



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:43 AM UTC

PDB ID : 9GNW / pdb\_00009gnw  
EMDB ID : EMD-51482  
Title : Universal PSII assembly intermediate  
Authors : Fadeeva, M.; Klaiman, D.; Nelson, N.  
Deposited on : 2024-09-04  
Resolution : 2.93 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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

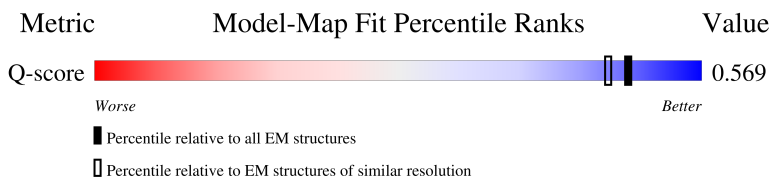
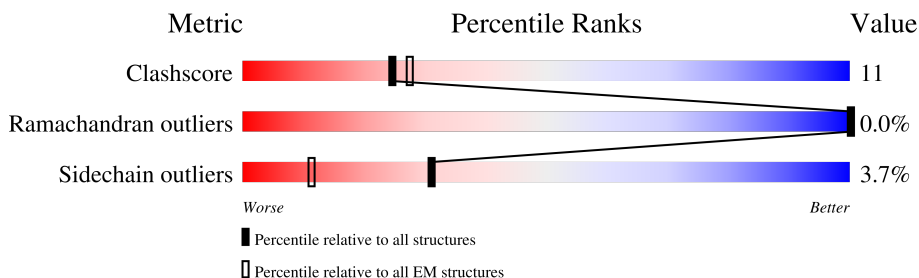
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.93 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.




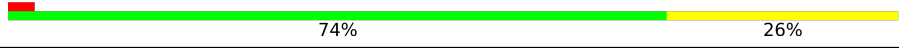



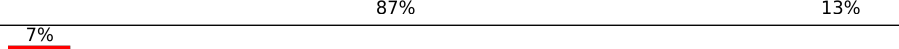
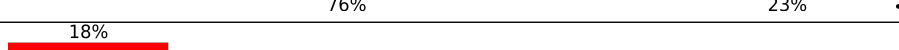

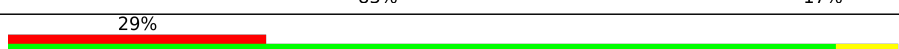
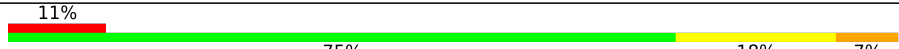

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13037 ( 2.43 - 3.43 )

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	336	<div> <div>9%</div> <div>74%</div> <div>26%</div> <div>.</div> </div>
2	B	484	<div> <div>79%</div> <div>20%</div> <div>.</div> </div>
3	V	33	<div> <div>82%</div> <div>18%</div> </div>
4	C	449	<div> <div>79%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	348	
6	E	76	
7	F	31	
8	H	67	
9	I	33	
10	J	36	
11	K	37	
12	L	36	
13	M	31	
14	O	238	
15	P	187	
16	T	30	
17	W	45	
18	X	33	
19	Z	61	
20	U	28	

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
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	408	X	-	-	-
24	CLA	B	501	X	-	-	-
24	CLA	B	502	X	-	-	-
24	CLA	B	503	X	-	-	-
24	CLA	B	504	X	-	-	-
24	CLA	B	505	X	-	-	-
24	CLA	B	506	X	-	-	-
24	CLA	B	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	508	X	-	-	-
24	CLA	B	509	X	-	-	-
24	CLA	B	510	X	-	-	-
24	CLA	B	511	X	-	-	-
24	CLA	B	512	X	-	-	-
24	CLA	B	513	X	-	-	-
24	CLA	B	514	X	-	-	-
24	CLA	B	515	X	-	-	-
24	CLA	B	516	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
26	BCR	A	409	-	X	-	-

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 24204 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 protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	33	Total	C	N	O	S	0	0
			235	157	38	39	1		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			265	182	39	43	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			265	181	40	44		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total	C	N	O	0	0
			300	201	49	50		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			235	161	33	41		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1819	1148	295	370	6		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	101	ASP	ASN	conflict	UNP A0A7S3QTM3
O	103	LYS	ARG	conflict	UNP A0A7S3QTM3
O	150	ASN	GLY	conflict	UNP A0A7S3QTM3
O	151	ASN	GLY	conflict	UNP A0A7S3QTM3
O	156	GLU	GLN	conflict	UNP A0A7S3QTM3
O	160	ASP	GLU	conflict	UNP A0A7S3QTM3
O	219	ALA	SER	conflict	UNP A0A7S3QTM3
O	220	THR	SER	conflict	UNP A0A7S3QTM3
O	226	ILE	VAL	conflict	UNP A0A7S3QTM3
O	240	LEU	VAL	conflict	UNP A0A7S3QTM3
O	244	SER	THR	conflict	UNP A0A7S3QTM3
O	248	GLY	SER	conflict	UNP A0A7S3QTM3
O	261	THR	ALA	conflict	UNP A0A7S3QTM3
O	272	SER	THR	conflict	UNP A0A7S3QTM3
O	285	ALA	SER	conflict	UNP A0A7S3QTM3

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1453	923	243	286	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	96	GLN	GLU	conflict	UNP A0A9J4RF14
P	100	GLU	ASP	conflict	UNP A0A9J4RF14
P	107	GLU	ALA	conflict	UNP A0A9J4RF14
P	116	LEU	VAL	conflict	UNP A0A9J4RF14
P	119	VAL	ILE	conflict	UNP A0A9J4RF14
P	120	GLU	ALA	conflict	UNP A0A9J4RF14

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Chain	Residue	Modelled	Actual	Comment	Reference
P	121	ASP	GLN	conflict	UNP A0A9J4RF14
P	122	LYS	ASP	conflict	UNP A0A9J4RF14
P	123	SER	THR	conflict	UNP A0A9J4RF14
P	129	GLU	GLN	conflict	UNP A0A9J4RF14
P	130	ALA	ASP	conflict	UNP A0A9J4RF14
P	133	THR	SER	conflict	UNP A0A9J4RF14
P	147	LYS	ARG	conflict	UNP A0A9J4RF14
P	164	ARG	LYS	conflict	UNP A0A9J4RF14
P	167	ASN	SER	conflict	UNP A0A9J4RF14
P	191	THR	SER	conflict	UNP A0A9J4RF14

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	45	Total	C	N	O	S	0	0
			335	217	54	63	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	104	GLY	-	expression tag	UNP A0A9J4RF15

- Molecule 18 is a protein called Photosystem II PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	33	Total	C	N	O	0	0
			225	148	36	41		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	81	VAL	THR	conflict	UNP A0A7S3VKF3

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

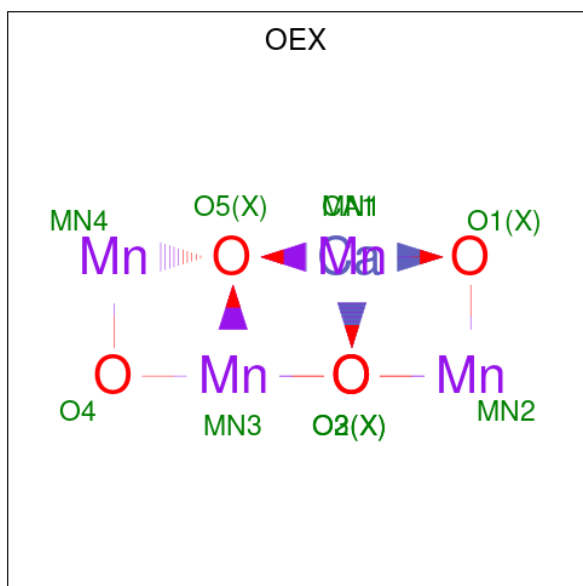


Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Photosystem II reaction center protein U, PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	28	Total	C	N	O	S	0	0
			235	141	46	47	1		

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

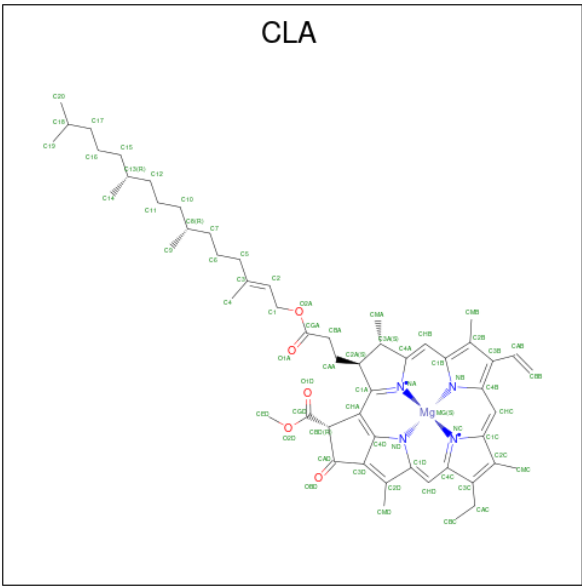
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
			Total	C	Mg	N	O	
			65	55	1	4	5	
			Total	C	Mg	N	O	
24	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
			65	55	1	4	5	
			Total	C	Mg	N	O	
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
			Total	C	Mg	N	O	
			65	55	1	4	5	
			Total	C	Mg	N	O	
24	B	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
			65	55	1	4	5	
			Total	C	Mg	N	O	
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
			Total	C	Mg	N	O	
			65	55	1	4	5	
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
			65	55	1	4	5	
			Total	C	Mg	N	O	
			65	55	1	4	5	

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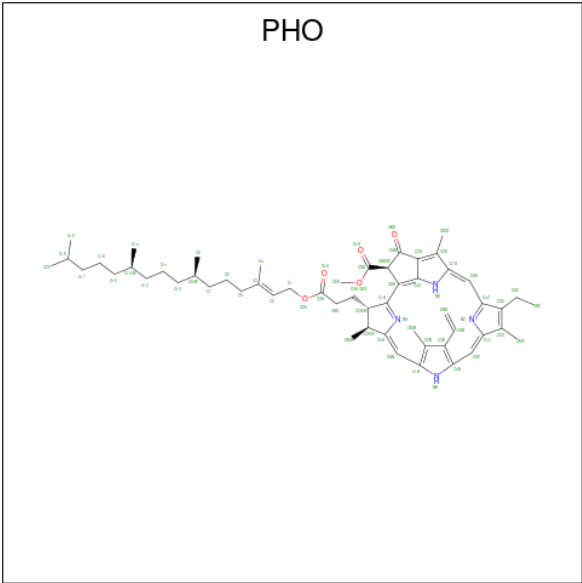
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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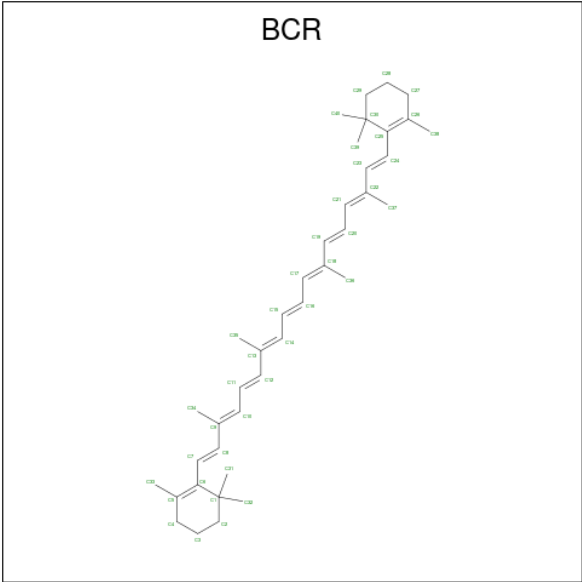
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	D	1	60	50	1	4	5	0

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



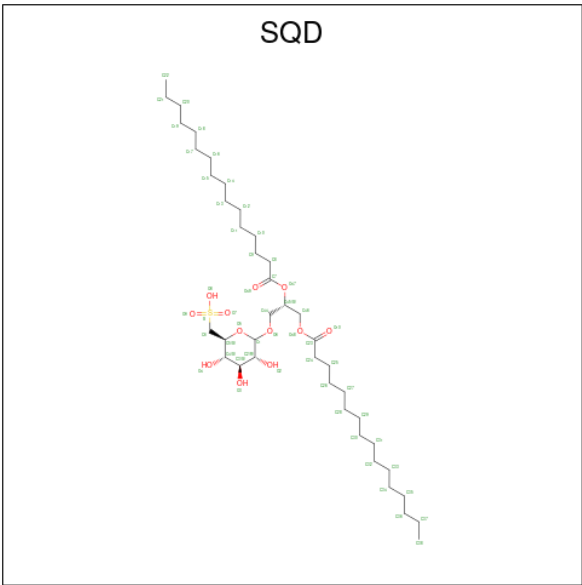
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
25	A	1	64	55	4	5	0
25	D	1	64	55	4	5	0

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



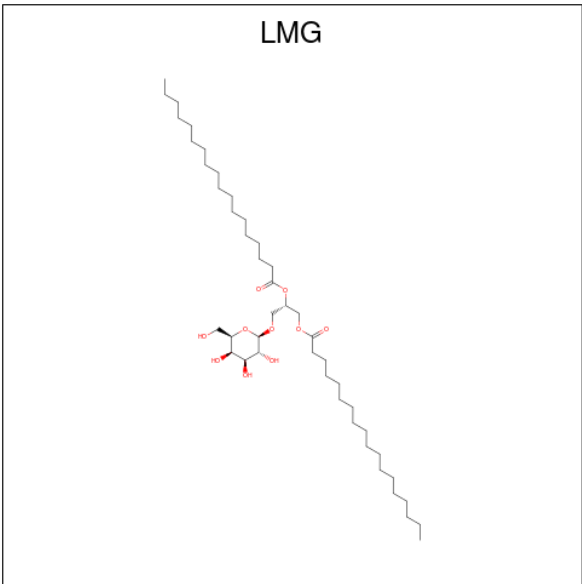
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	D	1	Total C 40 40	0
26	J	1	Total C 40 40	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	S	0
			42	29	12	1	
27	M	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			34	24	10	

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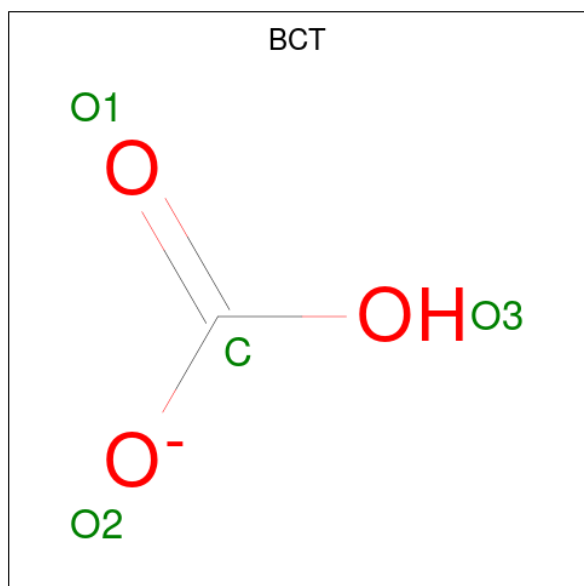
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Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			37	27	10	
28	B	1	Total	C	O	0
			44	34	10	
28	C	1	Total	C	O	0
			40	30	10	
28	C	1	Total	C	O	0
			47	37	10	
28	C	1	Total	C	O	0
			33	24	9	
28	D	1	Total	C	O	0
			42	32	10	
28	H	1	Total	C	O	0
			48	38	10	

- Molecule 29 is SODIUM ION (CCD ID: NA) (formula: Na).

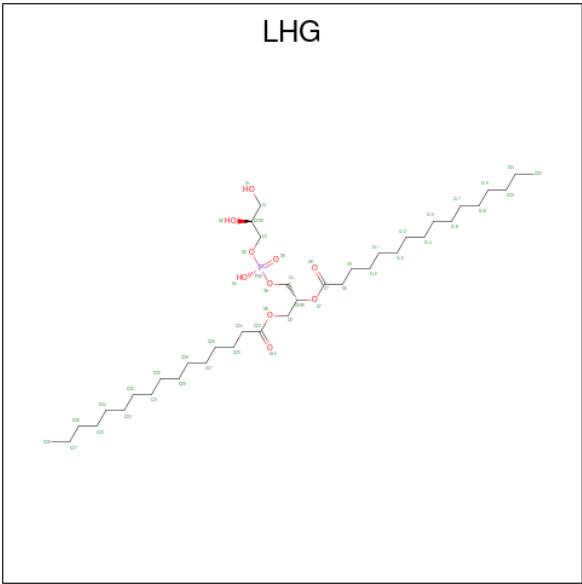
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Na	0
			1	1	

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			4	1	3	

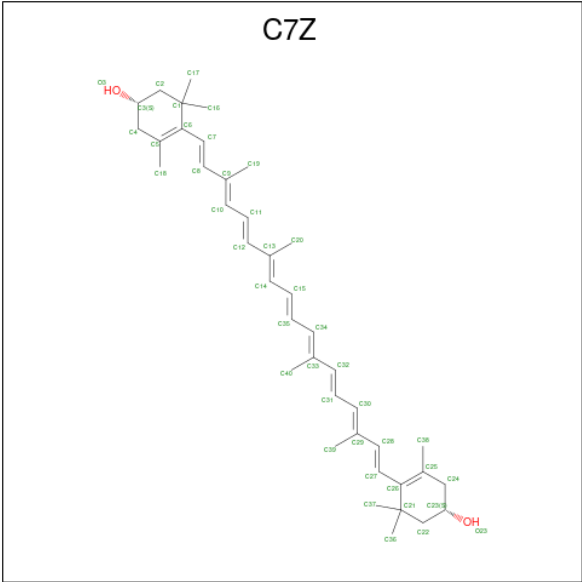
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			39	28	10	1	
31	D	1	Total	C	O	P	0
			44	33	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			39	28	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	

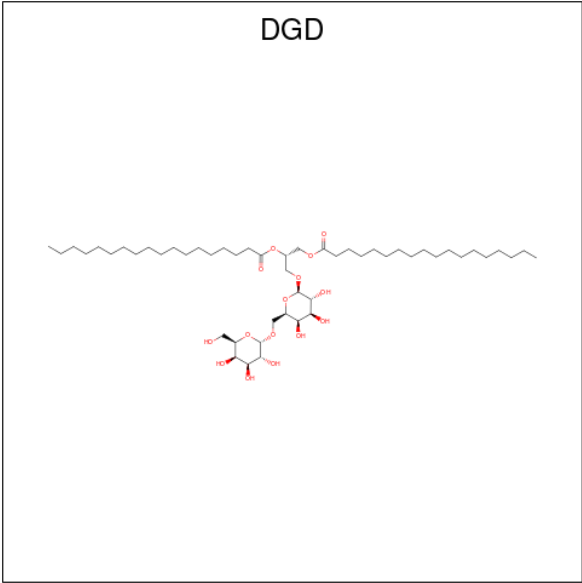
- Molecule 32 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			42	40	2	

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



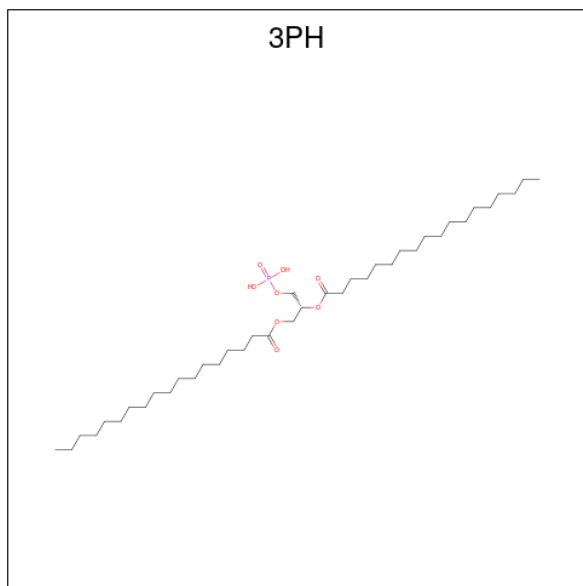
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			43	28	15	
33	C	1	Total	C	O	0
			44	29	15	

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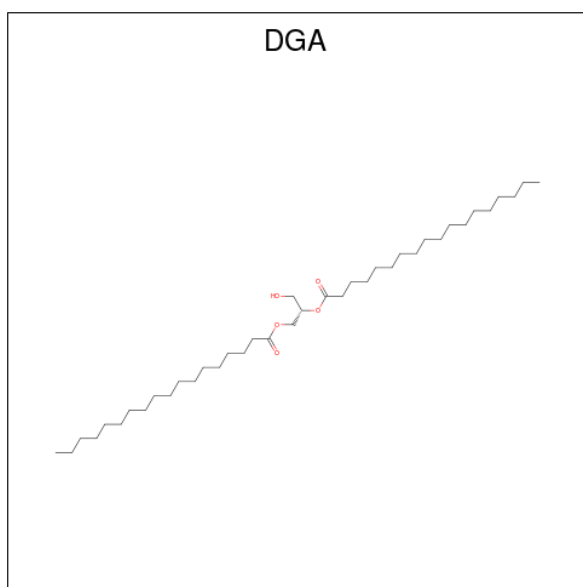
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			53	38	15	
33	C	1	Total	C	O	0
			53	38	15	

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



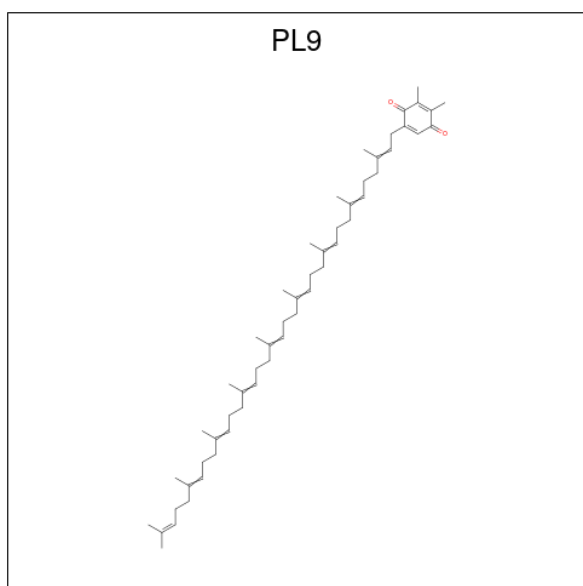
Mol	Chain	Residues	Atoms				AltConf
34	B	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 35 is DIACYL GLYCEROL (CCD ID: DGA) (formula:  $C_{39}H_{76}O_5$ ).



Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			37	32	5	

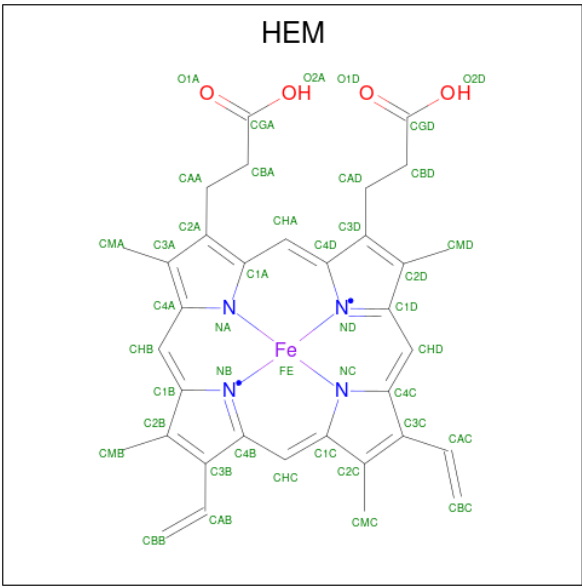
- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ).



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

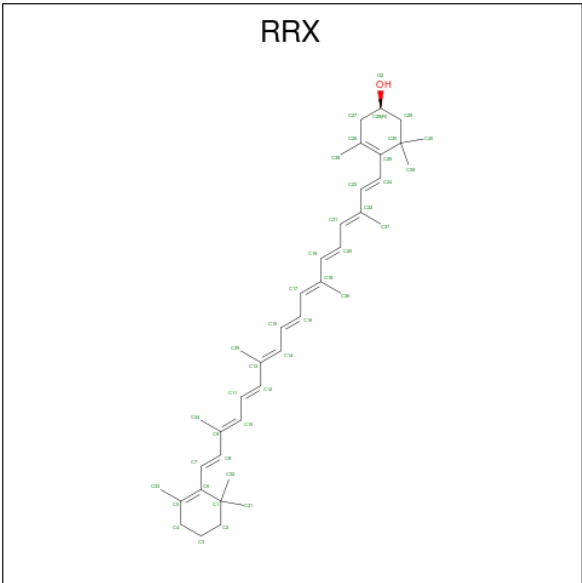
- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



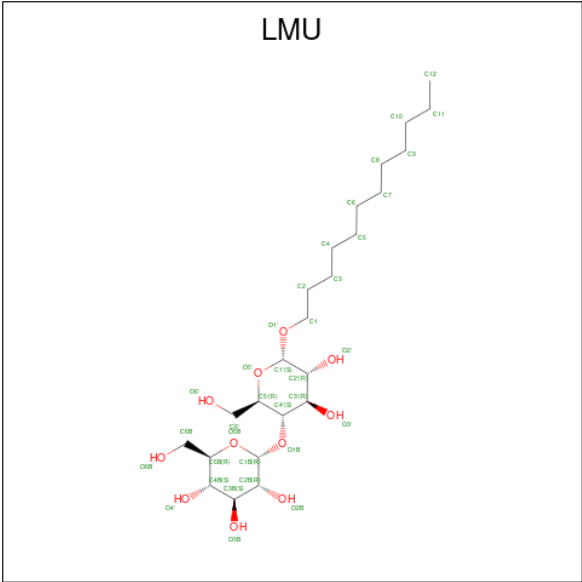
Mol	Chain	Residues	Atoms					AltConf
37	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



Mol	Chain	Residues	Atoms			AltConf
38	H	1	Total	C	O	0
			41	40	1	

- Molecule 39 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
39	J	1	Total	C	O	0
			35	24	11	

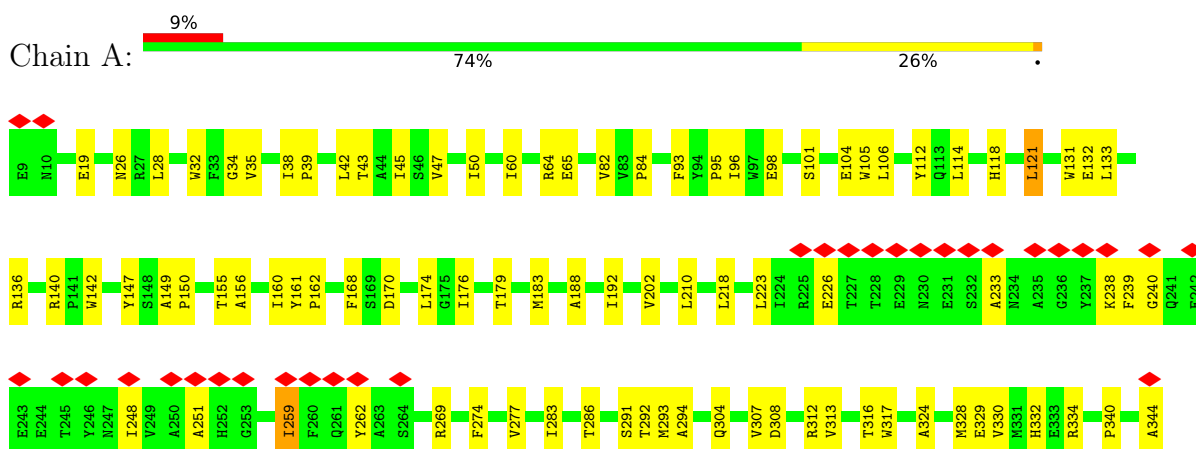
- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	6	Total	O	0
			6	6	
40	B	3	Total	O	0
			3	3	
40	C	1	Total	O	0
			1	1	
40	D	1	Total	O	0
			1	1	

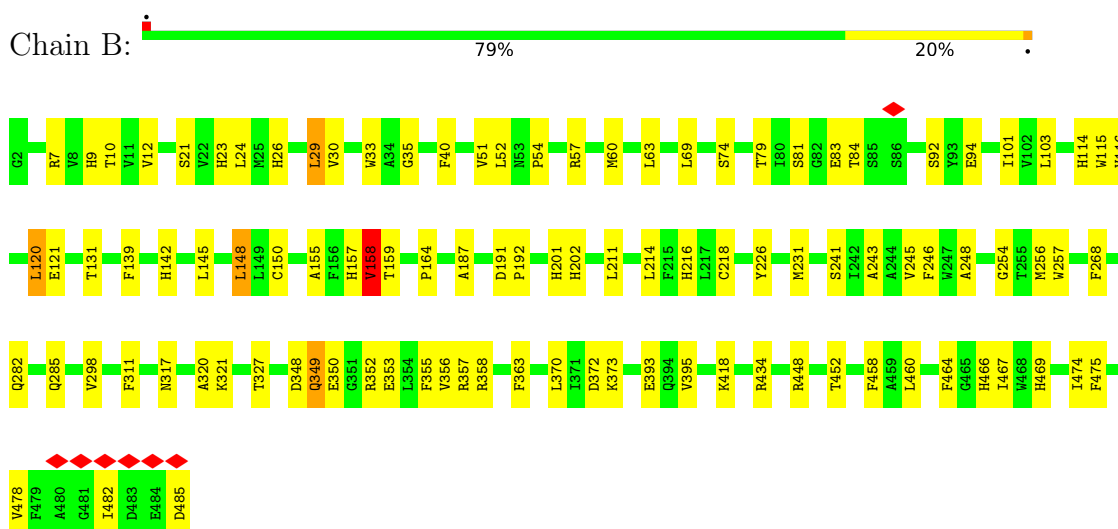
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

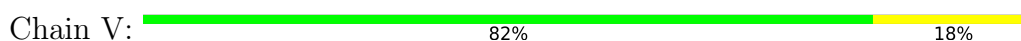
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



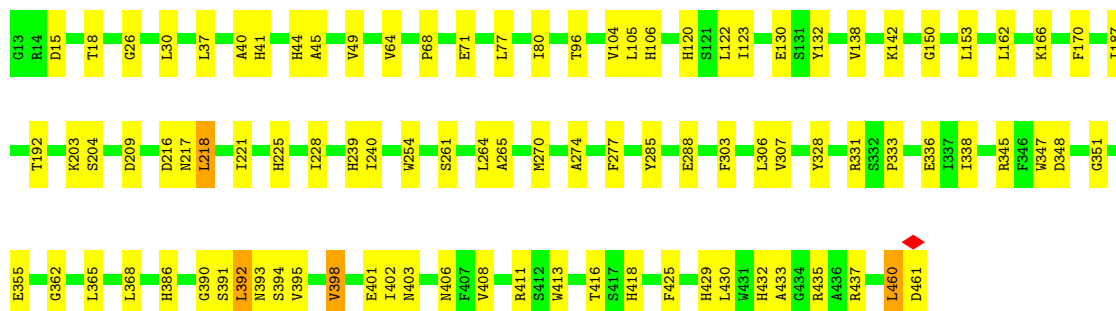
- Molecule 3: Photosystem II reaction center protein Psb30





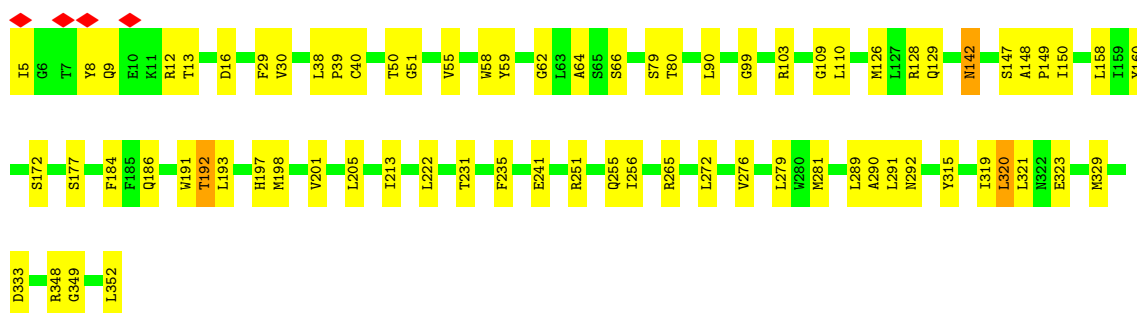
• Molecule 4: Photosystem II CP43 reaction center protein

Chain C: 79% 20%



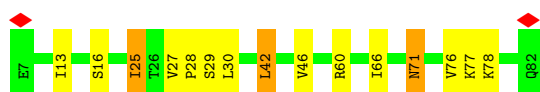
• Molecule 5: Photosystem II D2 protein

Chain D: 79% 20%



• Molecule 6: Cytochrome b559 subunit alpha

Chain E: 80% 16%



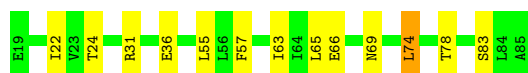
• Molecule 7: Cytochrome b559 subunit beta

Chain F: 74% 26%



• Molecule 8: Photosystem II reaction center protein H

Chain H: 81% 18%



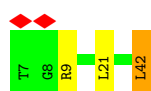
• Molecule 9: Photosystem II reaction center protein I

Chain I: 88% 12%



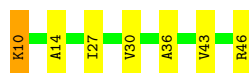
• Molecule 10: Photosystem II reaction center protein J

Chain J: 6% 92% 6%



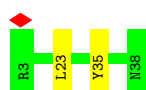
• Molecule 11: Photosystem II reaction center protein K

Chain K: 81% 16%



• Molecule 12: Photosystem II reaction center protein L

Chain L: 94% 6%



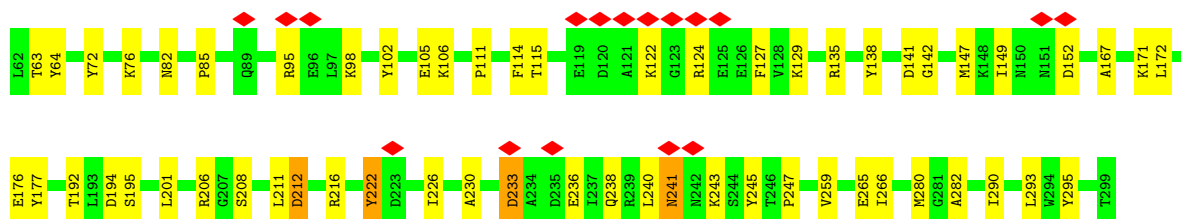
• Molecule 13: Photosystem II reaction center protein M

Chain M: 6% 87% 13%



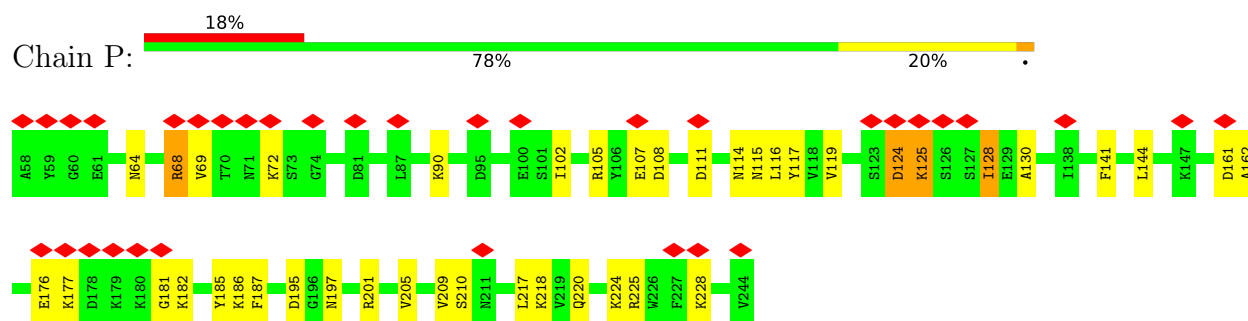
• Molecule 14: PsbO

Chain O: 7% 76% 23%

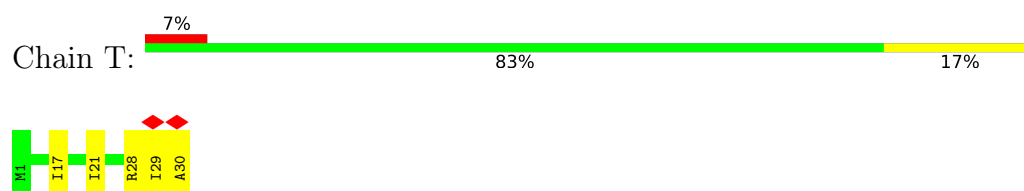




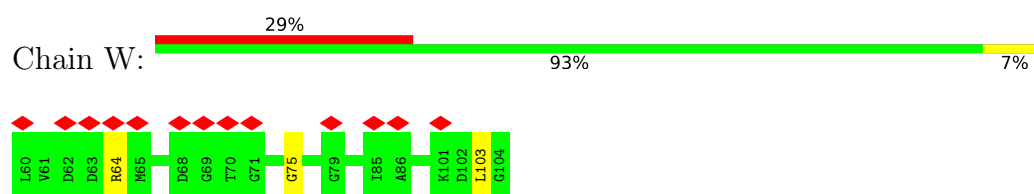
- Molecule 15: PsbP



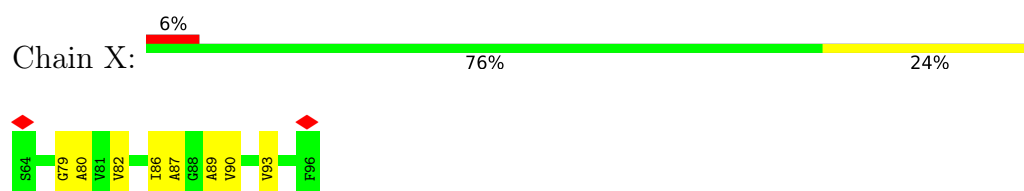
- Molecule 16: Photosystem II reaction center protein T



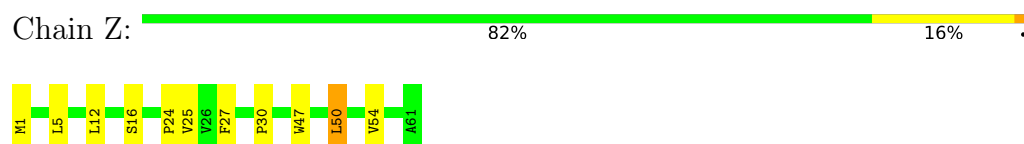
- Molecule 17: PSII 6.1 kDa protein



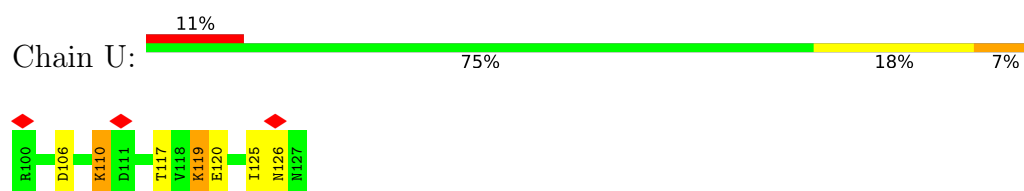
- Molecule 18: Photosystem II PsbX



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein U, PsbU



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	118340	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0047	Depositor
Map size ( $\text{\AA}$ )	193.5, 193.5, 193.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.645, 0.645, 0.645	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RRX, BCR, CLA, OEX, 3PH, LHG, SQD, CSD, NA, FE2, BCT, C7Z, PHO, HEM, PL9, LMU, DGA, CL, LMG, DGD

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	0.26	0/2717	0.34	0/3707
2	B	0.22	0/3906	0.31	0/5319
3	V	0.16	0/236	0.24	0/321
4	C	0.30	0/3602	0.37	0/4913
5	D	0.31	0/2860	0.37	0/3899
6	E	0.18	0/639	0.31	0/870
7	F	0.19	0/259	0.29	0/351
8	H	0.19	0/513	0.24	0/703
9	I	0.21	0/273	0.29	0/370
10	J	0.25	0/271	0.29	0/368
11	K	0.23	0/308	0.36	0/423
12	L	0.21	0/308	0.26	0/418
13	M	0.17	0/238	0.24	0/324
14	O	0.21	0/1854	0.31	0/2503
15	P	0.13	0/1482	0.26	0/1999
16	T	0.18	0/254	0.23	0/342
17	W	0.14	0/342	0.26	0/465
18	X	0.18	0/227	0.27	0/311
19	Z	0.15	0/469	0.25	0/641
20	U	0.15	0/235	0.25	0/311
All	All	0.24	0/20993	0.32	0/28558

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2635	0	2536	84	0
2	B	3785	0	3662	85	0
3	V	235	0	273	8	0
4	C	3483	0	3376	76	0
5	D	2766	0	2655	58	0
6	E	621	0	605	8	0
7	F	252	0	265	6	0
8	H	503	0	532	11	0
9	I	265	0	272	2	0
10	J	265	0	282	4	0
11	K	297	0	312	6	0
12	L	300	0	308	2	0
13	M	235	0	262	3	0
14	O	1819	0	1772	39	0
15	P	1453	0	1416	27	0
16	T	247	0	260	7	0
17	W	335	0	326	3	0
18	X	225	0	244	5	0
19	Z	457	0	478	10	0
20	U	235	0	244	6	0
21	A	10	0	0	0	0
22	A	1	0	0	0	0
23	A	2	0	0	0	0
24	A	190	0	203	16	0
24	B	1017	0	1095	82	0
24	C	794	0	824	53	0
24	D	190	0	203	20	0
25	A	64	0	74	5	0
25	D	64	0	74	5	0
26	A	40	0	56	5	0
26	B	80	0	112	6	0
26	C	120	0	168	9	0
26	D	40	0	56	1	0
26	J	40	0	56	2	0
27	A	42	0	47	0	0
27	M	42	0	47	4	0
28	A	71	0	82	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	44	0	58	2	0
28	C	120	0	156	7	0
28	D	42	0	54	1	0
28	H	48	0	66	5	0
29	A	1	0	0	0	0
30	A	4	0	1	0	0
31	A	39	0	48	3	0
31	D	132	0	185	11	0
31	L	49	0	74	1	0
32	B	42	0	0	3	0
33	B	43	0	44	2	0
33	C	150	0	174	7	0
34	B	48	0	75	4	0
35	B	37	0	56	3	0
36	D	55	0	80	1	0
37	E	43	0	30	2	0
38	H	41	0	56	6	0
39	J	35	0	46	4	0
40	A	6	0	0	0	0
40	B	3	0	0	0	0
40	C	1	0	0	0	0
40	D	1	0	0	0	0
All	All	24204	0	24380	513	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 11.

All (513) 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)
2:B:24:LEU:HD21	24:B:516:CLA:HAB	1.56	0.88
5:D:192:THR:HG23	24:D:403:CLA:HBC2	1.67	0.77
24:B:514:CLA:H18	26:B:517:BCR:H11C	1.68	0.75
4:C:187:ILE:HD11	4:C:218:LEU:HD23	1.68	0.74
1:A:26:ASN:HA	28:A:415:LMG:HC71	1.68	0.73
2:B:142:HIS:HE1	24:B:515:CLA:ND	1.87	0.73
2:B:469:HIS:HE1	24:B:511:CLA:NA	1.89	0.70
1:A:42:LEU:HB3	26:A:409:BCR:H353	1.74	0.70
14:O:240:LEU:O	14:O:241:ASN:ND2	2.26	0.69
1:A:106:LEU:HD11	26:A:409:BCR:H402	1.74	0.69
24:B:502:CLA:H2	24:B:502:CLA:HBD	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HH12	5:D:222:LEU:HD12	1.56	0.69
5:D:186:GLN:HB2	24:D:403:CLA:HBC1	1.74	0.69
4:C:392:LEU:HD12	33:C:520:DGD:HB51	1.74	0.68
5:D:55:VAL:O	5:D:66:SER:HB3	1.94	0.68
5:D:129:GLN:NE2	25:D:402:PHO:OBD	2.27	0.68
20:U:106:ASP:OD1	20:U:110:LYS:NZ	2.26	0.68
5:D:5:ILE:N	5:D:8:TYR:O	2.27	0.67
3:V:26:LEU:HB3	3:V:33:LEU:HD21	1.75	0.67
31:D:408:LHG:H272	12:L:23:LEU:HD22	1.78	0.66
15:P:182:LYS:HZ1	15:P:210:SER:HB3	1.60	0.66
24:B:501:CLA:H122	38:H:101:RRX:H50	1.78	0.65
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.78	0.65
1:A:26:ASN:HB3	28:A:415:LMG:HC91	1.78	0.65
5:D:279:LEU:HD22	25:D:402:PHO:HBC3	1.78	0.65
4:C:104:VAL:HG11	26:C:515:BCR:HC42	1.78	0.65
24:B:501:CLA:H143	24:B:501:CLA:H12	1.79	0.64
14:O:172:LEU:HB2	14:O:176:GLU:HB2	1.79	0.64
14:O:233:ASP:OD1	14:O:233:ASP:N	2.21	0.64
1:A:233:ALA:O	5:D:265:ARG:NH1	2.31	0.64
2:B:202:HIS:HE1	24:B:503:CLA:NA	1.94	0.63
8:H:69:ASN:ND2	28:H:102:LMG:O10	2.29	0.63
2:B:30:VAL:HG12	24:B:505:CLA:HHD	1.80	0.63
1:A:334:ARG:HB3	14:O:211:LEU:HD12	1.80	0.63
1:A:64:ARG:NH1	14:O:167:ALA:O	2.32	0.63
1:A:28:LEU:HD12	28:A:415:LMG:H312	1.80	0.62
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.32	0.62
24:C:507:CLA:HBB2	24:C:508:CLA:H52	1.82	0.62
4:C:71:GLU:OE2	4:C:386:HIS:NE2	2.32	0.62
31:D:408:LHG:H281	31:D:408:LHG:H131	1.82	0.62
10:J:21:LEU:HD21	26:J:101:BCR:H361	1.81	0.62
26:B:518:BCR:H14C	34:B:522:3PH:H2E1	1.82	0.62
24:D:404:CLA:NB	31:D:410:LHG:H202	2.15	0.61
15:P:107:GLU:HG3	15:P:115:ASN:HB3	1.81	0.61
4:C:461:ASP:O	5:D:251:ARG:NH2	2.34	0.61
15:P:128:ILE:HG12	15:P:209:VAL:HG23	1.81	0.61
24:A:405:CLA:H143	25:A:407:PHO:H72	1.81	0.60
1:A:43:THR:HA	26:A:409:BCR:H15C	1.83	0.60
26:C:516:BCR:H332	9:I:20:ILE:HG23	1.83	0.60
10:J:42:LEU:OXT	15:P:72:LYS:NZ	2.34	0.60
28:C:521:LMG:H172	39:J:102:LMU:H51	1.82	0.60
7:F:44:ARG:NH2	10:J:42:LEU:OXT	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:348:ARG:NH1	5:D:352:LEU:OXT	2.33	0.60
2:B:285:GLN:HG3	20:U:110:LYS:HE2	1.83	0.60
24:D:404:CLA:C1B	31:D:410:LHG:H202	2.32	0.59
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.84	0.59
13:M:28:LYS:HE3	27:M:101:SQD:H462	1.85	0.59
24:A:405:CLA:H112	24:D:401:CLA:HBB1	1.84	0.59
2:B:74:SER:HA	2:B:92:SER:HB2	1.83	0.59
24:B:508:CLA:H162	24:D:404:CLA:HBA1	1.83	0.59
4:C:285:TYR:O	4:C:411:ARG:NH2	2.36	0.59
2:B:157:HIS:O	2:B:159:THR:N	2.32	0.59
2:B:256:MET:O	2:B:448:ARG:NH1	2.35	0.59
14:O:95:ARG:NH1	14:O:194:ASP:OD1	2.35	0.59
1:A:93:PHE:HZ	24:A:408:CLA:HAA1	1.66	0.58
2:B:474:ILE:HD11	24:B:508:CLA:HAA2	1.85	0.58
4:C:432:HIS:HE1	24:C:509:CLA:NA	2.01	0.58
28:C:501:LMG:HC2	17:W:75:GLY:HA3	1.83	0.58
1:A:133:LEU:HD23	5:D:256:ILE:HG12	1.85	0.58
4:C:221:ILE:HA	26:C:516:BCR:H282	1.85	0.58
4:C:390:GLY:HA3	4:C:408:VAL:HG22	1.85	0.58
15:P:141:PHE:HB3	15:P:144:LEU:HD13	1.86	0.58
2:B:350:GLU:OE1	2:B:352:ARG:NH2	2.37	0.58
2:B:434:ARG:NH1	14:O:230:ALA:O	2.36	0.58
5:D:79:SER:HA	5:D:172:SER:HB3	1.86	0.58
7:F:43:GLN:O	15:P:64:ASN:ND2	2.32	0.58
24:D:404:CLA:H43	18:X:79:GLY:HA3	1.86	0.57
14:O:243:LYS:HD2	14:O:280:MET:HE2	1.86	0.57
2:B:79:THR:HG22	2:B:81:SER:H	1.69	0.57
14:O:259:VAL:HG22	14:O:266:ILE:HG22	1.87	0.57
37:E:101:HEM:HBC2	37:E:101:HEM:HMC2	1.85	0.57
4:C:68:PRO:HD2	4:C:71:GLU:HG3	1.85	0.57
4:C:430:LEU:HD21	24:C:506:CLA:HMB2	1.86	0.57
14:O:147:MET:HE2	14:O:149:ILE:HD11	1.86	0.57
1:A:47:VAL:HG21	1:A:114:LEU:HD22	1.87	0.57
24:A:408:CLA:HBB1	24:A:408:CLA:HMB3	1.86	0.57
4:C:331:ARG:NH2	14:O:82:ASN:HA	2.19	0.57
14:O:212:ASP:OD1	14:O:216:ARG:N	2.36	0.57
2:B:321:LYS:NZ	2:B:363:PHE:O	2.38	0.56
24:B:503:CLA:HMB2	24:B:503:CLA:H51	1.86	0.56
4:C:239:HIS:HE1	24:C:507:CLA:C1A	2.19	0.56
5:D:126:MET:HE1	5:D:147:SER:HA	1.88	0.56
1:A:118:HIS:HE1	24:A:408:CLA:C4D	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HB2	24:A:408:CLA:HAB	1.88	0.56
3:V:22:VAL:HG23	19:Z:25:VAL:HG23	1.87	0.56
4:C:398:VAL:O	4:C:401:GLU:HG2	2.05	0.56
24:C:512:CLA:H202	26:C:517:BCR:H17C	1.88	0.56
13:M:17:ILE:HB	13:M:18:PRO:HD3	1.86	0.56
14:O:122:LYS:H	14:O:122:LYS:HD3	1.71	0.56
4:C:395:VAL:CG1	4:C:403:ASN:HA	2.36	0.55
24:B:511:CLA:H52	24:B:513:CLA:HED3	1.89	0.55
4:C:30:LEU:HD21	24:C:512:CLA:H2A	1.89	0.55
14:O:122:LYS:HE2	14:O:124:ARG:HB2	1.89	0.55
24:B:513:CLA:OBD	24:B:514:CLA:HAB	2.06	0.55
2:B:355:PHE:HZ	2:B:373:LYS:HZ3	1.54	0.55
4:C:391:SER:OG	4:C:393:ASN:OD1	2.20	0.55
4:C:45:ALA:O	4:C:49:VAL:HG23	2.06	0.55
32:B:519:C7Z:C4	33:B:521:DGD:HA31	2.37	0.54
24:C:511:CLA:H191	11:K:30:VAL:HG12	1.87	0.54
15:P:225:ARG:HH11	15:P:228:LYS:HZ1	1.56	0.54
2:B:121:GLU:OE1	8:H:31:ARG:NH2	2.41	0.54
2:B:327:THR:HG22	24:B:507:CLA:H11	1.88	0.54
15:P:125:LYS:HB3	15:P:130:ALA:HB3	1.89	0.54
1:A:45:ILE:HD11	25:A:407:PHO:H51	1.88	0.53
1:A:84:PRO:HA	1:A:112:TYR:CG	2.43	0.53
24:B:502:CLA:H42	28:H:102:LMG:H131	1.91	0.53
3:V:26:LEU:HD21	19:Z:25:VAL:HA	1.91	0.53
2:B:35:GLY:HA3	2:B:101:ILE:HG12	1.89	0.53
5:D:193:LEU:O	12:L:35:TYR:OH	2.24	0.53
1:A:240:GLY:H	16:T:30:ALA:H	1.57	0.53
26:D:405:BCR:H20C	28:D:409:LMG:H321	1.91	0.53
1:A:93:PHE:CE2	1:A:95:PRO:HG3	2.44	0.53
1:A:283:ILE:HA	1:A:286:THR:HG22	1.89	0.53
3:V:5:LEU:HD22	39:J:102:LMU:H6'1	1.91	0.53
5:D:201:VAL:HG22	24:D:403:CLA:C2B	2.39	0.53
24:B:510:CLA:H112	24:B:515:CLA:HAA1	1.90	0.53
5:D:172:SER:HB2	5:D:177:SER:HB2	1.90	0.53
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.91	0.53
2:B:202:HIS:HE1	24:B:503:CLA:C1A	2.22	0.53
2:B:357:ARG:NH1	2:B:358:ARG:O	2.42	0.52
2:B:458:PHE:HB3	24:B:504:CLA:HBC2	1.89	0.52
1:A:223:LEU:HD11	5:D:265:ARG:NH1	2.25	0.52
2:B:282:GLN:HA	20:U:110:LYS:HD3	1.92	0.52
33:C:519:DGD:HO2D	39:J:102:LMU:H2O2	1.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:21:PHE:HD1	27:M:101:SQD:H271	1.73	0.52
15:P:68:ARG:HD3	15:P:69:VAL:N	2.25	0.52
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.52
24:C:507:CLA:H43	26:C:516:BCR:H10C	1.90	0.52
7:F:19:TRP:HE3	7:F:20:LEU:HD22	1.74	0.52
2:B:372:ASP:OD1	2:B:373:LYS:N	2.41	0.52
3:V:33:LEU:OXT	11:K:46:ARG:NH2	2.39	0.52
14:O:115:THR:HB	14:O:127:PHE:HB3	1.90	0.52
24:B:510:CLA:H101	24:B:515:CLA:HBA2	1.90	0.52
1:A:179:THR:O	1:A:183:MET:HG3	2.10	0.52
5:D:99:GLY:HA2	31:D:410:LHG:HC62	1.91	0.52
24:D:404:CLA:H102	18:X:80:ALA:HB2	1.91	0.52
2:B:7:ARG:O	2:B:10:THR:OG1	2.20	0.52
2:B:393:GLU:OE2	2:B:418:LYS:NZ	2.39	0.52
2:B:348:ASP:OD1	2:B:352:ARG:N	2.43	0.52
2:B:216:HIS:HE1	24:B:509:CLA:NC	2.07	0.51
24:B:505:CLA:HMA3	24:B:506:CLA:H3A	1.92	0.51
4:C:331:ARG:HH21	14:O:82:ASN:HA	1.74	0.51
4:C:432:HIS:HE1	24:C:509:CLA:C1A	2.23	0.51
24:D:404:CLA:H8	8:H:55:LEU:HD11	1.92	0.51
1:A:101:SER:HA	28:A:411:LMG:HC61	1.91	0.51
5:D:103:ARG:HD2	6:E:76:VAL:HG13	1.93	0.51
37:E:101:HEM:HBB2	37:E:101:HEM:HMB2	1.92	0.51
15:P:177:LYS:NZ	15:P:181:GLY:O	2.41	0.51
4:C:225:HIS:HE1	24:C:502:CLA:NA	2.09	0.51
5:D:5:ILE:O	5:D:9:GLN:NE2	2.43	0.51
24:B:514:CLA:H71	26:B:517:BCR:H20C	1.94	0.50
5:D:201:VAL:HG13	24:D:403:CLA:HMB2	1.92	0.50
1:A:308:ASP:OD1	1:A:312:ARG:N	2.44	0.50
2:B:12:VAL:HG23	24:B:512:CLA:HMC2	1.93	0.50
4:C:26:GLY:HA3	24:C:512:CLA:HMD2	1.93	0.50
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.92	0.50
5:D:142:ASN:HD22	5:D:142:ASN:H	1.60	0.50
24:B:507:CLA:H202	28:B:520:LMG:H351	1.92	0.50
2:B:201:HIS:HE1	24:B:502:CLA:C1D	2.16	0.50
34:B:522:3PH:H3H1	34:B:522:3PH:H2I3	1.93	0.50
1:A:269:ARG:HD2	5:D:235:PHE:HB2	1.92	0.50
33:C:519:DGD:O2D	39:J:102:LMU:O2'	2.26	0.50
31:D:408:LHG:H191	16:T:17:ILE:HD11	1.94	0.50
8:H:65:LEU:HD11	28:H:102:LMG:H302	1.94	0.50
11:K:14:ALA:HB1	19:Z:5:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:HIS:HE1	24:B:516:CLA:C1D	2.25	0.49
24:B:508:CLA:HBB1	24:B:508:CLA:HMB1	1.93	0.49
5:D:58:TRP:O	5:D:62:GLY:HA2	2.12	0.49
2:B:452:THR:HB	5:D:291:LEU:HD11	1.94	0.49
26:B:517:BCR:H383	27:M:101:SQD:H162	1.94	0.49
4:C:239:HIS:HE1	24:C:507:CLA:NA	2.05	0.49
4:C:40:ALA:HB2	24:C:512:CLA:HMA2	1.95	0.49
26:C:517:BCR:H391	11:K:36:ALA:HB2	1.93	0.49
1:A:223:LEU:HD21	5:D:265:ARG:NE	2.27	0.49
24:B:508:CLA:H92	35:B:523:DGA:HBH1	1.93	0.49
15:P:205:VAL:HG22	15:P:218:LYS:HG3	1.94	0.49
1:A:64:ARG:O	14:O:206:ARG:NH2	2.44	0.49
1:A:176:ILE:HD13	24:D:401:CLA:HED3	1.94	0.49
31:A:414:LHG:O1	4:C:435:ARG:NE	2.29	0.49
26:C:515:BCR:H332	19:Z:54:VAL:HG12	1.94	0.49
5:D:148:ALA:HB2	5:D:276:VAL:HG13	1.94	0.49
1:A:160:ILE:HD11	33:C:518:DGD:HB82	1.94	0.49
1:A:340:PRO:HB2	15:P:224:LYS:HB2	1.94	0.49
24:B:509:CLA:H42	35:B:523:DGA:HB71	1.94	0.49
14:O:238:GLN:NE2	14:O:282:ALA:O	2.46	0.49
4:C:288:GLU:OE1	4:C:288:GLU:N	2.41	0.48
15:P:161:ASP:OD1	15:P:162:ALA:N	2.42	0.48
2:B:29:LEU:HD21	26:B:517:BCR:H19C	1.95	0.48
2:B:464:PHE:HD2	24:B:511:CLA:HAC2	1.76	0.48
4:C:122:LEU:HD21	24:C:512:CLA:H2	1.95	0.48
1:A:170:ASP:OD2	4:C:345:ARG:NH1	2.40	0.48
24:C:502:CLA:H121	24:C:508:CLA:H92	1.95	0.48
10:J:9:ARG:H	10:J:9:ARG:HD2	1.78	0.48
2:B:349:GLN:NE2	2:B:395:VAL:O	2.47	0.48
3:V:22:VAL:HG21	19:Z:24:PRO:HB2	1.94	0.48
15:P:114:ASN:HA	15:P:220:GLN:O	2.14	0.48
2:B:214:LEU:O	2:B:218:CSD:OD2	2.29	0.48
4:C:418:HIS:CD2	24:C:503:CLA:ND	2.80	0.48
4:C:41:HIS:CD2	24:C:510:CLA:NA	2.82	0.48
4:C:80:ILE:HD11	24:C:504:CLA:HED3	1.95	0.48
14:O:236:GLU:HB3	14:O:240:LEU:HD13	1.95	0.48
24:B:504:CLA:CMB	24:B:507:CLA:HAB	2.44	0.48
1:A:93:PHE:CZ	24:A:408:CLA:HAA1	2.47	0.48
4:C:394:SER:HA	4:C:408:VAL:HG23	1.96	0.48
2:B:257:TRP:HB2	2:B:452:THR:HG21	1.96	0.48
4:C:264:LEU:HD21	24:C:509:CLA:CAB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:VAL:HG12	2:B:52:LEU:HG	1.94	0.47
2:B:142:HIS:HA	2:B:145:LEU:HD12	1.95	0.47
4:C:274:ALA:HB2	24:C:503:CLA:HMD2	1.96	0.47
2:B:356:VAL:HG22	2:B:370:LEU:HG	1.96	0.47
4:C:153:LEU:HD11	24:C:507:CLA:HAB	1.95	0.47
8:H:78:THR:OG1	8:H:83:SER:OG	2.31	0.47
24:A:405:CLA:HBA1	24:A:405:CLA:H3A	1.64	0.47
2:B:21:SER:OG	2:B:115:TRP:HB2	2.13	0.47
24:B:504:CLA:HBB1	24:B:504:CLA:HMB1	1.97	0.47
4:C:425:PHE:HA	24:C:509:CLA:HMC2	1.97	0.47
5:D:29:PHE:O	5:D:128:ARG:NH1	2.41	0.47
1:A:239:PHE:HB3	16:T:29:ILE:HA	1.96	0.47
4:C:338:ILE:HG21	4:C:347:TRP:HB2	1.96	0.47
1:A:155:THR:HG22	1:A:160:ILE:HG12	1.97	0.47
4:C:132:TYR:CE1	24:C:514:CLA:HAA2	2.50	0.47
15:P:185:TYR:HB3	15:P:187:PHE:CZ	2.50	0.47
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.97	0.47
25:A:407:PHO:HAB	5:D:205:LEU:HD13	1.97	0.47
4:C:265:ALA:HB2	4:C:429:HIS:CG	2.49	0.47
31:D:408:LHG:H322	16:T:21:ILE:HD11	1.96	0.47
14:O:85:PRO:HG2	14:O:295:TYR:CD2	2.49	0.47
2:B:157:HIS:CD2	2:B:164:PRO:HD2	2.49	0.47
2:B:191:ASP:OD2	8:H:83:SER:OG	2.32	0.47
2:B:348:ASP:OD2	2:B:352:ARG:NH1	2.48	0.47
5:D:50:THR:HG22	7:F:32:PHE:HZ	1.79	0.47
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.97	0.47
1:A:26:ASN:O	5:D:255:GLN:NE2	2.45	0.47
2:B:23:HIS:CD2	24:B:512:CLA:NB	2.82	0.47
24:C:502:CLA:H93	24:C:502:CLA:H112	1.73	0.47
2:B:60:MET:HB3	2:B:63:LEU:HB2	1.96	0.46
5:D:90:LEU:HD13	5:D:109:GLY:HA2	1.98	0.46
1:A:50:ILE:HG22	26:A:409:BCR:H271	1.97	0.46
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.50	0.46
2:B:268:PHE:HB3	2:B:448:ARG:HB3	1.98	0.46
4:C:261:SER:HB2	4:C:433:ALA:HB2	1.98	0.46
4:C:333:PRO:HB3	14:O:135:ARG:HD3	1.96	0.46
6:E:71:ASN:OD1	6:E:71:ASN:N	2.46	0.46
1:A:334:ARG:HD3	5:D:320:LEU:HD23	1.97	0.46
24:B:502:CLA:H61	24:B:502:CLA:H41	1.37	0.46
24:B:512:CLA:H102	24:B:512:CLA:H61	1.68	0.46
1:A:316:THR:HG23	5:D:64:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:HIS:HA	5:D:321:LEU:HD21	1.97	0.46
2:B:24:LEU:HD21	24:B:516:CLA:CAB	2.36	0.46
2:B:201:HIS:HB2	24:B:502:CLA:C1B	2.45	0.46
24:B:508:CLA:H3A	24:B:508:CLA:HBA2	1.60	0.46
24:B:508:CLA:H61	24:B:508:CLA:H41	1.60	0.46
8:H:63:ILE:HD13	38:H:101:RRX:H45	1.96	0.46
14:O:63:THR:OG1	14:O:64:TYR:N	2.49	0.46
4:C:406:ASN:HD21	33:C:519:DGD:HD4	1.79	0.46
4:C:413:TRP:CD1	24:C:505:CLA:HMA2	2.50	0.46
31:D:407:LHG:H111	31:D:407:LHG:H141	1.70	0.46
2:B:245:VAL:HG12	24:B:504:CLA:HAC1	1.98	0.46
24:C:510:CLA:H91	24:C:510:CLA:H111	1.73	0.46
24:C:513:CLA:H51	24:C:513:CLA:H11	1.75	0.46
5:D:198:MET:SD	24:D:401:CLA:HED2	2.56	0.46
26:C:516:BCR:H15C	26:C:516:BCR:H351	1.80	0.46
2:B:120:LEU:HD12	8:H:22:ILE:HB	1.98	0.46
2:B:349:GLN:OE1	2:B:350:GLU:N	2.48	0.46
24:B:507:CLA:C2B	28:B:520:LMG:H162	2.45	0.46
19:Z:16:SER:OG	19:Z:47:TRP:NE1	2.37	0.46
4:C:153:LEU:CD1	24:C:507:CLA:HAB	2.47	0.45
24:C:504:CLA:H61	24:C:504:CLA:H41	1.83	0.45
1:A:28:LEU:HB2	28:A:415:LMG:H301	1.98	0.45
24:D:404:CLA:H41	24:D:404:CLA:H62	1.41	0.45
6:E:25:ILE:O	6:E:29:SER:OG	2.29	0.45
24:A:408:CLA:H2	9:I:12:VAL:HG11	1.99	0.45
4:C:306:LEU:HD12	4:C:328:TYR:HB3	1.96	0.45
15:P:182:LYS:NZ	15:P:210:SER:HB3	2.30	0.45
1:A:269:ARG:NH1	5:D:231:THR:O	2.50	0.45
2:B:83:GLU:HG2	2:B:84:THR:H	1.82	0.45
24:B:516:CLA:H52	24:B:516:CLA:H11	1.69	0.45
25:D:402:PHO:HBA1	25:D:402:PHO:H3A	1.36	0.45
24:B:511:CLA:H193	24:B:511:CLA:H162	1.74	0.45
3:V:31:GLY:HA2	19:Z:30:PRO:HD3	1.99	0.45
1:A:307:VAL:HG23	7:F:44:ARG:HD3	1.98	0.45
2:B:116:VAL:HG21	32:B:519:C7Z:O23	2.15	0.45
6:E:27:VAL:HB	6:E:28:PRO:HD3	1.98	0.45
1:A:202:VAL:HG11	24:A:406:CLA:C3D	2.47	0.45
24:B:501:CLA:HBB2	38:H:101:RRX:H28	1.99	0.45
4:C:120:HIS:HE1	24:C:514:CLA:NA	2.09	0.45
1:A:43:THR:HG23	26:A:409:BCR:H362	1.99	0.45
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLN:HG2	1:A:313:VAL:HG11	1.98	0.45
2:B:69:LEU:HA	2:B:69:LEU:HD12	1.75	0.45
2:B:192:PRO:HB3	24:B:502:CLA:O1A	2.17	0.45
2:B:469:HIS:HE1	24:B:511:CLA:C1A	2.29	0.45
4:C:395:VAL:HG11	4:C:403:ASN:HA	1.99	0.45
14:O:201:LEU:HD11	14:O:247:PRO:HB2	1.99	0.45
2:B:9:HIS:CG	24:B:512:CLA:HBB2	2.52	0.45
4:C:270:MET:HE1	24:C:508:CLA:H11	1.98	0.45
6:E:13:ILE:O	6:E:16:SER:OG	2.29	0.45
2:B:40:PHE:HD1	34:B:522:3PH:H3B2	1.82	0.44
24:D:403:CLA:H41	24:D:403:CLA:H62	1.74	0.44
1:A:210:LEU:HD13	24:A:406:CLA:H43	1.98	0.44
24:B:514:CLA:H141	24:B:514:CLA:H161	1.66	0.44
5:D:323:GLU:OE2	14:O:222:TYR:OH	2.29	0.44
1:A:240:GLY:HA3	16:T:29:ILE:HG13	1.99	0.44
24:B:503:CLA:H152	8:H:57:PHE:HE2	1.82	0.44
24:B:510:CLA:H141	24:B:510:CLA:H162	1.70	0.44
5:D:12:ARG:HG3	5:D:16:ASP:HB2	1.99	0.44
5:D:320:LEU:HD12	5:D:320:LEU:HA	1.81	0.44
14:O:98:LYS:O	14:O:102:TYR:OH	2.22	0.44
15:P:68:ARG:HD3	15:P:69:VAL:H	1.83	0.44
2:B:320:ALA:HB1	5:D:292:ASN:HD22	1.82	0.44
26:B:517:BCR:H15C	26:B:517:BCR:H351	1.72	0.44
4:C:150:GLY:HA3	4:C:240:ILE:HG13	1.99	0.44
5:D:40:CYS:SG	24:D:404:CLA:HBB1	2.57	0.44
15:P:197:ASN:HD22	15:P:201:ARG:HH21	1.65	0.44
15:P:197:ASN:ND2	15:P:201:ARG:HH21	2.15	0.44
24:B:505:CLA:H102	24:B:510:CLA:H42	1.98	0.44
1:A:174:LEU:HD22	25:A:407:PHO:H143	2.00	0.44
24:B:502:CLA:H201	5:D:158:LEU:HD23	2.00	0.44
24:B:503:CLA:H141	24:B:503:CLA:H161	1.79	0.44
14:O:105:GLU:HG3	14:O:106:LYS:HG2	2.00	0.44
20:U:110:LYS:N	20:U:110:LYS:HE3	2.33	0.44
1:A:344:ALA:O	4:C:345:ARG:NH1	2.51	0.44
2:B:157:HIS:O	2:B:158:VAL:HG22	2.17	0.44
24:C:508:CLA:H62	24:C:508:CLA:H41	1.63	0.44
15:P:68:ARG:HH11	15:P:69:VAL:H	1.64	0.44
20:U:117:THR:HG22	20:U:119:LYS:H	1.82	0.44
31:A:414:LHG:H342	24:C:509:CLA:HBC2	1.99	0.44
2:B:478:VAL:HB	2:B:482:ILE:HG22	2.00	0.44
24:C:502:CLA:H41	24:C:502:CLA:H61	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:510:CLA:H62	24:C:510:CLA:H101	1.64	0.44
5:D:38:LEU:HB2	5:D:39:PRO:HD3	1.99	0.44
14:O:265:GLU:OE1	14:O:295:TYR:OH	2.32	0.44
24:B:504:CLA:HAB	24:B:511:CLA:H191	1.99	0.44
25:D:402:PHO:H112	25:D:402:PHO:H72	1.80	0.44
16:T:28:ARG:CZ	16:T:28:ARG:HA	2.48	0.44
25:A:407:PHO:H8	25:A:407:PHO:H121	1.78	0.43
24:B:508:CLA:HMC2	24:B:509:CLA:H142	2.00	0.43
24:B:515:CLA:H93	24:B:515:CLA:H62	1.69	0.43
24:C:510:CLA:H142	24:C:510:CLA:H112	1.75	0.43
5:D:329:MET:HG2	5:D:333:ASP:HB2	1.99	0.43
38:H:101:RRX:H40	38:H:101:RRX:H36	1.83	0.43
31:L:101:LHG:HC81	31:L:101:LHG:H112	1.52	0.43
1:A:149:ALA:HB3	1:A:150:PRO:HD3	2.00	0.43
14:O:135:ARG:HA	17:W:64:ARG:NH2	2.33	0.43
14:O:208:SER:HA	14:O:245:TYR:CZ	2.53	0.43
4:C:395:VAL:HG13	4:C:403:ASN:HA	2.00	0.43
5:D:51:GLY:HA2	5:D:55:VAL:HB	2.00	0.43
1:A:132:GLU:O	1:A:136:ARG:HG2	2.18	0.43
1:A:316:THR:HG22	1:A:317:TRP:H	1.84	0.43
1:A:324:ALA:O	1:A:328:MET:HG3	2.19	0.43
2:B:248:ALA:HA	24:B:503:CLA:H42	2.00	0.43
24:B:510:CLA:H161	24:B:510:CLA:H192	1.72	0.43
4:C:216:ASP:OD1	4:C:216:ASP:N	2.48	0.43
4:C:351:GLY:O	4:C:355:GLU:HG2	2.19	0.43
24:C:507:CLA:HBA1	24:C:507:CLA:H3A	1.88	0.43
1:A:140:ARG:HH21	1:A:142:TRP:HZ3	1.66	0.43
2:B:30:VAL:HG22	24:B:513:CLA:C3C	2.49	0.43
2:B:466:HIS:CE1	24:B:508:CLA:C4D	3.02	0.43
24:B:503:CLA:H193	24:B:503:CLA:H162	1.68	0.43
24:B:504:CLA:H92	24:B:504:CLA:H41	2.00	0.43
24:B:505:CLA:H41	24:B:505:CLA:H62	1.55	0.43
1:A:32:TRP:O	1:A:35:VAL:HG22	2.18	0.43
2:B:150:CYS:HB2	24:B:503:CLA:CMC	2.49	0.43
24:B:504:CLA:H92	24:B:504:CLA:H61	1.83	0.43
4:C:26:GLY:HA3	24:C:512:CLA:C2D	2.49	0.43
18:X:87:ALA:O	18:X:90:VAL:HG12	2.19	0.43
2:B:475:PHE:HB3	2:B:478:VAL:HG22	2.00	0.43
4:C:105:LEU:HB2	28:C:522:LMG:H171	2.01	0.43
24:C:508:CLA:H193	24:C:508:CLA:H162	1.76	0.43
14:O:141:ASP:OD1	14:O:141:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:O	2:B:30:VAL:HG23	2.19	0.42
24:B:504:CLA:H41	24:B:504:CLA:H61	1.71	0.42
24:D:401:CLA:H62	24:D:401:CLA:H92	1.81	0.42
4:C:204:SER:HB2	28:C:501:LMG:HC71	2.00	0.42
24:C:504:CLA:H61	24:C:504:CLA:H101	1.88	0.42
4:C:365:LEU:HD12	14:O:142:GLY:HA3	2.01	0.42
5:D:59:TYR:O	6:E:66:ILE:HG12	2.20	0.42
19:Z:12:LEU:HA	19:Z:50:LEU:HD23	2.01	0.42
2:B:74:SER:HG	2:B:94:GLU:CD	2.27	0.42
24:B:514:CLA:H3A	24:B:514:CLA:HBA2	1.50	0.42
5:D:160:TYR:HA	5:D:290:ALA:HB2	2.01	0.42
1:A:104:GLU:CD	17:W:64:ARG:HH12	2.28	0.42
4:C:15:ASP:OD1	4:C:18:THR:OG1	2.35	0.42
5:D:55:VAL:HG21	5:D:110:LEU:HD22	2.02	0.42
2:B:460:LEU:HD23	2:B:460:LEU:HA	1.88	0.42
24:B:513:CLA:H92	24:B:513:CLA:H61	1.82	0.42
24:B:513:CLA:CAD	24:B:514:CLA:HAB	2.48	0.42
15:P:124:ASP:OD1	15:P:124:ASP:N	2.51	0.42
20:U:110:LYS:HG2	20:U:117:THR:HG21	2.01	0.42
1:A:329:GLU:O	1:A:332:HIS:ND1	2.52	0.42
31:A:414:LHG:H331	31:A:414:LHG:H361	1.68	0.42
24:B:503:CLA:H91	24:B:503:CLA:H111	1.83	0.42
24:B:504:CLA:HBD	24:B:505:CLA:H42	2.02	0.42
24:B:513:CLA:HBB1	24:B:513:CLA:HMB1	2.02	0.42
35:B:523:DGA:HBE2	35:B:523:DGA:HB81	1.38	0.42
5:D:148:ALA:HB3	5:D:149:PRO:HD3	2.01	0.42
15:P:105:ARG:HG3	15:P:117:TYR:HB3	2.01	0.42
1:A:156:ALA:HA	1:A:160:ILE:HB	2.02	0.42
24:A:406:CLA:HBB1	25:D:402:PHO:H122	2.01	0.42
2:B:485:ASP:OD1	2:B:485:ASP:N	2.51	0.42
24:B:511:CLA:H142	24:B:511:CLA:H111	1.82	0.42
24:B:512:CLA:H3A	24:B:512:CLA:HBA2	1.62	0.42
34:B:522:3PH:H361	34:B:522:3PH:H331	1.71	0.42
4:C:106:HIS:CE1	28:C:522:LMG:H202	2.55	0.42
4:C:142:LYS:HZ2	4:C:254:TRP:CG	2.37	0.42
4:C:203:LYS:HG2	4:C:209:ASP:HB3	2.02	0.42
5:D:191:TRP:CE2	5:D:197:HIS:HB2	2.55	0.42
11:K:10:LYS:NZ	11:K:10:LYS:HB3	2.34	0.42
18:X:89:ALA:O	18:X:93:VAL:HG23	2.20	0.42
3:V:18:ALA:HB3	26:J:101:BCR:H12C	2.01	0.42
4:C:460:LEU:HD22	4:C:460:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:77:LYS:HE3	6:E:77:LYS:HB2	1.91	0.42
14:O:72:TYR:CE2	14:O:76:LYS:HD2	2.54	0.42
14:O:152:ASP:OD1	14:O:152:ASP:N	2.51	0.42
14:O:192:THR:HG23	14:O:195:SER:H	1.85	0.42
14:O:226:ILE:H	14:O:226:ILE:HG13	1.66	0.42
15:P:176:GLU:OE2	15:P:186:LYS:HD3	2.20	0.42
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.42
4:C:44:HIS:HE1	24:C:511:CLA:C4B	2.33	0.42
24:C:504:CLA:H203	24:C:511:CLA:HAB	2.01	0.42
8:H:63:ILE:CD1	38:H:101:RRX:H45	2.50	0.42
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.02	0.41
1:A:274:PHE:HA	1:A:277:VAL:HG12	2.00	0.41
2:B:226:TYR:HA	2:B:231:MET:SD	2.60	0.41
24:B:501:CLA:HBB1	38:H:101:RRX:H34	2.01	0.41
4:C:49:VAL:HG12	4:C:106:HIS:O	2.20	0.41
24:D:401:CLA:HBA2	24:D:401:CLA:H3A	1.54	0.41
14:O:171:LYS:HD2	14:O:177:TYR:HE1	1.85	0.41
1:A:259:ILE:HG22	24:A:406:CLA:H201	2.01	0.41
1:A:291:SER:O	1:A:294:ALA:HB3	2.19	0.41
5:D:191:TRP:CE3	5:D:289:LEU:HD11	2.55	0.41
31:D:407:LHG:H102	31:D:407:LHG:H362	2.02	0.41
15:P:102:ILE:HG12	15:P:119:VAL:HG22	2.01	0.41
19:Z:1:MET:SD	19:Z:1:MET:N	2.89	0.41
1:A:147:TYR:O	1:A:150:PRO:HD2	2.21	0.41
1:A:161:TYR:HA	1:A:294:ALA:HB1	2.02	0.41
1:A:218:LEU:HD12	1:A:251:ALA:HB1	2.02	0.41
15:P:108:ASP:HB3	15:P:111:ASP:O	2.20	0.41
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	2.01	0.41
2:B:103:LEU:HB2	24:B:506:CLA:H71	2.02	0.41
24:B:505:CLA:HBB2	32:B:519:C7Z:C19	2.51	0.41
4:C:264:LEU:HD21	24:C:509:CLA:HAB	2.01	0.41
24:A:405:CLA:H141	24:A:405:CLA:H162	1.72	0.41
2:B:74:SER:OG	2:B:94:GLU:OE2	2.34	0.41
24:B:502:CLA:H92	24:B:502:CLA:H62	1.79	0.41
4:C:44:HIS:HE1	24:C:511:CLA:NB	2.14	0.41
4:C:303:PHE:O	4:C:307:VAL:HG13	2.20	0.41
28:C:501:LMG:H322	28:C:501:LMG:H291	1.76	0.41
24:C:507:CLA:H8	26:C:516:BCR:H14C	2.03	0.41
4:C:406:ASN:HB2	33:C:520:DGD:O3E	2.20	0.41
6:E:42:LEU:O	6:E:46:VAL:HG22	2.21	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:HE1	24:A:408:CLA:ND	2.16	0.41
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.91	0.41
4:C:362:GLY:HA2	14:O:72:TYR:CE1	2.56	0.41
24:C:511:CLA:H111	24:C:511:CLA:H152	1.69	0.41
5:D:201:VAL:HG22	24:D:403:CLA:C1B	2.50	0.41
1:A:34:GLY:O	1:A:38:ILE:HG12	2.21	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.91	0.41
1:A:238:LYS:HB3	16:T:30:ALA:HA	2.01	0.41
1:A:238:LYS:HE2	1:A:238:LYS:HB2	1.83	0.41
1:A:330:VAL:O	5:D:349:GLY:N	2.47	0.41
24:C:502:CLA:H191	24:C:508:CLA:HBB1	2.03	0.41
24:C:510:CLA:H161	24:C:510:CLA:H141	1.84	0.41
5:D:160:TYR:HA	5:D:290:ALA:CB	2.51	0.41
11:K:27:ILE:O	11:K:30:VAL:HG22	2.21	0.41
14:O:111:PRO:HD2	14:O:138:TYR:HD1	1.86	0.41
14:O:114:PHE:HD1	14:O:290:ILE:HG12	1.85	0.41
15:P:195:ASP:OD1	15:P:195:ASP:N	2.53	0.41
2:B:254:GLY:HA2	28:H:102:LMG:H212	2.02	0.41
4:C:433:ALA:HB1	24:C:506:CLA:HED2	2.03	0.41
5:D:315:TYR:O	5:D:319:ILE:HG12	2.21	0.41
18:X:82:VAL:O	18:X:86:ILE:HG12	2.21	0.41
1:A:131:TRP:CH2	24:C:506:CLA:HAA2	2.56	0.40
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.91	0.40
2:B:187:ALA:HB1	8:H:74:LEU:HD23	2.03	0.40
2:B:466:HIS:HE1	24:B:508:CLA:C4D	2.33	0.40
24:B:511:CLA:H112	24:B:511:CLA:H72	1.68	0.40
33:B:521:DGD:HG31	33:B:521:DGD:HD2	1.68	0.40
4:C:15:ASP:OD1	4:C:15:ASP:N	2.54	0.40
4:C:336:GLU:OE1	4:C:336:GLU:N	2.54	0.40
5:D:184:PHE:HA	5:D:329:MET:HE1	2.03	0.40
31:D:410:LHG:H112	31:D:410:LHG:H142	1.49	0.40
27:M:101:SQD:H81	27:M:101:SQD:H112	1.86	0.40
2:B:241:SER:O	2:B:245:VAL:HG23	2.22	0.40
2:B:467:ILE:HD13	2:B:467:ILE:HA	1.83	0.40
4:C:166:LYS:HA	4:C:170:PHE:HB2	2.03	0.40
33:C:519:DGD:HB61	33:C:519:DGD:HB32	1.84	0.40
24:D:401:CLA:HMA2	36:D:406:PL9:H411	2.02	0.40
31:D:410:LHG:H131	31:D:410:LHG:H161	1.81	0.40
1:A:226:GLU:HB2	5:D:265:ARG:HH22	1.87	0.40
1:A:292:THR:HA	4:C:416:THR:HG22	2.04	0.40
4:C:37:LEU:HD12	4:C:37:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:123:ILE:HD11	19:Z:27:PHE:O	2.21	0.40
7:F:27:VAL:HB	7:F:28:PRO:HD3	2.04	0.40
28:H:102:LMG:O4	28:H:102:LMG:O5	2.36	0.40
15:P:177:LYS:HA	15:P:177:LYS:HE2	2.03	0.40
2:B:33:TRP:HE1	24:B:507:CLA:C3C	2.35	0.40
2:B:148:LEU:HD22	2:B:148:LEU:HA	1.96	0.40
24:A:408:CLA:O1A	28:C:501:LMG:H131	2.21	0.40
2:B:139:PHE:HE2	2:B:216:HIS:CD2	2.39	0.40
2:B:311:PHE:O	2:B:317:ASN:ND2	2.54	0.40
24:C:512:CLA:H141	24:C:512:CLA:H162	1.90	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	334/336 (99%)	322 (96%)	12 (4%)	0	100	100
2	B	481/484 (99%)	466 (97%)	14 (3%)	1 (0%)	43	65
3	V	31/33 (94%)	31 (100%)	0	0	100	100
4	C	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
5	D	346/348 (99%)	336 (97%)	10 (3%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	65 (100%)	0	0	100	100
9	I	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	34/36 (94%)	33 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	29/31 (94%)	29 (100%)	0	0	100	100
14	O	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
15	P	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
17	W	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
18	X	31/33 (94%)	31 (100%)	0	0	100	100
19	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
20	U	26/28 (93%)	26 (100%)	0	0	100	100
All	All	2578/2619 (98%)	2498 (97%)	79 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	VAL

### 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	275/275 (100%)	270 (98%)	5 (2%)	51	72
2	B	387/387 (100%)	378 (98%)	9 (2%)	44	68
3	V	26/26 (100%)	26 (100%)	0	100	100
4	C	350/350 (100%)	332 (95%)	18 (5%)	21	45
5	D	279/279 (100%)	268 (96%)	11 (4%)	28	53
6	E	68/68 (100%)	62 (91%)	6 (9%)	9	23
7	F	25/25 (100%)	24 (96%)	1 (4%)	28	53
8	H	56/56 (100%)	52 (93%)	4 (7%)	13	31
9	I	30/30 (100%)	28 (93%)	2 (7%)	15	34
10	J	27/27 (100%)	26 (96%)	1 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	33/33 (100%)	31 (94%)	2 (6%)	17	38
12	L	34/34 (100%)	34 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	189 (97%)	6 (3%)	35	60
15	P	152/152 (100%)	145 (95%)	7 (5%)	24	49
16	T	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	33 (97%)	1 (3%)	37	62
18	X	24/24 (100%)	24 (100%)	0	100	100
19	Z	50/50 (100%)	49 (98%)	1 (2%)	48	70
20	U	27/27 (100%)	22 (82%)	5 (18%)	1	3
All	All	2124/2124 (100%)	2045 (96%)	79 (4%)	31	55

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	121	LEU
1	A	248	ILE
1	A	259	ILE
1	A	262	TYR
2	B	29	LEU
2	B	120	LEU
2	B	131	THR
2	B	148	LEU
2	B	158	VAL
2	B	211	LEU
2	B	298	VAL
2	B	349	GLN
2	B	353	GLU
4	C	64	VAL
4	C	77	LEU
4	C	96	THR
4	C	130	GLU
4	C	138	VAL
4	C	162	LEU
4	C	192	THR
4	C	217	ASN
4	C	218	LEU

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Mol	Chain	Res	Type
4	C	228	ILE
4	C	277	PHE
4	C	348	ASP
4	C	368	LEU
4	C	392	LEU
4	C	398	VAL
4	C	402	ILE
4	C	437	ARG
4	C	460	LEU
5	D	13	THR
5	D	30	VAL
5	D	80	THR
5	D	142	ASN
5	D	150	ILE
5	D	192	THR
5	D	213	ILE
5	D	241	GLU
5	D	272	LEU
5	D	281	MET
5	D	320	LEU
6	E	25	ILE
6	E	30	LEU
6	E	42	LEU
6	E	60	ARG
6	E	71	ASN
6	E	78	LYS
7	F	25	ILE
8	H	24	THR
8	H	36	GLU
8	H	66	GLU
8	H	74	LEU
9	I	6	ILE
9	I	23	PHE
10	J	42	LEU
11	K	10	LYS
11	K	43	VAL
14	O	129	LYS
14	O	212	ASP
14	O	222	TYR
14	O	233	ASP
14	O	241	ASN
14	O	293	LEU

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Mol	Chain	Res	Type
15	P	68	ARG
15	P	90	LYS
15	P	116	LEU
15	P	124	ASP
15	P	125	LYS
15	P	128	ILE
15	P	217	LEU
17	W	103	LEU
19	Z	50	LEU
20	U	110	LYS
20	U	119	LYS
20	U	120	GLU
20	U	125	ILE
20	U	126	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
2	B	317	ASN
2	B	394	GLN
4	C	403	ASN
4	C	406	ASN
5	D	83	ASN
5	D	142	ASN
5	D	336	HIS
8	H	79	ASN
9	I	31	ASN
14	O	242	ASN
15	P	71	ASN
15	P	115	ASN
15	P	197	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CSD	B	218	2	4,7,8	1.09	0	1,8,10	0.14	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
2	CSD	B	218	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	218	CSD	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 77 ligands modelled in this entry, 4 are monoatomic - leaving 73 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$
31	LHG	D	408	-	48,48,48	0.40	0	51,54,54	1.10	3 (5%)
26	BCR	C	515	-	41,41,41	4.91	26 (63%)	56,56,56	2.26	20 (35%)
24	CLA	D	404	-	64,68,73	1.42	7 (10%)	76,107,113	2.01	18 (23%)
24	CLA	B	506	-	61,65,73	1.45	6 (9%)	72,103,113	1.96	17 (23%)
27	SQD	A	410	-	40,42,54	0.86	1 (2%)	50,53,65	0.93	2 (4%)
24	CLA	B	509	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
30	BCT	A	413	22	3,3,3	1.16	0	2,3,3	4.14	2 (100%)
31	LHG	D	407	-	43,43,48	0.42	0	46,49,54	1.07	3 (6%)
24	CLA	B	504	-	64,68,73	1.44	7 (10%)	76,107,113	1.98	16 (21%)
25	PHO	A	407	-	58,69,69	2.07	11 (18%)	55,99,99	1.47	6 (10%)
24	CLA	A	405	-	69,73,73	1.36	6 (8%)	82,113,113	1.88	20 (24%)
33	DGD	C	519	-	54,54,67	1.09	4 (7%)	68,68,81	1.21	5 (7%)
34	3PH	B	522	-	47,47,47	0.86	4 (8%)	50,52,52	1.17	2 (4%)
28	LMG	C	501	-	40,40,55	0.84	2 (5%)	48,48,63	1.24	6 (12%)
26	BCR	C	516	-	41,41,41	4.87	26 (63%)	56,56,56	2.45	23 (41%)
28	LMG	D	409	-	42,42,55	0.85	2 (4%)	50,50,63	1.09	3 (6%)
31	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.14	4 (7%)
39	LMU	J	102	-	36,36,36	0.40	0	47,47,47	0.78	1 (2%)
24	CLA	C	506	-	58,62,73	1.50	7 (12%)	68,99,113	2.04	17 (25%)
24	CLA	B	513	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	17 (20%)
24	CLA	B	501	-	69,73,73	1.35	7 (10%)	82,113,113	1.94	20 (24%)
24	CLA	C	503	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	19 (23%)
24	CLA	C	507	-	69,73,73	1.37	6 (8%)	82,113,113	1.87	19 (23%)
26	BCR	A	409	-	41,41,41	4.93	27 (65%)	56,56,56	3.02	26 (46%)
31	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.21	5 (12%)
33	DGD	B	521	-	44,44,67	0.86	2 (4%)	58,58,81	0.95	2 (3%)
26	BCR	J	101	-	41,41,41	4.93	26 (63%)	56,56,56	2.42	19 (33%)
26	BCR	B	517	-	41,41,41	4.89	27 (65%)	56,56,56	2.52	18 (32%)
24	CLA	C	505	-	59,63,73	1.46	7 (11%)	70,101,113	2.06	19 (27%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LMG	A	411	-	34,34,55	0.47	0	42,42,63	1.28	5 (11%)
24	CLA	B	514	-	69,73,73	1.37	6 (8%)	82,113,113	1.90	18 (21%)
24	CLA	A	408	-	64,68,73	1.41	7 (10%)	76,107,113	2.08	20 (26%)
35	DGA	B	523	-	36,36,43	1.19	3 (8%)	38,38,45	1.41	3 (7%)
24	CLA	B	507	40	69,73,73	1.36	7 (10%)	82,113,113	1.89	17 (20%)
37	HEM	E	101	7,6	50,50,50	1.38	7 (14%)	67,82,82	0.98	1 (1%)
33	DGD	C	518	-	45,45,67	0.81	1 (2%)	59,59,81	1.12	4 (6%)
33	DGD	C	520	-	54,54,67	1.01	4 (7%)	68,68,81	1.17	6 (8%)
24	CLA	B	512	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	17 (20%)
36	PL9	D	406	-	55,55,55	1.38	5 (9%)	68,69,69	1.49	13 (19%)
24	CLA	C	510	-	69,73,73	1.37	6 (8%)	82,113,113	1.87	16 (19%)
26	BCR	B	518	-	41,41,41	4.90	27 (65%)	56,56,56	2.28	21 (37%)
24	CLA	C	511	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	18 (21%)
24	CLA	C	502	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	19 (23%)
28	LMG	H	102	-	48,48,55	1.12	5 (10%)	56,56,63	1.14	3 (5%)
27	SQD	M	101	-	40,42,54	0.85	0	50,53,65	0.86	2 (4%)
21	OEX	A	401	4,1	0,15,15	-	-	-	-	-
24	CLA	B	515	-	69,73,73	1.34	7 (10%)	82,113,113	1.89	19 (23%)
24	CLA	B	503	-	69,73,73	1.38	7 (10%)	82,113,113	1.85	17 (20%)
24	CLA	C	512	4	69,73,73	1.37	7 (10%)	82,113,113	1.93	22 (26%)
24	CLA	C	514	-	49,53,73	1.61	6 (12%)	58,89,113	2.07	16 (27%)
31	LHG	A	414	-	38,38,48	0.43	0	41,44,54	1.21	4 (9%)
24	CLA	D	401	40	69,73,73	1.36	6 (8%)	82,113,113	1.93	18 (21%)
24	CLA	A	406	40	69,73,73	1.37	7 (10%)	82,113,113	1.89	21 (25%)
28	LMG	C	521	-	47,47,55	1.08	4 (8%)	55,55,63	1.10	3 (5%)
24	CLA	B	508	-	69,73,73	1.37	6 (8%)	82,113,113	1.83	17 (20%)
24	CLA	C	504	-	69,73,73	1.37	6 (8%)	82,113,113	1.88	19 (23%)
38	RRX	H	101	-	42,42,42	5.13	24 (57%)	56,58,58	2.58	21 (37%)
28	LMG	B	520	-	44,44,55	0.98	3 (6%)	52,52,63	1.15	2 (3%)
24	CLA	C	513	-	59,63,73	1.47	7 (11%)	70,101,113	1.98	18 (25%)
26	BCR	D	405	-	41,41,41	4.91	26 (63%)	56,56,56	2.24	20 (35%)
24	CLA	B	505	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
28	LMG	A	415	-	37,37,55	0.63	1 (2%)	45,45,63	1.08	3 (6%)
26	BCR	C	517	-	41,41,41	4.92	26 (63%)	56,56,56	2.42	18 (32%)
28	LMG	C	522	-	33,33,55	1.04	2 (6%)	40,40,63	1.10	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PHO	D	402	-	58,69,69	2.09	10 (17%)	55,99,99	1.47	7 (12%)
24	CLA	C	509	-	69,73,73	1.38	6 (8%)	82,113,113	1.87	17 (20%)
24	CLA	B	510	40	69,73,73	1.36	6 (8%)	82,113,113	1.88	17 (20%)
24	CLA	B	511	-	69,73,73	1.36	6 (8%)	82,113,113	1.86	19 (23%)
24	CLA	D	403	-	69,73,73	1.36	6 (8%)	82,113,113	1.83	16 (19%)
24	CLA	B	502	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	20 (24%)
24	CLA	C	508	40	69,73,73	1.37	7 (10%)	82,113,113	1.91	17 (20%)
24	CLA	B	516	-	59,63,73	1.47	6 (10%)	70,101,113	1.95	16 (22%)
32	C7Z	B	519	-	43,43,43	5.40	27 (62%)	56,60,60	2.39	17 (30%)

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
31	LHG	D	408	-	-	26/53/53/53	-
26	BCR	C	515	-	-	13/29/63/63	0/2/2/2
24	CLA	D	404	-	1/1/14/20	15/33/109/115	-
24	CLA	B	506	-	1/1/13/20	5/30/106/115	-
27	SQD	A	410	-	-	6/37/57/69	0/1/1/1
24	CLA	B	509	-	1/1/15/20	14/39/115/115	-
31	LHG	D	407	-	-	22/48/48/53	-
24	CLA	B	504	-	1/1/14/20	16/33/109/115	-
25	PHO	A	407	-	-	11/37/103/103	0/5/6/6
24	CLA	A	405	-	1/1/15/20	14/39/115/115	-
33	DGD	C	519	-	-	15/42/82/95	0/2/2/2
34	3PH	B	522	-	-	25/49/49/49	-
28	LMG	C	501	-	-	8/35/55/70	0/1/1/1
26	BCR	C	516	-	-	9/29/63/63	0/2/2/2
28	LMG	D	409	-	-	8/37/57/70	0/1/1/1
31	LHG	L	101	-	-	30/53/53/53	-
39	LMU	J	102	-	-	6/21/61/61	0/2/2/2
24	CLA	C	506	-	1/1/12/20	11/26/102/115	-
24	CLA	B	513	-	1/1/15/20	16/39/115/115	-
24	CLA	B	501	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	503	-	1/1/15/20	13/39/115/115	-
24	CLA	C	507	-	1/1/15/20	14/39/115/115	-
26	BCR	A	409	-	-	13/29/63/63	0/2/2/2
31	LHG	D	410	-	-	25/43/43/53	-
33	DGD	B	521	-	-	13/32/72/95	0/2/2/2
26	BCR	J	101	-	-	11/29/63/63	0/2/2/2
26	BCR	B	517	-	-	10/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/13/20	7/27/103/115	-
28	LMG	A	411	-	-	8/29/49/70	0/1/1/1
24	CLA	B	514	-	1/1/15/20	16/39/115/115	-
24	CLA	A	408	-	1/1/14/20	15/33/109/115	-
35	DGA	B	523	-	-	24/38/38/45	-
24	CLA	B	507	40	1/1/15/20	22/39/115/115	-
37	HEM	E	101	7,6	-	2/14/54/54	-
33	DGD	C	518	-	-	8/33/73/95	0/2/2/2
33	DGD	C	520	-	-	9/42/82/95	0/2/2/2
24	CLA	B	512	-	1/1/15/20	13/39/115/115	-
36	PL9	D	406	-	-	7/53/73/73	0/1/1/1
24	CLA	C	510	-	1/1/15/20	8/39/115/115	-
26	BCR	B	518	-	-	13/29/63/63	0/2/2/2
24	CLA	C	511	-	1/1/15/20	13/39/115/115	-
24	CLA	C	502	-	1/1/15/20	18/39/115/115	-
28	LMG	H	102	-	-	13/43/63/70	0/1/1/1
27	SQD	M	101	-	-	15/37/57/69	0/1/1/1
31	LHG	A	414	-	-	25/43/43/53	-
24	CLA	B	515	-	1/1/15/20	18/39/115/115	-
24	CLA	B	503	-	1/1/15/20	21/39/115/115	-
24	CLA	C	512	4	1/1/15/20	11/39/115/115	-
24	CLA	C	514	-	1/1/11/20	7/15/91/115	-
24	CLA	D	401	40	1/1/15/20	18/39/115/115	-
24	CLA	A	406	40	1/1/15/20	11/39/115/115	-
28	LMG	C	521	-	-	9/42/62/70	0/1/1/1
24	CLA	B	508	-	1/1/15/20	14/39/115/115	-
24	CLA	C	504	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	RRX	H	101	-	-	6/29/65/65	0/2/2/2
28	LMG	B	520	-	-	10/39/59/70	0/1/1/1
24	CLA	C	513	-	1/1/13/20	10/27/103/115	-
26	BCR	D	405	-	-	8/29/63/63	0/2/2/2
24	CLA	B	505	-	1/1/15/20	14/39/115/115	-
28	LMG	A	415	-	-	4/32/52/70	0/1/1/1
26	BCR	C	517	-	-	9/29/63/63	0/2/2/2
28	LMG	C	522	-	-	8/27/47/70	0/1/1/1
25	PHO	D	402	-	-	7/37/103/103	0/5/6/6
24	CLA	C	509	-	1/1/15/20	13/39/115/115	-
24	CLA	B	510	40	1/1/15/20	18/39/115/115	-
24	CLA	B	511	-	1/1/15/20	14/39/115/115	-
24	CLA	D	403	-	1/1/15/20	10/39/115/115	-
24	CLA	B	502	-	1/1/15/20	12/39/115/115	-
24	CLA	C	508	40	1/1/15/20	15/39/115/115	-
24	CLA	B	516	-	1/1/13/20	15/27/103/115	-
32	C7Z	B	519	-	-	12/29/67/67	0/2/2/2

All (559) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	519	C7Z	C25-C26	16.36	1.61	1.34
26	A	409	BCR	C26-C25	15.94	1.61	1.34
26	D	405	BCR	C26-C25	15.91	1.61	1.34
26	J	101	BCR	C26-C25	15.90	1.61	1.34
26	B	518	BCR	C26-C25	15.88	1.61	1.34
26	C	517	BCR	C26-C25	15.86	1.61	1.34
26	C	516	BCR	C26-C25	15.81	1.61	1.34
38	H	101	RRX	C26-C25	15.58	1.60	1.34
26	B	517	BCR	C26-C25	15.52	1.60	1.34
26	C	515	BCR	C26-C25	15.52	1.60	1.34
32	B	519	C7Z	C5-C6	15.24	1.60	1.34
38	H	101	RRX	C5-C6	14.54	1.58	1.34
26	J	101	BCR	C5-C6	14.48	1.58	1.34
26	A	409	BCR	C5-C6	14.47	1.58	1.34
26	C	515	BCR	C5-C6	14.43	1.58	1.34
26	C	517	BCR	C5-C6	14.41	1.58	1.34
26	B	518	BCR	C5-C6	14.31	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	405	BCR	C5-C6	14.22	1.58	1.34
26	B	517	BCR	C5-C6	14.07	1.58	1.34
26	C	516	BCR	C5-C6	13.99	1.58	1.34
32	B	519	C7Z	C22-C23	-11.43	1.36	1.52
32	B	519	C7Z	C24-C23	11.27	1.72	1.52
38	H	101	RRX	C29-C28	-10.86	1.36	1.52
32	B	519	C7Z	C2-C3	-10.22	1.37	1.52
25	D	402	PHO	C1B-C2B	9.12	1.49	1.39
25	A	407	PHO	C1B-C2B	9.05	1.49	1.39
25	D	402	PHO	C3B-C4B	8.26	1.49	1.41
32	B	519	C7Z	C4-C3	8.19	1.66	1.52
25	A	407	PHO	C3B-C4B	8.14	1.49	1.41
38	H	101	RRX	C30-C25	-7.88	1.43	1.53
26	B	517	BCR	C30-C25	-7.87	1.43	1.53
38	H	101	RRX	C27-C28	7.87	1.66	1.52
26	C	517	BCR	C30-C25	-7.71	1.43	1.53
26	C	515	BCR	C30-C25	-7.68	1.43	1.53
26	B	517	BCR	C1-C6	-7.64	1.44	1.53
26	D	405	BCR	C30-C25	-7.61	1.44	1.53
26	C	516	BCR	C1-C6	-7.57	1.44	1.53
26	C	516	BCR	C30-C25	-7.51	1.44	1.53
26	J	101	BCR	C1-C6	-7.50	1.44	1.53
26	B	518	BCR	C30-C25	-7.38	1.44	1.53
26	J	101	BCR	C30-C25	-7.32	1.44	1.53
38	H	101	RRX	C1-C6	-7.30	1.44	1.53
26	D	405	BCR	C1-C6	-7.28	1.44	1.53
26	A	409	BCR	C30-C25	-7.27	1.44	1.53
26	C	515	BCR	C1-C6	-7.24	1.44	1.53
26	C	517	BCR	C1-C6	-7.12	1.44	1.53
26	J	101	BCR	C2-C3	-7.08	1.35	1.52
26	A	409	BCR	C2-C3	-7.08	1.35	1.52
26	C	517	BCR	C2-C3	-7.02	1.36	1.52
26	B	517	BCR	C2-C3	-7.00	1.36	1.52
38	H	101	RRX	C2-C3	-7.00	1.36	1.52
26	A	409	BCR	C1-C6	-7.00	1.44	1.53
26	D	405	BCR	C2-C3	-7.00	1.36	1.52
26	B	518	BCR	C1-C6	-6.96	1.44	1.53
26	B	518	BCR	C2-C3	-6.95	1.36	1.52
26	C	515	BCR	C2-C3	-6.91	1.36	1.52
26	C	516	BCR	C2-C3	-6.83	1.36	1.52
26	A	409	BCR	C29-C28	-6.78	1.36	1.52
26	B	518	BCR	C29-C28	-6.75	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	517	BCR	C29-C28	-6.74	1.36	1.52
26	C	516	BCR	C29-C28	-6.72	1.36	1.52
26	J	101	BCR	C29-C28	-6.71	1.36	1.52
26	B	517	BCR	C29-C28	-6.70	1.36	1.52
26	C	515	BCR	C29-C28	-6.55	1.37	1.52
26	D	405	BCR	C29-C28	-6.53	1.37	1.52
24	C	504	CLA	MG-NA	6.26	2.21	2.06
24	C	508	CLA	MG-NA	6.26	2.21	2.06
24	B	516	CLA	MG-NA	6.24	2.21	2.06
24	B	504	CLA	MG-NA	6.24	2.21	2.06
24	C	506	CLA	MG-NA	6.23	2.21	2.06
24	B	510	CLA	MG-NA	6.21	2.21	2.06
24	C	512	CLA	MG-NA	6.21	2.21	2.06
24	C	507	CLA	MG-NA	6.20	2.21	2.06
24	B	501	CLA	MG-NA	6.16	2.20	2.06
24	C	509	CLA	MG-NA	6.15	2.20	2.06
24	C	514	CLA	MG-NA	6.15	2.20	2.06
24	C	513	CLA	MG-NA	6.15	2.20	2.06
24	D	404	CLA	MG-NA	6.15	2.20	2.06
24	C	503	CLA	MG-NA	6.13	2.20	2.06
24	B	514	CLA	MG-NA	6.13	2.20	2.06
24	A	406	CLA	MG-NA	6.12	2.20	2.06
24	B	503	CLA	MG-NA	6.12	2.20	2.06
24	C	502	CLA	MG-NA	6.11	2.20	2.06
24	B	508	CLA	MG-NA	6.11	2.20	2.06
24	B	507	CLA	MG-NA	6.11	2.20	2.06
24	B	502	CLA	MG-NA	6.08	2.20	2.06
24	B	511	CLA	MG-NA	6.07	2.20	2.06
24	A	408	CLA	MG-NA	6.05	2.20	2.06
24	D	403	CLA	MG-NA	6.05	2.20	2.06
24	B	515	CLA	MG-NA	6.04	2.20	2.06
24	B	513	CLA	MG-NA	6.03	2.20	2.06
24	C	510	CLA	MG-NA	6.03	2.20	2.06
24	C	511	CLA	MG-NA	6.02	2.20	2.06
24	C	505	CLA	MG-NA	6.02	2.20	2.06
24	B	505	CLA	MG-NA	6.00	2.20	2.06
24	B	509	CLA	MG-NA	6.00	2.20	2.06
24	B	506	CLA	MG-NA	5.98	2.20	2.06
24	B	512	CLA	MG-NA	5.96	2.20	2.06
24	D	401	CLA	MG-NA	5.96	2.20	2.06
24	A	405	CLA	MG-NA	5.93	2.20	2.06
32	B	519	C7Z	C12-C13	5.83	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	519	C7Z	C1-C6	-5.82	1.46	1.53
38	H	101	RRX	C19-C18	5.70	1.58	1.46
26	C	517	BCR	C12-C13	5.68	1.58	1.46
26	A	409	BCR	C12-C13	5.67	1.58	1.46
26	C	515	BCR	C12-C13	5.62	1.58	1.46
26	J	101	BCR	C12-C13	5.56	1.57	1.46
26	B	517	BCR	C12-C13	5.55	1.57	1.46
26	D	405	BCR	C12-C13	5.48	1.57	1.46
26	B	518	BCR	C12-C13	5.45	1.57	1.46
26	C	516	BCR	C12-C13	5.40	1.57	1.46
26	C	515	BCR	C8-C9	5.31	1.57	1.46
26	A	409	BCR	C8-C9	5.28	1.57	1.46
26	D	405	BCR	C8-C9	5.25	1.57	1.46
26	C	515	BCR	C29-C30	5.25	1.66	1.54
26	J	101	BCR	C8-C9	5.23	1.57	1.46
26	C	517	BCR	C8-C9	5.21	1.57	1.46
26	D	405	BCR	C29-C30	5.20	1.66	1.54
26	B	518	BCR	C8-C9	5.19	1.57	1.46
26	B	517	BCR	C8-C9	5.19	1.57	1.46
26	J	101	BCR	C29-C30	5.17	1.65	1.54
26	C	516	BCR	C8-C9	5.14	1.57	1.46
26	A	409	BCR	C23-C22	5.12	1.56	1.46
26	B	518	BCR	C23-C22	5.09	1.56	1.46
26	B	518	BCR	C29-C30	5.08	1.65	1.54
26	J	101	BCR	C23-C22	5.07	1.56	1.46
26	B	517	BCR	C29-C30	5.07	1.65	1.54
26	C	515	BCR	C23-C22	5.07	1.56	1.46
26	D	405	BCR	C23-C22	5.06	1.56	1.46
26	A	409	BCR	C29-C30	5.04	1.65	1.54
32	B	519	C7Z	C24-C25	-5.01	1.43	1.51
26	C	516	BCR	C29-C30	5.00	1.65	1.54
26	C	517	BCR	C29-C30	4.96	1.65	1.54
26	C	517	BCR	C23-C22	4.95	1.56	1.46
26	B	517	BCR	C23-C22	4.91	1.56	1.46
26	A	409	BCR	C15-C14	4.91	1.58	1.43
26	C	516	BCR	C23-C22	4.86	1.56	1.46
26	C	517	BCR	C15-C14	4.81	1.58	1.43
38	H	101	RRX	C8-C9	4.80	1.56	1.46
26	C	515	BCR	C15-C14	4.78	1.58	1.43
38	H	101	RRX	C12-C13	4.73	1.56	1.46
26	B	518	BCR	C15-C14	4.72	1.57	1.43
26	J	101	BCR	C15-C14	4.67	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	517	BCR	C15-C14	4.66	1.57	1.43
26	D	405	BCR	C15-C14	4.66	1.57	1.43
38	H	101	RRX	C2-C1	4.61	1.64	1.54
26	C	516	BCR	C15-C14	4.61	1.57	1.43
26	C	515	BCR	C19-C18	4.54	1.55	1.46
26	C	517	BCR	C2-C1	4.50	1.64	1.54
26	D	405	BCR	C2-C1	4.48	1.64	1.54
32	B	519	C7Z	C28-C29	4.48	1.55	1.46
38	H	101	RRX	C24-C25	4.48	1.60	1.45
26	B	518	BCR	C19-C18	4.43	1.55	1.46
26	C	516	BCR	C2-C1	4.42	1.64	1.54
26	C	517	BCR	C19-C18	4.42	1.55	1.46
32	B	519	C7Z	C31-C30	4.41	1.56	1.43
26	B	517	BCR	C2-C1	4.40	1.64	1.54
38	H	101	RRX	C23-C22	4.39	1.55	1.46
26	B	518	BCR	C2-C1	4.39	1.64	1.54
24	C	506	CLA	CBB-CAB	4.39	1.51	1.30
24	B	507	CLA	CBB-CAB	4.38	1.51	1.30
24	D	404	CLA	CBB-CAB	4.38	1.51	1.30
26	D	405	BCR	C19-C18	4.38	1.55	1.46
24	B	509	CLA	CBB-CAB	4.37	1.51	1.30
24	C	504	CLA	CBB-CAB	4.37	1.51	1.30
26	J	101	BCR	C19-C18	4.37	1.55	1.46
24	B	514	CLA	CBB-CAB	4.37	1.51	1.30
24	B	505	CLA	CBB-CAB	4.37	1.51	1.30
38	H	101	RRX	C27-C26	-4.37	1.44	1.51
24	C	505	CLA	CBB-CAB	4.37	1.51	1.30
24	B	513	CLA	CBB-CAB	4.37	1.51	1.30
24	B	504	CLA	CBB-CAB	4.37	1.51	1.30
24	B	502	CLA	CBB-CAB	4.37	1.51	1.30
26	C	515	BCR	C2-C1	4.37	1.64	1.54
24	B	503	CLA	CBB-CAB	4.36	1.51	1.30
24	B	515	CLA	CBB-CAB	4.36	1.51	1.30
24	B	510	CLA	CBB-CAB	4.36	1.51	1.30
24	B	508	CLA	CBB-CAB	4.36	1.51	1.30
24	C	503	CLA	CBB-CAB	4.35	1.51	1.30
24	C	507	CLA	CBB-CAB	4.35	1.51	1.30
24	C	511	CLA	CBB-CAB	4.35	1.51	1.30
24	C	512	CLA	CBB-CAB	4.35	1.51	1.30
24	A	405	CLA	CBB-CAB	4.35	1.51	1.30
24	C	514	CLA	CBB-CAB	4.35	1.51	1.30
24	C	509	CLA	CBB-CAB	4.35	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	CBB-CAB	4.34	1.51	1.30
26	C	515	BCR	C20-C21	4.34	1.56	1.43
24	B	506	CLA	CBB-CAB	4.34	1.51	1.30
26	J	101	BCR	C2-C1	4.34	1.64	1.54
24	C	513	CLA	CBB-CAB	4.34	1.51	1.30
24	C	502	CLA	CBB-CAB	4.33	1.51	1.30
26	B	518	BCR	C20-C21	4.32	1.56	1.43
24	A	406	CLA	CBB-CAB	4.32	1.51	1.30
24	B	511	CLA	CBB-CAB	4.31	1.51	1.30
26	A	409	BCR	C19-C18	4.31	1.55	1.46
24	B	516	CLA	CBB-CAB	4.31	1.51	1.30
24	D	401	CLA	CBB-CAB	4.30	1.51	1.30
24	B	501	CLA	CBB-CAB	4.30	1.51	1.30
26	B	517	BCR	C19-C18	4.30	1.55	1.46
38	H	101	RRX	C3-C4	4.30	1.65	1.52
38	H	101	RRX	C11-C10	4.30	1.56	1.43
24	A	408	CLA	CBB-CAB	4.29	1.51	1.30
24	B	512	CLA	CBB-CAB	4.29	1.51	1.30
24	C	510	CLA	CBB-CAB	4.29	1.51	1.30
26	A	409	BCR	C2-C1	4.28	1.63	1.54
26	C	517	BCR	C20-C21	4.27	1.56	1.43
26	D	405	BCR	C28-C27	4.27	1.65	1.52
26	J	101	BCR	C20-C21	4.27	1.56	1.43
33	C	518	DGD	O1G-C1A	4.26	1.45	1.33
24	D	403	CLA	CBB-CAB	4.25	1.50	1.30
33	B	521	DGD	O1G-C1A	4.24	1.45	1.33
26	A	409	BCR	C20-C21	4.23	1.56	1.43
36	D	406	PL9	C3-C4	-4.22	1.42	1.49
26	C	516	BCR	C19-C18	4.22	1.55	1.46
26	D	405	BCR	C20-C21	4.21	1.56	1.43
26	B	517	BCR	C20-C21	4.20	1.56	1.43
26	C	515	BCR	C28-C27	4.16	1.65	1.52
33	C	519	DGD	O1G-C1A	4.15	1.45	1.33
24	B	513	CLA	MG-ND	-4.13	1.97	2.05
26	B	517	BCR	C28-C27	4.13	1.65	1.52
26	C	517	BCR	C28-C27	4.11	1.65	1.52
26	C	516	BCR	C28-C27	4.11	1.65	1.52
26	A	409	BCR	C28-C27	4.10	1.65	1.52
26	B	518	BCR	C28-C27	4.10	1.65	1.52
26	J	101	BCR	C28-C27	4.10	1.65	1.52
24	B	508	CLA	MG-ND	-4.10	1.97	2.05
24	C	513	CLA	MG-ND	-4.09	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	516	BCR	C20-C21	4.09	1.55	1.43
38	H	101	RRX	C29-C30	4.08	1.67	1.54
24	B	512	CLA	MG-ND	-4.07	1.97	2.05
32	B	519	C7Z	C32-C33	4.06	1.54	1.46
24	C	510	CLA	MG-ND	-4.05	1.97	2.05
24	B	504	CLA	MG-ND	-4.04	1.97	2.05
24	B	503	CLA	MG-ND	-4.04	1.97	2.05
24	C	509	CLA	MG-ND	-4.03	1.97	2.05
33	C	520	DGD	O1G-C1A	4.03	1.45	1.33
24	D	403	CLA	MG-ND	-4.02	1.97	2.05
24	C	503	CLA	MG-ND	-4.01	1.97	2.05
24	C	508	CLA	MG-ND	-3.99	1.97	2.05
24	B	516	CLA	MG-ND	-3.98	1.97	2.05
24	B	506	CLA	MG-ND	-3.98	1.97	2.05
24	C	507	CLA	MG-ND	-3.96	1.97	2.05
24	D	401	CLA	MG-ND	-3.96	1.97	2.05
24	A	406	CLA	MG-ND	-3.96	1.97	2.05
38	H	101	RRX	C15-C14	3.96	1.55	1.43
24	C	511	CLA	MG-ND	-3.96	1.97	2.05
24	B	507	CLA	MG-ND	-3.95	1.98	2.05
24	C	512	CLA	MG-ND	-3.95	1.98	2.05
32	B	519	C7Z	C4-C5	-3.95	1.44	1.51
32	B	519	C7Z	C22-C21	3.94	1.66	1.54
24	B	515	CLA	MG-ND	-3.94	1.98	2.05
24	B	501	CLA	MG-ND	-3.94	1.98	2.05
24	B	514	CLA	MG-ND	-3.93	1.98	2.05
24	A	405	CLA	MG-ND	-3.93	1.98	2.05
26	C	516	BCR	C3-C4	3.92	1.64	1.52
24	D	404	CLA	MG-ND	-3.92	1.98	2.05
24	B	505	CLA	MG-ND	-3.92	1.98	2.05
24	B	510	CLA	MG-ND	-3.91	1.98	2.05
24	C	506	CLA	MG-ND	-3.91	1.98	2.05
24	C	514	CLA	MG-ND	-3.89	1.98	2.05
24	B	509	CLA	MG-ND	-3.88	1.98	2.05
26	B	518	BCR	C3-C4	3.87	1.64	1.52
26	C	515	BCR	C3-C4	3.86	1.64	1.52
26	B	517	BCR	C3-C4	3.85	1.64	1.52
26	A	409	BCR	C16-C17	3.85	1.55	1.43
32	B	519	C7Z	C11-C10	3.84	1.55	1.43
24	B	511	CLA	MG-ND	-3.82	1.98	2.05
24	C	505	CLA	MG-ND	-3.81	1.98	2.05
38	H	101	RRX	C16-C17	3.81	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	519	C7Z	C15-C14	3.80	1.55	1.43
24	C	504	CLA	MG-ND	-3.79	1.98	2.05
26	A	409	BCR	C11-C10	3.79	1.55	1.43
26	D	405	BCR	C3-C4	3.78	1.64	1.52
26	J	101	BCR	C3-C4	3.78	1.64	1.52
32	B	519	C7Z	C27-C26	3.77	1.58	1.45
24	C	502	CLA	MG-ND	-3.76	1.98	2.05
28	B	520	LMG	C22-C21	-3.76	1.33	1.51
26	B	518	BCR	C16-C17	3.76	1.54	1.43
26	A	409	BCR	C27-C26	-3.75	1.44	1.51
33	C	519	DGD	CAB-C9B	-3.75	1.33	1.51
26	C	517	BCR	C11-C10	3.75	1.54	1.43
26	C	517	BCR	C3-C4	3.75	1.64	1.52
26	A	409	BCR	C3-C4	3.74	1.64	1.52
26	C	515	BCR	C16-C17	3.74	1.54	1.43
28	C	522	LMG	C19-C18	-3.74	1.33	1.51
28	C	521	LMG	C19-C18	-3.74	1.33	1.51
33	C	519	DGD	CDB-CCB	-3.73	1.33	1.51
28	C	522	LMG	C22-C21	-3.73	1.33	1.51
26	C	517	BCR	C16-C17	3.73	1.54	1.43
26	D	405	BCR	C4-C5	-3.73	1.44	1.51
33	C	520	DGD	CAA-C9A	-3.73	1.33	1.51
26	C	515	BCR	C11-C10	3.73	1.54	1.43
28	B	520	LMG	C19-C18	-3.72	1.33	1.51
24	A	408	CLA	MG-ND	-3.72	1.98	2.05
38	H	101	RRX	C20-C21	3.72	1.54	1.43
26	B	517	BCR	C11-C10	3.71	1.54	1.43
28	H	102	LMG	C19-C18	-3.71	1.33	1.51
28	C	521	LMG	C40-C39	-3.71	1.33	1.51
28	C	521	LMG	C37-C36	-3.69	1.33	1.51
26	D	405	BCR	C24-C25	3.68	1.57	1.45
24	B	502	CLA	MG-ND	-3.68	1.98	2.05
26	A	409	BCR	C24-C25	3.68	1.57	1.45
26	A	409	BCR	C4-C5	-3.68	1.44	1.51
26	D	405	BCR	C16-C17	3.68	1.54	1.43
26	J	101	BCR	C16-C17	3.68	1.54	1.43
28	D	409	LMG	C19-C18	-3.68	1.33	1.51
28	H	102	LMG	C40-C39	-3.67	1.33	1.51
26	C	515	BCR	C27-C26	-3.67	1.44	1.51
32	B	519	C7Z	C2-C1	3.67	1.65	1.54
26	J	101	BCR	C11-C10	3.66	1.54	1.43
26	C	517	BCR	C4-C5	-3.66	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	517	BCR	C16-C17	3.66	1.54	1.43
26	B	518	BCR	C24-C25	3.66	1.57	1.45
26	C	516	BCR	C4-C5	-3.65	1.44	1.51
28	C	501	LMG	C19-C18	-3.65	1.33	1.51
26	D	405	BCR	C11-C10	3.64	1.54	1.43
28	H	102	LMG	C37-C36	-3.64	1.33	1.51
26	B	517	BCR	C27-C26	-3.64	1.44	1.51
26	J	101	BCR	C24-C25	3.63	1.57	1.45
26	C	516	BCR	C27-C26	-3.63	1.44	1.51
25	D	402	PHO	C1D-C2D	3.61	1.43	1.39
24	D	401	CLA	C1C-NC	-3.60	1.32	1.37
26	J	101	BCR	C4-C5	-3.60	1.44	1.51
26	C	517	BCR	C27-C26	-3.59	1.44	1.51
26	C	517	BCR	C24-C25	3.59	1.57	1.45
26	C	516	BCR	C24-C25	3.59	1.57	1.45
26	B	518	BCR	C11-C10	3.59	1.54	1.43
32	B	519	C7Z	C35-C34	3.57	1.54	1.43
26	C	516	BCR	C16-C17	3.56	1.54	1.43
26	C	515	BCR	C4-C5	-3.56	1.44	1.51
26	B	518	BCR	C4-C5	-3.56	1.44	1.51
26	B	517	BCR	C24-C25	3.55	1.57	1.45
26	B	518	BCR	C27-C26	-3.55	1.44	1.51
26	C	515	BCR	C24-C25	3.55	1.57	1.45
26	B	517	BCR	C4-C5	-3.54	1.44	1.51
25	D	402	PHO	C4D-CHA	3.54	1.44	1.39
26	C	516	BCR	C11-C10	3.53	1.54	1.43
26	J	101	BCR	C27-C26	-3.53	1.44	1.51
24	B	505	CLA	C1C-NC	-3.52	1.32	1.37
24	B	511	CLA	C1C-NC	-3.52	1.32	1.37
24	A	405	CLA	C1C-NC	-3.52	1.32	1.37
35	B	523	DGA	OG2-CB1	3.50	1.44	1.34
25	A	407	PHO	C1D-C2D	3.48	1.43	1.39
24	C	509	CLA	C1C-NC	-3.46	1.32	1.37
24	C	505	CLA	C1C-NC	-3.45	1.32	1.37
32	B	519	C7Z	C18-C5	3.44	1.56	1.50
38	H	101	RRX	C7-C6	3.44	1.56	1.45
24	A	406	CLA	C1C-NC	-3.44	1.32	1.37
24	C	503	CLA	C1C-NC	-3.44	1.32	1.37
24	B	506	CLA	C1C-NC	-3.43	1.32	1.37
24	B	512	CLA	C1C-NC	-3.43	1.32	1.37
24	B	510	CLA	C1C-NC	-3.43	1.32	1.37
24	B	504	CLA	C1C-NC	-3.43	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	H	101	RRX	C4-C5	-3.42	1.44	1.51
32	B	519	C7Z	C21-C26	-3.42	1.49	1.53
36	D	406	PL9	C7-C3	-3.40	1.46	1.51
26	D	405	BCR	C27-C26	-3.40	1.44	1.51
24	B	502	CLA	C1C-NC	-3.39	1.32	1.37
24	C	510	CLA	C1C-NC	-3.38	1.32	1.37
24	C	507	CLA	C1C-NC	-3.38	1.32	1.37
36	D	406	PL9	C6-C1	-3.37	1.42	1.48
24	B	507	CLA	C1C-NC	-3.37	1.32	1.37
24	C	512	CLA	C1C-NC	-3.37	1.32	1.37
24	C	514	CLA	C1C-NC	-3.37	1.32	1.37
24	D	404	CLA	C1C-NC	-3.37	1.32	1.37
24	B	501	CLA	C1C-NC	-3.36	1.32	1.37
24	B	514	CLA	C1C-NC	-3.36	1.32	1.37
24	B	509	CLA	C1C-NC	-3.36	1.32	1.37
24	C	506	CLA	C1C-NC	-3.36	1.32	1.37
25	A	407	PHO	C4D-CHA	3.35	1.44	1.39
24	B	503	CLA	C1C-NC	-3.35	1.32	1.37
24	A	408	CLA	C1C-NC	-3.33	1.32	1.37
24	C	502	CLA	C1C-NC	-3.32	1.32	1.37
35	B	523	DGA	OG1-CA1	3.32	1.43	1.33
24	C	511	CLA	C1C-NC	-3.32	1.32	1.37
32	B	519	C7Z	C7-C6	3.30	1.56	1.45
24	B	508	CLA	C1C-NC	-3.28	1.32	1.37
24	C	504	CLA	C1C-NC	-3.28	1.32	1.37
24	B	516	CLA	C1C-NC	-3.26	1.32	1.37
24	C	508	CLA	C1C-NC	-3.26	1.32	1.37
24	B	513	CLA	C1C-NC	-3.24	1.32	1.37
24	D	401	CLA	C4B-NB	-3.24	1.33	1.37
24	C	513	CLA	C1C-NC	-3.21	1.32	1.37
24	D	403	CLA	C1C-NC	-3.20	1.32	1.37
24	A	408	CLA	C4B-NB	-3.20	1.33	1.37
24	C	510	CLA	C4B-NB	-3.17	1.33	1.37
24	B	515	CLA	C1C-NC	-3.17	1.32	1.37
32	B	519	C7Z	C8-C9	3.14	1.52	1.46
24	B	511	CLA	C4B-NB	-3.13	1.33	1.37
24	B	504	CLA	C4B-NB	-3.13	1.33	1.37
24	A	405	CLA	C4B-NB	-3.11	1.33	1.37
37	E	101	HEM	FE-NA	3.10	2.05	1.95
24	B	502	CLA	C4B-NB	-3.09	1.33	1.37
24	C	509	CLA	C4B-NB	-3.08	1.33	1.37
24	A	406	CLA	C4B-NB	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	512	CLA	C4B-NB	-3.06	1.33	1.37
24	B	514	CLA	C4B-NB	-3.05	1.33	1.37
24	C	506	CLA	C4B-NB	-3.04	1.33	1.37
24	B	506	CLA	C4B-NB	-3.03	1.33	1.37
37	E	101	HEM	CAB-C3B	3.02	1.55	1.47
24	C	503	CLA	C4B-NB	-3.01	1.33	1.37
24	C	512	CLA	C4B-NB	-2.98	1.33	1.37
24	C	505	CLA	C4B-NB	-2.97	1.34	1.37
24	C	508	CLA	C4B-NB	-2.97	1.34	1.37
24	C	504	CLA	C4B-NB	-2.95	1.34	1.37
24	B	509	CLA	C4B-NB	-2.95	1.34	1.37
37	E	101	HEM	FE-ND	2.95	2.04	1.94
24	C	514	CLA	C4B-NB	-2.94	1.34	1.37
24	D	404	CLA	C4B-NB	-2.93	1.34	1.37
28	D	409	LMG	C37-C36	-2.93	1.33	1.51
24	B	515	CLA	C4B-NB	-2.92	1.34	1.37
24	C	507	CLA	C4B-NB	-2.92	1.34	1.37
37	E	101	HEM	CAC-C3C	2.91	1.55	1.47
24	B	503	CLA	C4B-NB	-2.89	1.34	1.37
25	A	407	PHO	CMC-C2C	-2.89	1.46	1.50
24	B	507	CLA	C4B-NB	-2.88	1.34	1.37
26	A	409	BCR	C34-C9	2.88	1.56	1.50
24	C	511	CLA	C4B-NB	-2.87	1.34	1.37
24	B	508	CLA	C4B-NB	-2.87	1.34	1.37
24	B	513	CLA	C4B-NB	-2.86	1.34	1.37
25	D	402	PHO	CMC-C2C	-2.85	1.46	1.50
26	B	517	BCR	C34-C9	2.84	1.56	1.50
24	B	516	CLA	C4B-NB	-2.80	1.34	1.37
26	C	515	BCR	C34-C9	2.79	1.56	1.50
24	B	505	CLA	C4B-NB	-2.79	1.34	1.37
26	C	515	BCR	C7-C6	2.77	1.54	1.45
24	C	513	CLA	C4B-NB	-2.76	1.34	1.37
37	E	101	HEM	FE-NC	2.74	2.04	1.95
26	B	518	BCR	C34-C9	2.73	1.56	1.50
26	J	101	BCR	C34-C9	2.70	1.56	1.50
26	J	101	BCR	C7-C6	2.70	1.54	1.45
26	D	405	BCR	C7-C6	2.70	1.54	1.45
26	A	409	BCR	C7-C6	2.69	1.54	1.45
26	B	518	BCR	C7-C6	2.69	1.54	1.45
26	C	516	BCR	C34-C9	2.68	1.56	1.50
26	D	405	BCR	C34-C9	2.67	1.56	1.50
25	D	402	PHO	CMD-C2D	-2.66	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	517	BCR	C7-C6	2.66	1.54	1.45
24	B	510	CLA	C4B-NB	-2.65	1.34	1.37
25	A	407	PHO	CMD-C2D	-2.64	1.46	1.51
26	B	517	BCR	C7-C6	2.63	1.54	1.45
26	C	516	BCR	C7-C6	2.63	1.54	1.45
24	C	502	CLA	C4B-NB	-2.63	1.34	1.37
24	D	403	CLA	C4B-NB	-2.60	1.34	1.37
26	C	517	BCR	C34-C9	2.60	1.56	1.50
37	E	101	HEM	FE-NB	2.58	2.02	1.94
26	C	516	BCR	C39-C30	-2.57	1.48	1.53
25	A	407	PHO	CMB-C2B	-2.55	1.46	1.51
36	D	406	PL9	C53-C6	-2.55	1.45	1.50
25	D	402	PHO	CMB-C2B	-2.55	1.46	1.51
25	D	402	PHO	CAC-C3C	-2.52	1.47	1.51
24	B	501	CLA	C4B-NB	-2.51	1.34	1.37
26	C	517	BCR	C39-C30	-2.51	1.49	1.53
25	A	407	PHO	CAC-C3C	-2.50	1.47	1.51
32	B	519	C7Z	C38-C25	2.47	1.54	1.50
26	J	101	BCR	C39-C30	-2.47	1.49	1.53
32	B	519	C7Z	C20-C13	2.45	1.55	1.50
36	D	406	PL9	C52-C5	-2.44	1.45	1.50
26	C	515	BCR	C39-C30	-2.44	1.49	1.53
34	B	522	3PH	O31-C31	2.42	1.40	1.33
33	C	520	DGD	CDA-CCA	-2.41	1.33	1.50
28	H	102	LMG	C22-C21	-2.41	1.33	1.50
33	C	520	DGD	CAB-C9B	-2.41	1.33	1.50
33	C	519	DGD	CGB-CFB	-2.40	1.33	1.50
28	A	415	LMG	C37-C36	-2.39	1.33	1.50
28	B	520	LMG	C25-C24	-2.39	1.33	1.50
28	C	501	LMG	C22-C21	-2.39	1.33	1.50
28	C	521	LMG	C43-C42	-2.39	1.33	1.50
26	A	409	BCR	C39-C30	-2.38	1.49	1.53
28	H	102	LMG	C43-C42	-2.37	1.33	1.50
26	B	518	BCR	C39-C30	-2.37	1.49	1.53
26	C	516	BCR	C36-C18	2.37	1.55	1.50
26	B	517	BCR	C39-C30	-2.36	1.49	1.53
26	D	405	BCR	C39-C30	-2.36	1.49	1.53
34	B	522	3PH	O21-C2	-2.36	1.41	1.46
25	A	407	PHO	C4D-ND	-2.36	1.35	1.38
38	H	101	RRX	C34-C9	2.35	1.55	1.50
26	C	515	BCR	C36-C18	2.34	1.55	1.50
26	J	101	BCR	C36-C18	2.32	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C3D-C4D	-2.32	1.39	1.44
24	B	503	CLA	C3D-C4D	-2.30	1.39	1.44
24	A	406	CLA	C3D-C4D	-2.30	1.39	1.44
32	B	519	C7Z	C40-C33	2.30	1.55	1.50
26	B	517	BCR	C36-C18	2.29	1.55	1.50
26	B	518	BCR	C36-C18	2.28	1.55	1.50
26	D	405	BCR	C36-C18	2.28	1.55	1.50
26	C	517	BCR	C36-C18	2.26	1.55	1.50
24	C	502	CLA	C3D-C4D	-2.26	1.39	1.44
24	C	510	CLA	C3D-C4D	-2.25	1.39	1.44
24	C	511	CLA	C3D-C4D	-2.25	1.39	1.44
24	A	408	CLA	C3D-C4D	-2.24	1.39	1.44
26	D	405	BCR	C38-C26	2.23	1.54	1.50
24	D	401	CLA	C3D-C4D	-2.23	1.39	1.44
24	B	504	CLA	C3D-C4D	-2.23	1.39	1.44
34	B	522	3PH	O31-C3	-2.22	1.40	1.45
24	A	405	CLA	C3D-C4D	-2.22	1.39	1.44
24	C	509	CLA	C3D-C4D	-2.21	1.39	1.44
32	B	519	C7Z	C19-C9	2.21	1.55	1.50
34	B	522	3PH	O21-C21	2.20	1.40	1.34
25	D	402	PHO	C3D-C4D	2.20	1.44	1.41
24	B	508	CLA	C3D-C4D	-2.20	1.39	1.44
24	C	504	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	505	CLA	C3D-C4D	-2.19	1.39	1.44
24	C	512	CLA	C3D-C4D	-2.18	1.39	1.44
24	B	506	CLA	C3D-C4D	-2.18	1.39	1.44
24	B	514	CLA	C3D-C4D	-2.17	1.39	1.44
24	B	512	CLA	C3D-C4D	-2.17	1.39	1.44
26	A	409	BCR	C36-C18	2.17	1.55	1.50
24	C	514	CLA	C3D-C4D	-2.17	1.39	1.44
24	C	506	CLA	C3D-C4D	-2.16	1.39	1.44
24	B	511	CLA	C3D-C4D	-2.16	1.39	1.44
25	D	402	PHO	C4D-ND	-2.15	1.35	1.38
24	B	516	CLA	C3D-C4D	-2.15	1.39	1.44
35	B	523	DGA	OG2-CG2	-2.15	1.41	1.46
24	B	501	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	502	CLA	C3D-C4D	-2.14	1.39	1.44
38	H	101	RRX	C33-C5	2.14	1.54	1.50
24	C	508	CLA	C3D-C4D	-2.14	1.39	1.44
24	C	507	CLA	C3D-C4D	-2.13	1.39	1.44
26	A	409	BCR	C37-C22	2.13	1.55	1.50
24	D	404	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	507	CLA	C1A-CHA	2.13	1.51	1.43
24	B	513	CLA	C3D-C4D	-2.12	1.39	1.44
24	B	507	CLA	C3D-C4D	-2.11	1.39	1.44
24	B	510	CLA	C3D-C4D	-2.11	1.39	1.44
24	C	503	CLA	C3D-C4D	-2.10	1.39	1.44
26	B	518	BCR	C38-C26	2.10	1.54	1.50
24	A	408	CLA	C1A-CHA	2.09	1.51	1.43
24	B	509	CLA	C3D-C4D	-2.09	1.39	1.44
26	J	101	BCR	C38-C26	2.09	1.54	1.50
24	B	515	CLA	C3D-C4D	-2.09	1.39	1.44
26	C	515	BCR	C38-C26	2.08	1.54	1.50
25	A	407	PHO	C3B-C2B	-2.08	1.37	1.40
26	C	517	BCR	C38-C26	2.08	1.54	1.50
24	C	513	CLA	C3D-C4D	-2.07	1.39	1.44
24	C	505	CLA	C1A-CHA	2.06	1.51	1.43
26	B	518	BCR	C37-C22	2.06	1.55	1.50
25	A	407	PHO	C3D-C4D	2.06	1.44	1.41
24	B	504	CLA	C1A-CHA	2.06	1.51	1.43
24	B	503	CLA	C1A-CHA	2.05	1.51	1.43
24	A	406	CLA	C1A-CHA	2.05	1.51	1.43
26	C	516	BCR	C38-C26	2.05	1.54	1.50
24	D	404	CLA	C1A-CHA	2.03	1.51	1.43
26	A	409	BCR	C38-C26	2.03	1.54	1.50
37	E	101	HEM	C2A-C3A	-2.03	1.33	1.38
24	B	515	CLA	C1A-CHA	2.03	1.51	1.43
24	C	506	CLA	C1A-CHA	2.02	1.51	1.43
26	B	517	BCR	C38-C26	2.02	1.54	1.50
33	B	521	DGD	O3G-C1D	2.02	1.43	1.40
24	B	509	CLA	C1A-CHA	2.02	1.51	1.43
26	B	517	BCR	C37-C22	2.02	1.54	1.50
27	A	410	SQD	O47-C45	-2.02	1.41	1.46
24	C	513	CLA	C1A-CHA	2.01	1.51	1.43
24	B	501	CLA	C1A-CHA	2.01	1.51	1.43
24	B	513	CLA	C1A-CHA	2.01	1.51	1.43
24	C	508	CLA	C1A-CHA	2.00	1.51	1.43
24	C	503	CLA	C1A-CHA	2.00	1.51	1.43
24	C	512	CLA	C1A-CHA	2.00	1.51	1.43

All (938) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	BCR	C7-C8-C9	-9.89	111.60	126.23
24	A	408	CLA	C4A-NA-C1A	9.61	111.06	106.68
24	B	512	CLA	C4A-NA-C1A	9.57	111.05	106.68
24	D	404	CLA	C4A-NA-C1A	9.47	111.00	106.68
24	B	509	CLA	C4A-NA-C1A	9.36	110.95	106.68
24	B	513	CLA	C4A-NA-C1A	9.28	110.91	106.68
24	B	507	CLA	C4A-NA-C1A	9.22	110.89	106.68
24	C	505	CLA	C4A-NA-C1A	9.20	110.88	106.68
24	B	506	CLA	C4A-NA-C1A	9.12	110.84	106.68
24	A	405	CLA	C4A-NA-C1A	9.09	110.83	106.68
24	B	515	CLA	C4A-NA-C1A	9.06	110.81	106.68
24	C	503	CLA	C4A-NA-C1A	9.05	110.81	106.68
24	C	512	CLA	C4A-NA-C1A	9.03	110.80	106.68
24	C	508	CLA	C4A-NA-C1A	8.94	110.76	106.68
24	C	511	CLA	C4A-NA-C1A	8.94	110.76	106.68
24	C	514	CLA	C4A-NA-C1A	8.86	110.72	106.68
24	C	510	CLA	C4A-NA-C1A	8.84	110.71	106.68
24	B	510	CLA	C4A-NA-C1A	8.82	110.70	106.68
24	B	514	CLA	C4A-NA-C1A	8.82	110.70	106.68
24	C	513	CLA	C4A-NA-C1A	8.74	110.67	106.68
24	D	401	CLA	C4A-NA-C1A	8.71	110.65	106.68
24	B	501	CLA	C4A-NA-C1A	8.69	110.64	106.68
24	C	506	CLA	C4A-NA-C1A	8.68	110.64	106.68
24	B	502	CLA	C4A-NA-C1A	8.66	110.63	106.68
24	C	507	CLA	C4A-NA-C1A	8.63	110.61	106.68
24	B	508	CLA	C4A-NA-C1A	8.57	110.59	106.68
24	A	406	CLA	C4A-NA-C1A	8.57	110.59	106.68
24	B	511	CLA	C4A-NA-C1A	8.52	110.56	106.68
24	B	504	CLA	C4A-NA-C1A	8.51	110.56	106.68
26	A	409	BCR	C15-C14-C13	-8.51	115.34	127.28
24	B	503	CLA	C4A-NA-C1A	8.47	110.54	106.68
24	C	502	CLA	C4A-NA-C1A	8.38	110.50	106.68
24	B	505	CLA	C4A-NA-C1A	8.29	110.46	106.68
24	B	516	CLA	C4A-NA-C1A	8.27	110.45	106.68
24	C	504	CLA	C4A-NA-C1A	8.23	110.44	106.68
38	H	101	RRX	C11-C10-C9	-8.02	116.03	127.28
24	C	509	CLA	C4A-NA-C1A	7.95	110.31	106.68
24	D	403	CLA	C4A-NA-C1A	7.84	110.26	106.68
26	C	517	BCR	C7-C8-C9	-7.33	115.38	126.23
26	A	409	BCR	C20-C21-C22	-6.85	117.68	127.28
26	B	517	BCR	C33-C5-C6	-6.76	117.11	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	H	101	RRX	C20-C21-C22	-6.45	118.24	127.28
24	A	408	CLA	O2D-CGD-CBD	6.37	122.37	111.23
26	B	517	BCR	C15-C14-C13	-6.35	118.37	127.28
24	B	501	CLA	O2D-CGD-CBD	6.17	122.02	111.23
38	H	101	RRX	C15-C14-C13	-6.12	118.70	127.28
26	A	409	BCR	C33-C5-C6	-6.06	117.88	124.48
24	C	510	CLA	O2D-CGD-CBD	6.02	121.76	111.23
25	A	407	PHO	C4D-CHA-CBD	-6.01	105.57	108.45
32	B	519	C7Z	C11-C10-C9	-5.99	118.88	127.28
24	C	502	CLA	CMD-C2D-C1D	5.88	135.09	124.73
26	B	517	BCR	C11-C10-C9	-5.85	119.08	127.28
25	D	402	PHO	C4D-CHA-CBD	-5.81	105.67	108.45
26	C	515	BCR	C16-C17-C18	-5.71	119.27	127.28
24	D	404	CLA	O2D-CGD-CBD	5.70	121.20	111.23
24	B	512	CLA	O2D-CGD-CBD	5.68	121.15	111.23
24	C	509	CLA	O2D-CGD-CBD	5.67	121.14	111.23
24	C	511	CLA	CMD-C2D-C1D	5.63	134.64	124.73
24	C	502	CLA	O2D-CGD-CBD	5.63	121.07	111.23
24	C	512	CLA	CMD-C2D-C1D	5.62	134.63	124.73
24	C	513	CLA	O2D-CGD-CBD	5.61	121.04	111.23
24	B	507	CLA	CMD-C2D-C1D	5.61	134.61	124.73
24	D	401	CLA	CMD-C2D-C1D	5.60	134.58	124.73
24	B	510	CLA	O2D-CGD-CBD	5.60	121.01	111.23
24	C	514	CLA	O2D-CGD-CBD	5.58	120.99	111.23
24	B	506	CLA	CMD-C2D-C1D	5.58	134.55	124.73
24	B	505	CLA	O2D-CGD-CBD	5.57	120.96	111.23
24	C	503	CLA	O2D-CGD-CBD	5.56	120.95	111.23
24	B	504	CLA	O2D-CGD-CBD	5.56	120.94	111.23
24	C	508	CLA	O2D-CGD-CBD	5.54	120.91	111.23
24	B	509	CLA	O2D-CGD-CBD	5.53	120.90	111.23
24	B	505	CLA	CMD-C2D-C1D	5.52	134.45	124.73
30	A	413	BCT	O2-C-O1	5.51	133.76	119.68
24	C	505	CLA	O2D-CGD-CBD	5.50	120.84	111.23
24	B	503	CLA	CMD-C2D-C1D	5.48	134.39	124.73
24	C	504	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	B	501	CLA	CMD-C2D-C1D	5.48	134.38	124.73
26	C	516	BCR	C15-C14-C13	-5.47	119.61	127.28
24	B	504	CLA	CMD-C2D-C1D	5.47	134.36	124.73
24	B	506	CLA	O2D-CGD-CBD	5.46	120.78	111.23
24	C	510	CLA	CMD-C2D-C1D	5.44	134.31	124.73
24	B	515	CLA	O2D-CGD-CBD	5.43	120.72	111.23
24	B	514	CLA	CMD-C2D-C1D	5.41	134.26	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	CMD-C2D-C1D	5.41	134.25	124.73
24	C	506	CLA	O2D-CGD-CBD	5.41	120.69	111.23
26	A	409	BCR	C10-C11-C12	-5.40	107.54	123.20
24	C	511	CLA	O2D-CGD-CBD	5.39	120.66	111.23
26	C	517	BCR	C20-C21-C22	-5.39	119.71	127.28
26	C	517	BCR	C11-C10-C9	-5.39	119.72	127.28
24	B	502	CLA	CMD-C2D-C1D	5.38	134.21	124.73
24	C	514	CLA	CMD-C2D-C1D	5.38	134.21	124.73
24	C	508	CLA	CMD-C2D-C1D	5.37	134.18	124.73
32	B	519	C7Z	C15-C14-C13	-5.35	119.77	127.28
24	A	405	CLA	CMD-C2D-C1D	5.35	134.14	124.73
24	A	408	CLA	CMD-C2D-C1D	5.35	134.14	124.73
24	C	507	CLA	CMD-C2D-C1D	5.34	134.14	124.73
24	C	505	CLA	CMD-C2D-C1D	5.34	134.14	124.73
24	D	403	CLA	CMD-C2D-C1D	5.33	134.12	124.73
26	A	409	BCR	C8-C9-C10	5.32	127.38	119.01
26	J	101	BCR	C24-C23-C22	-5.30	118.39	126.23
24	C	506	CLA	CMD-C2D-C1D	5.28	134.02	124.73
24	B	513	CLA	CMD-C2D-C1D	5.26	134.00	124.73
24	C	512	CLA	O2D-CGD-CBD	5.26	120.43	111.23
24	A	406	CLA	O2D-CGD-CBD	5.23	120.38	111.23
24	B	511	CLA	O2D-CGD-CBD	5.23	120.38	111.23
26	J	101	BCR	C11-C10-C9	-5.23	119.95	127.28
24	D	404	CLA	CMD-C2D-C1D	5.22	133.92	124.73
26	C	516	BCR	C38-C26-C25	-5.22	118.79	124.48
26	J	101	BCR	C16-C17-C18	-5.19	120.00	127.28
24	B	509	CLA	CMD-C2D-C1D	5.19	133.87	124.73
24	B	502	CLA	O2D-CGD-CBD	5.18	120.28	111.23
24	C	504	CLA	O2D-CGD-CBD	5.17	120.26	111.23
24	B	508	CLA	O2D-CGD-CBD	5.16	120.25	111.23
24	B	516	CLA	CMD-C2D-C1D	5.15	133.80	124.73
24	B	511	CLA	CMD-C2D-C1D	5.15	133.80	124.73
24	B	503	CLA	O2D-CGD-CBD	5.15	120.23	111.23
24	B	515	CLA	CMD-C2D-C1D	5.14	133.78	124.73
26	J	101	BCR	C33-C5-C6	-5.12	118.89	124.48
24	C	509	CLA	CMD-C2D-C1D	5.12	133.74	124.73
24	B	516	CLA	O2D-CGD-CBD	5.11	120.17	111.23
24	C	507	CLA	O2D-CGD-CBD	5.10	120.15	111.23
26	C	516	BCR	C1-C6-C5	-5.10	115.67	122.64
26	C	516	BCR	C11-C10-C9	-5.09	120.14	127.28
26	C	515	BCR	C24-C23-C22	-5.09	118.70	126.23
24	D	403	CLA	O2D-CGD-CBD	5.09	120.13	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	507	CLA	O2D-CGD-CBD	5.07	120.10	111.23
24	B	510	CLA	CMD-C2D-C1D	5.06	133.64	124.73
24	B	513	CLA	O2D-CGD-CBD	5.03	120.03	111.23
26	B	517	BCR	C38-C26-C25	-5.00	119.03	124.48
24	B	514	CLA	O2D-CGD-CBD	5.00	119.96	111.23
24	C	503	CLA	CMD-C2D-C1D	4.98	133.50	124.73
24	D	401	CLA	O2D-CGD-CBD	4.97	119.92	111.23
26	D	405	BCR	C16-C17-C18	-4.96	120.32	127.28
26	C	516	BCR	C4-C5-C6	-4.95	116.01	122.70
32	B	519	C7Z	C35-C34-C33	-4.94	120.34	127.28
24	B	512	CLA	CMD-C2D-C1D	4.92	133.39	124.73
24	C	513	CLA	CMD-C2D-C1D	4.90	133.36	124.73
26	B	518	BCR	C38-C26-C25	-4.90	119.14	124.48
26	B	518	BCR	C33-C5-C6	-4.86	119.18	124.48
26	C	517	BCR	C16-C17-C18	-4.85	120.47	127.28
26	J	101	BCR	C7-C8-C9	-4.85	119.06	126.23
32	B	519	C7Z	C1-C6-C5	-4.84	116.02	122.64
26	J	101	BCR	C38-C26-C25	-4.84	119.20	124.48
26	C	517	BCR	C38-C26-C25	-4.83	119.21	124.48
26	B	518	BCR	C20-C21-C22	-4.80	120.54	127.28
24	B	508	CLA	CMD-C2D-C1D	4.77	133.13	124.73
26	C	516	BCR	C16-C17-C18	-4.77	120.59	127.28
24	A	405	CLA	O2D-CGD-CBD	4.75	119.53	111.23
26	B	518	BCR	C15-C14-C13	-4.73	120.65	127.28
28	B	520	LMG	O7-C10-C11	4.71	121.67	111.48
36	D	406	PL9	C7-C3-C4	4.68	120.76	116.91
32	B	519	C7Z	C18-C5-C6	-4.64	119.42	124.48
26	J	101	BCR	C15-C14-C13	-4.62	120.80	127.28
32	B	519	C7Z	C31-C30-C29	-4.59	120.84	127.28
26	B	517	BCR	C7-C8-C9	-4.55	119.50	126.23
32	B	519	C7Z	C27-C28-C29	-4.55	119.51	126.23
38	H	101	RRX	C1-C6-C5	-4.53	116.45	122.64
38	H	101	RRX	C4-C5-C6	-4.50	116.62	122.70
38	H	101	RRX	C24-C23-C22	-4.50	119.58	126.23
28	C	501	LMG	O7-C10-C11	4.50	121.21	111.48
26	C	516	BCR	C33-C5-C6	-4.50	119.58	124.48
26	B	518	BCR	C16-C17-C18	-4.48	120.99	127.28
32	B	519	C7Z	C38-C25-C26	-4.48	119.59	124.48
26	C	515	BCR	C20-C21-C22	-4.48	120.99	127.28
26	D	405	BCR	C20-C21-C22	-4.47	121.01	127.28
24	C	511	CLA	C1-C2-C3	-4.45	118.90	126.20
24	B	504	CLA	C1-C2-C3	-4.45	118.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	519	C7Z	C7-C8-C9	-4.42	119.70	126.23
31	D	410	LHG	O7-C7-C8	4.41	121.02	111.48
26	B	517	BCR	C4-C5-C6	-4.36	116.82	122.70
26	C	515	BCR	C27-C26-C25	-4.36	116.82	122.70
38	H	101	RRX	C16-C17-C18	-4.33	121.21	127.28
24	D	401	CLA	C1-C2-C3	-4.31	119.13	126.20
26	A	409	BCR	C34-C9-C10	-4.31	115.83	122.82
31	A	414	LHG	O7-C7-C8	4.31	120.80	111.48
33	C	518	DGD	O2G-C1B-C2B	4.30	120.78	111.48
28	A	411	LMG	O7-C10-C11	4.28	120.74	111.48
31	L	101	LHG	O7-C7-C8	4.27	120.71	111.48
38	H	101	RRX	C33-C5-C6	-4.26	119.84	124.48
28	C	522	LMG	O7-C10-C11	4.24	120.65	111.48
26	J	101	BCR	C20-C21-C22	-4.22	121.36	127.28
34	B	522	3PH	O21-C21-C22	4.20	120.57	111.48
26	D	405	BCR	C30-C25-C26	-4.19	116.91	122.64
35	B	523	DGA	OG2-CB1-CB2	4.18	120.51	111.48
24	D	404	CLA	C1-C2-C3	-4.17	119.36	126.20
26	B	518	BCR	C24-C23-C22	-4.17	120.07	126.23
24	C	503	CLA	C1-C2-C3	-4.16	119.39	126.20
26	C	517	BCR	C24-C23-C22	-4.15	120.10	126.23
28	H	102	LMG	O7-C10-C11	4.14	120.44	111.48
24	B	514	CLA	C1-C2-C3	-4.10	119.48	126.20
26	D	405	BCR	C27-C26-C25	-4.10	117.17	122.70
26	B	518	BCR	C4-C5-C6	-4.09	117.17	122.70
26	A	409	BCR	C11-C10-C9	4.08	133.00	127.28
24	A	406	CLA	C1-C2-C3	-4.07	119.52	126.20
28	A	415	LMG	O7-C10-C11	4.05	120.24	111.48
24	A	405	CLA	O2A-C1-C2	4.04	123.65	108.11
33	C	519	DGD	O2G-C1B-C2B	4.03	120.20	111.48
24	C	509	CLA	C1-C2-C3	-4.02	119.62	126.20
35	B	523	DGA	CDB-CCB-CBB	-3.99	80.21	115.25
31	D	408	LHG	O7-C7-C8	3.99	120.10	111.48
28	C	521	LMG	O7-C10-C11	3.97	120.07	111.48
24	B	508	CLA	C1-C2-C3	-3.97	119.70	126.20
33	C	520	DGD	O2G-C1B-C2B	3.97	120.06	111.48
24	C	509	CLA	O2A-C1-C2	3.95	123.32	108.11
28	D	409	LMG	O7-C10-C11	3.95	120.03	111.48
26	D	405	BCR	C33-C5-C6	-3.95	120.18	124.48
26	C	515	BCR	C7-C8-C9	-3.95	120.39	126.23
26	J	101	BCR	C1-C6-C5	-3.92	117.27	122.64
24	B	514	CLA	O2A-C1-C2	3.92	123.20	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	O2A-C1-C2	3.91	123.17	108.11
33	B	521	DGD	O2G-C1B-C2B	3.90	119.93	111.48
26	B	517	BCR	C16-C17-C18	-3.90	121.80	127.28
31	D	407	LHG	O7-C7-C8	3.89	119.89	111.48
24	C	505	CLA	C1-C2-C3	-3.88	119.84	126.20
24	B	513	CLA	C1-C2-C3	-3.88	119.85	126.20
26	D	405	BCR	C15-C14-C13	-3.87	121.85	127.28
26	B	517	BCR	C27-C26-C25	-3.86	117.49	122.70
24	A	406	CLA	O2A-C1-C2	3.84	122.90	108.11
24	A	408	CLA	O2A-C1-C2	3.83	122.86	108.11
26	B	518	BCR	C1-C6-C5	-3.82	117.42	122.64
26	C	516	BCR	C7-C8-C9	-3.81	120.59	126.23
26	C	515	BCR	C4-C5-C6	-3.81	117.55	122.70
26	C	517	BCR	C27-C26-C25	-3.81	117.56	122.70
26	B	517	BCR	C30-C25-C26	-3.81	117.44	122.64
26	B	518	BCR	C11-C10-C9	-3.80	121.95	127.28
24	C	505	CLA	O2A-C1-C2	3.80	122.71	108.11
26	C	515	BCR	C1-C6-C5	-3.80	117.45	122.64
26	A	409	BCR	C27-C26-C25	-3.79	117.58	122.70
24	D	404	CLA	O2A-C1-C2	3.78	122.66	108.11
24	B	508	CLA	O2A-C1-C2	3.78	122.65	108.11
24	C	504	CLA	C1-C2-C3	-3.77	120.01	126.20
24	B	505	CLA	C1-C2-C3	-3.76	120.03	126.20
24	D	401	CLA	O2A-C1-C2	3.75	122.52	108.11
26	D	405	BCR	C38-C26-C25	-3.73	120.41	124.48
24	B	511	CLA	C1-C2-C3	-3.73	120.08	126.20
38	H	101	RRX	C30-C25-C26	-3.73	117.54	122.64
26	D	405	BCR	C1-C6-C5	-3.72	117.55	122.64
26	C	515	BCR	C38-C26-C25	-3.72	120.43	124.48
24	B	505	CLA	O2A-C1-C2	3.71	122.40	108.11
24	B	515	CLA	C1-C2-C3	-3.71	120.11	126.20
24	B	507	CLA	O2A-C1-C2	3.71	122.38	108.11
24	C	511	CLA	O2A-C1-C2	3.71	122.37	108.11
38	H	101	RRX	C38-C26-C25	-3.70	120.44	124.48
26	C	515	BCR	C15-C14-C13	-3.70	122.09	127.28
36	D	406	PL9	C7-C3-C2	-3.68	119.05	123.39
24	C	504	CLA	O2A-C1-C2	3.67	122.24	108.11
24	C	507	CLA	O2A-C1-C2	3.67	122.24	108.11
26	C	516	BCR	C27-C26-C25	-3.67	117.75	122.70
26	B	517	BCR	C23-C24-C25	-3.67	117.20	127.00
26	A	409	BCR	C12-C13-C14	3.65	124.75	119.01
24	B	501	CLA	O2A-C1-C2	3.65	122.15	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	516	CLA	C1-C2-C3	-3.64	120.24	126.20
24	C	512	CLA	C1-C2-C3	-3.64	120.24	126.20
26	C	516	BCR	C23-C24-C25	-3.63	117.29	127.00
24	C	508	CLA	O2A-C1-C2	3.63	122.08	108.11
24	B	513	CLA	O2A-C1-C2	3.60	121.96	108.11
24	D	403	CLA	O2A-C1-C2	3.59	121.92	108.11
24	C	512	CLA	O2A-C1-C2	3.58	121.87	108.11
24	D	403	CLA	C1-C2-C3	-3.57	120.34	126.20
24	B	504	CLA	O2A-C1-C2	3.57	121.85	108.11
24	C	506	CLA	C1-C2-C3	-3.56	120.37	126.20
24	B	511	CLA	O2A-C1-C2	3.54	121.74	108.11
24	C	506	CLA	O2A-C1-C2	3.54	121.74	108.11
24	B	516	CLA	O2A-C1-C2	3.54	121.74	108.11
26	C	517	BCR	C4-C5-C6	-3.54	117.92	122.70
26	D	405	BCR	C4-C5-C6	-3.54	117.92	122.70
24	C	502	CLA	C1-C2-C3	-3.51	120.44	126.20
24	B	509	CLA	O2A-C1-C2	3.51	121.60	108.11
24	C	508	CLA	C1-C2-C3	-3.47	120.51	126.20
24	B	501	CLA	C1-C2-C3	-3.46	120.53	126.20
24	B	503	CLA	O2A-C1-C2	3.44	121.35	108.11
24	D	403	CLA	C3B-C4B-NB	-3.43	107.46	110.53
24	B	510	CLA	O2A-C1-C2	3.43	121.32	108.11
26	A	409	BCR	C4-C5-C6	-3.43	118.07	122.70
24	B	515	CLA	O2A-C1-C2	3.42	121.29	108.11
25	A	407	PHO	C2B-C1B-NB	-3.38	106.99	109.43
25	D	402	PHO	C2B-C1B-NB	-3.38	106.99	109.43
26	C	515	BCR	C11-C10-C9	-3.37	122.55	127.28
26	C	517	BCR	C1-C6-C5	-3.35	118.05	122.64
26	C	515	BCR	C33-C5-C6	-3.35	120.83	124.48
24	C	512	CLA	CMA-C3A-C4A	3.35	120.77	111.77
26	B	518	BCR	C8-C7-C6	-3.34	118.06	127.00
25	D	402	PHO	O1D-CGD-CBD	3.33	129.78	124.72
24	C	502	CLA	O2A-C1-C2	3.33	120.91	108.11
26	D	405	BCR	C11-C10-C9	-3.32	122.62	127.28
24	C	510	CLA	O2A-C1-C2	3.32	120.88	108.11
38	H	101	RRX	C8-C7-C6	-3.30	118.18	127.00
26	C	516	BCR	C20-C21-C22	-3.29	122.66	127.28
26	C	517	BCR	C30-C25-C26	-3.28	118.16	122.64
24	A	408	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
24	B	512	CLA	C1-C2-C3	-3.26	120.85	126.20
26	A	409	BCR	C23-C24-C25	-3.26	118.29	127.00
24	C	507	CLA	C1-C2-C3	-3.23	120.90	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	405	BCR	C8-C7-C6	-3.23	118.36	127.00
26	D	405	BCR	C24-C23-C22	-3.22	121.47	126.23
24	B	510	CLA	C1-C2-C3	-3.22	120.93	126.20
26	D	405	BCR	C7-C8-C9	-3.21	121.48	126.23
24	B	509	CLA	C1-C2-C3	-3.21	120.94	126.20
26	B	517	BCR	C21-C20-C19	-3.20	113.92	123.20
26	C	517	BCR	C15-C14-C13	-3.20	122.79	127.28
26	C	516	BCR	C21-C20-C19	-3.19	113.96	123.20
26	C	515	BCR	C38-C26-C27	3.16	120.33	113.60
26	C	517	BCR	C15-C16-C17	-3.15	117.08	123.52
26	D	405	BCR	C23-C24-C25	-3.14	118.61	127.00
24	A	405	CLA	C1-C2-C3	-3.14	121.06	126.20
26	A	409	BCR	C1-C6-C5	-3.12	118.37	122.64
26	C	517	BCR	C2-C1-C6	3.12	114.97	110.44
26	J	101	BCR	C29-C30-C25	3.11	114.96	110.44
24	B	504	CLA	CMA-C3A-C4A	3.11	120.13	111.77
24	B	503	CLA	C1-C2-C3	-3.10	121.11	126.20
26	A	409	BCR	C16-C15-C14	-3.10	117.17	123.52
26	B	517	BCR	C15-C16-C17	-3.10	117.17	123.52
26	B	517	BCR	C1-C6-C5	-3.10	118.41	122.64
26	C	516	BCR	C8-C7-C6	-3.09	118.74	127.00
25	D	402	PHO	CMB-C2B-C3B	3.09	130.86	124.68
24	B	512	CLA	O2A-C1-C2	3.08	119.95	108.11
28	A	411	LMG	C8-O7-C10	-3.07	110.45	117.80
33	C	519	DGD	O1G-C1A-C2A	3.05	121.14	111.83
33	C	518	DGD	O1G-C1A-C2A	3.05	121.14	111.83
38	H	101	RRX	C23-C24-C25	-3.04	118.87	127.00
31	D	410	LHG	O8-C23-C24	3.03	121.08	111.83
26	A	409	BCR	C38-C26-C25	-3.03	121.18	124.48
24	B	515	CLA	C2C-C1C-NC	3.03	113.16	109.98
24	C	504	CLA	CMA-C3A-C4A	3.02	119.90	111.77
32	B	519	C7Z	C18-C5-C4	3.02	119.97	114.42
31	L	101	LHG	O8-C23-C24	3.00	121.00	111.83
25	A	407	PHO	O1D-CGD-CBD	3.00	129.28	124.72
24	C	506	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
31	D	407	LHG	O8-C23-C24	2.99	120.95	111.83
25	D	402	PHO	O2D-CGD-O1D	-2.99	118.04	123.85
28	H	102	LMG	O8-C28-C29	2.98	120.93	111.83
26	C	515	BCR	C30-C25-C26	-2.98	118.56	122.64
33	C	519	DGD	C1D-O6D-C5D	2.98	119.54	113.72
24	B	502	CLA	O2A-CGA-CBA	2.98	120.91	111.83
31	D	408	LHG	O8-C23-C24	2.98	120.91	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	406	PL9	C7-C8-C9	-2.97	121.71	126.83
24	D	401	CLA	O2A-CGA-CBA	2.96	120.88	111.83
32	B	519	C7Z	C8-C7-C6	-2.95	119.11	127.00
24	C	502	CLA	C3B-C4B-NB	-2.95	107.89	110.53
24	B	516	CLA	C2C-C1C-NC	2.95	113.08	109.98
24	B	507	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	C	513	CLA	O2A-C1-C2	2.94	119.44	108.11
33	C	520	DGD	O1G-C1A-C2A	2.94	120.80	111.83
24	B	510	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
26	C	516	BCR	C33-C5-C4	2.93	119.85	113.60
24	C	513	CLA	C1-C2-C3	-2.93	121.40	126.20
24	C	506	CLA	C3B-C4B-NB	-2.93	107.92	110.53
26	J	101	BCR	C30-C25-C26	-2.92	118.64	122.64
28	B	520	LMG	O8-C28-C29	2.92	120.74	111.83
24	C	508	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
24	C	510	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	C	510	CLA	C2C-C1C-NC	2.92	113.04	109.98
24	C	508	CLA	C2C-C1C-NC	2.90	113.03	109.98
32	B	519	C7Z	C38-C25-C24	2.90	119.75	114.42
24	C	507	CLA	C2C-C1C-NC	2.89	113.02	109.98
24	B	505	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	C	511	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
24	B	504	CLA	C2C-C1C-NC	2.88	113.01	109.98
33	C	519	DGD	O6D-C5D-C6D	2.88	112.40	106.69
24	A	408	CLA	C1-C2-C3	-2.88	121.48	126.20
25	A	407	PHO	O2D-CGD-O1D	-2.88	118.25	123.85
38	H	101	RRX	C11-C12-C13	-2.87	118.48	126.36
24	A	408	CLA	C2C-C1C-NC	2.87	113.00	109.98
24	B	512	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
24	B	501	CLA	CMA-C3A-C4A	2.86	119.46	111.77
26	B	517	BCR	C38-C26-C27	2.86	119.69	113.60
31	L	101	LHG	C5-O7-C7	-2.86	110.96	117.80
24	C	503	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	B	504	CLA	O2A-CGA-CBA	2.85	120.52	111.83
24	B	513	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
26	C	517	BCR	C33-C5-C6	-2.85	121.38	124.48
24	B	513	CLA	C2C-C1C-NC	2.84	112.97	109.98
24	B	502	CLA	O2A-C1-C2	2.84	119.03	108.11
36	D	406	PL9	C22-C23-C24	-2.83	121.14	127.62
24	C	513	CLA	C2C-C1C-NC	2.83	112.96	109.98
24	C	513	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
26	B	518	BCR	C27-C26-C25	-2.83	118.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	501	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
24	D	404	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
24	B	501	CLA	C3B-C4B-NB	-2.82	108.01	110.53
26	C	517	BCR	C23-C24-C25	-2.82	119.46	127.00
26	C	517	BCR	C21-C20-C19	-2.82	115.03	123.20
24	B	502	CLA	C1C-C2C-C3C	-2.82	104.02	106.98
28	C	521	LMG	O8-C28-C29	2.81	120.41	111.83
24	D	403	CLA	O2A-CGA-CBA	2.81	120.40	111.83
26	J	101	BCR	C27-C26-C25	-2.81	118.91	122.70
31	A	414	LHG	C5-O7-C7	-2.81	111.08	117.80
26	D	405	BCR	C33-C5-C4	2.80	119.58	113.60
26	C	516	BCR	C15-C16-C17	-2.80	117.78	123.52
24	A	408	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
24	B	507	CLA	C1-C2-C3	-2.80	121.61	126.20
24	C	505	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
38	H	101	RRX	C7-C8-C9	-2.79	122.10	126.23
31	A	414	LHG	O8-C23-C24	2.79	120.35	111.83
24	B	506	CLA	O2A-C1-C2	2.79	118.83	108.11
24	B	505	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
24	C	513	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	B	517	BCR	C8-C7-C6	-2.78	119.58	127.00
26	B	518	BCR	C29-C30-C25	2.77	114.46	110.44
24	B	503	CLA	O2A-CGA-CBA	2.77	120.27	111.83
24	B	510	CLA	C2C-C1C-NC	2.76	112.89	109.98
26	B	517	BCR	C20-C21-C22	-2.76	123.40	127.28
24	B	514	CLA	C1-O2A-CGA	2.76	123.33	116.65
26	B	518	BCR	C23-C24-C25	-2.76	119.63	127.00
24	D	401	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
26	D	405	BCR	C10-C11-C12	-2.76	115.22	123.20
24	A	408	CLA	CAA-C2A-C3A	-2.75	105.56	113.00
24	B	510	CLA	C3B-C4B-NB	-2.75	108.07	110.53
26	C	515	BCR	C16-C15-C14	-2.75	117.90	123.52
24	B	510	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
24	C	512	CLA	C2C-C1C-NC	2.74	112.86	109.98
24	C	510	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
24	B	504	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
24	C	502	CLA	CMA-C3A-C4A	2.74	119.13	111.77
24	B	501	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
24	B	516	CLA	C3B-C4B-NB	-2.73	108.09	110.53
27	A	410	SQD	O7-S-C6	-2.72	102.69	106.76
24	B	504	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
26	J	101	BCR	C4-C5-C6	-2.72	119.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	501	CLA	O2A-CGA-CBA	2.72	120.12	111.83
28	D	409	LMG	O8-C28-C29	2.72	120.12	111.83
24	C	505	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
26	J	101	BCR	C38-C26-C27	2.72	119.39	113.60
24	C	503	CLA	C2C-C1C-NC	2.71	112.83	109.98
24	C	508	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
24	C	511	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	D	403	CLA	C1D-ND-C4D	-2.70	104.42	106.31
24	B	508	CLA	CMA-C3A-C4A	2.70	119.03	111.77
24	C	514	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	B	510	CLA	C4B-CHC-C1C	2.70	132.59	126.25
25	A	407	PHO	CMB-C2B-C3B	2.69	130.06	124.68
24	B	516	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
24	B	512	CLA	C2C-C1C-NC	2.69	112.81	109.98
24	D	401	CLA	C2C-C1C-NC	2.69	112.81	109.98
26	A	409	BCR	C30-C25-C26	-2.69	118.96	122.64
24	A	406	CLA	CMA-C3A-C4A	2.69	118.99	111.77
24	B	510	CLA	CMA-C3A-C4A	2.69	118.99	111.77
24	B	514	CLA	CMA-C3A-C4A	2.68	118.98	111.77
24	B	508	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
35	B	523	DGA	OG1-CA1-CA2	2.68	120.00	111.83
34	B	522	3PH	O31-C31-C32	2.68	120.00	111.83
24	B	515	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
24	C	514	CLA	CMA-C3A-C4A	2.67	118.96	111.77
24	A	406	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	C	507	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	D	404	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
24	B	508	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
24	C	511	CLA	C2C-C1C-NC	2.67	112.78	109.98
26	B	518	BCR	C7-C8-C9	-2.67	122.29	126.23
26	A	409	BCR	C29-C30-C25	2.67	114.31	110.44
32	B	519	C7Z	C28-C27-C26	-2.67	119.88	127.00
24	B	511	CLA	C2C-C1C-NC	2.65	112.77	109.98
24	A	408	CLA	CMA-C3A-C4A	2.65	118.91	111.77
26	B	517	BCR	C24-C23-C22	-2.65	122.31	126.23
32	B	519	C7Z	C4-C5-C6	-2.65	115.31	120.76
24	C	512	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
24	B	514	CLA	C2C-C1C-NC	2.65	112.77	109.98
24	B	509	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
33	B	521	DGD	O1G-C1A-C2A	2.64	119.89	111.83
24	B	509	CLA	C2C-C1C-NC	2.64	112.75	109.98
24	B	512	CLA	C1C-C2C-C3C	-2.64	104.21	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	404	CLA	C2C-C1C-NC	2.63	112.75	109.98
24	B	505	CLA	C4B-CHC-C1C	2.63	132.43	126.25
24	B	514	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
24	C	513	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
24	A	406	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	B	508	CLA	C2C-C1C-NC	2.62	112.73	109.98
26	B	518	BCR	C15-C16-C17	-2.62	118.17	123.52
24	B	505	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
24	B	507	CLA	C2C-C1C-NC	2.61	112.73	109.98
24	C	505	CLA	C2C-C1C-NC	2.61	112.73	109.98
24	B	511	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
24	B	502	CLA	C2C-C1C-NC	2.61	112.72	109.98
24	C	502	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
26	C	517	BCR	C33-C5-C4	2.61	119.15	113.60
24	C	509	CLA	C2C-C1C-NC	2.60	112.72	109.98
24	B	504	CLA	CHA-C4D-ND	2.60	137.92	132.55
24	A	406	CLA	C2C-C1C-NC	2.60	112.72	109.98
26	A	409	BCR	C35-C13-C14	-2.60	118.60	122.82
24	B	506	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
24	B	513	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
33	C	520	DGD	O3G-C3G-C2G	-2.59	104.51	110.82
36	D	406	PL9	C27-C28-C29	-2.59	121.69	127.62
24	C	503	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
24	C	514	CLA	C2C-C1C-NC	2.59	112.70	109.98
24	C	509	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
24	B	505	CLA	C2C-C1C-NC	2.58	112.70	109.98
24	B	503	CLA	CMA-C3A-C4A	2.58	118.72	111.77
24	C	503	CLA	CMA-C3A-C4A	2.58	118.72	111.77
24	C	514	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
26	D	405	BCR	C38-C26-C27	2.58	119.10	113.60
26	C	515	BCR	C8-C7-C6	-2.58	120.10	127.00
24	B	501	CLA	C2C-C1C-NC	2.58	112.69	109.98
24	B	507	CLA	CHA-C4D-ND	2.58	137.87	132.55
24	B	502	CLA	CMA-C3A-C4A	2.58	118.69	111.77
24	C	502	CLA	C4B-CHC-C1C	2.57	132.30	126.25
26	D	405	BCR	C16-C15-C14	-2.57	118.25	123.52
24	B	502	CLA	C1D-ND-C4D	-2.57	104.51	106.31
24	B	509	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
24	B	506	CLA	C2C-C1C-NC	2.57	112.68	109.98
25	D	402	PHO	C1-C2-C3	-2.57	121.99	126.20
24	B	511	CLA	O2A-CGA-CBA	2.57	119.67	111.83
24	B	501	CLA	C4B-CHC-C1C	2.57	132.29	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	503	CLA	CHA-C4D-ND	2.57	137.84	132.55
24	C	509	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
24	C	511	CLA	O2A-CGA-CBA	2.56	119.64	111.83
24	C	502	CLA	CMD-C2D-C3D	-2.56	121.83	127.69
24	C	506	CLA	O2A-CGA-CBA	2.56	119.63	111.83
24	C	502	CLA	C1C-C2C-C3C	-2.55	104.29	106.98
24	B	515	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
24	C	502	CLA	C1D-ND-C4D	-2.55	104.52	106.31
24	C	502	CLA	O2A-CGA-CBA	2.55	119.61	111.83
26	A	409	BCR	C38-C26-C27	2.55	119.03	113.60
28	C	501	LMG	C8-O7-C10	-2.54	111.71	117.80
24	C	504	CLA	C1C-C2C-C3C	-2.54	104.30	106.98
24	B	506	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
26	J	101	BCR	C8-C7-C6	-2.54	120.22	127.00
24	D	404	CLA	CMA-C3A-C4A	2.53	118.59	111.77
26	C	515	BCR	C33-C5-C4	2.53	118.99	113.60
28	A	411	LMG	O8-C28-C29	2.53	119.54	111.83
24	C	508	CLA	CMA-C3A-C4A	2.53	118.56	111.77
24	B	514	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	C	507	CLA	C3B-C4B-NB	-2.52	108.28	110.53
32	B	519	C7Z	C15-C35-C34	-2.52	118.36	123.52
24	B	505	CLA	C1D-ND-C4D	-2.52	104.55	106.31
24	C	504	CLA	C4B-CHC-C1C	2.51	132.16	126.25
39	J	102	LMU	C1B-O1B-C4'	-2.51	112.02	117.98
26	B	518	BCR	C30-C25-C26	-2.51	119.20	122.64
24	C	511	CLA	CHD-C1D-ND	-2.51	121.27	124.80
24	B	501	CLA	CHA-C4D-ND	2.51	137.73	132.55
24	C	502	CLA	CHD-C1D-ND	-2.51	121.27	124.80
24	B	502	CLA	C4B-CHC-C1C	2.51	132.15	126.25
24	D	403	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	B	507	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
24	B	507	CLA	CMA-C3A-C4A	2.51	118.51	111.77
24	C	506	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
24	B	506	CLA	CHA-C4D-ND	2.50	137.72	132.55
24	C	506	CLA	CHA-C4D-ND	2.50	137.71	132.55
26	B	518	BCR	C33-C5-C4	2.50	118.93	113.60
38	H	101	RRX	C38-C26-C27	2.50	119.02	114.42
24	D	403	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
24	C	505	CLA	CHD-C1D-ND	-2.50	121.29	124.80
24	C	507	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
24	C	507	CLA	O2A-CGA-CBA	2.49	119.44	111.83
24	D	401	CLA	CHD-C1D-ND	-2.49	121.29	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	CHA-C4D-ND	2.49	137.68	132.55
24	B	503	CLA	C2C-C1C-NC	2.48	112.59	109.98
24	B	503	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
24	C	512	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	C	504	CLA	C3B-C4B-NB	-2.48	108.31	110.53
24	B	501	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
24	C	510	CLA	C4B-CHC-C1C	2.48	132.08	126.25
27	M	101	SQD	O7-S-C6	-2.48	103.06	106.76
24	C	509	CLA	CAA-C2A-C3A	-2.48	106.31	113.00
24	A	408	CLA	C1D-ND-C4D	-2.47	104.58	106.31
31	D	408	LHG	C5-O7-C7	-2.47	111.88	117.80
24	C	511	CLA	CHA-C4D-ND	2.47	137.65	132.55
24	C	504	CLA	O2A-CGA-CBA	2.47	119.37	111.83
24	B	503	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
24	B	516	CLA	CHA-C4D-ND	2.47	137.64	132.55
24	C	508	CLA	CHA-C4D-ND	2.47	137.64	132.55
24	D	403	CLA	CHA-C4D-ND	2.47	137.64	132.55
26	B	518	BCR	C38-C26-C27	2.47	118.85	113.60
24	B	502	CLA	CHD-C1D-ND	-2.47	121.33	124.80
28	A	415	LMG	O8-C28-C29	2.47	119.35	111.83
24	C	509	CLA	CMA-C3A-C4A	2.46	118.39	111.77
24	B	505	CLA	CHA-C4D-ND	2.46	137.63	132.55
24	C	506	CLA	C2C-C1C-NC	2.46	112.57	109.98
24	D	404	CLA	C3B-C4B-NB	-2.46	108.33	110.53
26	C	516	BCR	C30-C25-C26	-2.46	119.28	122.64
24	B	505	CLA	O2A-CGA-CBA	2.46	119.33	111.83
24	D	401	CLA	C4B-CHC-C1C	2.46	132.03	126.25
24	C	504	CLA	CHA-C4D-ND	2.46	137.62	132.55
26	C	515	BCR	C23-C24-C25	-2.46	120.44	127.00
24	C	502	CLA	CHA-C4D-ND	2.45	137.61	132.55
24	D	403	CLA	C4B-CHC-C1C	2.45	132.02	126.25
24	C	504	CLA	C2C-C1C-NC	2.45	112.56	109.98
24	B	502	CLA	C3B-C4B-NB	-2.45	108.34	110.53
24	B	504	CLA	C4B-CHC-C1C	2.45	132.00	126.25
24	B	516	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
24	C	505	CLA	CMA-C3A-C4A	2.44	118.34	111.77
24	C	506	CLA	CMA-C3A-C4A	2.44	118.33	111.77
28	C	501	LMG	C7-O1-C1	-2.44	108.57	113.80
24	B	514	CLA	CHA-C4D-ND	2.44	137.57	132.55
33	C	520	DGD	C2G-O2G-C1B	-2.44	111.97	117.80
24	C	507	CLA	CHA-C4D-ND	2.43	137.57	132.55
24	C	504	CLA	O2D-CGD-O1D	-2.43	119.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	513	CLA	CHD-C1D-ND	-2.43	121.38	124.80
24	B	502	CLA	C1-C2-C3	-2.43	122.21	126.20
24	C	503	CLA	C4B-CHC-C1C	2.43	131.96	126.25
31	D	410	LHG	C5-O7-C7	-2.43	111.98	117.80
24	C	509	CLA	C4B-CHC-C1C	2.43	131.96	126.25
24	B	506	CLA	CMA-C3A-C4A	2.43	118.30	111.77
24	C	510	CLA	CHD-C1D-ND	-2.43	121.39	124.80
24	B	503	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
24	C	508	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	B	506	CLA	CHD-C1D-ND	-2.42	121.40	124.80
24	B	503	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	A	406	CLA	C4B-CHC-C1C	2.42	131.93	126.25
24	B	503	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
24	B	509	CLA	O2A-CGA-CBA	2.42	119.20	111.83
24	B	513	CLA	CHA-C4D-ND	2.42	137.53	132.55
24	A	405	CLA	C4B-CHC-C1C	2.41	131.92	126.25
24	B	516	CLA	C4B-CHC-C1C	2.41	131.92	126.25
38	H	101	RRX	C20-C19-C18	-2.41	119.75	126.36
24	B	504	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
24	C	514	CLA	CHA-C4D-ND	2.41	137.52	132.55
24	D	401	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
24	D	404	CLA	CHD-C1D-ND	-2.40	121.42	124.80
28	C	501	LMG	O8-C28-C29	2.40	119.16	111.83
26	A	409	BCR	C21-C20-C19	-2.40	116.25	123.20
24	B	509	CLA	C4B-CHC-C1C	2.40	131.88	126.25
24	A	405	CLA	CHA-C4D-ND	2.40	137.49	132.55
24	B	516	CLA	CHD-C1D-ND	-2.39	121.43	124.80
26	J	101	BCR	C11-C12-C13	-2.39	119.80	126.36
24	C	506	CLA	C4B-CHC-C1C	2.39	131.87	126.25
24	A	408	CLA	C4B-CHC-C1C	2.39	131.86	126.25
26	A	409	BCR	C1-C6-C7	2.39	122.12	115.65
24	C	507	CLA	C4B-CHC-C1C	2.38	131.85	126.25
24	A	405	CLA	C1C-C2C-C3C	-2.38	104.47	106.98
24	A	406	CLA	CHD-C1D-ND	-2.38	121.45	124.80
24	B	511	CLA	CMA-C3A-C4A	2.38	118.17	111.77
24	D	404	CLA	CHA-C4D-ND	2.38	137.46	132.55
24	A	406	CLA	CHA-C4D-ND	2.38	137.46	132.55
24	D	401	CLA	CHA-C4D-ND	2.38	137.45	132.55
24	A	405	CLA	C1D-ND-C4D	-2.38	104.64	106.31
24	B	511	CLA	C1D-ND-C4D	-2.38	104.64	106.31
24	C	504	CLA	C1D-ND-C4D	-2.37	104.65	106.31
24	B	510	CLA	CHA-C4D-ND	2.37	137.45	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	CHA-C4D-ND	2.37	137.44	132.55
24	B	502	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
24	C	503	CLA	CHA-C4D-ND	2.37	137.44	132.55
32	B	519	C7Z	C21-C26-C25	-2.37	119.40	122.64
24	B	503	CLA	C4B-CHC-C1C	2.37	131.81	126.25
24	C	511	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
24	C	514	CLA	C4B-CHC-C1C	2.37	131.81	126.25
24	C	513	CLA	CHA-C4D-ND	2.36	137.43	132.55
24	A	408	CLA	O2A-CGA-CBA	2.36	119.04	111.83
24	A	406	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	B	515	CLA	CHA-C4D-ND	2.36	137.42	132.55
24	A	405	CLA	C2C-C1C-NC	2.36	112.46	109.98
24	C	510	CLA	CHA-C4D-ND	2.36	137.41	132.55
24	B	516	CLA	O2A-CGA-CBA	2.36	119.02	111.83
24	B	506	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
24	C	509	CLA	O2A-CGA-CBA	2.35	119.01	111.83
24	B	507	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
38	H	101	RRX	C15-C16-C17	-2.35	118.71	123.52
24	B	507	CLA	O2A-CGA-CBA	2.35	119.00	111.83
24	B	511	CLA	C4B-CHC-C1C	2.35	131.78	126.25
24	C	512	CLA	C4B-CHC-C1C	2.35	131.77	126.25
24	C	510	CLA	C1-C2-C3	-2.35	122.35	126.20
24	B	512	CLA	C4B-CHC-C1C	2.35	131.77	126.25
36	D	406	PL9	O1-C4-C3	-2.35	118.26	120.73
24	C	502	CLA	C2C-C1C-NC	2.34	112.44	109.98
24	B	512	CLA	CHA-C4D-ND	2.34	137.39	132.55
24	C	510	CLA	O2A-CGA-CBA	2.34	118.98	111.83
24	C	512	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
36	D	406	PL9	C20-C19-C21	2.34	119.29	115.23
24	B	505	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
24	C	507	CLA	CMA-C3A-C4A	2.33	118.05	111.77
28	C	521	LMG	C8-O7-C10	-2.33	112.21	117.80
24	D	404	CLA	C4B-CHC-C1C	2.33	131.73	126.25
38	H	101	RRX	C35-C13-C14	-2.33	119.04	122.82
24	B	513	CLA	O2A-CGA-CBA	2.33	118.94	111.83
24	A	405	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
24	C	508	CLA	C4B-CHC-C1C	2.33	131.72	126.25
24	B	512	CLA	O2A-CGA-CBA	2.33	118.93	111.83
24	B	509	CLA	CHA-C4D-ND	2.32	137.34	132.55
24	C	513	CLA	C4B-CHC-C1C	2.32	131.71	126.25
24	C	512	CLA	CHD-C1D-ND	-2.32	121.53	124.80
24	D	401	CLA	C6-C5-C3	-2.32	107.81	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	505	CLA	CHD-C1D-ND	-2.32	121.53	124.80
24	B	508	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	B	514	CLA	C4B-CHC-C1C	2.32	131.70	126.25
38	H	101	RRX	C34-C9-C10	-2.32	119.06	122.82
24	B	511	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
24	B	515	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	B	507	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	B	511	CLA	CHA-C4D-ND	2.31	137.32	132.55
24	C	511	CLA	C3B-C4B-NB	-2.31	108.47	110.53
24	C	512	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
24	B	502	CLA	CHA-C4D-ND	2.31	137.32	132.55
24	B	514	CLA	CHD-C1D-ND	-2.31	121.56	124.80
24	B	507	CLA	C4B-CHC-C1C	2.31	131.67	126.25
24	C	514	CLA	CHD-C1D-ND	-2.31	121.56	124.80
36	D	406	PL9	O2-C1-C6	2.30	124.15	120.48
24	C	513	CLA	O2A-CGA-CBA	2.30	118.86	111.83
24	B	510	CLA	C1D-ND-C4D	-2.30	104.70	106.31
24	C	503	CLA	C1-O2A-CGA	2.30	122.22	116.65
24	D	401	CLA	CMA-C3A-C4A	2.30	117.95	111.77
24	D	401	CLA	C1-O2A-CGA	2.30	122.21	116.65
26	J	101	BCR	C23-C24-C25	-2.30	120.86	127.00
24	D	403	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
36	D	406	PL9	C37-C38-C39	-2.30	122.37	127.62
24	C	512	CLA	O2A-CGA-CBA	2.29	118.83	111.83
24	C	505	CLA	C4B-CHC-C1C	2.29	131.64	126.25
24	B	508	CLA	CHA-C4D-ND	2.29	137.28	132.55
24	B	506	CLA	O2A-CGA-CBA	2.29	118.81	111.83
27	M	101	SQD	O3-C3-C2	-2.28	104.99	110.38
24	B	511	CLA	CHD-C1D-ND	-2.28	121.59	124.80
26	C	516	BCR	C1-C6-C7	2.28	121.84	115.65
24	D	403	CLA	CHD-C1D-ND	-2.28	121.59	124.80
24	A	405	CLA	O2A-CGA-CBA	2.28	118.78	111.83
24	B	509	CLA	C3B-C4B-NB	-2.28	108.50	110.53
24	B	508	CLA	C1D-ND-C4D	-2.27	104.72	106.31
24	C	504	CLA	CHD-C1D-ND	-2.27	121.60	124.80
24	A	406	CLA	O2A-CGA-CBA	2.27	118.77	111.83
24	B	506	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
24	C	509	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
24	B	512	CLA	C3B-C4B-NB	-2.27	108.51	110.53
36	D	406	PL9	C12-C13-C14	-2.26	122.44	127.62
24	C	510	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
24	A	406	CLA	C1D-ND-C4D	-2.26	104.72	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	CHD-C1D-ND	-2.26	121.62	124.80
25	A	407	PHO	C1-C2-C3	-2.26	122.50	126.20
27	A	410	SQD	O3-C3-C2	-2.26	105.06	110.38
24	B	515	CLA	CHD-C1D-ND	-2.26	121.63	124.80
24	C	511	CLA	C4B-CHC-C1C	2.25	131.55	126.25
26	A	409	BCR	C24-C23-C22	-2.25	122.90	126.23
24	C	513	CLA	CHD-C1D-ND	-2.25	121.63	124.80
26	C	515	BCR	C10-C11-C12	-2.25	116.69	123.20
28	A	415	LMG	C8-O7-C10	-2.24	112.42	117.80
24	D	401	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
24	B	507	CLA	C3B-C4B-NB	-2.24	108.53	110.53
38	H	101	RRX	C27-C26-C25	-2.24	116.16	120.76
24	C	510	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
26	J	101	BCR	C16-C15-C14	-2.24	118.94	123.52
24	B	515	CLA	C4B-CHC-C1C	2.24	131.51	126.25
24	B	509	CLA	C2D-C1D-ND	2.24	112.34	110.13
24	B	508	CLA	C4B-CHC-C1C	2.24	131.51	126.25
24	B	513	CLA	C4B-CHC-C1C	2.24	131.50	126.25
24	A	408	CLA	CHA-C4D-ND	2.23	137.16	132.55
26	C	515	BCR	C20-C19-C18	-2.23	120.24	126.36
24	B	510	CLA	CHD-C1D-ND	-2.23	121.66	124.80
24	B	501	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
24	A	408	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
24	C	514	CLA	C1D-ND-C4D	-2.23	104.75	106.31
24	B	515	CLA	CMA-C3A-C4A	2.22	117.75	111.77
24	B	514	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
24	C	509	CLA	CHA-C1A-NA	-2.22	121.36	126.39
24	B	512	CLA	CMA-C3A-C4A	2.22	117.74	111.77
24	C	507	CLA	CHD-C1D-ND	-2.22	121.68	124.80
24	C	504	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
26	C	516	BCR	C37-C22-C23	2.22	121.47	118.09
24	C	502	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
24	C	514	CLA	C3B-C4B-NB	-2.21	108.56	110.53
26	A	409	BCR	C7-C6-C5	-2.21	116.47	121.56
24	C	505	CLA	O2A-CGA-CBA	2.21	118.57	111.83
24	B	516	CLA	CHA-C1A-NA	-2.21	121.39	126.39
24	B	506	CLA	C4B-CHC-C1C	2.21	131.44	126.25
24	C	503	CLA	C6-C5-C3	-2.21	108.09	113.47
26	C	516	BCR	C11-C12-C13	-2.21	120.31	126.36
24	B	502	CLA	C2D-C1D-ND	2.21	112.31	110.13
24	B	510	CLA	C2D-C1D-ND	2.20	112.31	110.13
24	B	506	CLA	C3B-C4B-NB	-2.20	108.56	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
24	C	507	CLA	CHA-C1A-NA	-2.20	121.41	126.39
24	D	401	CLA	C1D-ND-C4D	-2.20	104.77	106.31
26	B	517	BCR	C37-C22-C23	2.20	121.45	118.09
32	B	519	C7Z	C11-C12-C13	-2.20	120.34	126.36
24	C	509	CLA	C3B-C4B-NB	-2.20	108.57	110.53
24	A	406	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
24	B	508	CLA	C1-O2A-CGA	2.20	121.97	116.65
24	B	504	CLA	CHA-C1A-NA	-2.19	121.42	126.39
24	A	405	CLA	CMA-C3A-C4A	2.19	117.67	111.77
24	A	406	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
25	D	402	PHO	O2A-CGA-O1A	-2.19	118.15	123.63
24	A	405	CLA	CHD-C1D-ND	-2.19	121.72	124.80
24	B	509	CLA	C1D-ND-C4D	-2.18	104.78	106.31
24	B	509	CLA	CHD-C1D-ND	-2.18	121.73	124.80
24	B	511	CLA	C3B-C4B-NB	-2.18	108.58	110.53
24	B	514	CLA	C3B-C4B-NB	-2.18	108.58	110.53
24	B	515	CLA	CHA-C1A-NA	-2.18	121.45	126.39
24	C	513	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
24	C	506	CLA	C1D-ND-C4D	-2.18	104.78	106.31
24	C	503	CLA	C3B-C4B-NB	-2.18	108.58	110.53
26	C	516	BCR	C24-C23-C22	-2.18	123.01	126.23
24	C	512	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
24	B	506	CLA	C1-O2A-CGA	2.18	121.92	116.65
24	C	503	CLA	C2D-C1D-ND	2.18	112.28	110.13
24	C	511	CLA	C1D-ND-C4D	-2.17	104.79	106.31
24	B	514	CLA	C1D-ND-C4D	-2.17	104.79	106.31
24	B	507	CLA	C1-O2A-CGA	2.17	121.90	116.65
24	C	508	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
28	C	522	LMG	C8-O7-C10	-2.17	112.61	117.80
24	C	510	CLA	CMA-C3A-C4A	2.17	117.59	111.77
24	A	405	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	B	516	CLA	CMA-C3A-C4A	2.16	117.58	111.77
31	D	410	LHG	O7-C7-O9	-2.16	118.65	123.70
24	D	404	CLA	O2A-CGA-CBA	2.16	118.42	111.83
24	B	502	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
31	D	407	LHG	C5-O7-C7	-2.16	112.63	117.80
24	D	403	CLA	C2D-C1D-ND	2.16	112.26	110.13
24	C	513	CLA	C6-C5-C3	-2.16	108.22	113.47
24	C	513	CLA	CHA-C1A-NA	-2.15	121.51	126.39
24	A	405	CLA	C2D-C1D-ND	2.15	112.26	110.13
24	C	512	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	408	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
26	B	518	BCR	C11-C12-C13	-2.15	120.47	126.36
24	B	505	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
24	C	509	CLA	CHD-C1D-ND	-2.15	121.78	124.80
26	D	405	BCR	C20-C19-C18	-2.15	120.47	126.36
24	C	507	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
24	B	511	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
24	B	510	CLA	O2A-CGA-CBA	2.14	118.37	111.83
24	D	403	CLA	C2C-C1C-NC	2.14	112.23	109.98
24	C	503	CLA	CHD-C1D-ND	-2.14	121.79	124.80
28	A	411	LMG	O7-C10-O9	-2.14	118.70	123.70
24	D	401	CLA	C3B-C4B-NB	-2.14	108.62	110.53
24	B	505	CLA	C2D-C1D-ND	2.14	112.24	110.13
24	C	508	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	C	504	CLA	C2D-C1D-ND	2.14	112.24	110.13
24	A	405	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
24	B	509	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
24	C	513	CLA	CMA-C3A-C4A	2.14	117.52	111.77
33	C	518	DGD	C2G-O2G-C1B	-2.14	112.68	117.80
24	A	408	CLA	C3B-C4B-NB	-2.14	108.62	110.53
24	C	505	CLA	CMD-C2D-C3D	-2.14	122.79	127.69
24	B	513	CLA	C2D-C1D-ND	2.13	112.24	110.13
24	C	506	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
24	B	506	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
26	C	516	BCR	C16-C15-C14	-2.13	119.17	123.52
24	B	512	CLA	CHD-C1D-ND	-2.13	121.81	124.80
24	C	503	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	B	515	CLA	O2A-CGA-CBA	2.12	118.30	111.83
24	B	512	CLA	C2D-C1D-ND	2.12	112.22	110.13
24	B	505	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
24	C	503	CLA	CHA-C1A-NA	-2.12	121.59	126.39
24	B	511	CLA	C2D-C1D-ND	2.11	112.22	110.13
24	A	406	CLA	CHA-C1A-NA	-2.11	121.61	126.39
24	B	508	CLA	O2A-CGA-CBA	2.11	118.27	111.83
26	C	515	BCR	C29-C30-C25	2.11	113.50	110.44
24	A	406	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
24	C	503	CLA	C1D-ND-C4D	-2.10	104.84	106.31
31	L	101	LHG	O8-C23-O10	-2.10	118.39	123.63
24	B	513	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
24	C	512	CLA	C1D-ND-C4D	-2.09	104.84	106.31
28	D	409	LMG	C8-O7-C10	-2.09	112.79	117.80
24	B	509	CLA	O1D-CGD-CBD	-2.09	120.39	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	518	BCR	C21-C20-C19	-2.09	117.14	123.20
24	A	408	CLA	C1-O2A-CGA	2.09	121.71	116.65
24	B	515	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
24	B	501	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	A	408	CLA	CHD-C1D-ND	-2.08	121.87	124.80
24	B	501	CLA	C1D-ND-C4D	-2.08	104.85	106.31
24	A	408	CLA	C2D-C1D-ND	2.08	112.19	110.13
26	A	409	BCR	C37-C22-C21	-2.08	119.44	122.82
24	C	507	CLA	C1D-ND-C4D	-2.08	104.85	106.31
24	B	501	CLA	C2D-C1D-ND	2.08	112.19	110.13
26	A	409	BCR	C2-C1-C6	2.08	113.46	110.44
24	C	514	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
24	B	508	CLA	CHD-C1D-ND	-2.08	121.88	124.80
24	B	508	CLA	C2D-C1D-ND	2.08	112.18	110.13
24	B	503	CLA	CHD-C1D-ND	-2.07	121.89	124.80
24	C	506	CLA	C2D-C1D-ND	2.07	112.17	110.13
33	C	520	DGD	O2G-C1B-O1B	-2.07	118.87	123.70
24	C	508	CLA	O2A-CGA-CBA	2.07	118.14	111.83
24	C	513	CLA	C2D-C1D-ND	2.07	112.17	110.13
24	D	404	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
38	H	101	RRX	C8-C9-C10	2.07	122.26	119.01
26	C	517	BCR	C38-C26-C27	2.07	118.00	113.60
24	B	511	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
24	C	504	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
24	B	509	CLA	CHA-C1A-NA	-2.06	121.72	126.39
33	C	520	DGD	O1G-C1A-O1A	-2.06	118.47	123.63
24	C	507	CLA	C1-O2A-CGA	2.06	121.64	116.65
24	C	505	CLA	C1D-ND-C4D	-2.06	104.87	106.31
24	C	506	CLA	CHD-C1D-ND	-2.06	121.90	124.80
24	B	512	CLA	C1D-ND-C4D	-2.06	104.87	106.31
24	C	511	CLA	C2D-C1D-ND	2.06	112.16	110.13
24	B	509	CLA	CMA-C3A-C4A	2.06	117.30	111.77
24	C	512	CLA	CHA-C1A-NA	-2.06	121.73	126.39
24	D	404	CLA	C2D-C1D-ND	2.05	112.16	110.13
24	C	510	CLA	CHA-C1A-NA	-2.05	121.75	126.39
36	D	406	PL9	O2-C1-C2	-2.05	117.17	121.83
24	C	505	CLA	C2D-C1D-ND	2.05	112.15	110.13
28	H	102	LMG	C8-O7-C10	-2.05	112.90	117.80
24	B	515	CLA	C2D-C1D-ND	2.05	112.15	110.13
24	B	502	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
24	A	405	CLA	C1-O2A-CGA	2.05	121.61	116.65
24	C	512	CLA	C1-O2A-CGA	2.05	121.61	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	CHA-C1A-NA	-2.04	121.76	126.39
24	B	501	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
24	A	406	CLA	C6-C5-C3	-2.04	108.49	113.47
24	B	501	CLA	CHA-C1A-NA	-2.04	121.77	126.39
24	C	512	CLA	C2D-C1D-ND	2.04	112.15	110.13
24	C	512	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	B	514	CLA	CHA-C1A-NA	-2.04	121.77	126.39
24	B	502	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
26	D	405	BCR	C2-C1-C6	2.04	113.40	110.44
24	B	511	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
24	D	404	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
24	C	514	CLA	C2D-C1D-ND	2.04	112.14	110.13
24	C	508	CLA	O1D-CGD-CBD	-2.03	120.50	124.52
24	B	510	CLA	CHA-C1A-NA	-2.03	121.79	126.39
24	B	513	CLA	CHA-C1A-NA	-2.03	121.79	126.39
24	B	513	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
33	C	518	DGD	C3G-C2G-C1G	-2.03	107.05	111.78
24	B	514	CLA	C2D-C1D-ND	2.03	112.14	110.13
24	C	512	CLA	C6-C5-C3	-2.03	108.53	113.47
28	A	411	LMG	C9-C8-C7	-2.03	107.06	111.78
24	D	404	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	D	410	LHG	O8-C23-O10	-2.03	118.56	123.63
28	C	501	LMG	O1-C1-C2	2.02	111.35	108.27
24	B	515	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	C	505	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	C	505	CLA	C3B-C4B-NB	-2.02	108.72	110.53
33	C	519	DGD	C2G-O2G-C1B	-2.02	112.96	117.80
24	A	405	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
37	E	101	HEM	C3B-C2B-C1B	2.02	107.93	106.41
24	B	513	CLA	C3B-C4B-NB	-2.02	108.73	110.53
31	A	414	LHG	O7-C7-O9	-2.02	118.98	123.70
26	A	409	BCR	C11-C12-C13	2.02	131.90	126.36
24	B	504	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
24	B	515	CLA	C1D-ND-C4D	-2.02	104.90	106.31
24	C	511	CLA	CAA-CBA-CGA	-2.02	107.48	113.21
24	B	503	CLA	CHA-C1A-NA	-2.02	121.83	126.39
36	D	406	PL9	C32-C33-C34	-2.02	123.01	127.62
24	B	516	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	A	405	CLA	CAC-C3C-C4C	2.01	127.41	124.79
24	C	514	CLA	CHA-C1A-NA	-2.01	121.83	126.39
36	D	406	PL9	C40-C39-C41	2.01	118.72	115.23
26	J	101	BCR	C33-C5-C4	2.01	117.89	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	C	502	CLA	C2D-C1D-ND	2.01	112.12	110.13
26	C	516	BCR	C36-C18-C19	2.01	121.16	118.09
26	B	518	BCR	C10-C11-C12	-2.01	117.38	123.20
24	B	504	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
24	C	511	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
26	C	516	BCR	C10-C11-C12	-2.01	117.39	123.20
24	B	502	CLA	CAA-C2A-C3A	-2.01	107.58	113.00
24	A	406	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
30	A	413	BCT	O3-C-O1	-2.01	114.55	119.68
24	C	507	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
28	C	501	LMG	O7-C10-O9	-2.00	119.02	123.70
24	B	507	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
24	C	505	CLA	C6-C5-C3	-2.00	108.59	113.47
24	B	512	CLA	O1D-CGD-CBD	-2.00	120.57	124.52

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	408	CLA	ND
24	B	501	CLA	ND
24	B	502	CLA	ND
24	B	503	CLA	ND
24	B	504	CLA	ND
24	B	505	CLA	ND
24	B	506	CLA	ND
24	B	507	CLA	ND
24	B	508	CLA	ND
24	B	509	CLA	ND
24	B	510	CLA	ND
24	B	511	CLA	ND
24	B	512	CLA	ND
24	B	513	CLA	ND
24	B	514	CLA	ND
24	B	515	CLA	ND
24	B	516	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND

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Mol	Chain	Res	Type	Atom
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	401	CLA	ND
24	D	403	CLA	ND
24	D	404	CLA	ND

All (926) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C1A-C2A-CAA-CBA
24	A	405	CLA	C3A-C2A-CAA-CBA
24	A	406	CLA	C1A-C2A-CAA-CBA
24	A	408	CLA	C1A-C2A-CAA-CBA
24	A	408	CLA	CHA-CBD-CGD-O1D
24	A	408	CLA	CHA-CBD-CGD-O2D
24	B	501	CLA	C2-C1-O2A-CGA
24	B	501	CLA	CHA-CBD-CGD-O1D
24	B	501	CLA	CHA-CBD-CGD-O2D
24	B	503	CLA	CBD-CGD-O2D-CED
24	B	504	CLA	CAD-CBD-CGD-O1D
24	B	504	CLA	CAD-CBD-CGD-O2D
24	B	504	CLA	C6-C7-C8-C9
24	B	506	CLA	CBD-CGD-O2D-CED
24	B	507	CLA	C1A-C2A-CAA-CBA
24	B	507	CLA	C3A-C2A-CAA-CBA
24	B	507	CLA	CAD-CBD-CGD-O1D
24	B	507	CLA	CAD-CBD-CGD-O2D
24	B	508	CLA	C1A-C2A-CAA-CBA
24	B	508	CLA	C3A-C2A-CAA-CBA
24	B	508	CLA	CBD-CGD-O2D-CED
24	B	508	CLA	C4-C3-C5-C6
24	B	509	CLA	C1A-C2A-CAA-CBA
24	B	509	CLA	C3A-C2A-CAA-CBA
24	B	509	CLA	CAD-CBD-CGD-O2D
24	B	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	B	510	CLA	CHA-CBD-CGD-O1D
24	B	510	CLA	CHA-CBD-CGD-O2D
24	B	511	CLA	CBD-CGD-O2D-CED
24	B	512	CLA	C1A-C2A-CAA-CBA
24	B	512	CLA	C3A-C2A-CAA-CBA
24	B	512	CLA	C2-C1-O2A-CGA
24	B	514	CLA	C1A-C2A-CAA-CBA
24	B	514	CLA	C3A-C2A-CAA-CBA
24	B	514	CLA	CBD-CGD-O2D-CED
24	B	516	CLA	CHA-CBD-CGD-O1D
24	B	516	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	C2-C3-C5-C6
24	C	502	CLA	C4-C3-C5-C6
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CBD-CGD-O2D-CED
24	C	505	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	C2-C1-O2A-CGA
24	C	507	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CBD-CGD-O2D-CED
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	C4-C3-C5-C6
24	C	509	CLA	CBD-CGD-O2D-CED
24	C	512	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C1A-C2A-CAA-CBA
24	C	514	CLA	C3A-C2A-CAA-CBA
24	C	514	CLA	CBD-CGD-O2D-CED
24	D	401	CLA	C1A-C2A-CAA-CBA
24	D	401	CLA	C3A-C2A-CAA-CBA
24	D	404	CLA	C1A-C2A-CAA-CBA
24	D	404	CLA	C3A-C2A-CAA-CBA
25	D	402	PHO	C3A-C2A-CAA-CBA
26	A	409	BCR	C5-C6-C7-C8
26	A	409	BCR	C11-C12-C13-C14
26	A	409	BCR	C11-C12-C13-C35
26	A	409	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
26	A	409	BCR	C36-C18-C19-C20
26	B	517	BCR	C11-C12-C13-C14
26	B	517	BCR	C11-C12-C13-C35
26	B	517	BCR	C17-C18-C19-C20
26	B	517	BCR	C36-C18-C19-C20
26	B	517	BCR	C21-C22-C23-C24
26	B	518	BCR	C7-C8-C9-C10
26	B	518	BCR	C7-C8-C9-C34
26	B	518	BCR	C9-C10-C11-C12
26	B	518	BCR	C17-C18-C19-C20
26	B	518	BCR	C36-C18-C19-C20
26	B	518	BCR	C19-C20-C21-C22
26	C	515	BCR	C7-C8-C9-C10
26	C	515	BCR	C7-C8-C9-C34
26	C	515	BCR	C11-C12-C13-C14
26	C	515	BCR	C11-C12-C13-C35
26	C	515	BCR	C17-C18-C19-C20
26	C	516	BCR	C17-C18-C19-C20
26	C	516	BCR	C36-C18-C19-C20
26	C	516	BCR	C19-C20-C21-C22
26	C	517	BCR	C7-C8-C9-C10
26	C	517	BCR	C7-C8-C9-C34
26	D	405	BCR	C19-C20-C21-C22
26	J	101	BCR	C11-C12-C13-C14
26	J	101	BCR	C11-C12-C13-C35
27	A	410	SQD	O5-C5-C6-S
27	M	101	SQD	O5-C1-O6-C44
28	A	411	LMG	C11-C10-O7-C8
28	B	520	LMG	O9-C10-O7-C8
28	B	520	LMG	C11-C10-O7-C8
28	C	521	LMG	O7-C8-C9-O8
31	A	414	LHG	O1-C1-C2-C3
31	A	414	LHG	C4-O6-P-O3
31	A	414	LHG	C4-O6-P-O4
31	A	414	LHG	C4-O6-P-O5
31	D	407	LHG	C1-C2-C3-O3
31	D	407	LHG	C3-O3-P-O6
31	D	408	LHG	O1-C1-C2-O2
31	D	408	LHG	O1-C1-C2-C3
31	D	408	LHG	C1-C2-C3-O3
31	D	408	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	C4-O6-P-O5
31	D	410	LHG	C2-C3-O3-P
31	D	410	LHG	C3-O3-P-O4
31	D	410	LHG	C3-O3-P-O6
31	D	410	LHG	C4-O6-P-O3
31	L	101	LHG	O1-C1-C2-C3
31	L	101	LHG	C3-O3-P-O5
31	L	101	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
32	B	519	C7Z	C21-C26-C27-C28
32	B	519	C7Z	C7-C8-C9-C19
32	B	519	C7Z	C7-C8-C9-C10
32	B	519	C7Z	C11-C12-C13-C14
32	B	519	C7Z	C31-C32-C33-C34
33	B	521	DGD	O6E-C1E-O5D-C6D
33	C	520	DGD	O6D-C1D-O3G-C3G
34	B	522	3PH	C1-O11-P-O14
34	B	522	3PH	C2-C1-O11-P
34	B	522	3PH	C22-C21-O21-C2
35	B	523	DGA	CB2-CB1-OG2-CG2
35	B	523	DGA	OB1-CB1-OG2-CG2
36	D	406	PL9	C37-C38-C39-C41
38	H	101	RRX	C37-C22-C23-C24
38	H	101	RRX	C21-C22-C23-C24
24	A	405	CLA	O1D-CGD-O2D-CED
24	A	405	CLA	CBD-CGD-O2D-CED
24	B	502	CLA	CBD-CGD-O2D-CED
24	B	505	CLA	CBD-CGD-O2D-CED
24	B	507	CLA	CBD-CGD-O2D-CED
24	B	513	CLA	CBD-CGD-O2D-CED
24	B	515	CLA	CBD-CGD-O2D-CED
24	C	503	CLA	CBD-CGD-O2D-CED
24	C	505	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
24	D	403	CLA	CBD-CGD-O2D-CED
24	B	510	CLA	O1A-CGA-O2A-C1
24	D	401	CLA	O1A-CGA-O2A-C1
28	A	411	LMG	O10-C28-O8-C9
24	B	505	CLA	O1D-CGD-O2D-CED
24	B	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	B	501	CLA	CBA-CGA-O2A-C1
24	B	510	CLA	CBA-CGA-O2A-C1
24	D	401	CLA	CBA-CGA-O2A-C1
28	A	411	LMG	C29-C28-O8-C9
24	B	501	CLA	O1A-CGA-O2A-C1
24	C	506	CLA	O1A-CGA-O2A-C1
28	C	521	LMG	O10-C28-O8-C9
24	B	506	CLA	O1D-CGD-O2D-CED
24	C	509	CLA	O1D-CGD-O2D-CED
24	B	503	CLA	O1D-CGD-O2D-CED
24	B	508	CLA	O1D-CGD-O2D-CED
24	B	514	CLA	O1D-CGD-O2D-CED
24	C	504	CLA	O1D-CGD-O2D-CED
24	C	512	CLA	O1D-CGD-O2D-CED
24	A	408	CLA	CBD-CGD-O2D-CED
24	B	516	CLA	CBD-CGD-O2D-CED
28	A	411	LMG	O9-C10-O7-C8
28	C	521	LMG	O9-C10-O7-C8
31	D	410	LHG	O9-C7-O7-C5
34	B	522	3PH	O22-C21-O21-C2
24	B	511	CLA	O1D-CGD-O2D-CED
24	A	408	CLA	C3-C5-C6-C7
24	B	502	CLA	C3-C5-C6-C7
24	B	504	CLA	C3-C5-C6-C7
24	C	505	CLA	C3-C5-C6-C7
24	C	513	CLA	C3-C5-C6-C7
25	D	402	PHO	C3-C5-C6-C7
24	B	502	CLA	CBA-CGA-O2A-C1
33	C	518	DGD	C2A-C1A-O1G-C1G
34	B	522	3PH	C32-C31-O31-C3
24	B	501	CLA	CBD-CGD-O2D-CED
24	B	510	CLA	CBD-CGD-O2D-CED
24	B	512	CLA	CBD-CGD-O2D-CED
24	D	404	CLA	CBD-CGD-O2D-CED
31	D	410	LHG	C8-C7-O7-C5
24	B	509	CLA	O1D-CGD-O2D-CED
24	C	502	CLA	O1D-CGD-O2D-CED
24	C	505	CLA	O1D-CGD-O2D-CED
24	C	507	CLA	O1D-CGD-O2D-CED
24	C	514	CLA	O1D-CGD-O2D-CED
24	A	408	CLA	C4-C3-C5-C6
24	B	503	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	505	CLA	C4-C3-C5-C6
24	B	509	CLA	C4-C3-C5-C6
24	A	408	CLA	C2-C3-C5-C6
24	B	503	CLA	C2-C3-C5-C6
24	B	508	CLA	C2-C3-C5-C6
24	C	508	CLA	C2-C3-C5-C6
24	C	508	CLA	CBD-CGD-O2D-CED
24	B	502	CLA	O1D-CGD-O2D-CED
24	B	507	CLA	O1D-CGD-O2D-CED
24	B	515	CLA	C3-C5-C6-C7
24	B	512	CLA	CBA-CGA-O2A-C1
24	C	506	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	CBA-CGA-O2A-C1
28	B	520	LMG	C29-C28-O8-C9
28	C	521	LMG	C29-C28-O8-C9
28	B	520	LMG	C17-C18-C19-C20
28	D	409	LMG	C17-C18-C19-C20
28	H	102	LMG	C35-C36-C37-C38
26	A	409	BCR	C19-C20-C21-C22
26	C	515	BCR	C13-C14-C15-C16
26	C	517	BCR	C13-C14-C15-C16
24	B	502	CLA	O1A-CGA-O2A-C1
33	C	518	DGD	O1A-C1A-O1G-C1G
28	C	501	LMG	C17-C18-C19-C20
28	C	521	LMG	C35-C36-C37-C38
28	C	522	LMG	C17-C18-C19-C20
28	H	102	LMG	C38-C39-C40-C41
33	C	519	DGD	CBB-CCB-CDB-CEB
31	A	414	LHG	O2-C2-C3-O3
24	B	515	CLA	O1D-CGD-O2D-CED
24	C	511	CLA	O1D-CGD-O2D-CED
24	D	403	CLA	O1D-CGD-O2D-CED
24	C	510	CLA	CBA-CGA-O2A-C1
33	B	521	DGD	C2A-C1A-O1G-C1G
28	B	520	LMG	O10-C28-O8-C9
34	B	522	3PH	O32-C31-O31-C3
31	D	410	LHG	C13-C14-C15-C16
24	C	503	CLA	O1D-CGD-O2D-CED
28	C	521	LMG	C11-C10-O7-C8
24	C	513	CLA	CBD-CGD-O2D-CED
24	D	404	CLA	C4-C3-C5-C6
24	B	505	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	509	CLA	C2-C3-C5-C6
24	D	404	CLA	C2-C3-C5-C6
24	C	513	CLA	O1A-CGA-O2A-C1
33	B	521	DGD	O1A-C1A-O1G-C1G
36	D	406	PL9	C39-C41-C42-C43
31	D	407	LHG	C11-C12-C13-C14
24	C	514	CLA	C2A-CAA-CBA-CGA
24	B	512	CLA	O1A-CGA-O2A-C1
24	B	516	CLA	O1D-CGD-O2D-CED
24	C	507	CLA	CBA-CGA-O2A-C1
24	A	406	CLA	CBD-CGD-O2D-CED
24	C	506	CLA	CBD-CGD-O2D-CED
31	D	407	LHG	C28-C29-C30-C31
27	M	101	SQD	C8-C7-O47-C45
26	B	517	BCR	C9-C10-C11-C12
24	C	507	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	O1A-CGA-O2A-C1
31	D	410	LHG	C1-C2-C3-O3
31	L	101	LHG	C1-C2-C3-O3
24	A	406	CLA	CBA-CGA-O2A-C1
24	B	507	CLA	CBA-CGA-O2A-C1
31	D	410	LHG	C11-C12-C13-C14
24	A	408	CLA	O1D-CGD-O2D-CED
24	B	502	CLA	C4-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	B	502	CLA	C2-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	A	406	CLA	C11-C12-C13-C14
24	B	503	CLA	C14-C13-C15-C16
24	B	510	CLA	C14-C13-C15-C16
24	B	511	CLA	C11-C12-C13-C14
24	B	515	CLA	C6-C7-C8-C9
24	C	502	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C10-C8-C9
25	A	407	PHO	C6-C7-C8-C9
24	B	512	CLA	O1D-CGD-O2D-CED
24	D	404	CLA	O1D-CGD-O2D-CED
33	B	521	DGD	C2E-C1E-O5D-C6D
31	D	407	LHG	O2-C2-C3-O3
31	D	408	LHG	O2-C2-C3-O3
24	B	510	CLA	O1D-CGD-O2D-CED
26	A	409	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	B	517	BCR	C37-C22-C23-C24
26	C	515	BCR	C36-C18-C19-C20
26	C	516	BCR	C7-C8-C9-C34
26	C	517	BCR	C36-C18-C19-C20
26	D	405	BCR	C37-C22-C23-C24
32	B	519	C7Z	C11-C12-C13-C20
32	B	519	C7Z	C31-C32-C33-C40
32	B	519	C7Z	C27-C28-C29-C39
38	H	101	RRX	C7-C8-C9-C34
26	A	409	BCR	C21-C22-C23-C24
26	C	516	BCR	C7-C8-C9-C10
26	C	517	BCR	C17-C18-C19-C20
26	D	405	BCR	C21-C22-C23-C24
32	B	519	C7Z	C27-C28-C29-C30
38	H	101	RRX	C7-C8-C9-C10
39	J	102	LMU	O5B-C5B-C6B-O6B
24	B	510	CLA	C13-C15-C16-C17
28	A	415	LMG	C11-C10-O7-C8
24	B	515	CLA	C5-C6-C7-C8
24	B	509	CLA	C2-C1-O2A-CGA
24	B	515	CLA	C2-C1-O2A-CGA
24	B	516	CLA	C2-C1-O2A-CGA
24	D	404	CLA	C2-C1-O2A-CGA
24	B	501	CLA	O1D-CGD-O2D-CED
24	B	503	CLA	C15-C16-C17-C18
24	B	513	CLA	C5-C6-C7-C8
31	D	407	LHG	O1-C1-C2-O2
39	J	102	LMU	C4B-C5B-C6B-O6B
24	B	501	CLA	C8-C10-C11-C12
28	C	522	LMG	C10-C11-C12-C13
31	A	414	LHG	C23-C24-C25-C26
26	A	409	BCR	C13-C14-C15-C16
26	C	515	BCR	C15-C16-C17-C18
26	C	515	BCR	C19-C20-C21-C22
26	C	517	BCR	C15-C16-C17-C18
26	C	517	BCR	C19-C20-C21-C22
27	M	101	SQD	O49-C7-O47-C45
24	C	507	CLA	C15-C16-C17-C18
28	B	520	LMG	C10-C11-C12-C13
31	L	101	LHG	C7-C8-C9-C10
24	B	505	CLA	C15-C16-C17-C18
24	B	507	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	B	512	CLA	C15-C16-C17-C18
24	B	515	CLA	C15-C16-C17-C18
24	C	502	CLA	C10-C11-C12-C13
37	E	101	HEM	C3D-CAD-CBD-CGD
24	B	506	CLA	C2A-CAA-CBA-CGA
24	C	506	CLA	C2A-CAA-CBA-CGA
24	B	508	CLA	C15-C16-C17-C18
24	B	512	CLA	C13-C15-C16-C17
24	B	513	CLA	C10-C11-C12-C13
24	B	514	CLA	C13-C15-C16-C17
24	D	401	CLA	C15-C16-C17-C18
31	D	410	LHG	C7-C8-C9-C10
31	D	410	LHG	C23-C24-C25-C26
35	B	523	DGA	CA1-CA2-CA3-CA4
24	A	406	CLA	O1A-CGA-O2A-C1
24	B	507	CLA	O1A-CGA-O2A-C1
35	B	523	DGA	CBB-CAB-CB9-CB8
24	A	405	CLA	C15-C16-C17-C18
24	B	501	CLA	C10-C11-C12-C13
24	B	502	CLA	C13-C15-C16-C17
24	B	503	CLA	C5-C6-C7-C8
24	B	504	CLA	C8-C10-C11-C12
24	B	507	CLA	C5-C6-C7-C8
24	B	508	CLA	C13-C15-C16-C17
24	B	510	CLA	C15-C16-C17-C18
24	B	511	CLA	C13-C15-C16-C17
24	C	502	CLA	C8-C10-C11-C12
24	C	504	CLA	C15-C16-C17-C18
24	D	404	CLA	C10-C11-C12-C13
31	D	410	LHG	O2-C2-C3-O3
31	L	101	LHG	O2-C2-C3-O3
24	A	408	CLA	C8-C10-C11-C12
28	A	415	LMG	O9-C10-O7-C8
28	D	409	LMG	C35-C36-C37-C38
36	D	406	PL9	C37-C38-C39-C40
24	C	508	CLA	O1D-CGD-O2D-CED
24	B	511	CLA	C15-C16-C17-C18
24	A	408	CLA	C10-C11-C12-C13
24	C	511	CLA	CBA-CGA-O2A-C1
24	B	508	CLA	C5-C6-C7-C8
26	A	409	BCR	C15-C16-C17-C18
31	A	414	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C2A-CAA-CBA-CGA
24	A	406	CLA	C2A-CAA-CBA-CGA
24	A	408	CLA	C2A-CAA-CBA-CGA
33	C	519	DGD	C2A-C1A-O1G-C1G
31	L	101	LHG	C11-C10-C9-C8
24	B	510	CLA	C5-C6-C7-C8
24	B	510	CLA	C10-C11-C12-C13
24	B	511	CLA	C8-C10-C11-C12
24	D	404	CLA	C8-C10-C11-C12
24	C	502	CLA	C15-C16-C17-C18
24	C	511	CLA	C15-C16-C17-C18
24	B	513	CLA	CBA-CGA-O2A-C1
24	D	404	CLA	CBA-CGA-O2A-C1
24	D	404	CLA	C3-C5-C6-C7
24	C	513	CLA	O1D-CGD-O2D-CED
28	C	522	LMG	C2-C1-O1-C7
31	L	101	LHG	C23-C24-C25-C26
24	C	502	CLA	C16-C17-C18-C20
24	B	509	CLA	C5-C6-C7-C8
26	B	518	BCR	C11-C12-C13-C35
26	C	517	BCR	C37-C22-C23-C24
26	D	405	BCR	C36-C18-C19-C20
26	J	101	BCR	C37-C22-C23-C24
26	B	518	BCR	C11-C12-C13-C14
26	D	405	BCR	C17-C18-C19-C20
26	J	101	BCR	C21-C22-C23-C24
24	C	502	CLA	C2A-CAA-CBA-CGA
31	D	407	LHG	O1-C1-C2-C3
31	D	410	LHG	O1-C1-C2-C3
27	M	101	SQD	C7-C8-C9-C10
34	B	522	3PH	C3-C2-O21-C21
33	C	519	DGD	O1A-C1A-O1G-C1G
24	C	509	CLA	C5-C6-C7-C8
24	C	511	CLA	C13-C15-C16-C17
33	C	519	DGD	C9B-CAB-CBB-CCB
31	A	414	LHG	O7-C5-C6-O8
24	C	504	CLA	CBA-CGA-O2A-C1
33	C	520	DGD	C2A-C1A-O1G-C1G
24	C	508	CLA	C8-C10-C11-C12
28	B	520	LMG	C28-C29-C30-C31
24	A	405	CLA	C2-C1-O2A-CGA
24	A	408	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	B	507	CLA	C2-C1-O2A-CGA
24	B	513	CLA	C2-C1-O2A-CGA
24	B	514	CLA	C2-C1-O2A-CGA
24	C	503	CLA	C2-C1-O2A-CGA
24	C	508	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C1-O2A-CGA
24	D	401	CLA	C2-C1-O2A-CGA
24	C	511	CLA	O1A-CGA-O2A-C1
33	C	518	DGD	C2G-C1G-O1G-C1A
31	L	101	LHG	C13-C14-C15-C16
33	C	520	DGD	C2A-C3A-C4A-C5A
35	B	523	DGA	CB1-CB2-CB3-CB4
31	L	101	LHG	C26-C27-C28-C29
35	B	523	DGA	CA6-CA7-CA8-CA9
31	A	414	LHG	O1-C1-C2-O2
31	L	101	LHG	O1-C1-C2-O2
24	C	506	CLA	O1D-CGD-O2D-CED
24	B	516	CLA	C6-C7-C8-C9
24	B	516	CLA	C6-C7-C8-C10
31	A	414	LHG	C28-C29-C30-C31
34	B	522	3PH	C29-C2A-C2B-C2C
24	B	507	CLA	C8-C10-C11-C12
24	B	516	CLA	C5-C6-C7-C8
24	B	513	CLA	O1A-CGA-O2A-C1
24	D	404	CLA	O1A-CGA-O2A-C1
24	B	510	CLA	C3A-C2A-CAA-CBA
39	J	102	LMU	C6-C7-C8-C9
28	D	409	LMG	C13-C14-C15-C16
33	C	520	DGD	O1A-C1A-O1G-C1G
24	A	406	CLA	O1D-CGD-O2D-CED
24	B	505	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C7-C8-C9-C10
31	D	410	LHG	C10-C11-C12-C13
35	B	523	DGA	CB3-CB4-CB5-CB6
31	A	414	LHG	C11-C10-C9-C8
24	C	506	CLA	C5-C6-C7-C8
28	H	102	LMG	C16-C17-C18-C19
24	C	504	CLA	O1A-CGA-O2A-C1
26	A	409	BCR	C1-C6-C7-C8
26	B	518	BCR	C1-C6-C7-C8
26	C	516	BCR	C1-C6-C7-C8
26	J	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	J	101	BCR	C23-C24-C25-C26
32	B	519	C7Z	C1-C6-C7-C8
32	B	519	C7Z	C25-C26-C27-C28
27	A	410	SQD	C11-C10-C9-C8
28	C	501	LMG	C11-C10-O7-C8
24	B	516	CLA	C3-C5-C6-C7
31	D	407	LHG	C13-C14-C15-C16
31	L	101	LHG	C34-C35-C36-C37
34	B	522	3PH	C39-C3A-C3B-C3C
28	C	501	LMG	O9-C10-O7-C8
24	B	504	CLA	C4-C3-C5-C6
31	A	414	LHG	C26-C27-C28-C29
31	D	410	LHG	C14-C15-C16-C17
24	B	516	CLA	CBA-CGA-O2A-C1
31	A	414	LHG	C25-C26-C27-C28
24	C	512	CLA	C10-C11-C12-C13
27	M	101	SQD	C24-C25-C26-C27
35	B	523	DGA	CB5-CB6-CB7-CB8
27	M	101	SQD	C2-C1-O6-C44
24	A	405	CLA	C13-C15-C16-C17
24	B	503	CLA	C8-C10-C11-C12
24	B	513	CLA	C13-C15-C16-C17
24	C	509	CLA	C13-C15-C16-C17
31	L	101	LHG	C11-C12-C13-C14
31	D	408	LHG	C23-C24-C25-C26
33	C	519	DGD	C5D-C6D-O5D-C1E
24	D	404	CLA	C2A-CAA-CBA-CGA
24	C	502	CLA	C16-C17-C18-C19
31	A	414	LHG	C24-C25-C26-C27
31	L	101	LHG	C33-C34-C35-C36
28	D	409	LMG	C12-C13-C14-C15
24	B	505	CLA	O1A-CGA-O2A-C1
24	B	510	CLA	C8-C10-C11-C12
24	C	508	CLA	C13-C15-C16-C17
24	D	401	CLA	C8-C10-C11-C12
34	B	522	3PH	C31-C32-C33-C34
24	C	508	CLA	C15-C16-C17-C18
33	C	519	DGD	CCB-CDB-CEB-CFB
24	B	512	CLA	C10-C11-C12-C13
31	D	408	LHG	C34-C35-C36-C37
33	B	521	DGD	C3A-C4A-C5A-C6A
34	B	522	3PH	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
31	A	414	LHG	C31-C32-C33-C34
24	B	509	CLA	C8-C10-C11-C12
24	C	503	CLA	C8-C10-C11-C12
24	C	508	CLA	C5-C6-C7-C8
31	D	408	LHG	C13-C14-C15-C16
35	B	523	DGA	CB9-CAB-CBB-CCB
24	C	507	CLA	C3-C5-C6-C7
24	B	503	CLA	C13-C15-C16-C17
28	B	520	LMG	C11-C12-C13-C14
24	B	501	CLA	C13-C15-C16-C17
28	H	102	LMG	C33-C34-C35-C36
24	B	504	CLA	C1A-C2A-CAA-CBA
24	B	510	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C1A-C2A-CAA-CBA
24	C	504	CLA	C1A-C2A-CAA-CBA
24	B	505	CLA	C8-C10-C11-C12
34	B	522	3PH	C3A-C3B-C3C-C3D
31	D	408	LHG	C28-C29-C30-C31
31	D	408	LHG	C33-C34-C35-C36
24	B	504	CLA	C6-C7-C8-C10
24	B	513	CLA	C11-C10-C8-C7
24	B	513	CLA	C11-C12-C13-C15
24	C	502	CLA	C6-C7-C8-C10
24	C	509	CLA	C11-C12-C13-C15
24	C	511	CLA	C6-C7-C8-C10
24	C	511	CLA	C11-C10-C8-C7
24	C	511	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C12-C13-C15
24	B	516	CLA	O1A-CGA-O2A-C1
33	C	520	DGD	O6E-C5E-C6E-O5E
24	B	504	CLA	C2-C3-C5-C6
24	B	504	CLA	C10-C11-C12-C13
24	B	502	CLA	C2A-CAA-CBA-CGA
24	B	507	CLA	C14-C13-C15-C16
24	B	513	CLA	C11-C12-C13-C14
24	C	502	CLA	C6-C7-C8-C9
24	C	511	CLA	C11-C10-C8-C9
24	C	511	CLA	C14-C13-C15-C16
33	C	519	DGD	C3A-C4A-C5A-C6A
31	D	408	LHG	C9-C10-C11-C12
24	C	505	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	C	512	CLA	CBA-CGA-O2A-C1
27	A	410	SQD	C28-C29-C30-C31
31	L	101	LHG	C31-C32-C33-C34
35	B	523	DGA	CAB-CBB-CCB-CDB
33	B	521	DGD	C2D-C1D-O3G-C3G
31	D	407	LHG	C7-C8-C9-C10
31	D	407	LHG	C4-C5-C6-O8
33	C	519	DGD	O6D-C5D-C6D-O5D
28	D	409	LMG	O6-C5-C6-O5
31	D	408	LHG	C11-C12-C13-C14
24	C	504	CLA	C8-C10-C11-C12
24	C	509	CLA	C8-C10-C11-C12
24	C	502	CLA	CBA-CGA-O2A-C1
24	A	405	CLA	C16-C17-C18-C19
24	D	401	CLA	C13-C15-C16-C17
24	C	502	CLA	O1A-CGA-O2A-C1
31	D	408	LHG	C11-C10-C9-C8
26	B	517	BCR	C7-C8-C9-C34
26	B	518	BCR	C37-C22-C23-C24
33	C	518	DGD	O6E-C5E-C6E-O5E
26	B	517	BCR	C7-C8-C9-C10
26	B	518	BCR	C21-C22-C23-C24
26	J	101	BCR	C7-C8-C9-C10
24	B	502	CLA	C15-C16-C17-C18
24	B	507	CLA	C13-C15-C16-C17
31	A	414	LHG	C33-C34-C35-C36
33	B	521	DGD	C2A-C3A-C4A-C5A
27	M	101	SQD	C46-C45-O47-C7
31	D	407	LHG	C27-C28-C29-C30
26	C	516	BCR	C9-C10-C11-C12
34	B	522	3PH	C27-C28-C29-C2A
35	B	523	DGA	CA2-CA3-CA4-CA5
31	D	410	LHG	C17-C18-C19-C20
33	C	519	DGD	O1G-C1G-C2G-O2G
24	B	503	CLA	C2A-CAA-CBA-CGA
24	B	507	CLA	C2A-CAA-CBA-CGA
27	A	410	SQD	C24-C25-C26-C27
24	B	507	CLA	C16-C17-C18-C20
31	D	410	LHG	C18-C19-C20-C21
24	C	505	CLA	O1A-CGA-O2A-C1
24	B	503	CLA	CBA-CGA-O2A-C1
24	B	514	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	A	407	PHO	C3-C5-C6-C7
31	A	414	LHG	C34-C35-C36-C37
31	A	414	LHG	C24-C23-O8-C6
24	C	512	CLA	C3-C5-C6-C7
24	B	513	CLA	C11-C10-C8-C9
24	B	514	CLA	C6-C7-C8-C9
24	B	515	CLA	C11-C12-C13-C14
24	C	503	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
24	D	403	CLA	C11-C12-C13-C14
24	B	501	CLA	C5-C6-C7-C8
24	C	512	CLA	O1A-CGA-O2A-C1
24	C	508	CLA	C4B-C3B-CAB-CBB
24	B	515	CLA	C13-C15-C16-C17
24	C	510	CLA	C13-C15-C16-C17
31	D	410	LHG	C11-C10-C9-C8
24	A	406	CLA	C11-C10-C8-C7
24	B	503	CLA	C11-C12-C13-C15
24	B	504	CLA	C11-C10-C8-C7
24	B	507	CLA	C12-C13-C15-C16
24	B	508	CLA	C11-C12-C13-C15
24	B	514	CLA	C6-C7-C8-C10
24	B	515	CLA	C11-C12-C13-C15
24	C	503	CLA	C12-C13-C15-C16
24	B	515	CLA	C8-C10-C11-C12
24	C	507	CLA	C3A-C2A-CAA-CBA
36	D	406	PL9	C40-C39-C41-C42
25	A	407	PHO	C2-C3-C5-C6
28	C	522	LMG	O6-C1-O1-C7
24	B	511	CLA	CBA-CGA-O2A-C1
24	B	515	CLA	CBA-CGA-O2A-C1
32	B	519	C7Z	C9-C10-C11-C12
26	C	517	BCR	C21-C22-C23-C24
31	A	414	LHG	C30-C31-C32-C33
34	B	522	3PH	C25-C26-C27-C28
28	A	411	LMG	O1-C7-C8-C9
28	C	521	LMG	C7-C8-C9-O8
31	A	414	LHG	C4-C5-C6-O8
31	D	408	LHG	C4-C5-C6-O8
33	B	521	DGD	C1G-C2G-C3G-O3G
35	B	523	DGA	OG1-CG1-CG2-CG3
35	B	523	DGA	CG1-CG2-CG3-OXT

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Mol	Chain	Res	Type	Atoms
25	A	407	PHO	C4-C3-C5-C6
31	D	407	LHG	C23-C24-C25-C26
31	D	410	LHG	O6-C4-C5-O7
33	C	520	DGD	O6D-C5D-C6D-O5D
26	D	405	BCR	C23-C24-C25-C30
24	B	511	CLA	C5-C6-C7-C8
24	B	514	CLA	CAA-CBA-CGA-O2A
25	D	402	PHO	C2A-CAA-CBA-CGA
28	A	411	LMG	O1-C7-C8-O7
28	H	102	LMG	O7-C8-C9-O8
35	B	523	DGA	CBB-CCB-CDB-CEB
24	B	507	CLA	C16-C17-C18-C19
24	B	504	CLA	C5-C6-C7-C8
24	B	514	CLA	C3-C5-C6-C7
24	B	508	CLA	C11-C12-C13-C14
24	C	509	CLA	C11-C12-C13-C14
31	D	408	LHG	C19-C20-C21-C22
39	J	102	LMU	C9-C10-C11-C12
33	C	520	DGD	C2D-C1D-O3G-C3G
35	B	523	DGA	OG2-CG2-CG3-OXT
34	B	522	3PH	C24-C25-C26-C27
25	A	407	PHO	C13-C15-C16-C17
26	D	405	BCR	C9-C10-C11-C12
28	C	522	LMG	C15-C16-C17-C18
31	D	407	LHG	C35-C36-C37-C38
24	B	513	CLA	C3-C5-C6-C7
31	A	414	LHG	O6-C4-C5-C6
31	D	407	LHG	O6-C4-C5-C6
24	A	405	CLA	C8-C10-C11-C12
25	A	407	PHO	C10-C11-C12-C13
26	C	515	BCR	C37-C22-C23-C24
26	J	101	BCR	C7-C8-C9-C34
31	D	408	LHG	C25-C26-C27-C28
24	B	508	CLA	C6-C7-C8-C10
33	C	519	DGD	C6B-C7B-C8B-C9B
26	C	515	BCR	C21-C22-C23-C24
34	B	522	3PH	C1-O11-P-O13
35	B	523	DGA	CB7-CB8-CB9-CAB
24	B	503	CLA	O1A-CGA-O2A-C1
35	B	523	DGA	CG1-CG2-OG2-CB1
24	B	515	CLA	O1A-CGA-O2A-C1
24	A	405	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C16-C17-C18-C19
24	B	511	CLA	O1A-CGA-O2A-C1
31	A	414	LHG	O10-C23-O8-C6
31	A	414	LHG	O6-C4-C5-O7
31	D	407	LHG	O6-C4-C5-O7
31	L	101	LHG	O6-C4-C5-O7
28	H	102	LMG	C7-C8-C9-O8
28	H	102	LMG	C36-C37-C38-C39
24	C	503	CLA	C3-C5-C6-C7
31	D	407	LHG	C31-C32-C33-C34
31	D	407	LHG	O7-C5-C6-O8
31	L	101	LHG	O7-C5-C6-O8
24	B	508	CLA	C6-C7-C8-C9
24	C	508	CLA	C16-C17-C18-C19
28	H	102	LMG	C32-C33-C34-C35
31	D	407	LHG	C34-C35-C36-C37
34	B	522	3PH	C32-C33-C34-C35
34	B	522	3PH	C2A-C2B-C2C-C2D
31	L	101	LHG	C10-C11-C12-C13
24	C	510	CLA	C8-C10-C11-C12
24	D	401	CLA	C3-C5-C6-C7
33	C	518	DGD	C1B-C2B-C3B-C4B
24	B	516	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C4B-C3B-CAB-CBB
24	B	509	CLA	CBA-CGA-O2A-C1
24	D	401	CLA	C2A-CAA-CBA-CGA
31	L	101	LHG	O6-C4-C5-C6
33	B	521	DGD	O1B-C1B-O2G-C2G
33	C	520	DGD	O1B-C1B-O2G-C2G
27	M	101	SQD	C5-C6-S-O9
24	B	503	CLA	C12-C13-C15-C16
24	B	507	CLA	C6-C7-C8-C10
24	B	510	CLA	C12-C13-C15-C16
24	B	515	CLA	C11-C10-C8-C7
24	D	401	CLA	C11-C12-C13-C15
24	D	401	CLA	C12-C13-C15-C16
24	B	503	CLA	C16-C17-C18-C19
24	C	504	CLA	C16-C17-C18-C20
33	B	521	DGD	C2B-C1B-O2G-C2G
24	A	406	CLA	C11-C10-C8-C9
24	B	501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	B	504	CLA	C11-C10-C8-C9
24	B	509	CLA	O1A-CGA-O2A-C1
31	D	408	LHG	O7-C5-C6-O8
33	B	521	DGD	O2G-C2G-C3G-O3G
35	B	523	DGA	OG1-CG1-CG2-OG2
24	B	505	CLA	CAD-CBD-CGD-O2D
24	B	512	CLA	CAD-CBD-CGD-O2D
28	C	501	LMG	O10-C28-O8-C9
28	C	501	LMG	C29-C28-O8-C9
24	C	507	CLA	C16-C17-C18-C20
24	B	505	CLA	CAD-CBD-CGD-O1D
24	B	509	CLA	CAD-CBD-CGD-O1D
24	B	512	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
25	D	402	PHO	CHA-CBD-CGD-O2D
26	J	101	BCR	C9-C10-C11-C12
26	J	101	BCR	C15-C16-C17-C18
31	A	414	LHG	C3-O3-P-O5
31	D	407	LHG	C3-O3-P-O5
31	D	408	LHG	C3-O3-P-O5
31	D	408	LHG	C4-O6-P-O4
31	D	410	LHG	C4-O6-P-O5
38	H	101	RRX	C15-C16-C17-C18
24	C	509	CLA	C3-C5-C6-C7
24	B	516	CLA	C2B-C3B-CAB-CBB
24	C	513	CLA	C2B-C3B-CAB-CBB
35	B	523	DGA	CB2-CB3-CB4-CB5
31	A	414	LHG	C2-C3-O3-P
24	B	502	CLA	CAA-CBA-CGA-O2A
28	H	102	LMG	O7-C10-C11-C12
34	B	522	3PH	C1-O11-P-O12
35	B	523	DGA	CB6-CB7-CB8-CB9
31	D	410	LHG	O1-C1-C2-O2
33	B	521	DGD	C1A-C2A-C3A-C4A
24	C	503	CLA	C16-C17-C18-C20
28	B	520	LMG	C9-C8-O7-C10
24	B	510	CLA	C16-C17-C18-C19
31	D	410	LHG	O6-C4-C5-C6
31	L	101	LHG	C28-C29-C30-C31
24	A	405	CLA	C11-C12-C13-C14
24	B	503	CLA	C11-C12-C13-C14
24	B	514	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	D	401	CLA	C11-C12-C13-C14
24	D	401	CLA	C14-C13-C15-C16
24	D	403	CLA	C14-C13-C15-C16
24	A	405	CLA	C11-C12-C13-C15
24	B	501	CLA	C12-C13-C15-C16
24	B	503	CLA	C6-C7-C8-C10
24	B	515	CLA	C6-C7-C8-C10
28	A	415	LMG	O6-C1-O1-C7
31	L	101	LHG	O8-C23-C24-C25
33	C	519	DGD	C2D-C1D-O3G-C3G
24	C	509	CLA	CBA-CGA-O2A-C1
24	B	516	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	C10-C11-C12-C13
28	D	409	LMG	C31-C32-C33-C34
24	B	505	CLA	C16-C17-C18-C20
33	C	519	DGD	C4D-C5D-C6D-O5D
24	B	514	CLA	C10-C11-C12-C13
31	D	410	LHG	C9-C10-C11-C12
33	C	519	DGD	O1G-C1G-C2G-C3G
24	A	405	CLA	CAA-CBA-CGA-O2A
33	C	520	DGD	C2B-C1B-O2G-C2G
39	J	102	LMU	C1-C2-C3-C4
24	B	503	CLA	C3-C5-C6-C7
28	A	415	LMG	C8-C7-O1-C1
24	D	401	CLA	C16-C17-C18-C19
31	D	407	LHG	C26-C27-C28-C29
27	M	101	SQD	C23-C24-C25-C26
24	B	513	CLA	C4-C3-C5-C6
24	B	511	CLA	C10-C11-C12-C13
28	A	411	LMG	C28-C29-C30-C31
24	B	503	CLA	C6-C7-C8-C9
25	A	407	PHO	C11-C10-C8-C9
31	D	407	LHG	C9-C10-C11-C12
24	A	406	CLA	C10-C11-C12-C13
24	C	509	CLA	O1A-CGA-O2A-C1
24	B	510	CLA	C16-C17-C18-C20
35	B	523	DGA	CA5-CA6-CA7-CA8
31	D	410	LHG	C25-C26-C27-C28
24	C	507	CLA	C16-C17-C18-C19
36	D	406	PL9	C38-C39-C41-C42
34	B	522	3PH	C28-C29-C2A-C2B
26	A	409	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
27	M	101	SQD	C25-C26-C27-C28
24	C	512	CLA	C2-C1-O2A-CGA
26	J	101	BCR	C13-C14-C15-C16
39	J	102	LMU	C5-C6-C7-C8
24	B	507	CLA	C6-C7-C8-C9
24	C	507	CLA	C11-C10-C8-C9
24	C	510	CLA	C11-C10-C8-C9
24	C	503	CLA	C13-C15-C16-C17
24	B	501	CLA	C3-C5-C6-C7
26	C	515	BCR	C9-C10-C11-C12
24	C	503	CLA	C16-C17-C18-C19
24	B	504	CLA	O1A-CGA-O2A-C1
24	B	503	CLA	C1A-C2A-CAA-CBA
26	A	409	BCR	C11-C10-C9-C8
24	B	514	CLA	C16-C17-C18-C20
28	C	522	LMG	O9-C10-O7-C8
24	C	509	CLA	C10-C11-C12-C13
24	D	404	CLA	C2B-C3B-CAB-CBB
26	B	517	BCR	C23-C24-C25-C26
26	B	518	BCR	C23-C24-C25-C26
26	C	515	BCR	C23-C24-C25-C30
31	L	101	LHG	C9-C10-C11-C12
35	B	523	DGA	CA9-CAA-CBA-CCA
24	B	506	CLA	C6-C7-C8-C10
24	C	502	CLA	C11-C10-C8-C7
25	A	407	PHO	C6-C7-C8-C10
25	A	407	PHO	C11-C10-C8-C7
25	D	402	PHO	C6-C7-C8-C10
24	B	511	CLA	C16-C17-C18-C19
31	L	101	LHG	C24-C25-C26-C27
27	M	101	SQD	O47-C7-C8-C9
34	B	522	3PH	C2C-C2D-C2E-C2F
24	A	408	CLA	C11-C10-C8-C9
24	B	505	CLA	C11-C12-C13-C14
31	L	101	LHG	C35-C36-C37-C38
24	C	503	CLA	C4-C3-C5-C6
24	D	401	CLA	C5-C6-C7-C8
31	L	101	LHG	C4-C5-C6-O8
28	H	102	LMG	C30-C31-C32-C33
24	D	403	CLA	CAA-CBA-CGA-O2A
24	B	511	CLA	C4-C3-C5-C6
38	H	101	RRX	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
24	C	514	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	C11-C12-C13-C14
24	D	404	CLA	C4B-C3B-CAB-CBB
25	A	407	PHO	CHA-CBD-CGD-O1D
25	D	402	PHO	CHA-CBD-CGD-O1D
31	L	101	LHG	C30-C31-C32-C33
31	L	101	LHG	C2-C3-O3-P
24	A	408	CLA	C11-C10-C8-C7
26	B	518	BCR	C15-C16-C17-C18
24	B	504	CLA	CBA-CGA-O2A-C1
24	C	502	CLA	C11-C12-C13-C14
24	C	512	CLA	C6-C7-C8-C9
27	M	101	SQD	C5-C6-S-O8
33	C	518	DGD	C5D-C6D-O5D-C1E
24	B	513	CLA	C16-C17-C18-C20
24	A	406	CLA	C3A-C2A-CAA-CBA
24	C	514	CLA	CAA-CBA-CGA-O1A
31	D	407	LHG	C12-C13-C14-C15
24	B	514	CLA	CAA-CBA-CGA-O1A
24	A	408	CLA	C11-C12-C13-C15
24	D	401	CLA	C16-C17-C18-C20
24	D	403	CLA	C15-C16-C17-C18
28	C	501	LMG	C31-C32-C33-C34
24	B	512	CLA	C8-C10-C11-C12
31	D	408	LHG	C30-C31-C32-C33
27	A	410	SQD	C10-C11-C12-C13
24	B	502	CLA	C14-C13-C15-C16
24	B	505	CLA	C11-C10-C8-C9
24	B	515	CLA	C11-C10-C8-C9
28	C	501	LMG	O7-C10-C11-C12
24	B	505	CLA	C11-C12-C13-C15
24	C	510	CLA	C6-C7-C8-C10
24	B	515	CLA	C2B-C3B-CAB-CBB
24	C	508	CLA	C2B-C3B-CAB-CBB
26	C	516	BCR	C5-C6-C7-C8
26	D	405	BCR	C5-C6-C7-C8
34	B	522	3PH	O21-C21-C22-C23
24	B	503	CLA	C2-C1-O2A-CGA
24	B	510	CLA	C2-C1-O2A-CGA
24	B	511	CLA	C2-C1-O2A-CGA
31	D	408	LHG	C32-C33-C34-C35
36	D	406	PL9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
36	D	406	PL9	C13-C14-C16-C17
28	C	521	LMG	O7-C10-C11-C12
27	A	410	SQD	C25-C26-C27-C28
27	M	101	SQD	C4-C5-C6-S
33	C	519	DGD	O2G-C1B-C2B-C3B
24	B	513	CLA	C2-C3-C5-C6
35	B	523	DGA	CA7-CA8-CA9-CAA
28	A	411	LMG	C31-C32-C33-C34
24	B	501	CLA	C14-C13-C15-C16
24	B	506	CLA	C6-C7-C8-C9
25	D	402	PHO	C6-C7-C8-C9
31	D	408	LHG	C2-C3-O3-P
24	B	507	CLA	CAA-CBA-CGA-O2A
28	H	102	LMG	C12-C13-C14-C15
24	B	515	CLA	C4B-C3B-CAB-CBB
24	C	506	CLA	C4B-C3B-CAB-CBB
24	D	403	CLA	C4B-C3B-CAB-CBB
28	C	522	LMG	C11-C10-O7-C8
31	D	410	LHG	C24-C23-O8-C6
24	C	506	CLA	CAA-CBA-CGA-O2A
24	C	511	CLA	C16-C17-C18-C20
27	M	101	SQD	C5-C6-S-O7
24	D	403	CLA	C4-C3-C5-C6
24	B	511	CLA	C11-C12-C13-C15
24	C	512	CLA	C6-C7-C8-C10
24	D	401	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
28	C	501	LMG	C16-C17-C18-C19
24	C	509	CLA	CAA-CBA-CGA-O2A
24	B	514	CLA	C2A-CAA-CBA-CGA
24	C	513	CLA	CAA-CBA-CGA-O2A
24	C	510	CLA	C4-C3-C5-C6
33	C	519	DGD	O1B-C1B-C2B-C3B
35	B	523	DGA	CA4-CA5-CA6-CA7
24	B	516	CLA	C2A-CAA-CBA-CGA
28	H	102	LMG	C40-C41-C42-C43
26	C	516	BCR	C15-C16-C17-C18
28	C	521	LMG	O9-C10-C11-C12
34	B	522	3PH	O22-C21-C22-C23
34	B	522	3PH	O31-C31-C32-C33
27	M	101	SQD	O5-C5-C6-S
31	D	408	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	C	518	DGD	O6D-C5D-C6D-O5D
33	B	521	DGD	O2G-C1B-C2B-C3B
24	C	508	CLA	C16-C17-C18-C20
37	E	101	HEM	CAA-CBA-CGA-O2A
24	C	506	CLA	CAA-CBA-CGA-O1A
28	H	102	LMG	C14-C15-C16-C17
25	A	407	PHO	C15-C16-C17-C18
24	C	509	CLA	CAA-CBA-CGA-O1A
24	C	504	CLA	CAA-CBA-CGA-O2A
24	B	507	CLA	CAA-CBA-CGA-O1A
28	C	522	LMG	O7-C10-C11-C12
33	C	518	DGD	O2G-C1B-C2B-C3B
24	B	508	CLA	CAA-CBA-CGA-O2A
24	C	513	CLA	CAA-CBA-CGA-O1A
24	B	504	CLA	CAA-CBA-CGA-O2A
24	B	509	CLA	CAA-CBA-CGA-O2A
34	B	522	3PH	O32-C31-C32-C33
28	B	520	LMG	C14-C15-C16-C17

There are no ring outliers.

70 monomers are involved in 245 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	408	LHG	4	0
26	C	515	BCR	2	0
24	D	404	CLA	8	0
24	B	506	CLA	2	0
24	B	509	CLA	3	0
31	D	407	LHG	2	0
24	B	504	CLA	9	0
25	A	407	PHO	5	0
24	A	405	CLA	4	0
33	C	519	DGD	4	0
34	B	522	3PH	4	0
28	C	501	LMG	4	0
26	C	516	BCR	5	0
28	D	409	LMG	1	0
31	L	101	LHG	1	0
39	J	102	LMU	4	0
24	C	506	CLA	3	0
24	B	513	CLA	6	0
24	B	501	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	503	CLA	2	0
24	C	507	CLA	8	0
26	A	409	BCR	5	0
31	D	410	LHG	5	0
33	B	521	DGD	2	0
26	J	101	BCR	2	0
26	B	517	BCR	5	0
24	C	505	CLA	1	0
28	A	411	LMG	1	0
24	B	514	CLA	6	0
24	A	408	CLA	8	0
35	B	523	DGA	3	0
24	B	507	CLA	5	0
37	E	101	HEM	2	0
33	C	518	DGD	1	0
33	C	520	DGD	2	0
24	B	512	CLA	5	0
36	D	406	PL9	1	0
24	C	510	CLA	6	0
26	B	518	BCR	1	0
24	C	511	CLA	5	0
24	C	502	CLA	5	0
28	H	102	LMG	5	0
27	M	101	SQD	4	0
24	B	515	CLA	4	0
24	B	503	CLA	9	0
24	C	512	CLA	7	0
24	C	514	CLA	2	0
31	A	414	LHG	3	0
24	D	401	CLA	6	0
24	A	406	CLA	4	0
28	C	521	LMG	1	0
24	B	508	CLA	9	0
24	C	504	CLA	4	0
38	H	101	RRX	6	0
28	B	520	LMG	2	0
24	C	513	CLA	1	0
26	D	405	BCR	1	0
24	B	505	CLA	6	0
28	A	415	LMG	4	0
26	C	517	BCR	2	0
28	C	522	LMG	2	0

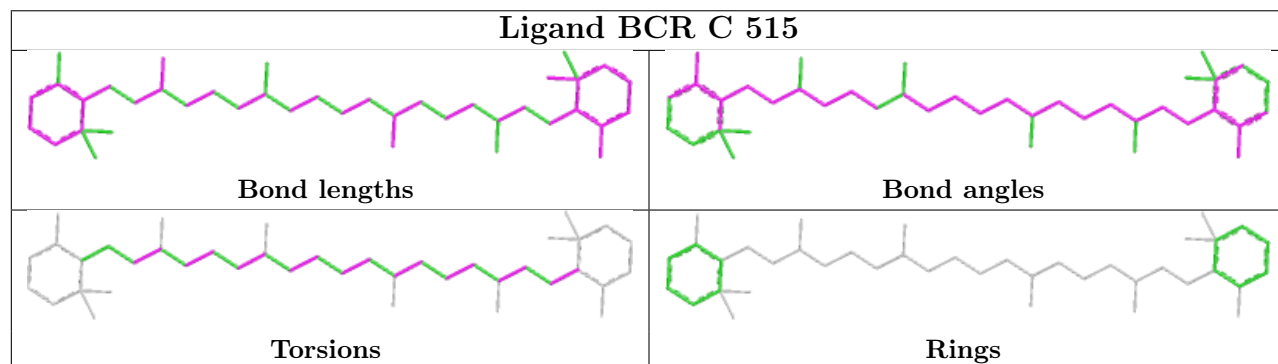
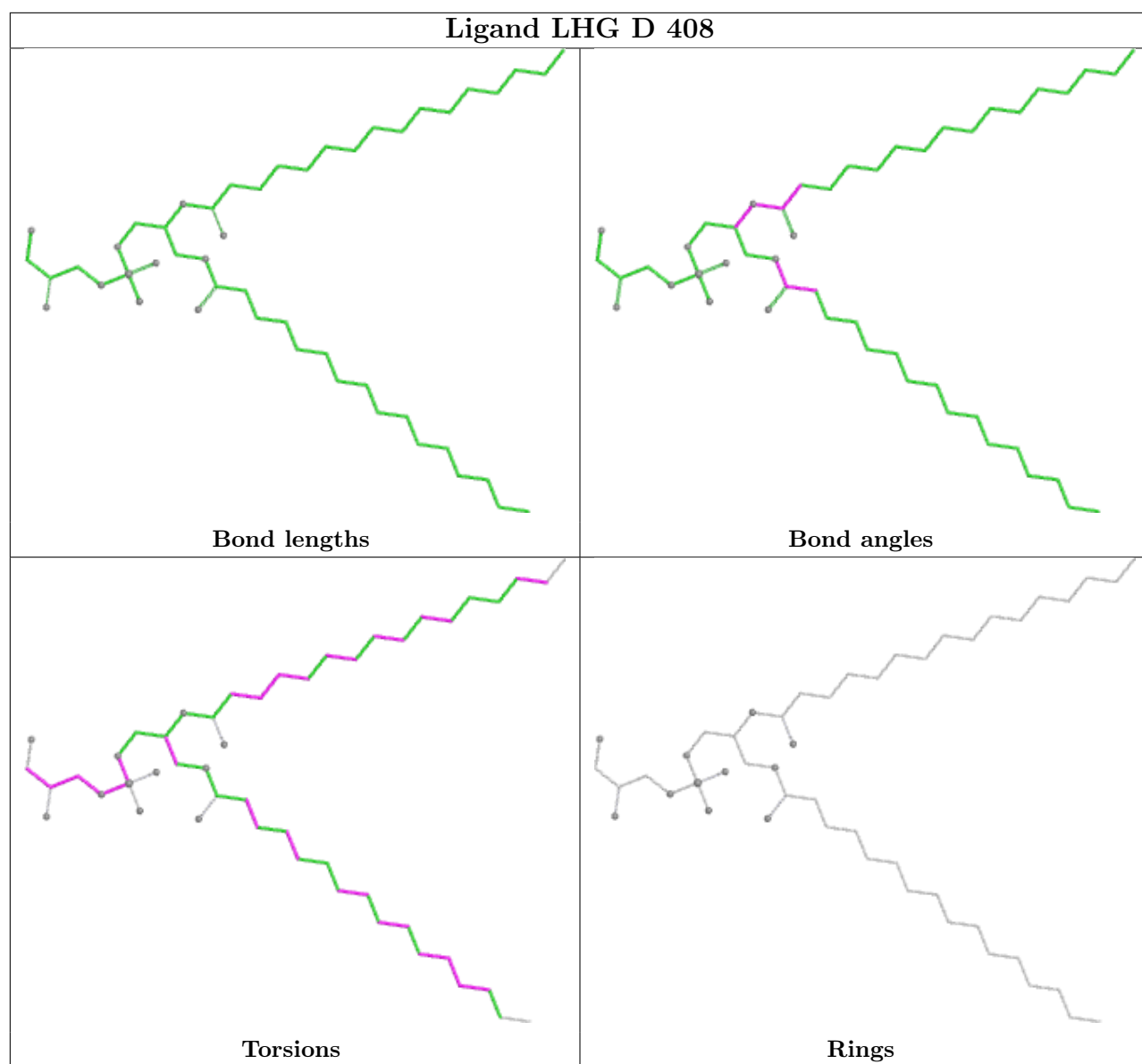
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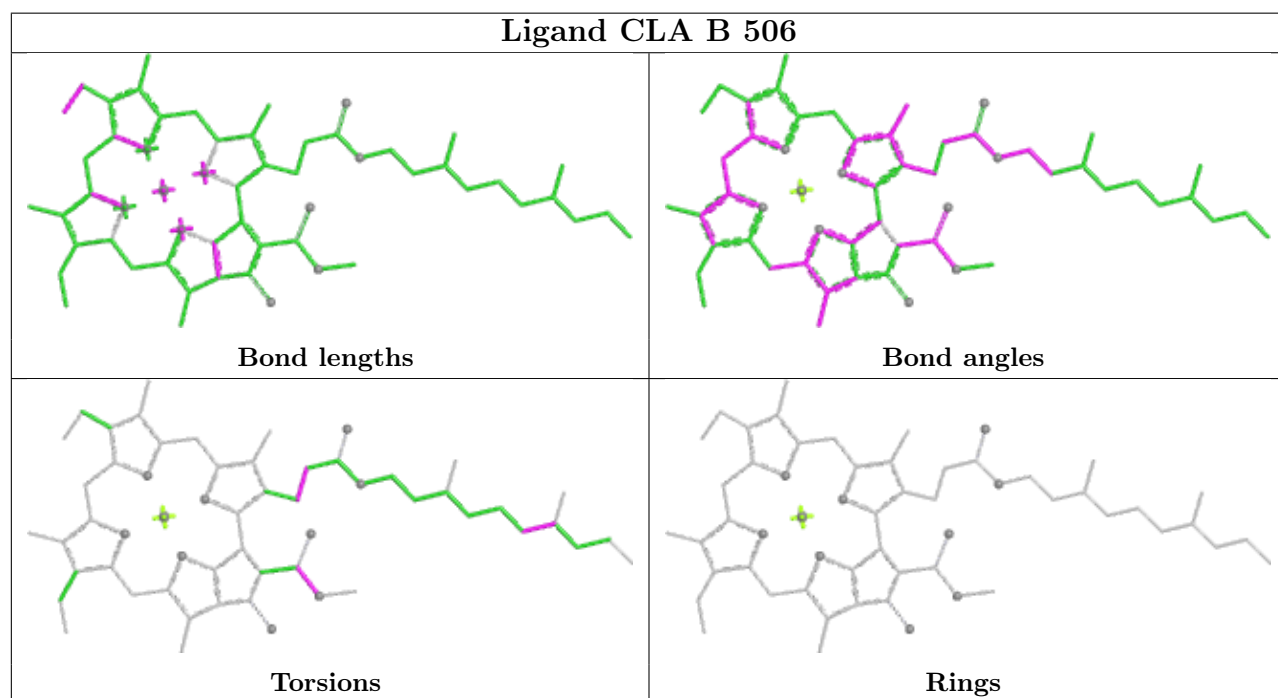
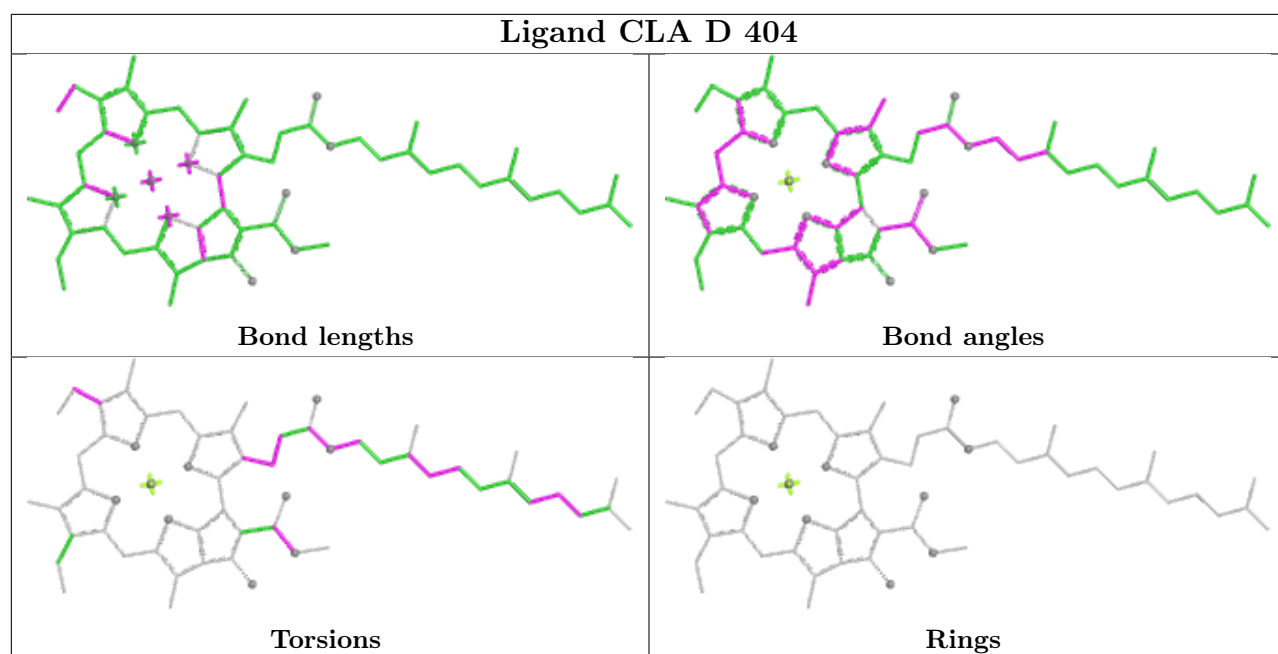


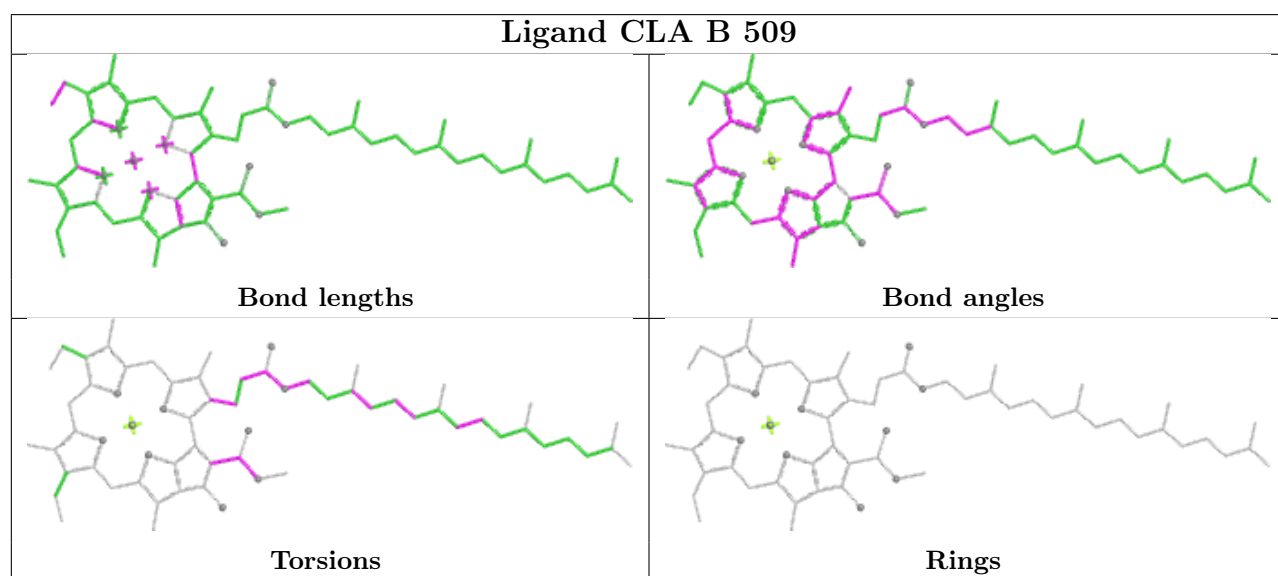
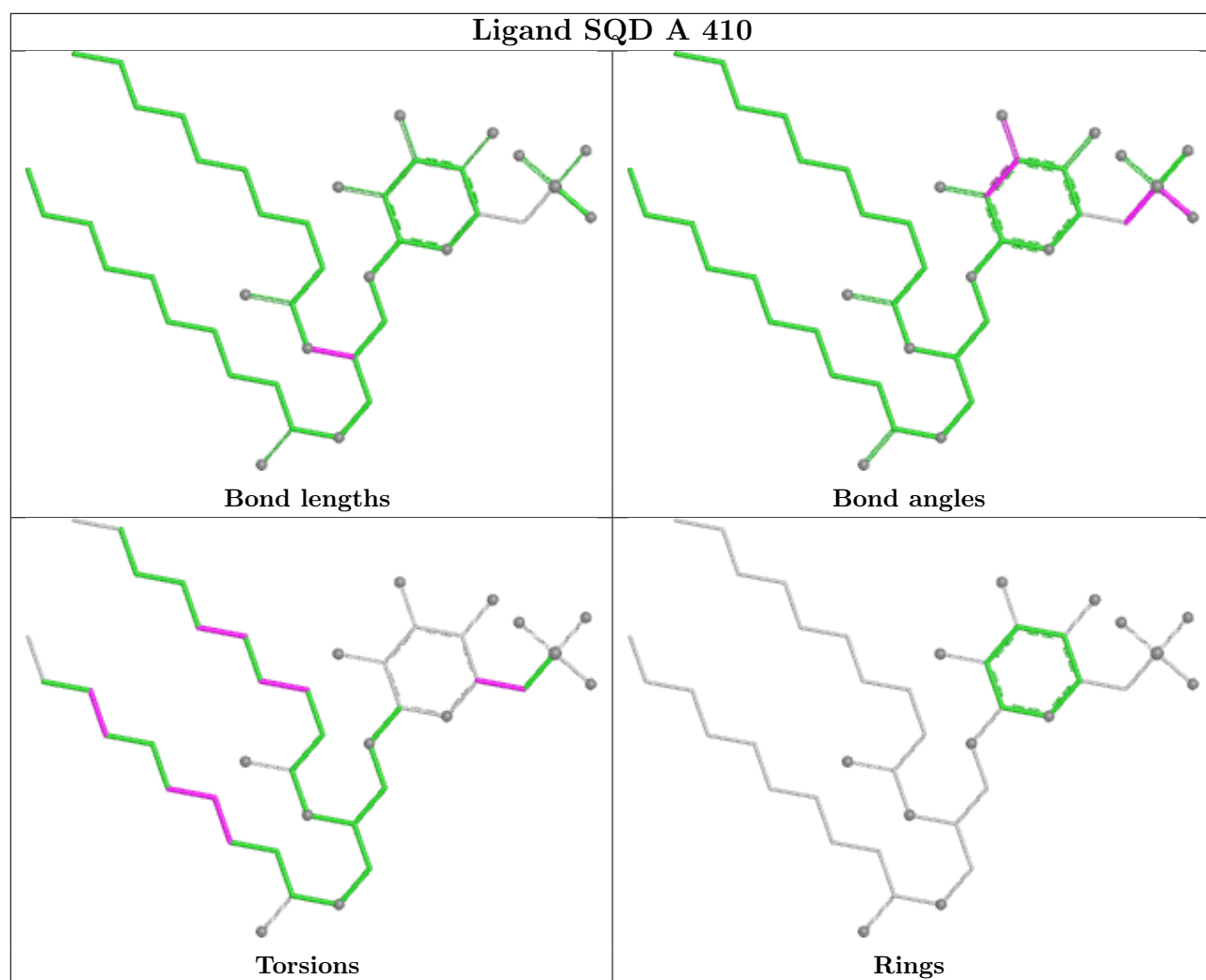
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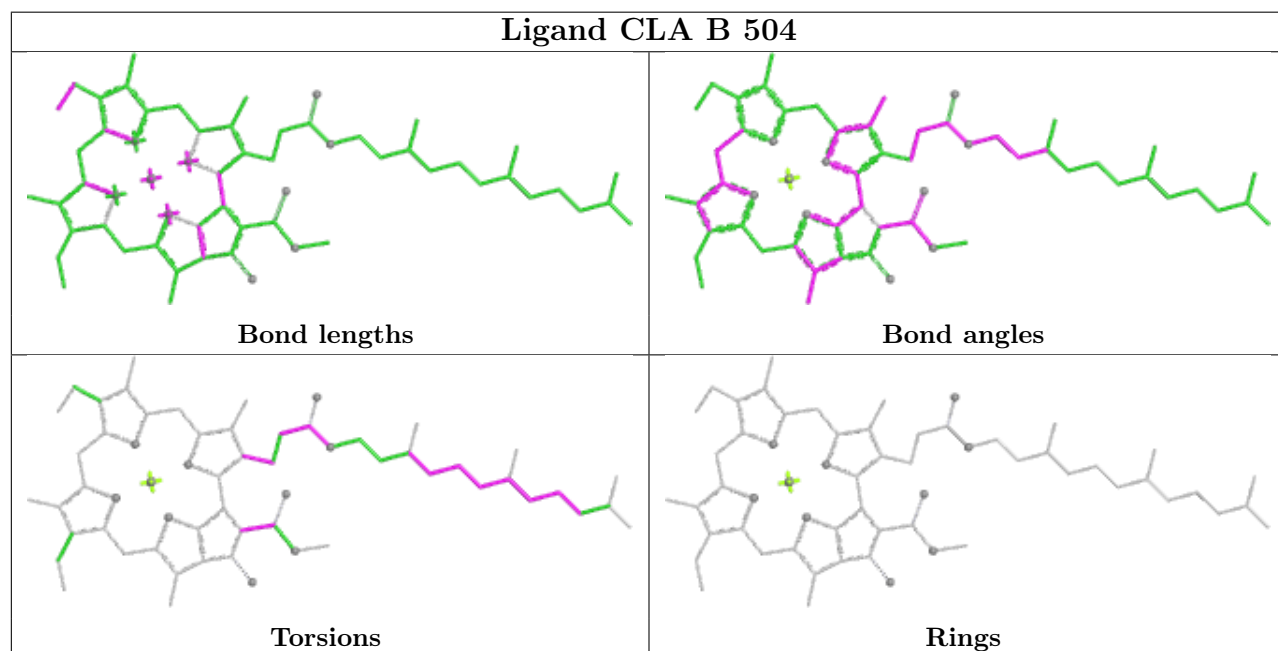
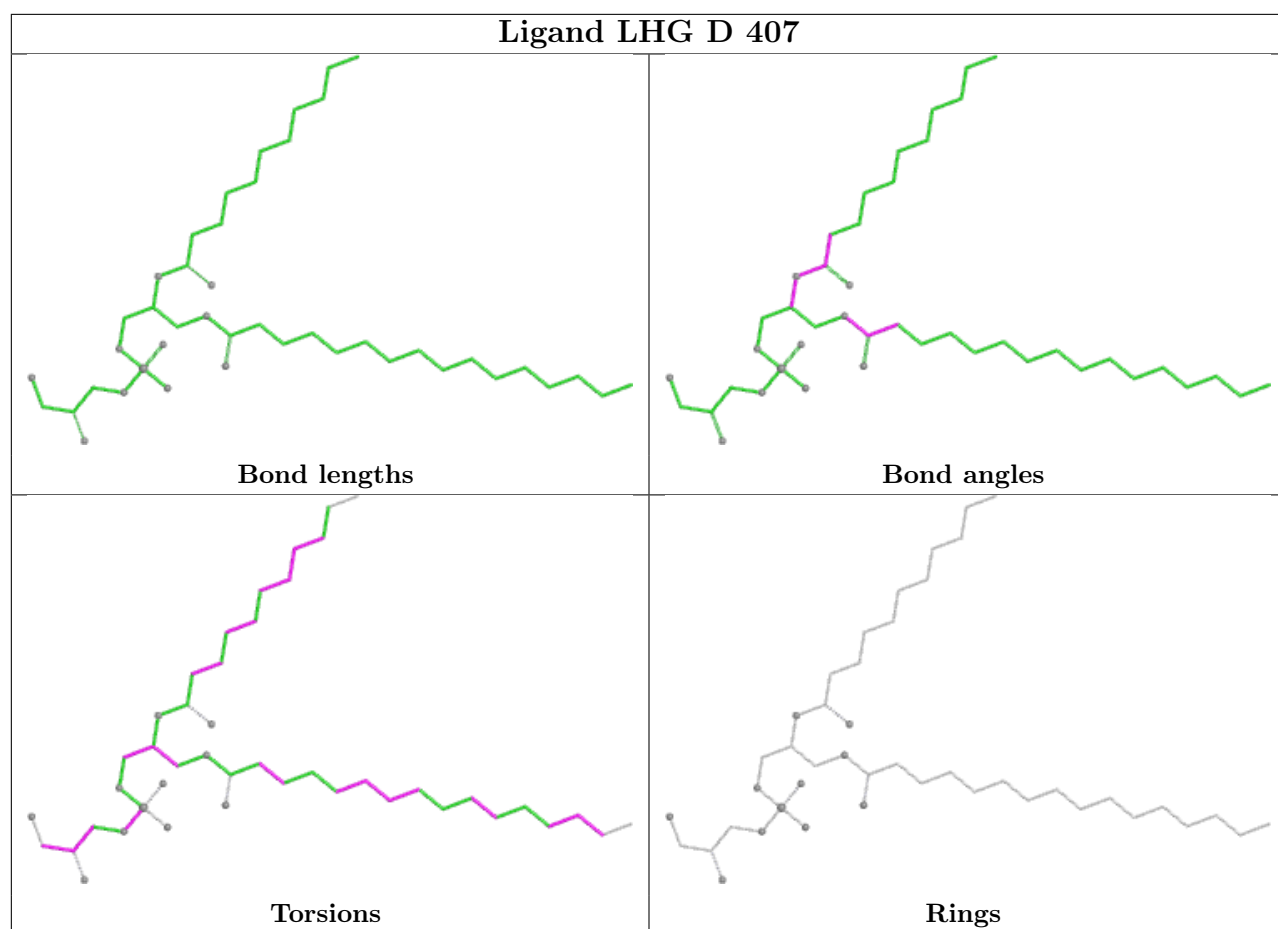
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	402	PHO	5	0
24	C	509	CLA	7	0
24	B	510	CLA	5	0
24	B	511	CLA	8	0
24	D	403	CLA	6	0
24	B	502	CLA	8	0
24	C	508	CLA	6	0
24	B	516	CLA	4	0
32	B	519	C7Z	3	0

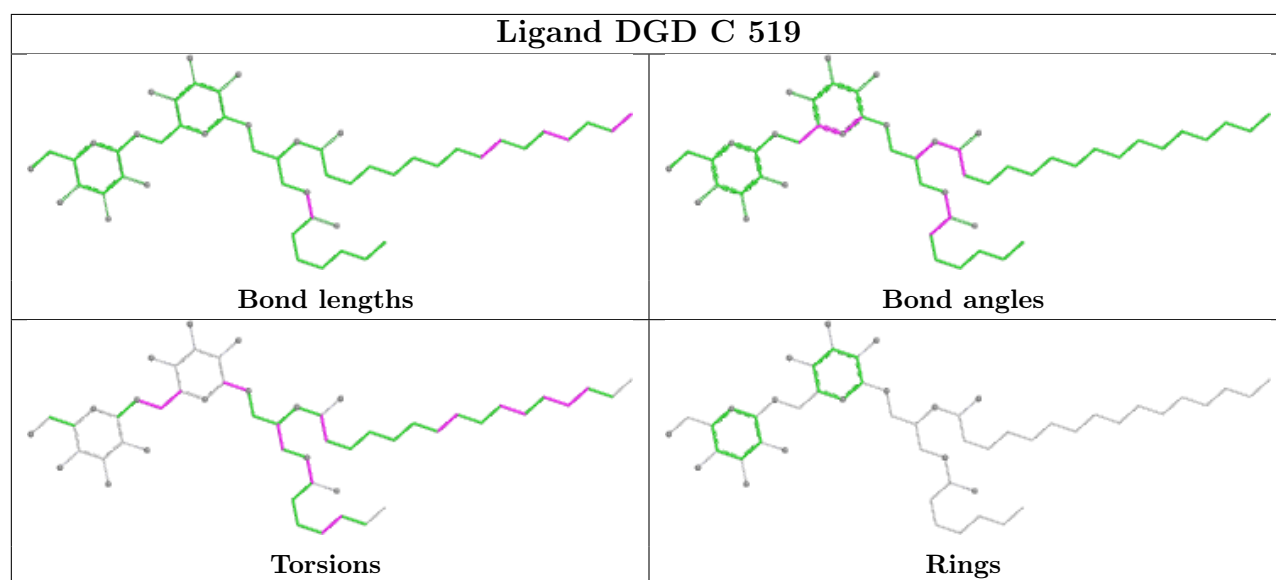
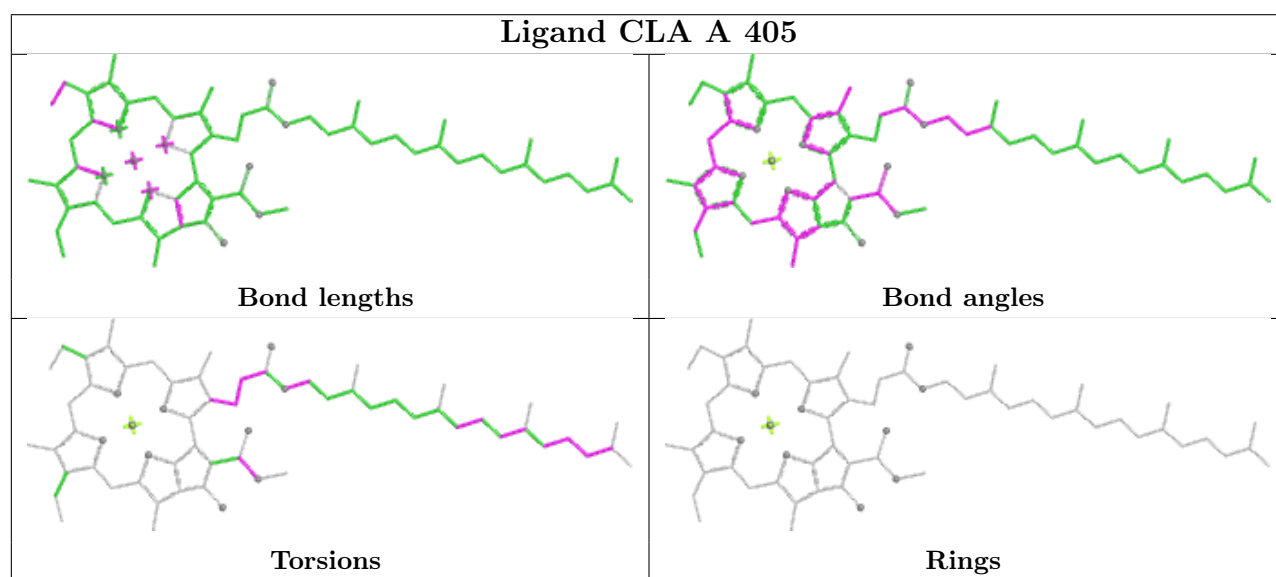
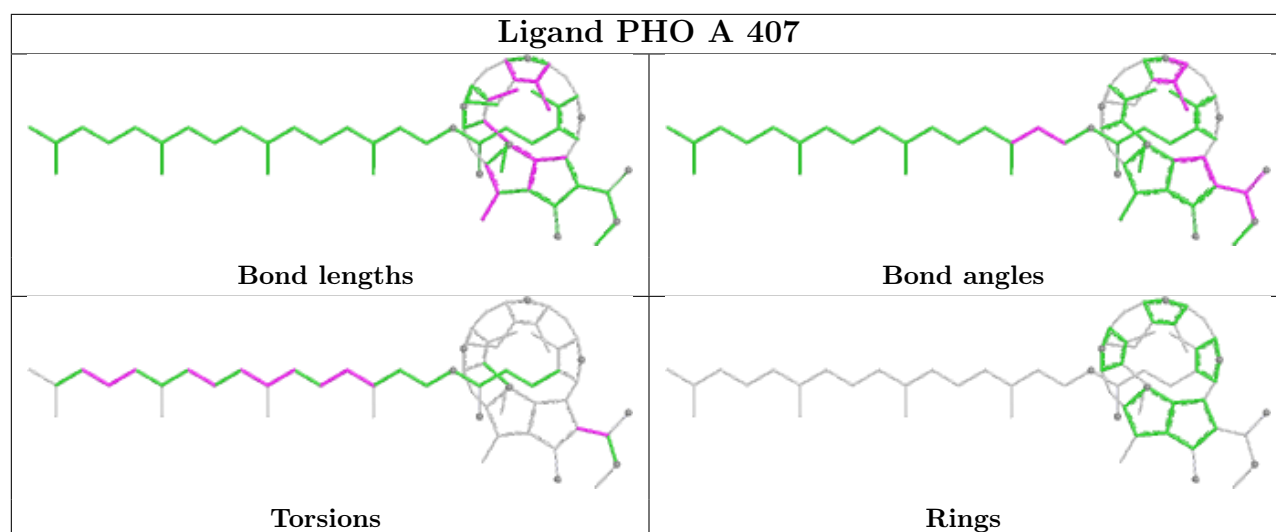
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

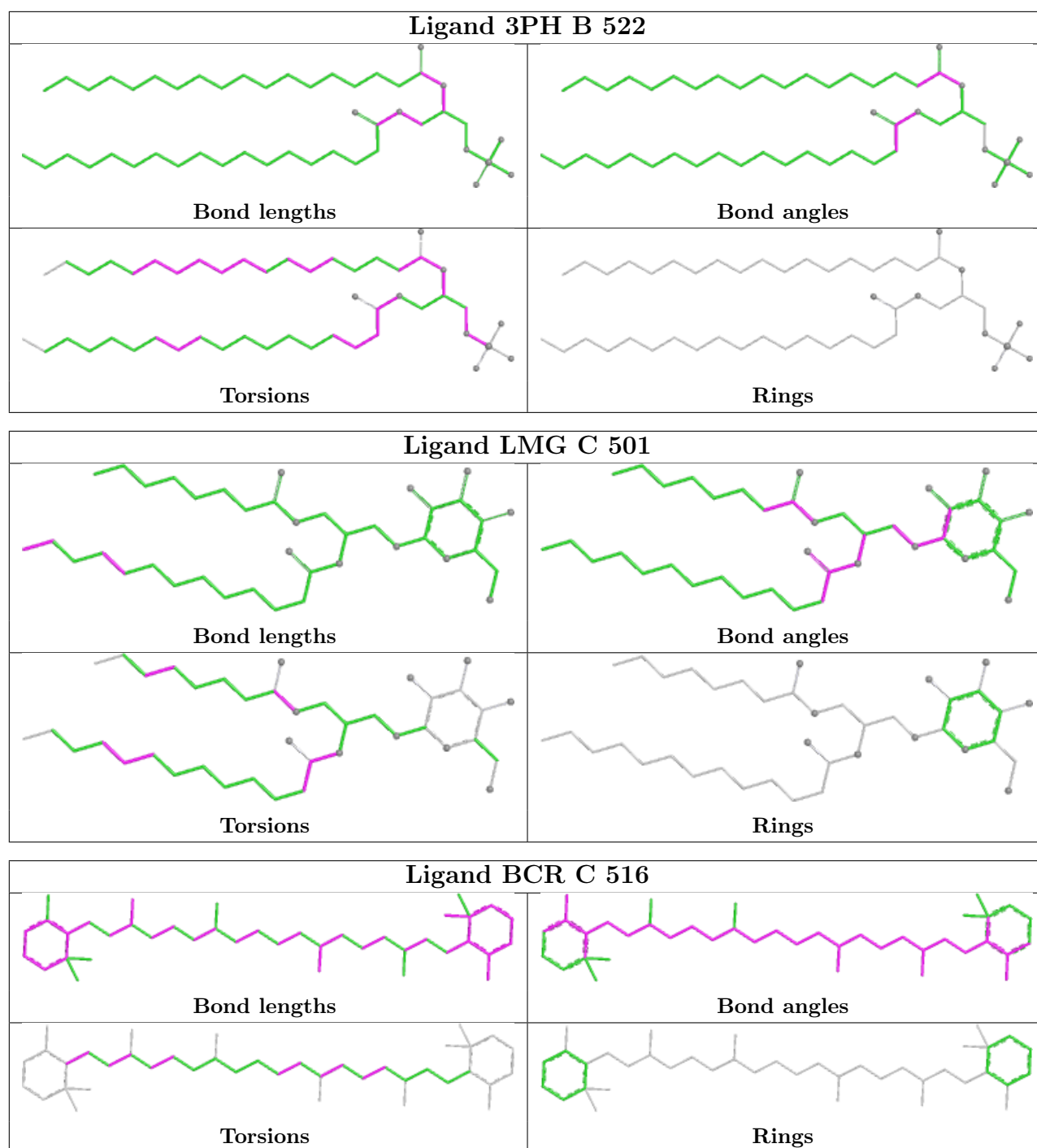


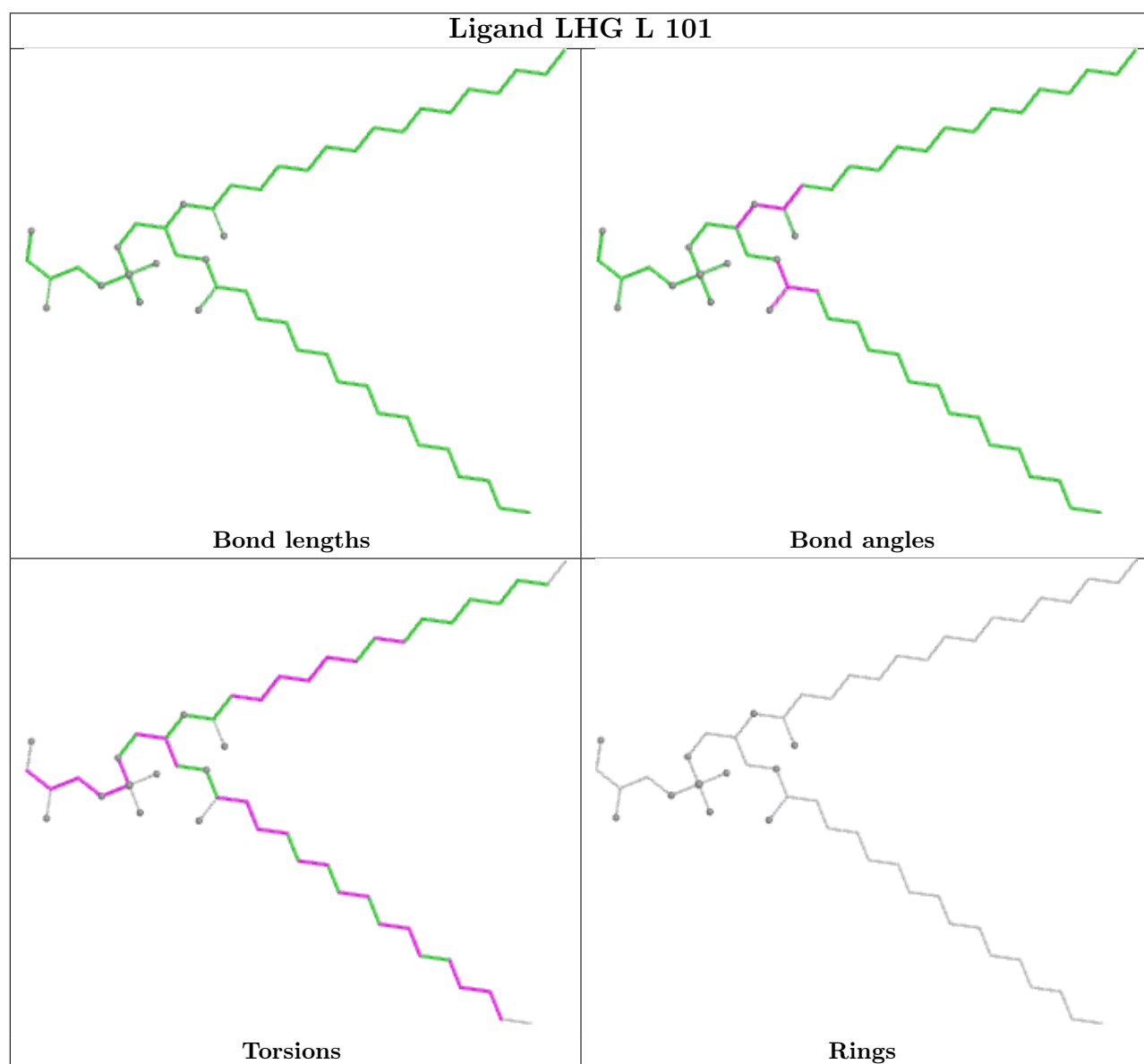
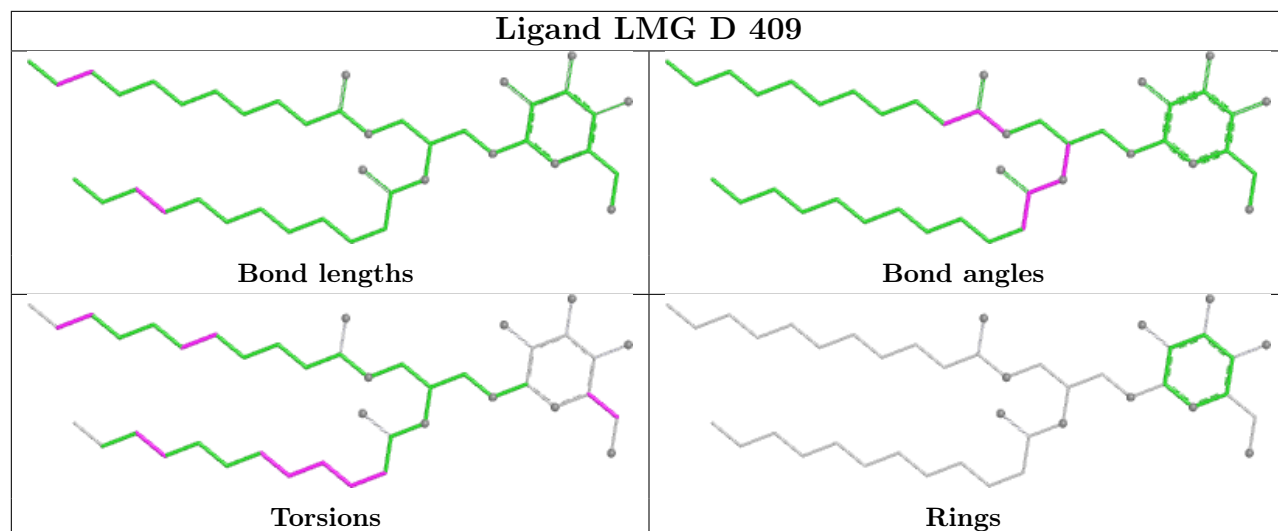




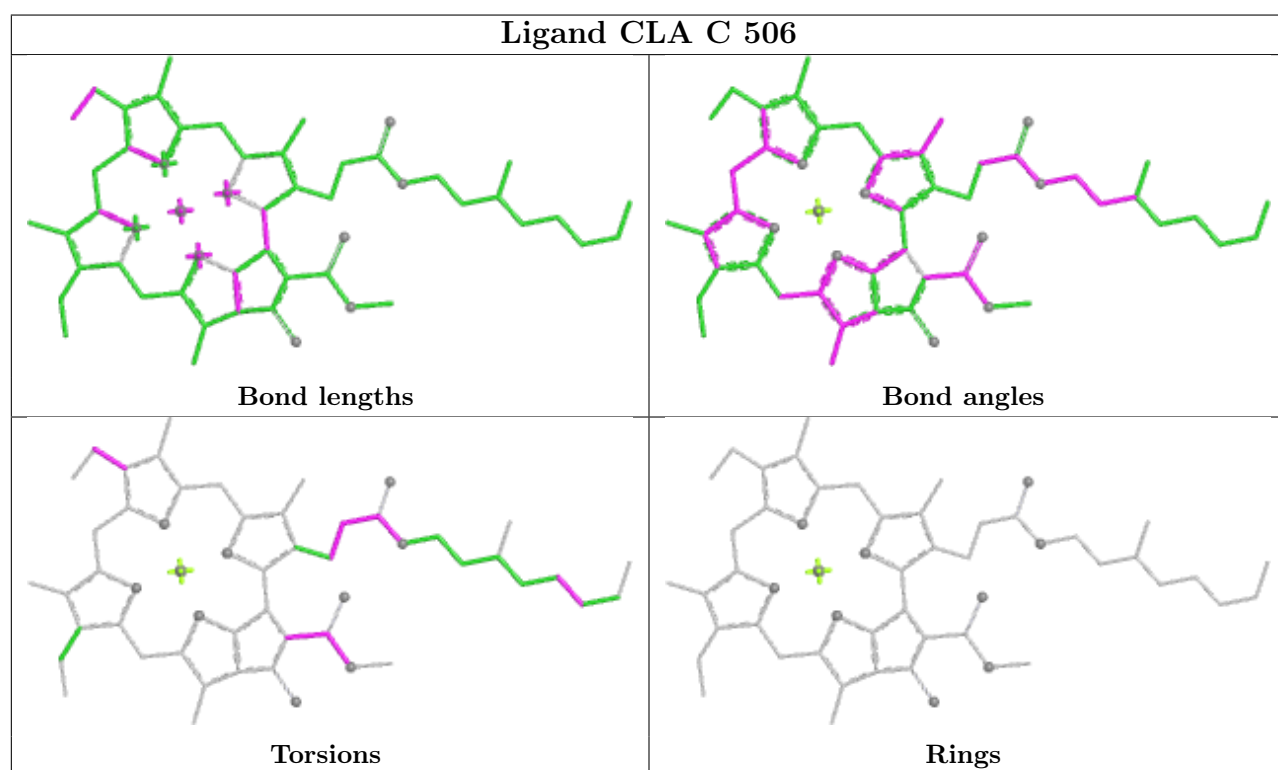
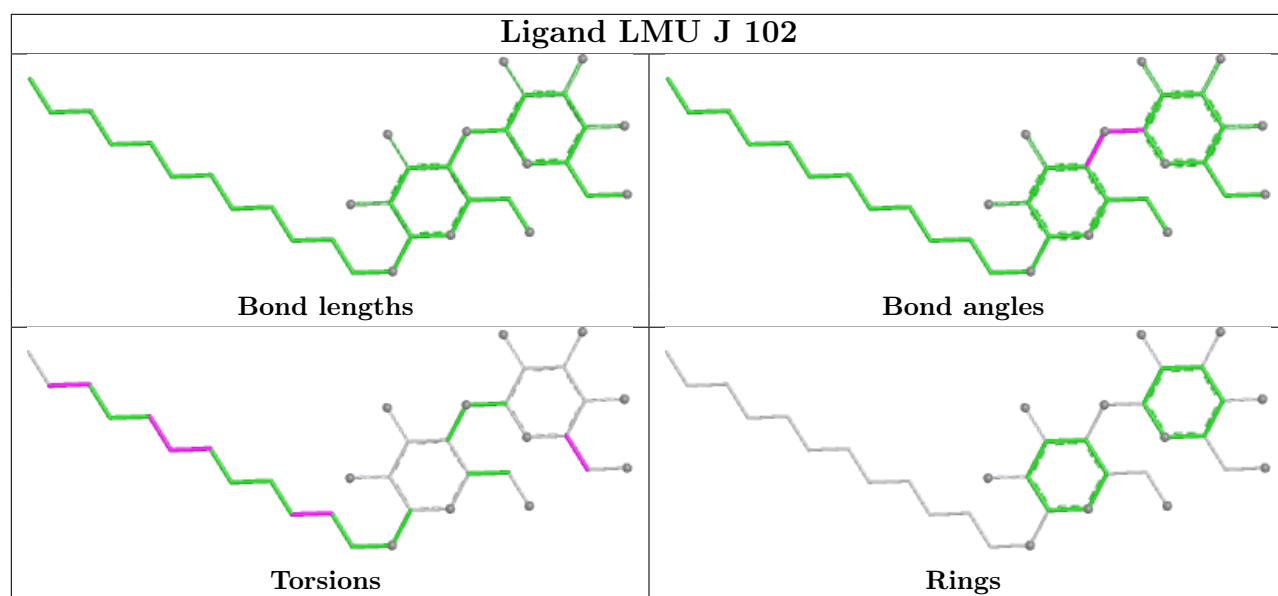


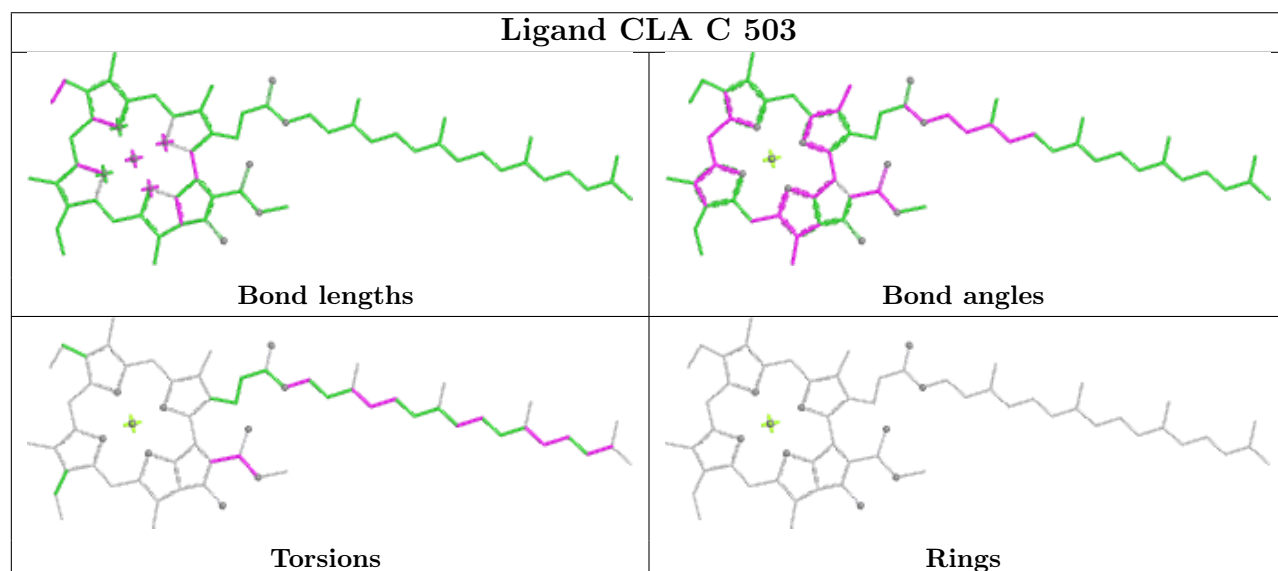
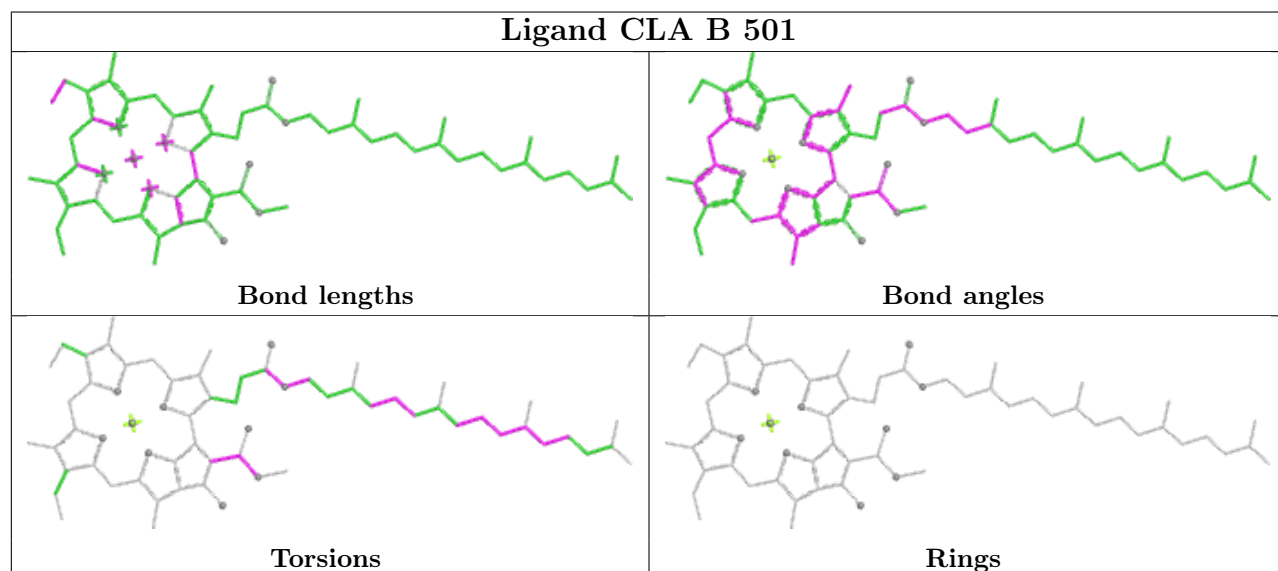
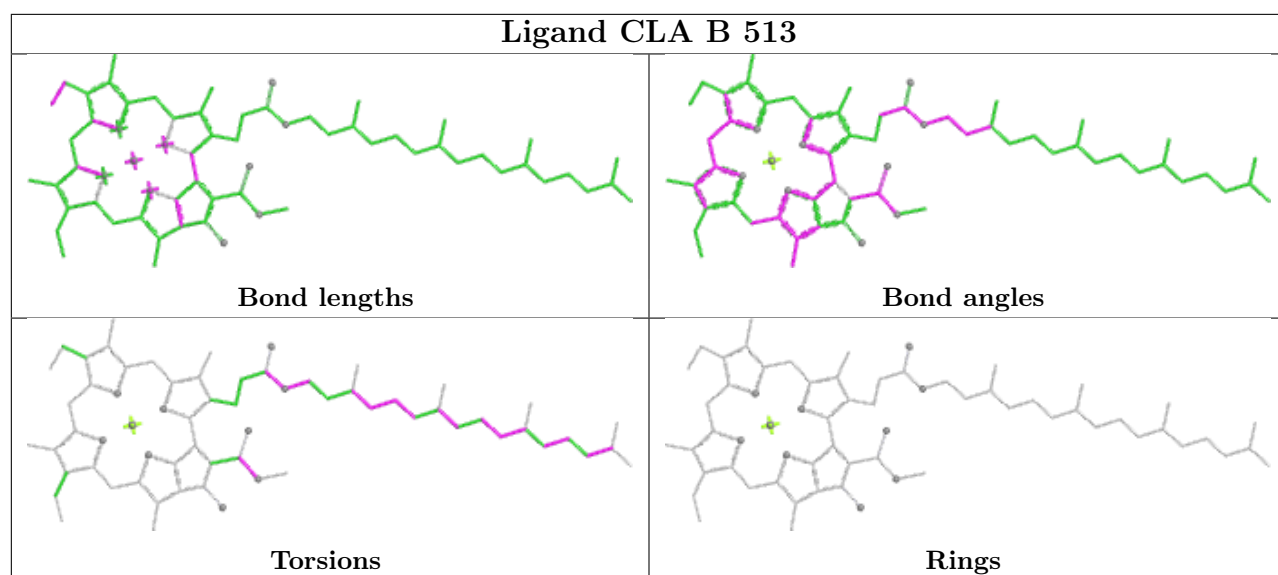


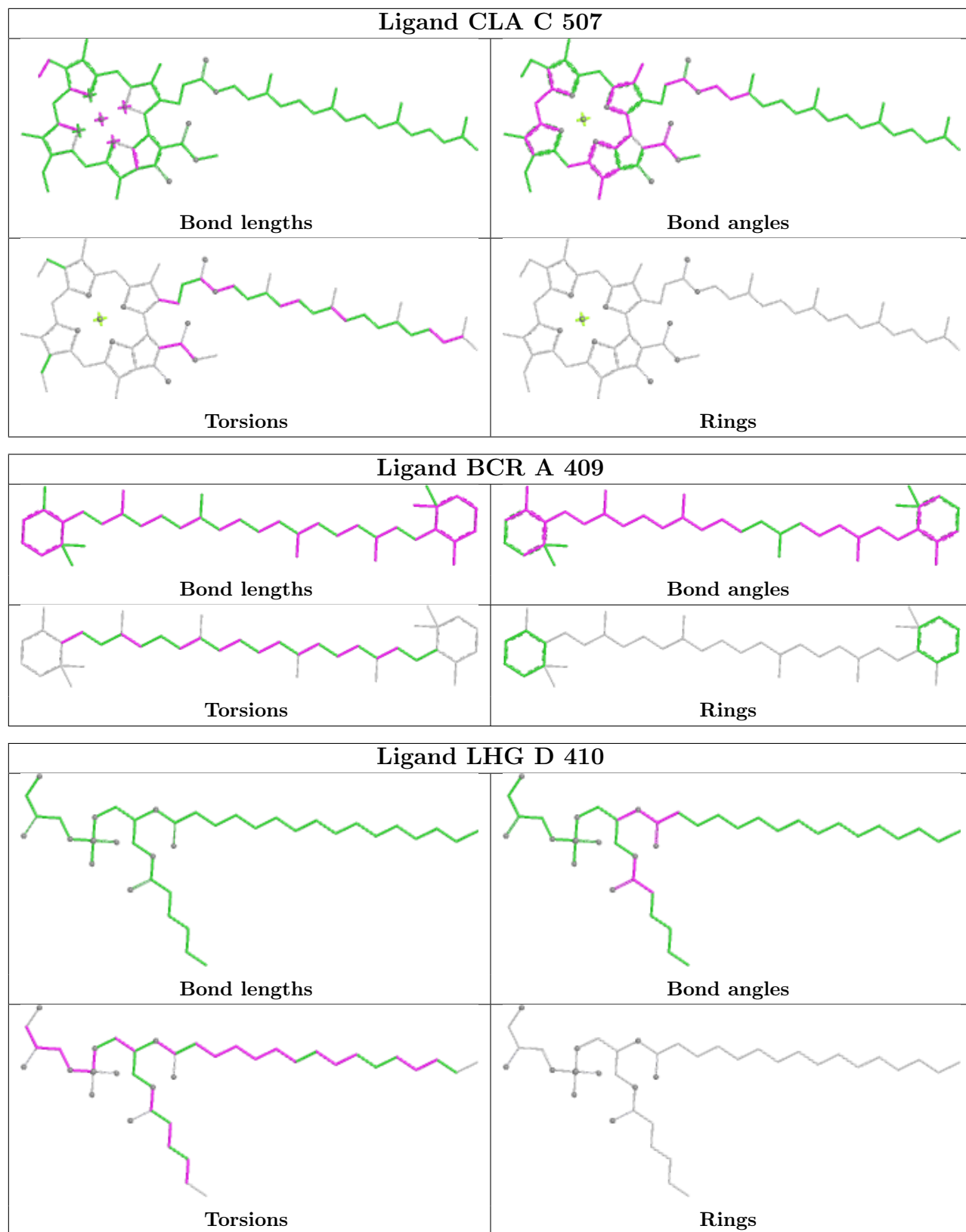


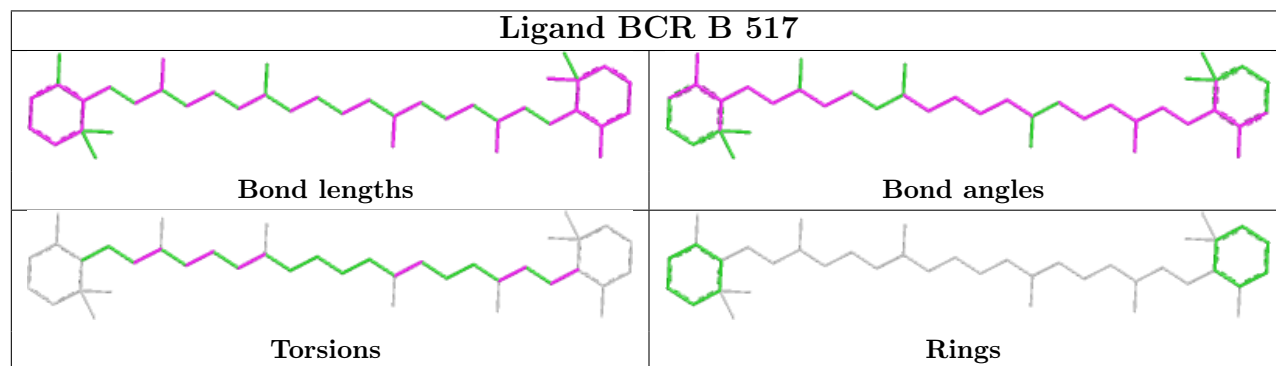
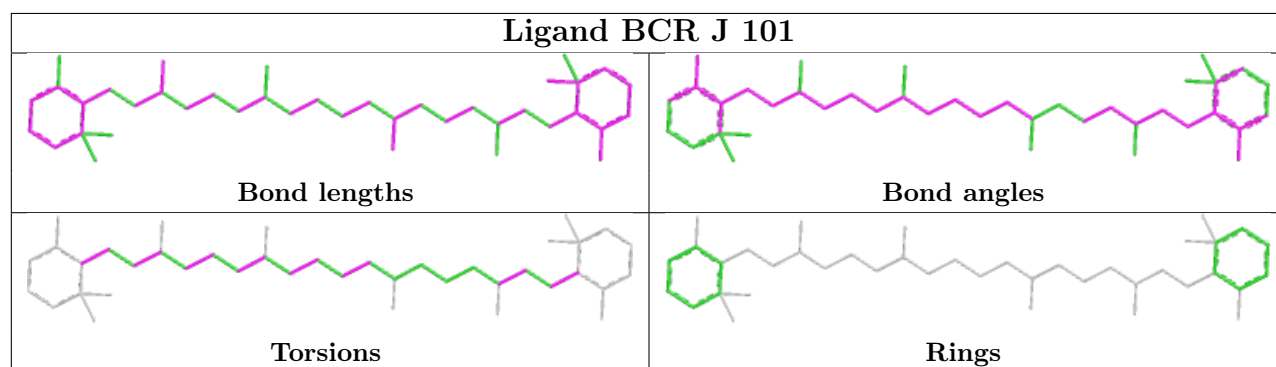
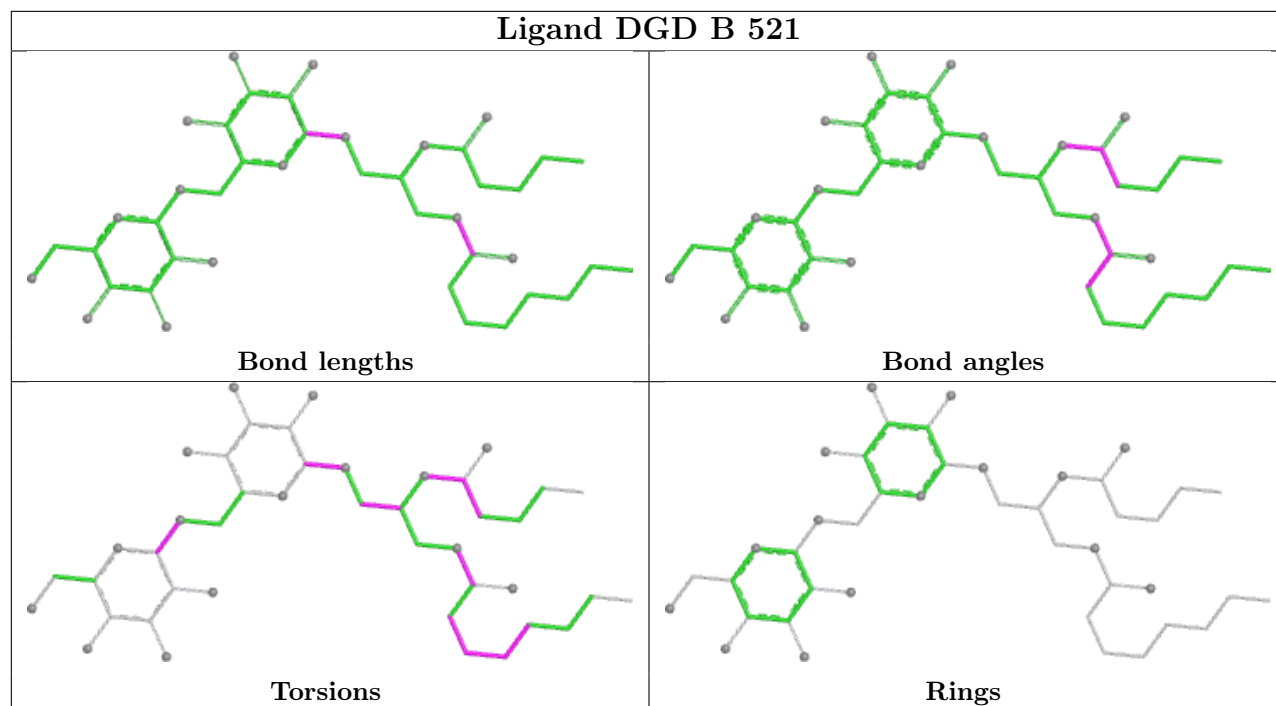


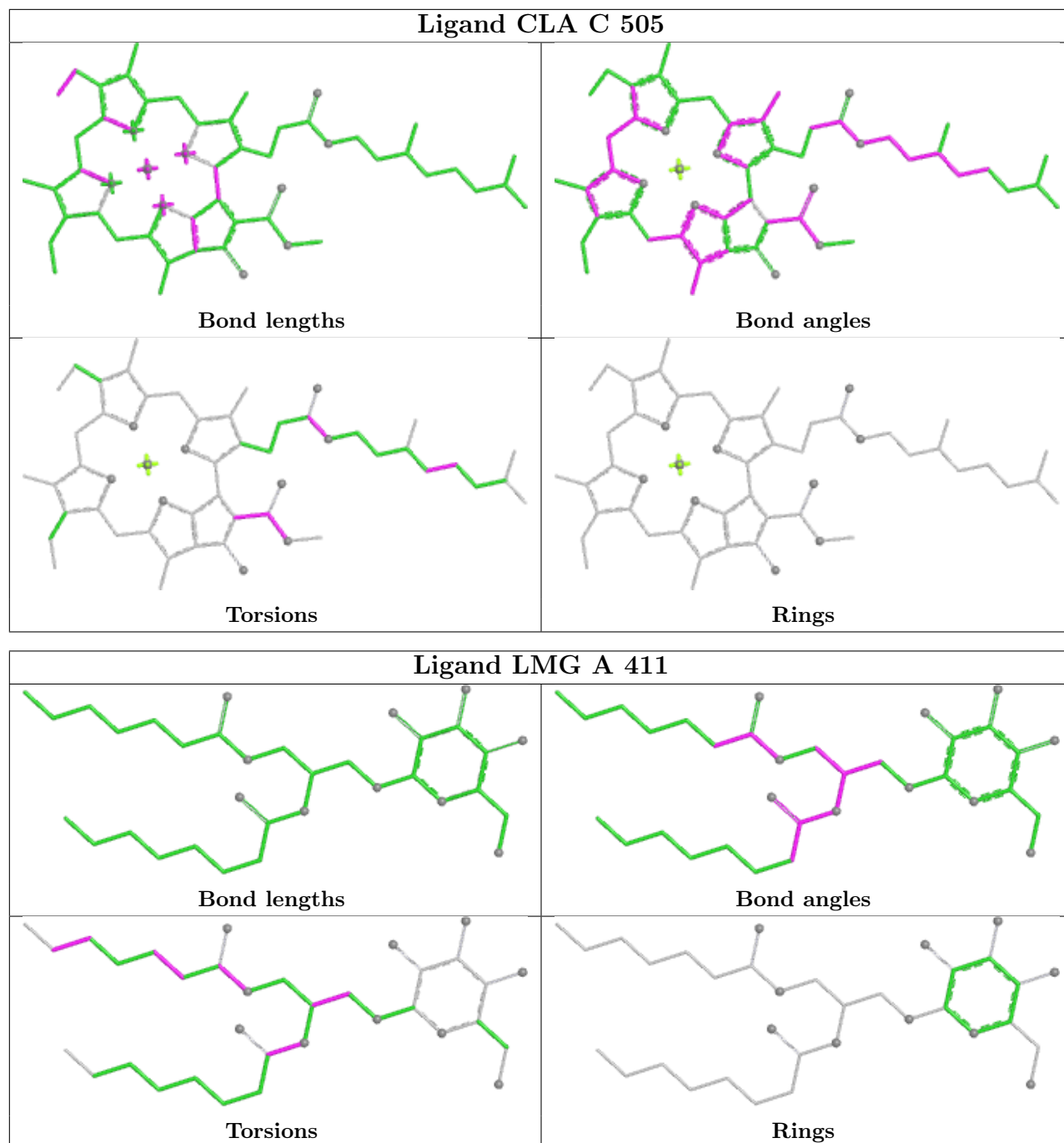


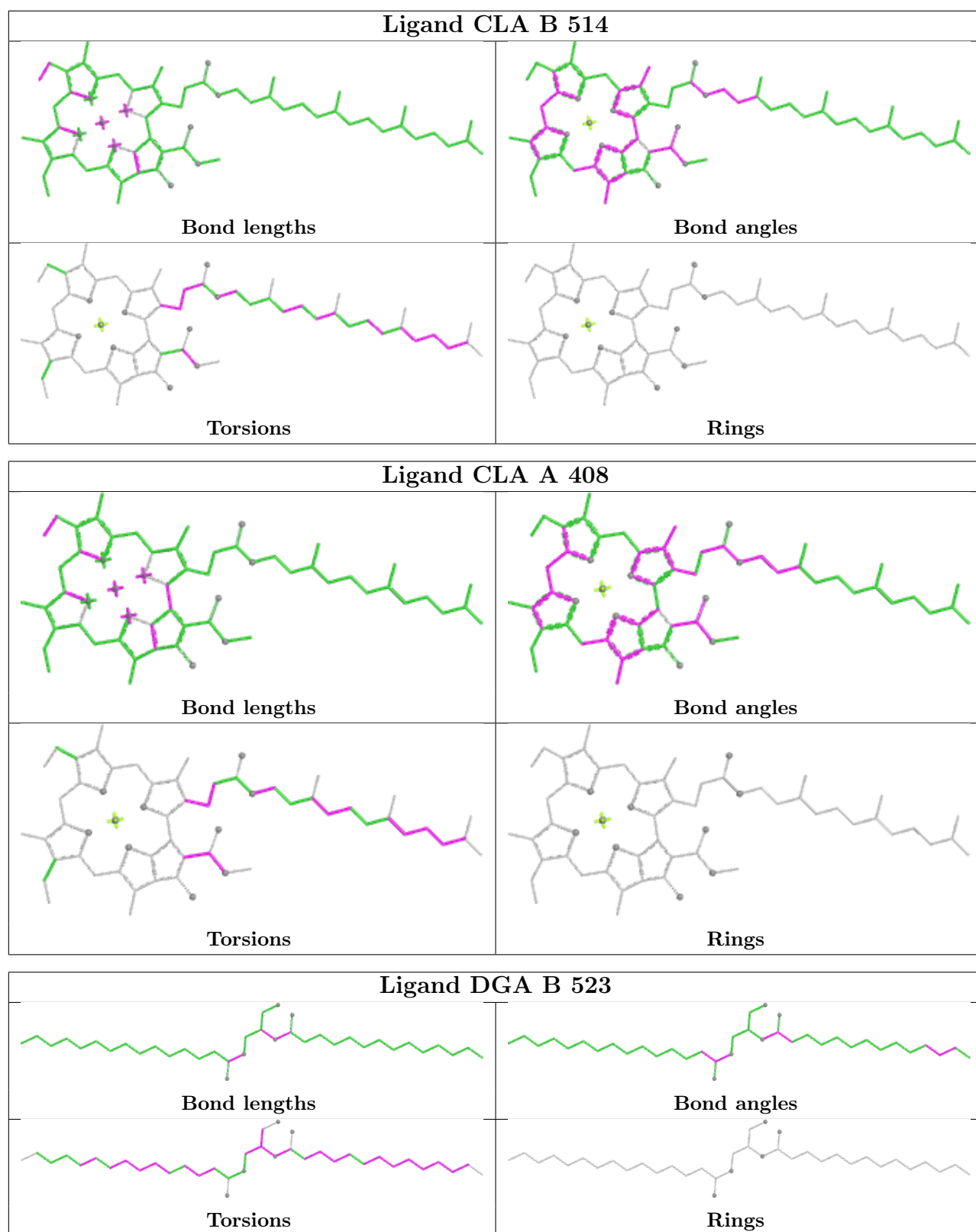




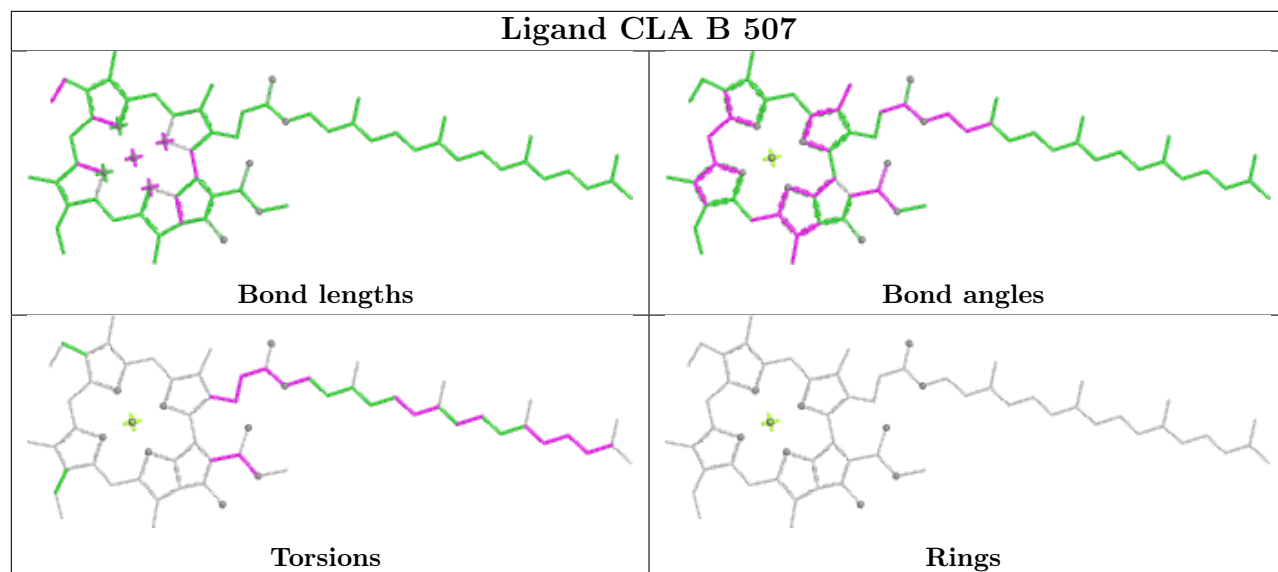




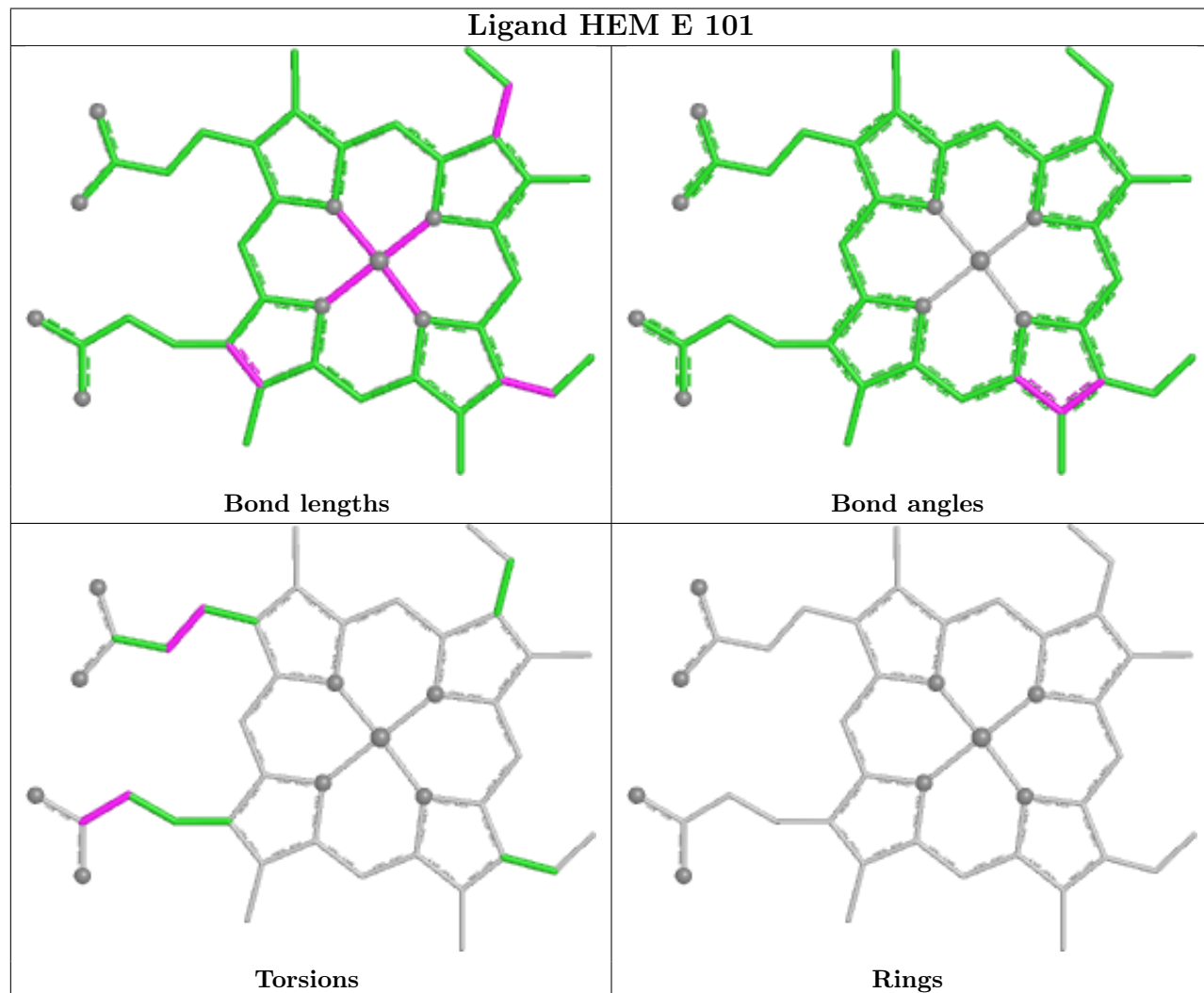


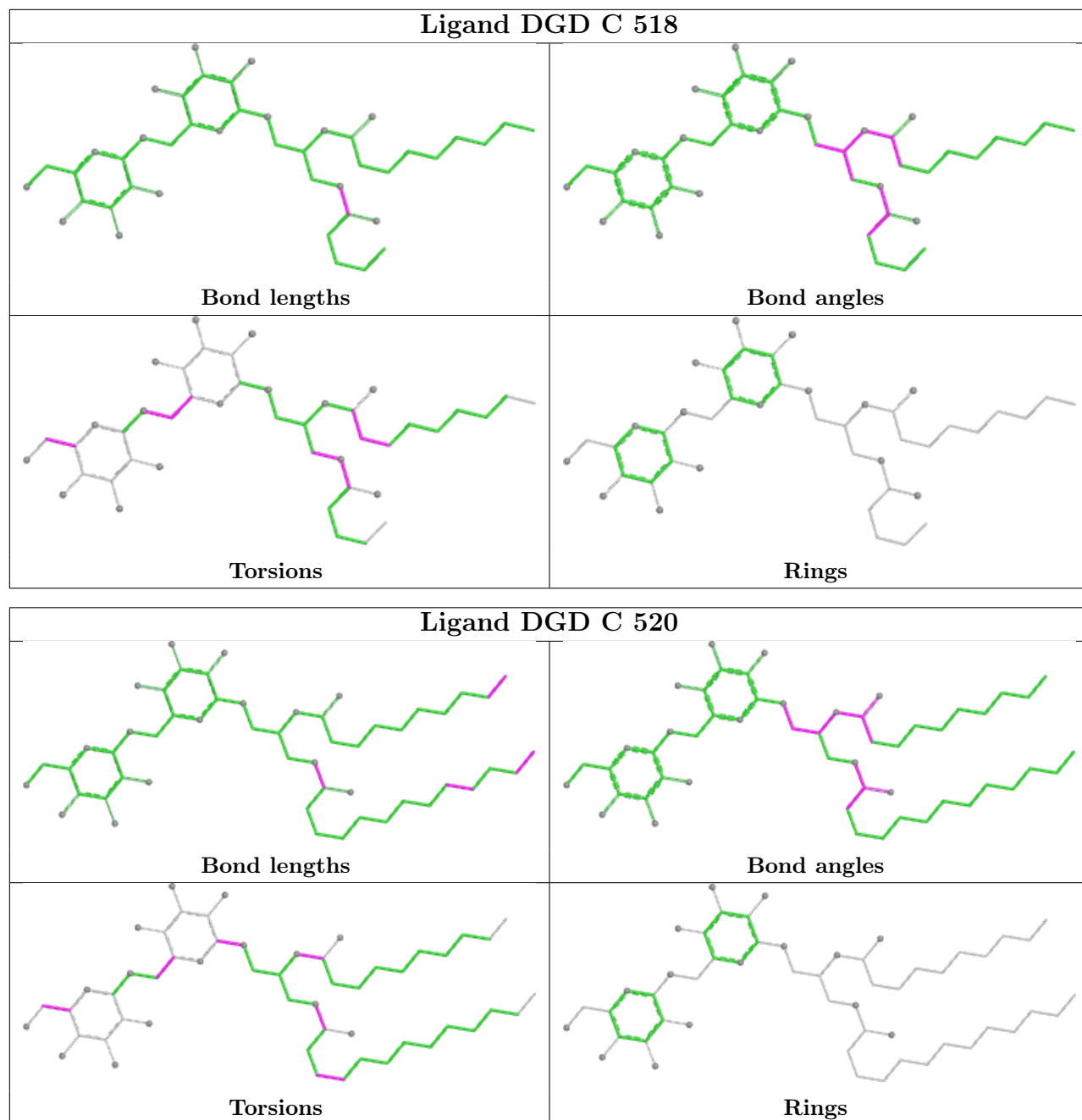


## Ligand CLA B 507

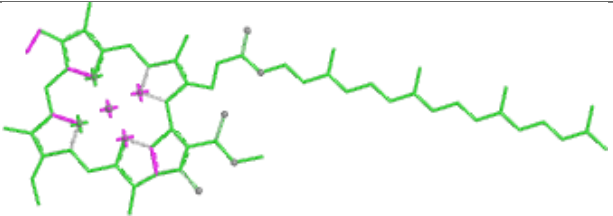
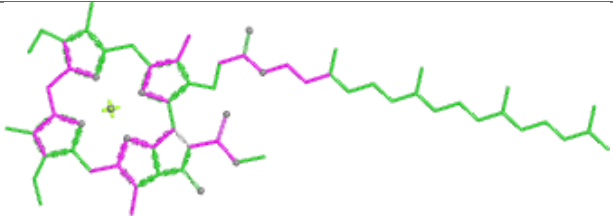
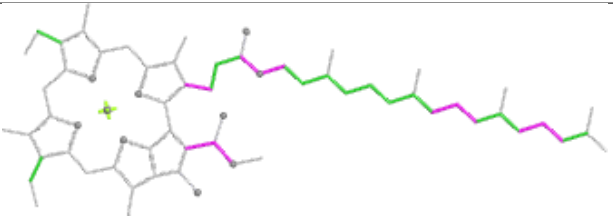
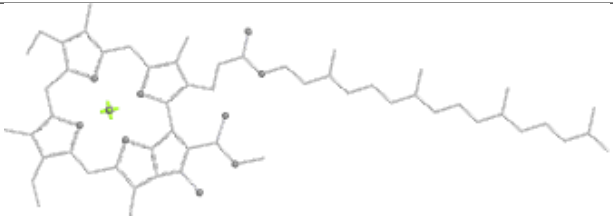
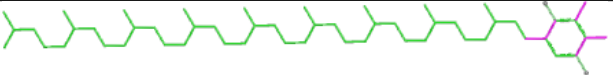
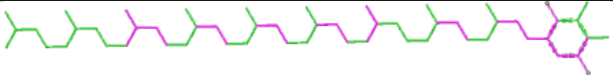
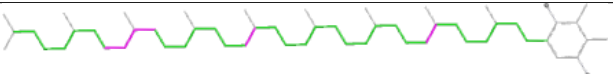
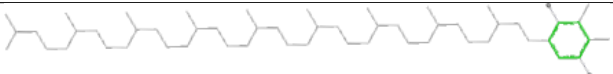
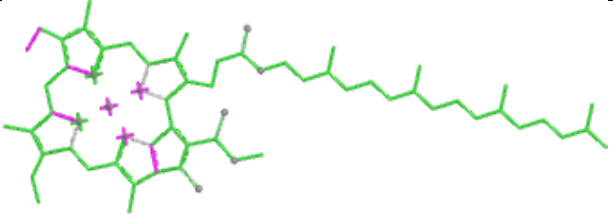
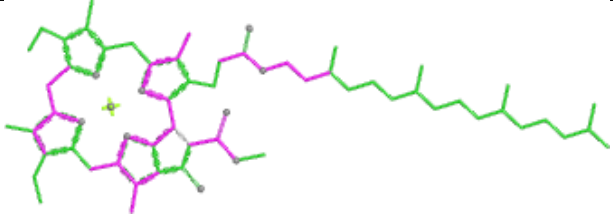
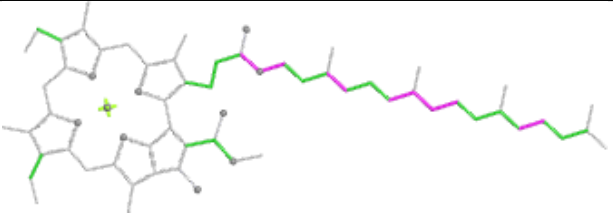
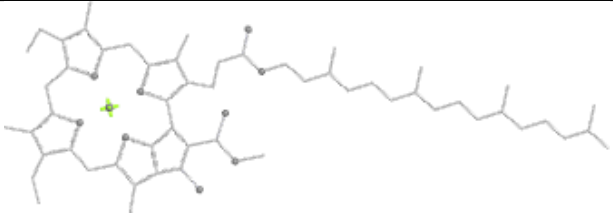


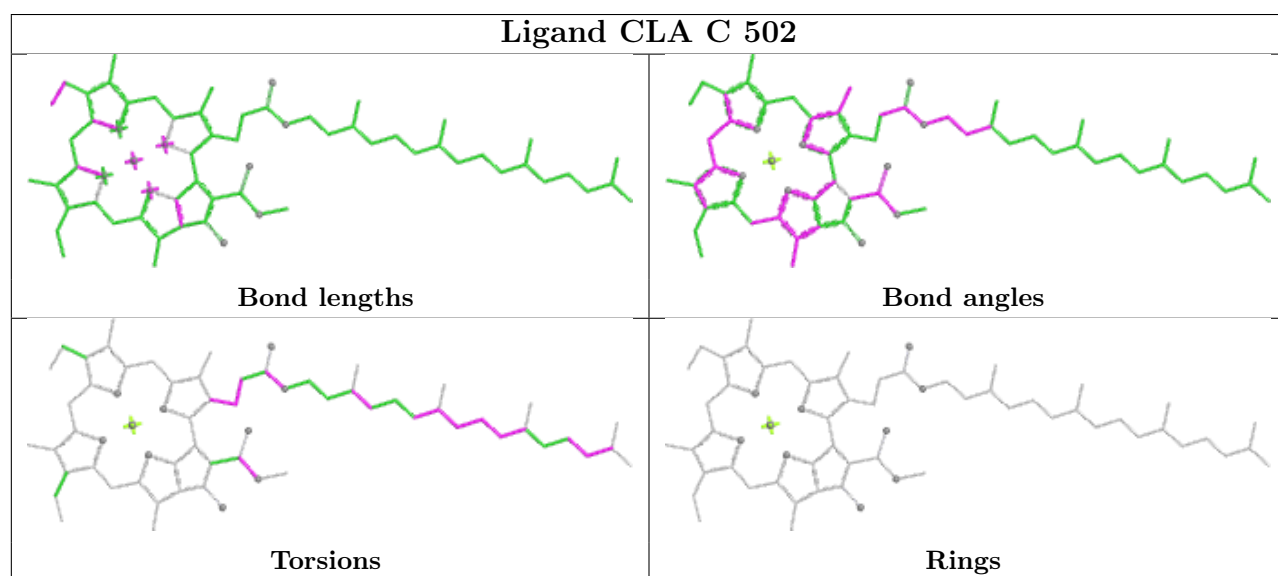
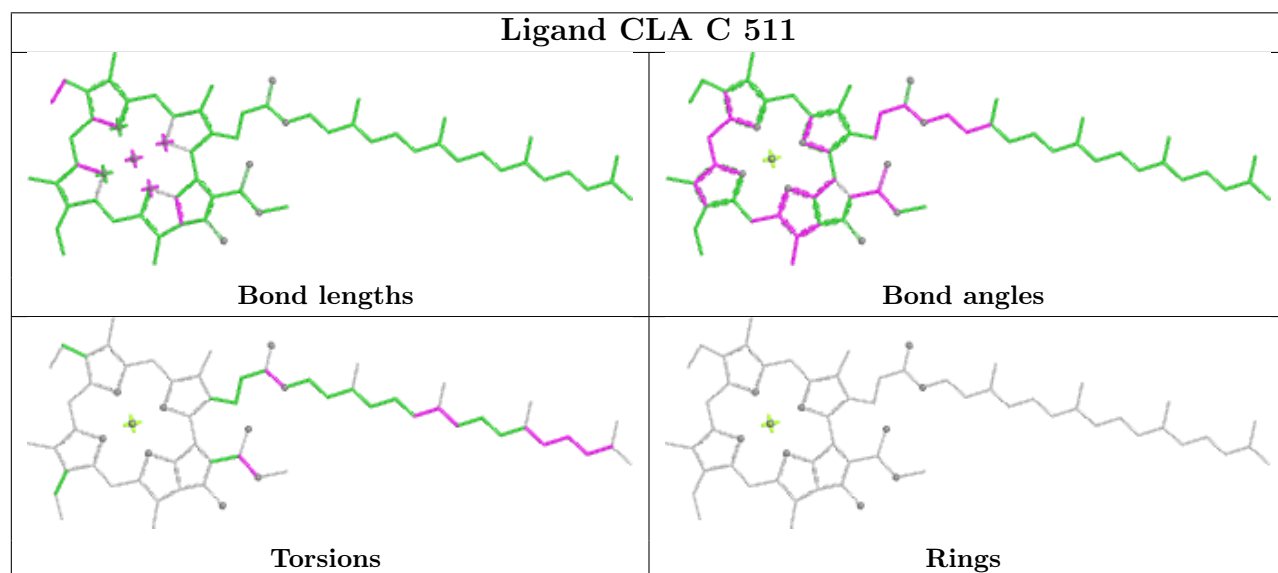
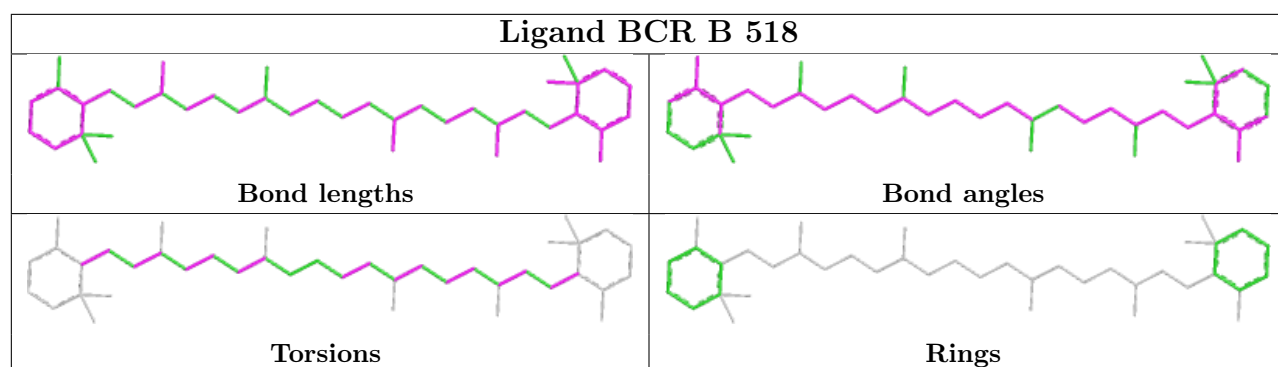
## Ligand HEM E 101

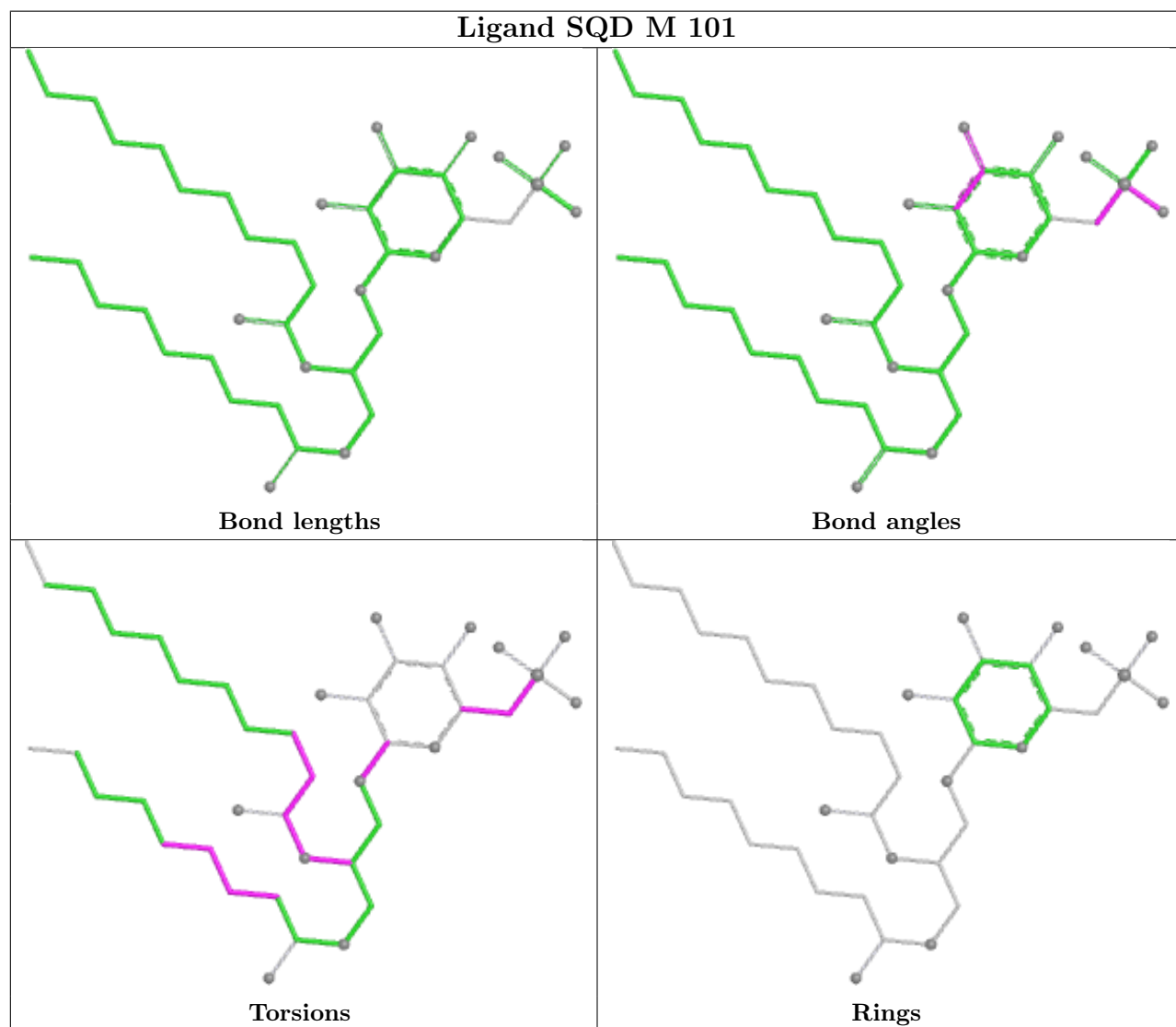
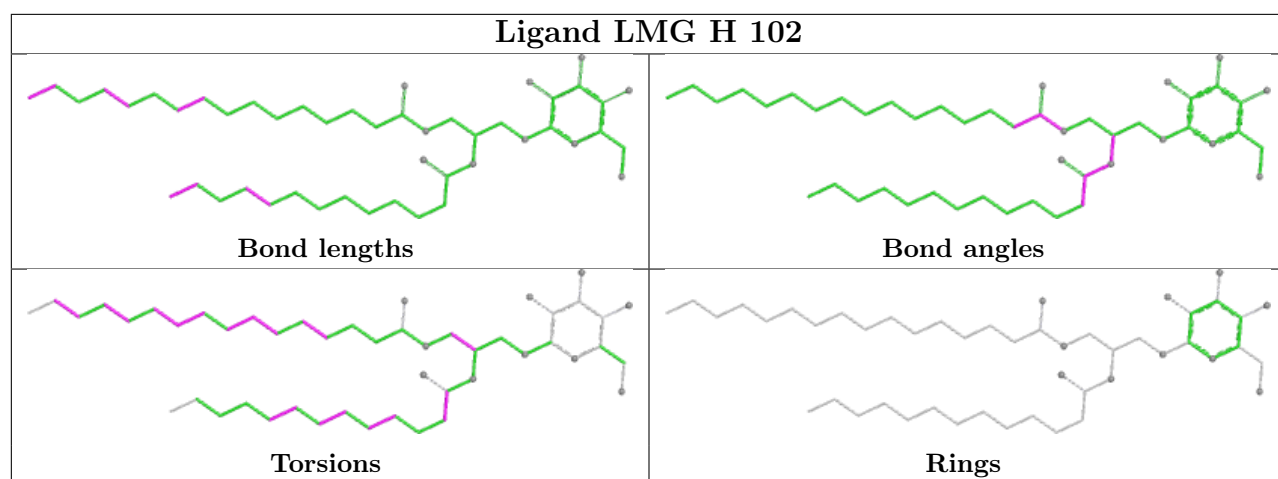


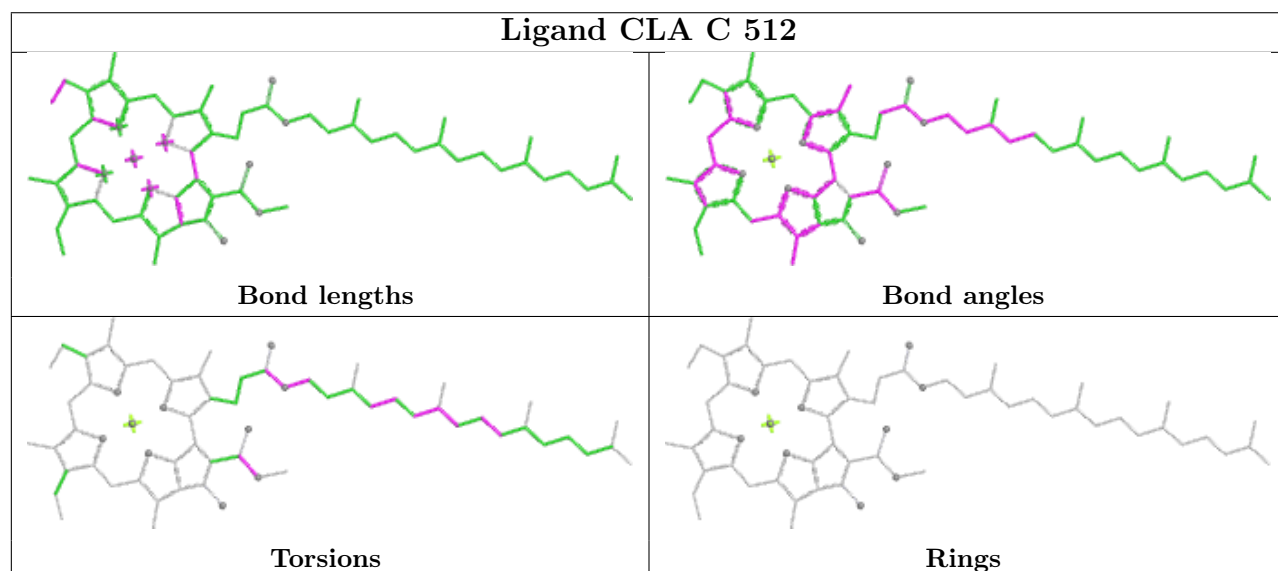
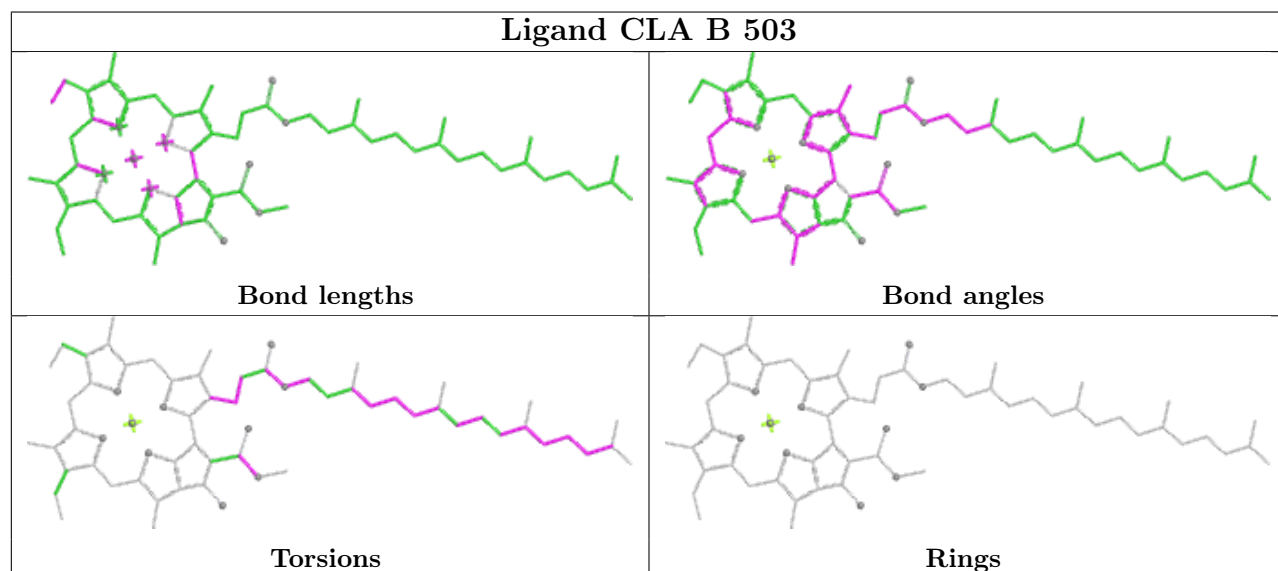
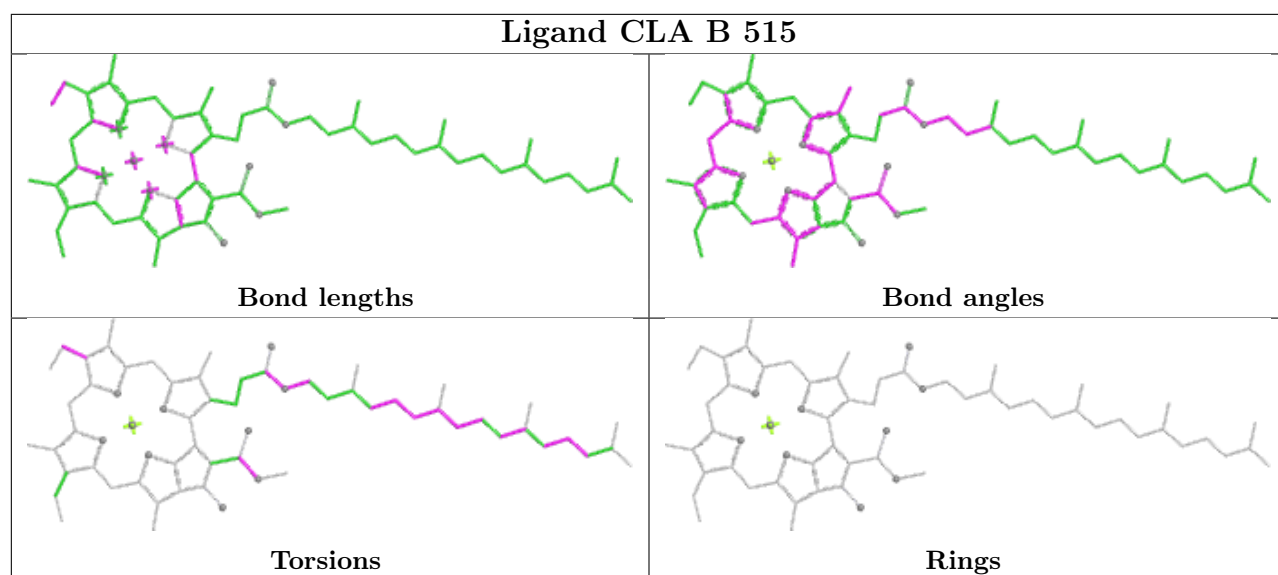




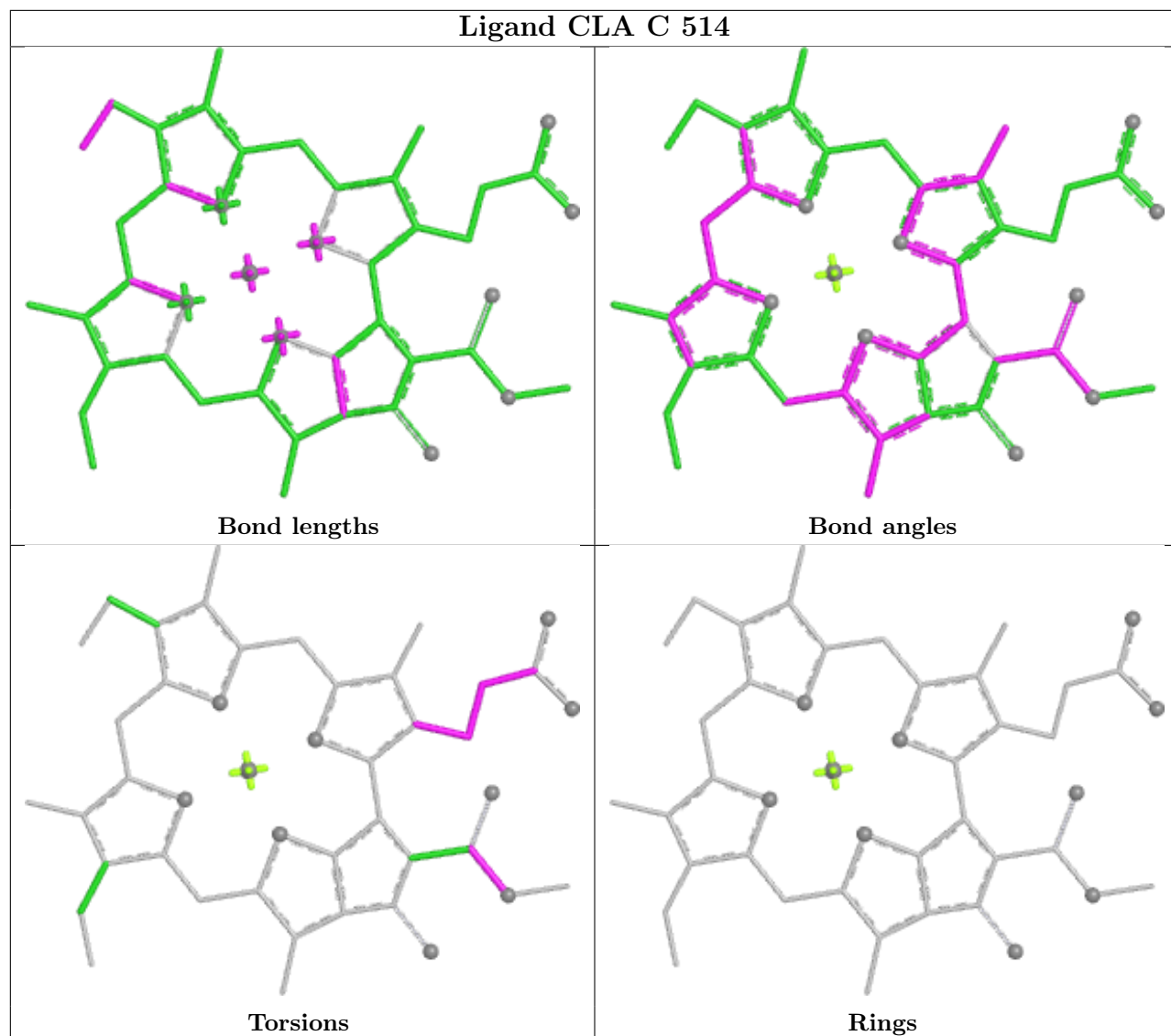
Ligand CLA B 512	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 D 406	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA C 510	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

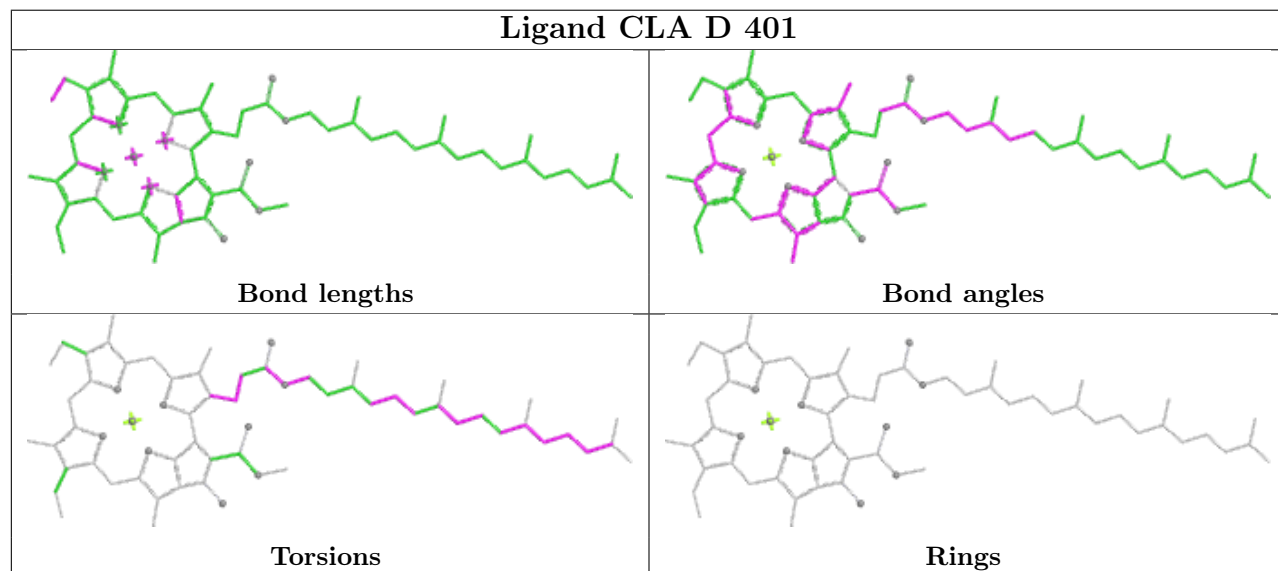
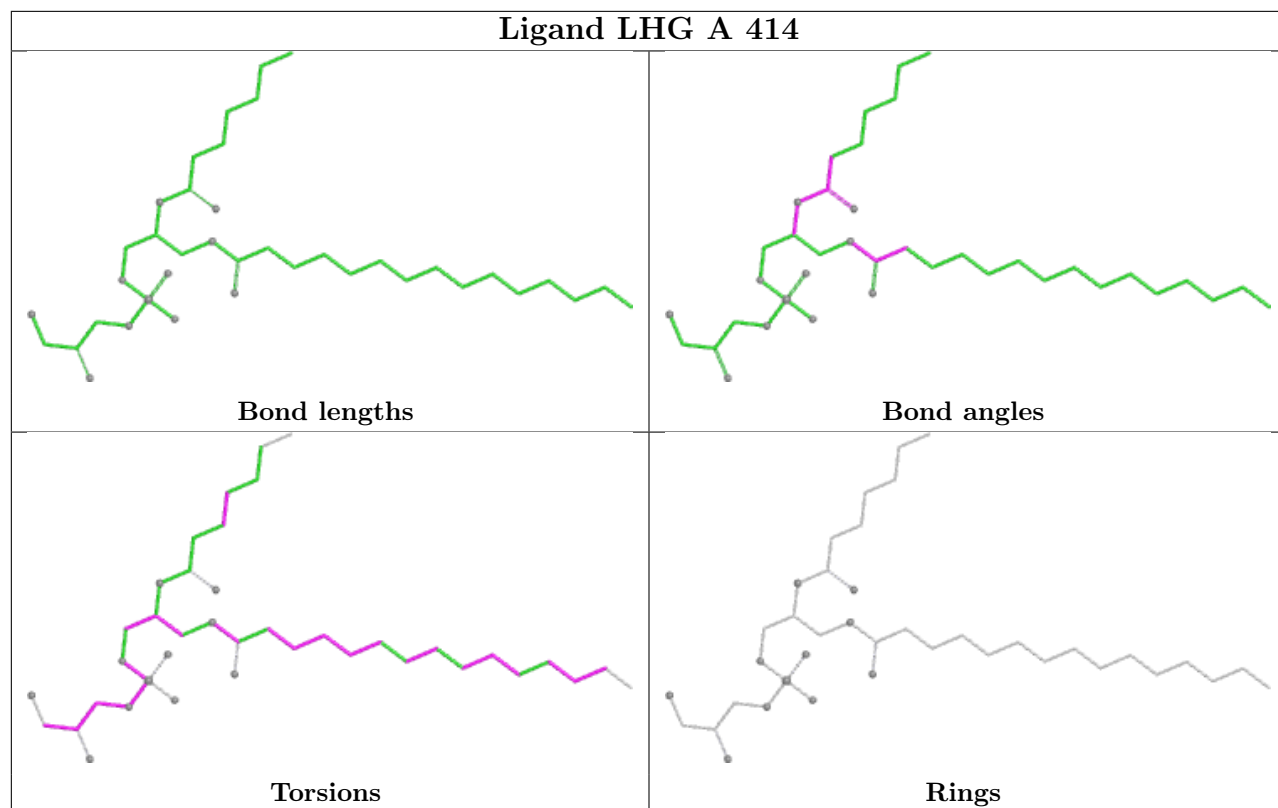


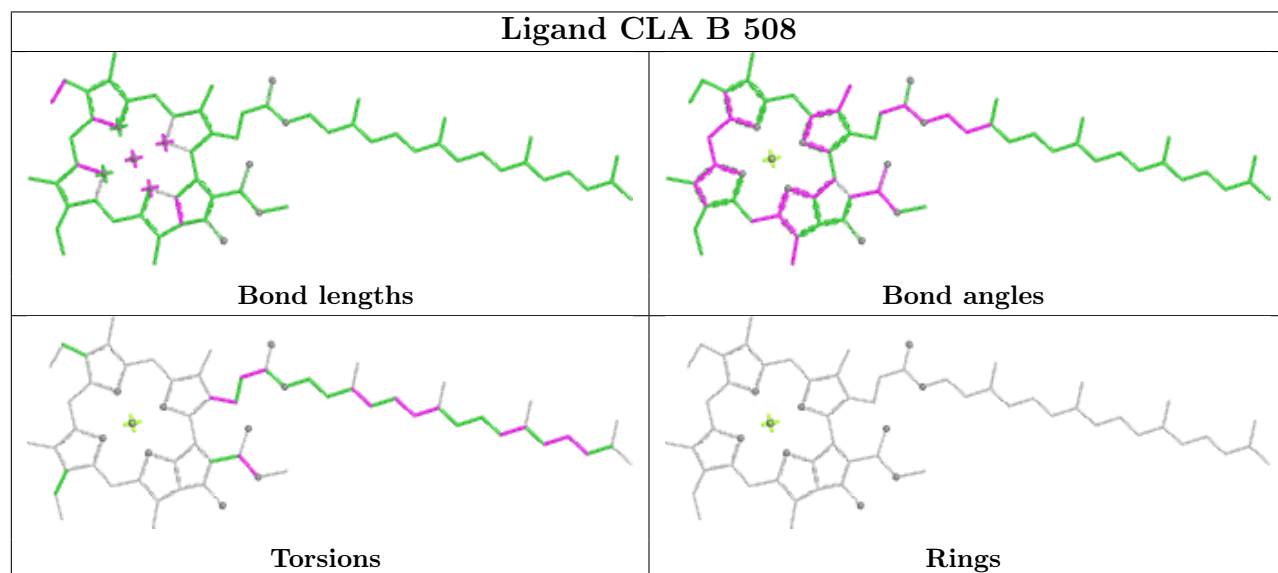
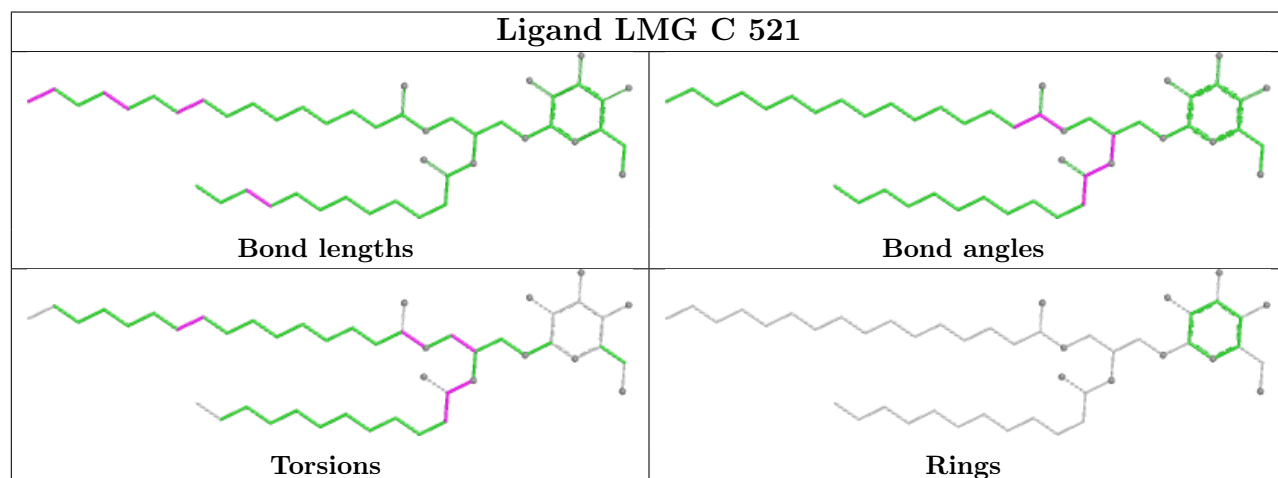
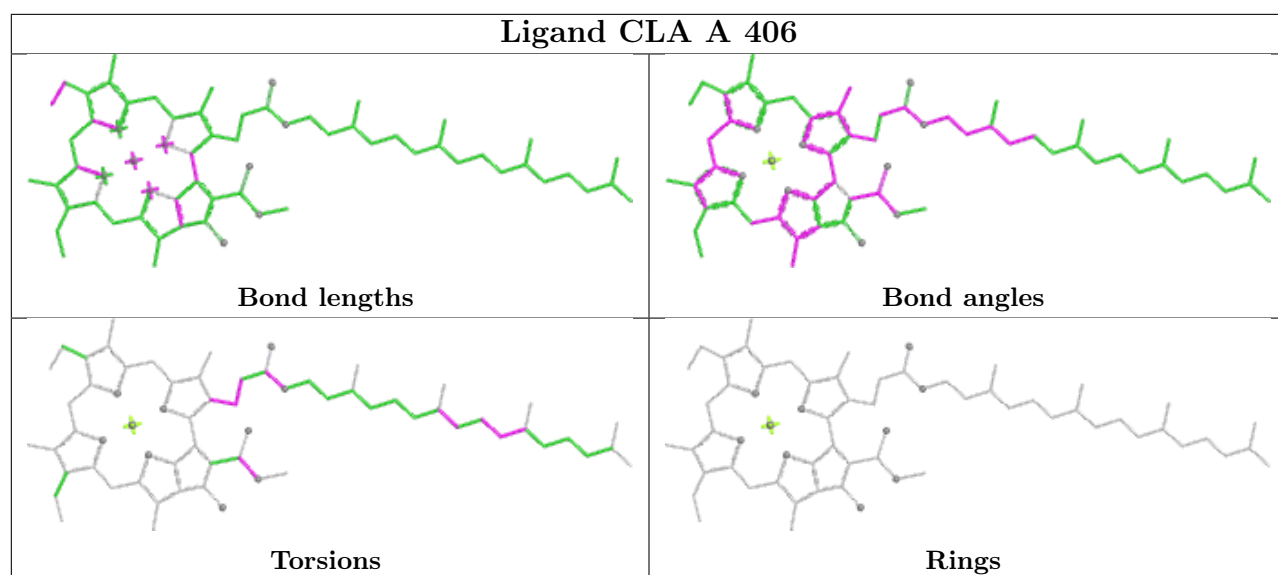


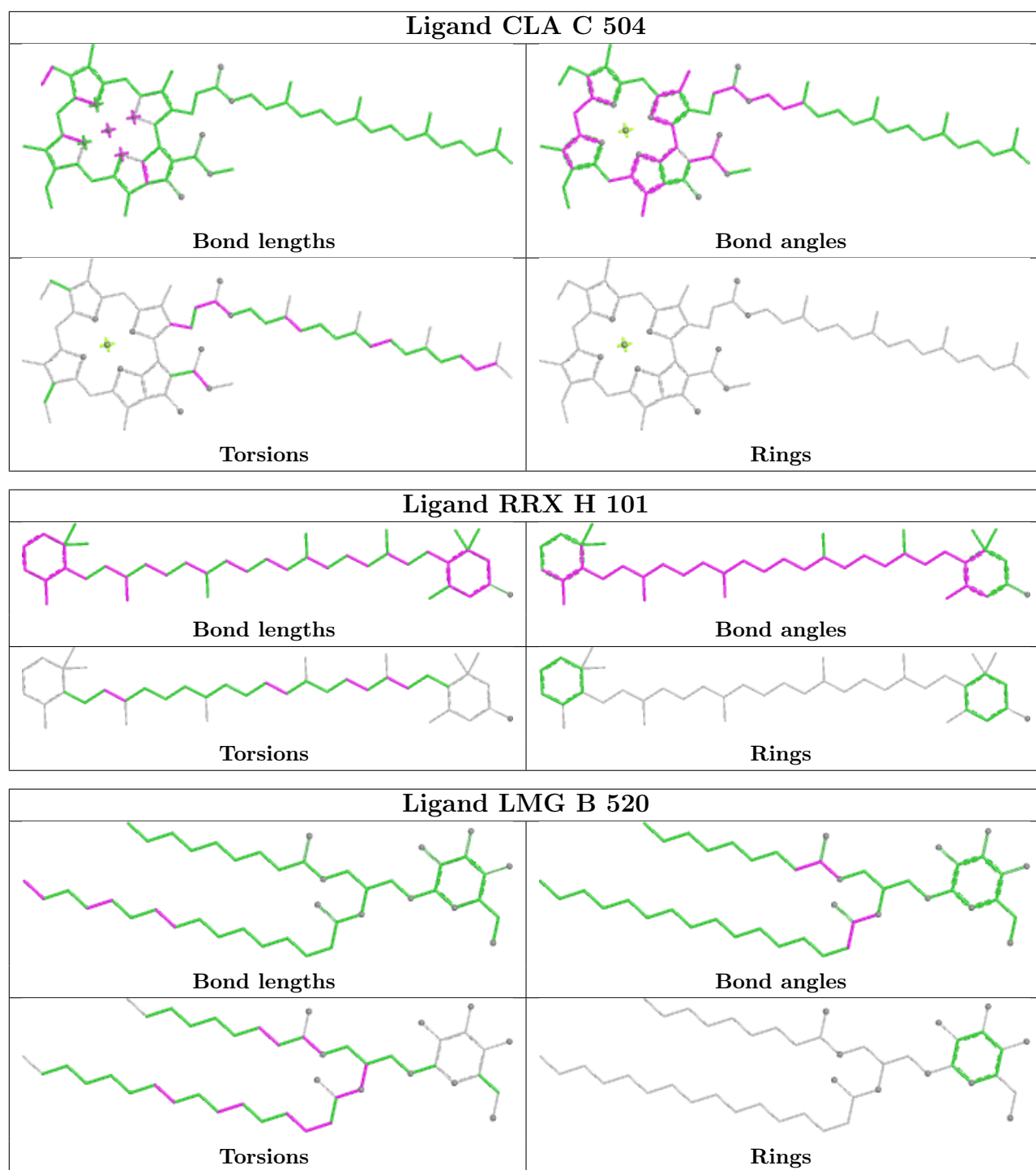


## Ligand CLA C 514

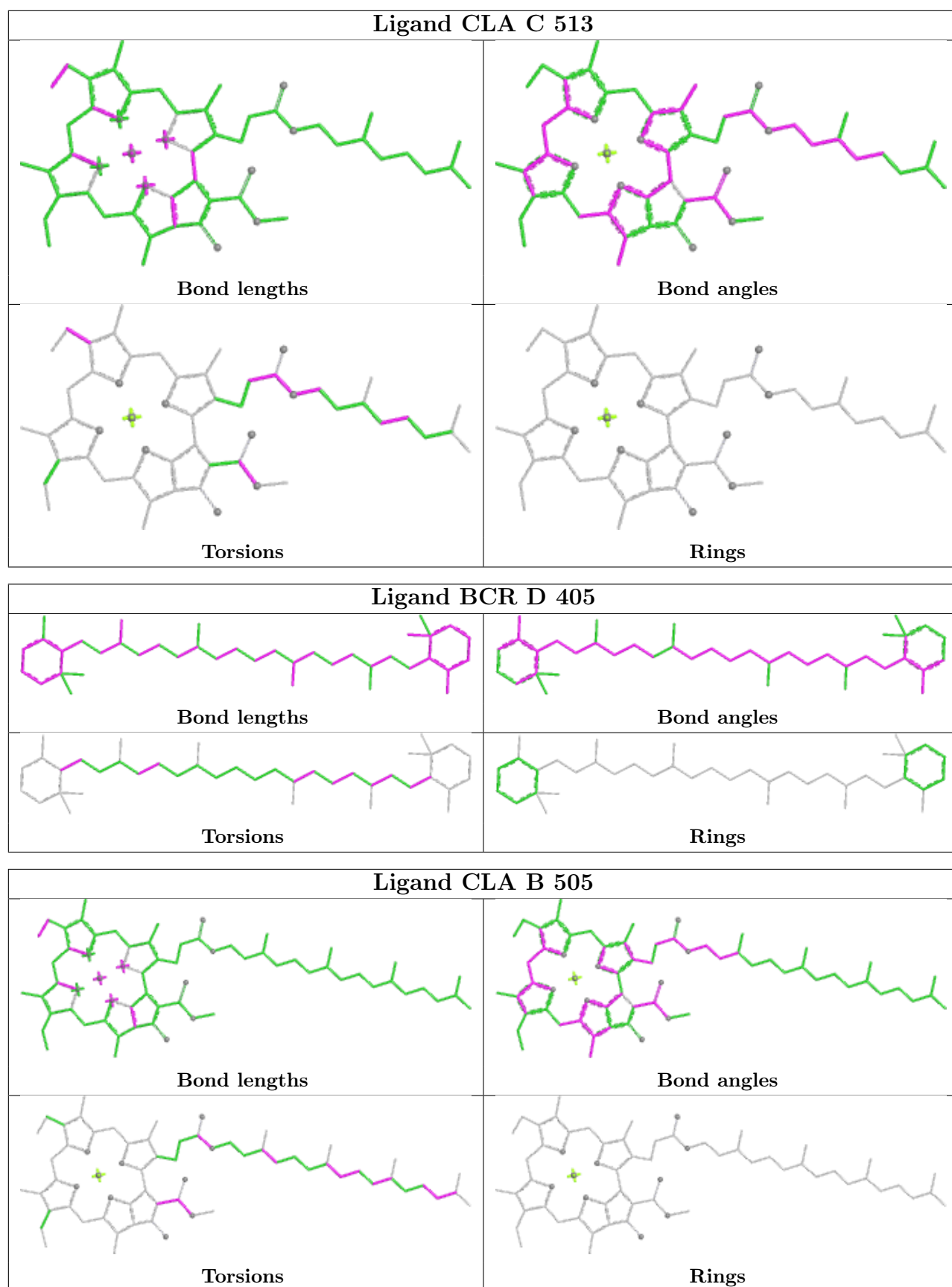


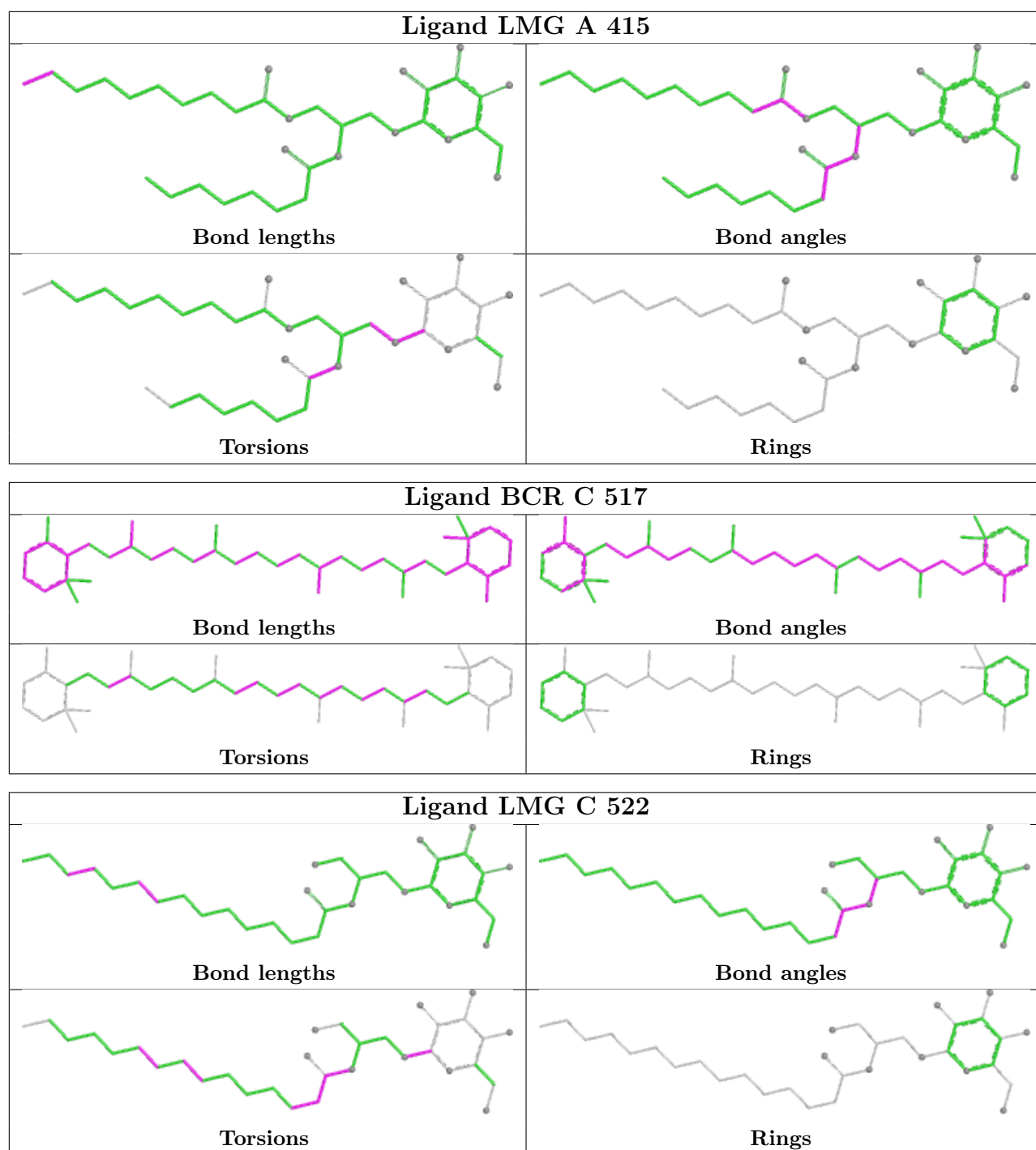


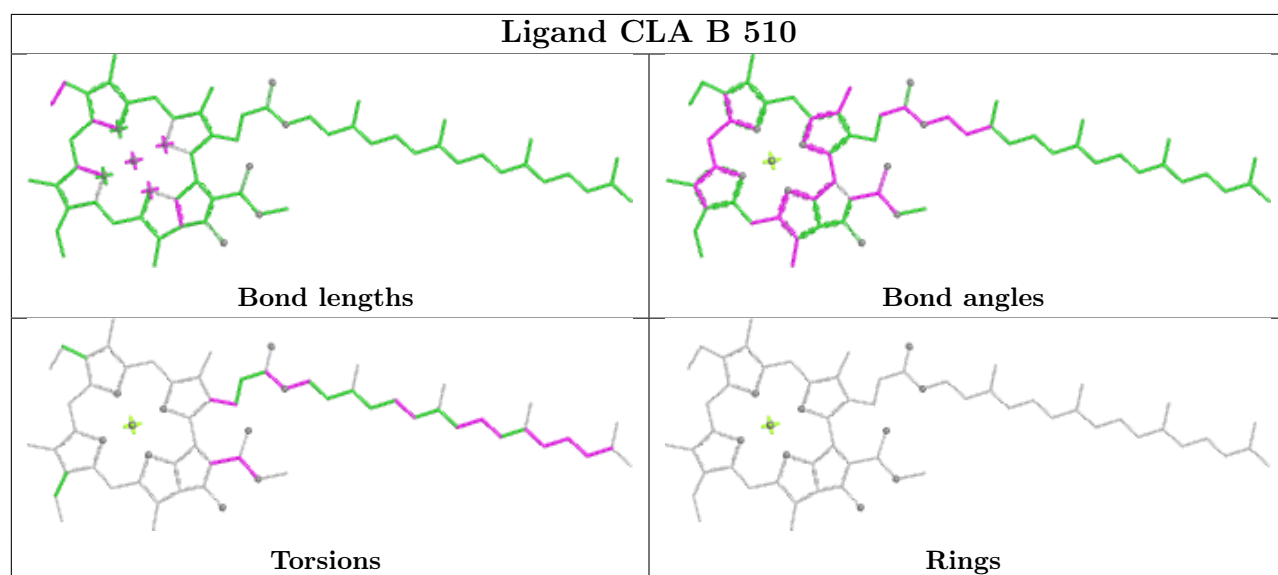
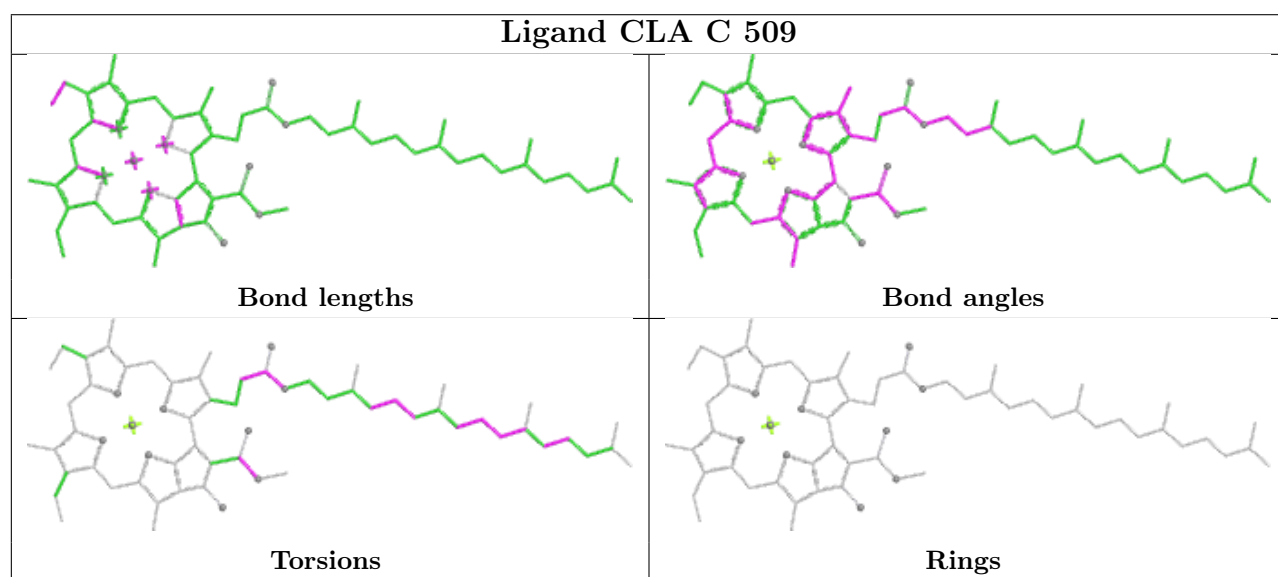
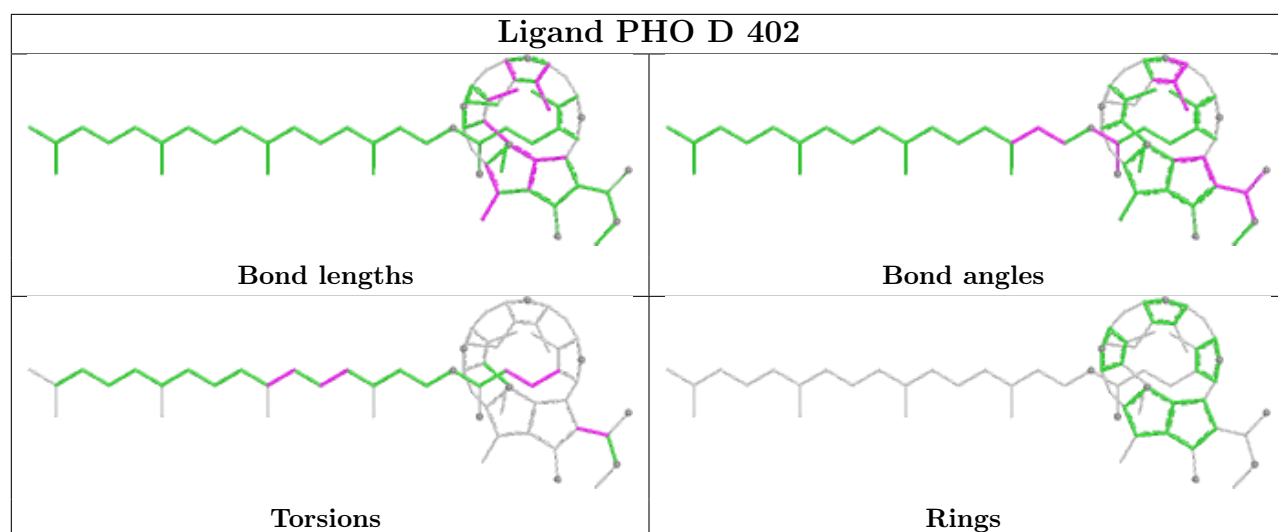


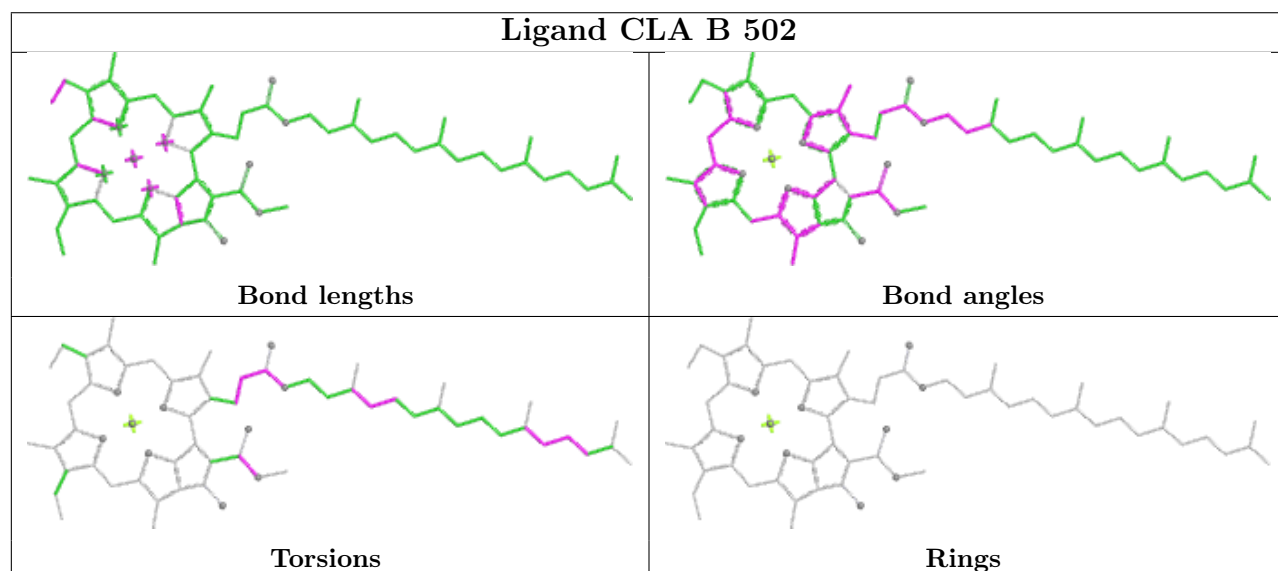
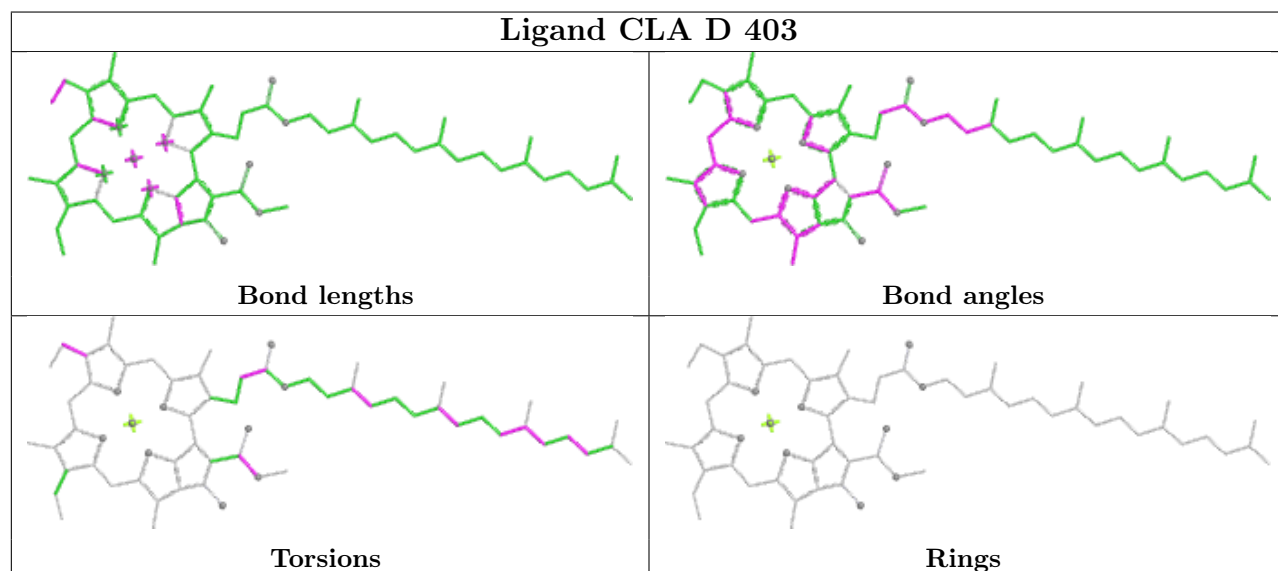
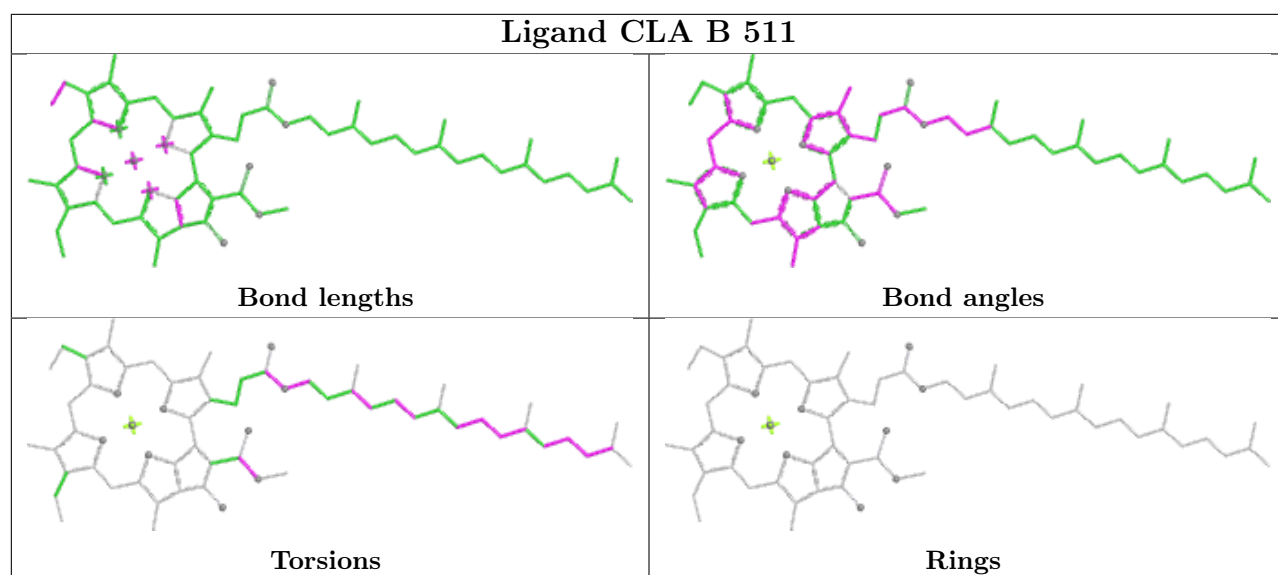


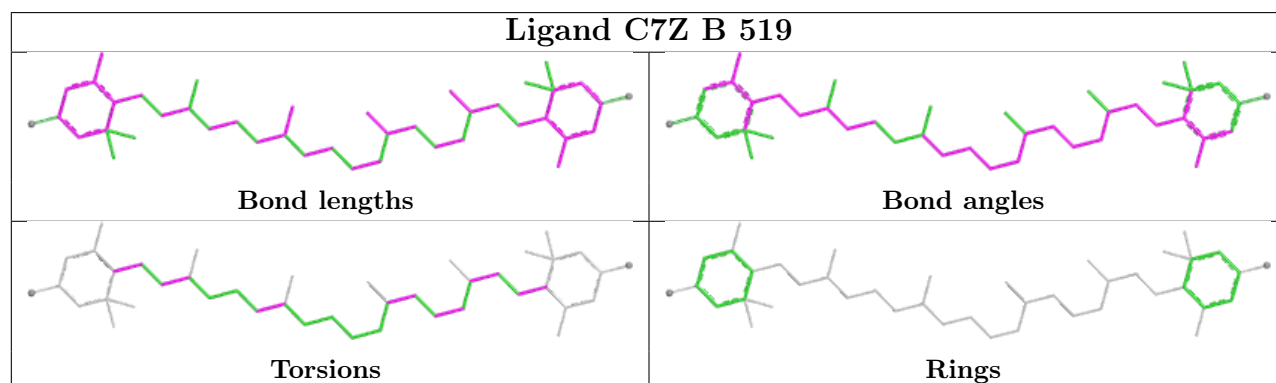
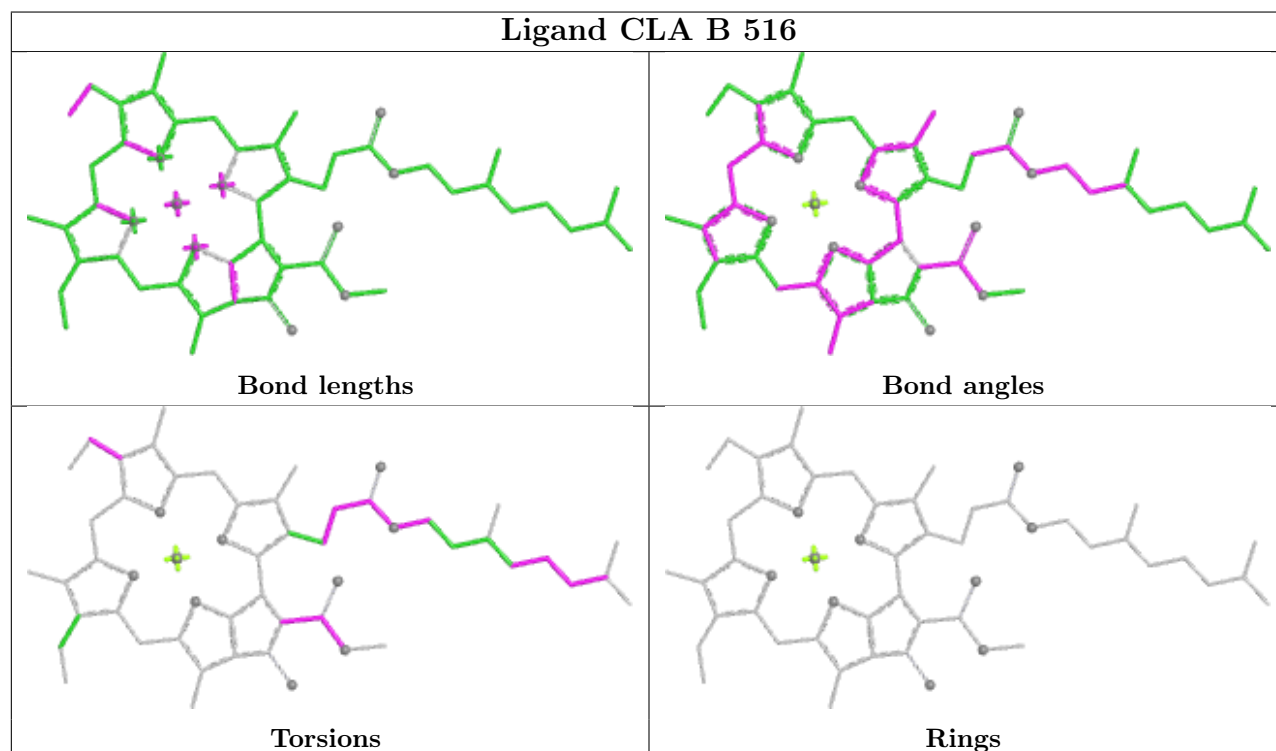
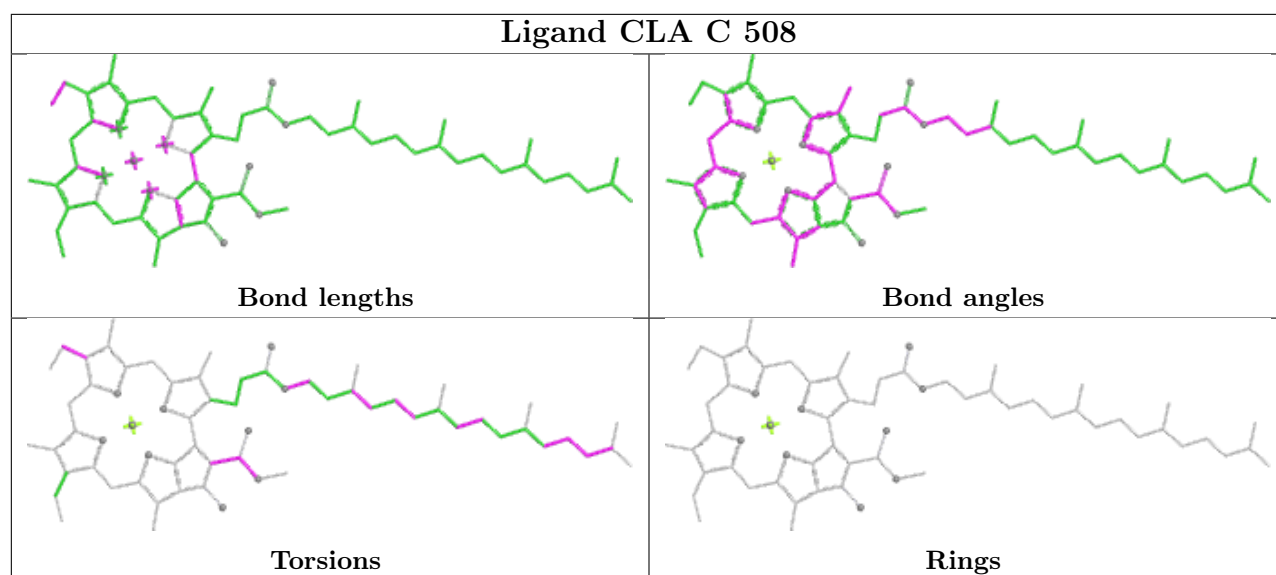












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

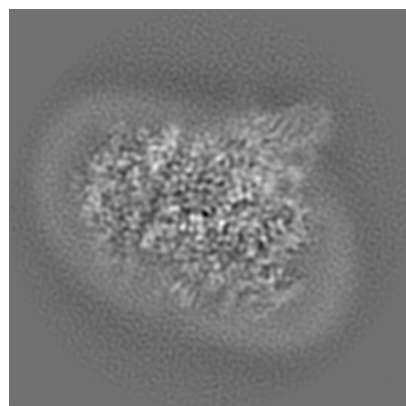
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51482. These allow visual inspection of the internal detail of the map and identification of artifacts.

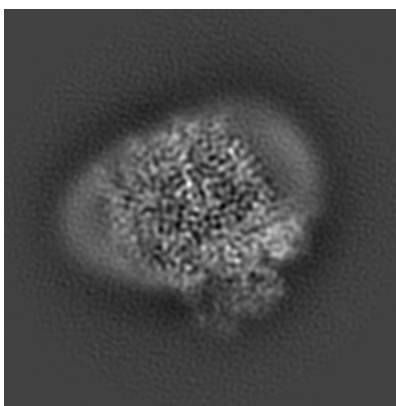
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

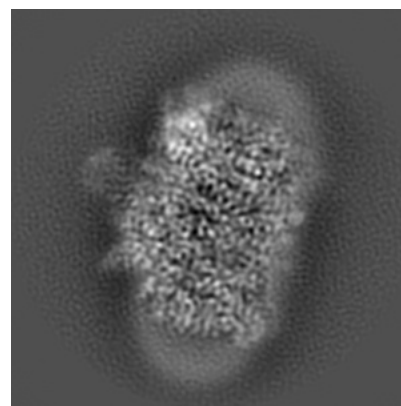
#### 6.1.1 Primary map



X

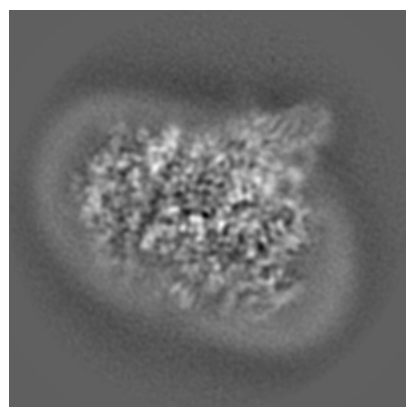


Y

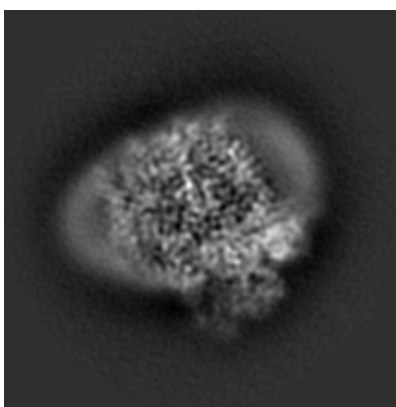


Z

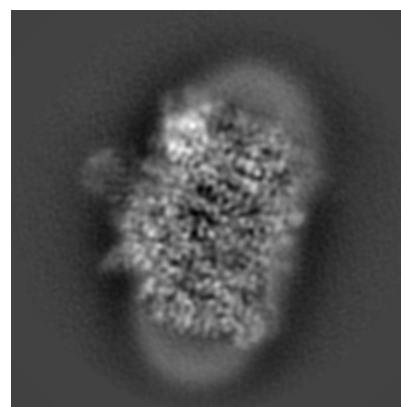
#### 6.1.2 Raw map



X



Y

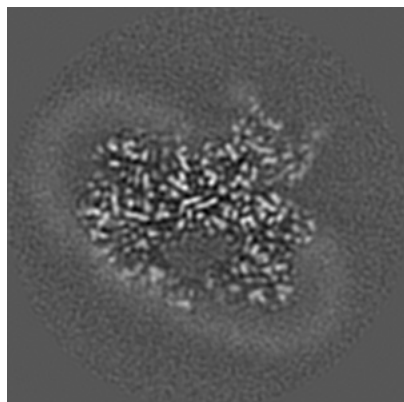


Z

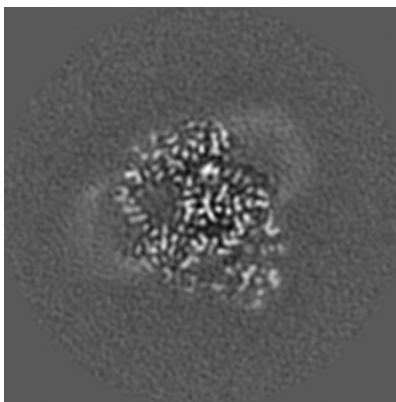
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

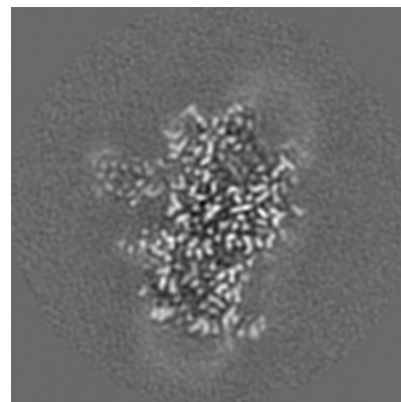
### 6.2.1 Primary map



X Index: 150

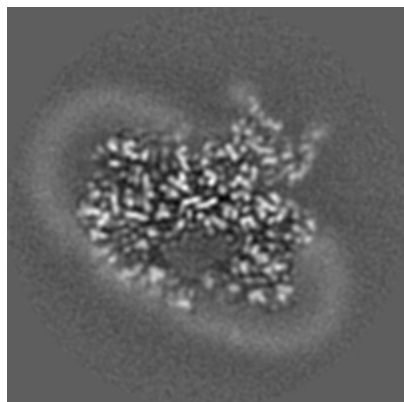


Y Index: 150

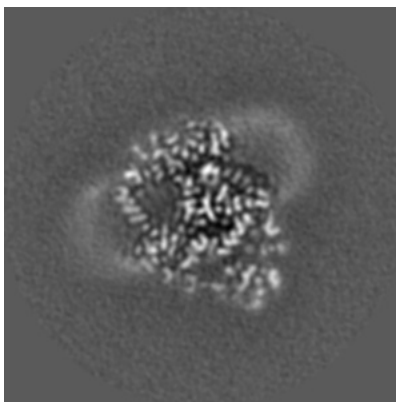


Z Index: 150

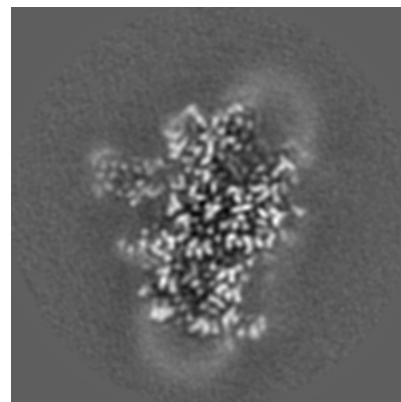
### 6.2.2 Raw map



X Index: 150



Y Index: 150



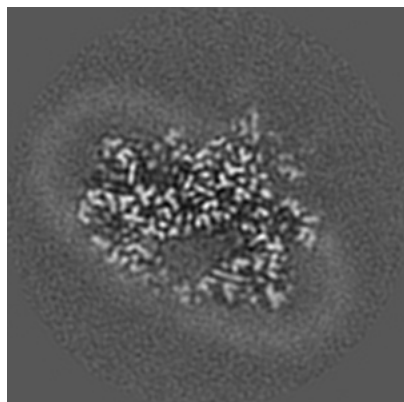
Z Index: 150

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

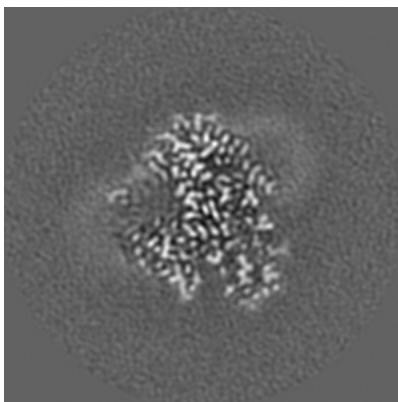


## 6.3 Largest variance slices [i](#)

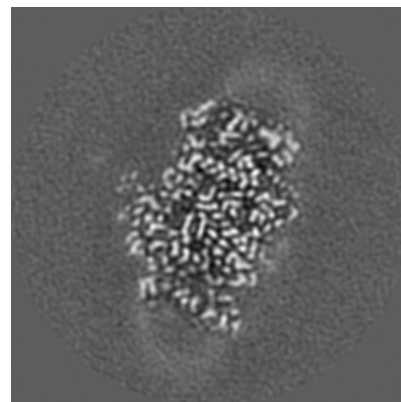
### 6.3.1 Primary map



X Index: 154

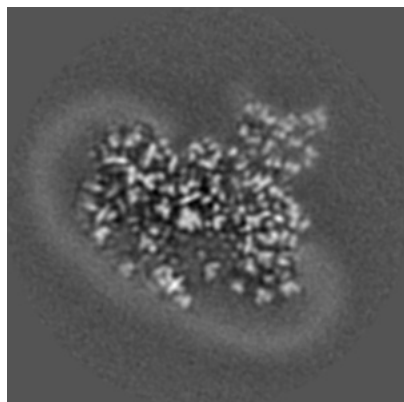


Y Index: 143

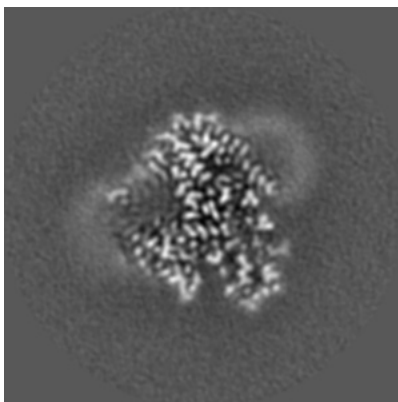


Z Index: 137

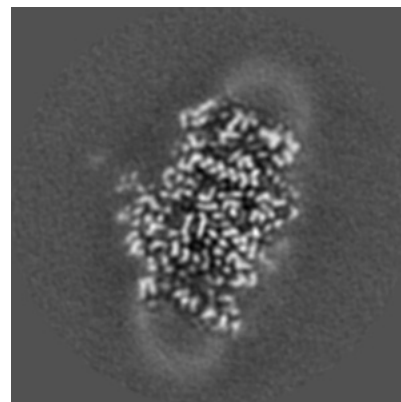
### 6.3.2 Raw map



X Index: 142



Y Index: 143

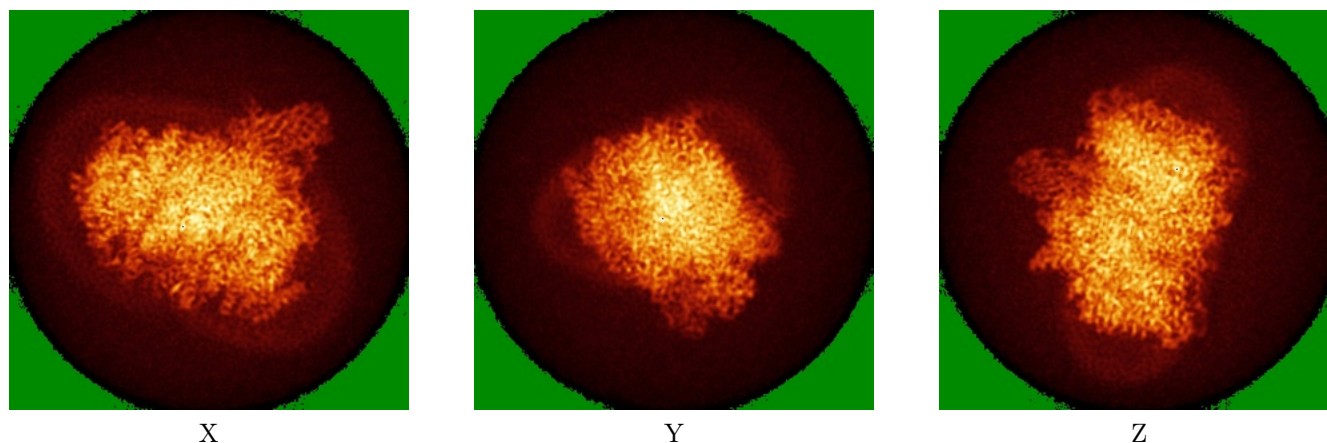


Z Index: 137

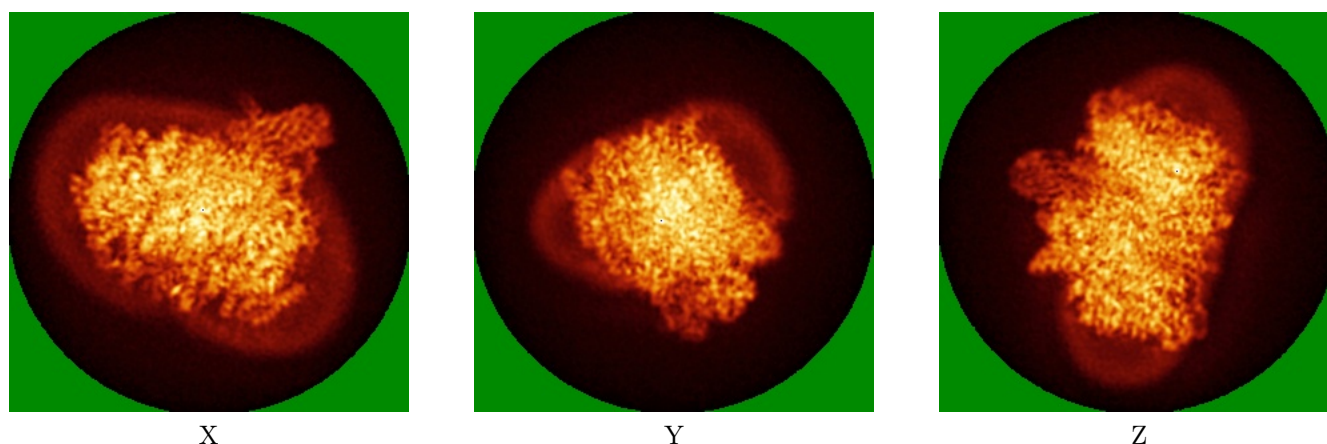
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

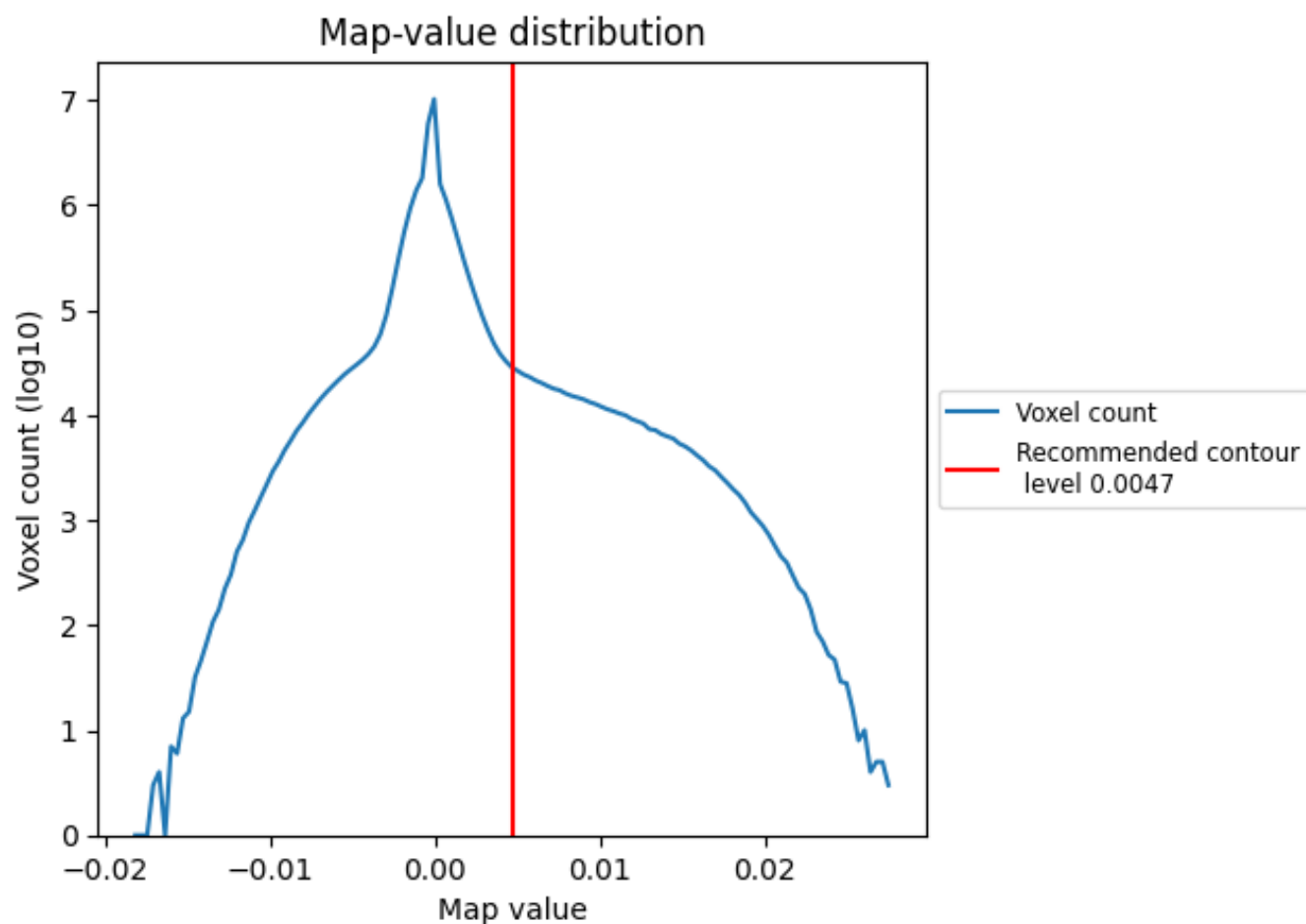
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

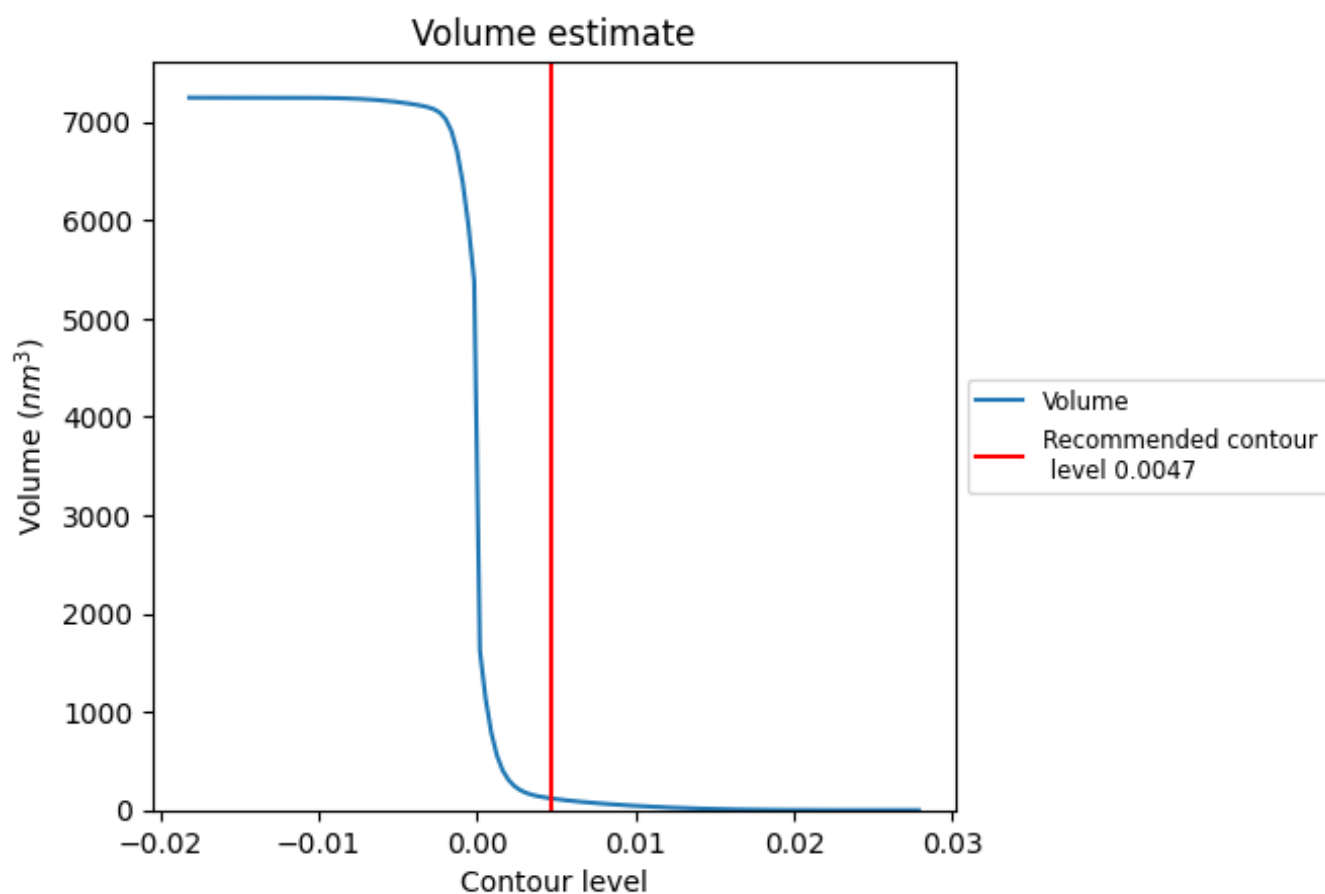
This section contains the results of statistical analysis of the map.

### 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.

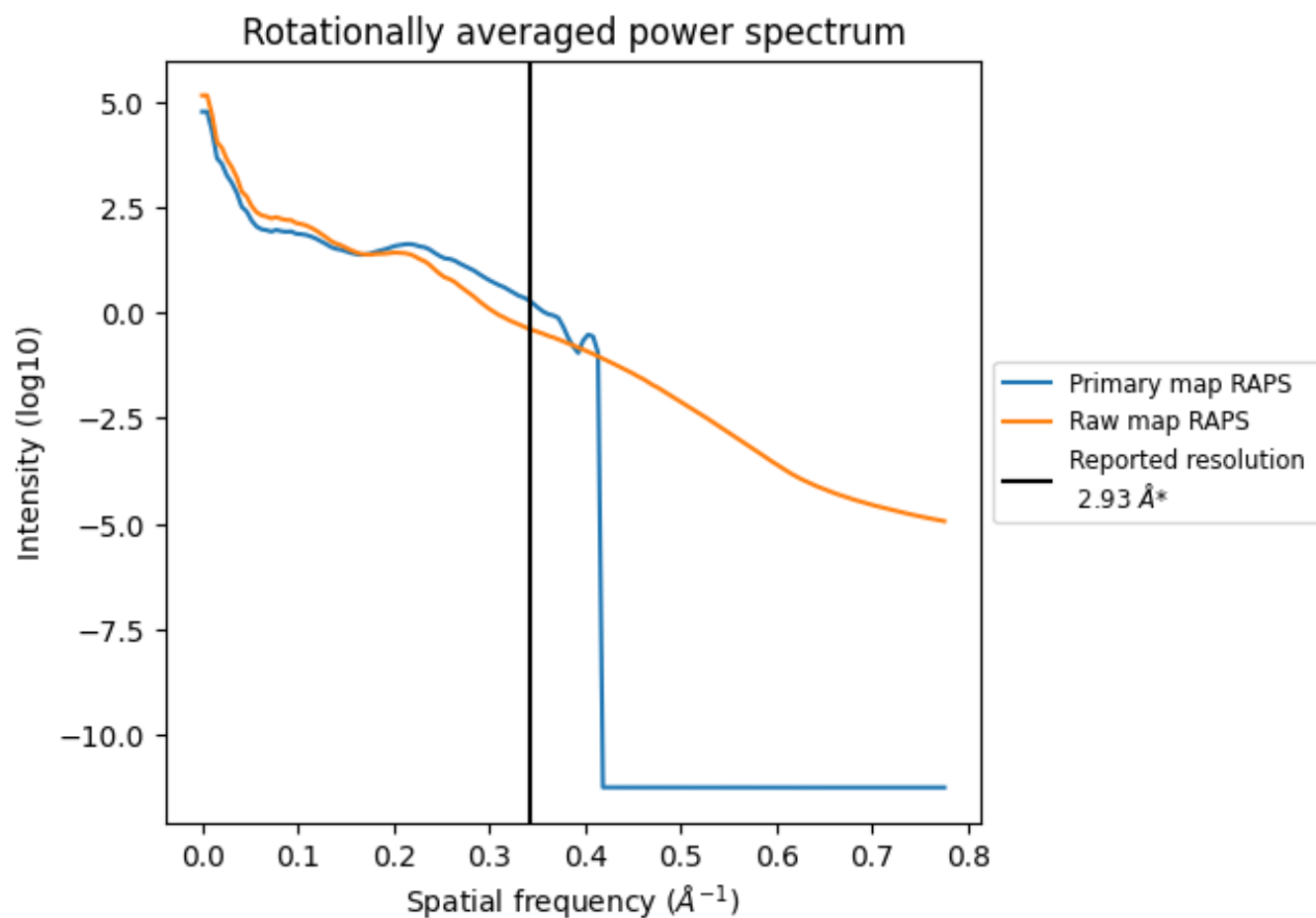
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm<sup>3</sup>; this corresponds to an approximate mass of 107 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 ⓘ

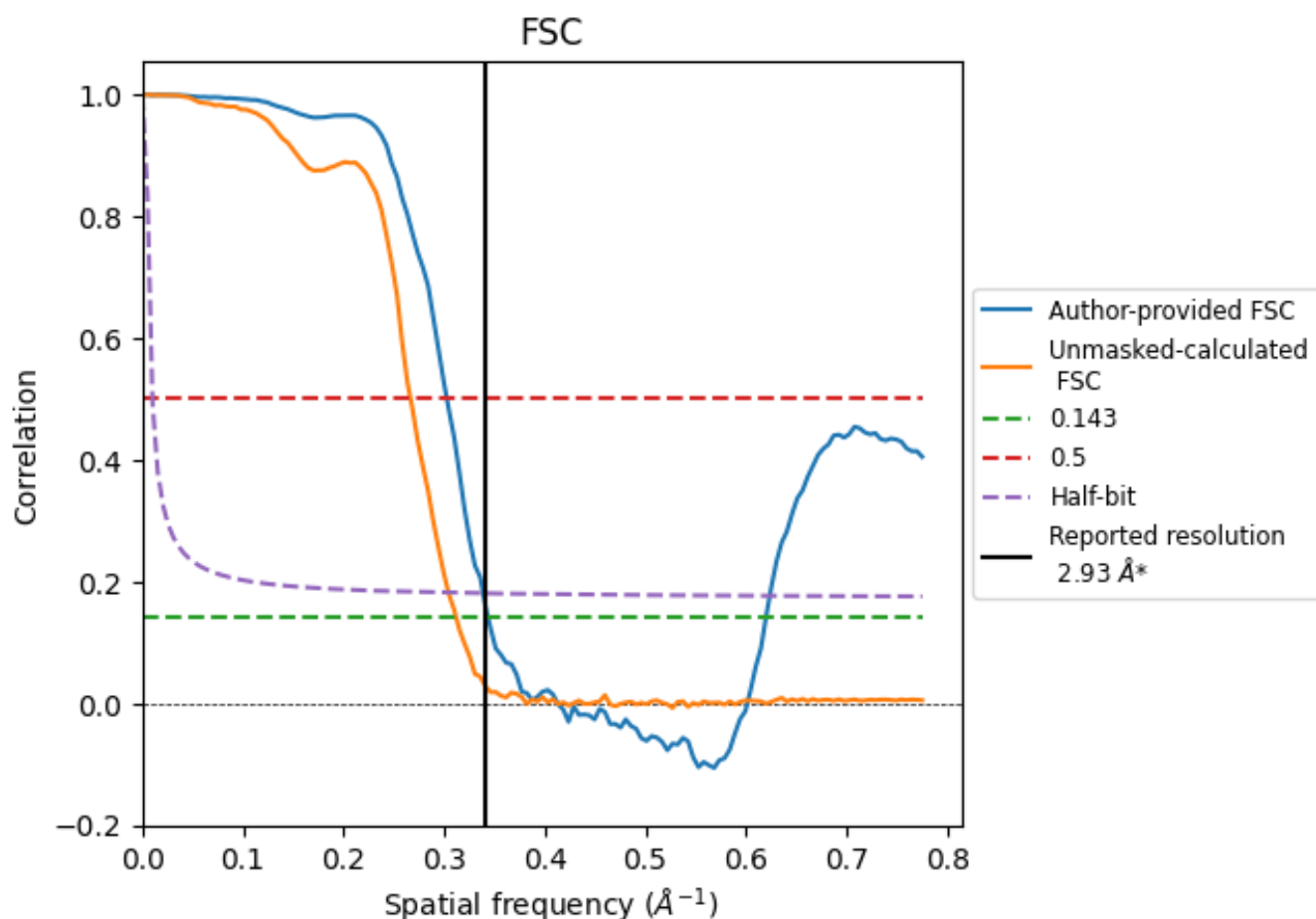


\*Reported resolution corresponds to spatial frequency of 0.341 Å<sup>-1</sup>

## 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 0.341 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

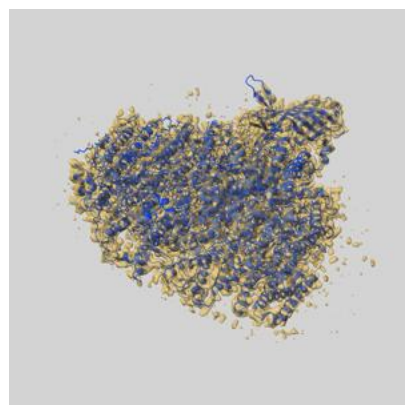
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.91	3.30	2.95
Unmasked-calculated*	3.21	3.75	3.28

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

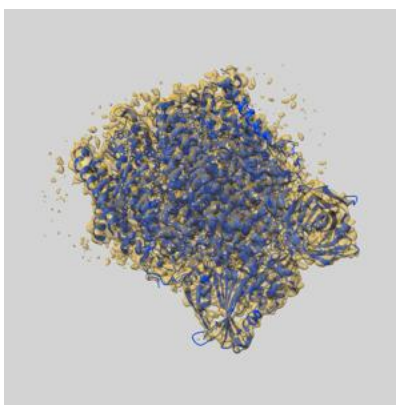
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51482 and PDB model 9GNW. Per-residue inclusion information can be found in section 3 on page 22.

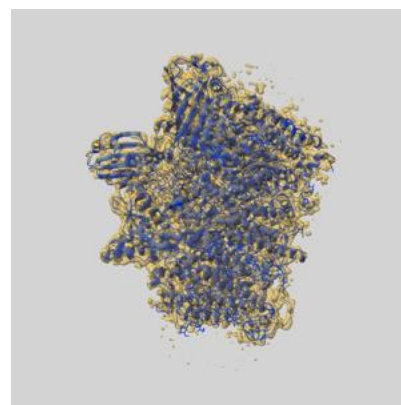
### 9.1 Map-model overlay [i](#)



X



Y

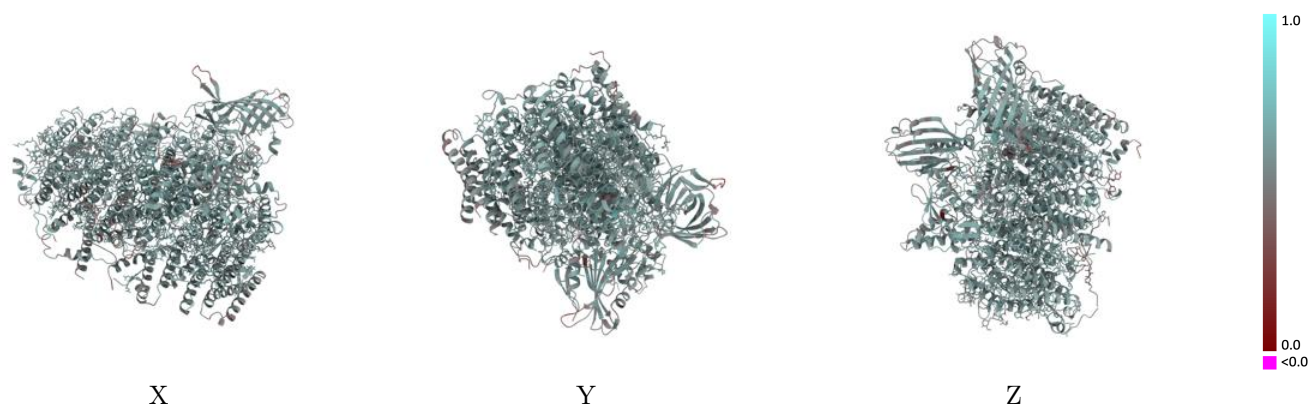


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0047 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.

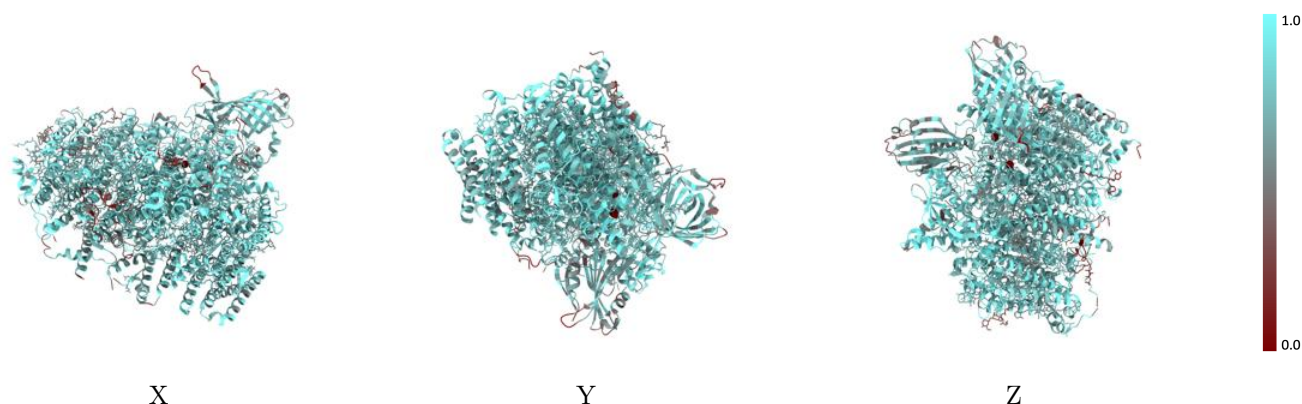


## 9.2 Q-score mapped to coordinate model [i](#)



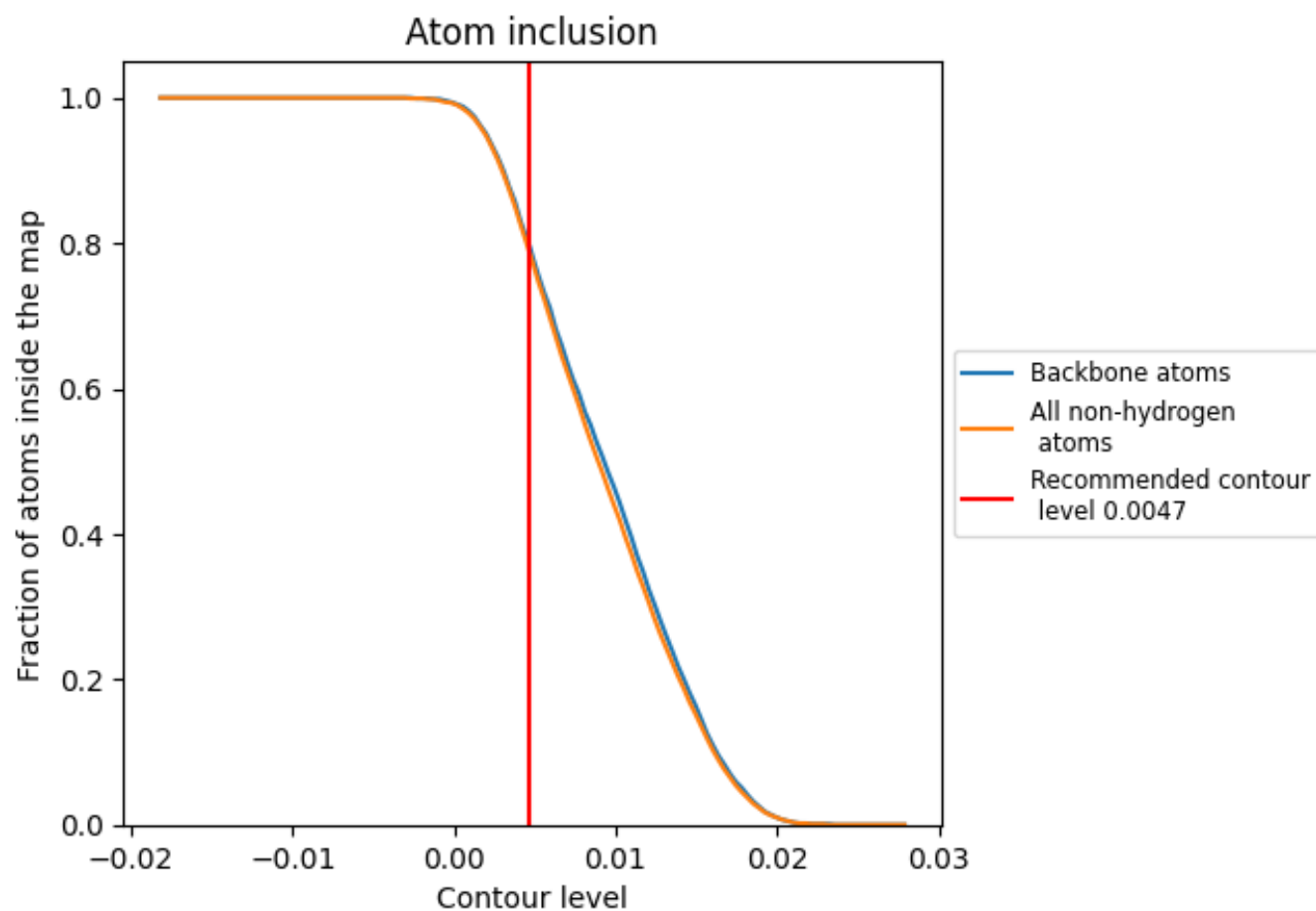
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0047).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.0047) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.5690
A	 0.7720	 0.5710
B	 0.8280	 0.5800
C	 0.8450	 0.5850
D	 0.8440	 0.5940
E	 0.8120	 0.5530
F	 0.7850	 0.5490
H	 0.8020	 0.5590
I	 0.8740	 0.5830
J	 0.7080	 0.5580
K	 0.8120	 0.5530
L	 0.8280	 0.5780
M	 0.6450	 0.5220
O	 0.7270	 0.5420
P	 0.5960	 0.5350
T	 0.7560	 0.5580
U	 0.6040	 0.4710
V	 0.7470	 0.5420
W	 0.5480	 0.5110
X	 0.7200	 0.5210
Z	 0.7280	 0.5050

