



## Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 12:12 PM JST

PDB ID : 9JOW / pdb\_00009jow  
EMDB ID : EMD-61687  
Title : Cryo-EM structure of the myxol-bound light-driven chloride ion-pumping rhodopsin, NM-R3  
Authors : Hosaka, T.; Shirouzu, M.  
Deposited on : 2024-09-25  
Resolution : 2.48 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

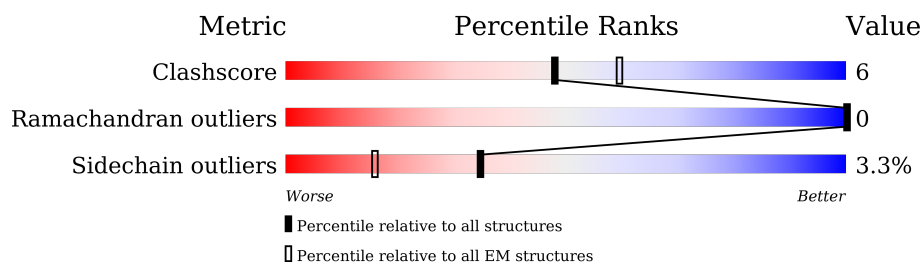
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.48 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	279	 83% 10% • 5%
1	B	279	 82% 9% • 5%
1	C	279	 82% 11% • 5%
1	D	279	 81% 12% • 5%
1	E	279	 82% 11% • 5%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11677 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 Chloride pumping rhodopsin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	264	Total 2065	C 1373	N 318	O 359	S 15	0	0
1	B	264	Total 2065	C 1373	N 318	O 359	S 15	0	0
1	C	264	Total 2065	C 1373	N 318	O 359	S 15	0	0
1	D	264	Total 2065	C 1373	N 318	O 359	S 15	0	0
1	E	264	Total 2065	C 1373	N 318	O 359	S 15	0	0

There are 35 discrepancies between the modelled and reference sequences:

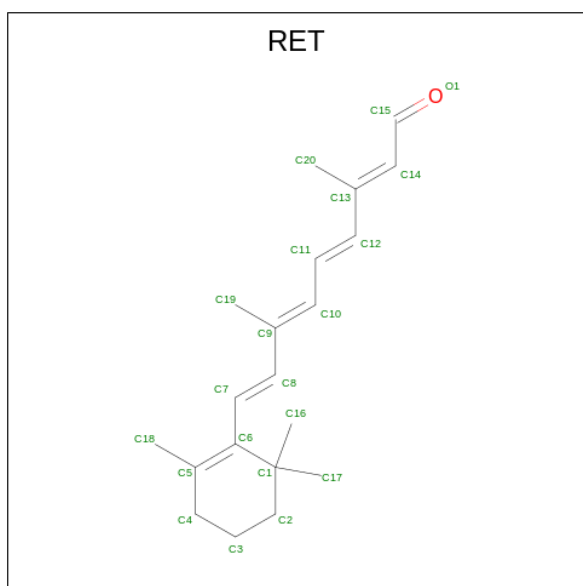
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP W8VZW3
A	-5	SER	-	expression tag	UNP W8VZW3
A	-4	SER	-	expression tag	UNP W8VZW3
A	-3	GLY	-	expression tag	UNP W8VZW3
A	-2	SER	-	expression tag	UNP W8VZW3
A	-1	SER	-	expression tag	UNP W8VZW3
A	0	GLY	-	expression tag	UNP W8VZW3
B	-6	GLY	-	expression tag	UNP W8VZW3
B	-5	SER	-	expression tag	UNP W8VZW3
B	-4	SER	-	expression tag	UNP W8VZW3
B	-3	GLY	-	expression tag	UNP W8VZW3
B	-2	SER	-	expression tag	UNP W8VZW3
B	-1	SER	-	expression tag	UNP W8VZW3
B	0	GLY	-	expression tag	UNP W8VZW3
C	-6	GLY	-	expression tag	UNP W8VZW3
C	-5	SER	-	expression tag	UNP W8VZW3
C	-4	SER	-	expression tag	UNP W8VZW3
C	-3	GLY	-	expression tag	UNP W8VZW3
C	-2	SER	-	expression tag	UNP W8VZW3
C	-1	SER	-	expression tag	UNP W8VZW3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP W8VZW3
D	-6	GLY	-	expression tag	UNP W8VZW3
D	-5	SER	-	expression tag	UNP W8VZW3
D	-4	SER	-	expression tag	UNP W8VZW3
D	-3	GLY	-	expression tag	UNP W8VZW3
D	-2	SER	-	expression tag	UNP W8VZW3
D	-1	SER	-	expression tag	UNP W8VZW3
D	0	GLY	-	expression tag	UNP W8VZW3
E	-6	GLY	-	expression tag	UNP W8VZW3
E	-5	SER	-	expression tag	UNP W8VZW3
E	-4	SER	-	expression tag	UNP W8VZW3
E	-3	GLY	-	expression tag	UNP W8VZW3
E	-2	SER	-	expression tag	UNP W8VZW3
E	-1	SER	-	expression tag	UNP W8VZW3
E	0	GLY	-	expression tag	UNP W8VZW3

- Molecule 2 is RETINAL (CCD ID: RET) (formula:  $C_{20}H_{28}O$ ) (labeled as "Ligand of Interest" by depositor).



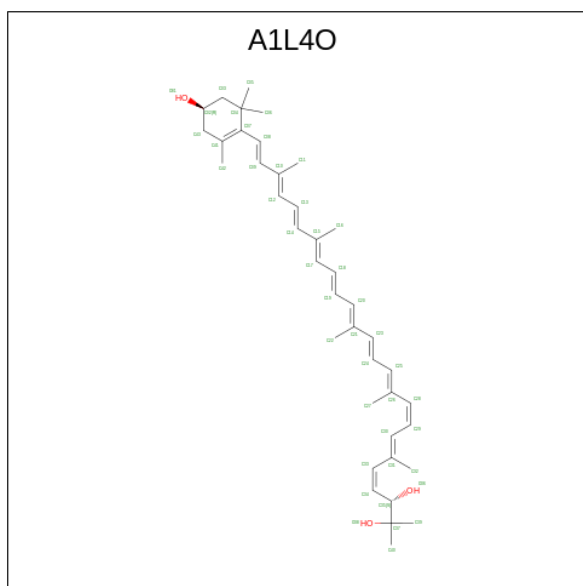
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C 20 20	0
2	B	1	Total C 20 20	0
2	C	1	Total C 20 20	0

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Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total	C	0
			20	20	
2	E	1	Total	C	0
			20	20	

- Molecule 3 is (3 {S},4 {Z},6 {E},8 {Z},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E})-2,6,10,14,19,23-hexamethyl-25-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]pentacos-4,6,8,10,12,14,16,18,20,22,24-undecaene-2,3-diol (CCD ID: A1L4O) (formula:  $C_{40}H_{56}O_3$ ).

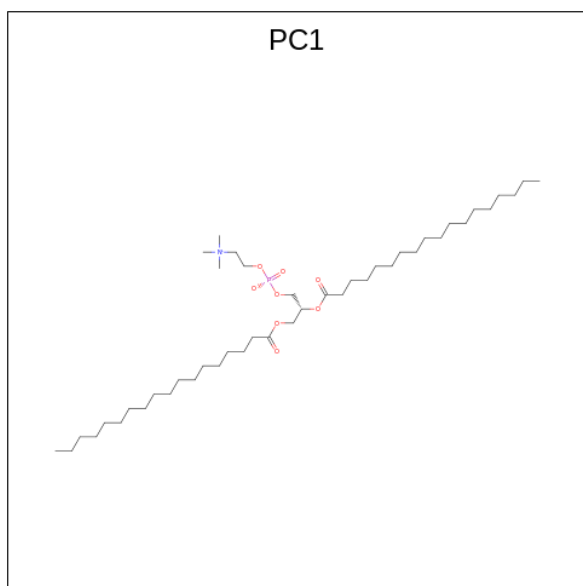


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			43	40	3	
3	B	1	Total	C	O	0
			43	40	3	
3	C	1	Total	C	O	0
			43	40	3	
3	D	1	Total	C	O	0
			43	40	3	
3	E	1	Total	C	O	0
			43	40	3	

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

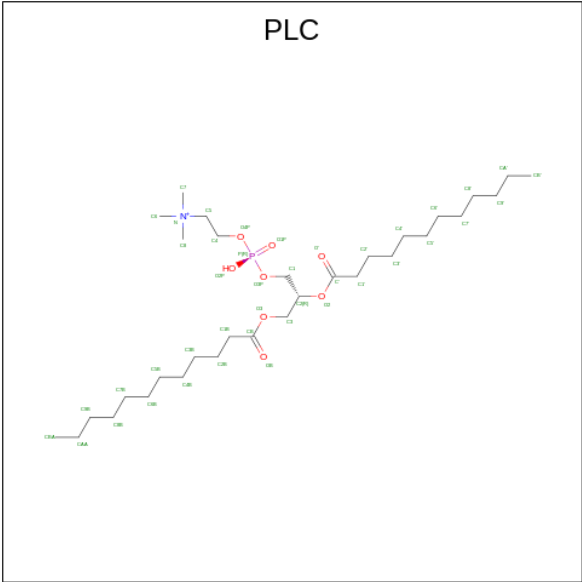
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Cl	0
			2	2	
4	B	2	Total	Cl	0
			2	2	
4	C	2	Total	Cl	0
			2	2	
4	D	2	Total	Cl	0
			2	2	
4	E	2	Total	Cl	0
			2	2	

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



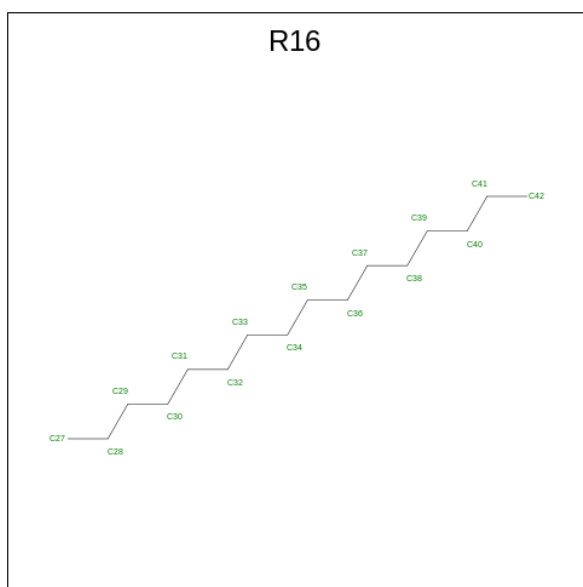
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	E	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 6 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula:  $C_{32}H_{65}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
6	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
6	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
6	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
6	D	1	Total	C	N	O	P	0
			42	32	1	8	1	

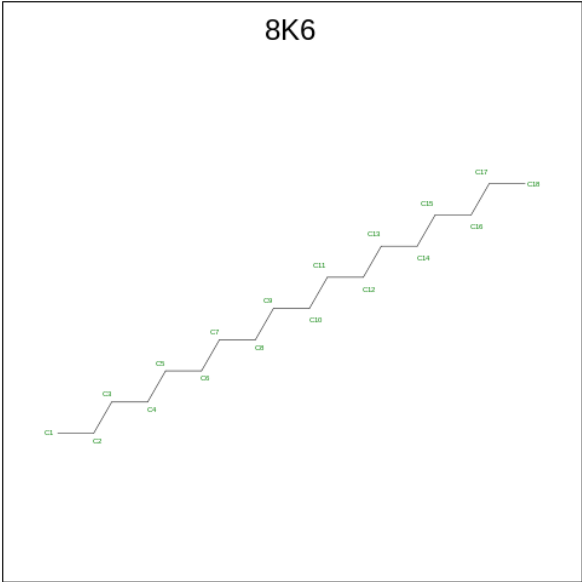
- Molecule 7 is HEXADECANE (CCD ID: R16) (formula: C<sub>16</sub>H<sub>34</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0
7	B	1	Total C 16 16	0
7	B	1	Total C 16 16	0
7	B	1	Total C 16 16	0
7	D	1	Total C 16 16	0
7	D	1	Total C 16 16	0
7	D	1	Total C 16 16	0
7	E	1	Total C 16 16	0
7	E	1	Total C 16 16	0

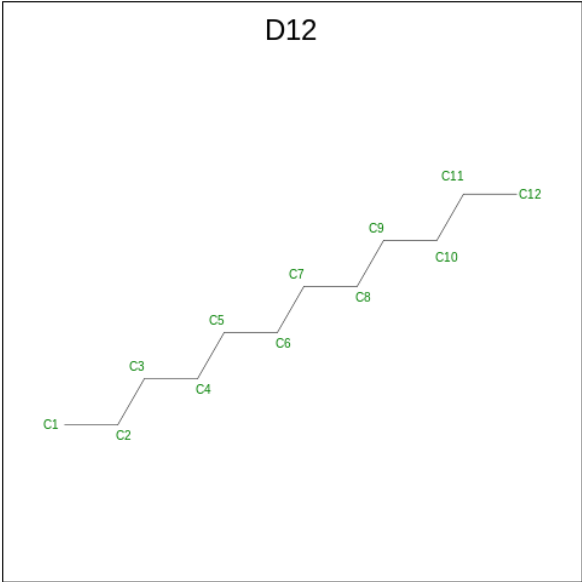
- Molecule 8 is Octadecane (CCD ID: 8K6) (formula: C<sub>18</sub>H<sub>38</sub>) (labeled as "Ligand of Interest" by depositor).





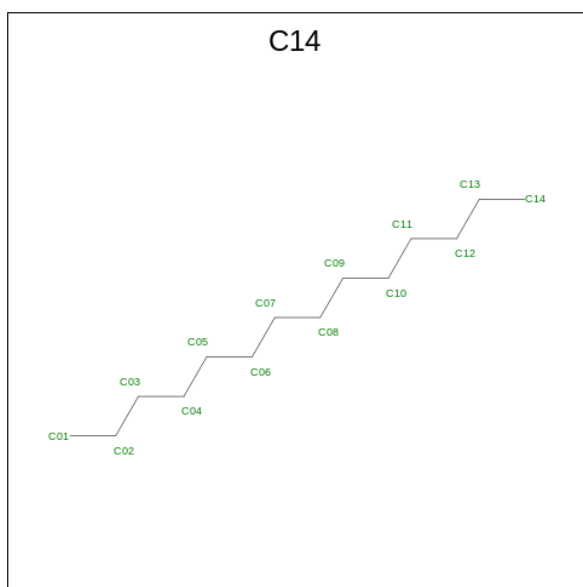
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	C	0
			18	18	
8	B	1	Total	C	0
			18	18	
8	C	1	Total	C	0
			18	18	

- Molecule 9 is DODECANE (CCD ID: D12) (formula: C<sub>12</sub>H<sub>26</sub>) (labeled as "Ligand of Interest" by depositor).



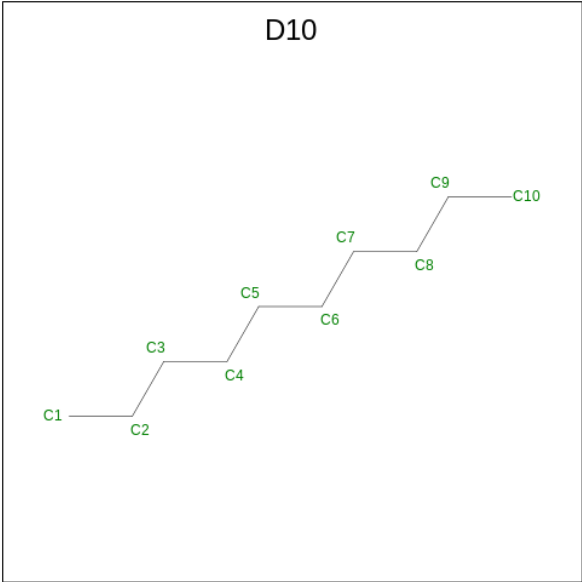
Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C 12 12	0
9	D	1	Total C 12 12	0
9	E	1	Total C 12 12	0

- Molecule 10 is TETRADECANE (CCD ID: C14) (formula:  $C_{14}H_{30}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
10	B	1	Total C 14 14	0
10	B	1	Total C 14 14	0
10	C	1	Total C 14 14	0
10	C	1	Total C 14 14	0
10	E	1	Total C 14 14	0
10	E	1	Total C 14 14	0

- Molecule 11 is DECANE (CCD ID: D10) (formula:  $C_{10}H_{22}$ ) (labeled as "Ligand of Interest" by depositor).

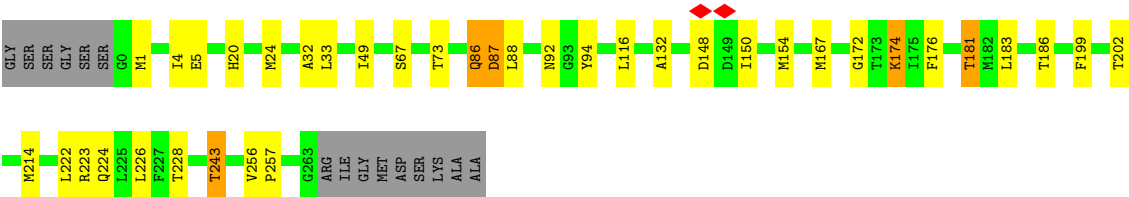


Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	C	0
			10	10	

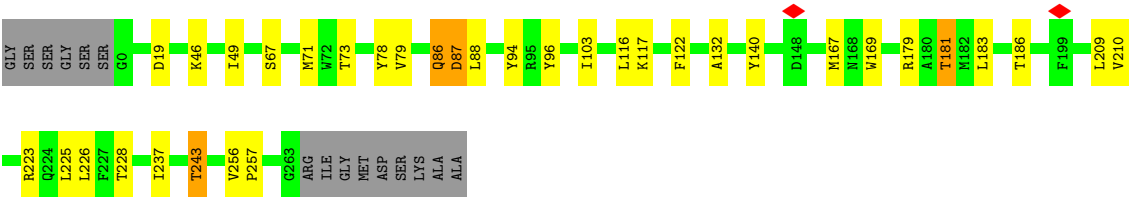
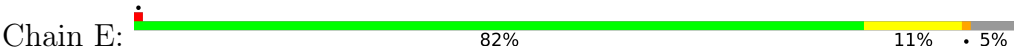
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	36	Total	O	0
			36	36	
12	B	36	Total	O	0
			36	36	
12	C	39	Total	O	0
			39	39	
12	D	37	Total	O	0
			37	37	
12	E	39	Total	O	0
			39	39	





• Molecule 1: Chloride pumping rhodopsin



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	791219	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 ( $e^-/\text{\AA}^2$ )	60.425	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.042	Depositor
Map size (Å)	182.26999, 182.26999, 182.26999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, PLC, A1L4O, D12, CL, 8K6, R16, C14, D10, RET

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	0.85	0/2117	1.19	6/2886 (0.2%)
1	B	0.85	0/2117	1.20	9/2886 (0.3%)
1	C	0.83	0/2117	1.18	7/2886 (0.2%)
1	D	0.82	0/2117	1.20	8/2886 (0.3%)
1	E	0.83	0/2117	1.19	7/2886 (0.2%)
All	All	0.84	0/10585	1.19	37/14430 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	2
All	All	0	5

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	GLN	CB-CA-C	-12.28	95.62	111.70
1	C	86	GLN	CB-CA-C	-12.21	95.70	111.70
1	D	86	GLN	CB-CA-C	-12.15	95.79	111.70
1	B	86	GLN	CB-CA-C	-12.12	95.83	111.70
1	E	86	GLN	CB-CA-C	-11.99	95.99	111.70
1	D	181	THR	CA-CB-OG1	-8.02	97.57	109.60
1	B	181	THR	CA-CB-OG1	-7.75	97.97	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	181	THR	CA-CB-OG1	-7.27	98.69	109.60
1	C	181	THR	CA-CB-OG1	-7.00	99.10	109.60
1	B	243	THR	OG1-CB-CG2	-6.85	95.59	109.30
1	C	116	LEU	N-CA-CB	6.73	120.52	110.29
1	A	243	THR	OG1-CB-CG2	-6.65	96.00	109.30
1	D	243	THR	OG1-CB-CG2	-6.35	96.60	109.30
1	D	116	LEU	N-CA-CB	6.32	119.27	110.17
1	D	174	LYS	CB-CG-CD	6.28	125.75	111.30
1	D	88	LEU	N-CA-CB	-6.10	101.72	111.43
1	E	116	LEU	N-CA-CB	5.98	118.78	110.17
1	E	243	THR	OG1-CB-CG2	-5.91	97.48	109.30
1	A	88	LEU	N-CA-CB	-5.79	102.23	111.43
1	B	116	LEU	N-CA-CB	5.71	118.40	110.17
1	A	116	LEU	N-CA-CB	5.60	118.24	110.17
1	B	88	LEU	N-CA-CB	-5.60	102.54	111.62
1	C	88	LEU	N-CA-CB	-5.60	102.52	111.43
1	B	228	THR	CA-CB-OG1	-5.57	101.24	109.60
1	B	202	THR	CA-CB-OG1	-5.42	101.46	109.60
1	E	228	THR	CA-CB-OG1	-5.41	101.49	109.60
1	B	103	ILE	N-CA-CB	5.40	113.90	110.50
1	C	103	ILE	N-CA-CB	5.39	113.90	110.50
1	E	103	ILE	N-CA-CB	5.30	113.84	110.50
1	A	202	THR	CA-CB-OG1	-5.29	101.67	109.60
1	D	228	THR	CA-CB-OG1	-5.23	101.76	109.60
1	D	202	THR	CA-CB-OG1	-5.22	101.77	109.60
1	E	88	LEU	N-CA-CB	-5.15	103.28	111.62
1	C	202	THR	CA-CB-OG1	-5.13	101.90	109.60
1	B	2	LYS	CG-CD-CE	5.09	123.00	111.30
1	A	228	THR	CA-CB-OG1	-5.05	102.02	109.60
1	C	197	MET	CG-SD-CE	-5.05	89.79	100.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ARG	Sidechain
1	C	223	ARG	Sidechain
1	D	223	ARG	Sidechain
1	E	179	ARG	Sidechain
1	E	223	ARG	Sidechain



## 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	2065	0	2096	19	0
1	B	2065	0	2096	19	0
1	C	2065	0	2096	23	0
1	D	2065	0	2096	19	0
1	E	2065	0	2096	18	0
2	A	20	0	27	3	0
2	B	20	0	27	4	0
2	C	20	0	27	2	0
2	D	20	0	27	2	0
2	E	20	0	27	1	0
3	A	43	0	0	1	0
3	B	43	0	0	0	0
3	C	43	0	0	0	0
3	D	43	0	0	0	0
3	E	43	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	1	0
5	A	54	0	88	5	0
5	B	54	0	88	3	0
5	C	54	0	88	6	0
5	D	54	0	88	3	0
5	E	54	0	88	10	0
6	A	84	0	128	0	0
6	B	42	0	64	2	0
6	C	42	0	64	1	0
6	D	42	0	64	0	0
7	A	48	0	102	3	0
7	B	48	0	102	3	0
7	D	48	0	102	5	0
7	E	32	0	68	1	0
8	A	18	0	38	0	0
8	B	18	0	38	1	0
8	C	18	0	38	2	0
9	A	12	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	12	0	26	1	0
9	E	12	0	26	1	0
10	B	28	0	60	0	0
10	C	28	0	60	4	0
10	E	28	0	60	2	0
11	C	10	0	22	2	0
12	A	36	0	0	0	0
12	B	36	0	0	0	0
12	C	39	0	0	2	0
12	D	37	0	0	0	0
12	E	39	0	0	2	0
All	All	11677	0	12143	134	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 (134) 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)
5:E:306:PC1:H32	5:E:306:PC1:C22	1.60	1.12
5:E:306:PC1:O11	5:E:306:PC1:O32	1.70	1.09
5:E:306:PC1:H221	5:E:306:PC1:C3	1.93	0.97
5:E:306:PC1:H32	5:E:306:PC1:H221	0.97	0.95
5:E:306:PC1:O32	5:E:306:PC1:C1	2.25	0.83
1:A:1:MET:HE1	1:A:89:THR:HG21	1.63	0.78
5:A:305:PC1:H3I1	5:A:305:PC1:H2E1	1.66	0.77
1:D:214:MET:HE1	1:D:222:LEU:HD22	1.71	0.72
1:C:140:TYR:OH	1:D:20:HIS:HD2	1.75	0.69
1:D:199:PHE:HB2	7:D:308:R16:H282	1.74	0.69
1:E:96:TYR:OH	12:E:401:HOH:O	2.07	0.68
1:B:87:ASP:OD1	1:B:87:ASP:C	2.37	0.67
1:A:132:ALA:HA	1:A:167:MET:HE1	1.77	0.67
1:E:132:ALA:HA	1:E:167:MET:HE1	1.78	0.66
1:A:1:MET:HE3	1:A:1:MET:HA	1.77	0.65
1:D:132:ALA:HA	1:D:167:MET:HE1	1.78	0.65
6:C:306:PLC:H1'1	6:C:306:PLC:H32	1.78	0.65
1:B:132:ALA:HA	1:B:167:MET:HE1	1.78	0.65
1:C:132:ALA:HA	1:C:167:MET:HE1	1.77	0.65
5:A:305:PC1:H3E1	7:A:312:R16:H421	1.79	0.64
5:E:306:PC1:C1	5:E:306:PC1:C31	2.76	0.62
5:E:306:PC1:O22	5:E:306:PC1:H242	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:311:R16:H402	10:C:307:C14:H122	1.82	0.62
1:E:86:GLN:O	1:E:87:ASP:OD1	2.18	0.61
2:D:302:RET:H161	2:D:302:RET:H8	1.84	0.60
1:C:92:ASN:OD1	12:C:401:HOH:O	2.17	0.59
1:A:214:MET:HE1	1:A:222:LEU:HD22	1.84	0.59
2:C:301:RET:H161	2:C:301:RET:H8	1.84	0.59
1:C:244:TYR:CD1	5:C:305:PC1:H321	2.38	0.59
1:D:214:MET:HE1	1:D:222:LEU:CD2	2.34	0.58
1:A:19:ASP:OD2	1:E:94:TYR:OH	2.21	0.57
1:C:198:MET:HB3	10:C:308:C14:H112	1.86	0.57
2:A:301:RET:H8	2:A:301:RET:H171	1.87	0.57
1:A:1:MET:HA	1:A:1:MET:CE	2.36	0.56
1:E:71:MET:HG2	12:E:428:HOH:O	2.06	0.56
8:C:310:8K6:H183	7:D:301:R16:C27	2.36	0.55
1:D:199:PHE:HB2	7:D:308:R16:C28	2.37	0.55
1:B:94:TYR:OH	1:C:19:ASP:OD2	2.19	0.54
5:E:306:PC1:O22	5:E:306:PC1:C24	2.51	0.53
2:B:302:RET:H8	2:B:302:RET:H161	1.91	0.53
1:C:127:TRP:CG	11:C:309:D10:H61	2.44	0.53
1:C:127:TRP:CD2	11:C:309:D10:H61	2.44	0.53
1:B:163:PHE:HE1	7:B:310:R16:H311	1.75	0.51
1:E:132:ALA:HA	1:E:167:MET:CE	2.41	0.51
1:C:198:MET:HB3	10:C:308:C14:C11	2.41	0.51
1:D:132:ALA:HA	1:D:167:MET:CE	2.41	0.51
1:A:132:ALA:HA	1:A:167:MET:CE	2.40	0.50
7:A:312:R16:H271	10:E:310:C14:H143	1.93	0.50
5:B:306:PC1:H31	5:B:306:PC1:H342	1.93	0.50
1:C:101:ALA:HB2	5:D:306:PC1:H2I1	1.93	0.50
1:A:20:HIS:HD2	1:E:140:TYR:OH	1.95	0.49
1:B:132:ALA:HA	1:B:167:MET:CE	2.41	0.49
1:D:49:ILE:HD12	1:D:49:ILE:H	1.77	0.49
1:C:140:TYR:OH	1:D:20:HIS:CD2	2.62	0.49
1:E:49:ILE:HD12	1:E:49:ILE:H	1.78	0.49
1:B:183:LEU:O	1:B:186:THR:OG1	2.30	0.48
5:A:305:PC1:C3D	5:A:305:PC1:H3I2	2.43	0.48
1:A:1:MET:HE1	1:A:89:THR:CG2	2.40	0.48
1:B:244:TYR:CD1	5:B:306:PC1:O32	2.67	0.48
1:C:132:ALA:HA	1:C:167:MET:CE	2.41	0.48
6:B:307:PLC:H2A2	1:C:247:ILE:HD12	1.96	0.48
1:B:71:MET:HE3	1:B:88:LEU:CD2	2.44	0.48
1:C:49:ILE:H	1:C:49:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:VAL:N	1:B:257:PRO:CD	2.77	0.47
1:E:256:VAL:N	1:E:257:PRO:CD	2.78	0.47
1:A:68:GLN:HE21	1:A:68:GLN:HA	1.80	0.47
1:A:214:MET:HE1	1:A:222:LEU:CD2	2.45	0.47
5:B:306:PC1:H3B1	5:B:306:PC1:H382	1.34	0.47
8:C:310:8K6:H183	7:D:301:R16:H273	1.97	0.47
1:C:256:VAL:N	1:C:257:PRO:CD	2.79	0.46
5:C:305:PC1:O32	5:C:305:PC1:C2	2.55	0.46
1:B:137:ILE:HG12	7:B:311:R16:H371	1.98	0.46
1:B:49:ILE:H	1:B:49:ILE:HD12	1.81	0.45
1:A:150:ILE:O	1:A:154:MET:HG2	2.17	0.45
7:A:312:R16:C27	10:E:310:C14:H143	2.46	0.45
1:B:86:GLN:O	1:B:87:ASP:OD1	2.34	0.45
5:E:306:PC1:C31	5:E:306:PC1:H12	2.44	0.45
1:C:86:GLN:O	1:C:87:ASP:OD2	2.35	0.45
1:D:86:GLN:O	1:D:87:ASP:OD2	2.35	0.45
1:A:49:ILE:HD12	1:A:49:ILE:H	1.81	0.45
5:C:305:PC1:H2B1	5:C:305:PC1:H281	1.85	0.45
1:A:256:VAL:N	1:A:257:PRO:CD	2.80	0.44
1:D:256:VAL:N	1:D:257:PRO:CD	2.80	0.44
1:B:2:LYS:HD2	1:B:144:LEU:HD22	1.99	0.44
1:E:169:TRP:CE3	3:E:303:A1L4O:C27	3.01	0.44
5:D:306:PC1:H3C1	5:D:306:PC1:H3F2	1.78	0.44
1:A:183:LEU:O	1:A:186:THR:OG1	2.30	0.44
1:A:86:GLN:O	1:A:87:ASP:OD2	2.35	0.44
1:D:32:ALA:O	1:D:33:LEU:C	2.60	0.44
1:E:237:ILE:HD13	5:E:306:PC1:H381	2.00	0.43
2:A:301:RET:H171	2:A:301:RET:C8	2.48	0.43
1:D:92:ASN:HD21	1:D:224:GLN:HE22	1.67	0.43
1:E:183:LEU:O	1:E:186:THR:OG1	2.31	0.43
1:C:71:MET:HE1	1:C:89:THR:O	2.19	0.43
1:D:150:ILE:O	1:D:154:MET:HG2	2.19	0.43
1:C:218:ASP:OD1	10:C:307:C14:H011	2.19	0.43
5:D:306:PC1:H322	5:D:306:PC1:H31	1.72	0.43
1:A:94:TYR:OH	1:B:19:ASP:OD2	2.31	0.42
5:A:305:PC1:H3I2	5:A:305:PC1:C3C	2.49	0.42
9:D:310:D12:H123	7:E:301:R16:H271	2.01	0.42
3:E:303:A1L4O:C39	3:E:303:A1L4O:C33	2.97	0.42
5:C:305:PC1:O32	5:C:305:PC1:H2	2.19	0.42
2:E:302:RET:H161	2:E:302:RET:H8	2.02	0.42
2:B:302:RET:H7	2:B:302:RET:H181	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLN:HA	1:B:68:GLN:HE21	1.86	0.41
1:C:46:LYS:NZ	12:C:405:HOH:O	2.42	0.41
1:D:24:MET:HE1	7:D:301:R16:H423	2.02	0.41
1:A:169:TRP:HA	3:A:302:A1L4O:C27	2.50	0.41
1:B:150:ILE:O	1:B:154:MET:HG2	2.21	0.41
1:C:150:ILE:HD13	1:C:150:ILE:HA	1.88	0.41
1:D:183:LEU:O	1:D:186:THR:OG1	2.31	0.41
1:D:4:ILE:O	1:D:5:GLU:C	2.63	0.41
2:D:302:RET:H181	2:D:302:RET:H7	1.69	0.41
1:C:150:ILE:O	1:C:154:MET:HG2	2.20	0.41
5:C:305:PC1:H2D2	5:C:305:PC1:H2G1	1.89	0.41
1:A:4:ILE:O	1:A:5:GLU:C	2.63	0.41
1:B:103:ILE:N	1:B:104:PRO:CD	2.83	0.41
2:C:301:RET:H181	2:C:301:RET:H7	1.91	0.41
1:E:225:LEU:CD2	9:E:307:D12:H71	2.51	0.41
2:A:301:RET:H8	2:A:301:RET:H161	2.02	0.41
9:A:310:D12:H122	8:B:301:8K6:H162	2.02	0.41
5:A:305:PC1:H143	1:E:122:PHE:CD1	2.56	0.40
2:B:302:RET:H161	2:B:302:RET:C8	2.50	0.40
1:D:172:GLY:O	1:D:176:PHE:HD2	2.03	0.40
1:B:122:PHE:CZ	6:B:307:PLC:H1'1	2.56	0.40
1:C:4:ILE:O	1:C:5:GLU:C	2.63	0.40
1:E:46:LYS:N	4:E:305:CL:CL	2.84	0.40
1:E:209:LEU:O	1:E:210:VAL:C	2.65	0.40
1:B:64:ILE:HG23	1:B:64:ILE:HD12	1.86	0.40
2:B:302:RET:H8	2:B:302:RET:H171	2.02	0.40
1:D:94:TYR:OH	1:E:19:ASP:OD2	2.33	0.40
1:E:78:TYR:C	1:E:79:VAL:HG23	2.47	0.40
1:C:32:ALA:O	1:C:33:LEU:C	2.63	0.40
5:C:305:PC1:H382	5:C:305:PC1:H3B1	1.71	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 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	262/279 (94%)	256 (98%)	6 (2%)	0	100	100
1	B	262/279 (94%)	257 (98%)	5 (2%)	0	100	100
1	C	262/279 (94%)	256 (98%)	6 (2%)	0	100	100
1	D	262/279 (94%)	256 (98%)	6 (2%)	0	100	100
1	E	262/279 (94%)	256 (98%)	6 (2%)	0	100	100
All	All	1310/1395 (94%)	1281 (98%)	29 (2%)	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	216/226 (96%)	209 (97%)	7 (3%)	34	57
1	B	216/226 (96%)	208 (96%)	8 (4%)	29	52
1	C	216/226 (96%)	211 (98%)	5 (2%)	45	69
1	D	216/226 (96%)	207 (96%)	9 (4%)	25	46
1	E	216/226 (96%)	209 (97%)	7 (3%)	34	57
All	All	1080/1130 (96%)	1044 (97%)	36 (3%)	35	56

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	46	LYS
1	A	67	SER
1	A	73	THR
1	A	87	ASP
1	A	117	LYS
1	A	243	THR

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Mol	Chain	Res	Type
1	B	1	MET
1	B	67	SER
1	B	73	THR
1	B	87	ASP
1	B	150	ILE
1	B	181	THR
1	B	226	LEU
1	B	243	THR
1	C	67	SER
1	C	73	THR
1	C	87	ASP
1	C	181	THR
1	C	243	THR
1	D	1	MET
1	D	67	SER
1	D	73	THR
1	D	87	ASP
1	D	148	ASP
1	D	174	LYS
1	D	181	THR
1	D	226	LEU
1	D	243	THR
1	E	67	SER
1	E	73	THR
1	E	87	ASP
1	E	117	LYS
1	E	181	THR
1	E	226	LEU
1	E	243	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	20	HIS
1	A	68	GLN
1	A	86	GLN
1	A	178	ASN
1	B	41	GLN
1	B	68	GLN
1	B	109	GLN
1	B	224	GLN

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Mol	Chain	Res	Type
1	B	248	GLN
1	B	260	GLN
1	C	168	ASN
1	C	259	GLN
1	D	20	HIS
1	D	29	HIS
1	D	92	ASN
1	D	109	GLN
1	D	152	GLN
1	D	248	GLN
1	D	259	GLN
1	E	92	ASN
1	E	109	GLN
1	E	152	GLN
1	E	224	GLN
1	E	248	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 54 ligands modelled in this entry, 10 are monoatomic - leaving 44 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
5	PC1	E	306	-	53,53,53	0.58	0	59,61,61	0.91	4 (6%)
10	C14	E	310	-	13,13,13	0.32	0	12,12,12	0.31	0
2	RET	E	302	1	20,20,21	2.21	4 (20%)	27,27,28	1.62	5 (18%)
7	R16	A	308	-	15,15,15	0.15	0	14,14,14	0.15	0
7	R16	D	309	-	15,15,15	0.19	0	14,14,14	0.22	0
3	A1L4O	C	302	-	42,43,43	0.80	0	53,58,58	2.26	15 (28%)
7	R16	E	301	-	15,15,15	0.21	0	14,14,14	0.27	0
8	8K6	B	301	-	17,17,17	0.36	0	16,16,16	0.40	0
10	C14	B	308	-	13,13,13	0.31	0	12,12,12	0.21	0
9	D12	A	310	-	11,11,11	0.28	0	10,10,10	0.17	0
8	8K6	A	309	-	17,17,17	0.28	0	16,16,16	0.23	0
7	R16	E	309	-	15,15,15	0.19	0	14,14,14	0.13	0
3	A1L4O	D	303	-	42,43,43	0.84	0	53,58,58	2.15	21 (39%)
10	C14	C	307	-	13,13,13	0.27	0	12,12,12	0.26	0
6	PLC	D	307	-	41,41,41	0.43	0	47,49,49	0.61	0
6	PLC	C	306	-	41,41,41	0.50	0	47,49,49	1.12	3 (6%)
2	RET	D	302	1	20,20,21	1.80	3 (15%)	27,27,28	1.55	3 (11%)
3	A1L4O	B	303	-	42,43,43	0.86	1 (2%)	53,58,58	2.31	17 (32%)
5	PC1	D	306	-	53,53,53	0.47	0	59,61,61	0.57	0
7	R16	B	310	-	15,15,15	0.18	0	14,14,14	0.19	0
7	R16	D	301	-	15,15,15	0.34	0	14,14,14	0.33	0
10	C14	E	308	-	13,13,13	0.28	0	12,12,12	0.23	0
7	R16	B	311	-	15,15,15	0.29	0	14,14,14	0.37	0
3	A1L4O	A	302	-	42,43,43	1.01	2 (4%)	53,58,58	2.77	19 (35%)
9	D12	E	307	-	11,11,11	0.22	0	10,10,10	0.33	0
6	PLC	A	306	-	41,41,41	0.47	0	47,49,49	0.62	0
8	8K6	C	310	-	17,17,17	0.33	0	16,16,16	0.27	0
2	RET	A	301	1	20,20,21	1.93	4 (20%)	27,27,28	1.49	6 (22%)
7	R16	A	307	-	15,15,15	0.23	0	14,14,14	0.18	0
10	C14	B	312	-	13,13,13	0.26	0	12,12,12	0.25	0
6	PLC	A	311	-	41,41,41	0.45	0	47,49,49	0.54	1 (2%)
2	RET	C	301	1	20,20,21	2.78	4 (20%)	27,27,28	1.60	5 (18%)
3	A1L4O	E	303	-	42,43,43	0.92	2 (4%)	53,58,58	2.63	20 (37%)
5	PC1	B	306	-	53,53,53	0.75	1 (1%)	59,61,61	0.76	1 (1%)
7	R16	A	312	-	15,15,15	0.24	0	14,14,14	0.32	0
11	D10	C	309	-	9,9,9	0.17	0	8,8,8	0.19	0
5	PC1	C	305	-	53,53,53	0.51	0	59,61,61	0.58	1 (1%)
6	PLC	B	307	-	41,41,41	0.50	0	47,49,49	0.64	0
10	C14	C	308	-	13,13,13	0.26	0	12,12,12	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	RET	B	302	1	20,20,21	2.27	3 (15%)	27,27,28	1.65	3 (11%)
7	R16	D	308	-	15,15,15	0.17	0	14,14,14	0.21	0
7	R16	B	309	-	15,15,15	0.25	0	14,14,14	0.16	0
9	D12	D	310	-	11,11,11	0.16	0	10,10,10	0.13	0
5	PC1	A	305	-	53,53,53	0.57	1 (1%)	59,61,61	0.49	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
5	PC1	E	306	-	-	30/57/57/57	-
10	C14	E	310	-	-	5/11/11/11	-
2	RET	E	302	1	-	0/13/30/31	0/1/1/1
7	R16	A	308	-	-	10/13/13/13	-
7	R16	D	309	-	-	7/13/13/13	-
3	A1L4O	C	302	-	-	12/41/60/60	0/1/1/1
7	R16	E	301	-	-	6/13/13/13	-
8	8K6	B	301	-	-	9/15/15/15	-
10	C14	B	308	-	-	6/11/11/11	-
9	D12	A	310	-	-	7/9/9/9	-
8	8K6	A	309	-	-	6/15/15/15	-
7	R16	E	309	-	-	9/13/13/13	-
3	A1L4O	D	303	-	-	9/41/60/60	0/1/1/1
10	C14	C	307	-	-	11/11/11/11	-
6	PLC	D	307	-	-	23/45/45/45	-
6	PLC	C	306	-	-	24/45/45/45	-
2	RET	D	302	1	-	0/13/30/31	0/1/1/1
3	A1L4O	B	303	-	-	16/41/60/60	0/1/1/1
5	PC1	D	306	-	-	35/57/57/57	-
7	R16	B	310	-	-	9/13/13/13	-
7	R16	D	301	-	-	8/13/13/13	-
10	C14	E	308	-	-	8/11/11/11	-
7	R16	B	311	-	-	11/13/13/13	-
3	A1L4O	A	302	-	-	14/41/60/60	0/1/1/1
9	D12	E	307	-	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLC	A	306	-	-	27/45/45/45	-
8	8K6	C	310	-	-	9/15/15/15	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
7	R16	A	307	-	-	7/13/13/13	-
10	C14	B	312	-	-	7/11/11/11	-
6	PLC	A	311	-	-	26/45/45/45	-
2	RET	C	301	1	-	1/13/30/31	0/1/1/1
3	A1L4O	E	303	-	-	13/41/60/60	0/1/1/1
5	PC1	B	306	-	-	32/57/57/57	-
7	R16	A	312	-	-	9/13/13/13	-
11	D10	C	309	-	-	4/7/7/7	-
5	PC1	C	305	-	-	30/57/57/57	-
6	PLC	B	307	-	-	25/45/45/45	-
10	C14	C	308	-	-	8/11/11/11	-
2	RET	B	302	1	-	0/13/30/31	0/1/1/1
7	R16	D	308	-	-	7/13/13/13	-
7	R16	B	309	-	-	8/13/13/13	-
9	D12	D	310	-	-	5/9/9/9	-
5	PC1	A	305	-	-	31/57/57/57	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	RET	C14-C13	10.44	1.41	1.33
2	B	302	RET	C14-C13	7.83	1.39	1.33
2	E	302	RET	C14-C13	7.22	1.39	1.33
2	A	301	RET	C14-C13	5.21	1.37	1.33
2	D	302	RET	C14-C13	5.05	1.37	1.33
2	B	302	RET	C10-C9	4.97	1.42	1.35
2	A	301	RET	C10-C9	4.62	1.41	1.35
2	D	302	RET	C10-C9	4.46	1.41	1.35
2	E	302	RET	C10-C9	4.19	1.41	1.35
2	C	301	RET	C12-C13	-3.60	1.38	1.45
5	B	306	PC1	C33-C32	-3.17	1.40	1.52
3	A	302	A1L4O	C17-C15	-3.13	1.31	1.35
2	C	301	RET	C10-C9	2.93	1.39	1.35
2	E	302	RET	C12-C13	-2.87	1.39	1.45
2	C	301	RET	C2-C3	-2.62	1.46	1.52
2	D	302	RET	C11-C10	-2.60	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	303	A1L4O	C17-C15	-2.55	1.32	1.35
5	A	305	PC1	C23-C22	-2.42	1.43	1.52
3	E	303	A1L4O	C35-C34	2.39	1.53	1.50
3	A	302	A1L4O	C35-C34	2.20	1.53	1.50
2	A	301	RET	C11-C10	-2.16	1.36	1.43
2	B	302	RET	C12-C13	-2.14	1.41	1.45
2	A	301	RET	C8-C9	-2.13	1.41	1.45
3	B	303	A1L4O	C35-C34	2.03	1.52	1.50
2	E	302	RET	C2-C3	-2.00	1.47	1.52

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	A1L4O	C08-C09-C10	-7.71	114.59	126.23
3	A	302	A1L4O	C24-C25-C26	-6.94	117.40	127.31
3	A	302	A1L4O	C08-C09-C10	-6.75	116.04	126.23
3	A	302	A1L4O	C18-C17-C15	-6.63	117.85	127.31
3	E	303	A1L4O	C39-C37-C35	6.24	118.69	110.62
3	E	303	A1L4O	C09-C08-C07	-6.12	110.01	127.20
3	E	303	A1L4O	C08-C09-C10	-6.12	116.99	126.23
3	A	302	A1L4O	C19-C18-C17	-5.91	111.37	123.47
3	A	302	A1L4O	C09-C08-C07	-5.80	110.91	127.20
3	B	303	A1L4O	C08-C09-C10	-5.70	117.63	126.23
3	C	302	A1L4O	C39-C37-C35	5.62	117.88	110.62
6	C	306	PLC	O2-C'-C1'	5.52	123.39	111.50
3	D	303	A1L4O	C09-C08-C07	-5.50	111.76	127.20
3	A	302	A1L4O	C42-C41-C07	-5.39	118.48	124.53
3	E	303	A1L4O	C19-C18-C17	-5.39	112.44	123.47
3	B	303	A1L4O	C09-C08-C07	-5.31	112.28	127.20
3	E	303	A1L4O	C24-C25-C26	-5.23	119.85	127.31
3	B	303	A1L4O	C29-C30-C31	-5.06	120.08	127.31
3	C	302	A1L4O	C29-C30-C31	-4.95	120.25	127.31
3	B	303	A1L4O	C18-C17-C15	-4.87	120.36	127.31
2	B	302	RET	C19-C9-C10	-4.70	116.34	122.92
3	C	302	A1L4O	C18-C17-C15	-4.67	120.64	127.31
3	B	303	A1L4O	C13-C12-C10	-4.55	120.81	127.31
3	D	303	A1L4O	C29-C30-C31	-4.54	120.83	127.31
3	D	303	A1L4O	C08-C09-C10	-4.53	119.38	126.23
3	E	303	A1L4O	C13-C12-C10	-4.48	120.91	127.31
2	D	302	RET	C19-C9-C8	4.48	125.13	118.08
3	B	303	A1L4O	C19-C18-C17	-4.48	114.30	123.47
3	E	303	A1L4O	C19-C20-C21	-4.46	120.94	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	A1L4O	C42-C41-C43	4.40	122.52	114.36
2	C	301	RET	C19-C9-C10	-4.39	116.78	122.92
3	E	303	A1L4O	C16-C15-C14	4.38	124.97	118.08
3	E	303	A1L4O	C18-C17-C15	-4.34	121.12	127.31
3	A	302	A1L4O	C19-C20-C21	-4.24	121.26	127.31
5	E	306	PC1	O21-C21-C22	4.18	120.51	111.50
2	B	302	RET	C19-C9-C8	4.07	124.48	118.08
2	E	302	RET	C19-C9-C10	-4.03	117.28	122.92
3	D	303	A1L4O	C18-C17-C15	-3.94	121.68	127.31
3	B	303	A1L4O	C24-C25-C26	-3.91	121.73	127.31
3	A	302	A1L4O	C29-C30-C31	-3.87	121.79	127.31
3	E	303	A1L4O	C05-C04-C07	3.85	116.54	110.30
3	C	302	A1L4O	C19-C20-C21	-3.79	121.90	127.31
3	B	303	A1L4O	C19-C20-C21	-3.72	122.01	127.31
3	A	302	A1L4O	C16-C15-C14	3.63	123.79	118.08
3	B	303	A1L4O	C16-C15-C14	3.62	123.79	118.08
2	A	301	RET	C19-C9-C10	-3.55	117.95	122.92
3	C	302	A1L4O	C29-C28-C26	-3.52	116.52	126.42
3	D	303	A1L4O	O01-C02-C43	3.48	117.13	109.68
3	D	303	A1L4O	C42-C41-C07	-3.46	120.64	124.53
3	D	303	A1L4O	C24-C25-C26	-3.40	122.46	127.31
2	D	302	RET	C19-C9-C10	-3.36	118.21	122.92
3	D	303	A1L4O	C29-C28-C26	-3.30	117.14	126.42
3	B	303	A1L4O	C29-C28-C26	-3.23	117.34	126.42
3	E	303	A1L4O	C23-C21-C20	-3.22	114.00	118.94
3	C	302	A1L4O	C16-C15-C14	3.22	123.15	118.08
3	D	303	A1L4O	C42-C41-C43	3.20	120.29	114.36
3	E	303	A1L4O	C16-C15-C17	-3.20	118.44	122.92
2	E	302	RET	C19-C9-C8	3.11	122.98	118.08
3	E	303	A1L4O	C30-C29-C28	-3.09	113.58	123.22
2	A	301	RET	C19-C9-C8	3.09	122.94	118.08
3	D	303	A1L4O	C16-C15-C14	3.05	122.89	118.08
3	A	302	A1L4O	C16-C15-C17	-2.97	118.76	122.92
3	C	302	A1L4O	C19-C18-C17	-2.93	117.47	123.47
3	C	302	A1L4O	C24-C25-C26	-2.91	123.16	127.31
5	B	306	PC1	O21-C21-C22	2.88	117.70	111.50
5	E	306	PC1	O21-C2-C3	-2.87	98.02	108.40
3	A	302	A1L4O	C13-C14-C15	-2.83	118.47	126.42
2	E	302	RET	C1-C6-C5	-2.73	118.77	122.61
3	C	302	A1L4O	C16-C15-C17	-2.73	119.10	122.92
2	A	301	RET	C11-C10-C9	2.68	131.13	127.31
3	C	302	A1L4O	C09-C08-C07	-2.66	119.72	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	303	A1L4O	C42-C41-C43	2.66	119.28	114.36
3	A	302	A1L4O	C13-C12-C10	-2.65	123.53	127.31
2	C	301	RET	C7-C8-C9	-2.65	122.23	126.23
3	D	303	A1L4O	C19-C18-C17	-2.65	118.05	123.47
3	A	302	A1L4O	C24-C23-C21	-2.65	118.98	126.42
3	A	302	A1L4O	C23-C21-C20	-2.63	114.91	118.94
3	D	303	A1L4O	C33-C31-C30	-2.63	114.91	118.94
2	C	301	RET	C19-C9-C8	2.62	122.21	118.08
6	C	306	PLC	O2-C2-C3	2.62	117.87	108.40
3	E	303	A1L4O	C13-C14-C15	-2.59	119.15	126.42
3	B	303	A1L4O	C13-C14-C15	-2.58	119.18	126.42
3	A	302	A1L4O	C11-C10-C09	2.56	122.11	118.08
3	D	303	A1L4O	C32-C31-C33	2.55	122.09	118.08
3	D	303	A1L4O	C16-C15-C17	-2.53	119.37	122.92
6	C	306	PLC	O'-C'-C1'	-2.50	113.98	123.73
3	E	303	A1L4O	C29-C30-C31	-2.49	123.75	127.31
3	A	302	A1L4O	C30-C29-C28	-2.47	115.51	123.22
3	B	303	A1L4O	C42-C41-C43	2.42	118.83	114.36
3	D	303	A1L4O	C19-C20-C21	-2.41	123.86	127.31
3	E	303	A1L4O	C29-C28-C26	-2.40	119.67	126.42
3	B	303	A1L4O	C14-C15-C17	-2.39	115.28	118.94
3	A	302	A1L4O	C29-C28-C26	-2.38	119.73	126.42
3	B	303	A1L4O	C12-C13-C14	-2.37	115.81	123.22
3	D	303	A1L4O	C24-C23-C21	-2.33	119.86	126.42
5	E	306	PC1	C3-C2-C1	2.32	117.27	111.79
5	E	306	PC1	O21-C21-O22	-2.26	118.25	123.70
2	A	301	RET	C1-C6-C7	2.23	122.08	115.78
3	D	303	A1L4O	C39-C37-C35	2.21	113.48	110.62
2	D	302	RET	C7-C6-C5	-2.21	116.11	121.46
2	A	301	RET	C1-C6-C5	-2.20	119.51	122.61
3	A	302	A1L4O	C04-C03-C02	-2.20	108.67	113.64
3	B	303	A1L4O	C05-C04-C07	2.19	113.85	110.30
2	C	301	RET	C1-C6-C5	-2.16	119.58	122.61
3	D	303	A1L4O	C04-C03-C02	-2.15	108.78	113.64
3	B	303	A1L4O	C23-C21-C20	-2.12	115.69	118.94
3	C	302	A1L4O	C04-C03-C02	-2.11	108.87	113.64
3	D	303	A1L4O	C03-C02-C43	-2.11	107.42	110.30
3	C	302	A1L4O	C03-C02-C43	-2.11	107.42	110.30
3	C	302	A1L4O	C13-C12-C10	-2.10	124.31	127.31
5	C	305	PC1	C3-C2-C1	2.10	116.76	111.79
3	E	303	A1L4O	C24-C23-C21	-2.10	120.52	126.42
3	D	303	A1L4O	C23-C21-C20	-2.10	115.72	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	A1L4O	C42-C41-C07	-2.10	122.17	124.53
2	E	302	RET	C2-C1-C6	2.07	113.67	110.48
2	B	302	RET	C18-C5-C6	2.07	126.85	124.53
2	E	302	RET	C18-C5-C6	2.06	126.84	124.53
3	D	303	A1L4O	C12-C13-C14	-2.04	116.84	123.22
3	E	303	A1L4O	C33-C31-C30	-2.04	115.81	118.94
2	A	301	RET	C2-C1-C6	2.03	113.61	110.48
2	C	301	RET	C2-C1-C6	2.02	113.60	110.48
3	C	302	A1L4O	C11-C10-C09	2.01	121.25	118.08
6	A	311	PLC	O2-C'-C1'	-2.01	107.16	111.50
3	E	303	A1L4O	C25-C24-C23	-2.01	116.95	123.22

There are no chirality outliers.

All (528) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	A1L4O	C33-C34-C35-C37
3	A	302	A1L4O	C34-C35-C37-C39
3	A	302	A1L4O	C34-C35-C37-C40
3	A	302	A1L4O	C34-C35-C37-O38
3	A	302	A1L4O	O36-C35-C37-C39
3	A	302	A1L4O	O36-C35-C37-C40
3	A	302	A1L4O	O36-C35-C37-O38
3	B	303	A1L4O	C08-C09-C10-C12
3	B	303	A1L4O	C13-C14-C15-C17
3	B	303	A1L4O	C33-C34-C35-C37
3	B	303	A1L4O	C34-C35-C37-C39
3	B	303	A1L4O	C34-C35-C37-C40
3	B	303	A1L4O	C34-C35-C37-O38
3	B	303	A1L4O	O36-C35-C37-C39
3	B	303	A1L4O	O36-C35-C37-O38
3	C	302	A1L4O	C30-C31-C33-C34
3	C	302	A1L4O	C32-C31-C33-C34
3	C	302	A1L4O	C33-C34-C35-C37
3	C	302	A1L4O	C33-C34-C35-O36
3	C	302	A1L4O	C34-C35-C37-C39
3	C	302	A1L4O	C34-C35-C37-C40
3	C	302	A1L4O	C34-C35-C37-O38
3	C	302	A1L4O	O36-C35-C37-C39
3	C	302	A1L4O	O36-C35-C37-C40
3	C	302	A1L4O	O36-C35-C37-O38
3	D	303	A1L4O	C08-C09-C10-C11

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Mol	Chain	Res	Type	Atoms
3	D	303	A1L4O	C08-C09-C10-C12
3	D	303	A1L4O	C04-C07-C08-C09
3	D	303	A1L4O	C34-C35-C37-C39
3	D	303	A1L4O	C34-C35-C37-C40
3	D	303	A1L4O	C34-C35-C37-O38
3	D	303	A1L4O	O36-C35-C37-C39
3	D	303	A1L4O	O36-C35-C37-C40
3	D	303	A1L4O	O36-C35-C37-O38
3	E	303	A1L4O	C08-C09-C10-C11
3	E	303	A1L4O	C08-C09-C10-C12
3	E	303	A1L4O	C33-C34-C35-C37
3	E	303	A1L4O	C34-C35-C37-C39
3	E	303	A1L4O	C34-C35-C37-C40
3	E	303	A1L4O	C34-C35-C37-O38
3	E	303	A1L4O	O36-C35-C37-C39
3	E	303	A1L4O	O36-C35-C37-C40
3	E	303	A1L4O	O36-C35-C37-O38
5	A	305	PC1	C1-O11-P-O14
5	A	305	PC1	O13-C11-C12-N
5	B	306	PC1	C1-O11-P-O12
5	B	306	PC1	C1-O11-P-O14
5	B	306	PC1	O13-C11-C12-N
5	C	305	PC1	O13-C11-C12-N
5	D	306	PC1	C1-O11-P-O12
5	D	306	PC1	O11-C1-C2-O21
5	D	306	PC1	O32-C31-O31-C3
5	D	306	PC1	C32-C31-O31-C3
5	E	306	PC1	O13-C11-C12-N
5	E	306	PC1	O22-C21-O21-C2
6	A	306	PLC	C1-O3P-P-O2P
6	A	311	PLC	C1-O3P-P-O1P
6	A	311	PLC	C1-O3P-P-O2P
6	A	311	PLC	C4-O4P-P-O1P
6	A	311	PLC	C4-O4P-P-O2P
6	B	307	PLC	C1-O3P-P-O2P
6	B	307	PLC	C4-O4P-P-O1P
6	B	307	PLC	C4-O4P-P-O3P
6	C	306	PLC	O4P-C4-C5-N
6	C	306	PLC	C1'-C'-O2-C2
6	C	306	PLC	O'-C'-O2-C2
6	C	306	PLC	C1B-CB-O3-C3
6	C	306	PLC	OB-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
6	C	306	PLC	C1-O3P-P-O1P
6	C	306	PLC	C1-O3P-P-O2P
6	C	306	PLC	C1-O3P-P-O4P
6	C	306	PLC	C4-O4P-P-O1P
6	D	307	PLC	C1-O3P-P-O1P
6	D	307	PLC	C1-O3P-P-O2P
6	D	307	PLC	C1-O3P-P-O4P
5	B	306	PC1	O32-C31-O31-C3
5	B	306	PC1	C32-C31-O31-C3
5	E	306	PC1	C22-C21-O21-C2
5	C	305	PC1	C2-C3-O31-C31
5	B	306	PC1	C38-C39-C3A-C3B
8	A	309	8K6	C12-C13-C14-C15
5	C	305	PC1	C28-C29-C2A-C2B
5	E	306	PC1	C27-C28-C29-C2A
6	A	311	PLC	C2-C1-O3P-P
9	A	310	D12	C3-C4-C5-C6
5	D	306	PC1	C3C-C3D-C3E-C3F
3	A	302	A1L4O	C08-C09-C10-C11
3	B	303	A1L4O	C08-C09-C10-C11
3	B	303	A1L4O	C13-C14-C15-C16
3	B	303	A1L4O	C32-C31-C33-C34
3	C	302	A1L4O	C08-C09-C10-C11
3	A	302	A1L4O	C08-C09-C10-C12
3	B	303	A1L4O	C30-C31-C33-C34
3	C	302	A1L4O	C08-C09-C10-C12
5	D	306	PC1	C22-C21-O21-C2
5	C	305	PC1	C24-C25-C26-C27
7	D	309	R16	C37-C38-C39-C40
6	D	307	PLC	C'-C1'-C2'-C3'
5	E	306	PC1	C32-C31-O31-C3
6	C	306	PLC	C'-C1'-C2'-C3'
5	C	305	PC1	C38-C39-C3A-C3B
5	C	305	PC1	C21-C22-C23-C24
5	E	306	PC1	C31-C32-C33-C34
6	A	306	PLC	C'-C1'-C2'-C3'
3	B	303	A1L4O	C33-C34-C35-O36
5	D	306	PC1	C3A-C3B-C3C-C3D
5	A	305	PC1	C1-O11-P-O13
5	B	306	PC1	C1-O11-P-O13
6	A	306	PLC	C1-O3P-P-O4P
6	A	311	PLC	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
6	A	311	PLC	C4-O4P-P-O3P
5	C	305	PC1	C2D-C2E-C2F-C2G
5	D	306	PC1	C31-C32-C33-C34
6	B	307	PLC	C'-C1'-C2'-C3'
6	A	306	PLC	O'-C'-O2-C2
5	C	305	PC1	C34-C35-C36-C37
7	B	310	R16	C29-C30-C31-C32
5	B	306	PC1	C22-C21-O21-C2
6	A	306	PLC	C1'-C'-O2-C2
5	A	305	PC1	C3D-C3E-C3F-C3G
6	A	311	PLC	C6B-C7B-C8B-C9B
6	B	307	PLC	C6B-C7B-C8B-C9B
6	D	307	PLC	C3'-C4'-C5'-C6'
7	B	310	R16	C36-C37-C38-C39
7	B	311	R16	C30-C31-C32-C33
7	D	301	R16	C31-C32-C33-C34
10	B	308	C14	C08-C09-C10-C11
10	B	312	C14	C05-C06-C07-C08
5	D	306	PC1	C3B-C3C-C3D-C3E
5	E	306	PC1	C22-C23-C24-C25
5	E	306	PC1	C24-C25-C26-C27
7	B	309	R16	C33-C34-C35-C36
8	C	310	8K6	C4-C5-C6-C7
9	D	310	D12	C5-C6-C7-C8
5	E	306	PC1	C3-C2-O21-C21
5	A	305	PC1	C3B-C3C-C3D-C3E
5	E	306	PC1	C3E-C3F-C3G-C3H
7	A	308	R16	C37-C38-C39-C40
7	D	308	R16	C37-C38-C39-C40
7	E	309	R16	C30-C31-C32-C33
8	A	309	8K6	C10-C11-C12-C13
8	B	301	8K6	C7-C8-C9-C10
5	A	305	PC1	C2B-C2C-C2D-C2E
5	A	305	PC1	C33-C34-C35-C36
5	D	306	PC1	C25-C26-C27-C28
6	B	307	PLC	C1'-C2'-C3'-C4'
6	C	306	PLC	C4'-C5'-C6'-C7'
9	A	310	D12	C11-C10-C9-C8
9	D	310	D12	C4-C5-C6-C7
7	B	310	R16	C31-C32-C33-C34
9	A	310	D12	C7-C8-C9-C10
5	D	306	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
5	D	306	PC1	C36-C37-C38-C39
6	A	306	PLC	C6B-C7B-C8B-C9B
7	B	311	R16	C33-C34-C35-C36
7	D	301	R16	C32-C33-C34-C35
7	D	301	R16	C34-C35-C36-C37
9	E	307	D12	C4-C5-C6-C7
10	B	308	C14	C02-C03-C04-C05
5	A	305	PC1	C3C-C3D-C3E-C3F
5	B	306	PC1	C2E-C2F-C2G-C2H
7	B	311	R16	C35-C36-C37-C38
7	B	311	R16	C36-C37-C38-C39
7	B	311	R16	C37-C38-C39-C40
7	B	311	R16	C38-C39-C40-C41
5	B	306	PC1	C31-C32-C33-C34
5	A	305	PC1	C32-C33-C34-C35
5	E	306	PC1	C2E-C2F-C2G-C2H
6	D	307	PLC	C7B-C8B-C9B-CAA
7	A	308	R16	C33-C34-C35-C36
7	B	309	R16	C34-C35-C36-C37
7	D	309	R16	C28-C29-C30-C31
5	B	306	PC1	C23-C24-C25-C26
5	E	306	PC1	C3A-C3B-C3C-C3D
7	B	309	R16	C36-C37-C38-C39
7	B	309	R16	C38-C39-C40-C41
7	D	301	R16	C36-C37-C38-C39
3	A	302	A1L4O	C30-C31-C33-C34
6	A	311	PLC	C'-C1'-C2'-C3'
5	A	305	PC1	C23-C24-C25-C26
5	B	306	PC1	C29-C2A-C2B-C2C
5	C	305	PC1	C36-C37-C38-C39
5	D	306	PC1	C2A-C2B-C2C-C2D
5	E	306	PC1	C3B-C3C-C3D-C3E
7	A	307	R16	C36-C37-C38-C39
7	E	301	R16	C33-C34-C35-C36
7	E	309	R16	C32-C33-C34-C35
10	B	312	C14	C04-C05-C06-C07
10	E	308	C14	C10-C11-C12-C13
5	C	305	PC1	O11-C1-C2-C3
5	B	306	PC1	C2D-C2E-C2F-C2G
6	C	306	PLC	C5'-C6'-C7'-C8'
6	C	306	PLC	C7B-C8B-C9B-CAA
7	A	308	R16	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
7	A	312	R16	C33-C34-C35-C36
7	A	312	R16	C38-C39-C40-C41
7	D	309	R16	C33-C34-C35-C36
8	B	301	8K6	C11-C12-C13-C14
10	E	308	C14	C08-C09-C10-C11
5	A	305	PC1	C2A-C2B-C2C-C2D
6	A	306	PLC	C5B-C6B-C7B-C8B
6	A	311	PLC	C3B-C4B-C5B-C6B
6	D	307	PLC	C2'-C3'-C4'-C5'
10	E	308	C14	C04-C05-C06-C07
10	C	307	C14	C05-C06-C07-C08
5	B	306	PC1	C39-C3A-C3B-C3C
10	C	307	C14	C08-C09-C10-C11
6	A	306	PLC	C3B-C4B-C5B-C6B
7	A	312	R16	C35-C36-C37-C38
7	A	308	R16	C34-C35-C36-C37
7	A	308	R16	C36-C37-C38-C39
7	D	309	R16	C34-C35-C36-C37
7	D	308	R16	C38-C39-C40-C41
10	C	307	C14	C10-C11-C12-C13
5	B	306	PC1	C3B-C3C-C3D-C3E
6	B	307	PLC	C1B-C2B-C3B-C4B
7	B	310	R16	C34-C35-C36-C37
5	C	305	PC1	C2C-C2D-C2E-C2F
6	A	306	PLC	C4'-C5'-C6'-C7'
7	B	311	R16	C29-C30-C31-C32
8	A	309	8K6	C15-C16-C17-C18
5	D	306	PC1	C34-C35-C36-C37
10	C	308	C14	C09-C10-C11-C12
10	C	307	C14	C02-C03-C04-C05
6	A	311	PLC	C4B-C5B-C6B-C7B
10	B	312	C14	C02-C03-C04-C05
6	A	306	PLC	CB-C1B-C2B-C3B
5	D	306	PC1	C26-C27-C28-C29
5	A	305	PC1	C39-C3A-C3B-C3C
5	A	305	PC1	C3F-C3G-C3H-C3I
5	C	305	PC1	C2A-C2B-C2C-C2D
5	E	306	PC1	C37-C38-C39-C3A
5	E	306	PC1	C38-C39-C3A-C3B
7	B	310	R16	C28-C29-C30-C31
3	A	302	A1L4O	C04-C07-C08-C09
3	B	303	A1L4O	C04-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
3	E	303	A1L4O	C04-C07-C08-C09
3	E	303	A1L4O	C41-C07-C08-C09
6	A	306	PLC	C2'-C3'-C4'-C5'
7	A	312	R16	C37-C38-C39-C40
5	C	305	PC1	C26-C27-C28-C29
8	C	310	8K6	C5-C6-C7-C8
9	A	310	D12	C5-C6-C7-C8
5	C	305	PC1	C37-C38-C39-C3A
7	B	309	R16	C28-C29-C30-C31
7	A	308	R16	C35-C36-C37-C38
9	D	310	D12	C1-C2-C3-C4
7	B	311	R16	C28-C29-C30-C31
9	A	310	D12	C1-C2-C3-C4
5	C	305	PC1	C2E-C2F-C2G-C2H
5	E	306	PC1	C2C-C2D-C2E-C2F
9	D	310	D12	C6-C7-C8-C9
5	E	306	PC1	C2B-C2C-C2D-C2E
6	A	306	PLC	C5'-C6'-C7'-C8'
7	B	310	R16	C38-C39-C40-C41
6	D	307	PLC	C6B-C7B-C8B-C9B
6	A	311	PLC	C1'-C'-O2-C2
6	D	307	PLC	C1'-C'-O2-C2
5	D	306	PC1	C3D-C3E-C3F-C3G
10	E	310	C14	C03-C04-C05-C06
5	D	306	PC1	O22-C21-O21-C2
6	A	311	PLC	O'-C'-O2-C2
6	D	307	PLC	O'-C'-O2-C2
5	B	306	PC1	C35-C36-C37-C38
6	A	306	PLC	O2-C2-C3-O3
6	A	311	PLC	O2-C2-C3-O3
5	B	306	PC1	C22-C23-C24-C25
6	D	307	PLC	C3B-C4B-C5B-C6B
5	B	306	PC1	C2B-C2C-C2D-C2E
6	A	306	PLC	C7'-C8'-C9'-CA'
6	B	307	PLC	C5'-C6'-C7'-C8'
6	B	307	PLC	C4B-C5B-C6B-C7B
7	A	307	R16	C30-C31-C32-C33
10	C	307	C14	C04-C05-C06-C07
10	C	307	C14	C07-C08-C09-C10
10	E	308	C14	C02-C03-C04-C05
3	E	303	A1L4O	C32-C31-C33-C34
5	D	306	PC1	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
7	E	309	R16	C36-C37-C38-C39
5	D	306	PC1	C2B-C2C-C2D-C2E
5	B	306	PC1	C11-O13-P-O11
5	D	306	PC1	C11-O13-P-O11
5	D	306	PC1	C1-O11-P-O13
6	B	307	PLC	C1-O3P-P-O4P
6	C	306	PLC	C4-O4P-P-O3P
5	A	305	PC1	C31-C32-C33-C34
5	C	305	PC1	C3B-C3C-C3D-C3E
6	D	307	PLC	C1B-C2B-C3B-C4B
5	D	306	PC1	O11-C1-C2-C3
6	C	306	PLC	O3P-C1-C2-C3
5	C	305	PC1	C23-C24-C25-C26
5	C	305	PC1	C2F-C2G-C2H-C2I
5	B	306	PC1	C37-C38-C39-C3A
6	A	311	PLC	C2'-C3'-C4'-C5'
6	B	307	PLC	C2'-C3'-C4'-C5'
5	B	306	PC1	O22-C21-O21-C2
5	C	305	PC1	C35-C36-C37-C38
6	C	306	PLC	C3B-C4B-C5B-C6B
10	C	308	C14	C02-C03-C04-C05
5	B	306	PC1	C32-C33-C34-C35
6	A	306	PLC	C1-C2-C3-O3
6	A	311	PLC	C8'-C9'-CA'-CB'
6	C	306	PLC	C3'-C4'-C5'-C6'
6	C	306	PLC	C2B-C3B-C4B-C5B
7	A	308	R16	C27-C28-C29-C30
5	B	306	PC1	C3F-C3G-C3H-C3I
8	A	309	8K6	C7-C8-C9-C10
10	E	308	C14	C03-C04-C05-C06
5	A	305	PC1	C2F-C2G-C2H-C2I
5	B	306	PC1	C26-C27-C28-C29
6	B	307	PLC	C3'-C4'-C5'-C6'
6	D	307	PLC	C7'-C8'-C9'-CA'
8	C	310	8K6	C10-C11-C12-C13
10	E	310	C14	C10-C11-C12-C13
10	B	308	C14	C03-C04-C05-C06
7	A	307	R16	C37-C38-C39-C40
7	D	308	R16	C39-C40-C41-C42
6	C	306	PLC	C8'-C9'-CA'-CB'
7	D	309	R16	C39-C40-C41-C42
5	D	306	PC1	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
10	C	307	C14	C01-C02-C03-C04
7	E	309	R16	C35-C36-C37-C38
8	C	310	8K6	C15-C16-C17-C18
9	A	310	D12	C9-C10-C11-C12
6	D	307	PLC	C8B-C9B-CAA-CBA
8	C	310	8K6	C13-C14-C15-C16
7	E	301	R16	C30-C31-C32-C33
10	C	307	C14	C11-C12-C13-C14
10	C	308	C14	C11-C12-C13-C14
10	E	308	C14	C01-C02-C03-C04
5	B	306	PC1	O11-C1-C2-O21
7	B	309	R16	C30-C31-C32-C33
7	E	309	R16	C31-C32-C33-C34
10	B	308	C14	C04-C05-C06-C07
10	B	312	C14	C08-C09-C10-C11
7	E	301	R16	C38-C39-C40-C41
5	B	306	PC1	O21-C2-C3-O31
6	C	306	PLC	C4B-C5B-C6B-C7B
3	B	303	A1L4O	O36-C35-C37-C40
7	E	301	R16	C39-C40-C41-C42
5	D	306	PC1	C2E-C2F-C2G-C2H
10	C	307	C14	C03-C04-C05-C06
6	B	307	PLC	C2B-C3B-C4B-C5B
2	C	301	RET	C12-C13-C14-C15
7	D	308	R16	C27-C28-C29-C30
5	A	305	PC1	C34-C35-C36-C37
5	A	305	PC1	C38-C39-C3A-C3B
6	A	311	PLC	C8B-C9B-CAA-CBA
7	A	312	R16	C30-C31-C32-C33
6	C	306	PLC	C7'-C8'-C9'-CA'
7	D	301	R16	C29-C30-C31-C32
5	D	306	PC1	C28-C29-C2A-C2B
7	D	308	R16	C31-C32-C33-C34
10	B	312	C14	C06-C07-C08-C09
5	B	306	PC1	C3A-C3B-C3C-C3D
5	D	306	PC1	C3F-C3G-C3H-C3I
5	A	305	PC1	C1-C2-C3-O31
5	C	305	PC1	C1-C2-C3-O31
6	A	311	PLC	C1-C2-C3-O3
5	C	305	PC1	O31-C31-C32-C33
8	A	309	8K6	C6-C7-C8-C9
9	A	310	D12	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	E	306	PC1	C23-C24-C25-C26
6	A	306	PLC	O3P-C1-C2-O2
5	E	306	PC1	C33-C34-C35-C36
7	B	311	R16	C39-C40-C41-C42
5	C	305	PC1	O21-C2-C3-O31
6	A	306	PLC	C2-C1-O3P-P
9	D	310	D12	C11-C10-C9-C8
6	A	311	PLC	C5'-C6'-C7'-C8'
5	A	305	PC1	C21-C22-C23-C24
5	E	306	PC1	C32-C33-C34-C35
7	A	312	R16	C39-C40-C41-C42
5	E	306	PC1	O32-C31-O31-C3
7	A	308	R16	C39-C40-C41-C42
5	B	306	PC1	O11-C1-C2-C3
6	A	306	PLC	O3P-C1-C2-C3
6	D	307	PLC	O3P-C1-C2-C3
7	A	308	R16	C29-C30-C31-C32
7	B	309	R16	C32-C33-C34-C35
10	E	310	C14	C06-C07-C08-C09
7	B	311	R16	C31-C32-C33-C34
6	B	307	PLC	C5B-C6B-C7B-C8B
8	B	301	8K6	C2-C3-C4-C5
7	E	301	R16	C27-C28-C29-C30
8	C	310	8K6	C11-C10-C9-C8
7	E	309	R16	C38-C39-C40-C41
5	B	306	PC1	C1-C2-C3-O31
5	C	305	PC1	O11-C1-C2-O21
6	C	306	PLC	O3P-C1-C2-O2
5	E	306	PC1	C2D-C2E-C2F-C2G
6	B	307	PLC	C3B-C4B-C5B-C6B
5	A	305	PC1	O21-C2-C3-O31
8	C	310	8K6	C14-C15-C16-C17
5	E	306	PC1	C2A-C2B-C2C-C2D
6	A	306	PLC	C1B-C2B-C3B-C4B
8	B	301	8K6	C13-C14-C15-C16
5	E	306	PC1	C21-C22-C23-C24
5	A	305	PC1	C25-C26-C27-C28
8	A	309	8K6	C11-C10-C9-C8
8	B	301	8K6	C9-C10-C11-C12
7	D	309	R16	C29-C30-C31-C32
3	A	302	A1L4O	C32-C31-C33-C34
3	E	303	A1L4O	C30-C31-C33-C34

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Mol	Chain	Res	Type	Atoms
5	A	305	PC1	C29-C2A-C2B-C2C
5	C	305	PC1	C32-C33-C34-C35
6	D	307	PLC	C4-O4P-P-O3P
6	A	306	PLC	C8B-C9B-CAA-CBA
5	C	305	PC1	C39-C3A-C3B-C3C
5	A	305	PC1	C1-O11-P-O12
5	D	306	PC1	C1-O11-P-O14
6	B	307	PLC	C1-O3P-P-O1P
6	A	306	PLC	C8'-C9'-CA'-CB'
7	B	311	R16	C32-C33-C34-C35
8	B	301	8K6	C3-C4-C5-C6
5	D	306	PC1	C35-C36-C37-C38
11	C	309	D10	C3-C4-C5-C6
10	B	308	C14	C09-C10-C11-C12
5	A	305	PC1	C12-C11-O13-P
5	B	306	PC1	C12-C11-O13-P
5	D	306	PC1	C12-C11-O13-P
6	B	307	PLC	C5-C4-O4P-P
6	D	307	PLC	C5-C4-O4P-P
7	D	309	R16	C31-C32-C33-C34
8	B	301	8K6	C1-C2-C3-C4
7	A	307	R16	C38-C39-C40-C41
6	D	307	PLC	O3P-C1-C2-O2
7	E	301	R16	C34-C35-C36-C37
6	B	307	PLC	O4P-C4-C5-N
6	D	307	PLC	O4P-C4-C5-N
5	C	305	PC1	C25-C26-C27-C28
9	E	307	D12	C7-C8-C9-C10
6	B	307	PLC	C7B-C8B-C9B-CAA
7	D	301	R16	C33-C34-C35-C36
6	B	307	PLC	OB-CB-O3-C3
10	C	307	C14	C09-C10-C11-C12
5	E	306	PC1	C26-C27-C28-C29
5	D	306	PC1	C23-C24-C25-C26
10	C	308	C14	C05-C06-C07-C08
6	B	307	PLC	C1B-CB-O3-C3
10	C	307	C14	C06-C07-C08-C09
5	E	306	PC1	C28-C29-C2A-C2B
6	D	307	PLC	C5B-C6B-C7B-C8B
5	C	305	PC1	C3C-C3D-C3E-C3F
10	E	308	C14	C05-C06-C07-C08
7	A	307	R16	C32-C33-C34-C35

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
6	B	307	PLC	CB-C1B-C2B-C3B
5	D	306	PC1	C38-C39-C3A-C3B
6	A	306	PLC	C2B-C3B-C4B-C5B
11	C	309	D10	C7-C8-C9-C10
5	C	305	PC1	C22-C23-C24-C25
5	E	306	PC1	C29-C2A-C2B-C2C
7	A	312	R16	C34-C35-C36-C37
6	A	306	PLC	C7B-C8B-C9B-CAA
7	A	307	R16	C29-C30-C31-C32
7	D	308	R16	C28-C29-C30-C31
8	C	310	8K6	C9-C10-C11-C12
6	A	311	PLC	C2B-C1B-CB-O3
6	A	311	PLC	C1-C2-O2-C'
6	D	307	PLC	C1-C2-O2-C'
6	B	307	PLC	C2B-C1B-CB-O3
10	B	308	C14	C07-C08-C09-C10
7	D	301	R16	C35-C36-C37-C38
5	E	306	PC1	C3F-C3G-C3H-C3I
5	A	305	PC1	C35-C36-C37-C38
9	E	307	D12	C11-C10-C9-C8
5	A	305	PC1	C28-C29-C2A-C2B
7	E	309	R16	C27-C28-C29-C30
7	A	308	R16	C32-C33-C34-C35
7	B	309	R16	C39-C40-C41-C42
7	D	301	R16	C39-C40-C41-C42
3	A	302	A1L4O	C13-C14-C15-C17
9	E	307	D12	C9-C10-C11-C12
10	C	308	C14	C01-C02-C03-C04
5	B	306	PC1	C2C-C2D-C2E-C2F
10	B	312	C14	C09-C10-C11-C12
8	B	301	8K6	C6-C7-C8-C9
6	B	307	PLC	C2-C1-O3P-P
7	B	310	R16	C33-C34-C35-C36
5	D	306	PC1	O31-C31-C32-C33
5	A	305	PC1	C3E-C3F-C3G-C3H
6	A	306	PLC	C2B-C1B-CB-O3
6	A	306	PLC	C3'-C4'-C5'-C6'
6	C	306	PLC	C2B-C1B-CB-O3
11	C	309	D10	C1-C2-C3-C4
10	E	310	C14	C11-C12-C13-C14
6	D	307	PLC	O2-C'-C1'-C2'
6	A	311	PLC	C5B-C6B-C7B-C8B

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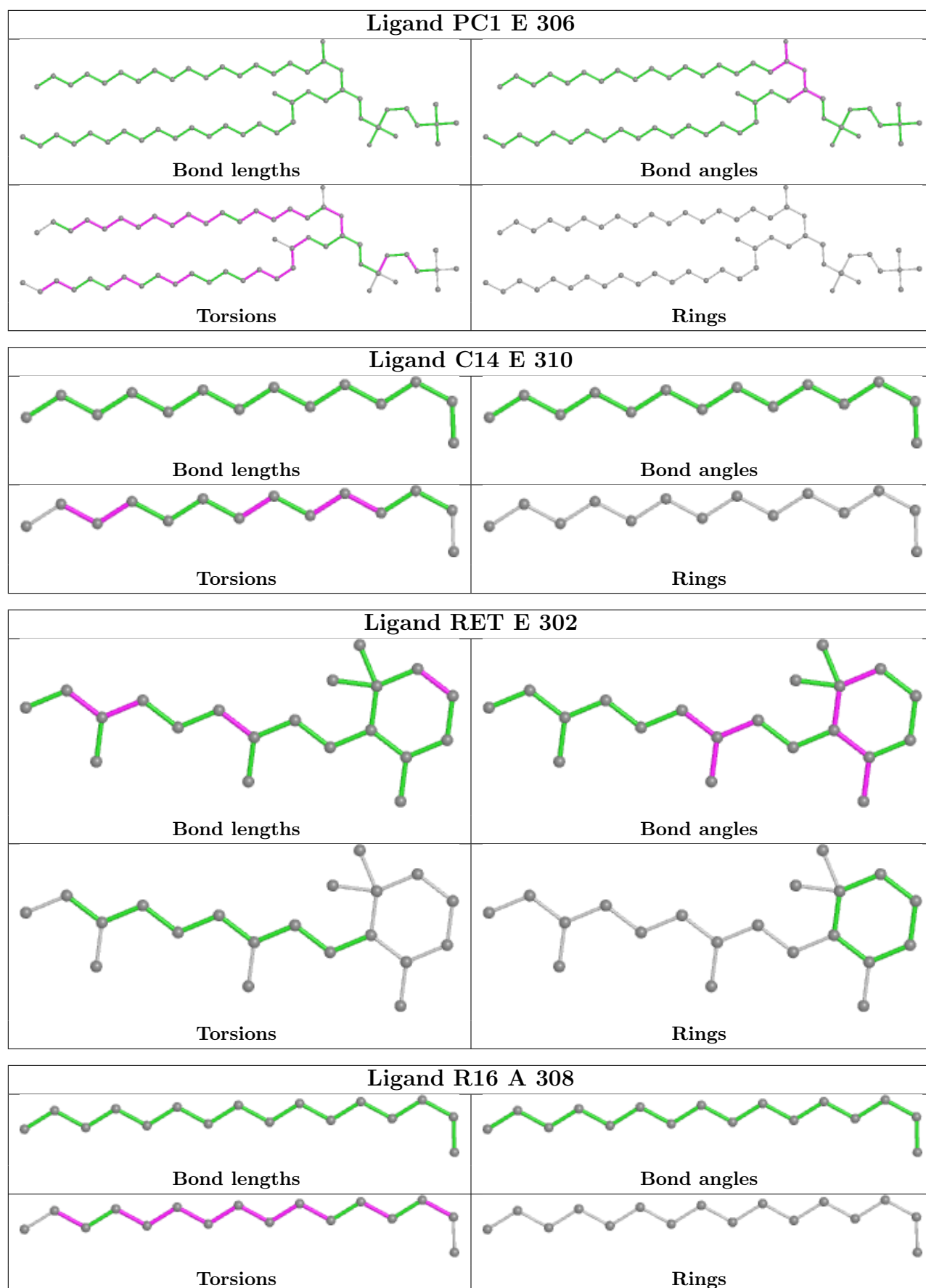
Mol	Chain	Res	Type	Atoms
7	A	312	R16	C27-C28-C29-C30
8	B	301	8K6	C12-C13-C14-C15
7	A	307	R16	C28-C29-C30-C31
10	C	308	C14	C08-C09-C10-C11
5	D	306	PC1	C2C-C2D-C2E-C2F
7	D	308	R16	C30-C31-C32-C33
8	C	310	8K6	C7-C8-C9-C10
7	A	312	R16	C28-C29-C30-C31
6	D	307	PLC	O'-C'-C1'-C2'
6	A	311	PLC	C4'-C5'-C6'-C7'
7	E	309	R16	C37-C38-C39-C40
10	C	308	C14	C04-C05-C06-C07
6	A	311	PLC	OB-CB-O3-C3
7	B	310	R16	C30-C31-C32-C33
7	E	309	R16	C33-C34-C35-C36
5	E	306	PC1	O32-C31-C32-C33
10	E	308	C14	C07-C08-C09-C10
6	C	306	PLC	C2B-C1B-CB-OB
5	A	305	PC1	C11-O13-P-O14
5	B	306	PC1	C11-O13-P-O14
5	C	305	PC1	C1-O11-P-O14
5	D	306	PC1	C11-O13-P-O14
5	E	306	PC1	C11-O13-P-O14
5	C	305	PC1	O32-C31-C32-C33
6	A	306	PLC	C2B-C1B-CB-OB
7	B	310	R16	C35-C36-C37-C38
3	A	302	A1L4O	C41-C07-C08-C09
3	B	303	A1L4O	C41-C07-C08-C09
10	E	310	C14	C04-C05-C06-C07
5	D	306	PC1	O32-C31-C32-C33
5	A	305	PC1	C24-C25-C26-C27
6	A	306	PLC	C5-C4-O4P-P
5	A	305	PC1	C2D-C2E-C2F-C2G
10	C	308	C14	C06-C07-C08-C09
10	B	312	C14	C10-C11-C12-C13
11	C	309	D10	C2-C3-C4-C5
5	A	305	PC1	C2C-C2D-C2E-C2F
6	A	311	PLC	O3P-C1-C2-O2
6	B	307	PLC	C6'-C7'-C8'-C9'
6	A	311	PLC	C1B-CB-O3-C3

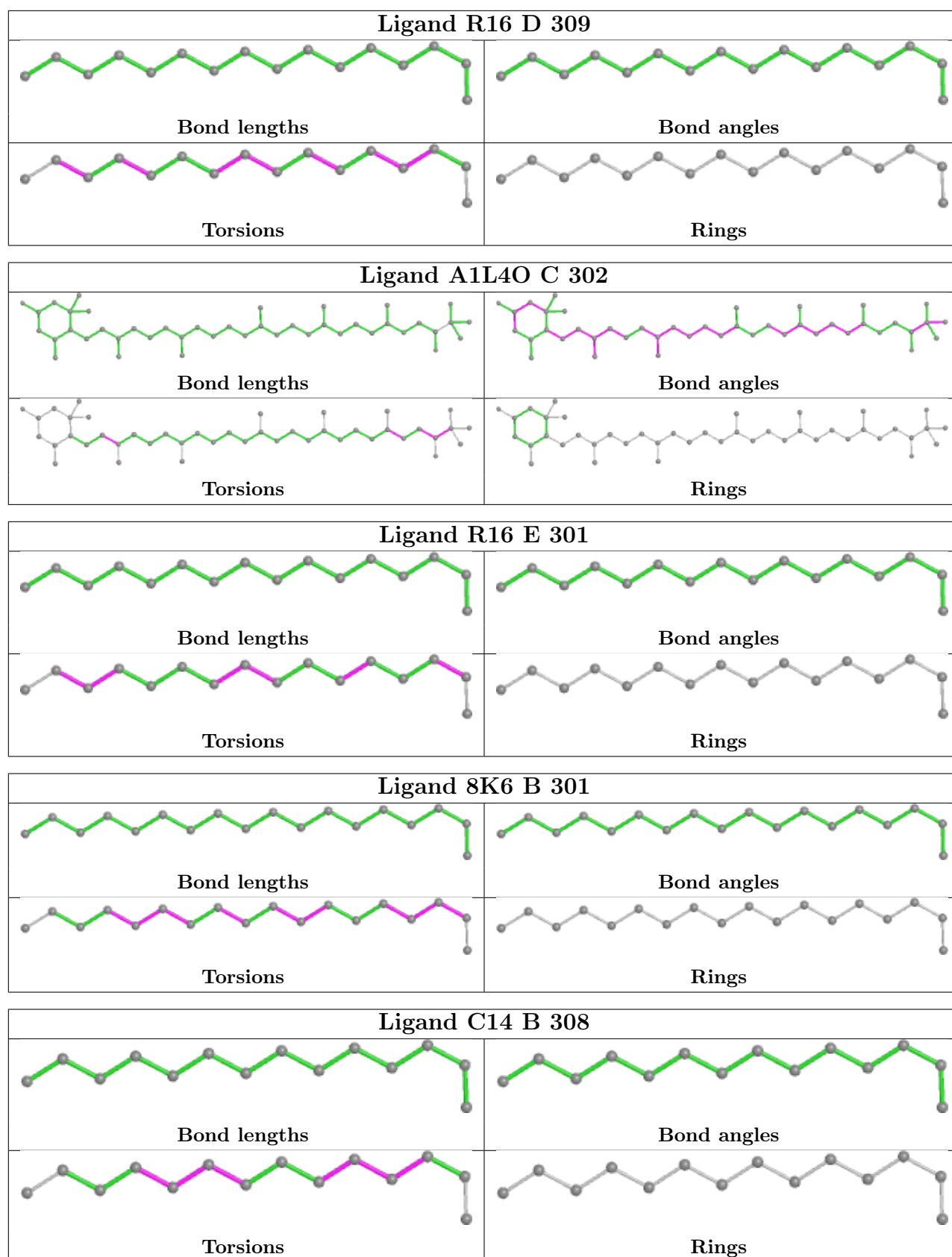
There are no ring outliers.

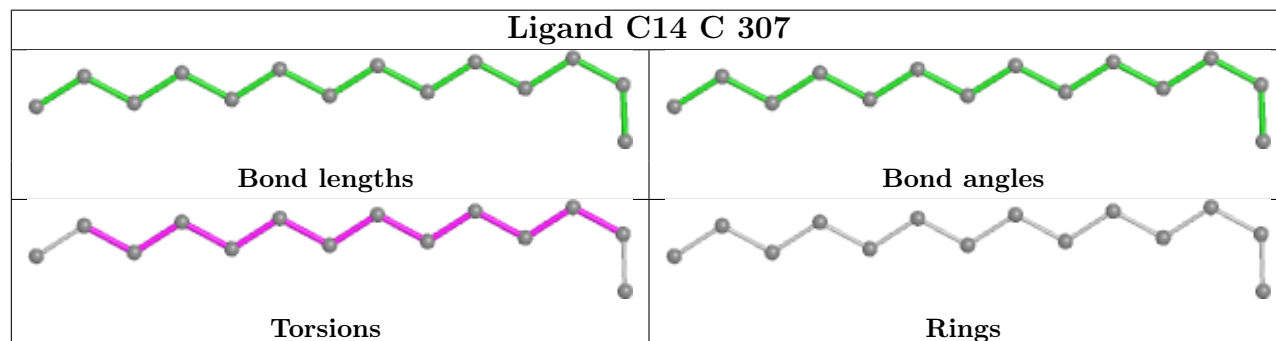
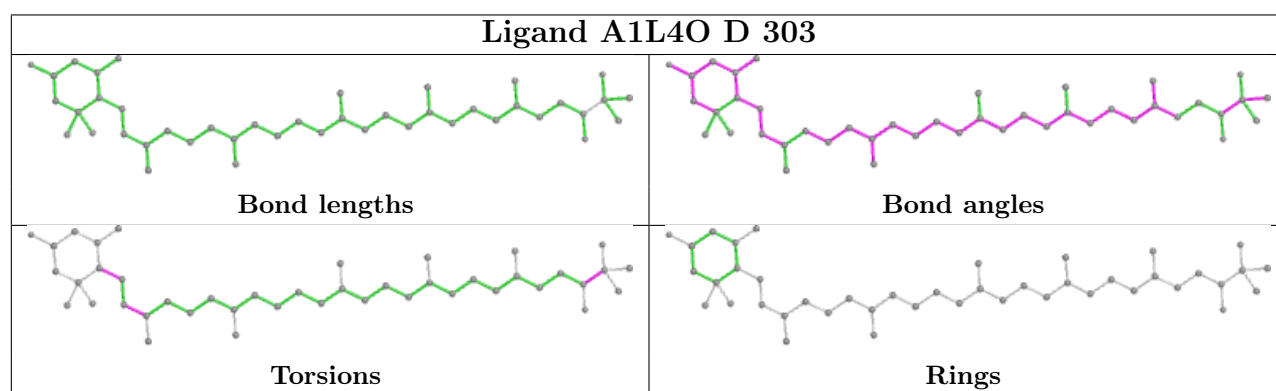
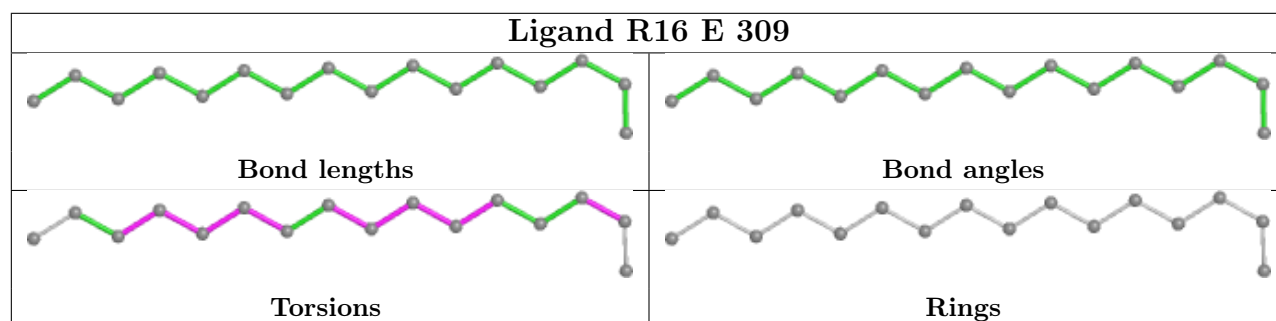
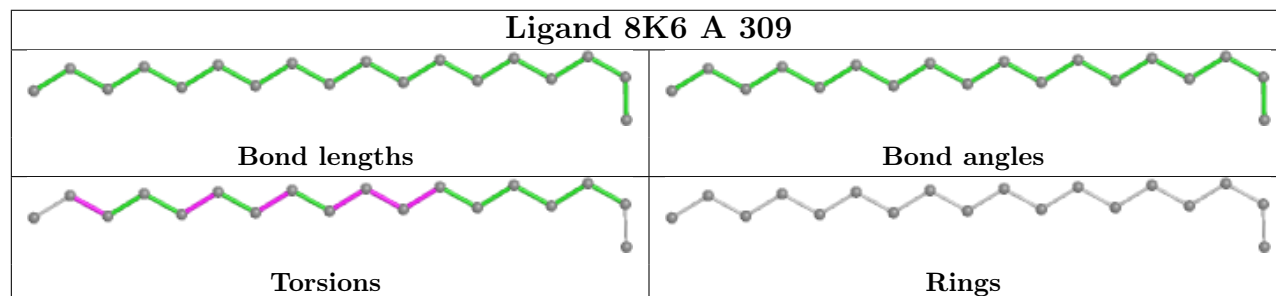
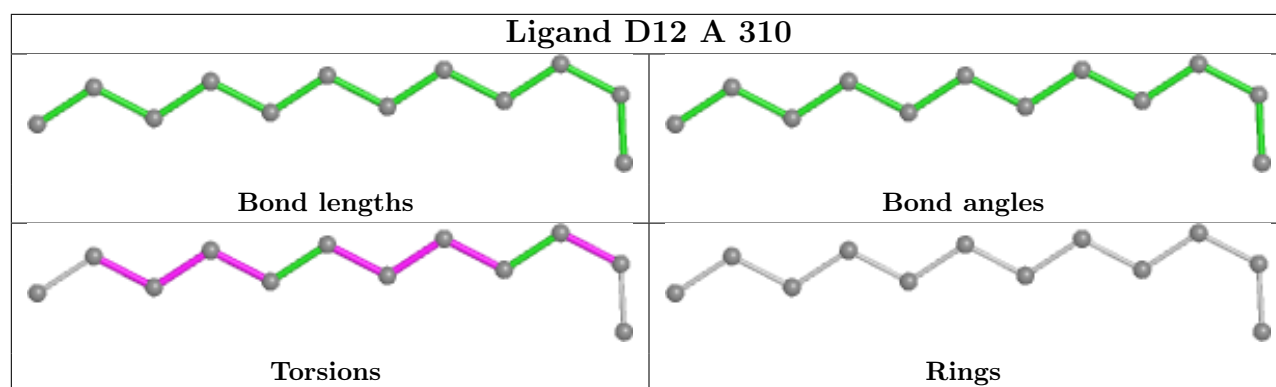
29 monomers are involved in 63 short contacts:

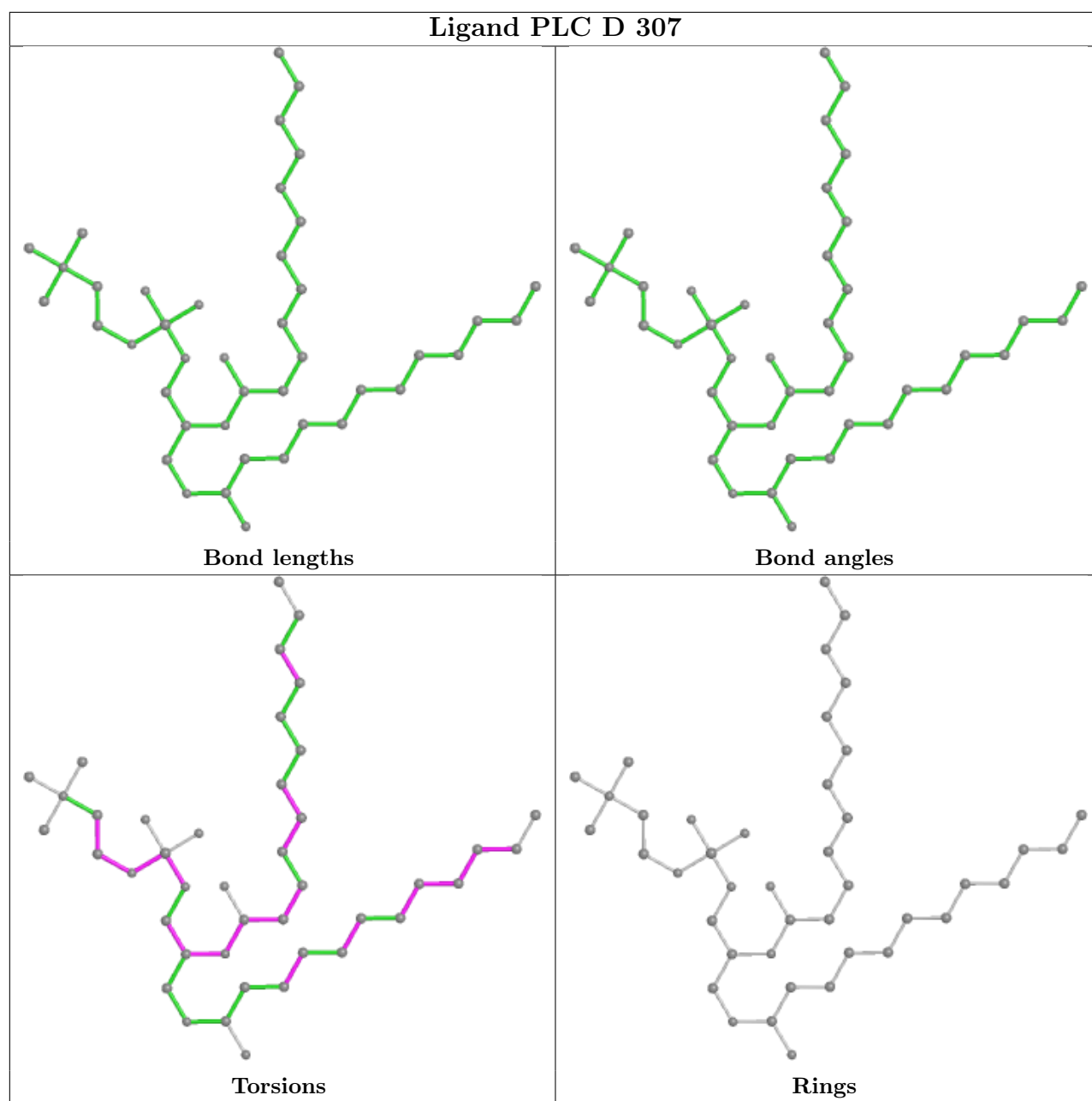
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	306	PC1	10	0
10	E	310	C14	2	0
2	E	302	RET	1	0
7	E	301	R16	1	0
8	B	301	8K6	1	0
9	A	310	D12	1	0
10	C	307	C14	2	0
6	C	306	PLC	1	0
2	D	302	RET	2	0
5	D	306	PC1	3	0
7	B	310	R16	1	0
7	D	301	R16	3	0
7	B	311	R16	2	0
3	A	302	A1L4O	1	0
9	E	307	D12	1	0
8	C	310	8K6	2	0
2	A	301	RET	3	0
2	C	301	RET	2	0
3	E	303	A1L4O	2	0
5	B	306	PC1	3	0
7	A	312	R16	3	0
11	C	309	D10	2	0
5	C	305	PC1	6	0
6	B	307	PLC	2	0
10	C	308	C14	2	0
2	B	302	RET	4	0
7	D	308	R16	2	0
9	D	310	D12	1	0
5	A	305	PC1	5	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.

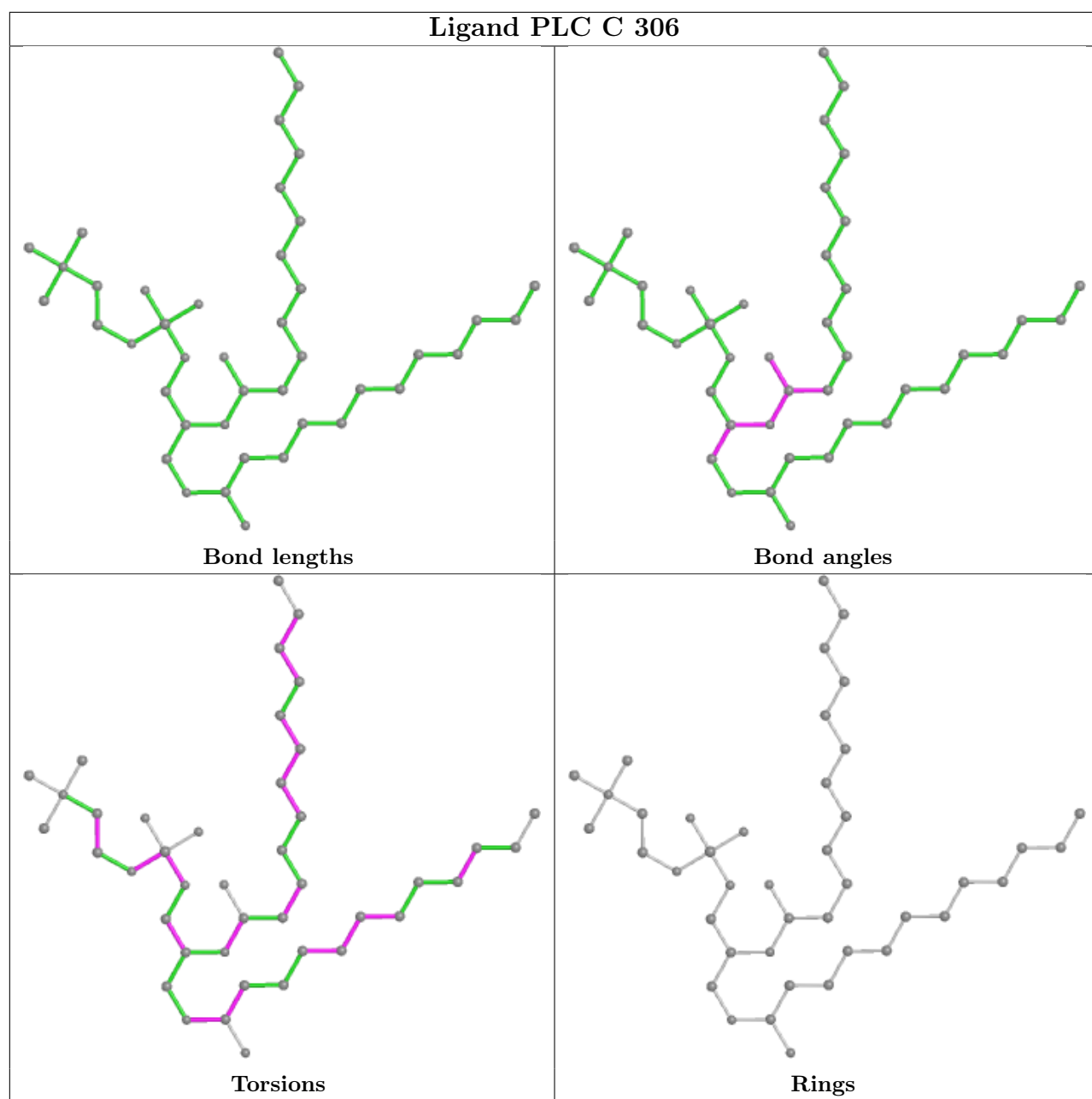


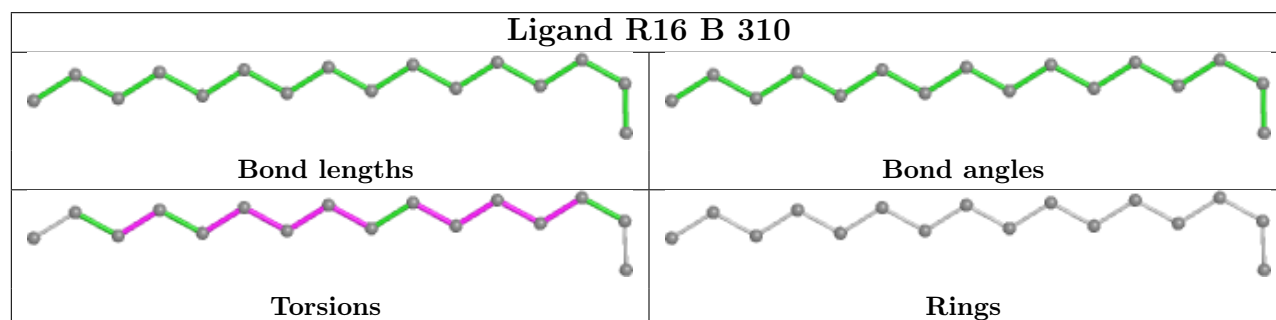
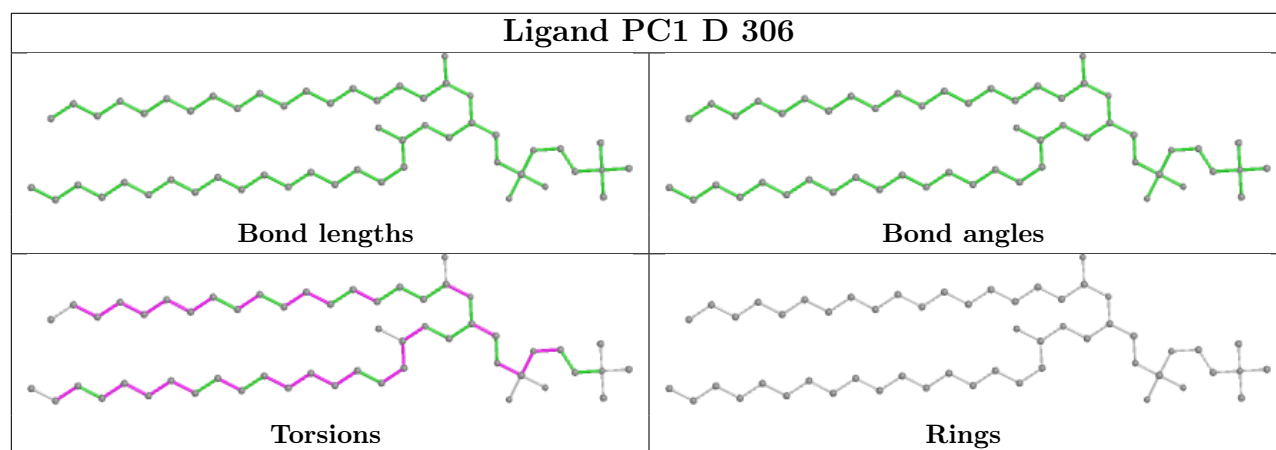
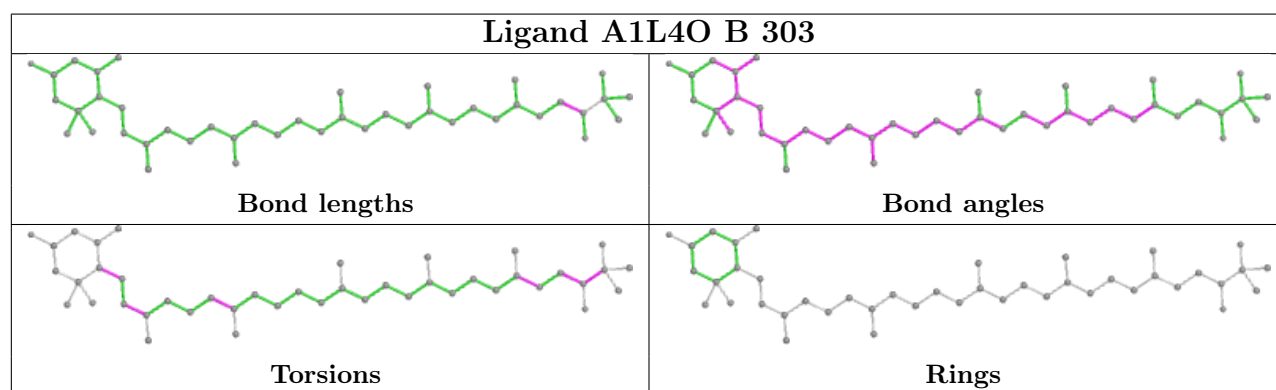
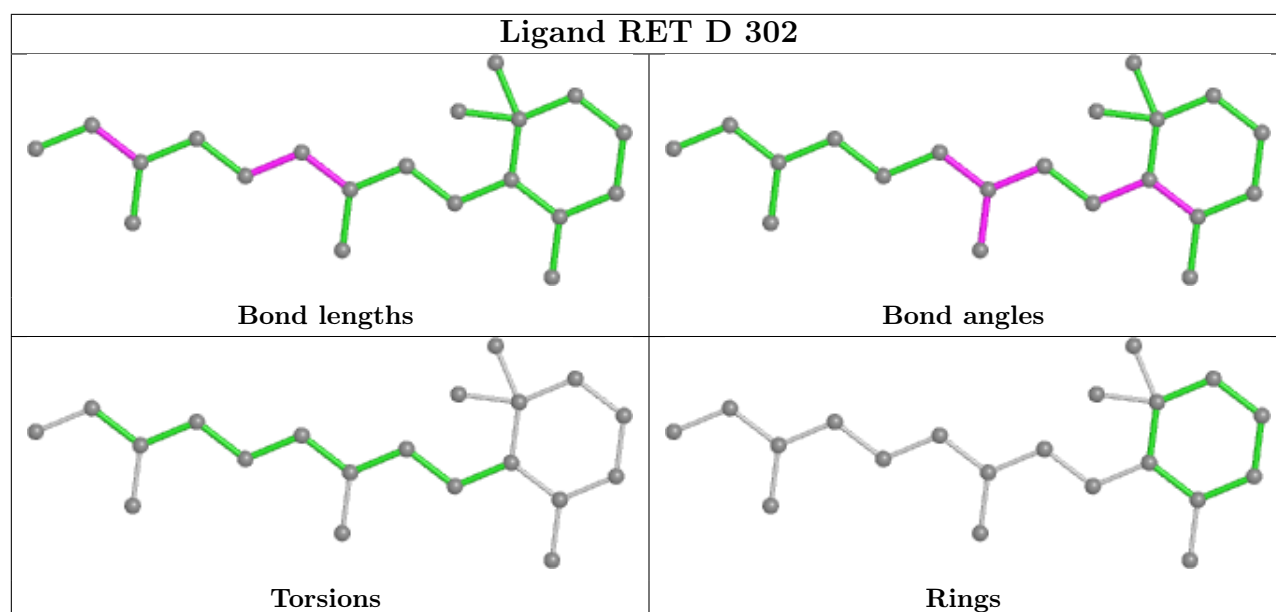


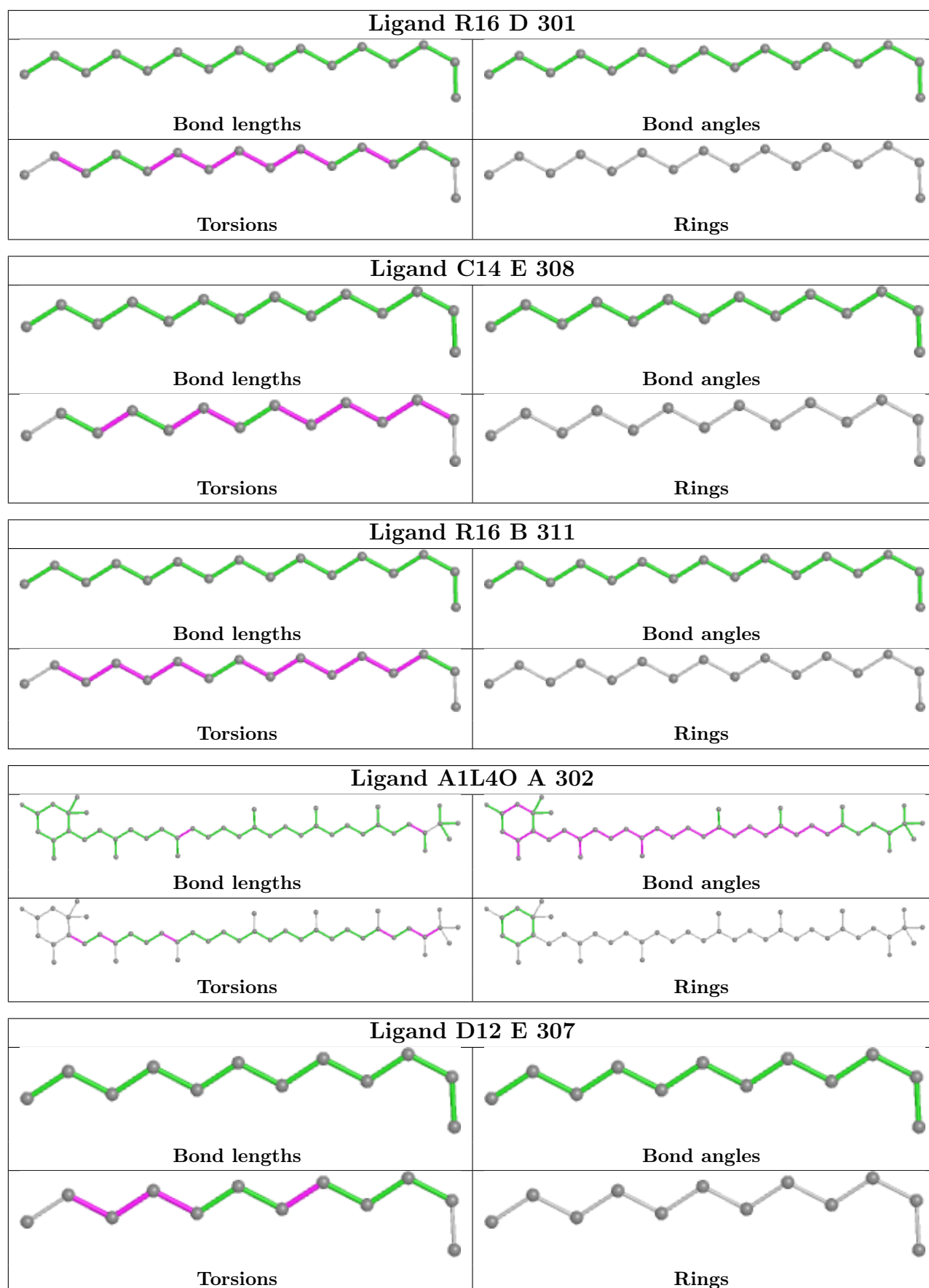


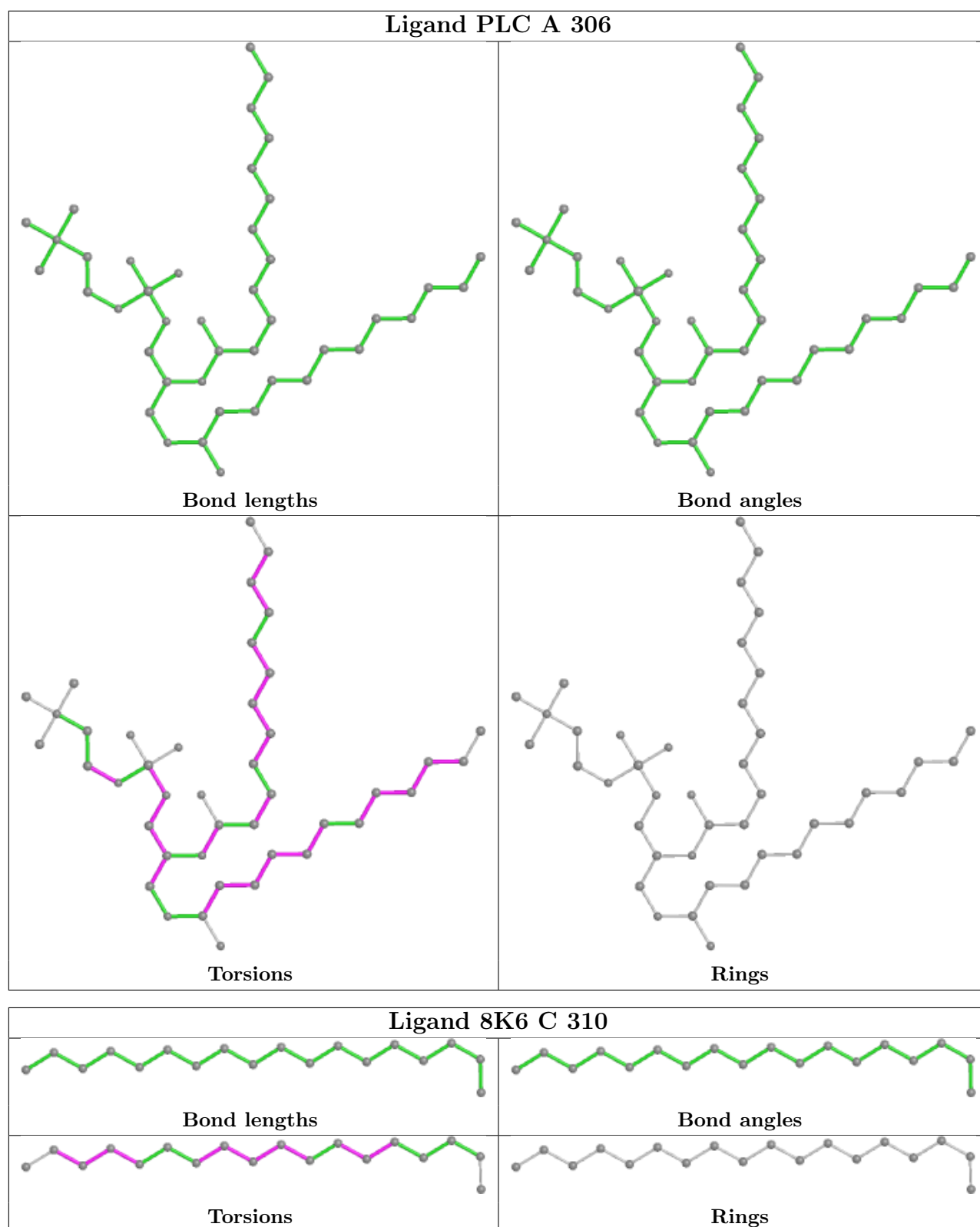


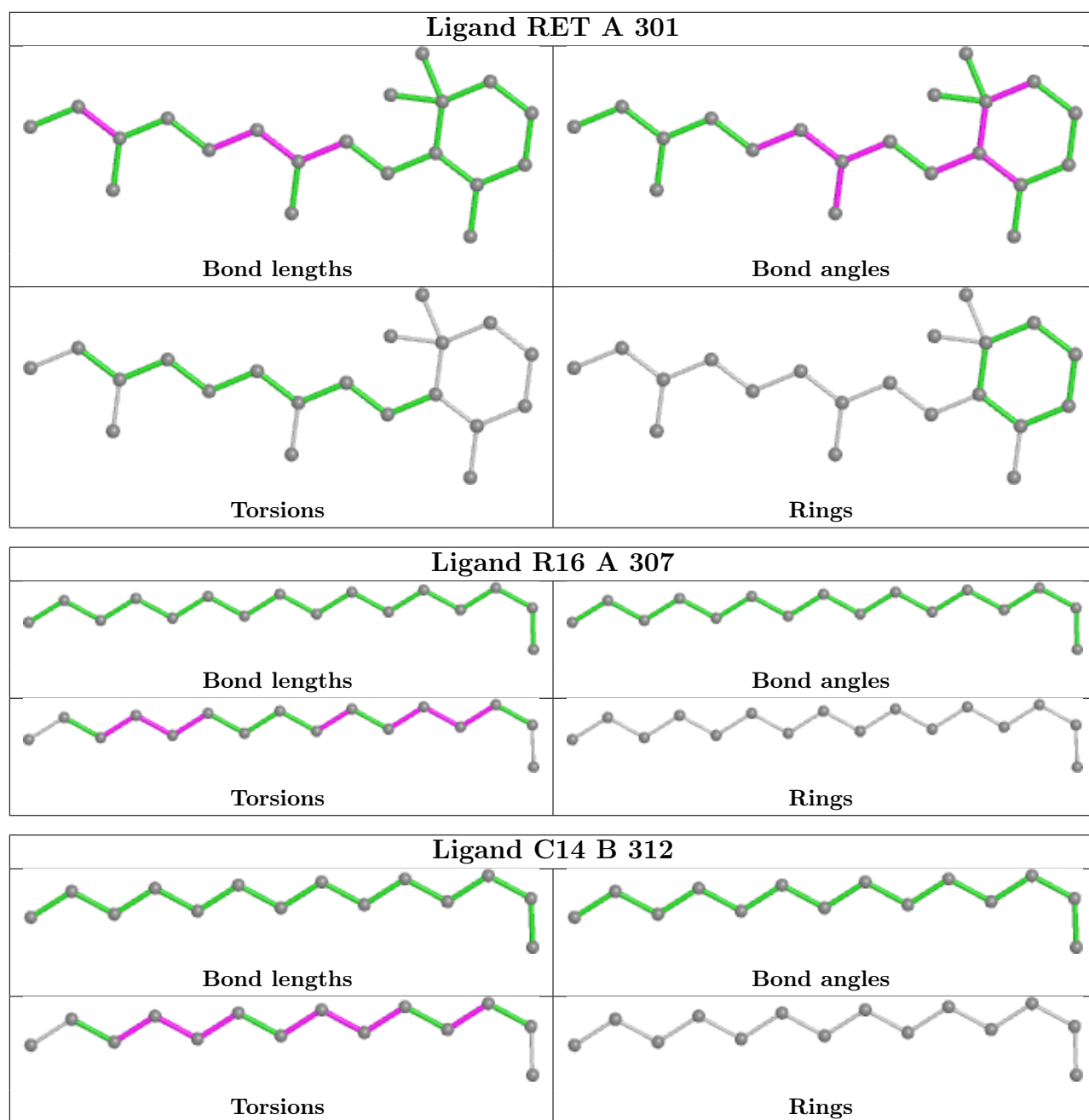


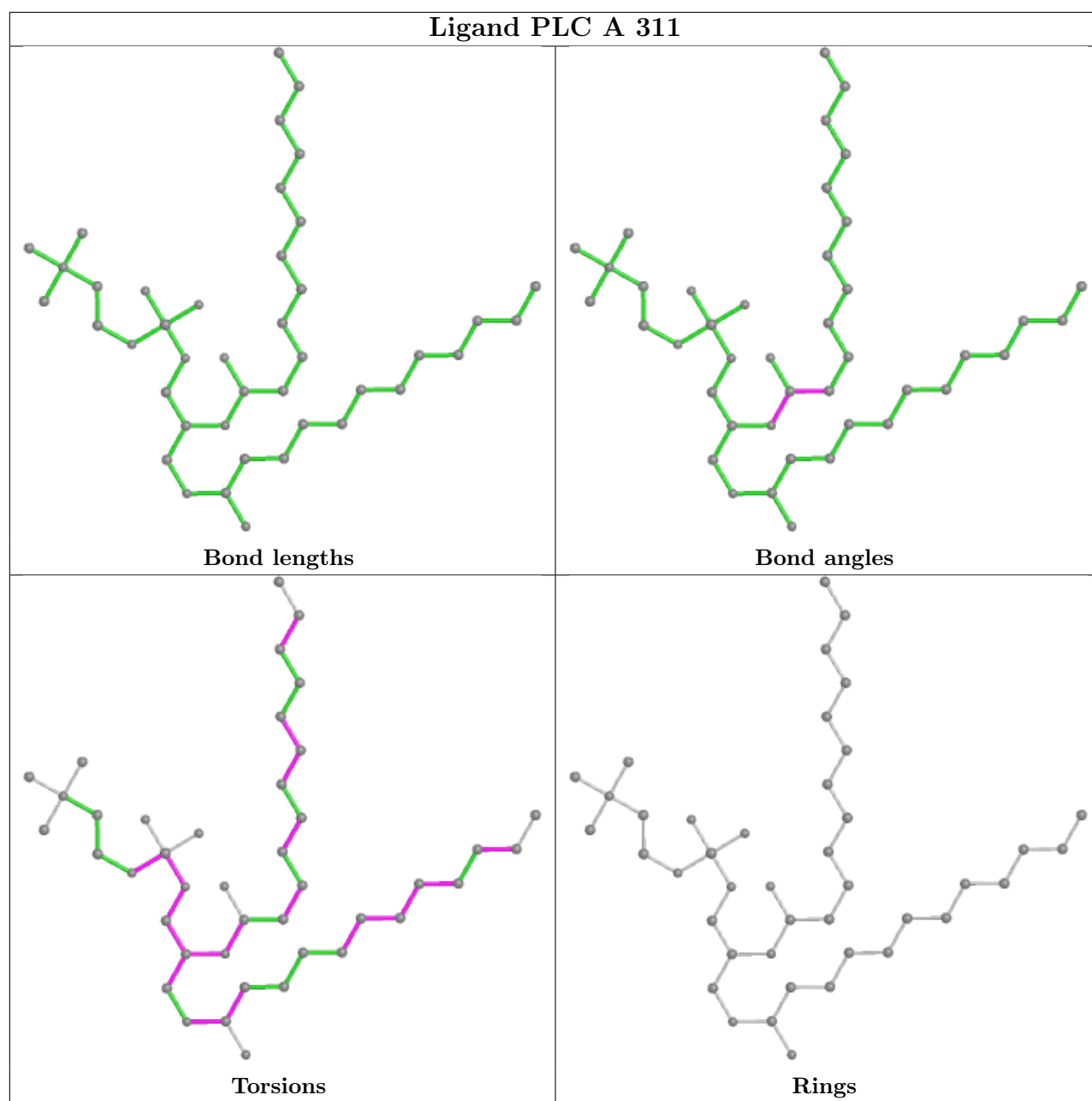


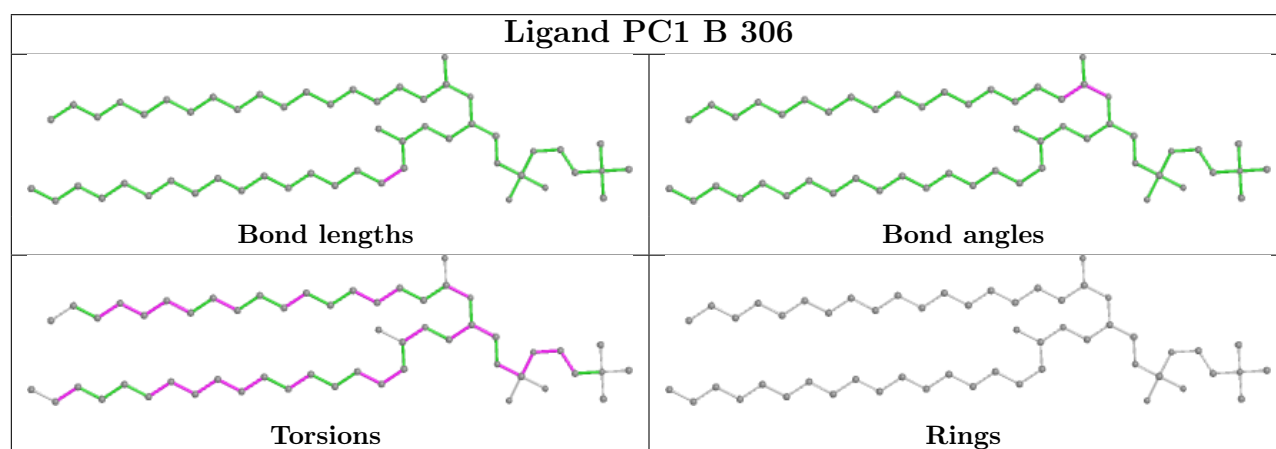
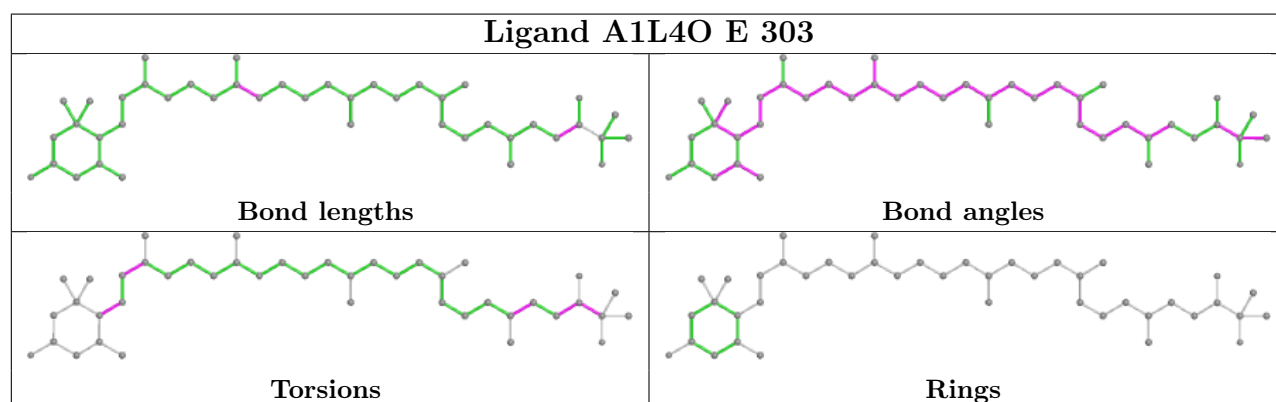
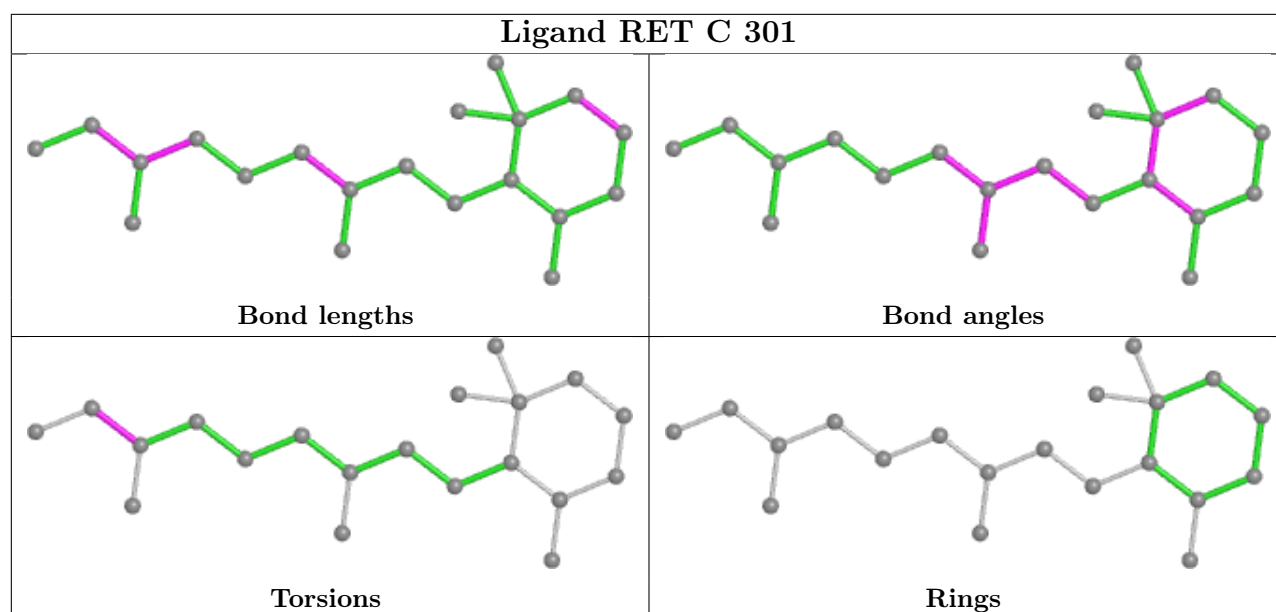


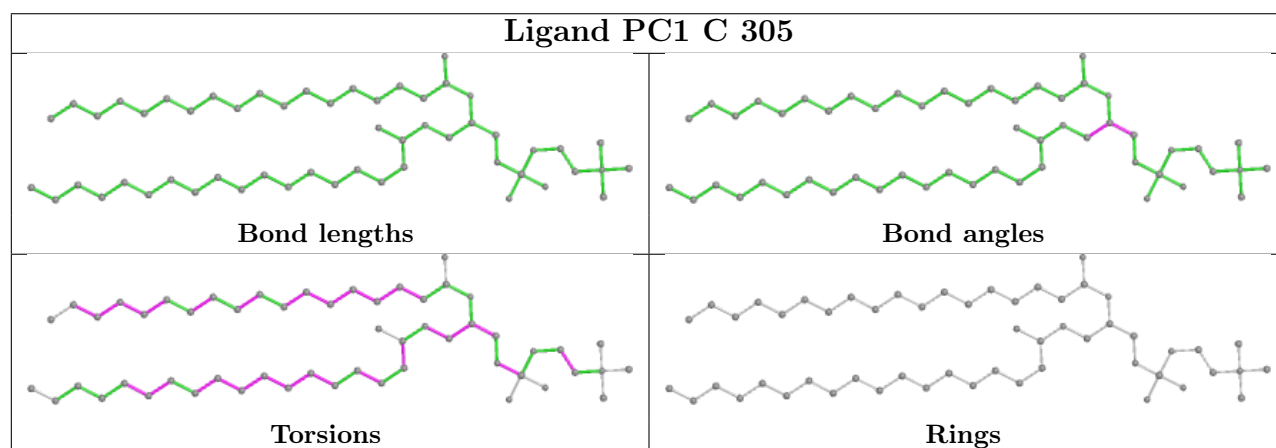
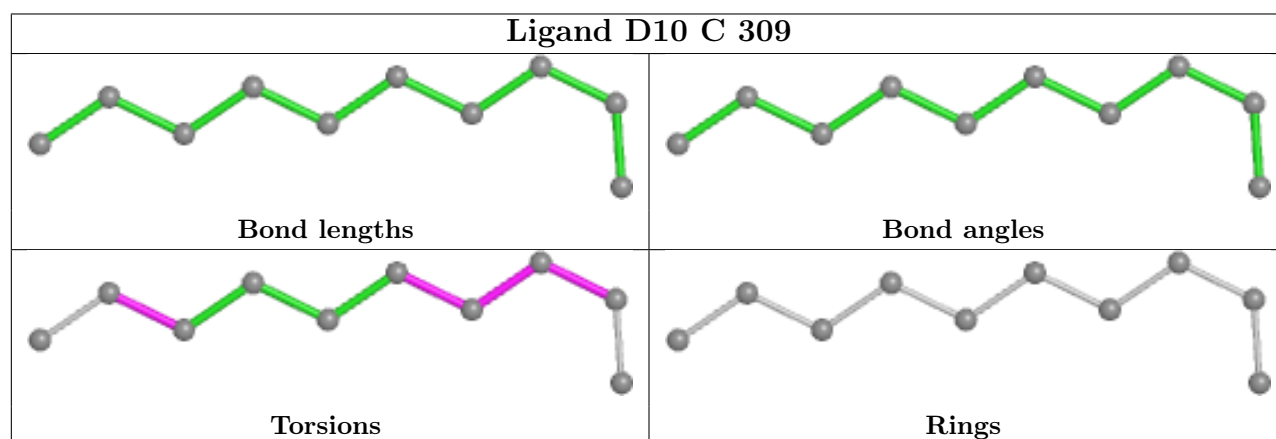
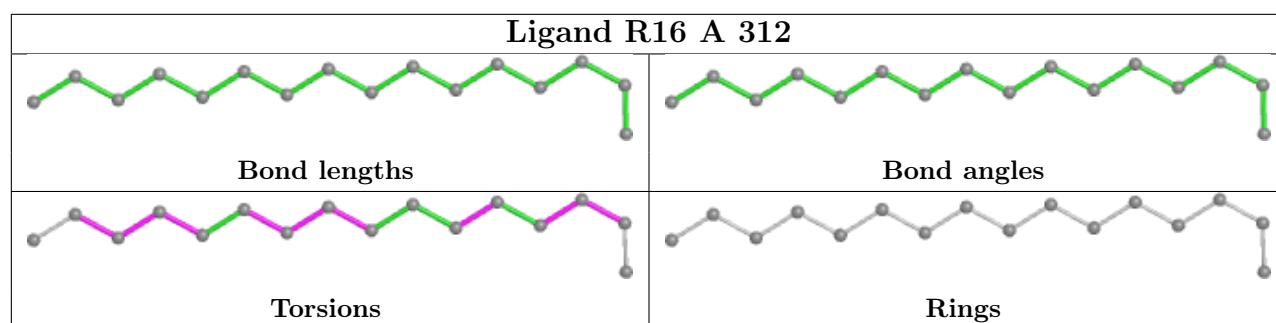




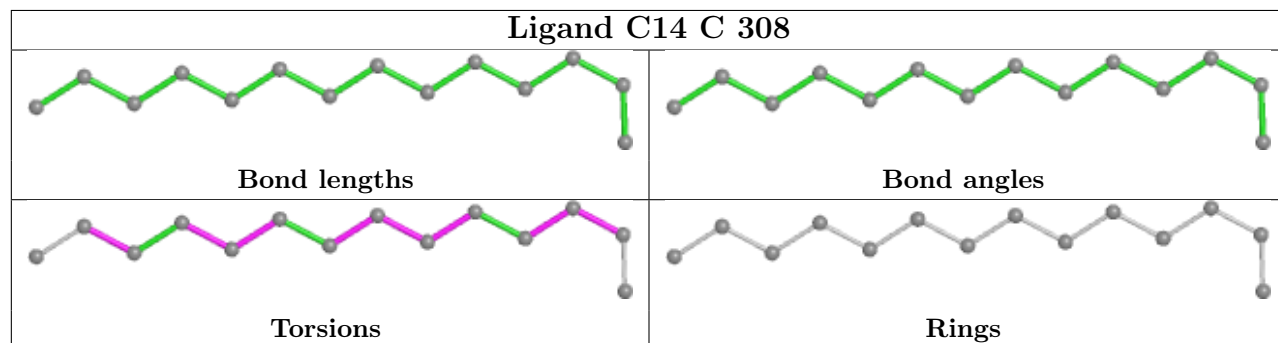
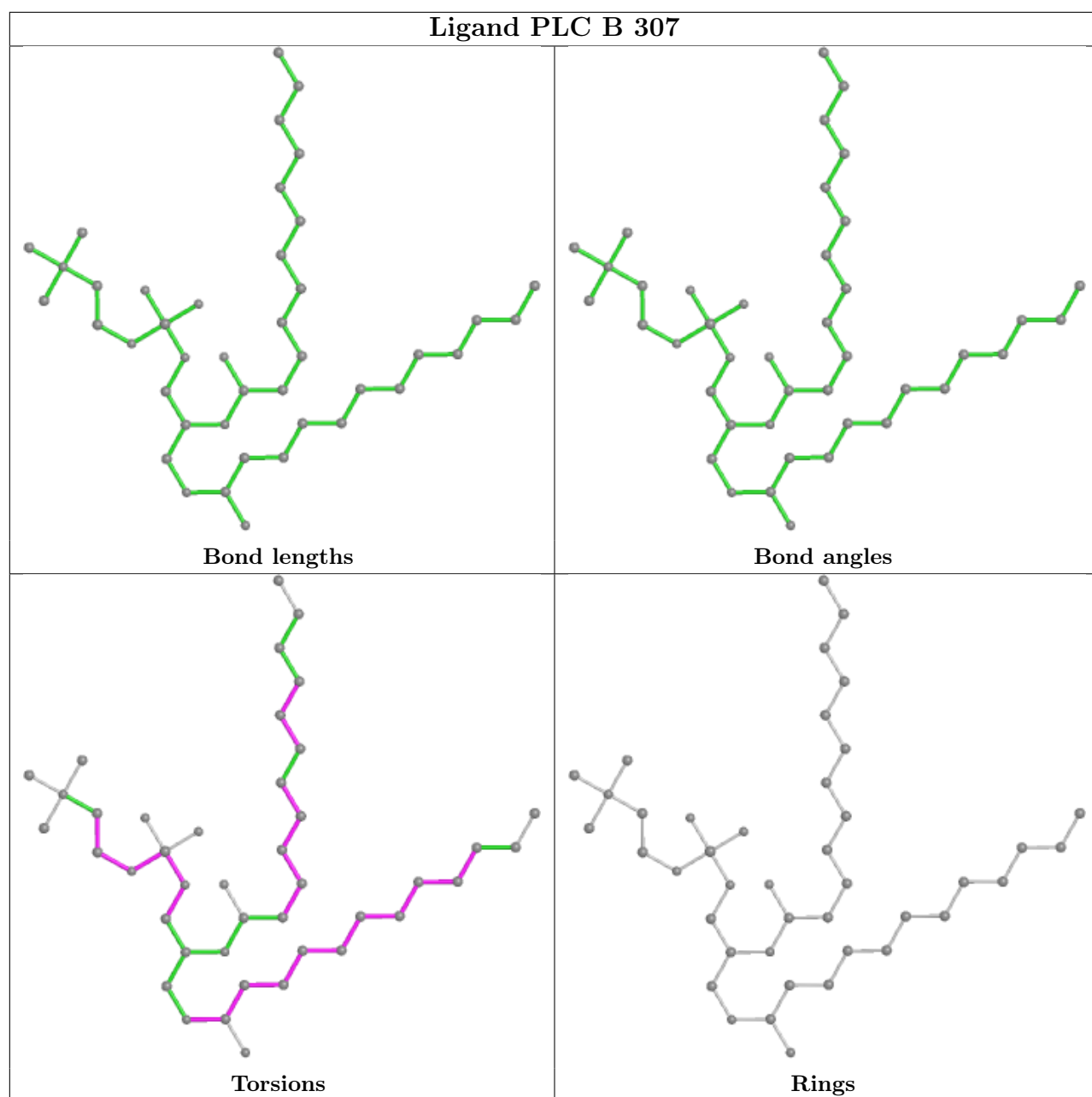


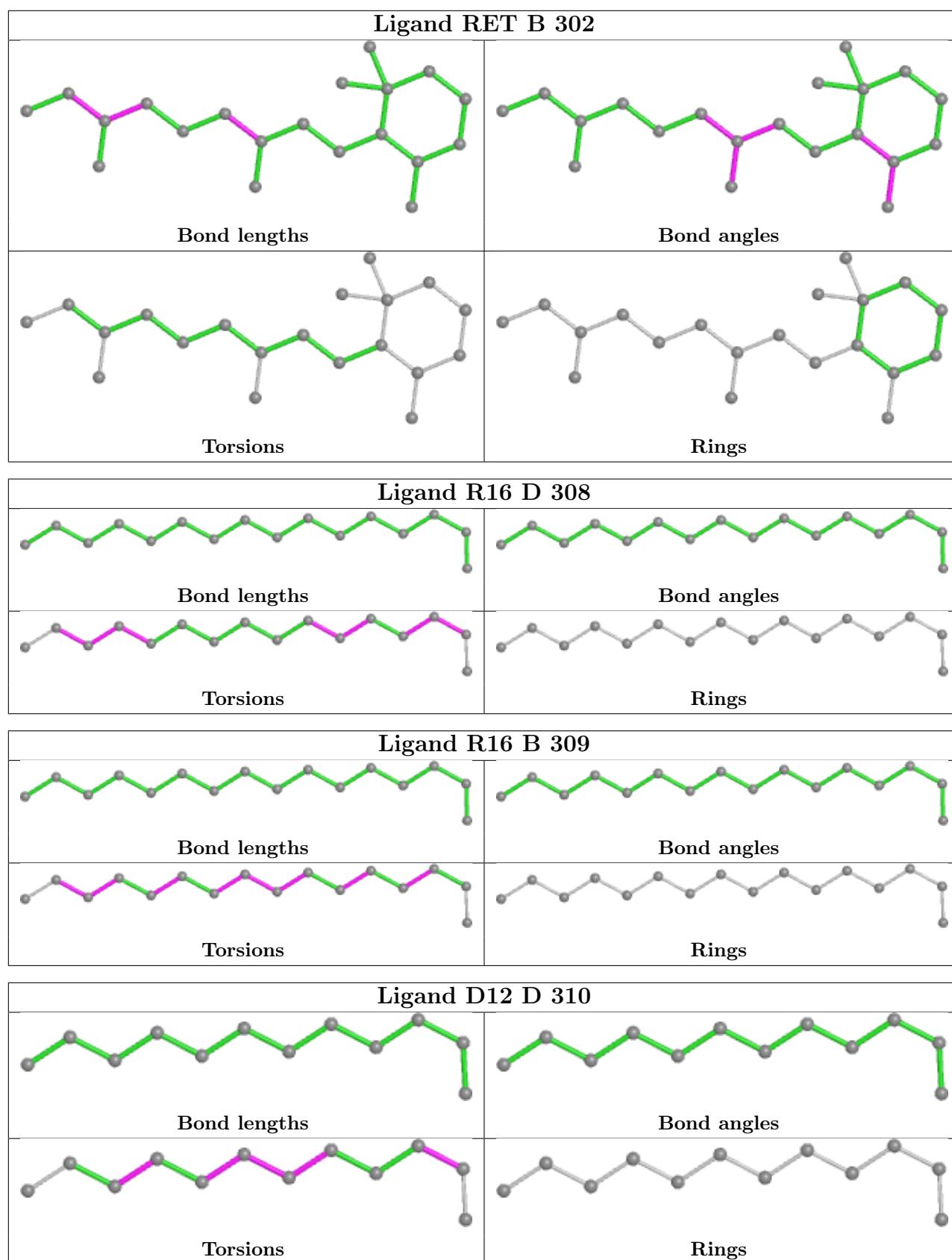


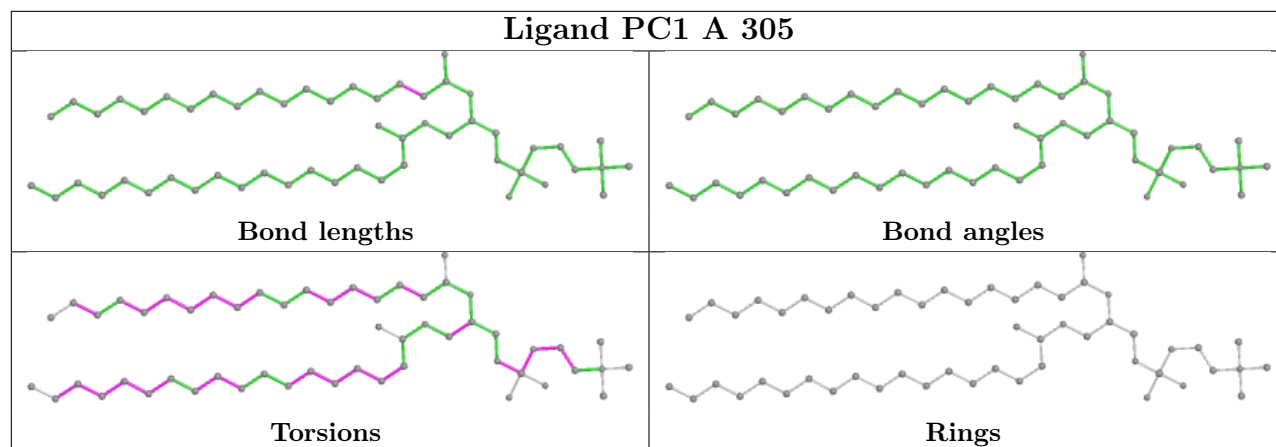












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

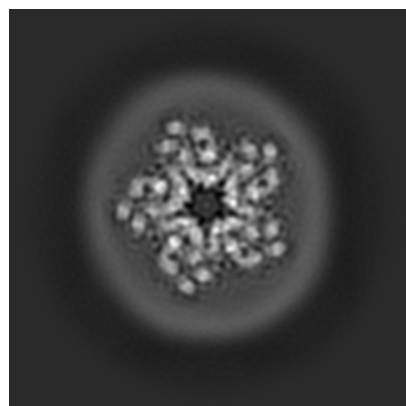
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61687. These allow visual inspection of the internal detail of the map and identification of artifacts.

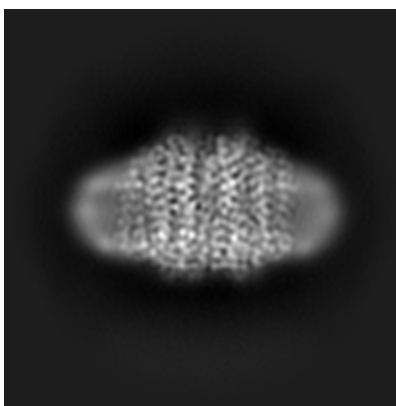
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

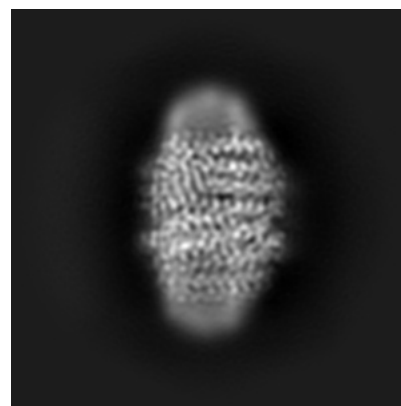
#### 6.1.1 Primary map



X

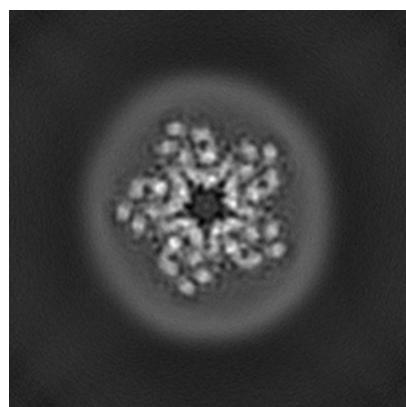


Y

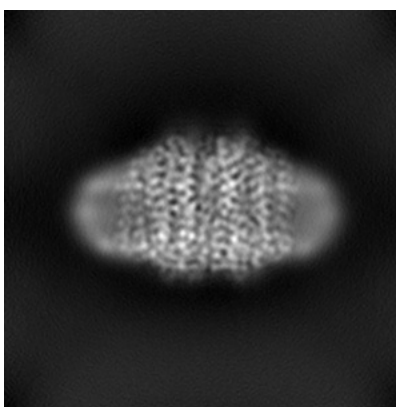


Z

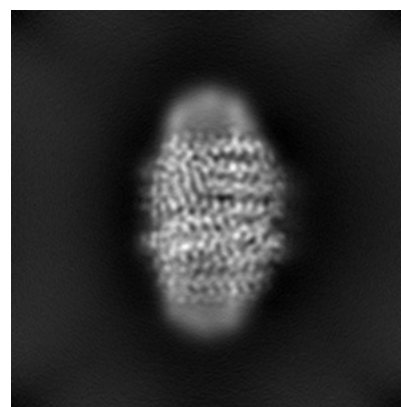
#### 6.1.2 Raw map



X



Y

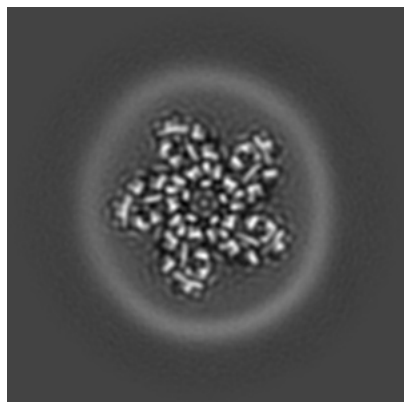


Z

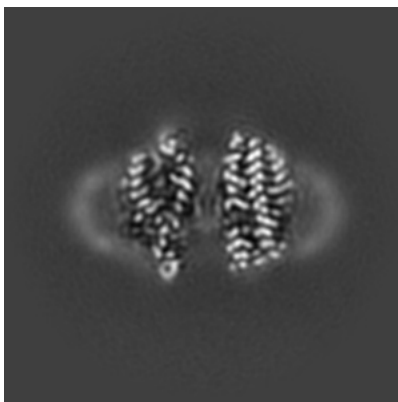
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

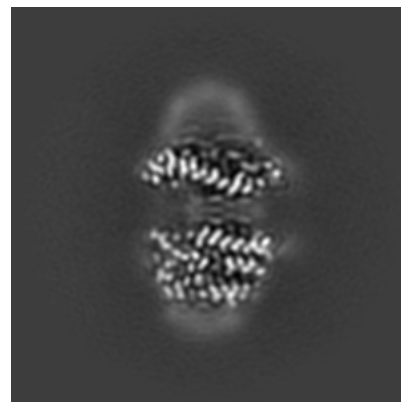
### 6.2.1 Primary map



X Index: 110

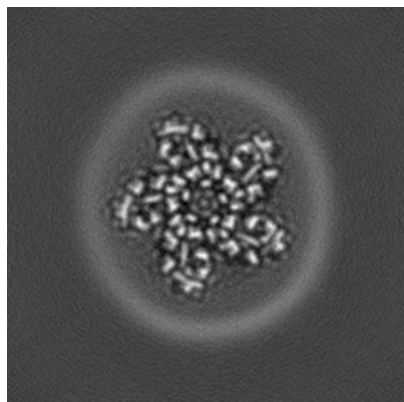


Y Index: 110

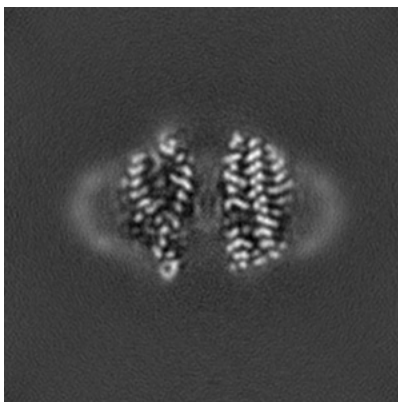


Z Index: 110

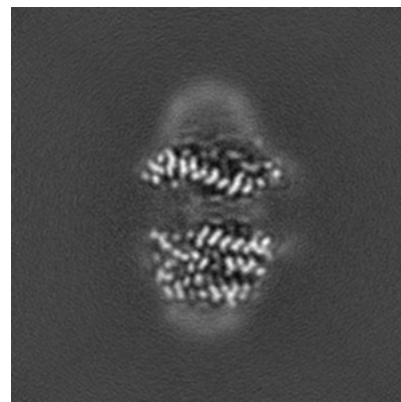
### 6.2.2 Raw map



X Index: 110



Y Index: 110

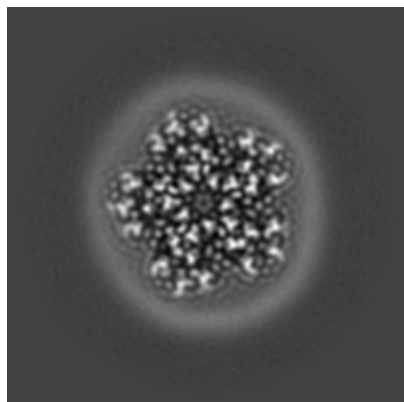


Z Index: 110

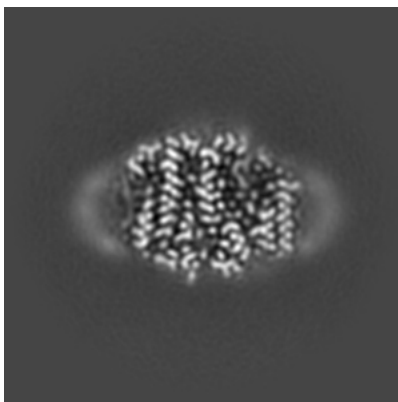
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

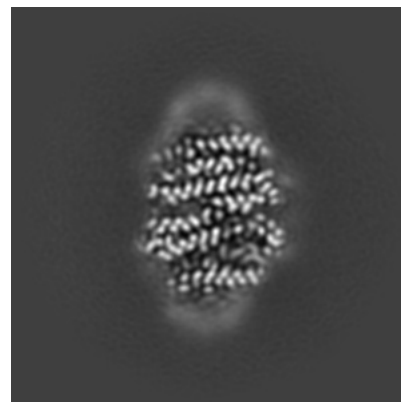
### 6.3.1 Primary map



X Index: 122

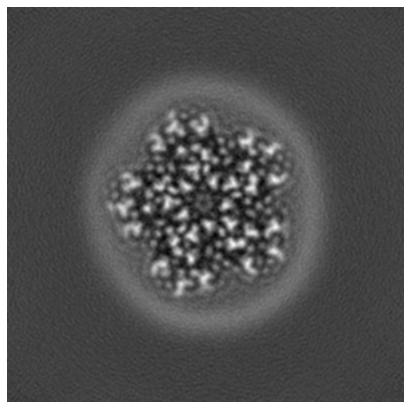


Y Index: 90

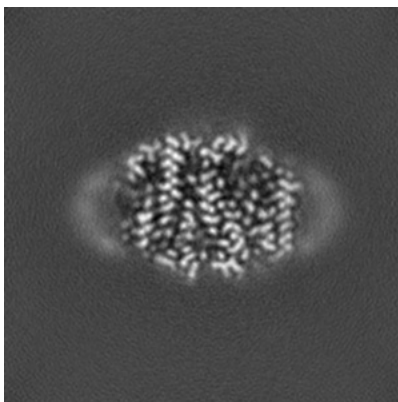


Z Index: 100

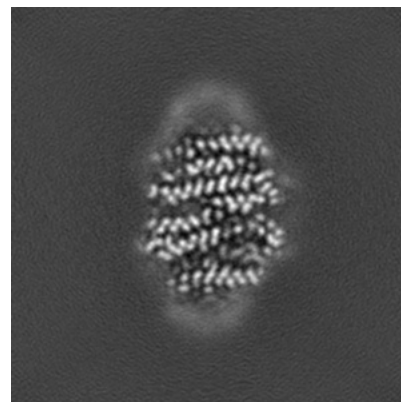
### 6.3.2 Raw map



X Index: 122



Y Index: 91

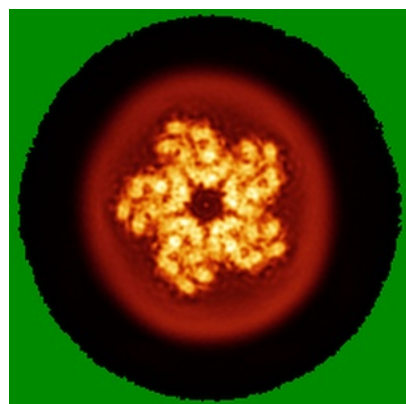


Z Index: 100

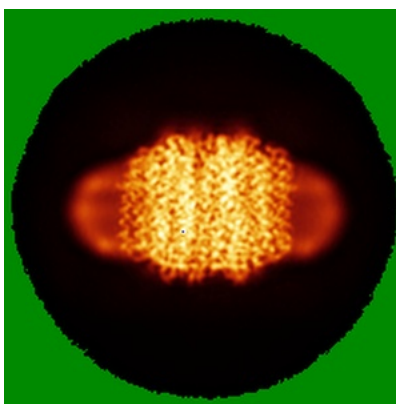
The images above show the largest variance slices of the map in three orthogonal directions.

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

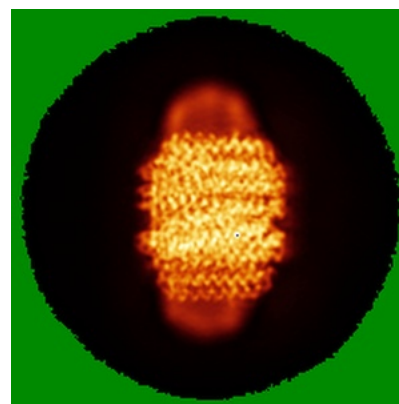
### 6.4.1 Primary map



X

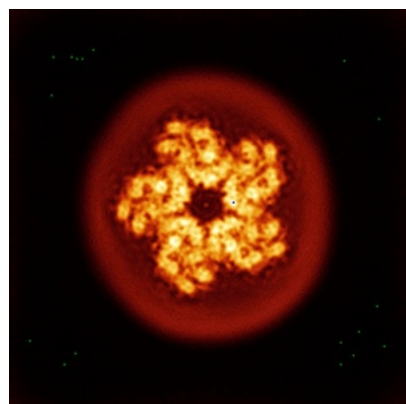


Y

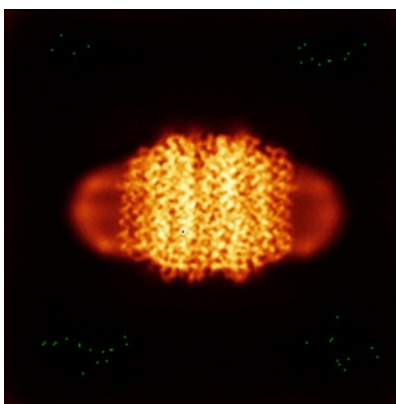


Z

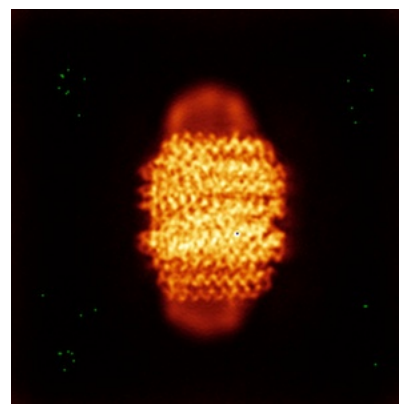
### 6.4.2 Raw map



X



Y



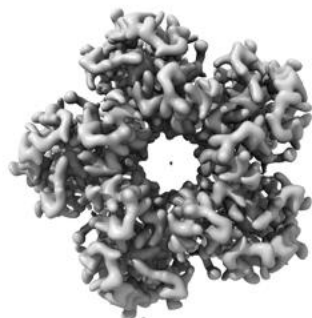
Z

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.

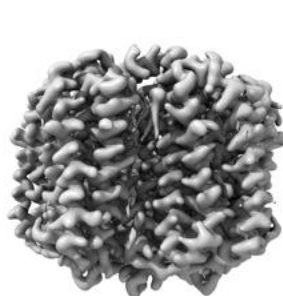


## 6.5 Orthogonal surface views [i](#)

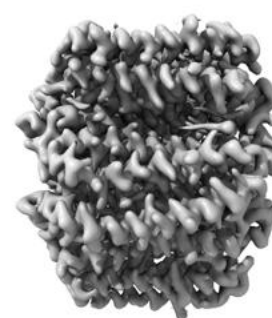
### 6.5.1 Primary map



X



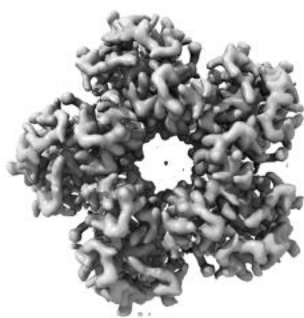
Y



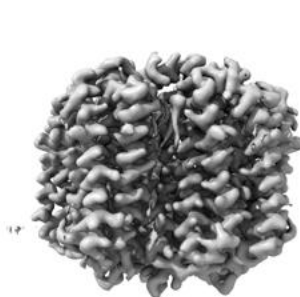
Z

The images above show the 3D surface view of the map at the recommended contour level 0.042. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

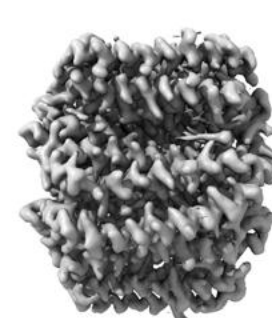
### 6.5.2 Raw map



X



Y



Z

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.



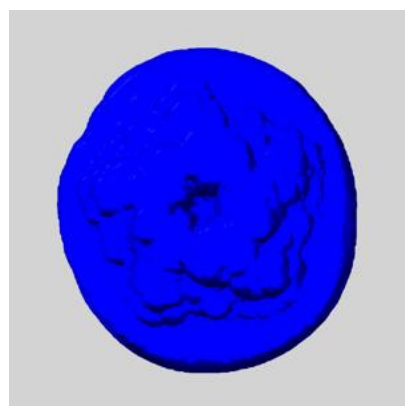
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

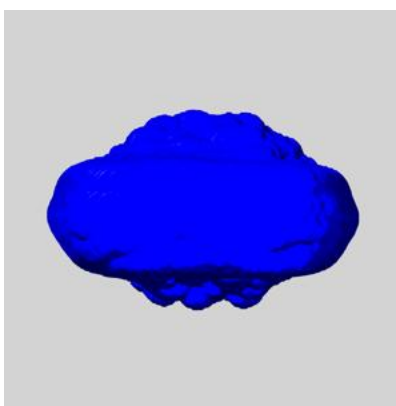
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

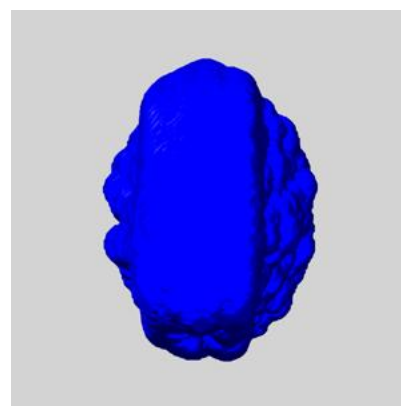
### 6.6.1 emd\_61687\_msk\_1.map [i](#)



X



Y

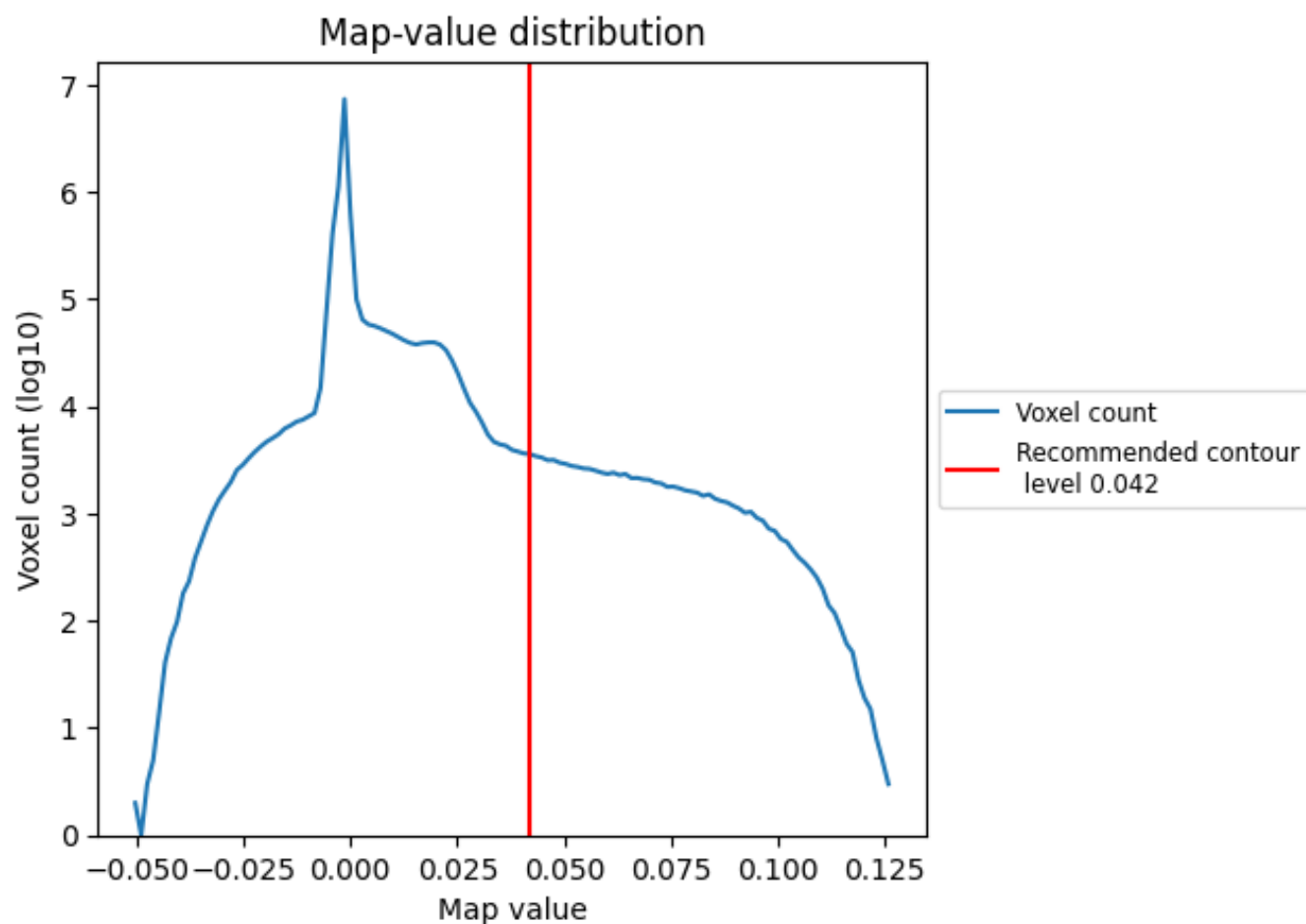


Z

## 7 Map analysis [i](#)

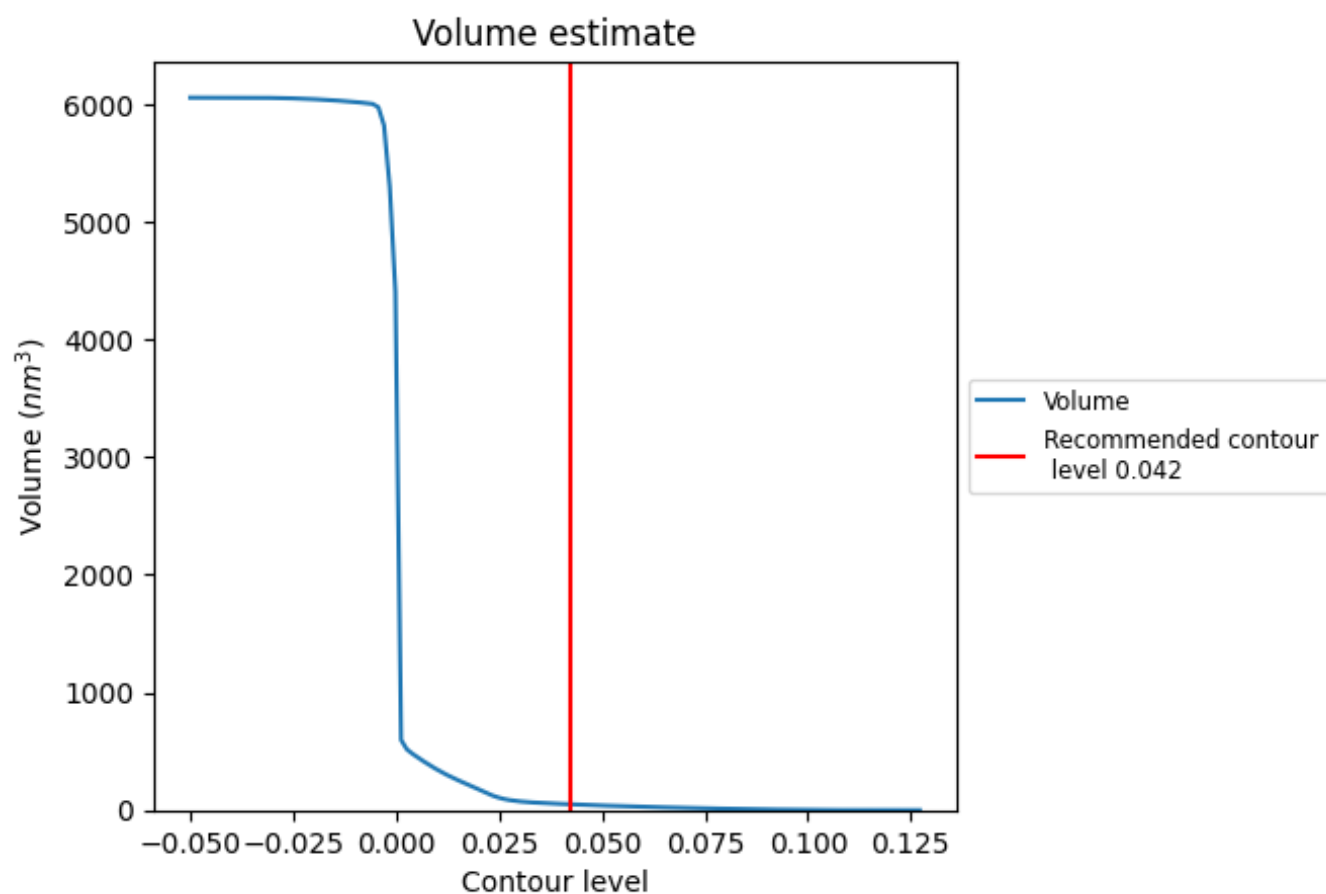
This section contains the results of statistical analysis of the map.

### 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.

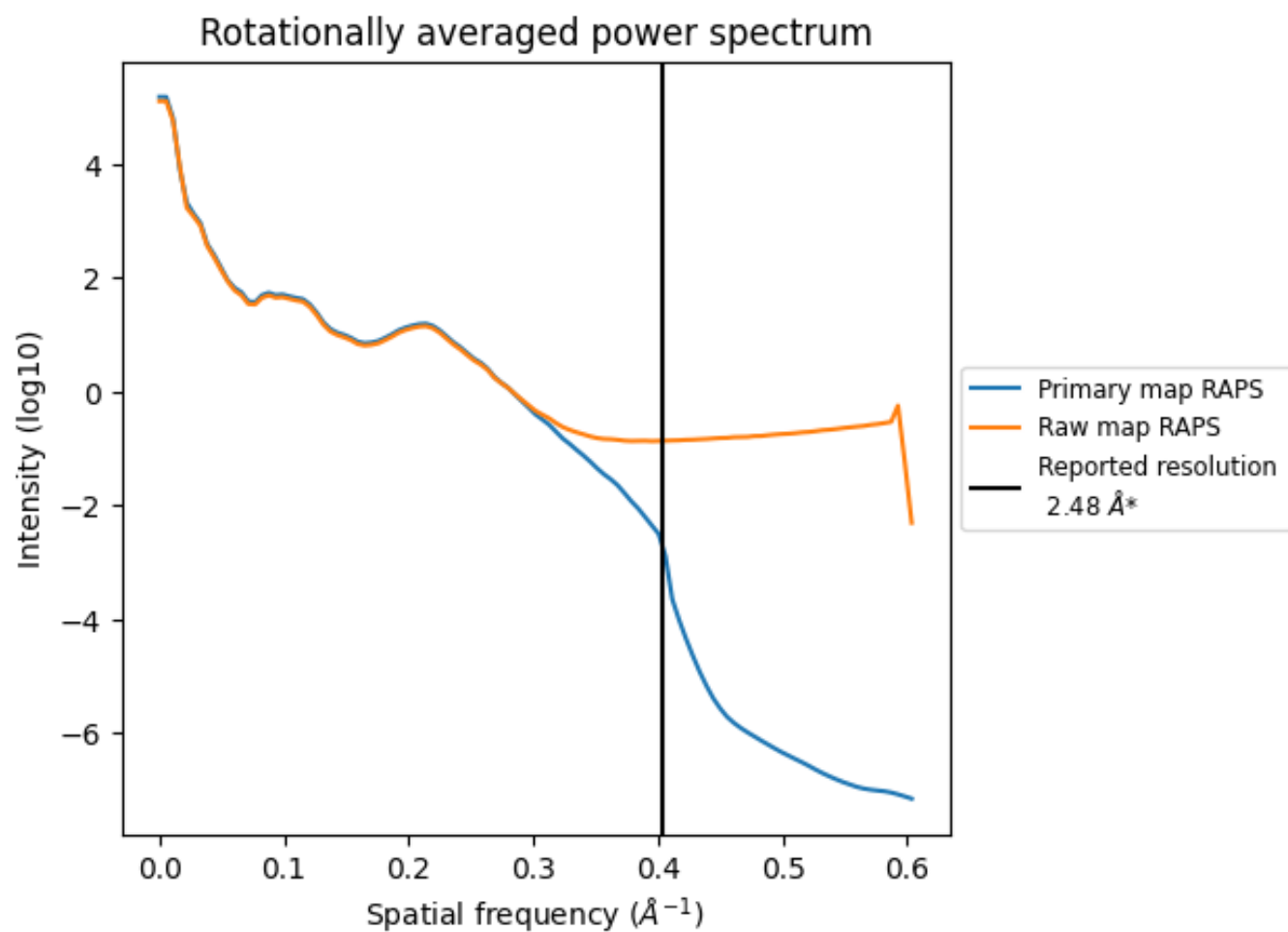
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50  $\text{nm}^3$ ; this corresponds to an approximate mass of 45 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 ⓘ

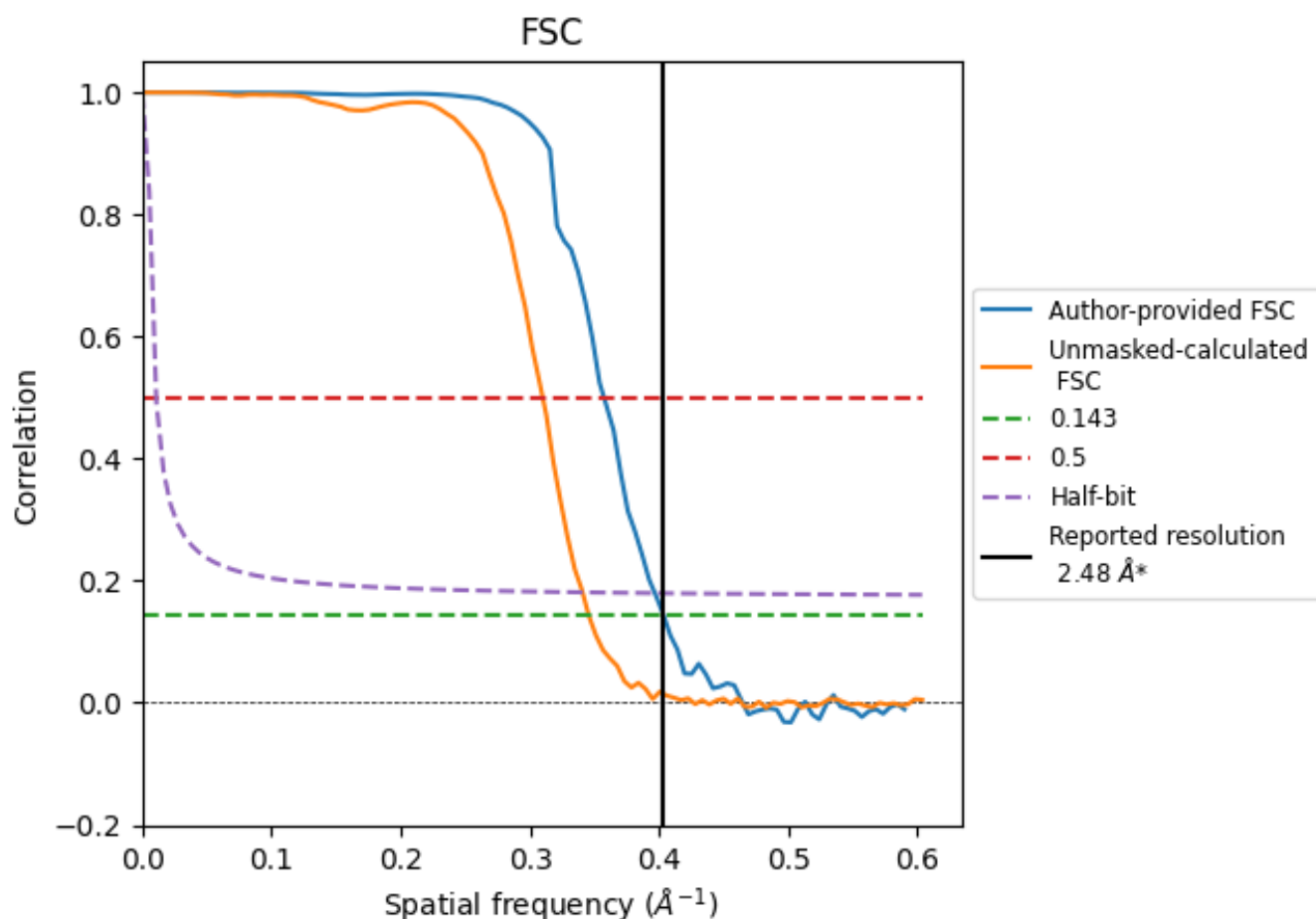


\*Reported resolution corresponds to spatial frequency of 0.403 Å<sup>-1</sup>

## 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 0.403  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

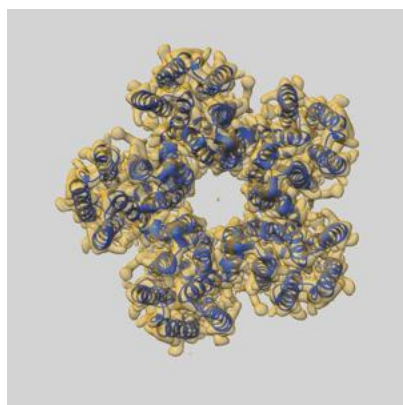
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.48	2.80	2.52
Unmasked-calculated*	2.89	3.23	2.94

\*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 2.89 differs from the reported value 2.48 by more than 10 %

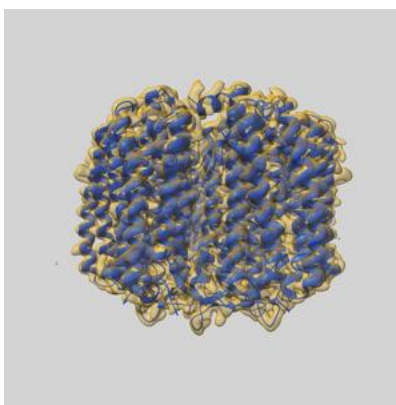
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61687 and PDB model 9JOW. Per-residue inclusion information can be found in section [3](#) on page [12](#).

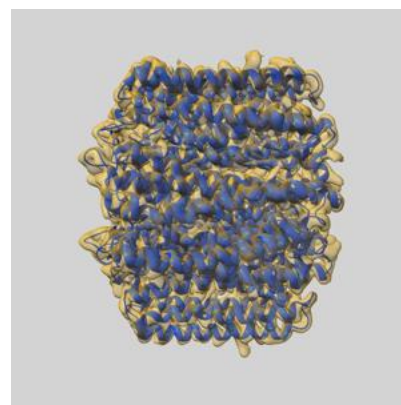
### 9.1 Map-model overlay [i](#)



X



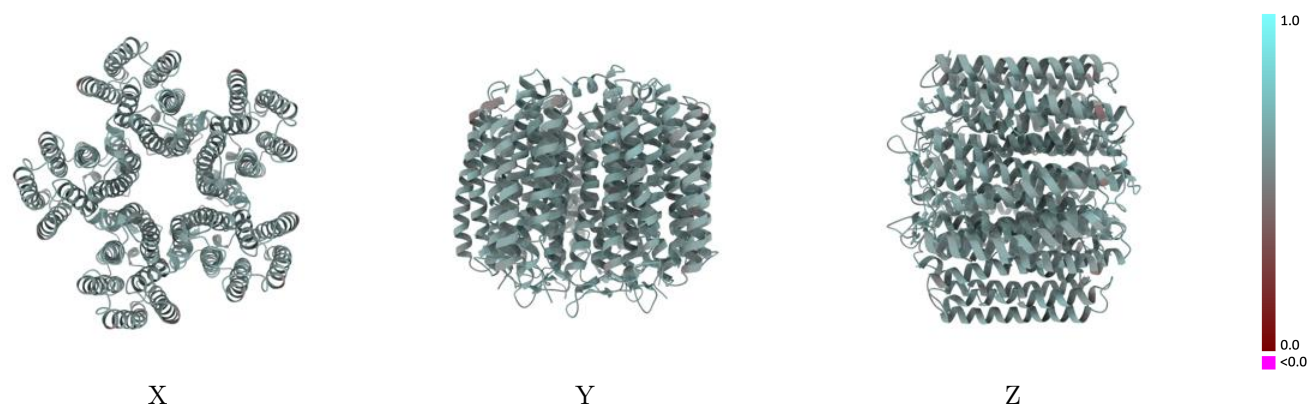
Y



Z

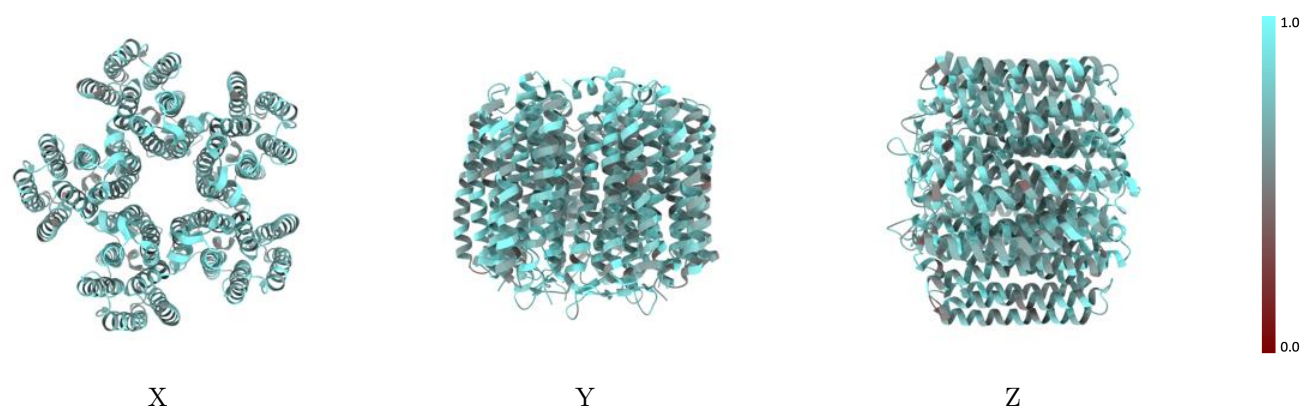
The images above show the 3D surface view of the map at the recommended contour level 0.042 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

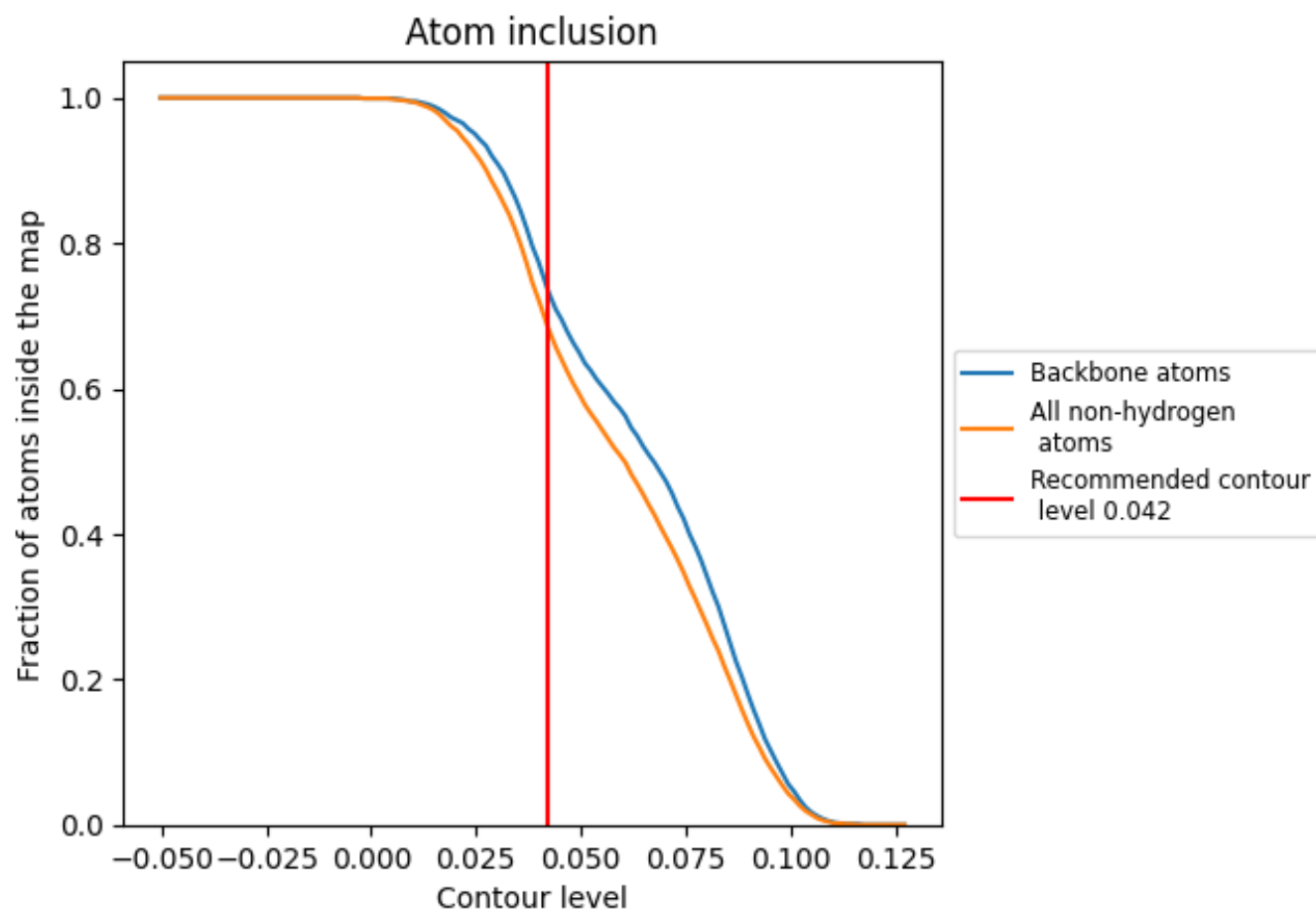
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.042).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 69% 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 (0.042) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6870	<div></div> 0.5760
A	<div></div> 0.6990	<div></div> 0.5780
B	<div></div> 0.6890	<div></div> 0.5760
C	<div></div> 0.6830	<div></div> 0.5750
D	<div></div> 0.6880	<div></div> 0.5760
E	<div></div> 0.7040	<div></div> 0.5740

