



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 7NHQ / pdb_00007nhq
EMDB ID : EMD-12337
Title : Structure of PSII-I prime (PSII with Psb28, and Psb34)
Authors : Zabret, J.; Bohn, S.; Schuller, S.K.; Arnolds, O.; Chan, A.; Tajkhorshid, E.;
Stoll, R.; Engel, B.D.; Rudack, T.; Schuller, J.M.; Nowaczyk, M.M.
Deposited on : 2021-02-11
Resolution : 2.68 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:

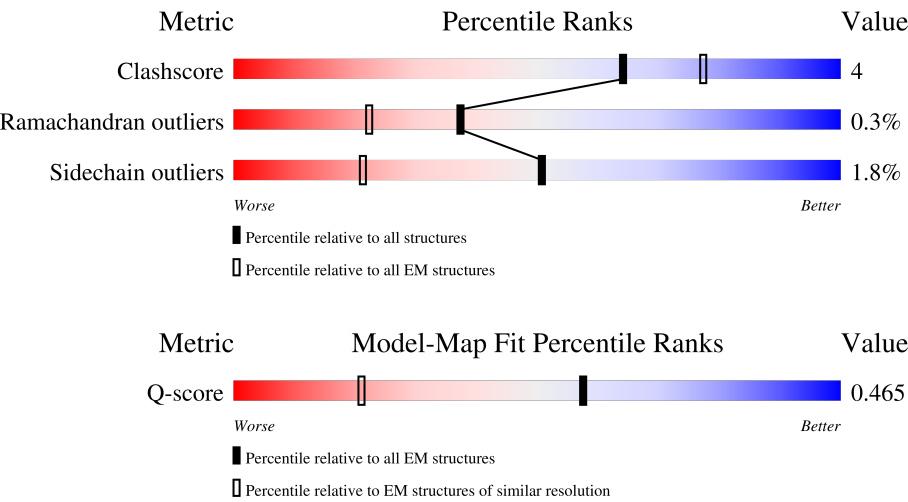
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.68 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9255 (2.18 - 3.18)

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	360	6% 87% 6% • 7%
2	B	510	• 94% • •
3	C	461	5% 84% 10% • 6%
4	D	352	• 89% 7% • •

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Mol	Chain	Length	Quality of chain
5	E	84	
6	F	45	
7	H	66	
8	I	38	
9	K	46	
10	L	37	
11	M	36	
12	T	32	
13	X	41	
14	y	46	
15	Z	62	
16	2	116	
17	3	56	

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	PHO	A	404	X	-	-	-
21	PHO	D	406	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	517	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	407	X	-	-	-
22	CLA	D	408	X	-	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 20946 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	335	Total	C	N	O	S	0	0
			2627	1720	432	460	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	496	Total	C	N	O	S	0	0
			3909	2569	649	678	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	432	Total	C	N	O	S	0	0
			3345	2197	561	575	12		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2717	1800	444	461	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	77	Total	C	N	O	0	0
			635	417	103	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	38	Total	C	N	O	S	0	0
			307	207	50	49	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			511	341	82	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	26	Total	C	N	O	S	0	0
			211	150	27	33	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			293	204	43	46		

- 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	34	Total	C	N	O	S	0	0
			267	178	40	48	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	28	Total	C	N	O	S	0	0
			241	170	34	35	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	35	Total	C	N	O	0	0
			254	172	38	44		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	28	Total	C	N	O	S	0	0
			208	137	36	32	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	60	Total	C	N	O	S	0	0
			463	318	70	74	1		

- Molecule 16 is a protein called Photosystem II reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	112	Total	C	N	O	S	0	0
			897	562	156	173	6		

- Molecule 17 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	56	Total	C	N	O	S	0	0
			419	269	74	75	1		

- Molecule 18 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

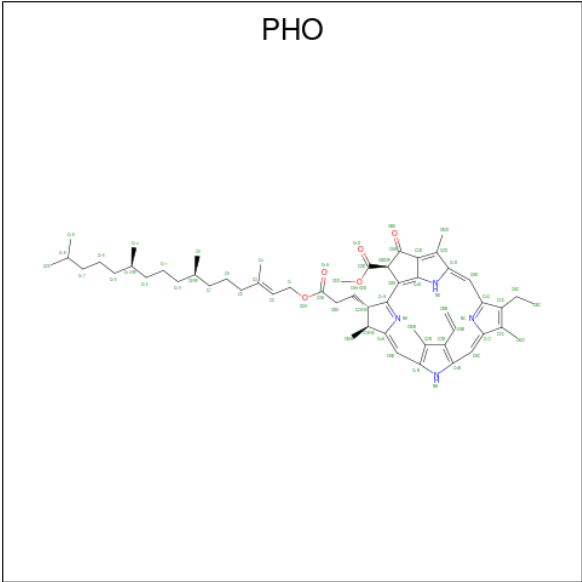
- Molecule 19 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mn	0
			1	1	

- Molecule 20 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

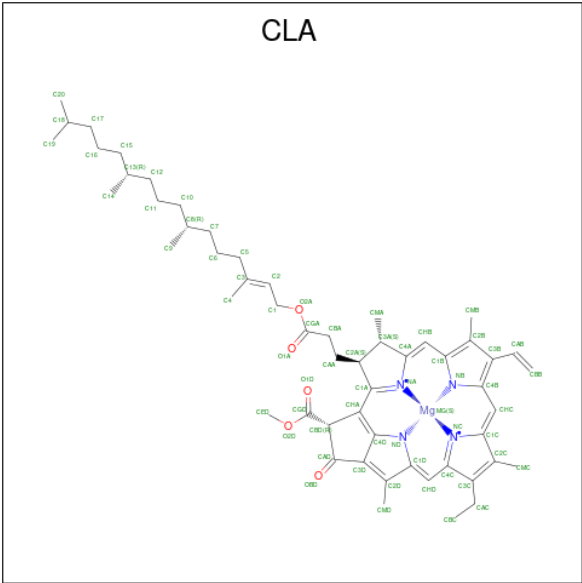
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Cl	0
			1	1	

- Molecule 21 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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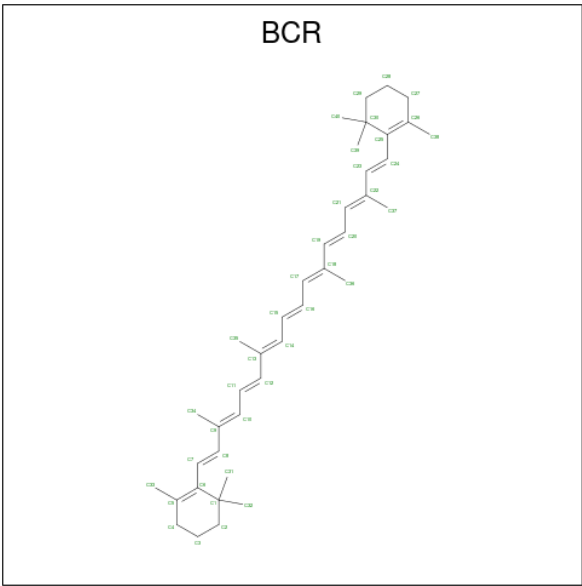
Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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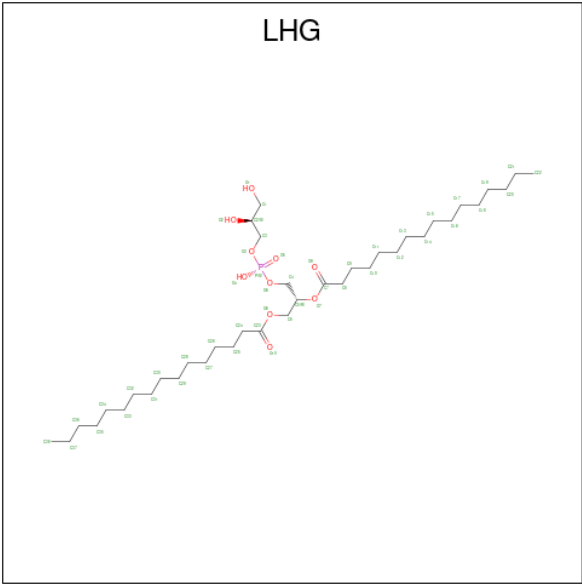
Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



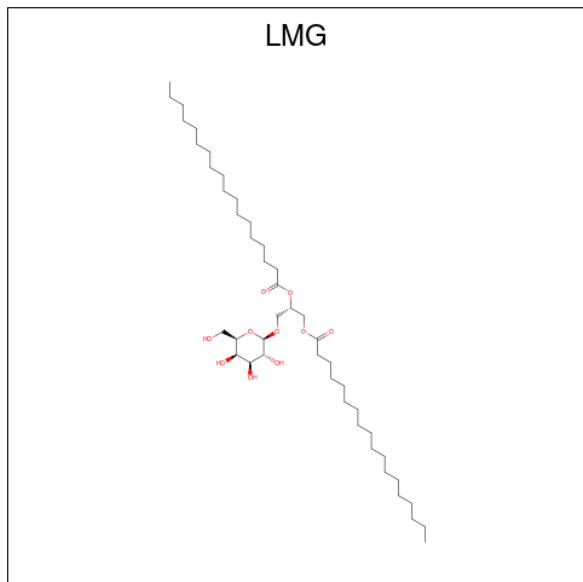
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	C	1	Total	C	0
			40	40	
23	C	1	Total	C	0
			40	40	
23	C	1	Total	C	0
			40	40	
23	F	1	Total	C	0
			40	40	
23	H	1	Total	C	0
			40	40	
23	K	1	Total	C	0
			40	40	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



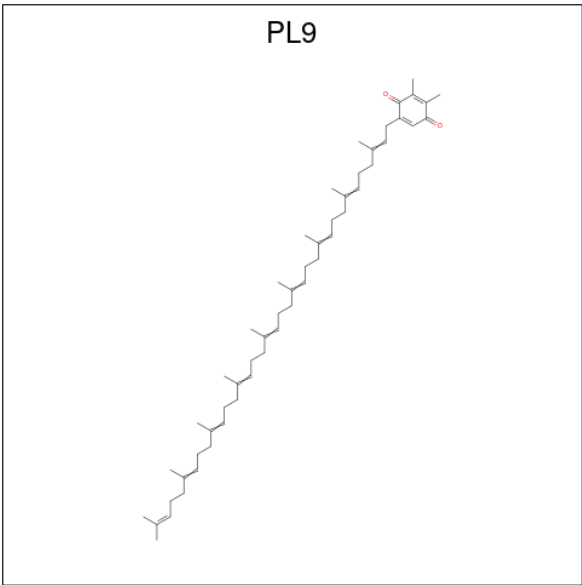
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



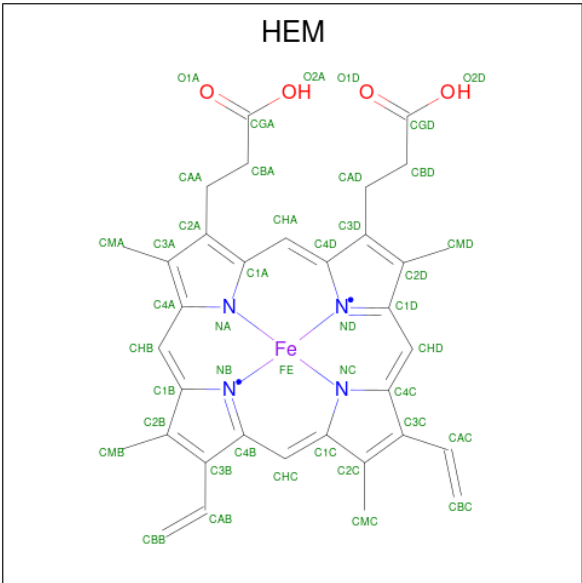
Mol	Chain	Residues	Atoms			AltConf
25	C	1	Total	C	O	0
			55	45	10	
25	C	1	Total	C	O	0
			55	45	10	
25	D	1	Total	C	O	0
			55	45	10	
25	D	1	Total	C	O	0
			55	45	10	
25	F	1	Total	C	O	0
			55	45	10	
25	I	1	Total	C	O	0
			55	45	10	
25	3	1	Total	C	O	0
			55	45	10	

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



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

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

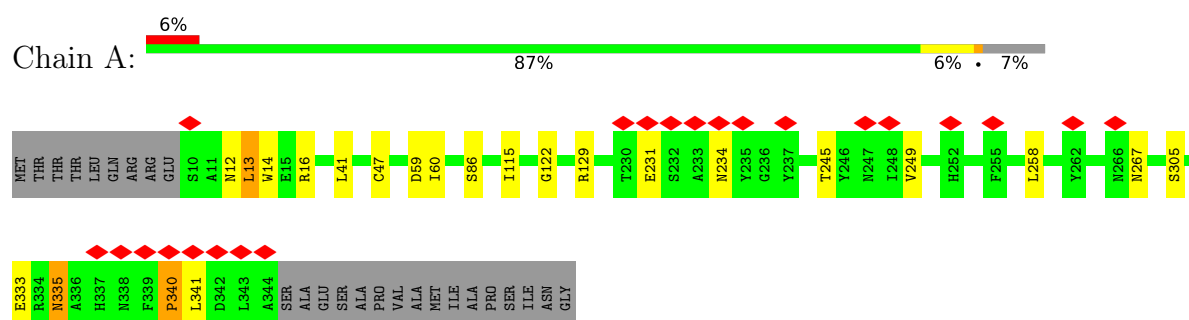


Mol	Chain	Residues	Atoms					AltConf
27	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

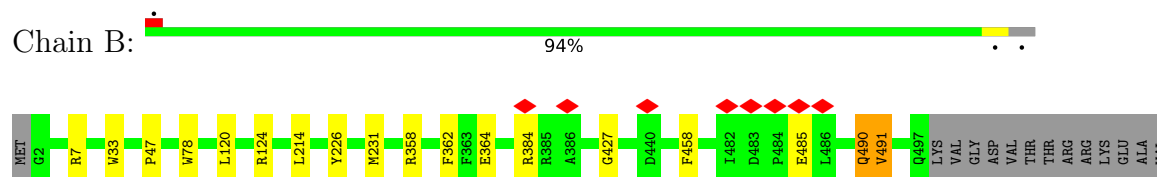
3 Residue-property plots [i](#)

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.

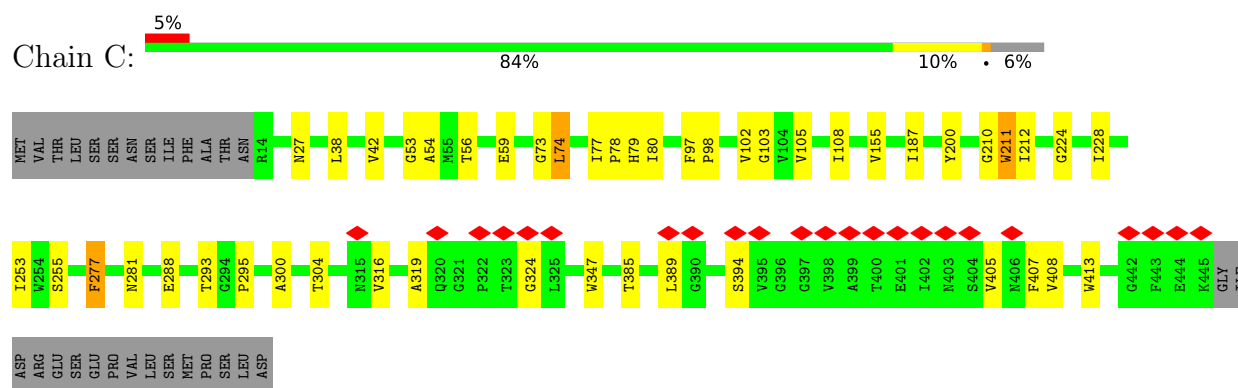
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein

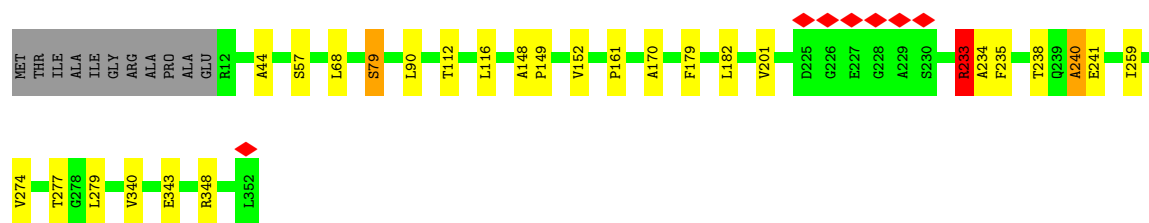


- Molecule 3: Photosystem II CP43 reaction center protein

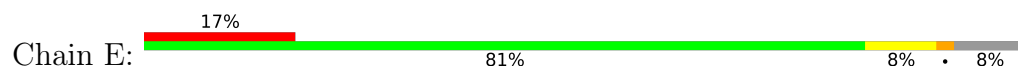


- Molecule 4: Photosystem II D2 protein





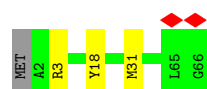
• Molecule 5: Cytochrome b559 subunit alpha



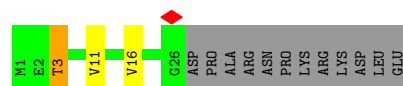
• Molecule 6: Cytochrome b559 subunit beta



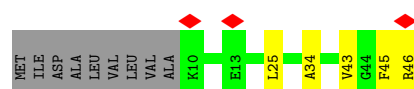
• Molecule 7: Photosystem II reaction center protein H



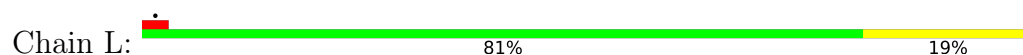
• Molecule 8: Photosystem II reaction center protein I

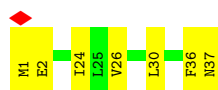


• Molecule 9: Photosystem II reaction center protein K

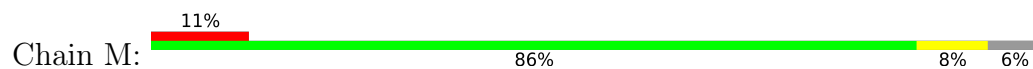


• Molecule 10: Photosystem II reaction center protein L

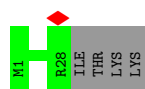




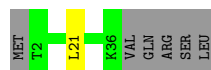
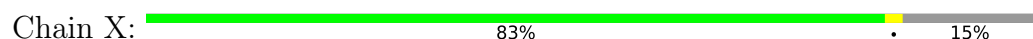
- Molecule 11: Photosystem II reaction center protein M



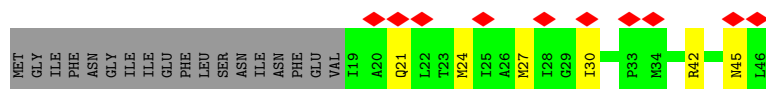
- Molecule 12: Photosystem II reaction center protein T



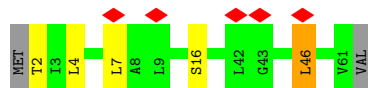
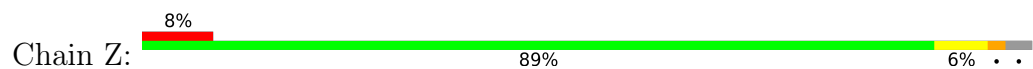
- Molecule 13: Photosystem II reaction center X protein



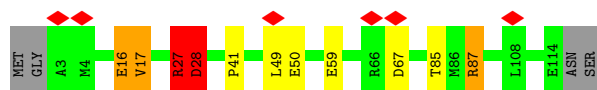
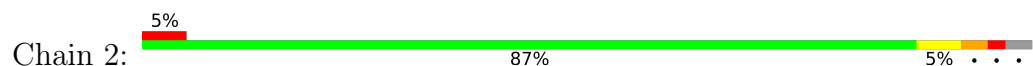
- Molecule 14: Photosystem II reaction center protein Ycf12



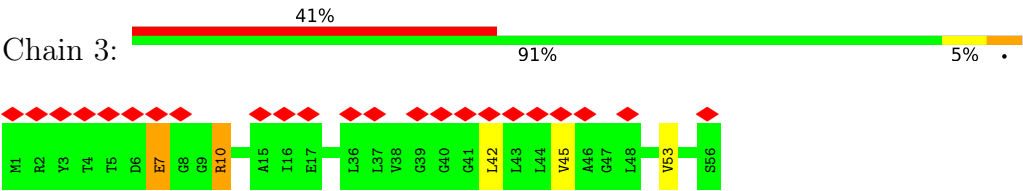
- Molecule 15: Photosystem II reaction center protein Z



- Molecule 16: Photosystem II reaction center Psb28 protein



- Molecule 17: Tsl0063 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	283.4, 283.4, 283.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, CL, HEM, LMG, PL9, CLA, BCR, MN, FE

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	0.41	0/2712	0.80	1/3700 (0.0%)
2	B	0.41	0/4049	0.79	4/5519 (0.1%)
3	C	0.39	0/3456	0.82	5/4706 (0.1%)
4	D	0.39	0/2812	0.80	4/3832 (0.1%)
5	E	0.40	0/654	0.87	0/891
6	F	0.55	0/317	1.11	2/433 (0.5%)
7	H	0.38	0/524	0.80	0/713
8	I	0.51	0/216	1.03	0/292
9	K	0.50	0/303	0.78	0/416
10	L	0.42	0/311	0.72	0/422
11	M	0.44	0/270	0.91	0/367
12	T	0.53	0/250	0.85	0/338
13	X	0.51	0/257	0.96	0/348
14	y	0.62	0/209	1.15	0/279
15	Z	0.48	0/474	0.97	2/649 (0.3%)
16	2	0.52	0/914	1.06	2/1231 (0.2%)
17	3	0.51	0/426	1.14	3/578 (0.5%)
All	All	0.42	0/18154	0.85	23/24714 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
4	D	0	1
5	E	0	1
14	y	0	1
16	2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	7	GLU	CA-CB-CG	9.94	133.98	114.10
17	3	7	GLU	CB-CG-CD	9.63	128.97	112.60
2	B	491	VAL	N-CA-CB	-7.09	99.54	111.23
3	C	212	ILE	N-CA-C	-6.90	106.06	112.96
2	B	490	GLN	CB-CG-CD	6.62	123.86	112.60
16	2	17	VAL	CA-C-N	-6.59	116.98	123.04
16	2	17	VAL	C-N-CA	-6.59	116.98	123.04
3	C	211	TRP	N-CA-C	6.59	124.83	110.80
17	3	7	GLU	CB-CA-C	-6.25	96.93	109.99
15	Z	46	LEU	CB-CA-C	-6.17	100.94	110.81
2	B	491	VAL	N-CA-C	6.02	121.87	109.34
4	D	233	ARG	CA-C-N	5.92	132.36	121.70
4	D	233	ARG	C-N-CA	5.92	132.36	121.70
2	B	490	GLN	CA-CB-CG	5.80	125.71	114.10
6	F	8	GLN	CB-CG-CD	5.67	122.23	112.60
6	F	8	GLN	CA-CB-CG	5.63	125.36	114.10
3	C	210	GLY	CA-C-N	5.57	132.17	121.54
3	C	210	GLY	C-N-CA	5.57	132.17	121.54
15	Z	46	LEU	N-CA-CB	5.52	118.16	109.94
1	A	249	VAL	CG1-CB-CG2	-5.14	99.49	110.80
3	C	324	GLY	N-CA-C	-5.12	108.39	114.48
4	D	238	THR	CA-C-N	5.08	131.24	121.54
4	D	238	THR	C-N-CA	5.08	131.24	121.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	2	27	ARG	Peptide
16	2	67	ASP	Sidechain
1	A	335	ASN	Sidechain
2	B	364	GLU	Sidechain
2	B	485	GLU	Sidechain
2	B	490	GLN	Mainchain
4	D	233	ARG	Peptide

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Mol	Chain	Res	Type	Group
5	E	10	PHE	Sidechain
14	y	45	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2524	14	0
2	B	3909	0	3763	9	0
3	C	3345	0	3273	33	0
4	D	2717	0	2621	20	0
5	E	635	0	625	5	0
6	F	307	0	312	4	0
7	H	511	0	532	2	0
8	I	211	0	227	2	0
9	K	293	0	305	7	0
10	L	304	0	316	6	0
11	M	267	0	289	2	0
12	T	241	0	244	0	0
13	X	254	0	282	0	0
14	y	208	0	237	2	0
15	Z	463	0	495	2	0
16	2	897	0	859	8	0
17	3	419	0	438	4	0
18	A	1	0	0	0	0
19	A	1	0	0	0	0
20	A	1	0	0	0	0
21	A	64	0	73	0	0
21	D	64	0	73	1	0
22	A	130	0	140	1	0
22	B	1040	0	1121	27	0
22	C	845	0	909	16	0
22	D	260	0	279	10	0
23	A	40	0	56	1	0
23	B	120	0	168	3	0
23	C	120	0	168	7	0
23	F	40	0	56	1	0
23	H	40	0	56	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K	40	0	56	11	0
24	A	49	0	74	0	0
25	3	55	0	86	2	0
25	C	110	0	172	0	0
25	D	110	0	172	2	0
25	F	55	0	86	0	0
25	I	55	0	86	2	0
26	D	55	0	80	4	0
27	E	43	0	30	3	0
All	All	20946	0	21283	175	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:609:CLA:C4B	23:H:101:BCR:H333	1.79	1.12
23:C:515:BCR:H353	23:K:101:BCR:H332	1.25	1.08
22:B:609:CLA:C3B	23:H:101:BCR:H333	1.95	0.96
23:K:101:BCR:C38	23:K:101:BCR:H23C	2.02	0.90
23:H:101:BCR:C38	23:H:101:BCR:H23C	2.03	0.89
22:B:602:CLA:HED2	22:B:603:CLA:H43	1.57	0.87
23:C:515:BCR:C35	23:K:101:BCR:H332	2.05	0.86
1:A:341:LEU:HD13	3:C:385:THR:HA	1.62	0.82
23:C:515:BCR:H353	23:K:101:BCR:C33	2.08	0.80
4:D:116:LEU:HD13	22:D:408:CLA:HBA1	1.65	0.78
22:B:602:CLA:HBA2	22:B:602:CLA:HMA2	1.69	0.74
23:H:101:BCR:H23C	23:H:101:BCR:H382	1.69	0.74
22:B:607:CLA:H142	22:B:607:CLA:H101	1.71	0.72
23:K:101:BCR:H23C	23:K:101:BCR:H382	1.69	0.72
1:A:341:LEU:CD1	3:C:385:THR:HA	2.21	0.70
22:B:609:CLA:C3B	23:H:101:BCR:C33	2.69	0.69
6:F:45:ARG:OXT	6:F:45:ARG:HD2	1.92	0.69
27:E:101:HEM:HMB2	27:E:101:HEM:HBB2	1.75	0.69
9:K:34:ALA:HB1	23:K:101:BCR:H21C	1.75	0.69
3:C:59:GLU:HG3	3:C:74:LEU:HD12	1.75	0.67
22:C:511:CLA:HMA3	22:C:517:CLA:HMA1	1.77	0.65
22:D:402:CLA:H41	22:D:402:CLA:H92	1.78	0.65
3:C:408:VAL:HG13	3:C:413:TRP:HE1	1.64	0.61
22:B:601:CLA:HMA3	23:H:101:BCR:H382	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:405:PL9:H352	10:L:26:VAL:HG12	1.83	0.59
2:B:33:TRP:HE1	22:B:607:CLA:HBC2	1.67	0.59
22:B:609:CLA:NB	23:H:101:BCR:H333	2.18	0.59
22:C:504:CLA:H42	22:C:505:CLA:H172	1.85	0.59
22:C:517:CLA:HBB1	22:C:517:CLA:HMB3	1.85	0.59
16:2:85:THR:O	16:2:87:ARG:NH1	2.36	0.59
4:D:116:LEU:HD13	22:D:408:CLA:CBA	2.32	0.57
17:3:42:LEU:O	17:3:45:VAL:HG12	2.04	0.56
3:C:288:GLU:N	3:C:288:GLU:OE1	2.39	0.56
17:3:42:LEU:HA	17:3:45:VAL:HG12	1.86	0.56
22:B:603:CLA:HAB	22:B:605:CLA:H171	1.88	0.56
3:C:293:THR:HG22	3:C:295:PRO:HD2	1.87	0.54
3:C:102:VAL:HG21	22:C:505:CLA:HMA3	1.90	0.54
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.89	0.54
22:C:503:CLA:H93	22:C:503:CLA:HMB2	1.90	0.53
3:C:108:ILE:HD11	23:C:518:BCR:H10C	1.90	0.53
22:C:509:CLA:H72	22:C:509:CLA:H41	1.90	0.53
23:K:101:BCR:H23C	23:K:101:BCR:H383	1.89	0.53
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.91	0.52
22:D:402:CLA:HAA1	22:D:402:CLA:CGD	2.40	0.52
9:K:34:ALA:HB1	23:K:101:BCR:C21	2.39	0.52
22:B:614:CLA:HAA1	22:B:614:CLA:CGD	2.39	0.52
1:A:231:GLU:HB2	1:A:234:ASN:OD1	2.10	0.52
4:D:343:GLU:H	4:D:343:GLU:CD	2.18	0.51
1:A:12:ASN:O	1:A:14:TRP:N	2.43	0.51
22:B:604:CLA:H72	22:B:604:CLA:H41	1.92	0.51
3:C:405:VAL:HG22	3:C:407:PHE:H	1.76	0.51
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.92	0.51
3:C:253:ILE:HG22	3:C:255:SER:H	1.76	0.51
4:D:233:ARG:HA	4:D:234:ALA:O	2.11	0.51
22:B:609:CLA:C2B	23:H:101:BCR:H333	2.38	0.51
25:D:403:LMG:H453	10:L:24:ILE:HD12	1.94	0.50
27:E:101:HEM:HBB2	27:E:101:HEM:CMB	2.41	0.50
9:K:25:LEU:CD2	23:K:101:BCR:H322	2.41	0.50
23:B:619:BCR:C8	23:B:619:BCR:H331	2.41	0.50
26:D:405:PL9:H202	26:D:405:PL9:H162	1.93	0.50
6:F:28:VAL:HG23	6:F:29:PRO:HD3	1.93	0.50
1:A:59:ASP:O	1:A:86:SER:HB3	2.11	0.49
4:D:234:ALA:HA	4:D:235:PHE:HB2	1.94	0.49
23:B:617:BCR:H392	23:B:617:BCR:H23C	1.95	0.49
4:D:240:ALA:O	4:D:241:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:CD1	3:C:385:THR:HG22	2.43	0.48
22:B:608:CLA:HBA1	22:B:608:CLA:HBD	1.95	0.48
3:C:389:LEU:O	3:C:408:VAL:HG23	2.13	0.48
9:K:43:VAL:HG12	9:K:43:VAL:O	2.13	0.48
22:B:609:CLA:H41	7:H:31:MET:SD	2.54	0.48
22:B:613:CLA:OBD	22:B:614:CLA:HHC	2.14	0.48
4:D:279:LEU:HD22	22:D:407:CLA:HBA2	1.96	0.48
22:D:408:CLA:HAA1	22:D:408:CLA:CGD	2.44	0.48
9:K:45:PHE:C	9:K:46:ARG:O	2.57	0.48
22:B:613:CLA:OBD	22:B:614:CLA:CAB	2.62	0.47
11:M:21:PHE:CE1	11:M:25:LEU:HD11	2.48	0.47
4:D:201:VAL:HG11	22:D:401:CLA:C3D	2.44	0.47
5:E:14:ILE:HD12	5:E:19:TYR:CZ	2.49	0.47
23:H:101:BCR:C8	23:H:101:BCR:H311	2.44	0.47
3:C:316:VAL:HB	3:C:319:ALA:HB3	1.97	0.47
1:A:340:PRO:O	1:A:341:LEU:HG	2.15	0.47
23:K:101:BCR:C8	23:K:101:BCR:H311	2.42	0.47
22:B:609:CLA:HHC	22:B:609:CLA:HBB1	1.96	0.47
4:D:57:SER:HB3	4:D:79:SER:OG	2.15	0.47
1:A:13:LEU:HA	1:A:16:ARG:HE	1.79	0.46
22:B:612:CLA:H93	22:B:612:CLA:CGA	2.45	0.46
3:C:77:ILE:N	3:C:78:PRO:CD	2.78	0.46
3:C:53:GLY:O	3:C:56:THR:HG22	2.16	0.46
22:B:610:CLA:HAA1	22:B:610:CLA:CGD	2.46	0.46
14:y:42:ARG:N	14:y:42:ARG:HD2	2.30	0.46
1:A:341:LEU:HD12	3:C:385:THR:HG22	1.97	0.46
3:C:56:THR:CG2	3:C:103:GLY:HA2	2.45	0.46
23:H:101:BCR:H23C	23:H:101:BCR:H383	1.91	0.46
22:A:406:CLA:HMA2	22:A:406:CLA:HBA2	1.98	0.46
2:B:47:PRO:HG3	2:B:78:TRP:CD2	2.51	0.45
3:C:79:HIS:CE1	22:C:504:CLA:HAA2	2.52	0.45
3:C:42:VAL:HG23	22:C:513:CLA:HED1	1.97	0.45
5:E:10:PHE:HA	5:E:13:ILE:HB	1.99	0.45
26:D:405:PL9:H371	10:L:30:LEU:HB2	1.98	0.45
6:F:44:GLN:H	6:F:44:GLN:CD	2.25	0.45
16:2:59:GLU:H	16:2:59:GLU:CD	2.24	0.45
3:C:224:GLY:O	3:C:228:ILE:HG13	2.16	0.45
16:2:28:ASP:N	16:2:28:ASP:OD1	2.50	0.45
17:3:10:ARG:CZ	25:3:101:LMG:HC4	2.47	0.45
23:A:407:BCR:C8	23:A:407:BCR:H331	2.47	0.44
4:D:340:VAL:HG23	4:D:340:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:TYR:O	3:C:211:TRP:O	2.36	0.44
23:C:515:BCR:H371	23:C:515:BCR:H24C	1.78	0.44
8:I:11:VAL:HG12	25:I:101:LMG:H273	2.00	0.44
15:Z:4:LEU:HA	15:Z:7:LEU:HG	2.00	0.44
3:C:277:PHE:CE1	3:C:281:ASN:ND2	2.85	0.44
4:D:152:VAL:HG21	22:D:407:CLA:HBA1	1.98	0.44
5:E:82:GLN:O	5:E:83:LEU:HB2	2.17	0.44
22:C:503:CLA:H93	22:C:503:CLA:CMB	2.48	0.44
3:C:155:VAL:HG21	22:C:513:CLA:HMA1	2.00	0.44
22:D:401:CLA:HMA2	25:3:101:LMG:H271	2.00	0.44
10:L:1:MET:HE2	10:L:2:GLU:O	2.18	0.44
22:B:609:CLA:C1B	23:H:101:BCR:H333	2.48	0.43
1:A:41:LEU:CD1	1:A:122:GLY:HA3	2.48	0.43
1:A:60:ILE:HA	1:A:86:SER:HA	2.00	0.43
22:B:615:CLA:HBA1	22:B:615:CLA:HMA2	2.00	0.43
22:C:514:CLA:HAA1	22:C:514:CLA:CGD	2.48	0.43
22:C:517:CLA:HAA1	22:C:517:CLA:CGD	2.48	0.43
1:A:258:LEU:HD12	1:A:258:LEU:N	2.33	0.43
4:D:179:PHE:HA	4:D:182:LEU:HD12	2.01	0.43
11:M:21:PHE:CZ	11:M:25:LEU:HD11	2.53	0.43
2:B:458:PHE:CE1	22:B:613:CLA:H101	2.53	0.43
22:B:609:CLA:HMA2	22:B:609:CLA:HBA2	2.00	0.43
22:D:407:CLA:HBB1	22:D:407:CLA:HHC	2.01	0.43
16:2:16:GLU:H	16:2:16:GLU:CD	2.26	0.43
2:B:120:LEU:HA	7:H:3:ARG:H	1.83	0.43
22:C:505:CLA:HMD2	22:C:505:CLA:H191	2.00	0.42
23:F:102:BCR:C8	23:F:102:BCR:H331	2.48	0.42
16:2:17:VAL:HG21	16:2:41:PRO:HA	2.01	0.42
23:H:101:BCR:HC31	23:H:101:BCR:H323	1.82	0.42
9:K:43:VAL:O	9:K:43:VAL:CG1	2.67	0.42
2:B:384:ARG:HH12	4:D:348:ARG:HH11	1.67	0.42
3:C:300:ALA:O	3:C:304:THR:HG22	2.20	0.42
23:H:101:BCR:C38	23:H:101:BCR:C23	2.82	0.42
22:B:603:CLA:H92	22:B:605:CLA:H122	2.01	0.42
3:C:77:ILE:HA	3:C:80:ILE:HD12	2.01	0.42
4:D:274:VAL:HG22	26:D:405:PL9:H253	2.01	0.42
16:2:50:GLU:CD	16:2:50:GLU:N	2.78	0.42
2:B:226:TYR:HA	2:B:231:MET:HE3	2.02	0.42
3:C:73:GLY:HA3	22:C:506:CLA:HBA1	2.01	0.42
8:I:3:THR:HG21	25:I:101:LMG:HC1	2.02	0.42
3:C:102:VAL:HA	3:C:105:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:27:ARG:O	16:2:28:ASP:O	2.38	0.42
3:C:228:ILE:HD11	23:C:516:BCR:H392	2.02	0.42
1:A:47:CYS:SG	1:A:115:ILE:HG13	2.59	0.42
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.85	0.42
10:L:36:PHE:C	10:L:37:ASN:O	2.63	0.41
3:C:56:THR:HG21	3:C:103:GLY:HA2	2.03	0.41
3:C:347:TRP:CD1	3:C:347:TRP:N	2.89	0.41
4:D:68:LEU:HD11	5:E:44:TYR:CE2	2.55	0.41
2:B:7:ARG:HA	22:B:611:CLA:HBA1	2.01	0.41
4:D:259:ILE:C	4:D:259:ILE:HD12	2.45	0.41
10:L:36:PHE:O	10:L:37:ASN:O	2.38	0.41
16:2:50:GLU:CD	16:2:50:GLU:H	2.28	0.41
23:B:617:BCR:C8	23:B:617:BCR:H331	2.51	0.41
4:D:44:ALA:HB1	21:D:406:PHO:H92	2.01	0.41
1:A:129:ARG:HH12	25:D:404:LMG:H441	1.86	0.41
23:C:516:BCR:H20C	23:C:516:BCR:H361	1.87	0.41
23:K:101:BCR:H331	23:K:101:BCR:HC7	1.50	0.41
17:3:42:LEU:HA	17:3:45:VAL:CG1	2.51	0.41
2:B:358:ARG:CZ	2:B:427:GLY:HA2	2.51	0.41
22:B:609:CLA:C1B	23:H:101:BCR:HC42	2.51	0.41
27:E:101:HEM:C4D	6:F:24:HIS:HE1	2.39	0.41
15:Z:2:THR:CG2	15:Z:4:LEU:HD23	2.51	0.41
14:y:27:MET:HA	14:y:30:ILE:HG22	2.03	0.40
3:C:27:ASN:OD1	22:C:510:CLA:H42	2.21	0.40
3:C:97:PHE:HB3	3:C:98:PRO:HD3	2.03	0.40
22:C:503:CLA:H2	22:C:504:CLA:OBD	2.22	0.40
3:C:54:ALA:HB1	9:K:25:LEU:HB3	2.04	0.40
4:D:90:LEU:HD12	4:D:112:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	314 (94%)	17 (5%)	2 (1%)	21	41
2	B	494/510 (97%)	470 (95%)	23 (5%)	1 (0%)	43	65
3	C	430/461 (93%)	405 (94%)	25 (6%)	0	100	100
4	D	339/352 (96%)	321 (95%)	17 (5%)	1 (0%)	36	57
5	E	75/84 (89%)	71 (95%)	4 (5%)	0	100	100
6	F	36/45 (80%)	32 (89%)	4 (11%)	0	100	100
7	H	63/66 (96%)	57 (90%)	5 (8%)	1 (2%)	7	18
8	I	24/38 (63%)	24 (100%)	0	0	100	100
9	K	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
10	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	M	32/36 (89%)	32 (100%)	0	0	100	100
12	T	26/32 (81%)	24 (92%)	2 (8%)	0	100	100
13	X	33/41 (80%)	32 (97%)	1 (3%)	0	100	100
14	y	26/46 (56%)	22 (85%)	4 (15%)	0	100	100
15	Z	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
16	2	110/116 (95%)	102 (93%)	6 (6%)	2 (2%)	6	15
17	3	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
All	All	2203/2388 (92%)	2083 (95%)	113 (5%)	7 (0%)	37	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	491	VAL
4	D	240	ALA
16	2	28	ASP
1	A	13	LEU
16	2	27	ARG
1	A	340	PRO
7	H	18	TYR

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	271/291 (93%)	266 (98%)	5 (2%)	51	76
2	B	395/407 (97%)	393 (100%)	2 (0%)	81	91
3	C	335/362 (92%)	330 (98%)	5 (2%)	57	79
4	D	276/283 (98%)	274 (99%)	2 (1%)	76	89
5	E	69/73 (94%)	68 (99%)	1 (1%)	59	80
6	F	32/39 (82%)	30 (94%)	2 (6%)	16	35
7	H	54/55 (98%)	54 (100%)	0	100	100
8	I	24/35 (69%)	22 (92%)	2 (8%)	10	24
9	K	30/37 (81%)	30 (100%)	0	100	100
10	L	35/35 (100%)	35 (100%)	0	100	100
11	M	31/33 (94%)	30 (97%)	1 (3%)	34	61
12	T	25/29 (86%)	25 (100%)	0	100	100
13	X	28/34 (82%)	27 (96%)	1 (4%)	31	57
14	y	21/37 (57%)	19 (90%)	2 (10%)	8	18
15	Z	50/52 (96%)	48 (96%)	2 (4%)	28	53
16	2	94/97 (97%)	90 (96%)	4 (4%)	26	51
17	3	42/42 (100%)	39 (93%)	3 (7%)	13	30
All	All	1812/1941 (93%)	1780 (98%)	32 (2%)	51	76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	THR
1	A	267	ASN
1	A	305	SER
1	A	333	GLU
1	A	335	ASN
2	B	214	LEU
2	B	362	PHE
3	C	38	LEU
3	C	74	LEU
3	C	187	ILE
3	C	277	PHE
3	C	394	SER
4	D	79	SER

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Mol	Chain	Res	Type
4	D	277	THR
5	E	14	ILE
6	F	8	GLN
6	F	30	THR
8	I	3	THR
8	I	16	VAL
11	M	9	ILE
13	X	21	LEU
14	y	21	GLN
14	y	24	MET
15	Z	16	SER
15	Z	46	LEU
16	2	16	GLU
16	2	28	ASP
16	2	49	LEU
16	2	87	ARG
17	3	7	GLU
17	3	10	ARG
17	3	53	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	198	HIS
1	A	304	HIS
1	A	322	ASN
1	A	332	HIS
1	A	335	ASN
2	B	58	GLN
2	B	274	GLN
2	B	455	HIS
2	B	466	HIS
3	C	106	HIS
3	C	370	ASN
3	C	393	ASN
3	C	432	HIS
4	D	87	HIS
4	D	106	GLN
4	D	129	GLN
4	D	186	GLN
4	D	194	ASN

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Mol	Chain	Res	Type
4	D	250	ASN
4	D	255	GLN
4	D	301	GLN
4	D	334	GLN
5	E	23	HIS
5	E	58	GLN
7	H	15	ASN
7	H	50	ASN
13	X	33	GLN
16	2	48	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 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	$\# Z > 2$
22	CLA	B	601	-	69,73,73	1.37	12 (17%)	82,113,113	2.54	21 (25%)
22	CLA	B	605	-	69,73,73	1.22	8 (11%)	82,113,113	2.29	18 (21%)
22	CLA	B	609	-	69,73,73	1.52	11 (15%)	82,113,113	2.69	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	K	101	-	41,41,41	2.94	9 (21%)	56,56,56	3.79	32 (57%)
22	CLA	B	616	-	69,73,73	1.47	13 (18%)	82,113,113	3.01	21 (25%)
22	CLA	C	514	-	69,73,73	1.42	10 (14%)	82,113,113	2.30	20 (24%)
22	CLA	C	511	-	69,73,73	1.32	10 (14%)	82,113,113	2.57	21 (25%)
22	CLA	C	517	22	69,73,73	1.46	12 (17%)	82,113,113	2.80	25 (30%)
22	CLA	A	405	-	69,73,73	1.29	9 (13%)	82,113,113	2.10	22 (26%)
22	CLA	B	610	-	69,73,73	1.42	14 (20%)	82,113,113	2.78	19 (23%)
26	PL9	D	405	-	55,55,55	1.15	3 (5%)	68,69,69	1.38	13 (19%)
22	CLA	C	507	-	69,73,73	1.52	13 (18%)	82,113,113	2.75	25 (30%)
22	CLA	B	607	-	69,73,73	1.29	10 (14%)	82,113,113	2.15	24 (29%)
23	BCR	B	618	-	41,41,41	1.04	2 (4%)	56,56,56	1.17	5 (8%)
22	CLA	C	505	-	69,73,73	1.28	10 (14%)	82,113,113	2.78	29 (35%)
25	LMG	C	501	-	55,55,55	0.94	0	63,63,63	1.13	5 (7%)
23	BCR	H	101	-	41,41,41	3.18	10 (24%)	56,56,56	4.02	31 (55%)
22	CLA	B	604	-	69,73,73	1.32	10 (14%)	82,113,113	2.71	19 (23%)
22	CLA	A	406	-	69,73,73	1.29	11 (15%)	82,113,113	2.20	18 (21%)
22	CLA	B	608	-	69,73,73	1.38	9 (13%)	82,113,113	2.53	22 (26%)
23	BCR	B	619	-	41,41,41	0.96	2 (4%)	56,56,56	1.29	8 (14%)
25	LMG	F	101	-	55,55,55	1.05	2 (3%)	63,63,63	1.00	3 (4%)
22	CLA	C	506	-	69,73,73	1.30	11 (15%)	82,113,113	2.38	18 (21%)
22	CLA	D	408	-	69,73,73	1.29	9 (13%)	82,113,113	2.11	18 (21%)
23	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	6 (10%)
23	BCR	C	516	-	41,41,41	0.97	2 (4%)	56,56,56	1.22	8 (14%)
22	CLA	B	611	-	69,73,73	1.40	10 (14%)	82,113,113	2.32	21 (25%)
25	LMG	C	502	-	55,55,55	1.09	3 (5%)	63,63,63	0.99	5 (7%)
22	CLA	B	612	-	69,73,73	1.41	15 (21%)	82,113,113	2.82	22 (26%)
22	CLA	B	606	-	69,73,73	1.30	11 (15%)	82,113,113	2.27	26 (31%)
23	BCR	A	407	-	41,41,41	0.95	2 (4%)	56,56,56	1.10	3 (5%)
22	CLA	C	513	-	69,73,73	1.34	11 (15%)	82,113,113	2.71	23 (28%)
22	CLA	D	407	-	69,73,73	1.33	10 (14%)	82,113,113	2.00	23 (28%)
23	BCR	C	515	-	41,41,41	1.03	2 (4%)	56,56,56	1.45	11 (19%)
22	CLA	C	512	-	69,73,73	1.46	10 (14%)	82,113,113	2.72	24 (29%)
21	PHO	D	406	-	58,69,69	2.18	11 (18%)	55,99,99	1.98	11 (20%)
22	CLA	B	613	-	69,73,73	1.46	12 (17%)	82,113,113	2.67	25 (30%)
22	CLA	D	402	-	69,73,73	1.30	10 (14%)	82,113,113	2.30	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	504	-	69,73,73	1.35	12 (17%)	82,113,113	2.16	19 (23%)
25	LMG	I	101	-	55,55,55	1.01	2 (3%)	63,63,63	1.09	4 (6%)
21	PHO	A	404	-	58,69,69	2.26	11 (18%)	55,99,99	1.65	9 (16%)
22	CLA	C	510	22	69,73,73	1.49	12 (17%)	82,113,113	2.58	23 (28%)
22	CLA	B	615	-	69,73,73	1.37	9 (13%)	82,113,113	2.56	23 (28%)
22	CLA	C	509	-	69,73,73	1.32	10 (14%)	82,113,113	2.46	15 (18%)
23	BCR	C	518	-	41,41,41	1.03	2 (4%)	56,56,56	1.51	12 (21%)
22	CLA	D	401	-	69,73,73	1.24	9 (13%)	82,113,113	2.03	21 (25%)
25	LMG	D	404	-	55,55,55	0.99	2 (3%)	63,63,63	1.08	4 (6%)
25	LMG	3	101	-	55,55,55	0.95	1 (1%)	63,63,63	1.07	5 (7%)
22	CLA	C	508	-	69,73,73	1.45	11 (15%)	82,113,113	2.14	16 (19%)
22	CLA	B	614	-	69,73,73	1.47	12 (17%)	82,113,113	2.56	21 (25%)
22	CLA	C	503	-	69,73,73	1.36	10 (14%)	82,113,113	1.92	24 (29%)
22	CLA	B	602	-	69,73,73	1.40	12 (17%)	82,113,113	2.47	17 (20%)
23	BCR	F	102	-	41,41,41	0.87	0	56,56,56	1.18	7 (12%)
25	LMG	D	403	-	55,55,55	0.99	1 (1%)	63,63,63	1.05	3 (4%)
27	HEM	E	101	6,5	50,50,50	1.28	4 (8%)	67,82,82	0.91	0
24	LHG	A	408	-	48,48,48	0.84	1 (2%)	51,54,54	0.92	2 (3%)
22	CLA	B	603	-	69,73,73	1.26	9 (13%)	82,113,113	2.26	19 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	601	-	3/3/15/20	10/39/115/115	-
22	CLA	B	605	-	2/2/15/20	7/39/115/115	-
22	CLA	B	609	-	2/2/15/20	7/39/115/115	-
23	BCR	K	101	-	-	15/29/63/63	0/2/2/2
22	CLA	B	616	-	4/4/15/20	11/39/115/115	-
22	CLA	C	514	-	3/3/15/20	9/39/115/115	-
22	CLA	C	511	-	3/3/15/20	9/39/115/115	-
22	CLA	C	517	22	3/3/15/20	10/39/115/115	-
22	CLA	A	405	-	2/2/15/20	12/39/115/115	-
22	CLA	B	610	-	2/2/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PL9	D	405	-	-	13/53/73/73	0/1/1/1
22	CLA	C	507	-	2/2/15/20	12/39/115/115	-
22	CLA	B	607	-	2/2/15/20	13/39/115/115	-
23	BCR	B	618	-	-	5/29/63/63	0/2/2/2
22	CLA	C	505	-	1/1/15/20	18/39/115/115	-
25	LMG	C	501	-	-	17/50/70/70	0/1/1/1
23	BCR	H	101	-	-	15/29/63/63	0/2/2/2
22	CLA	B	604	-	1/1/15/20	8/39/115/115	-
22	CLA	A	406	-	2/2/15/20	9/39/115/115	-
22	CLA	B	608	-	-	7/39/115/115	-
23	BCR	B	619	-	-	6/29/63/63	0/2/2/2
25	LMG	F	101	-	-	7/50/70/70	0/1/1/1
22	CLA	C	506	-	3/3/15/20	9/39/115/115	-
22	CLA	D	408	-	3/3/15/20	5/39/115/115	-
23	BCR	B	617	-	-	14/29/63/63	0/2/2/2
23	BCR	C	516	-	-	12/29/63/63	0/2/2/2
22	CLA	B	611	-	1/1/15/20	13/39/115/115	-
25	LMG	C	502	-	-	7/50/70/70	0/1/1/1
22	CLA	B	612	-	4/4/15/20	9/39/115/115	-
22	CLA	B	606	-	2/2/15/20	13/39/115/115	-
23	BCR	A	407	-	-	8/29/63/63	0/2/2/2
22	CLA	C	513	-	3/3/15/20	6/39/115/115	-
22	CLA	D	407	-	2/2/15/20	9/39/115/115	-
23	BCR	C	515	-	-	9/29/63/63	0/2/2/2
22	CLA	C	512	-	1/1/15/20	9/39/115/115	-
21	PHO	D	406	-	1/1/17/22	5/37/103/103	0/5/6/6
22	CLA	B	613	-	3/3/15/20	8/39/115/115	-
22	CLA	D	402	-	2/2/15/20	10/39/115/115	-
22	CLA	C	504	-	2/2/15/20	12/39/115/115	-
25	LMG	I	101	-	-	5/50/70/70	0/1/1/1
21	PHO	A	404	-	1/1/17/22	6/37/103/103	0/5/6/6
22	CLA	C	510	22	1/1/15/20	11/39/115/115	-
22	CLA	B	615	-	3/3/15/20	11/39/115/115	-
22	CLA	C	509	-	2/2/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	C	518	-	-	7/29/63/63	0/2/2/2
22	CLA	D	401	-	-	10/39/115/115	-
25	LMG	D	404	-	-	11/50/70/70	0/1/1/1
25	LMG	3	101	-	-	8/50/70/70	0/1/1/1
22	CLA	C	508	-	1/1/15/20	2/39/115/115	-
22	CLA	B	614	-	3/3/15/20	8/39/115/115	-
22	CLA	C	503	-	-	7/39/115/115	-
22	CLA	B	602	-	2/2/15/20	8/39/115/115	-
23	BCR	F	102	-	-	3/29/63/63	0/2/2/2
25	LMG	D	403	-	-	5/50/70/70	0/1/1/1
27	HEM	E	101	6,5	-	4/14/54/54	-
24	LHG	A	408	-	-	8/53/53/53	-
22	CLA	B	603	-	3/3/15/20	10/39/115/115	-

All (451) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	101	BCR	C1-C6	-10.62	1.40	1.53
21	A	404	PHO	C3B-C4B	10.58	1.52	1.41
23	H	101	BCR	C5-C6	-10.02	1.17	1.34
23	K	101	BCR	C1-C6	-9.78	1.41	1.53
21	D	406	PHO	C1B-C2B	9.70	1.50	1.39
21	A	404	PHO	C1B-C2B	8.67	1.49	1.39
23	K	101	BCR	C5-C6	-8.61	1.20	1.34
21	D	406	PHO	C3B-C4B	8.54	1.50	1.41
23	H	101	BCR	C33-C5	-7.63	1.38	1.50
23	H	101	BCR	C30-C25	-6.95	1.44	1.53
23	K	101	BCR	C30-C25	-6.81	1.45	1.53
23	K	101	BCR	C33-C5	-6.75	1.40	1.50
23	H	101	BCR	C31-C1	-5.51	1.43	1.53
23	K	101	BCR	C31-C1	-5.16	1.44	1.53
22	C	510	CLA	C3D-CAD	4.64	1.61	1.45
22	B	615	CLA	C4B-NB	4.38	1.43	1.37
22	B	609	CLA	C3D-C4D	4.34	1.54	1.44
22	C	514	CLA	C4B-NB	4.34	1.43	1.37
22	B	616	CLA	C3D-C4D	4.31	1.53	1.44
21	A	404	PHO	C1D-C2D	4.26	1.44	1.39
22	C	512	CLA	C4B-NB	4.25	1.43	1.37
22	C	507	CLA	C3D-CAD	4.20	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	C3D-C4D	4.17	1.53	1.44
22	D	408	CLA	C4B-NB	4.15	1.43	1.37
21	D	406	PHO	C1D-C2D	4.15	1.44	1.39
22	B	614	CLA	C3D-CAD	4.10	1.59	1.45
22	C	507	CLA	C3D-C4D	4.10	1.53	1.44
22	B	614	CLA	C3D-C4D	4.09	1.53	1.44
22	C	517	CLA	C3D-CAD	4.08	1.59	1.45
22	C	512	CLA	C3D-C4D	4.02	1.53	1.44
22	B	612	CLA	CMD-C2D	-3.97	1.42	1.50
22	B	602	CLA	CMD-C2D	-3.96	1.42	1.50
22	B	611	CLA	C3D-CAD	3.95	1.58	1.45
22	B	609	CLA	C4B-NB	3.95	1.43	1.37
22	B	613	CLA	C3D-CAD	3.94	1.58	1.45
22	B	616	CLA	C4B-NB	3.92	1.43	1.37
22	C	508	CLA	C3D-CAD	3.91	1.58	1.45
22	C	508	CLA	C4B-NB	3.88	1.43	1.37
23	K	101	BCR	C37-C22	-3.88	1.43	1.50
22	A	405	CLA	C4B-NB	3.86	1.42	1.37
23	H	101	BCR	C37-C22	-3.85	1.43	1.50
22	B	608	CLA	C3D-CAD	3.82	1.58	1.45
22	B	609	CLA	C3D-CAD	3.82	1.58	1.45
22	B	606	CLA	CMD-C2D	-3.79	1.43	1.50
22	C	511	CLA	C4B-NB	3.78	1.42	1.37
22	C	507	CLA	C4B-NB	3.73	1.42	1.37
22	C	508	CLA	C3D-C4D	3.72	1.52	1.44
22	B	601	CLA	C4B-NB	3.64	1.42	1.37
22	C	503	CLA	C4B-NB	3.63	1.42	1.37
22	B	607	CLA	C4B-NB	3.62	1.42	1.37
22	B	608	CLA	C3D-C4D	3.61	1.52	1.44
22	B	610	CLA	C3D-C4D	3.60	1.52	1.44
22	C	512	CLA	C3D-CAD	3.60	1.57	1.45
22	C	513	CLA	C4B-NB	3.59	1.42	1.37
22	C	517	CLA	C3D-C4D	3.58	1.52	1.44
22	B	608	CLA	C4B-NB	3.58	1.42	1.37
22	B	604	CLA	C4B-NB	3.55	1.42	1.37
22	B	613	CLA	C3D-C4D	3.49	1.52	1.44
22	B	602	CLA	CAA-C2A	-3.48	1.47	1.54
22	B	613	CLA	C4B-NB	3.47	1.42	1.37
22	C	517	CLA	C4B-NB	3.47	1.42	1.37
22	D	407	CLA	C4B-NB	3.45	1.42	1.37
23	B	617	BCR	C1-C6	-3.43	1.49	1.53
22	C	513	CLA	CMD-C2D	-3.42	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	514	CLA	C3D-C4D	3.41	1.51	1.44
22	B	611	CLA	C3D-C4D	3.39	1.51	1.44
22	D	401	CLA	C4B-NB	3.38	1.42	1.37
22	C	512	CLA	CMD-C2D	-3.37	1.43	1.50
22	B	616	CLA	CMD-C2D	-3.37	1.43	1.50
22	B	615	CLA	C3D-C4D	3.35	1.51	1.44
22	B	601	CLA	CMD-C2D	-3.35	1.43	1.50
22	D	402	CLA	C4B-NB	3.35	1.42	1.37
21	D	406	PHO	C4D-ND	-3.33	1.33	1.38
22	C	509	CLA	C4B-NB	3.32	1.42	1.37
22	B	614	CLA	C4B-NB	3.32	1.42	1.37
22	B	604	CLA	C3D-C4D	3.31	1.51	1.44
22	B	611	CLA	C4B-NB	3.30	1.42	1.37
22	C	505	CLA	C4B-NB	3.30	1.42	1.37
22	B	605	CLA	C1D-ND	3.28	1.42	1.37
22	C	514	CLA	C3D-CAD	3.27	1.56	1.45
22	B	610	CLA	C4B-NB	3.27	1.42	1.37
22	B	609	CLA	CAA-C2A	-3.27	1.48	1.54
22	C	507	CLA	C1D-C2D	3.27	1.51	1.45
23	K	101	BCR	C32-C1	-3.26	1.47	1.53
22	B	610	CLA	CMD-C2D	-3.26	1.44	1.50
22	B	614	CLA	CAA-C2A	-3.25	1.48	1.54
22	C	510	CLA	C4B-NB	3.25	1.42	1.37
22	C	504	CLA	C1D-ND	3.25	1.42	1.37
22	B	604	CLA	CMD-C2D	-3.23	1.44	1.50
22	B	603	CLA	C1D-ND	3.23	1.42	1.37
22	C	503	CLA	MG-NB	-3.22	1.99	2.05
22	B	613	CLA	CMD-C2D	-3.18	1.44	1.50
22	B	606	CLA	C4B-NB	3.18	1.42	1.37
22	C	510	CLA	C1D-C2D	3.17	1.51	1.45
23	B	619	BCR	C1-C6	-3.17	1.49	1.53
23	B	618	BCR	C30-C25	-3.15	1.49	1.53
22	B	615	CLA	C1D-ND	3.13	1.42	1.37
22	B	609	CLA	C3B-C4B	3.12	1.51	1.42
22	C	506	CLA	C4B-NB	3.11	1.42	1.37
22	B	607	CLA	CMD-C2D	-3.11	1.44	1.50
22	B	611	CLA	CMD-C2D	-3.10	1.44	1.50
22	C	512	CLA	C1B-C2B	3.09	1.50	1.43
26	D	405	PL9	C3-C4	-3.09	1.44	1.49
22	C	509	CLA	CMD-C2D	-3.08	1.44	1.50
22	C	504	CLA	CMD-C2D	-3.08	1.44	1.50
22	B	602	CLA	C3D-C4D	3.08	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	610	CLA	CBD-CAD	3.07	1.69	1.56
23	C	515	BCR	C1-C6	-3.07	1.49	1.53
22	A	405	CLA	C1B-C2B	3.06	1.50	1.43
22	B	603	CLA	CMD-C2D	-3.05	1.44	1.50
22	B	614	CLA	CMD-C2D	-3.05	1.44	1.50
22	C	514	CLA	CAA-C2A	-3.03	1.48	1.54
22	C	505	CLA	C3D-C4D	3.02	1.51	1.44
22	C	507	CLA	C1B-C2B	3.02	1.50	1.43
22	C	509	CLA	C1D-ND	3.01	1.41	1.37
22	D	402	CLA	C1D-ND	3.00	1.41	1.37
22	B	601	CLA	C1B-C2B	3.00	1.50	1.43
22	D	408	CLA	CMD-C2D	-3.00	1.44	1.50
22	C	506	CLA	C1D-ND	2.99	1.41	1.37
22	C	505	CLA	C1D-ND	2.99	1.41	1.37
22	B	602	CLA	C4B-NB	2.99	1.41	1.37
21	A	404	PHO	CMC-C2C	-2.99	1.46	1.50
22	C	511	CLA	C3D-C4D	2.98	1.50	1.44
22	C	503	CLA	CMD-C2D	-2.98	1.44	1.50
22	C	504	CLA	C1B-C2B	2.97	1.50	1.43
22	C	505	CLA	C1B-C2B	2.96	1.50	1.43
22	B	604	CLA	C1B-C2B	2.96	1.50	1.43
22	A	405	CLA	C1D-ND	2.96	1.41	1.37
22	C	509	CLA	C3D-C4D	2.96	1.50	1.44
22	C	504	CLA	C4B-NB	2.96	1.41	1.37
22	B	608	CLA	C1D-ND	2.94	1.41	1.37
22	D	401	CLA	CMD-C2D	-2.92	1.44	1.50
22	C	517	CLA	CMD-C2D	-2.92	1.44	1.50
22	C	511	CLA	CMD-C2D	-2.91	1.44	1.50
22	C	503	CLA	C1D-ND	2.91	1.41	1.37
22	B	615	CLA	CMD-C2D	-2.90	1.44	1.50
22	C	507	CLA	CMD-C2D	-2.88	1.44	1.50
21	D	406	PHO	CMC-C2C	-2.88	1.46	1.50
22	D	407	CLA	C1B-C2B	2.88	1.49	1.43
22	C	513	CLA	CBD-CAD	2.88	1.68	1.56
22	C	512	CLA	C3B-C4B	2.87	1.51	1.42
22	A	406	CLA	MG-ND	-2.87	2.00	2.05
24	A	408	LHG	P-O6	2.87	1.70	1.59
22	A	406	CLA	C1D-ND	2.86	1.41	1.37
22	B	601	CLA	C3D-C4D	2.86	1.50	1.44
22	C	513	CLA	C3D-C4D	2.85	1.50	1.44
23	C	518	BCR	C1-C6	-2.84	1.50	1.53
22	B	609	CLA	CMD-C2D	-2.84	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	406	CLA	C4B-NB	2.84	1.41	1.37
22	D	407	CLA	CMD-C2D	-2.84	1.45	1.50
22	A	406	CLA	CMD-C2D	-2.83	1.45	1.50
22	C	508	CLA	CMD-C2D	-2.83	1.45	1.50
22	A	405	CLA	CMD-C2D	-2.83	1.45	1.50
22	B	612	CLA	C4B-NB	2.83	1.41	1.37
22	B	607	CLA	C1B-C2B	2.82	1.49	1.43
22	C	517	CLA	C1B-C2B	2.82	1.49	1.43
22	B	605	CLA	CMD-C2D	-2.82	1.45	1.50
22	C	514	CLA	CMD-C2D	-2.82	1.45	1.50
22	B	612	CLA	CBD-CAD	2.81	1.68	1.56
22	C	505	CLA	CBD-CAD	2.81	1.68	1.56
22	B	609	CLA	C1B-C2B	2.81	1.49	1.43
22	C	510	CLA	CMD-C2D	-2.80	1.45	1.50
22	C	517	CLA	C1D-C2D	2.79	1.50	1.45
22	B	604	CLA	CBD-CAD	2.79	1.67	1.56
21	D	406	PHO	CMB-C2B	-2.79	1.46	1.51
22	D	407	CLA	C3D-CAD	2.79	1.54	1.45
22	B	616	CLA	CBD-CAD	2.78	1.67	1.56
22	B	616	CLA	C3D-CAD	2.78	1.54	1.45
22	B	615	CLA	C1B-C2B	2.78	1.49	1.43
22	C	506	CLA	CMD-C2D	-2.78	1.45	1.50
21	A	404	PHO	CBD-CGD	-2.77	1.49	1.52
22	B	612	CLA	CHC-C1C	2.77	1.44	1.38
22	C	514	CLA	C3B-C4B	2.77	1.50	1.42
22	B	615	CLA	C3B-C4B	2.77	1.50	1.42
22	C	508	CLA	CHC-C1C	2.76	1.44	1.38
22	B	610	CLA	MG-NC	2.76	2.12	2.06
21	A	404	PHO	C4D-CHA	2.75	1.43	1.39
22	C	514	CLA	C1B-C2B	2.74	1.49	1.43
22	C	509	CLA	C1B-C2B	2.74	1.49	1.43
25	F	101	LMG	C4-C5	2.74	1.58	1.53
22	B	602	CLA	CBD-CAD	2.73	1.67	1.56
22	C	505	CLA	CMD-C2D	-2.73	1.45	1.50
22	C	507	CLA	C1D-ND	2.73	1.41	1.37
22	C	504	CLA	C3D-C4D	2.73	1.50	1.44
22	A	405	CLA	C3B-C4B	2.73	1.50	1.42
22	D	401	CLA	C1B-C2B	2.72	1.49	1.43
22	A	405	CLA	CHC-C1C	2.71	1.43	1.38
22	A	406	CLA	MG-NB	-2.71	2.00	2.05
22	B	615	CLA	CHC-C1C	2.71	1.43	1.38
22	B	605	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	402	CLA	C1D-C2D	2.70	1.50	1.45
26	D	405	PL9	C46-C44	2.70	1.56	1.51
22	C	511	CLA	C3B-C4B	2.69	1.50	1.42
22	B	610	CLA	C1D-ND	2.68	1.41	1.37
22	C	517	CLA	C3B-C4B	2.68	1.50	1.42
22	C	517	CLA	CAA-C2A	-2.68	1.49	1.54
22	C	509	CLA	CBD-CAD	2.67	1.67	1.56
22	C	508	CLA	C3B-C4B	2.67	1.50	1.42
27	E	101	HEM	CAB-C3B	2.66	1.54	1.47
22	C	506	CLA	MG-NB	-2.66	2.00	2.05
22	B	607	CLA	C1D-ND	2.66	1.41	1.37
22	C	510	CLA	CHC-C1C	2.65	1.43	1.38
22	C	512	CLA	CHC-C1C	2.64	1.43	1.38
23	C	518	BCR	C30-C25	-2.64	1.50	1.53
22	C	510	CLA	C1D-ND	2.64	1.41	1.37
22	D	408	CLA	C1B-C2B	2.64	1.49	1.43
21	A	404	PHO	C4D-ND	-2.64	1.34	1.38
22	C	503	CLA	CMB-C2B	-2.64	1.45	1.50
22	B	607	CLA	C3B-C4B	2.64	1.50	1.42
22	B	610	CLA	C3B-C4B	2.63	1.50	1.42
23	H	101	BCR	C32-C1	-2.62	1.48	1.53
22	B	608	CLA	C1D-C2D	2.62	1.50	1.45
22	B	605	CLA	C4B-NB	2.62	1.41	1.37
22	B	612	CLA	MG-NB	-2.62	2.00	2.05
21	A	404	PHO	CAC-C3C	-2.62	1.47	1.51
22	B	602	CLA	C1B-C2B	2.61	1.49	1.43
22	B	616	CLA	C1D-ND	2.61	1.41	1.37
21	D	406	PHO	CAC-C3C	-2.61	1.47	1.51
22	D	402	CLA	CMB-C2B	-2.61	1.45	1.50
22	C	504	CLA	MG-NB	-2.60	2.00	2.05
22	B	612	CLA	MG-ND	-2.60	2.00	2.05
22	B	611	CLA	C3B-C4B	2.59	1.50	1.42
22	B	611	CLA	C1D-C2D	2.59	1.50	1.45
22	C	503	CLA	MG-NA	2.58	2.12	2.06
22	C	517	CLA	CMA-C3A	-2.57	1.47	1.53
21	A	404	PHO	CMB-C2B	-2.56	1.46	1.51
27	E	101	HEM	CAC-C3C	2.56	1.54	1.47
21	A	404	PHO	CMD-C2D	-2.56	1.46	1.51
22	C	504	CLA	CBD-CAD	2.56	1.66	1.56
22	C	506	CLA	CMB-C2B	-2.55	1.45	1.50
22	B	612	CLA	C3D-C4D	2.55	1.49	1.44
27	E	101	HEM	FE-NA	2.55	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	CMD-C2D	-2.54	1.45	1.50
22	B	608	CLA	C3B-C4B	2.54	1.50	1.42
22	D	408	CLA	C3B-C4B	2.54	1.50	1.42
22	B	614	CLA	C1B-C2B	2.54	1.49	1.43
23	C	516	BCR	C30-C25	-2.54	1.50	1.53
22	B	603	CLA	C4B-NB	2.54	1.41	1.37
22	B	604	CLA	C3B-C4B	2.54	1.50	1.42
22	C	514	CLA	CHC-C1C	2.54	1.43	1.38
22	B	611	CLA	CHC-C1C	2.53	1.43	1.38
22	C	511	CLA	CBD-CAD	2.53	1.66	1.56
22	B	613	CLA	C1B-C2B	2.52	1.49	1.43
22	C	503	CLA	MG-ND	-2.52	2.00	2.05
22	C	505	CLA	C3B-C4B	2.52	1.50	1.42
22	B	616	CLA	C3B-C4B	2.51	1.50	1.42
22	C	511	CLA	C1D-ND	2.51	1.41	1.37
22	C	517	CLA	CHC-C1C	2.50	1.43	1.38
22	B	606	CLA	C1B-C2B	2.50	1.49	1.43
23	A	407	BCR	C30-C25	-2.50	1.50	1.53
22	D	407	CLA	CMB-C2B	-2.50	1.45	1.50
22	B	615	CLA	CBD-CAD	2.49	1.66	1.56
22	B	603	CLA	C1B-C2B	2.48	1.49	1.43
22	B	613	CLA	C1D-C2D	2.48	1.50	1.45
22	C	517	CLA	C3A-C2A	-2.47	1.47	1.54
22	D	402	CLA	C3D-C4D	2.47	1.49	1.44
22	B	604	CLA	CMC-C2C	-2.47	1.45	1.50
22	D	401	CLA	CMA-C3A	-2.46	1.48	1.53
22	C	511	CLA	CMB-C2B	-2.45	1.45	1.50
22	C	510	CLA	C1B-C2B	2.45	1.48	1.43
22	C	504	CLA	MG-NA	2.45	2.12	2.06
22	B	603	CLA	C3B-C4B	2.45	1.49	1.42
22	D	401	CLA	CHC-C1C	2.45	1.43	1.38
22	D	402	CLA	C1B-C2B	2.44	1.48	1.43
22	D	407	CLA	C3D-C4D	2.44	1.49	1.44
22	B	612	CLA	C3A-C2A	-2.44	1.47	1.54
22	A	406	CLA	C1B-C2B	2.43	1.48	1.43
22	A	406	CLA	CHC-C1C	2.43	1.43	1.38
22	C	511	CLA	CHC-C1C	2.43	1.43	1.38
22	D	408	CLA	MG-NB	-2.43	2.01	2.05
22	B	616	CLA	C3A-C2A	-2.43	1.47	1.54
22	C	510	CLA	C3B-C4B	2.43	1.49	1.42
22	B	606	CLA	MG-ND	-2.43	2.01	2.05
22	B	610	CLA	MG-NA	2.43	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	CMB-C2B	-2.42	1.45	1.50
22	B	604	CLA	CHC-C1C	2.42	1.43	1.38
22	B	616	CLA	C1B-C2B	2.42	1.48	1.43
22	B	606	CLA	C3B-C4B	2.42	1.49	1.42
22	B	612	CLA	CMA-C3A	-2.41	1.48	1.53
22	B	614	CLA	C3B-C4B	2.41	1.49	1.42
22	C	508	CLA	CMB-C2B	-2.40	1.45	1.50
22	C	517	CLA	C1D-ND	2.40	1.41	1.37
22	B	613	CLA	CMB-C2B	-2.40	1.45	1.50
22	B	608	CLA	CHC-C1C	2.40	1.43	1.38
22	B	605	CLA	C3D-C4D	2.39	1.49	1.44
22	A	406	CLA	C3B-C4B	2.39	1.49	1.42
22	D	408	CLA	C1D-ND	2.39	1.41	1.37
22	C	508	CLA	C1D-ND	2.39	1.41	1.37
22	C	507	CLA	C4C-C3C	2.39	1.49	1.45
22	C	506	CLA	C3D-C4D	2.39	1.49	1.44
22	C	506	CLA	CBD-CAD	2.39	1.66	1.56
22	C	513	CLA	C1B-C2B	2.38	1.48	1.43
22	B	602	CLA	C3B-C4B	2.38	1.49	1.42
22	C	505	CLA	CMC-C2C	-2.38	1.45	1.50
22	B	611	CLA	CMB-C2B	-2.38	1.45	1.50
22	B	612	CLA	C3B-C4B	2.38	1.49	1.42
21	D	406	PHO	CBD-CGD	-2.37	1.49	1.52
25	C	502	LMG	C9-C8	2.37	1.58	1.50
22	D	402	CLA	CMD-C2D	-2.37	1.45	1.50
22	B	610	CLA	MG-NB	-2.37	2.01	2.05
22	B	616	CLA	CHC-C1C	2.36	1.43	1.38
22	B	607	CLA	MG-ND	-2.36	2.01	2.05
22	A	405	CLA	CMC-C2C	-2.36	1.45	1.50
22	B	612	CLA	CMB-C2B	-2.36	1.45	1.50
22	A	405	CLA	C3D-C4D	2.36	1.49	1.44
22	C	513	CLA	C3B-C4B	2.35	1.49	1.42
22	C	506	CLA	C1B-C2B	2.35	1.48	1.43
25	3	101	LMG	O7-C8	-2.34	1.41	1.46
22	D	402	CLA	C3D-CAD	2.34	1.53	1.45
22	B	602	CLA	C1D-ND	2.34	1.40	1.37
22	B	606	CLA	MG-NB	-2.34	2.01	2.05
23	H	101	BCR	C27-C26	-2.34	1.46	1.51
27	E	101	HEM	C2A-C3A	-2.33	1.32	1.38
22	D	402	CLA	C3B-C4B	2.33	1.49	1.42
22	D	407	CLA	C1D-ND	2.32	1.40	1.37
22	C	503	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CMC-C2C	-2.31	1.46	1.50
23	K	101	BCR	C27-C26	-2.31	1.46	1.51
22	B	605	CLA	C3B-C4B	2.30	1.49	1.42
22	D	408	CLA	CHC-C1C	2.30	1.43	1.38
22	C	509	CLA	C3B-C4B	2.29	1.49	1.42
22	B	616	CLA	CMB-C2B	-2.29	1.46	1.50
22	B	613	CLA	C3B-C4B	2.29	1.49	1.42
22	C	507	CLA	C3B-C4B	2.29	1.49	1.42
22	B	614	CLA	CMB-C2B	-2.28	1.46	1.50
22	B	609	CLA	C1D-C2D	2.28	1.49	1.45
21	D	406	PHO	C3B-C2B	-2.28	1.37	1.40
22	B	601	CLA	CAA-C2A	-2.28	1.49	1.54
22	B	609	CLA	C1D-ND	2.28	1.40	1.37
22	C	512	CLA	C1D-ND	2.27	1.40	1.37
22	A	406	CLA	CAA-C2A	-2.26	1.50	1.54
22	B	614	CLA	C2A-C1A	-2.26	1.47	1.52
22	C	514	CLA	C1D-C2D	2.26	1.49	1.45
21	D	406	PHO	CMD-C2D	-2.26	1.47	1.51
22	D	407	CLA	MG-NB	-2.26	2.01	2.05
22	B	601	CLA	CBD-CAD	2.26	1.65	1.56
22	B	603	CLA	CHC-C1C	2.26	1.43	1.38
22	C	507	CLA	CHC-C1C	2.25	1.43	1.38
23	B	619	BCR	C30-C25	-2.25	1.50	1.53
22	B	601	CLA	C1D-ND	2.25	1.40	1.37
22	B	601	CLA	CMB-C2B	-2.24	1.46	1.50
22	B	612	CLA	CAA-C2A	-2.24	1.50	1.54
22	A	406	CLA	CMB-C2B	-2.24	1.46	1.50
22	B	609	CLA	CMB-C2B	-2.23	1.46	1.50
25	D	404	LMG	C3-C2	2.23	1.58	1.52
22	B	606	CLA	CHC-C1C	2.23	1.42	1.38
25	C	502	LMG	C7-C8	2.22	1.57	1.50
22	B	601	CLA	CMC-C2C	-2.22	1.46	1.50
22	C	504	CLA	MG-NC	2.22	2.11	2.06
22	B	612	CLA	C3D-C2D	-2.22	1.32	1.39
22	C	510	CLA	C3C-C2C	2.22	1.41	1.36
22	B	610	CLA	CHC-C1C	2.21	1.42	1.38
23	A	407	BCR	C1-C6	-2.21	1.51	1.53
22	B	607	CLA	CHC-C1C	2.21	1.42	1.38
22	B	610	CLA	CMC-C2C	-2.21	1.46	1.50
22	C	509	CLA	MG-NB	-2.20	2.01	2.05
22	C	512	CLA	C1D-C2D	2.20	1.49	1.45
21	A	404	PHO	C3D-CAD	-2.20	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C1D-ND	2.20	1.40	1.37
22	B	610	CLA	CMB-C2B	-2.19	1.46	1.50
25	D	403	LMG	C3-C2	2.19	1.58	1.52
22	B	601	CLA	C3B-C4B	2.19	1.49	1.42
22	C	507	CLA	MG-NC	2.19	2.11	2.06
22	B	605	CLA	CBD-CAD	2.18	1.65	1.56
22	C	505	CLA	C3D-C2D	-2.18	1.33	1.39
22	C	503	CLA	CHC-C1C	2.18	1.42	1.38
22	D	408	CLA	CMB-C2B	-2.18	1.46	1.50
22	C	503	CLA	MG-NC	2.17	2.11	2.06
22	D	401	CLA	MG-NB	-2.17	2.01	2.05
22	B	606	CLA	CMB-C2B	-2.17	1.46	1.50
22	C	506	CLA	MG-ND	-2.17	2.01	2.05
22	C	509	CLA	C3D-C2D	-2.16	1.33	1.39
22	B	606	CLA	CMC-C2C	-2.16	1.46	1.50
22	B	613	CLA	C1B-NB	-2.16	1.35	1.37
22	B	603	CLA	CMB-C2B	-2.16	1.46	1.50
22	B	610	CLA	C4C-C3C	2.16	1.48	1.45
22	B	613	CLA	C1D-ND	2.16	1.40	1.37
22	D	408	CLA	MG-ND	-2.16	2.01	2.05
23	C	515	BCR	C35-C13	-2.15	1.46	1.50
22	D	401	CLA	CMB-C2B	-2.15	1.46	1.50
22	D	407	CLA	C1D-C2D	2.15	1.49	1.45
26	D	405	PL9	C52-C5	-2.15	1.46	1.50
22	C	506	CLA	O2D-CGD	2.15	1.38	1.33
22	C	508	CLA	C1B-C2B	2.14	1.48	1.43
25	D	404	LMG	C4-C3	2.14	1.57	1.52
22	C	510	CLA	C4C-C3C	2.14	1.48	1.45
22	C	504	CLA	C2A-C1A	2.14	1.57	1.52
22	B	605	CLA	CMC-C2C	-2.13	1.46	1.50
22	C	514	CLA	C1D-ND	2.13	1.40	1.37
22	B	601	CLA	CHC-C1C	2.13	1.42	1.38
22	B	602	CLA	MG-NB	-2.13	2.01	2.05
22	D	401	CLA	C3D-C4D	2.13	1.49	1.44
22	D	407	CLA	C4C-C3C	2.12	1.48	1.45
22	B	616	CLA	OBD-CAD	-2.12	1.18	1.22
25	I	101	LMG	C3-C2	2.12	1.57	1.52
22	C	504	CLA	MG-ND	-2.12	2.01	2.05
23	K	101	BCR	C36-C18	-2.12	1.46	1.50
22	B	602	CLA	C3D-C2D	-2.12	1.33	1.39
22	C	506	CLA	CAA-C2A	-2.12	1.50	1.54
22	B	602	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	617	BCR	C33-C5	-2.12	1.47	1.50
22	B	602	CLA	CMB-C2B	-2.11	1.46	1.50
22	C	504	CLA	CMB-C2B	-2.11	1.46	1.50
22	C	508	CLA	MG-NC	2.11	2.11	2.06
22	B	611	CLA	C1B-C2B	2.11	1.48	1.43
22	C	513	CLA	C1D-ND	2.11	1.40	1.37
22	A	406	CLA	MG-NC	2.11	2.11	2.06
22	D	402	CLA	CHC-C1C	2.11	1.42	1.38
22	C	505	CLA	CHC-C1C	2.11	1.42	1.38
22	C	508	CLA	C1D-C2D	2.11	1.49	1.45
22	C	509	CLA	CHC-C1C	2.10	1.42	1.38
23	H	101	BCR	C36-C18	-2.10	1.46	1.50
22	B	608	CLA	C1B-C2B	2.09	1.48	1.43
22	B	603	CLA	C3D-C4D	2.09	1.48	1.44
22	B	610	CLA	MG-ND	-2.08	2.01	2.05
23	B	618	BCR	C1-C6	-2.08	1.51	1.53
22	A	405	CLA	C3D-CAD	2.08	1.52	1.45
22	B	601	CLA	MG-NB	-2.08	2.01	2.05
22	B	612	CLA	CMC-C2C	-2.07	1.46	1.50
23	H	101	BCR	C29-C30	-2.07	1.49	1.54
22	C	513	CLA	CHC-C1C	2.07	1.42	1.38
22	C	513	CLA	C3A-C2A	-2.07	1.48	1.54
22	D	401	CLA	C3B-C4B	2.07	1.48	1.42
22	B	609	CLA	CBD-CGD	-2.07	1.46	1.52
22	B	613	CLA	CAA-C2A	-2.07	1.50	1.54
22	B	615	CLA	MG-NC	2.07	2.11	2.06
22	C	513	CLA	MG-NB	-2.06	2.01	2.05
22	B	616	CLA	CMA-C3A	-2.06	1.48	1.53
22	B	607	CLA	CBD-CAD	2.05	1.64	1.56
22	B	607	CLA	C3D-C2D	-2.05	1.33	1.39
22	B	604	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	612	CLA	CAB-C3B	-2.04	1.41	1.47
22	B	614	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	614	CLA	C1D-C2D	2.04	1.49	1.45
22	B	603	CLA	MG-NB	-2.04	2.01	2.05
22	B	614	CLA	C1D-ND	2.03	1.40	1.37
22	C	512	CLA	OBD-CAD	-2.03	1.19	1.22
25	F	101	LMG	C4-C3	2.03	1.57	1.52
22	C	507	CLA	CHD-C4C	2.03	1.43	1.39
23	C	516	BCR	C1-C6	-2.03	1.51	1.53
22	B	606	CLA	C3D-C4D	2.03	1.48	1.44
22	B	611	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	LMG	C3-C2	2.02	1.57	1.52
22	C	511	CLA	C1B-C2B	2.01	1.47	1.43
22	C	507	CLA	CMB-C2B	-2.01	1.46	1.50
22	C	510	CLA	CMB-C2B	-2.01	1.46	1.50
25	I	101	LMG	C4-C3	2.01	1.57	1.52
22	B	613	CLA	CHC-C1C	2.00	1.42	1.38
22	B	606	CLA	CBD-CAD	2.00	1.64	1.56
22	C	511	CLA	MG-NB	-2.00	2.01	2.05
21	D	406	PHO	C3D-C4D	2.00	1.44	1.41

All (933) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	C4A-NA-C1A	15.42	113.71	106.68
22	C	505	CLA	C4A-NA-C1A	15.03	113.53	106.68
23	H	101	BCR	C33-C5-C6	-13.60	109.64	124.48
22	B	616	CLA	C4A-NA-C1A	13.07	112.64	106.68
22	B	605	CLA	C4A-NA-C1A	12.58	112.42	106.68
22	B	616	CLA	C4D-C3D-CAD	12.53	121.71	108.11
22	C	517	CLA	C4A-NA-C1A	12.45	112.36	106.68
22	B	603	CLA	C4A-NA-C1A	12.34	112.31	106.68
22	C	512	CLA	C4D-C3D-CAD	12.10	121.25	108.11
22	B	615	CLA	C4A-NA-C1A	11.98	112.14	106.68
22	C	513	CLA	C4A-NA-C1A	11.63	111.98	106.68
22	C	512	CLA	C4A-NA-C1A	11.53	111.94	106.68
23	K	101	BCR	C33-C5-C6	-11.52	111.92	124.48
22	B	609	CLA	C4A-NA-C1A	11.51	111.93	106.68
22	B	601	CLA	C4A-NA-C1A	11.47	111.91	106.68
22	C	511	CLA	C4A-NA-C1A	11.40	111.88	106.68
22	C	510	CLA	C4A-NA-C1A	11.22	111.80	106.68
22	C	507	CLA	C4D-C3D-CAD	10.77	119.80	108.11
22	B	613	CLA	C4A-NA-C1A	10.69	111.56	106.68
22	C	507	CLA	C4A-NA-C1A	10.64	111.53	106.68
22	B	608	CLA	C4A-NA-C1A	10.44	111.44	106.68
22	C	509	CLA	C4A-NA-C1A	10.44	111.44	106.68
22	B	614	CLA	C4A-NA-C1A	10.34	111.40	106.68
22	B	612	CLA	C4A-NA-C1A	10.30	111.38	106.68
22	B	602	CLA	C4A-NA-C1A	10.27	111.36	106.68
22	B	609	CLA	C4D-C3D-CAD	10.08	119.05	108.11
22	B	610	CLA	C4A-NA-C1A	9.92	111.21	106.68
22	C	513	CLA	CAA-C2A-C3A	9.78	139.43	113.00
22	B	606	CLA	C4A-NA-C1A	9.73	111.12	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	C4A-NA-C1A	9.66	111.09	106.68
22	B	607	CLA	C4A-NA-C1A	9.65	111.08	106.68
23	H	101	BCR	C37-C22-C23	-9.61	103.41	118.09
22	C	504	CLA	C4A-NA-C1A	9.53	111.03	106.68
22	D	402	CLA	C4A-NA-C1A	9.52	111.02	106.68
23	K	101	BCR	C37-C22-C23	-9.52	103.55	118.09
22	B	602	CLA	C4D-C3D-CAD	9.51	118.44	108.11
22	B	609	CLA	C3A-C2A-C1A	9.46	115.51	101.34
22	B	610	CLA	C4D-C3D-CAD	9.41	118.33	108.11
22	B	610	CLA	C3A-C2A-C1A	9.26	115.21	101.34
22	C	517	CLA	C4D-C3D-CAD	9.08	117.96	108.11
22	C	509	CLA	C4D-C3D-CAD	9.05	117.94	108.11
22	B	615	CLA	C4D-C3D-CAD	9.03	117.91	108.11
22	B	601	CLA	C4D-C3D-CAD	9.02	117.91	108.11
22	B	614	CLA	C4D-C3D-CAD	9.02	117.90	108.11
22	B	616	CLA	CAA-C2A-C3A	9.01	137.34	113.00
22	C	510	CLA	C4D-C3D-CAD	8.99	117.87	108.11
22	A	405	CLA	C4A-NA-C1A	8.89	110.74	106.68
22	B	612	CLA	C4D-C3D-CAD	8.80	117.67	108.11
22	B	613	CLA	C4D-C3D-CAD	8.79	117.65	108.11
23	H	101	BCR	C1-C6-C5	-8.76	110.67	122.64
22	B	613	CLA	C3A-C2A-C1A	8.75	114.45	101.34
22	B	614	CLA	C3A-C2A-C1A	8.75	114.44	101.34
23	H	101	BCR	C2-C1-C6	8.58	122.90	110.44
22	B	604	CLA	C4D-C3D-CAD	8.50	117.33	108.11
22	B	602	CLA	C3A-C2A-C1A	8.48	114.05	101.34
22	B	612	CLA	CAA-C2A-C3A	8.47	135.88	113.00
23	K	101	BCR	C1-C6-C5	-8.46	111.08	122.64
22	D	408	CLA	C4A-NA-C1A	8.40	110.51	106.68
22	B	611	CLA	C4D-C3D-CAD	8.36	117.19	108.11
22	B	601	CLA	C3A-C2A-C1A	8.30	113.77	101.34
22	B	611	CLA	C4A-NA-C1A	8.23	110.43	106.68
22	A	406	CLA	C2A-C3A-C4A	-8.22	88.59	101.87
22	C	505	CLA	C4D-C3D-CAD	8.16	116.97	108.11
22	C	514	CLA	C4A-NA-C1A	8.16	110.40	106.68
22	B	606	CLA	C4D-C3D-CAD	8.14	116.94	108.11
23	K	101	BCR	C37-C22-C21	-8.13	109.65	122.82
22	D	401	CLA	C4A-NA-C1A	8.12	110.39	106.68
22	C	511	CLA	C3A-C2A-C1A	8.12	113.50	101.34
22	B	608	CLA	C4D-C3D-CAD	8.07	116.88	108.11
22	C	511	CLA	C4D-C3D-CAD	8.02	116.81	108.11
23	K	101	BCR	C2-C1-C6	7.98	122.04	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	C4D-C3D-CAD	7.93	116.72	108.11
22	C	514	CLA	C4D-C3D-CAD	7.92	116.71	108.11
23	H	101	BCR	C37-C22-C21	-7.86	110.08	122.82
22	C	506	CLA	C3A-C2A-C1A	7.84	113.08	101.34
22	C	505	CLA	C1D-ND-C4D	-7.83	100.82	106.31
22	C	517	CLA	CAA-C2A-C3A	7.82	134.13	113.00
22	D	407	CLA	C4A-NA-C1A	7.70	110.19	106.68
22	C	508	CLA	C4A-NA-C1A	7.45	110.08	106.68
21	A	404	PHO	C4D-CHA-CBD	-7.41	104.90	108.45
22	C	514	CLA	C3A-C2A-C1A	7.39	112.41	101.34
22	A	406	CLA	C2A-C1A-CHA	7.36	136.63	123.87
22	B	610	CLA	C2A-C1A-CHA	7.23	136.42	123.87
23	H	101	BCR	C32-C1-C6	-7.21	98.94	110.24
22	C	507	CLA	C3A-C2A-C1A	7.20	112.13	101.34
22	B	615	CLA	C3A-C2A-C1A	7.15	112.04	101.34
22	C	513	CLA	C4D-C3D-CAD	7.11	115.83	108.11
21	D	406	PHO	C4D-CHA-CBD	-7.08	105.06	108.45
22	C	509	CLA	C3A-C2A-C1A	6.96	111.77	101.34
22	B	604	CLA	CAA-C2A-C3A	6.90	131.66	113.00
22	B	612	CLA	C3B-C4B-NB	-6.90	104.37	110.53
22	C	504	CLA	C4D-C3D-CAD	6.84	115.53	108.11
22	B	603	CLA	C3A-C2A-C1A	6.70	111.38	101.34
22	A	406	CLA	C3A-C2A-C1A	6.70	111.37	101.34
22	C	509	CLA	C2A-C1A-CHA	6.69	135.48	123.87
22	C	506	CLA	C2A-C1A-CHA	6.60	135.32	123.87
21	D	406	PHO	C2B-C1B-NB	-6.57	104.68	109.43
22	B	616	CLA	C2A-C1A-CHA	6.55	135.23	123.87
22	C	507	CLA	C3D-C2D-C1D	6.54	114.76	105.83
22	D	408	CLA	CAA-C2A-C3A	6.53	130.64	113.00
22	A	406	CLA	CAA-C2A-C3A	6.52	130.62	113.00
22	C	511	CLA	C2A-C1A-CHA	6.40	134.98	123.87
22	C	510	CLA	C3D-C2D-C1D	6.34	114.48	105.83
22	B	605	CLA	C4D-C3D-CAD	6.33	114.98	108.11
22	B	614	CLA	C6-C7-C8	-6.24	95.24	115.97
22	B	613	CLA	C3D-C2D-C1D	6.23	114.33	105.83
22	C	512	CLA	C3A-C2A-C1A	6.21	110.64	101.34
22	C	513	CLA	C2A-C1A-CHA	6.16	134.56	123.87
22	B	610	CLA	C2A-C3A-C4A	-6.15	91.94	101.87
22	D	408	CLA	C3A-C2A-C1A	6.10	110.48	101.34
22	C	505	CLA	C3A-C2A-C1A	6.07	110.43	101.34
22	C	517	CLA	CHB-C4A-NA	6.06	133.15	124.40
22	B	611	CLA	C3D-C2D-C1D	6.05	114.09	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	C4D-C3D-CAD	6.05	114.68	108.11
22	D	402	CLA	C3A-C2A-C1A	6.02	110.36	101.34
22	D	408	CLA	C3B-C4B-NB	-6.02	105.16	110.53
22	B	612	CLA	C6-C7-C8	-6.02	95.96	115.97
22	B	604	CLA	CMA-C3A-C2A	6.01	137.22	113.98
22	B	616	CLA	CMA-C3A-C4A	6.00	127.89	111.77
22	C	512	CLA	C3D-C2D-C1D	5.96	113.96	105.83
22	C	517	CLA	CMA-C3A-C2A	5.89	136.74	113.98
22	B	614	CLA	C3D-C2D-C1D	5.82	113.78	105.83
22	B	612	CLA	C2A-C1A-CHA	5.81	133.94	123.87
22	B	613	CLA	C2A-C1A-CHA	5.77	133.88	123.87
22	D	401	CLA	C4D-C3D-CAD	5.77	114.38	108.11
22	B	601	CLA	C2A-C1A-CHA	5.76	133.87	123.87
22	C	508	CLA	CBA-CAA-C2A	5.75	130.91	113.79
22	C	517	CLA	C3D-C2D-C1D	5.75	113.68	105.83
22	C	503	CLA	C4D-C3D-CAD	5.75	114.35	108.11
23	H	101	BCR	C2-C3-C4	-5.70	98.74	111.28
23	K	101	BCR	C2-C3-C4	-5.69	98.76	111.28
22	C	510	CLA	C3D-C4D-ND	5.69	119.24	109.99
22	B	610	CLA	CBA-CAA-C2A	5.68	130.70	113.79
22	B	602	CLA	C2A-C1A-CHA	5.66	133.70	123.87
22	D	402	CLA	CAA-C2A-C3A	5.66	128.28	113.00
23	H	101	BCR	C31-C1-C6	-5.65	101.38	110.24
22	B	608	CLA	C6-C7-C8	-5.65	97.19	115.97
22	B	607	CLA	C4D-C3D-CAD	5.64	114.23	108.11
22	C	513	CLA	CMA-C3A-C2A	5.64	135.77	113.98
22	B	604	CLA	CHB-C4A-NA	5.63	132.53	124.40
23	K	101	BCR	C32-C1-C6	-5.63	101.42	110.24
22	B	609	CLA	C2A-C1A-CHA	5.63	133.63	123.87
23	K	101	BCR	C31-C1-C6	-5.60	101.46	110.24
22	B	612	CLA	CMA-C3A-C2A	5.58	135.54	113.98
22	C	504	CLA	CBA-CAA-C2A	5.56	130.32	113.79
22	B	609	CLA	C3D-C2D-C1D	5.55	113.41	105.83
22	C	514	CLA	C6-C7-C8	-5.54	97.56	115.97
22	C	503	CLA	C4A-NA-C1A	5.49	109.18	106.68
22	B	610	CLA	CAC-C3C-C4C	5.49	131.93	124.79
22	C	507	CLA	C6-C7-C8	-5.45	97.83	115.97
22	B	610	CLA	OBD-CAD-C3D	5.44	141.13	128.42
22	A	405	CLA	C4D-C3D-CAD	5.43	114.01	108.11
22	C	509	CLA	C2A-C3A-C4A	-5.35	93.23	101.87
22	B	610	CLA	C3B-C4B-NB	-5.35	105.75	110.53
22	D	402	CLA	C2A-C3A-C4A	-5.34	93.24	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	CMA-C3A-C2A	5.33	134.59	113.98
22	D	408	CLA	CBA-CAA-C2A	5.28	129.49	113.79
22	C	517	CLA	C3D-C4D-ND	5.28	118.56	109.99
22	B	616	CLA	OBD-CAD-C3D	5.27	140.73	128.42
23	H	101	BCR	C1-C6-C7	5.24	129.86	115.65
22	B	602	CLA	OBD-CAD-C3D	5.24	140.65	128.42
22	C	503	CLA	C3B-C4B-NB	-5.22	105.87	110.53
22	C	508	CLA	C3B-C4B-NB	-5.20	105.89	110.53
22	A	406	CLA	C3B-C4B-NB	-5.16	105.92	110.53
22	A	405	CLA	C3A-C2A-C1A	5.14	109.04	101.34
22	C	508	CLA	C3D-C4D-ND	5.14	118.34	109.99
22	A	406	CLA	C4A-NA-C1A	5.11	109.01	106.68
22	D	402	CLA	CBA-CAA-C2A	5.11	128.99	113.79
22	C	506	CLA	O2D-CGD-CBD	5.11	120.16	111.23
22	C	510	CLA	CHB-C4A-NA	5.06	131.71	124.40
22	C	512	CLA	C3D-C4D-ND	5.03	118.16	109.99
22	B	615	CLA	C2A-C1A-CHA	5.03	132.59	123.87
22	B	614	CLA	C3D-C4D-ND	5.02	118.14	109.99
22	C	510	CLA	CBA-CAA-C2A	5.02	128.72	113.79
22	C	506	CLA	C2A-C3A-C4A	-5.00	93.80	101.87
22	C	507	CLA	C3D-C4D-ND	4.99	118.10	109.99
22	B	611	CLA	C3D-C4D-ND	4.97	118.06	109.99
22	B	603	CLA	C4D-C3D-CAD	4.97	113.50	108.11
22	A	405	CLA	CAA-C2A-C3A	4.96	126.41	113.00
22	B	608	CLA	C3D-C2D-C1D	4.94	112.58	105.83
22	C	511	CLA	OBD-CAD-C3D	4.93	139.94	128.42
22	B	616	CLA	C3D-C2D-C1D	4.91	112.53	105.83
23	K	101	BCR	C1-C6-C7	4.90	128.94	115.65
22	D	407	CLA	C4D-C3D-CAD	4.90	113.42	108.11
22	B	615	CLA	OBD-CAD-C3D	4.89	139.86	128.42
22	B	609	CLA	C2A-C3A-C4A	-4.87	94.00	101.87
22	B	611	CLA	C3B-C4B-NB	-4.87	106.19	110.53
22	C	513	CLA	CMA-C3A-C4A	4.86	124.82	111.77
22	B	603	CLA	C2A-C1A-CHA	4.84	132.27	123.87
22	B	610	CLA	C6-C7-C8	-4.84	99.88	115.97
22	C	512	CLA	C1D-ND-C4D	-4.84	102.92	106.31
22	C	507	CLA	CAA-C2A-C3A	4.84	126.06	113.00
22	C	514	CLA	C3D-C2D-C1D	4.83	112.42	105.83
22	B	608	CLA	C3D-C4D-ND	4.81	117.81	109.99
22	C	509	CLA	OBD-CAD-C3D	4.78	139.58	128.42
22	B	607	CLA	C2A-C1A-CHA	4.73	132.08	123.87
22	C	511	CLA	C2A-C3A-C4A	-4.71	94.26	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	OBD-CAD-C3D	4.70	139.40	128.42
22	B	616	CLA	CMA-C3A-C2A	4.70	132.14	113.98
22	C	517	CLA	O2D-CGD-CBD	4.67	119.40	111.23
22	B	612	CLA	CHB-C4A-NA	4.67	131.14	124.40
22	C	510	CLA	C11-C10-C8	4.66	131.47	115.97
22	D	407	CLA	C3D-C2D-C1D	4.66	112.19	105.83
22	C	508	CLA	C3D-C2D-C1D	4.66	112.19	105.83
22	B	612	CLA	OBD-CAD-C3D	4.63	139.24	128.42
22	B	607	CLA	C3A-C2A-C1A	4.63	108.27	101.34
22	C	513	CLA	CHB-C4A-NA	4.63	131.08	124.40
22	B	607	CLA	CAA-C2A-C1A	4.60	127.06	111.97
22	B	612	CLA	CMA-C3A-C4A	4.59	124.11	111.77
22	A	406	CLA	CBA-CAA-C2A	4.57	127.38	113.79
22	C	503	CLA	CBA-CAA-C2A	4.56	127.36	113.79
22	C	506	CLA	CAA-C2A-C3A	4.56	125.31	113.00
23	H	101	BCR	C23-C22-C21	4.56	126.17	119.01
22	C	505	CLA	OBD-CAD-C3D	4.55	139.05	128.42
22	C	506	CLA	O2D-CGD-O1D	-4.54	115.02	123.85
22	B	601	CLA	CAA-C2A-C3A	4.50	125.15	113.00
22	C	514	CLA	C3D-C4D-ND	4.50	117.30	109.99
22	C	504	CLA	O2D-CGD-O1D	-4.48	115.13	123.85
22	D	402	CLA	C2A-C1A-CHA	4.48	131.63	123.87
22	C	511	CLA	C3B-C4B-NB	-4.47	106.54	110.53
22	B	613	CLA	C3D-C4D-ND	4.47	117.25	109.99
22	B	610	CLA	CAA-C2A-C3A	4.45	125.03	113.00
22	C	509	CLA	CAA-C2A-C3A	4.44	124.99	113.00
22	B	608	CLA	C3B-C4B-NB	-4.41	106.60	110.53
23	K	101	BCR	C23-C22-C21	4.40	125.93	119.01
22	D	401	CLA	CHB-C4A-NA	4.40	130.75	124.40
22	B	605	CLA	C3A-C2A-C1A	4.39	107.91	101.34
22	B	616	CLA	C1D-ND-C4D	-4.37	103.25	106.31
22	B	601	CLA	C3B-C4B-NB	-4.34	106.65	110.53
22	B	608	CLA	CAA-C2A-C3A	4.32	124.67	113.00
22	C	510	CLA	CMA-C3A-C2A	4.31	130.66	113.98
22	C	512	CLA	C3B-C4B-NB	-4.30	106.69	110.53
22	C	507	CLA	CBA-CAA-C2A	4.29	126.55	113.79
22	C	514	CLA	C3B-C4B-NB	-4.28	106.71	110.53
23	H	101	BCR	C4-C5-C6	4.28	128.48	122.70
22	C	513	CLA	C3B-C4B-NB	-4.26	106.73	110.53
22	B	604	CLA	C2A-C1A-CHA	4.25	131.24	123.87
22	B	601	CLA	CBA-CAA-C2A	4.25	126.43	113.79
22	B	604	CLA	OBD-CAD-C3D	4.23	138.31	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	C6-C5-C3	4.22	123.74	113.47
22	C	510	CLA	CBC-CAC-C3C	4.21	123.84	112.42
22	B	603	CLA	C3B-C4B-NB	-4.21	106.78	110.53
23	B	618	BCR	C2-C1-C6	4.20	116.54	110.44
22	C	508	CLA	C1D-ND-C4D	-4.20	103.36	106.31
22	B	609	CLA	C3D-C4D-ND	4.20	116.81	109.99
22	B	608	CLA	CAA-C2A-C1A	4.19	125.71	111.97
22	B	616	CLA	CHB-C4A-NA	4.19	130.44	124.40
22	B	608	CLA	C9-C8-C10	4.12	125.95	111.27
22	B	606	CLA	C3B-C4B-NB	-4.11	106.86	110.53
22	B	613	CLA	C2A-C3A-C4A	-4.11	95.23	101.87
23	K	101	BCR	C20-C21-C22	-4.11	121.52	127.28
22	C	517	CLA	C2A-C1A-CHA	4.10	130.99	123.87
22	D	407	CLA	C2D-C1D-ND	-4.09	106.08	110.13
22	B	603	CLA	CAA-C2A-C3A	4.09	124.05	113.00
22	B	611	CLA	CMA-C3A-C2A	-4.08	98.20	113.98
22	B	605	CLA	CAA-C2A-C1A	4.08	125.34	111.97
22	B	608	CLA	CHB-C4A-NA	4.08	130.28	124.40
22	B	614	CLA	C2A-C1A-CHA	4.07	130.93	123.87
22	B	615	CLA	C3B-C4B-NB	-4.06	106.90	110.53
22	C	514	CLA	CAA-C2A-C3A	4.06	123.97	113.00
23	K	101	BCR	C39-C30-C25	-4.05	103.89	110.24
22	C	509	CLA	C3B-C4B-NB	-4.04	106.92	110.53
22	C	504	CLA	C2A-C1A-CHA	4.04	130.87	123.87
22	B	613	CLA	C2D-C1D-ND	-4.04	106.13	110.13
22	C	506	CLA	OBD-CAD-C3D	4.03	137.83	128.42
22	C	507	CLA	C2D-C1D-ND	-4.02	106.15	110.13
22	D	402	CLA	C4D-C3D-CAD	4.01	112.47	108.11
22	C	511	CLA	CAA-C2A-C3A	4.00	123.81	113.00
21	D	406	PHO	CBC-CAC-C3C	4.00	118.60	112.87
23	H	101	BCR	C7-C8-C9	-4.00	120.32	126.23
22	D	401	CLA	C2A-C3A-C4A	4.00	108.33	101.87
22	B	612	CLA	CBA-CAA-C2A	3.99	125.67	113.79
22	B	609	CLA	CGD-CBD-CAD	-3.99	97.92	110.85
22	C	513	CLA	C11-C10-C8	3.98	129.21	115.97
23	K	101	BCR	C4-C5-C6	3.98	128.09	122.70
22	B	616	CLA	C3D-C4D-ND	3.98	116.46	109.99
22	C	506	CLA	CBA-CAA-C2A	3.98	125.64	113.79
23	H	101	BCR	C39-C30-C25	-3.98	104.00	110.24
22	B	606	CLA	C3A-C2A-C1A	3.97	107.29	101.34
22	B	611	CLA	C2D-C1D-ND	-3.96	106.20	110.13
22	C	505	CLA	C2A-C1A-CHA	3.95	130.73	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C3A-C2A-C1A	3.95	107.26	101.34
22	B	616	CLA	C3B-C4B-NB	-3.95	107.00	110.53
26	D	405	PL9	C7-C3-C4	3.94	120.16	116.91
22	D	408	CLA	C2A-C1A-CHA	3.94	130.70	123.87
22	D	407	CLA	CMA-C3A-C2A	-3.93	98.79	113.98
22	C	510	CLA	C3B-C4B-NB	-3.92	107.03	110.53
24	A	408	LHG	O4-P-O5	3.92	130.68	112.44
22	B	608	CLA	C2A-C1A-CHA	3.90	130.64	123.87
22	B	605	CLA	OBD-CAD-C3D	3.90	137.53	128.42
22	B	611	CLA	C6-C7-C8	-3.90	103.02	115.97
22	B	612	CLA	O2D-CGD-O1D	-3.89	116.27	123.85
22	C	513	CLA	O2D-CGD-O1D	-3.89	116.27	123.85
22	C	504	CLA	OBD-CAD-C3D	3.89	137.51	128.42
22	B	615	CLA	CAA-C2A-C3A	3.87	123.47	113.00
23	H	101	BCR	C33-C5-C4	3.87	121.86	113.60
22	C	517	CLA	C6-C7-C8	-3.87	103.09	115.97
22	C	507	CLA	CGD-CBD-CAD	-3.87	98.32	110.85
22	C	504	CLA	C3B-C4B-NB	-3.86	107.08	110.53
22	B	605	CLA	CMA-C3A-C2A	-3.86	99.06	113.98
22	B	614	CLA	C3B-C4B-NB	-3.85	107.10	110.53
22	B	601	CLA	OBD-CAD-C3D	3.84	137.40	128.42
22	C	505	CLA	CMD-C2D-C1D	3.84	131.49	124.73
22	B	609	CLA	CAA-C2A-C3A	3.84	123.37	113.00
22	B	603	CLA	CAA-C2A-C1A	3.84	124.54	111.97
22	D	407	CLA	CAA-C2A-C3A	3.83	123.36	113.00
22	C	506	CLA	C3B-C4B-NB	-3.83	107.11	110.53
22	B	611	CLA	CAC-C3C-C4C	3.82	129.76	124.79
22	B	616	CLA	C11-C10-C8	3.82	128.66	115.97
22	B	607	CLA	C3B-C4B-NB	-3.82	107.12	110.53
22	B	606	CLA	CBA-CAA-C2A	3.82	125.16	113.79
22	C	504	CLA	O2D-CGD-CBD	3.81	117.89	111.23
23	H	101	BCR	C20-C21-C22	-3.81	121.94	127.28
22	B	602	CLA	C3B-C4B-NB	-3.81	107.13	110.53
22	A	405	CLA	C3B-C4B-NB	-3.81	107.13	110.53
22	B	615	CLA	CAA-C2A-C1A	3.80	124.44	111.97
22	C	512	CLA	CAA-C2A-C3A	3.80	123.26	113.00
22	D	407	CLA	CAA-C2A-C1A	3.79	124.39	111.97
22	B	615	CLA	C11-C10-C8	-3.79	103.38	115.97
22	C	514	CLA	CGD-CBD-CAD	-3.79	98.59	110.85
23	K	101	BCR	C7-C8-C9	-3.76	120.67	126.23
22	C	503	CLA	CHB-C1B-NB	3.75	129.68	124.05
22	B	609	CLA	C3B-C4B-NB	-3.74	107.19	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	CBA-CAA-C2A	3.73	124.91	113.79
22	B	608	CLA	CBA-CAA-C2A	3.73	124.90	113.79
22	B	605	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
22	B	604	CLA	C1D-ND-C4D	-3.73	103.69	106.31
22	C	517	CLA	CMA-C3A-C4A	3.73	121.80	111.77
22	B	606	CLA	O2D-CGD-O1D	-3.72	116.60	123.85
22	B	613	CLA	C4D-CHA-C1A	-3.70	116.83	121.24
22	C	512	CLA	CMD-C2D-C3D	-3.70	119.21	127.69
22	B	616	CLA	CMD-C2D-C3D	-3.70	119.21	127.69
22	B	606	CLA	C6-C5-C3	3.70	122.47	113.47
21	A	404	PHO	C2B-C1B-NB	-3.69	106.76	109.43
22	B	614	CLA	C11-C10-C8	3.69	128.23	115.97
22	B	602	CLA	CAC-C3C-C4C	3.69	129.59	124.79
22	B	602	CLA	C2A-C3A-C4A	-3.68	95.92	101.87
21	D	406	PHO	C9-C8-C7	3.68	124.39	111.27
22	C	511	CLA	CAC-C3C-C4C	3.67	129.56	124.79
22	D	401	CLA	C3D-C4D-ND	3.66	115.94	109.99
22	C	508	CLA	CMA-C3A-C2A	-3.66	99.84	113.98
22	D	401	CLA	CMA-C3A-C2A	3.66	128.11	113.98
23	H	101	BCR	C23-C24-C25	-3.65	117.25	127.00
22	C	510	CLA	C2D-C1D-ND	-3.64	106.52	110.13
22	D	401	CLA	CBA-CAA-C2A	3.64	124.63	113.79
26	D	405	PL9	C36-C34-C33	-3.64	113.00	121.17
22	B	603	CLA	OBD-CAD-C3D	3.63	136.90	128.42
22	B	612	CLA	CAA-C2A-C1A	3.62	123.83	111.97
23	K	101	BCR	C36-C18-C17	-3.62	116.96	122.82
22	C	503	CLA	C11-C10-C8	3.61	127.97	115.97
23	K	101	BCR	C23-C24-C25	-3.61	117.36	127.00
23	H	101	BCR	C36-C18-C17	-3.60	116.98	122.82
22	B	602	CLA	CAA-C2A-C3A	3.60	122.73	113.00
23	K	101	BCR	C16-C17-C18	-3.60	122.23	127.28
23	H	101	BCR	C16-C17-C18	-3.59	122.24	127.28
22	A	405	CLA	C3D-C2D-C1D	3.59	110.73	105.83
22	C	512	CLA	OBD-CAD-C3D	3.57	136.77	128.42
22	C	517	CLA	C3B-C4B-NB	-3.57	107.34	110.53
22	C	514	CLA	C2A-C1A-CHA	3.56	130.05	123.87
22	C	503	CLA	CAA-C2A-C3A	3.54	122.57	113.00
23	B	619	BCR	C32-C1-C6	-3.53	104.70	110.24
22	B	605	CLA	CMD-C2D-C1D	3.52	130.93	124.73
22	B	608	CLA	CMA-C3A-C4A	3.52	121.24	111.77
22	A	405	CLA	CAC-C3C-C4C	3.52	129.37	124.79
23	C	515	BCR	C30-C25-C26	-3.51	117.84	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	CAA-C2A-C1A	3.50	123.46	111.97
22	B	615	CLA	C1-O2A-CGA	3.50	125.12	116.65
22	D	402	CLA	C6-C7-C8	-3.50	104.34	115.97
22	B	601	CLA	C2A-C3A-C4A	-3.49	96.24	101.87
22	C	512	CLA	CAA-C2A-C1A	3.48	123.39	111.97
22	B	606	CLA	C2A-C1A-CHA	3.47	129.89	123.87
22	B	607	CLA	CAA-C2A-C3A	3.47	122.37	113.00
22	D	407	CLA	C3D-C4D-ND	3.47	115.62	109.99
22	B	604	CLA	C3B-C4B-NB	-3.46	107.44	110.53
22	D	408	CLA	C2A-C3A-C4A	-3.45	96.30	101.87
22	B	605	CLA	C2A-C1A-CHA	3.44	129.84	123.87
21	D	406	PHO	C3B-C4B-NB	-3.44	105.22	107.46
22	C	509	CLA	CAA-C2A-C1A	3.44	123.24	111.97
23	H	101	BCR	C38-C26-C25	3.43	128.23	124.48
22	B	607	CLA	O2D-CGD-O1D	-3.43	117.16	123.85
22	D	401	CLA	CAA-C2A-C1A	3.43	123.22	111.97
22	D	402	CLA	C3D-C4D-ND	3.43	115.56	109.99
22	B	616	CLA	CBA-CAA-C2A	3.43	123.98	113.79
22	D	402	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
22	D	401	CLA	C3D-C2D-C1D	3.42	110.50	105.83
22	C	507	CLA	C2A-C1A-CHA	3.42	129.80	123.87
22	B	615	CLA	O2A-C1-C2	-3.42	94.96	108.11
22	D	407	CLA	C3B-C4B-NB	-3.41	107.49	110.53
22	D	401	CLA	C3B-C4B-NB	-3.41	107.49	110.53
22	C	514	CLA	CBA-CAA-C2A	3.40	123.91	113.79
22	B	606	CLA	OBD-CAD-C3D	3.39	136.33	128.42
22	B	614	CLA	C2A-C3A-C4A	-3.38	96.41	101.87
22	B	602	CLA	C3D-C2D-C1D	3.37	110.43	105.83
21	A	404	PHO	CMB-C2B-C3B	3.37	131.41	124.68
22	D	401	CLA	CMA-C3A-C4A	3.36	120.81	111.77
22	B	613	CLA	CAA-C2A-C3A	3.36	122.08	113.00
22	C	514	CLA	C11-C10-C8	3.36	127.13	115.97
23	B	617	BCR	C1-C6-C5	-3.36	118.05	122.64
22	C	503	CLA	C3A-C2A-C1A	3.36	106.37	101.34
22	B	612	CLA	O2D-CGD-CBD	3.34	117.07	111.23
22	C	517	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
22	B	606	CLA	CAA-C2A-C1A	3.34	122.90	111.97
23	K	101	BCR	C16-C15-C14	-3.33	116.70	123.52
22	B	613	CLA	CAC-C3C-C4C	3.33	129.12	124.79
22	B	604	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
22	B	607	CLA	OBD-CAD-C3D	3.32	136.17	128.42
22	B	605	CLA	CHB-C4A-NA	3.32	129.19	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	C9-C8-C10	3.31	123.08	111.27
23	H	101	BCR	C16-C15-C14	-3.31	116.75	123.52
22	C	504	CLA	C6-C7-C8	3.30	126.95	115.97
22	B	601	CLA	C11-C10-C8	3.30	126.95	115.97
22	B	611	CLA	O2A-C1-C2	3.30	120.82	108.11
23	K	101	BCR	C38-C26-C25	3.30	128.09	124.48
22	D	408	CLA	C4D-C3D-CAD	3.28	111.67	108.11
21	A	404	PHO	C9-C8-C7	3.28	122.97	111.27
22	C	517	CLA	CAA-C2A-C1A	3.28	122.72	111.97
22	D	402	CLA	C3B-C4B-NB	-3.28	107.60	110.53
22	B	607	CLA	C6-C7-C8	3.27	126.84	115.97
22	C	511	CLA	CAA-C2A-C1A	3.27	122.68	111.97
22	C	512	CLA	C2A-C1A-CHA	3.26	129.53	123.87
22	C	503	CLA	CAA-C2A-C1A	3.26	122.67	111.97
23	H	101	BCR	C29-C28-C27	-3.26	104.11	111.28
22	B	605	CLA	C3B-C4B-NB	-3.25	107.63	110.53
22	B	606	CLA	C7-C6-C5	-3.25	104.61	113.26
22	C	508	CLA	C3A-C2A-C1A	3.24	106.19	101.34
23	K	101	BCR	C29-C28-C27	-3.24	104.16	111.28
22	B	614	CLA	C1D-ND-C4D	-3.23	104.05	106.31
22	C	504	CLA	CAA-C2A-C1A	3.23	122.55	111.97
22	C	517	CLA	C1D-ND-C4D	-3.23	104.05	106.31
22	C	503	CLA	CMD-C2D-C1D	3.22	130.40	124.73
22	A	405	CLA	C9-C8-C10	3.21	122.71	111.27
22	C	510	CLA	O1D-CGD-CBD	3.20	130.84	124.52
22	C	507	CLA	C2A-C3A-C4A	-3.20	96.70	101.87
22	C	505	CLA	CAA-C2A-C3A	3.20	121.63	113.00
22	C	505	CLA	CHB-C4A-NA	3.19	129.00	124.40
22	C	509	CLA	CMD-C2D-C1D	3.19	130.34	124.73
22	B	610	CLA	C3D-C2D-C1D	3.19	110.18	105.83
22	B	611	CLA	C11-C10-C8	3.18	126.53	115.97
22	B	608	CLA	CHB-C1B-NB	3.18	128.82	124.05
23	B	617	BCR	C39-C30-C25	3.18	115.22	110.24
22	C	511	CLA	C4-C3-C5	3.18	120.74	115.23
22	B	611	CLA	C1-C2-C3	3.17	131.39	126.20
22	C	508	CLA	CAA-C2A-C3A	3.17	121.56	113.00
21	D	406	PHO	C3D-C4D-ND	3.17	111.77	107.71
22	D	402	CLA	C4-C3-C2	-3.16	115.50	123.63
22	D	408	CLA	C6-C7-C8	3.16	126.47	115.97
25	C	501	LMG	C3-C4-C5	-3.16	104.51	110.23
22	B	612	CLA	C3D-C2D-C1D	3.15	110.13	105.83
22	D	401	CLA	C9-C8-C7	3.15	122.49	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	C4D-CHA-C1A	-3.14	117.49	121.24
22	C	512	CLA	C11-C10-C8	3.14	126.40	115.97
22	D	408	CLA	C9-C8-C7	3.14	122.45	111.27
23	C	518	BCR	C2-C1-C6	3.13	114.98	110.44
23	C	518	BCR	C30-C25-C26	-3.12	118.37	122.64
22	B	608	CLA	C1D-ND-C4D	-3.11	104.13	106.31
22	C	505	CLA	C6-C7-C8	-3.11	105.62	115.97
22	A	405	CLA	C3D-C4D-ND	3.11	115.04	109.99
22	B	611	CLA	C3A-C2A-C1A	3.11	105.99	101.34
22	C	514	CLA	C1D-ND-C4D	-3.10	104.14	106.31
22	B	612	CLA	C9-C8-C10	3.09	122.30	111.27
22	D	401	CLA	C1D-ND-C4D	-3.09	104.14	106.31
22	B	616	CLA	C6-C7-C8	3.09	126.23	115.97
22	B	614	CLA	CAA-C2A-C3A	3.08	121.33	113.00
22	B	601	CLA	C9-C8-C10	3.08	122.26	111.27
22	B	615	CLA	CMD-C2D-C1D	3.08	130.15	124.73
22	C	512	CLA	CBA-CAA-C2A	3.07	122.94	113.79
22	C	511	CLA	CBA-CAA-C2A	3.07	122.92	113.79
22	D	402	CLA	C3D-C2D-C1D	3.06	110.01	105.83
22	B	602	CLA	CBA-CAA-C2A	3.06	122.89	113.79
22	B	613	CLA	CHD-C4C-C3C	3.06	129.23	124.77
22	B	614	CLA	CMD-C2D-C1D	-3.05	119.35	124.73
22	C	512	CLA	O1D-CGD-CBD	3.05	130.54	124.52
22	D	408	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
22	B	604	CLA	CBA-CAA-C2A	3.05	122.86	113.79
22	B	615	CLA	CBA-CAA-C2A	3.04	122.85	113.79
22	C	513	CLA	O2D-CGD-CBD	3.04	116.55	111.23
22	C	510	CLA	C2A-C3A-C4A	3.04	106.78	101.87
22	B	606	CLA	CMA-C3A-C4A	3.04	119.94	111.77
23	F	102	BCR	C31-C1-C6	3.04	115.01	110.24
22	D	407	CLA	CAC-C3C-C4C	3.04	128.74	124.79
22	B	612	CLA	CAC-C3C-C4C	3.04	128.74	124.79
23	K	101	BCR	C24-C23-C22	-3.03	121.75	126.23
23	C	518	BCR	C12-C13-C14	3.03	123.78	119.01
22	C	505	CLA	C2D-C1D-ND	3.03	113.12	110.13
22	C	508	CLA	CHB-C1B-NB	3.02	128.58	124.05
22	C	517	CLA	C4D-CHA-C1A	-3.02	117.65	121.24
23	H	101	BCR	C21-C20-C19	-3.02	114.46	123.20
22	B	614	CLA	C10-C8-C7	3.01	127.34	112.07
23	C	515	BCR	C35-C13-C14	-3.01	117.94	122.82
23	H	101	BCR	C24-C23-C22	-3.01	121.79	126.23
25	3	101	LMG	C1-C2-C3	-3.00	103.69	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	101	BCR	C21-C20-C19	-3.00	114.51	123.20
23	C	515	BCR	C33-C5-C6	-3.00	121.21	124.48
23	K	101	BCR	C33-C5-C4	3.00	119.99	113.60
22	C	510	CLA	C1D-ND-C4D	-3.00	104.21	106.31
22	C	517	CLA	C2D-C1D-ND	-2.99	107.17	110.13
22	C	504	CLA	CMA-C3A-C4A	2.98	119.79	111.77
23	B	619	BCR	C39-C30-C25	2.98	114.92	110.24
22	B	607	CLA	C9-C8-C7	2.98	121.89	111.27
22	C	507	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	B	601	CLA	C6-C5-C3	2.96	120.68	113.47
25	3	101	LMG	C1-O6-C5	-2.96	107.94	113.72
22	B	604	CLA	C6-C7-C8	2.96	125.79	115.97
22	B	604	CLA	C9-C8-C7	2.96	121.81	111.27
22	B	615	CLA	C9-C8-C7	2.95	121.80	111.27
22	B	606	CLA	CHB-C4A-NA	2.95	128.66	124.40
23	C	518	BCR	C37-C22-C21	-2.94	118.05	122.82
22	B	606	CLA	CAC-C3C-C4C	2.93	128.61	124.79
22	B	603	CLA	CMD-C2D-C1D	2.93	129.89	124.73
22	C	503	CLA	C9-C8-C7	2.93	121.72	111.27
22	B	611	CLA	CBA-CAA-C2A	2.93	122.51	113.79
22	B	616	CLA	CAA-C2A-C1A	2.92	121.56	111.97
22	C	513	CLA	C4D-CHA-C1A	-2.91	117.77	121.24
22	B	607	CLA	C11-C10-C8	2.91	125.64	115.97
22	C	511	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
22	B	608	CLA	C11-C10-C8	2.91	125.62	115.97
22	B	604	CLA	O1D-CGD-CBD	2.90	130.25	124.52
22	B	608	CLA	CHB-C1B-C2B	-2.90	119.01	127.43
23	C	515	BCR	C40-C30-C25	2.90	114.79	110.24
22	C	513	CLA	C10-C8-C7	2.90	126.74	112.07
22	C	512	CLA	C4D-CHA-C1A	-2.89	117.79	121.24
22	B	613	CLA	CHB-C4A-NA	2.89	128.57	124.40
23	C	518	BCR	C35-C13-C14	-2.88	118.14	122.82
23	H	101	BCR	C32-C1-C31	2.88	116.89	108.63
23	H	101	BCR	C38-C26-C27	-2.88	107.46	113.60
22	C	507	CLA	CMD-C2D-C3D	-2.87	121.10	127.69
23	K	101	BCR	C38-C26-C27	-2.86	107.49	113.60
22	D	402	CLA	CAA-C2A-C1A	2.86	121.35	111.97
22	C	505	CLA	C3D-C4D-ND	2.86	114.64	109.99
22	D	407	CLA	CGD-CBD-CAD	-2.86	101.59	110.85
22	B	602	CLA	C9-C8-C10	2.86	121.45	111.27
22	C	506	CLA	CAA-C2A-C1A	2.85	121.32	111.97
22	C	513	CLA	C3D-C2D-C1D	2.85	109.72	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	511	CLA	CAA-CBA-CGA	-2.84	105.13	113.21
22	C	503	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
22	B	605	CLA	C6-C7-C8	2.84	125.39	115.97
22	B	609	CLA	OBD-CAD-C3D	2.84	135.04	128.42
22	B	609	CLA	CBA-CAA-C2A	2.83	122.22	113.79
22	B	605	CLA	C11-C10-C8	2.83	125.36	115.97
22	B	606	CLA	C3D-C2D-C1D	2.83	109.69	105.83
22	D	401	CLA	C6-C7-C8	2.82	125.35	115.97
22	C	504	CLA	C9-C8-C7	2.82	121.33	111.27
23	B	619	BCR	C2-C1-C6	2.82	114.53	110.44
26	D	405	PL9	C35-C34-C36	2.81	120.10	115.23
22	A	405	CLA	C4D-CHA-C1A	-2.80	117.90	121.24
22	B	616	CLA	C10-C8-C7	2.80	126.27	112.07
22	B	606	CLA	C9-C8-C7	2.80	121.25	111.27
22	D	407	CLA	C2B-C1B-NB	-2.79	107.43	110.33
22	B	602	CLA	C4-C3-C5	2.79	120.08	115.23
23	B	617	BCR	C7-C6-C5	2.79	127.99	121.56
22	C	512	CLA	C2A-C3A-C4A	-2.79	97.36	101.87
22	B	613	CLA	CAA-C2A-C1A	2.79	121.12	111.97
23	B	619	BCR	C27-C26-C25	2.79	126.47	122.70
22	B	615	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
22	C	508	CLA	C9-C8-C10	2.78	121.19	111.27
22	A	406	CLA	C9-C8-C7	2.78	121.18	111.27
22	A	405	CLA	C2D-C1D-ND	-2.78	107.38	110.13
22	C	507	CLA	CAA-C2A-C1A	2.78	121.07	111.97
22	D	401	CLA	C9-C8-C10	2.77	121.14	111.27
25	C	501	LMG	C1-C2-C3	-2.76	104.19	110.01
23	H	101	BCR	C8-C9-C10	-2.76	114.66	119.01
22	D	408	CLA	C6-C5-C3	2.76	120.20	113.47
22	D	407	CLA	C3A-C2A-C1A	2.76	105.47	101.34
22	C	509	CLA	CMD-C2D-C3D	-2.76	121.36	127.69
22	B	611	CLA	CAA-C2A-C3A	2.76	120.45	113.00
22	D	402	CLA	C2D-C1D-ND	-2.76	107.40	110.13
22	C	509	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
22	B	612	CLA	C4D-CHA-C1A	-2.75	117.96	121.24
22	C	504	CLA	CHC-C4B-NB	2.75	128.17	124.05
22	B	613	CLA	C4-C3-C5	2.75	120.00	115.23
22	C	507	CLA	CHC-C4B-NB	2.75	128.17	124.05
22	B	611	CLA	C9-C8-C7	2.74	121.06	111.27
23	B	618	BCR	C27-C26-C25	2.74	126.40	122.70
22	B	615	CLA	CMD-C2D-C3D	-2.73	121.43	127.69
23	K	101	BCR	C32-C1-C31	2.73	116.44	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	C9-C8-C7	2.73	121.00	111.27
22	C	507	CLA	CHD-C1D-C2D	2.73	131.16	125.49
21	D	406	PHO	C6-C7-C8	2.72	125.01	115.97
23	K	101	BCR	C8-C9-C10	-2.72	114.73	119.01
23	H	101	BCR	C3-C4-C5	2.72	118.91	114.06
23	K	101	BCR	C3-C4-C5	2.72	118.90	114.06
22	B	613	CLA	O1D-CGD-CBD	2.72	129.88	124.52
22	B	611	CLA	CHB-C4A-NA	2.71	128.32	124.40
22	D	407	CLA	CHD-C4C-C3C	2.71	128.72	124.77
22	A	405	CLA	O1D-CGD-CBD	2.71	129.86	124.52
22	C	513	CLA	CAA-C2A-C1A	2.71	120.84	111.97
22	C	507	CLA	C9-C8-C10	2.70	120.91	111.27
25	C	502	LMG	C6-C5-C4	-2.70	106.38	113.02
22	B	609	CLA	C2D-C1D-ND	-2.70	107.45	110.13
22	D	407	CLA	CBA-CAA-C2A	2.70	121.81	113.79
22	C	505	CLA	CMD-C2D-C3D	-2.70	121.51	127.69
22	B	609	CLA	CHB-C4A-NA	2.69	128.29	124.40
22	C	507	CLA	CBC-CAC-C3C	2.69	119.70	112.42
23	B	619	BCR	C31-C1-C6	2.68	114.45	110.24
22	B	602	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
22	C	503	CLA	OBD-CAD-C3D	2.68	134.68	128.42
23	C	515	BCR	C15-C14-C13	-2.68	123.52	127.28
22	C	503	CLA	CMA-C3A-C4A	2.67	118.96	111.77
23	H	101	BCR	C24-C25-C26	2.67	127.71	121.56
23	C	516	BCR	C27-C26-C25	2.67	126.31	122.70
22	A	405	CLA	CGD-CBD-CAD	-2.67	102.20	110.85
22	C	512	CLA	CMA-C3A-C4A	2.66	118.93	111.77
22	B	609	CLA	C4D-CHA-C1A	-2.66	118.07	121.24
22	B	615	CLA	O2D-CGD-CBD	2.65	115.86	111.23
23	C	515	BCR	C27-C26-C25	2.64	126.28	122.70
22	C	509	CLA	CBA-CAA-C2A	2.64	121.66	113.79
22	B	610	CLA	CBC-CAC-C3C	2.64	119.58	112.42
22	C	505	CLA	O1D-CGD-CBD	2.64	129.72	124.52
22	C	517	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
22	C	512	CLA	C9-C8-C7	2.64	120.67	111.27
22	C	504	CLA	CMD-C2D-C1D	2.63	129.35	124.73
23	B	619	BCR	C33-C5-C6	-2.62	121.62	124.48
23	A	407	BCR	C29-C30-C25	2.62	114.24	110.44
22	D	402	CLA	C4-C3-C5	2.61	119.77	115.23
22	B	603	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
22	B	603	CLA	C6-C5-C3	2.61	119.83	113.47
22	B	606	CLA	CMA-C3A-C2A	-2.61	103.91	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	C6-C7-C8	2.60	124.61	115.97
23	K	101	BCR	C24-C25-C26	2.60	127.54	121.56
22	C	505	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
22	A	406	CLA	C11-C10-C8	2.59	124.59	115.97
22	B	607	CLA	O1D-CGD-CBD	2.59	129.63	124.52
22	B	615	CLA	C1D-ND-C4D	-2.59	104.49	106.31
21	A	404	PHO	C3B-C4B-NB	-2.59	105.78	107.46
22	C	517	CLA	C9-C8-C10	2.59	120.50	111.27
22	B	609	CLA	CAC-C3C-C4C	2.59	128.16	124.79
22	B	611	CLA	CHD-C1D-C2D	2.58	130.86	125.49
22	C	507	CLA	CHB-C4A-NA	2.58	128.13	124.40
22	B	613	CLA	O2A-C1-C2	-2.58	98.17	108.11
22	B	610	CLA	CHD-C4C-NC	-2.58	120.23	124.23
21	D	406	PHO	C4B-NB-C1B	2.57	112.57	108.82
22	B	615	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	B	603	CLA	CHB-C4A-NA	2.56	128.10	124.40
22	C	514	CLA	C4D-CHA-C1A	-2.56	118.19	121.24
22	D	407	CLA	C9-C8-C10	2.56	120.41	111.27
22	C	505	CLA	C3B-C4B-NB	-2.56	108.25	110.53
23	B	618	BCR	C12-C13-C14	2.56	123.03	119.01
22	D	402	CLA	CHD-C1D-C2D	2.56	130.81	125.49
22	C	511	CLA	CHB-C1B-NB	2.56	127.88	124.05
22	B	609	CLA	C9-C8-C10	2.56	120.39	111.27
21	D	406	PHO	C4D-ND-C1D	-2.55	105.81	108.87
22	C	510	CLA	C10-C8-C7	2.55	125.01	112.07
22	B	607	CLA	CMD-C2D-C1D	2.55	129.22	124.73
23	A	407	BCR	C2-C1-C6	2.55	114.14	110.44
23	C	516	BCR	C39-C30-C25	2.55	114.24	110.24
22	C	506	CLA	CMD-C2D-C1D	2.55	129.22	124.73
23	F	102	BCR	C27-C26-C25	2.54	126.13	122.70
22	C	514	CLA	C2A-C3A-C4A	-2.53	97.78	101.87
22	D	402	CLA	C9-C8-C7	2.53	120.29	111.27
25	D	403	LMG	O6-C1-O1	-2.53	104.07	110.04
22	B	609	CLA	C11-C10-C8	2.53	124.37	115.97
22	B	610	CLA	CHB-C1B-NB	2.53	127.84	124.05
22	C	507	CLA	CHD-C4C-C3C	2.53	128.46	124.77
22	A	405	CLA	C6-C7-C8	2.53	124.36	115.97
22	C	505	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
22	A	405	CLA	C4-C3-C2	-2.52	117.16	123.63
22	A	405	CLA	CMA-C3A-C2A	-2.52	104.24	113.98
26	D	405	PL9	O1-C4-C3	-2.52	118.08	120.73
23	C	518	BCR	C15-C14-C13	-2.52	123.75	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	LMG	C1-O6-C5	-2.52	108.81	113.72
22	C	510	CLA	CAA-CBA-CGA	2.51	120.34	113.21
22	B	603	CLA	CMA-C3A-C2A	-2.51	104.28	113.98
22	A	406	CLA	C1D-ND-C4D	2.51	108.07	106.31
22	C	506	CLA	C6-C5-C3	2.50	119.57	113.47
22	B	612	CLA	C9-C8-C7	2.49	120.17	111.27
23	C	516	BCR	C8-C7-C6	-2.49	120.33	127.00
22	B	607	CLA	C4D-CHA-C1A	-2.49	118.27	121.24
23	B	617	BCR	C24-C23-C22	-2.49	122.55	126.23
22	A	405	CLA	CHB-C4A-NA	2.49	128.00	124.40
25	F	101	LMG	O2-C2-C1	-2.49	104.15	110.08
22	D	407	CLA	O1D-CGD-CBD	2.48	129.42	124.52
22	B	613	CLA	C11-C10-C8	2.48	124.21	115.97
22	B	602	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
22	B	601	CLA	CBC-CAC-C3C	2.48	119.14	112.42
22	C	512	CLA	O2D-CGD-CBD	-2.47	106.91	111.23
22	C	510	CLA	C6-C7-C8	2.47	124.17	115.97
22	B	606	CLA	C6-C7-C8	2.46	124.16	115.97
25	D	403	LMG	C1-O6-C5	-2.46	108.91	113.72
22	B	612	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
22	B	614	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	C	516	BCR	C31-C1-C6	2.46	114.10	110.24
22	B	606	CLA	O1D-CGD-CBD	2.46	129.36	124.52
22	B	604	CLA	C6-C5-C3	2.45	119.45	113.47
22	A	406	CLA	O1D-CGD-CBD	2.45	129.36	124.52
22	C	510	CLA	CHD-C1D-C2D	2.45	130.59	125.49
22	C	517	CLA	CHD-C1D-C2D	2.45	130.58	125.49
25	C	502	LMG	O6-C1-O1	-2.45	104.26	110.04
22	C	509	CLA	C6-C7-C8	2.44	124.08	115.97
22	C	514	CLA	C9-C8-C7	2.44	119.96	111.27
26	D	405	PL9	C37-C38-C39	-2.44	122.05	127.62
22	B	615	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
26	D	405	PL9	C7-C3-C2	-2.43	120.52	123.39
22	B	608	CLA	CBC-CAC-C3C	2.43	119.01	112.42
22	B	606	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
22	C	509	CLA	C9-C8-C7	2.43	119.92	111.27
22	C	514	CLA	C10-C8-C7	2.42	124.34	112.07
22	C	510	CLA	CMA-C3A-C4A	2.42	118.28	111.77
22	B	614	CLA	C2D-C1D-ND	-2.42	107.73	110.13
23	C	518	BCR	C27-C26-C25	2.41	125.96	122.70
25	3	101	LMG	O6-C5-C6	2.41	112.41	106.44
22	D	408	CLA	C2B-C1B-NB	-2.41	107.83	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	C2D-C1D-ND	-2.41	107.74	110.13
22	B	611	CLA	CMA-C3A-C4A	2.41	118.24	111.77
23	C	515	BCR	C29-C30-C25	2.40	113.93	110.44
22	B	603	CLA	C9-C8-C7	2.40	119.84	111.27
22	C	513	CLA	C2A-C3A-C4A	-2.40	97.99	101.87
22	A	405	CLA	C9-C8-C7	2.40	119.83	111.27
26	D	405	PL9	C46-C44-C43	2.40	126.54	121.17
22	B	605	CLA	CBA-CAA-C2A	2.39	120.92	113.79
25	C	501	LMG	O6-C1-O1	-2.39	104.39	110.04
23	F	102	BCR	C39-C30-C25	2.39	113.99	110.24
23	A	407	BCR	C30-C25-C26	-2.39	119.37	122.64
22	C	505	CLA	C5-C3-C2	2.39	126.52	121.17
26	D	405	PL9	C8-C7-C3	2.37	118.17	112.03
22	C	510	CLA	OBD-CAD-C3D	2.37	133.96	128.42
22	B	611	CLA	CBC-CAC-C3C	2.37	118.84	112.42
25	C	501	LMG	C8-O7-C10	2.37	123.47	117.80
22	C	503	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
22	C	505	CLA	CGD-CBD-CAD	2.36	118.47	110.85
22	B	613	CLA	C3B-C4B-NB	-2.35	108.43	110.53
23	B	617	BCR	C15-C16-C17	-2.35	118.71	123.52
25	F	101	LMG	O6-C1-O1	-2.35	104.50	110.04
22	C	503	CLA	C1-C2-C3	2.35	130.04	126.20
23	B	618	BCR	C1-C6-C5	-2.34	119.43	122.64
22	B	605	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
22	D	402	CLA	CHD-C1D-ND	-2.34	121.51	124.80
22	B	601	CLA	C2B-C1B-NB	-2.34	107.90	110.33
22	C	511	CLA	C6-C7-C8	2.34	123.73	115.97
22	B	613	CLA	CHD-C1D-C2D	2.34	130.34	125.49
24	A	408	LHG	O8-C23-C24	2.33	118.94	111.83
22	C	517	CLA	CAA-CBA-CGA	-2.33	106.59	113.21
23	C	518	BCR	C8-C9-C10	2.33	122.67	119.01
23	C	516	BCR	C30-C25-C26	-2.33	119.45	122.64
22	B	605	CLA	C1D-ND-C4D	-2.33	104.68	106.31
25	C	502	LMG	O2-C2-C1	-2.33	104.53	110.08
22	B	612	CLA	O2A-C1-C2	-2.32	99.18	108.11
22	B	604	CLA	C3D-C2D-C1D	2.32	109.00	105.83
22	B	615	CLA	C9-C8-C10	2.32	119.55	111.27
22	A	405	CLA	CBA-CAA-C2A	2.32	120.68	113.79
22	C	503	CLA	CHC-C4B-NB	2.31	127.52	124.05
23	F	102	BCR	C35-C13-C14	-2.31	119.08	122.82
25	I	101	LMG	C1-O6-C5	-2.31	109.21	113.72
23	C	516	BCR	C19-C18-C17	2.31	122.64	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
22	C	513	CLA	CAC-C3C-C4C	2.30	127.78	124.79
26	D	405	PL9	O2-C1-C6	2.30	124.14	120.48
22	B	610	CLA	C4C-C3C-C2C	-2.30	103.54	106.89
23	C	515	BCR	C2-C1-C6	2.30	113.78	110.44
23	C	516	BCR	C29-C30-C25	2.30	113.78	110.44
22	C	514	CLA	CHB-C4A-NA	2.30	127.71	124.40
22	C	503	CLA	O1D-CGD-CBD	2.29	129.04	124.52
22	D	401	CLA	O2A-C1-C2	-2.29	99.29	108.11
22	C	510	CLA	C9-C8-C10	2.29	119.43	111.27
22	B	603	CLA	C9-C8-C10	2.29	119.43	111.27
22	C	508	CLA	CAA-C2A-C1A	2.29	119.47	111.97
22	D	402	CLA	CAC-C3C-C4C	2.29	127.76	124.79
22	C	507	CLA	OBD-CAD-C3D	2.29	133.76	128.42
25	C	501	LMG	C1-O6-C5	-2.28	109.26	113.72
22	C	508	CLA	CMA-C3A-C4A	2.28	117.91	111.77
23	C	518	BCR	C38-C26-C25	-2.28	122.00	124.48
22	C	505	CLA	O2A-C1-C2	2.28	116.86	108.11
25	D	404	LMG	O1-C7-C8	-2.27	105.29	110.82
23	F	102	BCR	C8-C7-C6	-2.27	120.94	127.00
22	B	603	CLA	C5-C3-C2	-2.27	116.08	121.17
22	B	604	CLA	C3D-C4D-ND	2.27	113.67	109.99
23	C	515	BCR	C1-C6-C5	-2.26	119.54	122.64
26	D	405	PL9	C45-C44-C46	-2.26	111.31	115.23
22	C	505	CLA	O2A-CGA-CBA	2.26	118.71	111.83
22	B	616	CLA	C9-C8-C7	2.26	119.32	111.27
22	B	614	CLA	CGD-CBD-CAD	-2.26	103.55	110.85
22	C	511	CLA	C10-C8-C7	2.24	123.44	112.07
22	D	401	CLA	CAC-C3C-C4C	2.24	127.71	124.79
22	D	408	CLA	CHB-C1B-NB	2.24	127.41	124.05
23	C	518	BCR	C34-C9-C8	-2.24	114.67	118.09
22	B	605	CLA	O1D-CGD-CBD	2.24	128.93	124.52
22	A	405	CLA	CBC-CAC-C3C	2.24	118.48	112.42
22	B	613	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
22	C	512	CLA	CGD-CBD-CAD	-2.23	103.62	110.85
22	C	503	CLA	CMA-C3A-C2A	-2.23	105.35	113.98
22	B	601	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
22	B	604	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
22	D	402	CLA	C3C-C4C-NC	-2.23	107.57	110.43
21	A	404	PHO	C9-C8-C10	2.23	119.22	111.27
22	B	601	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
22	C	513	CLA	CGD-CBD-CAD	2.22	118.04	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	CMD-C2D-C1D	2.22	128.64	124.73
22	D	407	CLA	CMD-C2D-C1D	-2.22	120.82	124.73
22	D	407	CLA	C2C-C1C-NC	2.22	112.31	109.98
22	A	406	CLA	C2D-C1D-ND	-2.22	107.93	110.13
22	C	513	CLA	C6-C7-C8	2.22	123.33	115.97
22	B	606	CLA	C4D-CHA-C1A	-2.22	118.60	121.24
25	D	403	LMG	O2-C2-C1	-2.21	104.80	110.08
22	B	607	CLA	CAC-C3C-C4C	2.21	127.67	124.79
25	I	101	LMG	C32-C31-C30	-2.21	103.18	114.37
22	C	517	CLA	C9-C8-C7	2.21	119.16	111.27
22	B	610	CLA	CAA-C2A-C1A	2.21	119.21	111.97
23	C	518	BCR	C33-C5-C6	-2.21	122.08	124.48
22	B	608	CLA	O1D-CGD-CBD	2.21	128.87	124.52
22	B	614	CLA	OBD-CAD-C3D	2.21	133.57	128.42
22	B	607	CLA	C2A-C3A-C4A	-2.21	98.31	101.87
22	B	603	CLA	C2A-C3A-C4A	-2.20	98.31	101.87
22	C	508	CLA	CGD-CBD-CAD	-2.20	103.74	110.85
25	D	404	LMG	C8-O7-C10	2.19	123.05	117.80
22	B	609	CLA	CMA-C3A-C4A	-2.19	105.88	111.77
22	C	511	CLA	O2A-C1-C2	-2.19	99.67	108.11
23	K	101	BCR	C34-C9-C8	2.19	121.44	118.09
22	C	510	CLA	CMD-C2D-C1D	-2.18	120.89	124.73
22	B	610	CLA	C10-C8-C7	2.18	123.12	112.07
22	C	503	CLA	C2A-C1A-CHA	2.18	127.64	123.87
22	A	406	CLA	CHA-C4D-ND	2.18	137.04	132.55
22	D	408	CLA	O1D-CGD-CBD	2.18	128.81	124.52
22	B	616	CLA	O1D-CGD-CBD	2.17	128.81	124.52
23	F	102	BCR	C2-C1-C6	2.17	113.59	110.44
22	B	615	CLA	C4D-CHA-C1A	-2.17	118.66	121.24
22	C	512	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
22	A	406	CLA	C4D-C3D-CAD	2.17	110.46	108.11
22	C	512	CLA	CHB-C4A-NA	2.17	127.53	124.40
22	B	601	CLA	C3D-C2D-C1D	2.17	108.79	105.83
22	B	613	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
22	B	606	CLA	C9-C8-C10	2.17	118.99	111.27
22	B	606	CLA	C1D-ND-C4D	-2.16	104.79	106.31
22	B	613	CLA	C1-C2-C3	-2.16	122.65	126.20
22	B	607	CLA	CBA-CAA-C2A	2.16	120.23	113.79
22	B	608	CLA	CAC-C3C-C4C	2.16	127.60	124.79
22	B	606	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
22	C	506	CLA	C9-C8-C7	2.16	118.97	111.27
23	H	101	BCR	C34-C9-C8	2.16	121.39	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
22	C	506	CLA	C9-C8-C10	2.16	118.96	111.27
22	C	505	CLA	CMA-C3A-C2A	-2.15	105.65	113.98
22	B	614	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
22	D	407	CLA	CHD-C1D-C2D	2.15	129.96	125.49
22	C	505	CLA	C9-C8-C7	2.15	118.95	111.27
22	D	407	CLA	CHC-C4B-NB	2.15	127.28	124.05
22	C	507	CLA	O1D-CGD-CBD	2.15	128.76	124.52
23	C	515	BCR	C39-C30-C25	-2.15	106.88	110.24
22	C	517	CLA	CHD-C1D-ND	-2.15	121.78	124.80
21	A	404	PHO	O2D-CGD-O1D	-2.15	119.67	123.85
22	C	504	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
26	D	405	PL9	C40-C39-C41	2.15	118.95	115.23
22	C	505	CLA	CED-O2D-CGD	2.14	120.78	115.92
22	B	612	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
22	A	406	CLA	C6-C7-C8	2.13	123.05	115.97
22	C	507	CLA	C1D-ND-C4D	-2.13	104.82	106.31
22	C	517	CLA	CBA-CAA-C2A	2.13	120.14	113.79
22	B	614	CLA	CBC-CAC-C3C	2.13	118.19	112.42
23	B	619	BCR	C1-C6-C5	-2.12	119.73	122.64
22	B	616	CLA	C2A-C3A-C4A	-2.12	98.44	101.87
22	D	402	CLA	O1D-CGD-CBD	2.12	128.70	124.52
22	D	401	CLA	C3A-C2A-C1A	-2.12	98.16	101.34
22	B	613	CLA	CAC-C3C-C2C	-2.12	123.67	127.56
22	C	517	CLA	C3A-C2A-C1A	-2.12	98.17	101.34
22	C	511	CLA	C9-C8-C7	2.11	118.81	111.27
22	B	611	CLA	CMD-C2D-C1D	-2.11	121.01	124.73
22	C	503	CLA	CHB-C1B-C2B	-2.11	121.30	127.43
22	B	606	CLA	CAA-C2A-C3A	2.11	118.70	113.00
23	K	101	BCR	C10-C11-C12	-2.11	117.09	123.20
22	D	408	CLA	CAA-C2A-C1A	2.11	118.88	111.97
23	B	617	BCR	C4-C5-C6	2.10	125.55	122.70
22	B	607	CLA	CHB-C4A-NA	2.10	127.43	124.40
22	B	607	CLA	CHA-C4D-ND	2.10	136.88	132.55
22	B	601	CLA	O2D-CGD-CBD	2.10	114.90	111.23
23	C	516	BCR	C23-C24-C25	-2.10	121.39	127.00
22	B	604	CLA	C10-C8-C7	2.10	122.71	112.07
22	C	503	CLA	C9-C8-C10	2.10	118.76	111.27
22	B	602	CLA	O2D-CGD-CBD	2.10	114.90	111.23
22	C	503	CLA	O2A-C1-C2	2.10	116.18	108.11
22	D	408	CLA	C9-C8-C10	2.10	118.75	111.27
21	A	404	PHO	C3D-C4D-ND	2.10	110.40	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	511	CLA	CMD-C2D-C1D	2.10	128.42	124.73
22	A	406	CLA	C2B-C1B-NB	-2.10	108.15	110.33
22	B	607	CLA	CED-O2D-CGD	2.09	120.67	115.92
22	D	408	CLA	C4D-CHA-C1A	-2.09	118.75	121.24
22	B	602	CLA	CHB-C4A-NA	2.09	127.42	124.40
22	C	514	CLA	C4-C3-C5	2.09	118.86	115.23
22	C	506	CLA	CHC-C4B-NB	2.09	127.18	124.05
22	A	406	CLA	C6-C5-C3	2.09	118.56	113.47
22	B	609	CLA	C1D-ND-C4D	-2.09	104.85	106.31
22	C	514	CLA	C2D-C1D-ND	-2.08	108.07	110.13
25	I	101	LMG	C1-C2-C3	-2.07	105.64	110.01
23	B	618	BCR	C29-C30-C25	2.07	113.45	110.44
21	D	406	PHO	C11-C10-C8	2.07	122.85	115.97
25	D	404	LMG	O6-C1-O1	-2.07	105.15	110.04
23	C	515	BCR	C35-C13-C12	2.07	121.25	118.09
21	A	404	PHO	O1D-CGD-CBD	2.06	127.85	124.72
22	B	606	CLA	C4-C3-C5	2.06	118.81	115.23
22	C	513	CLA	C6-C5-C3	-2.06	108.44	113.47
22	D	407	CLA	C6-C7-C8	2.06	122.82	115.97
22	C	508	CLA	C6-C7-C8	2.06	122.81	115.97
22	B	609	CLA	CMD-C2D-C1D	-2.06	121.10	124.73
22	B	603	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
23	F	102	BCR	C16-C15-C14	-2.06	119.31	123.52
22	D	401	CLA	C6-C5-C3	2.05	118.47	113.47
22	D	401	CLA	CHB-C1B-NB	2.05	127.13	124.05
23	K	101	BCR	C11-C10-C9	-2.05	124.40	127.28
22	B	603	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
22	C	505	CLA	CAA-CBA-CGA	2.05	119.02	113.21
22	C	505	CLA	CBA-CAA-C2A	2.05	119.89	113.79
23	B	619	BCR	C4-C5-C6	2.05	125.47	122.70
22	C	504	CLA	C10-C8-C7	2.05	122.43	112.07
22	C	512	CLA	C2D-C1D-ND	-2.05	108.10	110.13
23	C	518	BCR	C11-C10-C9	-2.05	124.41	127.28
25	3	101	LMG	C6-C5-C4	-2.04	108.00	113.02
22	B	610	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
22	C	504	CLA	C2B-C1B-NB	-2.04	108.21	110.33
22	D	401	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
25	3	101	LMG	O6-C1-O1	-2.04	105.23	110.04
22	B	607	CLA	C2D-C1D-ND	-2.04	108.11	110.13
22	D	402	CLA	CHB-C4A-NA	2.04	127.34	124.40
23	K	101	BCR	C28-C27-C26	-2.03	110.43	114.06
21	D	406	PHO	O2D-CGD-O1D	-2.03	119.89	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	CHD-C4C-C3C	2.03	127.73	124.77
26	D	405	PL9	O2-C1-C2	-2.03	117.21	121.83
22	C	505	CLA	C10-C8-C7	2.03	122.35	112.07
22	C	505	CLA	C9-C8-C10	2.02	118.49	111.27
25	C	502	LMG	C1-C2-C3	-2.02	105.76	110.01
22	B	607	CLA	C5-C3-C2	-2.02	116.63	121.17
22	B	605	CLA	C10-C8-C7	2.02	122.30	112.07
22	C	504	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
22	C	511	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
22	C	506	CLA	CHB-C4A-NA	2.02	127.31	124.40
25	C	502	LMG	O6-C5-C6	2.01	111.43	106.44
23	H	101	BCR	C28-C27-C26	-2.01	110.46	114.06
22	B	615	CLA	C2A-C3A-C4A	-2.01	98.62	101.87
22	C	503	CLA	CHA-C4D-ND	2.01	136.70	132.55
23	H	101	BCR	C10-C11-C12	-2.01	117.37	123.20
25	I	101	LMG	O2-C2-C1	-2.01	105.28	110.08
22	D	407	CLA	CHB-C4A-NA	2.01	127.30	124.40
22	A	405	CLA	C6-C5-C3	2.01	118.36	113.47
22	B	607	CLA	CMD-C2D-C3D	-2.00	123.09	127.69
26	D	405	PL9	C12-C13-C14	-2.00	123.04	127.62
22	A	406	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
25	F	101	LMG	O3-C3-C2	-2.00	105.66	110.38

All (75) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	404	PHO	C8
21	D	406	PHO	C8
22	A	405	CLA	C2A
22	A	405	CLA	ND
22	A	406	CLA	C2A
22	A	406	CLA	ND
22	B	601	CLA	C8
22	B	601	CLA	C2A
22	B	601	CLA	ND
22	B	602	CLA	C2A
22	B	602	CLA	ND
22	B	603	CLA	C2A
22	B	603	CLA	ND
22	B	603	CLA	C8
22	B	604	CLA	ND
22	B	605	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	605	CLA	C8
22	B	606	CLA	C8
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	607	CLA	C8
22	B	609	CLA	ND
22	B	609	CLA	C2A
22	B	610	CLA	C2A
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	C2A
22	B	612	CLA	ND
22	B	612	CLA	C8
22	B	612	CLA	C3A
22	B	613	CLA	C8
22	B	613	CLA	C2A
22	B	613	CLA	ND
22	B	614	CLA	C8
22	B	614	CLA	C2A
22	B	614	CLA	ND
22	B	615	CLA	C2A
22	B	615	CLA	ND
22	B	615	CLA	C8
22	B	616	CLA	C2A
22	B	616	CLA	C8
22	B	616	CLA	ND
22	B	616	CLA	C3A
22	C	504	CLA	ND
22	C	504	CLA	C8
22	C	505	CLA	C8
22	C	506	CLA	C2A
22	C	506	CLA	C8
22	C	506	CLA	ND
22	C	507	CLA	C2A
22	C	507	CLA	ND
22	C	508	CLA	C8
22	C	509	CLA	C2A
22	C	509	CLA	ND
22	C	510	CLA	C8
22	C	511	CLA	C2A
22	C	511	CLA	ND
22	C	511	CLA	C8

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Mol	Chain	Res	Type	Atom
22	C	512	CLA	ND
22	C	513	CLA	C2A
22	C	513	CLA	ND
22	C	513	CLA	C3A
22	C	514	CLA	C8
22	C	514	CLA	C2A
22	C	514	CLA	ND
22	C	517	CLA	C8
22	C	517	CLA	ND
22	C	517	CLA	C3A
22	D	402	CLA	C2A
22	D	402	CLA	ND
22	D	407	CLA	ND
22	D	407	CLA	C8
22	D	408	CLA	C2A
22	D	408	CLA	ND
22	D	408	CLA	C8

All (517) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C3A-C2A-CAA-CBA
22	A	406	CLA	C3A-C2A-CAA-CBA
22	A	406	CLA	C11-C10-C8-C7
22	B	601	CLA	C11-C10-C8-C9
22	B	603	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C11-C10-C8-C9
22	B	604	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C1A-C2A-CAA-CBA
22	B	610	CLA	C1A-C2A-CAA-CBA
22	B	611	CLA	C3A-C2A-CAA-CBA
22	B	613	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	B	616	CLA	C3A-C2A-CAA-CBA
22	B	616	CLA	C4B-C3B-CAB-CBB
22	C	503	CLA	O2A-C1-C2-C3
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	C3A-C2A-CAA-CBA
22	C	505	CLA	O2A-C1-C2-C3
22	C	506	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C3A-C2A-CAA-CBA
22	C	517	CLA	C1A-C2A-CAA-CBA
22	C	517	CLA	C3A-C2A-CAA-CBA
22	C	517	CLA	CHA-CBD-CGD-O1D
22	C	517	CLA	CHA-CBD-CGD-O2D
22	D	401	CLA	C1A-C2A-CAA-CBA
22	D	402	CLA	C1A-C2A-CAA-CBA
22	D	407	CLA	C3A-C2A-CAA-CBA
22	D	407	CLA	C11-C10-C8-C9
22	D	408	CLA	C3A-C2A-CAA-CBA
23	A	407	BCR	C21-C22-C23-C24
23	B	617	BCR	C7-C8-C9-C10
23	B	617	BCR	C9-C10-C11-C12
23	B	617	BCR	C11-C12-C13-C14
23	B	617	BCR	C11-C12-C13-C35
23	B	617	BCR	C15-C16-C17-C18
23	B	617	BCR	C17-C18-C19-C20
23	B	617	BCR	C21-C22-C23-C24
23	B	617	BCR	C37-C22-C23-C24
23	B	619	BCR	C13-C14-C15-C16
23	C	515	BCR	C7-C8-C9-C10
23	C	515	BCR	C7-C8-C9-C34
23	C	515	BCR	C11-C12-C13-C14
23	C	515	BCR	C11-C12-C13-C35
23	C	515	BCR	C17-C18-C19-C20
23	C	516	BCR	C11-C12-C13-C14
23	C	516	BCR	C11-C12-C13-C35
23	C	518	BCR	C7-C8-C9-C10
23	C	518	BCR	C7-C8-C9-C34
23	C	518	BCR	C15-C16-C17-C18
23	F	102	BCR	C21-C22-C23-C24
23	F	102	BCR	C37-C22-C23-C24
23	H	101	BCR	C5-C6-C7-C8
23	H	101	BCR	C17-C18-C19-C20
23	H	101	BCR	C20-C21-C22-C37
23	H	101	BCR	C23-C24-C25-C26
23	H	101	BCR	C23-C24-C25-C30
23	K	101	BCR	C7-C8-C9-C10
23	K	101	BCR	C17-C18-C19-C20
23	K	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	K	101	BCR	C23-C24-C25-C26
23	K	101	BCR	C23-C24-C25-C30
26	D	405	PL9	C35-C34-C36-C37
22	B	616	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	C4-C3-C5-C6
22	B	603	CLA	C2-C3-C5-C6
22	C	504	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	C	510	CLA	C2A-CAA-CBA-CGA
23	C	515	BCR	C19-C20-C21-C22
23	C	516	BCR	C13-C14-C15-C16
23	C	518	BCR	C13-C14-C15-C16
22	C	517	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C4-C3-C5-C6
22	B	609	CLA	CBD-CGD-O2D-CED
23	A	407	BCR	C19-C20-C21-C22
23	C	515	BCR	C13-C14-C15-C16
23	C	515	BCR	C15-C16-C17-C18
23	C	516	BCR	C15-C16-C17-C18
22	B	602	CLA	C2-C3-C5-C6
26	D	405	PL9	C33-C34-C36-C37
22	A	405	CLA	C6-C7-C8-C9
22	A	405	CLA	C11-C10-C8-C9
22	A	406	CLA	C6-C7-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C10-C8-C9
22	B	604	CLA	C6-C7-C8-C9
22	B	608	CLA	C11-C10-C8-C9
22	B	609	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	C	503	CLA	C6-C7-C8-C9
22	C	506	CLA	C11-C10-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	C	512	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	D	401	CLA	C6-C7-C8-C9
22	D	401	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	D	408	CLA	C11-C10-C8-C9
22	B	616	CLA	O1D-CGD-O2D-CED
23	A	407	BCR	C36-C18-C19-C20
23	A	407	BCR	C37-C22-C23-C24
23	B	617	BCR	C7-C8-C9-C34
23	B	617	BCR	C36-C18-C19-C20
23	B	618	BCR	C36-C18-C19-C20
23	B	619	BCR	C36-C18-C19-C20
23	C	515	BCR	C36-C18-C19-C20
23	C	518	BCR	C36-C18-C19-C20
23	C	518	BCR	C37-C22-C23-C24
23	H	101	BCR	C11-C12-C13-C35
23	H	101	BCR	C37-C22-C23-C24
23	K	101	BCR	C11-C12-C13-C35
23	K	101	BCR	C37-C22-C23-C24
23	A	407	BCR	C17-C18-C19-C20
23	C	516	BCR	C7-C8-C9-C10
23	H	101	BCR	C7-C8-C9-C10
23	H	101	BCR	C11-C12-C13-C14
23	K	101	BCR	C11-C12-C13-C14
22	B	615	CLA	CBA-CGA-O2A-C1
21	D	406	PHO	C8-C10-C11-C12
22	B	605	CLA	C3-C5-C6-C7
22	B	602	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
22	B	610	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C10-C8-C7
22	C	504	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	C	513	CLA	C6-C7-C8-C10
22	C	514	CLA	C11-C10-C8-C7
22	D	402	CLA	C11-C10-C8-C7
23	A	407	BCR	C9-C10-C11-C12
23	A	407	BCR	C13-C14-C15-C16
23	C	516	BCR	C9-C10-C11-C12
23	F	102	BCR	C19-C20-C21-C22
23	H	101	BCR	C19-C20-C21-C22
23	K	101	BCR	C19-C20-C21-C22
22	B	614	CLA	C3-C5-C6-C7
22	B	615	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	517	CLA	O1D-CGD-O2D-CED
23	B	617	BCR	C13-C14-C15-C16
22	A	405	CLA	C3-C5-C6-C7
23	B	619	BCR	C11-C12-C13-C35
23	B	619	BCR	C37-C22-C23-C24
23	C	516	BCR	C7-C8-C9-C34
23	C	516	BCR	C37-C22-C23-C24
23	H	101	BCR	C7-C8-C9-C34
23	K	101	BCR	C7-C8-C9-C34
23	B	619	BCR	C21-C22-C23-C24
25	D	404	LMG	O6-C1-O1-C7
22	C	507	CLA	O1D-CGD-O2D-CED
22	B	608	CLA	C4B-C3B-CAB-CBB
22	D	402	CLA	C4B-C3B-CAB-CBB
24	A	408	LHG	C32-C33-C34-C35
22	B	614	CLA	C2A-CAA-CBA-CGA
22	B	616	CLA	C6-C7-C8-C10
22	C	517	CLA	C11-C10-C8-C7
22	B	608	CLA	C3A-C2A-CAA-CBA
22	C	507	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C5-C6-C7-C8
23	H	101	BCR	C9-C10-C11-C12
22	B	601	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	CBA-CGA-O2A-C1
24	A	408	LHG	C11-C12-C13-C14
22	D	402	CLA	C2B-C3B-CAB-CBB
23	B	617	BCR	C23-C24-C25-C30
23	H	101	BCR	C1-C6-C7-C8
23	K	101	BCR	C1-C6-C7-C8
23	K	101	BCR	C5-C6-C7-C8
22	C	509	CLA	C3-C5-C6-C7
25	3	101	LMG	C37-C38-C39-C40
22	B	606	CLA	O1A-CGA-O2A-C1
25	D	403	LMG	C37-C38-C39-C40
23	K	101	BCR	C9-C10-C11-C12
25	C	501	LMG	C11-C10-O7-C8
25	I	101	LMG	C39-C40-C41-C42
25	3	101	LMG	C32-C33-C34-C35
22	B	602	CLA	C5-C6-C7-C8
25	I	101	LMG	C16-C17-C18-C19
25	C	501	LMG	C22-C23-C24-C25
26	D	405	PL9	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
25	C	502	LMG	C15-C16-C17-C18
22	B	616	CLA	C2-C3-C5-C6
26	D	405	PL9	C13-C14-C16-C17
22	D	401	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	C1A-C2A-CAA-CBA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	611	CLA	C1A-C2A-CAA-CBA
22	B	612	CLA	C1A-C2A-CAA-CBA
22	C	509	CLA	C1A-C2A-CAA-CBA
22	C	511	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	D	407	CLA	C1A-C2A-CAA-CBA
22	D	408	CLA	C1A-C2A-CAA-CBA
26	D	405	PL9	C47-C48-C49-C51
26	D	405	PL9	C46-C47-C48-C49
22	B	605	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C12-C13-C15
22	B	607	CLA	C6-C7-C8-C10
22	B	607	CLA	C11-C10-C8-C7
22	B	612	CLA	C6-C7-C8-C10
22	C	506	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C10-C8-C7
25	D	404	LMG	C13-C14-C15-C16
21	D	406	PHO	C11-C10-C8-C9
22	B	603	CLA	C6-C7-C8-C9
22	B	603	CLA	C11-C12-C13-C14
22	B	613	CLA	C11-C10-C8-C9
22	C	507	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C9
22	D	402	CLA	C6-C7-C8-C9
22	D	407	CLA	C6-C7-C8-C9
25	D	404	LMG	O1-C7-C8-C9
22	C	505	CLA	CBA-CGA-O2A-C1
25	I	101	LMG	O6-C5-C6-O5
23	B	618	BCR	C16-C17-C18-C36
22	B	616	CLA	C4-C3-C5-C6
23	H	101	BCR	C21-C22-C23-C24
23	K	101	BCR	C21-C22-C23-C24
21	A	404	PHO	O2A-C1-C2-C3
22	B	611	CLA	O2A-C1-C2-C3
22	C	514	CLA	O2A-C1-C2-C3
22	D	407	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	C	517	CLA	C8-C10-C11-C12
22	B	611	CLA	C5-C6-C7-C8
24	A	408	LHG	C27-C28-C29-C30
22	B	604	CLA	CBA-CGA-O2A-C1
22	B	610	CLA	CBA-CGA-O2A-C1
22	D	401	CLA	CBA-CGA-O2A-C1
25	C	501	LMG	O9-C10-O7-C8
21	A	404	PHO	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	B	606	CLA	C11-C10-C8-C9
22	B	609	CLA	C11-C10-C8-C9
22	B	611	CLA	C11-C10-C8-C9
22	B	616	CLA	C11-C10-C8-C9
22	C	508	CLA	C6-C7-C8-C9
22	C	512	CLA	C4B-C3B-CAB-CBB
22	A	405	CLA	C12-C13-C15-C16
22	B	601	CLA	C12-C13-C15-C16
22	B	610	CLA	C6-C7-C8-C10
22	C	504	CLA	C6-C7-C8-C10
22	C	507	CLA	C12-C13-C15-C16
25	3	101	LMG	C20-C21-C22-C23
22	B	603	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	610	CLA	C4-C3-C5-C6
22	B	612	CLA	C3A-C2A-CAA-CBA
22	D	401	CLA	C3A-C2A-CAA-CBA
26	D	405	PL9	C15-C14-C16-C17
23	H	101	BCR	C13-C14-C15-C16
23	K	101	BCR	C13-C14-C15-C16
22	C	505	CLA	O1A-CGA-O2A-C1
22	C	511	CLA	C2A-CAA-CBA-CGA
25	D	403	LMG	C22-C23-C24-C25
21	D	406	PHO	C4-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
22	D	401	CLA	O1A-CGA-O2A-C1
25	D	403	LMG	C12-C13-C14-C15
23	B	617	BCR	C23-C24-C25-C26
23	C	516	BCR	C23-C24-C25-C30
25	C	502	LMG	C18-C19-C20-C21
22	B	602	CLA	C8-C10-C11-C12
25	D	404	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
25	F	101	LMG	O1-C7-C8-O7
25	F	101	LMG	C15-C16-C17-C18
22	B	614	CLA	C6-C7-C8-C9
22	C	517	CLA	C6-C7-C8-C9
23	C	518	BCR	C6-C7-C8-C9
22	D	407	CLA	C2C-C3C-CAC-CBC
22	B	601	CLA	C4-C3-C5-C6
21	D	406	PHO	C2-C3-C5-C6
22	B	604	CLA	O1A-CGA-O2A-C1
22	B	610	CLA	O1A-CGA-O2A-C1
22	B	610	CLA	C2C-C3C-CAC-CBC
22	B	613	CLA	C5-C6-C7-C8
21	A	404	PHO	C11-C10-C8-C7
22	A	405	CLA	C6-C7-C8-C10
22	B	602	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C12-C13-C15
23	B	619	BCR	C17-C18-C19-C20
25	C	501	LMG	C40-C41-C42-C43
25	D	404	LMG	C8-C7-O1-C1
22	C	514	CLA	C2A-CAA-CBA-CGA
22	B	603	CLA	C3-C5-C6-C7
25	D	404	LMG	C9-C8-O7-C10
25	C	501	LMG	C29-C30-C31-C32
22	C	505	CLA	C8-C10-C11-C12
22	B	609	CLA	O1D-CGD-O2D-CED
22	A	405	CLA	C14-C13-C15-C16
22	B	612	CLA	C8-C10-C11-C12
25	D	404	LMG	C22-C23-C24-C25
26	D	405	PL9	C44-C46-C47-C48
22	B	604	CLA	C4B-C3B-CAB-CBB
22	B	606	CLA	C4B-C3B-CAB-CBB
22	C	511	CLA	C4B-C3B-CAB-CBB
22	C	513	CLA	C4B-C3B-CAB-CBB
22	C	514	CLA	C1A-C2A-CAA-CBA
22	D	407	CLA	C4C-C3C-CAC-CBC
22	C	505	CLA	C4-C3-C5-C6
22	C	511	CLA	C4-C3-C5-C6
25	3	101	LMG	C29-C30-C31-C32
22	A	405	CLA	C11-C12-C13-C15
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C6-C7-C8-C10
22	B	615	CLA	C6-C7-C8-C10
22	C	507	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C10-C8-C7
22	D	401	CLA	C6-C7-C8-C10
22	A	406	CLA	C4-C3-C5-C6
22	B	615	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C12-C13-C14
25	3	101	LMG	C13-C14-C15-C16
22	C	504	CLA	C3-C5-C6-C7
25	D	404	LMG	C39-C40-C41-C42
25	D	404	LMG	C14-C15-C16-C17
25	F	101	LMG	O1-C7-C8-C9
22	B	611	CLA	C4-C3-C5-C6
22	A	406	CLA	C2-C3-C5-C6
25	C	502	LMG	C28-C29-C30-C31
25	C	501	LMG	O6-C1-O1-C7
22	B	602	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CHA-CBD-CGD-O1D
22	C	514	CLA	CHA-CBD-CGD-O1D
22	C	514	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	C4-C3-C5-C6
22	B	616	CLA	C2B-C3B-CAB-CBB
22	C	511	CLA	C2B-C3B-CAB-CBB
22	B	601	CLA	C2-C3-C5-C6
22	B	606	CLA	C2-C3-C5-C6
26	D	405	PL9	C43-C44-C46-C47
24	A	408	LHG	C5-C4-O6-P
22	C	505	CLA	C16-C17-C18-C20
22	C	510	CLA	C8-C10-C11-C12
25	F	101	LMG	C7-C8-O7-C10
22	C	505	CLA	C2-C3-C5-C6
25	F	101	LMG	C10-C11-C12-C13
22	B	607	CLA	C11-C10-C8-C9
22	B	608	CLA	C6-C7-C8-C9
22	C	504	CLA	C6-C7-C8-C9
22	C	514	CLA	C6-C7-C8-C9
22	B	609	CLA	C11-C10-C8-C7
22	B	613	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C12-C13-C15-C16
22	C	511	CLA	C10-C11-C12-C13
25	D	404	LMG	C2-C1-O1-C7
22	C	504	CLA	C10-C11-C12-C13
21	A	404	PHO	C16-C17-C18-C19
22	B	607	CLA	C4-C3-C5-C6
22	B	616	CLA	C8-C10-C11-C12
23	B	618	BCR	C17-C18-C19-C20
22	C	510	CLA	O1A-CGA-O2A-C1
25	C	501	LMG	C12-C13-C14-C15
25	C	501	LMG	C15-C16-C17-C18
22	C	511	CLA	C2-C3-C5-C6
22	B	611	CLA	C6-C7-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	B	607	CLA	C4B-C3B-CAB-CBB
22	C	503	CLA	C4B-C3B-CAB-CBB
22	B	611	CLA	C2-C3-C5-C6
22	B	612	CLA	C12-C13-C15-C16
25	D	404	LMG	C40-C41-C42-C43
22	B	615	CLA	C5-C6-C7-C8
22	C	512	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C2-C3-C5-C6
22	D	402	CLA	C8-C10-C11-C12
22	B	616	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	D	408	CLA	C6-C7-C8-C9
25	C	501	LMG	C7-C8-O7-C10
25	C	501	LMG	C9-C8-O7-C10
22	B	603	CLA	C2C-C3C-CAC-CBC
27	E	101	HEM	CAD-CBD-CGD-O2D
22	A	405	CLA	C1A-C2A-CAA-CBA
22	B	609	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
24	A	408	LHG	O6-C4-C5-O7
22	B	606	CLA	C2B-C3B-CAB-CBB
22	B	608	CLA	C2B-C3B-CAB-CBB
22	C	505	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C2B-C3B-CAB-CBB
22	C	513	CLA	C2B-C3B-CAB-CBB
23	B	618	BCR	C23-C24-C25-C30
23	C	516	BCR	C1-C6-C7-C8
22	B	606	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	611	CLA	C6-C7-C8-C10
22	C	509	CLA	C6-C7-C8-C10
22	C	511	CLA	C11-C10-C8-C7
22	C	506	CLA	C13-C15-C16-C17
22	C	505	CLA	CAA-CBA-CGA-O2A
27	E	101	HEM	CAD-CBD-CGD-O1D
22	C	505	CLA	C11-C10-C8-C9
25	C	502	LMG	C23-C24-C25-C26
22	B	607	CLA	CBA-CGA-O2A-C1
21	A	404	PHO	C16-C17-C18-C20
22	B	607	CLA	O1A-CGA-O2A-C1
23	A	407	BCR	C11-C10-C9-C34
24	A	408	LHG	O6-C4-C5-C6
22	A	405	CLA	C11-C10-C8-C7
22	D	408	CLA	C6-C7-C8-C10
25	D	403	LMG	C40-C41-C42-C43
22	B	606	CLA	C11-C12-C13-C14
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C14
22	C	517	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	C2-C1-O2A-CGA
22	C	505	CLA	C2-C1-O2A-CGA
22	C	509	CLA	C2-C1-O2A-CGA
22	C	504	CLA	C3A-C2A-CAA-CBA
22	D	402	CLA	C3A-C2A-CAA-CBA
21	A	404	PHO	C10-C11-C12-C13
22	B	613	CLA	CAA-CBA-CGA-O2A
25	F	101	LMG	C9-C8-O7-C10
22	C	505	CLA	C10-C11-C12-C13
22	D	402	CLA	C13-C15-C16-C17
23	C	516	BCR	C12-C13-C14-C15
22	D	401	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
25	C	501	LMG	O1-C7-C8-O7
21	D	406	PHO	C6-C7-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	507	CLA	C6-C7-C8-C9
22	C	510	CLA	C16-C17-C18-C19
25	3	101	LMG	C40-C41-C42-C43
22	B	612	CLA	CAA-CBA-CGA-O2A
22	C	509	CLA	C2A-CAA-CBA-CGA
22	A	406	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C11-C10-C8-C7
22	B	608	CLA	C6-C7-C8-C10
22	B	613	CLA	C6-C7-C8-C10
22	B	614	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C10
27	E	101	HEM	CAA-CBA-CGA-O2A
22	B	607	CLA	C2B-C3B-CAB-CBB
23	B	618	BCR	C23-C24-C25-C26
23	C	516	BCR	C23-C24-C25-C26
22	B	613	CLA	C2-C1-O2A-CGA
26	D	405	PL9	C29-C31-C32-C33
26	D	405	PL9	C39-C41-C42-C43
22	B	611	CLA	CBA-CGA-O2A-C1
22	B	611	CLA	O1A-CGA-O2A-C1
22	D	402	CLA	CAA-CBA-CGA-O2A
25	I	101	LMG	C38-C39-C40-C41
25	C	501	LMG	C42-C43-C44-C45
22	B	614	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	CAA-CBA-CGA-O2A
22	B	603	CLA	C15-C16-C17-C18
26	D	405	PL9	C16-C17-C18-C19
22	B	606	CLA	C6-C7-C8-C9
22	B	615	CLA	C11-C10-C8-C9
25	C	501	LMG	O1-C7-C8-C9
22	B	614	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C4B-C3B-CAB-CBB
22	C	506	CLA	C4B-C3B-CAB-CBB
22	C	507	CLA	C4B-C3B-CAB-CBB
22	C	510	CLA	CBA-CGA-O2A-C1
25	F	101	LMG	O6-C5-C6-O5
25	C	501	LMG	O8-C28-C29-C30
22	B	611	CLA	CAA-CBA-CGA-O2A
25	3	101	LMG	C30-C31-C32-C33
22	C	512	CLA	C2A-CAA-CBA-CGA
27	E	101	HEM	CAA-CBA-CGA-O1A
26	D	405	PL9	C26-C27-C28-C29
22	D	407	CLA	CAA-CBA-CGA-O2A
25	C	502	LMG	O8-C28-C29-C30
22	B	608	CLA	C11-C10-C8-C7
22	C	503	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	D	401	CLA	C12-C13-C15-C16
22	B	601	CLA	C3-C5-C6-C7
25	I	101	LMG	C15-C16-C17-C18
22	C	512	CLA	C5-C6-C7-C8
22	C	514	CLA	C16-C17-C18-C20
22	B	612	CLA	CAA-CBA-CGA-O1A
25	3	101	LMG	C14-C15-C16-C17
25	C	502	LMG	C38-C39-C40-C41
22	A	405	CLA	C11-C12-C13-C14
22	A	406	CLA	C11-C10-C8-C9
22	B	615	CLA	C6-C7-C8-C9
25	C	501	LMG	O7-C10-C11-C12
22	D	402	CLA	CAA-CBA-CGA-O1A
22	B	614	CLA	CAA-CBA-CGA-O1A
25	C	502	LMG	O10-C28-C29-C30
22	A	406	CLA	CAA-CBA-CGA-O2A
22	C	510	CLA	CAA-CBA-CGA-O2A
25	C	501	LMG	O10-C28-C29-C30
23	B	617	BCR	C10-C11-C12-C13
22	D	407	CLA	CAA-CBA-CGA-O1A
25	C	501	LMG	O9-C10-C11-C12
22	C	506	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAA-CBA-CGA-O1A
24	A	408	LHG	C14-C15-C16-C17
22	A	406	CLA	CAA-CBA-CGA-O1A
22	B	611	CLA	CAA-CBA-CGA-O1A
22	A	405	CLA	CAA-CBA-CGA-O2A
25	D	403	LMG	C24-C25-C26-C27
22	B	607	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	O1A-CGA-O2A-C1
22	C	510	CLA	CAA-CBA-CGA-O1A
24	A	408	LHG	C29-C30-C31-C32

There are no ring outliers.

45 monomers are involved in 93 short contacts:

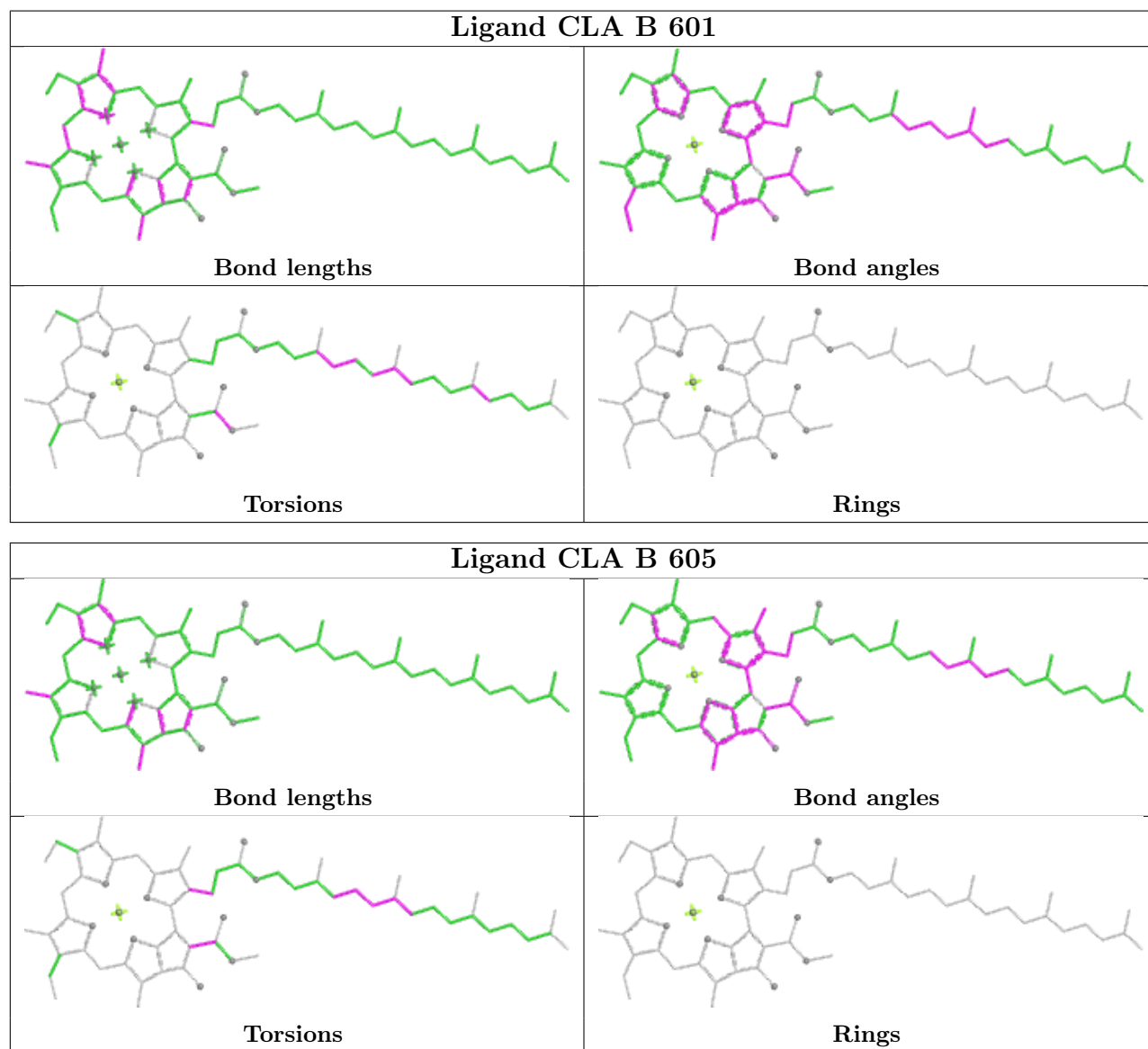
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	601	CLA	1	0
22	B	605	CLA	2	0
22	B	609	CLA	10	0

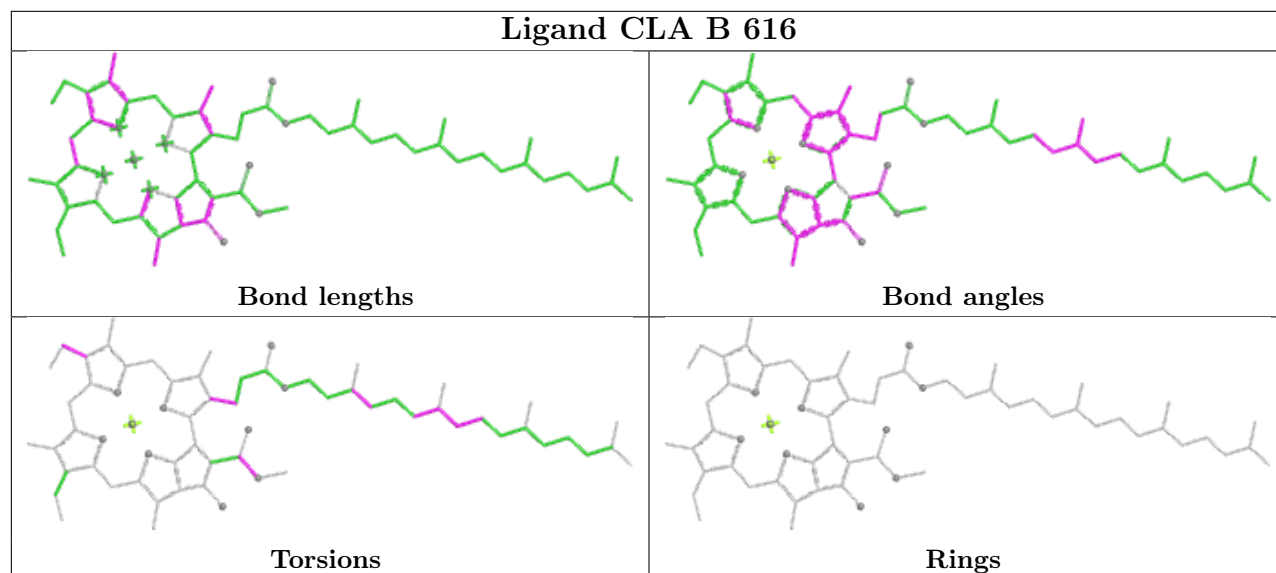
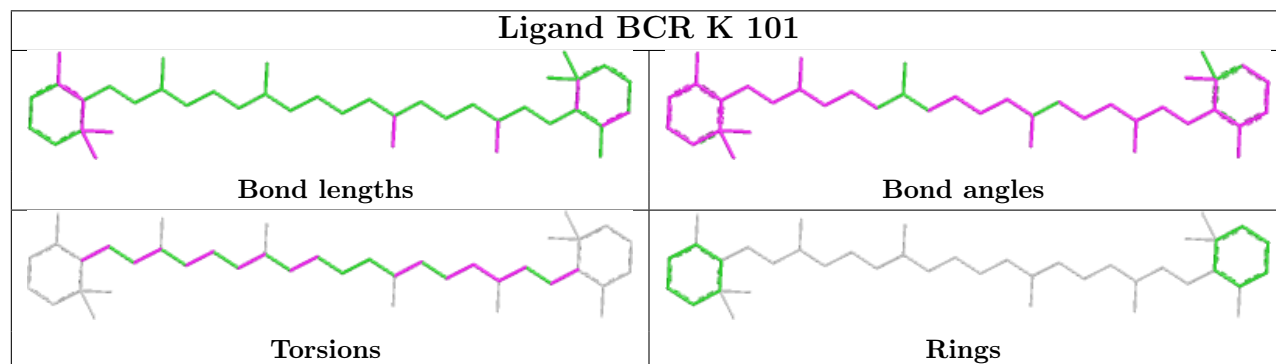
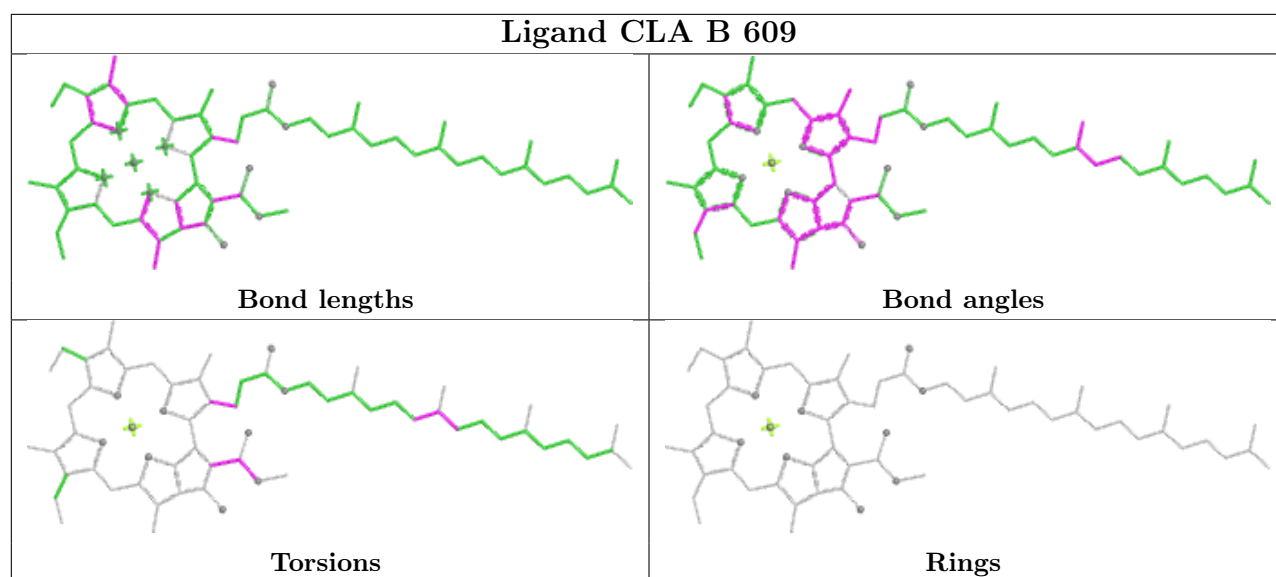
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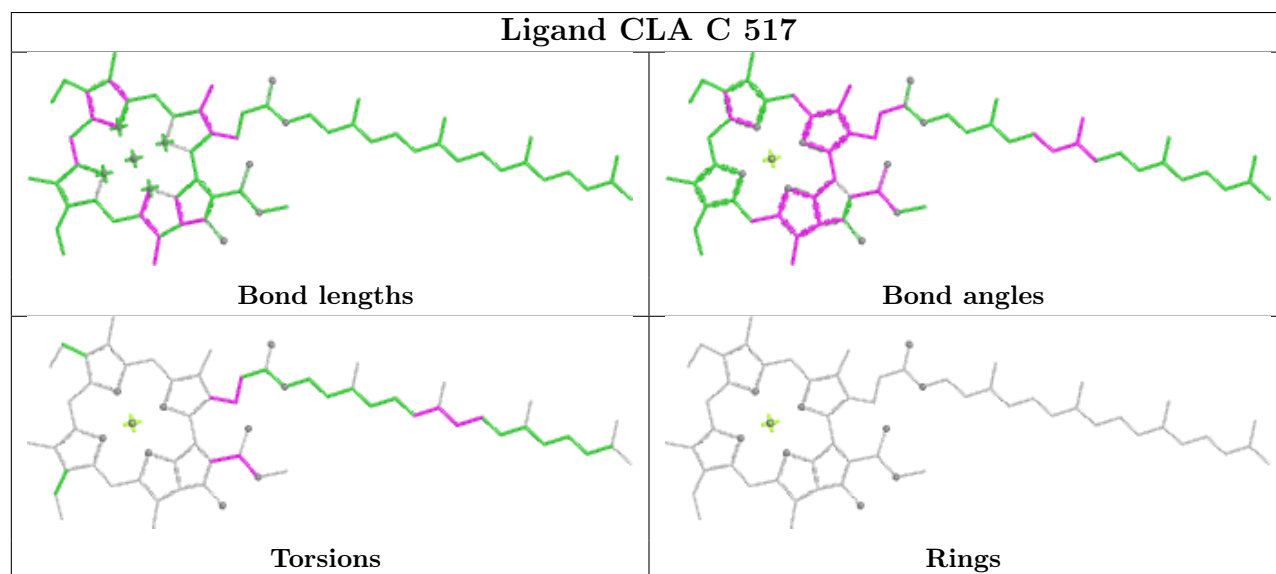
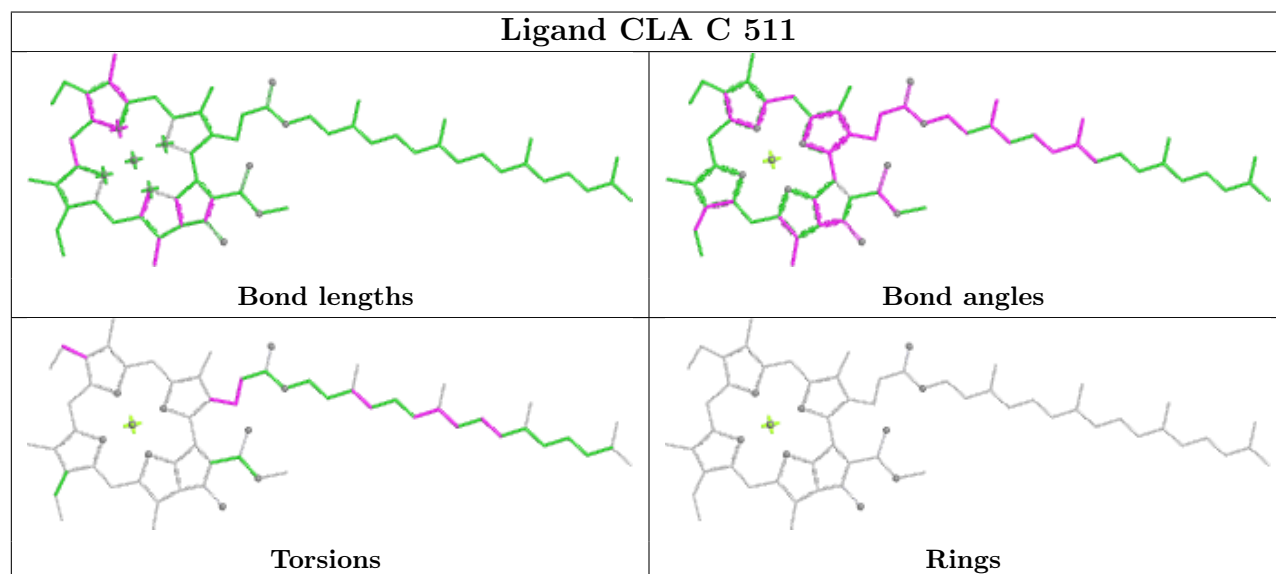
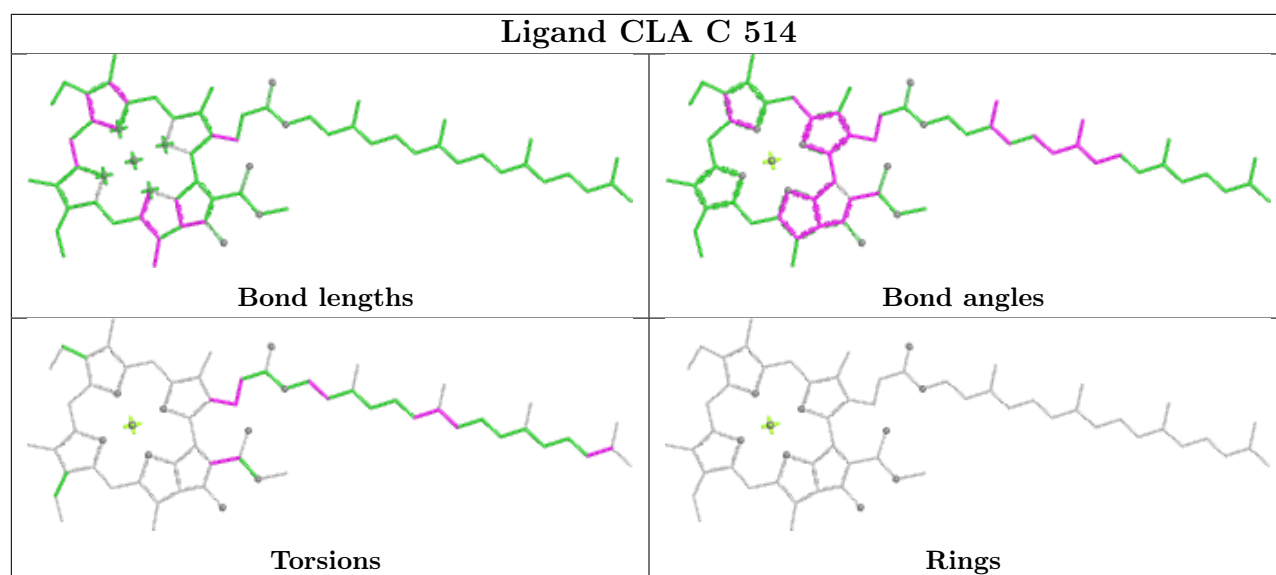
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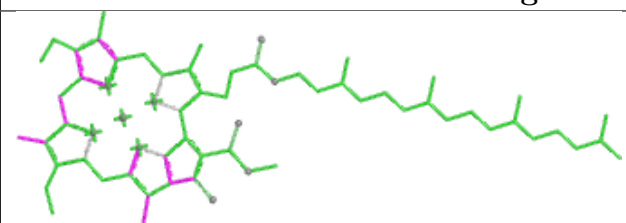
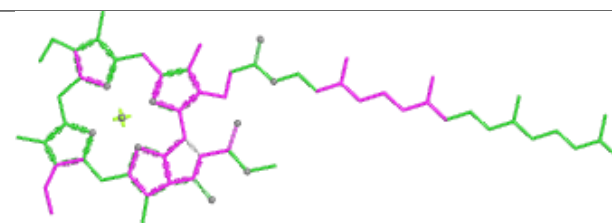
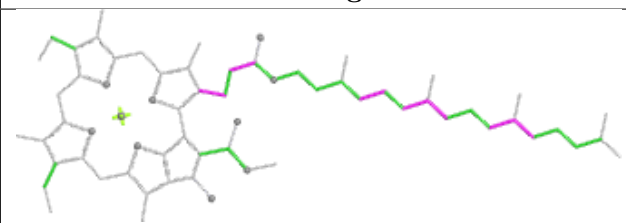
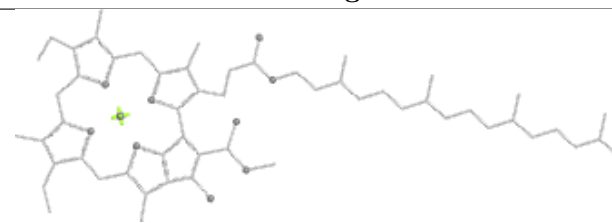
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	K	101	BCR	11	0
22	C	514	CLA	1	0
22	C	511	CLA	1	0
22	C	517	CLA	3	0
22	B	610	CLA	1	0
26	D	405	PL9	4	0
22	B	607	CLA	2	0
22	C	505	CLA	3	0
23	H	101	BCR	14	0
22	B	604	CLA	1	0
22	A	406	CLA	1	0
22	B	608	CLA	1	0
23	B	619	BCR	1	0
22	C	506	CLA	1	0
22	D	408	CLA	3	0
23	B	617	BCR	2	0
23	C	516	BCR	2	0
22	B	611	CLA	1	0
22	B	612	CLA	1	0
23	A	407	BCR	1	0
22	C	513	CLA	2	0
22	D	407	CLA	3	0
23	C	515	BCR	4	0
21	D	406	PHO	1	0
22	B	613	CLA	3	0
22	D	402	CLA	2	0
22	C	504	CLA	3	0
25	I	101	LMG	2	0
22	C	510	CLA	1	0
22	B	615	CLA	1	0
22	C	509	CLA	1	0
23	C	518	BCR	1	0
22	D	401	CLA	2	0
25	D	404	LMG	1	0
25	3	101	LMG	2	0
22	B	614	CLA	3	0
22	C	503	CLA	3	0
22	B	602	CLA	2	0
23	F	102	BCR	1	0
25	D	403	LMG	1	0
27	E	101	HEM	3	0
22	B	603	CLA	3	0

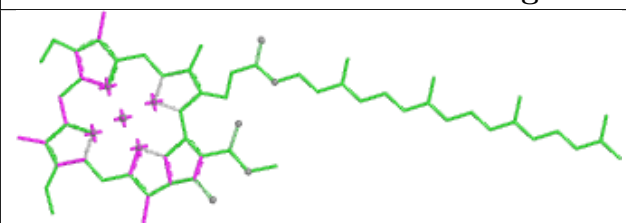
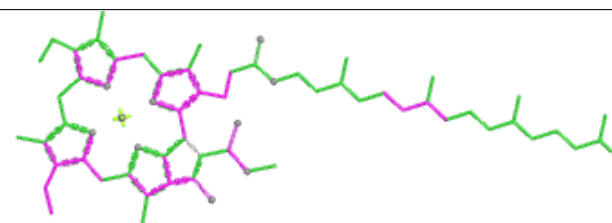
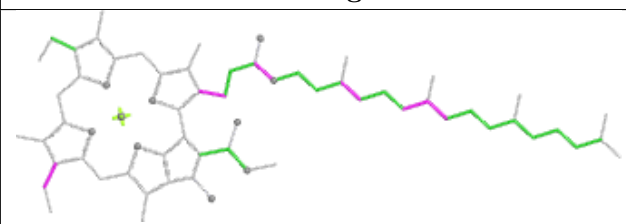
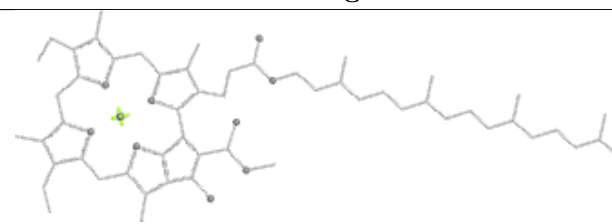
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



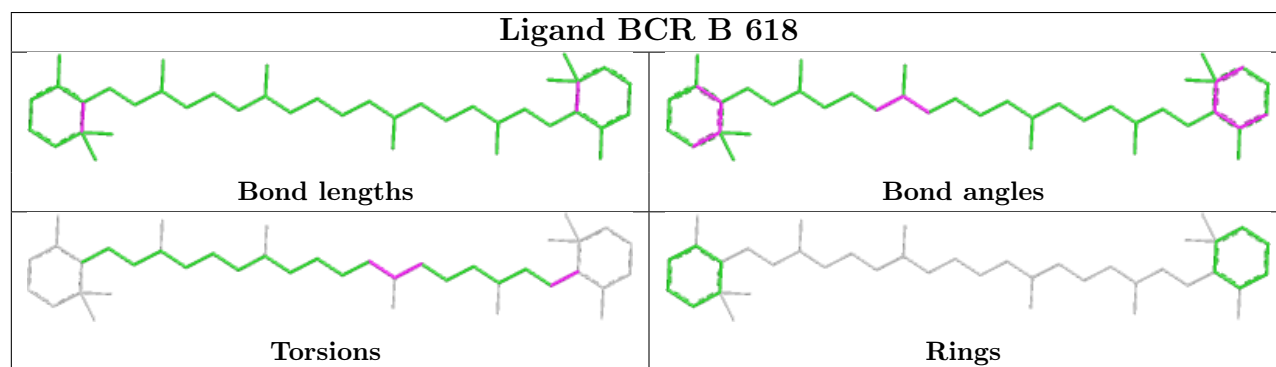
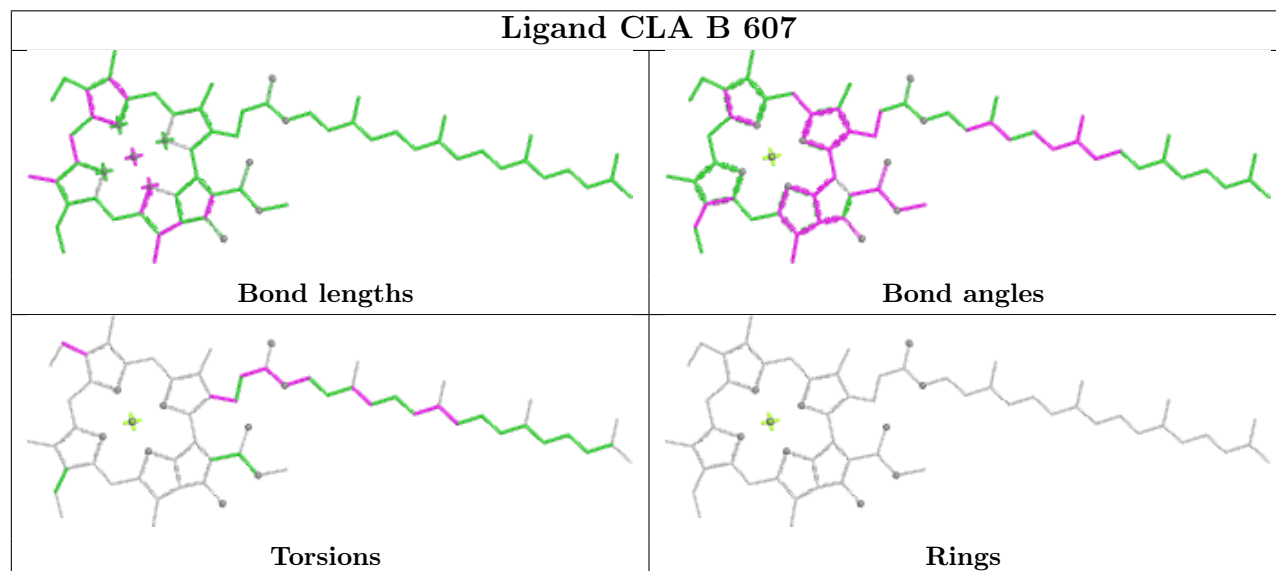
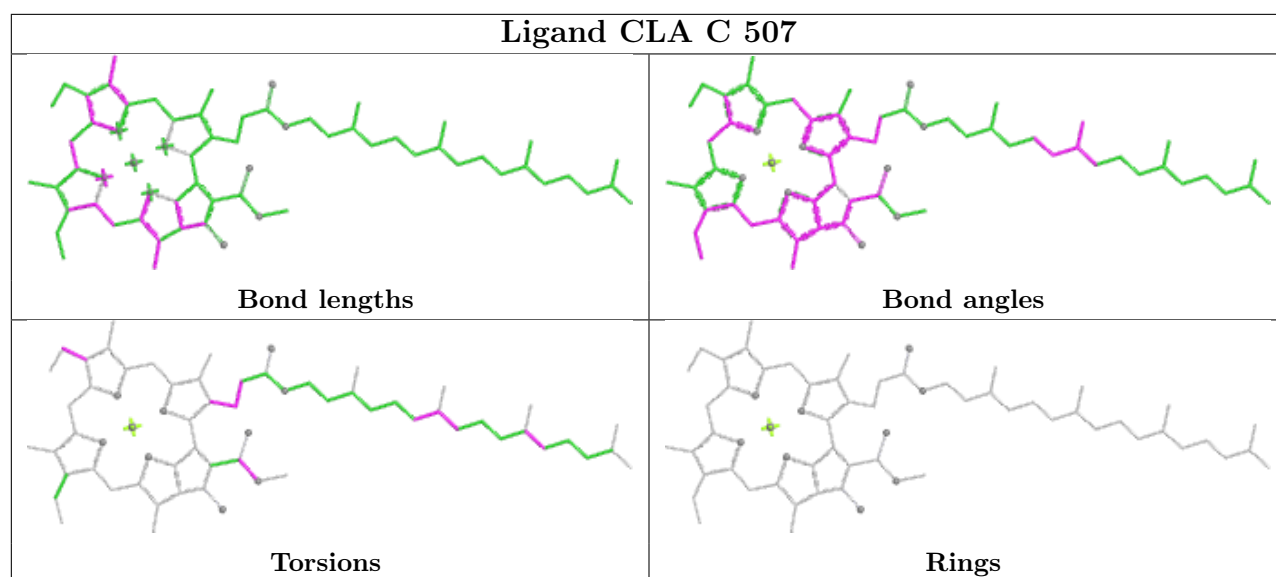


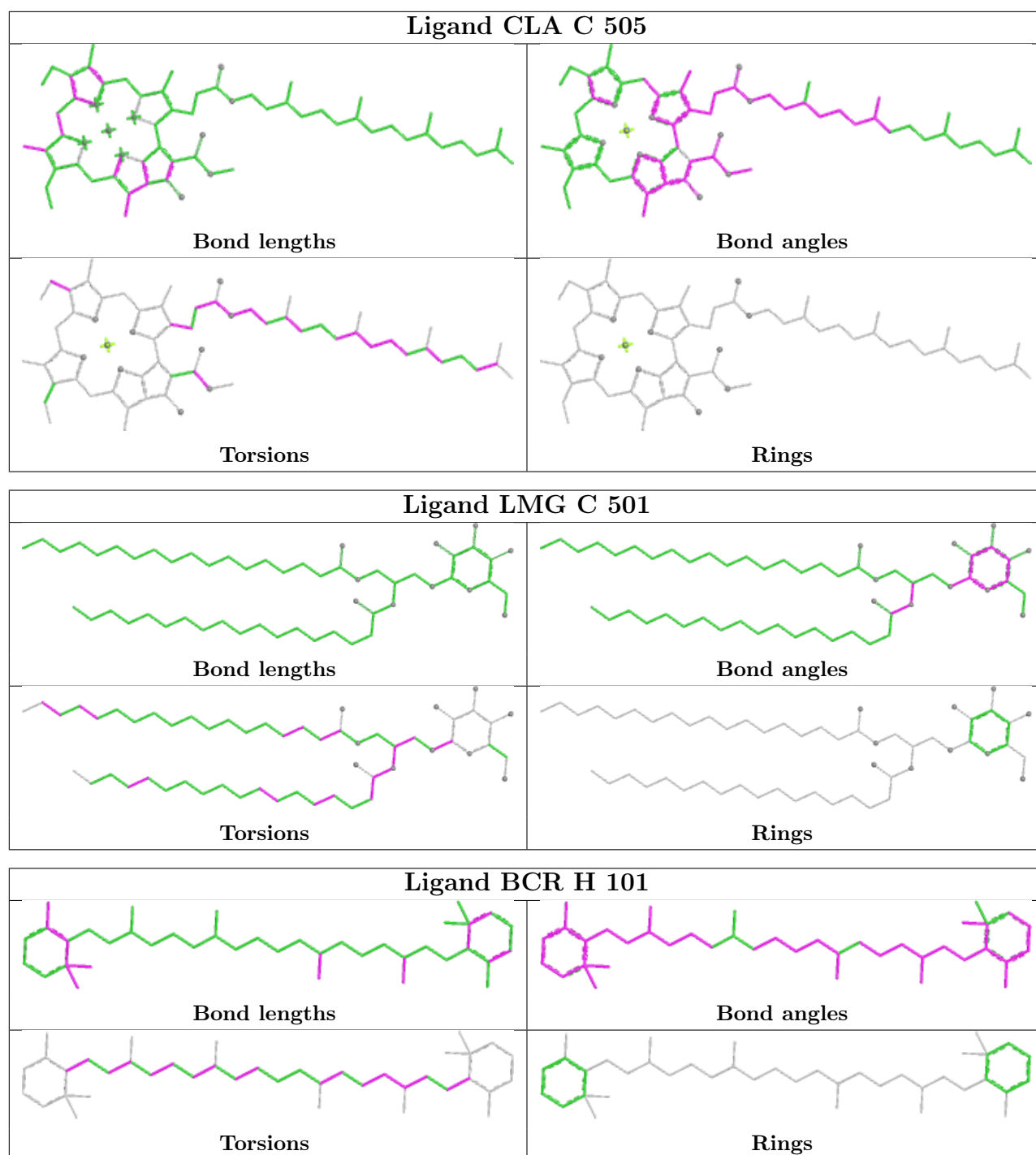


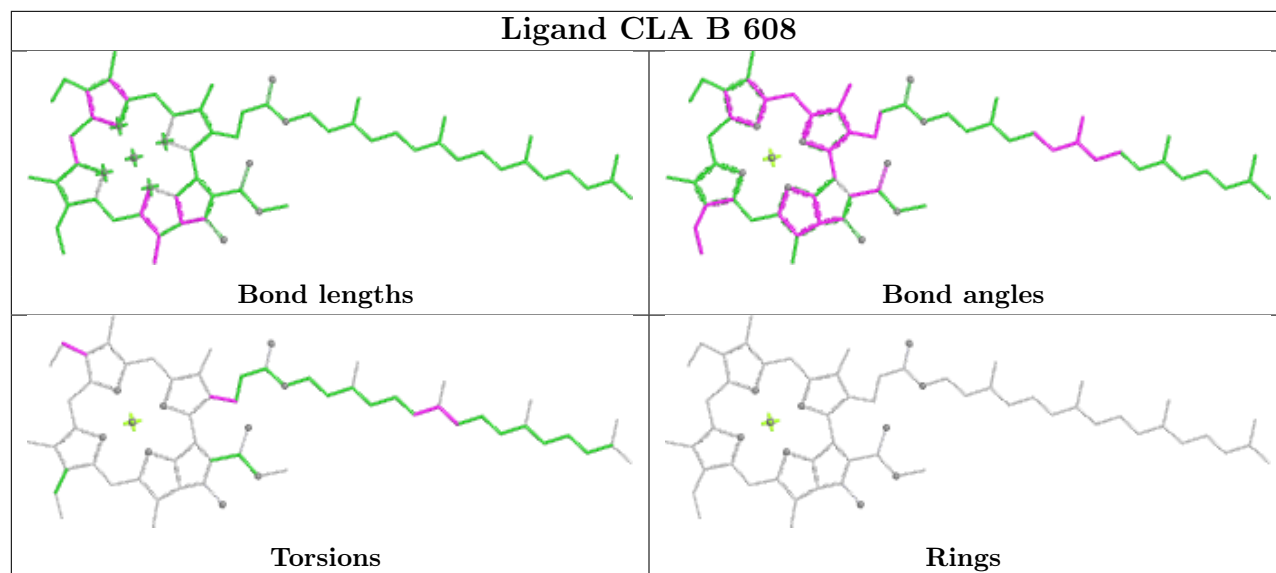
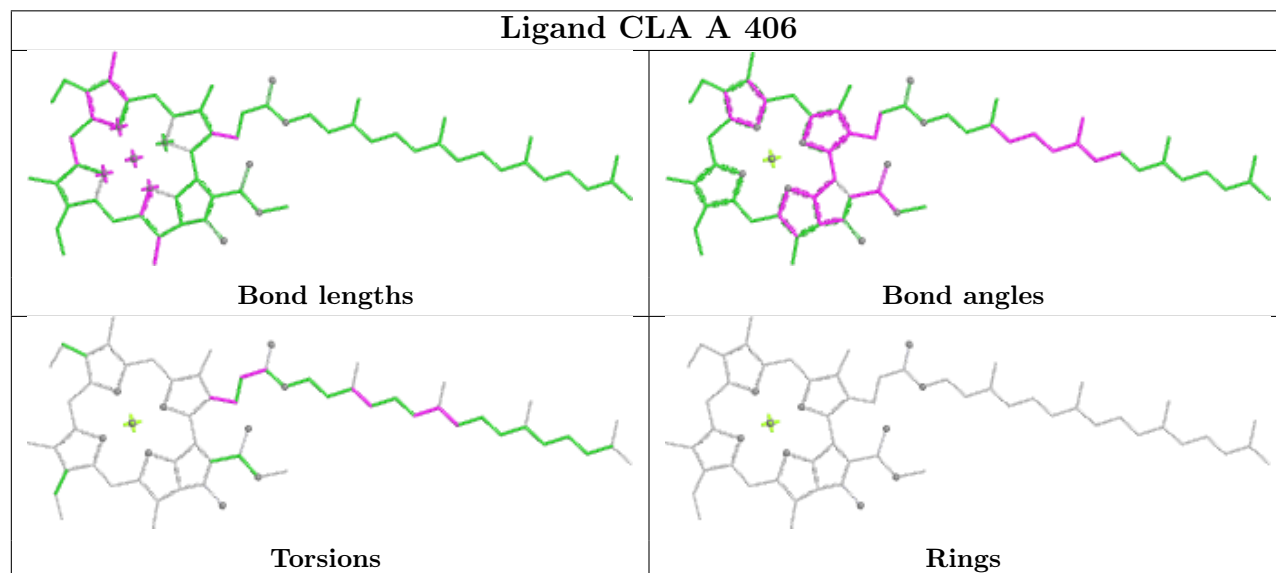
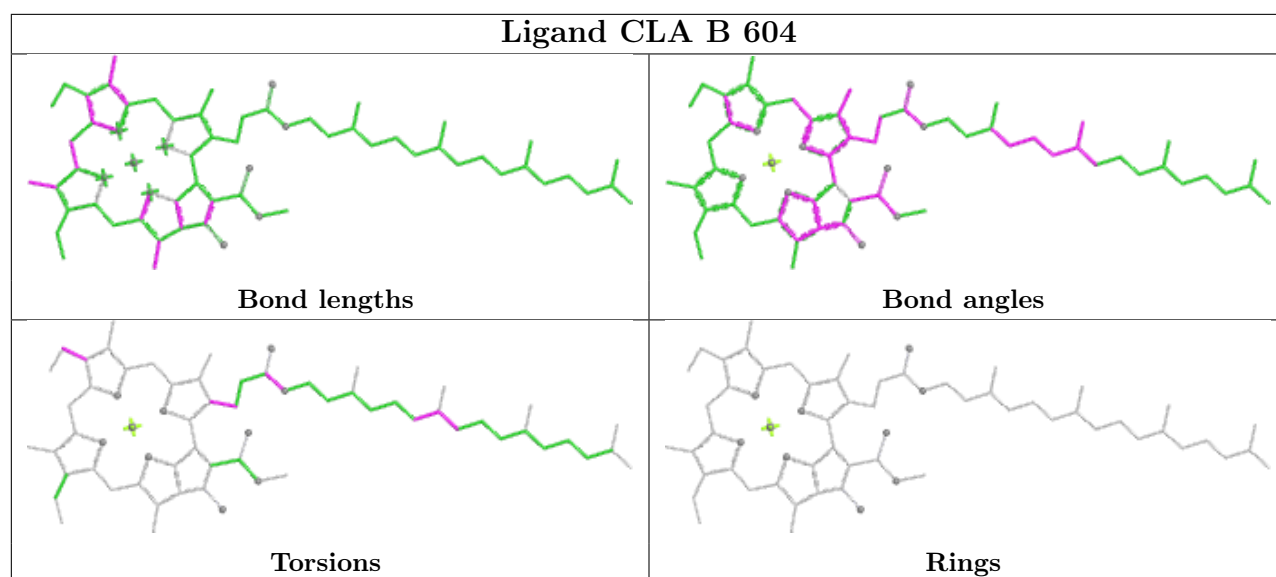
Ligand CLA A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

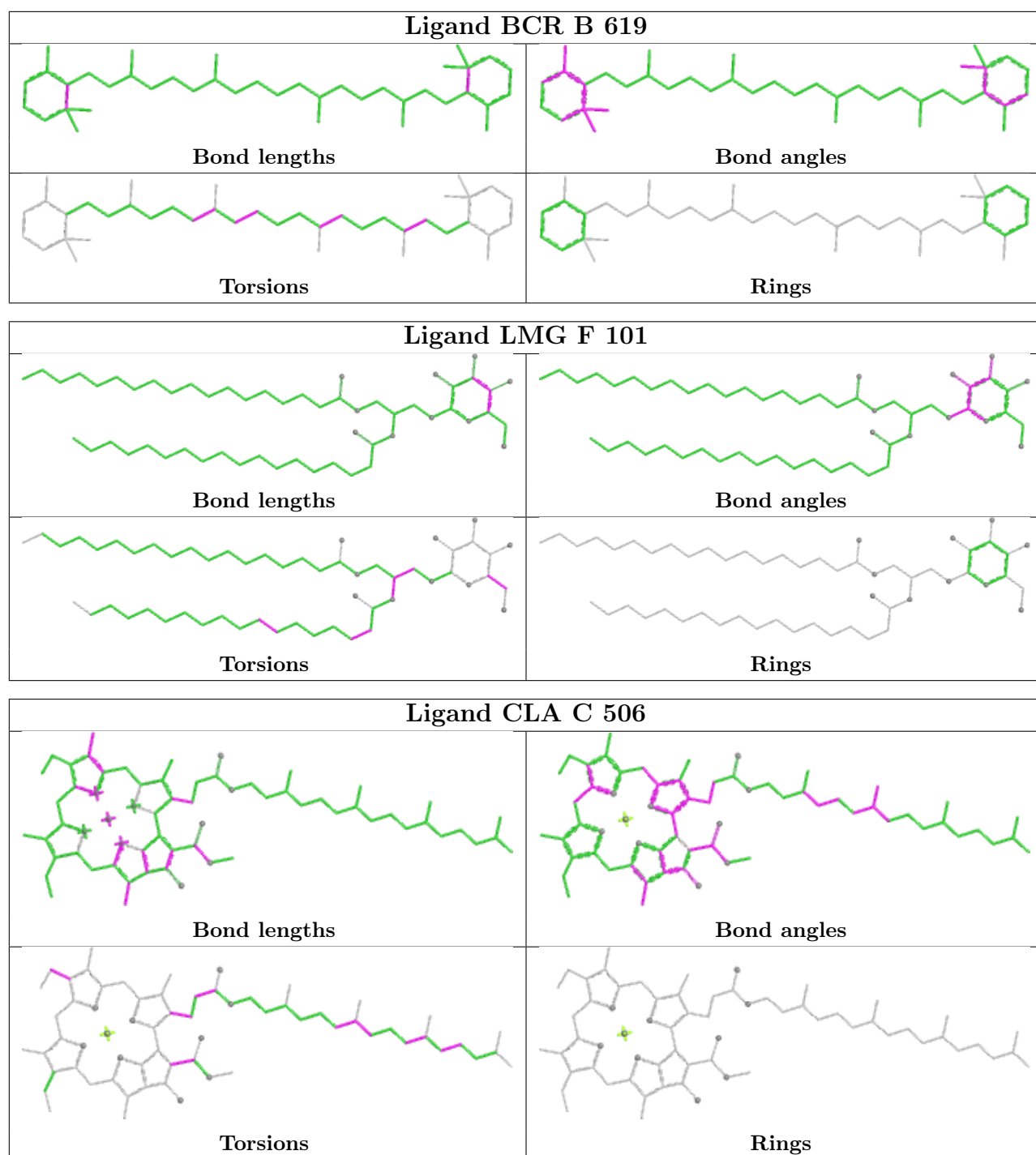
Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

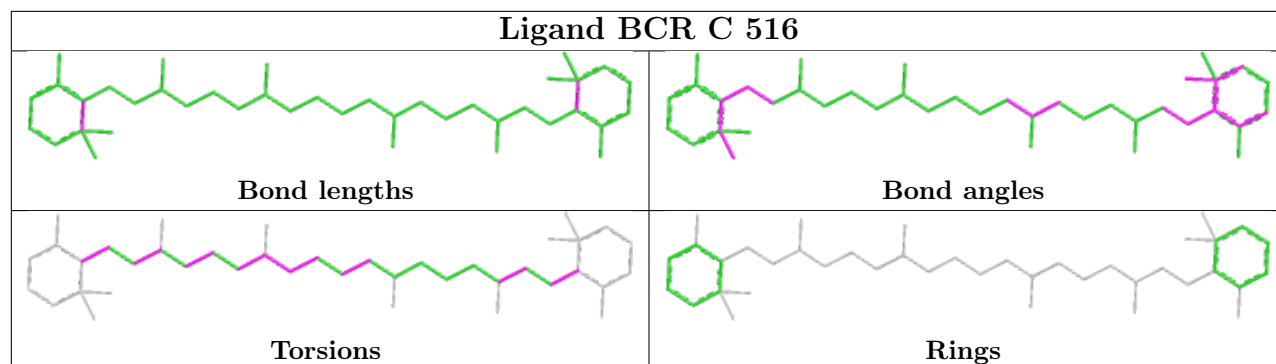
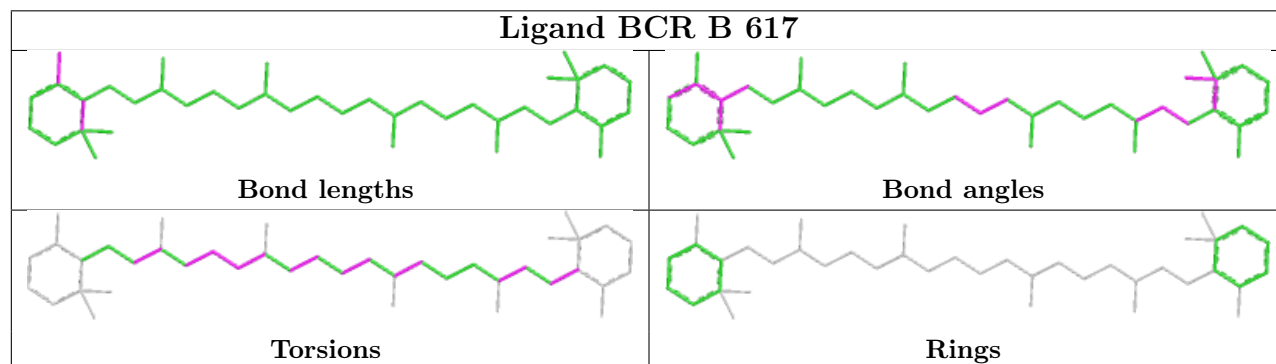
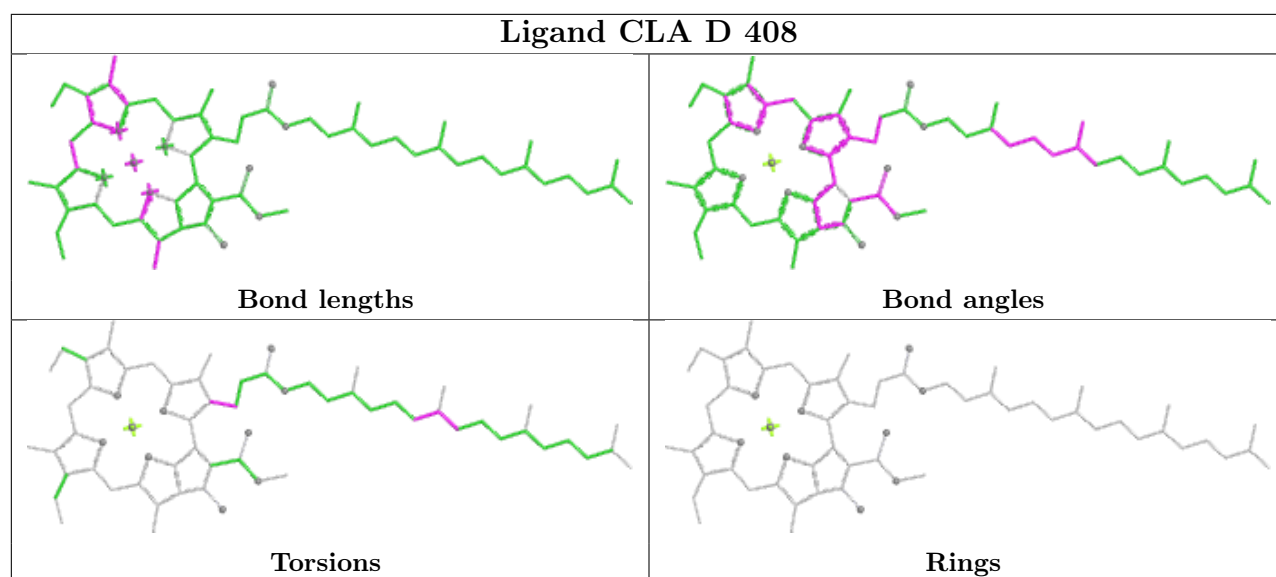
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

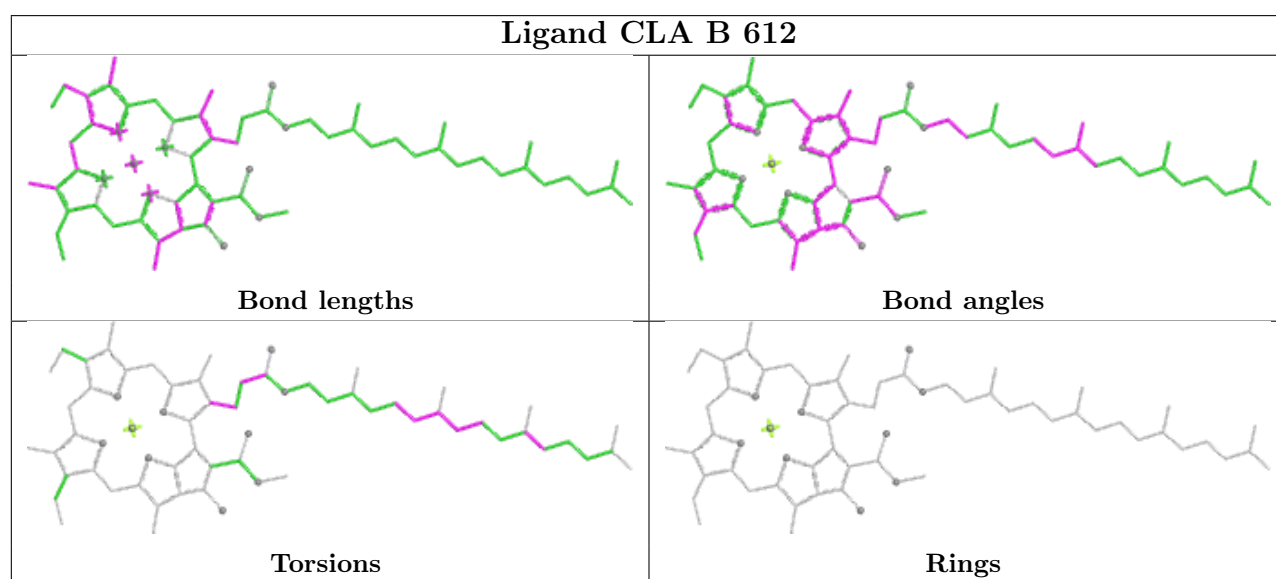
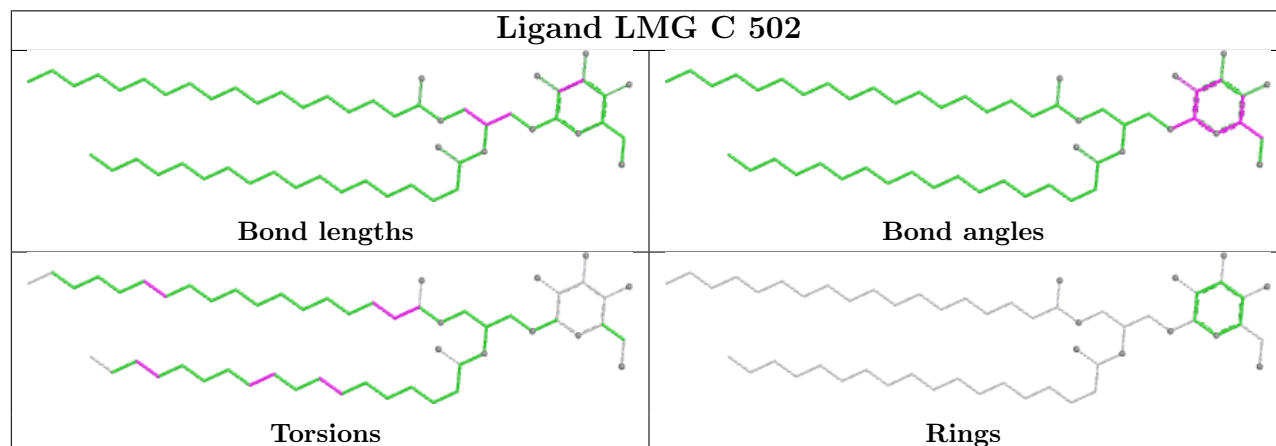
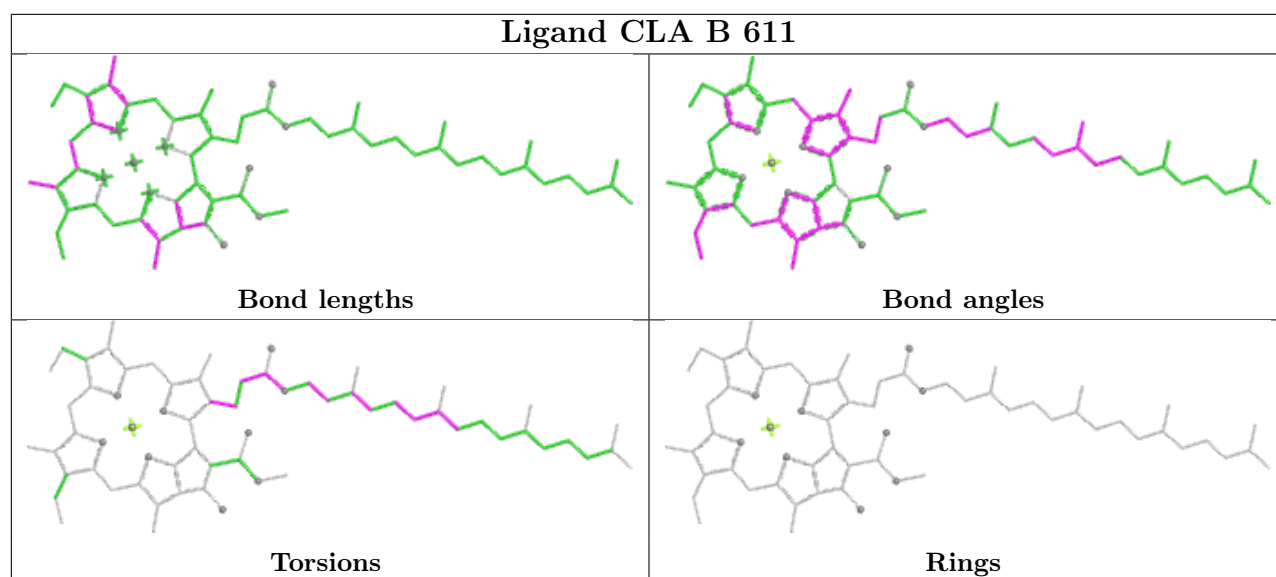


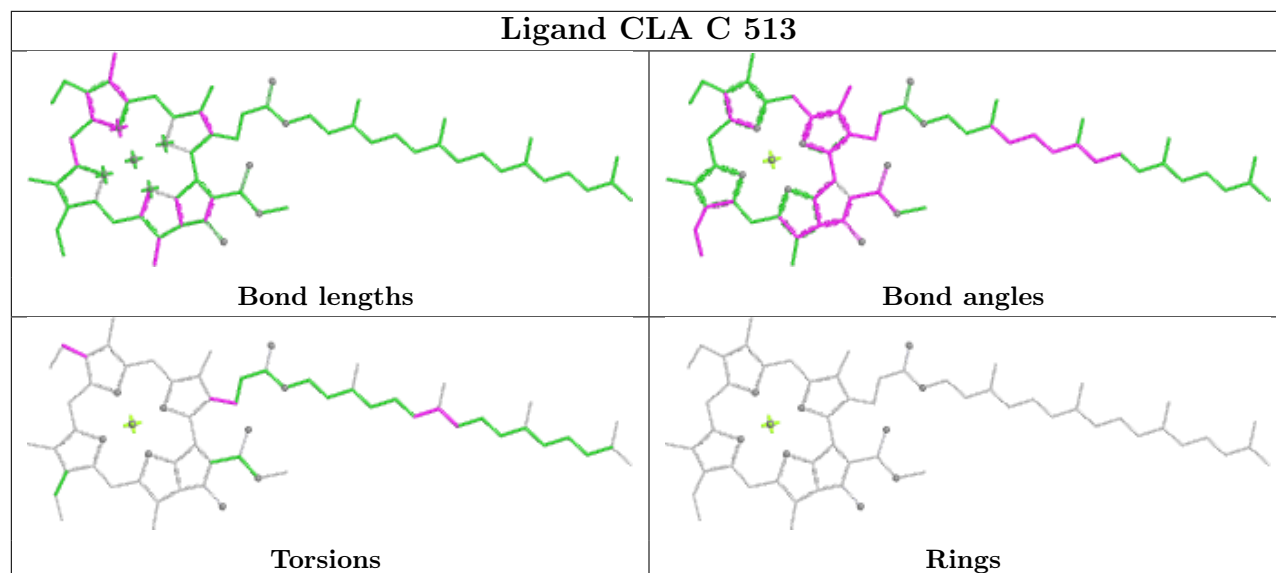
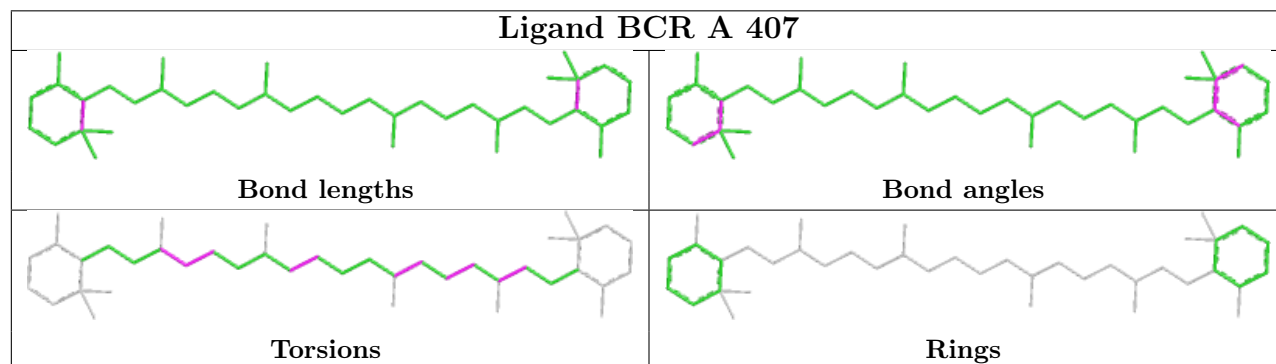
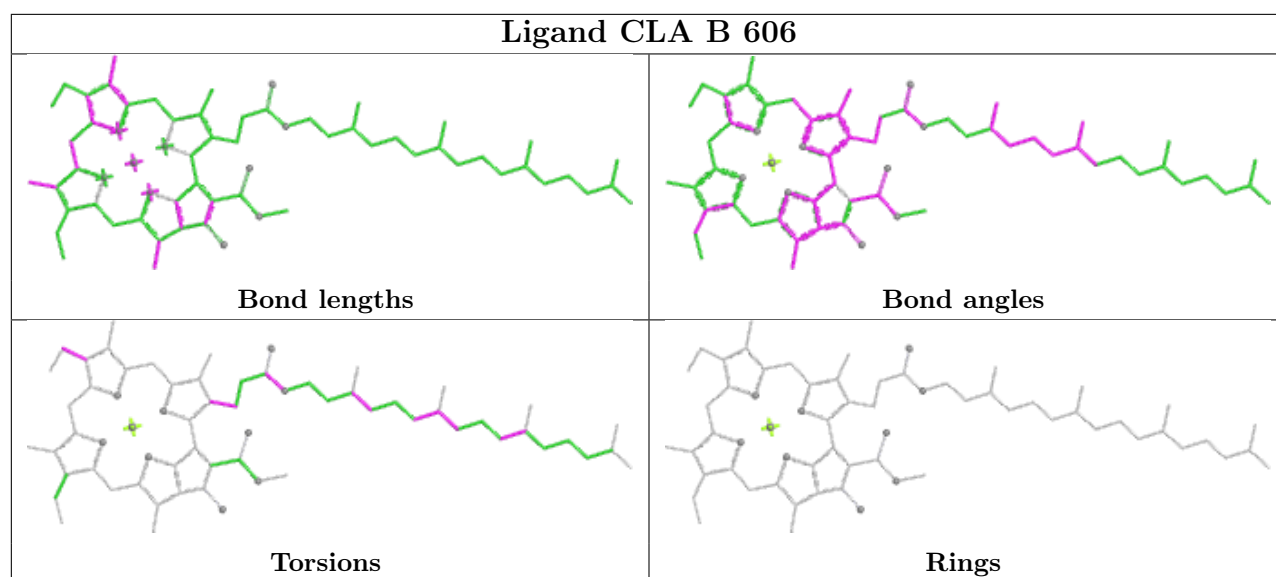


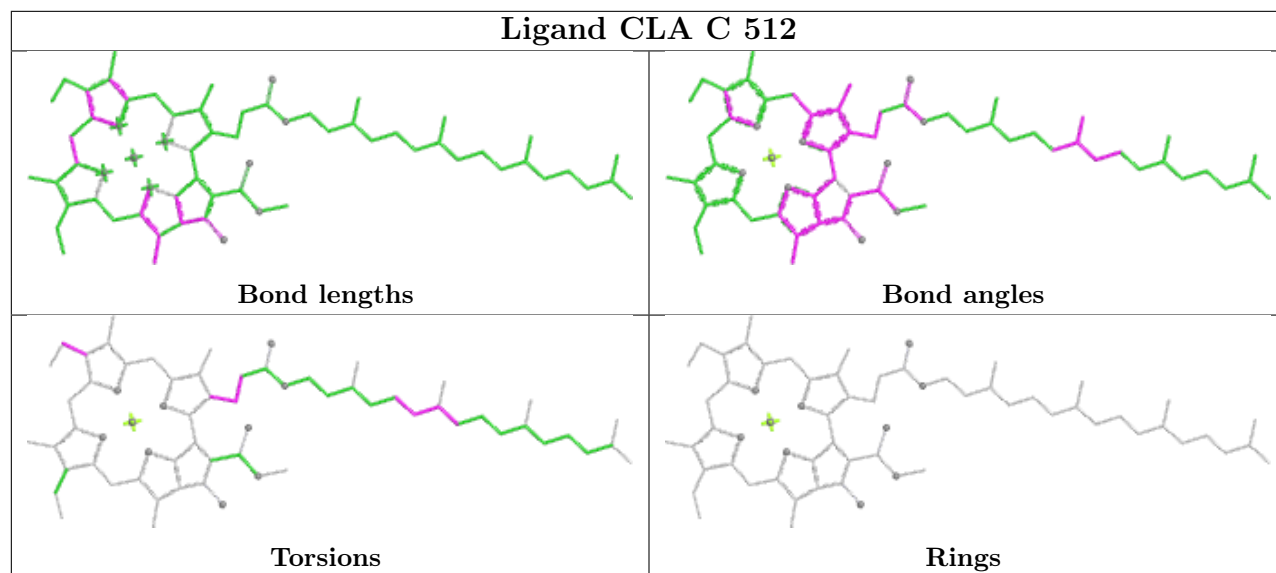
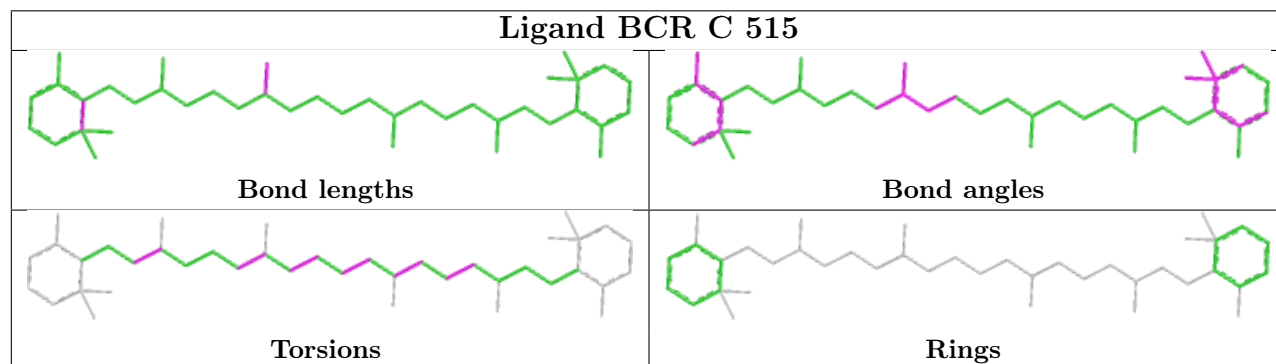
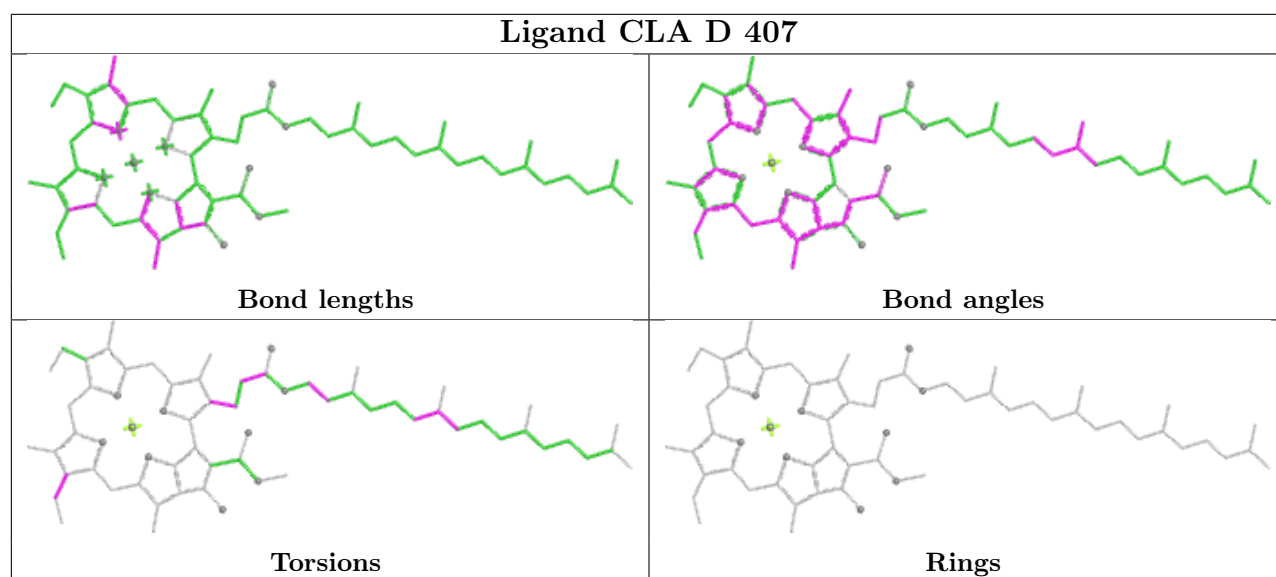


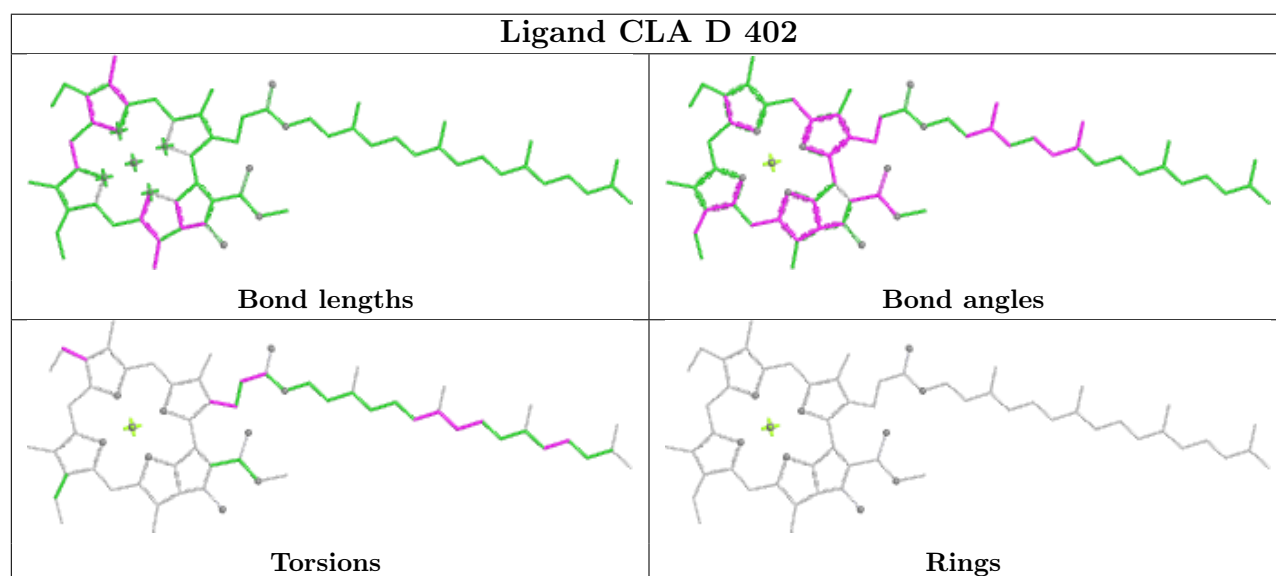
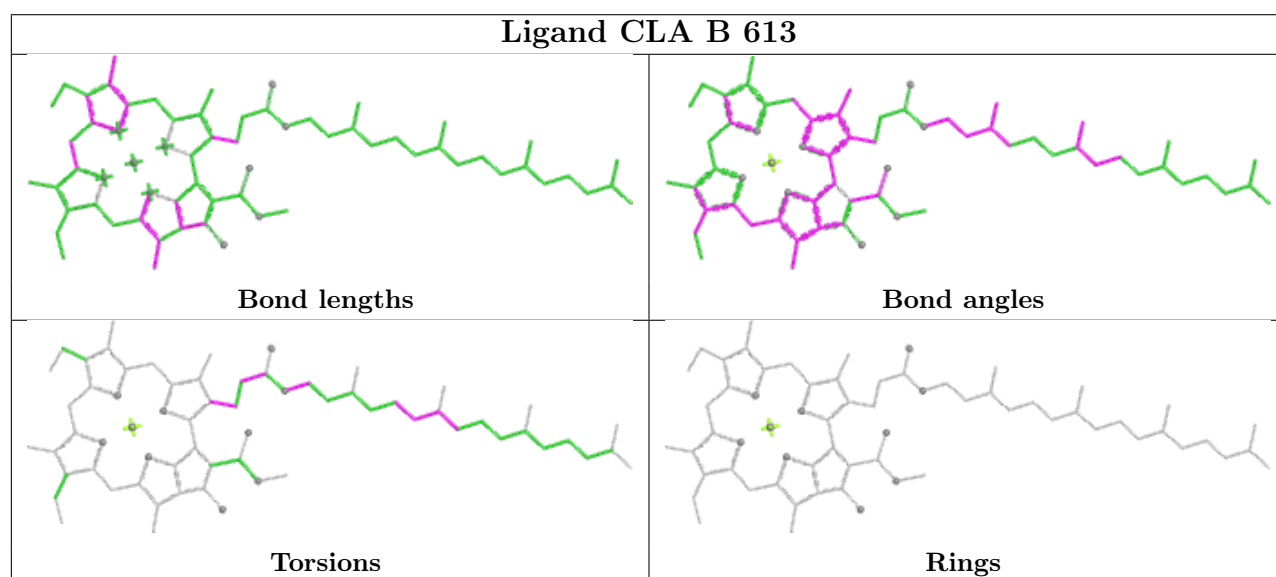
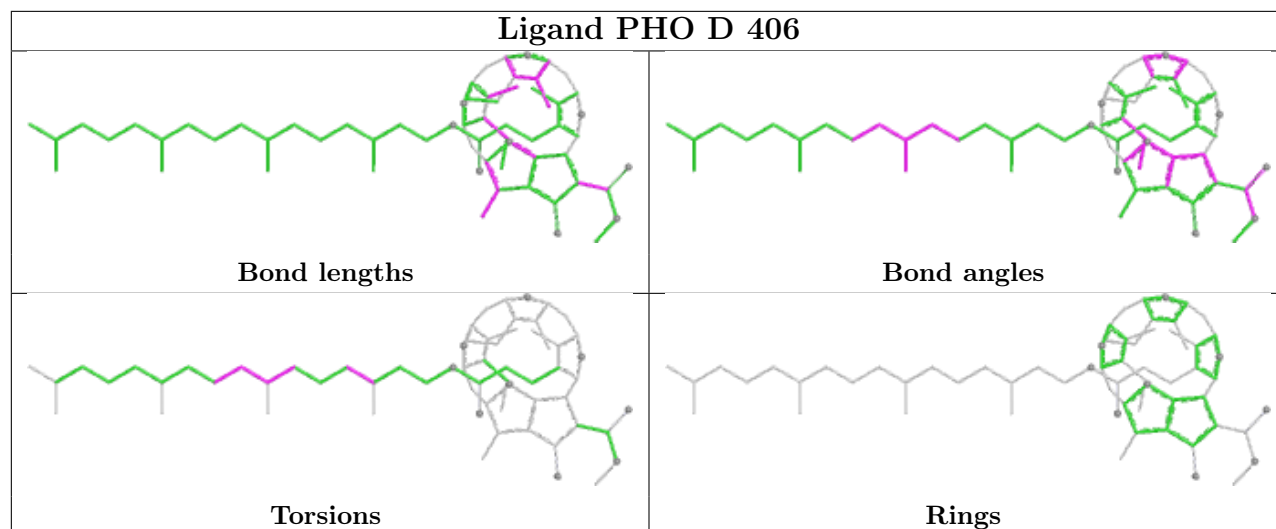


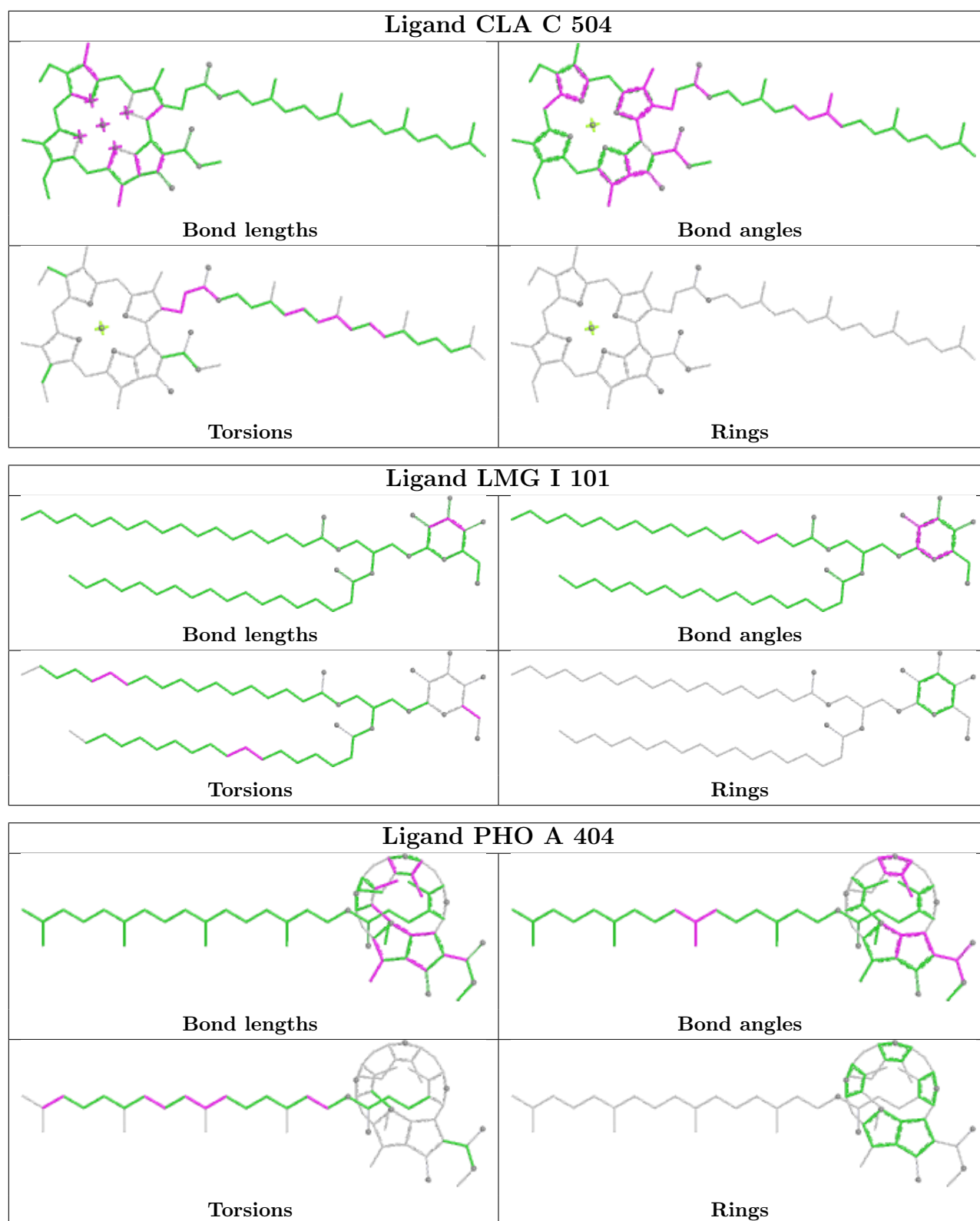


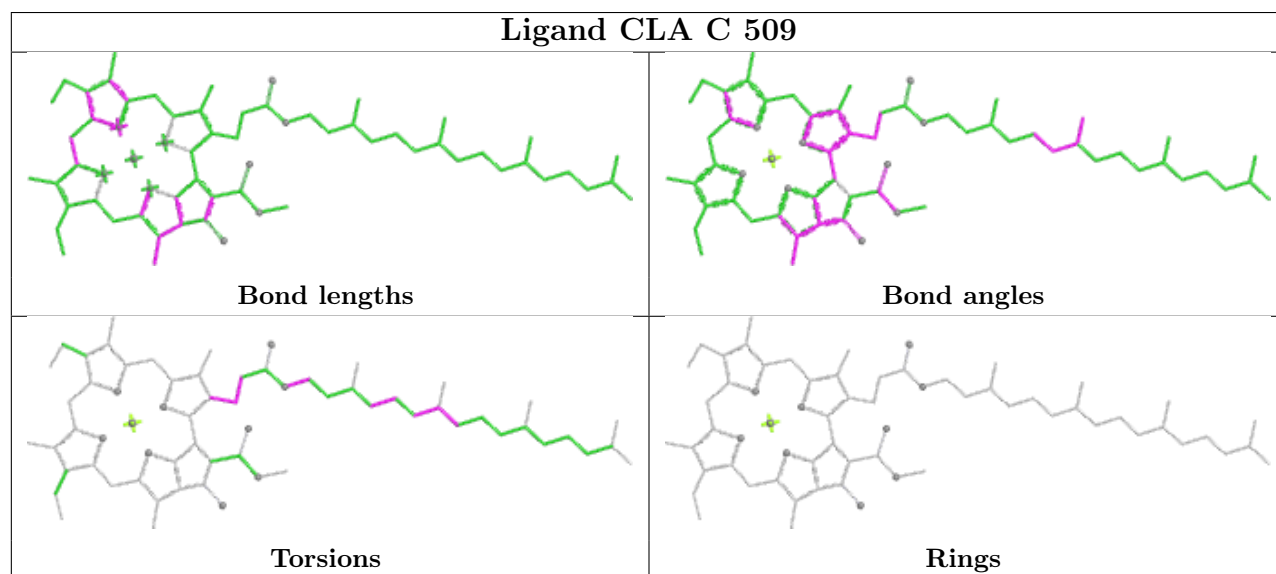
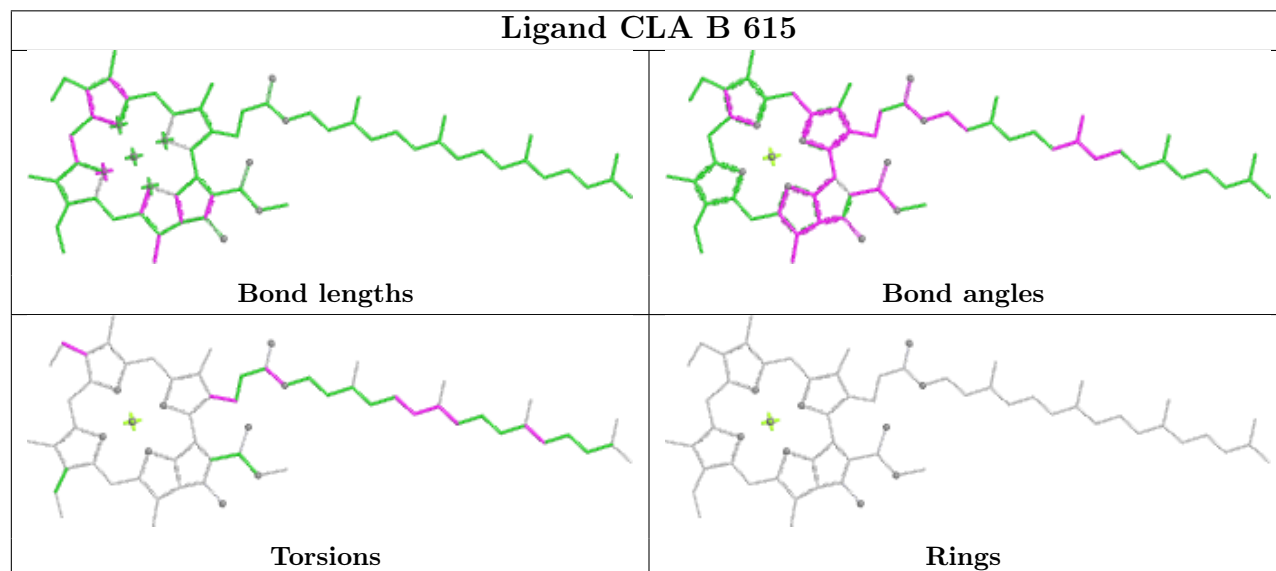
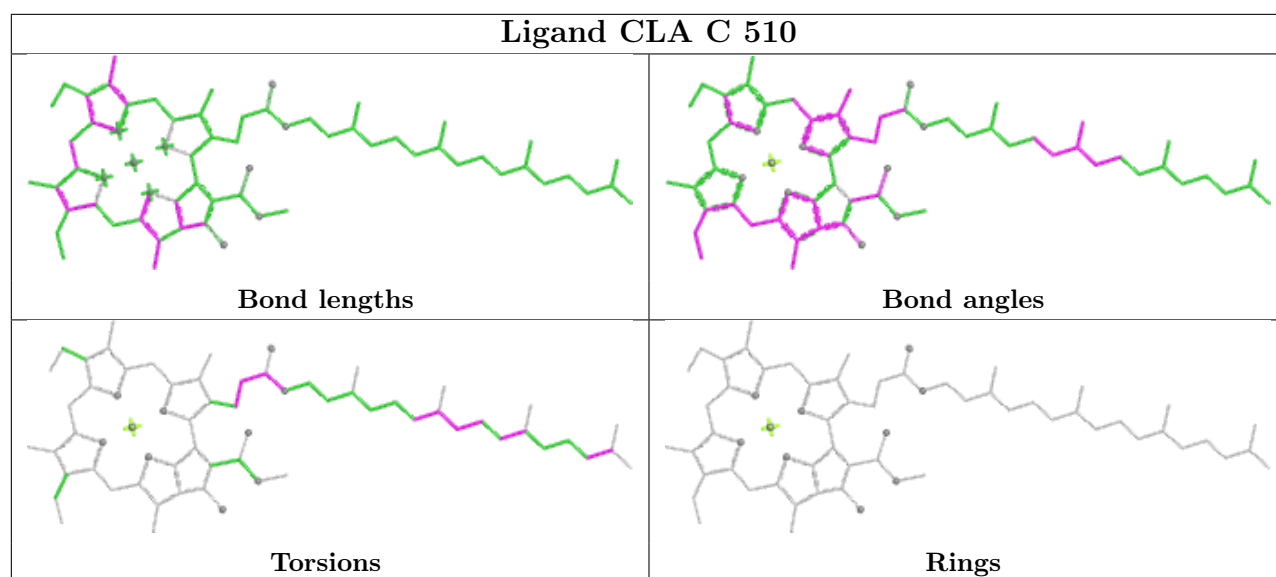


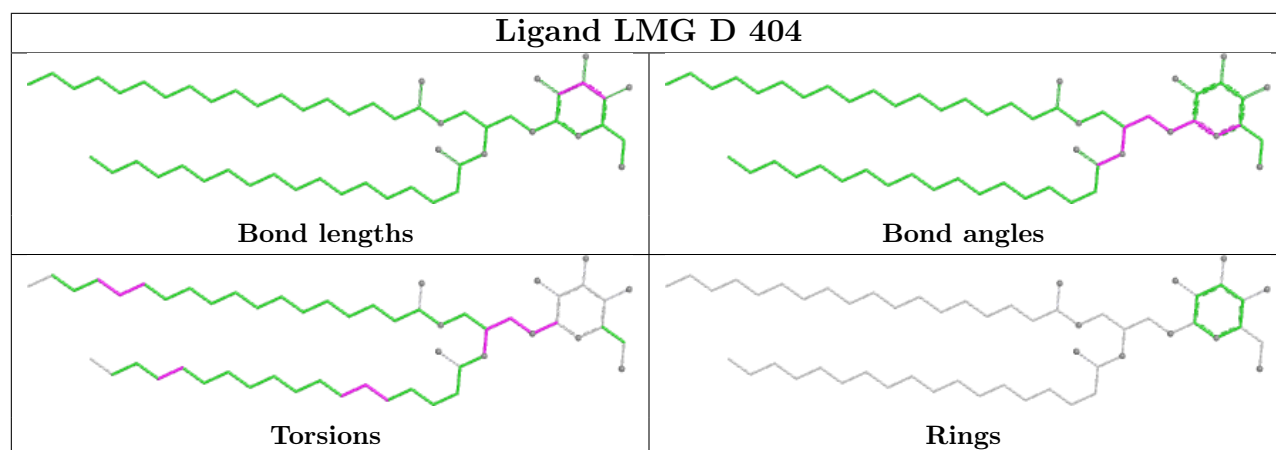
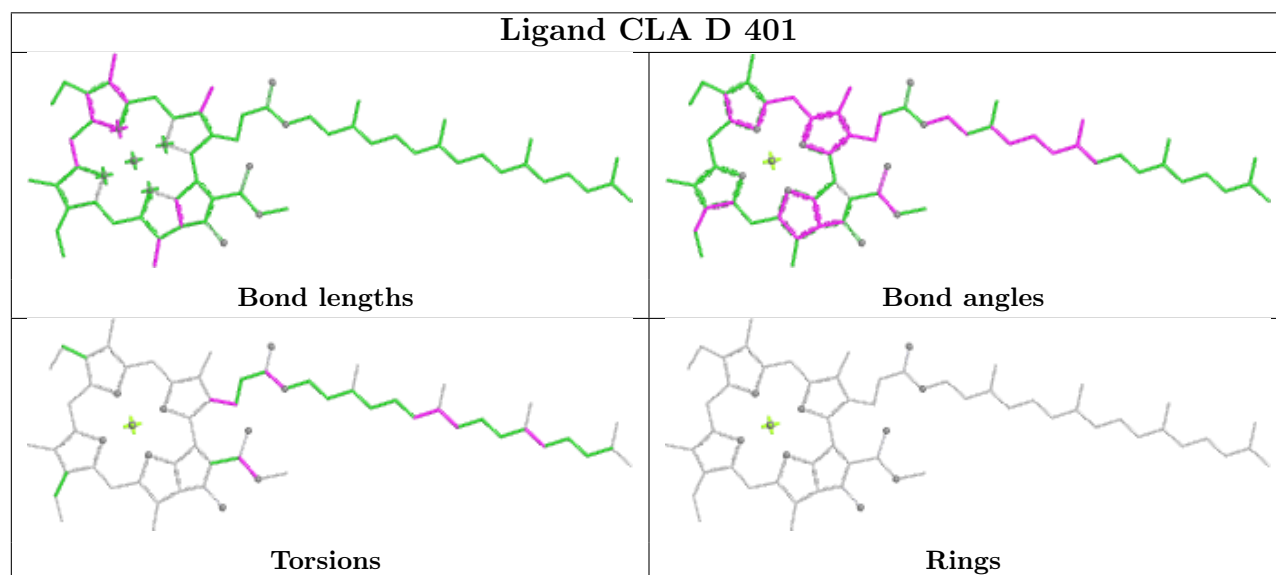
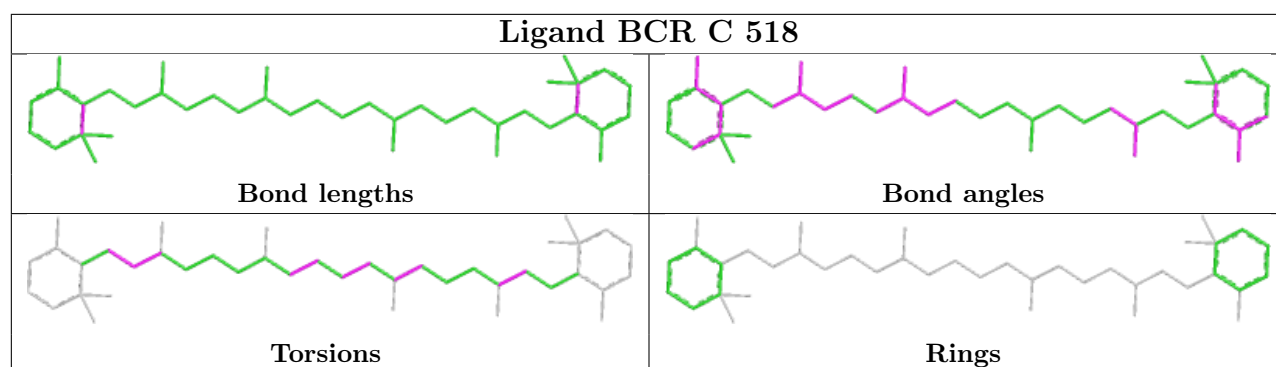




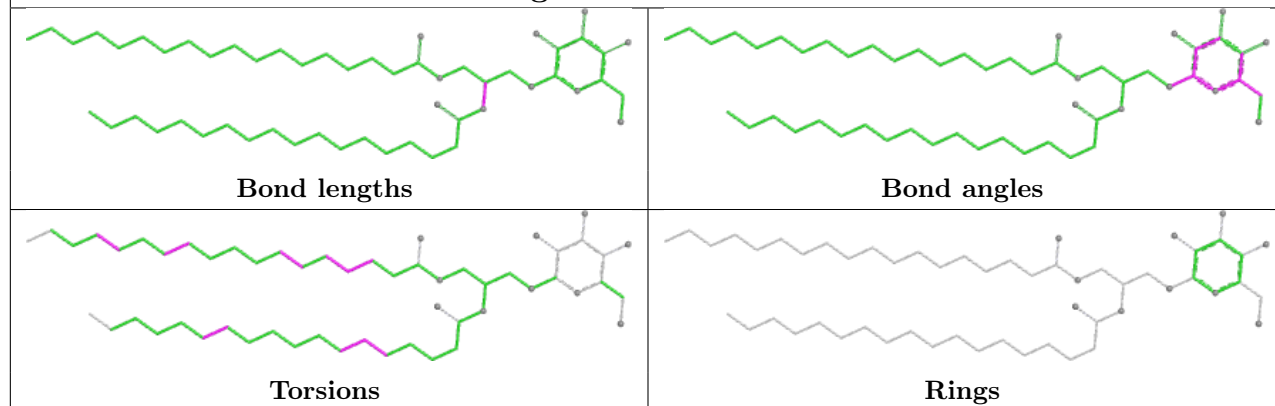




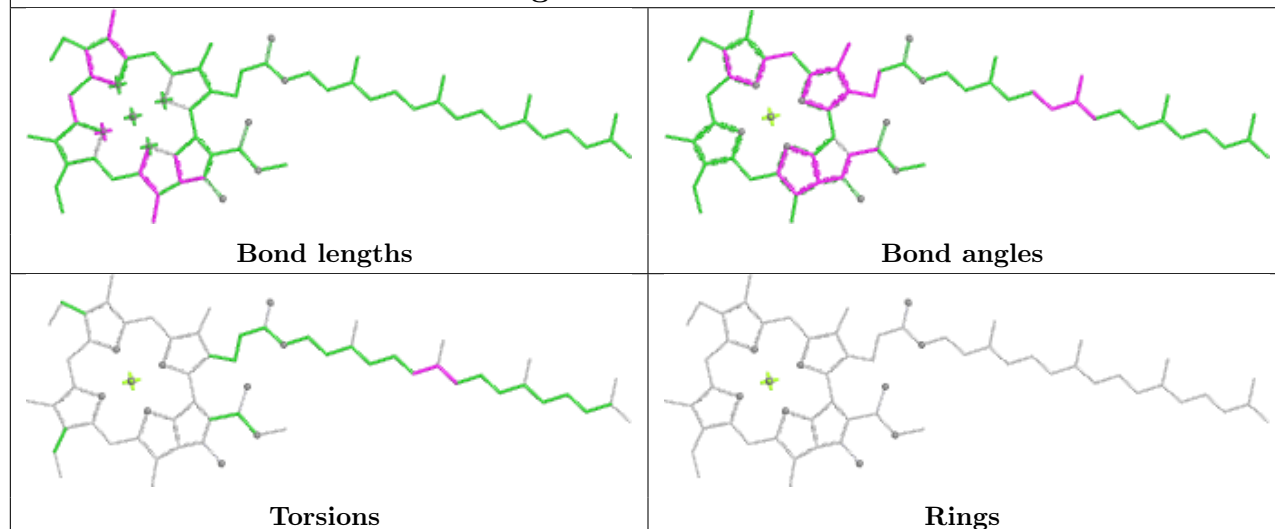




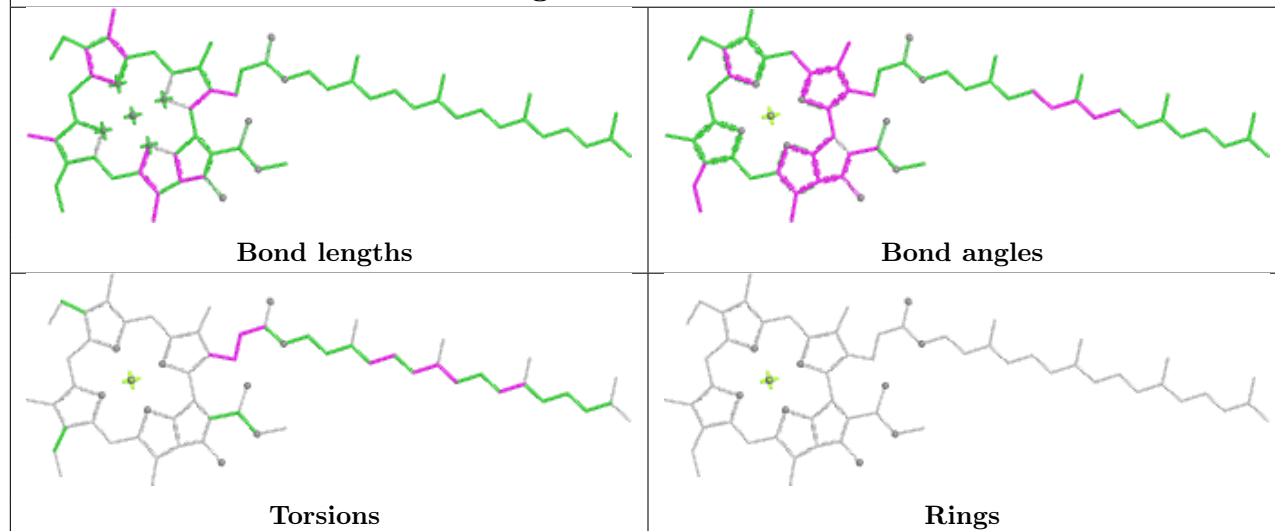
Ligand LMG 3 101

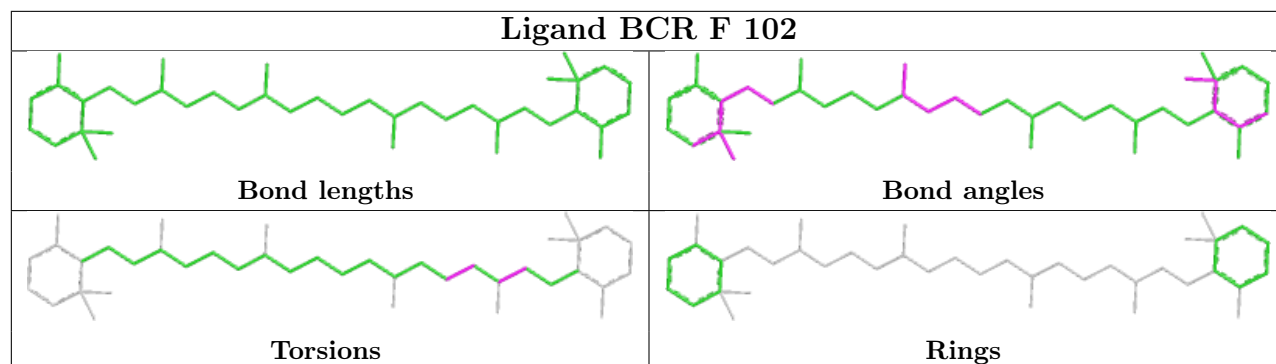
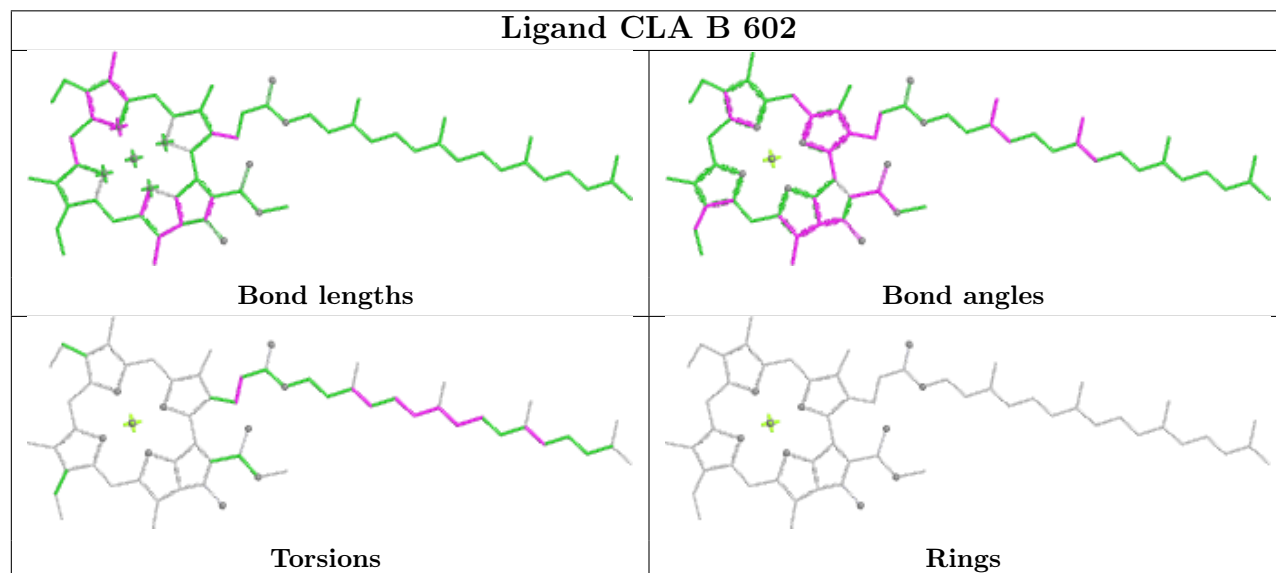
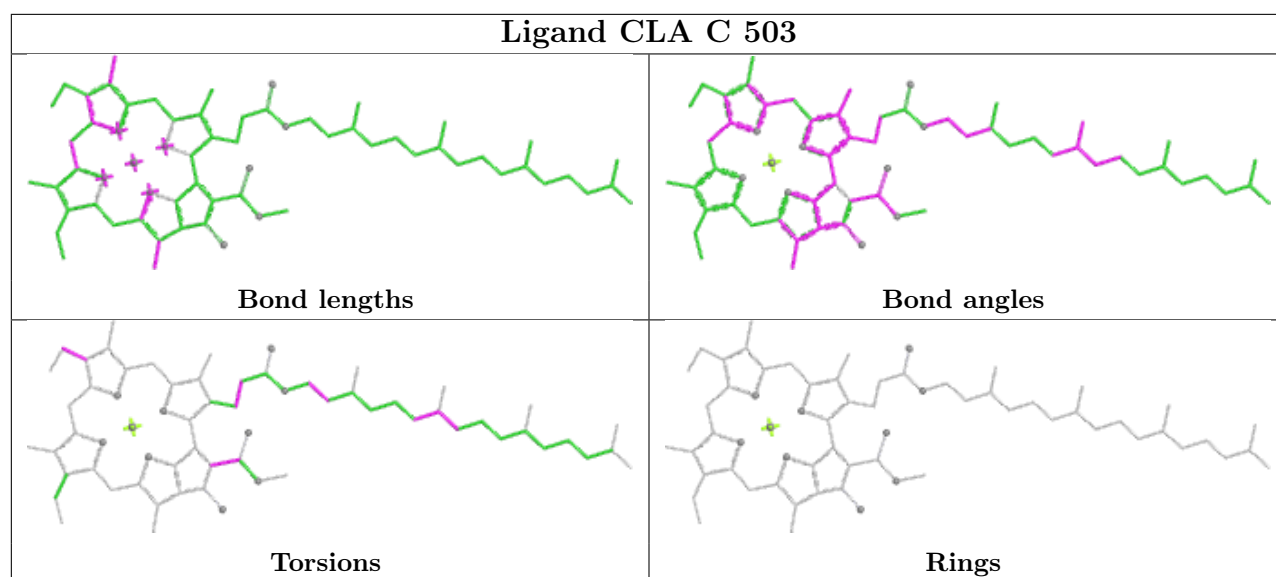


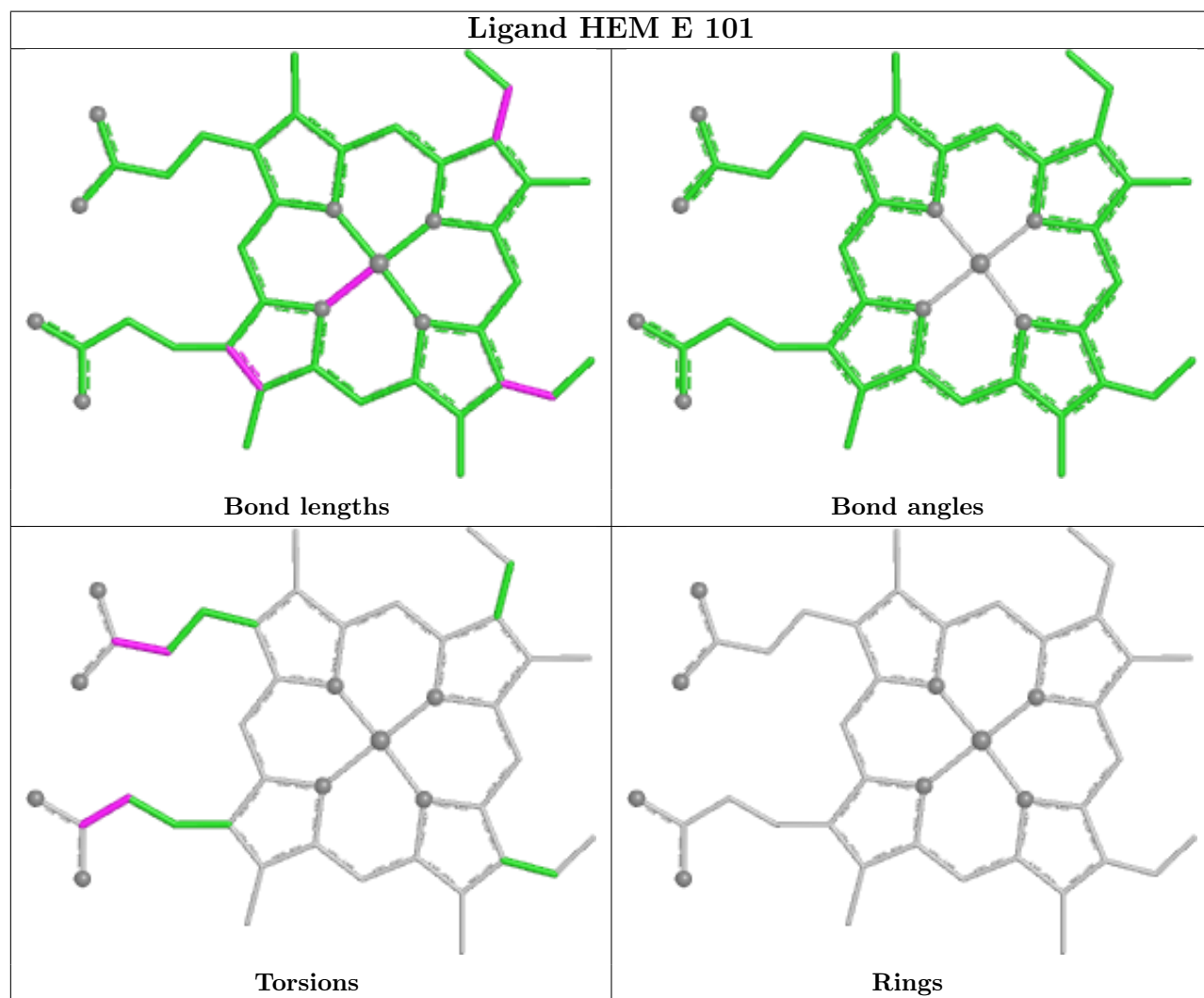
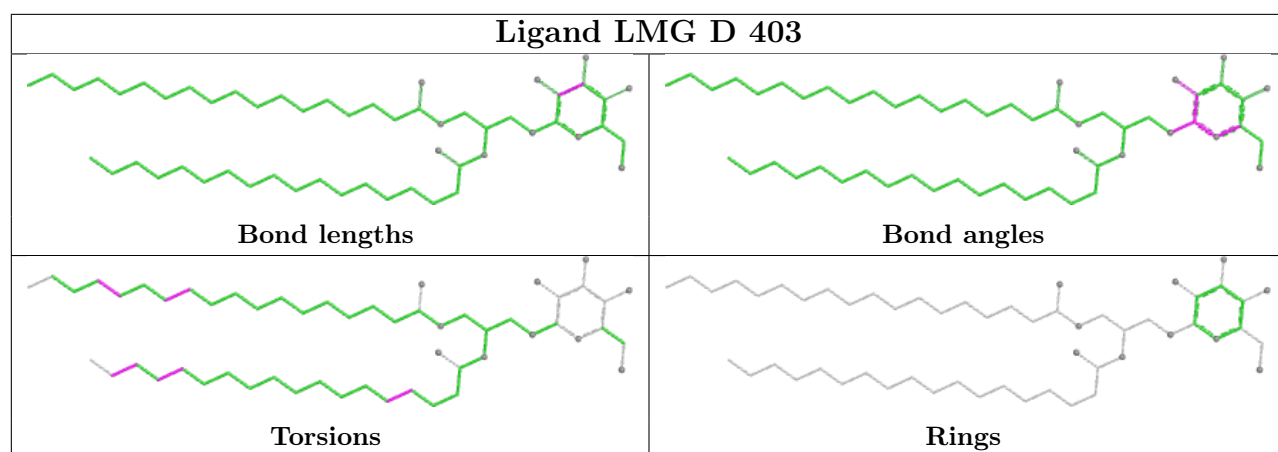
Ligand CLA C 508

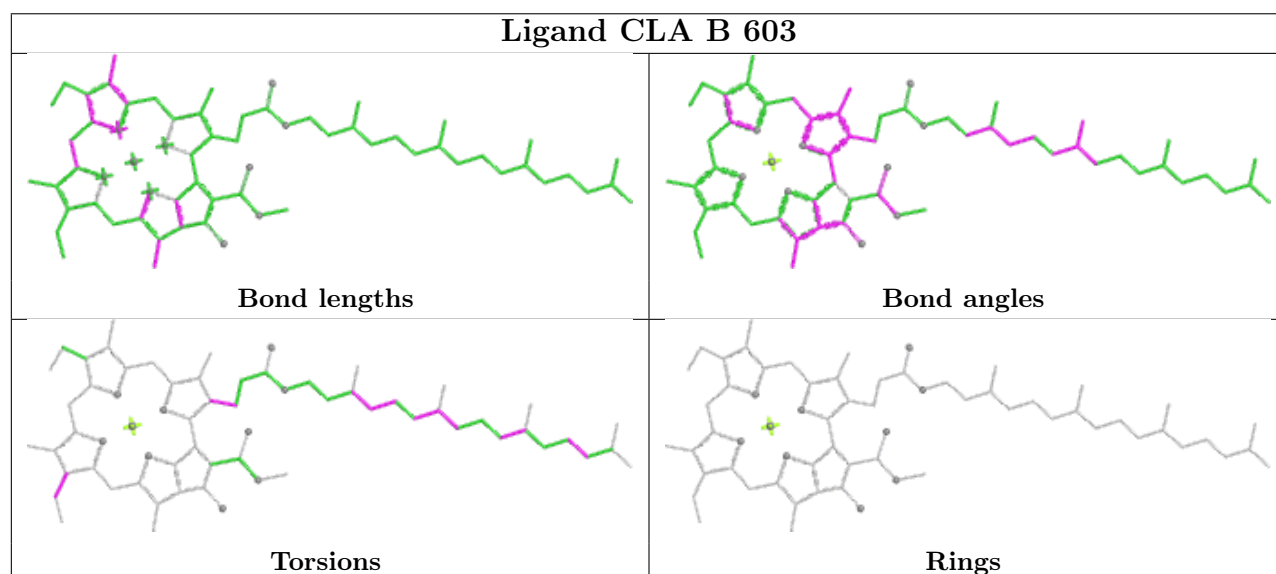
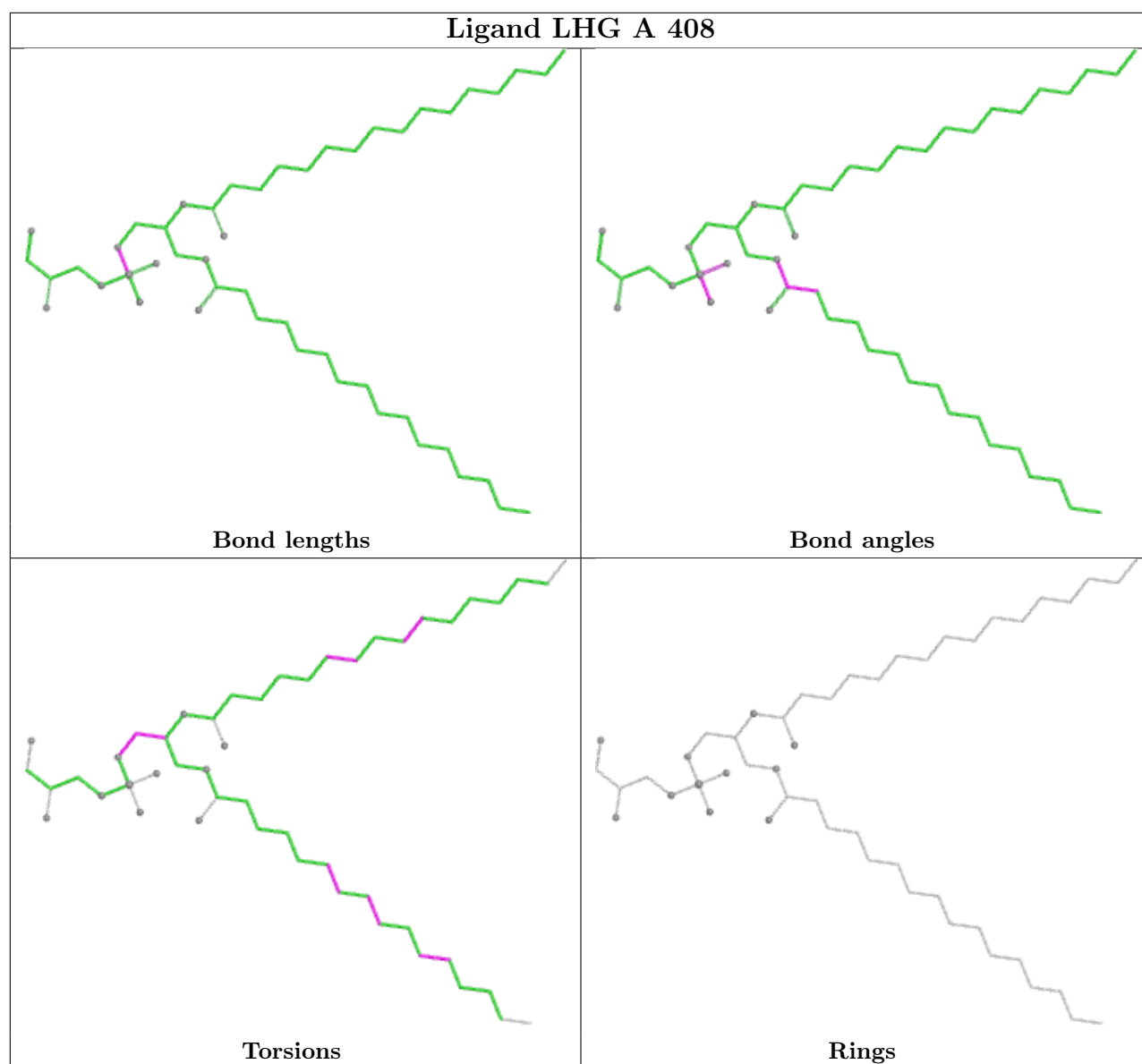


Ligand CLA B 614









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

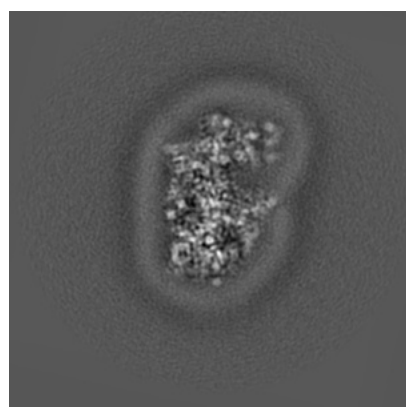
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12337. These allow visual inspection of the internal detail of the map and identification of artifacts.

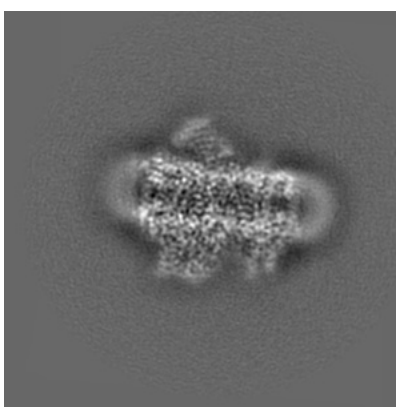
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

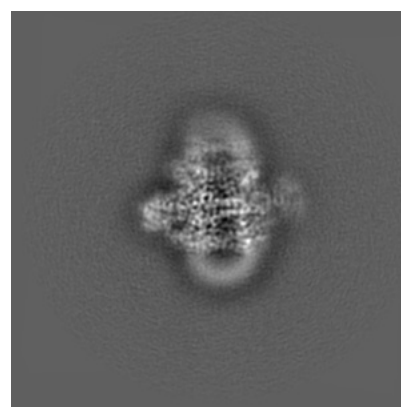
6.1.1 Primary map



X



Y

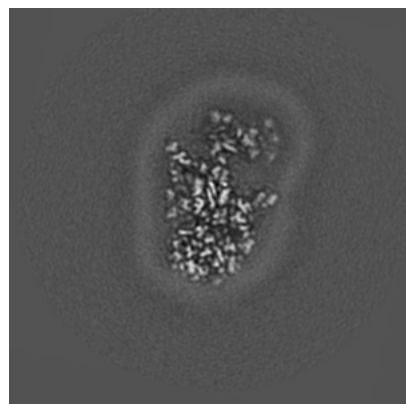


Z

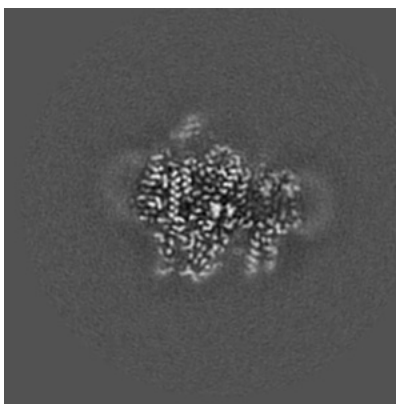
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

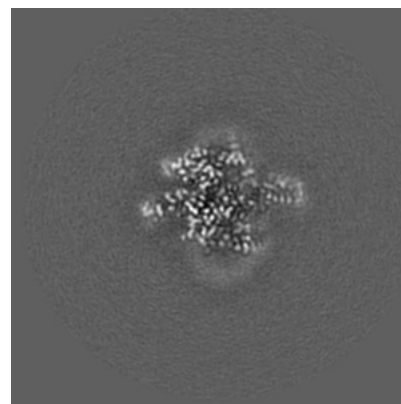
6.2.1 Primary map



X Index: 130



Y Index: 130

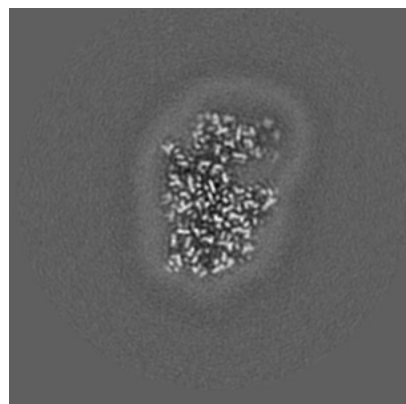


Z Index: 130

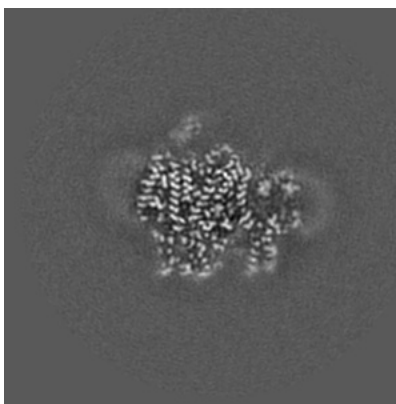
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

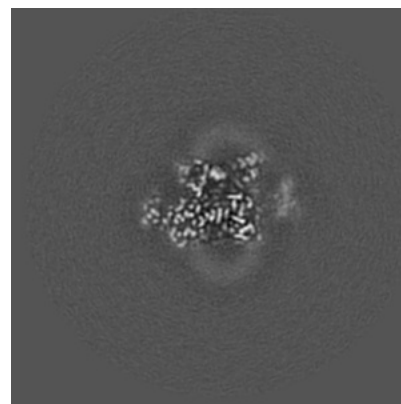
6.3.1 Primary map



X Index: 125



Y Index: 129

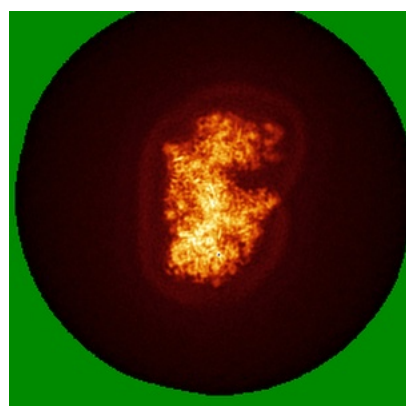


Z Index: 116

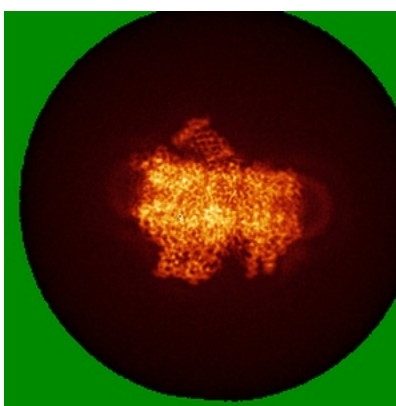
The images above show the largest variance slices of the map in three orthogonal directions.

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

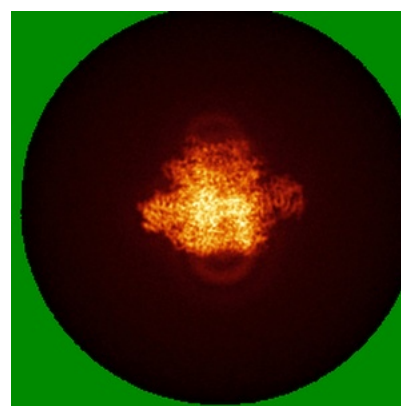
6.4.1 Primary map



X



Y

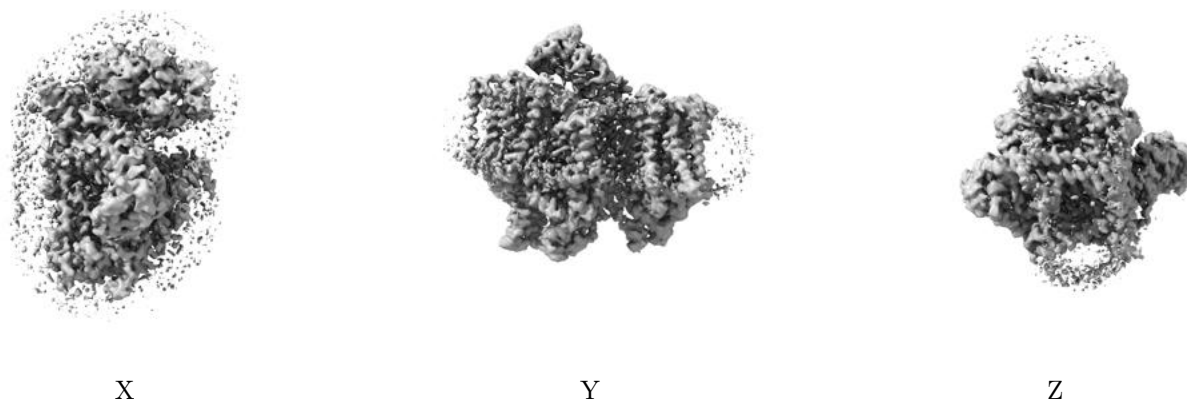


Z

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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

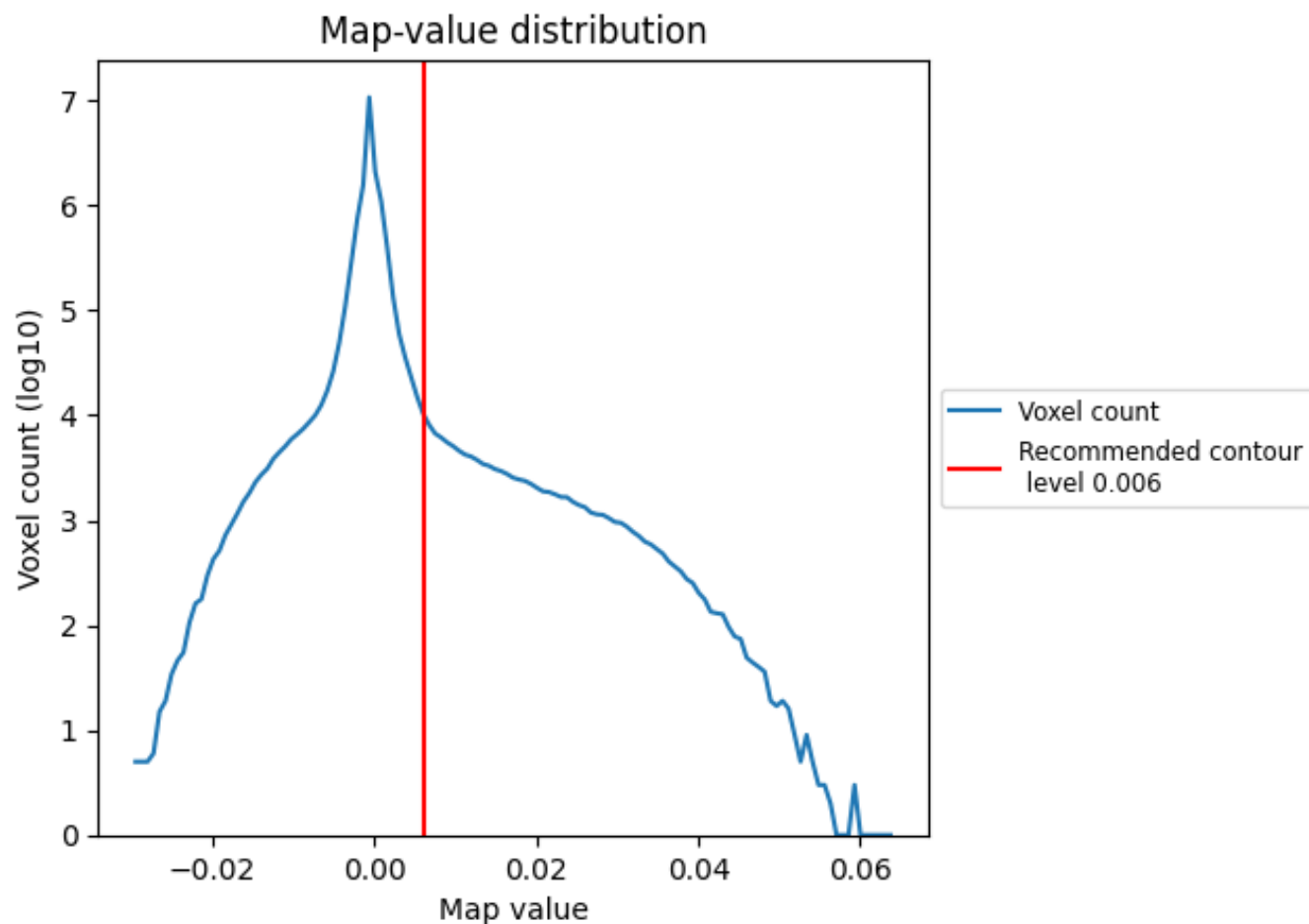
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

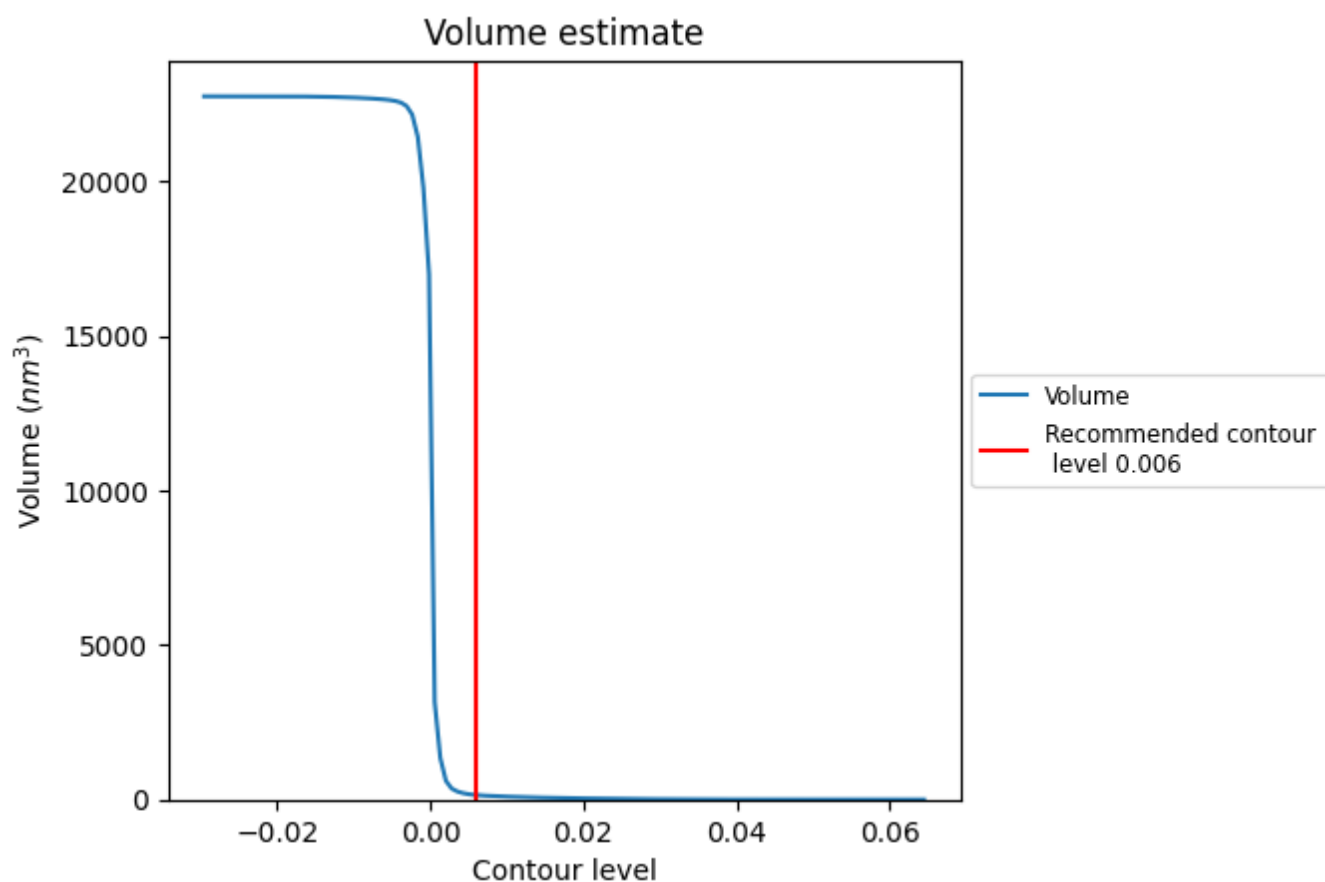
This section contains the results of statistical analysis of the map.

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.

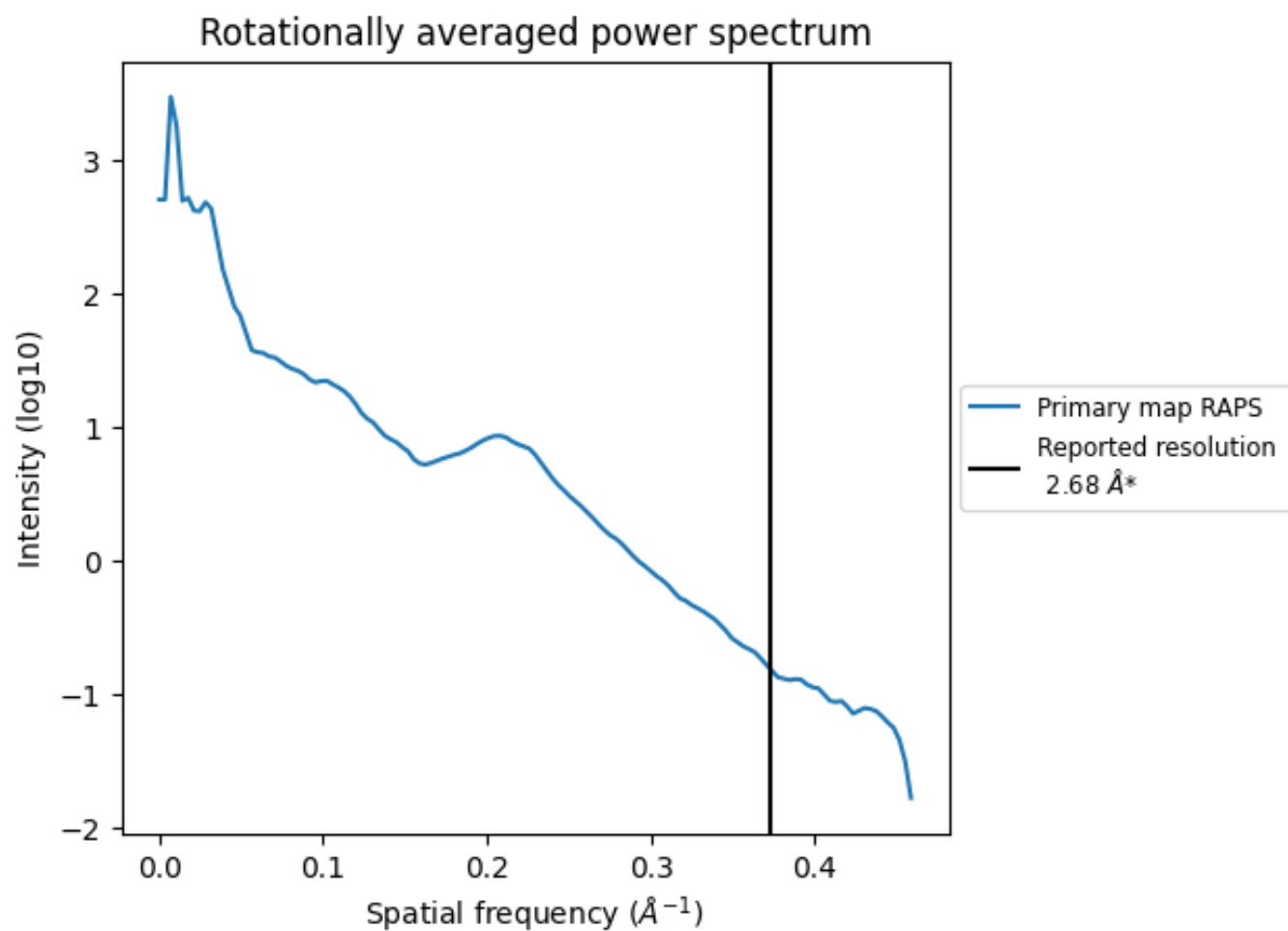
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm³; this corresponds to an approximate mass of 133 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 0.373 Å⁻¹

8 Fourier-Shell correlation

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

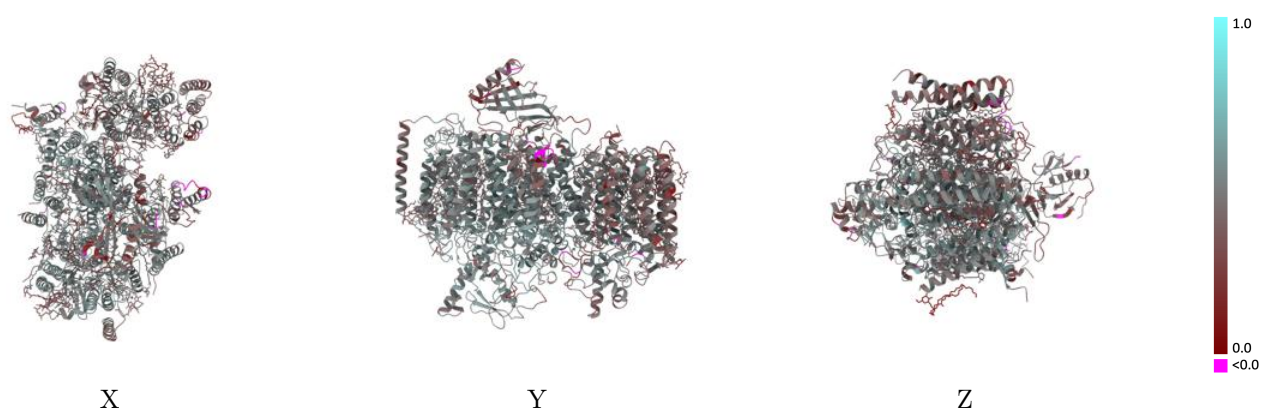
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12337 and PDB model 7NHQ. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

This section was not generated.

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

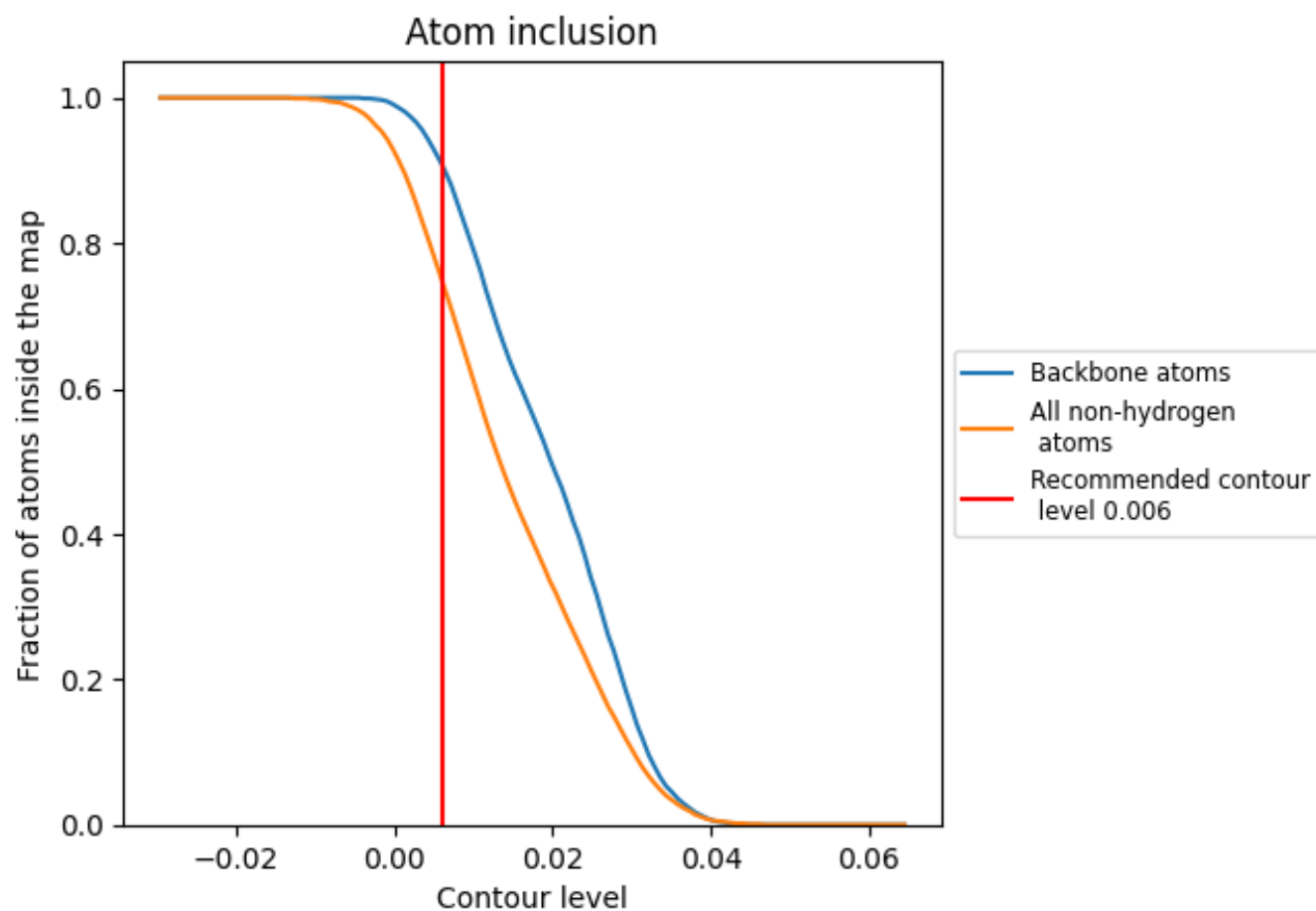


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 75% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4650
2	0.7490	0.3980
3	0.4990	0.4070
A	0.7660	0.4900
B	0.8120	0.4970
C	0.7050	0.4280
D	0.8150	0.5250
E	0.7010	0.3620
F	0.5680	0.3920
H	0.8410	0.4930
I	0.6230	0.3870
K	0.5780	0.3990
L	0.8020	0.5130
M	0.6800	0.4440
T	0.7420	0.4800
X	0.7790	0.4710
Z	0.6720	0.3760
y	0.5240	0.3410

