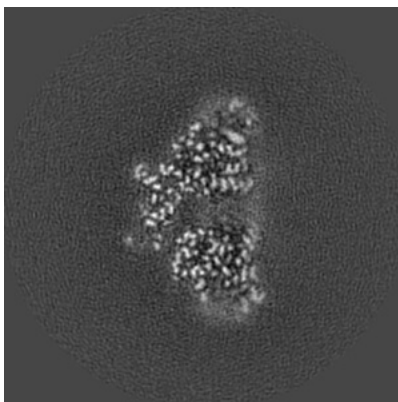


Z Index: 108

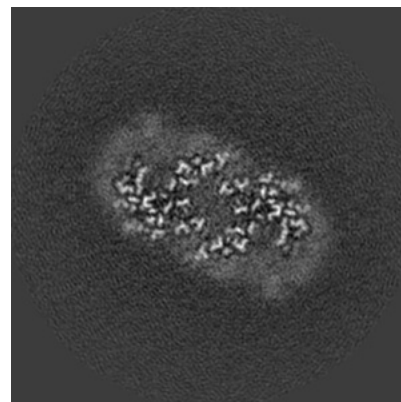
6.3.2 Raw map



X Index: 127



Y Index: 113

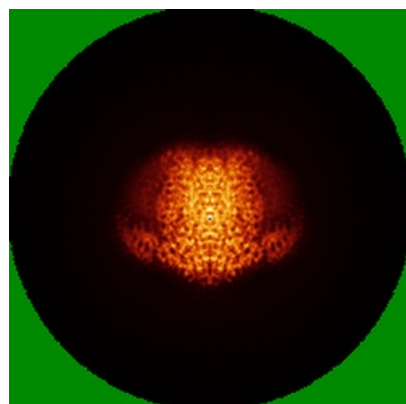


Z Index: 108

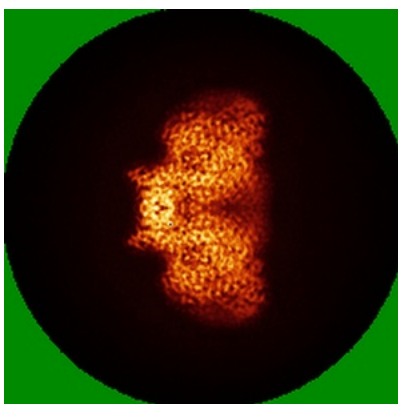
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

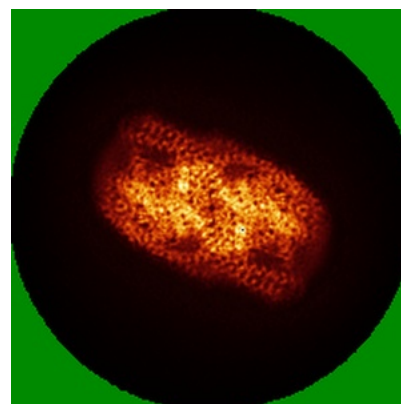
6.4.1 Primary map



X

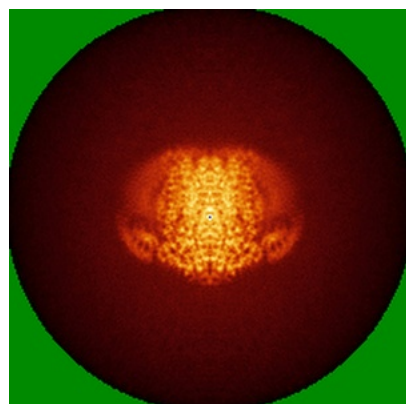


Y

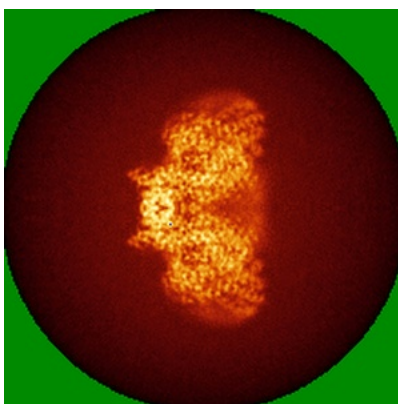


Z

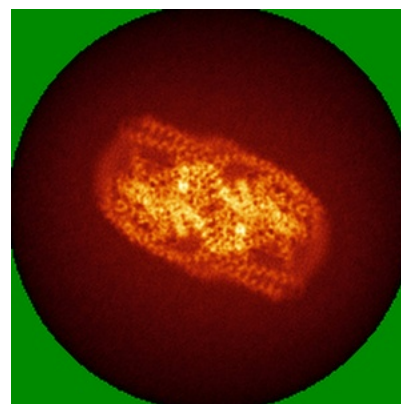
6.4.2 Raw map



X



Y

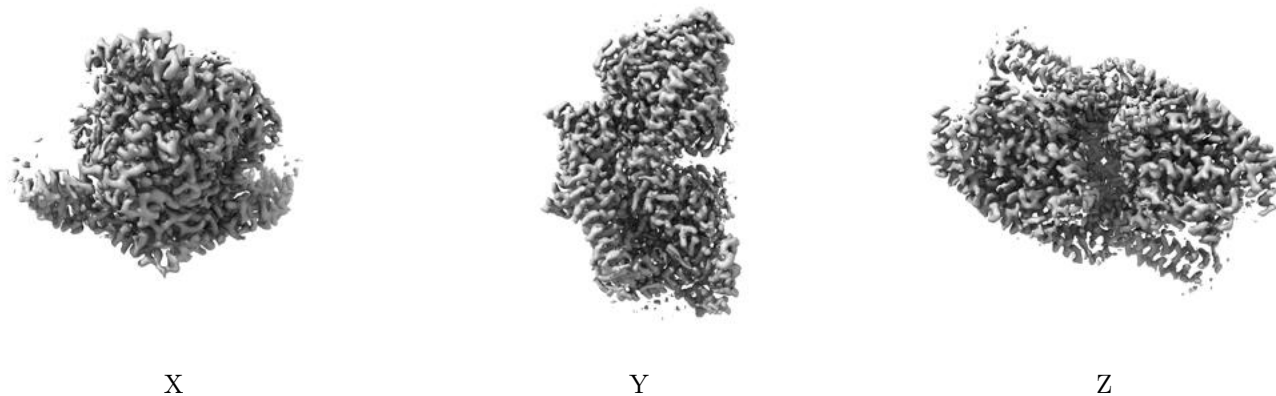


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

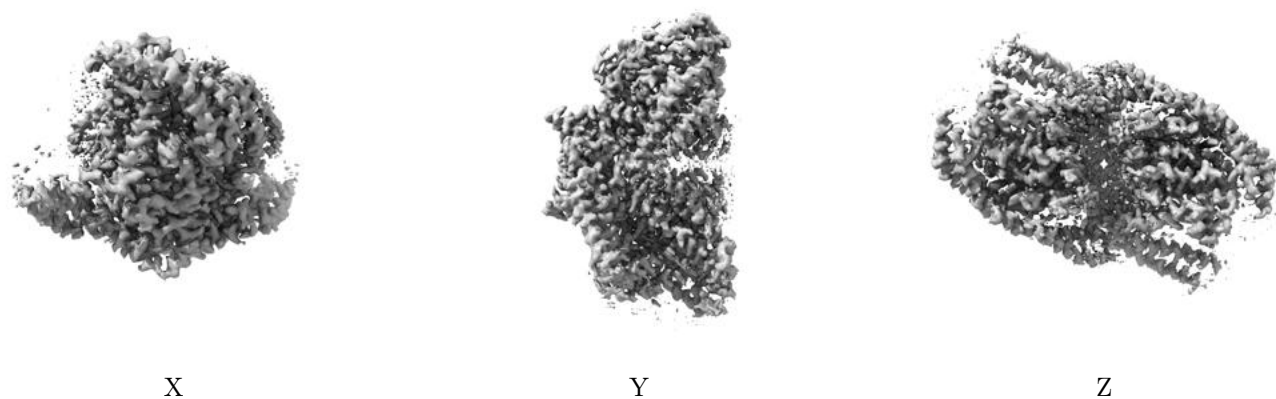
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0138. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

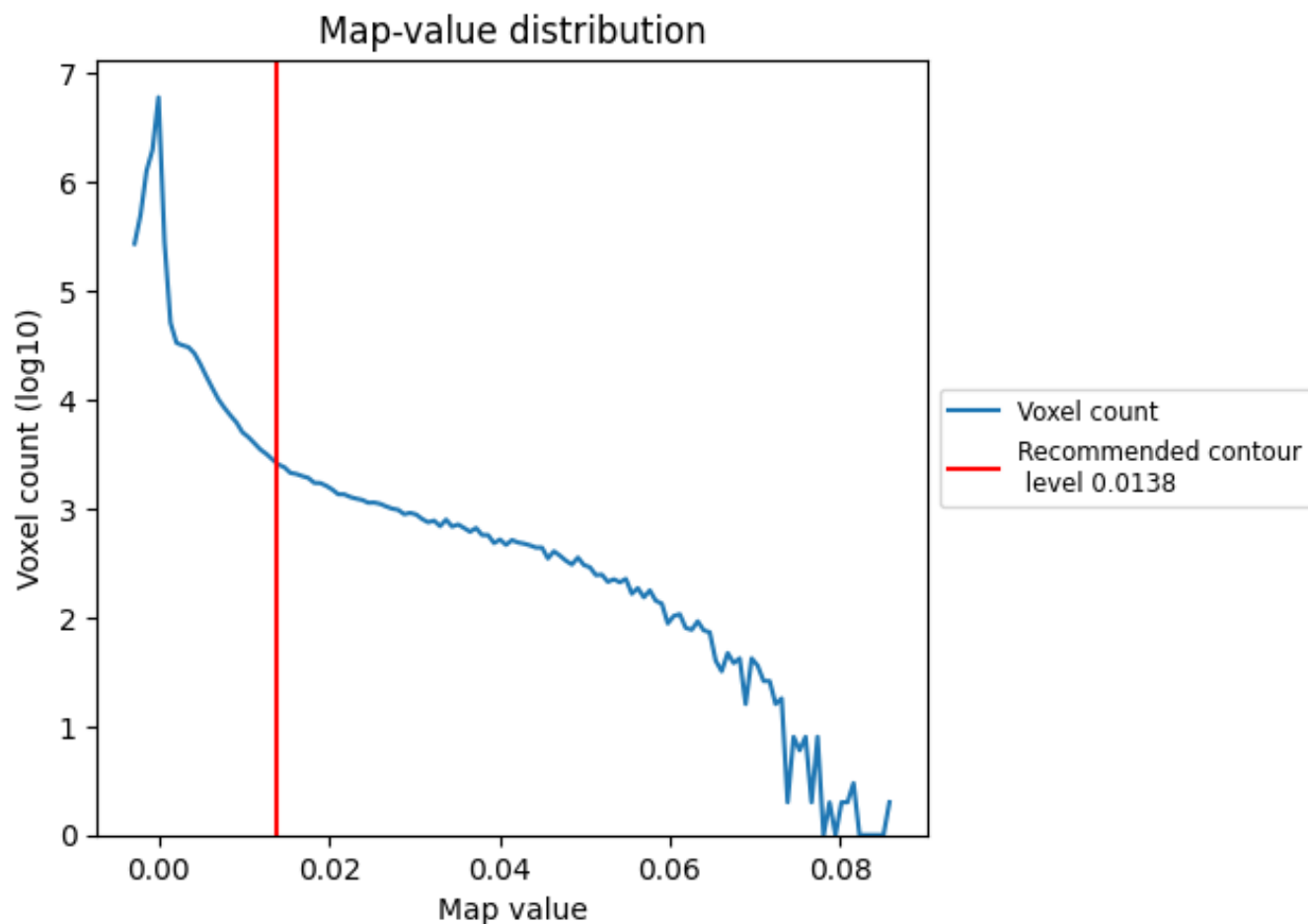
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

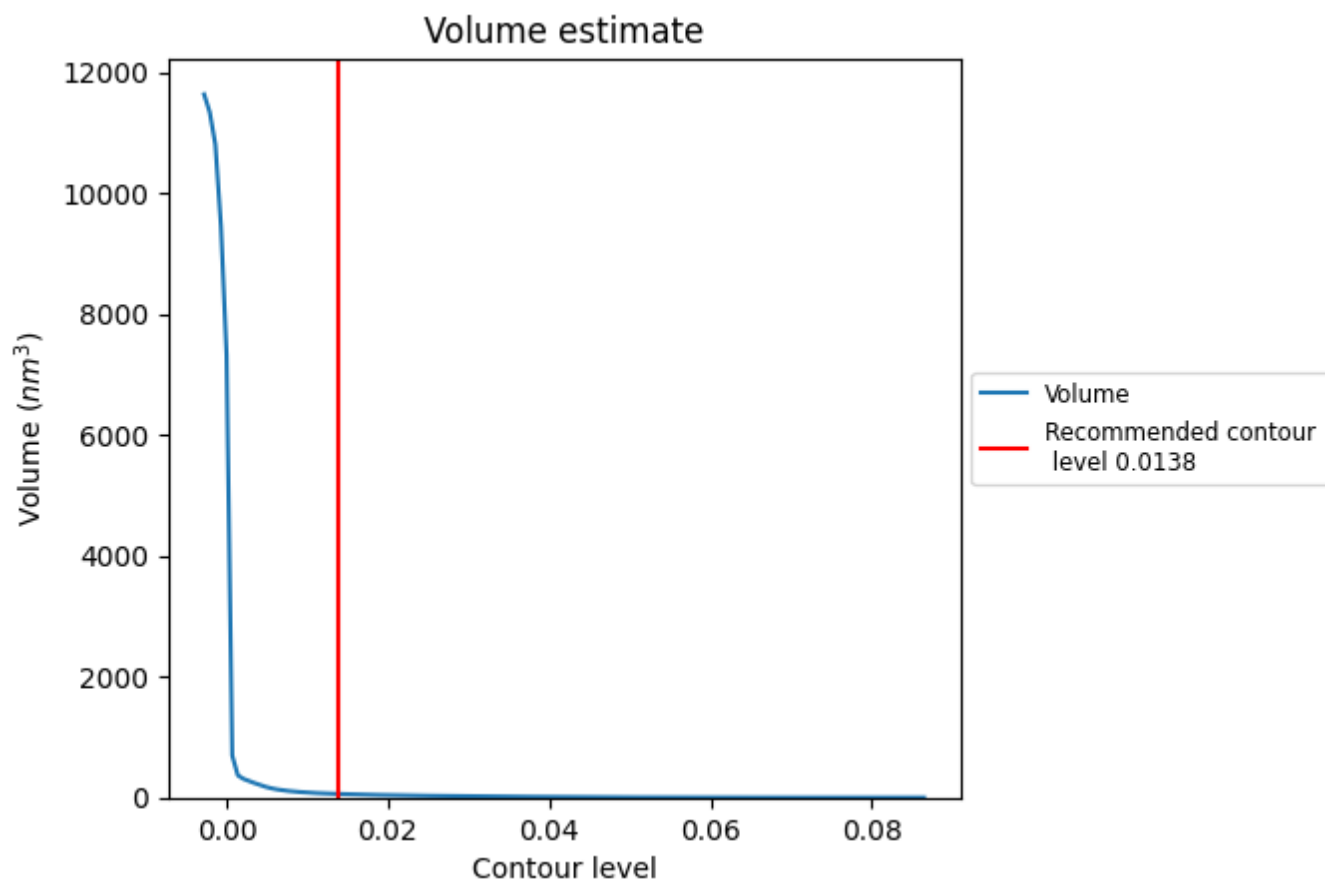
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

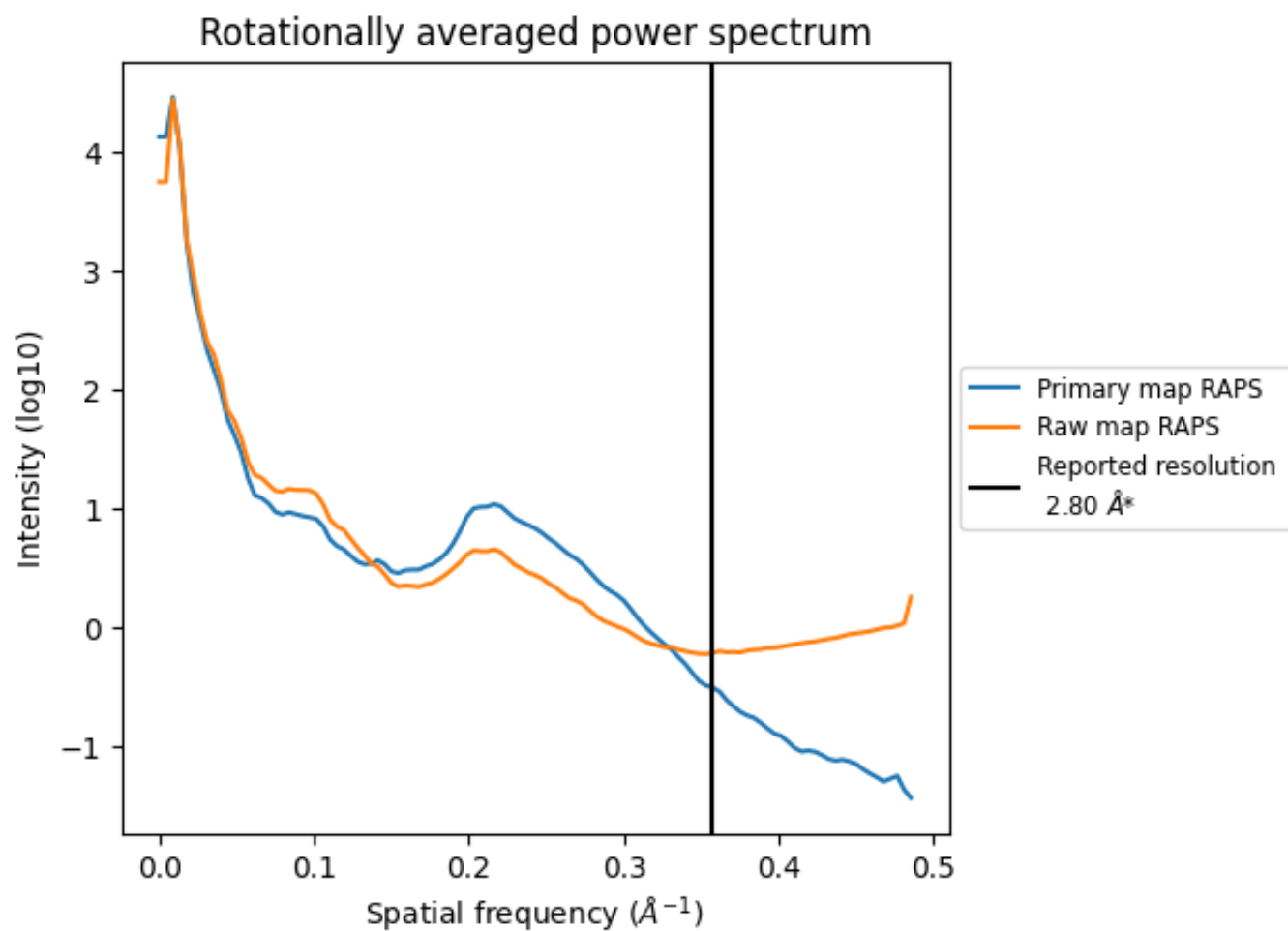
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 54 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

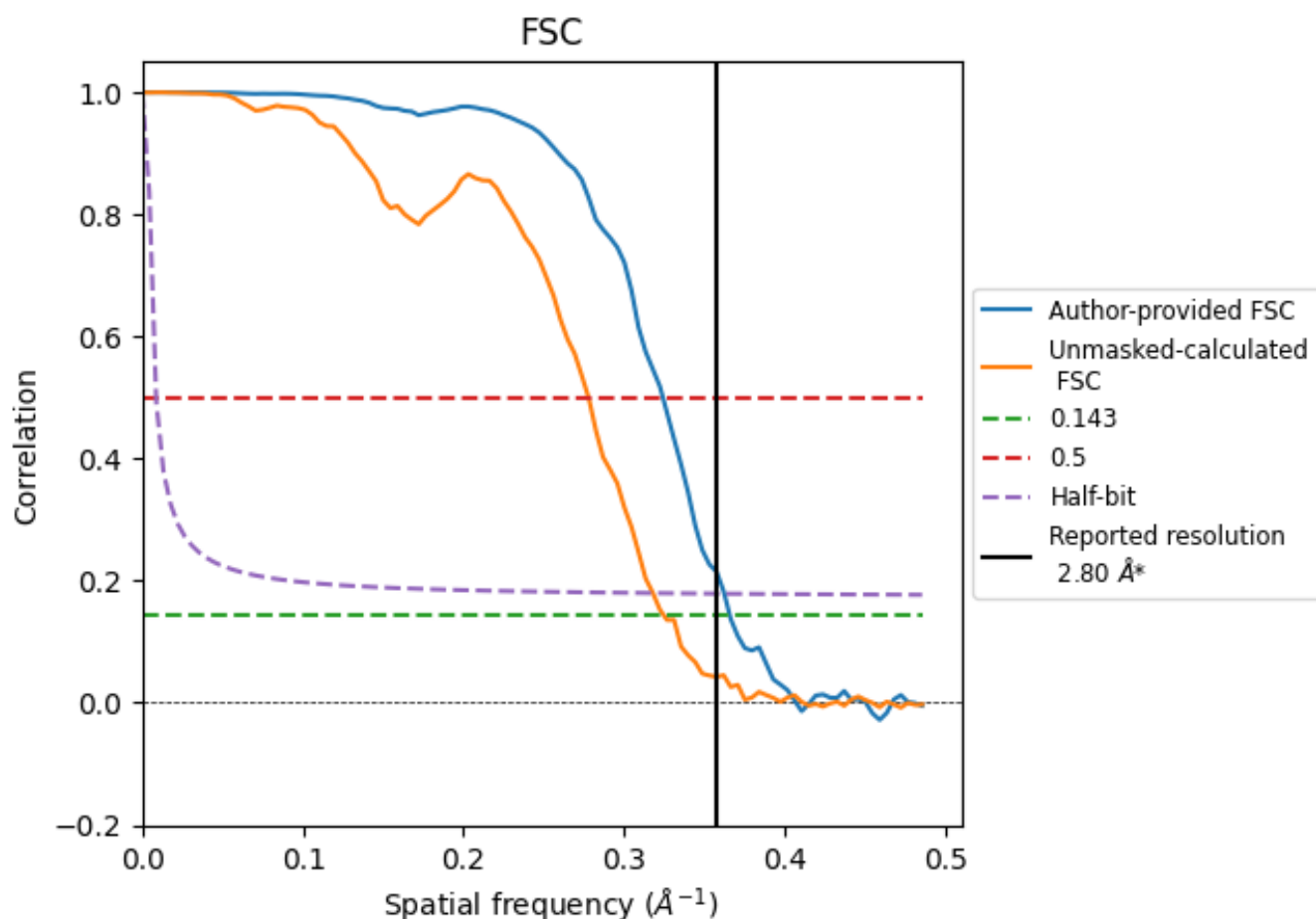


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

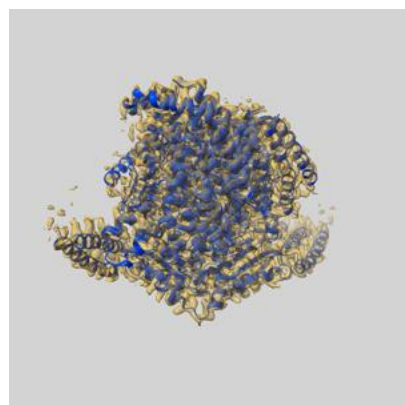
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.73	3.09	2.76
Unmasked-calculated*	3.08	3.60	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.08 differs from the reported value 2.8 by more than 10 %

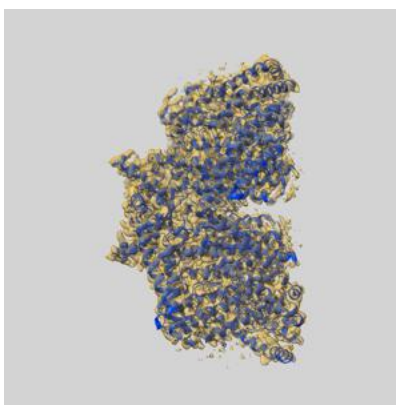
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41043 and PDB model 8T56. Per-residue inclusion information can be found in section [3](#) on page [9](#).

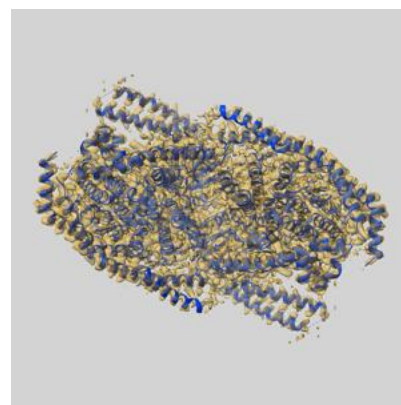
9.1 Map-model overlay [i](#)



X



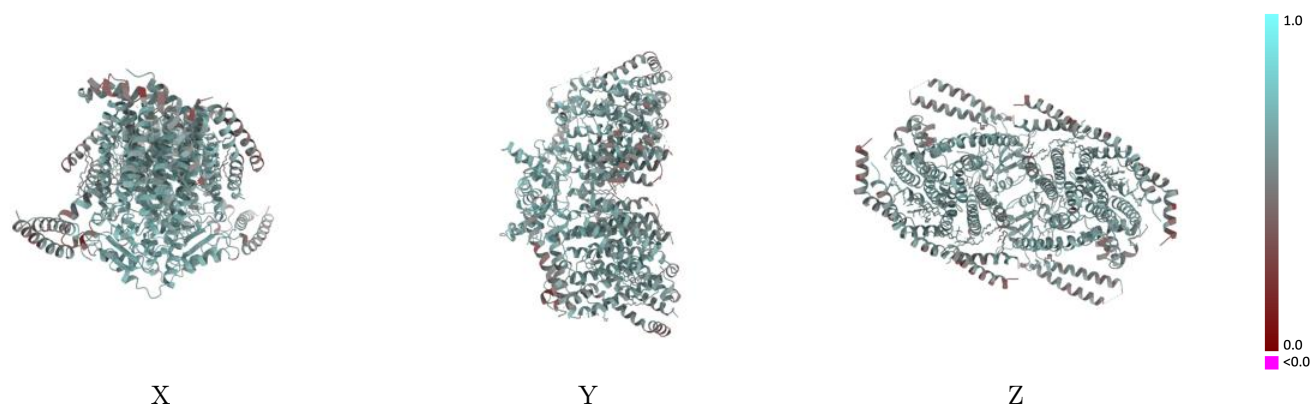
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0138 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

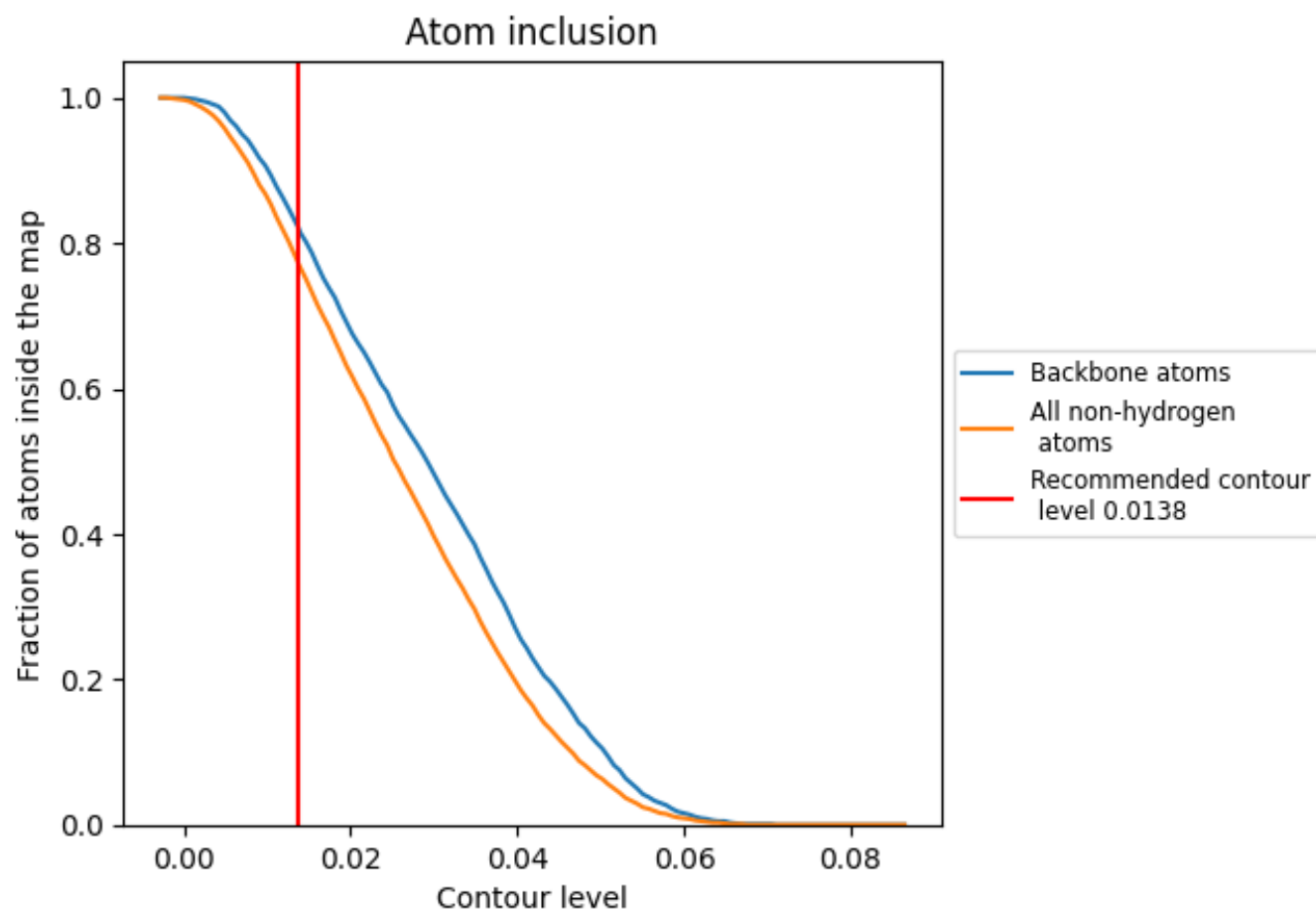


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0138) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7710	0.5840
A	0.8020	0.5980
B	0.8020	0.5980
C	0.6140	0.4990
D	0.7710	0.5770
E	0.6910	0.5450
F	0.3850	0.4460
G	0.6170	0.4940
H	0.7710	0.5840
I	0.6940	0.5410
J	0.3900	0.4580

1.0

0.0

<0.0