



Full wwPDB EM Validation Report ⓘ

May 27, 2024 – 11:39 AM JST

PDB ID : 7DXH
EMDB ID : EMD-30909
Title : Cryo-EM structure of PSII intermediate Psb28-PSII complex
Authors : Sui, S.F.; Shen, J.R.; Han, G.Y.; Xiao, Y.N.; Huang, G.Q.
Deposited on : 2021-01-18
Resolution : 3.14 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

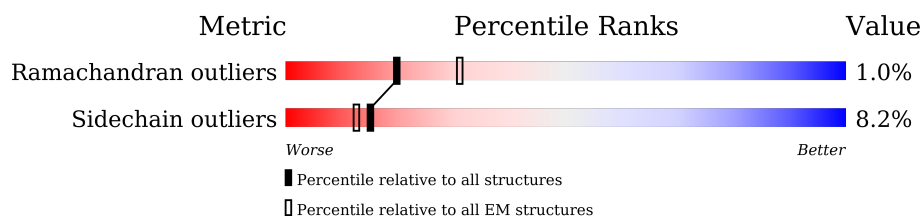
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	116	<div> <div>13%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
2	B	56	<div> <div>30%</div> <div>80%</div> <div>5%</div> <div>14%</div> </div>
3	a	360	<div> <div>76%</div> <div>6%</div> <div>18%</div> </div>
4	b	505	<div> <div>95%</div> <div>•</div> </div>
5	d	342	<div> <div>95%</div> <div>•</div> </div>
6	e	84	<div> <div>10%</div> <div>71%</div> <div>•</div> <div>25%</div> </div>
7	f	45	<div> <div>53%</div> <div>9%</div> <div>38%</div> </div>
8	h	65	<div> <div>85%</div> <div>9%</div> <div>•</div> <div>5%</div> </div>
9	i	38	<div> <div>11%</div> <div>66%</div> <div>11%</div> <div>24%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	l	37	
11	m	36	
12	t	32	
13	x	40	
14	c	451	
15	k	46	
16	z	62	
17	y	30	
18	C	23	

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
21	CLA	a	402	X	-	-	-
21	CLA	b	601	X	-	-	-
21	CLA	b	602	X	-	-	-
21	CLA	b	603	X	-	-	-
21	CLA	b	604	X	-	-	-
21	CLA	b	605	X	-	-	-
21	CLA	b	606	X	-	-	-
21	CLA	b	609	X	-	-	-
21	CLA	b	611	X	-	-	-
21	CLA	b	612	X	-	-	-
21	CLA	b	613	X	-	-	-
21	CLA	b	614	X	-	-	-
21	CLA	b	615	X	-	-	-
21	CLA	c	503	X	-	-	-
21	CLA	c	504	X	-	-	-
21	CLA	c	508	X	-	-	-
21	CLA	c	509	X	-	-	-
21	CLA	c	510	X	-	-	-
21	CLA	c	511	X	-	-	-
21	CLA	d	402	X	-	-	-
21	CLA	d	406	X	-	-	-

2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 20054 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	109	Total	C	N	O	S	0	0
			875	549	153	168	5		

- Molecule 2 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	48	Total	C	N	O	0	0
			349	227	63	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	297	Total	C	N	O	S	0	0
			2304	1515	381	393	15		

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	494	Total	C	N	O	S	0	0
			3886	2554	646	673	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	339	Total	C	N	O	S	0	0
			2694	1787	439	456	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	63	Total	C	N	O	0	0
			509	334	81	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	28	Total	C	N	O	S	0	0
			219	149	36	33	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	62	Total	C	N	O	S	0	0
			493	330	79	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	29	Total	C	N	O	S	0	0
			231	162	30	38	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	37	Total	C	N	O	S	0	0
			304	202	48	53	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	m	31	Total	C	N	O	0	0
			244	165	36	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	27	Total	C	N	O	S	0	0
			230	164	30	34	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	x	36	Total	C	N	O	0	0
			261	177	39	45		

- Molecule 14 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	403	Total	C	N	O	S	0	0
			3130	2071	520	527	12		

- Molecule 15 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	k	34	Total	C	N	O	0	0
			264	186	36	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	z	62	Total	C	N	O	S	0	0
			455	316	67	70	2		

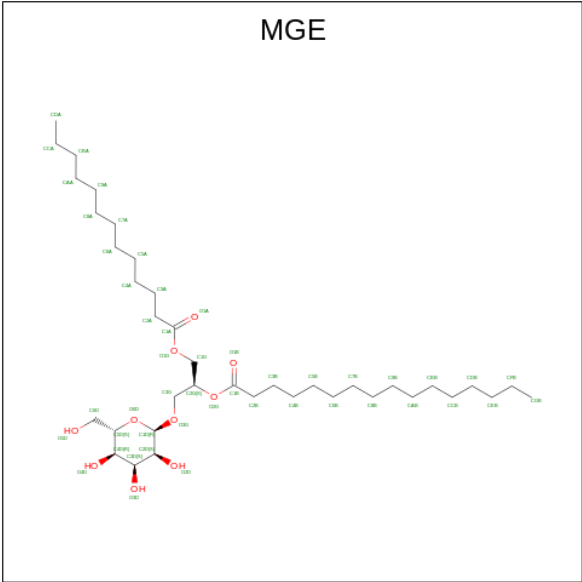
- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	y	28	Total	C	N	O	0	0
			137	81	28	28		

- Molecule 18 is a protein called unidentified transmembrane protein.

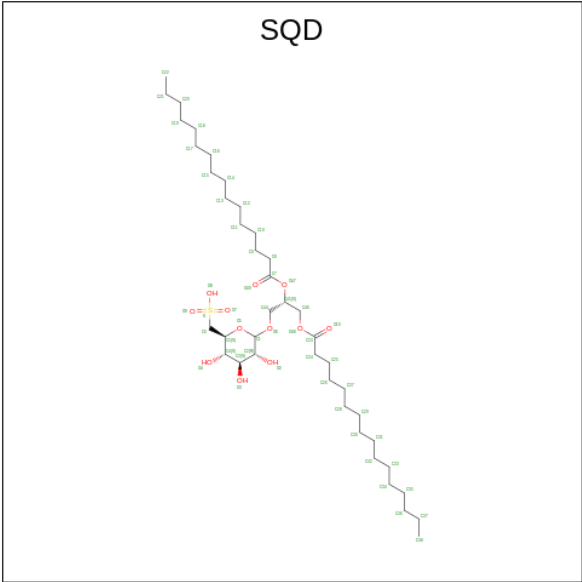
Mol	Chain	Residues	Atoms				AltConf	Trace
18	C	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 19 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: C₃₈H₇₂O₁₀).



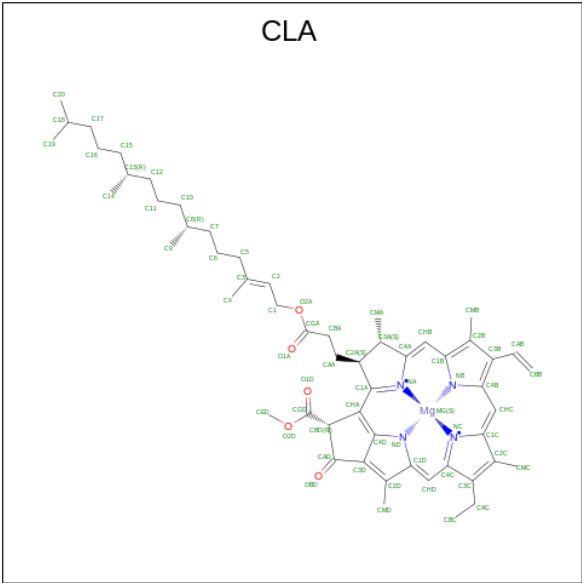
Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			48	38	10	
19	b	1	Total	C	O	0
			48	38	10	
19	b	1	Total	C	O	0
			41	31	10	
19	d	1	Total	C	O	0
			48	38	10	
19	f	1	Total	C	O	0
			47	37	10	
19	m	1	Total	C	O	0
			48	38	10	
19	c	1	Total	C	O	0
			48	38	10	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
20	a	1	Total	C	O	S	0
			26	13	12	1	
20	1	1	Total	C	O	S	0
			47	34	12	1	

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

Continued on next page...

Continued from previous page...

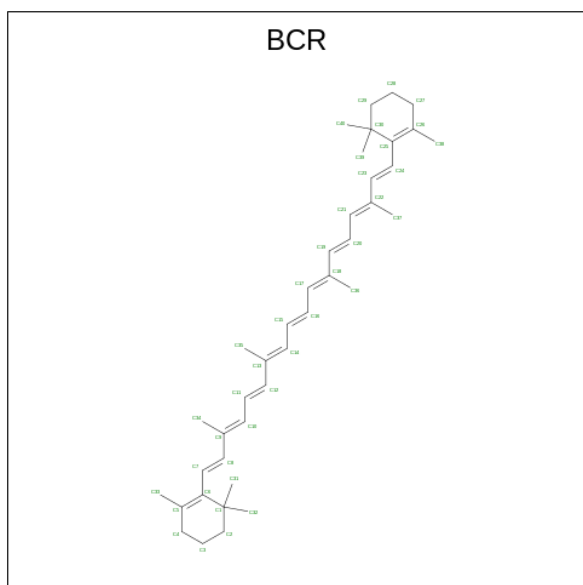
Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	d	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	h	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

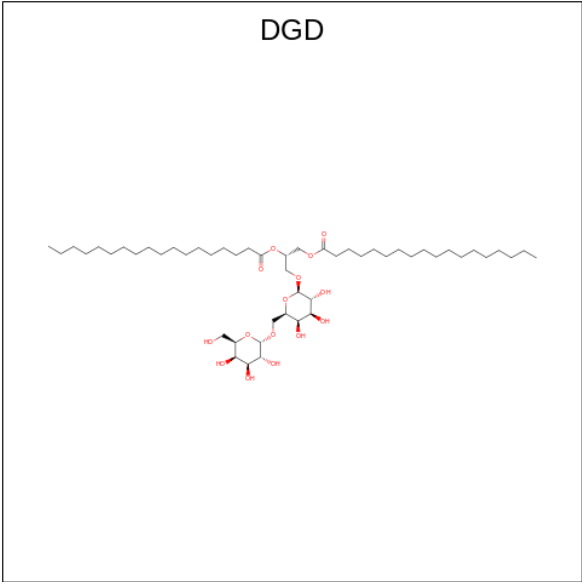


Mol	Chain	Residues	Atoms	AltConf
22	a	1	Total C 40 40	0
22	b	1	Total C 40 40	0
22	b	1	Total C 40 40	0
22	b	1	Total C 40 40	0
22	d	1	Total C 40 40	0
22	h	1	Total C 40 40	0
22	c	1	Total C 40 40	0
22	c	1	Total C 40 40	0
22	z	1	Total C 40 40	0

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

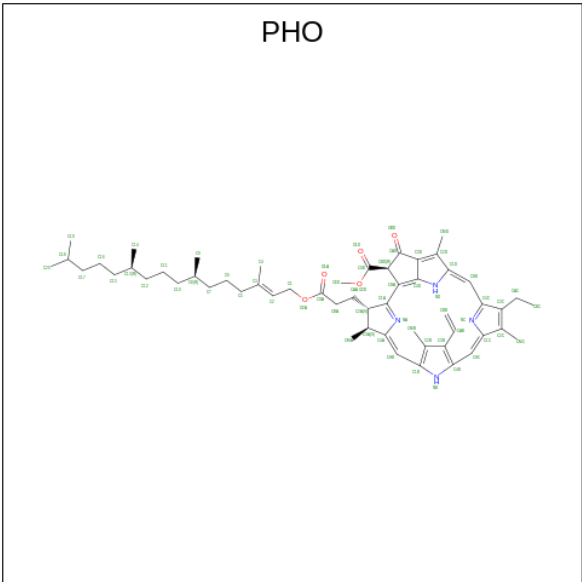
Mol	Chain	Residues	Atoms	AltConf
23	a	1	Total Cl 1 1	0
23	c	1	Total Cl 1 1	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



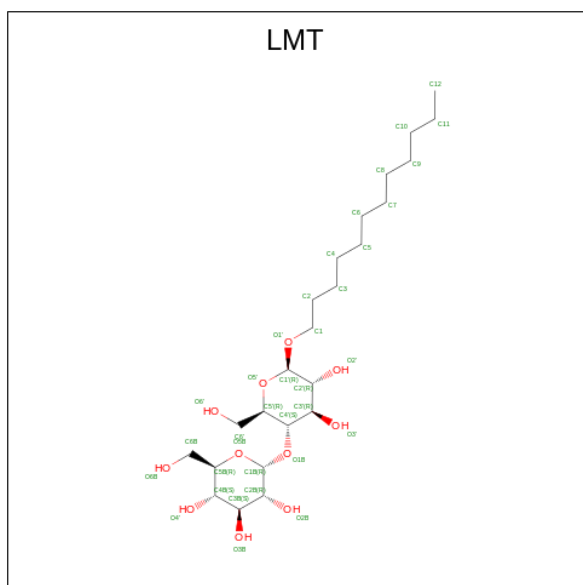
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			57	42	15	
24	h	1	Total	C	O	0
			54	39	15	
24	c	1	Total	C	O	0
			53	38	15	
24	c	1	Total	C	O	0
			47	32	15	

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

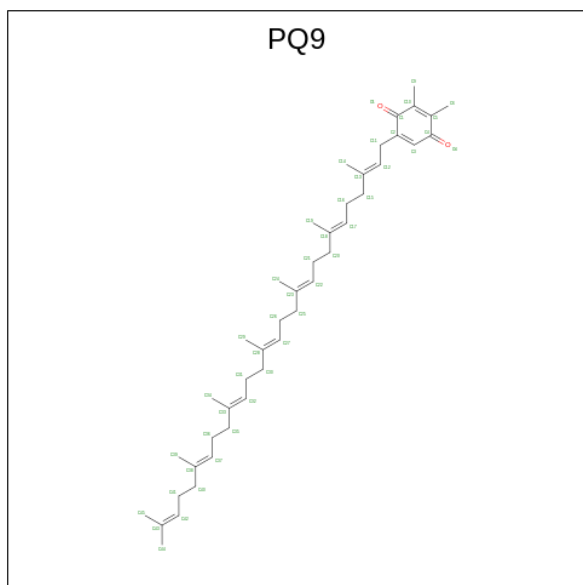


Mol	Chain	Residues	Atoms			AltConf
26	d	1	Total	C	O	0
			35	24	11	
26	m	1	Total	C	O	0
			35	24	11	
26	t	1	Total	C	O	0
			35	24	11	

- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
27	d	1	Total	Fe	0
			1	1	

- Molecule 28 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: $C_{43}H_{64}O_2$).

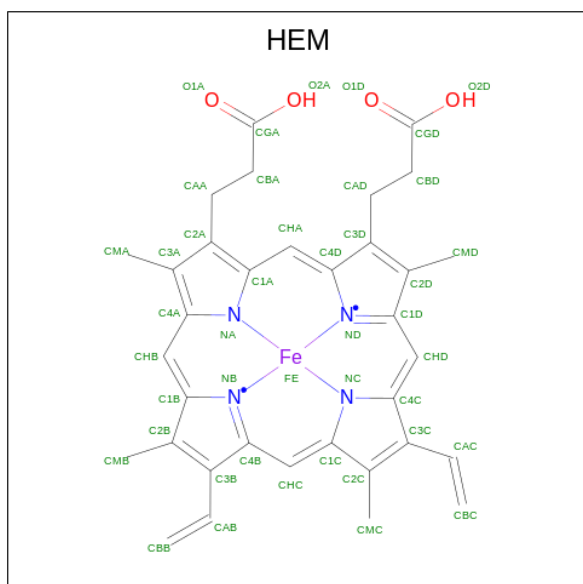


Mol	Chain	Residues	Atoms			AltConf
28	d	1	Total	C	O	0
			45	43	2	

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

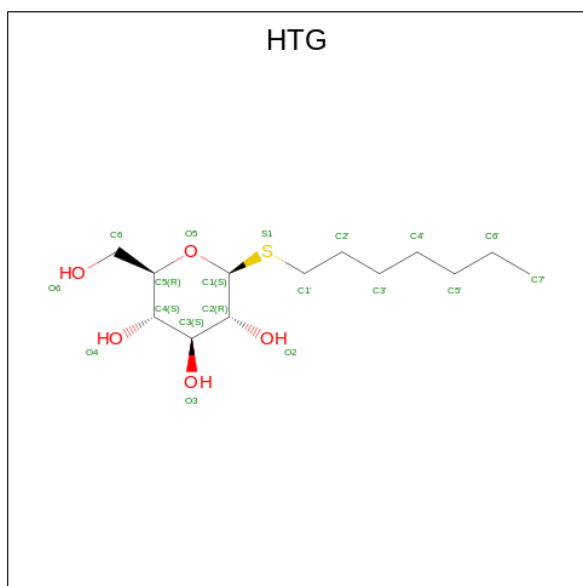
Mol	Chain	Residues	Atoms			AltConf
29	d	2	Total	C	O	0
			53	47	6	

- Molecule 30 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 31 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).

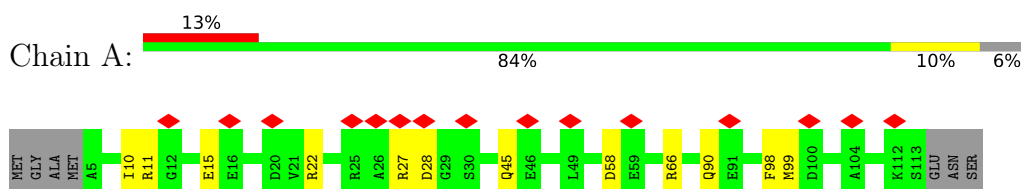


Mol	Chain	Residues	Atoms				AltConf
31	h	1	Total	C	O	S	0
			16	10	5	1	

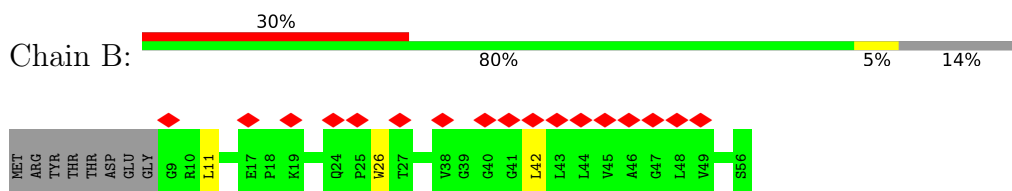
3 Residue-property plots [i](#)

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

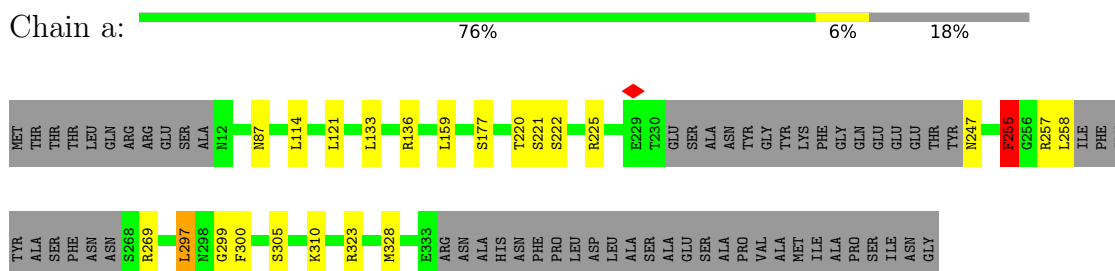
- Molecule 1: Photosystem II reaction center Psb28 protein



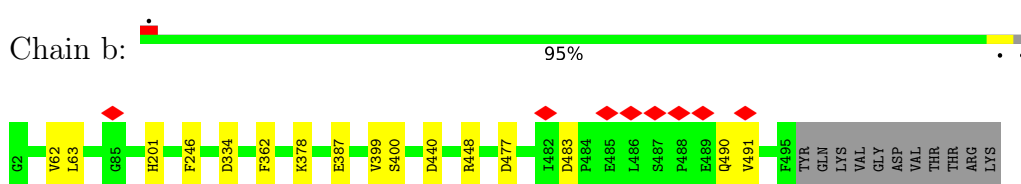
- Molecule 2: Tsl0063 protein



- Molecule 3: Photosystem II protein D1

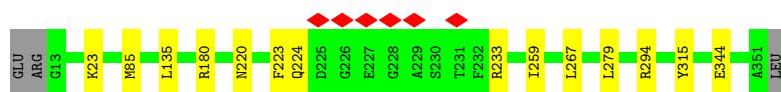


- Molecule 4: Photosystem II CP47 reaction center protein

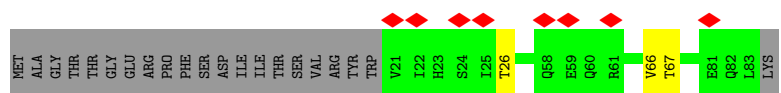


- Molecule 5: Photosystem II D2 protein

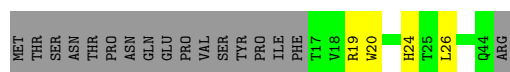




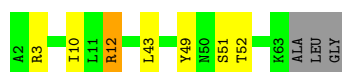
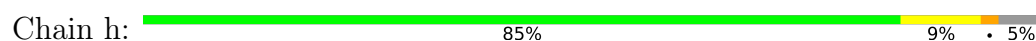
- Molecule 6: Cytochrome b559 subunit alpha



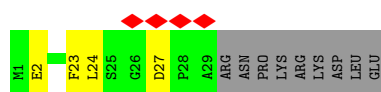
- Molecule 7: Cytochrome b559 subunit beta



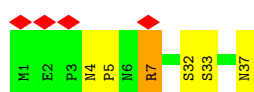
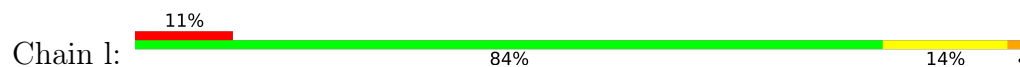
- Molecule 8: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein I



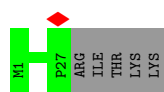
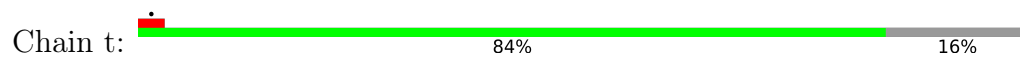
- Molecule 10: Photosystem II reaction center protein L



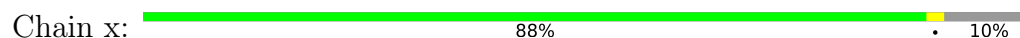
- Molecule 11: Photosystem II reaction center protein M



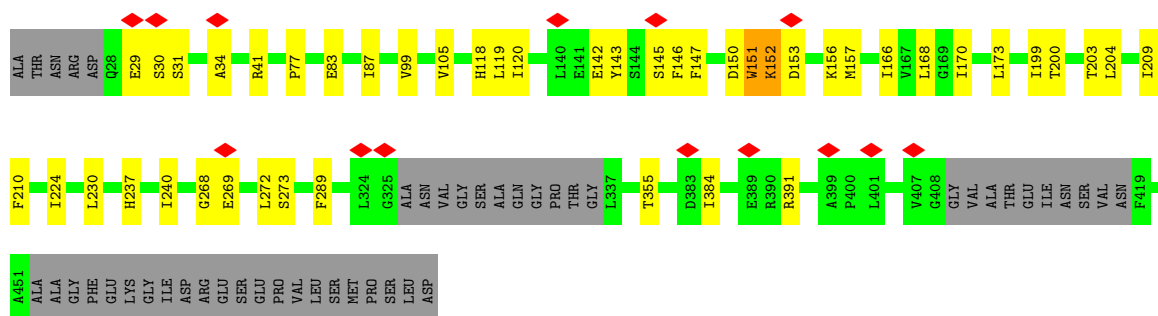
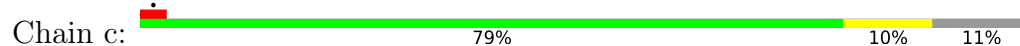
- Molecule 12: Photosystem II reaction center protein T



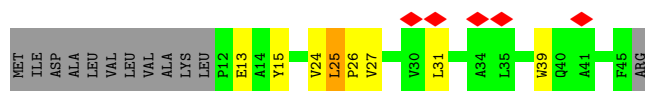
- Molecule 13: Photosystem II reaction center protein X



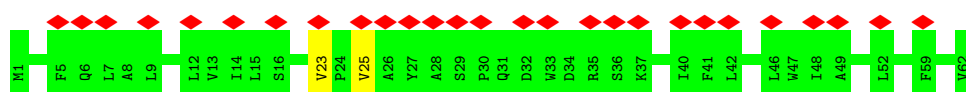
- Molecule 14: Photosystem II CP43 reaction center protein



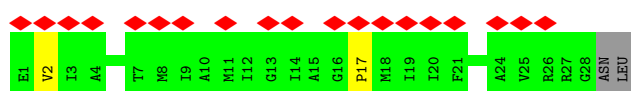
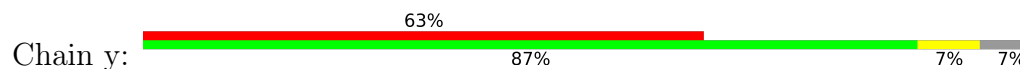
- Molecule 15: Photosystem II reaction center protein K



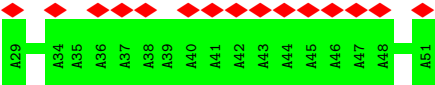
- Molecule 16: Photosystem II reaction center protein Z



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: unidentified transmembrane protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194738	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (\AA)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CLA, UNL, PHO, HTG, LMT, MGE, SQD, PQ9, DGD, BCR, CL, FE2

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	0.39	0/892	0.59	0/1202
2	B	0.28	0/355	0.65	1/484 (0.2%)
3	a	0.37	0/2376	0.62	2/3239 (0.1%)
4	b	0.39	0/4025	0.57	0/5486
5	d	0.42	0/2789	0.61	2/3803 (0.1%)
6	e	0.34	0/523	0.53	0/714
7	f	0.33	0/225	0.66	0/308
8	h	0.34	0/506	0.60	0/690
9	i	0.42	0/237	0.63	0/322
10	l	0.34	0/311	0.53	0/422
11	m	0.37	0/248	0.55	0/339
12	t	0.39	0/239	0.48	0/324
13	x	0.29	0/264	0.51	0/358
14	c	0.35	0/3237	0.56	0/4408
15	k	0.39	0/274	0.75	1/379 (0.3%)
16	z	0.33	0/466	0.65	0/641
17	y	0.34	0/136	0.77	1/187 (0.5%)
18	C	0.15	0/114	0.34	0/158
All	All	0.37	0/17217	0.59	7/23464 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	k	31	LEU	CA-CB-CG	7.04	131.48	115.30
3	a	297	LEU	N-CA-C	-6.51	93.44	111.00
17	y	17	PRO	N-CA-CB	6.11	110.64	103.30
5	d	267	LEU	CA-CB-CG	6.09	129.30	115.30
2	B	42	LEU	CA-CB-CG	5.46	127.85	115.30
5	d	267	LEU	CB-CG-CD2	-5.24	102.09	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	255	PHE	CB-CA-C	5.23	120.85	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	107/116 (92%)	95 (89%)	11 (10%)	1 (1%)	17	50
2	B	46/56 (82%)	44 (96%)	2 (4%)	0	100	100
3	a	291/360 (81%)	279 (96%)	10 (3%)	2 (1%)	22	56
4	b	492/505 (97%)	470 (96%)	21 (4%)	1 (0%)	47	78
5	d	337/342 (98%)	323 (96%)	14 (4%)	0	100	100
6	e	61/84 (73%)	56 (92%)	5 (8%)	0	100	100
7	f	26/45 (58%)	22 (85%)	4 (15%)	0	100	100
8	h	60/65 (92%)	54 (90%)	5 (8%)	1 (2%)	9	34
9	i	27/38 (71%)	25 (93%)	2 (7%)	0	100	100
10	l	35/37 (95%)	31 (89%)	2 (6%)	2 (6%)	1	9
11	m	29/36 (81%)	28 (97%)	1 (3%)	0	100	100
12	t	25/32 (78%)	24 (96%)	1 (4%)	0	100	100
13	x	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
14	c	397/451 (88%)	355 (89%)	32 (8%)	10 (2%)	5	25
15	k	32/46 (70%)	26 (81%)	4 (12%)	2 (6%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	z	60/62 (97%)	48 (80%)	10 (17%)	2 (3%)	4	19
17	y	26/30 (87%)	20 (77%)	5 (19%)	1 (4%)	3	17
18	C	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
All	All	2106/2368 (89%)	1950 (93%)	134 (6%)	22 (1%)	20	47

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	l	7	ARG
14	c	151	TRP
14	c	153	ASP
14	c	210	PHE
16	z	23	VAL
17	y	2	VAL
14	c	152	LYS
14	c	209	ILE
14	c	268	GLY
16	z	25	VAL
14	c	30	SER
14	c	34	ALA
14	c	147	PHE
15	k	26	PRO
1	A	45	GLN
3	a	299	GLY
10	l	5	PRO
14	c	77	PRO
15	k	25	LEU
3	a	255	PHE
4	b	491	VAL
8	h	12	ARG

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	92/97 (95%)	81 (88%)	11 (12%)	5	19
2	B	34/42 (81%)	32 (94%)	2 (6%)	19	48
3	a	236/290 (81%)	214 (91%)	22 (9%)	9	31
4	b	392/403 (97%)	377 (96%)	15 (4%)	33	64
5	d	272/277 (98%)	259 (95%)	13 (5%)	25	56
6	e	55/73 (75%)	52 (94%)	3 (6%)	21	51
7	f	22/39 (56%)	18 (82%)	4 (18%)	1	7
8	h	53/54 (98%)	46 (87%)	7 (13%)	4	16
9	i	26/35 (74%)	22 (85%)	4 (15%)	2	11
10	l	35/35 (100%)	30 (86%)	5 (14%)	3	13
11	m	28/33 (85%)	21 (75%)	7 (25%)	0	2
12	t	24/29 (83%)	24 (100%)	0	100	100
13	x	29/33 (88%)	28 (97%)	1 (3%)	37	67
14	c	312/352 (89%)	274 (88%)	38 (12%)	5	19
15	k	27/37 (73%)	21 (78%)	6 (22%)	1	4
16	z	45/52 (86%)	45 (100%)	0	100	100
All	All	1682/1881 (89%)	1544 (92%)	138 (8%)	15	36

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	11	ARG
1	A	15	GLU
1	A	22	ARG
1	A	27	ARG
1	A	28	ASP
1	A	58	ASP
1	A	66	ARG
1	A	90	GLN
1	A	98	PHE
1	A	99	MET
2	B	11	LEU
2	B	26	TRP
3	a	87	ASN
3	a	114	LEU
3	a	121	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	a	133	LEU
3	a	136	ARG
3	a	159	LEU
3	a	177	SER
3	a	220	THR
3	a	221	SER
3	a	222	SER
3	a	225	ARG
3	a	247	ASN
3	a	255	PHE
3	a	257	ARG
3	a	258	LEU
3	a	269	ARG
3	a	297	LEU
3	a	300	PHE
3	a	305	SER
3	a	310	LYS
3	a	323	ARG
3	a	328	MET
4	b	62	VAL
4	b	63	LEU
4	b	201	HIS
4	b	246	PHE
4	b	334	ASP
4	b	362	PHE
4	b	378	LYS
4	b	387	GLU
4	b	399	VAL
4	b	400	SER
4	b	440	ASP
4	b	448	ARG
4	b	477	ASP
4	b	483	ASP
4	b	490	GLN
5	d	23	LYS
5	d	85	MET
5	d	135	LEU
5	d	180	ARG
5	d	220	ASN
5	d	223	PHE
5	d	224	GLN
5	d	233	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	d	259	ILE
5	d	279	LEU
5	d	294	ARG
5	d	315	TYR
5	d	344	GLU
6	e	26	THR
6	e	66	VAL
6	e	67	THR
7	f	19	ARG
7	f	20	TRP
7	f	24	HIS
7	f	26	LEU
8	h	3	ARG
8	h	10	ILE
8	h	12	ARG
8	h	43	LEU
8	h	49	TYR
8	h	51	SER
8	h	52	THR
9	i	2	GLU
9	i	23	PHE
9	i	24	LEU
9	i	27	ASP
10	l	4	ASN
10	l	7	ARG
10	l	32	SER
10	l	33	SER
10	l	37	ASN
11	m	6	LEU
11	m	9	ILE
11	m	25	LEU
11	m	28	GLN
11	m	29	THR
11	m	31	SER
11	m	32	GLN
13	x	35	ASP
14	c	29	GLU
14	c	31	SER
14	c	41	ARG
14	c	83	GLU
14	c	87	ILE
14	c	99	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	c	105	VAL
14	c	118	HIS
14	c	119	LEU
14	c	120	ILE
14	c	142	GLU
14	c	143	TYR
14	c	145	SER
14	c	146	PHE
14	c	150	ASP
14	c	151	TRP
14	c	152	LYS
14	c	156	LYS
14	c	157	MET
14	c	166	ILE
14	c	168	LEU
14	c	170	ILE
14	c	173	LEU
14	c	199	ILE
14	c	200	THR
14	c	203	THR
14	c	204	LEU
14	c	224	ILE
14	c	230	LEU
14	c	237	HIS
14	c	240	ILE
14	c	269	GLU
14	c	272	LEU
14	c	273	SER
14	c	289	PHE
14	c	355	THR
14	c	384	ILE
14	c	391	ARG
15	k	13	GLU
15	k	15	TYR
15	k	24	VAL
15	k	25	LEU
15	k	27	VAL
15	k	39	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
2	B	24	GLN
3	a	113	GLN
3	a	118	HIS
3	a	190	HIS
3	a	198	HIS
3	a	215	HIS
3	a	332	HIS
4	b	58	GLN
4	b	179	GLN
4	b	331	ASN
4	b	374	ASN
4	b	394	GLN
4	b	409	GLN
4	b	455	HIS
5	d	129	GLN
5	d	332	GLN
7	f	41	GLN
11	m	28	GLN
14	c	118	HIS
14	c	293	ASN
14	c	441	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 3 are monoatomic and 2 are unknown - leaving 64 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	$\# Z > 2$
24	DGD	c	516	-	54,54,67	0.99	2 (3%)	68,68,81	1.48	14 (20%)
22	BCR	d	409	-	41,41,41	0.69	0	56,56,56	1.73	9 (16%)
21	CLA	b	605	-	65,73,73	2.42	19 (29%)	76,113,113	2.48	24 (31%)
21	CLA	b	601	-	65,73,73	2.12	13 (20%)	76,113,113	2.30	27 (35%)
21	CLA	c	509	-	63,71,73	2.38	21 (33%)	73,110,113	2.51	26 (35%)
19	MGE	b	620	-	41,41,48	1.03	2 (4%)	49,49,56	1.20	6 (12%)
21	CLA	b	603	-	65,73,73	2.09	16 (24%)	76,113,113	2.52	24 (31%)
21	CLA	b	606	-	65,73,73	2.22	15 (23%)	76,113,113	2.08	24 (31%)
21	CLA	b	608	-	65,73,73	2.25	18 (27%)	76,113,113	1.98	19 (25%)
21	CLA	b	604	-	65,73,73	1.90	14 (21%)	76,113,113	2.54	25 (32%)
21	CLA	k	501	-	46,54,73	2.32	13 (28%)	53,90,113	4.72	29 (54%)
20	SQD	a	401	-	25,26,54	1.68	4 (16%)	34,37,65	4.81	7 (20%)
22	BCR	a	404	-	41,41,41	0.70	0	56,56,56	2.29	17 (30%)
21	CLA	d	402	-	65,73,73	1.97	17 (26%)	76,113,113	2.17	22 (28%)
21	CLA	c	507	-	51,59,73	2.25	14 (27%)	59,96,113	3.60	27 (45%)
21	CLA	c	513	-	50,58,73	2.30	13 (26%)	58,95,113	3.81	34 (58%)
30	HEM	e	101	-	41,50,50	1.32	5 (12%)	45,82,82	1.76	9 (20%)
19	MGE	d	410	-	48,48,48	0.95	2 (4%)	56,56,56	1.28	5 (8%)
20	SQD	l	101	-	46,47,54	1.30	4 (8%)	55,58,65	3.86	9 (16%)
21	CLA	d	406	-	61,69,73	1.95	8 (13%)	71,108,113	3.91	31 (43%)
19	MGE	b	619	-	48,48,48	0.99	2 (4%)	56,56,56	1.18	5 (8%)
21	CLA	b	615	-	46,54,73	2.57	18 (39%)	53,90,113	2.76	24 (45%)
21	CLA	a	402	-	65,73,73	1.89	14 (21%)	76,113,113	2.31	24 (31%)
26	LMT	m	101	-	36,36,36	0.47	0	47,47,47	0.95	3 (6%)
25	PHO	d	403	-	51,69,69	1.54	8 (15%)	47,99,99	1.99	11 (23%)
22	BCR	b	618	-	41,41,41	0.71	0	56,56,56	2.04	17 (30%)
21	CLA	b	612	-	54,62,73	2.14	16 (29%)	62,99,113	2.54	21 (33%)
24	DGD	h	104	-	55,55,67	0.92	2 (3%)	69,69,81	1.06	4 (5%)
26	LMT	d	404	-	36,36,36	0.44	0	47,47,47	0.83	1 (2%)
19	MGE	c	502	-	48,48,48	0.97	2 (4%)	56,56,56	1.09	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	c	504	-	65,73,73	2.26	17 (26%)	76,113,113	2.59	26 (34%)
21	CLA	a	403	-	51,59,73	2.17	16 (31%)	59,96,113	2.86	29 (49%)
21	CLA	c	512	-	51,59,73	2.26	13 (25%)	59,96,113	4.15	26 (44%)
19	MGE	B	101	-	48,48,48	0.94	2 (4%)	56,56,56	1.29	6 (10%)
22	BCR	h	103	-	41,41,41	0.75	0	56,56,56	1.93	15 (26%)
22	BCR	c	515	-	41,41,41	0.82	1 (2%)	56,56,56	2.60	20 (35%)
24	DGD	c	517	-	48,48,67	1.02	2 (4%)	62,62,81	1.11	5 (8%)
21	CLA	b	602	-	65,73,73	2.03	16 (24%)	76,113,113	2.53	24 (31%)
21	CLA	c	506	-	46,54,73	2.35	14 (30%)	53,90,113	4.82	26 (49%)
21	CLA	b	607	-	65,73,73	2.06	17 (26%)	76,113,113	2.15	23 (30%)
21	CLA	h	101	-	41,49,73	2.47	12 (29%)	47,84,113	5.07	27 (57%)
21	CLA	c	510	-	46,54,73	2.86	20 (43%)	53,90,113	2.70	25 (47%)
21	CLA	b	614	-	65,73,73	2.12	16 (24%)	76,113,113	2.38	25 (32%)
31	HTG	h	102	-	16,16,19	1.18	2 (12%)	20,21,24	1.68	1 (5%)
21	CLA	d	407	-	50,58,73	2.22	12 (24%)	58,95,113	4.21	30 (51%)
21	CLA	b	610	-	65,73,73	2.08	15 (23%)	76,113,113	2.30	26 (34%)
21	CLA	b	613	-	52,60,73	2.10	16 (30%)	60,97,113	3.19	31 (51%)
19	MGE	m	102	-	48,48,48	0.99	2 (4%)	56,56,56	1.13	3 (5%)
21	CLA	c	505	-	65,73,73	2.51	18 (27%)	76,113,113	2.28	25 (32%)
22	BCR	b	617	-	41,41,41	0.69	0	56,56,56	1.86	15 (26%)
24	DGD	a	406	-	58,58,67	0.91	2 (3%)	72,72,81	1.00	4 (5%)
22	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.99	13 (23%)
28	PQ9	d	408	-	45,45,45	0.69	1 (2%)	56,57,57	1.49	13 (23%)
21	CLA	b	609	-	65,73,73	2.13	16 (24%)	76,113,113	2.47	20 (26%)
21	CLA	c	511	-	65,73,73	2.12	16 (24%)	76,113,113	2.12	23 (30%)
22	BCR	b	616	-	41,41,41	0.71	0	56,56,56	1.89	20 (35%)
26	LMT	t	301	-	36,36,36	0.49	0	47,47,47	0.89	1 (2%)
25	PHO	d	401	-	51,69,69	1.65	8 (15%)	47,99,99	1.88	9 (19%)
21	CLA	b	611	-	65,73,73	2.12	15 (23%)	76,113,113	2.55	21 (27%)
21	CLA	c	508	-	46,54,73	2.54	16 (34%)	53,90,113	2.95	24 (45%)
21	CLA	a	407	-	65,73,73	1.81	16 (24%)	76,113,113	2.37	29 (38%)
19	MGE	f	101	-	47,47,48	0.99	2 (4%)	55,55,56	1.33	7 (12%)
22	BCR	z	101	-	41,41,41	0.70	0	56,56,56	2.06	16 (28%)
21	CLA	c	503	-	65,73,73	2.12	16 (24%)	76,113,113	2.70	24 (31%)

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
24	DGD	c	516	-	-	12/42/82/95	0/2/2/2
22	BCR	d	409	-	-	8/29/63/63	0/2/2/2
21	CLA	b	605	-	1/1/15/20	12/37/115/115	-
21	CLA	b	601	-	1/1/15/20	4/37/115/115	-
21	CLA	c	509	-	1/1/14/20	7/35/113/115	-
19	MGE	b	620	-	-	6/36/56/63	0/1/1/1
21	CLA	b	603	-	1/1/15/20	7/37/115/115	-
21	CLA	b	606	-	1/1/15/20	2/37/115/115	-
21	CLA	b	608	-	-	0/37/115/115	-
21	CLA	b	604	-	1/1/15/20	4/37/115/115	-
21	CLA	k	501	-	-	7/15/93/115	-
20	SQD	a	401	-	-	4/19/39/69	0/1/1/1
22	BCR	a	404	-	-	10/29/63/63	0/2/2/2
21	CLA	d	402	-	1/1/15/20	5/37/115/115	-
21	CLA	c	507	-	-	10/21/99/115	-
21	CLA	c	513	-	-	9/19/97/115	-
30	HEM	e	101	-	-	5/12/54/54	-
19	MGE	d	410	-	-	14/43/63/63	0/1/1/1
21	CLA	d	406	-	1/1/14/20	9/33/111/115	-
20	SQD	l	101	-	-	7/42/62/69	0/1/1/1
19	MGE	b	619	-	-	9/43/63/63	0/1/1/1
21	CLA	b	615	-	1/1/11/20	2/15/93/115	-
21	CLA	a	402	-	1/1/15/20	5/37/115/115	-
26	LMT	m	101	-	-	2/21/61/61	0/2/2/2
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6
22	BCR	b	618	-	-	3/29/63/63	0/2/2/2
21	CLA	b	612	-	1/1/12/20	0/24/102/115	-
24	DGD	h	104	-	-	13/43/83/95	0/2/2/2
26	LMT	d	404	-	-	4/21/61/61	0/2/2/2
21	CLA	c	504	-	1/1/15/20	7/37/115/115	-
19	MGE	c	502	-	-	13/43/63/63	0/1/1/1
21	CLA	a	403	-	-	1/21/99/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	c	512	-	-	8/21/99/115	-
19	MGE	B	101	-	-	17/43/63/63	0/1/1/1
22	BCR	h	103	-	-	7/29/63/63	0/2/2/2
22	BCR	c	515	-	-	4/29/63/63	0/2/2/2
24	DGD	c	517	-	-	8/36/76/95	0/2/2/2
21	CLA	b	602	-	1/1/15/20	4/37/115/115	-
21	CLA	c	510	-	1/1/11/20	3/15/93/115	-
21	CLA	b	607	-	-	1/37/115/115	-
21	CLA	h	101	-	-	2/8/86/115	-
21	CLA	c	506	-	-	4/15/93/115	-
21	CLA	b	614	-	1/1/15/20	9/37/115/115	-
31	HTG	h	102	-	-	0/7/27/30	0/1/1/1
21	CLA	d	407	-	-	4/19/97/115	-
21	CLA	b	613	-	1/1/12/20	9/22/100/115	-
21	CLA	b	610	-	-	6/37/115/115	-
19	MGE	m	102	-	-	10/43/63/63	0/1/1/1
21	CLA	c	505	-	-	2/37/115/115	-
22	BCR	b	617	-	-	0/29/63/63	0/2/2/2
24	DGD	a	406	-	-	19/46/86/95	0/2/2/2
22	BCR	c	514	-	-	8/29/63/63	0/2/2/2
28	PQ9	d	408	-	-	7/41/61/61	0/1/1/1
21	CLA	b	609	-	1/1/15/20	4/37/115/115	-
21	CLA	c	511	-	1/1/15/20	9/37/115/115	-
22	BCR	b	616	-	-	0/29/63/63	0/2/2/2
26	LMT	t	301	-	-	7/21/61/61	0/2/2/2
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6
21	CLA	b	611	-	1/1/15/20	7/37/115/115	-
21	CLA	c	508	-	1/1/11/20	3/15/93/115	-
21	CLA	a	407	-	-	6/37/115/115	-
19	MGE	f	101	-	-	3/42/62/63	0/1/1/1
22	BCR	z	101	-	-	6/29/63/63	0/2/2/2
21	CLA	c	503	-	1/1/15/20	4/37/115/115	-

All (581) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	611	CLA	MG-NA	10.39	2.31	2.06
21	b	605	CLA	MG-NA	10.30	2.30	2.06
21	c	505	CLA	MG-NA	9.83	2.29	2.06
21	c	506	CLA	C1D-ND	8.70	1.48	1.37
21	c	505	CLA	MG-NC	8.62	2.26	2.06
21	b	614	CLA	MG-NA	8.39	2.26	2.06
21	b	610	CLA	MG-NA	8.37	2.26	2.06
21	d	406	CLA	C1D-ND	8.27	1.47	1.37
21	d	407	CLA	C1D-ND	8.24	1.47	1.37
21	b	603	CLA	MG-NA	8.24	2.25	2.06
21	h	101	CLA	C1D-ND	8.22	1.47	1.37
21	c	508	CLA	MG-ND	-8.19	1.89	2.05
21	c	512	CLA	C1D-ND	8.15	1.47	1.37
21	c	503	CLA	MG-NA	8.13	2.25	2.06
21	k	501	CLA	C1D-ND	8.09	1.47	1.37
21	c	513	CLA	C1D-ND	7.89	1.47	1.37
21	c	510	CLA	MG-NA	7.80	2.24	2.06
21	c	507	CLA	C1D-ND	7.80	1.47	1.37
21	b	607	CLA	MG-NA	7.70	2.24	2.06
21	c	504	CLA	MG-ND	-7.39	1.91	2.05
21	c	504	CLA	MG-NA	7.38	2.23	2.06
21	c	510	CLA	MG-ND	-7.34	1.91	2.05
21	b	606	CLA	MG-NA	7.13	2.23	2.06
21	c	510	CLA	OBD-CAD	6.89	1.34	1.22
21	b	608	CLA	MG-NC	6.78	2.22	2.06
21	c	509	CLA	MG-NA	6.57	2.21	2.06
21	c	509	CLA	MG-NC	6.53	2.21	2.06
21	c	511	CLA	MG-NC	6.47	2.21	2.06
21	b	608	CLA	CHC-C1C	6.35	1.51	1.35
21	d	402	CLA	MG-NA	6.33	2.21	2.06
21	a	402	CLA	MG-NA	6.32	2.21	2.06
21	b	601	CLA	MG-NC	6.17	2.20	2.06
21	c	509	CLA	MG-ND	6.11	2.17	2.05
21	b	609	CLA	MG-NA	6.10	2.20	2.06
21	b	606	CLA	C3C-C2C	6.08	1.49	1.36
21	b	606	CLA	CHC-C1C	6.01	1.50	1.35
21	b	615	CLA	CHC-C1C	5.98	1.50	1.35
21	b	612	CLA	MG-NA	5.97	2.20	2.06
21	b	601	CLA	C3C-C2C	5.97	1.49	1.36
21	c	503	CLA	C3B-C2B	5.92	1.48	1.40
21	b	604	CLA	C1D-ND	-5.83	1.30	1.37
21	b	615	CLA	MG-NA	5.83	2.20	2.06
21	b	602	CLA	MG-NA	5.70	2.19	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	606	CLA	MG-NC	5.66	2.19	2.06
21	b	608	CLA	O2D-CGD	5.65	1.47	1.33
21	b	609	CLA	C3C-C2C	5.65	1.48	1.36
21	b	605	CLA	C3B-C2B	5.64	1.48	1.40
21	c	509	CLA	C3C-C2C	5.56	1.48	1.36
21	b	611	CLA	C3C-C2C	5.54	1.48	1.36
21	d	402	CLA	CHC-C1C	5.53	1.49	1.35
21	c	505	CLA	C3C-C2C	5.52	1.48	1.36
21	c	504	CLA	C3B-C2B	5.51	1.48	1.40
21	b	602	CLA	CHC-C1C	5.51	1.49	1.35
21	c	508	CLA	O2D-CGD	5.46	1.46	1.33
21	b	603	CLA	CHC-C1C	5.45	1.48	1.35
21	b	613	CLA	MG-NA	5.43	2.19	2.06
21	b	608	CLA	C3C-C2C	5.41	1.48	1.36
21	b	605	CLA	MG-NC	5.33	2.18	2.06
21	b	601	CLA	CHC-C1C	5.31	1.48	1.35
21	b	602	CLA	C1D-ND	-5.30	1.31	1.37
21	b	602	CLA	C3C-C2C	5.28	1.48	1.36
21	h	101	CLA	O2D-CGD	5.25	1.46	1.33
21	b	604	CLA	CHC-C1C	5.23	1.48	1.35
21	c	505	CLA	CHC-C1C	5.21	1.48	1.35
21	a	403	CLA	CHC-C1C	5.18	1.48	1.35
21	c	509	CLA	CHC-C1C	5.16	1.48	1.35
21	b	612	CLA	CHC-C1C	5.15	1.48	1.35
21	c	513	CLA	O2D-CGD	5.15	1.45	1.33
21	b	609	CLA	O2D-CGD	5.14	1.45	1.33
21	b	601	CLA	C1D-ND	-5.12	1.31	1.37
21	b	610	CLA	CHD-C1D	5.11	1.48	1.38
21	b	608	CLA	CHD-C1D	5.11	1.48	1.38
21	b	603	CLA	C3C-C2C	5.10	1.47	1.36
21	b	612	CLA	O2D-CGD	5.07	1.45	1.33
21	c	512	CLA	O2D-CGD	5.07	1.45	1.33
21	c	511	CLA	O2D-CGD	5.06	1.45	1.33
21	b	604	CLA	MG-NA	5.06	2.18	2.06
21	c	507	CLA	O2D-CGD	5.05	1.45	1.33
21	a	403	CLA	MG-NA	5.05	2.18	2.06
21	k	501	CLA	O2D-CGD	5.05	1.45	1.33
21	c	504	CLA	O2D-CGD	5.05	1.45	1.33
21	b	601	CLA	OBD-CAD	5.04	1.31	1.22
21	c	508	CLA	C3B-C2B	5.04	1.47	1.40
21	b	614	CLA	C3C-C2C	5.02	1.47	1.36
21	b	604	CLA	O2D-CGD	5.00	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	505	CLA	C3B-C2B	5.00	1.47	1.40
20	l	101	SQD	O8-S	4.99	1.65	1.47
21	c	510	CLA	C3B-C2B	4.99	1.47	1.40
21	c	508	CLA	MG-NA	4.99	2.18	2.06
21	c	506	CLA	O2D-CGD	4.98	1.45	1.33
21	b	615	CLA	C1D-ND	-4.95	1.31	1.37
21	b	601	CLA	C3B-C2B	4.92	1.47	1.40
20	a	401	SQD	O8-S	4.92	1.65	1.47
21	c	510	CLA	O2D-CGD	4.91	1.45	1.33
21	a	407	CLA	CHC-C1C	4.88	1.47	1.35
21	b	604	CLA	C3C-C2C	4.88	1.47	1.36
21	d	406	CLA	O2D-CGD	4.88	1.45	1.33
20	a	401	SQD	O47-C7	4.87	1.46	1.35
21	c	508	CLA	C3C-C2C	4.86	1.47	1.36
21	a	402	CLA	OBD-CAD	4.85	1.30	1.22
21	c	511	CLA	C3C-C2C	4.84	1.47	1.36
21	d	402	CLA	C3C-C2C	4.84	1.47	1.36
21	b	615	CLA	C3C-C2C	4.82	1.47	1.36
21	d	406	CLA	C3D-C4D	-4.80	1.33	1.44
21	b	609	CLA	CHD-C1D	4.79	1.47	1.38
21	d	407	CLA	O2D-CGD	4.77	1.44	1.33
25	d	401	PHO	O2D-CGD	4.77	1.44	1.33
21	b	610	CLA	CHC-C1C	4.77	1.47	1.35
21	b	615	CLA	O2D-CGD	4.75	1.44	1.33
25	d	403	PHO	C3D-C2D	4.75	1.48	1.39
21	a	402	CLA	C3C-C2C	4.75	1.46	1.36
21	b	613	CLA	CHD-C1D	4.75	1.47	1.38
21	b	605	CLA	C3C-C2C	4.74	1.46	1.36
21	c	511	CLA	CHC-C1C	4.73	1.47	1.35
21	b	607	CLA	CHC-C1C	4.71	1.47	1.35
25	d	401	PHO	C3D-C2D	4.70	1.47	1.39
21	c	513	CLA	C3C-C2C	4.68	1.46	1.36
21	b	601	CLA	CHD-C4C	4.67	1.49	1.39
21	c	504	CLA	OBD-CAD	4.66	1.30	1.22
21	b	611	CLA	CHC-C1C	4.65	1.46	1.35
21	a	403	CLA	C3B-C2B	4.65	1.46	1.40
21	h	101	CLA	C3D-C4D	-4.64	1.33	1.44
21	c	505	CLA	CHD-C1D	4.63	1.47	1.38
21	a	403	CLA	C3C-C2C	4.63	1.46	1.36
21	b	614	CLA	O2D-CGD	4.62	1.44	1.33
21	k	501	CLA	C3D-C4D	-4.62	1.33	1.44
21	c	506	CLA	C3D-C4D	-4.62	1.33	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	615	CLA	C3B-C2B	4.61	1.46	1.40
21	b	607	CLA	C3B-C2B	4.60	1.46	1.40
21	b	609	CLA	MG-ND	-4.60	1.96	2.05
21	b	602	CLA	O2D-CGD	4.59	1.44	1.33
21	d	407	CLA	C3D-C4D	-4.56	1.33	1.44
21	b	614	CLA	C3B-C2B	4.56	1.46	1.40
21	c	512	CLA	C3D-C4D	-4.55	1.33	1.44
21	b	606	CLA	CHD-C1D	4.55	1.47	1.38
21	b	614	CLA	OBD-CAD	4.55	1.30	1.22
21	k	501	CLA	O2A-CGA	4.55	1.47	1.33
21	c	503	CLA	CHC-C1C	4.55	1.46	1.35
21	b	605	CLA	CHC-C1C	4.54	1.46	1.35
21	h	101	CLA	C3C-C2C	4.53	1.46	1.36
21	c	512	CLA	C3C-C2C	4.52	1.46	1.36
21	b	609	CLA	CHC-C1C	4.51	1.46	1.35
21	b	605	CLA	CHD-C1D	4.50	1.47	1.38
21	b	610	CLA	O2D-CGD	4.49	1.44	1.33
21	c	503	CLA	CHD-C1D	4.46	1.47	1.38
21	c	510	CLA	CHD-C1D	4.46	1.47	1.38
21	b	614	CLA	CHD-C4C	4.45	1.49	1.39
21	c	511	CLA	MG-NA	4.45	2.16	2.06
21	c	504	CLA	CHD-C1D	4.44	1.47	1.38
21	b	605	CLA	O2D-CGD	4.41	1.44	1.33
19	b	619	MGE	O2G-C1B	4.41	1.46	1.34
21	b	613	CLA	O2A-CGA	4.41	1.46	1.33
21	c	513	CLA	C3D-C4D	-4.41	1.34	1.44
21	b	612	CLA	C3C-C2C	4.39	1.46	1.36
21	c	507	CLA	C3C-C2C	4.38	1.46	1.36
21	c	507	CLA	C3D-C4D	-4.37	1.34	1.44
21	b	614	CLA	CHC-C1C	4.36	1.46	1.35
21	c	503	CLA	C3C-C2C	4.36	1.46	1.36
21	b	615	CLA	CHD-C1D	4.36	1.46	1.38
21	c	513	CLA	CHC-C1C	4.35	1.46	1.35
21	a	402	CLA	C3B-C2B	4.35	1.46	1.40
21	c	510	CLA	CHC-C1C	4.35	1.46	1.35
21	b	603	CLA	MG-ND	-4.34	1.97	2.05
21	a	407	CLA	C3C-C2C	4.33	1.45	1.36
21	c	504	CLA	CHC-C1C	4.33	1.46	1.35
21	c	513	CLA	O2A-CGA	4.32	1.46	1.33
21	c	505	CLA	O2D-CGD	4.30	1.43	1.33
21	b	607	CLA	C3C-C2C	4.30	1.45	1.36
21	b	601	CLA	CHD-C1D	4.30	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	d	402	CLA	CHD-C1D	4.28	1.46	1.38
21	c	511	CLA	C3B-C2B	4.27	1.46	1.40
20	l	101	SQD	O47-C7	4.27	1.46	1.34
25	d	403	PHO	O2D-CGD	4.26	1.43	1.33
21	c	512	CLA	O2A-CGA	4.26	1.45	1.33
21	d	407	CLA	C3C-C2C	4.26	1.45	1.36
21	c	510	CLA	C3C-C2C	4.26	1.45	1.36
21	k	501	CLA	C3C-C2C	4.25	1.45	1.36
21	b	613	CLA	CHC-C1C	4.24	1.45	1.35
19	b	619	MGE	O1G-C1A	4.24	1.45	1.33
19	m	102	MGE	O1G-C1A	4.23	1.45	1.33
21	k	501	CLA	CHC-C1C	4.23	1.45	1.35
21	b	612	CLA	O2A-CGA	4.22	1.45	1.33
19	b	620	MGE	O2G-C1B	4.22	1.46	1.34
21	c	507	CLA	O2A-CGA	4.21	1.45	1.33
19	c	502	MGE	O2G-C1B	4.20	1.46	1.34
21	d	407	CLA	O2A-CGA	4.20	1.45	1.33
21	c	507	CLA	CHC-C1C	4.17	1.45	1.35
19	m	102	MGE	O2G-C1B	4.17	1.46	1.34
20	l	101	SQD	O48-C23	4.17	1.45	1.33
21	b	607	CLA	OBD-CAD	4.16	1.29	1.22
21	a	407	CLA	MG-NA	4.15	2.16	2.06
19	f	101	MGE	O2G-C1B	4.15	1.46	1.34
21	b	605	CLA	C1B-NB	4.15	1.38	1.35
19	f	101	MGE	O1G-C1A	4.15	1.45	1.33
25	d	403	PHO	C3B-C2B	4.15	1.46	1.40
24	c	516	DGD	O2G-C1B	4.14	1.46	1.34
21	h	101	CLA	CHC-C1C	4.14	1.45	1.35
21	c	508	CLA	CHD-C4C	4.14	1.48	1.39
19	c	502	MGE	O1G-C1A	4.13	1.45	1.33
24	c	517	DGD	O2G-C1B	4.13	1.45	1.34
24	h	104	DGD	O1G-C1A	4.12	1.45	1.33
21	c	512	CLA	CHC-C1C	4.12	1.45	1.35
19	d	410	MGE	O1G-C1A	4.12	1.45	1.33
21	c	506	CLA	C3C-C2C	4.12	1.45	1.36
24	a	406	DGD	O1G-C1A	4.10	1.45	1.33
19	B	101	MGE	O2G-C1B	4.09	1.45	1.34
21	b	606	CLA	O2D-CGD	4.09	1.43	1.33
21	c	508	CLA	CHC-C1C	4.09	1.45	1.35
21	c	511	CLA	CHD-C1D	4.09	1.46	1.38
24	c	516	DGD	O1G-C1A	4.07	1.45	1.33
24	c	517	DGD	O1G-C1A	4.07	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	506	CLA	O2A-CGA	4.07	1.46	1.33
21	b	603	CLA	O2D-CGD	4.06	1.43	1.33
19	b	620	MGE	O1G-C1A	4.05	1.45	1.33
25	d	401	PHO	C3B-C2B	4.03	1.46	1.40
21	d	406	CLA	C3C-C2C	4.03	1.45	1.36
21	b	610	CLA	C3C-C2C	4.02	1.45	1.36
21	b	610	CLA	C3B-C2B	4.02	1.46	1.40
21	a	403	CLA	C1D-ND	-4.02	1.32	1.37
21	b	603	CLA	CHD-C1D	4.02	1.46	1.38
21	b	615	CLA	O2A-CGA	4.01	1.45	1.33
24	a	406	DGD	O2G-C1B	4.00	1.45	1.34
21	c	509	CLA	CHD-C1D	4.00	1.46	1.38
21	b	615	CLA	MG-ND	3.99	2.13	2.05
21	d	406	CLA	CHC-C1C	3.99	1.45	1.35
21	b	613	CLA	O2D-CGD	3.99	1.42	1.33
21	b	608	CLA	MG-NA	3.98	2.15	2.06
21	d	406	CLA	O2A-CGA	3.98	1.45	1.33
21	b	609	CLA	OBD-CAD	3.97	1.29	1.22
21	d	407	CLA	CHC-C1C	3.97	1.45	1.35
21	b	611	CLA	O2D-CGD	3.96	1.42	1.33
21	d	402	CLA	CHD-C4C	3.96	1.48	1.39
24	h	104	DGD	O2G-C1B	3.96	1.45	1.34
21	b	612	CLA	C3B-C2B	3.96	1.45	1.40
21	c	511	CLA	O2A-CGA	3.96	1.44	1.33
21	c	512	CLA	C3B-C2B	3.95	1.45	1.40
21	b	609	CLA	C4C-C3C	3.95	1.51	1.45
21	k	501	CLA	C3B-C2B	3.94	1.45	1.40
21	b	608	CLA	C3B-C2B	3.94	1.45	1.40
19	B	101	MGE	O1G-C1A	3.94	1.44	1.33
21	h	101	CLA	C3B-C2B	3.92	1.45	1.40
19	d	410	MGE	O2G-C1B	3.91	1.45	1.34
21	b	613	CLA	CHD-C4C	3.91	1.48	1.39
21	c	509	CLA	CHD-C4C	3.90	1.48	1.39
21	d	406	CLA	C3B-C2B	3.89	1.45	1.40
21	b	606	CLA	C1D-ND	-3.89	1.33	1.37
21	c	511	CLA	CHD-C4C	3.89	1.48	1.39
25	d	403	PHO	C3A-C2A	-3.87	1.51	1.54
21	a	402	CLA	O2D-CGD	3.87	1.42	1.33
21	c	506	CLA	CHC-C1C	3.85	1.44	1.35
21	c	503	CLA	O2D-CGD	3.85	1.42	1.33
31	h	102	HTG	C1'-S1	-3.84	1.76	1.81
21	c	503	CLA	O2A-CGA	3.83	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	605	CLA	CHD-C4C	3.82	1.47	1.39
21	b	609	CLA	CHD-C4C	3.80	1.47	1.39
21	b	607	CLA	CHD-C1D	3.80	1.45	1.38
21	c	508	CLA	O2A-CGA	3.78	1.45	1.33
21	b	602	CLA	CHD-C1D	3.77	1.45	1.38
21	c	507	CLA	C3B-C2B	3.76	1.45	1.40
21	b	606	CLA	C3D-C2D	3.76	1.49	1.39
21	c	505	CLA	CHD-C4C	3.75	1.47	1.39
21	c	506	CLA	C3B-C2B	3.74	1.45	1.40
21	b	607	CLA	CHD-C4C	3.73	1.47	1.39
21	b	606	CLA	MG-ND	3.72	2.13	2.05
21	a	403	CLA	CHD-C1D	3.71	1.45	1.38
21	d	407	CLA	C3B-C2B	3.70	1.45	1.40
21	a	403	CLA	O2A-CGA	3.68	1.44	1.33
21	c	507	CLA	OBD-CAD	3.68	1.28	1.22
21	h	101	CLA	OBD-CAD	3.68	1.28	1.22
21	b	608	CLA	O2A-CGA	3.66	1.44	1.33
21	b	602	CLA	OBD-CAD	3.64	1.28	1.22
21	b	614	CLA	C3D-C2D	3.62	1.49	1.39
21	b	603	CLA	MG-NC	3.62	2.14	2.06
21	a	402	CLA	CHC-C1C	3.61	1.44	1.35
21	b	607	CLA	C4B-NB	-3.61	1.32	1.35
21	b	612	CLA	OBD-CAD	3.61	1.28	1.22
21	c	509	CLA	O2A-CGA	3.60	1.43	1.33
21	b	611	CLA	CHD-C1D	3.58	1.45	1.38
21	b	613	CLA	C3C-C2C	3.57	1.44	1.36
21	b	610	CLA	CHD-C4C	3.57	1.47	1.39
21	b	610	CLA	O2A-CGA	3.57	1.43	1.33
21	a	407	CLA	O2D-CGD	3.57	1.41	1.33
25	d	403	PHO	O2A-CGA	3.56	1.43	1.33
21	c	509	CLA	O2D-CGD	3.55	1.41	1.33
21	c	503	CLA	CHD-C4C	3.55	1.47	1.39
21	c	511	CLA	MG-ND	-3.55	1.98	2.05
21	c	508	CLA	CHD-C1D	3.54	1.45	1.38
25	d	401	PHO	C3C-C2C	3.54	1.48	1.37
21	a	403	CLA	O2D-CGD	3.52	1.41	1.33
21	c	504	CLA	C3C-C2C	3.51	1.44	1.36
21	c	513	CLA	CHD-C4C	3.51	1.47	1.39
21	k	501	CLA	OBD-CAD	3.50	1.28	1.22
21	c	513	CLA	OBD-CAD	3.50	1.28	1.22
21	c	510	CLA	O2A-CGA	3.49	1.44	1.33
21	c	513	CLA	CHD-C1D	3.49	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	403	CLA	CHD-C4C	3.47	1.47	1.39
21	b	607	CLA	O2D-CGD	3.47	1.41	1.33
21	c	512	CLA	OBD-CAD	3.46	1.28	1.22
21	b	613	CLA	C3B-C2B	3.45	1.45	1.40
21	a	407	CLA	C4D-ND	-3.45	1.32	1.37
25	d	401	PHO	OBD-CAD	3.45	1.27	1.22
21	c	511	CLA	OBD-CAD	3.44	1.28	1.22
21	c	509	CLA	C3B-C2B	3.44	1.45	1.40
21	c	510	CLA	MG-NC	3.43	2.14	2.06
21	d	407	CLA	OBD-CAD	3.43	1.28	1.22
21	h	101	CLA	CHD-C1D	3.42	1.45	1.38
21	a	403	CLA	OBD-CAD	3.41	1.28	1.22
21	b	608	CLA	OBD-CAD	3.41	1.28	1.22
21	c	506	CLA	OBD-CAD	3.40	1.28	1.22
30	e	101	HEM	C1B-NB	-3.40	1.34	1.40
21	c	509	CLA	C3D-C2D	3.39	1.48	1.39
21	b	609	CLA	MG-NC	3.38	2.14	2.06
21	b	603	CLA	C3B-C2B	3.38	1.45	1.40
21	c	503	CLA	C4C-C3C	3.38	1.50	1.45
21	c	504	CLA	O2A-CGA	3.37	1.43	1.33
21	b	601	CLA	O2A-CGA	3.37	1.43	1.33
21	b	610	CLA	C1B-CHB	3.35	1.50	1.41
21	a	407	CLA	C3D-C2D	3.34	1.48	1.39
21	d	402	CLA	C1D-ND	-3.34	1.33	1.37
21	b	602	CLA	C3B-C2B	3.33	1.45	1.40
21	c	509	CLA	OBD-CAD	3.32	1.28	1.22
21	d	402	CLA	C3B-C2B	3.31	1.45	1.40
21	a	402	CLA	CHD-C4C	3.30	1.46	1.39
21	b	612	CLA	CHD-C1D	3.30	1.44	1.38
21	b	604	CLA	C3B-C2B	3.27	1.44	1.40
21	b	607	CLA	C1D-ND	-3.26	1.33	1.37
21	a	402	CLA	C4B-NB	-3.26	1.32	1.35
30	e	101	HEM	C4D-ND	-3.26	1.34	1.40
21	a	407	CLA	C1D-ND	-3.25	1.33	1.37
21	h	101	CLA	CHD-C4C	3.24	1.46	1.39
21	c	505	CLA	O2A-CGA	3.22	1.42	1.33
21	a	403	CLA	C1B-CHB	3.21	1.49	1.41
21	b	613	CLA	MG-ND	-3.21	1.99	2.05
21	b	602	CLA	CHD-C4C	3.20	1.46	1.39
21	b	608	CLA	CHD-C4C	3.20	1.46	1.39
21	b	605	CLA	C4D-CHA	3.19	1.49	1.38
21	c	513	CLA	C3D-C2D	3.18	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	407	CLA	C4D-CHA	3.18	1.49	1.38
21	d	406	CLA	OBD-CAD	3.17	1.27	1.22
21	c	509	CLA	C4D-CHA	3.17	1.49	1.38
21	b	611	CLA	O2A-CGA	3.17	1.42	1.33
21	a	407	CLA	CHD-C4C	3.15	1.46	1.39
21	c	513	CLA	C3B-C2B	3.15	1.44	1.40
21	c	505	CLA	C1B-CHB	3.15	1.49	1.41
21	b	603	CLA	CHD-C4C	3.15	1.46	1.39
21	b	615	CLA	OBD-CAD	3.15	1.27	1.22
21	b	615	CLA	C3D-C2D	3.14	1.47	1.39
21	d	402	CLA	O2A-CGA	3.13	1.42	1.33
21	c	507	CLA	C3D-C2D	3.12	1.47	1.39
21	c	503	CLA	OBD-CAD	3.11	1.27	1.22
21	a	407	CLA	C3B-C2B	3.11	1.44	1.40
21	c	504	CLA	CHD-C4C	3.09	1.46	1.39
21	c	503	CLA	C1B-CHB	3.09	1.49	1.41
21	c	512	CLA	CHD-C1D	3.08	1.44	1.38
21	c	509	CLA	C1D-ND	-3.07	1.34	1.37
21	c	510	CLA	C3D-C2D	3.07	1.47	1.39
21	c	513	CLA	C1D-C2D	3.06	1.51	1.45
21	b	608	CLA	C1D-ND	-3.06	1.34	1.37
21	b	610	CLA	C3D-C2D	3.05	1.47	1.39
21	b	608	CLA	C3D-C2D	3.05	1.47	1.39
21	b	614	CLA	CHD-C1D	3.04	1.44	1.38
21	d	407	CLA	CHD-C1D	3.03	1.44	1.38
21	c	505	CLA	C3D-C2D	3.03	1.47	1.39
21	c	505	CLA	C4D-CHA	3.03	1.49	1.38
21	b	606	CLA	CHD-C4C	3.02	1.46	1.39
21	c	504	CLA	C1B-CHB	3.01	1.49	1.41
21	c	507	CLA	CHD-C1D	3.00	1.44	1.38
21	c	507	CLA	CHD-C4C	2.99	1.46	1.39
21	b	615	CLA	C1C-C2C	2.98	1.50	1.44
21	d	402	CLA	OBD-CAD	2.98	1.27	1.22
21	b	612	CLA	C1D-ND	-2.96	1.34	1.37
21	b	611	CLA	C3D-C2D	2.96	1.47	1.39
21	b	615	CLA	CHD-C4C	2.95	1.46	1.39
21	a	407	CLA	CHD-C1D	2.95	1.44	1.38
21	b	610	CLA	C4D-CHA	2.93	1.48	1.38
21	b	611	CLA	MG-NC	-2.93	1.99	2.06
21	b	604	CLA	O2A-CGA	2.91	1.41	1.33
21	b	605	CLA	C3D-C2D	2.91	1.47	1.39
21	b	609	CLA	C3B-C2B	2.90	1.44	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	602	CLA	C3D-C2D	2.89	1.47	1.39
21	b	612	CLA	CHD-C4C	2.88	1.45	1.39
21	c	503	CLA	C4D-CHA	2.88	1.48	1.38
21	d	402	CLA	MG-ND	-2.88	2.00	2.05
21	a	407	CLA	O2A-CGA	2.88	1.41	1.33
21	b	602	CLA	C4D-CHA	2.88	1.48	1.38
21	a	402	CLA	O2A-CGA	2.87	1.41	1.33
21	b	613	CLA	C1B-CHB	2.87	1.49	1.41
30	e	101	HEM	FE-NB	2.86	2.11	1.96
25	d	403	PHO	C3C-C2C	2.86	1.46	1.37
21	c	505	CLA	C4C-C3C	2.85	1.50	1.45
21	b	606	CLA	C4D-CHA	2.85	1.48	1.38
21	a	402	CLA	C4D-CHA	2.85	1.48	1.38
21	c	508	CLA	C1C-C2C	2.85	1.50	1.44
21	b	614	CLA	C4D-CHA	2.84	1.48	1.38
21	b	607	CLA	C4D-CHA	2.84	1.48	1.38
21	c	510	CLA	CHD-C4C	2.83	1.45	1.39
21	c	511	CLA	C4D-CHA	2.83	1.48	1.38
21	d	407	CLA	CHD-C4C	2.82	1.45	1.39
21	c	509	CLA	C4B-CHC	2.82	1.48	1.41
21	c	509	CLA	C1B-CHB	2.81	1.48	1.41
21	b	604	CLA	CHD-C1D	2.81	1.43	1.38
21	c	506	CLA	CHD-C4C	2.80	1.45	1.39
21	c	509	CLA	C1C-C2C	2.80	1.50	1.44
21	b	612	CLA	C3D-C2D	2.80	1.46	1.39
21	b	608	CLA	C4D-CHA	2.79	1.48	1.38
25	d	401	PHO	CMA-C3A	2.79	1.58	1.53
21	c	504	CLA	C4D-CHA	2.78	1.48	1.38
21	c	512	CLA	CHD-C4C	2.78	1.45	1.39
21	b	606	CLA	C3B-C2B	2.78	1.44	1.40
21	b	603	CLA	C3D-C2D	2.76	1.46	1.39
21	b	604	CLA	OBD-CAD	2.75	1.27	1.22
21	b	615	CLA	C1C-NC	-2.75	1.33	1.37
21	b	605	CLA	O2A-CGA	2.74	1.41	1.33
21	a	402	CLA	CHD-C1D	2.74	1.43	1.38
21	c	510	CLA	C4D-ND	2.74	1.41	1.37
21	b	615	CLA	C4D-CHA	2.73	1.48	1.38
21	c	507	CLA	C1D-C2D	2.73	1.50	1.45
21	b	602	CLA	O2A-CGA	2.73	1.41	1.33
21	b	614	CLA	C1D-ND	-2.71	1.34	1.37
21	c	506	CLA	CHD-C1D	2.71	1.43	1.38
21	b	608	CLA	C4C-C3C	2.70	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	614	CLA	MG-NC	2.69	2.12	2.06
21	c	511	CLA	C1B-CHB	2.69	1.48	1.41
21	b	601	CLA	C4C-C3C	2.68	1.49	1.45
21	b	605	CLA	OBD-CAD	2.68	1.27	1.22
21	b	605	CLA	C1B-CHB	2.68	1.48	1.41
21	c	511	CLA	C3D-C2D	2.68	1.46	1.39
25	d	401	PHO	CBD-CGD	-2.68	1.48	1.52
21	b	604	CLA	CHD-C4C	2.67	1.45	1.39
21	b	606	CLA	O2A-CGA	2.67	1.41	1.33
21	c	509	CLA	C4B-NB	-2.66	1.32	1.35
21	b	601	CLA	C1B-CHB	2.66	1.48	1.41
21	b	605	CLA	C1C-NC	-2.65	1.33	1.37
21	b	612	CLA	C4D-CHA	2.65	1.47	1.38
21	b	607	CLA	O2A-CGA	2.64	1.41	1.33
21	h	101	CLA	C1D-C2D	2.64	1.50	1.45
21	b	615	CLA	C1B-CHB	2.63	1.48	1.41
21	b	614	CLA	O2A-CGA	2.63	1.41	1.33
21	c	512	CLA	C3D-C2D	2.62	1.46	1.39
21	b	613	CLA	MG-NC	2.62	2.12	2.06
22	c	515	BCR	C30-C25	-2.61	1.50	1.53
21	c	510	CLA	C1C-NC	-2.61	1.33	1.37
21	h	101	CLA	C3D-C2D	2.61	1.46	1.39
21	b	609	CLA	C4D-CHA	2.60	1.47	1.38
21	b	615	CLA	C4B-CHC	2.60	1.48	1.41
21	c	505	CLA	C1D-ND	-2.59	1.34	1.37
21	a	407	CLA	OBD-CAD	2.59	1.26	1.22
21	b	607	CLA	C1B-CHB	2.59	1.48	1.41
25	d	403	PHO	OBD-CAD	2.58	1.25	1.22
21	c	506	CLA	C1D-C2D	2.58	1.50	1.45
20	a	401	SQD	O48-C23	2.58	1.46	1.33
21	c	505	CLA	MG-ND	2.58	2.10	2.05
21	d	402	CLA	C1-C2	2.57	1.56	1.49
21	k	501	CLA	CHD-C1D	2.56	1.43	1.38
21	b	602	CLA	MG-ND	2.56	2.10	2.05
21	c	508	CLA	C1C-NC	-2.56	1.34	1.37
21	b	610	CLA	C1D-ND	-2.55	1.34	1.37
21	c	504	CLA	C1C-NC	-2.55	1.34	1.37
21	a	407	CLA	MG-ND	-2.55	2.00	2.05
21	c	510	CLA	C4D-CHA	2.55	1.47	1.38
21	c	508	CLA	OBD-CAD	2.55	1.26	1.22
21	c	505	CLA	C4B-CHC	2.54	1.48	1.41
21	b	612	CLA	C4C-C3C	2.54	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	l	101	SQD	C6-S	-2.54	1.68	1.77
21	a	407	CLA	C4C-C3C	2.54	1.49	1.45
21	b	603	CLA	C4D-CHA	2.54	1.47	1.38
21	b	607	CLA	C3D-C2D	2.54	1.46	1.39
21	b	613	CLA	C4B-CHC	2.54	1.48	1.41
21	b	605	CLA	MG-ND	2.53	2.10	2.05
21	b	611	CLA	OBD-CAD	2.52	1.26	1.22
21	b	603	CLA	C1C-NC	-2.50	1.34	1.37
21	b	603	CLA	C1B-CHB	2.48	1.47	1.41
21	b	601	CLA	C3D-C2D	2.48	1.45	1.39
21	b	605	CLA	C1C-C2C	2.48	1.49	1.44
21	b	608	CLA	C1B-CHB	2.47	1.47	1.41
21	b	609	CLA	O2A-CGA	2.47	1.40	1.33
21	h	101	CLA	C3A-C2A	-2.47	1.52	1.54
21	c	508	CLA	C3D-C2D	2.47	1.45	1.39
20	a	401	SQD	C6-S	-2.47	1.68	1.77
21	a	402	CLA	C1B-NB	2.47	1.37	1.35
21	k	501	CLA	CHD-C4C	2.46	1.44	1.39
21	d	402	CLA	O2D-CGD	2.46	1.39	1.33
21	b	609	CLA	C3D-C2D	2.46	1.45	1.39
21	d	407	CLA	C1D-C2D	2.45	1.50	1.45
21	c	503	CLA	MG-NC	2.44	2.12	2.06
21	b	601	CLA	C4D-CHA	2.44	1.47	1.38
21	b	614	CLA	C4D-ND	2.41	1.41	1.37
21	c	504	CLA	C3D-C2D	2.41	1.45	1.39
21	c	504	CLA	C4D-ND	2.41	1.41	1.37
21	c	504	CLA	C4C-C3C	2.40	1.49	1.45
21	b	604	CLA	C4D-CHA	2.39	1.46	1.38
21	b	609	CLA	C4B-CHC	2.39	1.47	1.41
21	c	511	CLA	C4B-CHC	2.39	1.47	1.41
28	d	408	PQ9	C10-C5	2.38	1.47	1.35
21	b	606	CLA	C1B-CHB	2.38	1.47	1.41
21	b	605	CLA	C4B-CHC	2.38	1.47	1.41
21	b	607	CLA	C4B-CHC	2.37	1.47	1.41
21	c	509	CLA	C1C-NC	-2.37	1.34	1.37
21	c	513	CLA	C4C-C3C	2.36	1.49	1.45
21	b	614	CLA	C4C-C3C	2.35	1.49	1.45
21	k	501	CLA	C1C-C2C	2.33	1.49	1.44
21	c	510	CLA	C1B-CHB	2.33	1.47	1.41
21	c	503	CLA	C3D-C2D	2.32	1.45	1.39
21	c	508	CLA	C4D-CHA	2.32	1.46	1.38
21	c	509	CLA	C4C-C3C	2.31	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	611	CLA	CHD-C4C	2.31	1.44	1.39
21	a	403	CLA	C4D-CHA	2.30	1.46	1.38
21	b	611	CLA	C4D-CHA	2.30	1.46	1.38
31	h	102	HTG	C1-S1	-2.29	1.77	1.80
21	d	407	CLA	C3D-C2D	2.29	1.45	1.39
21	c	510	CLA	C3D-C4D	-2.28	1.39	1.44
21	b	612	CLA	C3D-C4D	-2.27	1.39	1.44
21	b	612	CLA	C4B-CHC	2.26	1.47	1.41
21	c	510	CLA	C4C-C3C	2.25	1.48	1.45
21	b	609	CLA	C1B-CHB	2.25	1.47	1.41
21	b	613	CLA	C4D-CHA	2.25	1.46	1.38
21	c	510	CLA	C1C-C2C	2.25	1.48	1.44
21	b	611	CLA	C1D-ND	-2.24	1.35	1.37
21	c	506	CLA	C3D-C2D	2.24	1.45	1.39
21	b	611	CLA	C1B-CHB	2.24	1.47	1.41
21	c	503	CLA	C4B-CHC	2.24	1.47	1.41
21	c	510	CLA	C4B-NB	2.24	1.37	1.35
21	c	504	CLA	C3D-C4D	-2.23	1.39	1.44
21	a	402	CLA	C3D-C2D	2.22	1.45	1.39
21	b	604	CLA	C1B-NB	-2.22	1.33	1.35
21	b	602	CLA	C1B-NB	-2.22	1.33	1.35
25	d	403	PHO	CBD-CGD	-2.21	1.49	1.52
21	b	614	CLA	C4B-NB	2.21	1.37	1.35
21	b	603	CLA	O2A-CGA	2.20	1.39	1.33
21	d	402	CLA	C4D-CHA	2.20	1.46	1.38
21	b	602	CLA	MG-NC	-2.20	2.01	2.06
21	c	512	CLA	C1D-C2D	2.19	1.49	1.45
21	c	507	CLA	MG-ND	2.19	2.10	2.05
21	a	403	CLA	MG-ND	2.19	2.10	2.05
21	c	505	CLA	OBD-CAD	2.19	1.26	1.22
21	c	505	CLA	C1C-C2C	2.18	1.48	1.44
21	c	508	CLA	C1B-CHB	2.18	1.47	1.41
21	b	608	CLA	MG-ND	2.17	2.10	2.05
21	b	613	CLA	C4C-C3C	2.17	1.48	1.45
21	b	607	CLA	C1B-NB	-2.17	1.33	1.35
21	b	613	CLA	OBD-CAD	2.16	1.26	1.22
21	c	503	CLA	C1C-NC	-2.15	1.34	1.37
21	c	509	CLA	C1A-CHA	2.15	1.52	1.43
30	e	101	HEM	CHB-C1B	2.14	1.40	1.35
21	c	507	CLA	C4C-C3C	2.14	1.48	1.45
21	a	403	CLA	C4D-ND	2.14	1.40	1.37
21	c	506	CLA	C1C-C2C	2.13	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	k	501	CLA	C1D-C2D	2.12	1.49	1.45
21	c	512	CLA	C1C-C2C	2.11	1.48	1.44
30	e	101	HEM	C1D-ND	-2.11	1.34	1.38
21	b	605	CLA	C4C-C3C	2.11	1.48	1.45
21	b	604	CLA	C1C-NC	-2.10	1.34	1.37
21	a	407	CLA	C1B-CHB	2.09	1.46	1.41
21	b	606	CLA	C4B-CHC	2.09	1.46	1.41
21	a	402	CLA	C1C-NC	-2.09	1.34	1.37
21	d	402	CLA	C4C-C3C	2.09	1.48	1.45
21	b	608	CLA	C4B-CHC	2.08	1.46	1.41
21	k	501	CLA	C3D-C2D	2.07	1.44	1.39
25	d	401	PHO	C4B-NB	-2.07	1.32	1.38
21	b	612	CLA	C1-C2	2.07	1.55	1.49
21	b	610	CLA	MG-NC	2.07	2.11	2.06
21	a	403	CLA	C3D-C2D	2.06	1.44	1.39
21	b	607	CLA	CAA-C2A	2.06	1.57	1.54
21	a	403	CLA	C4C-C3C	2.06	1.48	1.45
21	b	613	CLA	C3D-C2D	2.05	1.44	1.39
21	c	506	CLA	MG-NC	2.05	2.11	2.06
21	d	402	CLA	CMD-C2D	2.05	1.55	1.50
21	b	611	CLA	C4B-CHC	2.05	1.46	1.41
21	b	610	CLA	C3D-C4D	-2.04	1.39	1.44
21	b	608	CLA	O2D-CED	-2.04	1.40	1.45
21	b	604	CLA	C3B-CAB	2.03	1.52	1.47
21	b	602	CLA	C1B-CHB	2.03	1.46	1.41
21	b	615	CLA	MG-NC	2.03	2.11	2.06
21	b	611	CLA	C3B-C2B	2.02	1.43	1.40
21	d	402	CLA	C1B-CHB	2.02	1.46	1.41
21	d	402	CLA	C3D-C2D	2.02	1.44	1.39
21	b	603	CLA	C1C-C2C	2.01	1.48	1.44
21	c	511	CLA	C4C-C3C	2.01	1.48	1.45
21	b	610	CLA	C4B-NB	2.01	1.37	1.35
21	c	508	CLA	C3D-C4D	-2.01	1.39	1.44
21	b	603	CLA	C1D-ND	-2.00	1.35	1.37

All (1134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	l	101	SQD	O9-S-C6	-19.47	83.80	106.94
20	a	401	SQD	O9-S-C6	-18.75	84.65	106.94
21	k	501	CLA	C1D-ND-C4D	-18.13	93.46	106.33
21	c	506	CLA	C1D-ND-C4D	-17.32	94.03	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	d	407	CLA	C1D-ND-C4D	-16.66	94.50	106.33
21	d	406	CLA	C1D-ND-C4D	-16.58	94.55	106.33
21	c	512	CLA	C1D-ND-C4D	-15.45	95.36	106.33
21	h	101	CLA	C1D-ND-C4D	-15.33	95.45	106.33
21	h	101	CLA	C1B-CHB-C4A	-14.99	100.44	130.12
20	l	101	SQD	O8-S-O9	-11.82	82.39	111.27
20	a	401	SQD	O8-S-O9	-11.81	82.41	111.27
21	b	605	CLA	C4A-NA-C1A	11.78	112.00	106.71
21	c	505	CLA	C4A-NA-C1A	10.65	111.50	106.71
21	c	506	CLA	C4A-NA-C1A	-10.51	101.98	106.71
21	d	406	CLA	C2C-C1C-NC	10.44	119.75	109.97
21	c	506	CLA	C2C-C1C-NC	10.08	119.41	109.97
21	c	503	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	k	501	CLA	C2D-C1D-ND	10.04	117.50	110.10
21	c	507	CLA	C4A-NA-C1A	-9.99	102.22	106.71
21	d	407	CLA	C2C-C1C-NC	9.86	119.21	109.97
21	b	603	CLA	C4A-NA-C1A	9.81	111.12	106.71
21	c	513	CLA	CHD-C1D-ND	-9.79	115.46	124.45
20	a	401	SQD	O7-S-C6	9.72	118.49	106.94
20	l	101	SQD	O7-S-C6	9.63	118.39	106.94
21	c	512	CLA	C2C-C1C-NC	9.54	118.91	109.97
21	h	101	CLA	CHD-C1D-ND	-9.53	115.70	124.45
21	c	507	CLA	C2C-C1C-NC	9.48	118.86	109.97
21	c	504	CLA	C2D-C1D-ND	9.43	117.05	110.10
21	c	512	CLA	C4A-NA-C1A	-9.34	102.51	106.71
21	b	613	CLA	C2D-C1D-ND	9.28	116.94	110.10
20	a	401	SQD	O9-S-O7	-9.11	82.43	113.95
21	c	513	CLA	C1D-ND-C4D	-9.02	99.93	106.33
21	k	501	CLA	C2C-C1C-NC	9.00	118.41	109.97
20	l	101	SQD	O9-S-O7	-9.00	82.80	113.95
21	h	101	CLA	C4D-CHA-C1A	-8.96	110.35	121.25
21	c	506	CLA	C2D-C1D-ND	8.92	116.68	110.10
21	b	609	CLA	C2D-C1D-ND	8.84	116.62	110.10
21	b	609	CLA	C4A-NA-C1A	8.80	110.66	106.71
21	d	406	CLA	C2D-C1D-ND	8.74	116.55	110.10
21	k	501	CLA	CMD-C2D-C1D	8.74	140.12	124.71
21	d	406	CLA	C3C-C4C-NC	8.71	120.34	110.57
21	h	101	CLA	C2C-C1C-NC	8.70	118.13	109.97
21	d	407	CLA	C2D-C1D-ND	8.66	116.49	110.10
21	c	513	CLA	C1D-CHD-C4C	-8.60	107.51	126.06
21	h	101	CLA	CMD-C2D-C1D	8.53	139.75	124.71
21	c	506	CLA	CMD-C2D-C1D	8.53	139.74	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	507	CLA	C1D-ND-C4D	-8.52	100.28	106.33
21	b	613	CLA	C4A-NA-C1A	8.52	110.54	106.71
22	c	515	BCR	C11-C10-C9	-8.47	115.22	127.31
21	b	611	CLA	CAC-C3C-C4C	8.40	135.71	124.81
21	d	406	CLA	CHD-C4C-C3C	-8.35	112.56	124.84
21	d	407	CLA	CMD-C2D-C1D	8.29	139.31	124.71
21	c	513	CLA	C2C-C1C-NC	8.19	117.64	109.97
21	c	506	CLA	C1B-CHB-C4A	-8.14	113.99	130.12
21	c	513	CLA	CMD-C2D-C1D	8.14	139.06	124.71
21	c	509	CLA	C4A-NA-C1A	8.11	110.35	106.71
21	k	501	CLA	C4D-CHA-C1A	-8.08	111.41	121.25
25	d	403	PHO	O2D-CGD-CBD	8.08	121.23	111.00
20	a	401	SQD	O8-S-C6	8.04	118.55	105.74
21	c	507	CLA	CMD-C2D-C1D	8.04	138.88	124.71
21	c	512	CLA	C2D-C1D-ND	8.03	116.02	110.10
21	b	610	CLA	C4A-NA-C1A	8.01	110.31	106.71
20	l	101	SQD	O8-S-C6	7.94	118.40	105.74
21	a	402	CLA	C2D-C1D-ND	7.93	115.95	110.10
22	c	515	BCR	C16-C17-C18	-7.92	116.01	127.31
21	k	501	CLA	C3C-C4C-NC	7.85	119.38	110.57
21	b	611	CLA	C4A-NA-C1A	7.84	110.23	106.71
21	a	403	CLA	C2C-C1C-NC	7.84	117.31	109.97
21	c	513	CLA	C4A-NA-C1A	-7.81	103.19	106.71
21	c	504	CLA	C1D-ND-C4D	-7.80	100.80	106.33
21	c	503	CLA	C2D-C1D-ND	7.76	115.82	110.10
21	d	406	CLA	CMD-C2D-C1D	7.67	138.24	124.71
21	k	501	CLA	C3D-C4D-ND	7.61	122.55	110.24
21	c	506	CLA	C3C-C4C-NC	7.61	119.10	110.57
21	k	501	CLA	CHD-C1D-ND	-7.57	117.50	124.45
21	h	101	CLA	C2D-C1D-ND	7.43	115.58	110.10
21	c	506	CLA	CHD-C1D-ND	-7.38	117.67	124.45
21	c	506	CLA	C3D-C4D-ND	7.37	122.17	110.24
21	d	407	CLA	CHD-C1D-ND	-7.33	117.71	124.45
21	c	510	CLA	C4A-NA-C1A	7.31	109.99	106.71
21	d	407	CLA	C3D-C4D-ND	7.27	121.99	110.24
21	c	512	CLA	C4D-CHA-C1A	-7.26	112.42	121.25
21	a	407	CLA	C2C-C1C-NC	7.25	116.76	109.97
21	c	508	CLA	C2D-C1D-ND	7.23	115.44	110.10
21	c	508	CLA	CHD-C4C-C3C	-7.20	114.26	124.84
21	c	506	CLA	C4D-CHA-C1A	-7.19	112.50	121.25
21	b	604	CLA	C2C-C1C-NC	7.19	116.70	109.97
21	b	602	CLA	CHD-C1D-ND	-7.16	117.88	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	512	CLA	CMD-C2D-C1D	7.14	137.29	124.71
21	c	507	CLA	C3C-C4C-NC	7.13	118.57	110.57
21	b	602	CLA	C2C-C1C-NC	7.13	116.65	109.97
25	d	401	PHO	O2D-CGD-CBD	7.07	119.95	111.00
21	b	614	CLA	C4A-NA-C1A	7.04	109.87	106.71
21	h	101	CLA	C3D-C4D-ND	7.03	121.61	110.24
21	b	604	CLA	CAC-C3C-C4C	6.98	133.87	124.81
21	c	511	CLA	C2D-C1D-ND	6.95	115.22	110.10
21	a	402	CLA	CAC-C3C-C4C	6.94	133.82	124.81
21	d	407	CLA	C3C-C4C-NC	6.91	118.33	110.57
21	b	613	CLA	C4D-CHA-C1A	-6.88	112.87	121.25
21	h	101	CLA	C4A-NA-C1A	-6.84	103.63	106.71
21	b	615	CLA	CHD-C4C-C3C	-6.83	114.81	124.84
21	c	512	CLA	C3D-C4D-ND	6.81	121.26	110.24
21	b	613	CLA	C1D-ND-C4D	-6.77	101.53	106.33
21	h	101	CLA	C3C-C4C-NC	6.71	118.09	110.57
21	c	504	CLA	C4A-NA-C1A	6.70	109.72	106.71
21	b	612	CLA	C2D-C1D-ND	6.67	115.02	110.10
21	d	402	CLA	C2D-C1D-ND	6.67	115.02	110.10
21	k	501	CLA	C3B-C4B-NB	6.67	117.83	109.21
21	c	513	CLA	C4D-CHA-C1A	-6.62	113.19	121.25
21	b	601	CLA	C2D-C1D-ND	6.58	114.96	110.10
21	b	602	CLA	C2D-C1D-ND	6.53	114.92	110.10
21	b	603	CLA	C2C-C1C-NC	6.49	116.06	109.97
21	c	507	CLA	C4D-CHA-C1A	-6.48	113.37	121.25
21	b	612	CLA	C4A-NA-C1A	6.47	109.61	106.71
21	c	508	CLA	C4D-CHA-C1A	-6.42	113.44	121.25
21	c	512	CLA	C3C-C4C-NC	6.38	117.73	110.57
21	b	604	CLA	C2D-C1D-ND	6.37	114.80	110.10
22	c	515	BCR	C7-C8-C9	-6.36	116.62	126.23
21	b	615	CLA	C2D-C1D-ND	6.35	114.79	110.10
21	b	612	CLA	C2C-C1C-NC	6.31	115.88	109.97
31	h	102	HTG	C1'-S1-C1	6.31	111.89	100.09
21	b	603	CLA	C2D-C1D-ND	6.27	114.72	110.10
21	b	613	CLA	O2D-CGD-CBD	6.26	122.39	111.27
21	c	509	CLA	O2D-CGD-CBD	6.25	122.37	111.27
21	c	512	CLA	C1B-CHB-C4A	-6.23	117.79	130.12
21	b	605	CLA	C2D-C1D-ND	6.22	114.69	110.10
21	c	513	CLA	C3C-C4C-NC	6.20	117.53	110.57
21	c	503	CLA	CHD-C1D-ND	-6.20	118.76	124.45
21	b	611	CLA	C2D-C1D-ND	6.19	114.67	110.10
21	b	615	CLA	O2D-CGD-CBD	6.19	122.27	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	403	CLA	C2D-C1D-ND	6.19	114.66	110.10
21	c	512	CLA	CHD-C1D-ND	-6.16	118.79	124.45
21	c	503	CLA	C1D-ND-C4D	-6.16	101.96	106.33
21	c	508	CLA	CHD-C1D-ND	-6.15	118.81	124.45
22	h	103	BCR	C7-C8-C9	-6.14	116.95	126.23
21	a	407	CLA	CAC-C3C-C4C	6.12	132.75	124.81
21	d	406	CLA	O2D-CGD-CBD	6.12	122.14	111.27
21	d	407	CLA	C4A-NA-C1A	-6.10	103.96	106.71
21	d	406	CLA	C3D-C4D-ND	6.10	120.10	110.24
21	a	403	CLA	CHD-C1D-ND	-6.10	118.85	124.45
21	b	604	CLA	CHD-C1D-ND	-6.10	118.85	124.45
21	k	501	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
21	k	501	CLA	C4A-NA-C1A	-6.04	103.99	106.71
21	d	407	CLA	C4D-CHA-C1A	-6.02	113.92	121.25
21	b	611	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
22	a	404	BCR	C11-C10-C9	-6.00	118.74	127.31
21	a	403	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
21	c	509	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
22	b	616	BCR	C28-C27-C26	-5.95	103.45	114.08
21	d	406	CLA	C4D-CHA-C1A	-5.90	114.06	121.25
21	d	402	CLA	C2C-C1C-NC	5.88	115.48	109.97
21	d	402	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
21	b	607	CLA	C2D-C1D-ND	5.85	114.42	110.10
21	d	407	CLA	C3B-C4B-NB	5.84	116.76	109.21
21	b	614	CLA	C2D-C1D-ND	5.83	114.40	110.10
22	a	404	BCR	C7-C8-C9	-5.82	117.44	126.23
21	c	513	CLA	CMA-C3A-C4A	-5.77	96.27	111.77
21	b	608	CLA	C2C-C1C-NC	5.77	115.38	109.97
21	a	403	CLA	CAC-C3C-C4C	5.77	132.29	124.81
21	b	614	CLA	C2C-C1C-NC	5.73	115.34	109.97
21	c	506	CLA	O2D-CGD-CBD	5.72	121.44	111.27
22	z	101	BCR	C16-C17-C18	-5.72	119.14	127.31
21	c	510	CLA	C2D-C1D-ND	5.70	114.31	110.10
21	c	507	CLA	CHD-C1D-ND	-5.70	119.22	124.45
21	c	509	CLA	C2D-C1D-ND	5.67	114.28	110.10
21	c	512	CLA	C3B-C4B-NB	5.66	116.53	109.21
21	b	602	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
21	c	506	CLA	C3B-C4B-NB	5.64	116.50	109.21
21	c	505	CLA	C2D-C1D-ND	5.62	114.25	110.10
21	d	406	CLA	C1C-C2C-C3C	-5.61	101.05	106.96
21	b	607	CLA	C2C-C1C-NC	5.58	115.20	109.97
21	c	506	CLA	CHD-C4C-C3C	-5.57	116.66	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	509	CLA	C2C-C1C-NC	5.56	115.18	109.97
21	b	611	CLA	C3C-C4C-NC	5.54	116.79	110.57
21	c	510	CLA	C4D-CHA-C1A	-5.53	114.52	121.25
21	c	504	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
21	c	503	CLA	C2C-C1C-NC	5.49	115.12	109.97
21	b	615	CLA	C4A-NA-C1A	5.46	109.16	106.71
21	b	612	CLA	CAC-C3C-C4C	5.45	131.88	124.81
21	c	512	CLA	C1C-C2C-C3C	-5.44	101.24	106.96
21	c	506	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
21	b	609	CLA	C2C-C1C-NC	5.42	115.05	109.97
21	b	611	CLA	C4D-CHA-C1A	-5.41	114.67	121.25
21	b	610	CLA	C2D-C1D-ND	5.40	114.09	110.10
21	b	601	CLA	CMB-C2B-C3B	5.38	134.75	124.68
22	c	514	BCR	C28-C27-C26	-5.38	104.46	114.08
21	k	501	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
22	c	514	BCR	C7-C8-C9	-5.34	118.17	126.23
21	d	406	CLA	C3B-C4B-NB	5.33	116.10	109.21
21	b	609	CLA	C1D-ND-C4D	-5.31	102.56	106.33
21	c	504	CLA	O2D-CGD-CBD	5.30	120.69	111.27
21	d	406	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
21	c	509	CLA	CHD-C1D-ND	-5.29	119.59	124.45
21	c	503	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
21	b	608	CLA	CAC-C3C-C4C	5.26	131.64	124.81
21	b	605	CLA	CHD-C1D-ND	-5.25	119.63	124.45
21	b	601	CLA	CHD-C1D-ND	-5.25	119.63	124.45
21	c	510	CLA	C2C-C1C-NC	5.24	114.88	109.97
21	c	507	CLA	C3B-C4B-NB	5.21	115.95	109.21
21	c	509	CLA	O2D-CGD-O1D	-5.21	113.66	123.84
21	h	101	CLA	C1D-CHD-C4C	-5.20	114.85	126.06
21	d	407	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
21	c	513	CLA	C1B-CHB-C4A	-5.18	119.85	130.12
21	b	611	CLA	C2C-C1C-NC	5.16	114.81	109.97
21	a	402	CLA	C2C-C1C-NC	5.16	114.81	109.97
21	b	614	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
22	d	409	BCR	C24-C23-C22	-5.14	118.46	126.23
21	b	602	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
22	a	404	BCR	C20-C21-C22	-5.09	120.04	127.31
21	c	508	CLA	CHD-C4C-NC	5.08	132.20	124.20
21	d	407	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
21	d	407	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
21	b	610	CLA	C2C-C1C-NC	5.02	114.67	109.97
21	b	602	CLA	O2D-CGD-O1D	-5.01	114.04	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	602	CLA	C4-C3-C5	5.00	123.67	115.27
22	a	404	BCR	C24-C23-C22	-4.98	118.70	126.23
19	d	410	MGE	O2G-C1B-C2B	4.95	122.18	111.50
21	h	101	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
21	b	603	CLA	C1C-C2C-C3C	-4.95	101.75	106.96
21	a	402	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
21	b	615	CLA	CHD-C1D-ND	-4.94	119.91	124.45
21	b	612	CLA	C1-C2-C3	-4.94	117.50	126.04
21	c	508	CLA	CMD-C2D-C1D	4.92	133.39	124.71
21	c	506	CLA	C1C-C2C-C3C	-4.92	101.79	106.96
22	b	618	BCR	C7-C8-C9	-4.91	118.82	126.23
21	b	607	CLA	O2D-CGD-CBD	4.89	119.97	111.27
21	b	604	CLA	C4-C3-C5	4.88	123.49	115.27
21	a	407	CLA	C1C-C2C-C3C	-4.87	101.83	106.96
21	b	606	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
21	b	612	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
21	d	406	CLA	C1D-CHD-C4C	-4.86	115.58	126.06
21	c	503	CLA	C4D-CHA-C1A	-4.85	115.34	121.25
21	b	607	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
21	b	604	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
21	c	512	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
21	b	613	CLA	O2D-CGD-O1D	-4.82	114.41	123.84
21	c	508	CLA	C1D-ND-C4D	-4.80	102.92	106.33
25	d	403	PHO	O2D-CGD-O1D	-4.80	114.45	123.84
21	b	611	CLA	C4C-C3C-C2C	-4.80	99.91	106.90
21	c	506	CLA	C1D-CHD-C4C	-4.79	115.73	126.06
21	a	407	CLA	C3C-C4C-NC	4.78	115.94	110.57
21	c	512	CLA	O2D-CGD-CBD	4.78	119.77	111.27
21	c	510	CLA	CHD-C4C-C3C	-4.78	117.82	124.84
21	b	604	CLA	C3C-C4C-NC	4.76	115.91	110.57
25	d	401	PHO	O2D-CGD-O1D	-4.76	114.53	123.84
21	b	603	CLA	CAC-C3C-C4C	4.76	130.98	124.81
21	c	503	CLA	O2D-CGD-O1D	-4.72	114.61	123.84
21	c	507	CLA	C1B-CHB-C4A	-4.72	120.78	130.12
21	d	407	CLA	O2D-CGD-CBD	4.71	119.64	111.27
21	b	612	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
21	c	507	CLA	C1D-CHD-C4C	-4.71	115.90	126.06
21	a	407	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
22	a	404	BCR	C11-C12-C13	-4.70	113.22	126.42
21	b	606	CLA	C2C-C1C-NC	4.70	114.37	109.97
22	c	515	BCR	C33-C5-C6	-4.69	119.26	124.53
21	b	601	CLA	O2D-CGD-CBD	4.69	119.60	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	k	501	CLA	O2D-CGD-CBD	4.68	119.59	111.27
21	h	101	CLA	C3B-C4B-NB	4.68	115.27	109.21
21	a	403	CLA	C4-C3-C5	4.68	121.33	115.98
21	c	503	CLA	O2D-CGD-CBD	4.68	119.58	111.27
21	b	613	CLA	C2C-C1C-NC	4.67	114.35	109.97
30	e	101	HEM	CHC-C4B-NB	4.64	129.48	124.43
21	c	507	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
21	k	501	CLA	C1D-CHD-C4C	-4.63	116.07	126.06
21	b	605	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
21	b	606	CLA	CAC-C3C-C4C	4.62	130.80	124.81
21	b	609	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
21	c	511	CLA	C4A-NA-C1A	4.61	108.78	106.71
21	c	505	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
21	c	505	CLA	C2C-C1C-NC	4.60	114.28	109.97
21	b	607	CLA	CHD-C4C-C3C	-4.60	118.08	124.84
21	b	603	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
21	a	407	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
21	c	513	CLA	O2D-CGD-CBD	4.55	119.36	111.27
21	b	608	CLA	O2D-CGD-CBD	4.55	119.36	111.27
24	h	104	DGD	O2G-C1B-C2B	4.53	121.27	111.50
21	c	504	CLA	C2C-C1C-NC	4.53	114.22	109.97
21	b	613	CLA	C1-C2-C3	-4.53	118.21	126.04
22	b	618	BCR	C24-C23-C22	-4.53	119.40	126.23
21	c	512	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
21	c	507	CLA	O2D-CGD-CBD	4.52	119.30	111.27
21	b	610	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
21	b	601	CLA	C2C-C1C-NC	4.51	114.19	109.97
21	b	614	CLA	C1D-CHD-C4C	-4.50	116.35	126.06
21	b	605	CLA	C2C-C1C-NC	4.50	114.19	109.97
21	b	615	CLA	C2C-C1C-NC	4.50	114.19	109.97
21	d	402	CLA	C1D-CHD-C4C	-4.50	116.36	126.06
21	b	604	CLA	O2D-CGD-CBD	4.48	119.23	111.27
21	a	402	CLA	CHD-C4C-C3C	-4.46	118.28	124.84
21	b	606	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
21	c	503	CLA	CHD-C4C-C3C	-4.46	118.28	124.84
21	b	614	CLA	CMB-C2B-C3B	4.46	133.02	124.68
21	b	608	CLA	C2D-C1D-ND	4.45	113.39	110.10
21	c	504	CLA	C1D-CHD-C4C	-4.45	116.47	126.06
21	c	503	CLA	CMD-C2D-C1D	4.44	132.54	124.71
21	c	507	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
21	k	501	CLA	C1C-C2C-C3C	-4.41	102.31	106.96
21	b	603	CLA	C3D-C2D-C1D	-4.41	99.81	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	z	101	BCR	C7-C8-C9	-4.41	119.58	126.23
21	h	101	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
22	c	514	BCR	C15-C14-C13	-4.40	121.03	127.31
21	b	606	CLA	C4A-NA-C1A	4.40	108.69	106.71
22	z	101	BCR	C24-C23-C22	4.40	132.88	126.23
22	d	409	BCR	C16-C17-C18	-4.38	121.06	127.31
21	b	601	CLA	O2D-CGD-O1D	-4.37	115.30	123.84
21	b	615	CLA	C3C-C4C-NC	4.37	115.47	110.57
21	b	604	CLA	CMD-C2D-C1D	4.36	132.41	124.71
30	e	101	HEM	C1B-NB-C4B	4.35	109.57	105.07
21	c	507	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
21	b	606	CLA	C2D-C1D-ND	4.34	113.30	110.10
22	b	618	BCR	C27-C26-C25	-4.33	116.44	122.73
22	z	101	BCR	C16-C15-C14	-4.33	114.61	123.47
21	c	511	CLA	C1D-ND-C4D	-4.32	103.26	106.33
19	B	101	MGE	O2G-C1B-C2B	4.32	120.82	111.50
21	b	613	CLA	CHD-C4C-C3C	-4.32	118.49	124.84
20	a	401	SQD	O47-C7-C8	4.31	119.03	111.09
22	c	514	BCR	C24-C23-C22	-4.30	119.73	126.23
30	e	101	HEM	CHD-C1D-ND	4.30	129.10	124.43
21	c	511	CLA	C4D-CHA-C1A	-4.30	116.02	121.25
21	c	509	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
21	b	610	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
21	c	511	CLA	C2C-C1C-NC	4.28	113.98	109.97
21	c	513	CLA	C3D-C4D-ND	4.27	117.15	110.24
21	b	607	CLA	CHD-C1D-ND	-4.27	120.53	124.45
21	b	602	CLA	CMB-C2B-C3B	4.26	132.65	124.68
21	c	513	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
21	h	101	CLA	O2D-CGD-CBD	4.23	118.79	111.27
22	z	101	BCR	C11-C10-C9	-4.23	121.28	127.31
22	c	515	BCR	C30-C25-C26	-4.22	116.67	122.61
21	c	508	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
25	d	401	PHO	CMB-C2B-C3B	4.21	132.55	124.68
21	a	403	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
21	a	403	CLA	O2D-CGD-CBD	4.20	118.73	111.27
21	b	604	CLA	C3D-C2D-C1D	-4.19	100.12	105.83
21	b	614	CLA	O2D-CGD-CBD	4.18	118.70	111.27
22	c	514	BCR	C20-C21-C22	-4.18	121.34	127.31
22	b	617	BCR	C24-C23-C22	-4.18	119.92	126.23
21	b	604	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
24	c	516	DGD	O2G-C1B-C2B	4.16	120.46	111.50
22	b	618	BCR	C11-C10-C9	-4.15	121.39	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	604	CLA	CMC-C2C-C1C	4.15	131.35	125.04
21	d	402	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
21	d	407	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
21	b	612	CLA	CHD-C1D-ND	-4.13	120.66	124.45
21	b	615	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
21	b	608	CLA	C4D-CHA-C1A	-4.13	116.23	121.25
22	d	409	BCR	C7-C8-C9	-4.12	120.02	126.23
21	c	513	CLA	C3B-C4B-NB	4.11	114.53	109.21
22	z	101	BCR	C37-C22-C23	4.10	124.54	118.08
21	b	610	CLA	CHA-C4D-ND	4.09	141.06	132.50
21	b	609	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
21	c	512	CLA	CHC-C1C-NC	-4.08	118.01	124.20
21	b	603	CLA	C3C-C4C-NC	4.08	115.15	110.57
21	b	614	CLA	CHD-C4C-C3C	-4.08	118.85	124.84
21	b	606	CLA	CHD-C1D-ND	-4.06	120.73	124.45
22	b	616	BCR	C15-C14-C13	-4.05	121.52	127.31
22	b	617	BCR	C15-C14-C13	-4.05	121.53	127.31
21	b	601	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
21	c	508	CLA	CHB-C4A-NA	4.04	130.10	124.51
21	c	509	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
21	b	602	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
21	b	614	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
21	a	402	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
21	b	613	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
21	b	605	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
21	b	610	CLA	C1-C2-C3	-4.00	119.12	126.04
21	b	606	CLA	C1D-ND-C4D	4.00	109.18	106.33
21	b	603	CLA	O2D-CGD-CBD	4.00	118.37	111.27
21	b	603	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
21	c	512	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
21	b	601	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
21	b	610	CLA	C4D-CHA-C1A	-3.99	116.40	121.25
19	m	102	MGE	O2G-C1B-C2B	3.98	120.08	111.50
22	c	514	BCR	C16-C17-C18	-3.97	121.64	127.31
21	c	510	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
21	c	505	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
21	b	607	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
24	a	406	DGD	O2G-C1B-C2B	3.95	120.02	111.50
21	b	607	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
21	b	605	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
21	c	504	CLA	C4D-CHA-C1A	-3.93	116.46	121.25
21	b	615	CLA	CAC-C3C-C4C	3.93	129.91	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	614	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
22	h	103	BCR	C8-C9-C10	3.93	124.97	118.94
22	a	404	BCR	C15-C14-C13	-3.92	121.72	127.31
21	b	604	CLA	C4D-CHA-C1A	-3.91	116.49	121.25
21	b	615	CLA	CMB-C2B-C3B	3.90	131.98	124.68
22	a	404	BCR	C1-C6-C5	-3.89	117.13	122.61
21	c	513	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
21	c	510	CLA	C1D-ND-C4D	-3.89	103.57	106.33
22	b	618	BCR	C38-C26-C27	3.86	121.03	113.62
21	c	505	CLA	CHA-C4D-ND	3.86	140.58	132.50
21	d	402	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
21	b	611	CLA	C3D-C2D-C1D	-3.86	100.57	105.83
21	b	612	CLA	CMD-C2D-C1D	3.85	131.49	124.71
19	f	101	MGE	C1D-O6D-C5D	3.84	121.23	113.69
21	a	407	CLA	C4-C3-C5	3.84	121.74	115.27
22	h	103	BCR	C11-C10-C9	-3.83	121.84	127.31
21	c	505	CLA	C1-C2-C3	-3.83	119.42	126.04
19	c	502	MGE	O2G-C1B-C2B	3.83	119.75	111.50
21	a	402	CLA	CHD-C1D-ND	-3.82	120.94	124.45
21	b	611	CLA	O2D-CGD-O1D	-3.82	116.38	123.84
21	a	407	CLA	C2D-C1D-ND	3.81	112.91	110.10
19	b	620	MGE	O2G-C1B-C2B	3.81	119.71	111.50
22	b	618	BCR	C16-C17-C18	-3.81	121.88	127.31
22	c	515	BCR	C16-C15-C14	-3.81	115.68	123.47
21	b	610	CLA	O2D-CGD-CBD	3.81	118.03	111.27
21	a	403	CLA	C3B-C4B-NB	3.80	114.13	109.21
21	b	608	CLA	CHD-C1D-ND	-3.80	120.96	124.45
21	c	509	CLA	C4-C3-C5	3.80	121.66	115.27
21	b	606	CLA	CHA-C4D-ND	3.80	140.44	132.50
21	b	603	CLA	CMC-C2C-C1C	3.79	130.81	125.04
21	c	508	CLA	C2C-C1C-NC	3.79	113.52	109.97
20	l	101	SQD	O47-C7-C8	3.79	119.67	111.50
21	h	101	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
22	c	514	BCR	C21-C20-C19	-3.79	111.40	123.22
21	c	508	CLA	CMC-C2C-C1C	3.78	130.80	125.04
21	c	511	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
21	b	601	CLA	CHD-C4C-C3C	-3.78	119.29	124.84
22	c	514	BCR	C15-C16-C17	-3.78	115.74	123.47
19	f	101	MGE	C4D-C3D-C2D	3.77	117.41	110.82
21	b	608	CLA	C3C-C4C-NC	3.77	114.79	110.57
21	b	609	CLA	CHD-C4C-C3C	-3.76	119.31	124.84
21	d	402	CLA	CHD-C4C-NC	3.76	130.13	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	613	CLA	CMD-C2D-C1D	3.75	131.33	124.71
21	b	614	CLA	CAC-C3C-C4C	3.75	129.68	124.81
21	c	508	CLA	CHA-C4D-ND	3.74	140.32	132.50
21	a	403	CLA	C3C-C4C-NC	3.74	114.76	110.57
21	b	602	CLA	CHD-C4C-NC	3.74	130.09	124.20
22	d	409	BCR	C11-C10-C9	-3.74	121.98	127.31
21	b	609	CLA	C4D-CHA-C1A	-3.73	116.70	121.25
21	b	613	CLA	O2A-CGA-O1A	-3.73	114.19	123.59
21	a	402	CLA	C1D-ND-C4D	-3.72	103.69	106.33
21	b	610	CLA	C3B-C4B-NB	3.72	114.01	109.21
22	c	514	BCR	C10-C11-C12	-3.72	111.62	123.22
21	b	611	CLA	C1-C2-C3	-3.71	119.63	126.04
21	a	407	CLA	C4D-CHA-C1A	-3.70	116.74	121.25
21	b	613	CLA	C6-C5-C3	-3.69	108.58	114.62
21	c	505	CLA	CHD-C4C-C3C	-3.69	119.41	124.84
21	d	402	CLA	C4D-CHA-C1A	-3.69	116.76	121.25
21	c	504	CLA	C3D-C2D-C1D	-3.69	100.80	105.83
21	c	507	CLA	C4C-C3C-C2C	-3.68	101.54	106.90
21	c	503	CLA	C3D-C2D-C1D	-3.67	100.83	105.83
21	k	501	CLA	C4C-C3C-C2C	-3.67	101.55	106.90
21	b	614	CLA	CMC-C2C-C1C	3.66	130.61	125.04
21	c	511	CLA	O2D-CGD-CBD	3.66	117.77	111.27
21	c	508	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
21	c	504	CLA	O2D-CGD-O1D	-3.65	116.69	123.84
21	b	609	CLA	O2D-CGD-CBD	3.65	117.76	111.27
21	b	613	CLA	CHD-C1D-ND	-3.65	121.10	124.45
21	b	610	CLA	CBC-CAC-C3C	-3.65	102.38	112.43
21	c	511	CLA	C3D-C2D-C1D	-3.63	100.87	105.83
25	d	403	PHO	C4-C3-C5	3.62	121.36	115.27
21	c	511	CLA	C4-C3-C5	3.62	121.36	115.27
21	b	601	CLA	CHA-C4D-ND	3.62	140.06	132.50
21	b	602	CLA	CHA-C4D-ND	3.61	140.06	132.50
21	c	510	CLA	C3B-C4B-NB	3.61	113.88	109.21
21	b	614	CLA	C1B-CHB-C4A	-3.61	122.97	130.12
21	c	513	CLA	CAC-C3C-C4C	3.60	129.48	124.81
21	c	510	CLA	CMD-C2D-C1D	3.59	131.05	124.71
21	b	613	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
21	d	406	CLA	C4A-NA-C1A	-3.59	105.09	106.71
21	b	602	CLA	CMC-C2C-C1C	3.59	130.50	125.04
21	b	609	CLA	CHD-C1D-ND	-3.58	121.17	124.45
21	c	513	CLA	C4C-C3C-C2C	-3.58	101.69	106.90
22	c	515	BCR	C38-C26-C27	3.57	120.47	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	511	CLA	CHD-C4C-C3C	-3.57	119.59	124.84
21	b	603	CLA	CHA-C4D-ND	3.56	139.95	132.50
21	a	407	CLA	CMD-C2D-C1D	3.56	130.99	124.71
21	b	608	CLA	CHD-C4C-C3C	-3.55	119.62	124.84
21	a	407	CLA	O2D-CGD-CBD	3.55	117.58	111.27
19	f	101	MGE	O2G-C1B-C2B	3.54	119.14	111.50
21	c	504	CLA	CHD-C4C-NC	3.54	129.79	124.20
21	a	403	CLA	C1-C2-C3	-3.54	119.92	126.04
21	b	602	CLA	CAC-C3C-C4C	3.54	129.40	124.81
21	c	508	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
21	c	509	CLA	CHD-C4C-NC	3.53	129.77	124.20
21	b	610	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
22	b	618	BCR	C20-C21-C22	-3.52	122.29	127.31
24	c	517	DGD	O2G-C1B-C2B	3.52	119.08	111.50
21	b	603	CLA	C6-C5-C3	-3.51	104.25	113.45
21	c	503	CLA	CHD-C4C-NC	3.51	129.73	124.20
21	c	510	CLA	O2D-CGD-CBD	3.51	117.50	111.27
22	c	515	BCR	C27-C26-C25	-3.51	117.64	122.73
21	b	615	CLA	CHD-C4C-NC	3.50	129.72	124.20
21	b	615	CLA	O1D-CGD-CBD	-3.50	117.31	124.48
21	b	602	CLA	C5-C3-C2	-3.50	114.03	121.12
19	d	410	MGE	C2G-O2G-C1B	-3.50	109.18	117.79
21	b	610	CLA	C3D-C2D-C1D	-3.49	101.07	105.83
21	c	513	CLA	CHC-C1C-C2C	-3.48	117.08	126.72
21	c	503	CLA	C3B-C4B-NB	3.48	113.71	109.21
21	d	406	CLA	C4C-C3C-C2C	-3.48	101.82	106.90
21	k	501	CLA	CMC-C2C-C1C	3.48	130.34	125.04
22	h	103	BCR	C16-C17-C18	-3.48	122.34	127.31
21	k	501	CLA	C1-O2A-CGA	3.48	127.58	116.11
21	c	507	CLA	CHC-C1C-C2C	-3.48	117.09	126.72
21	a	407	CLA	CHA-C4D-ND	3.48	139.77	132.50
22	b	617	BCR	C3-C4-C5	-3.48	107.87	114.08
21	d	402	CLA	CBC-CAC-C3C	-3.47	102.85	112.43
21	b	605	CLA	O2D-CGD-CBD	3.47	117.44	111.27
21	b	610	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
21	h	101	CLA	C4C-C3C-C2C	-3.46	101.85	106.90
21	c	506	CLA	CHC-C1C-C2C	-3.46	117.15	126.72
21	c	513	CLA	CMB-C2B-C3B	3.45	131.13	124.68
21	b	607	CLA	C4D-CHA-C1A	-3.44	117.06	121.25
21	c	507	CLA	C4-C3-C5	3.44	119.92	115.98
21	b	607	CLA	CHA-C4D-ND	3.44	139.70	132.50
21	c	505	CLA	CHD-C1D-ND	-3.43	121.30	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	d	406	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
19	b	619	MGE	O1G-C1A-C2A	3.43	122.66	111.91
24	c	516	DGD	C1D-C2D-C3D	3.42	117.12	110.00
21	b	602	CLA	C3B-C4B-NB	3.42	113.63	109.21
21	c	511	CLA	CHA-C4D-ND	3.42	139.65	132.50
21	b	601	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
21	c	504	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
21	c	507	CLA	CAC-C3C-C4C	3.41	129.23	124.81
21	a	407	CLA	C2A-C1A-CHA	-3.41	117.90	123.86
21	c	507	CLA	C1-C2-C3	-3.40	120.16	126.04
21	c	507	CLA	C3D-C4D-ND	3.40	115.73	110.24
21	d	406	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	b	614	CLA	CHA-C4D-ND	3.39	139.59	132.50
21	b	602	CLA	C4D-CHA-C1A	-3.39	117.12	121.25
21	c	510	CLA	C3C-C4C-NC	3.39	114.37	110.57
21	c	506	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
22	b	617	BCR	C11-C10-C9	-3.39	122.48	127.31
22	a	404	BCR	C21-C20-C19	3.38	133.75	123.22
21	a	402	CLA	C7-C6-C5	-3.37	104.20	113.36
21	c	510	CLA	CHA-C4D-ND	3.37	139.56	132.50
22	c	515	BCR	C20-C21-C22	-3.37	122.50	127.31
21	b	608	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
22	b	617	BCR	C20-C21-C22	-3.36	122.51	127.31
22	b	618	BCR	C15-C14-C13	-3.36	122.52	127.31
21	b	608	CLA	C1-C2-C3	-3.36	120.24	126.04
21	b	606	CLA	C4-C3-C5	3.35	120.91	115.27
21	b	613	CLA	C4-C3-C2	-3.35	115.08	123.68
21	a	402	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
22	d	409	BCR	C20-C21-C22	-3.35	122.53	127.31
21	a	403	CLA	C4D-CHA-C1A	-3.34	117.18	121.25
21	b	612	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
28	d	408	PQ9	C39-C38-C40	3.33	120.87	115.27
22	b	616	BCR	C16-C17-C18	-3.32	122.57	127.31
21	c	504	CLA	C1-C2-C3	-3.32	120.30	126.04
22	a	404	BCR	C16-C17-C18	-3.32	122.57	127.31
21	c	505	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
21	b	613	CLA	C3B-C4B-NB	3.30	113.48	109.21
21	k	501	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
21	b	614	CLA	CMD-C2D-C3D	3.30	135.20	127.61
21	h	101	CLA	CHC-C1C-C2C	-3.29	117.61	126.72
21	b	615	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
21	b	603	CLA	CMD-C2D-C1D	3.29	130.51	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	605	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
21	b	605	CLA	CMD-C2D-C1D	3.28	130.49	124.71
22	d	409	BCR	C16-C15-C14	-3.27	116.78	123.47
24	c	517	DGD	O6D-C5D-C6D	3.26	113.25	106.67
19	m	102	MGE	C1D-O6D-C5D	3.26	120.09	113.69
21	a	403	CLA	CMC-C2C-C1C	3.26	130.01	125.04
21	d	407	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
21	b	605	CLA	C4D-CHA-C1A	-3.26	117.28	121.25
21	c	504	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	z	101	BCR	C30-C25-C26	-3.26	118.03	122.61
22	h	103	BCR	C24-C23-C22	-3.25	121.33	126.23
21	c	512	CLA	CMC-C2C-C1C	3.25	129.98	125.04
24	c	516	DGD	C4D-C3D-C2D	3.24	116.48	110.82
21	d	407	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
21	b	603	CLA	C4D-CHA-C1A	-3.23	117.32	121.25
21	a	403	CLA	CMB-C2B-C3B	3.22	130.70	124.68
21	a	407	CLA	C1D-ND-C4D	3.22	108.62	106.33
21	b	601	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
21	b	607	CLA	O2A-CGA-O1A	-3.22	115.47	123.59
25	d	401	PHO	CBA-CAA-C2A	-3.21	104.44	113.81
21	c	510	CLA	C4D-C3D-CAD	3.20	111.87	108.10
22	a	404	BCR	C4-C5-C6	-3.20	118.08	122.73
21	c	513	CLA	CHD-C1D-C2D	3.20	132.18	125.48
22	b	617	BCR	C8-C7-C6	-3.19	118.24	127.20
21	a	407	CLA	C1-O2A-CGA	3.19	124.82	116.44
22	b	617	BCR	C16-C17-C18	-3.19	122.76	127.31
21	c	509	CLA	C3C-C4C-NC	3.19	114.15	110.57
21	b	601	CLA	C1-C2-C3	-3.19	120.53	126.04
21	b	609	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
21	b	614	CLA	C4-C3-C5	3.18	120.62	115.27
22	a	404	BCR	C36-C18-C19	3.18	123.09	118.08
21	a	403	CLA	C1D-ND-C4D	-3.18	104.08	106.33
22	c	515	BCR	C20-C19-C18	-3.17	117.51	126.42
21	b	607	CLA	C3C-C4C-NC	3.17	114.13	110.57
22	c	515	BCR	C36-C18-C17	-3.17	118.48	122.92
21	b	612	CLA	C3C-C4C-NC	3.17	114.12	110.57
25	d	401	PHO	C4C-NC-C1C	-3.17	100.60	107.09
21	b	613	CLA	CHB-C4A-NA	3.16	128.88	124.51
21	b	607	CLA	CMB-C2B-C3B	3.15	130.56	124.68
21	c	506	CLA	CAC-C3C-C4C	3.15	128.89	124.81
21	d	406	CLA	CHC-C1C-C2C	-3.15	118.02	126.72
22	b	616	BCR	C27-C26-C25	-3.14	118.17	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	605	CLA	CMC-C2C-C3C	3.14	134.64	126.12
21	b	604	CLA	CHA-C4D-ND	3.13	139.06	132.50
21	b	612	CLA	C4D-CHA-C1A	-3.13	117.43	121.25
21	b	610	CLA	CMC-C2C-C1C	3.13	129.80	125.04
22	b	617	BCR	C33-C5-C4	3.12	119.62	113.62
21	a	407	CLA	CBC-CAC-C3C	-3.12	103.84	112.43
21	c	509	CLA	CHA-C4D-ND	3.12	139.02	132.50
21	a	403	CLA	CHD-C4C-NC	3.12	129.11	124.20
21	d	406	CLA	O2A-CGA-CBA	3.12	121.68	111.91
22	z	101	BCR	C15-C14-C13	-3.11	122.87	127.31
21	a	403	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
21	b	611	CLA	C4-C3-C5	3.11	120.51	115.27
21	d	406	CLA	CAC-C3C-C4C	3.11	128.85	124.81
21	b	611	CLA	O2D-CGD-CBD	3.11	116.80	111.27
21	a	402	CLA	CMD-C2D-C1D	3.11	130.19	124.71
21	d	402	CLA	C1D-ND-C4D	-3.10	104.13	106.33
21	a	402	CLA	CAC-C3C-C2C	-3.10	122.22	127.53
21	b	609	CLA	CAA-CBA-CGA	-3.10	104.19	113.25
22	z	101	BCR	C28-C27-C26	-3.10	108.54	114.08
21	b	604	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
21	d	402	CLA	CHA-C4D-ND	3.10	138.98	132.50
21	c	511	CLA	CHD-C1D-ND	-3.09	121.61	124.45
21	d	406	CLA	CHB-C4A-NA	3.09	128.78	124.51
20	l	101	SQD	O8-S-O7	3.09	118.82	111.27
21	b	604	CLA	C3A-C2A-C1A	-3.09	96.72	101.34
30	e	101	HEM	CHB-C1B-NB	3.08	128.19	124.38
21	b	602	CLA	O2A-C1-C2	-3.07	100.55	108.64
21	b	608	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
20	a	401	SQD	O8-S-O7	3.07	118.77	111.27
21	a	403	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
21	b	612	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
21	b	601	CLA	C4-C3-C5	3.06	120.41	115.27
21	c	512	CLA	C2A-C3A-C4A	-3.05	96.94	101.87
21	b	613	CLA	CAC-C3C-C4C	3.05	128.77	124.81
21	c	511	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
20	l	101	SQD	O48-C23-C24	3.04	121.46	111.91
21	h	101	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	z	101	BCR	C23-C22-C21	-3.04	114.27	118.94
21	b	603	CLA	CMB-C2B-C3B	3.04	130.37	124.68
21	b	611	CLA	C3B-C4B-NB	3.04	113.14	109.21
22	b	617	BCR	C15-C16-C17	-3.04	117.25	123.47
24	h	104	DGD	O1G-C1A-C2A	3.04	121.44	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	601	CLA	CMD-C2D-C3D	3.03	134.59	127.61
21	h	101	CLA	CAC-C3C-C4C	3.03	128.74	124.81
22	d	409	BCR	C15-C14-C13	-3.03	122.98	127.31
21	b	606	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
21	b	605	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
21	c	505	CLA	OBD-CAD-C3D	-3.03	121.23	128.52
22	b	617	BCR	C4-C5-C6	-3.03	118.34	122.73
21	b	613	CLA	C1D-CHD-C4C	-3.02	119.53	126.06
22	c	515	BCR	C34-C9-C10	-3.02	118.70	122.92
22	c	515	BCR	C8-C9-C10	3.01	123.56	118.94
21	a	403	CLA	C3D-C2D-C1D	-3.01	101.72	105.83
21	b	606	CLA	CMD-C2D-C1D	3.01	130.01	124.71
22	z	101	BCR	C27-C26-C25	-3.01	118.36	122.73
19	b	619	MGE	O2G-C1B-C2B	3.01	117.98	111.50
22	b	617	BCR	C1-C6-C5	-3.00	118.39	122.61
21	k	501	CLA	CMB-C2B-C3B	3.00	130.29	124.68
21	b	607	CLA	C3B-C4B-NB	3.00	113.08	109.21
21	b	613	CLA	CHA-C4D-ND	3.00	138.76	132.50
21	b	612	CLA	C3B-C4B-NB	2.99	113.08	109.21
21	c	508	CLA	C3B-C4B-NB	2.99	113.08	109.21
21	b	602	CLA	O2D-CGD-CBD	2.99	116.57	111.27
21	k	501	CLA	CHB-C4A-NA	2.98	128.64	124.51
21	a	402	CLA	CHD-C4C-NC	2.98	128.90	124.20
21	b	605	CLA	C3B-C4B-NB	2.98	113.06	109.21
21	b	605	CLA	CHD-C4C-NC	2.98	128.89	124.20
21	b	609	CLA	CHB-C4A-NA	2.98	128.63	124.51
21	b	610	CLA	CHD-C1D-ND	-2.97	121.72	124.45
21	b	612	CLA	C1-O2A-CGA	2.97	124.24	116.44
21	b	603	CLA	O2A-CGA-O1A	-2.97	116.10	123.59
21	b	612	CLA	C2A-C1A-CHA	-2.97	118.67	123.86
21	c	507	CLA	C2A-C3A-C4A	-2.96	97.09	101.87
21	c	504	CLA	C3B-C4B-NB	2.96	113.03	109.21
21	d	407	CLA	CHB-C4A-NA	2.96	128.60	124.51
28	d	408	PQ9	C11-C12-C13	-2.95	121.88	126.79
21	b	614	CLA	C3B-C4B-NB	2.95	113.03	109.21
21	b	615	CLA	O2A-CGA-CBA	2.94	123.87	112.23
21	b	613	CLA	CHD-C4C-NC	2.94	128.84	124.20
21	c	504	CLA	CAC-C3C-C4C	2.94	128.63	124.81
21	a	407	CLA	C3B-C4B-NB	2.94	113.01	109.21
21	c	510	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
21	c	506	CLA	CMB-C2B-C3B	2.94	130.18	124.68
25	d	403	PHO	C1-C2-C3	-2.94	120.96	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	601	CLA	C2A-C3A-C4A	-2.93	97.13	101.87
21	b	606	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
22	a	404	BCR	C20-C19-C18	2.93	134.64	126.42
21	c	513	CLA	CMD-C2D-C3D	-2.93	120.88	127.61
21	b	614	CLA	CHD-C4C-NC	2.93	128.81	124.20
21	b	607	CLA	CAC-C3C-C4C	2.93	128.61	124.81
21	b	601	CLA	C4D-CHA-C1A	-2.92	117.69	121.25
22	c	515	BCR	C33-C5-C4	2.92	119.23	113.62
21	b	609	CLA	CHA-C4D-ND	2.92	138.61	132.50
21	a	402	CLA	C4D-CHA-C1A	-2.91	117.71	121.25
21	c	507	CLA	CAA-CBA-CGA	-2.90	104.77	113.25
21	c	507	CLA	CMB-C2B-C3B	2.90	130.11	124.68
19	b	619	MGE	C1D-O6D-C5D	2.90	119.37	113.69
21	c	510	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
21	c	503	CLA	CBC-CAC-C3C	-2.89	104.46	112.43
21	b	613	CLA	C1-O2A-CGA	2.89	124.02	116.44
21	b	606	CLA	CMB-C2B-C3B	2.89	130.08	124.68
28	d	408	PQ9	C19-C18-C20	2.89	120.12	115.27
21	b	604	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
21	c	512	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
30	e	101	HEM	CHA-C4D-ND	2.88	127.94	124.38
21	b	606	CLA	CHD-C4C-NC	2.87	128.73	124.20
19	B	101	MGE	O1G-C1A-C2A	2.87	120.92	111.91
21	b	604	CLA	CHC-C1C-NC	-2.87	119.84	124.20
21	b	615	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
21	c	510	CLA	C1D-CHD-C4C	-2.87	119.88	126.06
22	a	404	BCR	C36-C18-C17	-2.86	118.91	122.92
21	b	612	CLA	CMB-C2B-C3B	2.86	130.04	124.68
24	c	517	DGD	O1G-C1A-C2A	2.86	120.89	111.91
24	c	517	DGD	O5D-C6D-C5D	-2.86	103.75	109.05
21	c	504	CLA	CHA-C4D-ND	2.86	138.48	132.50
21	b	615	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
21	b	601	CLA	CMA-C3A-C4A	-2.85	104.11	111.77
21	d	407	CLA	CAC-C3C-C4C	2.85	128.50	124.81
28	d	408	PQ9	C11-C2-C1	2.84	119.19	116.88
22	c	515	BCR	C19-C18-C17	2.84	123.30	118.94
21	c	508	CLA	CED-O2D-CGD	2.84	122.36	115.94
22	z	101	BCR	C33-C5-C6	-2.84	121.34	124.53
21	b	604	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
24	c	516	DGD	C6E-C5E-C4E	2.82	119.62	113.00
19	b	620	MGE	O1G-C1A-C2A	2.82	120.76	111.91
21	b	613	CLA	C4-C3-C5	2.82	120.01	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	608	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
21	d	406	CLA	CMC-C2C-C1C	2.81	129.32	125.04
21	h	101	CLA	CMD-C2D-C3D	-2.80	121.17	127.61
21	c	510	CLA	CED-O2D-CGD	2.80	122.27	115.94
21	b	601	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
21	a	407	CLA	C1-C2-C3	-2.79	121.21	126.04
19	c	502	MGE	O1G-C1A-C2A	2.79	120.67	111.91
21	c	513	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
22	b	618	BCR	C33-C5-C4	2.79	118.98	113.62
22	h	103	BCR	C34-C9-C10	-2.79	119.02	122.92
19	b	619	MGE	C3G-O3G-C1D	-2.79	108.30	113.74
21	a	403	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	d	410	MGE	O1G-C1A-C2A	2.79	120.65	111.91
25	d	403	PHO	CMA-C3A-C4A	-2.79	108.28	114.38
22	h	103	BCR	C32-C1-C6	2.78	114.82	110.30
21	b	604	CLA	C4A-NA-C1A	-2.78	105.45	106.71
21	c	513	CLA	CMA-C3A-C2A	-2.78	102.60	113.83
21	c	513	CLA	O2A-CGA-CBA	2.78	120.64	111.91
21	d	406	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
21	b	602	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
21	c	506	CLA	CMC-C2C-C1C	2.77	129.25	125.04
21	c	509	CLA	CBC-CAC-C3C	-2.77	104.80	112.43
22	a	404	BCR	C15-C16-C17	-2.77	117.81	123.47
21	b	609	CLA	CMD-C2D-C1D	2.76	129.57	124.71
21	b	602	CLA	C1D-CHD-C4C	-2.76	120.11	126.06
21	c	507	CLA	CMC-C2C-C1C	2.76	129.24	125.04
21	b	609	CLA	CHD-C4C-NC	2.76	128.55	124.20
21	c	506	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
21	b	605	CLA	C1D-ND-C4D	-2.75	104.38	106.33
21	c	507	CLA	CMD-C2D-C3D	-2.75	121.29	127.61
21	b	606	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
21	c	510	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	h	103	BCR	C1-C6-C7	2.75	123.55	115.78
21	c	508	CLA	O2D-CGD-CBD	2.74	116.14	111.27
25	d	401	PHO	CAA-CBA-CGA	-2.74	105.24	113.25
28	d	408	PQ9	C6-C5-C4	2.74	120.59	114.99
24	c	516	DGD	C6D-C5D-C4D	-2.74	106.38	112.09
21	b	609	CLA	O2A-CGA-O1A	-2.73	116.69	123.59
21	d	406	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
25	d	403	PHO	O2A-CGA-O1A	-2.73	116.70	123.59
21	c	505	CLA	CMB-C2B-C3B	2.73	129.79	124.68
21	b	605	CLA	C1-O2A-CGA	2.73	123.61	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	k	501	CLA	CMD-C2D-C3D	-2.72	121.35	127.61
30	e	101	HEM	C4D-ND-C1D	2.72	107.89	105.07
21	a	402	CLA	CHA-C4D-ND	2.72	138.19	132.50
21	c	510	CLA	CHC-C1C-NC	-2.72	120.08	124.20
25	d	403	PHO	CMC-C2C-C3C	2.72	130.06	124.94
21	d	402	CLA	C3C-C4C-NC	2.72	113.62	110.57
22	b	616	BCR	C21-C20-C19	-2.72	114.74	123.22
21	a	402	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
22	c	515	BCR	C28-C27-C26	-2.72	109.23	114.08
21	b	609	CLA	C3B-C4B-NB	2.71	112.72	109.21
21	a	407	CLA	CBA-CAA-C2A	-2.71	105.85	113.86
21	b	608	CLA	C7-C6-C5	-2.71	106.00	113.36
24	c	516	DGD	C6D-O5D-C1E	-2.71	108.45	113.74
22	c	514	BCR	C29-C30-C25	2.71	114.65	110.48
19	B	101	MGE	C1D-O6D-C5D	2.71	119.00	113.69
22	b	616	BCR	C33-C5-C6	-2.71	121.49	124.53
21	b	615	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
21	a	407	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
21	c	508	CLA	C2A-C1A-CHA	-2.70	119.15	123.86
21	b	610	CLA	C14-C13-C15	-2.69	101.54	111.29
21	b	615	CLA	CHA-C4D-ND	2.69	138.13	132.50
21	a	402	CLA	O2A-CGA-O1A	-2.69	116.80	123.59
24	h	104	DGD	C1E-O6E-C5E	2.69	118.97	113.69
21	b	606	CLA	C4D-CHA-C1A	-2.69	117.98	121.25
21	b	603	CLA	CED-O2D-CGD	2.68	122.01	115.94
21	c	503	CLA	C3D-C4D-ND	2.68	114.58	110.24
19	f	101	MGE	O1G-C1A-C2A	2.68	120.32	111.91
21	d	406	CLA	CMB-C2B-C3B	2.68	129.69	124.68
21	c	506	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
21	b	612	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
21	d	407	CLA	CMC-C2C-C1C	2.67	129.10	125.04
21	d	402	CLA	C4A-NA-C1A	-2.67	105.51	106.71
21	b	606	CLA	C3B-C4B-NB	2.66	112.65	109.21
21	c	504	CLA	C3D-C4D-ND	2.66	114.54	110.24
25	d	401	PHO	CMA-C3A-C4A	-2.66	108.56	114.38
21	b	613	CLA	CBC-CAC-C3C	-2.66	105.11	112.43
21	a	407	CLA	CHC-C1C-C2C	-2.66	119.38	126.72
21	b	606	CLA	O2D-CGD-CBD	2.65	115.98	111.27
21	b	602	CLA	C7-C6-C5	-2.65	106.17	113.36
21	c	508	CLA	C3C-C4C-NC	2.64	113.53	110.57
21	c	509	CLA	O2A-CGA-CBA	2.64	120.18	111.91
21	b	608	CLA	CHA-C4D-ND	2.63	138.01	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	620	MGE	C1D-O6D-C5D	2.63	118.86	113.69
21	b	608	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
19	f	101	MGE	C3D-C4D-C5D	2.63	114.94	110.24
21	c	503	CLA	C4-C3-C5	2.63	119.70	115.27
21	b	603	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
21	c	513	CLA	CAA-C2A-C3A	2.62	119.95	112.78
21	b	611	CLA	O2A-CGA-CBA	2.62	120.12	111.91
21	k	501	CLA	CHC-C1C-NC	-2.62	120.23	124.20
21	c	505	CLA	CBC-CAC-C3C	-2.61	105.22	112.43
30	e	101	HEM	CHD-C1D-C2D	-2.61	120.90	124.98
21	a	402	CLA	C3B-C4B-NB	2.61	112.58	109.21
21	b	607	CLA	C1D-CHD-C4C	-2.61	120.43	126.06
21	b	601	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
21	d	406	CLA	CGD-CBD-CAD	-2.60	102.30	110.73
21	c	512	CLA	O2A-CGA-CBA	2.60	120.08	111.91
24	c	516	DGD	O1G-C1A-C2A	2.60	120.07	111.91
19	B	101	MGE	C2G-O2G-C1B	-2.60	111.40	117.79
21	a	403	CLA	CHA-C4D-ND	2.59	137.93	132.50
21	a	407	CLA	C3A-C2A-C1A	-2.59	97.45	101.34
21	b	606	CLA	C3C-C4C-NC	2.58	113.47	110.57
21	b	614	CLA	CMA-C3A-C4A	-2.58	104.84	111.77
21	c	510	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
21	b	612	CLA	O2A-CGA-CBA	2.58	120.00	111.91
21	b	609	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
19	m	102	MGE	O1G-C1A-C2A	2.57	119.98	111.91
22	b	616	BCR	C11-C10-C9	-2.57	123.64	127.31
21	k	501	CLA	C4D-C3D-CAD	2.57	111.12	108.10
24	a	406	DGD	C2G-O2G-C1B	-2.56	111.49	117.79
21	c	508	CLA	C3D-C4D-CHA	-2.56	106.87	112.72
21	b	613	CLA	O2A-CGA-CBA	2.55	119.92	111.91
21	d	407	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
21	b	601	CLA	CHD-C4C-NC	2.54	128.21	124.20
21	b	603	CLA	C3B-C4B-NB	2.54	112.49	109.21
21	b	606	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
21	c	512	CLA	CAC-C3C-C4C	2.54	128.10	124.81
21	b	615	CLA	CED-O2D-CGD	2.54	121.67	115.94
21	b	610	CLA	CHD-C4C-NC	2.54	128.20	124.20
21	b	613	CLA	CED-O2D-CGD	2.53	121.67	115.94
21	c	509	CLA	CAC-C3C-C4C	2.53	128.10	124.81
21	c	511	CLA	C3D-C4D-CHA	-2.53	106.93	112.72
19	f	101	MGE	O6D-C1D-C2D	2.53	115.70	110.35
22	b	618	BCR	C33-C5-C6	-2.53	121.69	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	504	CLA	C3C-C4C-NC	2.53	113.41	110.57
21	b	610	CLA	CMD-C2D-C1D	2.52	129.16	124.71
21	c	506	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
26	m	101	LMT	C2'-C3'-C4'	2.52	115.43	109.68
21	h	101	CLA	CHA-C1A-NA	-2.52	120.63	126.40
21	c	504	CLA	C3D-C4D-CHA	-2.52	106.97	112.72
21	c	508	CLA	C4A-NA-C1A	2.52	107.84	106.71
22	b	618	BCR	C30-C25-C26	-2.52	119.07	122.61
22	b	617	BCR	C29-C30-C25	2.51	114.35	110.48
21	d	407	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
21	a	403	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
22	z	101	BCR	C23-C24-C25	2.51	134.25	127.20
21	d	407	CLA	CHC-C1C-C2C	-2.51	119.79	126.72
22	b	618	BCR	C29-C28-C27	2.51	116.98	111.38
22	b	618	BCR	C28-C27-C26	-2.51	109.60	114.08
21	c	511	CLA	C3C-C4C-NC	2.50	113.38	110.57
21	c	505	CLA	C7-C6-C5	-2.50	106.57	113.36
21	b	615	CLA	C4D-CHA-C1A	-2.50	118.21	121.25
21	b	612	CLA	CHD-C4C-NC	2.49	128.13	124.20
21	b	615	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
21	b	603	CLA	C7-C6-C5	-2.49	106.59	113.36
21	b	615	CLA	C3B-C4B-NB	2.49	112.43	109.21
22	a	404	BCR	C33-C5-C4	2.49	118.40	113.62
21	b	608	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
22	b	616	BCR	C20-C21-C22	-2.49	123.76	127.31
21	k	501	CLA	CAC-C3C-C4C	2.48	128.03	124.81
21	c	509	CLA	CMD-C2D-C1D	2.48	129.09	124.71
21	b	605	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
21	b	614	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
21	c	505	CLA	CED-O2D-CGD	2.47	121.53	115.94
21	c	512	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
21	d	406	CLA	C4D-C3D-CAD	2.47	111.01	108.10
22	c	514	BCR	C27-C26-C25	-2.47	119.14	122.73
21	b	604	CLA	O2A-C1-C2	-2.47	102.14	108.64
22	h	103	BCR	C15-C14-C13	-2.47	123.79	127.31
21	d	407	CLA	CMD-C2D-C3D	-2.47	121.94	127.61
21	c	509	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
21	c	510	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
21	a	407	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
21	c	504	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
21	a	403	CLA	CHC-C1C-C2C	-2.46	119.93	126.72
21	b	606	CLA	C7-C6-C5	-2.46	106.69	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	606	CLA	CGD-CBD-CAD	-2.45	102.79	110.73
21	b	603	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	h	103	BCR	C28-C27-C26	-2.44	109.71	114.08
21	b	602	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
21	c	503	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
21	b	612	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	b	617	BCR	C39-C30-C25	-2.43	106.36	110.30
21	b	607	CLA	CMD-C2D-C1D	2.43	128.99	124.71
21	c	507	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
22	b	616	BCR	C38-C26-C27	2.43	118.28	113.62
21	d	402	CLA	C1-O2A-CGA	2.42	122.80	116.44
21	b	601	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
19	b	619	MGE	O1G-C1A-O1A	-2.42	117.49	123.59
21	c	503	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
21	b	611	CLA	CED-O2D-CGD	2.41	121.40	115.94
21	k	501	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
21	b	602	CLA	C3C-C4C-NC	2.41	113.28	110.57
22	h	103	BCR	C16-C15-C14	-2.41	118.54	123.47
21	c	511	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
21	b	601	CLA	O2A-CGA-CBA	2.41	119.46	111.91
25	d	401	PHO	C7-C6-C5	-2.41	106.83	113.36
22	b	618	BCR	C4-C5-C6	-2.40	119.24	122.73
22	h	103	BCR	C39-C30-C25	-2.40	106.40	110.30
21	c	508	CLA	O2A-CGA-O1A	-2.40	115.62	123.14
22	z	101	BCR	C38-C26-C27	2.40	118.22	113.62
21	c	513	CLA	C2A-C3A-C4A	-2.39	98.00	101.87
24	c	516	DGD	C4E-C3E-C2E	2.39	114.99	110.82
30	e	101	HEM	CMA-C3A-C4A	-2.39	124.80	128.46
21	c	509	CLA	C3B-C4B-NB	2.38	112.29	109.21
21	c	511	CLA	CAC-C3C-C4C	2.37	127.89	124.81
28	d	408	PQ9	C29-C28-C27	-2.37	117.59	123.68
21	c	511	CLA	C3B-C4B-NB	2.37	112.28	109.21
28	d	408	PQ9	C14-C13-C15	2.37	119.26	115.27
22	h	103	BCR	C30-C25-C26	-2.37	119.28	122.61
21	c	505	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
21	c	504	CLA	C16-C17-C18	-2.37	104.83	115.98
22	a	404	BCR	C8-C9-C10	2.36	122.57	118.94
21	b	610	CLA	C7-C6-C5	-2.36	106.95	113.36
22	b	616	BCR	C33-C5-C4	2.36	118.15	113.62
21	c	511	CLA	C4-C3-C2	-2.36	117.63	123.68
22	c	515	BCR	C38-C26-C25	-2.36	121.88	124.53
21	c	504	CLA	C4C-C3C-C2C	-2.36	103.46	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	d	402	CLA	C3B-C4B-NB	2.35	112.25	109.21
21	a	407	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
19	B	101	MGE	C4D-C3D-C2D	2.35	114.92	110.82
21	c	513	CLA	C2D-C1D-ND	2.35	111.83	110.10
24	a	406	DGD	O1G-C1A-C2A	2.35	119.27	111.91
21	d	407	CLA	CMB-C2B-C3B	2.35	129.07	124.68
22	b	616	BCR	C15-C16-C17	-2.34	118.67	123.47
21	b	614	CLA	C11-C10-C8	-2.34	108.34	115.92
22	c	514	BCR	C34-C9-C8	2.34	121.76	118.08
21	a	402	CLA	CMC-C2C-C3C	2.33	132.46	126.12
19	f	101	MGE	C3G-O3G-C1D	-2.33	109.18	113.74
21	c	511	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
22	b	616	BCR	C7-C8-C9	-2.33	122.71	126.23
22	h	103	BCR	C7-C6-C5	-2.33	115.82	121.46
24	c	516	DGD	O6D-C5D-C4D	-2.33	105.47	109.69
21	c	510	CLA	C3D-C4D-CHA	-2.32	107.42	112.72
21	b	610	CLA	C3C-C4C-NC	2.32	113.17	110.57
26	m	101	LMT	C1-O1'-C1'	-2.31	110.01	113.84
21	k	501	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
21	c	512	CLA	CMB-C2B-C3B	2.31	128.99	124.68
21	d	406	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
19	b	620	MGE	C3G-C2G-C1G	-2.30	106.34	111.79
26	m	101	LMT	O1'-C1'-C2'	2.30	111.90	108.30
24	c	516	DGD	C1E-O6E-C5E	2.30	118.21	113.69
21	c	513	CLA	CHD-C4C-C3C	-2.30	121.45	124.84
21	d	406	CLA	C4-C3-C5	2.30	119.14	115.27
21	b	604	CLA	C14-C13-C12	-2.30	102.96	111.29
22	b	616	BCR	C29-C30-C25	2.30	114.02	110.48
21	b	613	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
21	c	505	CLA	C4C-C3C-C2C	-2.30	103.55	106.90
21	c	504	CLA	CMB-C2B-C3B	2.30	128.97	124.68
21	b	601	CLA	C16-C17-C18	-2.30	105.16	115.98
22	b	618	BCR	C16-C15-C14	-2.30	118.77	123.47
22	b	616	BCR	C23-C24-C25	-2.30	120.75	127.20
21	c	510	CLA	CHD-C1D-ND	-2.29	122.35	124.45
22	c	515	BCR	C35-C13-C12	2.29	121.69	118.08
21	d	402	CLA	CHD-C1D-ND	-2.29	122.35	124.45
25	d	403	PHO	CMB-C2B-C3B	2.29	128.96	124.68
21	c	510	CLA	CHD-C4C-NC	2.29	127.81	124.20
21	c	512	CLA	C4-C3-C5	2.29	118.60	115.98
21	d	407	CLA	O2A-CGA-CBA	2.28	119.08	111.91
22	b	616	BCR	C1-C6-C5	-2.28	119.40	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	608	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
21	h	101	CLA	CHB-C4A-NA	-2.28	121.36	124.51
21	b	607	CLA	CHD-C4C-NC	2.27	127.79	124.20
28	d	408	PQ9	C24-C23-C25	2.27	119.10	115.27
21	c	509	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
21	a	407	CLA	O2A-CGA-CBA	2.27	119.03	111.91
21	b	611	CLA	CMC-C2C-C1C	2.27	128.49	125.04
21	c	503	CLA	CMB-C2B-C1B	2.26	131.94	128.46
21	c	511	CLA	O2A-C1-C2	-2.26	102.69	108.64
21	b	601	CLA	CED-O2D-CGD	2.26	121.05	115.94
28	d	408	PQ9	C31-C32-C33	-2.26	122.22	127.66
21	b	604	CLA	CAC-C3C-C2C	-2.25	123.67	127.53
21	b	613	CLA	C3D-C4D-CHA	-2.25	107.57	112.72
21	b	610	CLA	CAC-C3C-C4C	2.25	127.73	124.81
21	b	605	CLA	CHA-C4D-ND	2.25	137.21	132.50
21	b	601	CLA	C3D-C4D-CHA	-2.25	107.58	112.72
21	c	509	CLA	C4D-CHA-C1A	-2.25	118.51	121.25
21	b	615	CLA	C1-O2A-CGA	2.24	123.50	116.11
21	d	402	CLA	O2A-C1-C2	-2.24	102.75	108.64
22	b	617	BCR	C33-C5-C6	-2.24	122.01	124.53
25	d	403	PHO	C3D-CAD-CBD	2.24	110.55	107.61
21	c	509	CLA	C5-C3-C2	-2.23	116.60	121.12
21	a	402	CLA	O2A-CGA-CBA	2.23	118.92	111.91
21	c	505	CLA	O2A-CGA-CBA	2.23	118.91	111.91
21	c	503	CLA	C7-C6-C5	-2.23	107.31	113.36
19	d	410	MGE	O1G-C1A-O1A	-2.23	117.97	123.59
21	a	407	CLA	CED-O2D-CGD	2.23	120.97	115.94
21	d	406	CLA	C1-C2-C3	-2.22	122.20	126.04
21	b	614	CLA	CHD-C1D-ND	-2.22	122.41	124.45
21	c	509	CLA	C11-C12-C13	-2.22	108.74	115.92
21	b	605	CLA	C3C-C4C-NC	2.22	113.06	110.57
21	c	513	CLA	C1-C2-C3	-2.21	123.17	126.75
21	c	513	CLA	C5-C3-C4	2.21	119.49	114.60
24	h	104	DGD	O1G-C1A-O1A	-2.21	118.01	123.59
22	b	616	BCR	C24-C23-C22	-2.21	122.89	126.23
22	z	101	BCR	C19-C18-C17	2.21	122.33	118.94
21	a	403	CLA	O2A-CGA-CBA	2.20	118.83	111.91
21	h	101	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	c	517	DGD	O1G-C1A-O1A	-2.20	118.03	123.59
24	c	516	DGD	O6D-C1D-C2D	2.20	115.01	110.35
21	c	511	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
21	a	402	CLA	C1-C2-C3	-2.20	122.24	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	614	CLA	C1-O2A-CGA	2.20	122.21	116.44
21	a	407	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
22	b	616	BCR	C8-C7-C6	-2.19	121.05	127.20
21	c	512	CLA	C1-C2-C3	-2.19	122.26	126.04
21	b	605	CLA	O2A-CGA-CBA	2.18	118.75	111.91
21	a	407	CLA	C1D-CHD-C4C	-2.18	121.36	126.06
21	c	504	CLA	O2A-CGA-CBA	2.18	118.74	111.91
28	d	408	PQ9	C29-C28-C30	2.18	118.93	115.27
21	d	402	CLA	C4C-C3C-C2C	-2.18	103.73	106.90
21	k	501	CLA	C3D-C4D-CHA	-2.18	107.75	112.72
21	c	509	CLA	C1-O2A-CGA	2.17	122.15	116.44
21	c	513	CLA	CHD-C4C-NC	-2.17	120.78	124.20
21	c	505	CLA	C3C-C4C-NC	2.17	113.00	110.57
19	b	620	MGE	C3G-O3G-C1D	-2.17	109.50	113.74
22	d	409	BCR	C28-C27-C26	-2.17	110.21	114.08
21	b	605	CLA	C4-C3-C5	2.16	118.91	115.27
21	b	608	CLA	CMB-C2B-C3B	2.16	128.73	124.68
24	c	516	DGD	O5D-C1E-C2E	2.16	111.68	108.30
21	b	610	CLA	C16-C15-C13	2.16	122.91	115.92
21	c	508	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
22	c	515	BCR	C30-C25-C24	2.16	121.88	115.78
21	b	606	CLA	C1-C2-C3	-2.16	122.31	126.04
21	b	607	CLA	C6-C7-C8	-2.16	108.95	115.92
24	c	516	DGD	O2G-C1B-O1B	-2.16	118.49	123.70
21	h	101	CLA	CGD-CBD-CAD	2.15	117.71	110.73
21	d	402	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
21	c	510	CLA	CMC-C2C-C1C	2.15	128.32	125.04
21	c	509	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
21	d	402	CLA	CGD-CBD-CAD	-2.15	103.76	110.73
21	b	609	CLA	O2A-CGA-CBA	2.15	118.66	111.91
21	h	101	CLA	CED-O2D-CGD	2.15	120.80	115.94
22	b	617	BCR	C30-C25-C26	-2.15	119.59	122.61
19	c	502	MGE	C3G-C2G-C1G	-2.15	106.71	111.79
21	c	506	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
21	a	403	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	b	616	BCR	C10-C11-C12	-2.14	116.55	123.22
21	d	402	CLA	CMD-C2D-C3D	2.14	132.53	127.61
25	d	403	PHO	C16-C15-C13	-2.14	109.01	115.92
21	b	607	CLA	C3D-C4D-CHA	-2.14	107.84	112.72
21	c	513	CLA	CED-O2D-CGD	2.14	120.77	115.94
21	a	407	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
21	c	503	CLA	O2A-CGA-CBA	2.13	118.60	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	610	CLA	C3D-C4D-CHA	-2.13	107.84	112.72
21	b	610	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
21	d	402	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
25	d	403	PHO	CBA-CAA-C2A	-2.13	107.60	113.81
22	c	514	BCR	C33-C5-C6	-2.13	122.14	124.53
21	b	605	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
25	d	401	PHO	CMD-C2D-C3D	2.12	128.65	124.68
22	b	618	BCR	C1-C6-C5	-2.12	119.62	122.61
21	c	505	CLA	CHD-C4C-NC	2.12	127.55	124.20
26	d	404	LMT	C1'-O5'-C5'	2.12	117.85	113.69
21	b	613	CLA	C3D-C4D-ND	2.12	113.67	110.24
21	c	513	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
24	c	516	DGD	O4D-C4D-C5D	-2.12	104.04	109.30
26	t	301	LMT	C4B-C3B-C2B	2.12	114.52	110.82
21	c	505	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
21	d	407	CLA	CHC-C1C-NC	-2.11	121.00	124.20
24	a	406	DGD	C1E-O6E-C5E	2.11	117.83	113.69
19	B	101	MGE	O1G-C1A-O1A	-2.11	118.27	123.59
21	b	604	CLA	C1-C2-C3	-2.11	122.40	126.04
21	c	503	CLA	CHA-C4D-ND	2.11	136.91	132.50
21	c	511	CLA	C1-C2-C3	-2.10	122.40	126.04
21	c	504	CLA	C6-C5-C3	-2.10	107.94	113.45
21	c	506	CLA	C3D-C4D-CHA	-2.10	107.92	112.72
21	c	507	CLA	O2A-CGA-CBA	2.10	118.50	111.91
21	b	611	CLA	CHA-C4D-ND	2.10	136.89	132.50
21	b	603	CLA	C1D-CHD-C4C	-2.10	121.54	126.06
28	d	408	PQ9	C11-C2-C3	-2.09	120.54	123.30
22	b	616	BCR	C34-C9-C8	2.09	121.38	118.08
21	b	610	CLA	C17-C16-C15	-2.09	103.64	113.24
21	c	513	CLA	CHB-C4A-NA	-2.09	121.62	124.51
21	b	602	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
21	c	505	CLA	O2D-CGD-CBD	2.09	114.97	111.27
22	b	616	BCR	C16-C15-C14	-2.08	119.21	123.47
21	c	505	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
21	c	503	CLA	C1-O2A-CGA	2.08	121.91	116.44
21	b	601	CLA	C17-C16-C15	-2.07	103.70	113.24
21	b	614	CLA	C5-C3-C2	-2.07	116.92	121.12
21	b	611	CLA	CMD-C2D-C1D	2.07	128.37	124.71
21	b	604	CLA	C5-C3-C2	-2.07	116.92	121.12
22	a	404	BCR	C29-C28-C27	-2.06	106.76	111.38
21	b	614	CLA	CBC-CAC-C3C	-2.06	106.74	112.43
21	b	613	CLA	C4D-C3D-CAD	2.06	110.52	108.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	607	CLA	CMC-C2C-C1C	2.06	128.18	125.04
21	b	608	CLA	C4-C3-C5	2.06	118.73	115.27
21	b	605	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
21	k	501	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
22	h	103	BCR	C31-C1-C6	-2.06	106.96	110.30
19	c	502	MGE	O1G-C1A-O1A	-2.06	118.40	123.59
22	d	409	BCR	C33-C5-C6	-2.05	122.22	124.53
19	d	410	MGE	C1D-O6D-C5D	2.05	117.72	113.69
22	z	101	BCR	C20-C19-C18	-2.05	120.65	126.42
21	b	607	CLA	C6-C5-C3	-2.05	108.08	113.45
21	d	407	CLA	C3D-C4D-CHA	-2.05	108.04	112.72
21	c	505	CLA	CMD-C2D-C3D	2.04	132.32	127.61
21	c	505	CLA	C11-C10-C8	-2.04	109.31	115.92
19	b	620	MGE	O1G-C1A-O1A	-2.04	118.43	123.59
21	b	611	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
28	d	408	PQ9	C21-C22-C23	-2.04	122.75	127.66
21	d	406	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
21	a	402	CLA	O2D-CGD-CBD	2.04	114.89	111.27
21	c	509	CLA	CHC-C1C-NC	-2.03	121.12	124.20
21	h	101	CLA	CMC-C2C-C1C	2.03	128.14	125.04
21	a	403	CLA	C3A-C2A-C1A	2.03	104.39	101.34
21	a	403	CLA	OBD-CAD-C3D	-2.03	123.63	128.52
20	l	101	SQD	O48-C23-O10	-2.03	118.47	123.59
21	b	611	CLA	C1D-ND-C4D	-2.03	104.89	106.33
21	b	603	CLA	C6-C7-C8	-2.03	109.36	115.92
22	b	618	BCR	C20-C19-C18	-2.02	120.73	126.42
21	a	402	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
21	a	403	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
21	b	607	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
21	d	407	CLA	C1-C2-C3	-2.02	123.49	126.75
22	c	515	BCR	C37-C22-C23	2.02	121.25	118.08
28	d	408	PQ9	C31-C30-C28	-2.01	106.35	112.98
21	d	407	CLA	C5-C3-C4	2.01	119.05	114.60
21	a	403	CLA	C4A-NA-C1A	2.01	107.61	106.71
21	c	508	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
21	a	402	CLA	C3C-C4C-NC	2.00	112.82	110.57
30	e	101	HEM	CAD-CBD-CGD	-2.00	109.29	113.60
21	b	615	CLA	CMD-C2D-C1D	2.00	128.24	124.71

All (21) chirality outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
-----	-------	-----	------	------

Mol	Chain	Res	Type	Atom
21	a	402	CLA	ND
21	b	601	CLA	ND
21	b	602	CLA	ND
21	b	603	CLA	ND
21	b	604	CLA	ND
21	b	605	CLA	ND
21	b	606	CLA	ND
21	b	609	CLA	ND
21	b	611	CLA	ND
21	b	612	CLA	ND
21	b	613	CLA	ND
21	b	614	CLA	ND
21	b	615	CLA	ND
21	d	402	CLA	ND
21	d	406	CLA	C8
21	c	503	CLA	ND
21	c	504	CLA	ND
21	c	508	CLA	ND
21	c	509	CLA	ND
21	c	510	CLA	ND
21	c	511	CLA	ND

All (387) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	101	MGE	O2G-C2G-C3G-O3G
19	d	410	MGE	O6D-C1D-O3G-C3G
19	m	102	MGE	C2B-C1B-O2G-C2G
20	a	401	SQD	C5-C6-S-O8
20	l	101	SQD	O47-C45-C46-O48
20	l	101	SQD	C5-C6-S-O8
21	b	601	CLA	CHA-CBD-CGD-O1D
21	b	604	CLA	C2-C3-C5-C6
21	b	604	CLA	C4-C3-C5-C6
21	b	605	CLA	CHA-CBD-CGD-O1D
21	b	613	CLA	CHA-CBD-CGD-O2D
21	b	613	CLA	CAD-CBD-CGD-O1D
21	b	613	CLA	CAD-CBD-CGD-O2D
21	b	613	CLA	C3-C5-C6-C7
21	d	402	CLA	CHA-CBD-CGD-O2D
21	d	407	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	h	101	CLA	CBD-CGD-O2D-CED
21	c	504	CLA	CHA-CBD-CGD-O1D
21	c	504	CLA	CAD-CBD-CGD-O1D
21	c	507	CLA	C1A-C2A-CAA-CBA
21	c	507	CLA	C2A-CAA-CBA-CGA
21	c	507	CLA	CBD-CGD-O2D-CED
21	c	507	CLA	O2A-C1-C2-C3
21	c	512	CLA	C1A-C2A-CAA-CBA
21	c	512	CLA	C2-C3-C5-C6
21	c	512	CLA	C4-C3-C5-C6
22	a	404	BCR	C7-C8-C9-C34
22	a	404	BCR	C17-C18-C19-C20
22	a	404	BCR	C36-C18-C19-C20
22	b	618	BCR	C37-C22-C23-C24
22	d	409	BCR	C21-C22-C23-C24
22	d	409	BCR	C37-C22-C23-C24
22	h	103	BCR	C7-C8-C9-C10
22	h	103	BCR	C7-C8-C9-C34
22	c	514	BCR	C1-C6-C7-C8
22	c	515	BCR	C23-C24-C25-C26
22	z	101	BCR	C17-C18-C19-C20
22	z	101	BCR	C36-C18-C19-C20
22	z	101	BCR	C19-C20-C21-C22
22	z	101	BCR	C21-C22-C23-C24
22	z	101	BCR	C37-C22-C23-C24
24	c	516	DGD	O2G-C2G-C3G-O3G
28	d	408	PQ9	C37-C38-C40-C41
28	d	408	PQ9	C39-C38-C40-C41
28	d	408	PQ9	C38-C40-C41-C42
30	e	101	HEM	C2B-C3B-CAB-CBB
30	e	101	HEM	C4B-C3B-CAB-CBB
30	e	101	HEM	C3D-CAD-CBD-CGD
21	c	507	CLA	O1D-CGD-O2D-CED
21	c	513	CLA	CBD-CGD-O2D-CED
21	k	501	CLA	CBD-CGD-O2D-CED
21	c	507	CLA	O1A-CGA-O2A-C1
21	h	101	CLA	O1D-CGD-O2D-CED
21	k	501	CLA	CBA-CGA-O2A-C1
21	k	501	CLA	O1A-CGA-O2A-C1
21	c	507	CLA	CBA-CGA-O2A-C1
24	c	516	DGD	O6D-C5D-C6D-O5D
21	d	406	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	603	CLA	C3-C5-C6-C7
21	k	501	CLA	O1D-CGD-O2D-CED
19	m	102	MGE	O1B-C1B-O2G-C2G
22	c	515	BCR	C19-C20-C21-C22
24	a	406	DGD	O6E-C5E-C6E-O5E
26	d	404	LMT	O5'-C5'-C6'-O6'
26	t	301	LMT	C4B-C5B-C6B-O6B
21	b	613	CLA	C4-C3-C5-C6
21	b	613	CLA	C2-C3-C5-C6
24	c	516	DGD	C4D-C5D-C6D-O5D
26	m	101	LMT	C4'-C5'-C6'-O6'
21	c	513	CLA	O1D-CGD-O2D-CED
24	a	406	DGD	C2B-C1B-O2G-C2G
21	d	407	CLA	CBA-CGA-O2A-C1
21	b	603	CLA	C13-C15-C16-C17
26	t	301	LMT	O5B-C5B-C6B-O6B
21	d	406	CLA	C2-C3-C5-C6
22	a	404	BCR	C11-C12-C13-C35
22	d	409	BCR	C7-C8-C9-C34
22	c	514	BCR	C7-C8-C9-C34
22	a	404	BCR	C11-C12-C13-C14
22	c	514	BCR	C7-C8-C9-C10
21	d	407	CLA	O1A-CGA-O2A-C1
26	d	404	LMT	C4'-C5'-C6'-O6'
24	c	516	DGD	O6E-C5E-C6E-O5E
24	c	516	DGD	C4E-C5E-C6E-O5E
21	d	406	CLA	C8-C10-C11-C12
24	a	406	DGD	C1B-C2B-C3B-C4B
21	b	605	CLA	C11-C12-C13-C15
21	d	406	CLA	C10-C11-C12-C13
26	m	101	LMT	O5'-C5'-C6'-O6'
21	a	402	CLA	C15-C16-C17-C18
21	b	602	CLA	C5-C6-C7-C8
21	c	509	CLA	O1D-CGD-O2D-CED
24	a	406	DGD	O1B-C1B-O2G-C2G
21	b	605	CLA	C13-C15-C16-C17
19	f	101	MGE	O6D-C5D-C6D-O5D
22	h	103	BCR	C9-C10-C11-C12
22	c	514	BCR	C19-C20-C21-C22
21	b	614	CLA	C10-C11-C12-C13
21	c	511	CLA	C8-C10-C11-C12
19	d	410	MGE	C7A-C8A-C9A-CAA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	c	502	MGE	C3B-C4B-C5B-C6B
19	B	101	MGE	C8B-C9B-CAB-CBB
24	a	406	DGD	C5A-C6A-C7A-C8A
19	b	619	MGE	C8A-C9A-CAA-CBA
19	c	502	MGE	C1A-C2A-C3A-C4A
24	a	406	DGD	C2E-C1E-O5D-C6D
24	c	517	DGD	C2D-C1D-O3G-C3G
21	b	605	CLA	C16-C17-C18-C19
19	m	102	MGE	C7A-C8A-C9A-CAA
22	c	514	BCR	C11-C12-C13-C35
22	c	514	BCR	C11-C12-C13-C14
19	c	502	MGE	C4B-C5B-C6B-C7B
24	a	406	DGD	CBB-CCB-CDB-CEB
19	m	102	MGE	C1A-C2A-C3A-C4A
24	a	406	DGD	O6E-C1E-O5D-C6D
19	B	101	MGE	C5B-C6B-C7B-C8B
26	d	404	LMT	O1'-C1-C2-C3
21	a	407	CLA	C13-C15-C16-C17
24	c	517	DGD	C8A-C9A-CAA-CBA
26	t	301	LMT	O1'-C1-C2-C3
21	b	610	CLA	O1D-CGD-O2D-CED
21	d	407	CLA	C3A-C2A-CAA-CBA
21	c	506	CLA	C3A-C2A-CAA-CBA
21	c	507	CLA	C3A-C2A-CAA-CBA
26	d	404	LMT	C5-C6-C7-C8
21	c	504	CLA	C16-C17-C18-C19
21	c	504	CLA	C16-C17-C18-C20
21	c	511	CLA	C2-C3-C5-C6
19	B	101	MGE	C2B-C1B-O2G-C2G
19	d	410	MGE	C2B-C1B-O2G-C2G
19	b	619	MGE	C4A-C5A-C6A-C7A
26	t	301	LMT	C1-C2-C3-C4
24	c	517	DGD	C4A-C5A-C6A-C7A
24	h	104	DGD	C3B-C4B-C5B-C6B
21	b	607	CLA	C13-C15-C16-C17
21	a	402	CLA	C2C-C3C-CAC-CBC
22	a	404	BCR	C23-C24-C25-C26
22	a	404	BCR	C23-C24-C25-C30
22	d	409	BCR	C1-C6-C7-C8
22	d	409	BCR	C5-C6-C7-C8
22	d	409	BCR	C23-C24-C25-C26
22	d	409	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	h	103	BCR	C1-C6-C7-C8
22	h	103	BCR	C5-C6-C7-C8
22	h	103	BCR	C23-C24-C25-C26
22	h	103	BCR	C23-C24-C25-C30
22	c	514	BCR	C5-C6-C7-C8
22	c	515	BCR	C23-C24-C25-C30
19	c	502	MGE	C7B-C8B-C9B-CAB
21	a	407	CLA	C6-C7-C8-C10
21	b	605	CLA	C6-C7-C8-C10
22	a	404	BCR	C13-C14-C15-C16
21	c	503	CLA	O1D-CGD-O2D-CED
19	B	101	MGE	O1B-C1B-O2G-C2G
21	b	610	CLA	C13-C15-C16-C17
21	b	611	CLA	C13-C15-C16-C17
21	d	406	CLA	C5-C6-C7-C8
21	b	602	CLA	CBD-CGD-O2D-CED
19	d	410	MGE	O1B-C1B-O2G-C2G
21	d	402	CLA	C2C-C3C-CAC-CBC
19	b	620	MGE	O1G-C1G-C2G-O2G
24	c	517	DGD	O1G-C1G-C2G-O2G
24	a	406	DGD	C4E-C5E-C6E-O5E
21	c	511	CLA	C4-C3-C5-C6
21	a	407	CLA	C6-C7-C8-C9
21	b	605	CLA	C2A-CAA-CBA-CGA
19	d	410	MGE	C5B-C6B-C7B-C8B
19	m	102	MGE	C8A-C9A-CAA-CBA
21	c	506	CLA	C1A-C2A-CAA-CBA
21	c	513	CLA	C1A-C2A-CAA-CBA
21	b	601	CLA	C16-C17-C18-C19
21	b	605	CLA	C16-C17-C18-C20
19	b	620	MGE	C1B-C2B-C3B-C4B
21	b	613	CLA	O1D-CGD-O2D-CED
19	d	410	MGE	O6D-C5D-C6D-O5D
19	B	101	MGE	C1G-C2G-C3G-O3G
24	c	516	DGD	C1G-C2G-C3G-O3G
19	b	619	MGE	CBB-CCB-CDB-CEB
21	c	506	CLA	CAA-CBA-CGA-O2A
20	l	101	SQD	C24-C25-C26-C27
19	b	620	MGE	C8B-C9B-CAB-CBB
24	h	104	DGD	O6E-C5E-C6E-O5E
21	b	601	CLA	C16-C17-C18-C20
19	b	619	MGE	O2G-C2G-C3G-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	406	DGD	O2G-C2G-C3G-O3G
21	b	605	CLA	C12-C13-C15-C16
21	c	505	CLA	C6-C7-C8-C10
21	c	509	CLA	C11-C10-C8-C7
21	b	610	CLA	C14-C13-C15-C16
22	b	618	BCR	C21-C22-C23-C24
22	d	409	BCR	C7-C8-C9-C10
24	h	104	DGD	C2B-C1B-O2G-C2G
24	a	406	DGD	O6D-C1D-O3G-C3G
21	b	611	CLA	C3-C5-C6-C7
24	a	406	DGD	C4D-C5D-C6D-O5D
21	a	402	CLA	C4C-C3C-CAC-CBC
21	b	614	CLA	C5-C6-C7-C8
21	b	614	CLA	O1D-CGD-O2D-CED
19	c	502	MGE	C2A-C1A-O1G-C1G
21	c	512	CLA	C3A-C2A-CAA-CBA
21	b	614	CLA	C16-C17-C18-C20
19	b	619	MGE	O1G-C1G-C2G-C3G
19	b	620	MGE	O1G-C1G-C2G-C3G
20	l	101	SQD	C44-C45-C46-O48
24	a	406	DGD	C1G-C2G-C3G-O3G
24	c	517	DGD	O1G-C1G-C2G-C3G
19	d	410	MGE	C9B-CAB-CBB-CCB
20	l	101	SQD	C25-C26-C27-C28
21	d	402	CLA	C4C-C3C-CAC-CBC
24	h	104	DGD	CAA-CBA-CCA-CDA
24	h	104	DGD	C9A-CAA-CBA-CCA
21	a	402	CLA	C16-C17-C18-C20
19	c	502	MGE	O6D-C1D-O3G-C3G
21	c	509	CLA	C5-C6-C7-C8
21	b	609	CLA	C11-C12-C13-C14
21	c	509	CLA	C11-C10-C8-C9
19	d	410	MGE	C2A-C3A-C4A-C5A
24	h	104	DGD	C6A-C7A-C8A-C9A
22	a	404	BCR	C7-C8-C9-C10
21	a	407	CLA	C11-C10-C8-C7
21	b	603	CLA	C6-C7-C8-C10
21	b	610	CLA	C12-C13-C15-C16
21	b	614	CLA	C16-C17-C18-C19
21	b	603	CLA	CAD-CBD-CGD-O2D
21	c	503	CLA	CAD-CBD-CGD-O2D
25	d	401	PHO	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	f	101	MGE	C5B-C6B-C7B-C8B
24	c	517	DGD	O6D-C1D-O3G-C3G
19	c	502	MGE	O1G-C1G-C2G-C3G
24	h	104	DGD	O1G-C1G-C2G-C3G
19	c	502	MGE	C8B-C9B-CAB-CBB
19	b	620	MGE	C2B-C3B-C4B-C5B
24	h	104	DGD	O1B-C1B-O2G-C2G
21	c	504	CLA	CHA-CBD-CGD-O2D
21	c	509	CLA	CHA-CBD-CGD-O1D
21	c	512	CLA	CHA-CBD-CGD-O1D
21	c	512	CLA	CHA-CBD-CGD-O2D
21	c	513	CLA	CHA-CBD-CGD-O1D
21	c	513	CLA	CHA-CBD-CGD-O2D
19	c	502	MGE	C3A-C4A-C5A-C6A
19	b	619	MGE	O1G-C1G-C2G-O2G
19	c	502	MGE	O1G-C1G-C2G-O2G
19	c	502	MGE	O1A-C1A-O1G-C1G
21	b	605	CLA	C11-C12-C13-C14
21	a	403	CLA	O1D-CGD-O2D-CED
21	d	406	CLA	O1D-CGD-O2D-CED
19	B	101	MGE	C7A-C8A-C9A-CAA
21	b	604	CLA	CAD-CBD-CGD-O1D
21	b	606	CLA	CAD-CBD-CGD-O1D
21	c	507	CLA	CAD-CBD-CGD-O1D
21	c	508	CLA	CAD-CBD-CGD-O1D
24	a	406	DGD	O6D-C5D-C6D-O5D
19	B	101	MGE	C1A-C2A-C3A-C4A
24	h	104	DGD	C6B-C7B-C8B-C9B
21	c	509	CLA	C11-C12-C13-C15
21	b	614	CLA	C13-C15-C16-C17
24	c	517	DGD	C1A-C2A-C3A-C4A
19	b	619	MGE	C1G-C2G-C3G-O3G
20	a	401	SQD	O47-C45-C46-O48
24	c	516	DGD	C9A-CAA-CBA-CCA
21	b	605	CLA	C15-C16-C17-C18
24	a	406	DGD	C2A-C3A-C4A-C5A
21	a	407	CLA	C11-C10-C8-C9
21	b	603	CLA	C6-C7-C8-C9
21	b	605	CLA	C14-C13-C15-C16
21	c	509	CLA	C11-C12-C13-C14
22	a	404	BCR	C18-C19-C20-C21
22	c	515	BCR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	t	301	LMT	C5-C6-C7-C8
19	c	502	MGE	C5A-C6A-C7A-C8A
21	d	406	CLA	CAA-CBA-CGA-O2A
21	b	613	CLA	C2-C1-O2A-CGA
22	z	101	BCR	C23-C24-C25-C26
19	d	410	MGE	C2D-C1D-O3G-C3G
19	m	102	MGE	O1G-C1G-C2G-O2G
24	h	104	DGD	O1G-C1G-C2G-O2G
21	c	504	CLA	C11-C12-C13-C15
21	b	606	CLA	C3-C5-C6-C7
21	b	614	CLA	C14-C13-C15-C16
21	d	406	CLA	C6-C7-C8-C9
19	m	102	MGE	C2A-C3A-C4A-C5A
21	c	510	CLA	O1D-CGD-O2D-CED
21	b	611	CLA	CBA-CGA-O2A-C1
22	c	514	BCR	C15-C16-C17-C18
21	c	511	CLA	O1D-CGD-O2D-CED
28	d	408	PQ9	C13-C15-C16-C17
21	b	611	CLA	C10-C11-C12-C13
21	c	506	CLA	CAA-CBA-CGA-O1A
19	B	101	MGE	C7B-C8B-C9B-CAB
19	m	102	MGE	C4B-C5B-C6B-C7B
24	c	516	DGD	C3B-C4B-C5B-C6B
19	f	101	MGE	C1A-C2A-C3A-C4A
26	t	301	LMT	C7-C8-C9-C10
19	d	410	MGE	O1G-C1G-C2G-C3G
20	a	401	SQD	C44-C45-C46-O48
19	B	101	MGE	C4A-C5A-C6A-C7A
19	b	619	MGE	CAB-CBB-CCB-CDB
21	b	614	CLA	C12-C13-C15-C16
24	h	104	DGD	C4B-C5B-C6B-C7B
21	b	609	CLA	C2A-CAA-CBA-CGA
28	d	408	PQ9	C19-C18-C20-C21
24	a	406	DGD	C1A-C2A-C3A-C4A
22	b	618	BCR	C9-C10-C11-C12
21	c	507	CLA	C2-C1-O2A-CGA
21	c	504	CLA	C11-C12-C13-C14
21	d	402	CLA	C15-C16-C17-C18
19	d	410	MGE	O2G-C1B-C2B-C3B
21	b	609	CLA	C16-C17-C18-C20
21	c	503	CLA	C13-C15-C16-C17
19	B	101	MGE	C2G-C3G-O3G-C1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	d	410	MGE	C2G-C3G-O3G-C1D
19	c	502	MGE	C2G-C3G-O3G-C1D
20	l	101	SQD	C18-C19-C20-C21
30	e	101	HEM	CAA-CBA-CGA-O2A
19	m	102	MGE	C5B-C6B-C7B-C8B
21	d	406	CLA	C14-C13-C15-C16
19	B	101	MGE	C9B-CAB-CBB-CCB
19	B	101	MGE	C1B-C2B-C3B-C4B
19	d	410	MGE	C1B-C2B-C3B-C4B
30	e	101	HEM	CAA-CBA-CGA-O1A
21	c	513	CLA	CBA-CGA-O2A-C1
25	d	403	PHO	C4C-C3C-CAC-CBC
28	d	408	PQ9	C24-C23-C25-C26
24	c	516	DGD	O2G-C1B-C2B-C3B
26	t	301	LMT	C4-C5-C6-C7
21	b	614	CLA	C3A-C2A-CAA-CBA
21	a	402	CLA	CAD-CBD-CGD-O2D
21	b	609	CLA	CAD-CBD-CGD-O2D
21	b	615	CLA	CAD-CBD-CGD-O2D
21	c	508	CLA	CAD-CBD-CGD-O2D
21	c	510	CLA	CAD-CBD-CGD-O2D
21	c	511	CLA	CAD-CBD-CGD-O2D
20	a	401	SQD	O5-C1-O6-C44
28	d	408	PQ9	C17-C18-C20-C21
24	h	104	DGD	O2G-C1B-C2B-C3B
25	d	403	PHO	C2C-C3C-CAC-CBC
21	c	513	CLA	O1A-CGA-O2A-C1
21	b	603	CLA	O2A-C1-C2-C3
25	d	401	PHO	O2A-C1-C2-C3
24	c	517	DGD	C7A-C8A-C9A-CAA
21	a	407	CLA	CHA-CBD-CGD-O2D
21	b	601	CLA	CHA-CBD-CGD-O2D
21	b	604	CLA	CHA-CBD-CGD-O1D
21	b	605	CLA	CHA-CBD-CGD-O2D
21	b	610	CLA	CHA-CBD-CGD-O2D
21	b	613	CLA	CHA-CBD-CGD-O1D
21	b	615	CLA	CHA-CBD-CGD-O1D
21	c	505	CLA	CHA-CBD-CGD-O2D
21	c	508	CLA	CHA-CBD-CGD-O1D
21	c	510	CLA	CHA-CBD-CGD-O1D
21	c	511	CLA	CHA-CBD-CGD-O1D
21	k	501	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

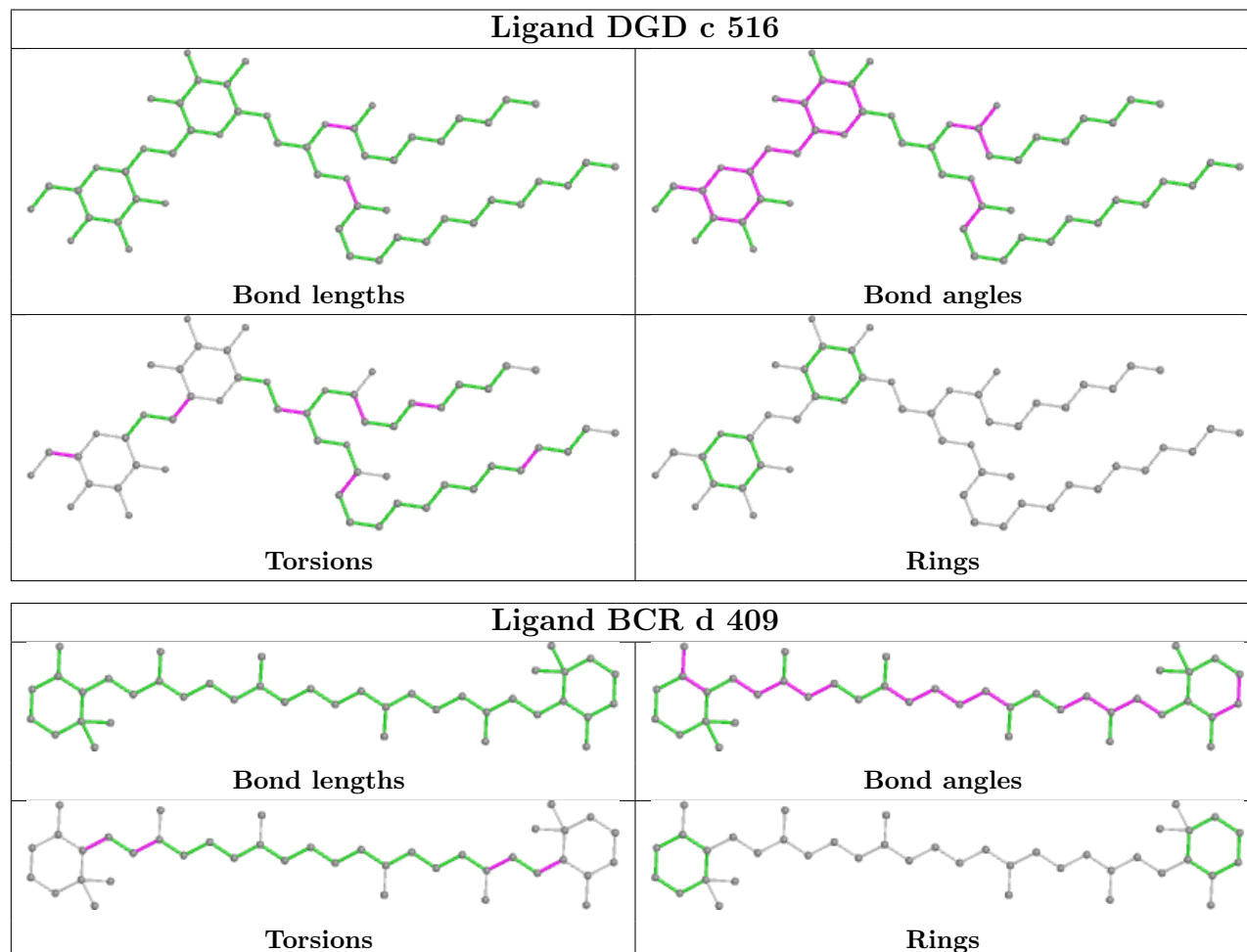
Mol	Chain	Res	Type	Atoms
21	k	501	CLA	CHA-CBD-CGD-O2D
21	c	512	CLA	CAA-CBA-CGA-O2A
21	k	501	CLA	CAA-CBA-CGA-O2A
24	c	516	DGD	O1G-C1A-C2A-C3A
21	c	513	CLA	CAA-CBA-CGA-O2A
25	d	403	PHO	CHA-CBD-CGD-O2D
21	c	511	CLA	C6-C7-C8-C10
21	d	402	CLA	C11-C12-C13-C14
21	c	511	CLA	C6-C7-C8-C9
19	B	101	MGE	C2A-C1A-O1G-C1G
21	b	602	CLA	C2A-CAA-CBA-CGA
19	d	410	MGE	C4B-C5B-C6B-C7B
24	c	516	DGD	O1B-C1B-C2B-C3B
24	h	104	DGD	C2B-C3B-C4B-C5B
19	B	101	MGE	O1A-C1A-O1G-C1G
19	m	102	MGE	O1G-C1G-C2G-C3G
21	c	512	CLA	CAA-CBA-CGA-O1A
21	b	602	CLA	C13-C15-C16-C17
21	c	513	CLA	CAA-CBA-CGA-O1A
19	b	620	MGE	C6B-C7B-C8B-C9B
19	B	101	MGE	O2G-C1B-C2B-C3B
21	c	503	CLA	CAA-CBA-CGA-O2A
21	c	511	CLA	C16-C17-C18-C20
20	l	101	SQD	C10-C11-C12-C13
21	b	603	CLA	C16-C17-C18-C19
24	c	516	DGD	O1A-C1A-C2A-C3A
21	b	611	CLA	C6-C7-C8-C9
21	b	611	CLA	C11-C10-C8-C9
24	a	406	DGD	CCB-CDB-CEB-CFB
19	b	619	MGE	C1A-C2A-C3A-C4A
24	a	406	DGD	C4A-C5A-C6A-C7A
21	b	611	CLA	C11-C10-C8-C7
19	B	101	MGE	O1B-C1B-C2B-C3B
24	a	406	DGD	O1G-C1A-C2A-C3A
21	b	610	CLA	C16-C17-C18-C20

There are no ring outliers.

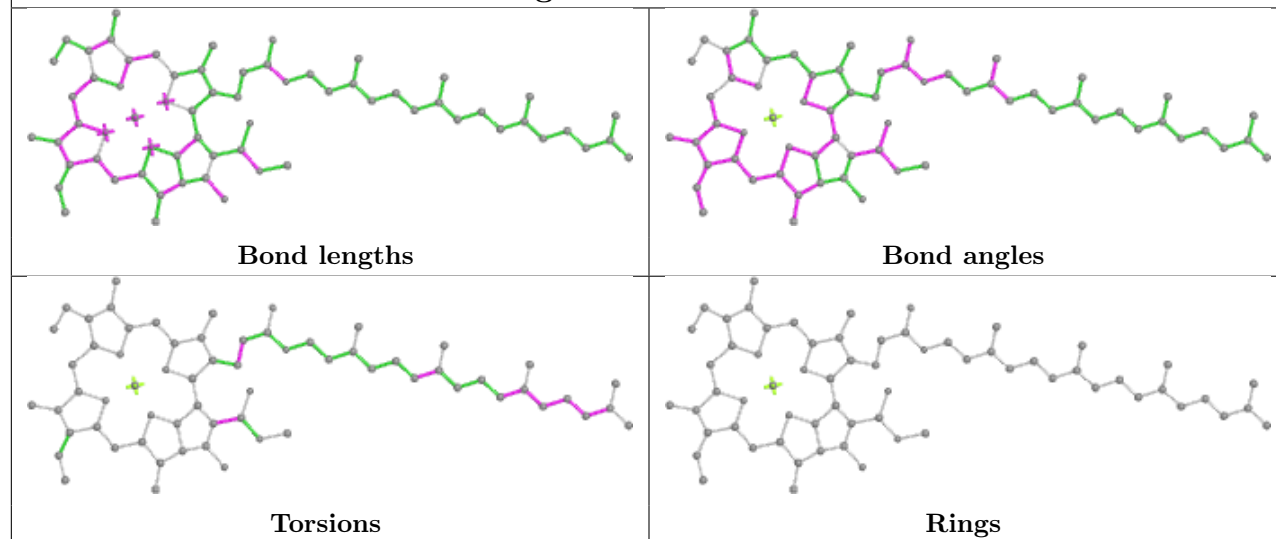
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

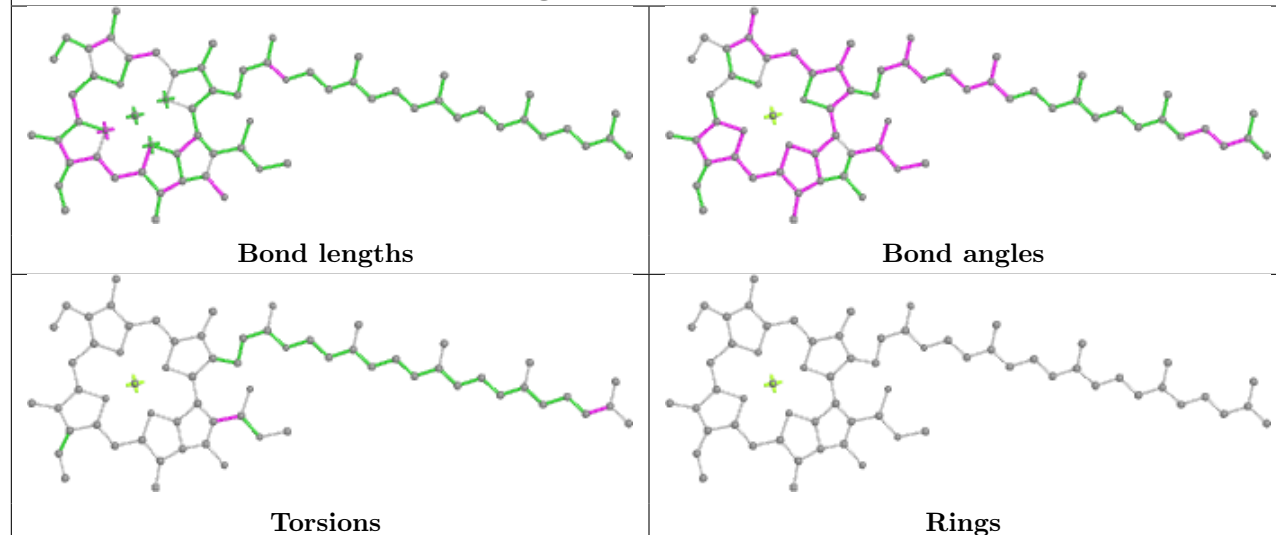
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



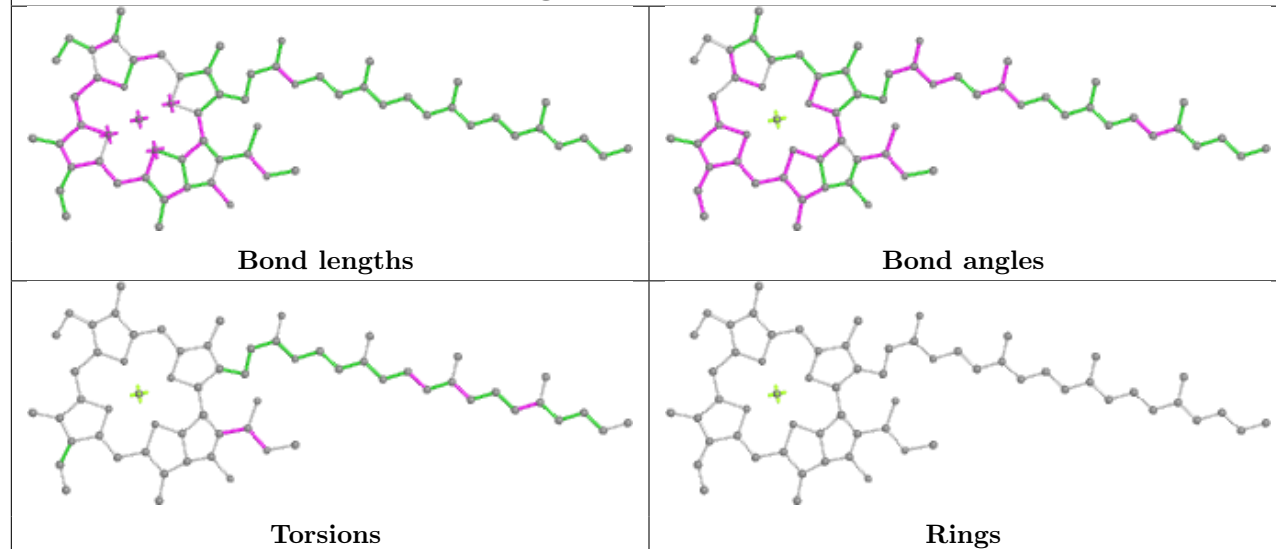
Ligand CLA b 605

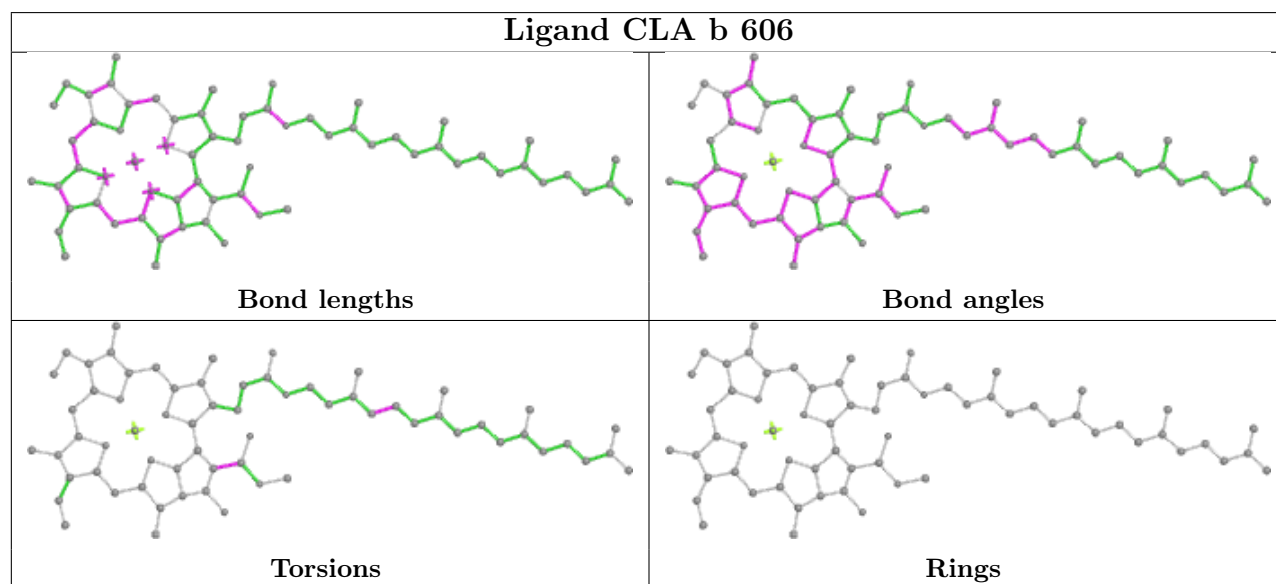
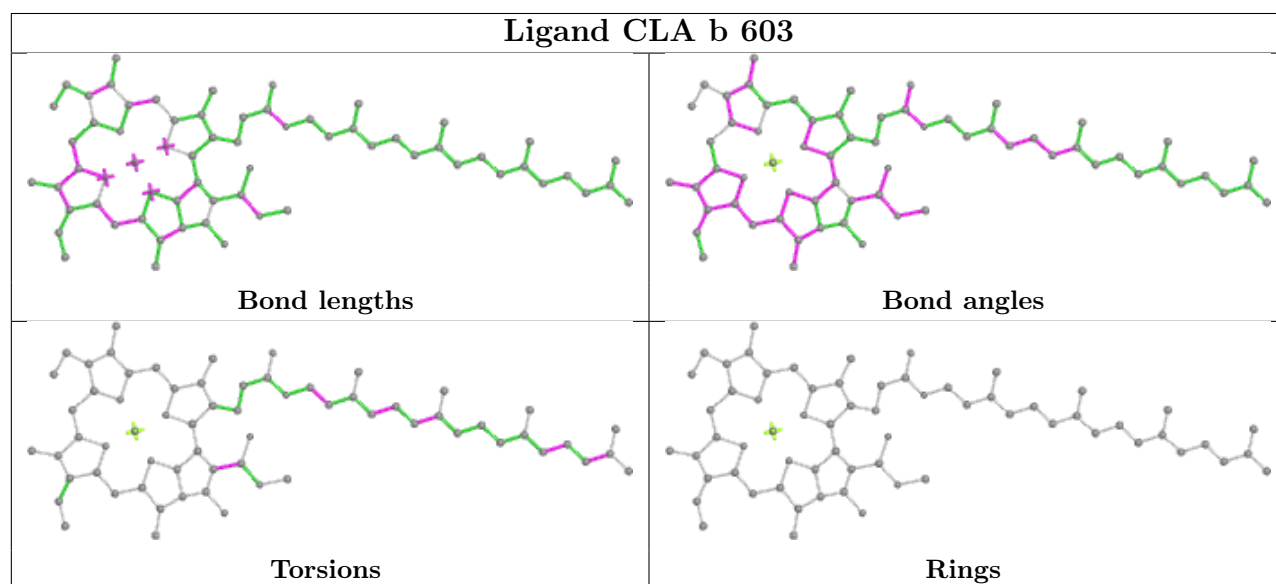
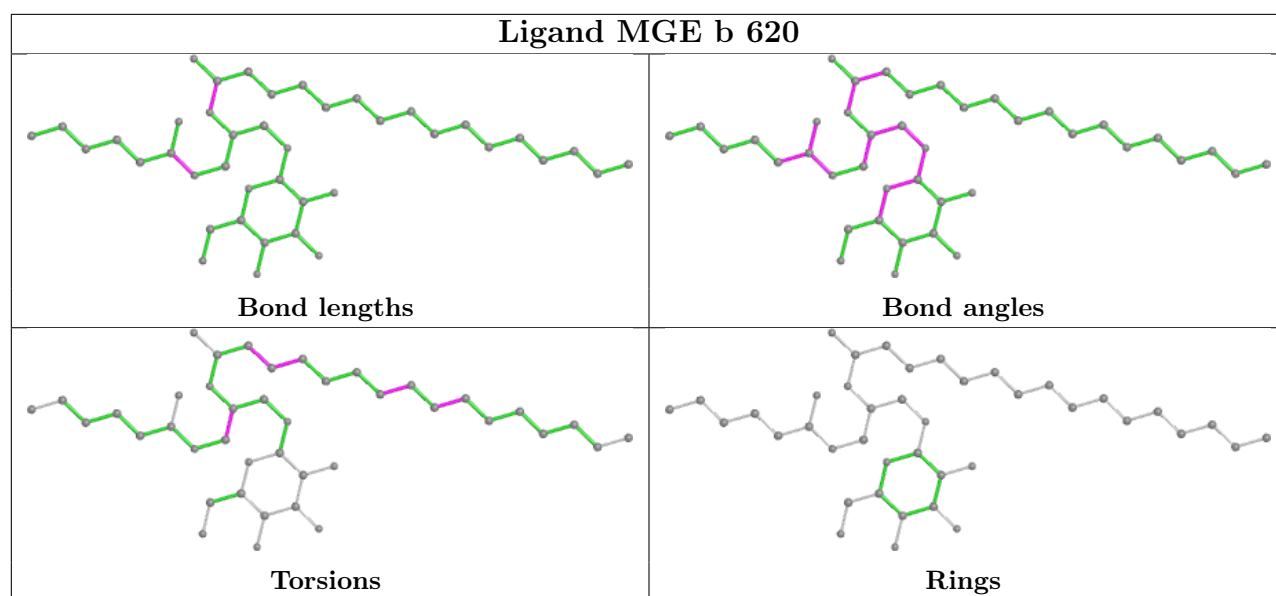


Ligand CLA b 601

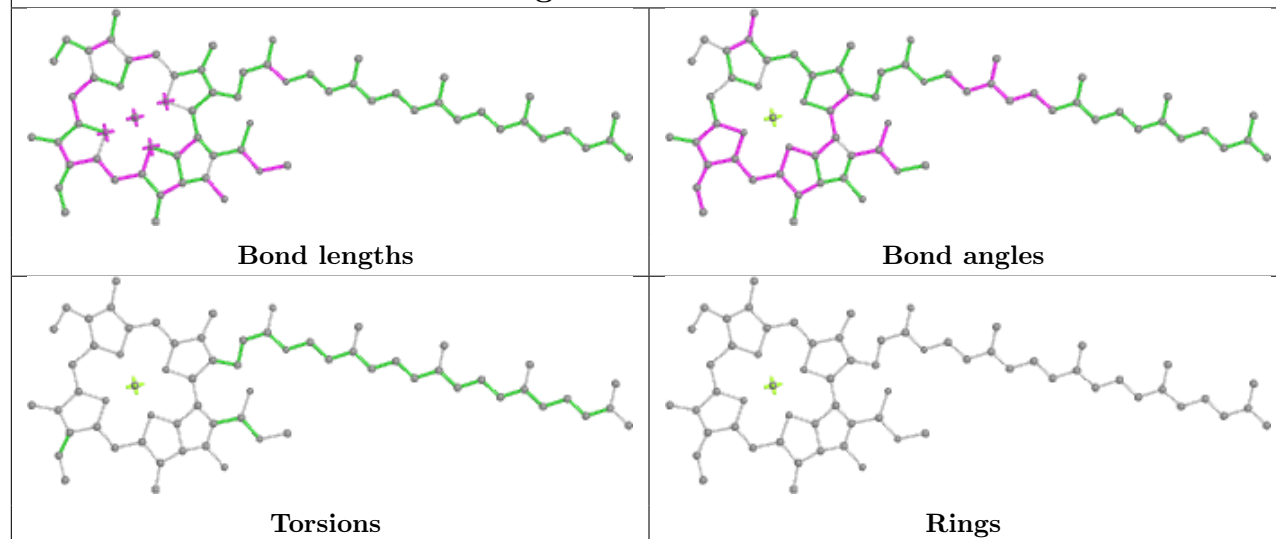


Ligand CLA c 509

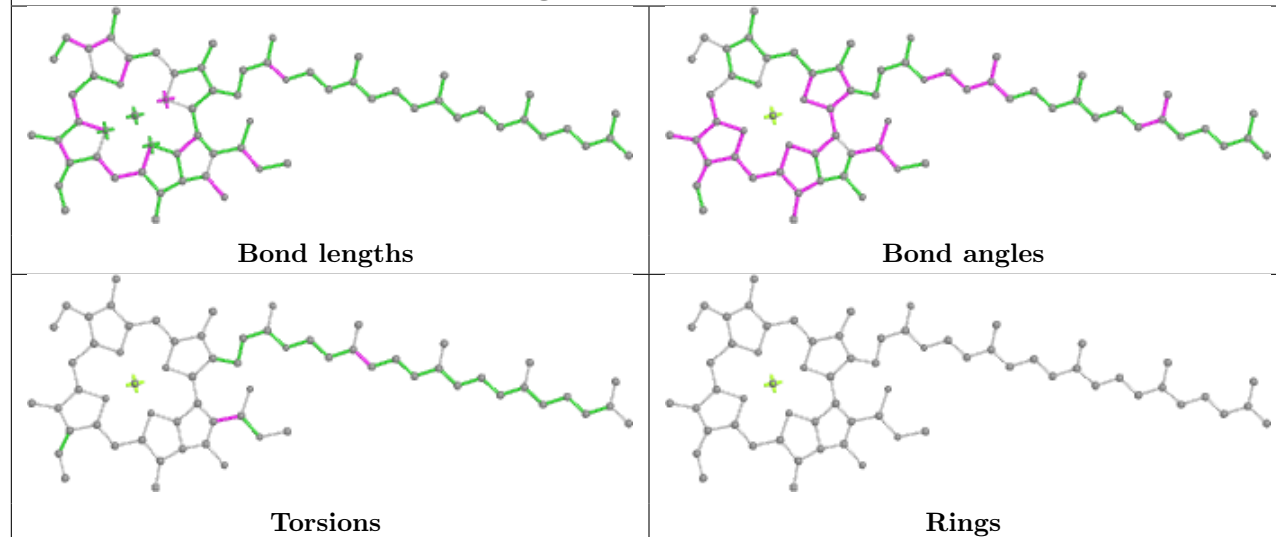




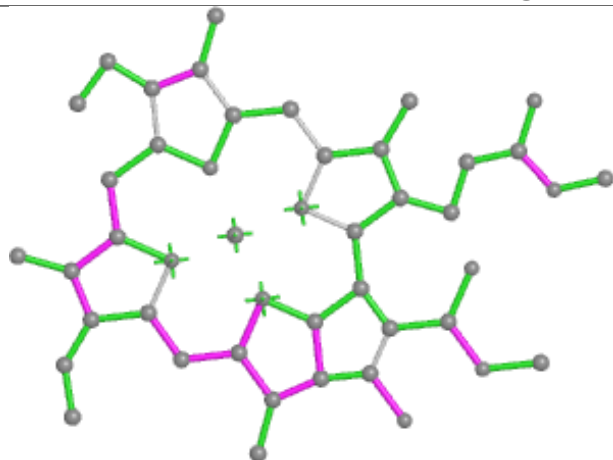
Ligand CLA b 608



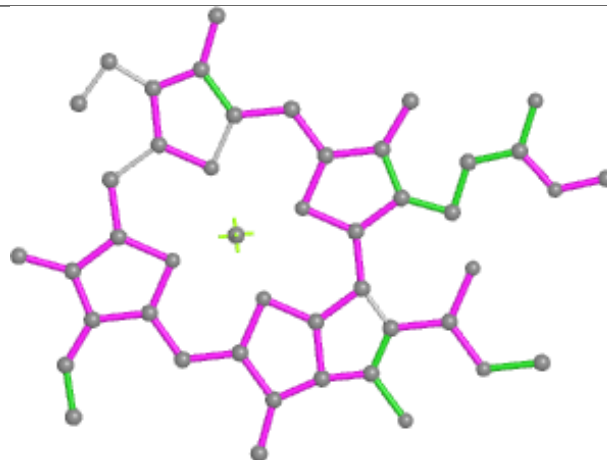
Ligand CLA b 604



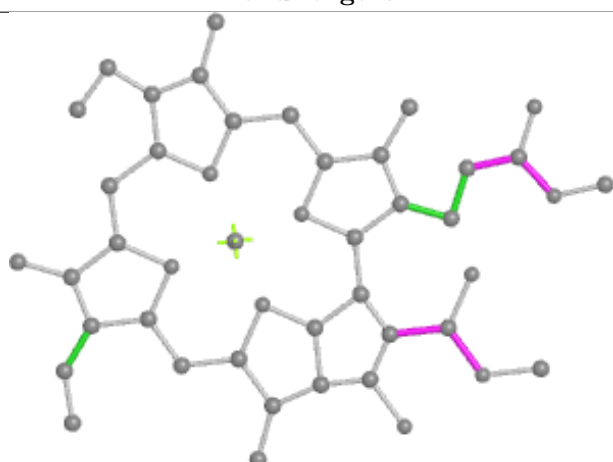
Ligand CLA k 501



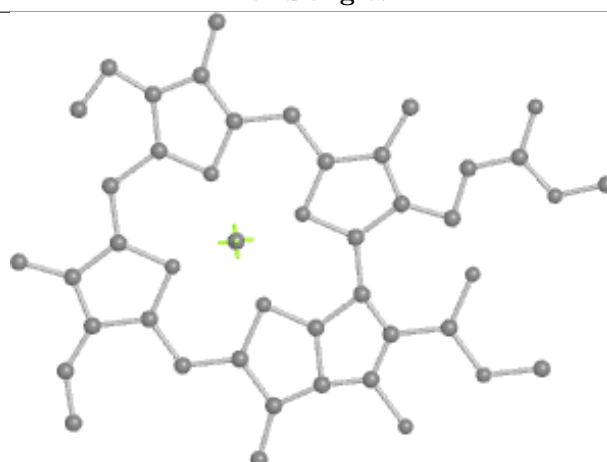
Bond lengths



Bond angles

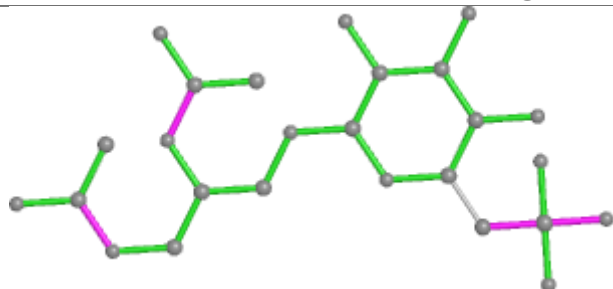


Torsions

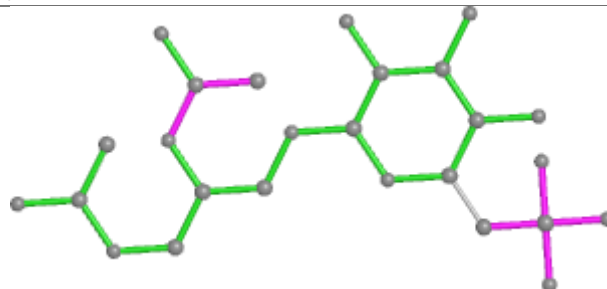


Rings

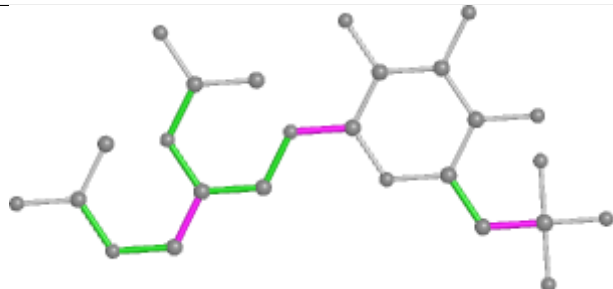
Ligand SQD a 401



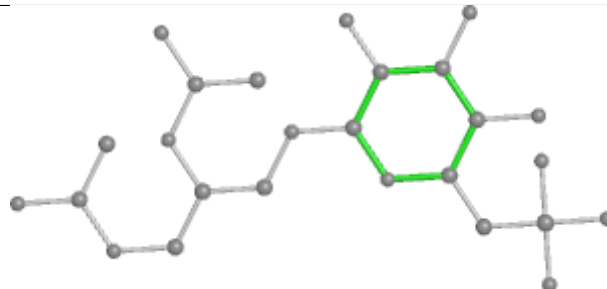
Bond lengths



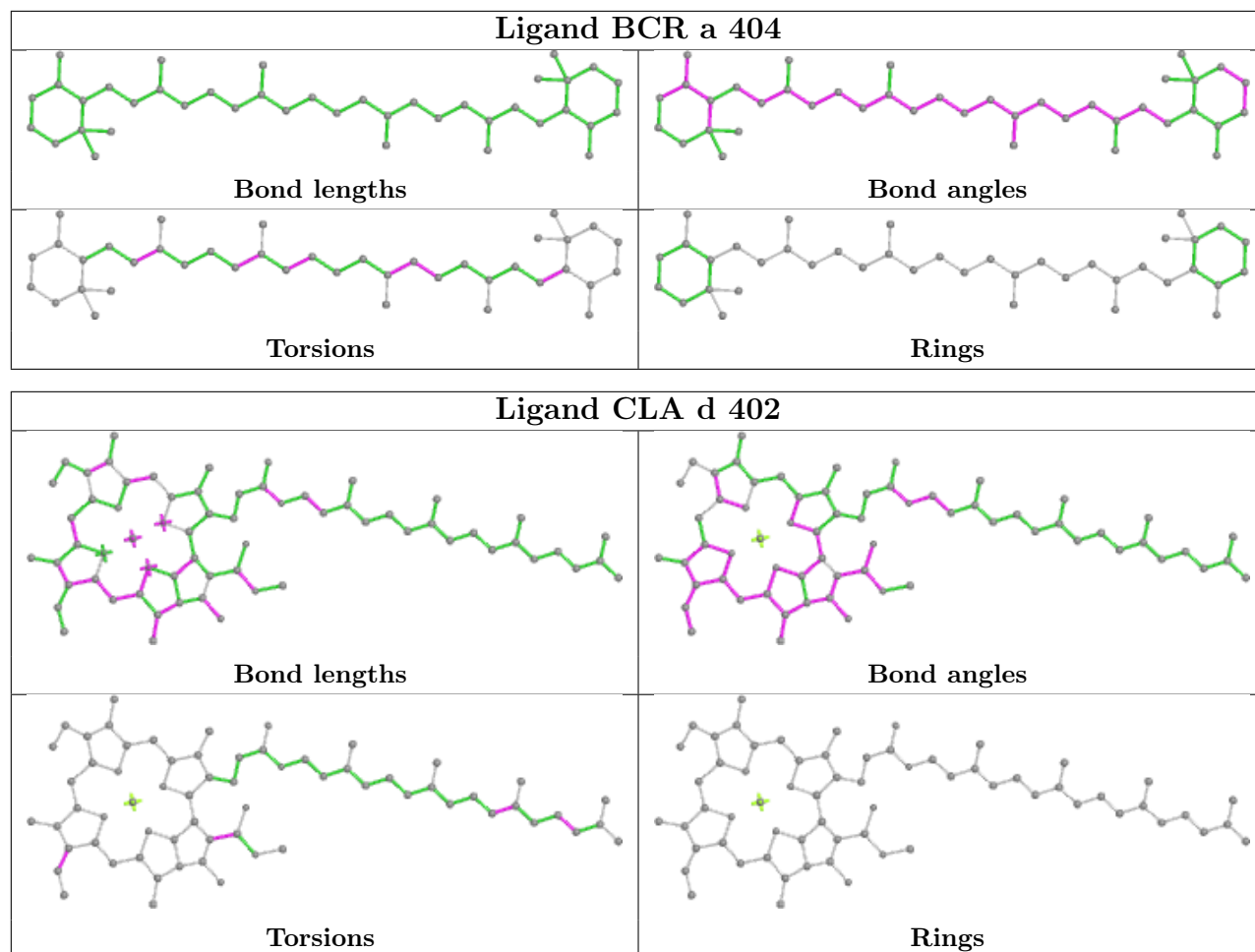
Bond angles



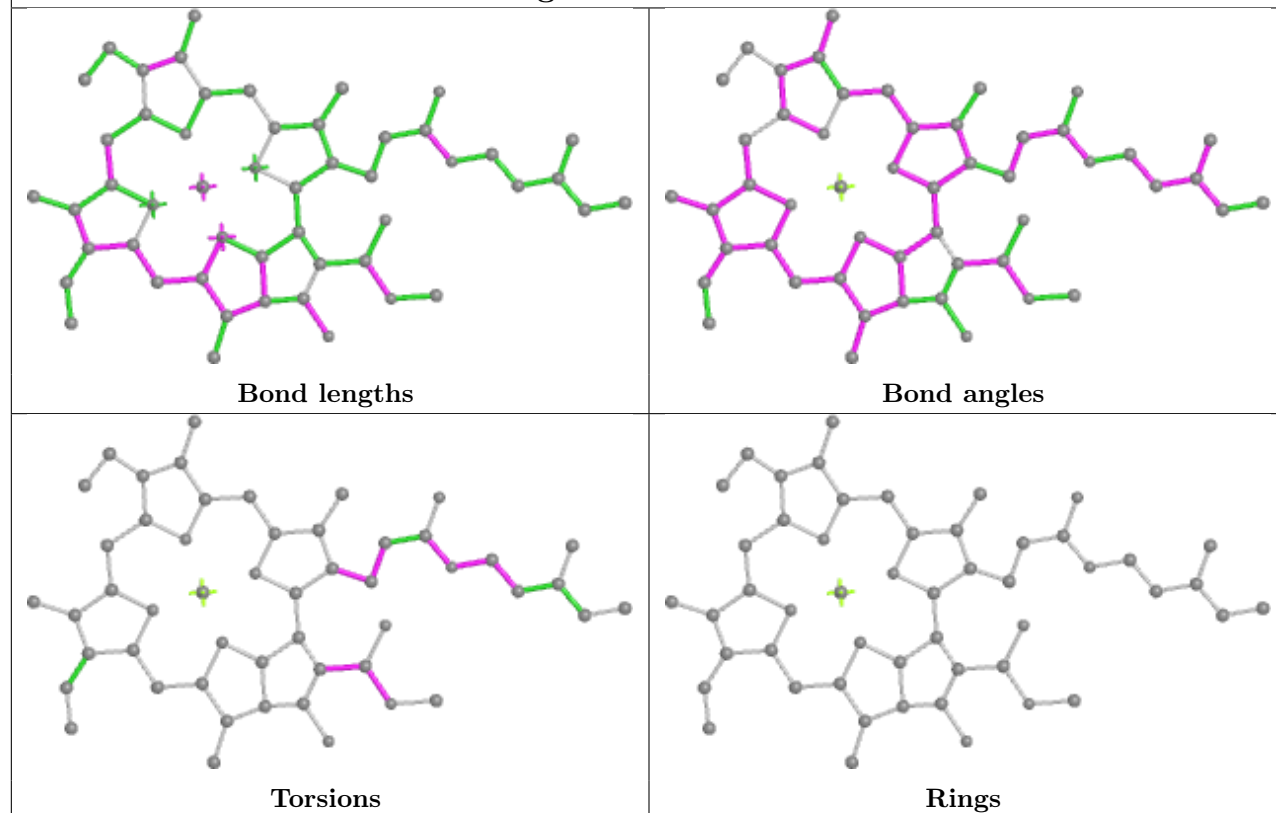
Torsions



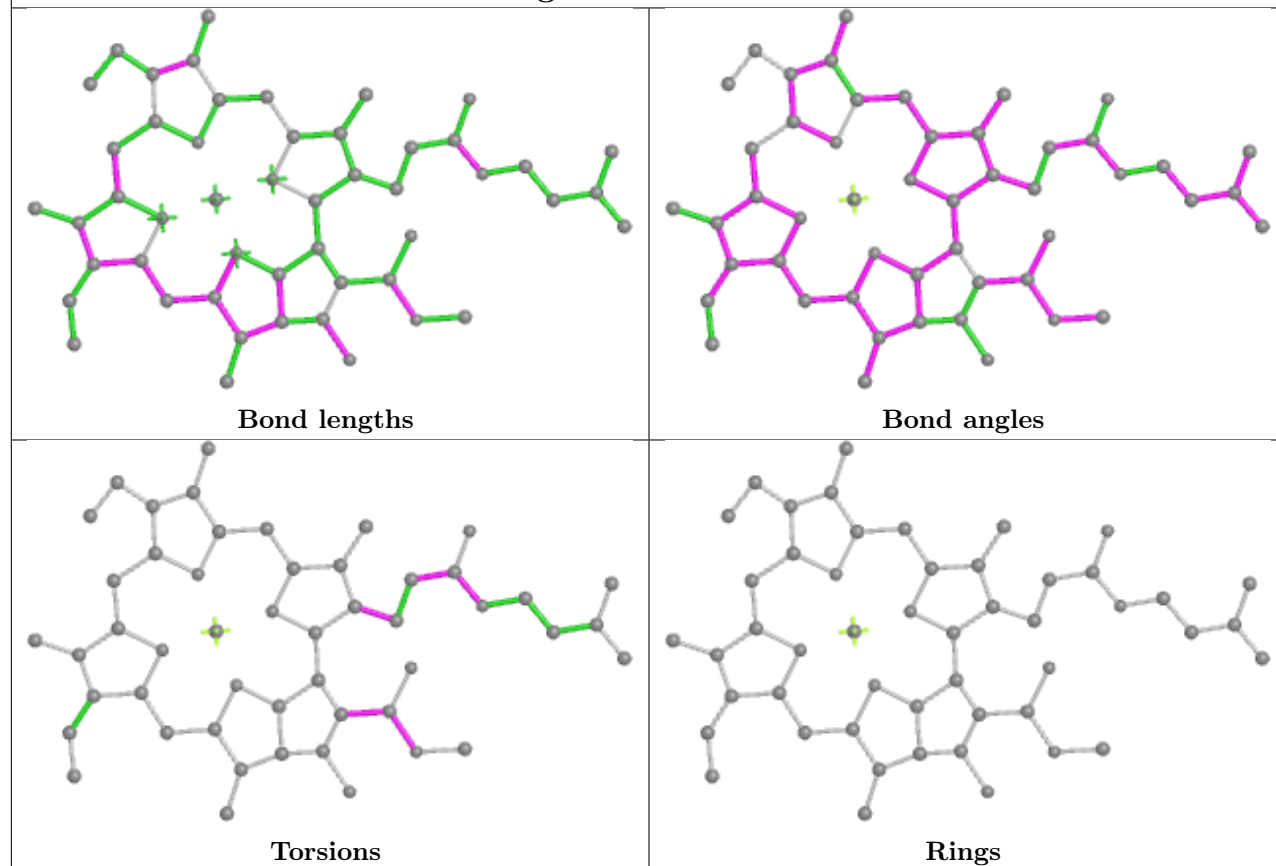
Rings

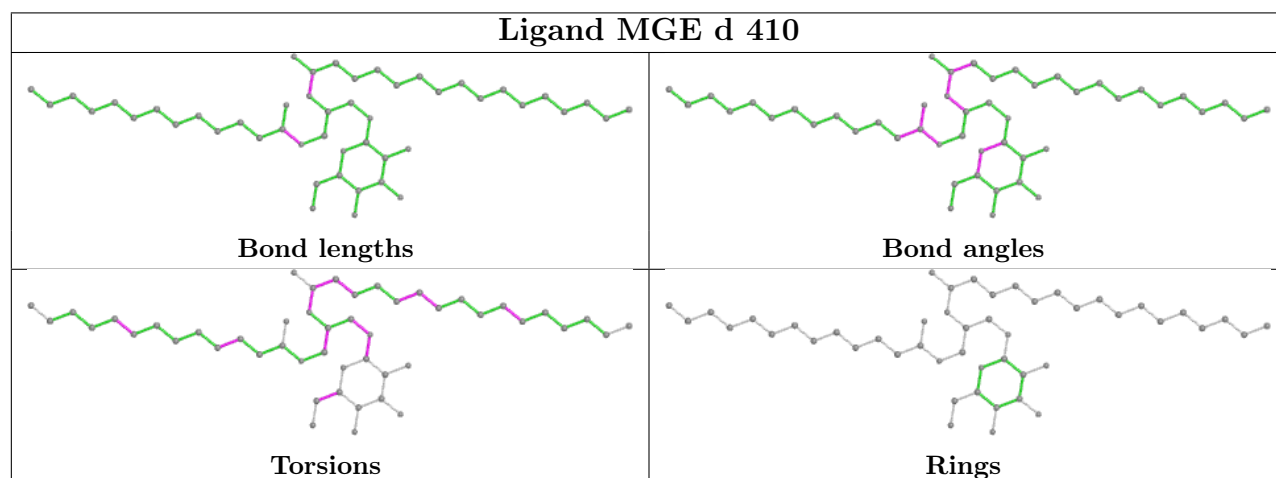
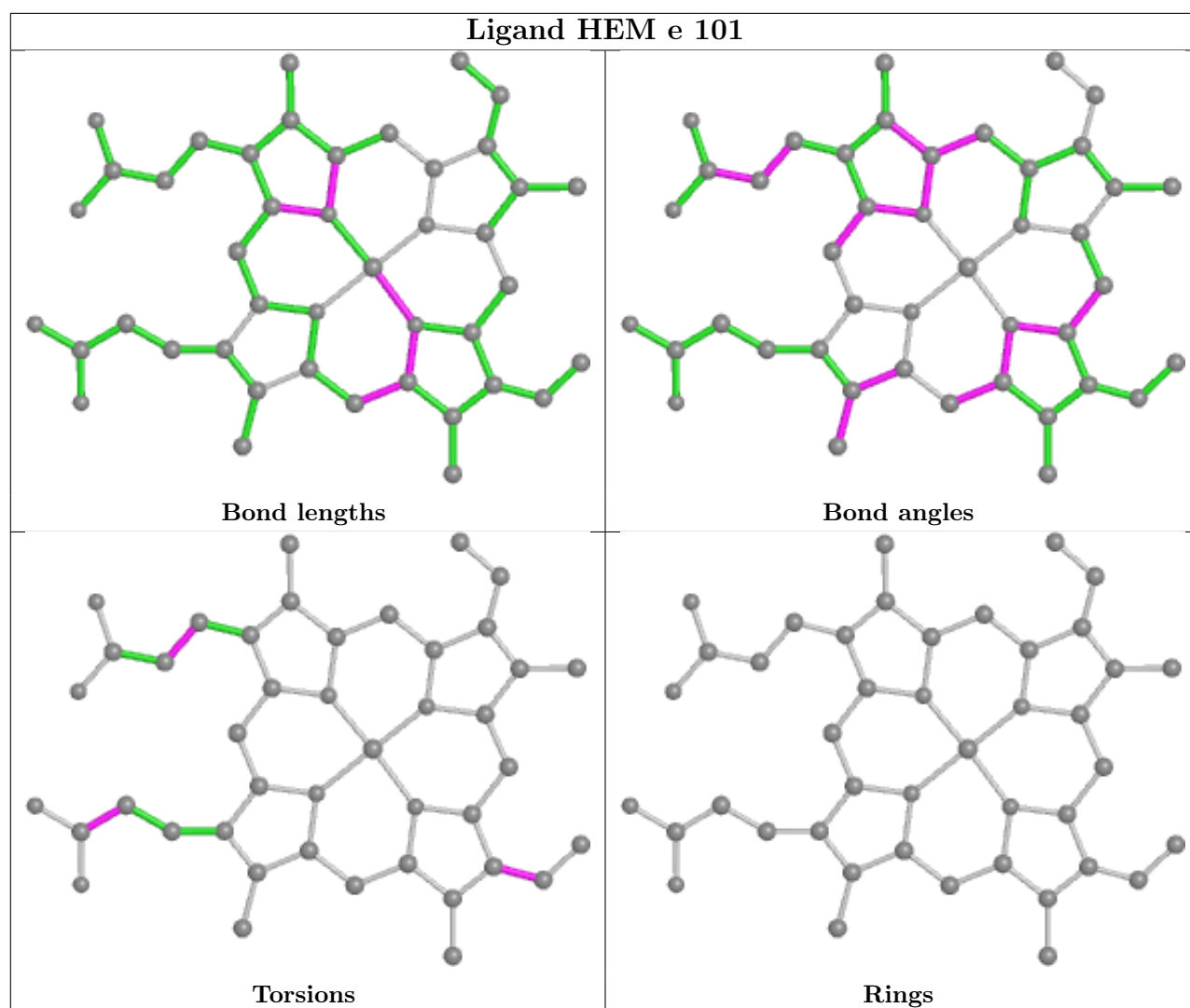


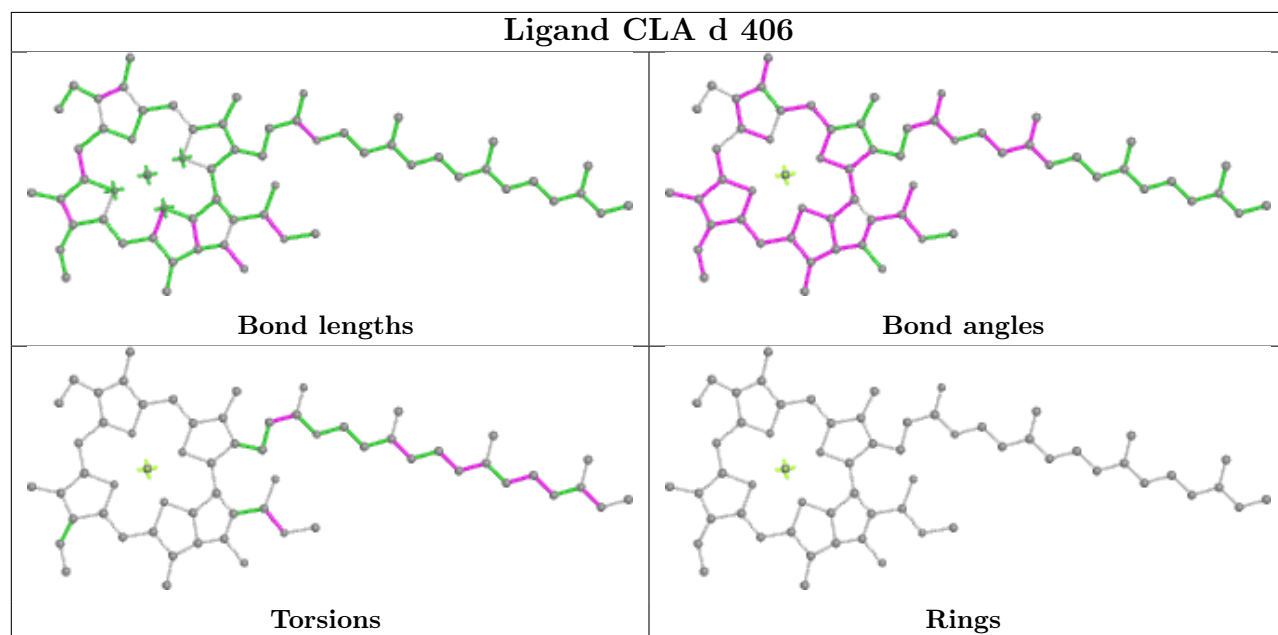
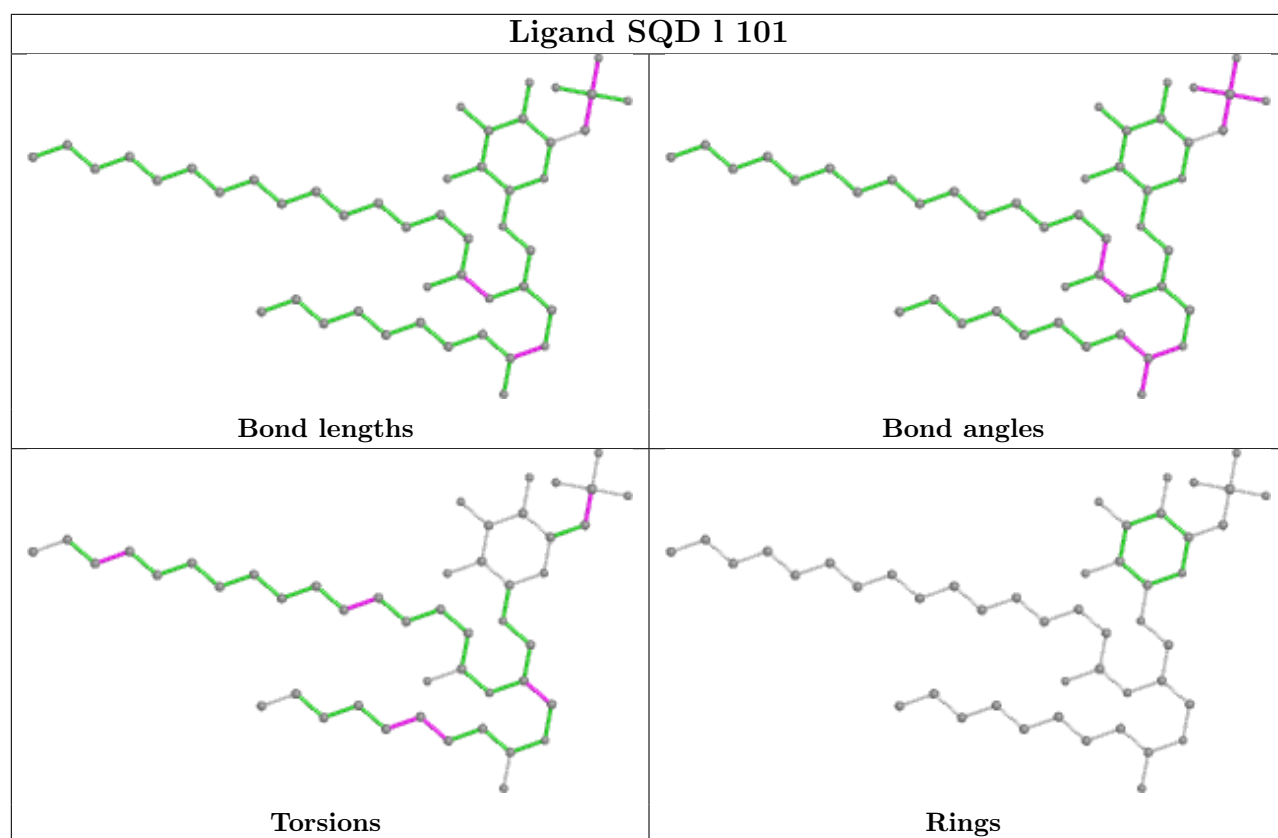
Ligand CLA c 507

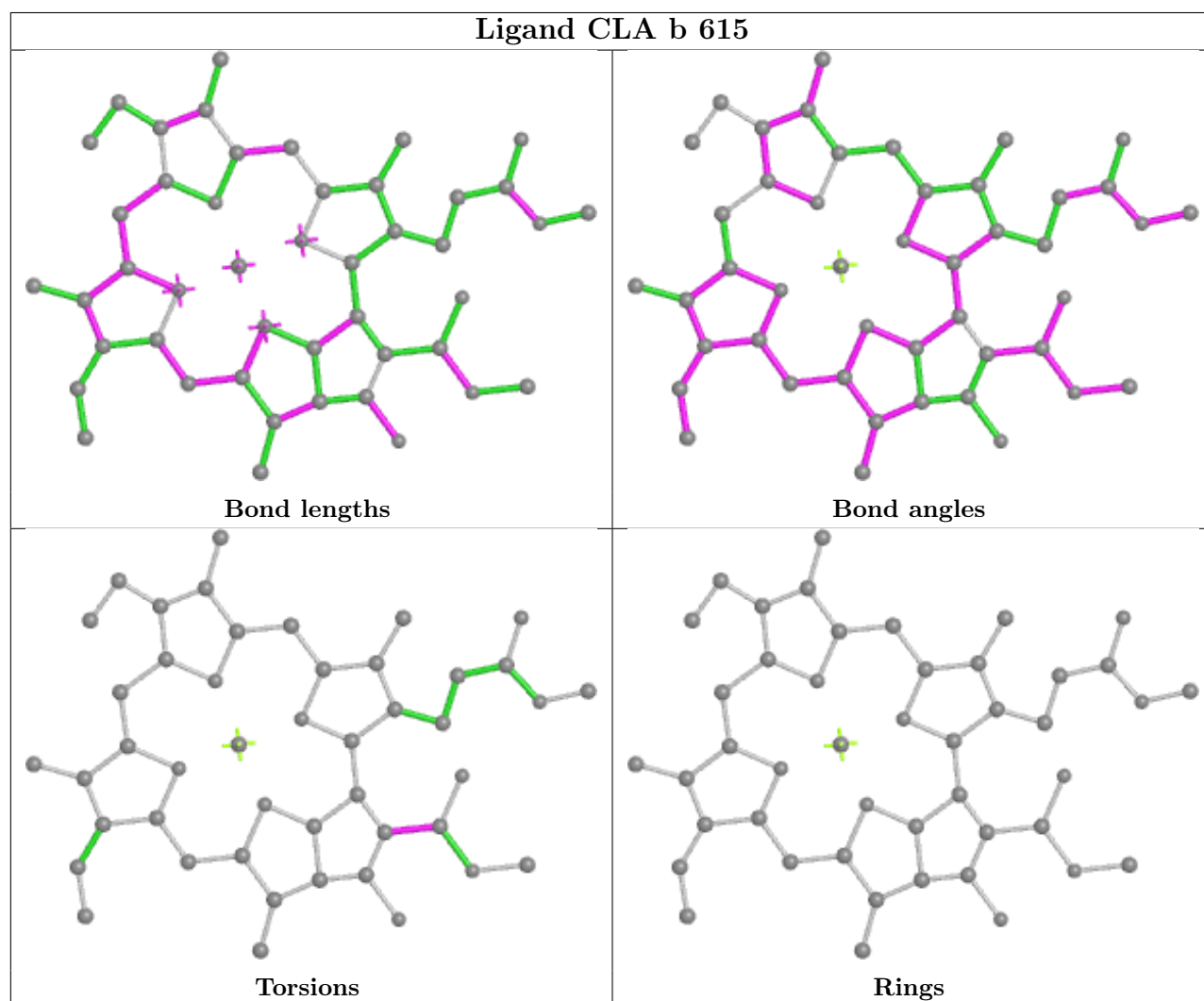
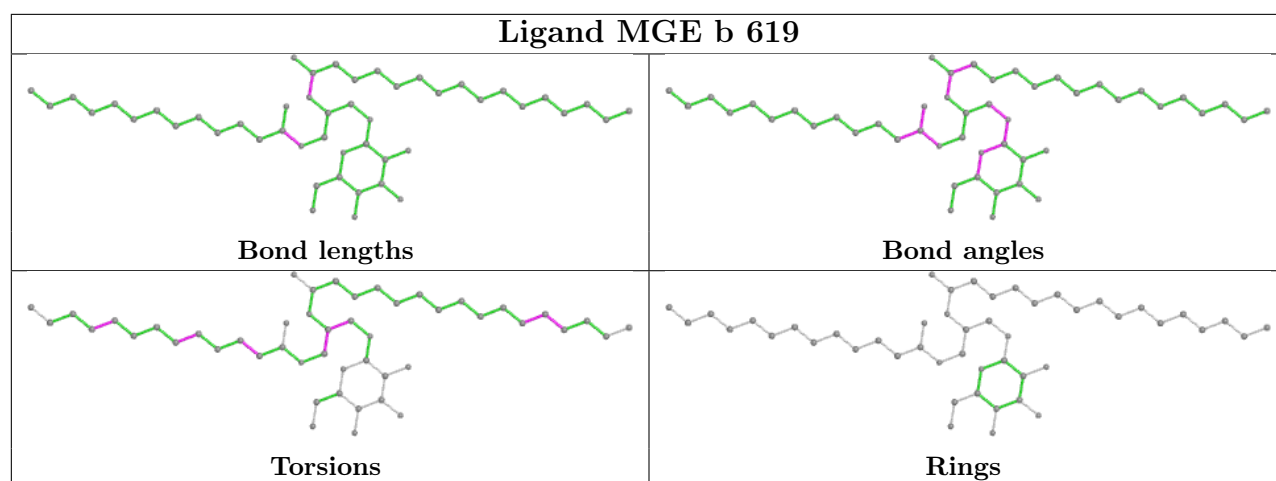


Ligand CLA c 513

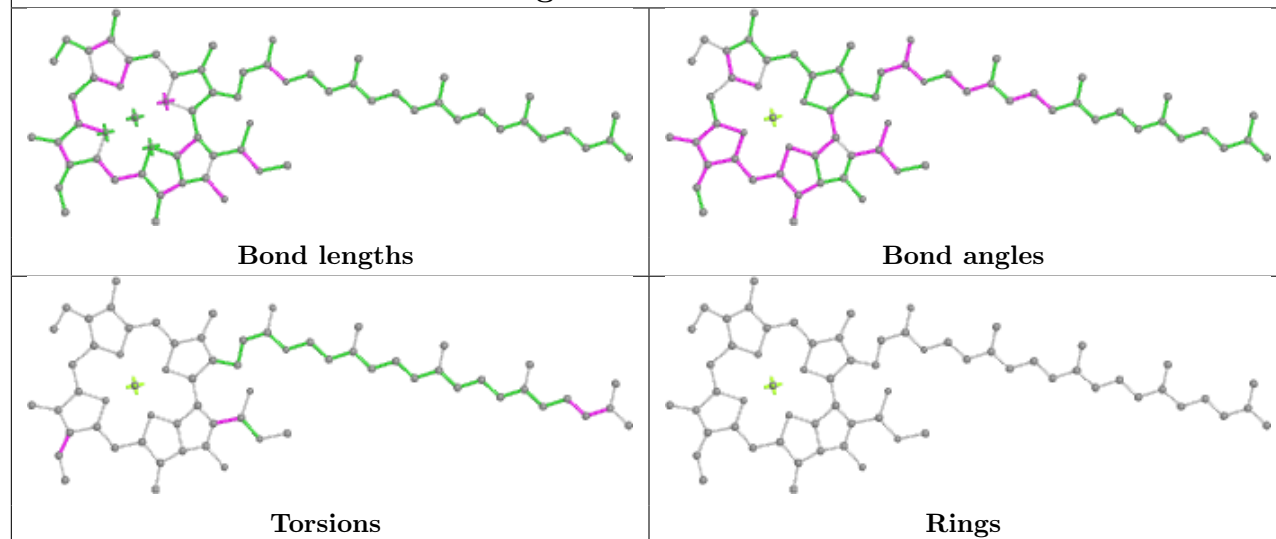




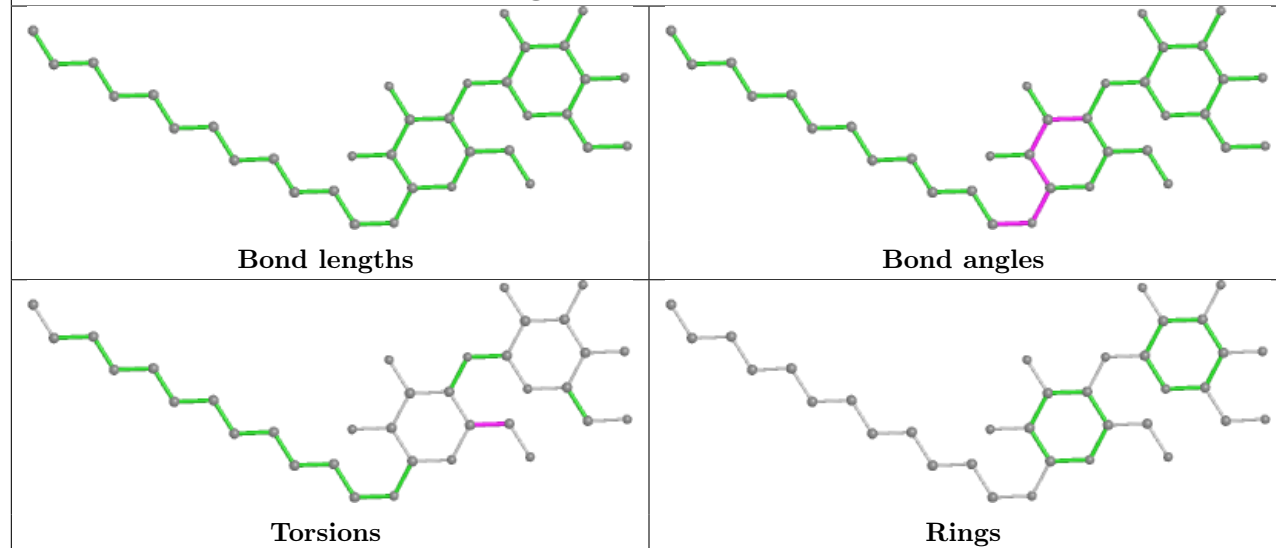




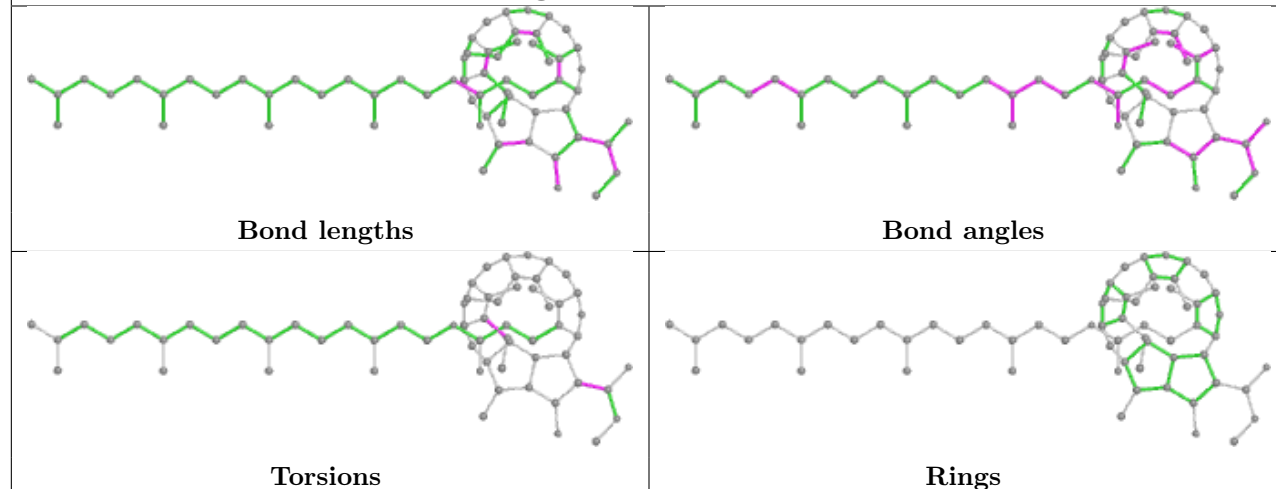
Ligand CLA a 402

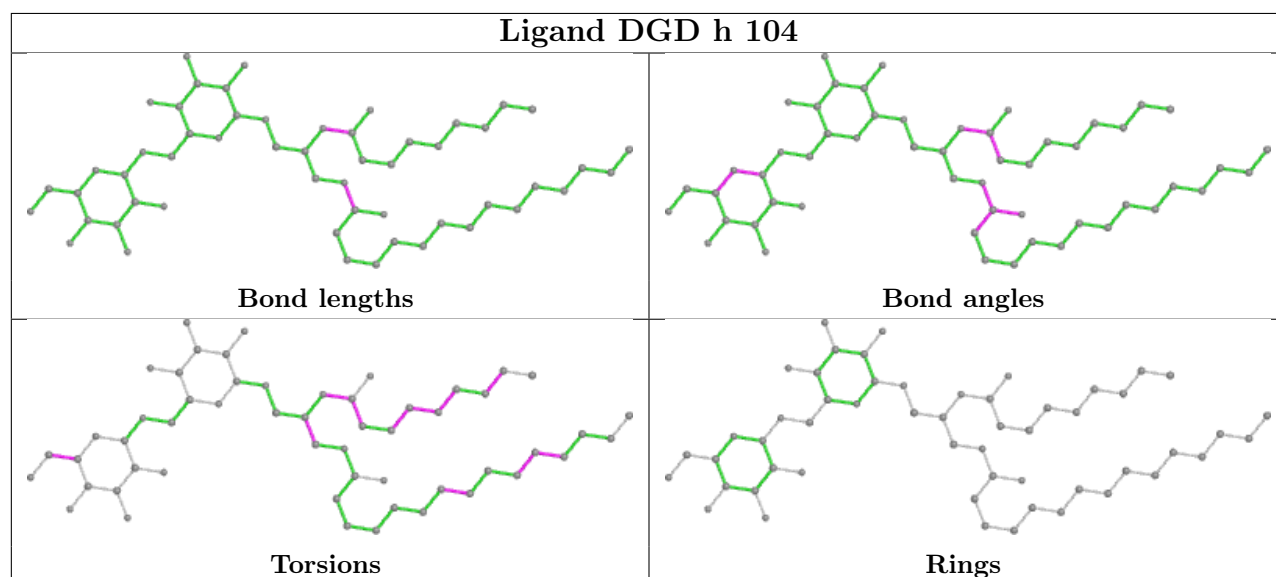
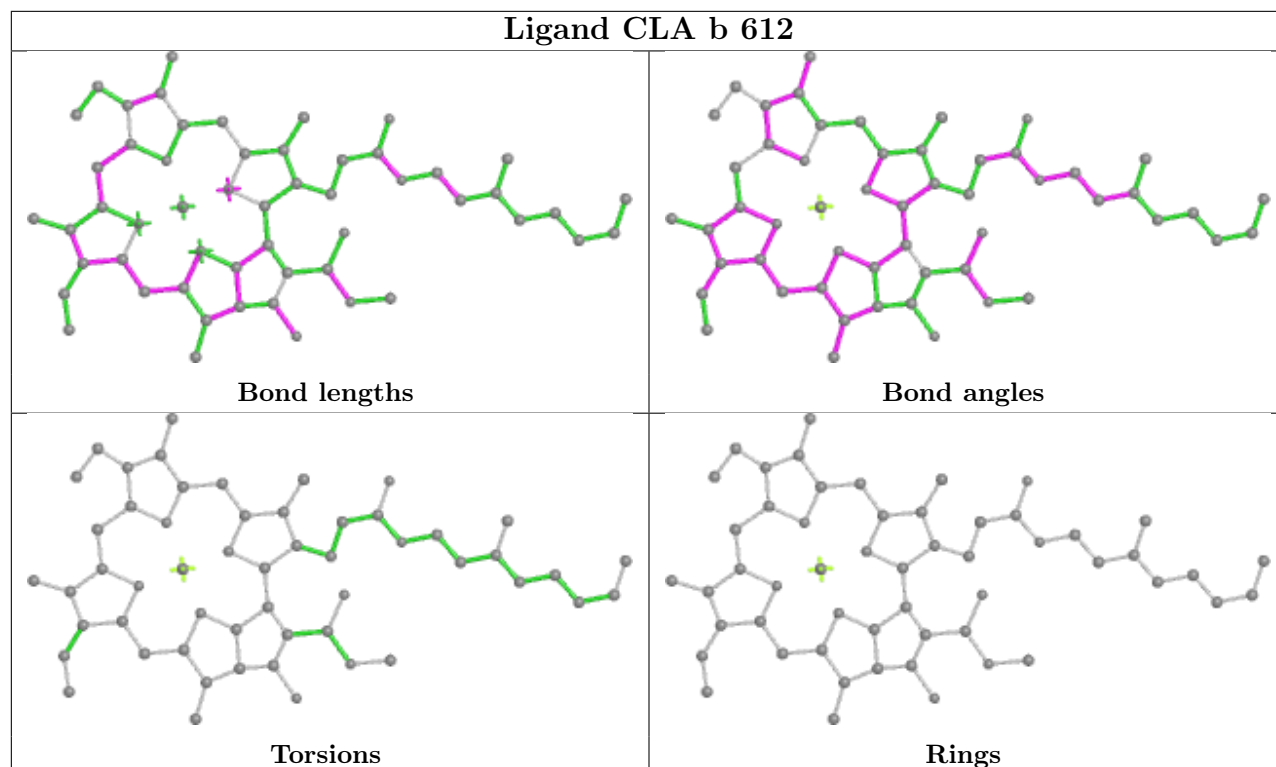
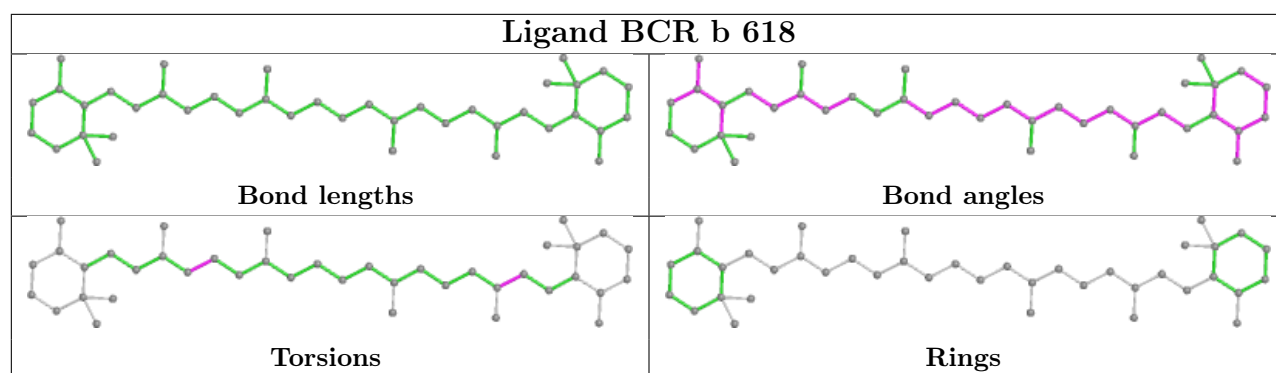


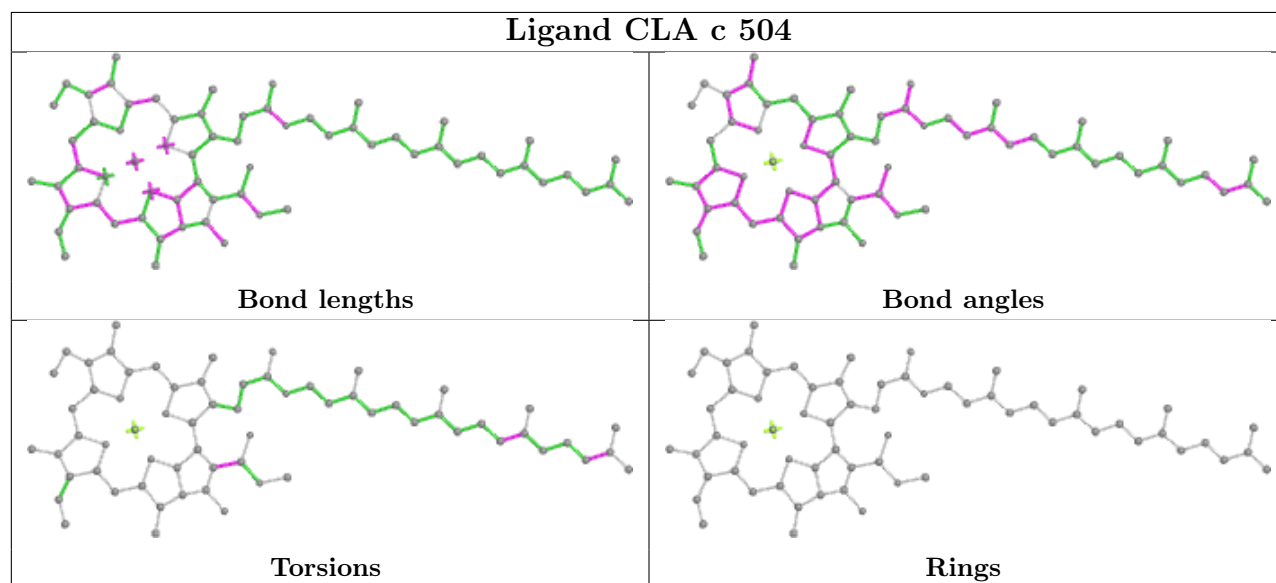
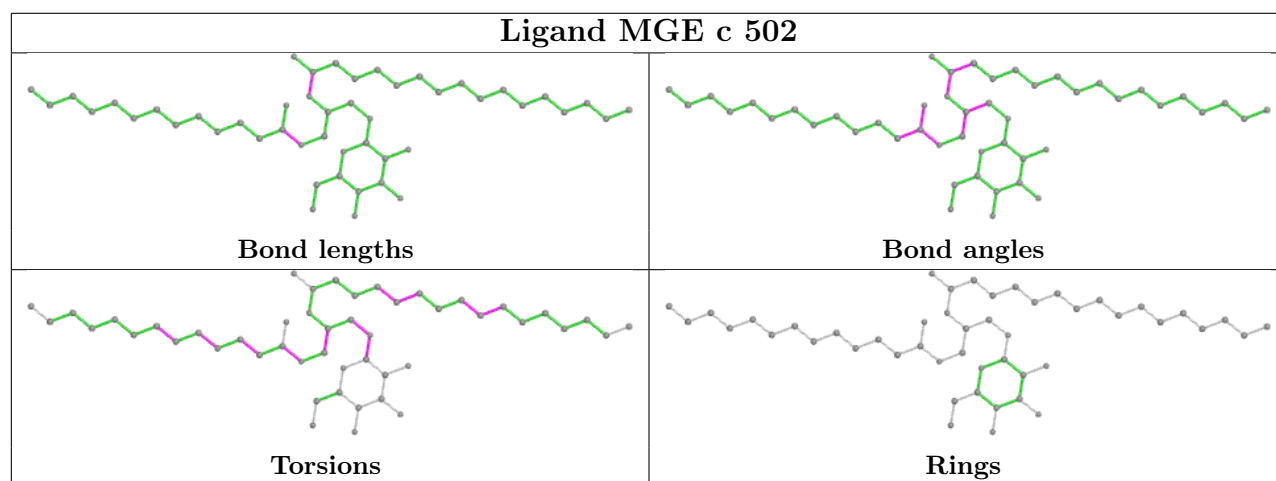
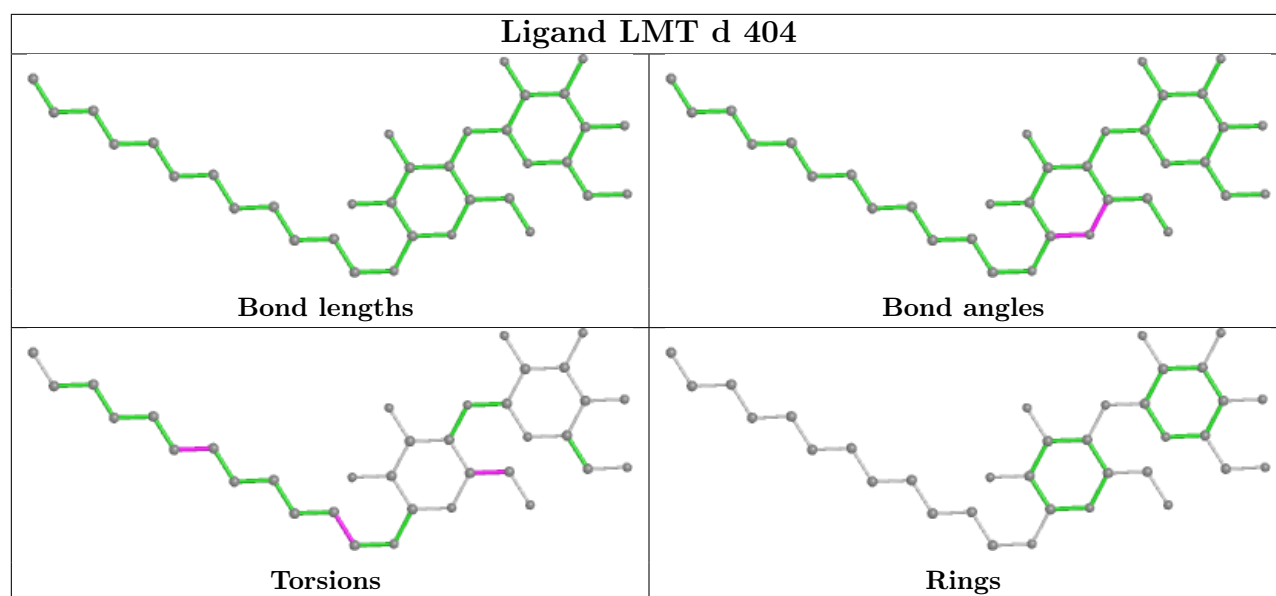
Ligand LMT m 101



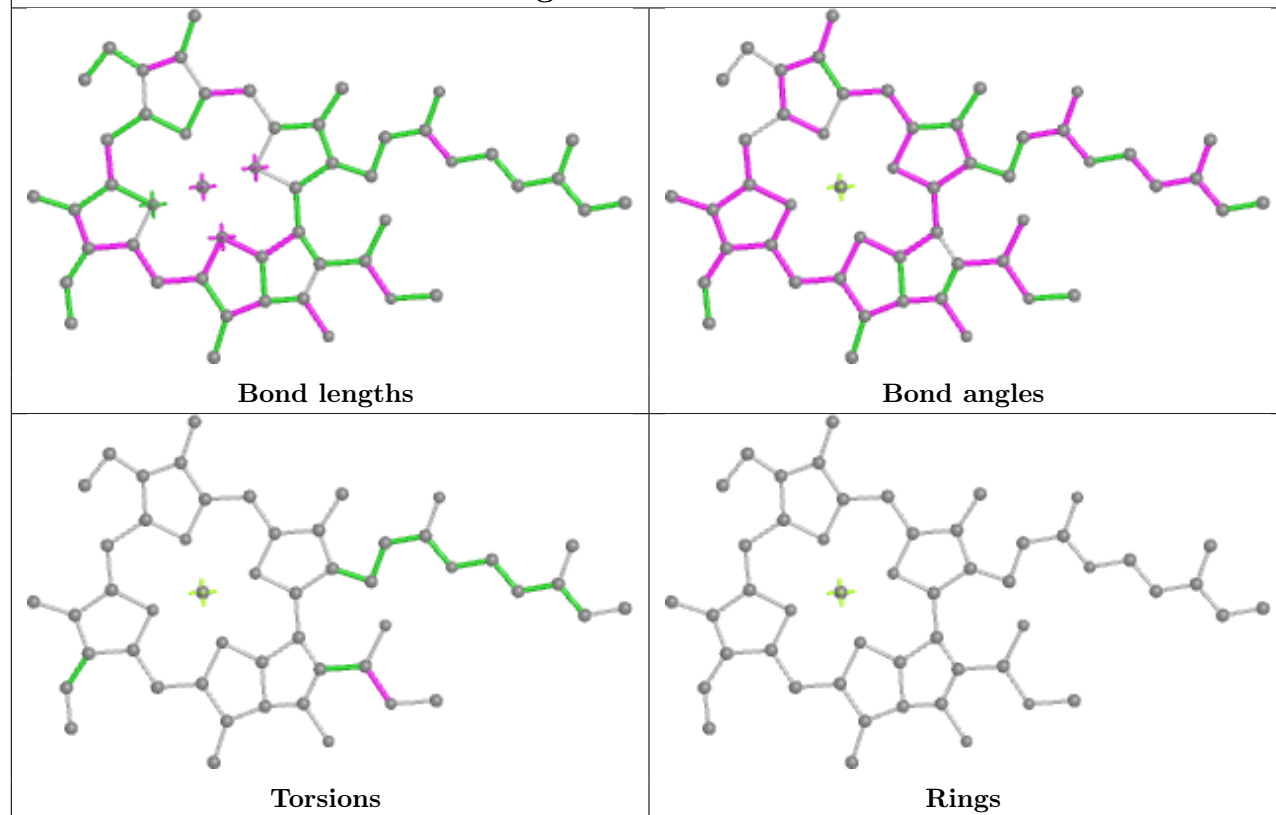
Ligand PHO d 403



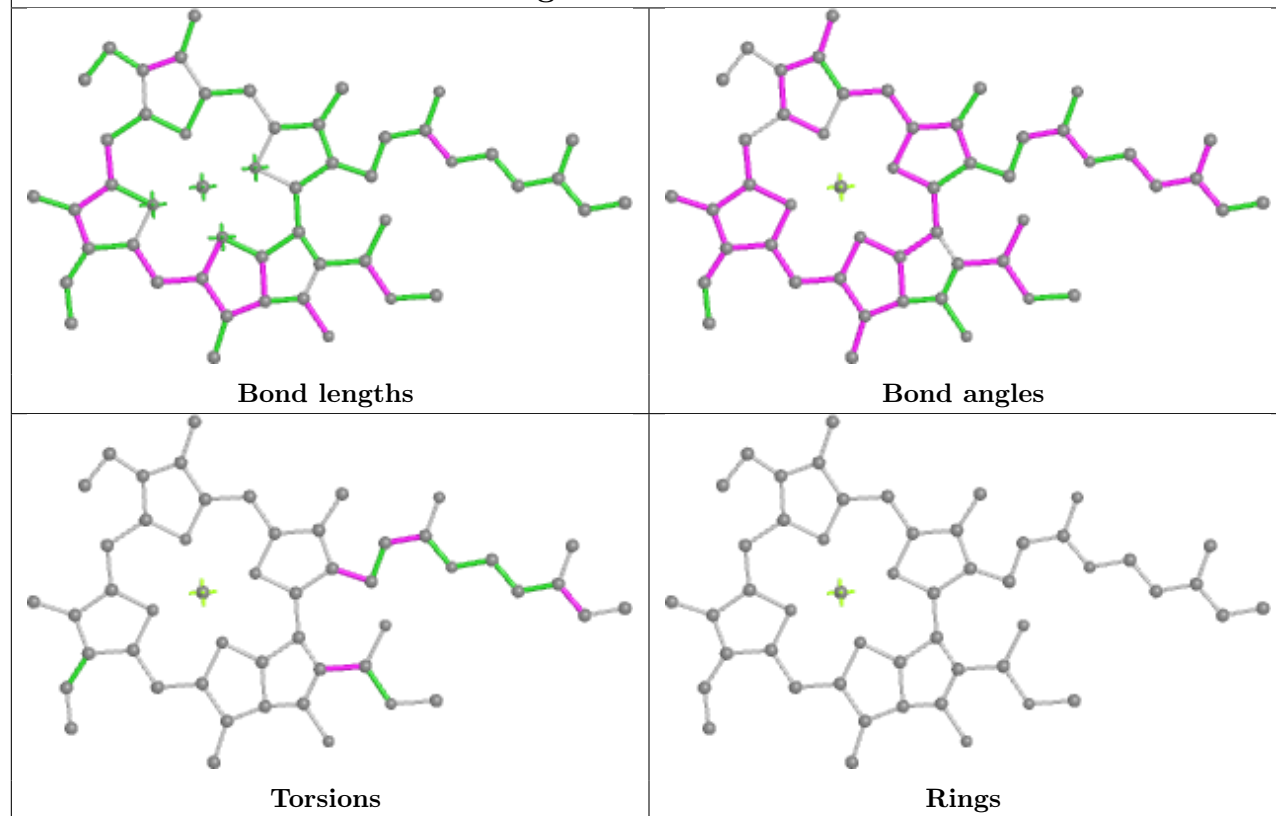


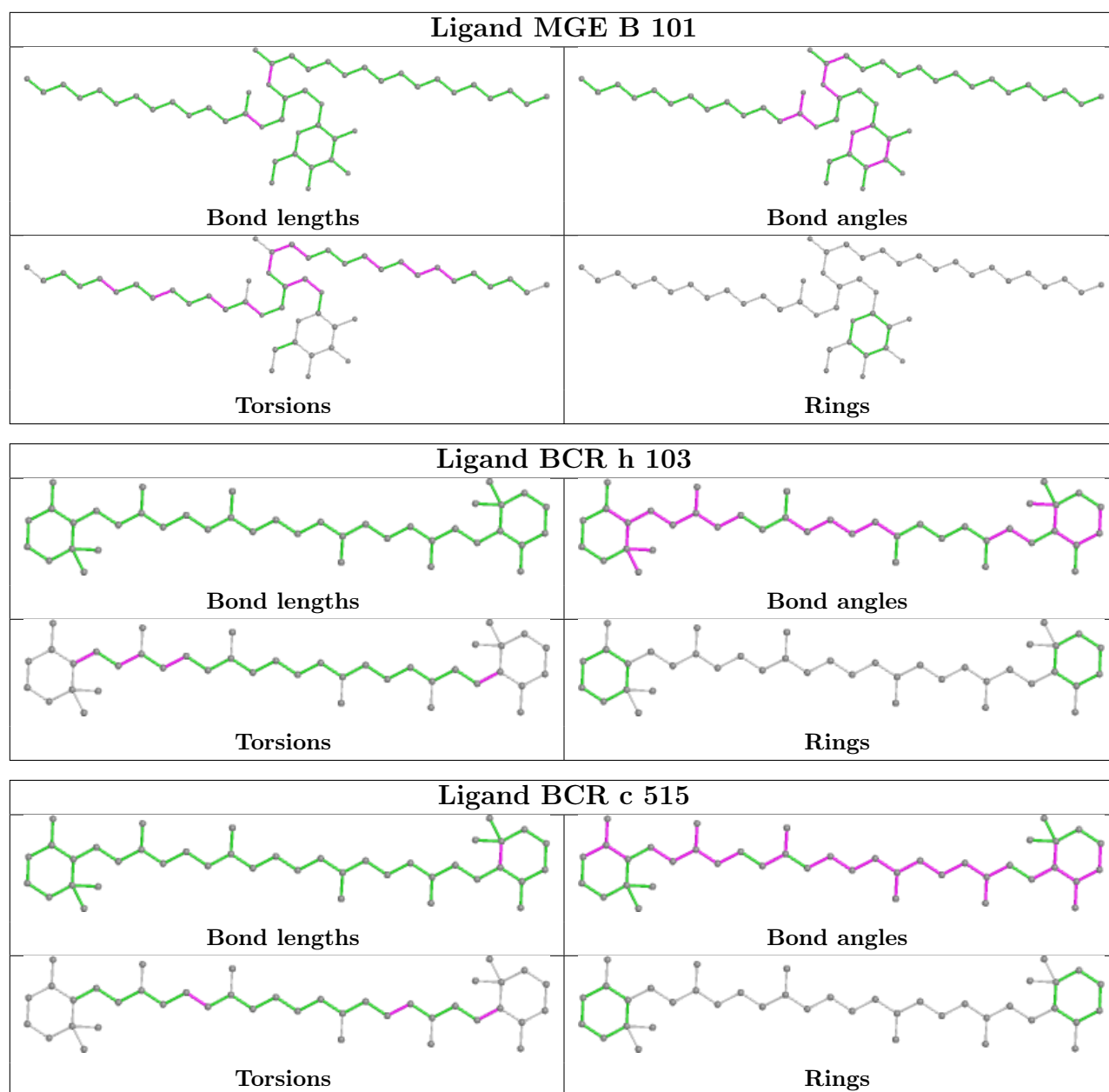


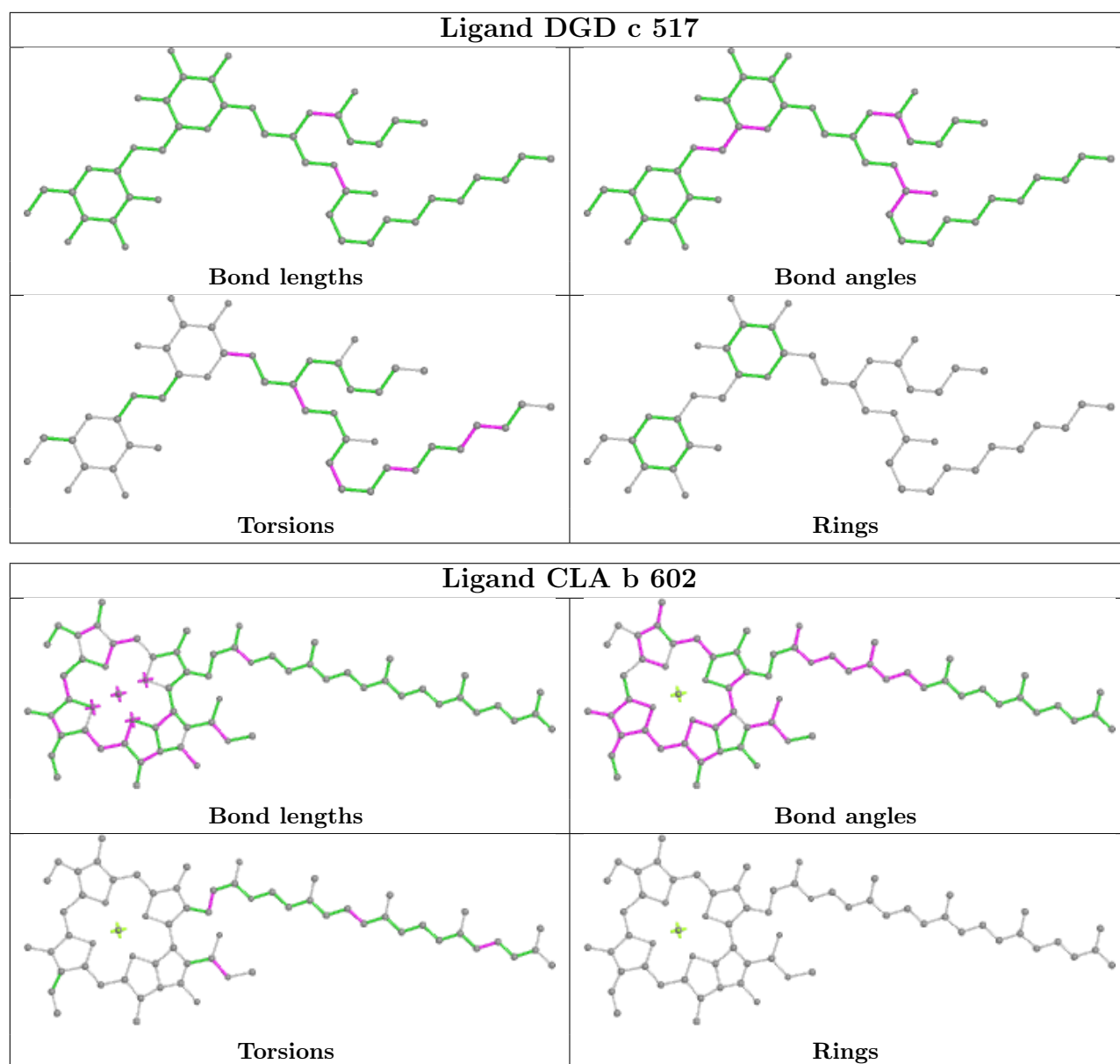
Ligand CLA a 403



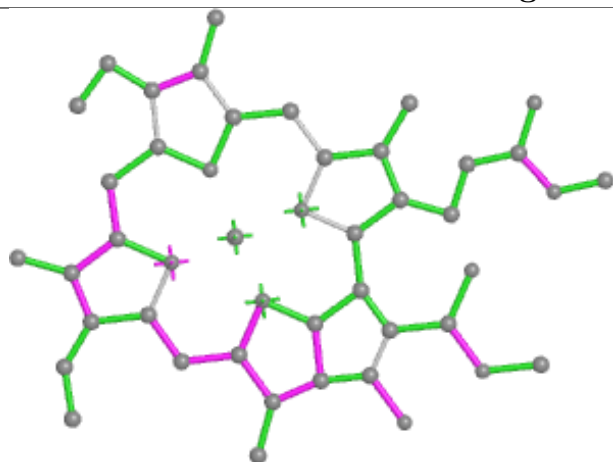
Ligand CLA c 512



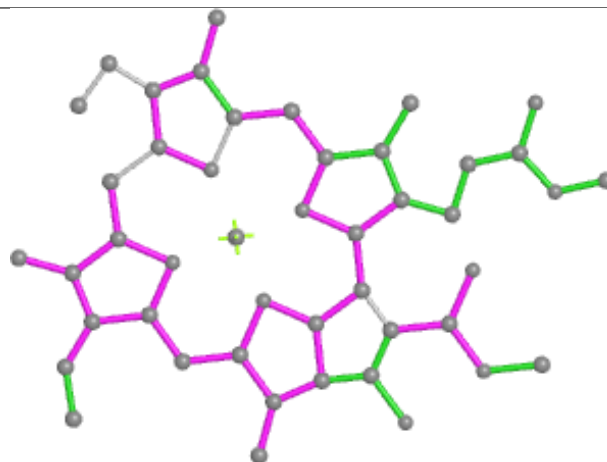




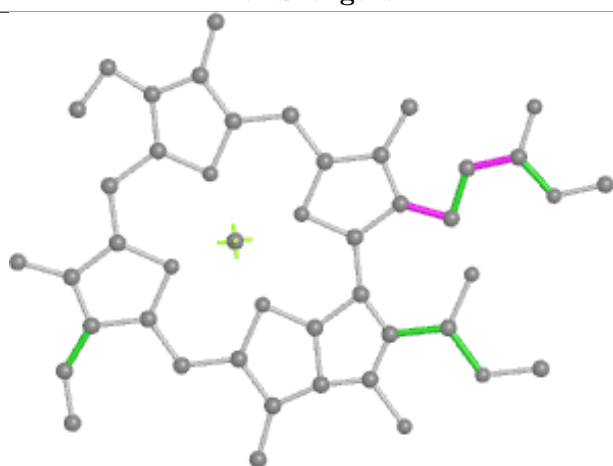
Ligand CLA c 506



Bond lengths



Bond angles

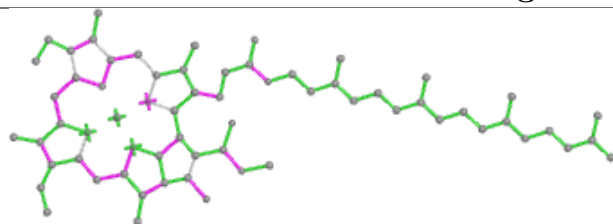


Torsions

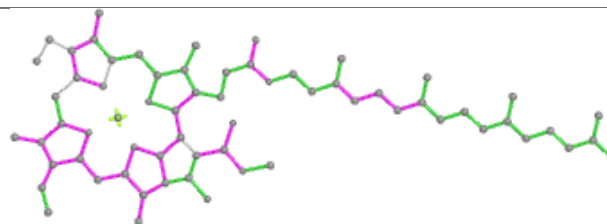


Rings

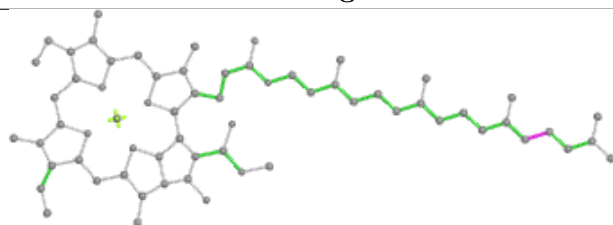
Ligand CLA b 607



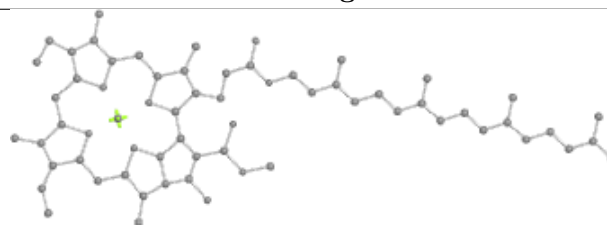
Bond lengths



Bond angles

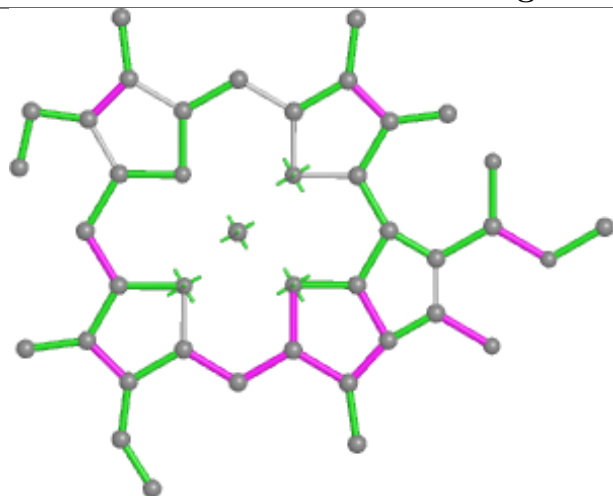


Torsions

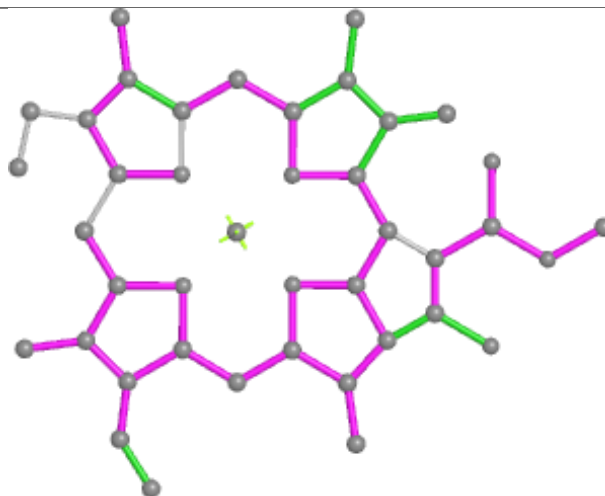


Rings

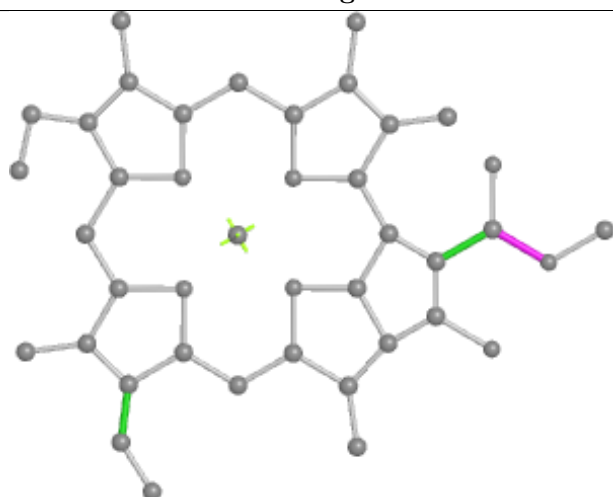
Ligand CLA h 101



Bond lengths



Bond angles

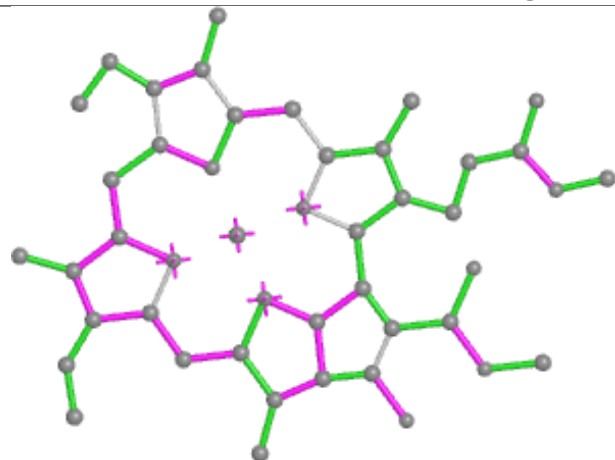


Torsions

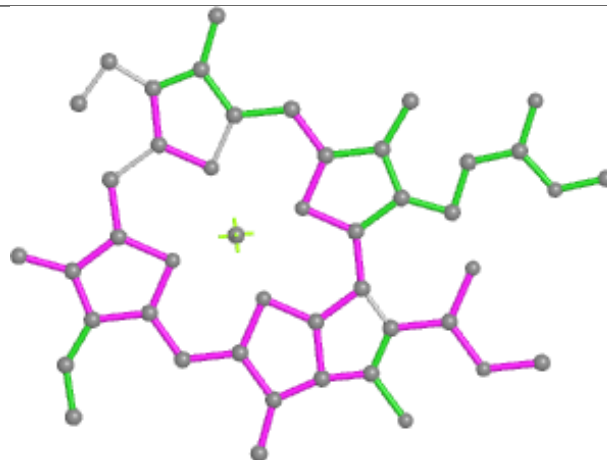


Rings

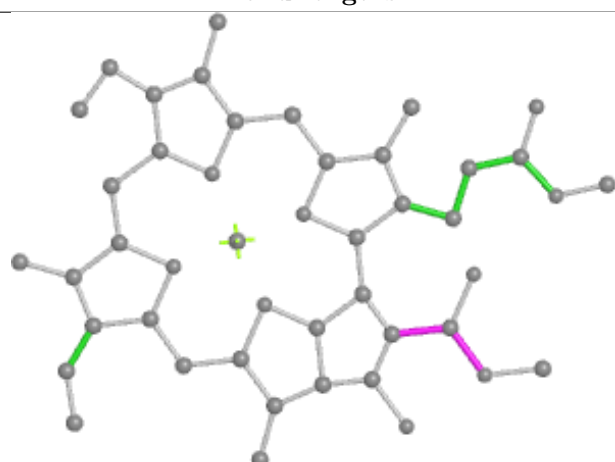
Ligand CLA c 510



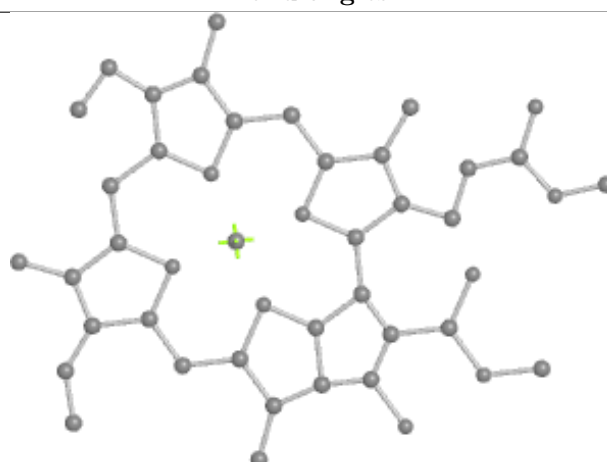
Bond lengths



Bond angles

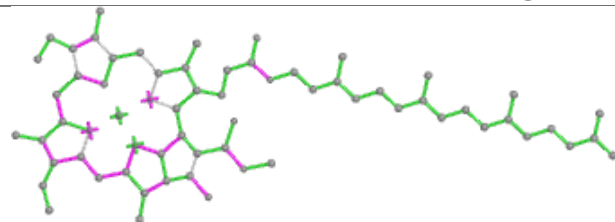


Torsions

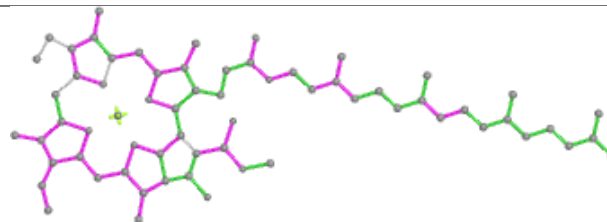


Rings

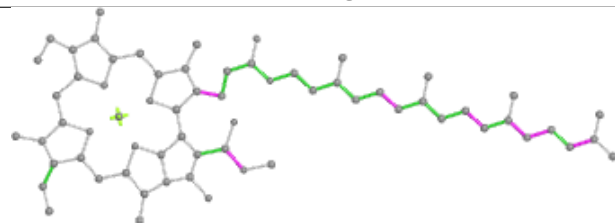
Ligand CLA b 614



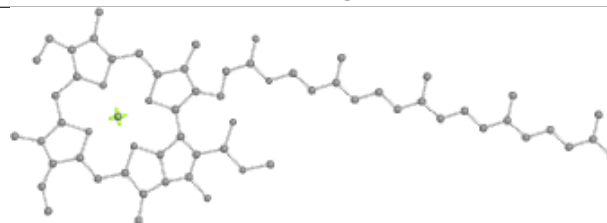
Bond lengths



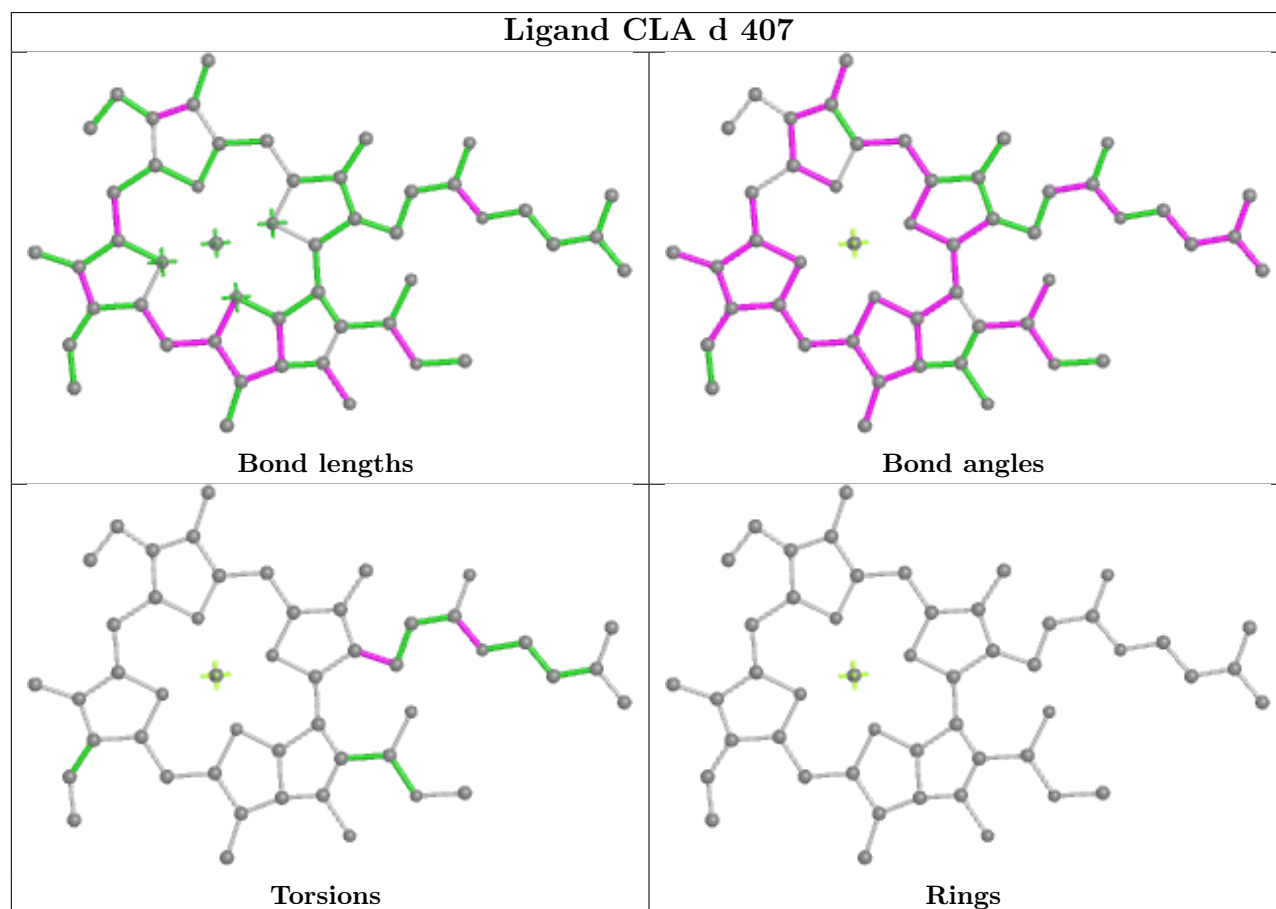
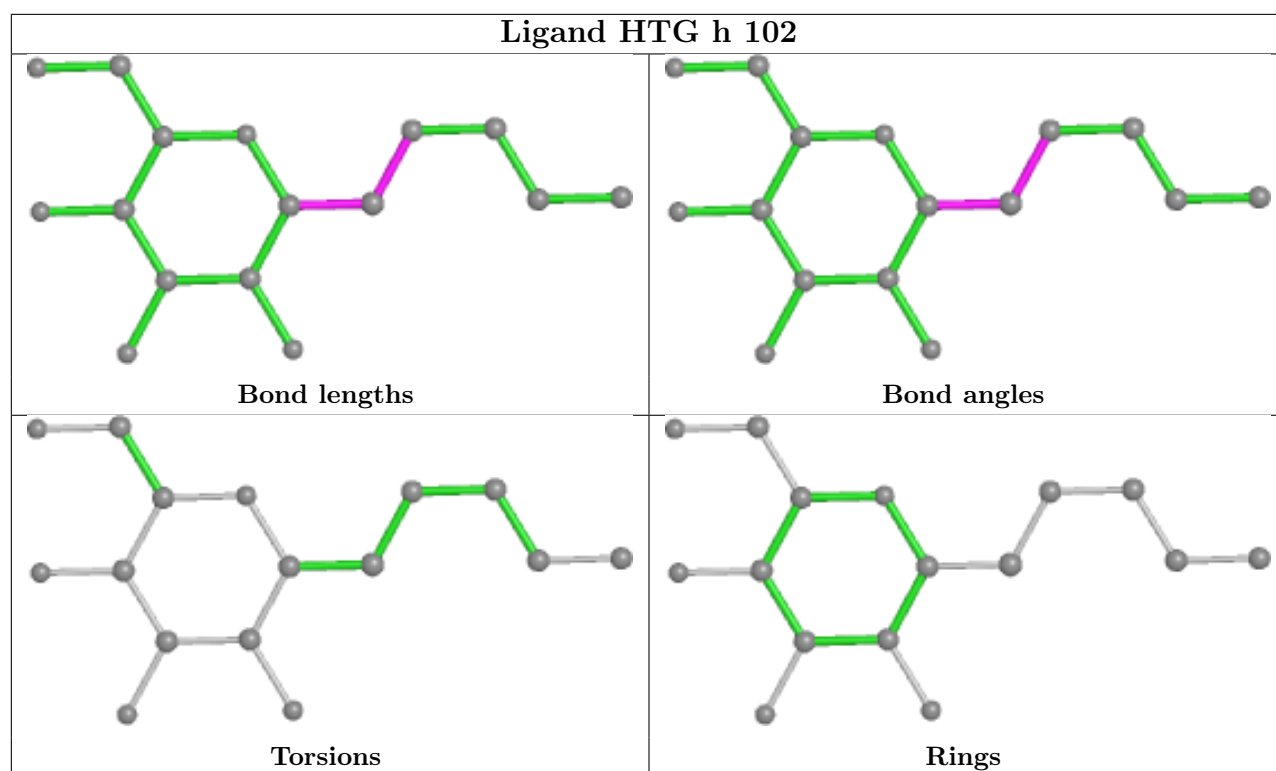
Bond angles



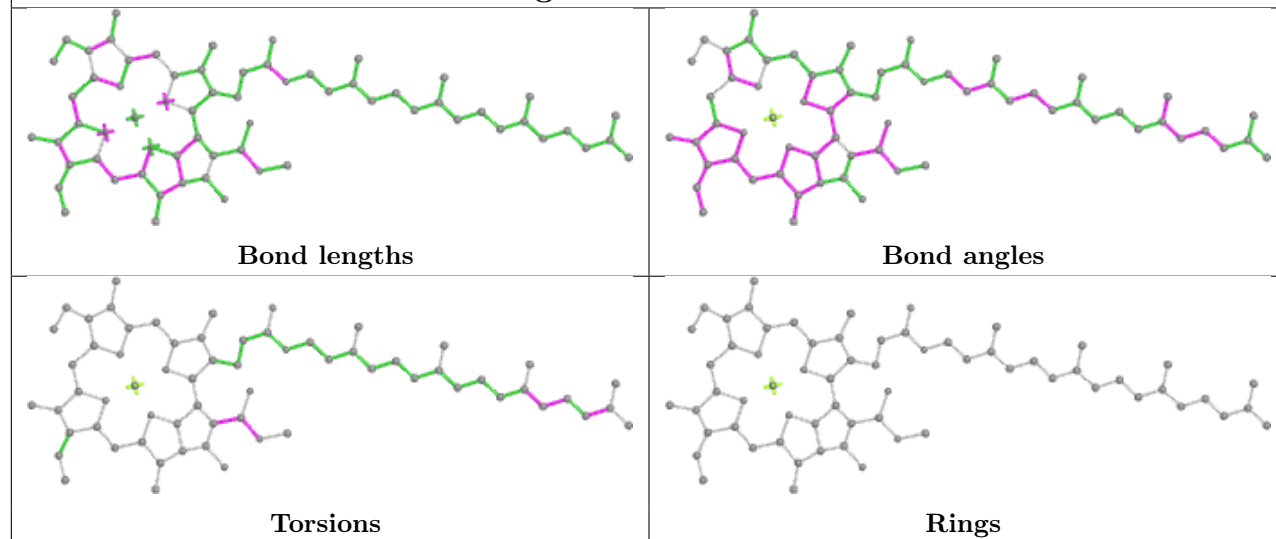
Torsions



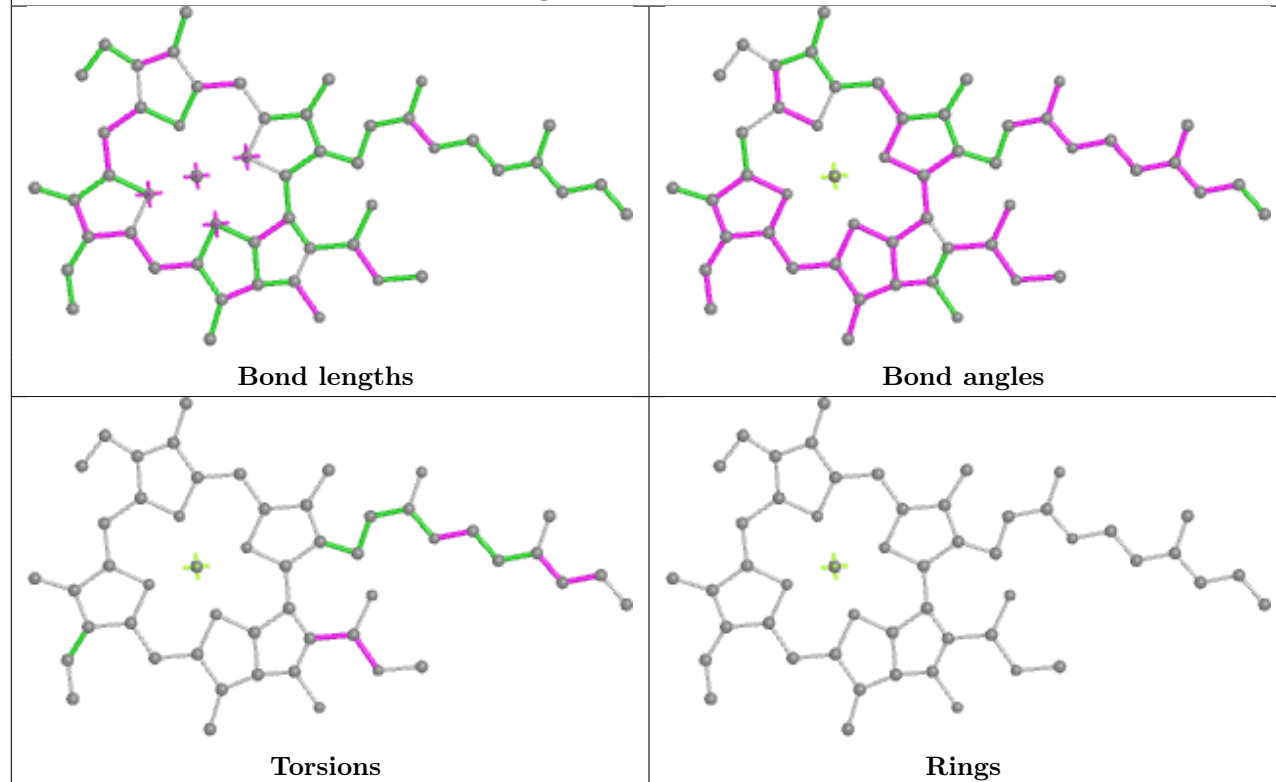
Rings

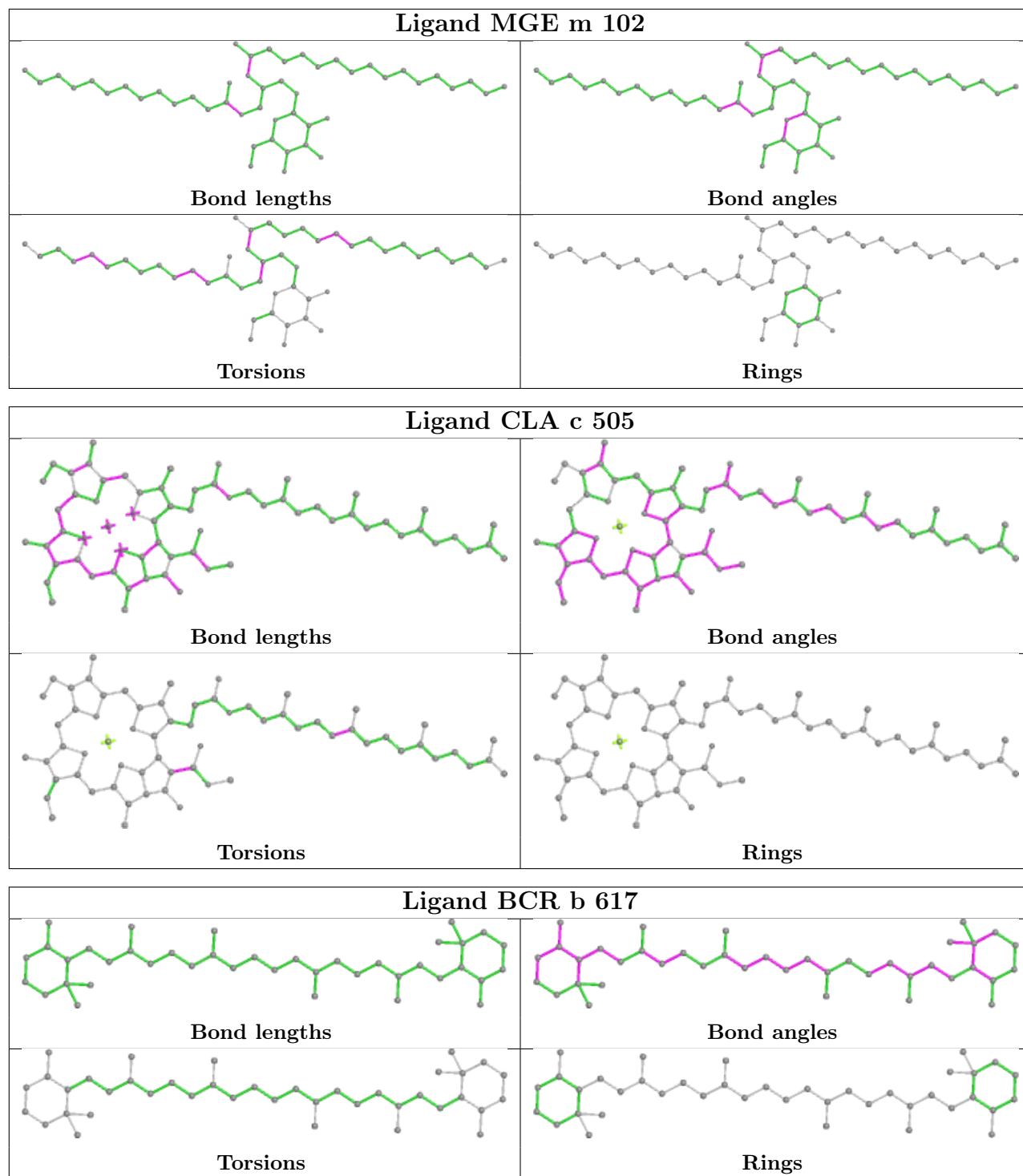


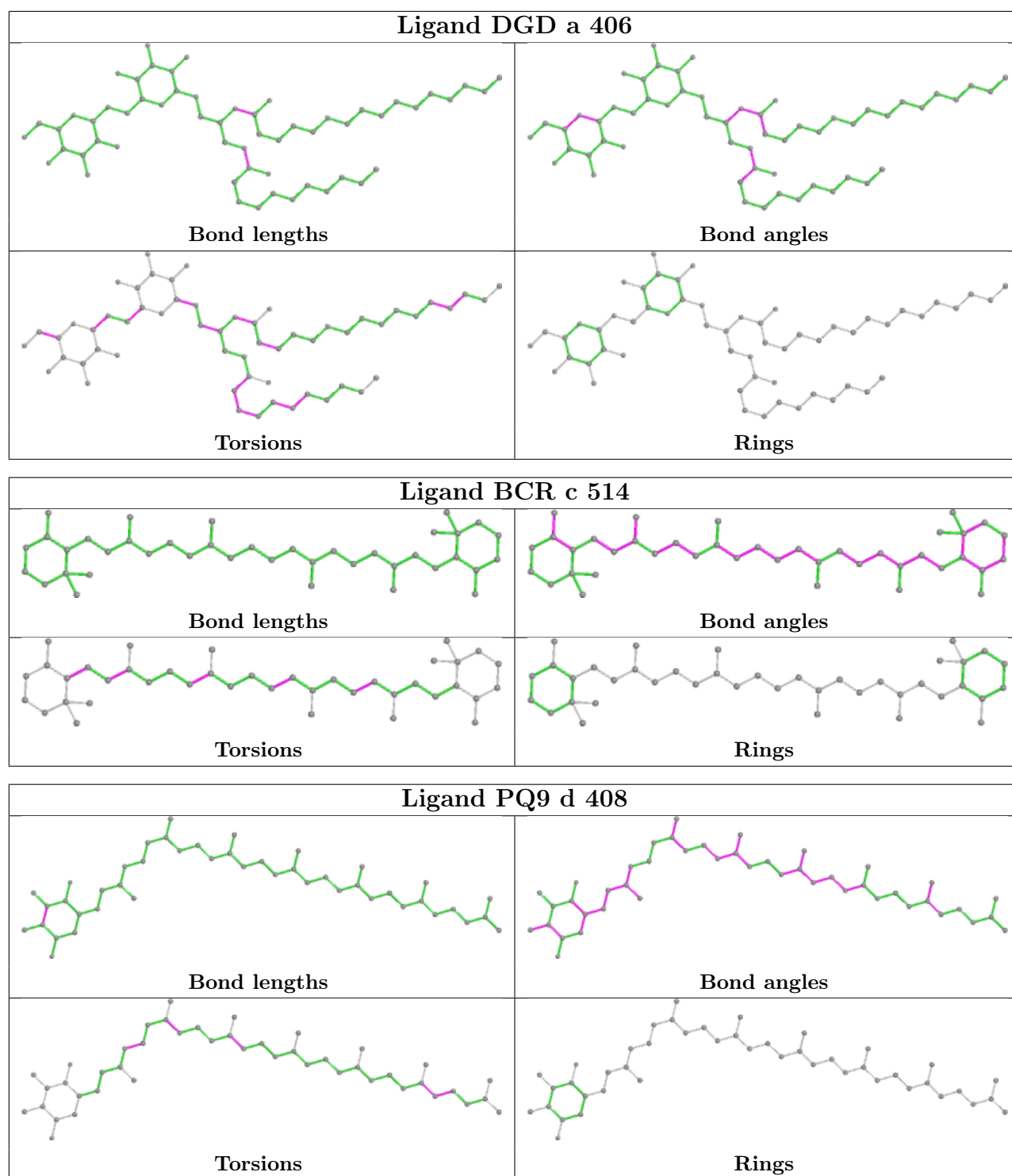
Ligand CLA b 610



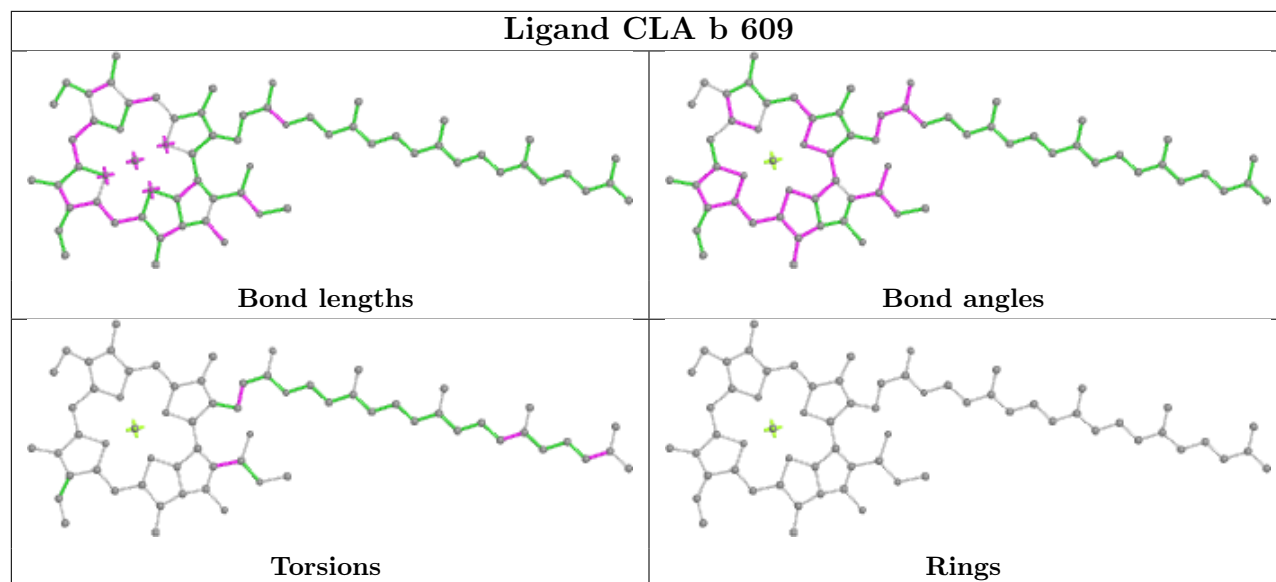
Ligand CLA b 613



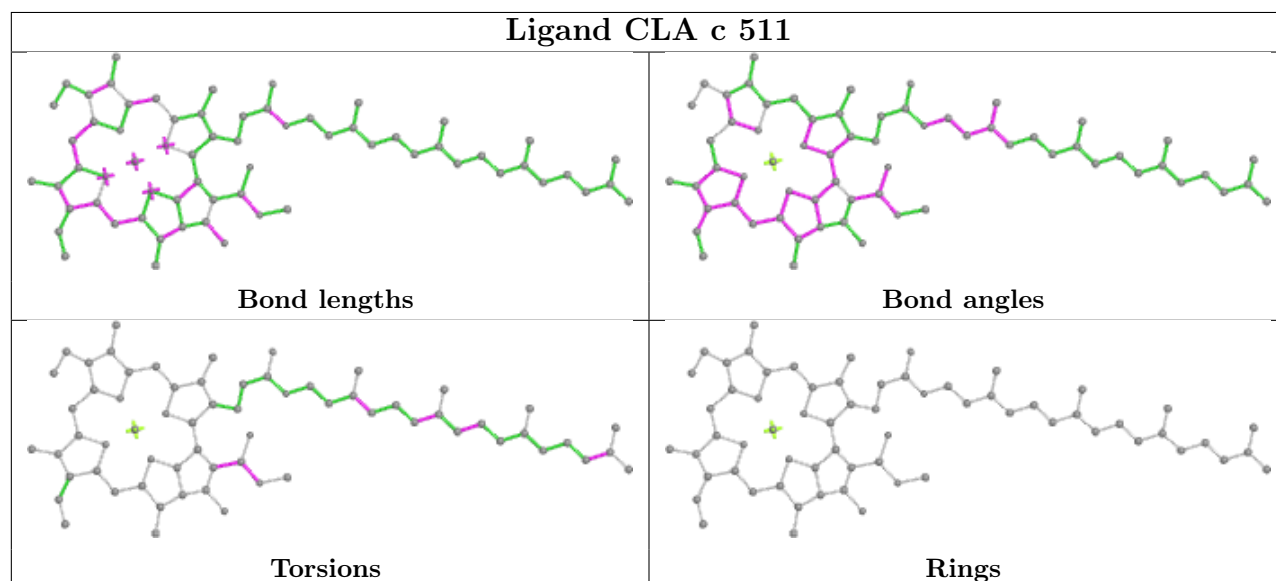




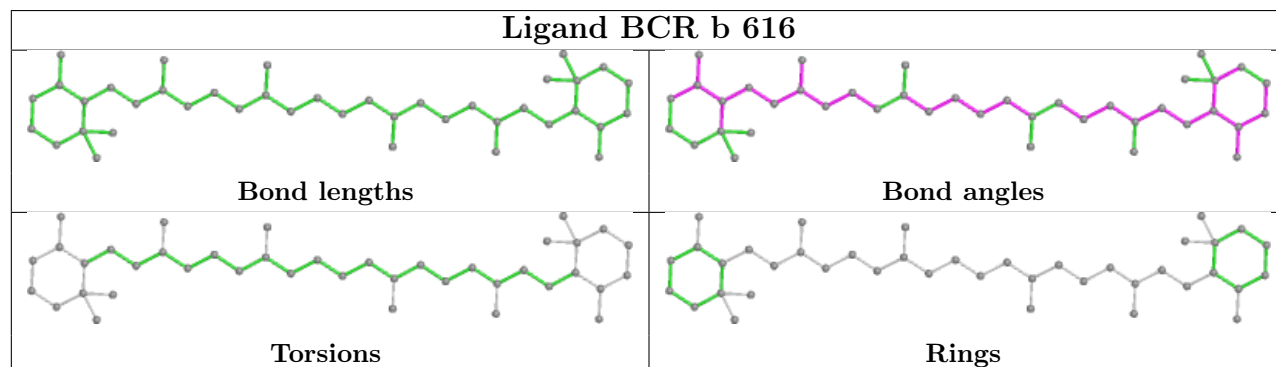
Ligand CLA b 609

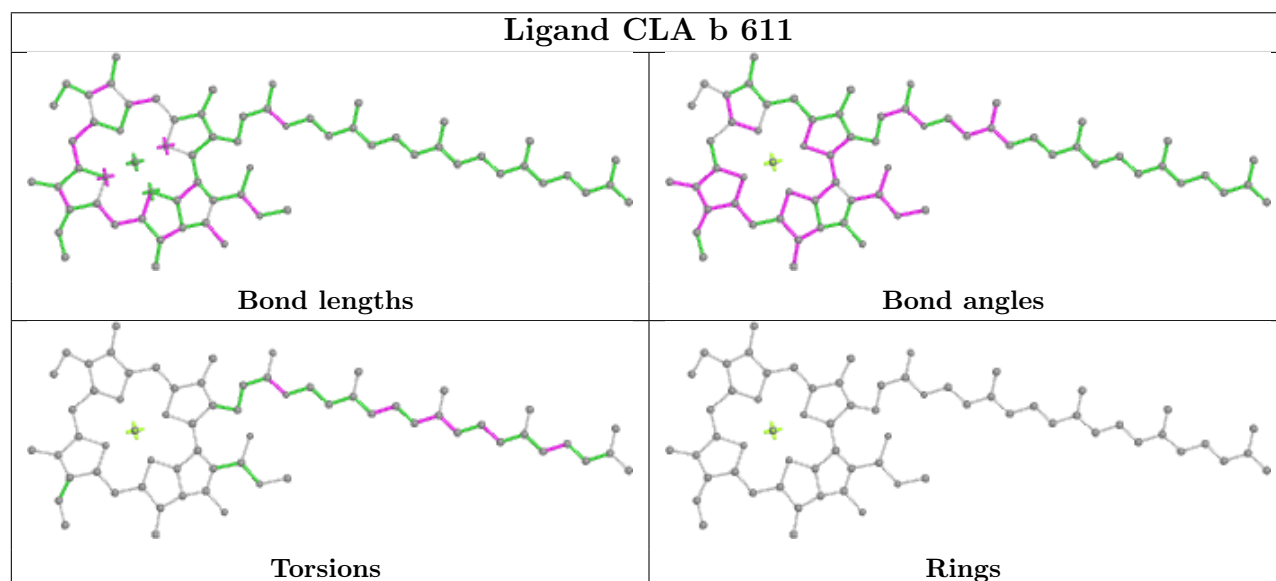
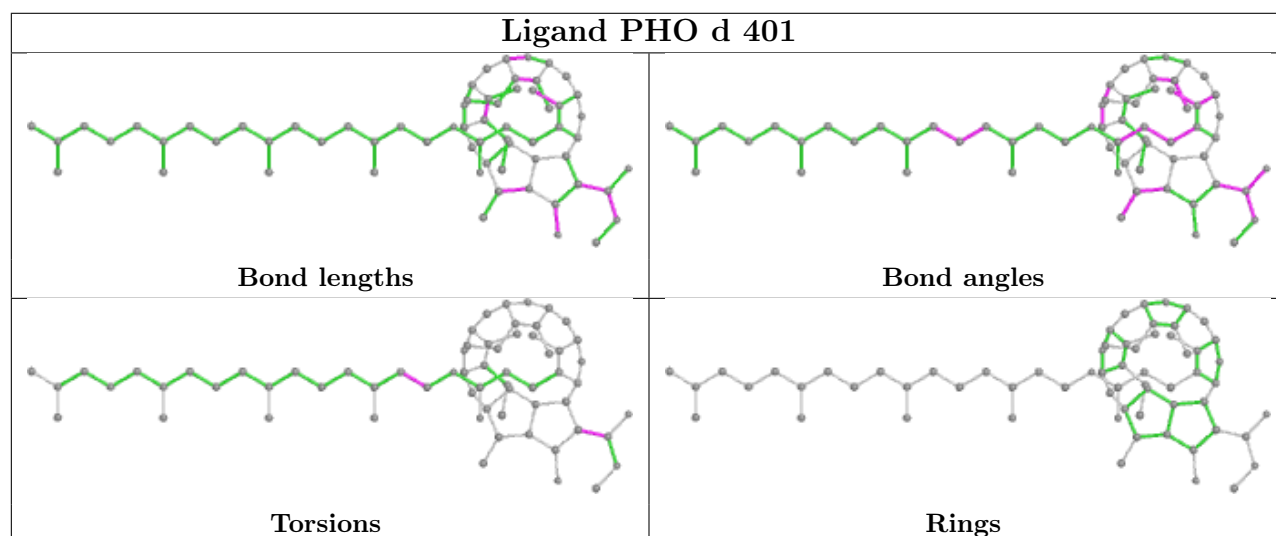
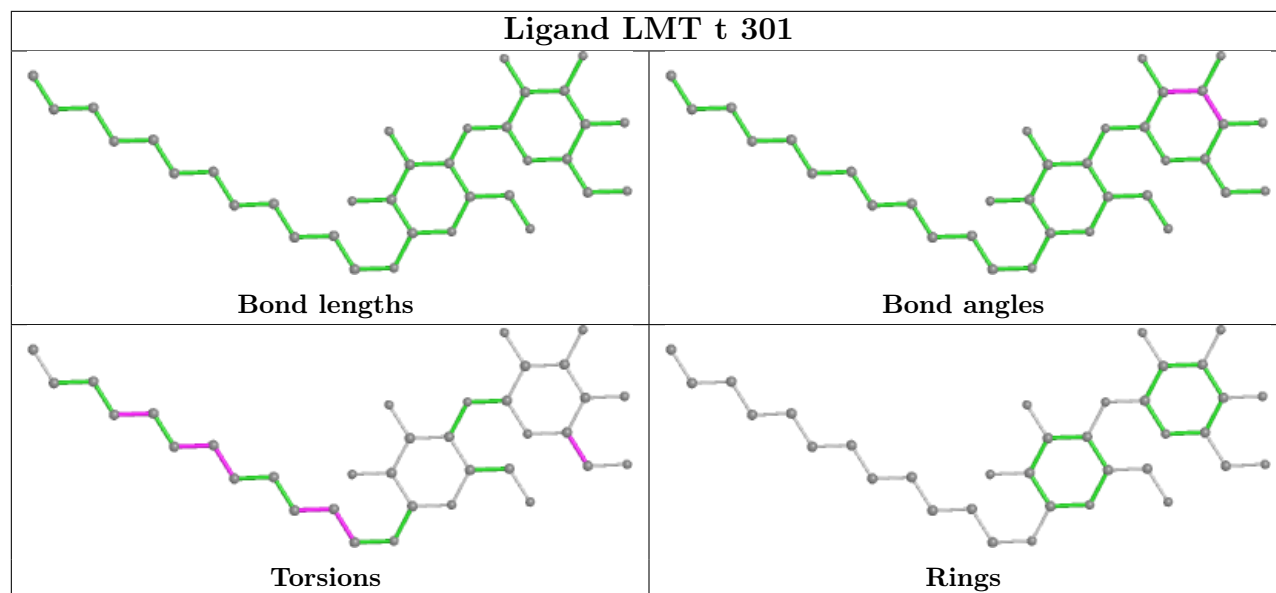


Ligand CLA c 511

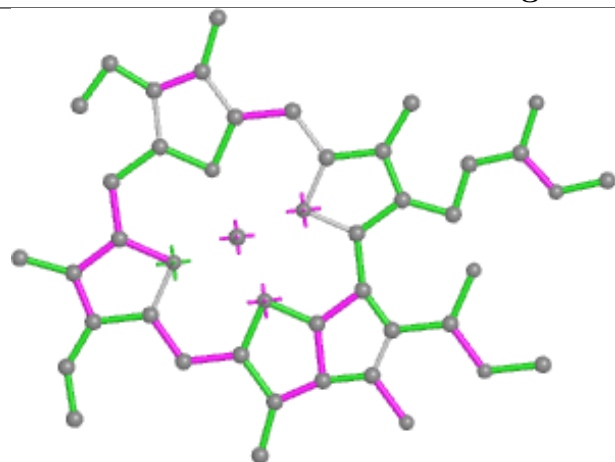


Ligand BCR b 616

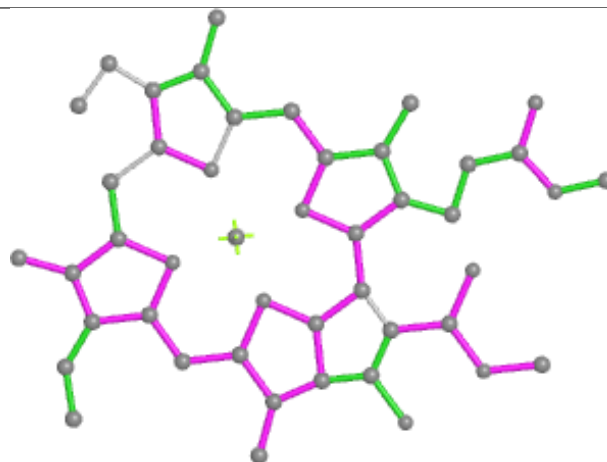




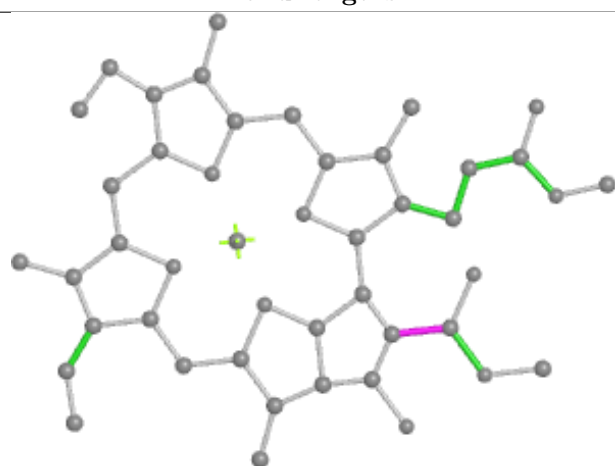
Ligand CLA c 508



Bond lengths



Bond angles

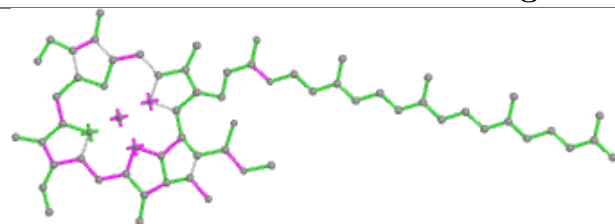


Torsions

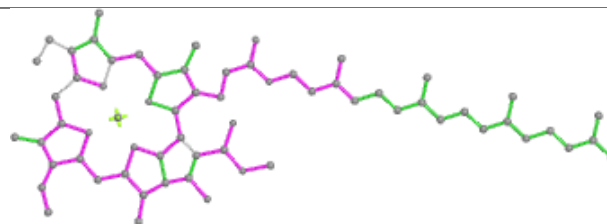


Rings

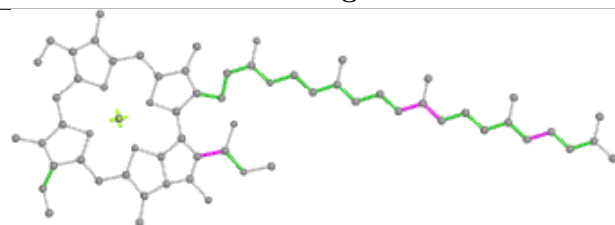
Ligand CLA a 407



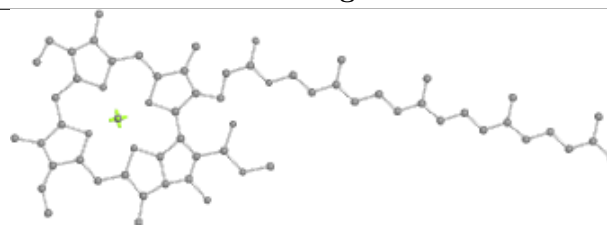
Bond lengths



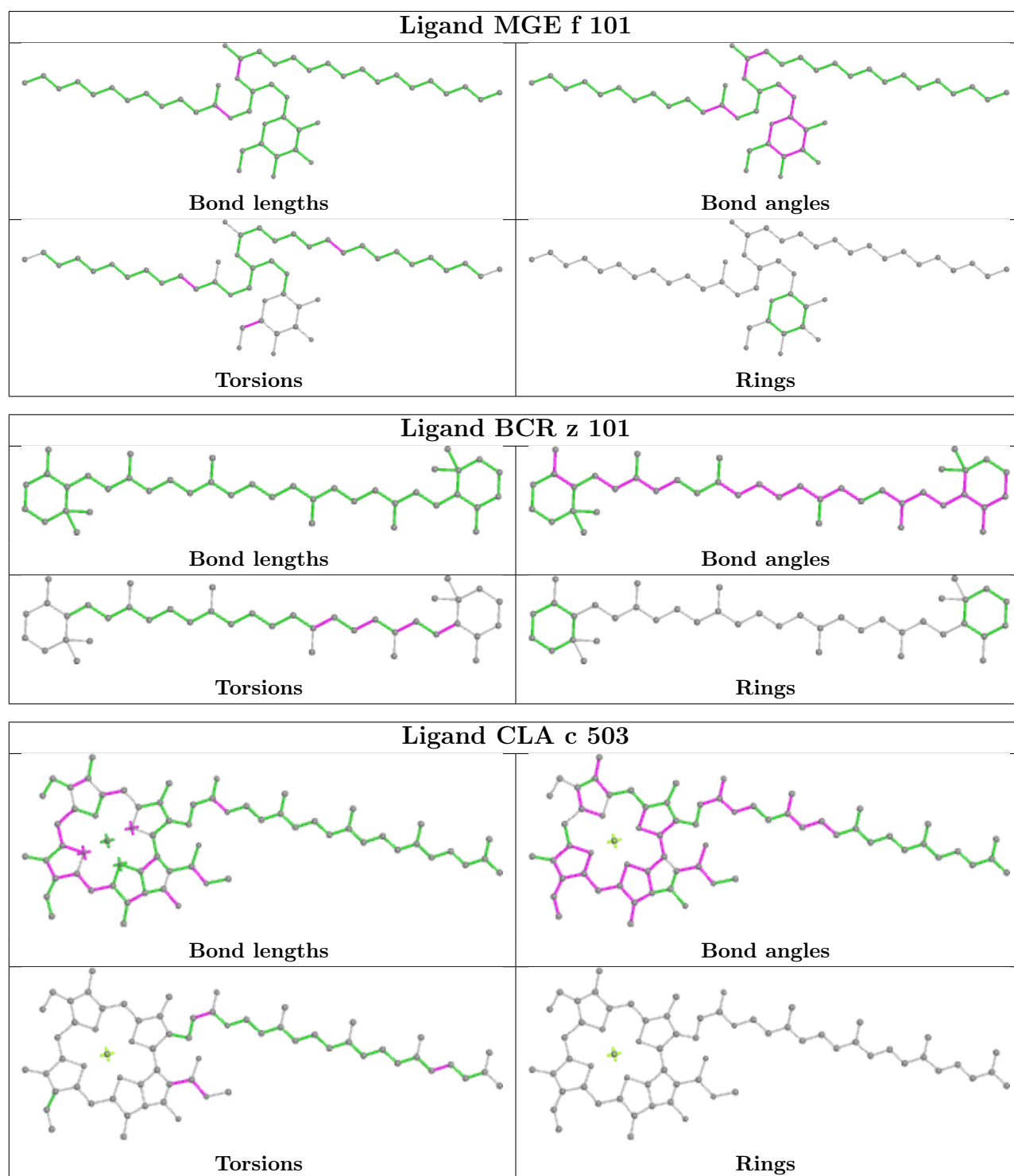
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

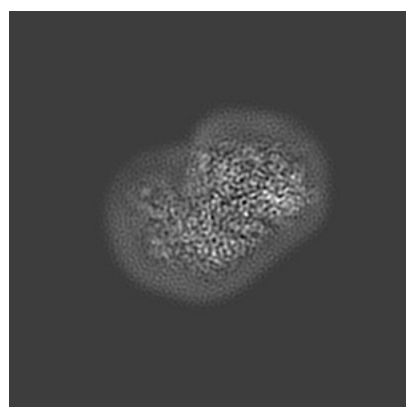
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30909. These allow visual inspection of the internal detail of the map and identification of artifacts.

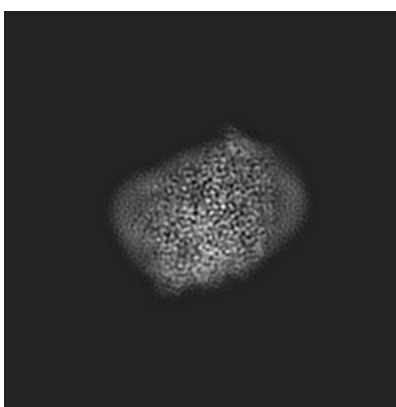
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

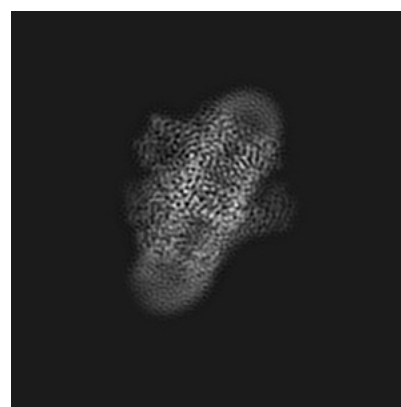
6.1.1 Primary map



X



Y

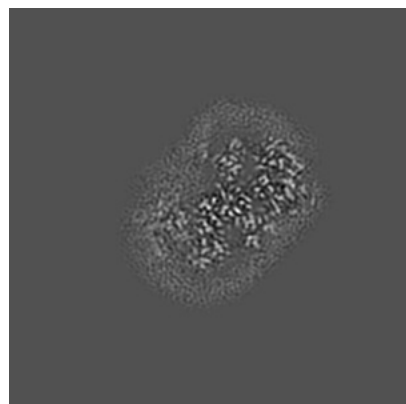


Z

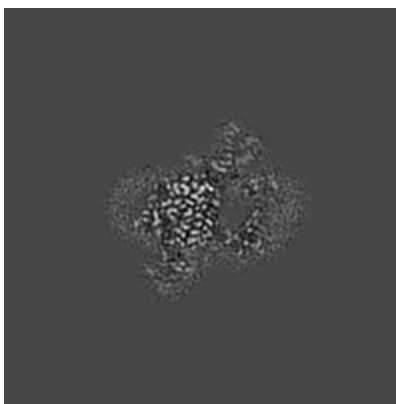
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

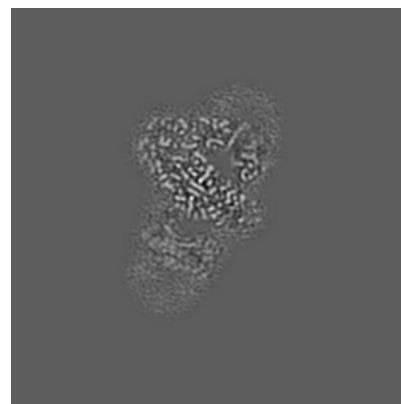
6.2.1 Primary map



X Index: 100



Y Index: 100

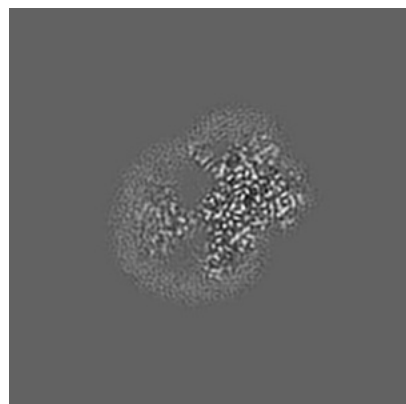


Z Index: 100

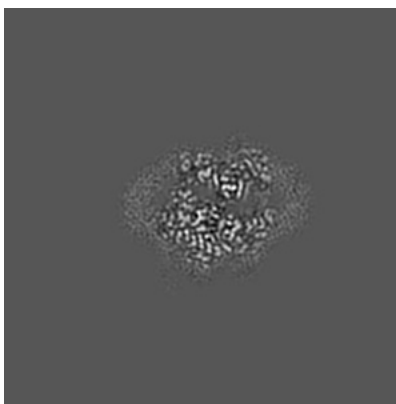
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

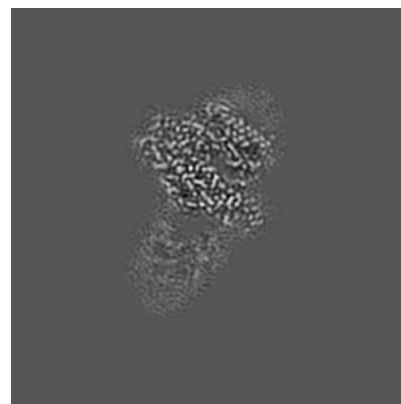
6.3.1 Primary map



X Index: 91



Y Index: 118

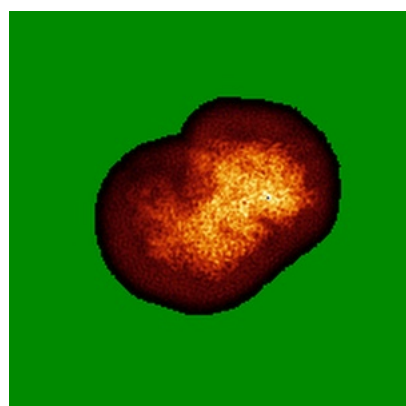


Z Index: 104

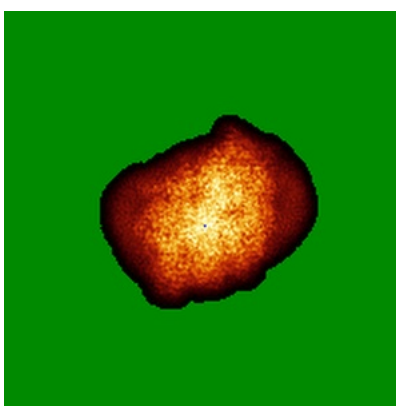
The images above show the largest variance slices of the map in three orthogonal directions.

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

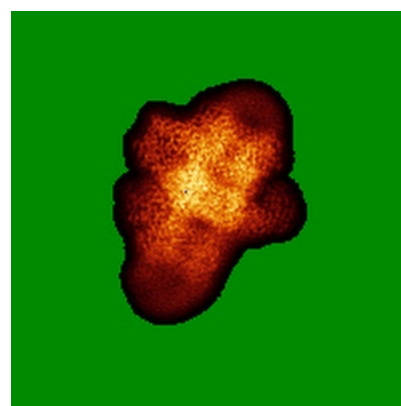
6.4.1 Primary map



X



Y

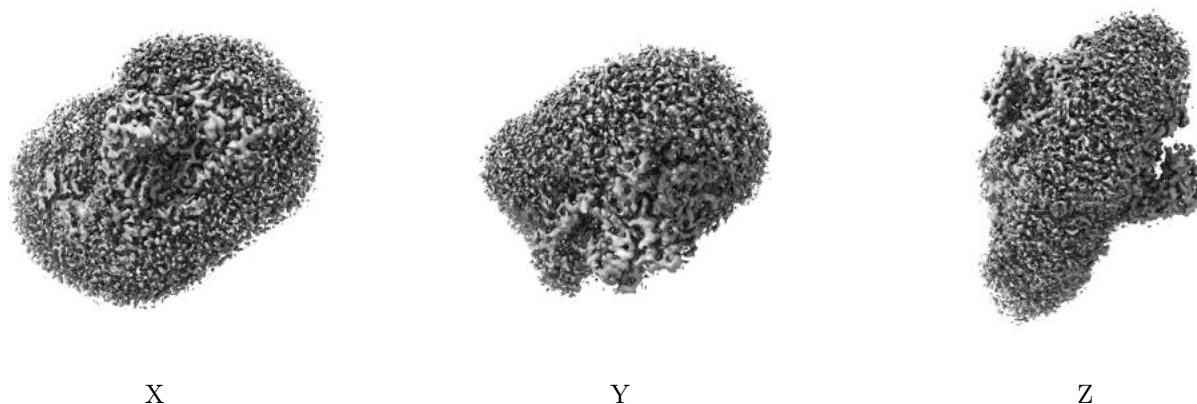


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

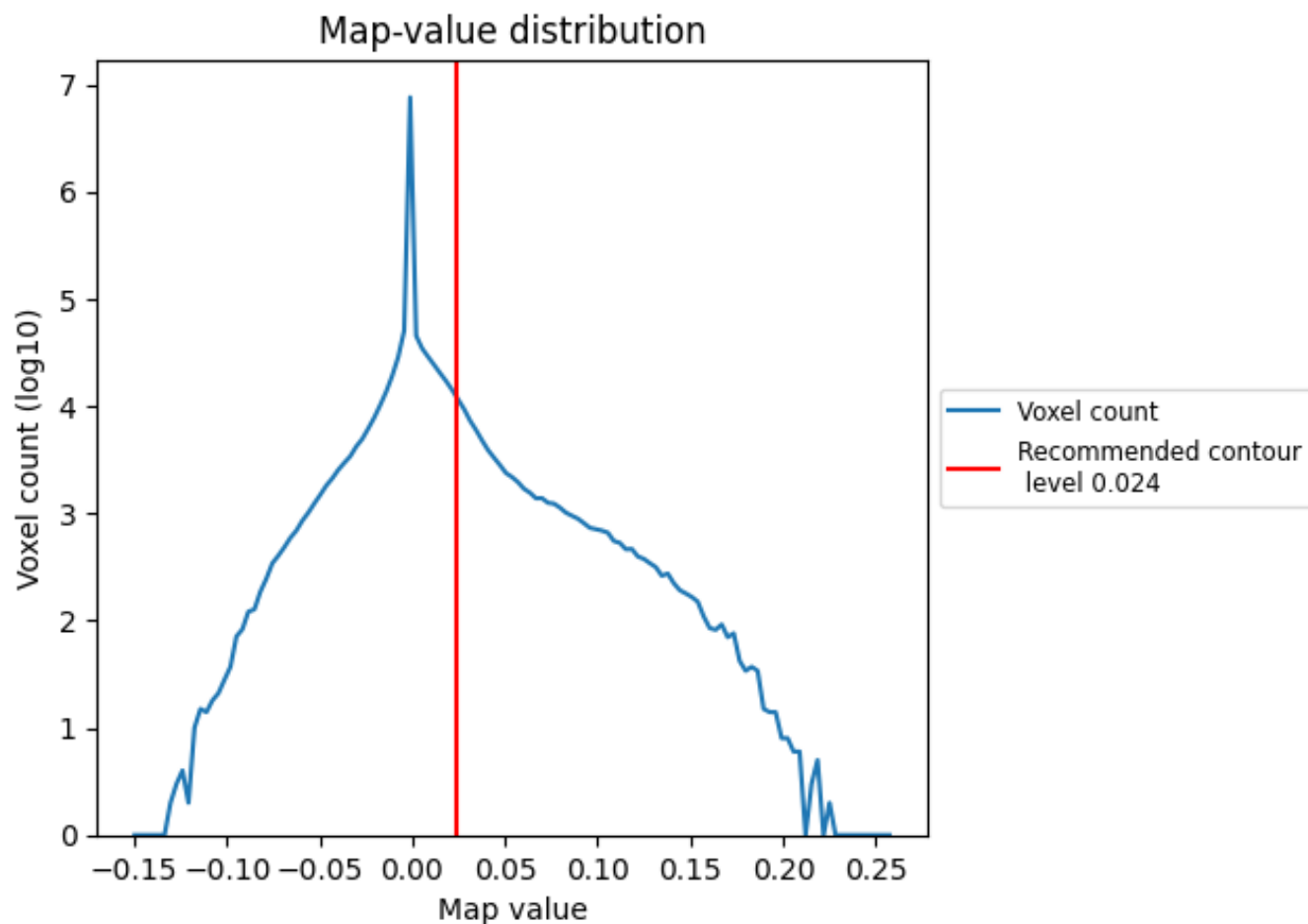
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

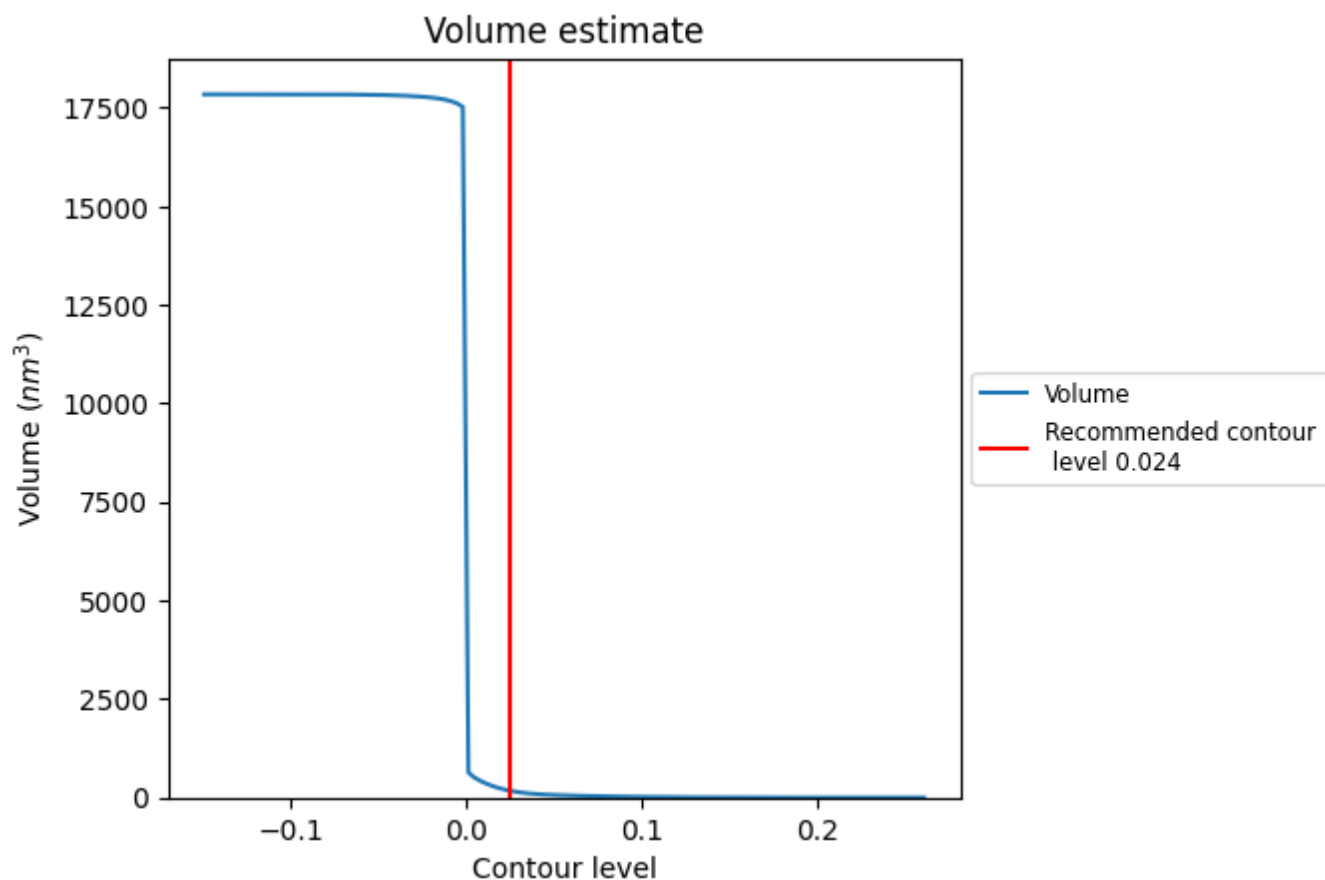
This section contains the results of statistical analysis of the map.

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.

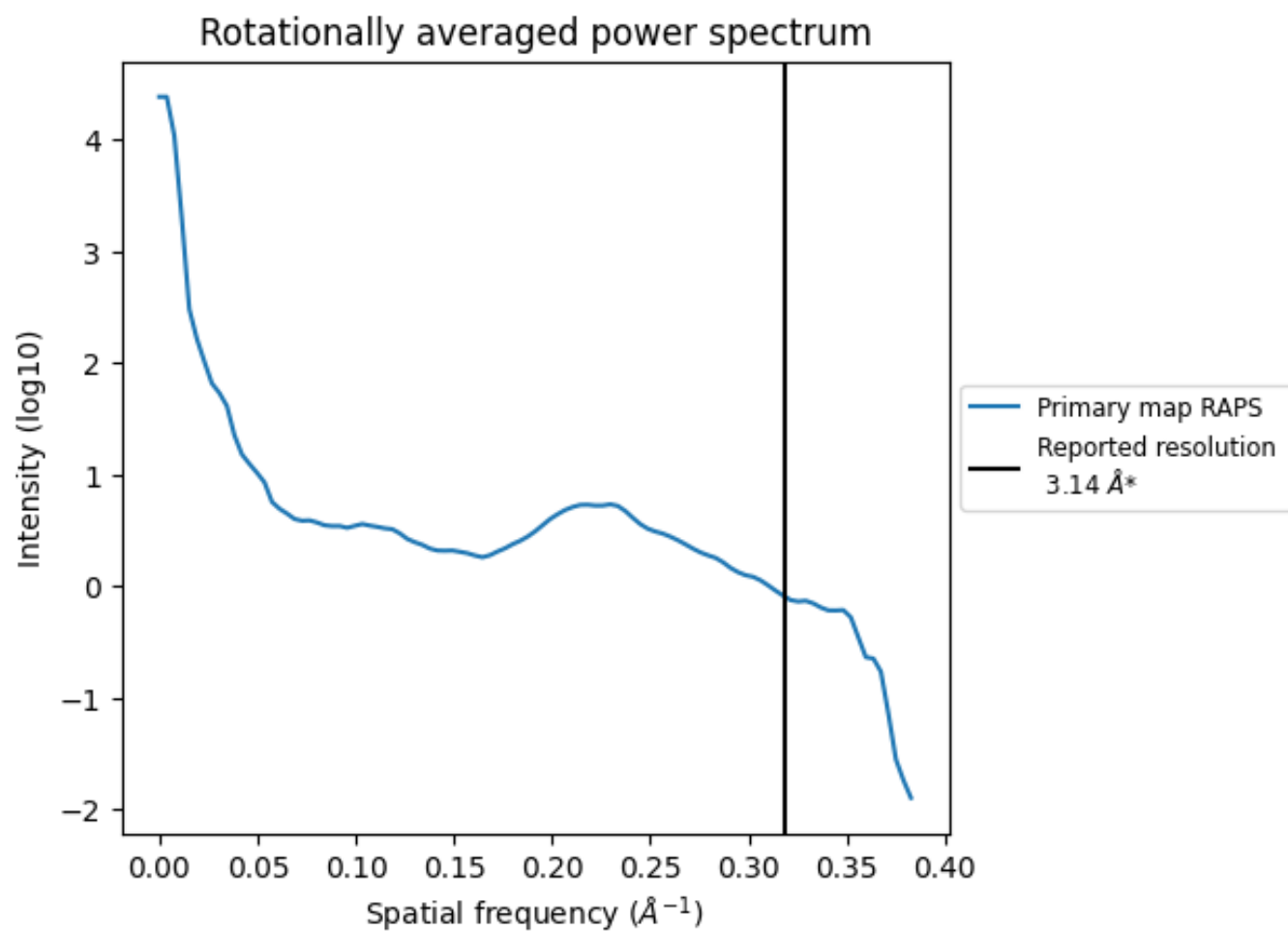
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179 nm^3 ; this corresponds to an approximate mass of 162 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 0.318 Å⁻¹

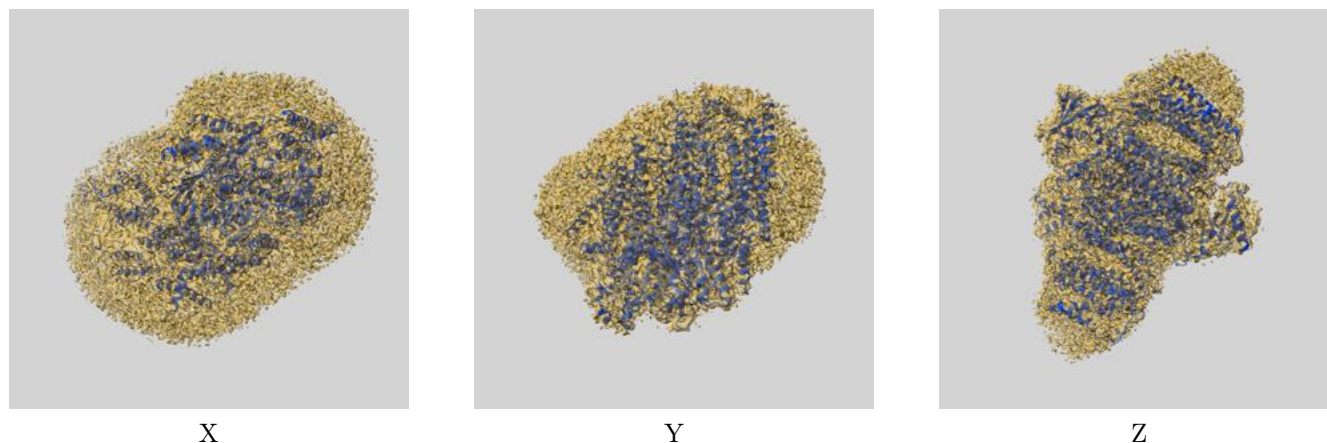
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

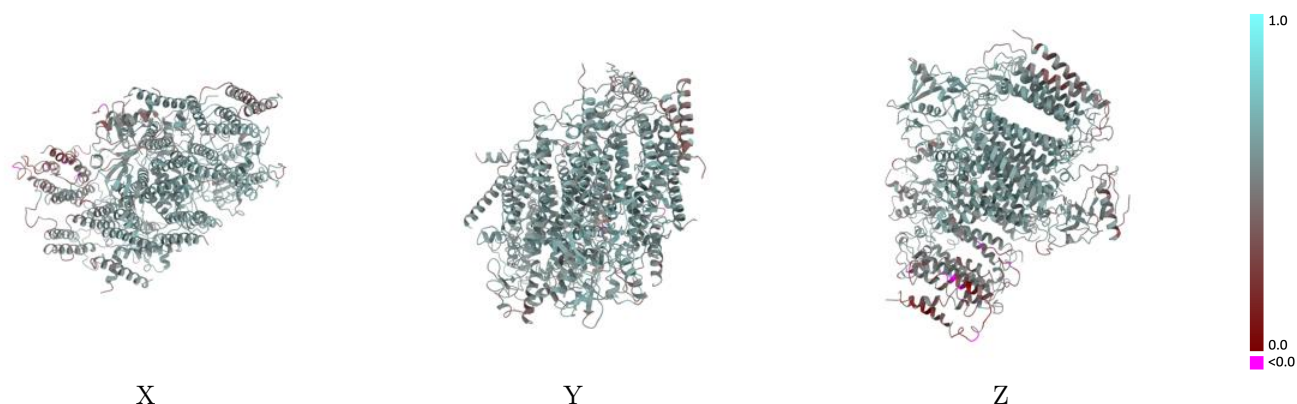
This section contains information regarding the fit between EMDB map EMD-30909 and PDB model 7DXH. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



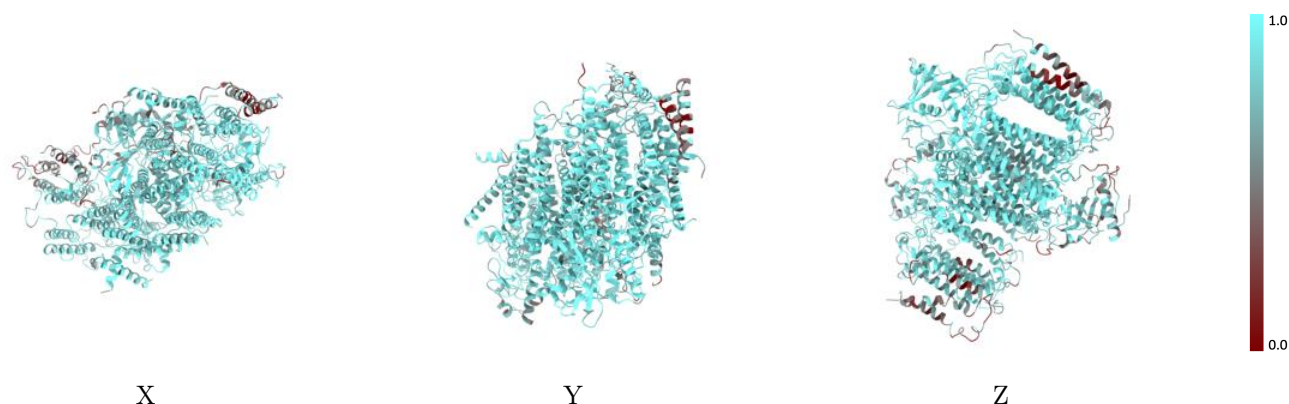
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



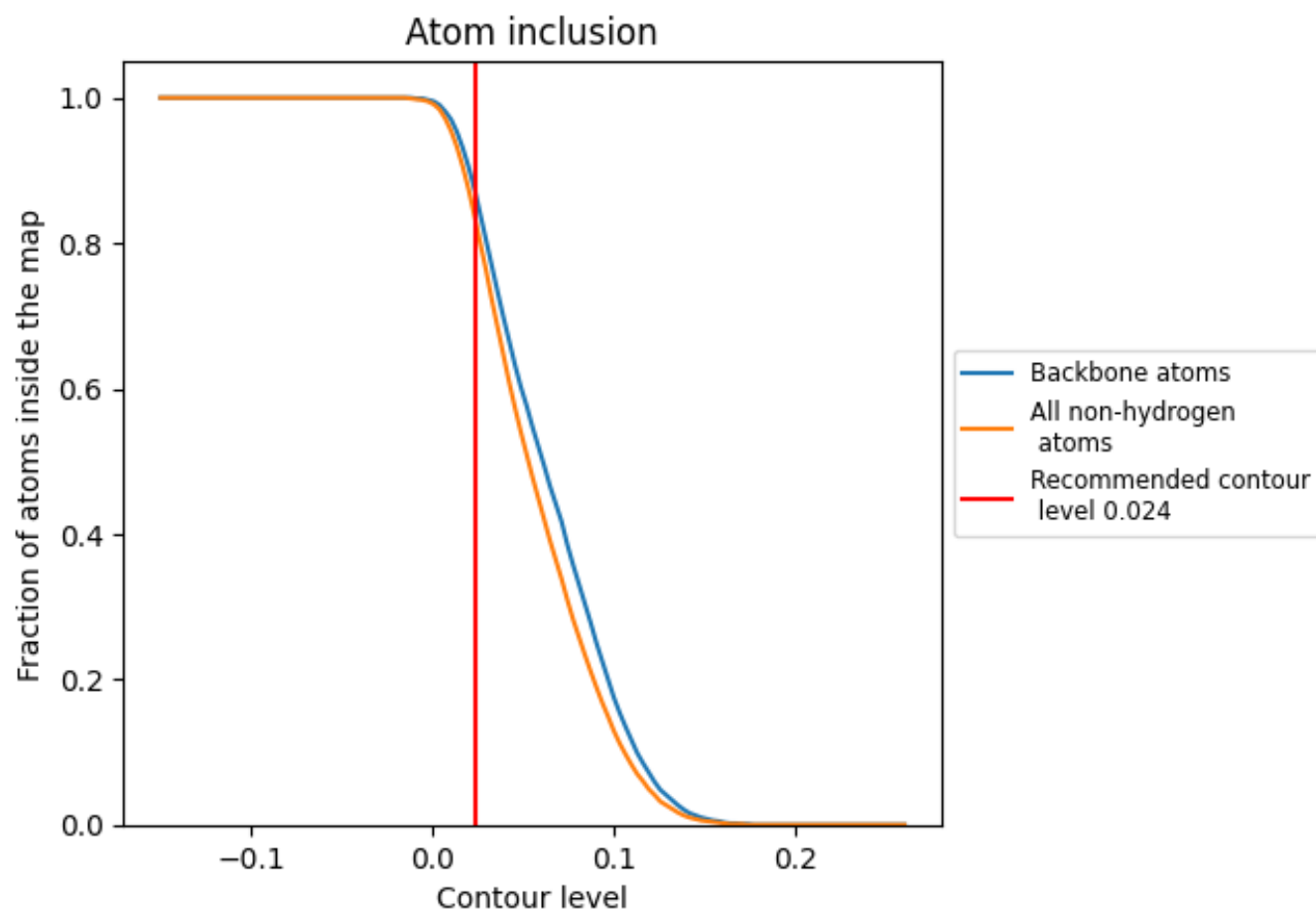
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8310	 0.5420
A	 0.6930	 0.4890
B	 0.5420	 0.4840
C	 0.4350	 0.4330
a	 0.8940	 0.5730
b	 0.8880	 0.5800
c	 0.8260	 0.5060
d	 0.9100	 0.5950
e	 0.7530	 0.4920
f	 0.8100	 0.5430
h	 0.8920	 0.5710
i	 0.8130	 0.5100
k	 0.6910	 0.4490
l	 0.7740	 0.5510
m	 0.6660	 0.5040
t	 0.7710	 0.5220
x	 0.8310	 0.5580
y	 0.3360	 0.2240
z	 0.4530	 0.3120

