



wwPDB EM Validation Summary Report ⓘ

Sep 14, 2026 – 10:53 AM JST

PDB ID : 9WFZ / pdb_00009wfz
EMDB ID : EMD-65941
Title : Cryo-EM structure of PSII PsbA3-S264V from *Thermosynechococcus vestitus* BP-1 (local refinement)
Authors : Fan, S.B.; Nakajima, Y.; Shen, J.R.
Deposited on : 2025-08-22
Resolution : 2.08 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

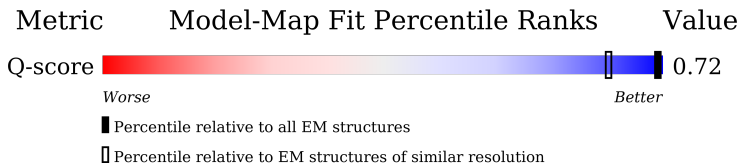
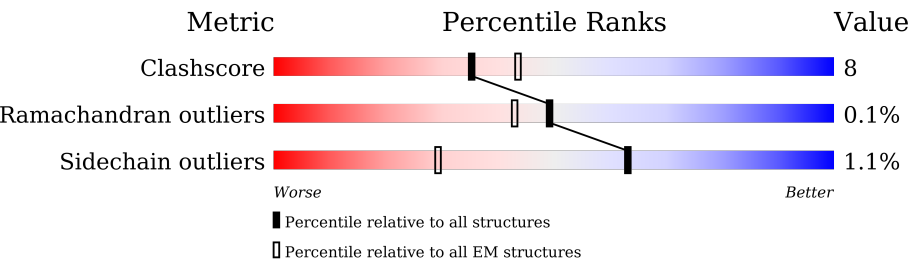
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.08 Å.

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



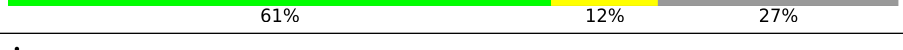
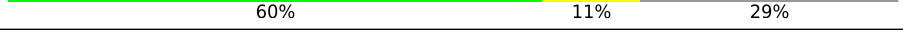
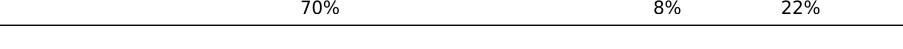
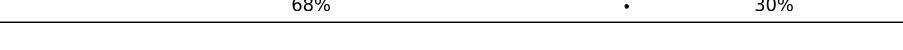
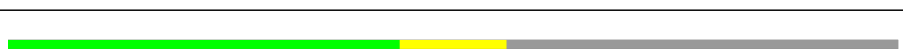
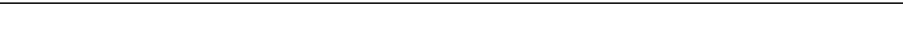
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1976 (1.58 - 2.58)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	38	92% 5%
2	K	46	61% 20% 20%
3	T	32	72% 19% 9%
4	V	163	73% 6% 20%

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Mol	Chain	Length	Quality of chain
5	Y	46	
6	A	360	
7	B	510	
7	b	510	
8	C	461	
9	D	352	
10	E	84	
11	F	45	
12	J	40	
13	L	37	
14	M	36	
15	O	272	
16	U	134	
17	X	41	
18	Z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	HEC	V	201	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 17446 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 Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	36	Total	C	N	O	S	0	0
			261	176	41	43	1		

- Molecule 2 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	37	Total	C	N	O	0	0
			275	193	42	40		

- Molecule 3 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	29	Total	C	N	O	S	0	0
			232	164	32	34	2		

- Molecule 4 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	130	Total	C	N	O	S	0	0
			931	603	161	163	4		

- Molecule 5 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	29	Total	C	N	O	S	0	0
			177	118	30	28	1		

- Molecule 6 is a protein called Photosystem II protein D1 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	327	Total	C	N	O	S	0	2
			2516	1661	411	430	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	VAL	SER	variant	UNP Q8DIV4

- Molecule 7 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	212	Total	C	N	O	S	1	7
			1517	1000	248	267	2		
7	b	42	Total	C	N	O		0	6
			237	153	39	45			

- Molecule 8 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	350	Total	C	N	O	S	0	9
			2514	1632	436	436	10		

- Molecule 9 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	333	Total	C	N	O	S	1	2
			2603	1728	427	436	12		

- Molecule 10 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	61	Total	C	N	O	0	0
			474	321	77	76		

- Molecule 11 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	32	Total	C	N	O	S	0	0
			258	179	42	36	1		

- Molecule 12 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	31	Total	C	N	O	S	0	0
			225	156	32	36	1		

- Molecule 13 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	L	26	Total	C	N	O	1	1
			212	149	30	33		

- Molecule 14 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	19	Total	C	N	O	S	0	3
			103	67	18	17	1		

- Molecule 15 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	188	Total	C	N	O	S	1	7
			1275	811	223	237	4		

- Molecule 16 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	U	94	Total	C	N	O	0	0
			683	445	120	118		

- Molecule 17 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	X	23	Total	C	N	O	0	6
			110	73	18	19		

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	47	Total	C	N	O	S	0	4
			270	183	43	43	1		

- Molecule 19 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

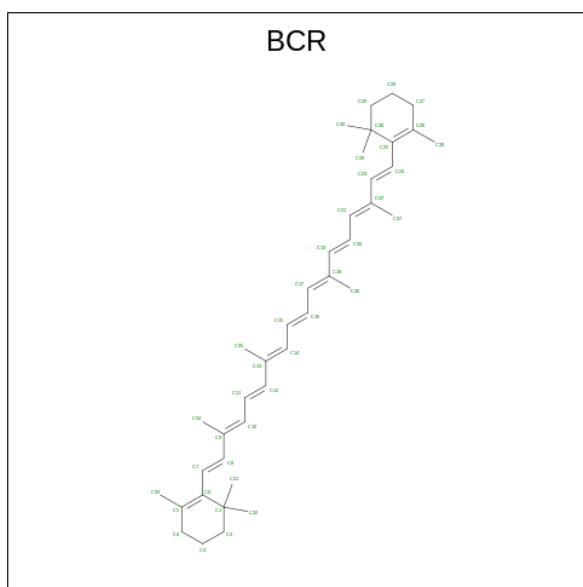
Mol	Chain	Residues	Atoms		AltConf
19	I	1	Total	C	0
			6	6	
19	K	1	Total	C	0
			13	13	

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Mol	Chain	Residues	Atoms	AltConf
19	T	1	Total C 5 5	0
19	A	1	Total C 8 8	0
19	D	1	Total C 7 7	0
19	X	1	Total C 9 9	0

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



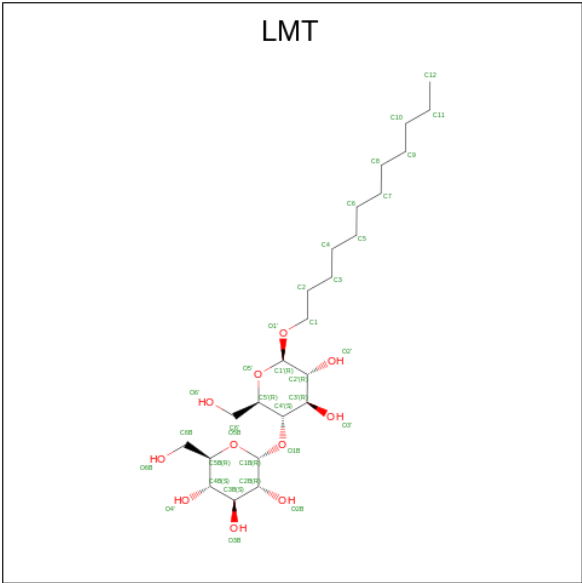
Mol	Chain	Residues	Atoms	AltConf
20	I	1	Total C 19 19	0
20	K	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	K	1	Total C 4 4	0
20	T	1	Total C 16 16	0
20	A	1	Total C 40 40	0
20	A	1	Total C 1 1	0

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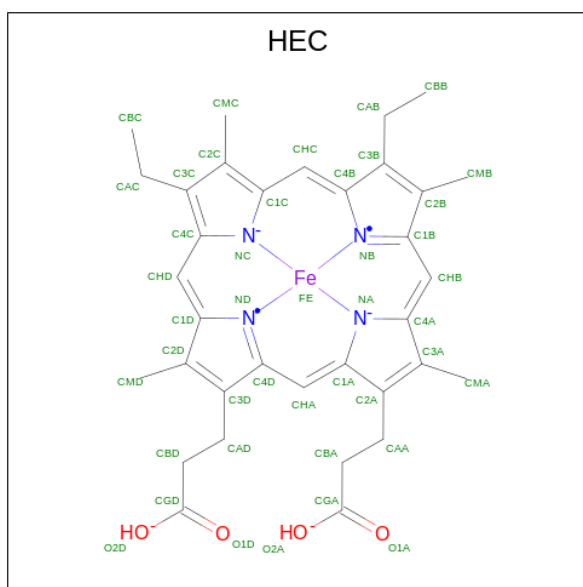
Mol	Chain	Residues	Atoms		AltConf
20	D	1	Total	C	0
			40	40	

- Molecule 21 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



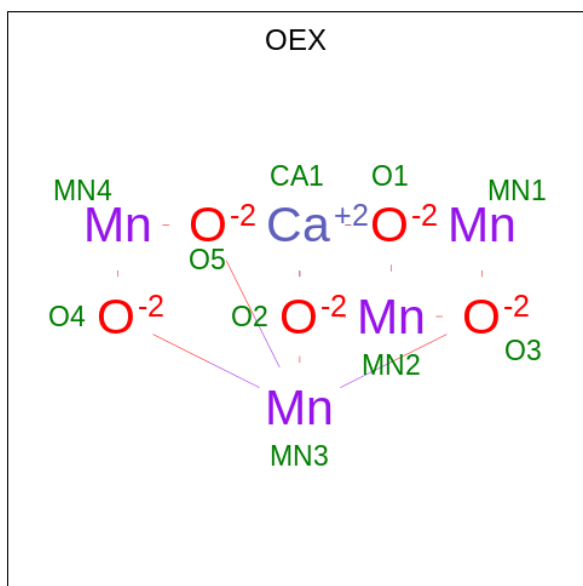
Mol	Chain	Residues	Atoms			AltConf
21	T	1	Total	C	O	0
			15	10	5	
21	J	1	Total	C	O	0
			24	18	6	
21	M	1	Total	O		0
			2	2		

- Molecule 22 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
22	V	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 23 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total 10	Ca 1	Mn 4	O 5	0

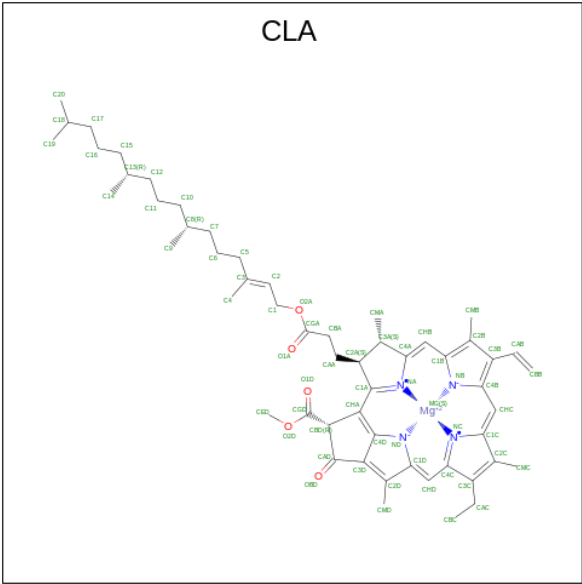
- Molecule 24 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Fe	0
			1	1	

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Cl	0
			2	2	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



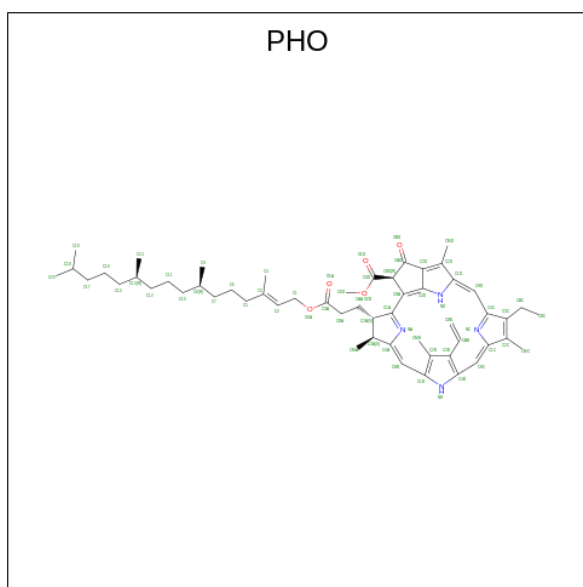
Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	O			0
			25	23	2			
26	B	1	Total	C	O			0
			3	2	1			
26	C	1	Total	C	N	O		0
			30	26	1	3		
26	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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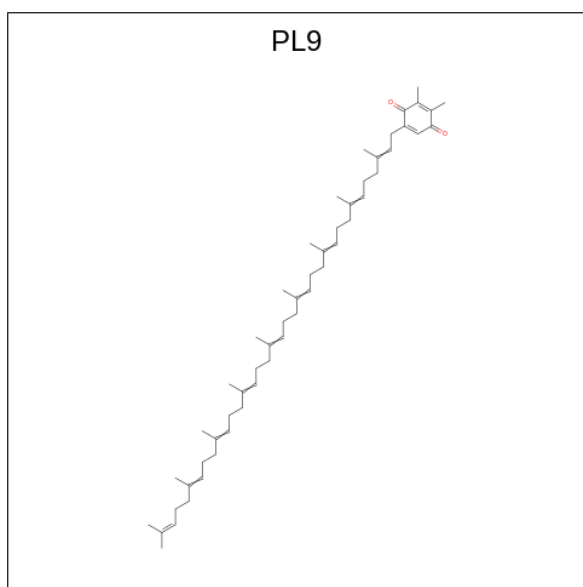
Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total 54	C 45	Mg 1	N 3	O 5	0
26	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	C	1	Total 21	C 16	Mg 1	N 2	O 2	0
26	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 4	C 2	O 2			0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 4	C 4				0
26	D	1	Total 10	C 10				0
26	D	1	Total 1	C 1				0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 44	C 35	Mg 1	N 4	O 4	0

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



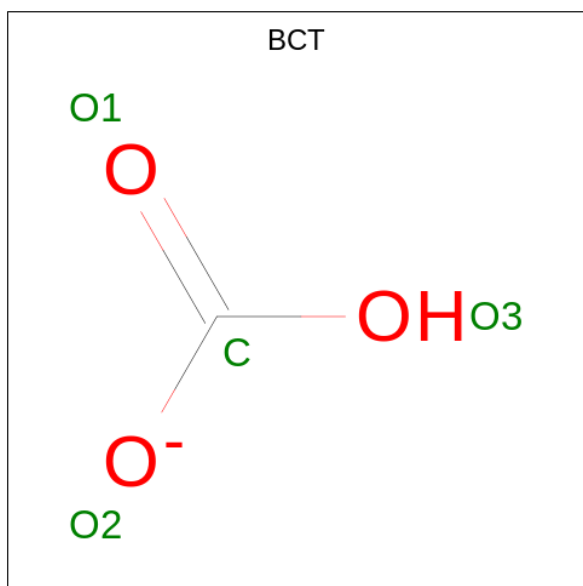
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			55	53	2	

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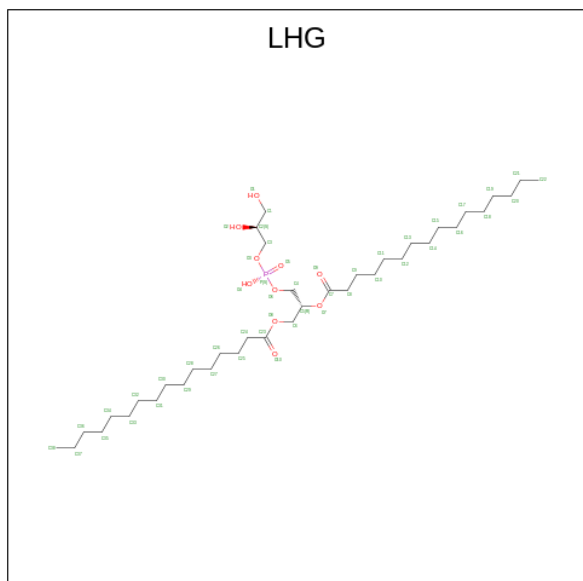
Mol	Chain	Residues	Atoms			AltConf
28	D	1	Total	C	O	0
			55	53	2	

- Molecule 29 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



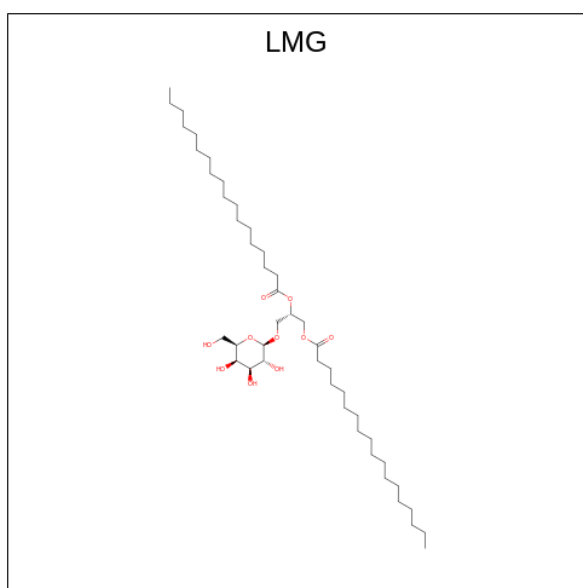
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	1
			4	1	3	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



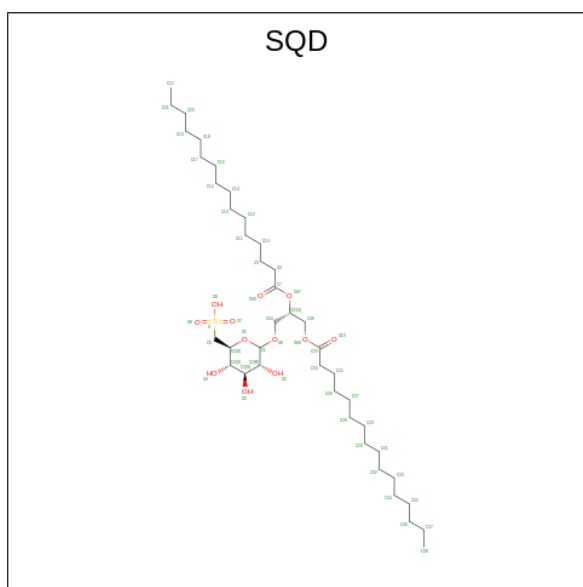
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			39	28	10	1	
30	A	1	Total	C	O	P	0
			31	22	8	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			42	31	10	1	
30	L	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



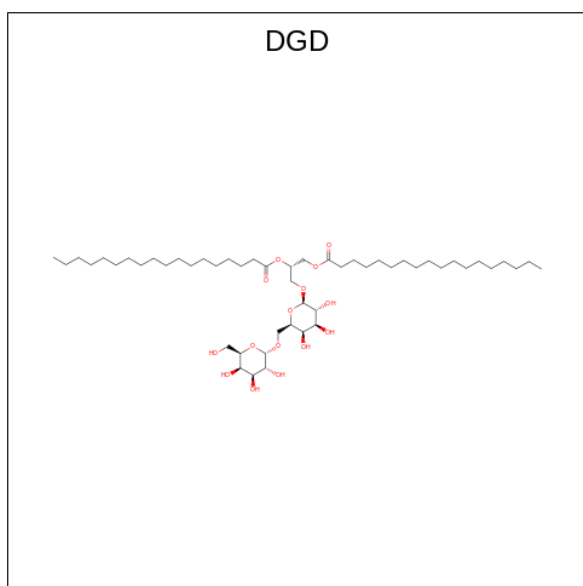
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			31	22	9	
31	C	1	Total	C	O	0
			47	37	10	
31	D	1	Total	C	O	0
			38	28	10	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
32	C	1	Total	C	O	S	0
			32	19	12	1	
32	F	1	Total	C	O	S	0
			23	11	11	1	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



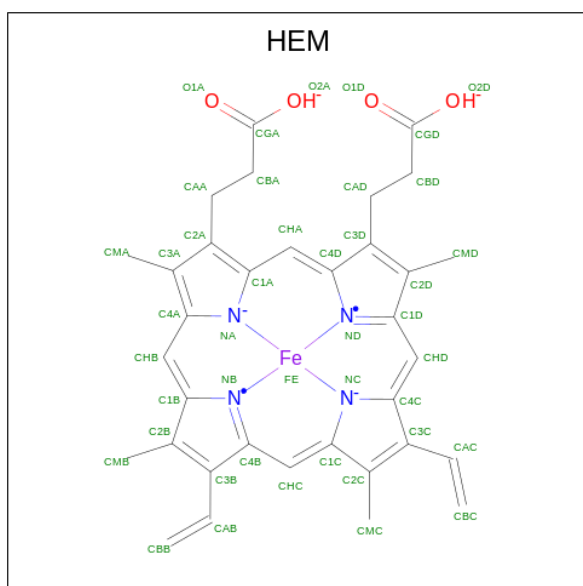
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			52	37	15	

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Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			50	35	15	
33	C	1	Total	C	O	0
			53	38	15	
33	D	1	Total	C	O	0
			54	40	14	

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
34	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	I	4	Total	O	0
			4	4	
35	K	2	Total	O	0
			2	2	
35	T	4	Total	O	0
			4	4	
35	V	10	Total	O	0
			10	10	
35	A	105	Total	O	2
			106	106	

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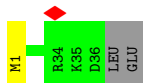
Mol	Chain	Residues	Atoms		AltConf
35	B	68	Total 68	O 68	0
35	C	85	Total 87	O 87	2
35	D	87	Total 88	O 88	1
35	E	6	Total 6	O 6	0
35	F	1	Total 1	O 1	0
35	J	3	Total 3	O 3	0
35	L	9	Total 9	O 9	0
35	M	4	Total 4	O 4	0
35	O	39	Total 39	O 39	1
35	U	7	Total 7	O 7	0
35	X	1	Total 1	O 1	0
35	b	5	Total 5	O 5	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Photosystem II reaction center protein I

Chain I: 



- Molecule 2: Photosystem II reaction center protein K

Chain K: 



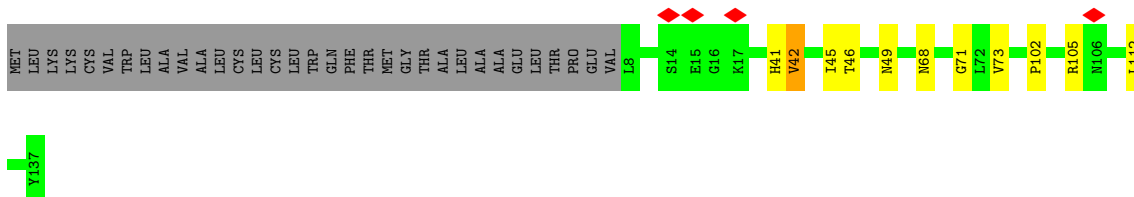
- Molecule 3: Photosystem II reaction center protein T

Chain T: 



- Molecule 4: Photosystem II extrinsic protein V

Chain V: 



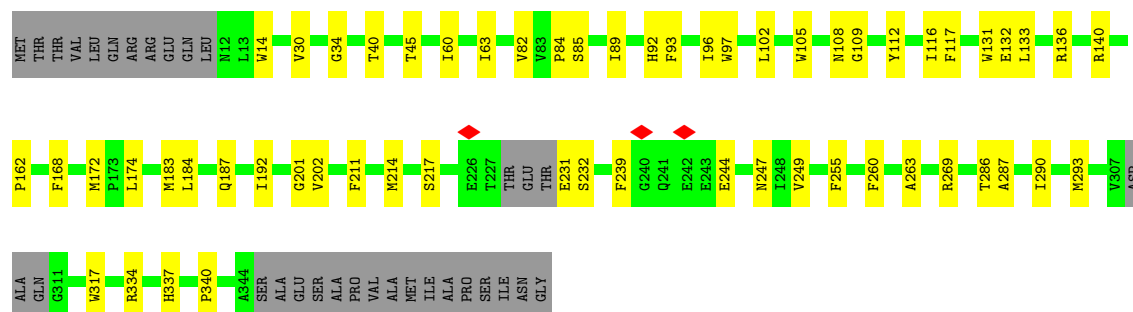
- Molecule 5: Photosystem II reaction center protein Psb30

Chain Y: 

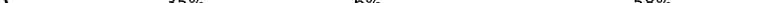


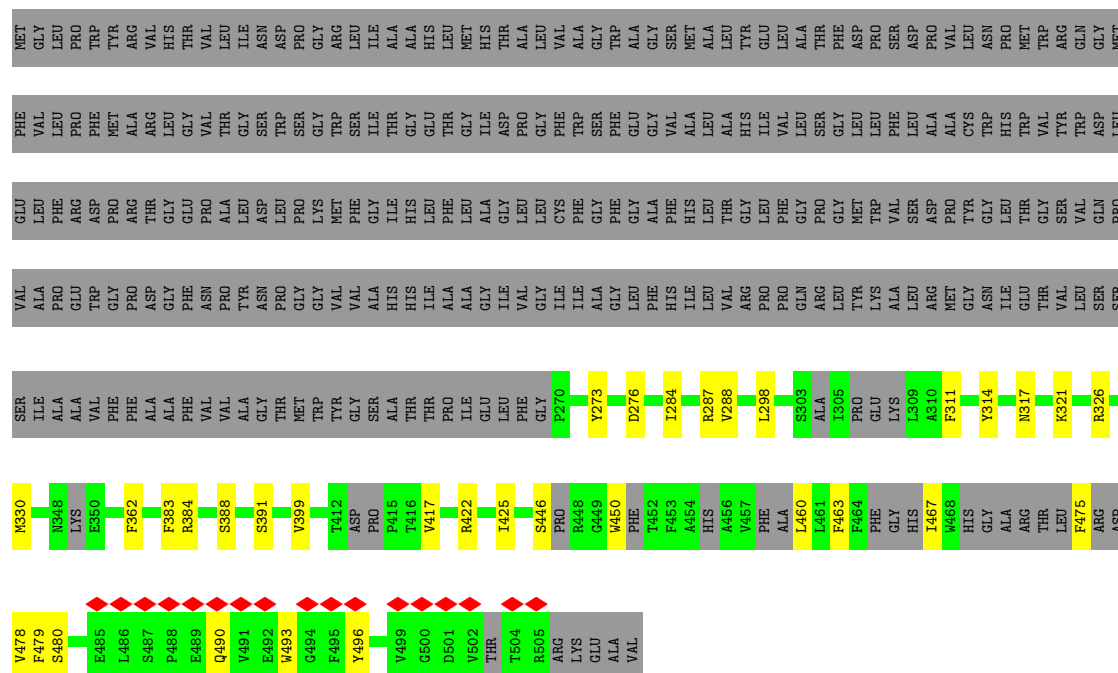
- Molecule 6: Photosystem II protein D1 3

Chain A: 75% 16% 9%



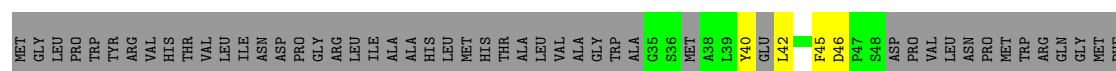
- Molecule 7: Photosystem II CP47 reaction center protein

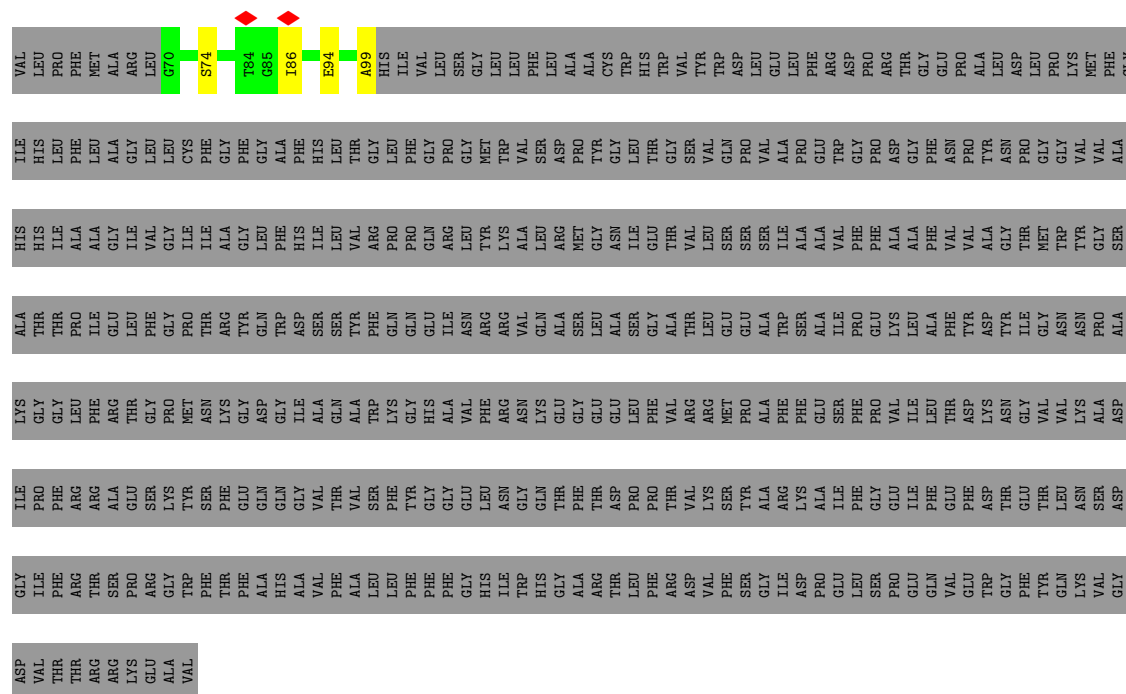
Chain B:  35% 6% 58%



- Molecule 7: Photosystem II CP47 reaction center protein

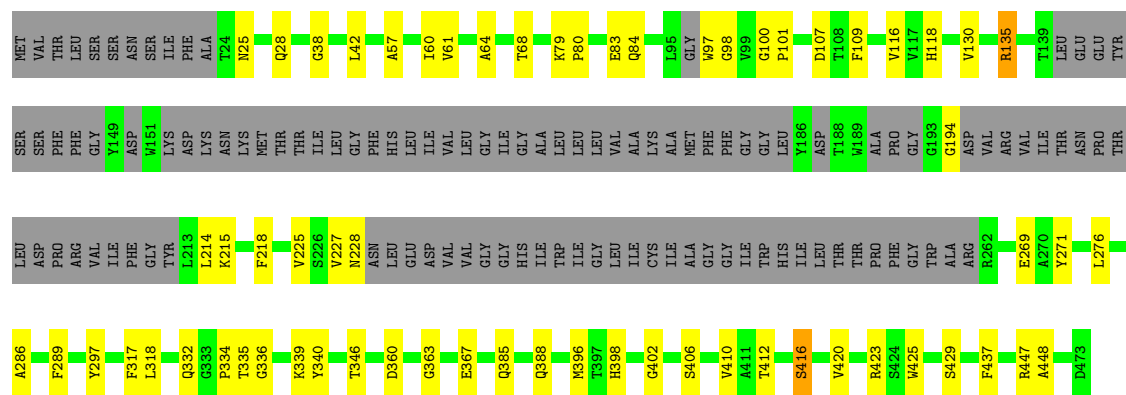
Chain b: 7% : 92%





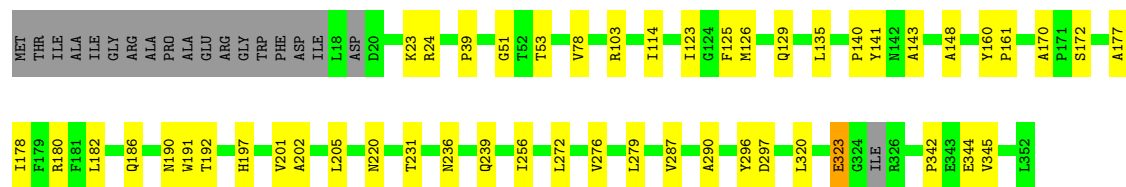
• Molecule 8: Photosystem II CP43 reaction center protein

Chain C: 62% 13% 24%



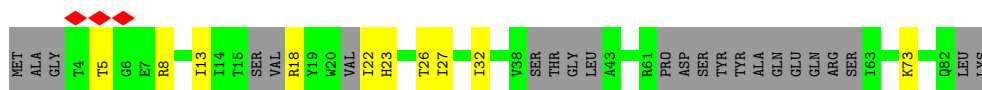
• Molecule 9: Photosystem II D2 protein

Chain D: 80% 14% 5%

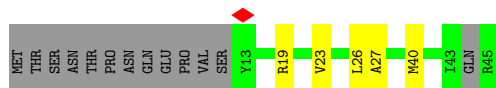


• Molecule 10: Cytochrome b559 subunit alpha

Chain E: 61% 12% 27%



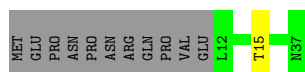
- Molecule 11: Cytochrome b559 subunit beta



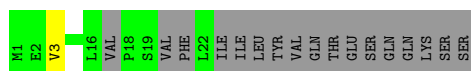
- Molecule 12: Photosystem II reaction center protein J



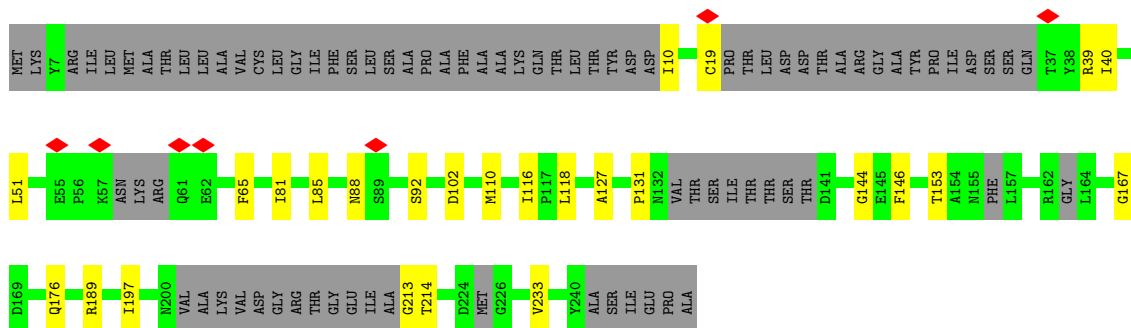
- Molecule 13: Photosystem II reaction center protein L



- Molecule 14: Photosystem II reaction center protein M

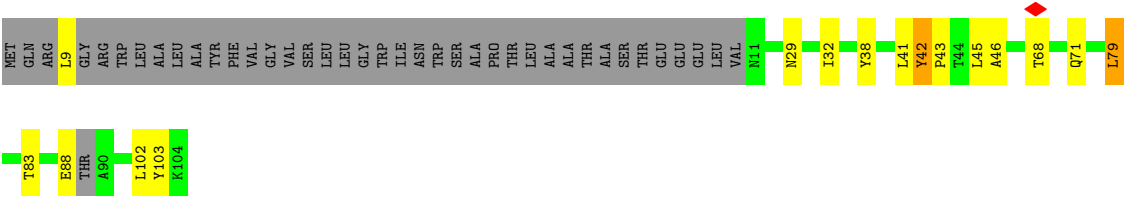


- Molecule 15: Photosystem II extrinsic protein O

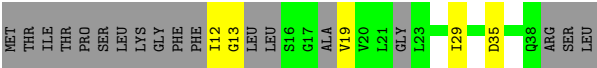


- Molecule 16: Photosystem II extrinsic protein U

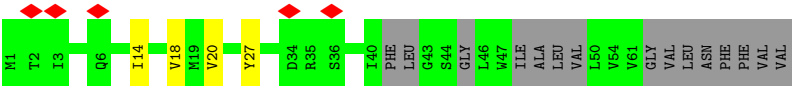




• Molecule 17: Photosystem II reaction center protein X



• Molecule 18: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.350	Depositor
Minimum map value	-0.726	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.129	Depositor
Map size (Å)	290.56, 290.56, 290.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5675, 0.5675, 0.5675	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, OEX, CL, FE2, PHO, LMT, HEM, LHG, UNL, DGD, CLA, BCT, LMG, HEC, SQD, BCR

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	I	0.11	0/267	0.26	0/363
2	K	0.16	0/285	0.37	0/395
3	T	0.13	0/239	0.28	0/324
4	V	0.26	0/951	0.40	0/1301
5	Y	0.14	0/178	0.25	0/243
6	A	0.16	0/2595	0.34	0/3542
7	B	0.12	0/1539	0.30	0/2048
7	b	0.13	0/233	0.32	0/306
8	C	0.12	0/2569	0.28	0/3472
9	D	0.14	0/2691	0.31	0/3666
10	E	0.22	0/485	0.41	0/657
11	F	0.25	0/266	0.34	0/363
12	J	0.12	0/230	0.26	0/312
13	L	0.11	0/218	0.21	0/294
14	M	0.14	0/99	0.25	0/129
15	O	0.12	0/1285	0.28	0/1734
16	U	0.27	0/692	0.48	1/941 (0.1%)
17	X	0.16	0/101	0.31	0/127
18	Z	0.11	0/269	0.25	0/364
All	All	0.16	0/15192	0.32	1/20581 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	U	42	TYR	CB-CA-C	5.60	116.76	108.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	261	0	251	1	0
2	K	275	0	272	5	0
3	T	232	0	224	5	0
4	V	931	0	910	6	0
5	Y	177	0	164	4	0
6	A	2516	0	2407	51	0
7	B	1517	0	1323	24	0
7	b	237	0	178	7	0
8	C	2514	0	2328	48	0
9	D	2603	0	2504	42	0
10	E	474	0	451	8	0
11	F	258	0	268	5	0
12	J	225	0	235	2	0
13	L	212	0	229	1	0
14	M	103	0	98	1	0
15	O	1275	0	1172	18	0
16	U	683	0	664	11	0
17	X	110	0	90	7	0
18	Z	270	0	224	3	0
19	A	8	0	0	0	0
19	D	7	0	0	0	0
19	I	6	0	0	0	0
19	K	13	0	0	0	0
19	T	5	0	0	0	0
19	X	9	0	0	0	0
20	A	41	0	56	0	0
20	D	40	0	56	2	0
20	I	19	0	26	0	0
20	K	84	0	117	8	0
20	T	16	0	22	1	0
21	J	24	0	35	1	0
21	M	2	0	0	0	0
21	T	15	0	14	0	0
22	V	43	0	32	0	0
23	A	10	0	0	1	0
24	A	1	0	0	0	0
25	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	237	0	236	16	0
26	B	28	0	41	1	0
26	C	530	0	526	29	0
26	D	124	0	122	7	0
27	A	64	0	74	1	0
27	D	64	0	74	5	0
28	A	55	0	80	7	0
28	D	55	0	80	2	0
29	A	4	0	0	0	0
30	A	70	0	84	4	0
30	D	91	0	128	3	0
30	L	39	0	51	1	0
31	B	31	0	28	0	0
31	C	47	0	64	3	0
31	D	38	0	46	0	0
32	C	32	0	28	1	0
32	F	23	0	16	0	0
33	C	155	0	184	6	0
33	D	54	0	66	3	0
34	E	43	0	30	2	0
35	A	106	0	0	3	0
35	B	68	0	0	0	0
35	C	87	0	0	0	0
35	D	88	0	0	0	0
35	E	6	0	0	0	0
35	F	1	0	0	0	0
35	I	4	0	0	0	0
35	J	3	0	0	0	0
35	K	2	0	0	0	0
35	L	9	0	0	0	0
35	M	4	0	0	0	0
35	O	39	0	0	0	0
35	T	4	0	0	0	0
35	U	7	0	0	0	0
35	V	10	0	0	0	0
35	X	1	0	0	0	0
35	b	5	0	0	0	0
All	All	17446	0	16308	262	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 262 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)
3:T:19:PHE:CD2	3:T:19:PHE:CZ	2.39	1.02
8:C:271:TYR:CE1	8:C:271:TYR:CE2	2.39	1.01
7:B:463:PHE:CG	7:B:463:PHE:CE1	2.40	1.00
8:C:109:PHE:CD1	8:C:109:PHE:CB	2.51	0.94
7:B:478:VAL:C	7:B:479:PHE:CA	2.41	0.94

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	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
2	K	35/46 (76%)	35 (100%)	0	0	100	100
3	T	27/32 (84%)	27 (100%)	0	0	100	100
4	V	128/163 (78%)	126 (98%)	2 (2%)	0	100	100
5	Y	27/46 (59%)	27 (100%)	0	0	100	100
6	A	319/360 (89%)	315 (99%)	4 (1%)	0	100	100
7	B	180/510 (35%)	177 (98%)	3 (2%)	0	100	100
7	b	28/510 (6%)	27 (96%)	0	1 (4%)	2	1
8	C	328/461 (71%)	321 (98%)	7 (2%)	0	100	100
9	D	329/352 (94%)	323 (98%)	6 (2%)	0	100	100
10	E	50/84 (60%)	49 (98%)	1 (2%)	0	100	100
11	F	29/45 (64%)	29 (100%)	0	0	100	100
12	J	27/40 (68%)	27 (100%)	0	0	100	100
13	L	24/37 (65%)	24 (100%)	0	0	100	100
14	M	12/36 (33%)	12 (100%)	0	0	100	100
15	O	168/272 (62%)	163 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	U	89/134 (66%)	88 (99%)	1 (1%)	0	100	100
17	X	12/41 (29%)	12 (100%)	0	0	100	100
18	Z	36/62 (58%)	36 (100%)	0	0	100	100
All	All	1882/3269 (58%)	1851 (98%)	30 (2%)	1 (0%)	49	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	b	86	ILE

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	I	25/35 (71%)	25 (100%)	0	100	100
2	K	25/37 (68%)	24 (96%)	1 (4%)	28	28
3	T	22/29 (76%)	22 (100%)	0	100	100
4	V	88/138 (64%)	87 (99%)	1 (1%)	65	73
5	Y	11/37 (30%)	11 (100%)	0	100	100
6	A	253/291 (87%)	253 (100%)	0	100	100
7	B	131/407 (32%)	128 (98%)	3 (2%)	44	49
7	b	18/407 (4%)	18 (100%)	0	100	100
8	C	228/362 (63%)	224 (98%)	4 (2%)	51	58
9	D	259/283 (92%)	258 (100%)	1 (0%)	84	89
10	E	45/73 (62%)	44 (98%)	1 (2%)	45	51
11	F	26/39 (67%)	25 (96%)	1 (4%)	29	30
12	J	22/28 (79%)	22 (100%)	0	100	100
13	L	24/35 (69%)	24 (100%)	0	100	100
14	M	9/33 (27%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	118/228 (52%)	118 (100%)	0	100	100
16	U	62/112 (55%)	59 (95%)	3 (5%)	23	22
17	X	6/34 (18%)	6 (100%)	0	100	100
18	Z	16/52 (31%)	16 (100%)	0	100	100
All	All	1388/2660 (52%)	1373 (99%)	15 (1%)	63	73

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	C	346	THR
16	U	79	LEU
8	C	416	SER
16	U	83	THR
11	F	23	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
8	C	311	GLN
16	U	29	ASN
8	C	388	GLN
15	O	228	HIS
8	C	378	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 64 ligands modelled in this entry, 6 are unknown, 2 are modelled with single atom and 3 are monoatomic - leaving 53 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
26	CLA	D	406	9	48,52,73	2.39	19 (39%)	56,87,113	3.28	27 (48%)
26	CLA	D	405	9	69,73,73	2.01	20 (28%)	83,113,113	2.82	29 (34%)
26	CLA	A	408	6	55,59,73	2.31	20 (36%)	66,96,113	3.16	31 (46%)
26	CLA	C	510	8	69,73,73	2.07	20 (28%)	83,113,113	2.78	30 (36%)
26	CLA	B	602	-	1,1,73	0.01	0	-		
23	OEX	A	401	35,6,8	0,14,14	-	-	-		
21	LMT	J	101	-	24,24,36	0.15	0	29,29,47	0.32	0
26	CLA	C	506	8	59,63,73	2.22	20 (33%)	71,101,113	3.00	30 (42%)
26	CLA	B	601	-	24,24,73	0.95	1 (4%)	28,28,113	1.26	3 (10%)
20	BCR	K	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	16 (28%)
33	DGD	C	515	-	54,54,67	0.91	2 (3%)	68,68,81	1.06	4 (5%)
32	SQD	C	501	-	31,32,54	1.28	3 (9%)	40,43,65	1.42	6 (15%)
30	LHG	A	415	-	30,30,48	1.00	2 (6%)	33,35,54	1.10	1 (3%)
26	CLA	C	512	-	0,1,73	-	-	-		
20	BCR	K	101	-	41,41,41	1.11	1 (2%)	56,56,56	1.76	15 (26%)
20	BCR	D	407	-	41,41,41	1.07	1 (2%)	56,56,56	1.99	10 (17%)
26	CLA	C	503	-	25,28,73	1.04	1 (4%)	28,35,113	2.18	4 (14%)
28	PL9	D	408	-	55,55,55	0.59	1 (1%)	68,69,69	1.76	20 (29%)
30	LHG	L	101	-	38,38,48	1.04	2 (5%)	41,44,54	1.13	3 (7%)
30	LHG	A	414	-	38,38,48	1.05	2 (5%)	41,44,54	1.12	3 (7%)
26	CLA	C	505	8	53,59,73	2.07	12 (22%)	60,86,113	3.18	19 (31%)
30	LHG	D	412	-	41,41,48	1.01	2 (4%)	44,47,54	1.08	3 (6%)
31	LMG	D	410	-	38,38,55	1.06	2 (5%)	46,46,63	1.12	4 (8%)
34	HEM	E	101	11,10	50,50,50	1.54	7 (14%)	66,82,82	1.71	12 (18%)
27	PHO	A	407	-	58,69,69	2.75	15 (25%)	56,99,99	2.82	17 (30%)
27	PHO	D	401	-	58,69,69	2.78	15 (25%)	56,99,99	2.80	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	C	516	35	69,73,73	2.07	21 (30%)	83,113,113	2.83	30 (36%)
20	BCR	I	102	-	19,19,41	0.58	0	26,26,56	1.65	8 (30%)
33	DGD	C	513	-	53,53,67	0.92	2 (3%)	67,67,81	1.05	3 (4%)
22	HEC	V	201	4	50,50,50	1.75	6 (12%)	68,82,82	1.41	6 (8%)
30	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	1.04	3 (5%)
29	BCT	A	413[A]	24	2,3,3	0.70	0	2,3,3	0.64	0
26	CLA	A	412	35	69,73,73	2.07	20 (28%)	83,113,113	2.80	28 (33%)
26	CLA	C	507	35	17,23,73	2.23	6 (35%)	18,34,113	2.91	5 (27%)
26	CLA	C	508	8	64,68,73	2.14	20 (31%)	77,107,113	2.92	28 (36%)
26	CLA	D	403	-	7,7,73	0.28	0	6,6,113	1.59	2 (33%)
26	CLA	C	509	8	63,67,73	2.18	20 (31%)	75,105,113	2.88	28 (37%)
20	BCR	T	102	-	16,16,41	1.42	1 (6%)	22,22,56	2.22	7 (31%)
20	BCR	K	104	-	3,3,41	0.21	0	2,2,56	0.65	0
31	LMG	C	502	-	47,47,55	0.97	2 (4%)	55,55,63	1.16	4 (7%)
28	PL9	A	410	-	55,55,55	0.61	1 (1%)	68,69,69	1.82	20 (29%)
33	DGD	D	413	-	53,53,67	0.68	1 (1%)	64,64,81	0.77	1 (1%)
21	LMT	T	103	-	12,12,36	0.17	0	11,11,47	0.58	0
26	CLA	C	511	8	69,73,73	2.06	20 (28%)	83,113,113	2.81	29 (34%)
33	DGD	C	514	-	51,51,67	0.95	2 (3%)	65,65,81	1.14	5 (7%)
26	CLA	A	406	35	60,64,73	2.23	21 (35%)	72,102,113	3.00	29 (40%)
31	LMG	B	603	-	29,29,55	1.52	3 (10%)	33,34,63	1.22	2 (6%)
26	CLA	A	405	6	69,73,73	2.03	19 (27%)	83,113,113	2.82	32 (38%)
26	CLA	C	504	8	54,58,73	2.32	20 (37%)	65,95,113	3.11	27 (41%)
32	SQD	F	101	-	22,23,54	1.03	2 (9%)	30,33,65	1.07	3 (10%)
26	CLA	D	402	-	3,3,73	0.03	0	3,3,113	0.08	0
20	BCR	A	409	-	41,41,41	1.07	1 (2%)	56,56,56	1.72	13 (23%)

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
26	CLA	D	406	9	-	0/13/90/115	-
26	CLA	D	405	9	-	4/39/115/115	-
26	CLA	A	408	6	-	5/23/99/115	-
26	CLA	C	510	8	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMT	J	101	-	-	0/15/35/61	0/1/1/2
26	CLA	C	506	8	-	10/27/103/115	-
26	CLA	B	601	-	-	4/26/26/115	-
20	BCR	K	102	-	-	0/29/63/63	0/2/2/2
33	DGD	C	515	-	-	2/42/82/95	0/2/2/2
32	SQD	C	501	-	-	7/27/47/69	0/1/1/1
30	LHG	A	415	-	-	8/33/33/53	-
20	BCR	K	101	-	-	7/29/63/63	0/2/2/2
20	BCR	D	407	-	-	8/29/63/63	0/2/2/2
26	CLA	C	503	-	-	6/24/40/115	0/1/1/9
28	PL9	D	408	-	-	10/53/73/73	0/1/1/1
30	LHG	L	101	-	-	11/43/43/53	-
30	LHG	A	414	-	-	13/43/43/53	-
26	CLA	C	505	8	-	5/37/89/115	0/6/6/9
30	LHG	D	412	-	-	23/46/46/53	-
31	LMG	D	410	-	-	3/33/53/70	0/1/1/1
34	HEM	E	101	11,10	-	9/14/54/54	-
27	PHO	A	407	-	-	6/37/103/103	0/5/6/6
27	PHO	D	401	-	-	0/37/103/103	0/5/6/6
26	CLA	C	516	35	-	13/39/115/115	-
20	BCR	I	102	-	-	2/11/28/63	0/1/1/2
33	DGD	C	513	-	-	9/41/81/95	0/2/2/2
22	HEC	V	201	4	1/1/3/7	4/14/54/54	-
30	LHG	D	409	-	-	9/53/53/53	-
26	CLA	A	412	35	-	7/39/115/115	-
26	CLA	C	507	35	-	1/7/31/115	0/3/3/9
26	CLA	C	508	8	-	8/33/109/115	-
26	CLA	D	403	-	-	2/2/1/115	-
26	CLA	C	509	8	-	8/31/107/115	-
20	BCR	T	102	-	-	2/8/25/63	0/1/1/2
20	BCR	K	104	-	-	1/1/1/63	-
31	LMG	C	502	-	-	6/42/62/70	0/1/1/1
28	PL9	A	410	-	-	11/53/73/73	0/1/1/1
33	DGD	D	413	-	-	3/38/74/95	0/2/2/2
21	LMT	T	103	-	-	0/10/10/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	C	511	8	-	5/39/115/115	-
33	DGD	C	514	-	-	7/39/79/95	0/2/2/2
26	CLA	A	406	35	-	5/29/105/115	-
31	LMG	B	603	-	-	1/21/38/70	0/1/1/1
26	CLA	A	405	6	-	6/39/115/115	-
26	CLA	C	504	8	-	3/21/97/115	-
32	SQD	F	101	-	-	3/15/35/69	0/1/1/1
20	BCR	A	409	-	-	2/29/63/63	0/2/2/2

The worst 5 of 359 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	401	PHO	C1D-C2D	8.91	1.49	1.39
27	A	407	PHO	C1D-C2D	8.81	1.49	1.39
27	A	407	PHO	C1B-C2B	8.74	1.49	1.39
27	D	401	PHO	C1B-C2B	8.66	1.49	1.39
22	V	201	HEC	C3D-C2D	7.98	1.53	1.36

The worst 5 of 615 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	505	CLA	C1C-C2C-C3C	-12.60	103.04	112.33
27	A	407	PHO	C2D-C1D-ND	11.11	117.20	109.53
27	D	401	PHO	C2D-C1D-ND	11.08	117.18	109.53
26	A	406	CLA	C1D-ND-C4D	-9.45	99.62	106.33
26	A	408	CLA	C1D-ND-C4D	-9.39	99.67	106.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	V	201	HEC	NA

5 of 266 torsion outliers are listed below:

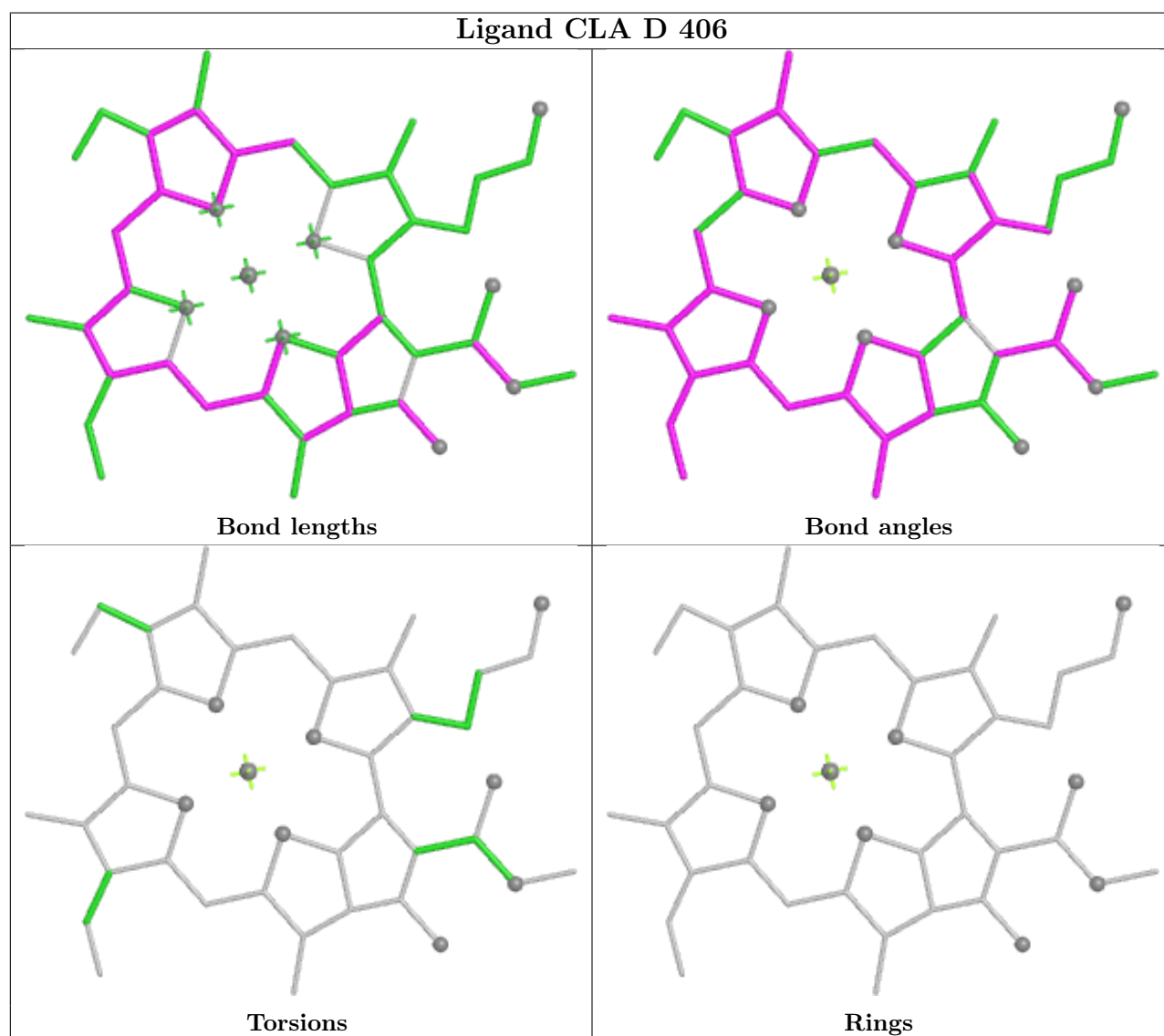
Mol	Chain	Res	Type	Atoms
20	I	102	BCR	C1-C6-C7-C8
20	K	101	BCR	C5-C6-C7-C8
20	K	101	BCR	C7-C8-C9-C34
20	D	407	BCR	C1-C6-C7-C8
20	D	407	BCR	C7-C8-C9-C34

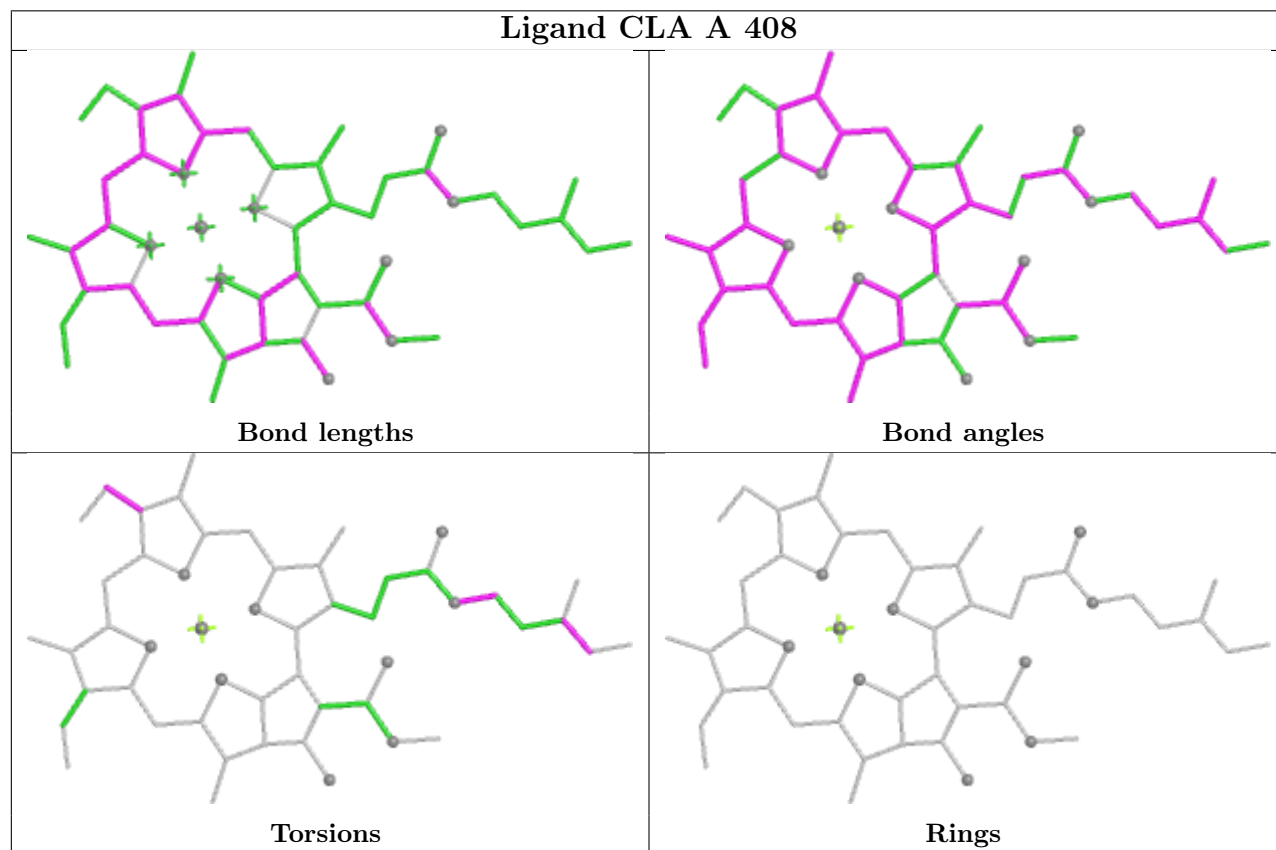
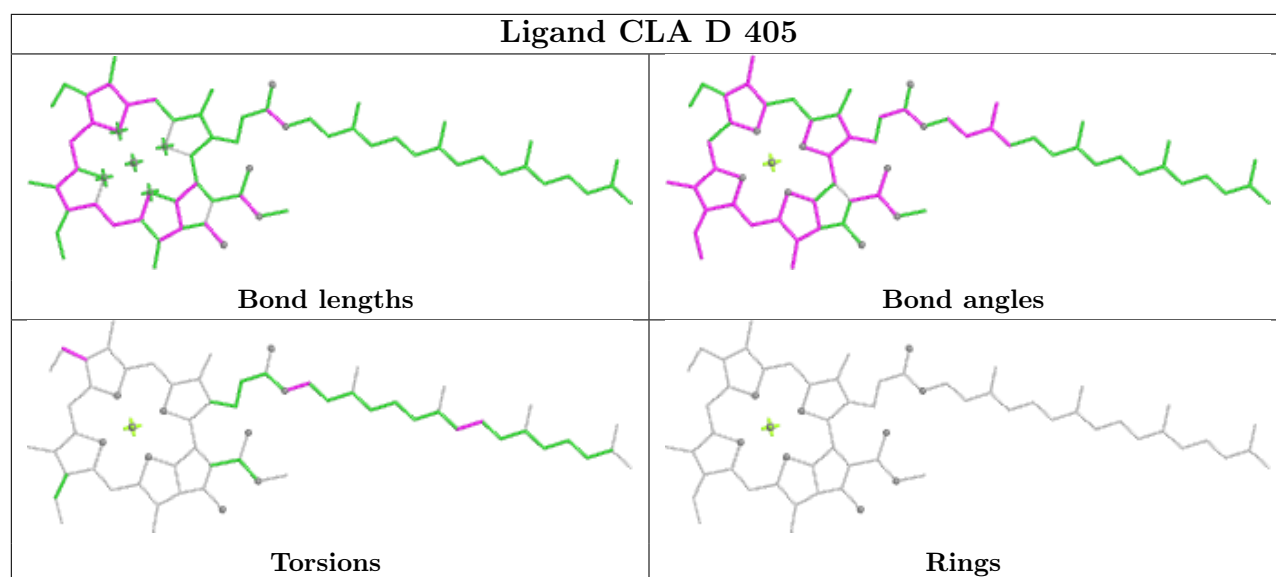
There are no ring outliers.

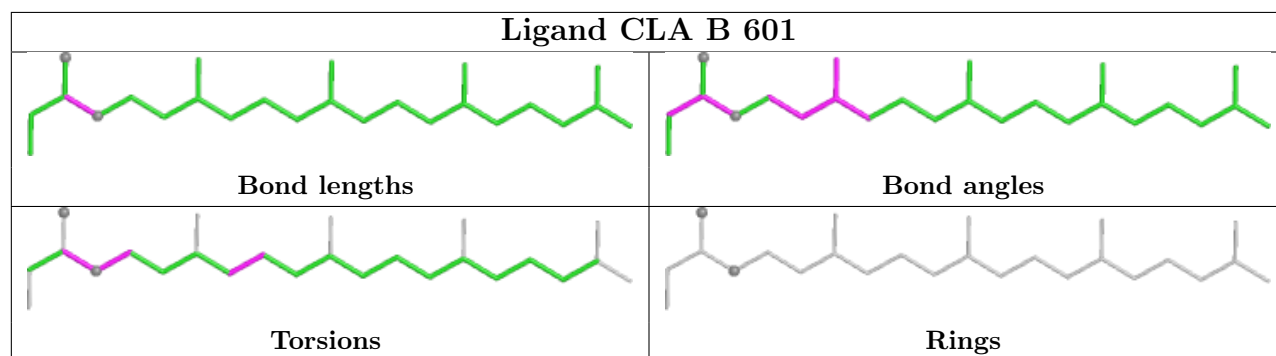
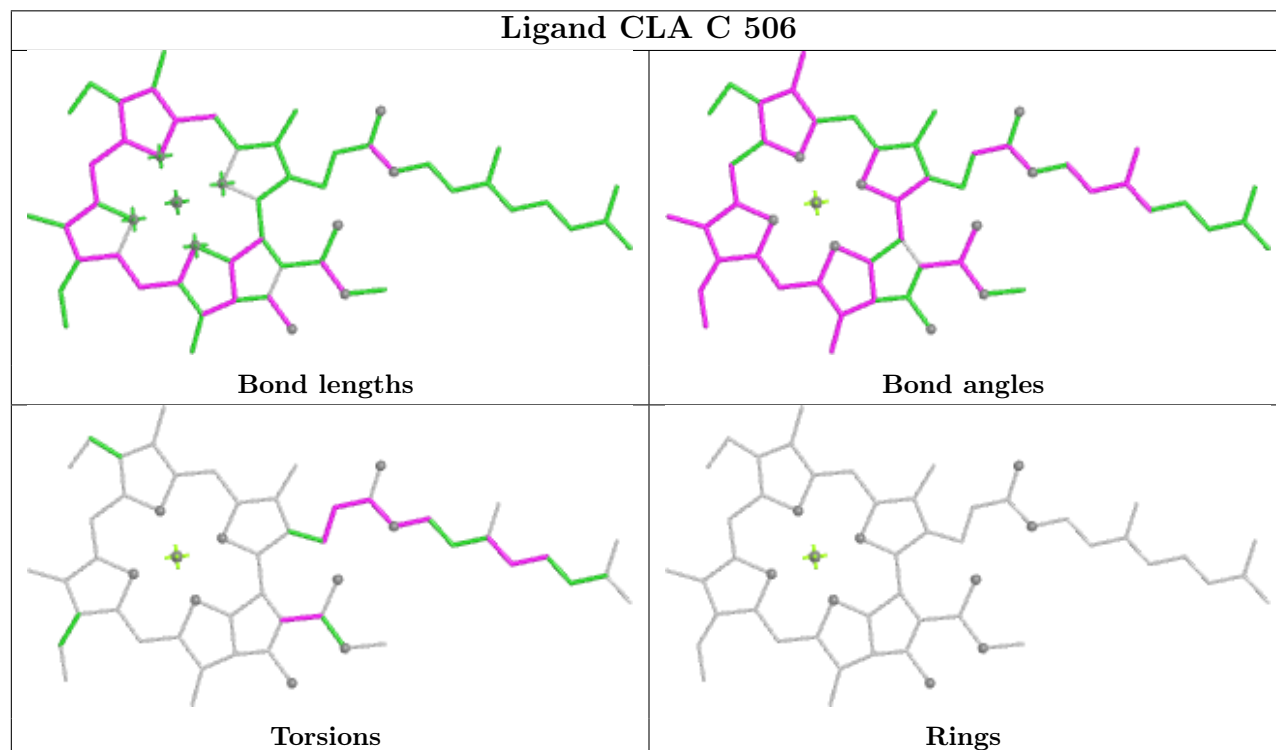
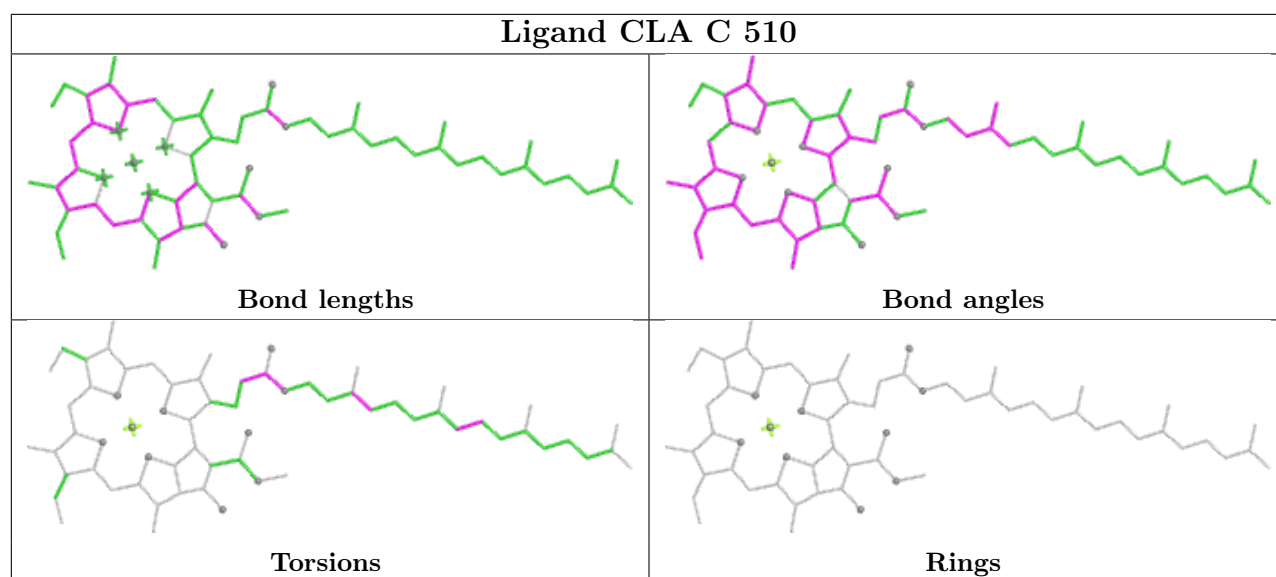
40 monomers are involved in 92 short contacts:

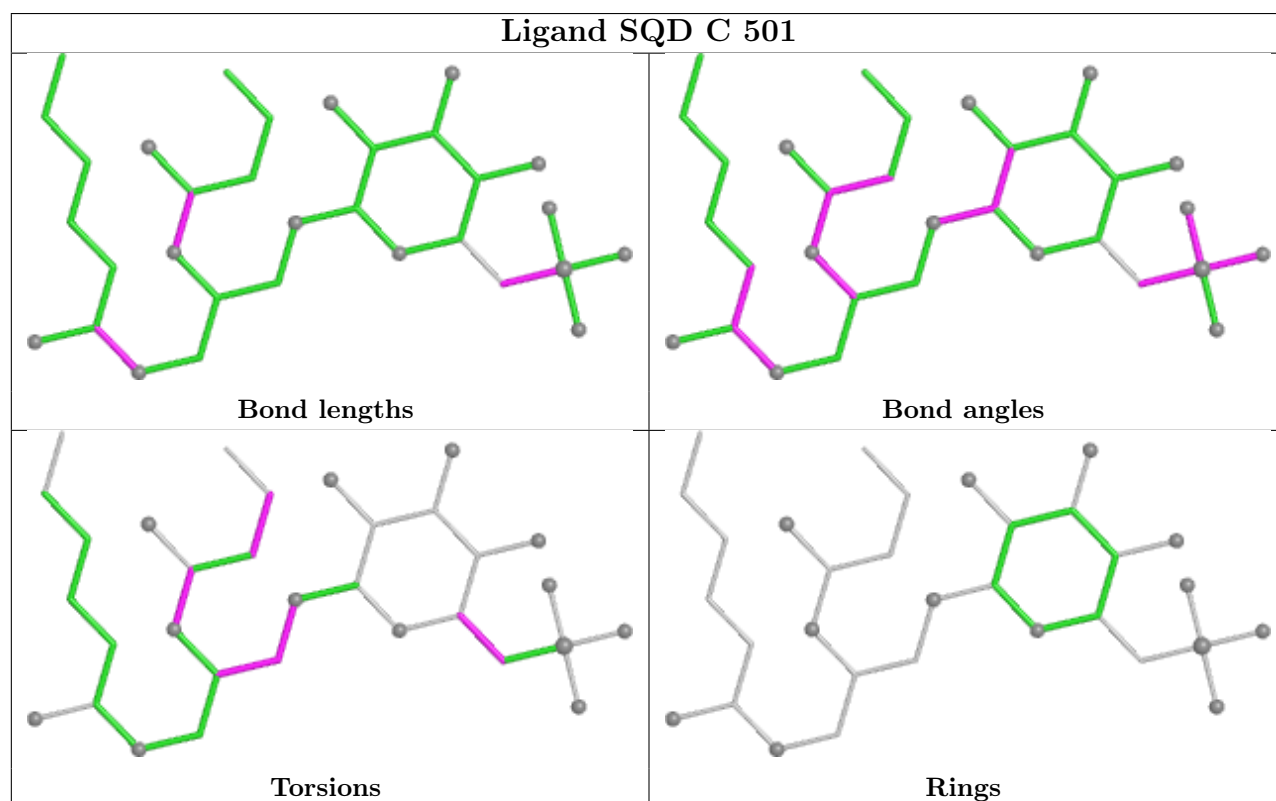
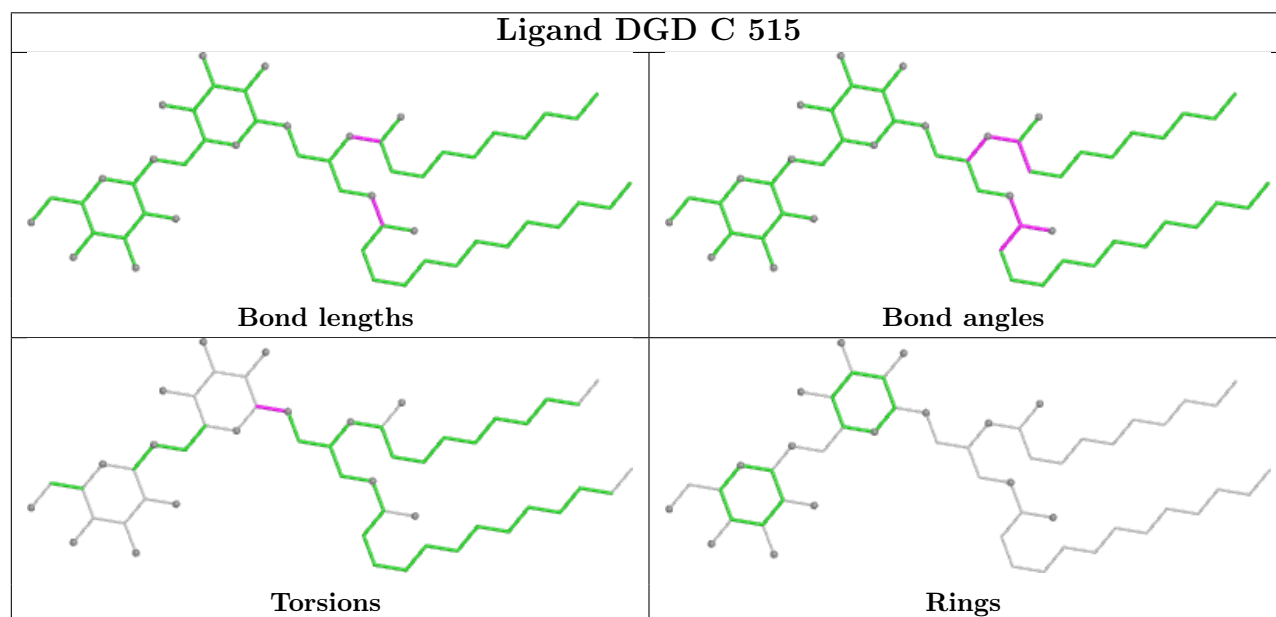
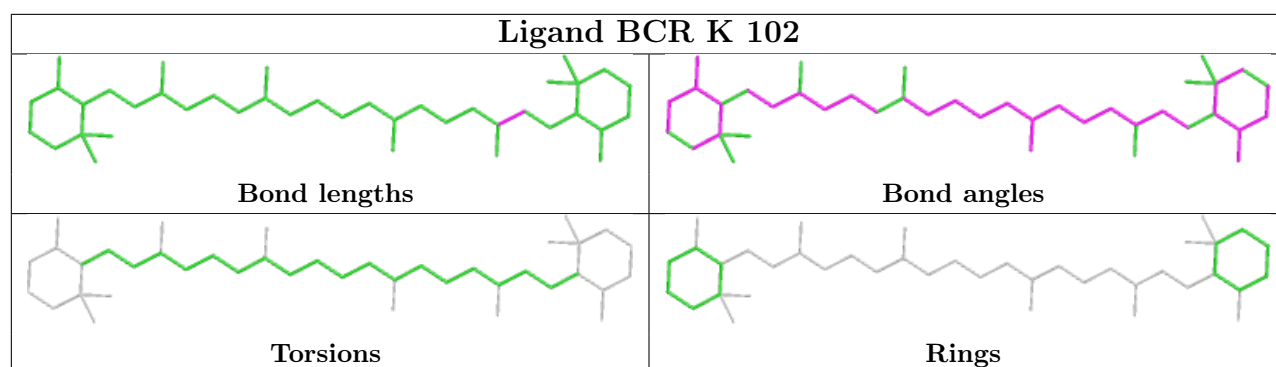
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	405	CLA	5	0
26	A	408	CLA	2	0
26	C	510	CLA	4	0
23	A	401	OEX	1	0
21	J	101	LMT	1	0
26	C	506	CLA	3	0
26	B	601	CLA	1	0
20	K	102	BCR	4	0
33	C	515	DGD	1	0
32	C	501	SQD	1	0
30	A	415	LHG	1	0
20	K	101	BCR	3	0
20	D	407	BCR	2	0
26	C	503	CLA	1	0
28	D	408	PL9	2	0
30	L	101	LHG	1	0
30	A	414	LHG	3	0
26	C	505	CLA	4	0
30	D	412	LHG	2	0
34	E	101	HEM	2	0
27	A	407	PHO	1	0
27	D	401	PHO	5	0
26	C	516	CLA	3	0
33	C	513	DGD	1	0
30	D	409	LHG	1	0
26	A	412	CLA	4	0
26	C	507	CLA	1	0
26	C	508	CLA	3	0
26	D	403	CLA	2	0
26	C	509	CLA	5	0
20	T	102	BCR	1	0
20	K	104	BCR	1	0
31	C	502	LMG	3	0
28	A	410	PL9	7	0
33	D	413	DGD	3	0
26	C	511	CLA	7	0
33	C	514	DGD	4	0
26	A	406	CLA	2	0
26	A	405	CLA	8	0
26	C	504	CLA	4	0

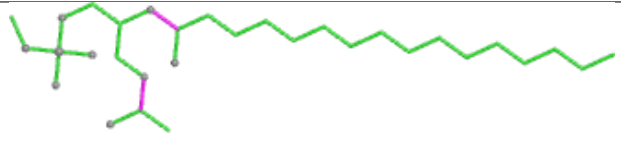
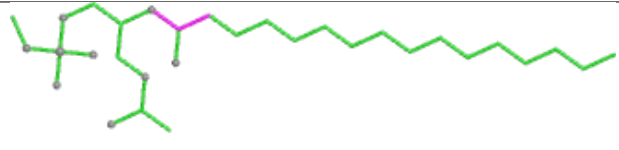
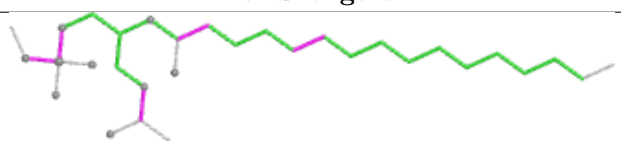
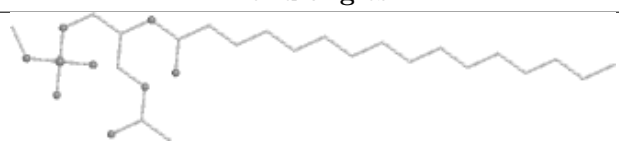
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

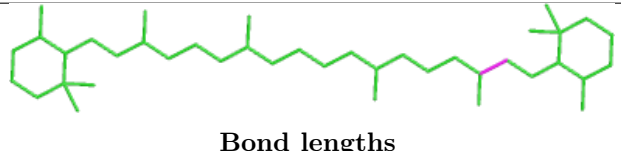
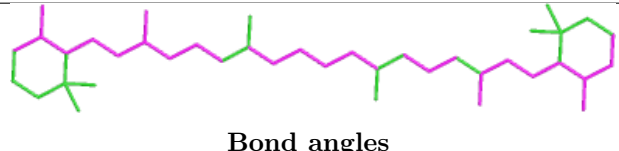
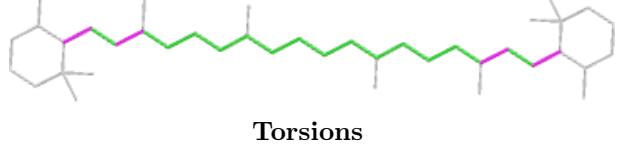
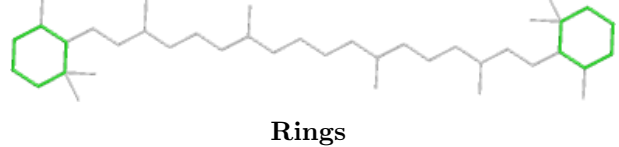


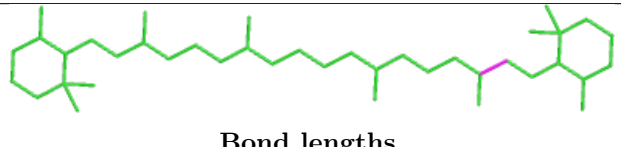
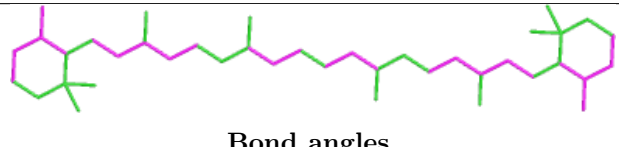
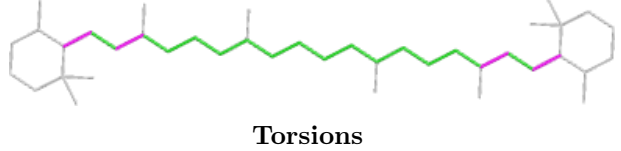
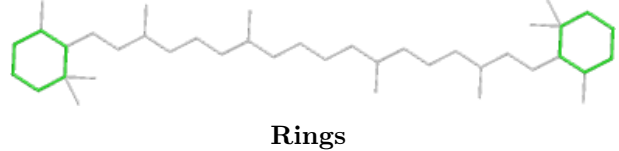


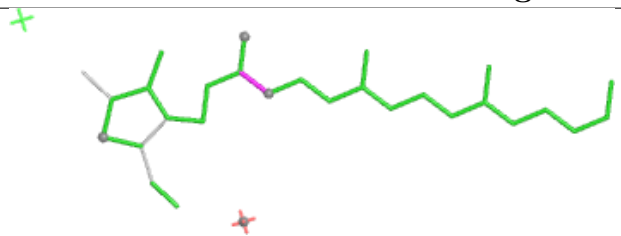
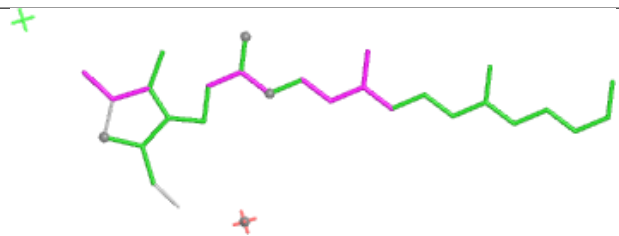
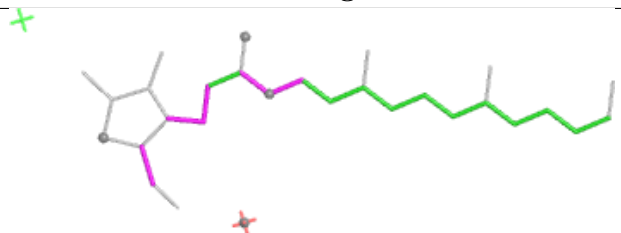
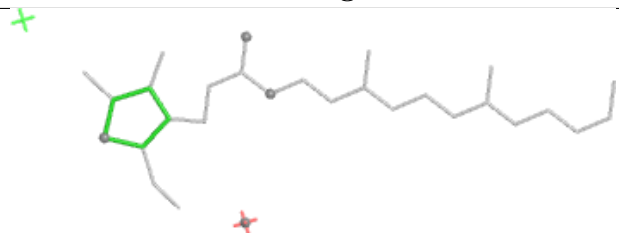


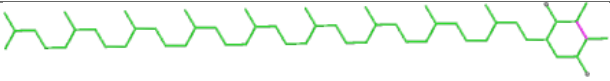
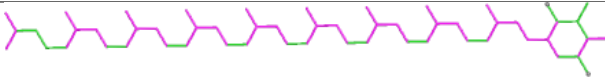
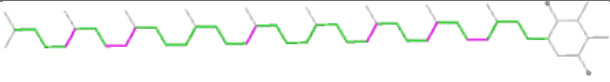
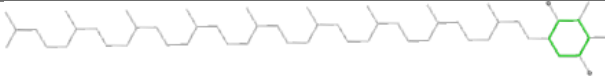
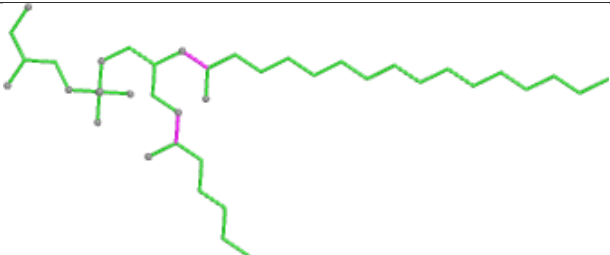
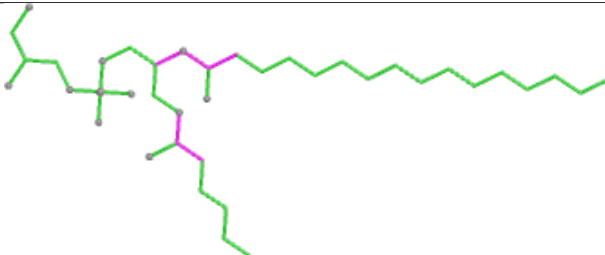
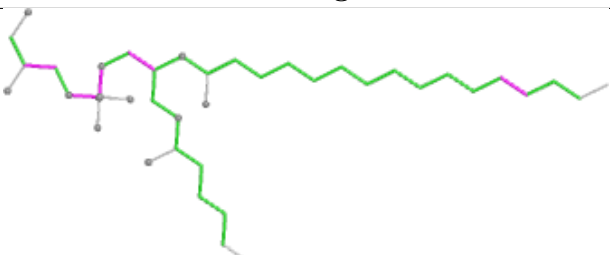
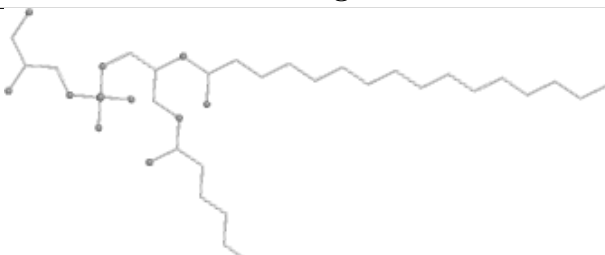


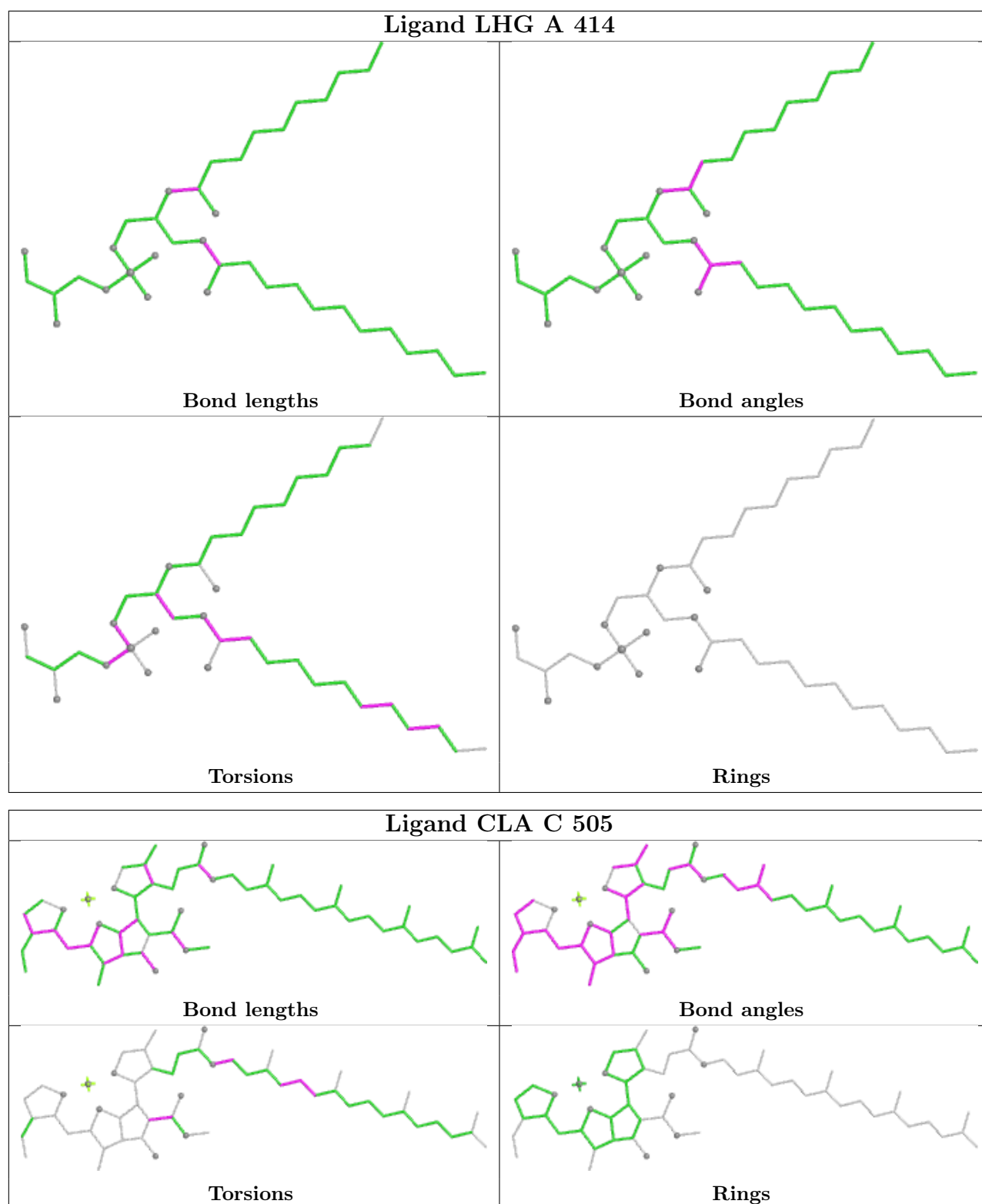
Ligand LHG A 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

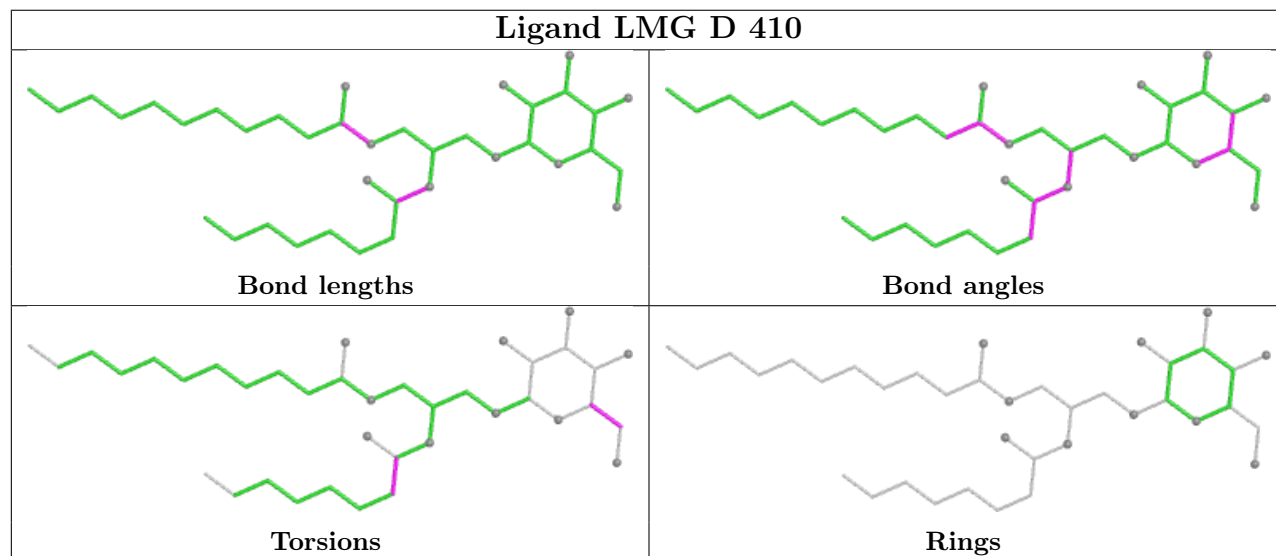
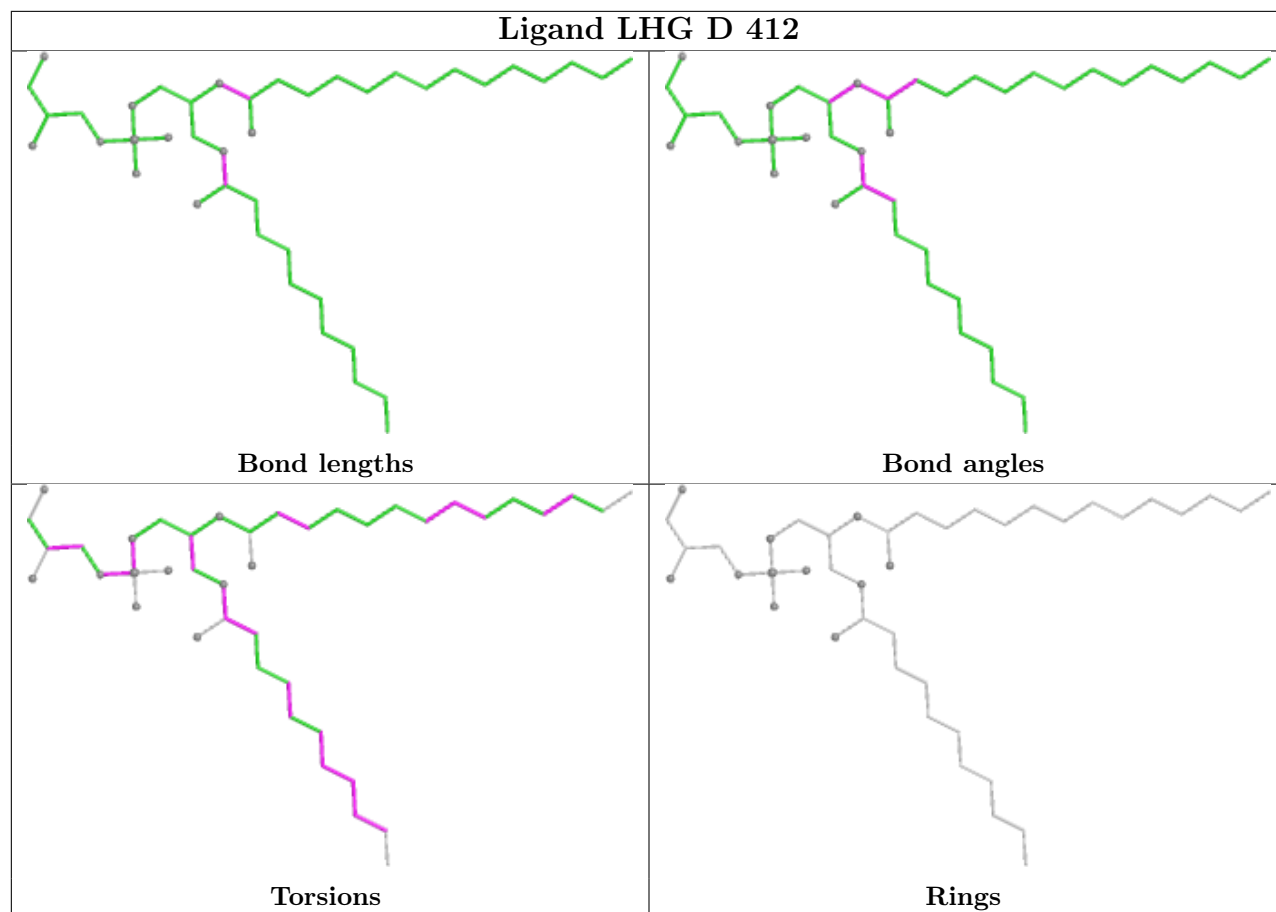
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

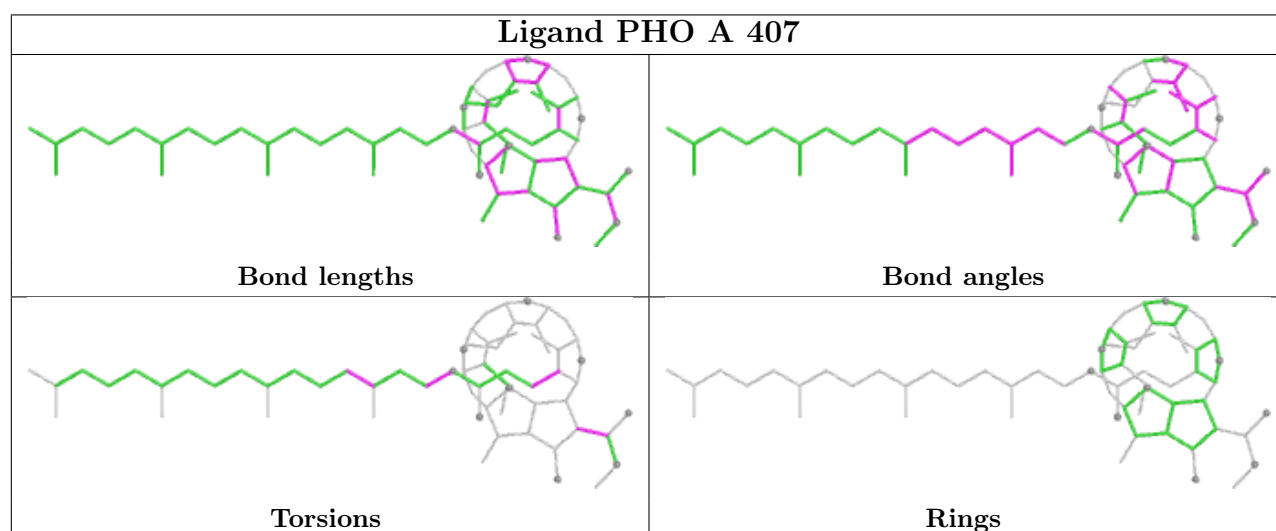
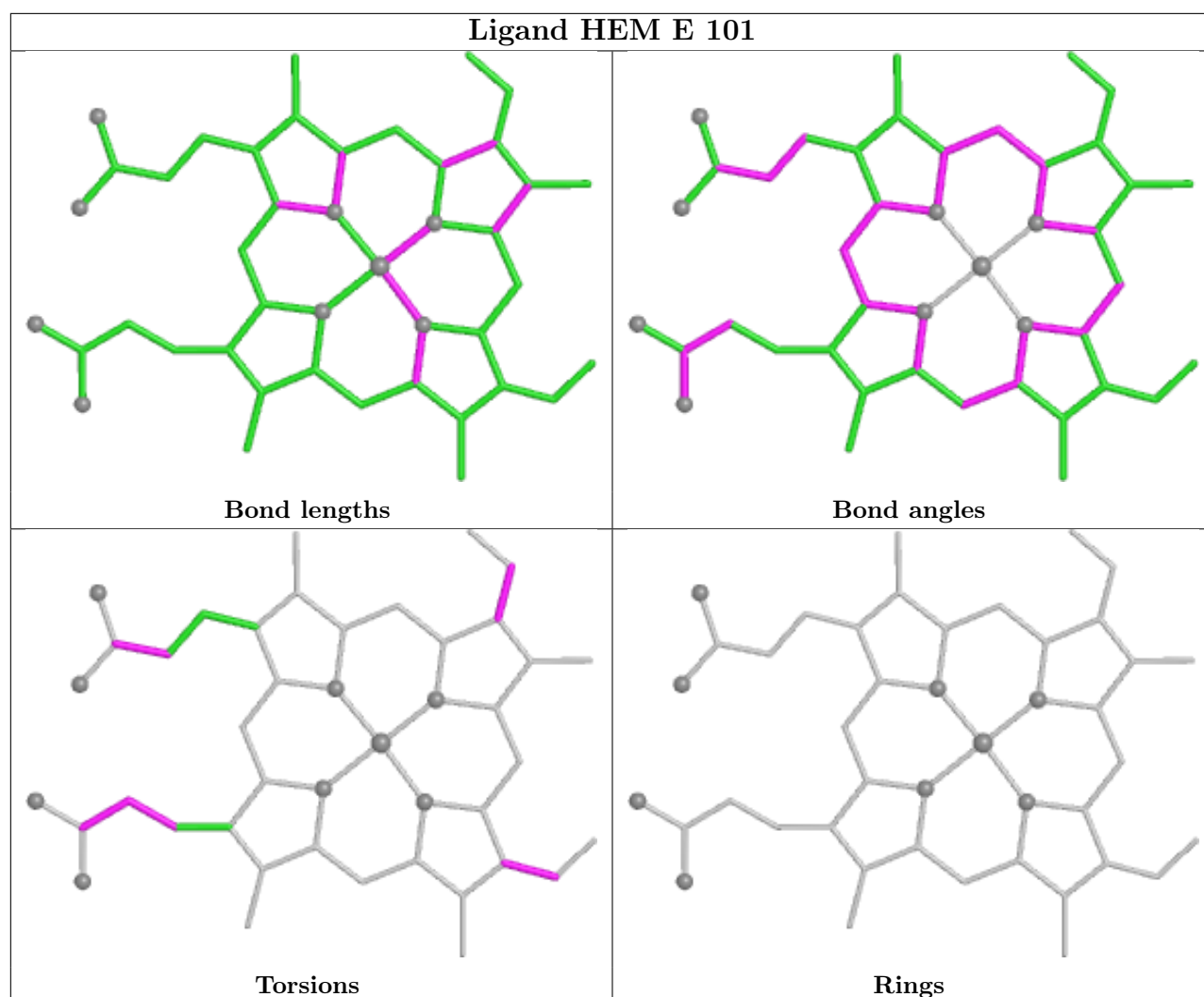
Ligand BCR D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

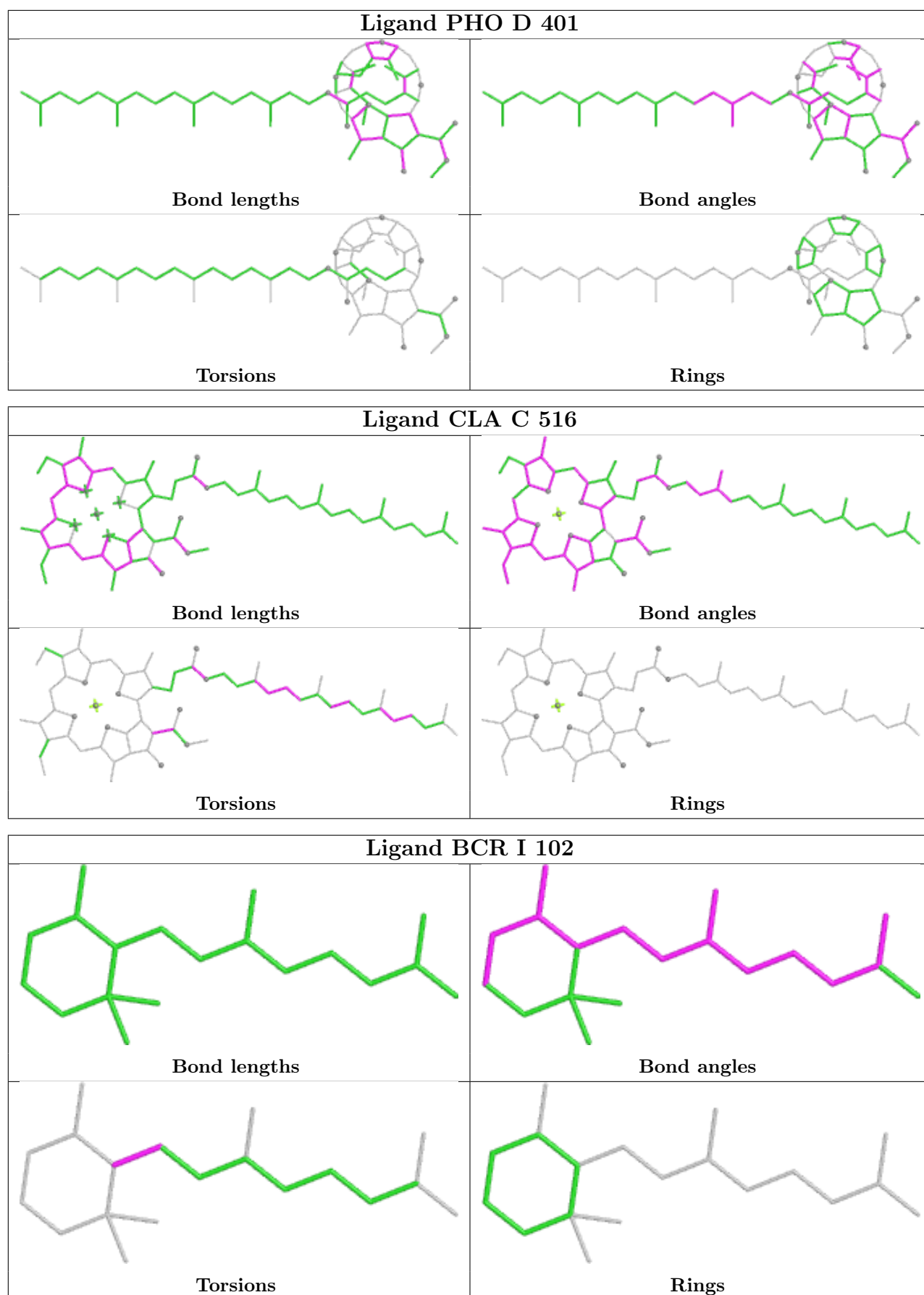
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

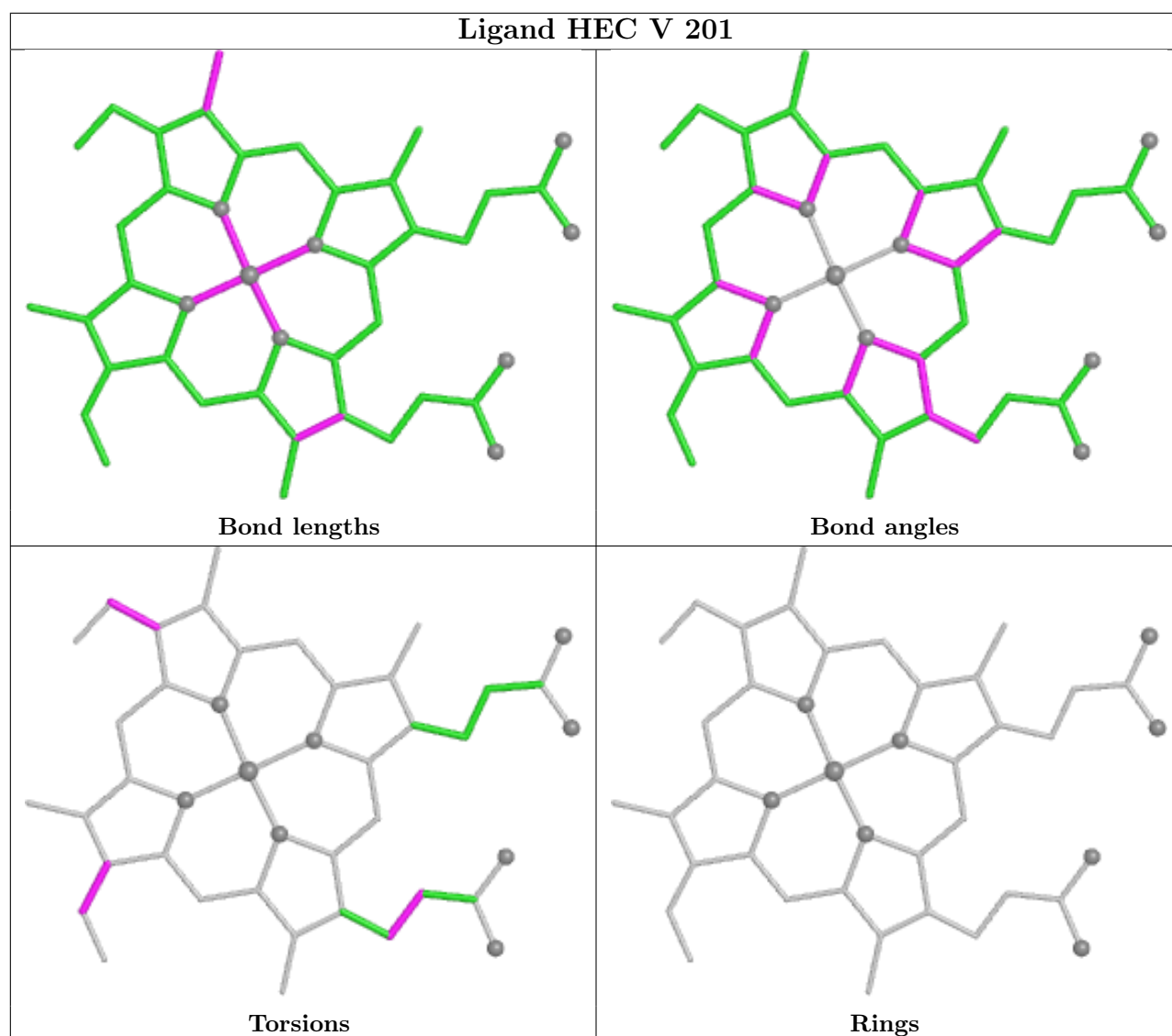
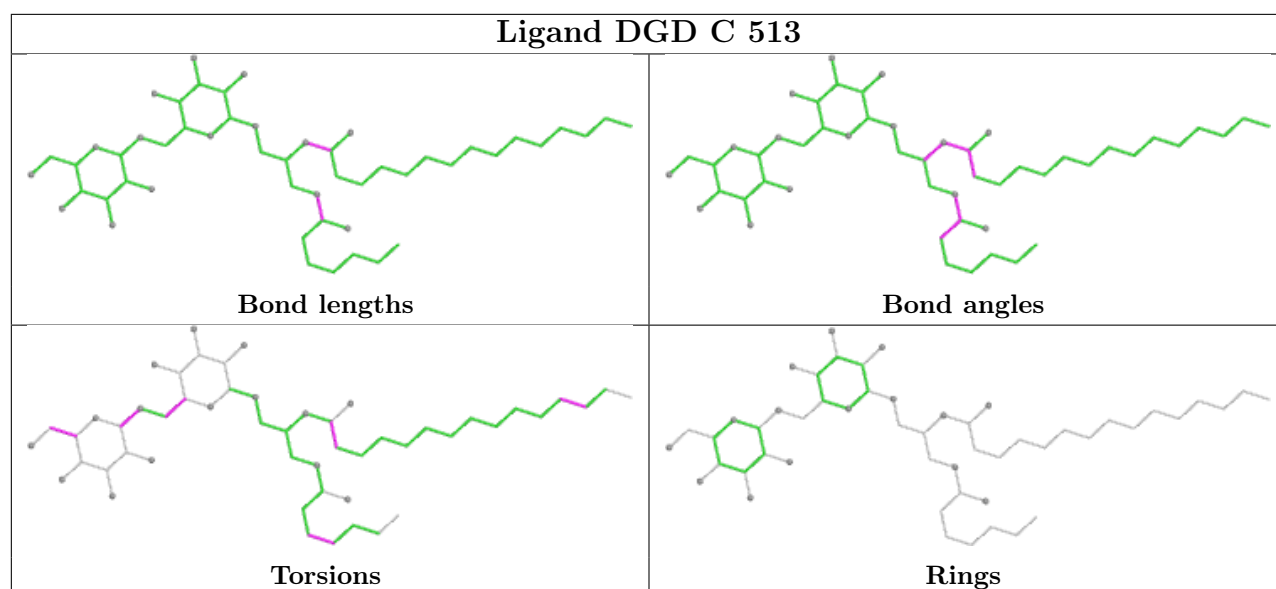
Ligand PL9 D 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LHG L 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

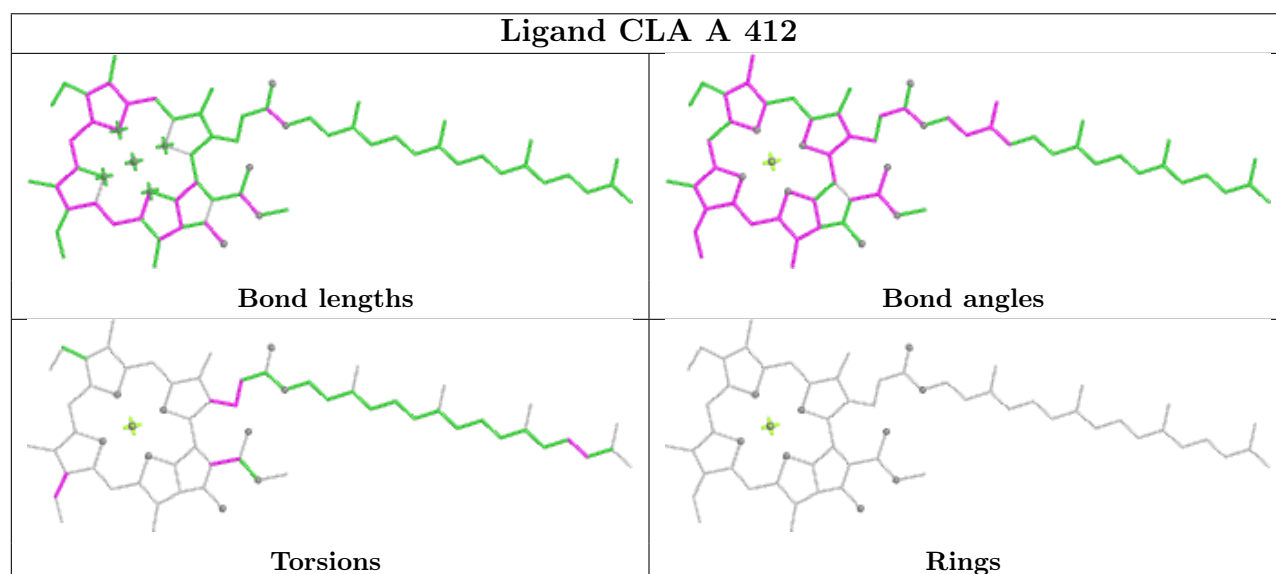
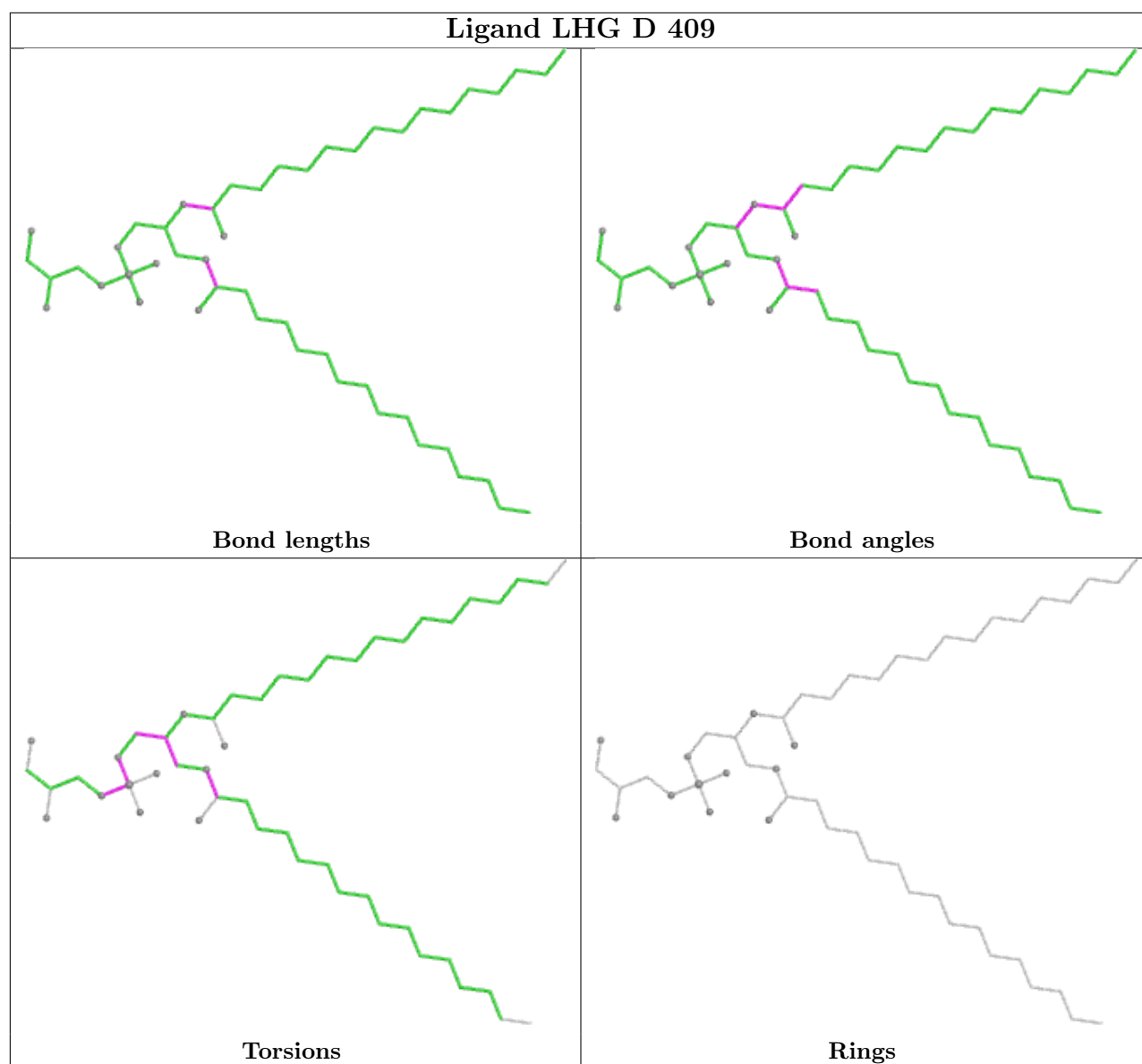


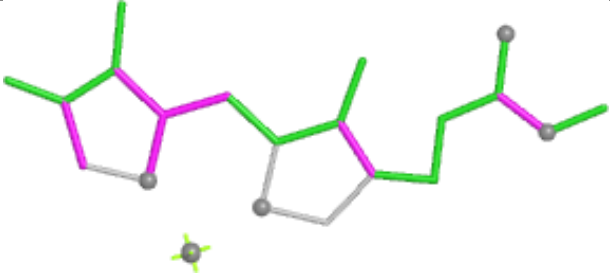
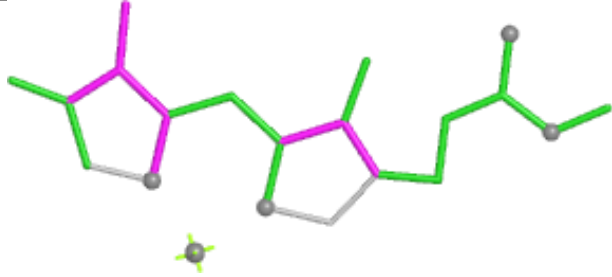
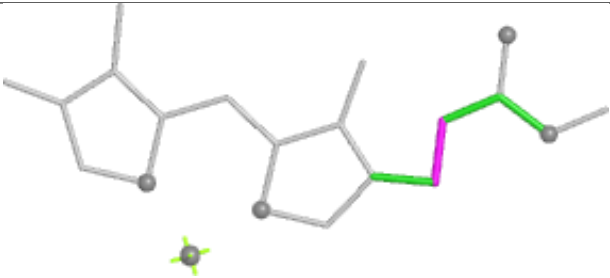
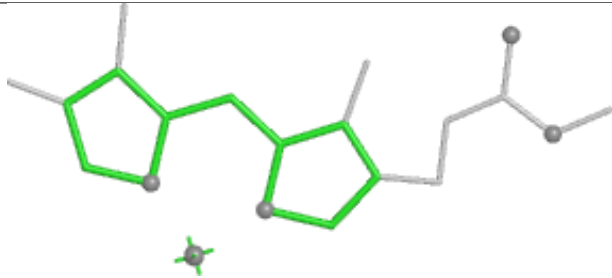
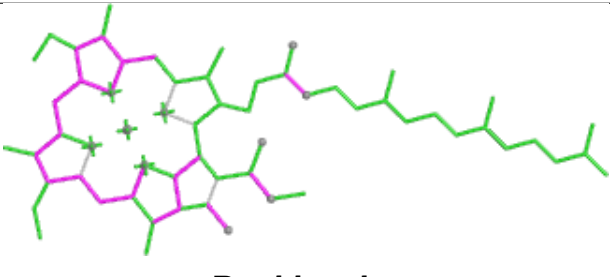
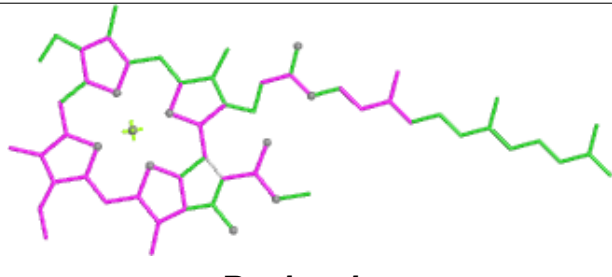
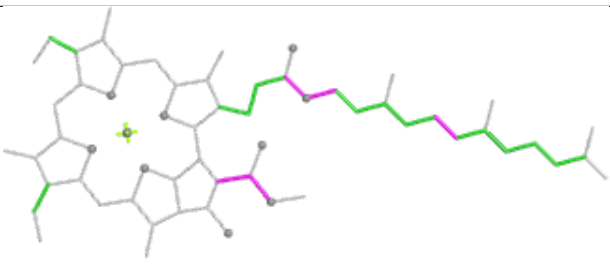
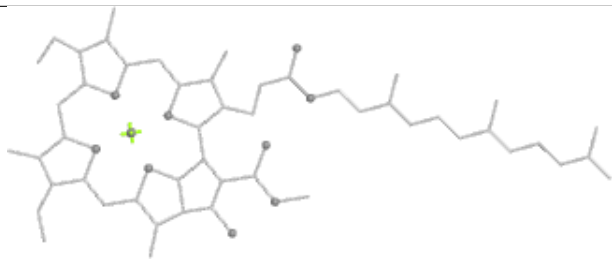
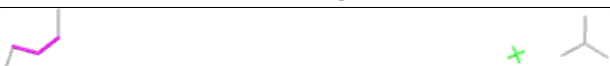
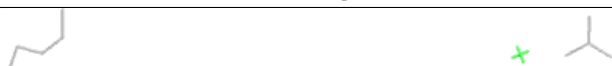


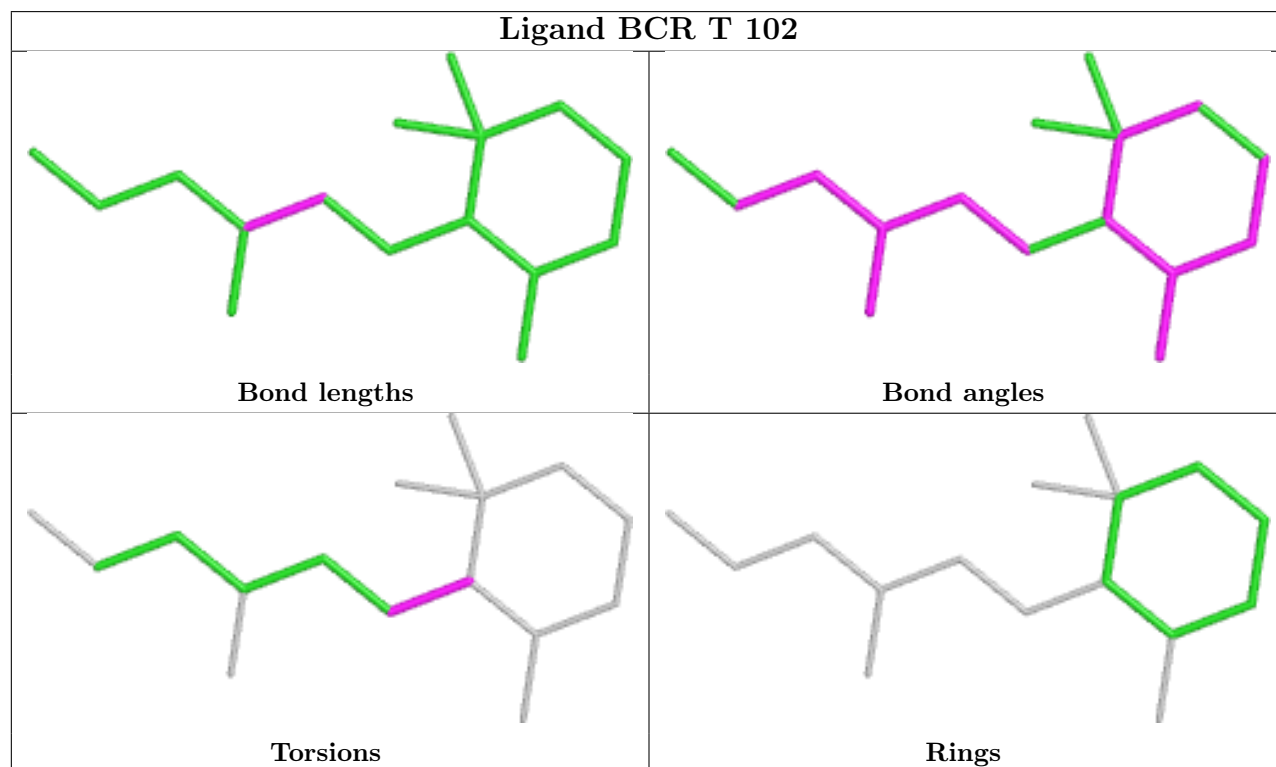
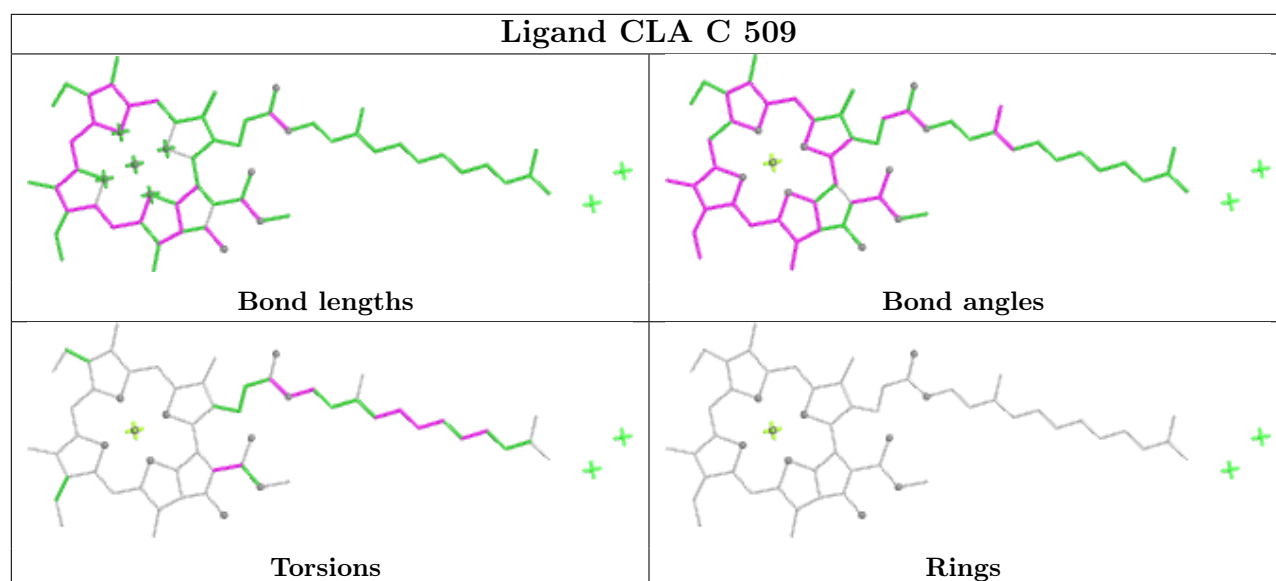


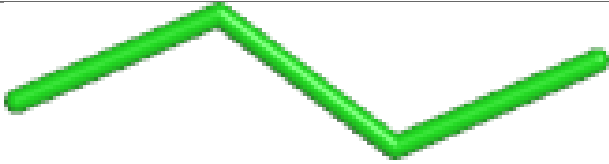
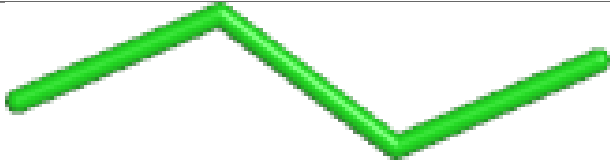
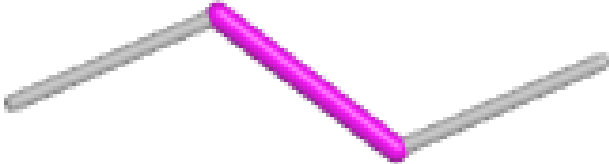
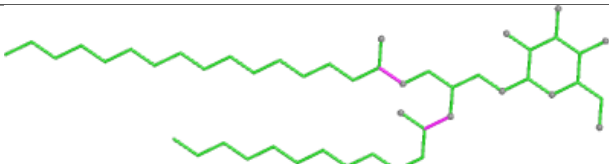
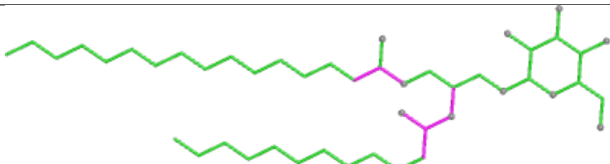
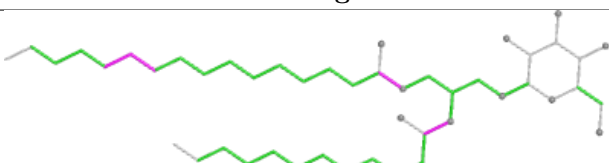
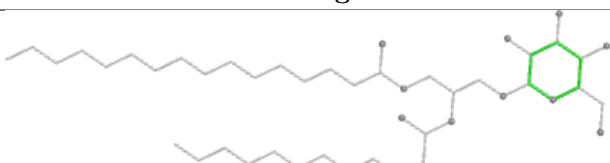
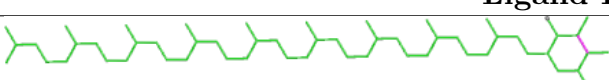
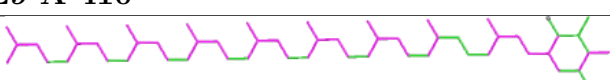
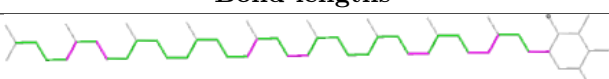
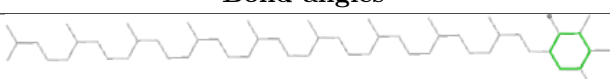


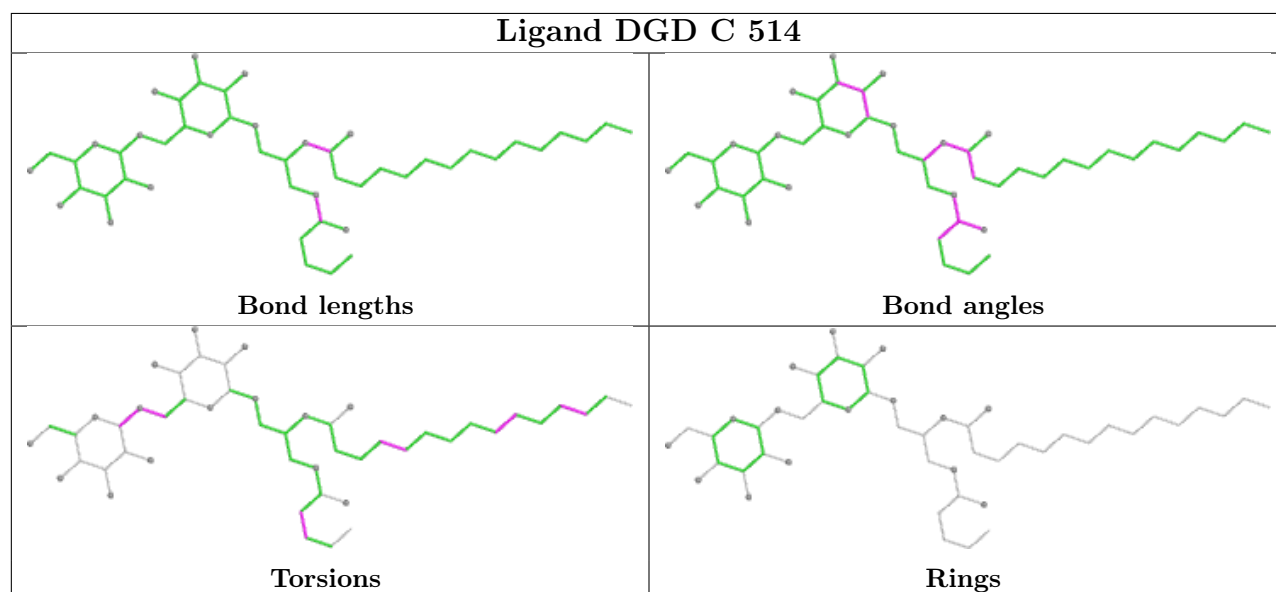
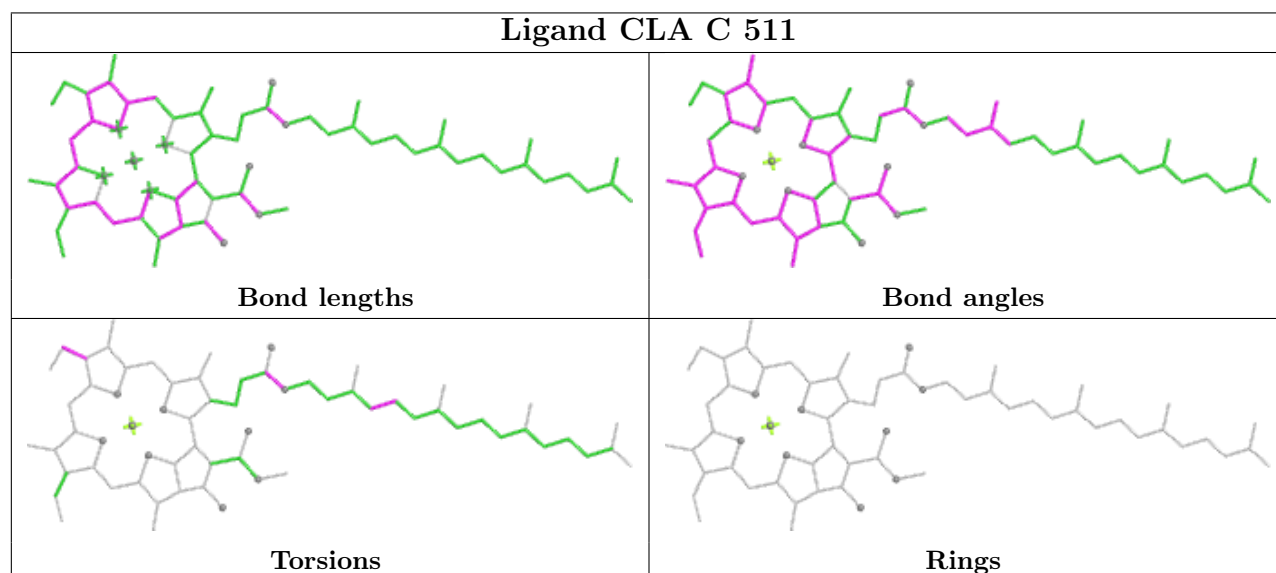
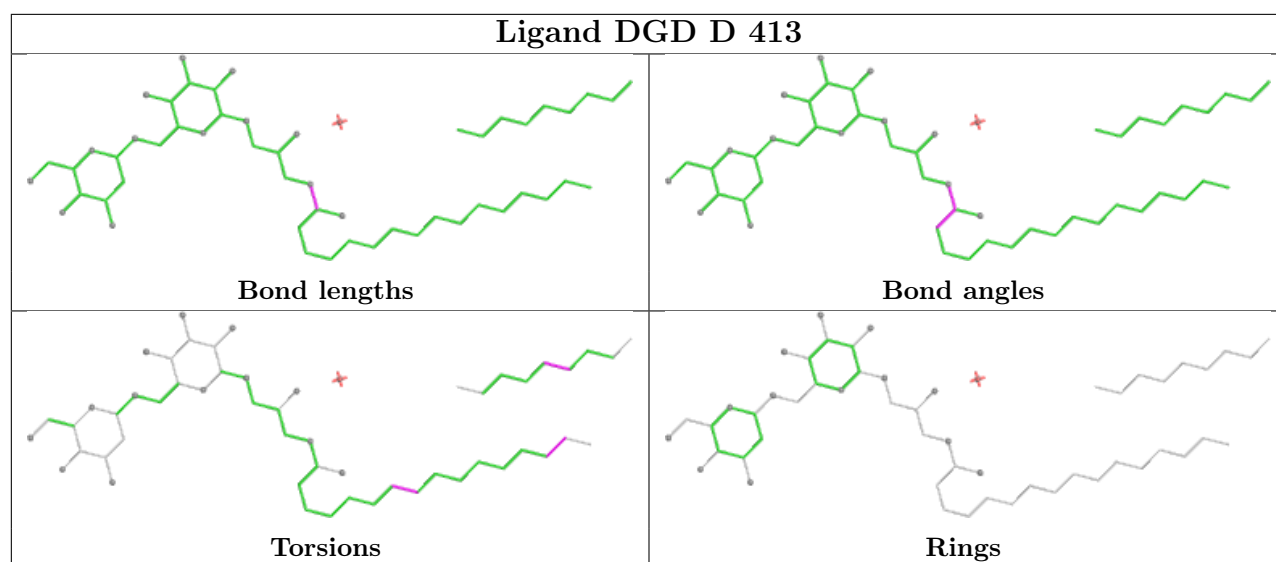


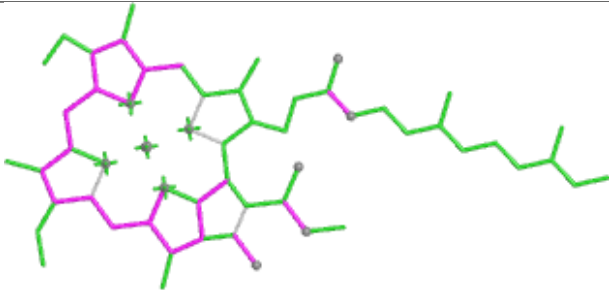
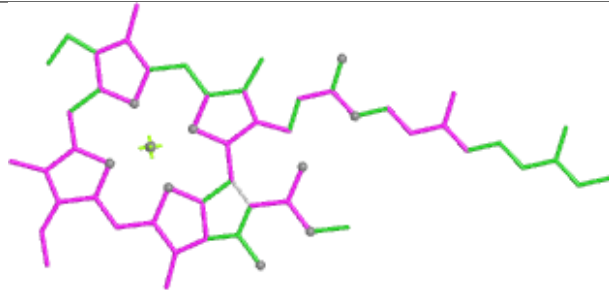
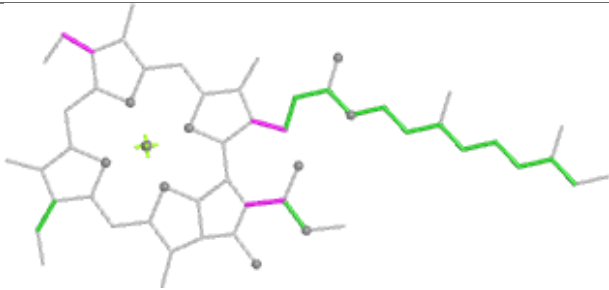
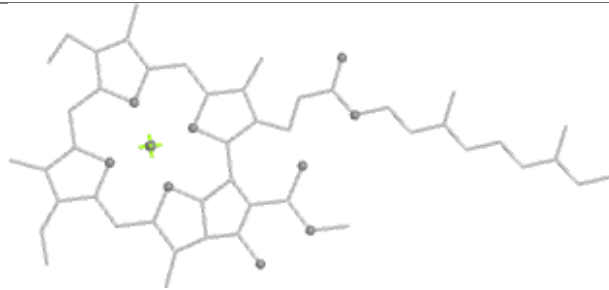
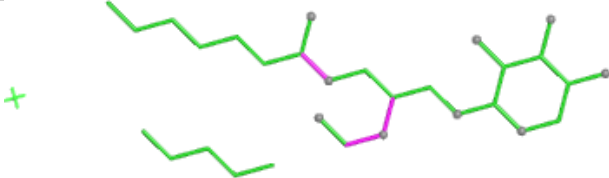
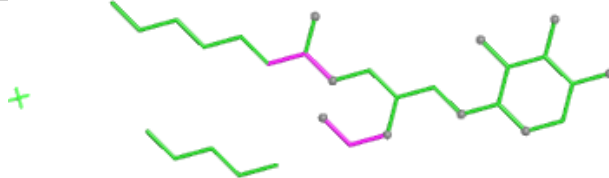
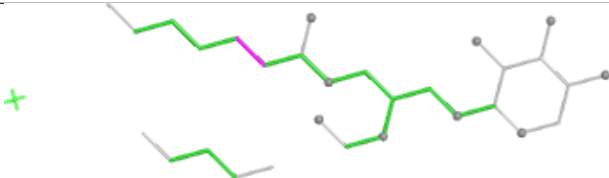
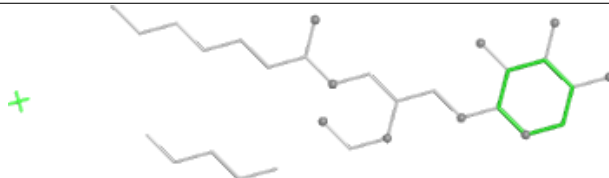


Ligand CLA C 507			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand CLA C 508			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand CLA D 403			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

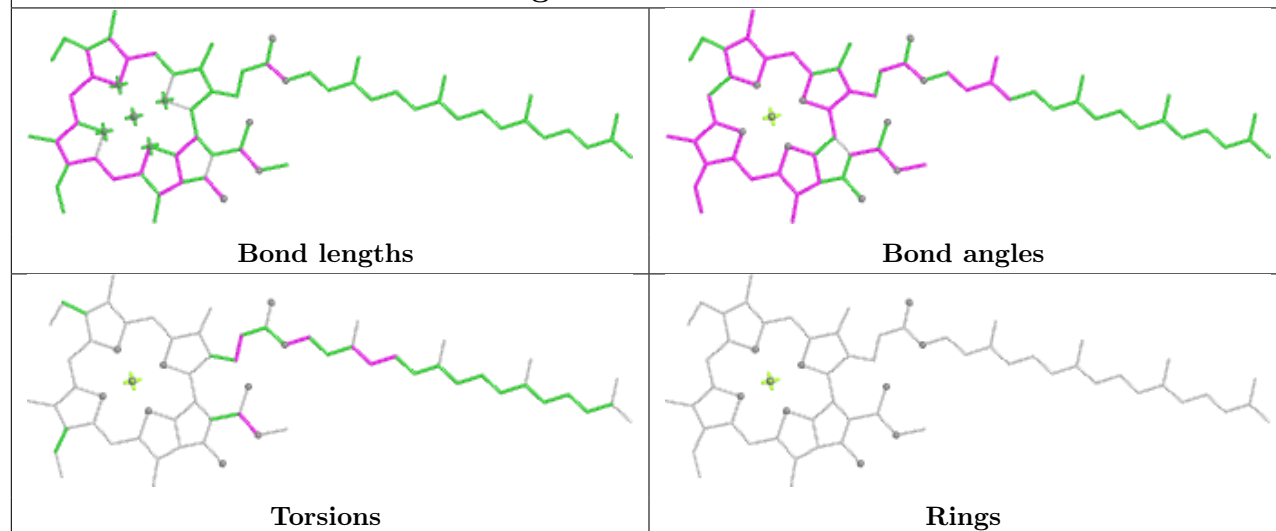


Ligand BCR K 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

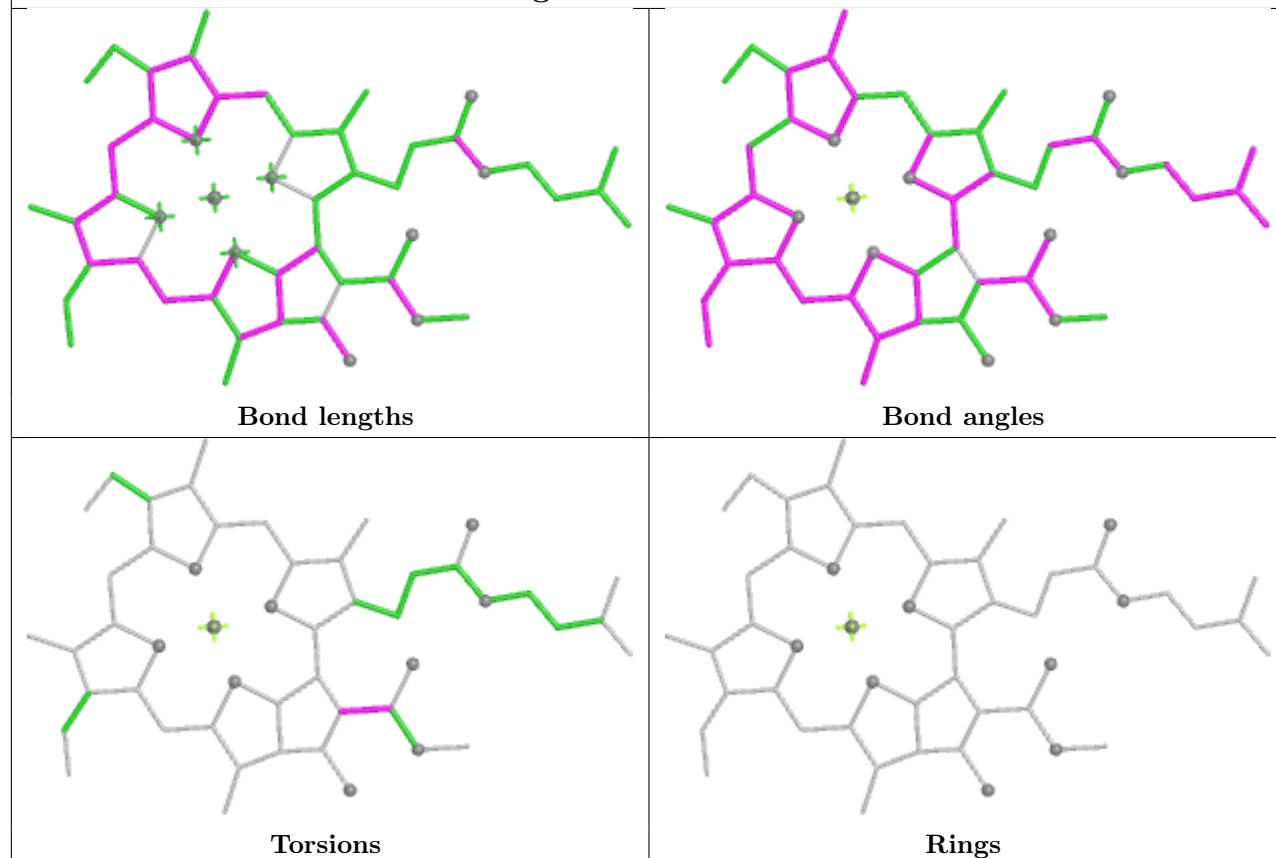


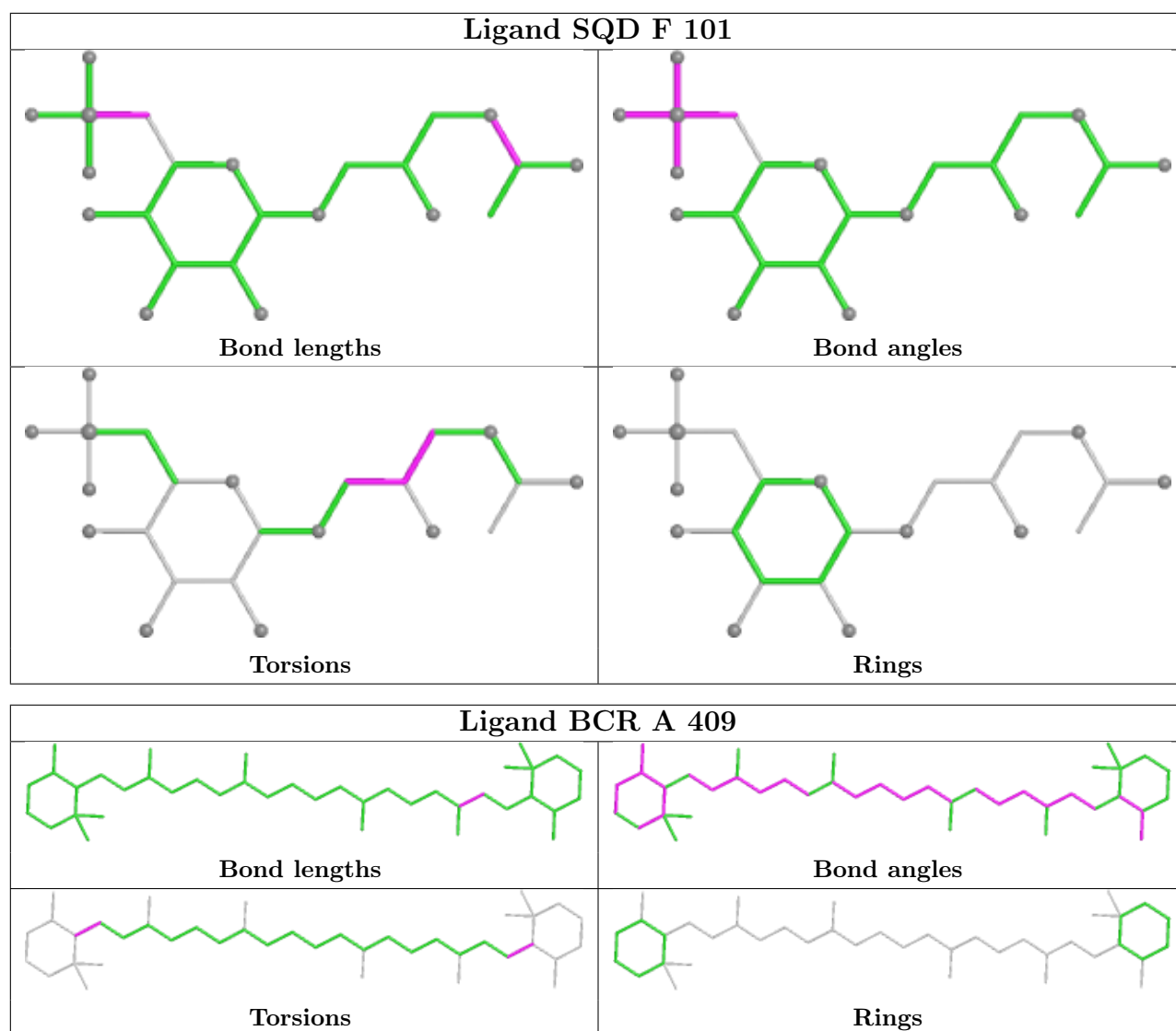
Ligand CLA A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LMG B 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 405



Ligand CLA C 504





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	50:PRO	C	61:ARG	N	16.06

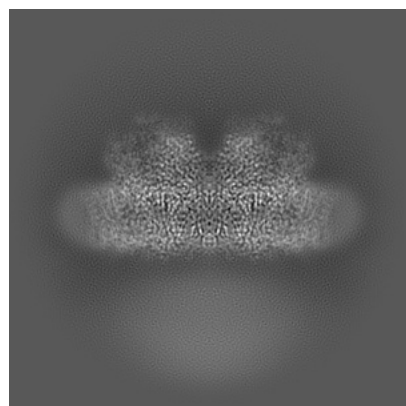
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65941. These allow visual inspection of the internal detail of the map and identification of artifacts.

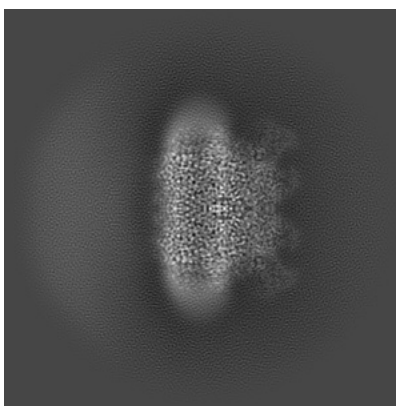
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

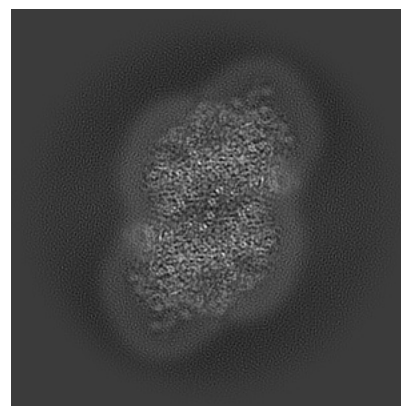
6.1.1 Primary map



X

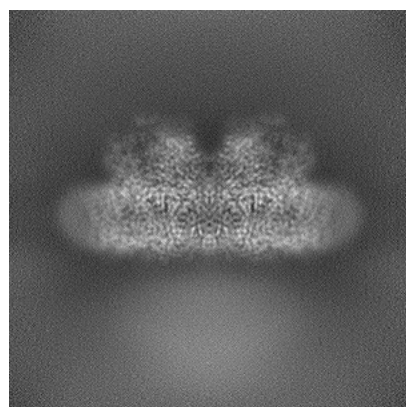


Y

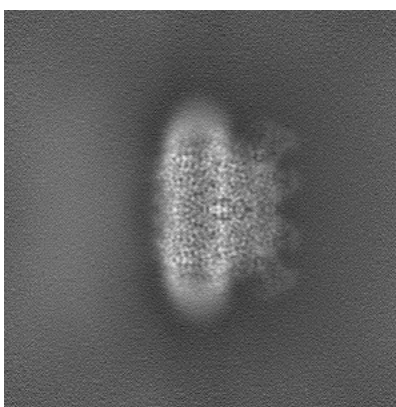


Z

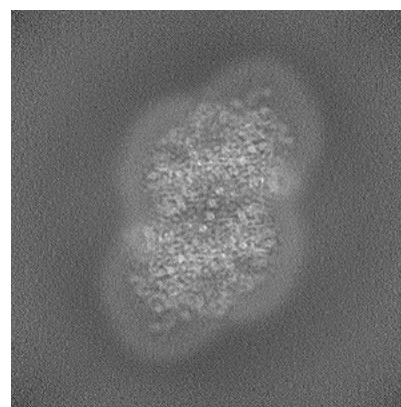
6.1.2 Raw map



X



Y

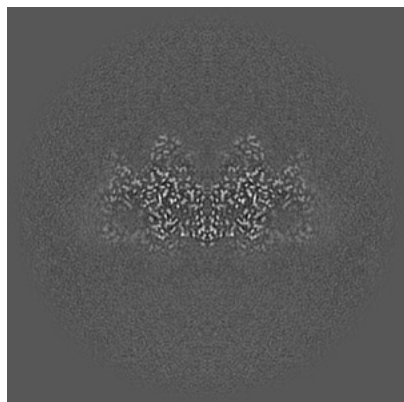


Z

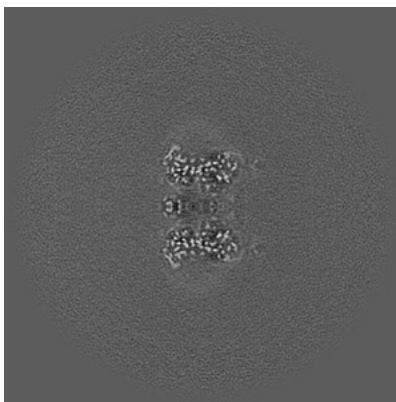
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

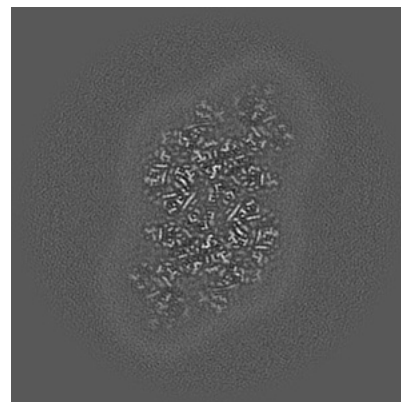
6.2.1 Primary map



X Index: 256

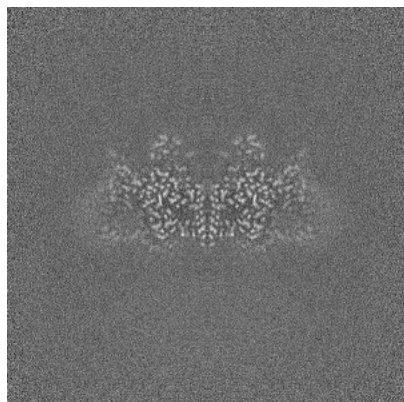


Y Index: 256

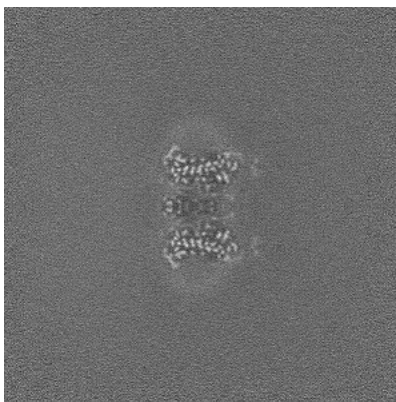


Z Index: 256

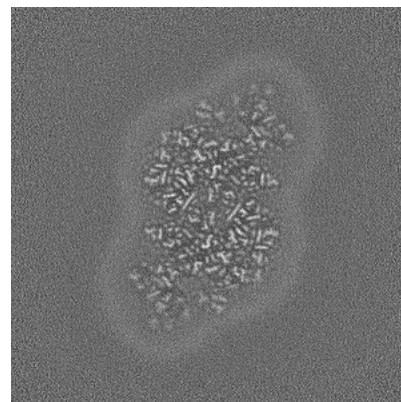
6.2.2 Raw map



X Index: 256



Y Index: 256

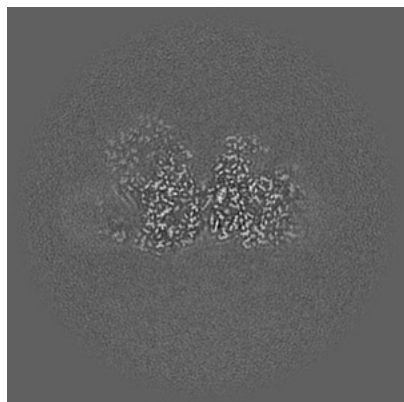


Z Index: 256

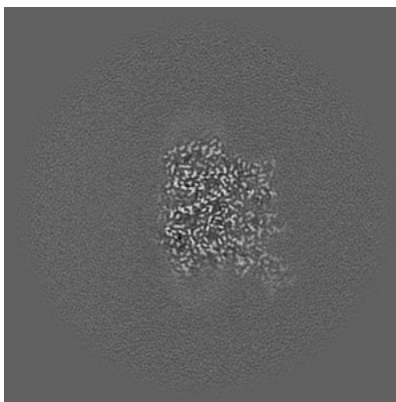
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

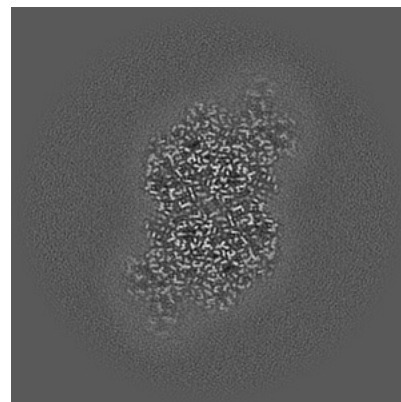
6.3.1 Primary map



X Index: 230

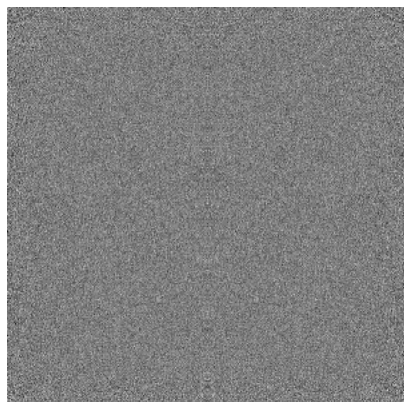


Y Index: 209

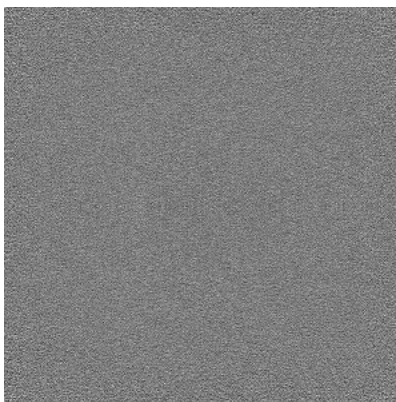


Z Index: 275

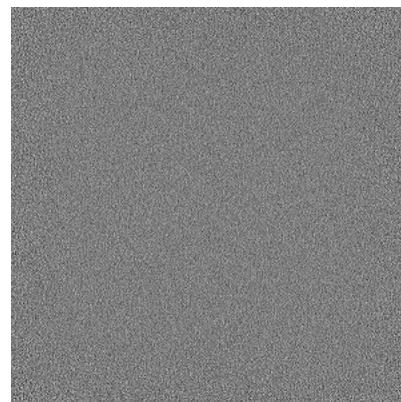
6.3.2 Raw map



X Index: 0



Y Index: 0

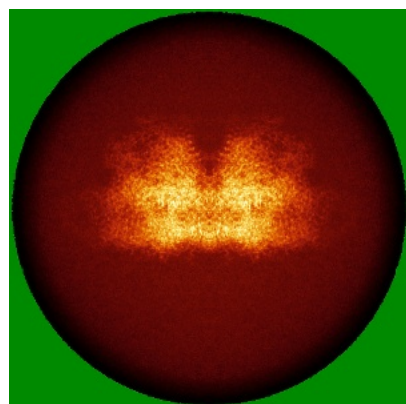


Z Index: 0

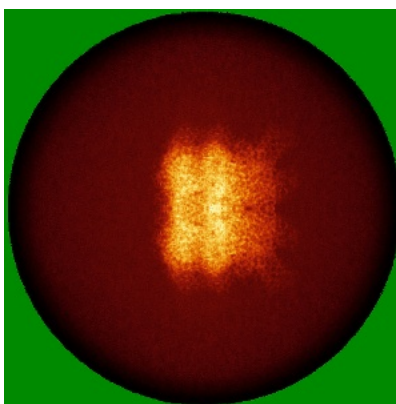
The images above show the largest variance slices of the map in three orthogonal directions.

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

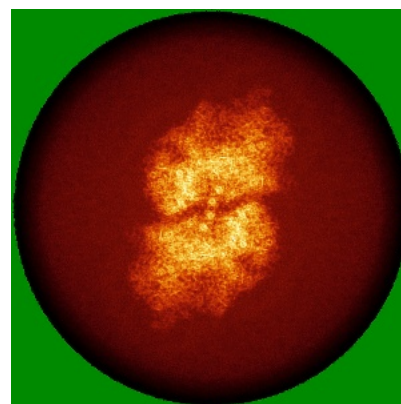
6.4.1 Primary map



X

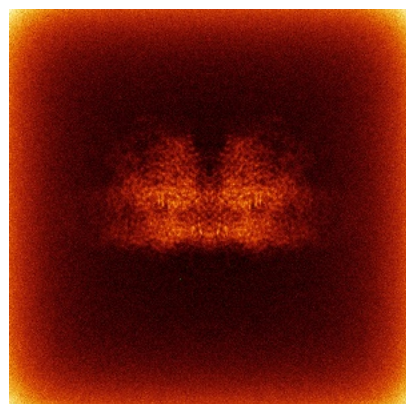


Y

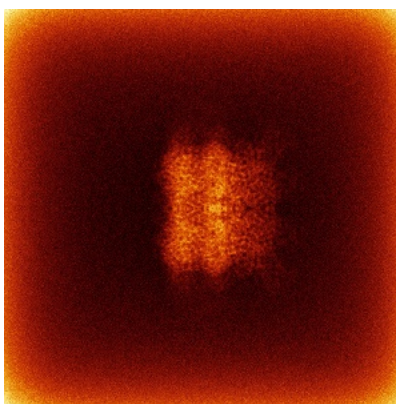


Z

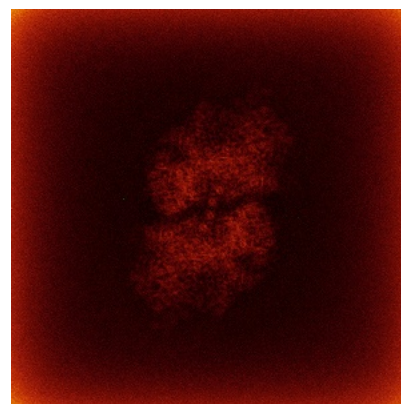
6.4.2 Raw map



X



Y

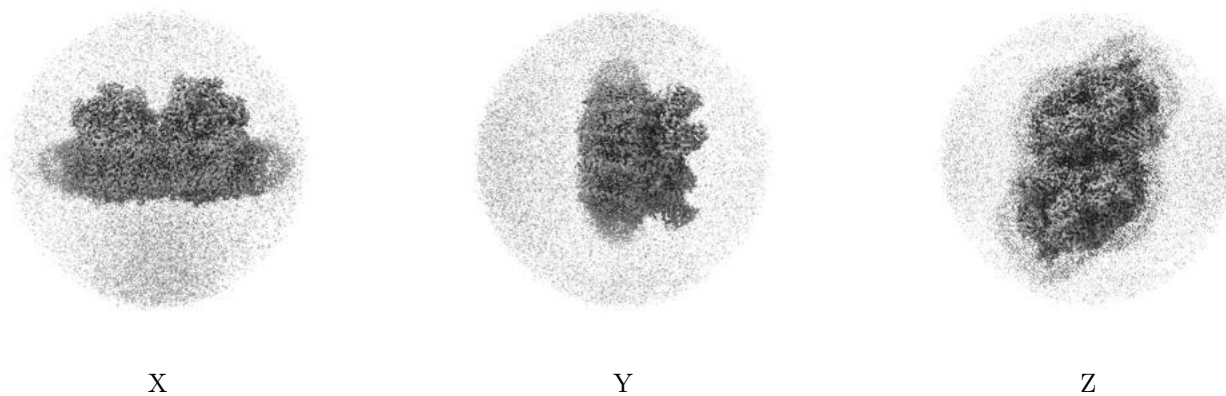


Z

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.

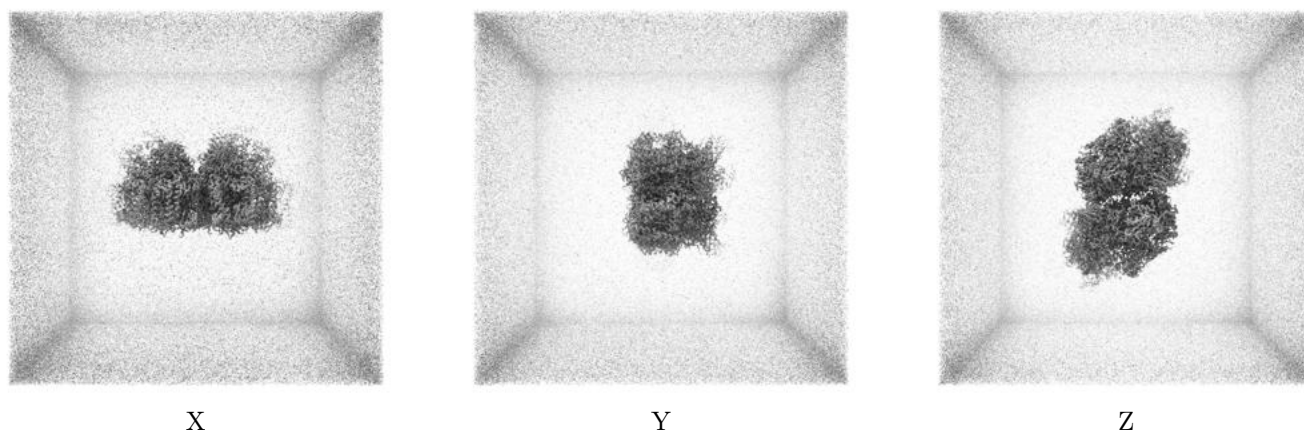
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

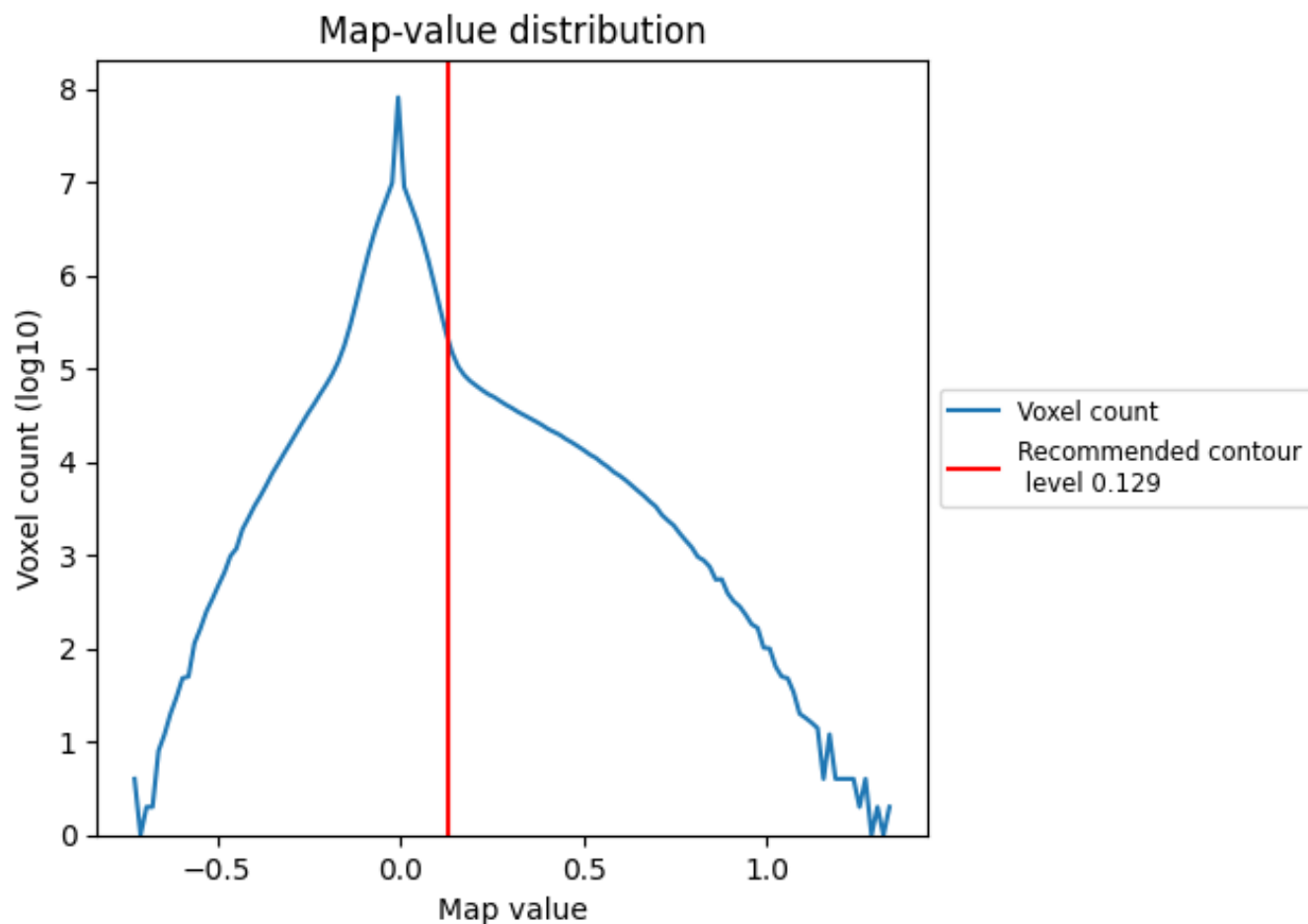
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

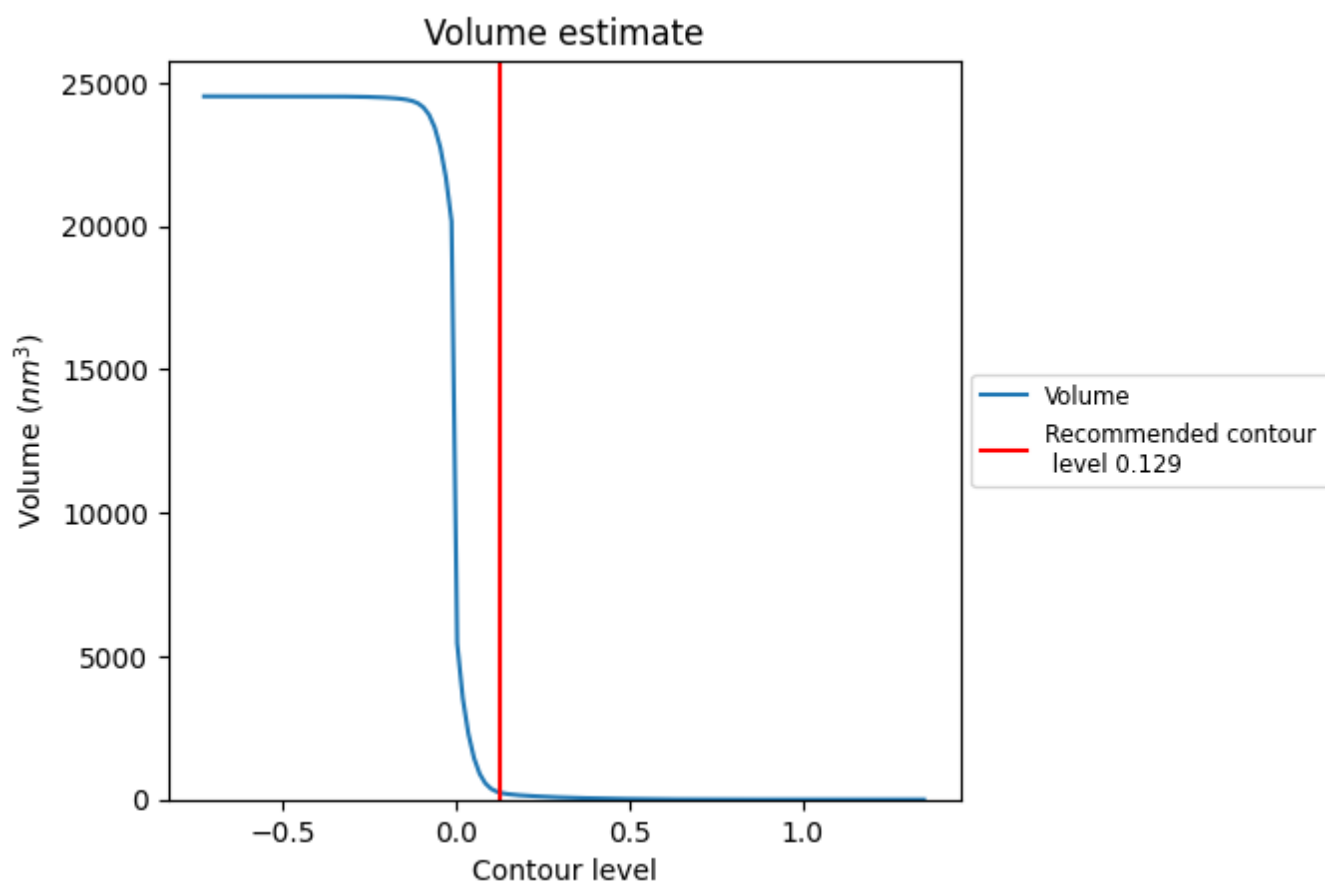
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

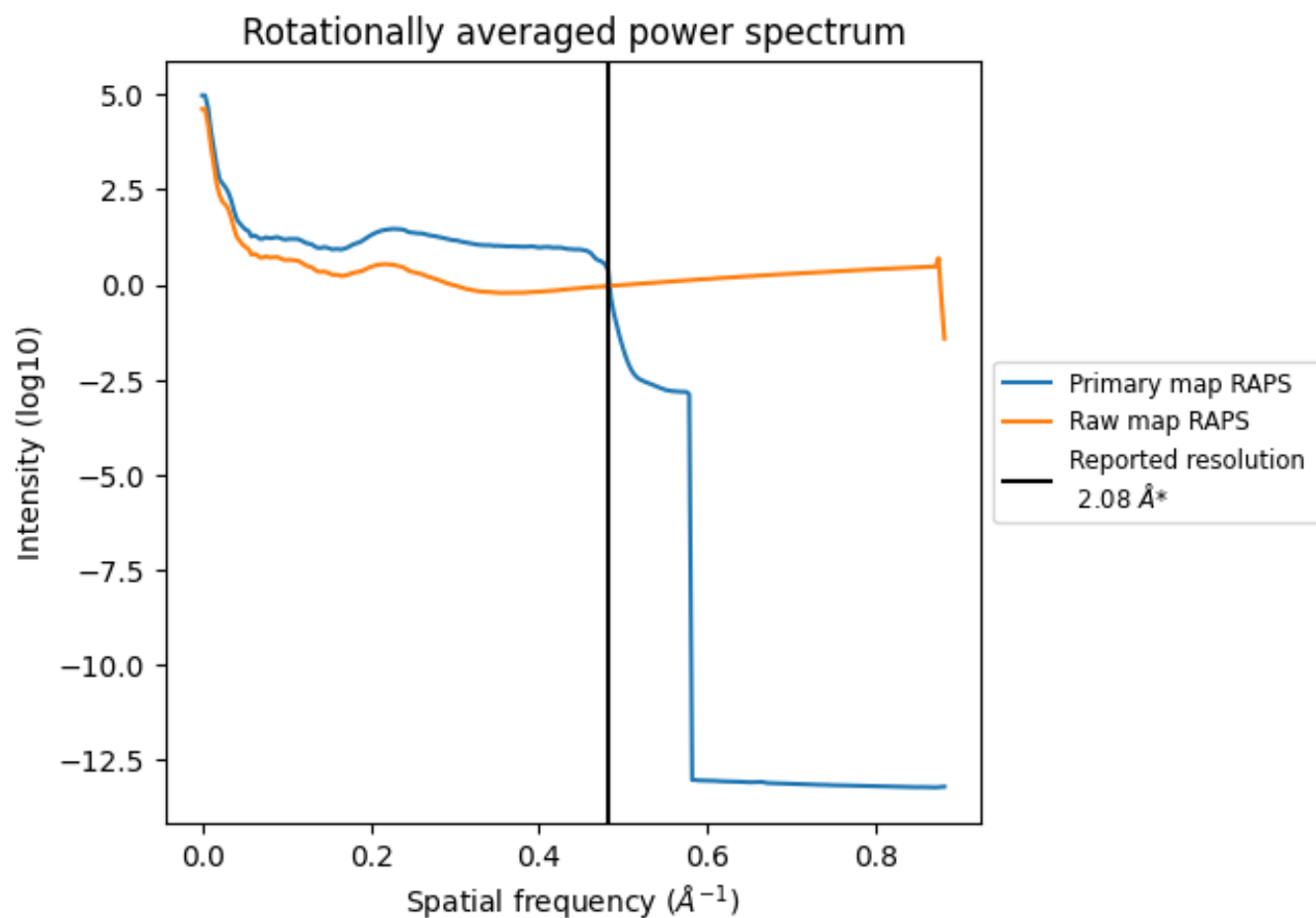
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm³; this corresponds to an approximate mass of 216 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 ⓘ

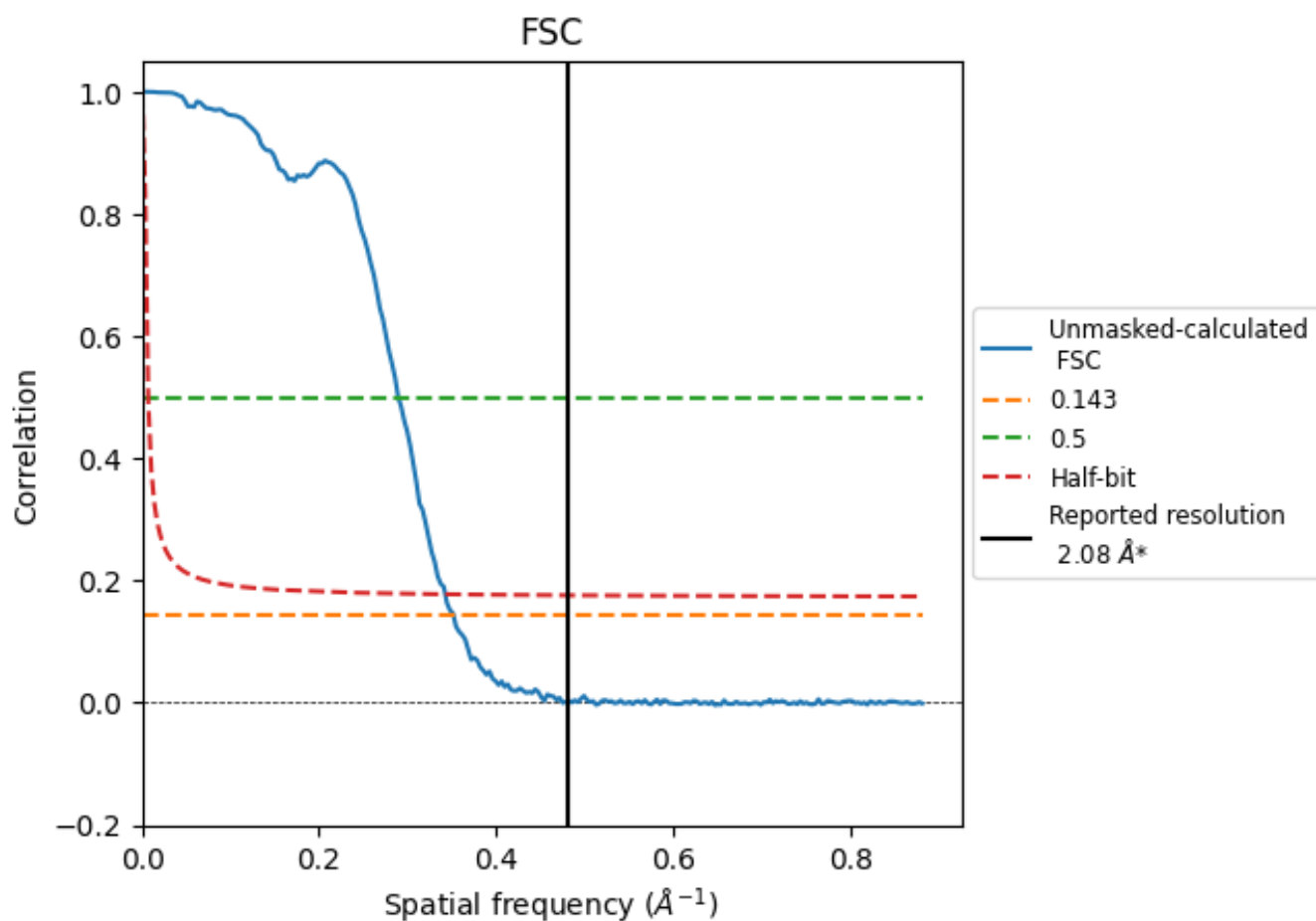


*Reported resolution corresponds to spatial frequency of 0.481 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.481 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	3.46	2.92

*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 2.84 differs from the reported value 2.08 by more than 10 %

9 Map-model fit [i](#)

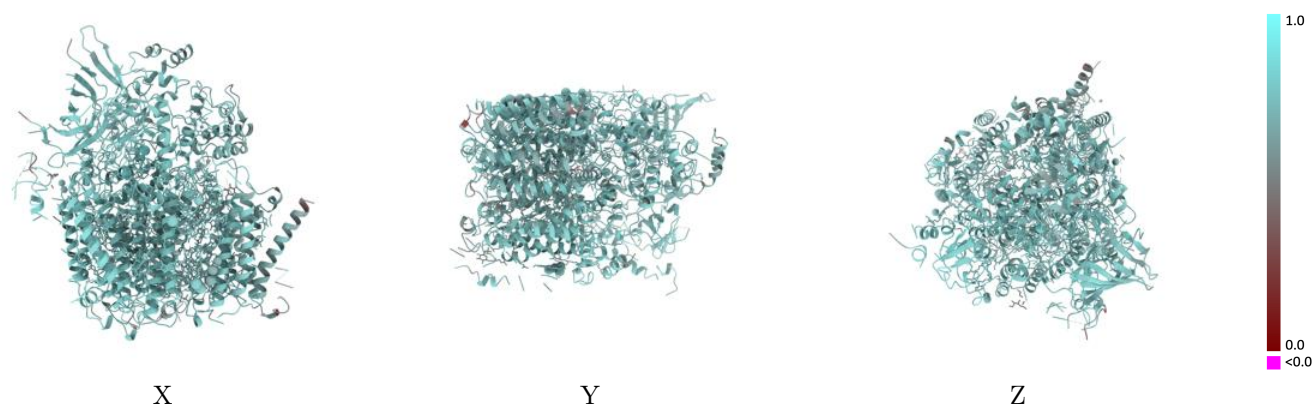
This section contains information regarding the fit between EMDB map EMD-65941 and PDB model 9WFZ. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



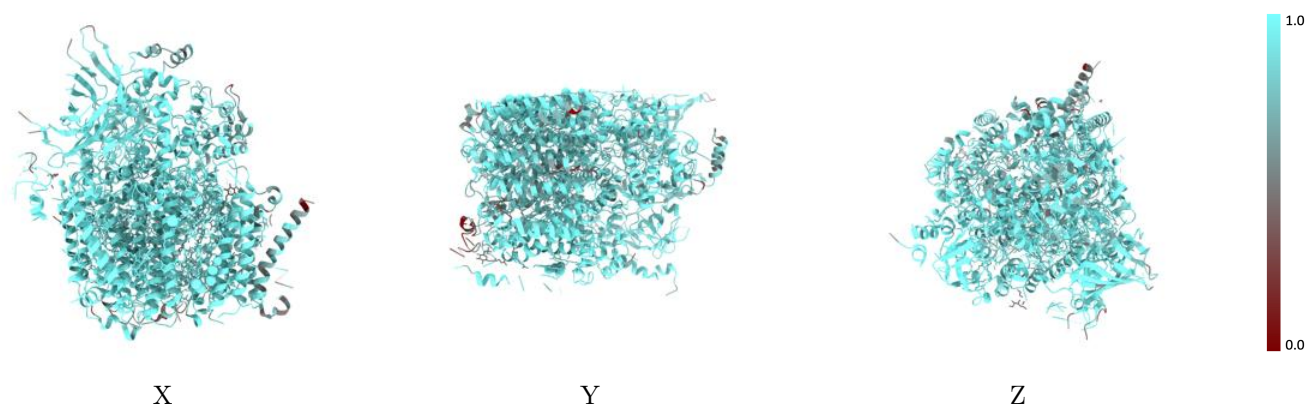
The images above show the 3D surface view of the map at the recommended contour level 0.129 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



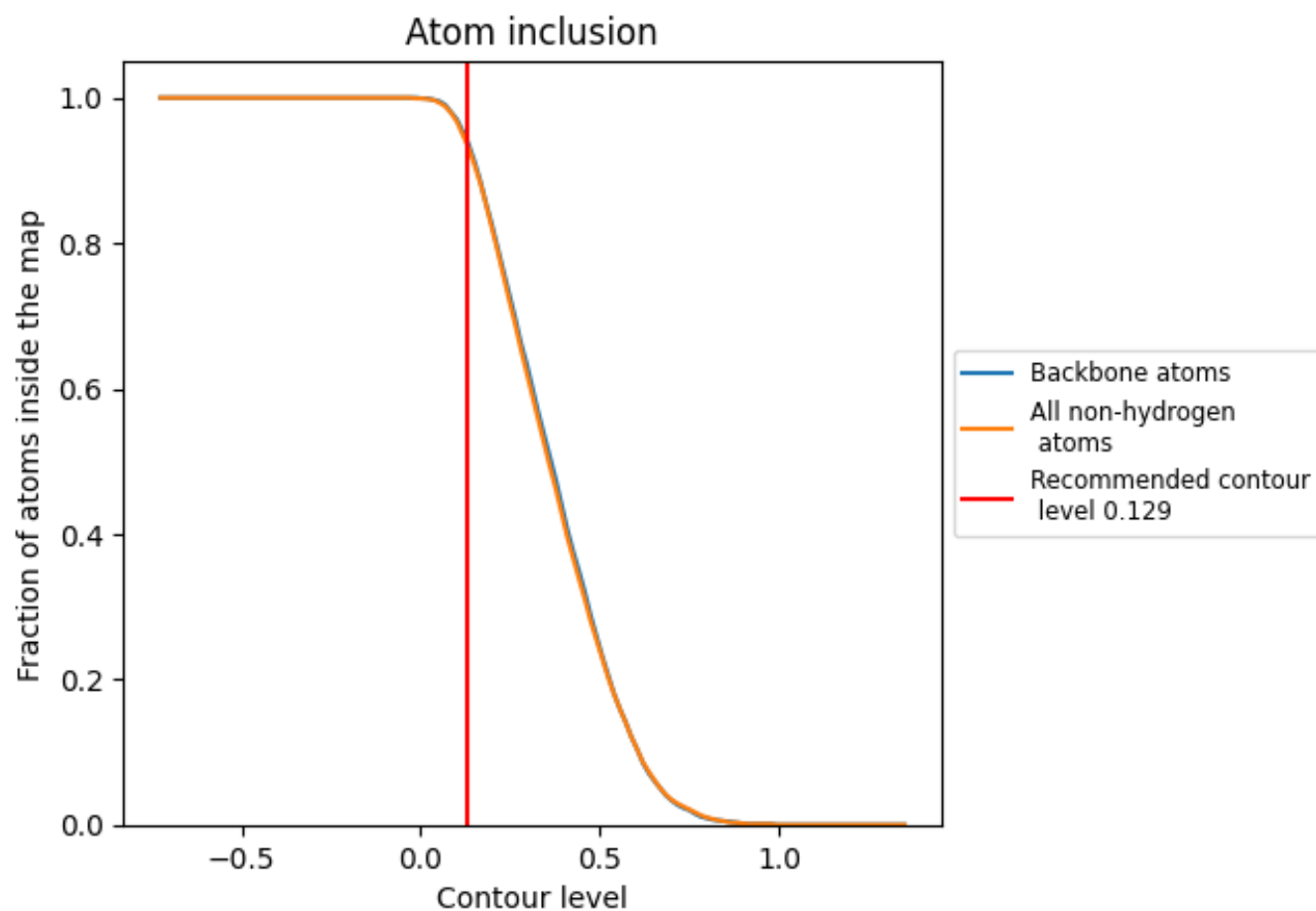
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.129).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.7200
A	 0.9620	 0.7420
B	 0.9240	 0.7250
C	 0.9610	 0.7240
D	 0.9810	 0.7440
E	 0.8930	 0.6830
F	 0.8800	 0.6860
I	 0.9650	 0.7140
J	 0.8780	 0.6860
K	 0.8700	 0.6780
L	 0.9960	 0.7580
M	 0.9910	 0.7370
O	 0.9270	 0.7120
T	 0.9400	 0.7230
U	 0.8780	 0.6910
V	 0.8670	 0.6860
X	 0.9330	 0.6770
Y	 0.7680	 0.6400
Z	 0.6750	 0.5920
b	 0.9570	 0.7060

