



## Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 12:12 PM JST

PDB ID : 9JOX / pdb\_00009jox  
EMDB ID : EMD-61688  
Title : Cryo-EM structure of the light-driven chloride ion-pumping rhodopsin, NM-R3  
Authors : Hosaka, T.; Shirouzu, M.  
Deposited on : 2024-09-25  
Resolution : 2.50 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

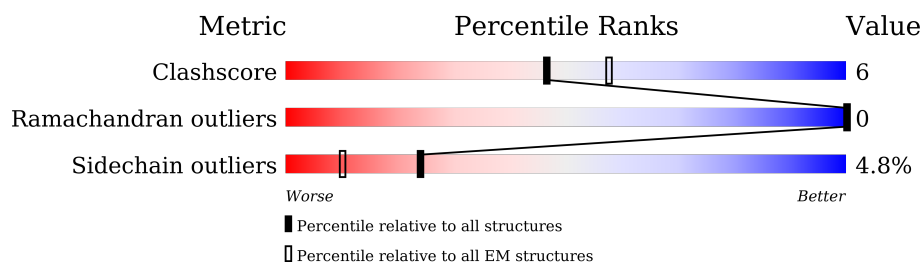
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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	 78% 14% • 6%
1	B	279	 78% 15% • 6%
1	C	279	 77% 15% • 6%
1	D	279	 78% 14% • 6%
1	E	279	 77% 15% • 6%

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11229 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	263	Total 2061	C 1371	N 317	O 358	S 15	0	0
1	B	263	Total 2061	C 1371	N 317	O 358	S 15	0	0
1	C	263	Total 2061	C 1371	N 317	O 358	S 15	0	0
1	D	263	Total 2061	C 1371	N 317	O 358	S 15	0	0
1	E	263	Total 2061	C 1371	N 317	O 358	S 15	0	0

There are 35 discrepancies between the modelled and reference sequences:

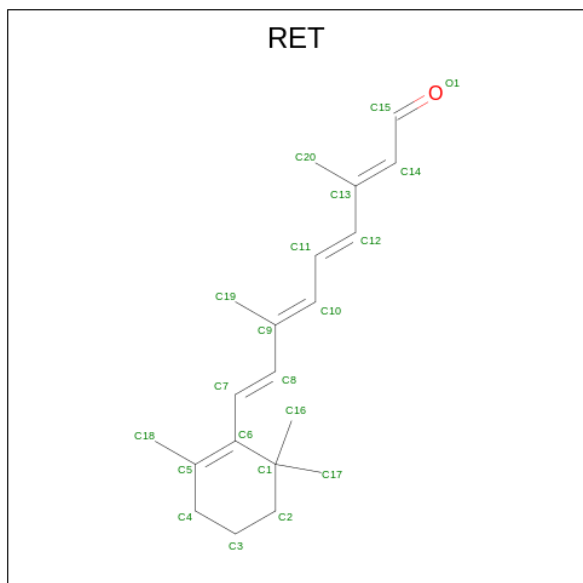
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP W8VZW3
A	-5	SER	-	expression tag	UNP W8VZW3
A	-4	SER	-	expression tag	UNP W8VZW3
A	-3	GLY	-	expression tag	UNP W8VZW3
A	-2	SER	-	expression tag	UNP W8VZW3
A	-1	SER	-	expression tag	UNP W8VZW3
A	0	GLY	-	expression tag	UNP W8VZW3
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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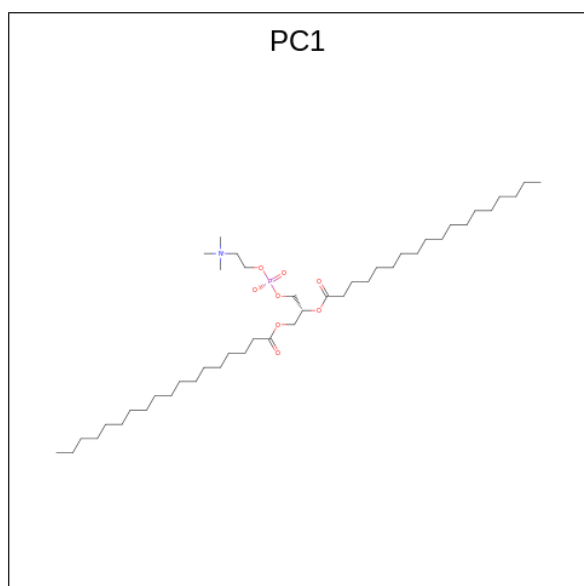
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Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total	C	0
			20	20	
2	E	1	Total	C	0
			20	20	

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



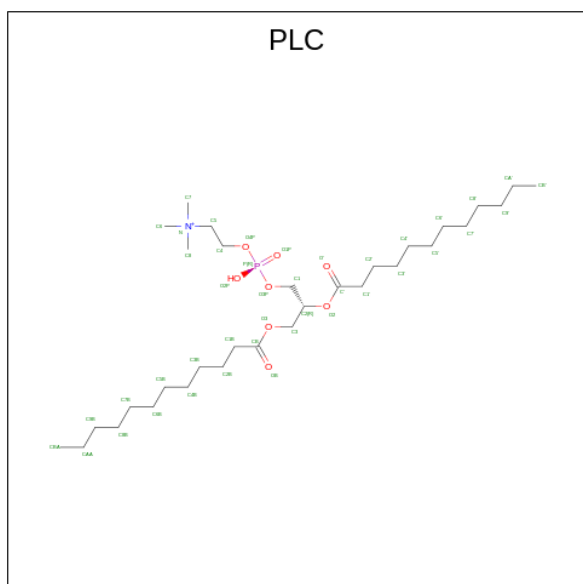
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

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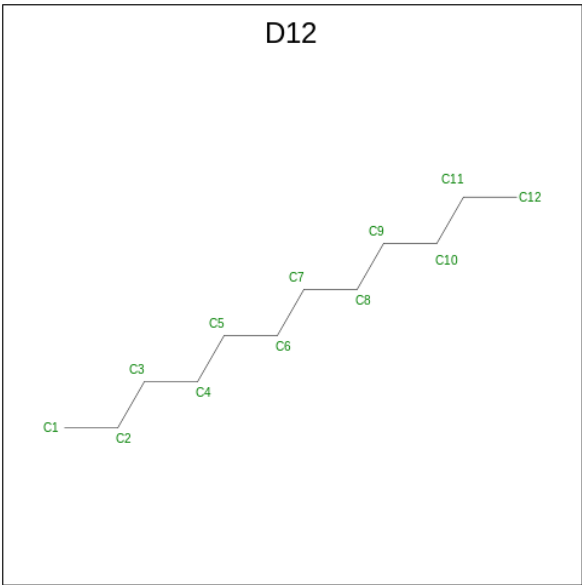
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	E	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 5 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula:  $C_{32}H_{65}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



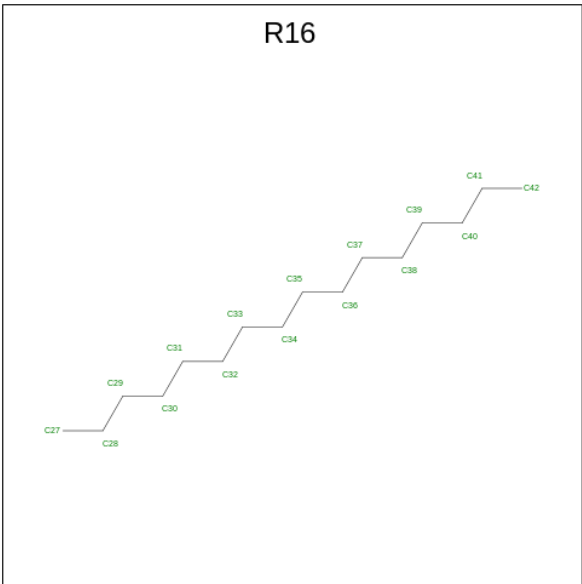
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
5	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
5	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
5	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
5	D	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 6 is DODECANE (CCD ID: D12) (formula:  $C_{12}H_{26}$ ) (labeled as "Ligand of Interest" by depositor).



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

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



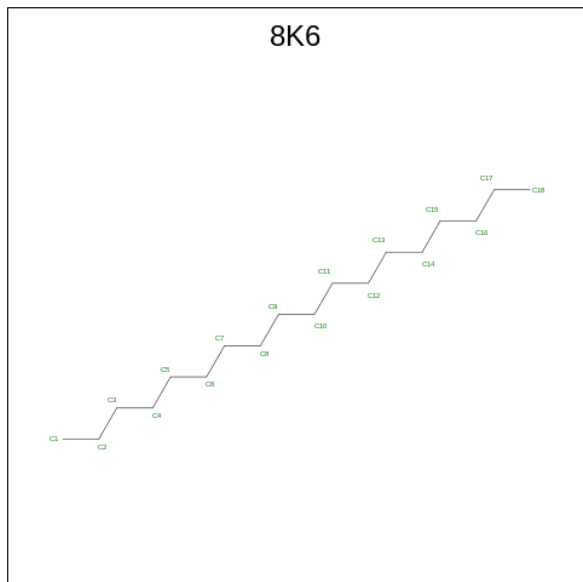
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	C	0
			16	16	

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

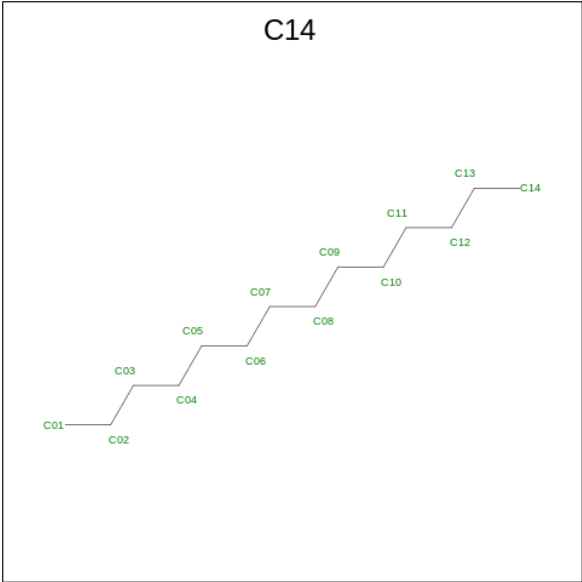
- Molecule 8 is Octadecane (CCD ID: 8K6) (formula:  $C_{18}H_{38}$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is TETRADECANE (CCD ID: C14) (formula:  $C_{14}H_{30}$ ) (labeled as "Ligand of Interest" by depositor).





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

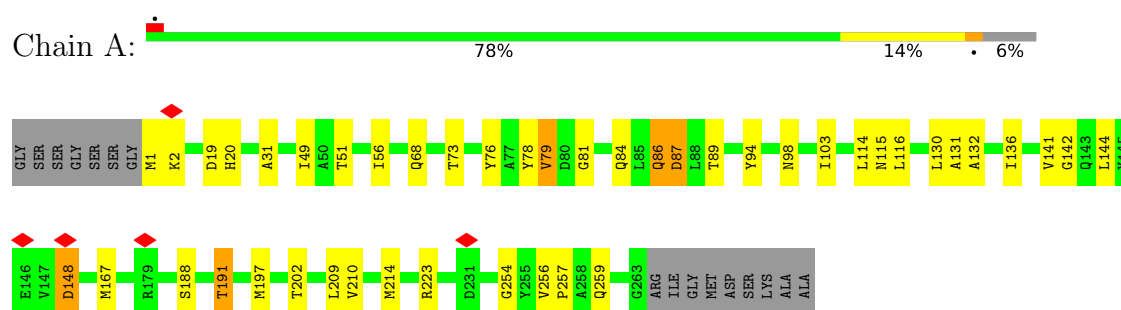
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	A	32	Total	O	0
			32	32	
10	B	28	Total	O	0
			28	28	
10	C	35	Total	O	0
			35	35	
10	D	30	Total	O	0
			30	30	
10	E	25	Total	O	0
			25	25	

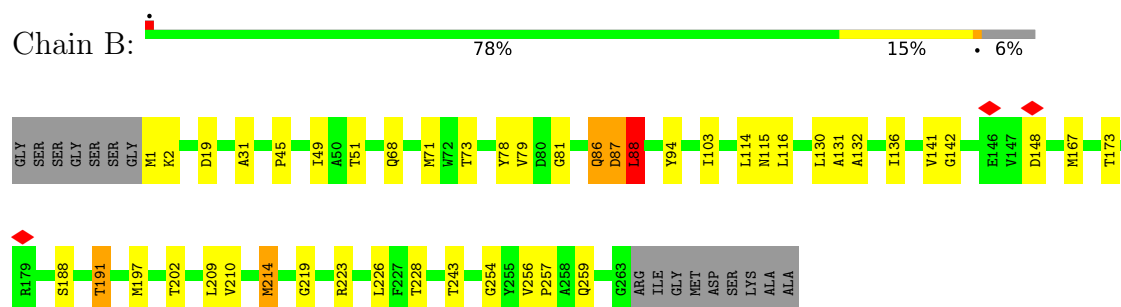
### 3 Residue-property plots

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.

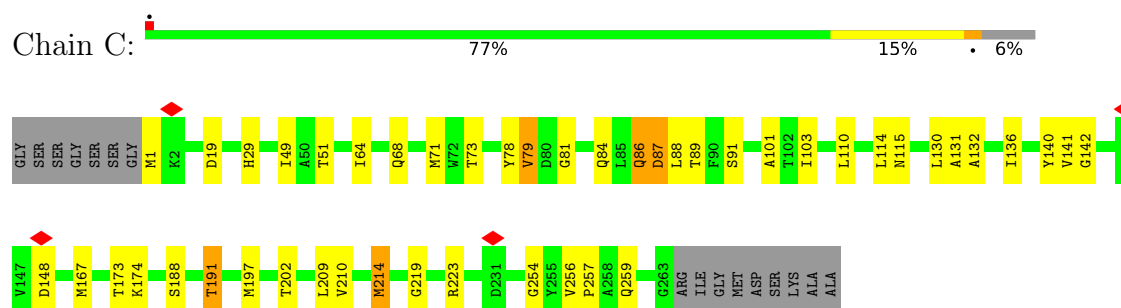
- Molecule 1: Chloride pumping rhodopsin



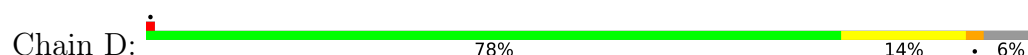
- Molecule 1: Chloride pumping rhodopsin

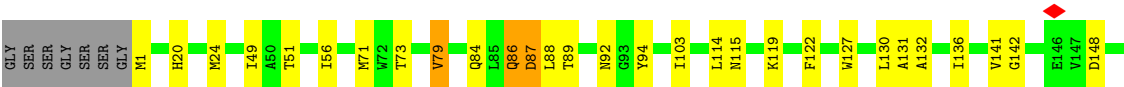


- Molecule 1: Chloride pumping rhodopsin

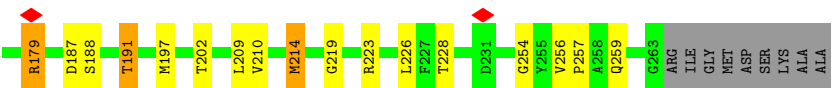
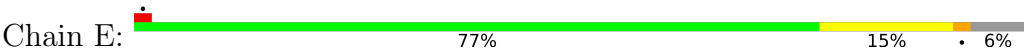


- Molecule 1: Chloride pumping rhodopsin





• 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	2081189	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 ( $e^-/\text{\AA}^2$ )	57.534	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	0.094	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.031	Depositor
Map size (Å)	165.7, 165.7, 165.7	wwPDB
Map dimensions	200, 200, 200	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: RET, 8K6, D12, C14, PLC, CL, PC1, R16

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	0.81	0/2113	1.19	7/2881 (0.2%)
1	B	0.78	0/2113	1.21	9/2881 (0.3%)
1	C	0.80	0/2113	1.19	7/2881 (0.2%)
1	D	0.79	0/2113	1.19	6/2881 (0.2%)
1	E	0.78	0/2113	1.18	6/2881 (0.2%)
All	All	0.79	0/10565	1.19	35/14405 (0.2%)

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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	GLN	CB-CA-C	-9.98	98.62	111.70
1	C	86	GLN	CB-CA-C	-9.52	99.23	111.70
1	E	86	GLN	CB-CA-C	-9.46	99.31	111.70
1	D	86	GLN	CB-CA-C	-9.18	98.84	111.51
1	B	202	THR	CA-CB-OG1	-8.65	96.63	109.60
1	A	86	GLN	CB-CA-C	-8.50	100.56	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	THR	CA-CB-OG1	-8.33	97.10	109.60
1	A	202	THR	CA-CB-OG1	-8.23	97.25	109.60
1	D	202	THR	CA-CB-OG1	-8.05	97.52	109.60
1	E	202	THR	CA-CB-OG1	-7.92	97.71	109.60
1	D	228	THR	CA-CB-OG1	-6.44	99.95	109.60
1	C	51	THR	CA-CB-OG1	-6.37	100.05	109.60
1	B	191	THR	CA-CB-OG1	-6.06	100.51	109.60
1	E	191	THR	CA-CB-OG1	-5.92	100.72	109.60
1	D	191	THR	CA-CB-OG1	-5.90	100.75	109.60
1	B	228	THR	CA-CB-OG1	-5.88	100.78	109.60
1	E	51	THR	CA-CB-OG1	-5.86	100.82	109.60
1	A	191	THR	CA-CB-OG1	-5.78	100.92	109.60
1	E	228	THR	CA-CB-OG1	-5.67	101.09	109.60
1	B	173	THR	CA-CB-OG1	-5.67	101.10	109.60
1	E	173	THR	CA-CB-OG1	-5.63	101.16	109.60
1	C	173	THR	CA-CB-OG1	-5.61	101.18	109.60
1	C	191	THR	CA-CB-OG1	-5.58	101.24	109.60
1	B	51	THR	CA-CB-OG1	-5.55	101.27	109.60
1	D	51	THR	CA-CB-OG1	-5.51	101.33	109.60
1	B	116	LEU	N-CA-CB	5.31	117.82	110.17
1	D	88	LEU	N-CA-CB	-5.16	102.57	111.55
1	A	51	THR	CA-CB-OG1	-5.15	101.87	109.60
1	C	88	LEU	N-CA-CB	-5.15	102.59	111.55
1	A	98	ASN	CA-CB-CG	-5.10	107.50	112.60
1	C	29	HIS	CA-CB-CG	-5.08	108.72	113.80
1	B	243	THR	CA-CB-OG1	-5.07	102.00	109.60
1	B	88	LEU	N-CA-CB	-5.07	102.73	111.55
1	A	116	LEU	N-CA-CB	5.03	117.42	110.17
1	A	148	ASP	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ARG	Sidechain
1	B	223	ARG	Sidechain
1	C	223	ARG	Sidechain
1	D	223	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	2061	0	2093	23	0
1	B	2061	0	2093	21	0
1	C	2061	0	2093	24	0
1	D	2061	0	2093	25	0
1	E	2061	0	2093	21	0
2	A	20	0	27	3	0
2	B	20	0	27	4	0
2	C	20	0	27	3	0
2	D	20	0	27	2	0
2	E	20	0	27	4	0
3	A	2	0	0	0	0
3	B	2	0	0	1	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
4	A	54	0	88	2	0
4	B	54	0	88	1	0
4	C	54	0	88	1	0
4	D	54	0	88	1	0
4	E	54	0	88	7	0
5	A	84	0	128	0	0
5	B	42	0	64	0	0
5	C	42	0	64	2	0
5	D	42	0	64	2	0
6	A	12	0	26	1	0
6	D	12	0	26	0	0
7	A	16	0	34	0	0
7	B	16	0	34	0	0
7	D	32	0	68	3	0
7	E	32	0	68	0	0
8	B	18	0	38	1	0
8	C	18	0	38	1	0
9	B	14	0	30	0	0
9	E	14	0	30	0	0
10	A	32	0	0	1	0
10	B	28	0	0	0	0
10	C	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	30	0	0	1	0
10	E	25	0	0	1	0
All	All	11229	0	11752	135	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 (135) 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)
4:E:305:PC1:H221	4:E:305:PC1:H32	1.40	1.00
4:E:305:PC1:H32	4:E:305:PC1:C22	1.92	0.97
4:E:305:PC1:O32	4:E:305:PC1:O11	1.88	0.91
4:E:305:PC1:H221	4:E:305:PC1:C3	2.07	0.83
4:A:304:PC1:H2E1	4:A:304:PC1:H3I1	1.62	0.79
1:A:1:MET:HE1	1:A:89:THR:HG21	1.62	0.79
2:B:302:RET:H8	2:B:302:RET:H161	1.78	0.66
1:C:140:TYR:OH	1:D:20:HIS:HD2	1.79	0.66
2:D:302:RET:H161	2:D:302:RET:H8	1.78	0.66
1:A:20:HIS:HD2	1:E:140:TYR:OH	1.80	0.65
1:A:76:TYR:O	10:A:401:HOH:O	2.16	0.63
2:E:302:RET:H171	2:E:302:RET:H8	1.81	0.62
1:B:94:TYR:OH	1:C:19:ASP:OD2	2.12	0.62
1:A:79:VAL:O	1:A:84:GLN:NE2	2.33	0.61
1:C:79:VAL:O	1:C:84:GLN:NE2	2.33	0.60
1:D:79:VAL:O	1:D:84:GLN:NE2	2.34	0.60
1:C:101:ALA:HB2	4:D:305:PC1:H2I1	1.84	0.59
1:D:122:PHE:CZ	5:D:306:PLC:H2A2	2.38	0.58
1:C:254:GLY:HA2	1:C:259:GLN:NE2	2.19	0.57
6:A:306:D12:H102	8:B:301:8K6:H162	1.86	0.57
8:C:306:8K6:H183	7:D:301:R16:C27	2.34	0.57
1:A:1:MET:HA	1:A:1:MET:HE2	1.86	0.56
1:C:91:SER:HB2	10:C:422:HOH:O	2.03	0.56
1:B:86:GLN:O	1:B:87:ASP:OD1	2.24	0.56
1:A:132:ALA:HA	1:A:167:MET:HE1	1.88	0.55
2:E:302:RET:H171	2:E:302:RET:C8	2.37	0.55
1:C:86:GLN:O	1:C:87:ASP:OD1	2.25	0.55
1:A:94:TYR:OH	1:B:19:ASP:OD2	2.19	0.55
1:E:49:ILE:HD12	1:E:49:ILE:H	1.72	0.55
1:A:86:GLN:O	1:A:87:ASP:OD1	2.25	0.54
1:E:86:GLN:O	1:E:87:ASP:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLN:O	1:D:87:ASP:OD1	2.25	0.54
1:A:49:ILE:HD12	1:A:49:ILE:H	1.73	0.54
1:D:71:MET:CE	1:D:89:THR:O	2.56	0.54
1:C:49:ILE:H	1:C:49:ILE:HD12	1.73	0.54
1:D:49:ILE:HD12	1:D:49:ILE:H	1.73	0.53
1:B:49:ILE:H	1:B:49:ILE:HD12	1.73	0.53
1:B:71:MET:CE	1:B:88:LEU:HG	2.39	0.53
1:E:179:ARG:HD3	1:E:187:ASP:HB2	1.90	0.53
1:A:19:ASP:OD2	1:E:94:TYR:OH	2.18	0.52
1:D:132:ALA:HA	1:D:167:MET:HE1	1.91	0.52
1:C:71:MET:CE	1:C:89:THR:O	2.58	0.51
1:C:103:ILE:HD12	1:C:136:ILE:HD11	1.92	0.51
2:C:301:RET:H171	2:C:301:RET:H8	1.91	0.51
1:D:94:TYR:OH	1:E:19:ASP:OD2	2.24	0.51
2:B:302:RET:H161	2:B:302:RET:C8	2.41	0.51
1:B:103:ILE:HD12	1:B:136:ILE:HD11	1.92	0.50
1:B:68:GLN:HA	1:B:68:GLN:HE21	1.76	0.50
1:D:119:LYS:HD2	4:E:305:PC1:H152	1.94	0.50
2:B:302:RET:H8	2:B:302:RET:H171	1.94	0.49
1:D:122:PHE:CE2	5:D:306:PLC:H2A2	2.47	0.49
1:E:114:LEU:O	1:E:115:ASN:HB2	2.12	0.49
1:A:103:ILE:HD12	1:A:136:ILE:HD11	1.94	0.49
1:C:132:ALA:HA	1:C:167:MET:HE1	1.94	0.49
1:E:103:ILE:HD12	1:E:136:ILE:HD11	1.95	0.49
1:A:114:LEU:O	1:A:115:ASN:HB2	2.11	0.49
4:B:305:PC1:H3B1	4:B:305:PC1:H382	1.52	0.49
1:D:24:MET:HE1	7:D:301:R16:H423	1.93	0.48
1:B:132:ALA:HA	1:B:167:MET:HE1	1.95	0.48
4:E:305:PC1:C22	4:E:305:PC1:C3	2.63	0.48
2:A:301:RET:H8	2:A:301:RET:H161	1.95	0.48
1:D:132:ALA:HA	1:D:167:MET:CE	2.44	0.48
1:A:68:GLN:HE21	1:A:68:GLN:HA	1.78	0.48
1:D:71:MET:HE1	1:D:89:THR:O	2.13	0.47
1:D:103:ILE:HD12	1:D:136:ILE:HD11	1.95	0.47
1:E:91:SER:HB2	10:E:411:HOH:O	2.13	0.47
1:D:114:LEU:O	1:D:115:ASN:HB2	2.15	0.47
1:A:132:ALA:HA	1:A:167:MET:CE	2.44	0.47
1:B:114:LEU:O	1:B:115:ASN:HB2	2.13	0.47
1:E:132:ALA:HA	1:E:167:MET:CE	2.45	0.47
1:E:132:ALA:HA	1:E:167:MET:HE1	1.95	0.47
2:B:302:RET:C8	2:B:302:RET:H171	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LEU:O	1:C:115:ASN:HB2	2.13	0.47
4:C:304:PC1:H3B1	4:C:304:PC1:H382	1.62	0.47
1:D:141:VAL:O	1:D:142:GLY:C	2.58	0.46
1:C:110:LEU:HD22	1:C:197:MET:HE1	1.97	0.46
2:D:302:RET:H161	2:D:302:RET:C8	2.46	0.46
1:E:141:VAL:O	1:E:142:GLY:C	2.58	0.46
4:E:305:PC1:O32	4:E:305:PC1:C1	2.64	0.46
1:C:141:VAL:O	1:C:142:GLY:C	2.59	0.45
1:E:160:SER:OG	2:E:302:RET:H41	2.16	0.45
1:B:130:LEU:O	1:B:131:ALA:C	2.56	0.45
1:A:141:VAL:O	1:A:142:GLY:C	2.59	0.45
1:E:256:VAL:N	1:E:257:PRO:CD	2.79	0.45
1:C:130:LEU:O	1:C:131:ALA:C	2.58	0.45
1:D:209:LEU:O	1:D:210:VAL:C	2.59	0.45
1:B:45:PRO:HD2	3:B:304:CL:CL	2.54	0.45
1:C:132:ALA:HA	1:C:167:MET:CE	2.46	0.45
1:A:2:LYS:HE2	1:A:144:LEU:HD22	1.99	0.45
1:A:254:GLY:HA2	1:A:259:GLN:NE2	2.32	0.45
1:E:254:GLY:HA2	1:E:259:GLN:NE2	2.32	0.45
1:C:71:MET:HE1	1:C:89:THR:O	2.17	0.44
1:B:132:ALA:HA	1:B:167:MET:CE	2.47	0.44
1:B:256:VAL:N	1:B:257:PRO:CD	2.79	0.44
1:D:92:ASN:HD21	1:D:224:GLN:HE22	1.64	0.44
2:E:302:RET:H8	2:E:302:RET:H161	1.99	0.44
1:C:209:LEU:O	1:C:210:VAL:C	2.60	0.44
1:C:256:VAL:N	1:C:257:PRO:CD	2.80	0.44
1:B:254:GLY:HA2	1:B:259:GLN:NE2	2.32	0.44
1:D:256:VAL:N	1:D:257:PRO:CD	2.81	0.44
1:B:141:VAL:O	1:B:142:GLY:C	2.59	0.43
1:A:256:VAL:N	1:A:257:PRO:CD	2.80	0.43
1:E:209:LEU:O	1:E:210:VAL:C	2.60	0.43
5:C:305:PLC:H32	5:C:305:PLC:H1'1	2.00	0.43
1:B:214:MET:HE2	1:B:219:GLY:N	2.34	0.43
5:C:305:PLC:H32	5:C:305:PLC:H1A1	1.89	0.43
1:D:130:LEU:O	1:D:131:ALA:C	2.58	0.43
2:A:301:RET:H7	2:A:301:RET:H181	1.84	0.42
1:A:130:LEU:O	1:A:131:ALA:C	2.57	0.42
1:C:64:ILE:HD13	1:C:64:ILE:HA	1.90	0.42
2:A:301:RET:H8	2:A:301:RET:H171	2.01	0.42
1:B:209:LEU:O	1:B:210:VAL:C	2.60	0.42
1:C:214:MET:HE2	1:C:219:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:MET:HE2	1:D:219:GLY:N	2.35	0.42
1:A:209:LEU:O	1:A:210:VAL:C	2.60	0.41
1:C:78:TYR:CZ	1:C:81:GLY:HA2	2.55	0.41
1:C:174:LYS:HA	1:C:174:LYS:HD3	1.95	0.41
1:E:64:ILE:HD13	1:E:64:ILE:HA	1.89	0.41
1:D:84:GLN:HA	10:D:406:HOH:O	2.20	0.41
1:E:130:LEU:O	1:E:131:ALA:C	2.57	0.41
1:C:68:GLN:NE2	10:C:401:HOH:O	2.47	0.41
1:E:214:MET:HE2	1:E:219:GLY:N	2.35	0.41
1:A:78:TYR:CZ	1:A:81:GLY:HA2	2.56	0.41
1:B:68:GLN:HA	1:B:68:GLN:NE2	2.35	0.41
2:C:301:RET:H171	2:C:301:RET:C8	2.50	0.41
2:C:301:RET:H181	2:C:301:RET:H7	1.81	0.41
1:D:56:ILE:HD13	1:D:56:ILE:HG21	1.88	0.41
1:B:256:VAL:N	1:B:257:PRO:HD2	2.36	0.41
1:A:56:ILE:HG23	1:B:31:ALA:HB1	2.02	0.41
1:A:31:ALA:HB1	1:E:56:ILE:HG23	2.03	0.40
4:A:304:PC1:H3I2	4:A:304:PC1:C3C	2.51	0.40
1:D:256:VAL:HB	1:D:257:PRO:HD3	2.03	0.40
1:B:78:TYR:CZ	1:B:81:GLY:HA2	2.56	0.40
1:D:127:TRP:CD1	7:D:307:R16:H391	2.55	0.40
1:E:78:TYR:CZ	1:E:81:GLY:HA2	2.56	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	261/279 (94%)	248 (95%)	13 (5%)	0	100	100
1	B	261/279 (94%)	248 (95%)	13 (5%)	0	100	100
1	C	261/279 (94%)	249 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	261/279 (94%)	248 (95%)	13 (5%)	0	100	100
1	E	261/279 (94%)	248 (95%)	13 (5%)	0	100	100
All	All	1305/1395 (94%)	1241 (95%)	64 (5%)	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%)	208 (96%)	8 (4%)	29	55
1	B	216/226 (96%)	204 (94%)	12 (6%)	17	36
1	C	216/226 (96%)	208 (96%)	8 (4%)	29	55
1	D	216/226 (96%)	205 (95%)	11 (5%)	20	40
1	E	216/226 (96%)	203 (94%)	13 (6%)	16	33
All	All	1080/1130 (96%)	1028 (95%)	52 (5%)	24	43

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	79	VAL
1	A	87	ASP
1	A	148	ASP
1	A	188	SER
1	A	191	THR
1	A	197	MET
1	A	214	MET
1	B	1	MET
1	B	2	LYS
1	B	73	THR
1	B	79	VAL
1	B	87	ASP

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Mol	Chain	Res	Type
1	B	88	LEU
1	B	148	ASP
1	B	188	SER
1	B	191	THR
1	B	197	MET
1	B	214	MET
1	B	226	LEU
1	C	1	MET
1	C	73	THR
1	C	79	VAL
1	C	87	ASP
1	C	148	ASP
1	C	188	SER
1	C	191	THR
1	C	214	MET
1	D	1	MET
1	D	73	THR
1	D	79	VAL
1	D	87	ASP
1	D	148	ASP
1	D	174	LYS
1	D	188	SER
1	D	191	THR
1	D	197	MET
1	D	214	MET
1	D	226	LEU
1	E	1	MET
1	E	2	LYS
1	E	73	THR
1	E	79	VAL
1	E	87	ASP
1	E	117	LYS
1	E	148	ASP
1	E	179	ARG
1	E	188	SER
1	E	191	THR
1	E	197	MET
1	E	214	MET
1	E	226	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) 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	115	ASN
1	A	178	ASN
1	A	260	GLN
1	B	41	GLN
1	B	68	GLN
1	B	84	GLN
1	B	109	GLN
1	B	115	ASN
1	B	224	GLN
1	B	248	GLN
1	B	260	GLN
1	C	41	GLN
1	C	115	ASN
1	C	168	ASN
1	C	178	ASN
1	C	260	GLN
1	D	20	HIS
1	D	29	HIS
1	D	41	GLN
1	D	92	ASN
1	D	109	GLN
1	D	152	GLN
1	D	178	ASN
1	D	248	GLN
1	D	259	GLN
1	D	260	GLN
1	E	84	GLN
1	E	92	ASN
1	E	109	GLN
1	E	115	ASN
1	E	152	GLN
1	E	224	GLN
1	E	248	GLN
1	E	260	GLN

### 5.3.3 RNA ⓘ

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 37 ligands modelled in this entry, 10 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PC1	A	304	-	53,53,53	0.32	0	59,61,61	0.45	0
8	8K6	B	301	-	17,17,17	0.19	0	16,16,16	0.14	0
4	PC1	D	305	-	53,53,53	0.41	0	59,61,61	0.56	0
7	R16	E	301	-	15,15,15	0.58	0	14,14,14	0.58	0
4	PC1	C	304	-	53,53,53	0.34	0	59,61,61	0.50	0
4	PC1	E	305	-	53,53,53	0.44	0	59,61,61	1.26	4 (6%)
7	R16	B	307	-	15,15,15	0.56	0	14,14,14	0.58	0
5	PLC	D	306	-	41,41,41	0.34	0	47,49,49	0.47	0
5	PLC	C	305	-	41,41,41	0.35	0	47,49,49	0.78	2 (4%)
2	RET	A	301	1	20,20,21	2.02	3 (15%)	27,27,28	1.46	5 (18%)
6	D12	A	306	-	11,11,11	0.12	0	10,10,10	0.13	0
8	8K6	C	306	-	17,17,17	0.24	0	16,16,16	0.19	0
5	PLC	B	306	-	41,41,41	0.36	0	47,49,49	0.37	0
4	PC1	B	305	-	53,53,53	0.46	0	59,61,61	0.51	1 (1%)
2	RET	E	302	1	20,20,21	2.75	5 (25%)	27,27,28	1.41	3 (11%)
7	R16	D	307	-	15,15,15	0.45	0	14,14,14	0.55	0
7	R16	E	306	-	15,15,15	0.47	0	14,14,14	0.52	0
7	R16	D	301	-	15,15,15	0.46	0	14,14,14	0.71	1 (7%)
6	D12	D	308	-	11,11,11	0.12	0	10,10,10	0.15	0
7	R16	A	308	-	15,15,15	0.52	0	14,14,14	0.43	0
9	C14	B	308	-	13,13,13	0.40	0	12,12,12	0.59	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	2.44	4 (20%)	27,27,28	1.41	4 (14%)
5	PLC	A	305	-	41,41,41	0.38	0	47,49,49	0.63	1 (2%)
2	RET	C	301	1	20,20,21	2.30	3 (15%)	27,27,28	1.58	2 (7%)
9	C14	E	307	-	13,13,13	0.46	0	12,12,12	0.58	0
2	RET	D	302	1	20,20,21	2.80	4 (20%)	27,27,28	1.44	4 (14%)
5	PLC	A	307	-	41,41,41	0.29	0	47,49,49	0.39	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	PC1	A	304	-	-	26/57/57/57	-
8	8K6	B	301	-	-	11/15/15/15	-
4	PC1	D	305	-	-	36/57/57/57	-
7	R16	E	301	-	-	5/13/13/13	-
4	PC1	C	304	-	-	32/57/57/57	-
4	PC1	E	305	-	-	28/57/57/57	-
7	R16	B	307	-	-	10/13/13/13	-
5	PLC	D	306	-	-	25/45/45/45	-
5	PLC	C	305	-	-	25/45/45/45	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
6	D12	A	306	-	-	7/9/9/9	-
8	8K6	C	306	-	-	9/15/15/15	-
5	PLC	B	306	-	-	19/45/45/45	-
4	PC1	B	305	-	-	29/57/57/57	-
2	RET	E	302	1	-	0/13/30/31	0/1/1/1
7	R16	D	307	-	-	6/13/13/13	-
7	R16	E	306	-	-	7/13/13/13	-
7	R16	D	301	-	-	6/13/13/13	-
6	D12	D	308	-	-	5/9/9/9	-
7	R16	A	308	-	-	7/13/13/13	-
9	C14	B	308	-	-	6/11/11/11	-
2	RET	B	302	1	-	0/13/30/31	0/1/1/1
5	PLC	A	305	-	-	25/45/45/45	-
2	RET	C	301	1	-	0/13/30/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	C14	E	307	-	-	6/11/11/11	-
2	RET	D	302	1	-	0/13/30/31	0/1/1/1
5	PLC	A	307	-	-	17/45/45/45	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	RET	C14-C13	10.48	1.41	1.33
2	E	302	RET	C14-C13	10.28	1.41	1.33
2	C	301	RET	C14-C13	8.68	1.40	1.33
2	B	302	RET	C14-C13	8.68	1.40	1.33
2	A	301	RET	C14-C13	5.92	1.38	1.33
2	A	301	RET	C10-C9	4.85	1.42	1.35
2	D	302	RET	C10-C9	4.38	1.41	1.35
2	B	302	RET	C10-C9	4.00	1.41	1.35
2	E	302	RET	C10-C9	3.74	1.40	1.35
2	B	302	RET	C12-C13	-2.94	1.39	1.45
2	E	302	RET	C12-C13	-2.88	1.39	1.45
2	C	301	RET	C12-C13	-2.81	1.39	1.45
2	D	302	RET	C12-C13	-2.78	1.40	1.45
2	C	301	RET	C10-C9	2.69	1.39	1.35
2	E	302	RET	C8-C9	-2.60	1.40	1.45
2	D	302	RET	C8-C9	-2.55	1.40	1.45
2	B	302	RET	C8-C9	-2.25	1.41	1.45
2	E	302	RET	C19-C9	-2.08	1.46	1.50
2	A	301	RET	C11-C12	2.08	1.39	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	305	PC1	O21-C21-C22	7.90	128.52	111.50
2	C	301	RET	C19-C9-C10	-4.85	116.13	122.92
2	C	301	RET	C19-C9-C8	4.37	124.97	118.08
2	E	302	RET	C19-C9-C10	-4.07	117.23	122.92
2	B	302	RET	C19-C9-C10	-3.82	117.58	122.92
5	C	305	PLC	O2-C'-C1'	3.71	119.51	111.50
2	A	301	RET	C19-C9-C10	-3.58	117.91	122.92
2	D	302	RET	C19-C9-C10	-3.45	118.09	122.92
2	D	302	RET	C7-C8-C9	-3.40	121.10	126.23
2	E	302	RET	C2-C1-C6	3.06	115.19	110.48
2	B	302	RET	C7-C8-C9	-2.87	121.90	126.23
4	E	305	PC1	O22-C21-C22	-2.77	112.92	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C19-C9-C8	2.60	122.18	118.08
5	A	305	PLC	O2-C2-C1	-2.32	100.02	108.40
2	D	302	RET	C19-C9-C8	2.31	121.72	118.08
4	E	305	PC1	C2-O21-C21	2.31	123.47	117.79
2	A	301	RET	C7-C8-C9	-2.26	122.82	126.23
2	B	302	RET	C11-C12-C13	2.16	132.47	126.42
2	A	301	RET	C18-C5-C4	-2.14	109.50	113.62
4	E	305	PC1	O21-C21-O22	-2.13	118.54	123.70
7	D	301	R16	C40-C39-C38	-2.11	103.74	114.42
2	A	301	RET	C1-C6-C5	-2.09	119.67	122.61
2	D	302	RET	C11-C10-C9	2.07	130.27	127.31
2	B	302	RET	C8-C9-C10	2.07	122.12	118.94
5	C	305	PLC	O2-C2-C3	2.05	115.81	108.40
4	B	305	PC1	O21-C2-C1	2.03	115.74	108.40
2	E	302	RET	C11-C10-C9	2.02	130.19	127.31

There are no chirality outliers.

All (347) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	PC1	C1-O11-P-O14
4	A	304	PC1	C12-C11-O13-P
4	A	304	PC1	O13-C11-C12-N
4	B	305	PC1	C1-O11-P-O12
4	B	305	PC1	C1-O11-P-O14
4	B	305	PC1	O13-C11-C12-N
4	B	305	PC1	O32-C31-O31-C3
4	B	305	PC1	C32-C31-O31-C3
4	C	304	PC1	O13-C11-C12-N
4	D	305	PC1	C1-O11-P-O12
4	D	305	PC1	C1-O11-P-O14
4	D	305	PC1	O11-C1-C2-O21
4	D	305	PC1	O32-C31-O31-C3
4	D	305	PC1	C32-C31-O31-C3
4	E	305	PC1	O13-C11-C12-N
4	E	305	PC1	O22-C21-O21-C2
4	E	305	PC1	C22-C21-O21-C2
5	A	305	PLC	C1-O3P-P-O1P
5	A	305	PLC	C1-O3P-P-O2P
5	A	305	PLC	C1-O3P-P-O4P
5	A	307	PLC	C1-O3P-P-O1P
5	B	306	PLC	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
5	B	306	PLC	C4-O4P-P-O1P
5	C	305	PLC	O4P-C4-C5-N
5	C	305	PLC	C1'-C'-O2-C2
5	C	305	PLC	O'-C'-O2-C2
5	C	305	PLC	C1B-CB-O3-C3
5	C	305	PLC	OB-CB-O3-C3
5	C	305	PLC	C1-O3P-P-O1P
5	D	306	PLC	C1-O3P-P-O1P
5	D	306	PLC	C1-O3P-P-O2P
5	D	306	PLC	C1-O3P-P-O4P
4	A	304	PC1	C2B-C2C-C2D-C2E
4	B	305	PC1	C38-C39-C3A-C3B
4	E	305	PC1	C27-C28-C29-C2A
4	C	304	PC1	C26-C27-C28-C29
4	A	304	PC1	C21-C22-C23-C24
4	C	304	PC1	C28-C29-C2A-C2B
7	D	301	R16	C36-C37-C38-C39
4	C	304	PC1	C21-C22-C23-C24
4	D	305	PC1	C38-C39-C3A-C3B
5	D	306	PLC	C'-C1'-C2'-C3'
4	C	304	PC1	C24-C25-C26-C27
4	A	304	PC1	C31-C32-C33-C34
4	E	305	PC1	C31-C32-C33-C34
4	C	304	PC1	C2D-C2E-C2F-C2G
4	D	305	PC1	C31-C32-C33-C34
5	C	305	PLC	C'-C1'-C2'-C3'
4	B	305	PC1	C31-C32-C33-C34
4	C	304	PC1	C38-C39-C3A-C3B
4	A	304	PC1	C1-O11-P-O13
4	B	305	PC1	C1-O11-P-O13
4	D	305	PC1	C1-O11-P-O13
5	A	307	PLC	C1-O3P-P-O4P
5	B	306	PLC	C4-O4P-P-O3P
5	B	306	PLC	C1B-C2B-C3B-C4B
5	D	306	PLC	C1B-C2B-C3B-C4B
4	B	305	PC1	C2D-C2E-C2F-C2G
4	B	305	PC1	C2E-C2F-C2G-C2H
4	D	305	PC1	C3B-C3C-C3D-C3E
4	E	305	PC1	C2C-C2D-C2E-C2F
5	C	305	PLC	C4'-C5'-C6'-C7'
5	C	305	PLC	C5'-C6'-C7'-C8'
8	C	306	8K6	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	B	308	C14	C04-C05-C06-C07
4	A	304	PC1	C33-C34-C35-C36
4	B	305	PC1	C23-C24-C25-C26
4	E	305	PC1	C3E-C3F-C3G-C3H
5	D	306	PLC	C3'-C4'-C5'-C6'
5	D	306	PLC	C3B-C4B-C5B-C6B
7	B	307	R16	C29-C30-C31-C32
7	D	307	R16	C28-C29-C30-C31
7	E	301	R16	C33-C34-C35-C36
7	E	306	R16	C30-C31-C32-C33
7	E	306	R16	C32-C33-C34-C35
4	A	304	PC1	C3B-C3C-C3D-C3E
5	A	305	PLC	C7'-C8'-C9'-CA'
5	A	305	PLC	C3B-C4B-C5B-C6B
7	B	307	R16	C37-C38-C39-C40
4	E	305	PC1	C22-C23-C24-C25
4	E	305	PC1	C3B-C3C-C3D-C3E
5	D	306	PLC	C7B-C8B-C9B-CAA
9	B	308	C14	C05-C06-C07-C08
4	A	304	PC1	C39-C3A-C3B-C3C
4	B	305	PC1	C2B-C2C-C2D-C2E
5	B	306	PLC	C4B-C5B-C6B-C7B
5	D	306	PLC	C2'-C3'-C4'-C5'
7	D	301	R16	C31-C32-C33-C34
5	A	307	PLC	C'-C1'-C2'-C3'
5	A	305	PLC	O2-C2-C3-O3
7	B	307	R16	C35-C36-C37-C38
4	A	304	PC1	C3D-C3E-C3F-C3G
4	B	305	PC1	C22-C23-C24-C25
4	A	304	PC1	C32-C33-C34-C35
4	B	305	PC1	C35-C36-C37-C38
4	E	305	PC1	C24-C25-C26-C27
5	C	305	PLC	C7B-C8B-C9B-CAA
5	D	306	PLC	C7'-C8'-C9'-CA'
4	A	304	PC1	C3C-C3D-C3E-C3F
4	B	305	PC1	C29-C2A-C2B-C2C
7	D	307	R16	C33-C34-C35-C36
5	A	305	PLC	O'-C'-O2-C2
4	B	305	PC1	C39-C3A-C3B-C3C
4	E	305	PC1	C3A-C3B-C3C-C3D
5	A	305	PLC	C3'-C4'-C5'-C6'
5	A	307	PLC	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
5	A	307	PLC	C4B-C5B-C6B-C7B
5	B	306	PLC	C5'-C6'-C7'-C8'
7	B	307	R16	C36-C37-C38-C39
9	B	308	C14	C02-C03-C04-C05
4	A	304	PC1	C25-C26-C27-C28
8	C	306	8K6	C5-C6-C7-C8
4	A	304	PC1	C24-C25-C26-C27
4	D	305	PC1	C2A-C2B-C2C-C2D
4	D	305	PC1	C2D-C2E-C2F-C2G
4	E	305	PC1	C23-C24-C25-C26
4	E	305	PC1	C37-C38-C39-C3A
6	A	306	D12	C4-C5-C6-C7
7	E	306	R16	C31-C32-C33-C34
5	B	306	PLC	C2'-C3'-C4'-C5'
5	D	306	PLC	C6B-C7B-C8B-C9B
9	E	307	C14	C04-C05-C06-C07
4	A	304	PC1	C3F-C3G-C3H-C3I
4	D	305	PC1	C33-C34-C35-C36
5	C	305	PLC	C2B-C3B-C4B-C5B
8	B	301	8K6	C9-C10-C11-C12
7	A	308	R16	C30-C31-C32-C33
7	B	307	R16	C32-C33-C34-C35
5	A	305	PLC	C4'-C5'-C6'-C7'
4	A	304	PC1	C29-C2A-C2B-C2C
4	C	304	PC1	C34-C35-C36-C37
4	D	305	PC1	C22-C21-O21-C2
5	A	305	PLC	C1'-C'-O2-C2
4	B	305	PC1	C37-C38-C39-C3A
5	A	305	PLC	C1'-C2'-C3'-C4'
6	D	308	D12	C4-C5-C6-C7
7	B	307	R16	C28-C29-C30-C31
4	A	304	PC1	C23-C24-C25-C26
4	C	304	PC1	C36-C37-C38-C39
7	A	308	R16	C33-C34-C35-C36
4	B	305	PC1	C26-C27-C28-C29
5	C	305	PLC	C3B-C4B-C5B-C6B
5	A	305	PLC	C5'-C6'-C7'-C8'
8	B	301	8K6	C11-C12-C13-C14
5	A	307	PLC	C2'-C3'-C4'-C5'
7	B	307	R16	C30-C31-C32-C33
4	C	304	PC1	C3B-C3C-C3D-C3E
5	A	307	PLC	C8B-C9B-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	B	308	C14	C06-C07-C08-C09
4	E	305	PC1	C32-C31-O31-C3
8	C	306	8K6	C10-C11-C12-C13
6	A	306	D12	C2-C3-C4-C5
8	B	301	8K6	C13-C14-C15-C16
4	E	305	PC1	C38-C39-C3A-C3B
6	D	308	D12	C5-C6-C7-C8
4	A	304	PC1	C22-C23-C24-C25
4	E	305	PC1	C2E-C2F-C2G-C2H
6	A	306	D12	C7-C8-C9-C10
4	D	305	PC1	C36-C37-C38-C39
5	A	305	PLC	C6B-C7B-C8B-C9B
5	A	307	PLC	C6B-C7B-C8B-C9B
4	B	305	PC1	C22-C21-O21-C2
4	B	305	PC1	O11-C1-C2-O21
5	B	306	PLC	C3'-C4'-C5'-C6'
5	B	306	PLC	CB-C1B-C2B-C3B
7	A	308	R16	C35-C36-C37-C38
4	B	305	PC1	C32-C33-C34-C35
8	B	301	8K6	C2-C3-C4-C5
4	C	304	PC1	C35-C36-C37-C38
4	C	304	PC1	C2E-C2F-C2G-C2H
4	B	305	PC1	C11-O13-P-O11
4	D	305	PC1	C11-O13-P-O11
5	C	305	PLC	C1-O3P-P-O4P
5	C	305	PLC	C1'-C2'-C3'-C4'
4	C	304	PC1	O11-C1-C2-C3
5	D	306	PLC	O3P-C1-C2-C3
6	D	308	D12	C6-C7-C8-C9
8	C	306	8K6	C7-C8-C9-C10
4	B	305	PC1	C3A-C3B-C3C-C3D
4	D	305	PC1	C2E-C2F-C2G-C2H
9	B	308	C14	C08-C09-C10-C11
6	D	308	D12	C1-C2-C3-C4
7	D	307	R16	C34-C35-C36-C37
4	A	304	PC1	C1-C2-C3-O31
4	E	305	PC1	C3D-C3E-C3F-C3G
4	E	305	PC1	C2A-C2B-C2C-C2D
8	B	301	8K6	C14-C15-C16-C17
4	C	304	PC1	C2C-C2D-C2E-C2F
7	D	301	R16	C29-C30-C31-C32
8	C	306	8K6	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
7	B	307	R16	C38-C39-C40-C41
7	D	301	R16	C32-C33-C34-C35
5	A	305	PLC	C1B-C2B-C3B-C4B
5	A	305	PLC	C'-C1'-C2'-C3'
5	B	306	PLC	C'-C1'-C2'-C3'
8	B	301	8K6	C1-C2-C3-C4
4	E	305	PC1	C3-C2-O21-C21
4	D	305	PC1	C25-C26-C27-C28
4	C	304	PC1	C37-C38-C39-C3A
6	A	306	D12	C6-C7-C8-C9
8	B	301	8K6	C6-C7-C8-C9
5	C	305	PLC	O3P-C1-C2-O2
4	E	305	PC1	C28-C29-C2A-C2B
5	A	307	PLC	O2-C2-C3-O3
7	A	308	R16	C38-C39-C40-C41
7	E	301	R16	C39-C40-C41-C42
4	D	305	PC1	C3F-C3G-C3H-C3I
5	D	306	PLC	C8B-C9B-CAA-CBA
4	B	305	PC1	C3F-C3G-C3H-C3I
4	D	305	PC1	C35-C36-C37-C38
8	B	301	8K6	C15-C16-C17-C18
4	B	305	PC1	O11-C1-C2-C3
4	A	304	PC1	C2F-C2G-C2H-C2I
4	D	305	PC1	C2B-C2C-C2D-C2E
5	A	305	PLC	C8B-C9B-CAA-CBA
5	C	305	PLC	C8'-C9'-CA'-CB'
9	E	307	C14	C06-C07-C08-C09
7	E	301	R16	C30-C31-C32-C33
4	C	304	PC1	C23-C24-C25-C26
5	A	307	PLC	C2-C1-O3P-P
4	D	305	PC1	C26-C27-C28-C29
8	C	306	8K6	C11-C10-C9-C8
4	D	305	PC1	C2F-C2G-C2H-C2I
4	D	305	PC1	C34-C35-C36-C37
5	A	305	PLC	C1-C2-C3-O3
5	A	307	PLC	C1-C2-C3-O3
4	C	304	PC1	C2F-C2G-C2H-C2I
4	E	305	PC1	C3F-C3G-C3H-C3I
5	A	305	PLC	C5B-C6B-C7B-C8B
7	E	306	R16	C36-C37-C38-C39
4	E	305	PC1	C2F-C2G-C2H-C2I
4	C	304	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
5	D	306	PLC	O3P-C1-C2-O2
5	A	307	PLC	C5'-C6'-C7'-C8'
4	A	304	PC1	O21-C2-C3-O31
4	C	304	PC1	C29-C2A-C2B-C2C
4	D	305	PC1	C28-C29-C2A-C2B
8	C	306	8K6	C14-C15-C16-C17
4	B	305	PC1	C3B-C3C-C3D-C3E
4	D	305	PC1	O22-C21-O21-C2
7	A	308	R16	C27-C28-C29-C30
7	B	307	R16	C39-C40-C41-C42
7	B	307	R16	C33-C34-C35-C36
4	D	305	PC1	O11-C1-C2-C3
5	A	305	PLC	C6'-C7'-C8'-C9'
4	C	304	PC1	C39-C3A-C3B-C3C
4	E	305	PC1	C33-C34-C35-C36
5	B	306	PLC	C1'-C2'-C3'-C4'
8	B	301	8K6	C11-C10-C9-C8
4	A	304	PC1	C34-C35-C36-C37
7	A	308	R16	C37-C38-C39-C40
4	C	304	PC1	C1-C2-C3-O31
4	C	304	PC1	C22-C21-O21-C2
5	A	305	PLC	O3P-C1-C2-O2
7	E	301	R16	C38-C39-C40-C41
5	B	306	PLC	C8B-C9B-CAA-CBA
6	A	306	D12	C1-C2-C3-C4
4	C	304	PC1	C32-C33-C34-C35
7	E	306	R16	C38-C39-C40-C41
4	C	304	PC1	C2B-C2C-C2D-C2E
7	E	306	R16	C35-C36-C37-C38
8	B	301	8K6	C7-C8-C9-C10
5	C	305	PLC	C4B-C5B-C6B-C7B
5	D	306	PLC	C5'-C6'-C7'-C8'
5	A	305	PLC	C2-C1-O3P-P
4	A	304	PC1	C1-O11-P-O12
4	D	305	PC1	C11-O13-P-O12
5	A	307	PLC	C1-O3P-P-O2P
5	C	305	PLC	C1-O3P-P-O2P
5	A	305	PLC	O3P-C1-C2-C3
9	E	307	C14	C03-C04-C05-C06
5	A	307	PLC	C8'-C9'-CA'-CB'
4	B	305	PC1	C12-C11-O13-P
4	D	305	PC1	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
5	B	306	PLC	C5-C4-O4P-P
4	B	305	PC1	O22-C21-O21-C2
4	E	305	PC1	C32-C33-C34-C35
5	B	306	PLC	C3B-C4B-C5B-C6B
5	A	305	PLC	C8'-C9'-CA'-CB'
7	D	301	R16	C34-C35-C36-C37
5	B	306	PLC	O4P-C4-C5-N
5	D	306	PLC	O4P-C4-C5-N
4	C	304	PC1	O21-C2-C3-O31
5	D	306	PLC	O2-C2-C3-O3
4	C	304	PC1	C2A-C2B-C2C-C2D
4	A	304	PC1	C38-C39-C3A-C3B
4	C	304	PC1	O31-C31-C32-C33
4	E	305	PC1	C2D-C2E-C2F-C2G
7	D	307	R16	C31-C32-C33-C34
5	A	307	PLC	C6'-C7'-C8'-C9'
8	C	306	8K6	C13-C14-C15-C16
5	D	306	PLC	C1-C2-O2-C'
7	D	301	R16	C33-C34-C35-C36
5	C	305	PLC	C4-O4P-P-O3P
5	D	306	PLC	C4-O4P-P-O3P
9	B	308	C14	C09-C10-C11-C12
4	C	304	PC1	C3C-C3D-C3E-C3F
5	D	306	PLC	C2-C1-O3P-P
4	E	305	PC1	C26-C27-C28-C29
7	E	301	R16	C34-C35-C36-C37
4	D	305	PC1	C3D-C3E-C3F-C3G
9	E	307	C14	C05-C06-C07-C08
5	A	305	PLC	CB-C1B-C2B-C3B
4	D	305	PC1	C21-C22-C23-C24
7	D	307	R16	C29-C30-C31-C32
4	D	305	PC1	C3A-C3B-C3C-C3D
5	D	306	PLC	CB-C1B-C2B-C3B
7	D	307	R16	C27-C28-C29-C30
5	D	306	PLC	C6'-C7'-C8'-C9'
5	C	305	PLC	C7'-C8'-C9'-CA'
6	D	308	D12	C11-C10-C9-C8
4	E	305	PC1	O32-C31-O31-C3
7	E	306	R16	C28-C29-C30-C31
6	A	306	D12	C5-C6-C7-C8
5	D	306	PLC	O2-C'-C1'-C2'
5	C	305	PLC	C2B-C1B-CB-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	306	PLC	C5B-C6B-C7B-C8B
9	E	307	C14	C11-C12-C13-C14
5	C	305	PLC	O3P-C1-C2-C3
5	B	306	PLC	C6B-C7B-C8B-C9B
5	C	305	PLC	O2-C2-C3-O3
7	A	308	R16	C32-C33-C34-C35
8	C	306	8K6	C9-C10-C11-C12
5	A	305	PLC	C7B-C8B-C9B-CAA
4	C	304	PC1	C2-C3-O31-C31
4	D	305	PC1	C2C-C2D-C2E-C2F
5	D	306	PLC	O'-C'-C1'-C2'
4	C	304	PC1	C3E-C3F-C3G-C3H
5	D	306	PLC	C1-C2-C3-O3
6	A	306	D12	C3-C4-C5-C6
4	A	304	PC1	C11-O13-P-O14
4	B	305	PC1	C11-O13-P-O14
4	C	304	PC1	C1-O11-P-O14
4	D	305	PC1	C11-O13-P-O14
4	E	305	PC1	C11-O13-P-O14
5	B	306	PLC	C1-O3P-P-O1P
5	C	305	PLC	C2B-C1B-CB-OB
5	A	307	PLC	C4'-C5'-C6'-C7'
5	A	307	PLC	C2B-C3B-C4B-C5B
5	C	305	PLC	C5-C4-O4P-P
4	D	305	PC1	C22-C23-C24-C25
4	D	305	PC1	O31-C31-C32-C33
8	B	301	8K6	C10-C11-C12-C13
9	E	307	C14	C10-C11-C12-C13
5	B	306	PLC	O3P-C1-C2-O2
4	D	305	PC1	O32-C31-C32-C33
4	C	304	PC1	O32-C31-C32-C33

There are no ring outliers.

17 monomers are involved in 36 short contacts:

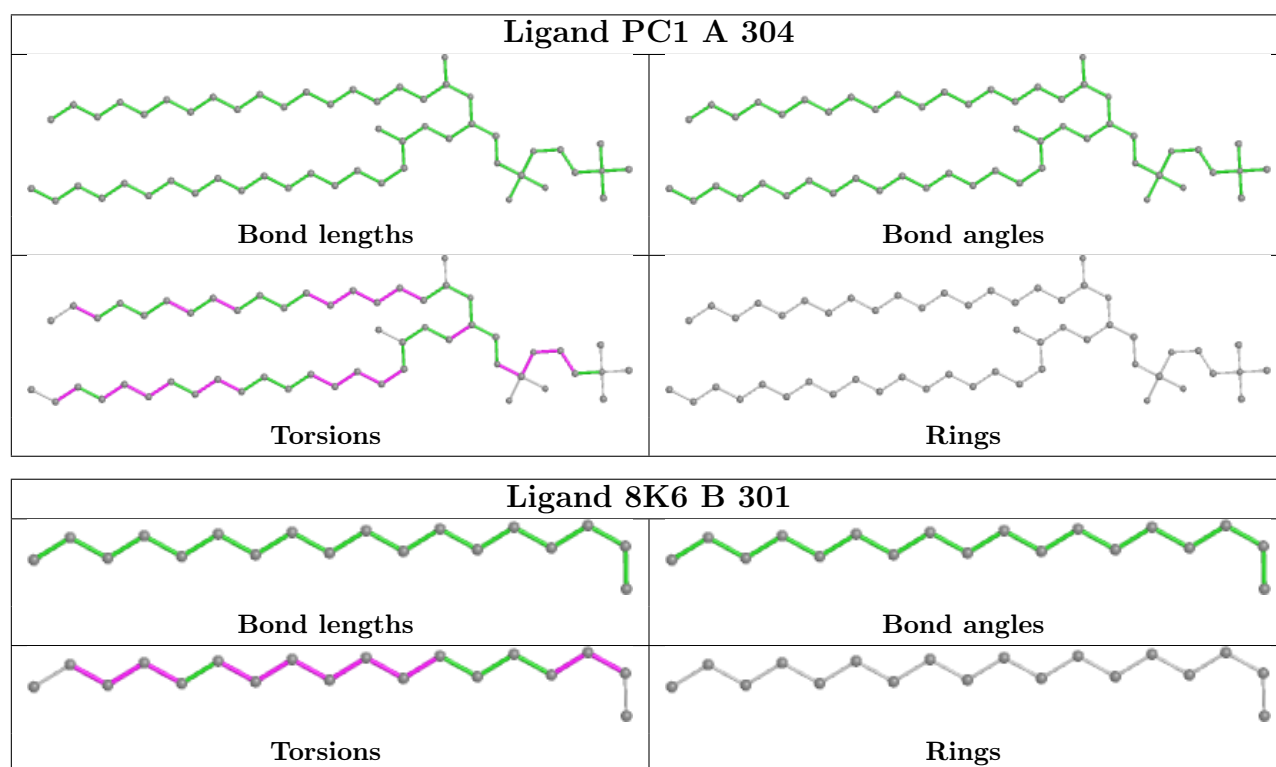
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	PC1	2	0
8	B	301	8K6	1	0
4	D	305	PC1	1	0
4	C	304	PC1	1	0
4	E	305	PC1	7	0
5	D	306	PLC	2	0

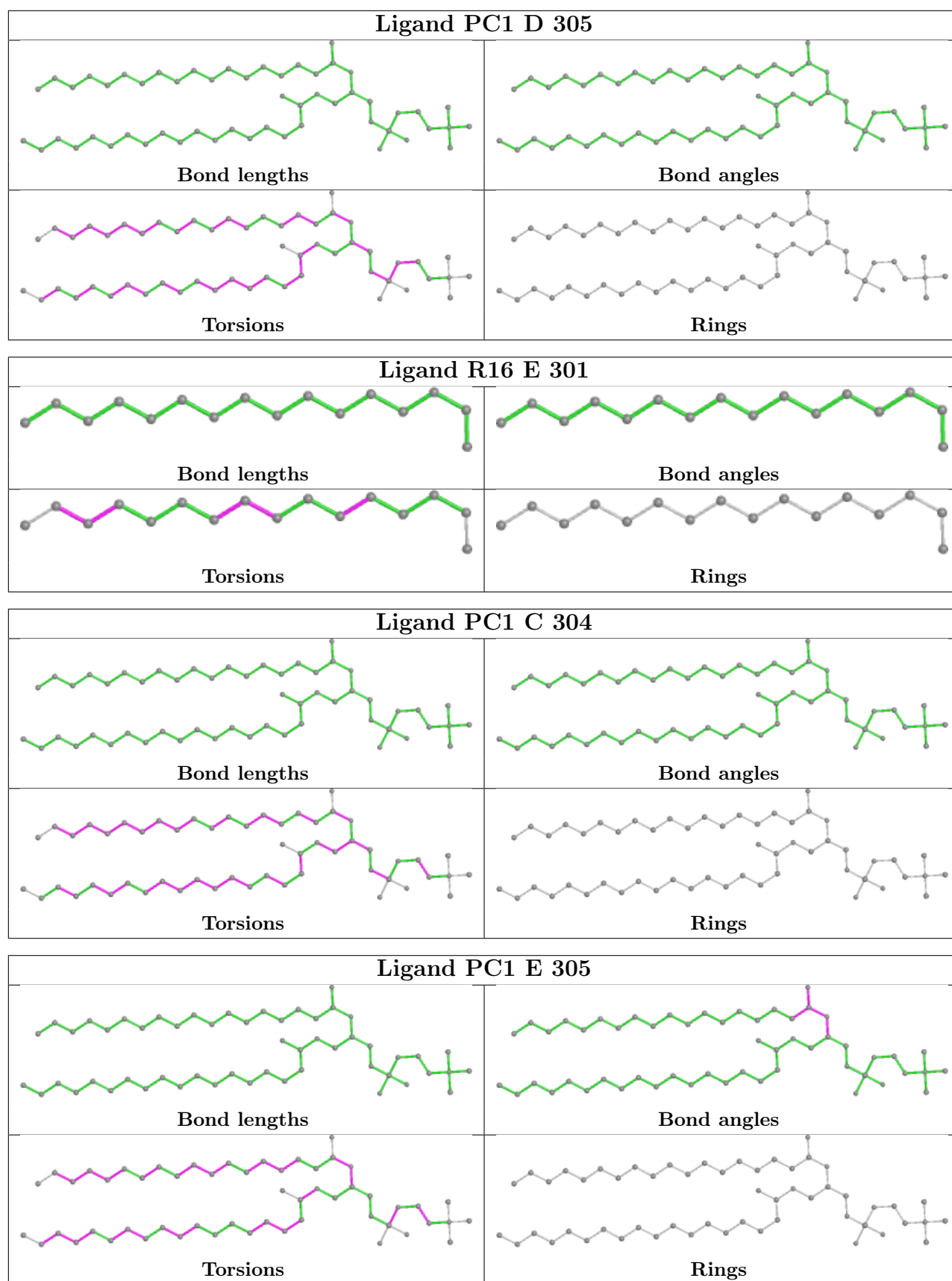
*Continued on next page...*

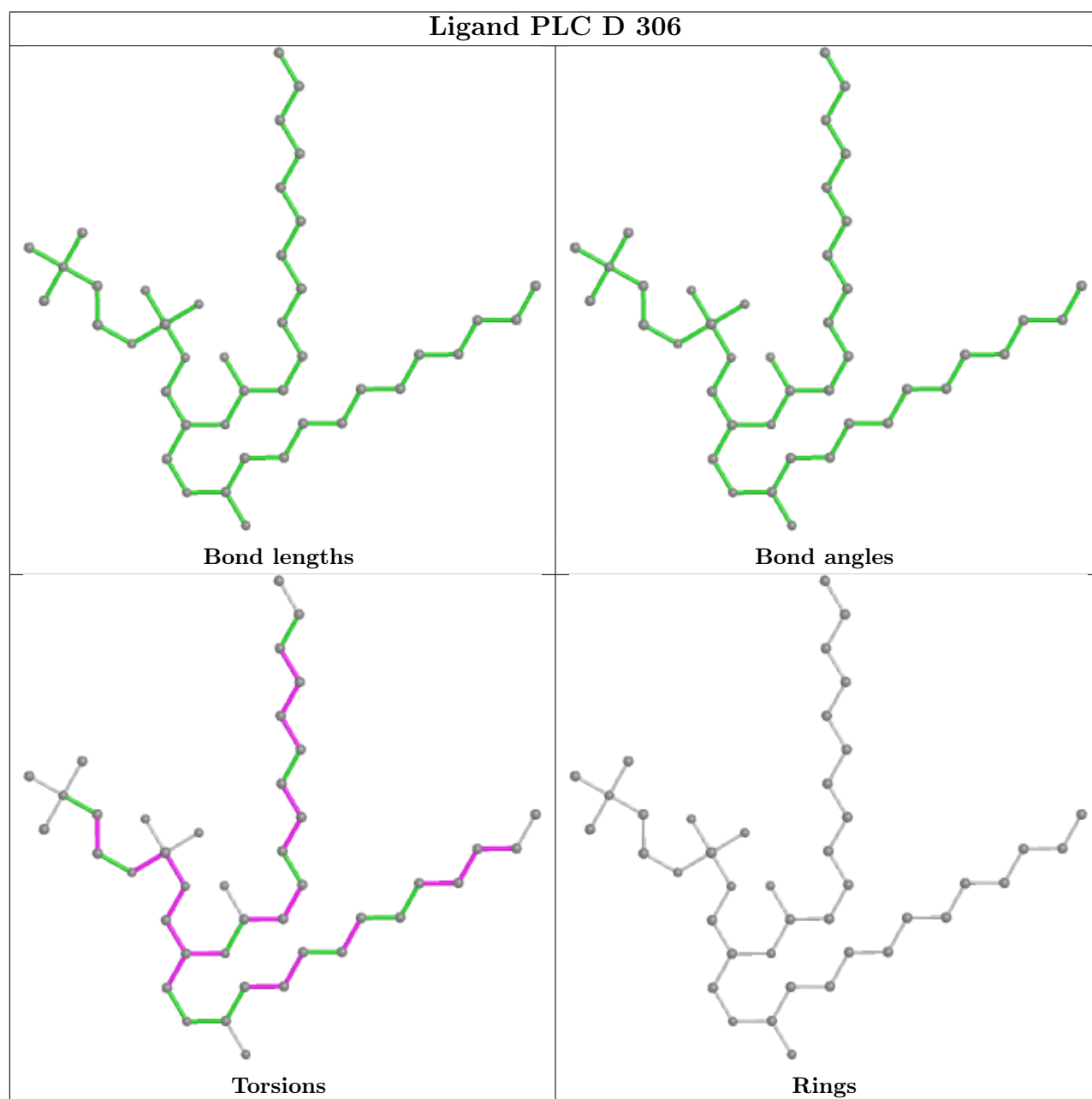
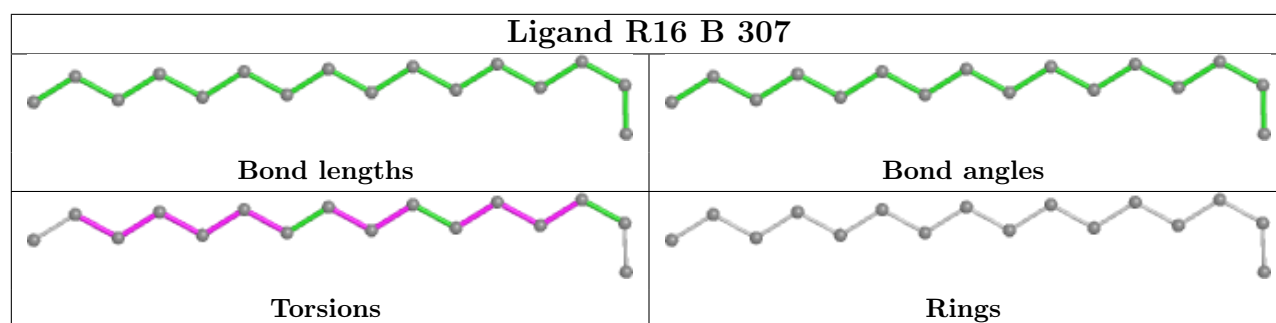
*Continued from previous page...*

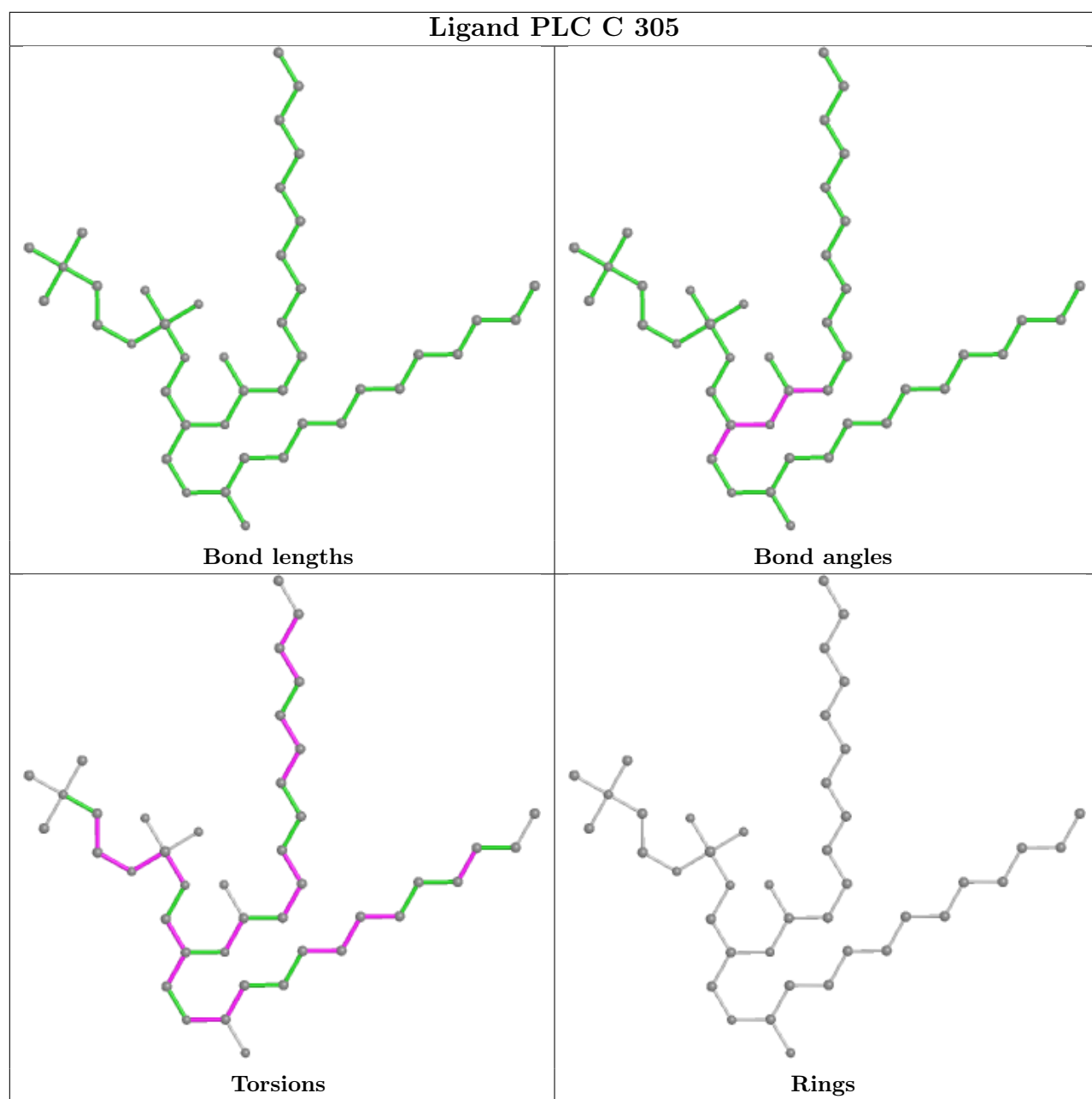
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	305	PLC	2	0
2	A	301	RET	3	0
6	A	306	D12	1	0
8	C	306	8K6	1	0
4	B	305	PC1	1	0
2	E	302	RET	4	0
7	D	307	R16	1	0
7	D	301	R16	2	0
2	B	302	RET	4	0
2	C	301	RET	3	0
2	D	302	RET	2	0

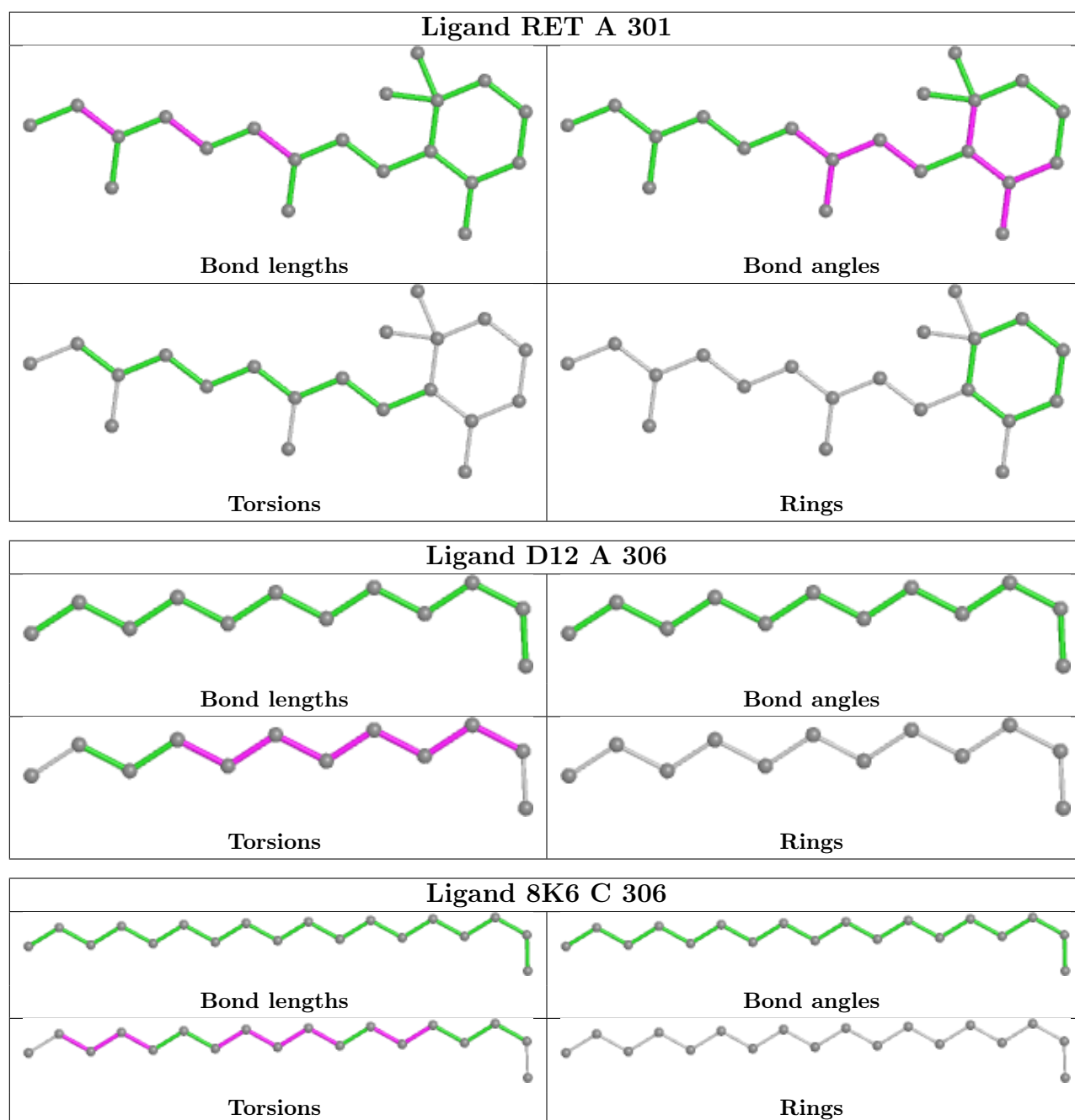
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

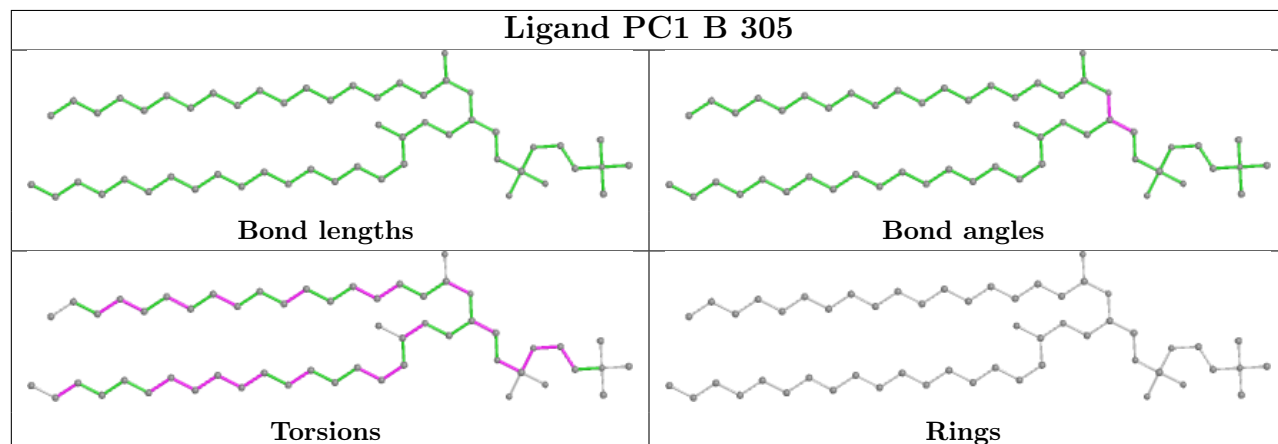
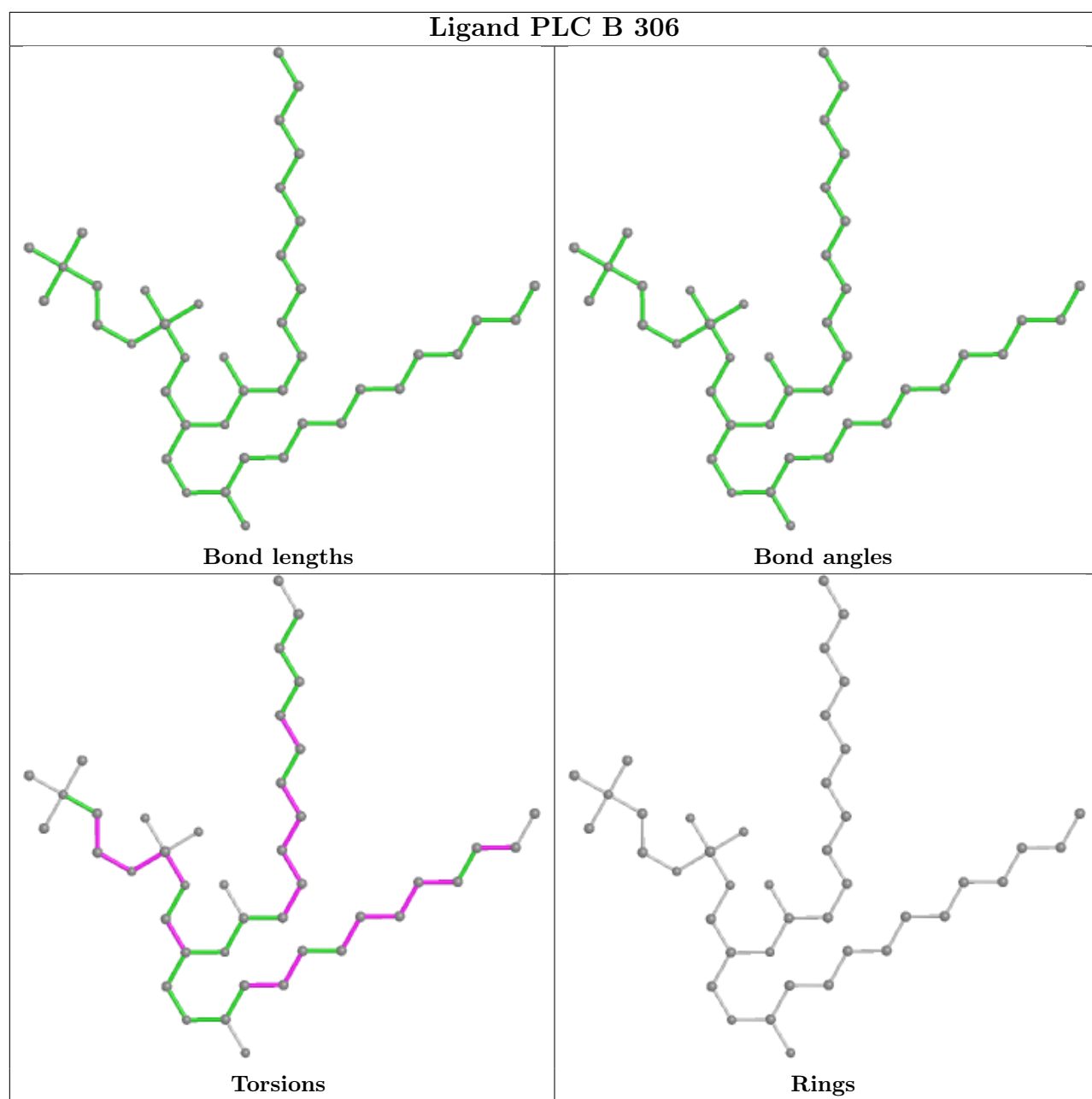




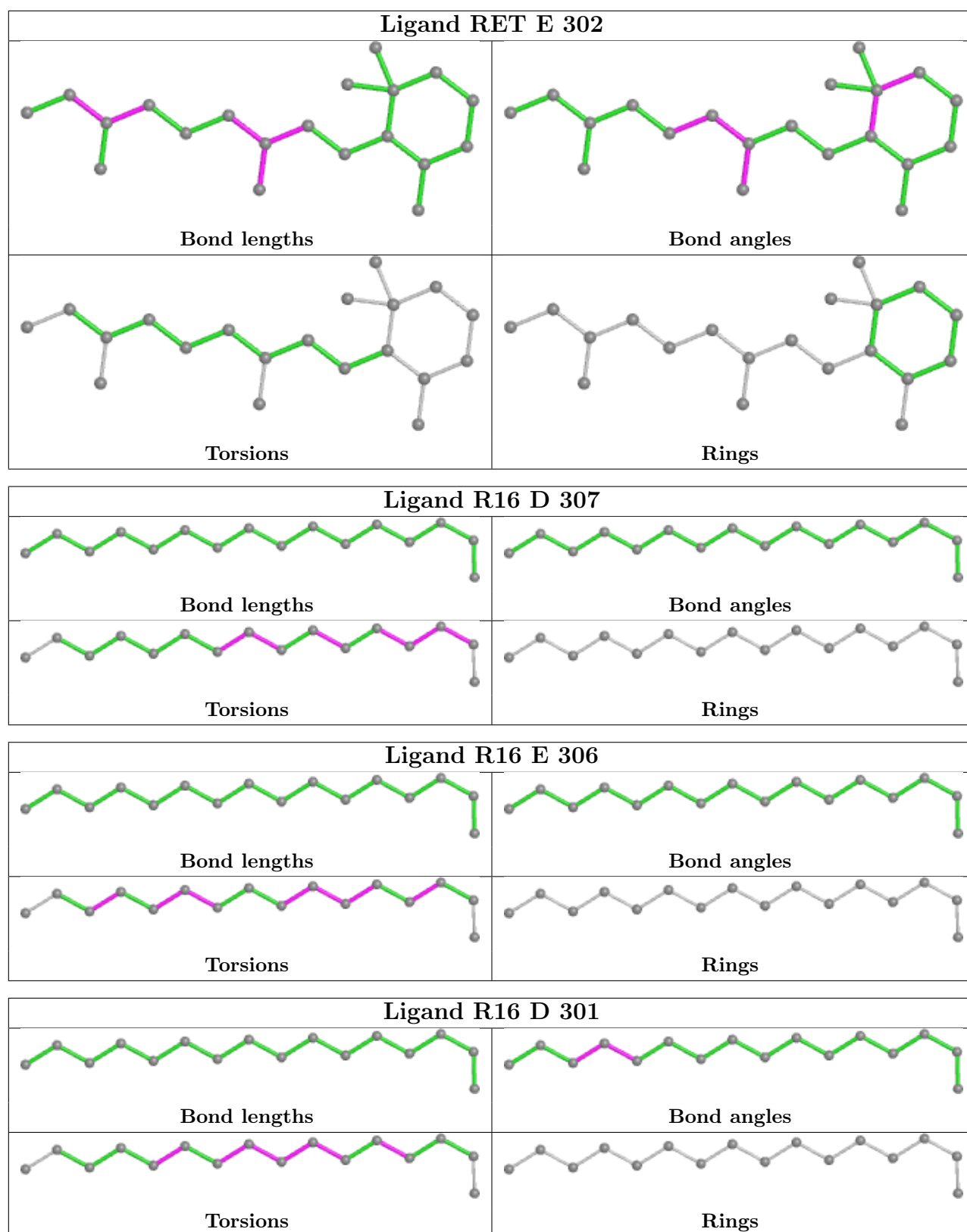


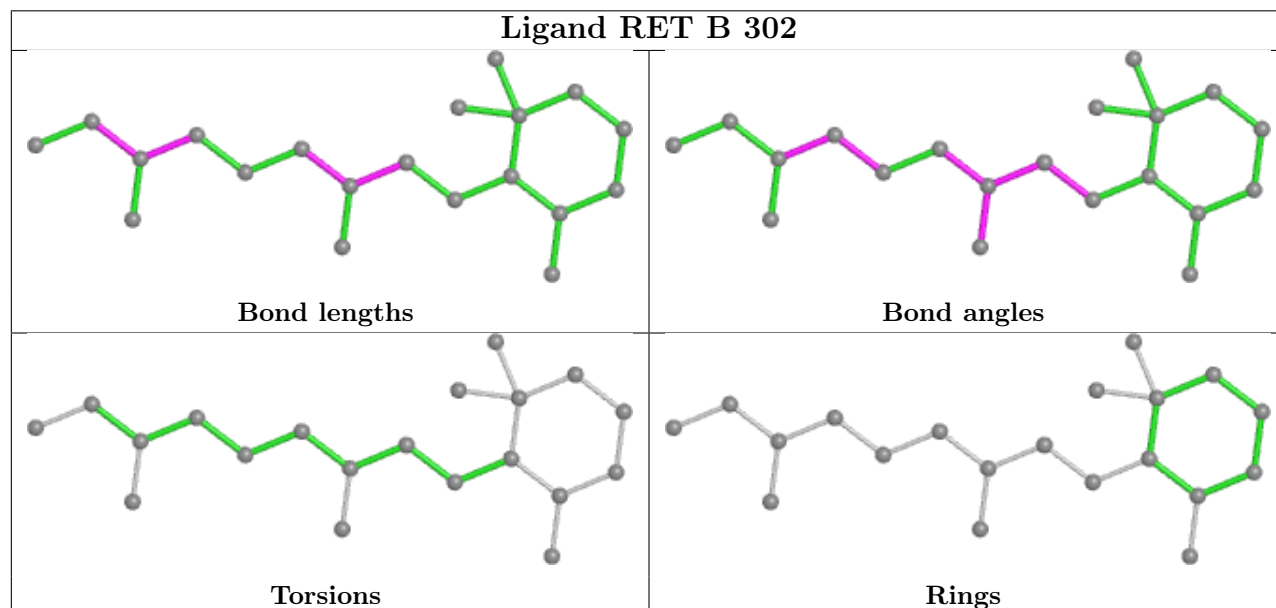
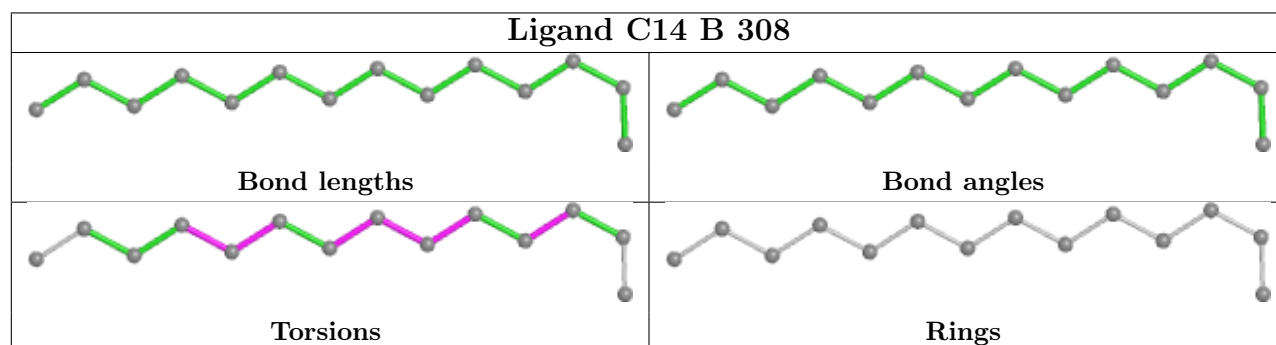
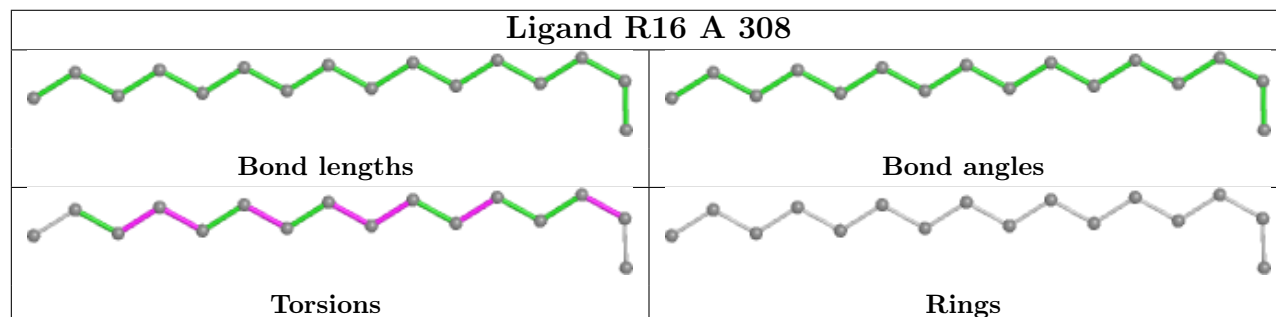
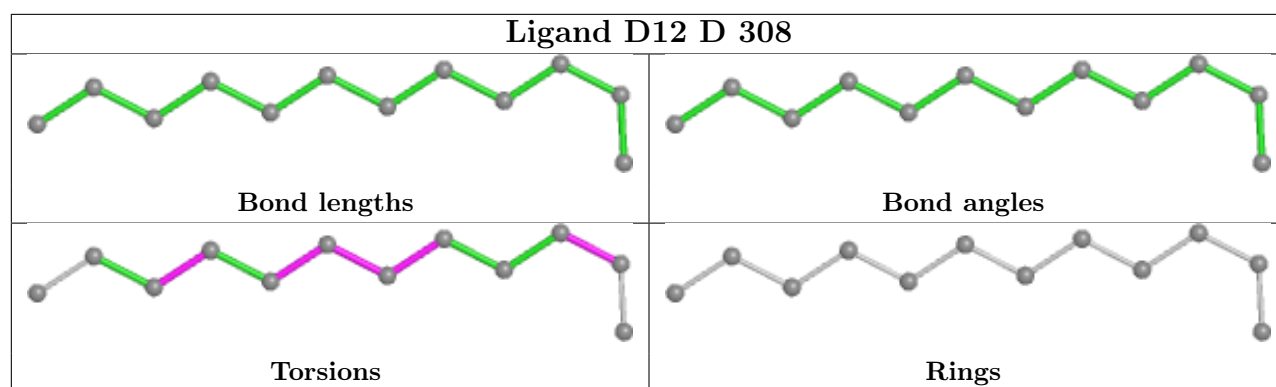


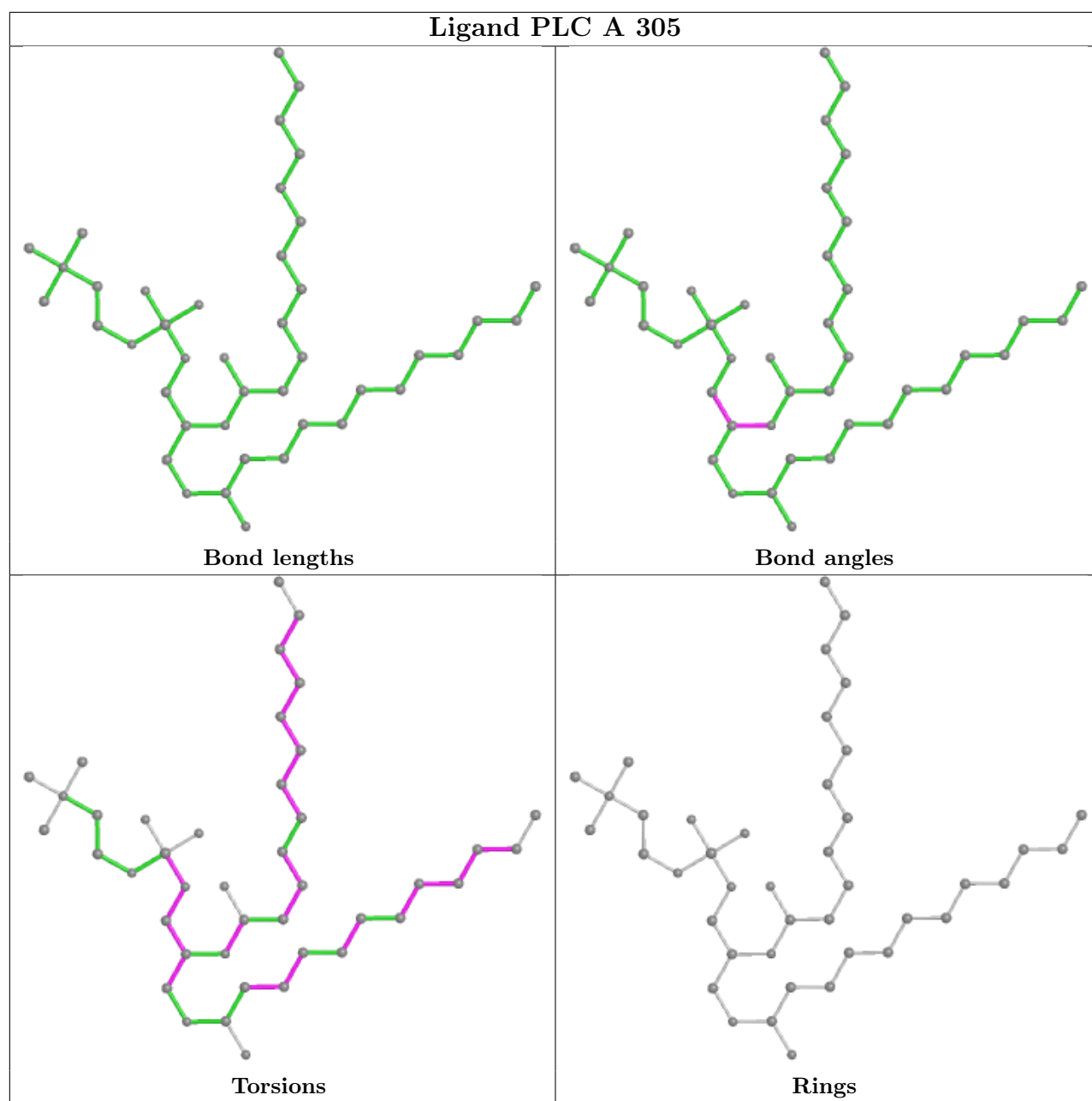


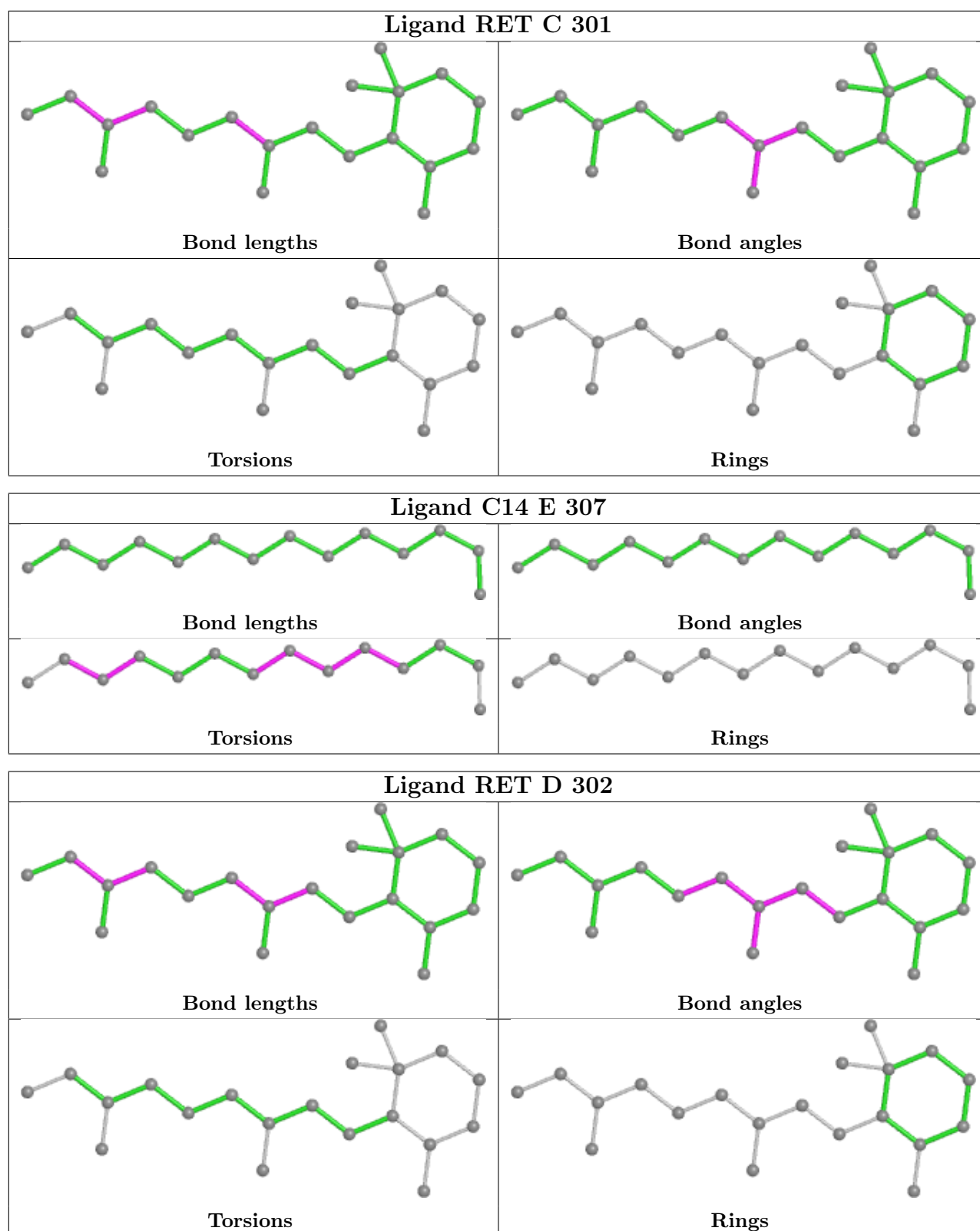


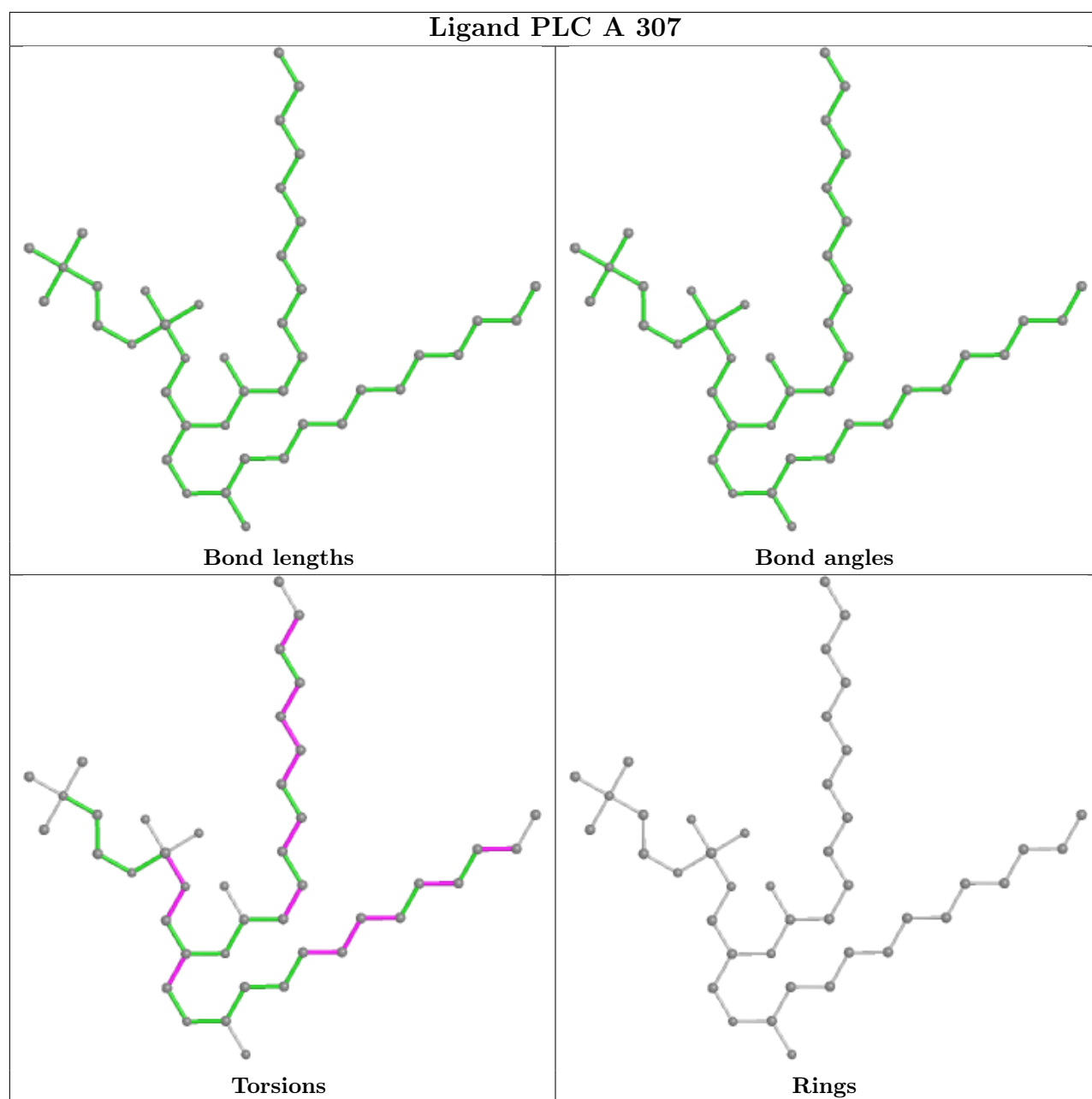












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

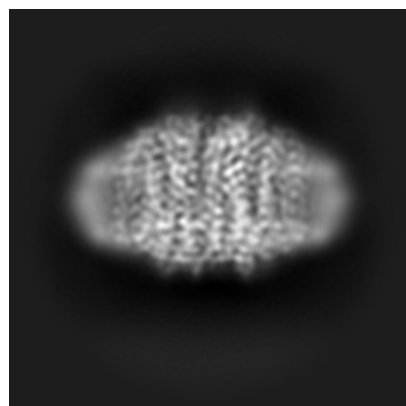
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61688. These allow visual inspection of the internal detail of the map and identification of artifacts.

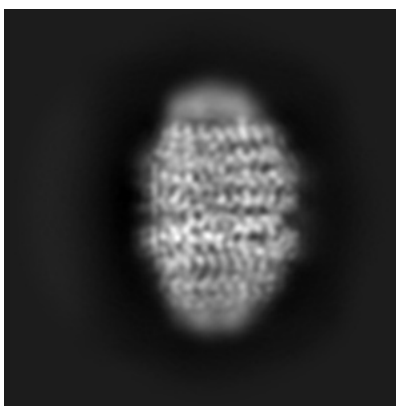
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

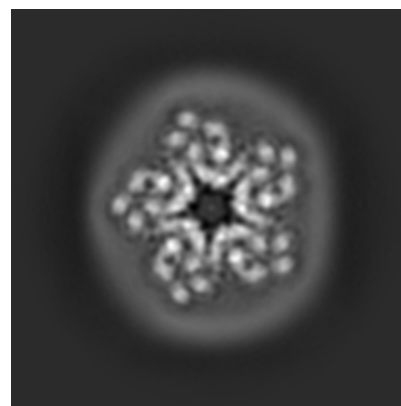
#### 6.1.1 Primary map



X

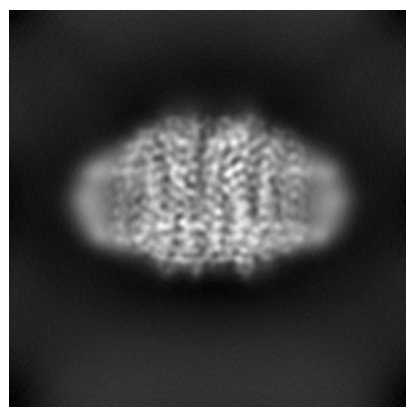


Y

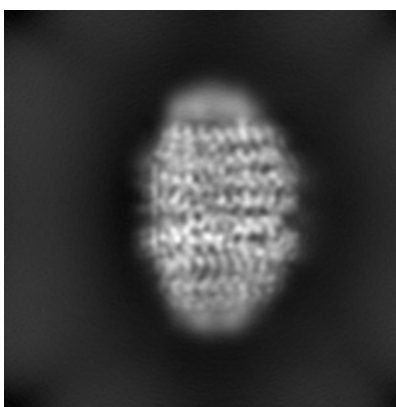


Z

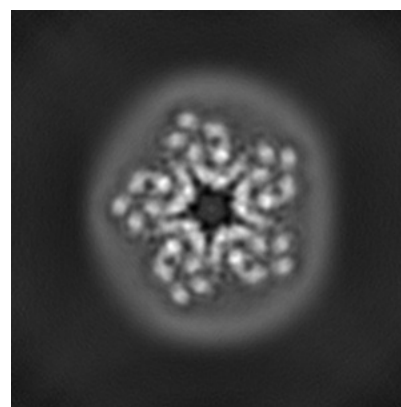
#### 6.1.2 Raw map



X



Y

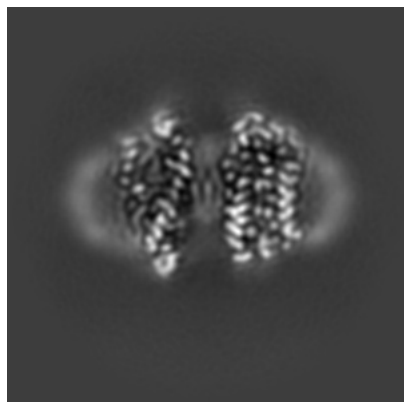


Z

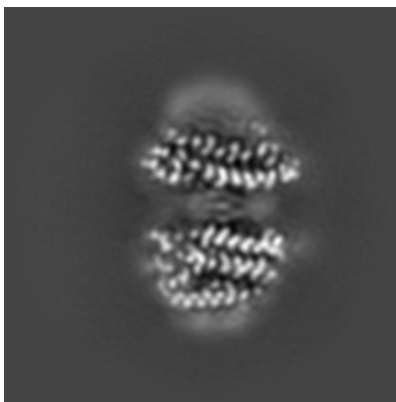
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

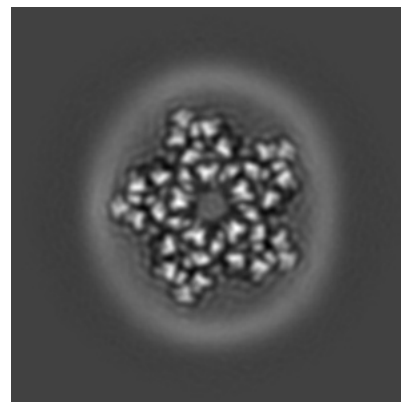
### 6.2.1 Primary map



X Index: 100

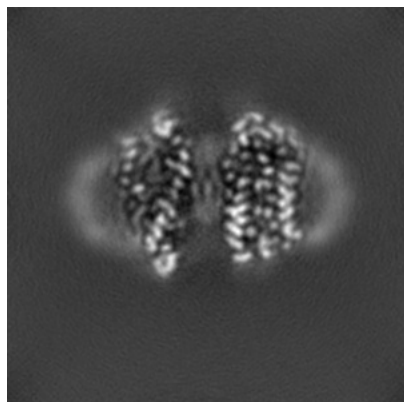


Y Index: 100

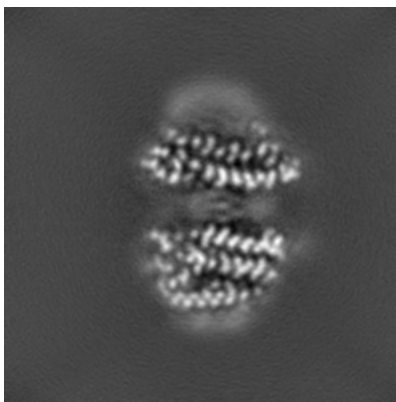


Z Index: 100

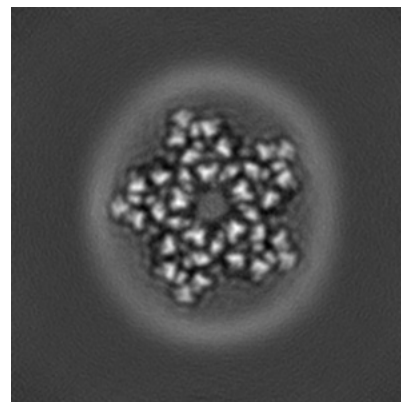
### 6.2.2 Raw map



X Index: 100



Y Index: 100

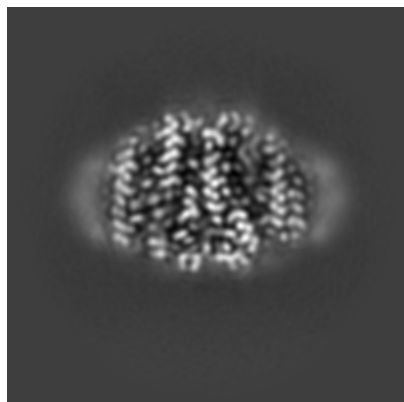


Z Index: 100

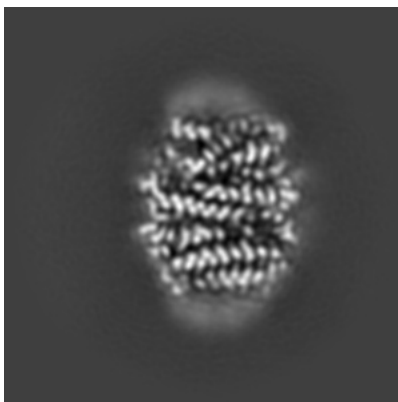
The images above show central slices of the map in three orthogonal directions.

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

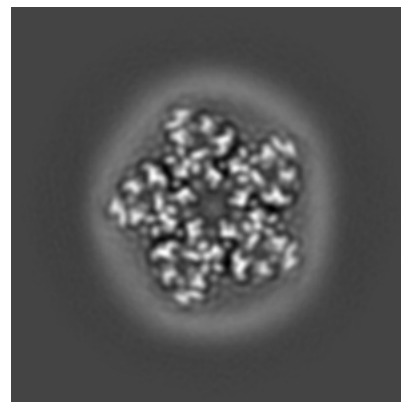
### 6.3.1 Primary map



X Index: 83

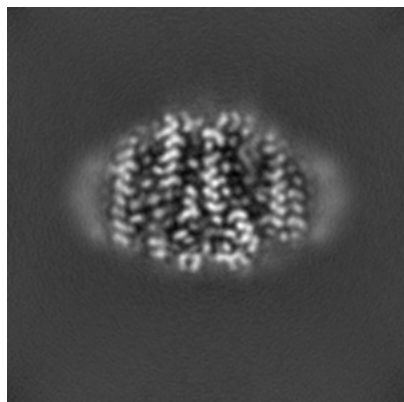


Y Index: 115

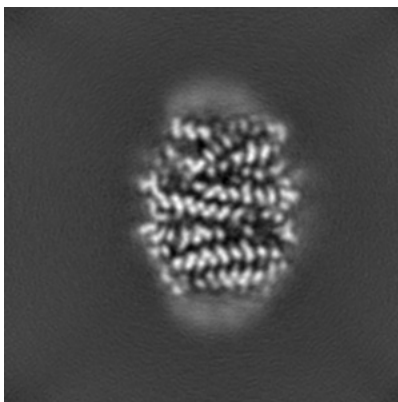


Z Index: 92

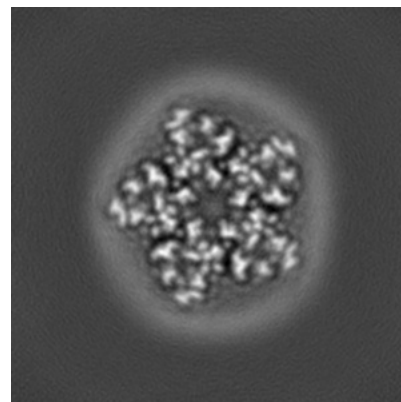
### 6.3.2 Raw map



X Index: 83



Y Index: 115



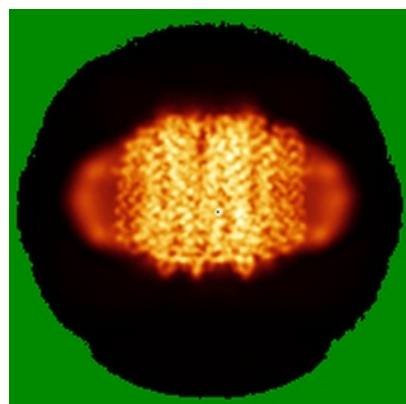
Z Index: 92

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

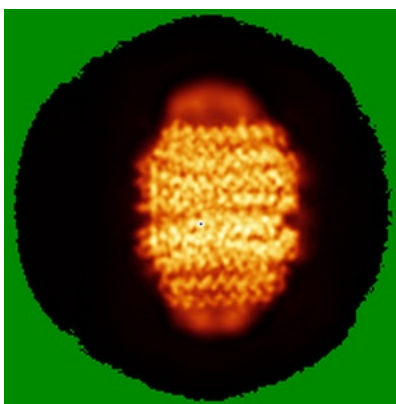


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

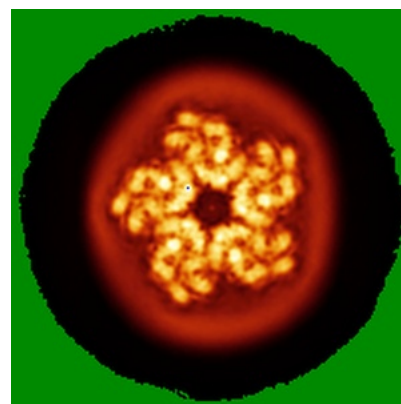
### 6.4.1 Primary map



X

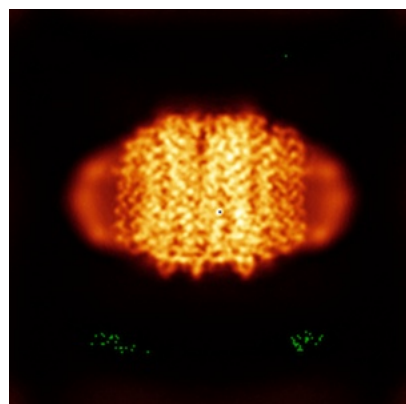


Y

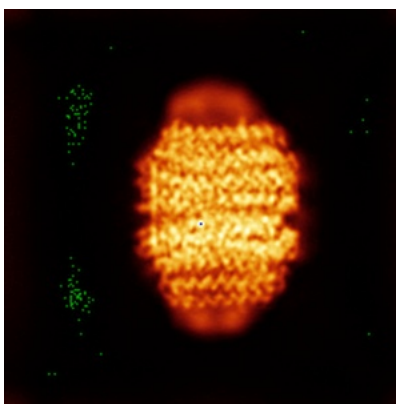


Z

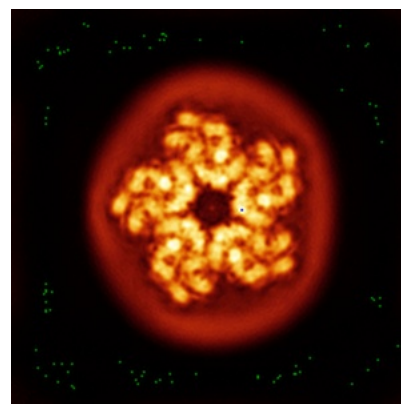
### 6.4.2 Raw map



X



Y

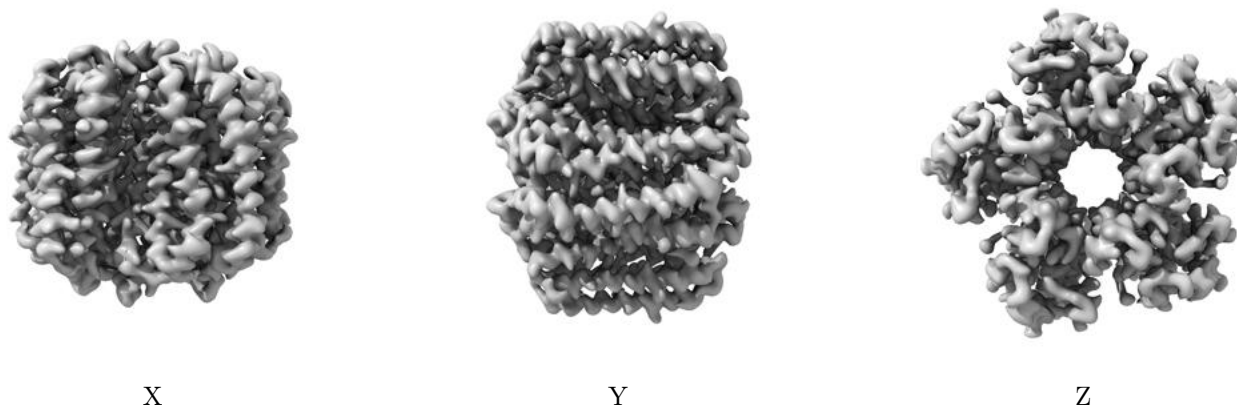


Z

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.

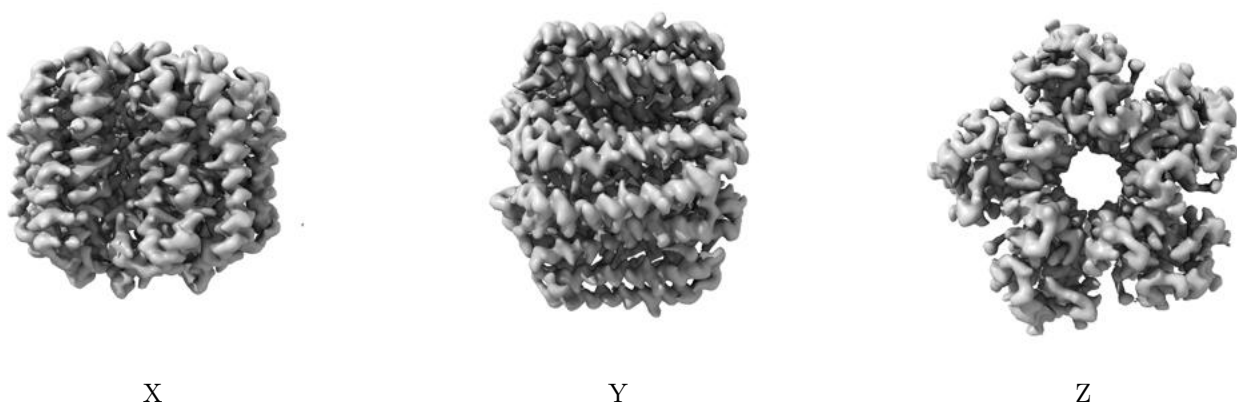
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.031. 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.

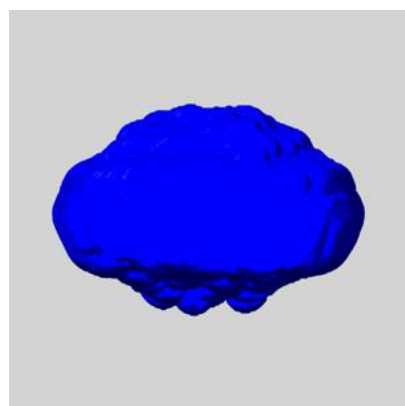
## 6.6 Mask visualisation [i](#)

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

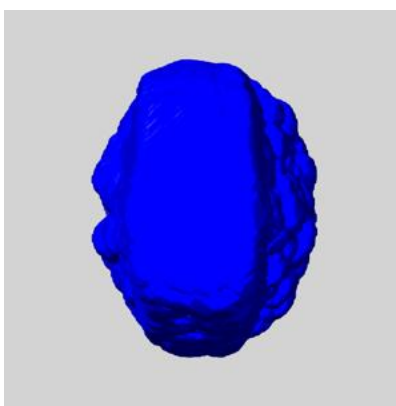
A mask typically either:

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

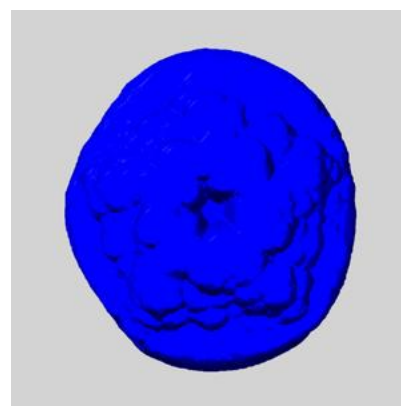
### 6.6.1 emd\_61688\_msk\_1.map [i](#)



X



Y

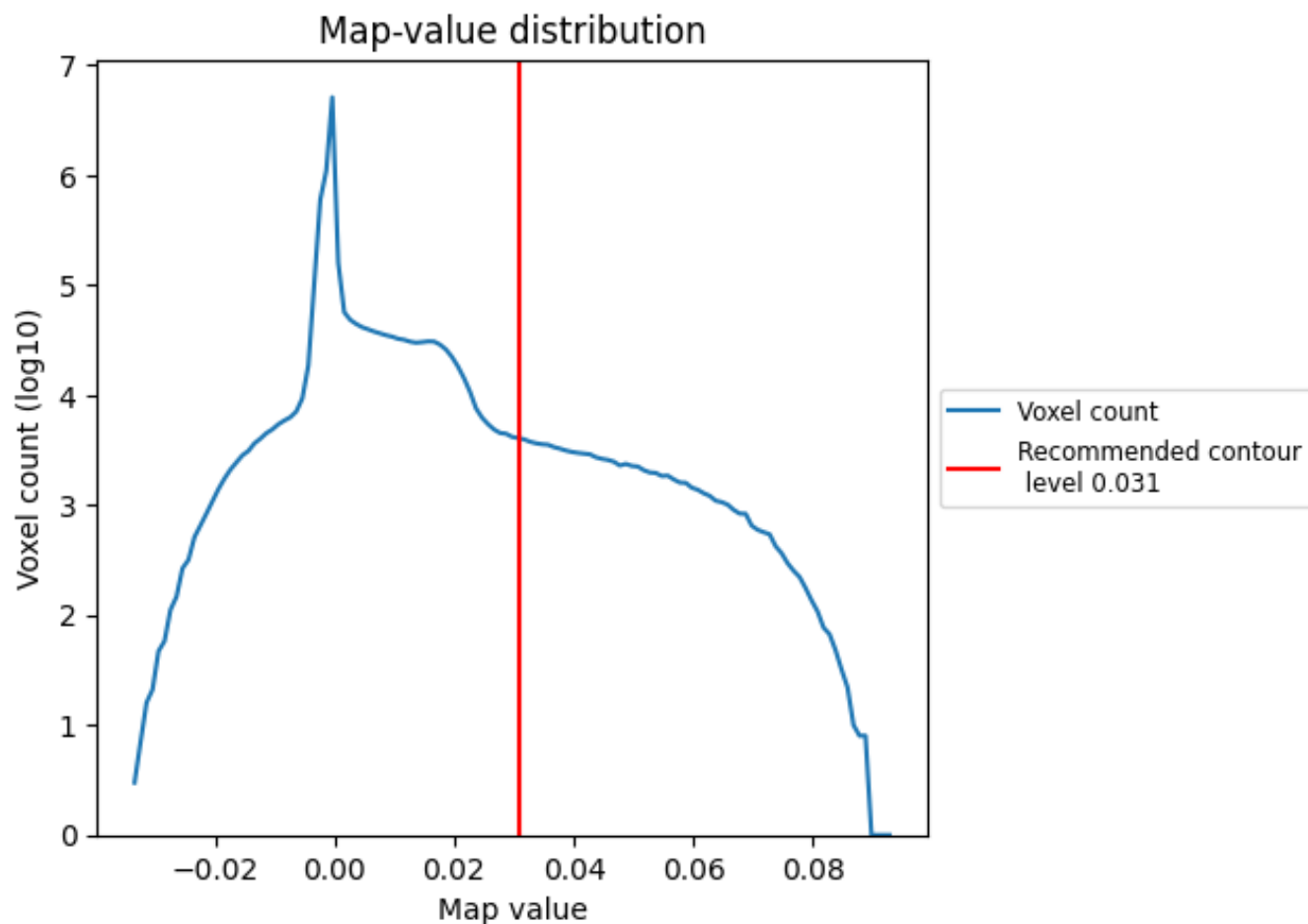


Z

## 7 Map analysis [i](#)

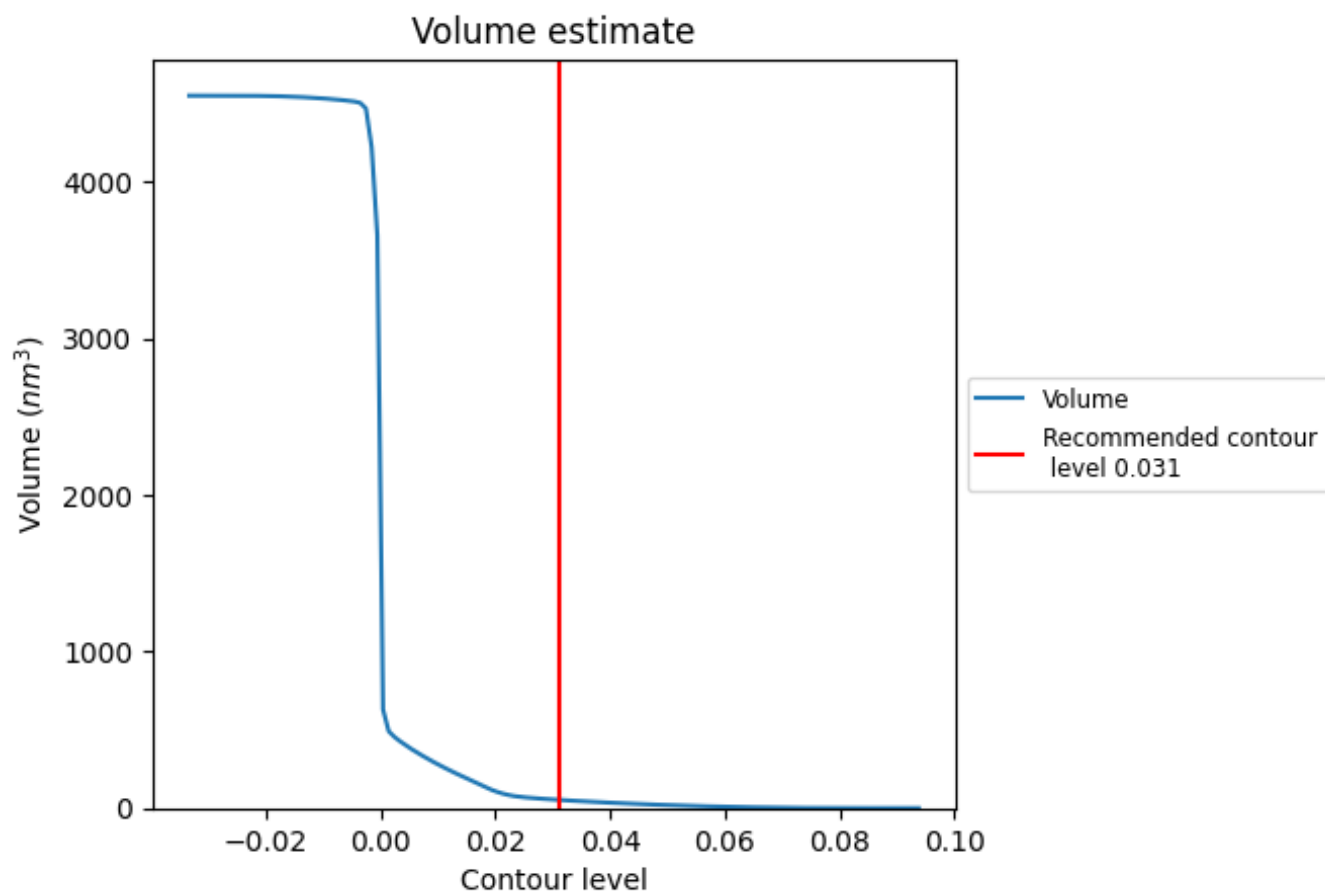
This section contains the results of statistical analysis of the map.

### 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.

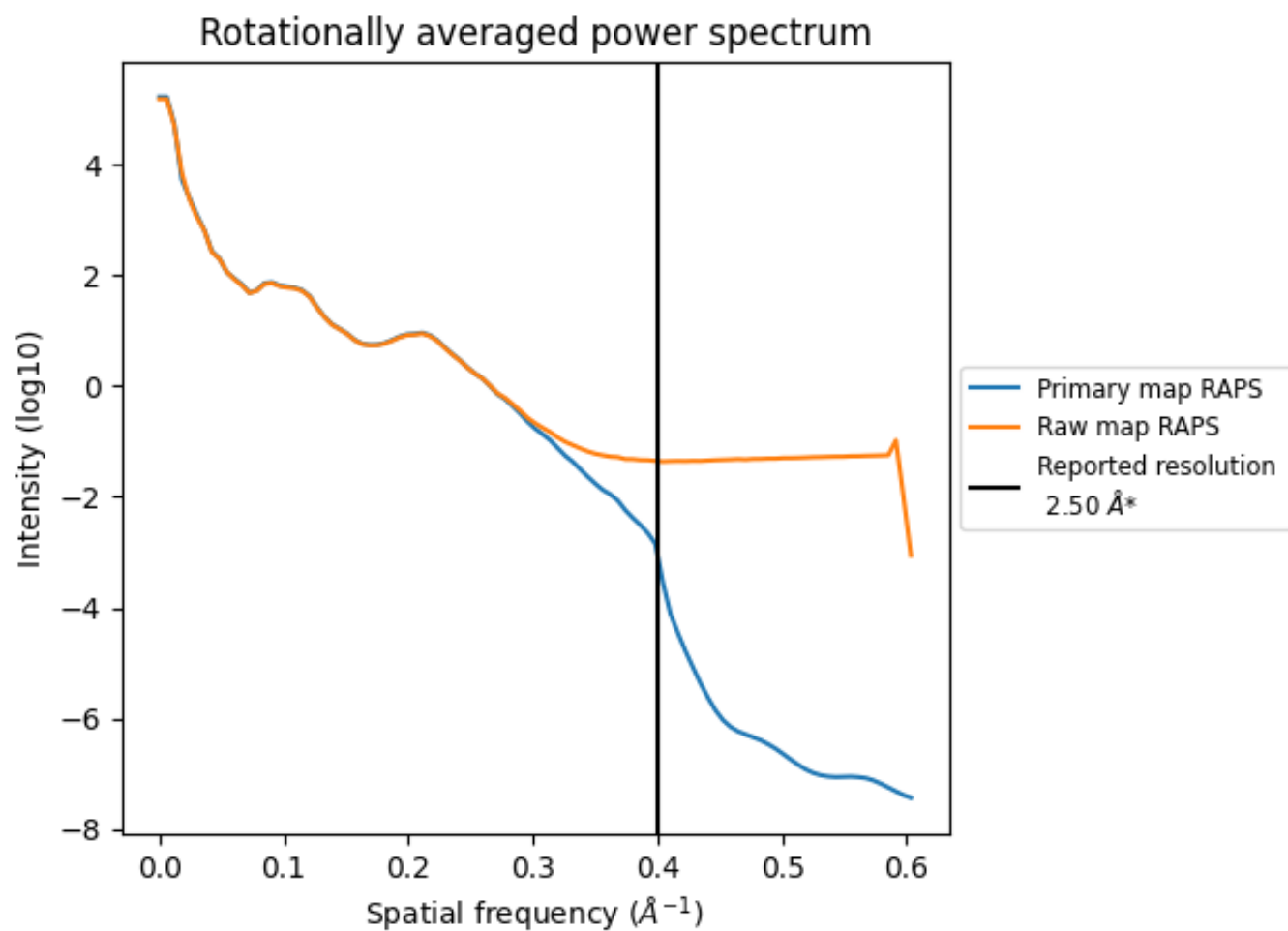
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53 nm<sup>3</sup>; this corresponds to an approximate mass of 48 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 ⓘ

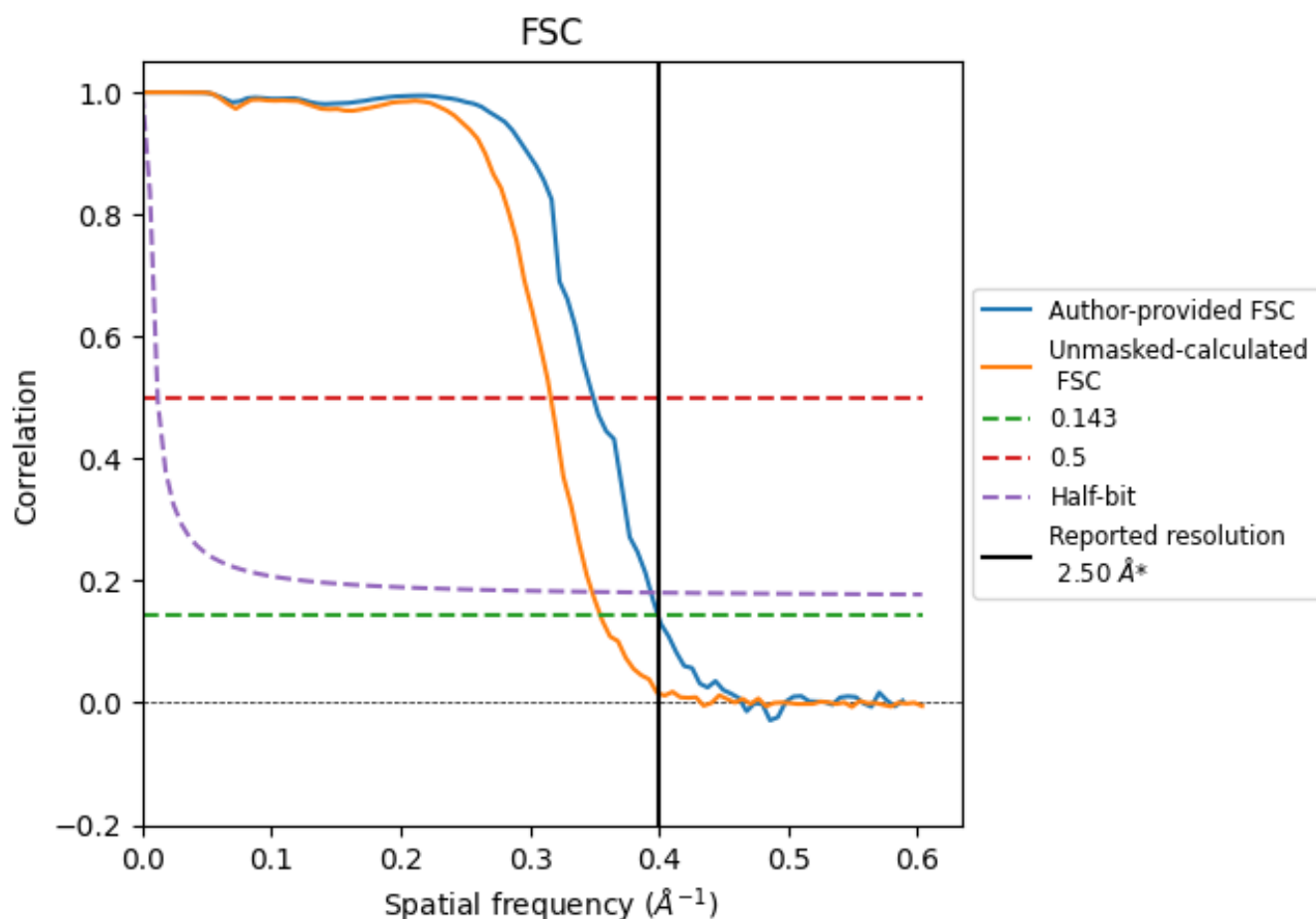


\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.51	2.86	2.54
Unmasked-calculated*	2.82	3.16	2.87

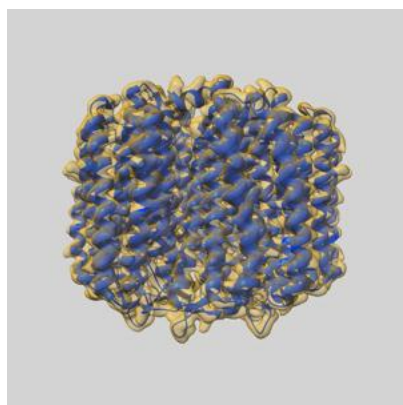
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.82 differs from the reported value 2.5 by more than 10 %



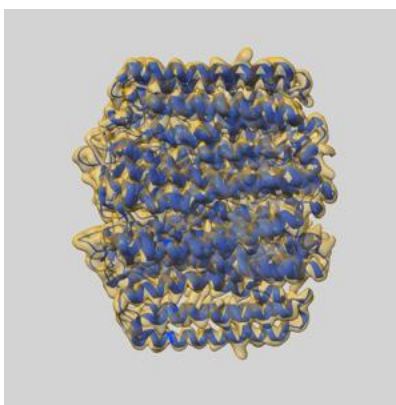
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61688 and PDB model 9JOX. Per-residue inclusion information can be found in section [3](#) on page [10](#).

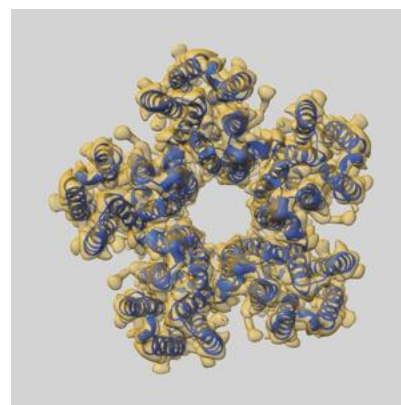
### 9.1 Map-model overlay [i](#)



X



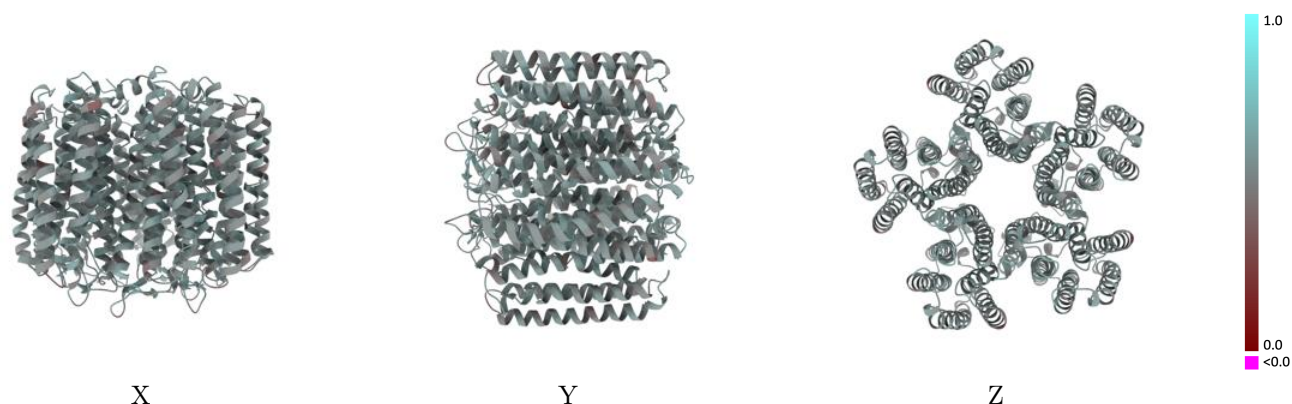
Y



Z

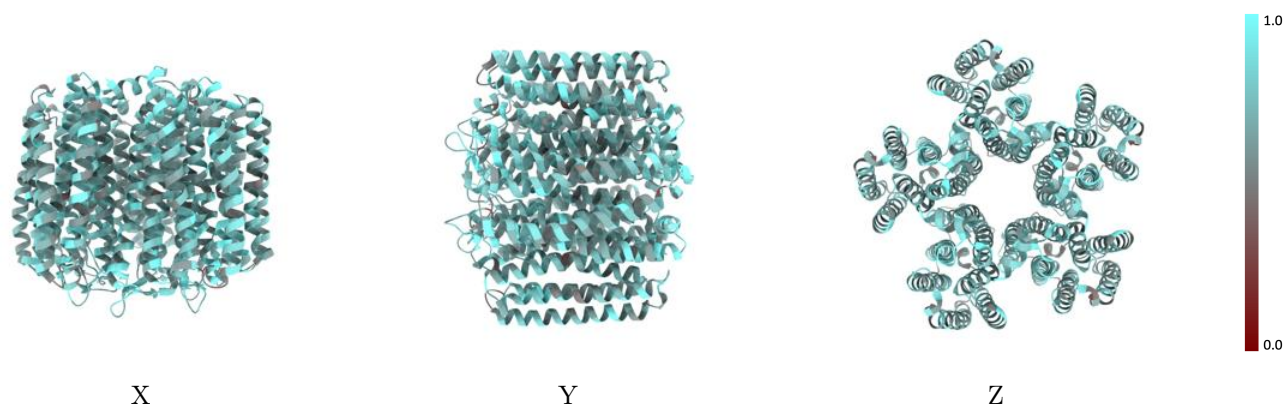
The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



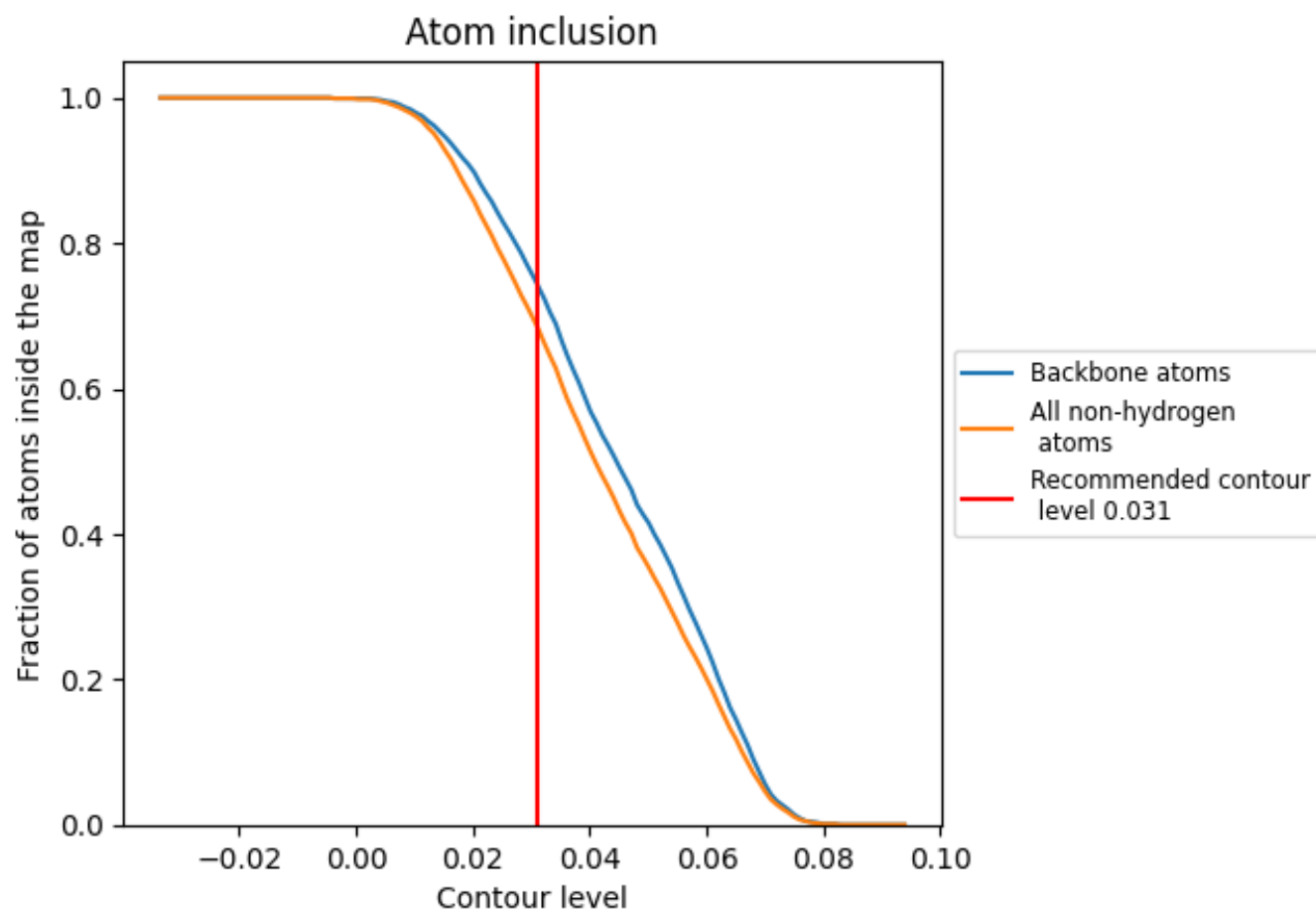
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.031).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6850	<div></div> 0.5360
A	<div></div> 0.6860	<div></div> 0.5340
B	<div></div> 0.6850	<div></div> 0.5350
C	<div></div> 0.7020	<div></div> 0.5340
D	<div></div> 0.6940	<div></div> 0.5380
E	<div></div> 0.6900	<div></div> 0.5370

