Full wwPDB EM Validation Report (i)

Nov 16, 2022 – 12:44 AM JST

PDB ID	:	6M32
EMDB ID	:	EMD-30069
Title	:	Cryo-EM structure of FMO-RC complex from green sulfur bacteria
Authors	:	Chen, J.H.; Zhang, X.
Deposited on	:	2020-03-02
Resolution	:	2.70 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 (i) 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 (1)) were used in the production of this report:

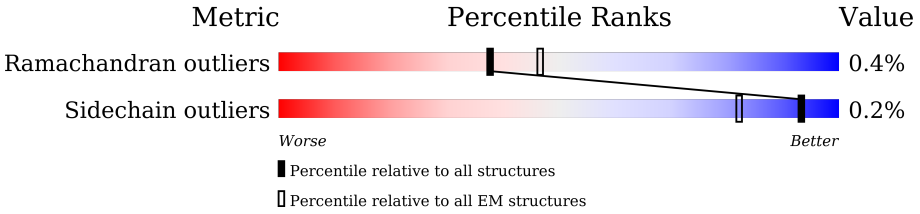
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	E	366	14% 99%
1	F	366	12% 98%
1	G	366	9% 97%
2	D	143	41% 64% 34%
3	B	231	10% 41% 59%
4	A	731	13% 85% 14%
4	a	731	17% 84% 14%

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
9	F39	A	817	-	X	-	-
9	F39	a	817	-	X	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 23566 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 Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	362	2815	1783	501	524	7	0	0
1	F	358	2789	1770	496	516	7	0	0
1	G	358	2789	1770	496	516	7	0	0

- Molecule 2 is a protein called P840 reaction center 17 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	94	766	484	137	141	4	0	0

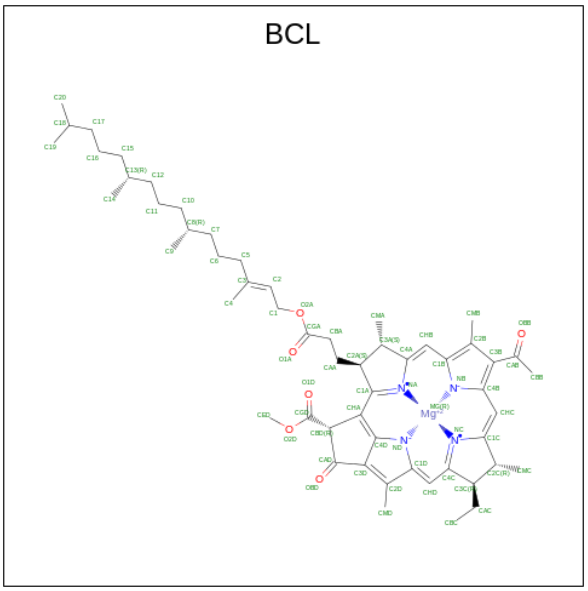
- Molecule 3 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	95	731	469	115	138	9	0	0

- Molecule 4 is a protein called Photosystem P840 reaction center, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	628	5030	3360	798	846	26	0	0
4	a	628	5030	3360	798	846	26	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	1
5	E	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	F	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	F	1	508	420	8	32	48	1
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	1
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0

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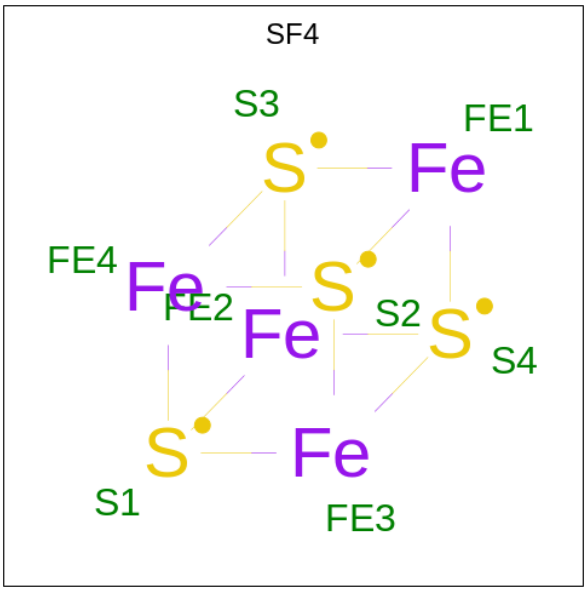
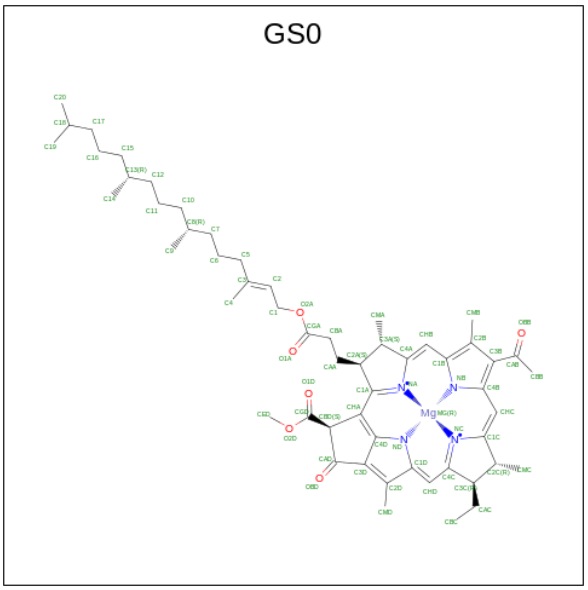
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
6	B	1	16	8	8	0
			Total	Fe	S	
6	B	1	16	8	8	0
			Total	Fe	S	
6	A	1	8	4	4	0

- Molecule 7 is Bacteriochlorophyll A isomer (three-letter code: GS0) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	A	1	66	55	1	4	6	0

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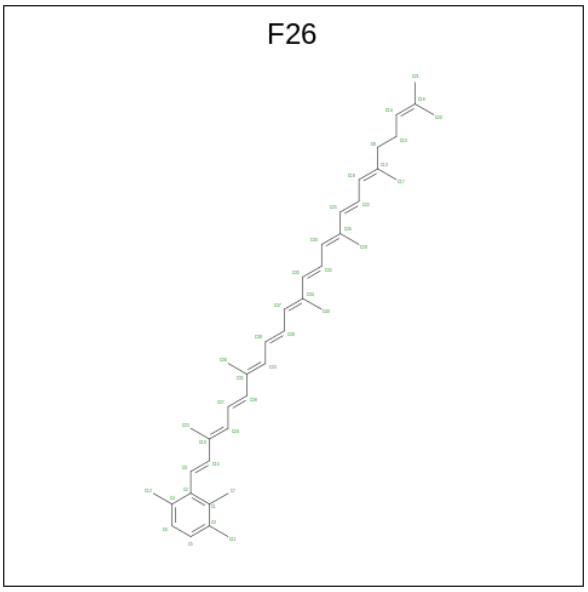
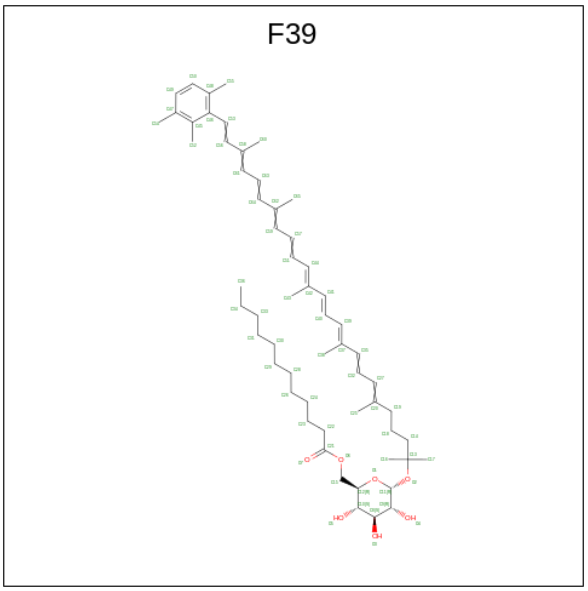
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	a	1	66	55	1	4	6	0

- Molecule 8 is 2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E,19E)-3,7,12,16,20,24-hexamethylpentacosa-1,3,5,7,9,11,13,15,17,19,23-undecaenyl]-1,3,4-trimethyl-benzene (three-letter code: F26) (formula: $C_{40}H_{52}$).



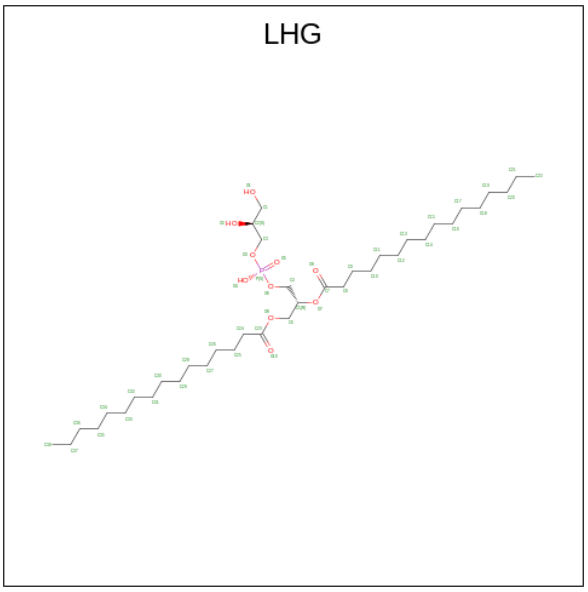
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
8	A	1	40	40	0
8	a	1	40	40	0

- Molecule 9 is [(2R,3S,4S,5R,6R)-6-[(10E,12E,14E)-2,6,10,14,19,23-hexamethyl-25-(2,3,6-trimethylphenyl)pentacosa-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl dodecanoate (three-letter code: F39) (formula: $C_{58}H_{86}O_7$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	A	1	65	58	7	0
			Total	C	O	
9	a	1	65	58	7	0

- Molecule 10 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
10	A	1	46	35	10	1	0

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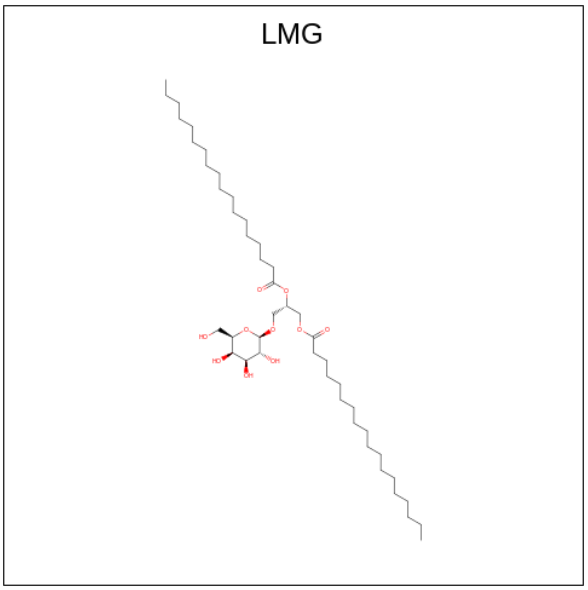
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
10	a	1	46	35	10	1	0

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

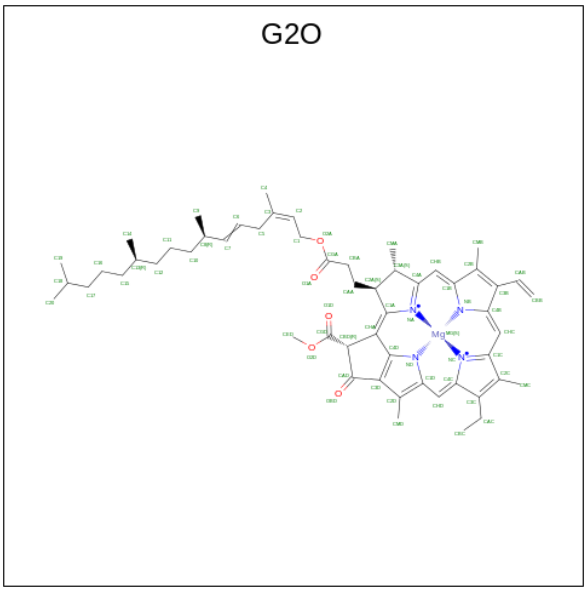


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	A	1	44	34	10	0
11	a	1	44	34	10	0

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
12	A	1	1	1	0
12	a	1	1	1	0

- Molecule 13 is Chlorophyll A ester (three-letter code: G2O) (formula: $C_{55}H_{70}MgN_4O_5$).



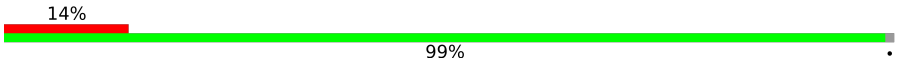
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	A	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
13	A	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
13	a	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
13	a	1	130	110	2	8	10	0

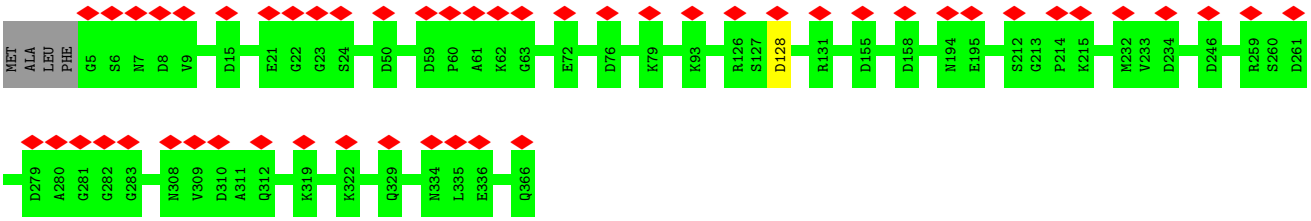
3 Residue-property plots (i)

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

- Molecule 1: Bacteriochlorophyll a protein

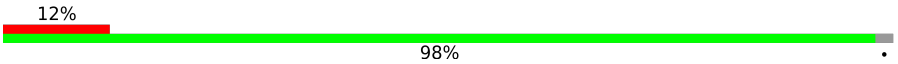
Chain E:

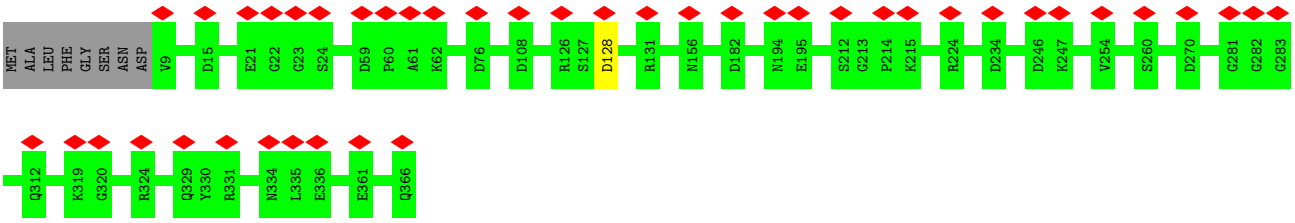




- Molecule 1: Bacteriochlorophyll a protein

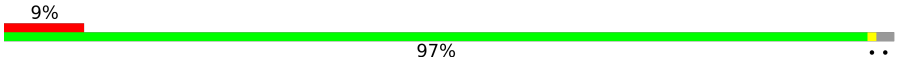
Chain F:

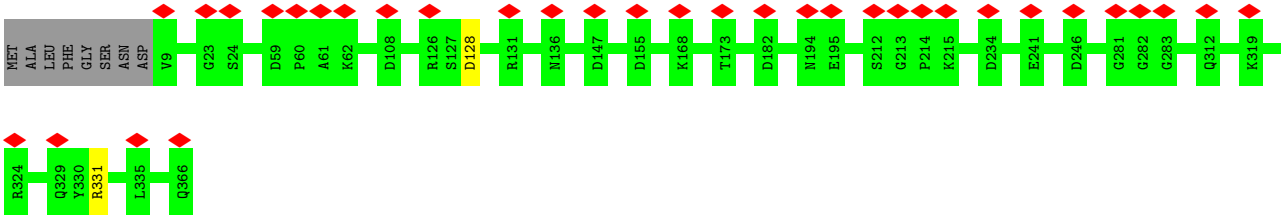




- Molecule 1: Bacteriochlorophyll a protein

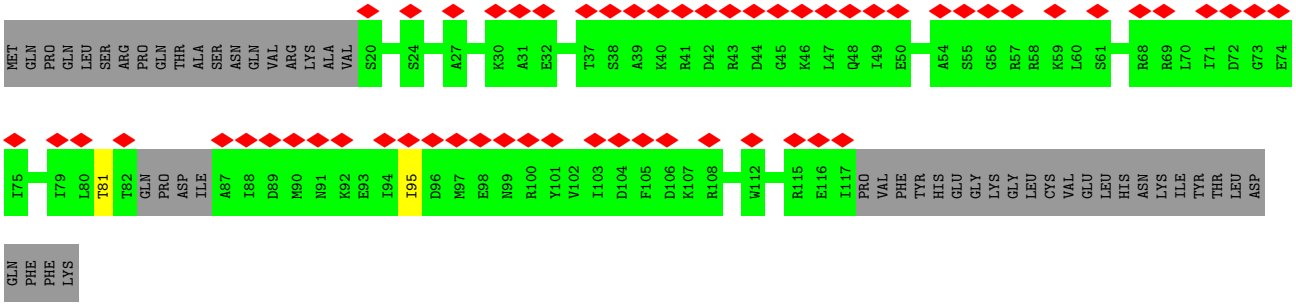
Chain G:





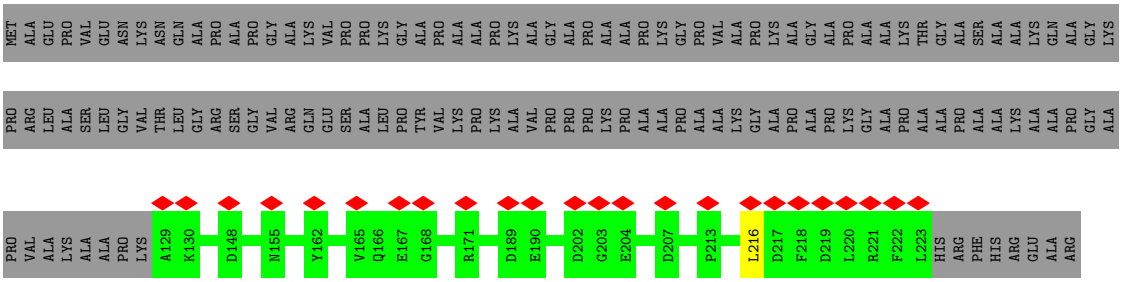
- Molecule 2: P840 reaction center 17 kDa protein

Chain D:



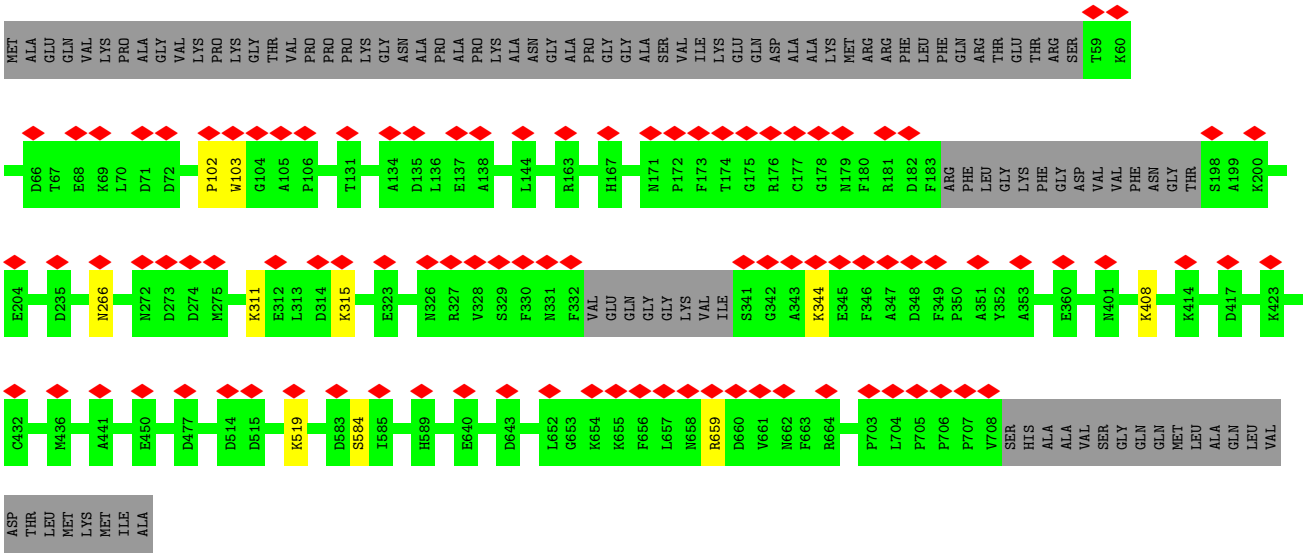
• Molecule 3: Photosystem P840 reaction center iron-sulfur protein

Chain B:



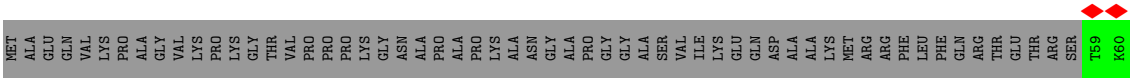
• Molecule 4: Photosystem P840 reaction center, large subunit

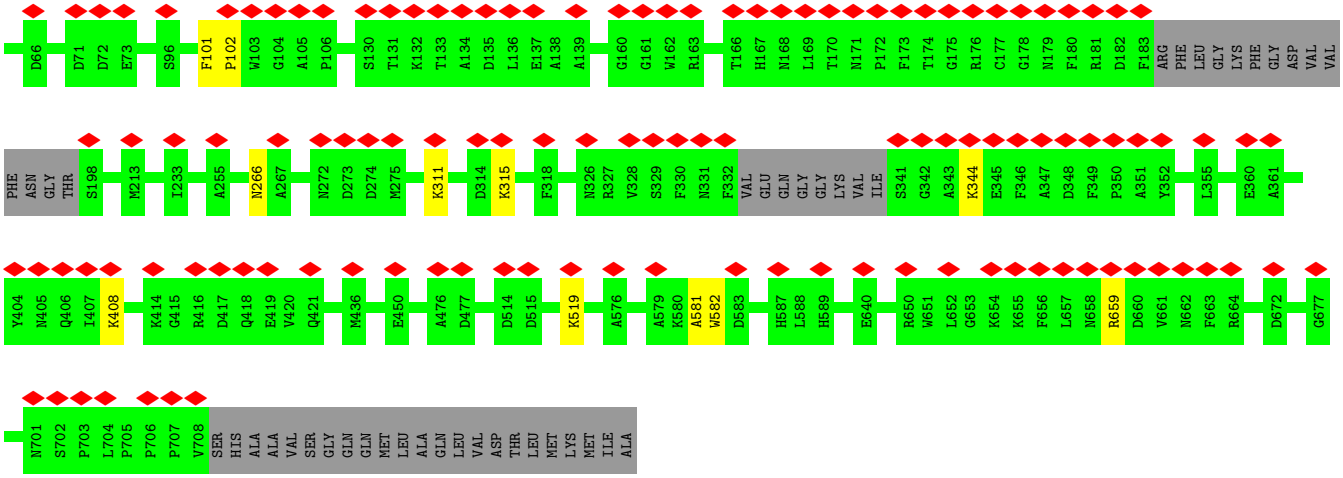
Chain A:



• Molecule 4: Photosystem P840 reaction center, large subunit

Chain a:




D56
D71 D72 E73
S96
F101 P102 W103 G104 A105 P106
S130 T131 K132 T133 A134 D135 L136 E137 A138 A139
G160 G161 W162 R163
T166 H167 N168 L169 T170 N171 P172 F173 T174 G175 R176 C177 G178 N179 F180 R181 D182 F183
ARG PHE LEU GLY LYS PHE GLY ASP VAL VAL
PHE ASN GLY THR
S198
M213
T233
A255
N266
A267
N272 D273 D274 M275
K311
D314 K315
F318
N326 R327 V328 S329 F330 N331 F332
VAL GLU GLN GLY GLY LYS VAL ILE
S341 G342 A343 K344 E345 F346 A347 D348 F349 P350 A351 Y352
L355
E360 A361
Y404 N405 Q406 I407 K408
K414 G415 R416 D417 Q418 E419 V420 Q421
M436
E450
A476 D477
D514 D515
K519
A576
A579 K580 A581 W582
D583
H587 L588 H589
E640
R650 W651 L652 G653 K654 K655 F656 L657 N658 R659 D660 V661 N662 F663 R664
D672
G677
N701 S702 P703 L704 P705 P706 P707 V708
SER HIS ALA ALA VAL SER GLY GLN GLN MET LEU ALA GLN LEU VAL ASP THR LEU MET LYS MET ILE ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	268430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	38244	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0341	Depositor
Map size (Å)	209.12001, 209.12001, 209.12001	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, LHG, CA, F39, LMG, F26, G2O, GS0, BCL

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	E	0.31	0/2885	0.53	1/3910 (0.0%)
1	F	0.31	0/2859	0.53	1/3875 (0.0%)
1	G	0.31	0/2859	0.53	1/3875 (0.0%)
2	D	0.28	0/778	0.56	0/1043
3	B	0.32	0/749	0.56	0/1013
4	A	0.32	0/5207	0.51	2/7097 (0.0%)
4	a	0.31	0/5207	0.50	2/7097 (0.0%)
All	All	0.31	0/20544	0.52	7/27910 (0.0%)

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
3	B	0	1
4	A	0	3
4	a	0	3
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	128	ASP	CB-CG-OD2	6.18	123.86	118.30
1	F	128	ASP	CB-CG-OD2	6.16	123.84	118.30
1	G	128	ASP	CB-CG-OD2	6.13	123.82	118.30
4	a	266	ASN	N-CA-C	5.76	126.56	111.00
4	A	266	ASN	N-CA-C	5.76	126.55	111.00
4	a	315	LYS	CD-CE-NZ	5.24	123.74	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	315	LYS	CD-CE-NZ	5.21	123.67	111.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	311	LYS	Peptide
4	A	344	LYS	Peptide
4	A	519	LYS	Peptide
3	B	216	LEU	Peptide
4	a	311	LYS	Peptide
4	a	344	LYS	Peptide
4	a	519	LYS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	360/366 (98%)	339 (94%)	21 (6%)	0	100	100
1	F	356/366 (97%)	338 (95%)	18 (5%)	0	100	100
1	G	356/366 (97%)	338 (95%)	18 (5%)	0	100	100
2	D	90/143 (63%)	71 (79%)	17 (19%)	2 (2%)	6	17
3	B	93/231 (40%)	76 (82%)	17 (18%)	0	100	100
4	A	622/731 (85%)	568 (91%)	51 (8%)	3 (0%)	29	54
4	a	622/731 (85%)	571 (92%)	46 (7%)	5 (1%)	19	43
All	All	2499/2934 (85%)	2301 (92%)	188 (8%)	10 (0%)	38	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	95	ILE
4	A	102	PRO
4	a	102	PRO
4	A	659	ARG
4	a	659	ARG
4	A	584	SER
4	a	581	ALA
4	a	582	TRP
2	D	81	THR
4	a	101	PHE

5.3.2 Protein sidechains (i)

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	E	299/302 (99%)	299 (100%)	0	100	100
1	F	296/302 (98%)	296 (100%)	0	100	100
1	G	296/302 (98%)	295 (100%)	1 (0%)	92	98
2	D	83/128 (65%)	83 (100%)	0	100	100
3	B	80/162 (49%)	80 (100%)	0	100	100
4	A	521/599 (87%)	519 (100%)	2 (0%)	91	97
4	a	521/599 (87%)	520 (100%)	1 (0%)	93	98
All	All	2096/2394 (88%)	2092 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	331	ARG
4	A	103	TRP
4	A	408	LYS
4	a	408	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	F	37	ASN
1	G	312	GLN
1	G	329	GLN
4	A	237	GLN
4	a	237	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 2 are monoatomic - leaving 65 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	$\#\|Z\| > 2$
8	F26	a	816	-	40,40,40	2.01	15 (37%)	46,50,50	2.00	10 (21%)
5	BCL	F	378[B]	1	38,54,74	1.88	7 (18%)	45,91,115	2.36	18 (40%)
5	BCL	E	376	-	58,74,74	1.59	8 (13%)	69,115,115	2.17	23 (33%)
5	BCL	E	375	1	58,74,74	1.60	8 (13%)	69,115,115	2.13	24 (34%)
5	BCL	A	804	-	38,54,74	1.89	8 (21%)	45,91,115	2.31	19 (42%)
5	BCL	a	809	4	38,54,74	1.86	6 (15%)	45,91,115	2.45	19 (42%)
11	LMG	a	819	4	44,44,55	0.78	1 (2%)	52,52,63	1.33	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	LHG	A	818	-	45,45,48	0.64	1 (2%)	48,51,54	1.27	6 (12%)
5	BCL	G	371	1	58,74,74	1.60	7 (12%)	69,115,115	2.31	25 (36%)
5	BCL	E	373	-	58,74,74	1.61	9 (15%)	69,115,115	2.20	24 (34%)
7	GS0	a	801	-	64,74,74	1.73	12 (18%)	78,115,115	2.17	24 (30%)
10	LHG	a	818	-	45,45,48	0.63	1 (2%)	48,51,54	1.27	6 (12%)
5	BCL	a	806	-	58,74,74	1.61	9 (15%)	69,115,115	2.10	24 (34%)
5	BCL	G	372	-	58,74,74	1.58	7 (12%)	69,115,115	2.14	24 (34%)
13	G2O	A	803	-	67,73,73	2.73	24 (35%)	75,113,113	1.56	10 (13%)
5	BCL	A	807	4	38,54,74	1.92	9 (23%)	45,91,115	2.32	17 (37%)
5	BCL	A	814	-	38,54,74	1.87	6 (15%)	45,91,115	2.41	19 (42%)
5	BCL	G	375	1	58,74,74	1.60	8 (13%)	69,115,115	2.13	24 (34%)
5	BCL	A	808	-	58,74,74	1.59	8 (13%)	69,115,115	2.05	21 (30%)
5	BCL	G	374	-	58,74,74	1.59	7 (12%)	69,115,115	2.14	24 (34%)
5	BCL	F	373	-	58,74,74	1.61	9 (15%)	69,115,115	2.20	24 (34%)
5	BCL	a	808	-	58,74,74	1.60	8 (13%)	69,115,115	2.05	21 (30%)
5	BCL	F	372	-	58,74,74	1.59	7 (12%)	69,115,115	2.14	24 (34%)
6	SF4	A	821	4	0,12,12	-	-	-		
9	F39	A	817	-	66,66,66	8.01	53 (80%)	79,85,85	4.33	29 (36%)
5	BCL	A	812	4	58,74,74	1.61	9 (15%)	69,115,115	2.08	23 (33%)
5	BCL	a	812	4	58,74,74	1.60	9 (15%)	69,115,115	2.08	23 (33%)
5	BCL	a	811	4	58,74,74	1.60	8 (13%)	69,115,115	2.18	23 (33%)
9	F39	a	817	-	66,66,66	8.01	53 (80%)	79,85,85	4.33	29 (36%)
5	BCL	G	373	-	58,74,74	1.61	9 (15%)	69,115,115	2.20	23 (33%)
5	BCL	F	371	1	58,74,74	1.60	7 (12%)	69,115,115	2.31	24 (34%)
13	G2O	A	802	4	67,73,73	2.70	24 (35%)	75,113,113	1.50	7 (9%)
5	BCL	a	810	4	38,54,74	1.82	8 (21%)	45,91,115	2.47	19 (42%)
6	SF4	B	302	3	0,12,12	-	-	-		
5	BCL	A	815	-	38,54,74	1.86	7 (18%)	45,91,115	2.44	19 (42%)
5	BCL	F	375	1	58,74,74	1.59	8 (13%)	69,115,115	2.13	25 (36%)
7	GS0	A	801	-	64,74,74	1.72	12 (18%)	78,115,115	2.17	24 (30%)
5	BCL	E	371	1	58,74,74	1.60	8 (13%)	69,115,115	2.30	25 (36%)
5	BCL	a	804	-	38,54,74	1.89	8 (21%)	45,91,115	2.32	19 (42%)
8	F26	A	816	-	40,40,40	2.00	15 (37%)	46,50,50	2.00	12 (26%)
5	BCL	a	805	-	48,64,74	1.76	8 (16%)	57,103,115	2.24	22 (38%)
6	SF4	B	301	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
11	LMG	A	819	4	44,44,55	0.78	1 (2%)	52,52,63	1.33	4 (7%)
5	BCL	F	376	-	58,74,74	1.60	7 (12%)	69,115,115	2.17	23 (33%)
5	BCL	A	810	4	38,54,74	1.82	8 (21%)	45,91,115	2.47	19 (42%)
5	BCL	E	377	-	58,74,74	1.59	8 (13%)	69,115,115	2.17	23 (33%)
13	G2O	a	803	-	67,73,73	2.73	24 (35%)	75,113,113	1.55	10 (13%)
5	BCL	E	374	-	58,74,74	1.59	7 (12%)	69,115,115	2.14	25 (36%)
5	BCL	A	805	-	48,64,74	1.76	9 (18%)	57,103,115	2.24	22 (38%)
13	G2O	a	802	4	67,73,73	2.70	24 (35%)	75,113,113	1.49	7 (9%)
5	BCL	E	378[B]	1	38,54,74	1.87	7 (18%)	45,91,115	2.36	17 (37%)
5	BCL	a	807	4	38,54,74	1.92	9 (23%)	45,91,115	2.32	17 (37%)
5	BCL	F	377	-	58,74,74	1.59	7 (12%)	69,115,115	2.16	23 (33%)
5	BCL	F	374	-	58,74,74	1.58	7 (12%)	69,115,115	2.14	24 (34%)
5	BCL	A	809	4	38,54,74	1.86	7 (18%)	45,91,115	2.46	19 (42%)
5	BCL	G	376	-	58,74,74	1.60	8 (13%)	69,115,115	2.17	23 (33%)
5	BCL	G	377	-	58,74,74	1.59	7 (12%)	69,115,115	2.17	23 (33%)
5	BCL	A	813	-	38,54,74	1.87	9 (23%)	45,91,115	2.33	18 (40%)
5	BCL	a	814	-	38,54,74	1.86	6 (15%)	45,91,115	2.40	18 (40%)
5	BCL	a	815	-	38,54,74	1.86	8 (21%)	45,91,115	2.44	19 (42%)
5	BCL	a	813	-	38,54,74	1.87	9 (23%)	45,91,115	2.33	17 (37%)
5	BCL	G	378[B]	1	38,54,74	1.87	8 (21%)	45,91,115	2.36	18 (40%)
5	BCL	E	372	-	58,74,74	1.59	8 (13%)	69,115,115	2.14	23 (33%)
5	BCL	A	806	-	58,74,74	1.62	9 (15%)	69,115,115	2.09	24 (34%)
5	BCL	A	811	4	58,74,74	1.60	8 (13%)	69,115,115	2.18	23 (33%)

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
8	F26	a	816	-	-	15/36/36/36	0/1/1/1
5	BCL	F	378[B]	1	-	3/13/113/137	-
5	BCL	E	376	-	-	11/37/137/137	-
5	BCL	E	375	1	-	11/37/137/137	-
5	BCL	A	804	-	-	11/13/113/137	-
5	BCL	a	809	4	-	4/13/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LMG	a	819	4	-	19/39/59/70	0/1/1/1
10	LHG	A	818	-	-	21/50/50/53	-
5	BCL	G	371	1	-	12/37/137/137	-
5	BCL	E	373	-	-	13/37/137/137	-
7	GS0	a	801	-	-	12/37/137/137	-
10	LHG	a	818	-	-	21/50/50/53	-
5	BCL	a	806	-	-	10/37/137/137	-
5	BCL	G	372	-	-	17/37/137/137	-
13	G2O	A	803	-	-	18/39/115/115	-
5	BCL	A	807	4	-	5/13/113/137	-
5	BCL	A	814	-	-	5/13/113/137	-
5	BCL	G	375	1	-	11/37/137/137	-
5	BCL	A	808	-	-	18/37/137/137	-
5	BCL	G	374	-	-	14/37/137/137	-
5	BCL	F	373	-	-	13/37/137/137	-
5	BCL	a	808	-	-	18/37/137/137	-
5	BCL	F	372	-	-	17/37/137/137	-
6	SF4	A	821	4	-	-	0/6/5/5
9	F39	A	817	-	-	40/58/78/78	0/2/2/2
5	BCL	A	812	4	-	14/37/137/137	-
5	BCL	a	812	4	-	14/37/137/137	-
5	BCL	a	811	4	-	17/37/137/137	-
9	F39	a	817	-	-	40/58/78/78	0/2/2/2
5	BCL	G	373	-	-	13/37/137/137	-
5	BCL	F	371	1	-	12/37/137/137	-
13	G2O	A	802	4	-	12/39/115/115	-
5	BCL	a	810	4	-	8/13/113/137	-
6	SF4	B	302	3	-	-	0/6/5/5
5	BCL	A	815	-	-	7/13/113/137	-
5	BCL	F	375	1	-	11/37/137/137	-
7	GS0	A	801	-	-	12/37/137/137	-
5	BCL	E	371	1	-	12/37/137/137	-
5	BCL	a	804	-	-	11/13/113/137	-
8	F26	A	816	-	-	15/36/36/36	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	a	805	-	-	12/25/125/137	-
6	SF4	B	301	3	-	-	0/6/5/5
11	LMG	A	819	4	-	19/39/59/70	0/1/1/1
5	BCL	F	376	-	-	11/37/137/137	-
5	BCL	A	810	4	-	8/13/113/137	-
5	BCL	E	377	-	-	12/37/137/137	-
13	G2O	a	803	-	-	18/39/115/115	-
5	BCL	E	374	-	-	14/37/137/137	-
5	BCL	A	805	-	-	12/25/125/137	-
13	G2O	a	802	4	-	12/39/115/115	-
5	BCL	E	378[B]	1	-	3/13/113/137	-
5	BCL	a	807	4	-	5/13/113/137	-
5	BCL	F	377	-	-	12/37/137/137	-
5	BCL	F	374	-	-	14/37/137/137	-
5	BCL	A	809	4	-	4/13/113/137	-
5	BCL	G	376	-	-	11/37/137/137	-
5	BCL	G	377	-	-	12/37/137/137	-
5	BCL	A	813	-	-	5/13/113/137	-
5	BCL	a	814	-	-	5/13/113/137	-
5	BCL	a	815	-	-	7/13/113/137	-
5	BCL	a	813	-	-	5/13/113/137	-
5	BCL	G	378[B]	1	-	3/13/113/137	-
5	BCL	E	372	-	-	17/37/137/137	-
5	BCL	A	806	-	-	10/37/137/137	-
5	BCL	A	811	4	-	17/37/137/137	-

All (636) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	817	F39	C27-C20	26.99	1.62	1.34
9	a	817	F39	C27-C20	26.91	1.62	1.34
9	a	817	F39	C39-C37	22.04	1.65	1.35
9	A	817	F39	C39-C37	22.01	1.65	1.35
9	A	817	F39	C44-C42	20.11	1.62	1.35
9	a	817	F39	C44-C42	20.07	1.62	1.35
9	a	817	F39	C61-C58	19.89	1.62	1.35
9	A	817	F39	C61-C58	19.80	1.62	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	817	F39	C59-C62	19.58	1.61	1.35
9	a	817	F39	C59-C62	19.57	1.61	1.35
9	A	817	F39	C40-C41	11.90	1.65	1.34
9	a	817	F39	C40-C41	11.90	1.65	1.34
9	A	817	F39	C32-C35	11.82	1.65	1.34
9	a	817	F39	C32-C35	11.81	1.65	1.34
9	A	817	F39	C56-C53	11.55	1.63	1.33
9	a	817	F39	C56-C53	11.54	1.63	1.33
9	A	817	F39	C63-C64	11.39	1.63	1.34
9	a	817	F39	C63-C64	11.38	1.63	1.34
9	a	817	F39	C57-C51	10.80	1.64	1.36
9	A	817	F39	C57-C51	10.76	1.64	1.36
13	a	803	G2O	CAA-C2A	-10.69	1.34	1.54
13	A	803	G2O	CAA-C2A	-10.64	1.34	1.54
13	A	802	G2O	CAA-C2A	-10.29	1.35	1.54
13	a	802	G2O	CAA-C2A	-10.23	1.35	1.54
9	A	817	F39	C35-C37	8.74	1.64	1.45
9	a	817	F39	C35-C37	8.74	1.64	1.45
9	a	817	F39	C14-C13	8.51	1.66	1.53
9	A	817	F39	C14-C13	8.48	1.66	1.53
13	a	802	G2O	CMA-C3A	-7.96	1.36	1.53
13	A	802	G2O	CMA-C3A	-7.96	1.36	1.53
13	A	803	G2O	CMA-C3A	-7.88	1.36	1.53
13	a	803	G2O	CMA-C3A	-7.84	1.36	1.53
9	A	817	F39	C41-C42	7.78	1.62	1.45
9	a	817	F39	C41-C42	7.75	1.62	1.45
9	a	817	F39	C64-C62	7.72	1.62	1.45
9	A	817	F39	C64-C62	7.71	1.62	1.45
9	A	817	F39	C56-C58	7.52	1.62	1.45
9	a	817	F39	C56-C58	7.52	1.62	1.45
9	a	817	F39	C46-C53	7.22	1.63	1.47
9	A	817	F39	C46-C53	7.22	1.63	1.47
9	a	817	F39	C51-C44	6.86	1.64	1.43
9	A	817	F39	C51-C44	6.85	1.64	1.43
9	a	817	F39	C57-C59	6.84	1.64	1.43
9	A	817	F39	C57-C59	6.83	1.64	1.43
9	a	817	F39	C40-C39	6.82	1.64	1.43
9	A	817	F39	C40-C39	6.79	1.64	1.43
9	a	817	F39	C63-C61	6.69	1.64	1.43
9	a	817	F39	C32-C27	6.65	1.64	1.43
9	A	817	F39	C63-C61	6.64	1.64	1.43
9	A	817	F39	C32-C27	6.64	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	802	G2O	CBD-CGD	-6.27	1.32	1.52
13	A	802	G2O	CBD-CGD	-6.25	1.32	1.52
13	A	803	G2O	CBD-CGD	-6.19	1.33	1.52
13	a	803	G2O	CBD-CGD	-6.16	1.33	1.52
7	a	801	GS0	MG-ND	-5.97	1.94	2.05
5	A	807	BCL	OBD-CAD	5.95	1.30	1.22
5	a	807	BCL	OBD-CAD	5.95	1.30	1.22
5	E	374	BCL	OBD-CAD	5.94	1.30	1.22
7	A	801	GS0	MG-ND	-5.93	1.94	2.05
5	G	374	BCL	OBD-CAD	5.90	1.30	1.22
5	A	811	BCL	OBD-CAD	5.89	1.30	1.22
5	E	375	BCL	OBD-CAD	5.88	1.30	1.22
5	F	373	BCL	OBD-CAD	5.88	1.30	1.22
5	a	805	BCL	OBD-CAD	5.87	1.30	1.22
5	a	811	BCL	OBD-CAD	5.87	1.30	1.22
5	F	374	BCL	OBD-CAD	5.86	1.30	1.22
5	A	805	BCL	OBD-CAD	5.86	1.30	1.22
5	A	814	BCL	OBD-CAD	5.86	1.30	1.22
5	a	808	BCL	OBD-CAD	5.86	1.30	1.22
5	E	371	BCL	OBD-CAD	5.85	1.30	1.22
5	G	376	BCL	OBD-CAD	5.85	1.30	1.22
5	F	371	BCL	OBD-CAD	5.84	1.30	1.22
5	A	812	BCL	OBD-CAD	5.84	1.30	1.22
5	G	371	BCL	OBD-CAD	5.83	1.30	1.22
5	G	375	BCL	OBD-CAD	5.83	1.30	1.22
5	G	373	BCL	OBD-CAD	5.83	1.30	1.22
5	a	814	BCL	OBD-CAD	5.83	1.30	1.22
5	F	376	BCL	OBD-CAD	5.82	1.30	1.22
5	F	377	BCL	OBD-CAD	5.81	1.30	1.22
5	E	373	BCL	OBD-CAD	5.80	1.30	1.22
5	A	808	BCL	OBD-CAD	5.80	1.30	1.22
5	F	372	BCL	OBD-CAD	5.79	1.30	1.22
5	G	378[B]	BCL	OBD-CAD	5.79	1.30	1.22
5	F	375	BCL	OBD-CAD	5.79	1.30	1.22
5	A	806	BCL	OBD-CAD	5.78	1.30	1.22
5	A	815	BCL	OBD-CAD	5.78	1.30	1.22
5	E	378[B]	BCL	OBD-CAD	5.78	1.30	1.22
5	E	376	BCL	OBD-CAD	5.78	1.30	1.22
5	a	813	BCL	OBD-CAD	5.78	1.30	1.22
5	F	378[B]	BCL	OBD-CAD	5.78	1.30	1.22
5	a	804	BCL	OBD-CAD	5.77	1.30	1.22
5	G	377	BCL	OBD-CAD	5.77	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	372	BCL	OBD-CAD	5.77	1.30	1.22
5	A	804	BCL	OBD-CAD	5.76	1.30	1.22
5	a	806	BCL	OBD-CAD	5.76	1.30	1.22
5	a	815	BCL	OBD-CAD	5.76	1.30	1.22
5	G	372	BCL	OBD-CAD	5.76	1.30	1.22
5	a	809	BCL	OBD-CAD	5.76	1.30	1.22
5	a	812	BCL	OBD-CAD	5.76	1.30	1.22
5	A	809	BCL	OBD-CAD	5.75	1.30	1.22
5	A	813	BCL	OBD-CAD	5.75	1.30	1.22
9	a	817	F39	C19-C20	5.69	1.63	1.51
9	A	817	F39	C19-C20	5.68	1.63	1.51
5	E	377	BCL	OBD-CAD	5.67	1.30	1.22
9	a	817	F39	O6-C21	5.42	1.49	1.33
9	A	817	F39	O6-C21	5.40	1.49	1.33
9	a	817	F39	C54-C47	5.34	1.61	1.51
9	A	817	F39	O1-C11	5.32	1.55	1.41
9	A	817	F39	C54-C47	5.31	1.61	1.51
9	a	817	F39	O1-C11	5.28	1.55	1.41
9	A	817	F39	C55-C48	5.24	1.61	1.51
9	A	817	F39	O2-C13	5.19	1.54	1.46
9	a	817	F39	O2-C13	5.18	1.54	1.46
5	A	810	BCL	OBD-CAD	5.17	1.29	1.22
13	a	803	G2O	C2A-C1A	-5.17	1.40	1.52
9	a	817	F39	C55-C48	5.16	1.61	1.51
5	a	810	BCL	OBD-CAD	5.15	1.29	1.22
13	A	803	G2O	C2A-C1A	-5.12	1.40	1.52
13	a	802	G2O	C2A-C1A	-4.91	1.41	1.52
9	a	817	F39	C38-C37	4.88	1.61	1.50
13	a	803	G2O	C3A-C2A	-4.87	1.40	1.54
13	A	803	G2O	C3A-C2A	-4.87	1.40	1.54
9	A	817	F39	C38-C37	4.86	1.60	1.50
13	A	802	G2O	C2A-C1A	-4.86	1.41	1.52
9	a	817	F39	O1-C12	4.82	1.56	1.44
9	A	817	F39	O1-C12	4.82	1.56	1.44
13	A	803	G2O	MG-NB	-4.78	1.96	2.05
13	a	803	G2O	MG-NB	-4.77	1.96	2.05
13	a	802	G2O	C3A-C2A	-4.77	1.41	1.54
13	a	802	G2O	MG-NB	-4.73	1.96	2.05
13	A	802	G2O	MG-NB	-4.73	1.96	2.05
13	A	802	G2O	C3A-C2A	-4.72	1.41	1.54
9	a	817	F39	C50-C49	4.63	1.47	1.38
9	A	817	F39	C50-C49	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	817	F39	C52-C45	4.55	1.61	1.51
9	a	817	F39	C52-C45	4.53	1.61	1.51
7	a	801	GS0	OBD-CAD	4.51	1.30	1.22
9	a	817	F39	O3-C8	4.50	1.53	1.43
7	A	801	GS0	OBD-CAD	4.49	1.30	1.22
9	A	817	F39	O3-C8	4.48	1.53	1.43
9	a	817	F39	C46-C45	4.44	1.47	1.41
7	A	801	GS0	C4D-ND	-4.41	1.31	1.37
7	a	801	GS0	C4D-ND	-4.37	1.31	1.37
9	A	817	F39	C46-C45	4.37	1.47	1.41
9	a	817	F39	C46-C48	4.27	1.47	1.41
9	A	817	F39	C46-C48	4.27	1.47	1.41
13	a	803	G2O	C1D-ND	4.22	1.39	1.35
13	a	802	G2O	C1D-ND	4.19	1.38	1.35
13	A	803	G2O	C1D-ND	4.19	1.38	1.35
8	A	816	F26	C30-C26	-4.17	1.30	1.35
13	A	802	G2O	C1D-ND	4.16	1.38	1.35
9	A	817	F39	C22-C21	4.14	1.62	1.50
13	a	802	G2O	C4B-NB	4.14	1.42	1.37
9	a	817	F39	C22-C21	4.14	1.62	1.50
5	A	815	BCL	O1D-CGD	-4.14	1.10	1.21
5	a	815	BCL	O1D-CGD	-4.14	1.10	1.21
9	a	817	F39	C60-C58	4.13	1.59	1.50
13	A	802	G2O	C4B-NB	4.12	1.42	1.37
9	A	817	F39	C60-C58	4.12	1.59	1.50
5	a	810	BCL	O1D-CGD	-4.11	1.10	1.21
7	a	801	GS0	O1D-CGD	-4.11	1.10	1.21
5	F	376	BCL	O1D-CGD	-4.10	1.10	1.21
8	a	816	F26	C30-C26	-4.10	1.30	1.35
5	E	371	BCL	O1D-CGD	-4.10	1.10	1.21
5	F	373	BCL	O1D-CGD	-4.09	1.11	1.21
5	A	809	BCL	O1D-CGD	-4.09	1.11	1.21
5	A	812	BCL	O1D-CGD	-4.09	1.11	1.21
5	G	373	BCL	O1D-CGD	-4.09	1.11	1.21
5	F	371	BCL	O1D-CGD	-4.09	1.11	1.21
5	A	810	BCL	O1D-CGD	-4.08	1.11	1.21
5	A	811	BCL	O1D-CGD	-4.08	1.11	1.21
5	G	372	BCL	O1D-CGD	-4.08	1.11	1.21
5	A	813	BCL	O1D-CGD	-4.07	1.11	1.21
5	a	811	BCL	O1D-CGD	-4.07	1.11	1.21
5	F	377	BCL	O1D-CGD	-4.07	1.11	1.21
5	G	374	BCL	O1D-CGD	-4.07	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	375	BCL	O1D-CGD	-4.07	1.11	1.21
5	E	372	BCL	O1D-CGD	-4.07	1.11	1.21
5	G	375	BCL	O1D-CGD	-4.06	1.11	1.21
7	A	801	GS0	O1D-CGD	-4.06	1.11	1.21
5	G	376	BCL	O1D-CGD	-4.06	1.11	1.21
5	a	813	BCL	O1D-CGD	-4.06	1.11	1.21
5	E	374	BCL	O1D-CGD	-4.06	1.11	1.21
5	F	372	BCL	O1D-CGD	-4.05	1.11	1.21
5	G	371	BCL	O1D-CGD	-4.04	1.11	1.21
5	a	805	BCL	O1D-CGD	-4.04	1.11	1.21
5	G	377	BCL	O1D-CGD	-4.04	1.11	1.21
5	a	812	BCL	O1D-CGD	-4.04	1.11	1.21
5	E	376	BCL	O1D-CGD	-4.04	1.11	1.21
5	E	373	BCL	O1D-CGD	-4.04	1.11	1.21
5	F	375	BCL	O1D-CGD	-4.04	1.11	1.21
5	a	808	BCL	O1D-CGD	-4.04	1.11	1.21
5	A	804	BCL	O1D-CGD	-4.04	1.11	1.21
5	F	374	BCL	O1D-CGD	-4.03	1.11	1.21
5	A	805	BCL	O1D-CGD	-4.03	1.11	1.21
5	E	377	BCL	O1D-CGD	-4.03	1.11	1.21
5	a	809	BCL	O1D-CGD	-4.03	1.11	1.21
5	a	804	BCL	O1D-CGD	-4.03	1.11	1.21
5	A	806	BCL	O1D-CGD	-4.03	1.11	1.21
5	a	806	BCL	O1D-CGD	-4.01	1.11	1.21
5	A	808	BCL	O1D-CGD	-4.01	1.11	1.21
9	A	817	F39	C17-C13	4.01	1.61	1.52
9	a	817	F39	C17-C13	4.00	1.61	1.52
5	F	378[B]	BCL	O1D-CGD	-4.00	1.11	1.21
5	G	378[B]	BCL	O1D-CGD	-4.00	1.11	1.21
5	A	814	BCL	O1D-CGD	-3.99	1.11	1.21
5	a	814	BCL	O1D-CGD	-3.99	1.11	1.21
8	a	816	F26	C37-C34	-3.98	1.30	1.35
5	E	378[B]	BCL	O1D-CGD	-3.97	1.11	1.21
8	A	816	F26	C37-C34	-3.94	1.30	1.35
5	A	807	BCL	O1D-CGD	-3.94	1.11	1.21
5	a	807	BCL	O1D-CGD	-3.94	1.11	1.21
9	A	817	F39	C16-C13	3.86	1.61	1.52
9	a	817	F39	C16-C13	3.86	1.61	1.52
9	A	817	F39	C18-C19	3.83	1.66	1.52
13	a	803	G2O	CHC-C4B	-3.81	1.31	1.38
13	A	803	G2O	C4B-NB	3.81	1.42	1.37
9	a	817	F39	C18-C19	3.81	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	803	G2O	C4B-NB	3.80	1.42	1.37
13	A	803	G2O	C4D-CHA	-3.80	1.40	1.45
13	A	803	G2O	CHC-C4B	-3.78	1.31	1.38
13	a	803	G2O	C10-C8	-3.76	1.42	1.54
9	a	817	F39	C65-C62	3.76	1.58	1.50
9	a	817	F39	C14-C18	3.75	1.65	1.52
13	a	802	G2O	C10-C8	-3.74	1.42	1.54
13	A	803	G2O	C10-C8	-3.74	1.42	1.54
9	A	817	F39	C14-C18	3.74	1.65	1.52
13	A	802	G2O	C10-C8	-3.74	1.42	1.54
9	A	817	F39	C65-C62	3.74	1.58	1.50
9	a	817	F39	C43-C42	3.73	1.58	1.50
13	a	803	G2O	C4D-CHA	-3.73	1.40	1.45
13	A	802	G2O	CHC-C4B	-3.73	1.31	1.38
9	a	817	F39	O5-C10	3.71	1.51	1.43
9	A	817	F39	C43-C42	3.70	1.58	1.50
13	a	802	G2O	CHC-C4B	-3.70	1.31	1.38
9	A	817	F39	O5-C10	3.68	1.51	1.43
9	A	817	F39	C10-C12	3.66	1.60	1.53
13	A	802	G2O	C4D-ND	-3.66	1.31	1.35
5	A	807	BCL	O2D-CED	3.65	1.53	1.45
9	a	817	F39	C10-C12	3.64	1.60	1.53
13	a	802	G2O	C4D-CHA	-3.64	1.40	1.45
5	a	807	BCL	O2D-CED	3.62	1.53	1.45
13	a	802	G2O	C4D-ND	-3.59	1.32	1.35
13	A	802	G2O	C4D-CHA	-3.55	1.40	1.45
13	a	803	G2O	C14-C13	-3.54	1.41	1.52
13	A	803	G2O	C14-C13	-3.53	1.41	1.52
5	a	810	BCL	O2D-CED	3.48	1.53	1.45
5	A	810	BCL	O2D-CED	3.46	1.53	1.45
5	a	806	BCL	C3D-C2D	-3.46	1.33	1.39
9	A	817	F39	C47-C45	3.45	1.47	1.40
5	A	806	BCL	C3D-C2D	-3.44	1.33	1.39
7	A	801	GS0	O2D-CED	3.43	1.53	1.45
5	A	805	BCL	C3D-C2D	-3.43	1.33	1.39
9	a	817	F39	C47-C45	3.43	1.47	1.40
5	G	374	BCL	O2D-CED	3.43	1.53	1.45
5	F	374	BCL	O2D-CED	3.43	1.53	1.45
5	E	373	BCL	O2D-CED	3.43	1.53	1.45
13	a	803	G2O	C4D-ND	-3.43	1.32	1.35
5	E	377	BCL	O2D-CED	3.42	1.53	1.45
13	a	802	G2O	C14-C13	-3.42	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	805	BCL	C3D-C2D	-3.42	1.33	1.39
13	A	802	G2O	C14-C13	-3.41	1.42	1.52
5	A	813	BCL	O2D-CED	3.41	1.53	1.45
5	G	375	BCL	O2D-CED	3.41	1.53	1.45
7	a	801	GS0	O2D-CED	3.41	1.53	1.45
5	E	375	BCL	C3D-C2D	-3.41	1.33	1.39
5	F	377	BCL	O2D-CED	3.41	1.53	1.45
5	A	814	BCL	O2D-CED	3.41	1.53	1.45
5	E	375	BCL	O2D-CED	3.40	1.53	1.45
5	a	804	BCL	O2D-CED	3.40	1.53	1.45
5	E	374	BCL	O2D-CED	3.40	1.53	1.45
5	A	811	BCL	O2D-CED	3.40	1.53	1.45
5	F	375	BCL	O2D-CED	3.40	1.53	1.45
5	G	373	BCL	O2D-CED	3.40	1.53	1.45
5	a	809	BCL	O2D-CED	3.39	1.53	1.45
5	a	805	BCL	O2D-CED	3.39	1.53	1.45
5	A	804	BCL	O2D-CED	3.39	1.53	1.45
5	A	805	BCL	O2D-CED	3.39	1.53	1.45
5	F	378[B]	BCL	O2D-CED	3.39	1.53	1.45
5	a	812	BCL	O2D-CED	3.39	1.53	1.45
5	A	806	BCL	O2D-CED	3.39	1.53	1.45
5	A	809	BCL	O2D-CED	3.38	1.53	1.45
5	a	806	BCL	O2D-CED	3.38	1.53	1.45
5	A	812	BCL	O2D-CED	3.38	1.53	1.45
5	a	804	BCL	C3D-C2D	-3.38	1.33	1.39
5	a	813	BCL	O2D-CED	3.38	1.53	1.45
5	F	378[B]	BCL	C3D-C2D	-3.38	1.33	1.39
5	G	375	BCL	C3D-C2D	-3.38	1.33	1.39
5	a	814	BCL	O2D-CED	3.38	1.53	1.45
5	A	815	BCL	O2D-CED	3.37	1.53	1.45
5	a	811	BCL	O2D-CED	3.37	1.53	1.45
5	G	377	BCL	O2D-CED	3.37	1.53	1.45
5	F	371	BCL	O2D-CED	3.37	1.53	1.45
5	F	373	BCL	O2D-CED	3.37	1.53	1.45
13	a	803	G2O	C3A-C4A	-3.36	1.40	1.51
5	F	375	BCL	C3D-C2D	-3.36	1.33	1.39
5	F	376	BCL	O2D-CED	3.36	1.53	1.45
5	a	815	BCL	O2D-CED	3.36	1.53	1.45
13	a	802	G2O	C9-C8	-3.36	1.41	1.53
5	G	378[B]	BCL	C3D-C2D	-3.35	1.33	1.39
5	G	371	BCL	C3D-C2D	-3.35	1.33	1.39
5	F	372	BCL	O2D-CED	3.35	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	371	BCL	O2D-CED	3.35	1.53	1.45
5	G	378[B]	BCL	O2D-CED	3.34	1.53	1.45
5	E	378[B]	BCL	O2D-CED	3.34	1.53	1.45
13	A	802	G2O	C9-C8	-3.34	1.41	1.53
5	G	372	BCL	O2D-CED	3.34	1.53	1.45
5	a	808	BCL	O2D-CED	3.34	1.53	1.45
9	a	817	F39	C49-C47	3.34	1.46	1.39
5	G	376	BCL	C3D-C2D	-3.34	1.33	1.39
5	F	376	BCL	C3D-C2D	-3.34	1.33	1.39
5	F	377	BCL	C3D-C2D	-3.34	1.33	1.39
5	E	371	BCL	O2D-CED	3.34	1.53	1.45
5	A	808	BCL	O2D-CED	3.34	1.53	1.45
5	E	378[B]	BCL	C3D-C2D	-3.34	1.33	1.39
5	A	815	BCL	C3D-C2D	-3.33	1.33	1.39
5	G	376	BCL	O2D-CED	3.33	1.53	1.45
13	A	803	G2O	C3A-C4A	-3.33	1.40	1.51
13	A	803	G2O	C4D-ND	-3.33	1.32	1.35
5	a	815	BCL	C3D-C2D	-3.33	1.33	1.39
5	A	814	BCL	C3D-C2D	-3.33	1.33	1.39
5	F	371	BCL	C3D-C2D	-3.32	1.33	1.39
5	E	376	BCL	C3D-C2D	-3.32	1.33	1.39
5	E	371	BCL	C3D-C2D	-3.32	1.33	1.39
5	E	372	BCL	O2D-CED	3.32	1.53	1.45
5	A	804	BCL	C3D-C2D	-3.32	1.33	1.39
5	G	373	BCL	C3D-C2D	-3.31	1.33	1.39
13	A	803	G2O	C9-C8	-3.31	1.41	1.53
9	A	817	F39	C49-C47	3.31	1.46	1.39
5	a	809	BCL	C3D-C2D	-3.31	1.33	1.39
5	G	377	BCL	C3D-C2D	-3.30	1.33	1.39
13	a	803	G2O	C9-C8	-3.30	1.41	1.53
5	A	813	BCL	C3D-C2D	-3.30	1.33	1.39
5	A	811	BCL	C3D-C2D	-3.30	1.33	1.39
9	A	817	F39	C50-C48	3.29	1.46	1.39
5	E	376	BCL	O2D-CED	3.29	1.53	1.45
5	E	373	BCL	C3D-C2D	-3.29	1.33	1.39
5	F	373	BCL	C3D-C2D	-3.29	1.33	1.39
9	a	817	F39	C50-C48	3.28	1.46	1.39
5	G	372	BCL	C3D-C2D	-3.28	1.33	1.39
5	a	811	BCL	C3D-C2D	-3.28	1.33	1.39
13	a	802	G2O	C3A-C4A	-3.28	1.41	1.51
5	F	372	BCL	C3D-C2D	-3.28	1.33	1.39
5	E	372	BCL	C3D-C2D	-3.28	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	813	BCL	C3D-C2D	-3.28	1.33	1.39
5	a	814	BCL	C3D-C2D	-3.27	1.33	1.39
13	A	802	G2O	C3A-C4A	-3.27	1.41	1.51
5	E	377	BCL	C3D-C2D	-3.27	1.33	1.39
5	A	812	BCL	C3D-C2D	-3.26	1.33	1.39
5	G	374	BCL	C3D-C2D	-3.22	1.33	1.39
8	a	816	F26	C24-C19	-3.22	1.31	1.35
5	A	809	BCL	C3D-C2D	-3.22	1.33	1.39
8	a	816	F26	C33-C31	-3.22	1.31	1.35
5	a	807	BCL	C3D-C2D	-3.22	1.33	1.39
5	A	807	BCL	C3D-C2D	-3.22	1.33	1.39
5	E	374	BCL	C3D-C2D	-3.20	1.33	1.39
5	F	374	BCL	C3D-C2D	-3.20	1.33	1.39
5	a	808	BCL	C3D-C2D	-3.19	1.33	1.39
8	A	816	F26	C15-C19	3.18	1.52	1.45
5	A	808	BCL	C3D-C2D	-3.18	1.33	1.39
8	a	816	F26	C15-C19	3.18	1.52	1.45
5	a	812	BCL	C3D-C2D	-3.18	1.33	1.39
8	A	816	F26	C33-C31	-3.14	1.31	1.35
8	A	816	F26	C24-C19	-3.12	1.31	1.35
9	a	817	F39	O4-C9	3.11	1.50	1.43
9	A	817	F39	O4-C9	3.11	1.50	1.43
5	A	811	BCL	O2A-CGA	-3.09	1.24	1.33
5	F	374	BCL	O2A-CGA	-3.08	1.24	1.33
5	G	374	BCL	O2A-CGA	-3.07	1.24	1.33
5	a	811	BCL	O2A-CGA	-3.06	1.24	1.33
5	E	372	BCL	O2A-CGA	-3.06	1.24	1.33
9	a	817	F39	C25-C20	3.05	1.58	1.50
5	E	371	BCL	O2A-CGA	-3.05	1.24	1.33
5	E	374	BCL	O2A-CGA	-3.05	1.24	1.33
5	A	806	BCL	O2A-CGA	-3.05	1.24	1.33
5	F	371	BCL	O2A-CGA	-3.05	1.24	1.33
5	A	812	BCL	O2A-CGA	-3.04	1.24	1.33
5	G	372	BCL	O2A-CGA	-3.04	1.24	1.33
5	F	372	BCL	O2A-CGA	-3.04	1.24	1.33
9	A	817	F39	C25-C20	3.04	1.58	1.50
5	E	373	BCL	O2A-CGA	-3.03	1.24	1.33
7	a	801	GS0	O2D-CGD	-3.03	1.25	1.33
5	F	373	BCL	O2A-CGA	-3.03	1.24	1.33
5	F	372	BCL	O2D-CGD	-3.02	1.25	1.33
5	G	371	BCL	O2A-CGA	-3.02	1.24	1.33
5	G	373	BCL	O2D-CGD	-3.02	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	372	BCL	O2D-CGD	-3.02	1.25	1.33
5	a	806	BCL	O2A-CGA	-3.01	1.24	1.33
7	A	801	GS0	O2D-CGD	-3.01	1.25	1.33
5	E	375	BCL	O2A-CGA	-3.01	1.24	1.33
5	A	808	BCL	O2D-CGD	-3.01	1.25	1.33
5	a	812	BCL	O2A-CGA	-3.01	1.24	1.33
5	E	372	BCL	O2D-CGD	-3.00	1.25	1.33
5	G	373	BCL	O2A-CGA	-3.00	1.24	1.33
5	E	371	BCL	O2D-CGD	-3.00	1.25	1.33
5	G	375	BCL	O2A-CGA	-3.00	1.24	1.33
7	a	801	GS0	O2A-CGA	-3.00	1.24	1.33
5	F	376	BCL	O2A-CGA	-3.00	1.24	1.33
5	a	808	BCL	O2D-CGD	-3.00	1.25	1.33
5	a	812	BCL	O2D-CGD	-3.00	1.25	1.33
5	G	376	BCL	O2A-CGA	-3.00	1.24	1.33
5	G	371	BCL	O2D-CGD	-2.99	1.25	1.33
7	A	801	GS0	O2A-CGA	-2.99	1.24	1.33
5	G	377	BCL	O2D-CGD	-2.99	1.25	1.33
5	E	373	BCL	O2D-CGD	-2.99	1.25	1.33
5	a	813	BCL	O2D-CGD	-2.99	1.25	1.33
5	E	376	BCL	O2A-CGA	-2.98	1.24	1.33
5	F	373	BCL	O2D-CGD	-2.98	1.25	1.33
5	F	377	BCL	O2D-CGD	-2.98	1.25	1.33
5	F	377	BCL	O2A-CGA	-2.98	1.24	1.33
5	G	376	BCL	O2D-CGD	-2.98	1.25	1.33
5	F	376	BCL	O2D-CGD	-2.98	1.25	1.33
5	G	377	BCL	O2A-CGA	-2.97	1.24	1.33
5	A	810	BCL	O2D-CGD	-2.97	1.26	1.33
5	A	812	BCL	O2D-CGD	-2.97	1.26	1.33
5	E	377	BCL	O2D-CGD	-2.97	1.26	1.33
5	a	804	BCL	O2D-CGD	-2.97	1.26	1.33
5	A	814	BCL	O2D-CGD	-2.96	1.26	1.33
5	F	375	BCL	O2A-CGA	-2.96	1.24	1.33
5	A	815	BCL	O2D-CGD	-2.96	1.26	1.33
5	a	810	BCL	O2D-CGD	-2.96	1.26	1.33
5	F	375	BCL	O2D-CGD	-2.95	1.26	1.33
5	E	377	BCL	O2A-CGA	-2.95	1.24	1.33
5	A	804	BCL	O2D-CGD	-2.95	1.26	1.33
5	a	811	BCL	O2D-CGD	-2.95	1.26	1.33
5	E	375	BCL	O2D-CGD	-2.95	1.26	1.33
5	A	811	BCL	O2D-CGD	-2.95	1.26	1.33
5	A	813	BCL	O2D-CGD	-2.95	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	375	BCL	O2D-CGD	-2.95	1.26	1.33
5	a	814	BCL	O2D-CGD	-2.95	1.26	1.33
5	F	371	BCL	O2D-CGD	-2.95	1.26	1.33
5	F	374	BCL	O2D-CGD	-2.94	1.26	1.33
5	E	376	BCL	O2D-CGD	-2.93	1.26	1.33
5	G	374	BCL	O2D-CGD	-2.93	1.26	1.33
5	F	378[B]	BCL	O2D-CGD	-2.93	1.26	1.33
8	a	816	F26	C28-C31	2.93	1.52	1.45
5	G	378[B]	BCL	O2D-CGD	-2.93	1.26	1.33
5	a	815	BCL	O2D-CGD	-2.93	1.26	1.33
5	a	809	BCL	O2D-CGD	-2.92	1.26	1.33
5	a	805	BCL	O2A-CGA	-2.92	1.24	1.33
5	A	805	BCL	O2A-CGA	-2.92	1.24	1.33
5	A	809	BCL	O2D-CGD	-2.92	1.26	1.33
8	a	816	F26	C39-C37	2.90	1.52	1.43
5	A	805	BCL	O2D-CGD	-2.90	1.26	1.33
5	E	374	BCL	O2D-CGD	-2.90	1.26	1.33
5	a	805	BCL	O2D-CGD	-2.89	1.26	1.33
8	A	816	F26	C39-C37	2.89	1.52	1.43
5	A	812	BCL	O1A-CGA	-2.88	1.14	1.22
8	A	816	F26	C28-C31	2.88	1.52	1.45
5	A	806	BCL	O2D-CGD	-2.88	1.26	1.33
5	a	806	BCL	O2D-CGD	-2.88	1.26	1.33
5	a	808	BCL	O2A-CGA	-2.87	1.24	1.33
5	a	806	BCL	O1A-CGA	-2.87	1.14	1.22
5	A	807	BCL	C4B-NB	2.87	1.37	1.35
5	E	372	BCL	O1A-CGA	-2.87	1.14	1.22
5	a	811	BCL	O1A-CGA	-2.87	1.14	1.22
5	E	378[B]	BCL	O2D-CGD	-2.87	1.26	1.33
5	A	811	BCL	O1A-CGA	-2.86	1.14	1.22
7	A	801	GS0	O1A-CGA	-2.86	1.14	1.22
5	G	373	BCL	O1A-CGA	-2.86	1.14	1.22
13	a	803	G2O	C8-C7	-2.86	1.42	1.51
5	a	812	BCL	O1A-CGA	-2.85	1.14	1.22
5	A	808	BCL	O2A-CGA	-2.85	1.25	1.33
5	A	810	BCL	C3D-C2D	-2.85	1.34	1.39
5	E	374	BCL	O1A-CGA	-2.85	1.14	1.22
5	A	806	BCL	O1A-CGA	-2.85	1.14	1.22
7	a	801	GS0	O1A-CGA	-2.85	1.14	1.22
5	G	376	BCL	O1A-CGA	-2.84	1.14	1.22
5	a	810	BCL	C3D-C2D	-2.84	1.34	1.39
5	E	373	BCL	O1A-CGA	-2.84	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	373	BCL	O1A-CGA	-2.84	1.14	1.22
5	F	376	BCL	O1A-CGA	-2.84	1.14	1.22
5	E	377	BCL	O1A-CGA	-2.83	1.14	1.22
13	A	803	G2O	C8-C7	-2.83	1.42	1.51
5	F	377	BCL	O1A-CGA	-2.83	1.14	1.22
5	G	372	BCL	O1A-CGA	-2.83	1.14	1.22
8	a	816	F26	C22-C18	2.83	1.52	1.43
9	a	817	F39	C23-C22	2.83	1.62	1.52
5	F	372	BCL	O1A-CGA	-2.82	1.14	1.22
5	a	808	BCL	O1A-CGA	-2.82	1.14	1.22
5	G	371	BCL	O1A-CGA	-2.82	1.14	1.22
5	F	371	BCL	O1A-CGA	-2.82	1.14	1.22
5	E	376	BCL	O1A-CGA	-2.81	1.14	1.22
13	A	803	G2O	C3D-CAD	-2.81	1.41	1.47
8	A	816	F26	C22-C18	2.81	1.52	1.43
5	G	377	BCL	O1A-CGA	-2.81	1.14	1.22
5	F	374	BCL	O1A-CGA	-2.81	1.14	1.22
5	a	807	BCL	C4B-NB	2.81	1.37	1.35
8	a	816	F26	C38-C33	2.81	1.52	1.43
5	G	374	BCL	O1A-CGA	-2.81	1.14	1.22
5	A	808	BCL	O1A-CGA	-2.81	1.14	1.22
13	a	803	G2O	C3D-CAD	-2.80	1.41	1.47
9	A	817	F39	C23-C22	2.80	1.62	1.52
13	a	802	G2O	C3D-CAD	-2.80	1.41	1.47
5	E	371	BCL	O1A-CGA	-2.80	1.14	1.22
5	a	805	BCL	O1A-CGA	-2.80	1.14	1.22
5	A	805	BCL	O1A-CGA	-2.79	1.14	1.22
8	A	816	F26	C38-C33	2.79	1.52	1.43
5	F	375	BCL	O1A-CGA	-2.78	1.14	1.22
8	a	816	F26	C32-C30	2.77	1.52	1.43
5	G	375	BCL	O1A-CGA	-2.77	1.14	1.22
8	A	816	F26	C32-C30	2.76	1.52	1.43
8	a	816	F26	C18-C13	-2.76	1.31	1.34
13	A	802	G2O	C3D-CAD	-2.75	1.41	1.47
9	A	817	F39	C11-C9	2.75	1.60	1.52
8	a	816	F26	C27-C24	2.75	1.52	1.43
5	E	375	BCL	O1A-CGA	-2.75	1.14	1.22
9	a	817	F39	C11-C9	2.74	1.60	1.52
13	A	802	G2O	MG-NA	2.74	2.12	2.06
8	A	816	F26	C27-C24	2.73	1.51	1.43
13	a	802	G2O	MG-NA	2.70	2.12	2.06
8	A	816	F26	C18-C13	-2.67	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	807	BCL	O2D-CGD	-2.66	1.26	1.33
13	A	803	G2O	MG-NA	2.64	2.12	2.06
8	A	816	F26	C35-C34	2.63	1.51	1.45
8	a	816	F26	C35-C34	2.63	1.51	1.45
13	a	803	G2O	MG-NA	2.62	2.12	2.06
5	A	807	BCL	O2D-CGD	-2.62	1.26	1.33
13	A	803	G2O	CMD-C2D	-2.59	1.46	1.51
13	a	803	G2O	CMD-C2D	-2.58	1.46	1.51
7	a	801	GS0	C1D-C2D	-2.56	1.40	1.45
13	a	802	G2O	CMB-C2B	-2.56	1.45	1.50
7	A	801	GS0	C1D-C2D	-2.53	1.40	1.45
13	A	802	G2O	C8-C7	-2.53	1.43	1.51
13	a	802	G2O	C8-C7	-2.52	1.43	1.51
13	A	802	G2O	CMB-C2B	-2.51	1.45	1.50
5	A	804	BCL	C3B-C2B	-2.49	1.35	1.39
13	a	803	G2O	CMB-C2B	-2.49	1.45	1.50
8	A	816	F26	C25-C26	2.48	1.51	1.45
5	a	804	BCL	C3B-C2B	-2.47	1.35	1.39
13	a	802	G2O	CMD-C2D	-2.47	1.46	1.51
13	A	802	G2O	C1B-C2B	2.46	1.50	1.45
8	a	816	F26	C25-C26	2.46	1.51	1.45
8	a	816	F26	C2-C9	2.44	1.53	1.47
5	a	808	BCL	C3B-C2B	-2.44	1.35	1.39
13	A	803	G2O	CMB-C2B	-2.44	1.45	1.50
13	a	802	G2O	C1B-C2B	2.43	1.50	1.45
5	E	378[B]	BCL	C4B-NB	2.43	1.37	1.35
5	A	808	BCL	C3B-C2B	-2.43	1.35	1.39
5	a	813	BCL	O1A-CGA	-2.42	1.14	1.22
8	A	816	F26	C2-C9	2.41	1.53	1.47
13	A	802	G2O	CMD-C2D	-2.41	1.46	1.51
5	A	810	BCL	O1A-CGA	-2.41	1.14	1.22
13	A	803	G2O	C1B-C2B	2.41	1.50	1.45
5	F	378[B]	BCL	O1A-CGA	-2.41	1.14	1.22
5	E	378[B]	BCL	O1A-CGA	-2.41	1.14	1.22
5	G	378[B]	BCL	O1A-CGA	-2.40	1.14	1.22
5	A	813	BCL	O1A-CGA	-2.40	1.14	1.22
5	a	810	BCL	O1A-CGA	-2.40	1.14	1.22
5	A	806	BCL	C4B-NB	2.39	1.37	1.35
5	A	810	BCL	C4B-NB	2.38	1.37	1.35
5	A	804	BCL	C4B-NB	2.38	1.37	1.35
5	a	807	BCL	O1A-CGA	-2.38	1.14	1.22
5	A	815	BCL	O1A-CGA	-2.38	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	809	BCL	O1A-CGA	-2.38	1.14	1.22
5	A	807	BCL	O1A-CGA	-2.38	1.14	1.22
5	a	804	BCL	O1A-CGA	-2.37	1.14	1.22
5	a	812	BCL	C4B-NB	2.37	1.37	1.35
5	A	804	BCL	O1A-CGA	-2.37	1.14	1.22
5	a	806	BCL	C3B-C2B	-2.37	1.35	1.39
5	F	373	BCL	C4B-NB	2.37	1.37	1.35
5	A	812	BCL	C4B-NB	2.36	1.37	1.35
5	a	804	BCL	C4B-NB	2.36	1.37	1.35
5	a	815	BCL	O1A-CGA	-2.36	1.14	1.22
13	a	803	G2O	C1B-C2B	2.35	1.50	1.45
5	A	813	BCL	C3B-C2B	-2.35	1.35	1.39
5	G	373	BCL	C4B-NB	2.35	1.37	1.35
5	A	809	BCL	O1A-CGA	-2.35	1.14	1.22
5	a	810	BCL	C4B-NB	2.34	1.37	1.35
5	E	373	BCL	C4B-NB	2.34	1.37	1.35
5	a	814	BCL	O1A-CGA	-2.34	1.14	1.22
5	A	814	BCL	O1A-CGA	-2.34	1.14	1.22
5	A	806	BCL	C3B-C2B	-2.34	1.35	1.39
5	a	813	BCL	C3B-C2B	-2.33	1.35	1.39
5	a	810	BCL	C3B-C2B	-2.32	1.35	1.39
5	A	810	BCL	C3B-C2B	-2.32	1.35	1.39
5	a	806	BCL	C4B-NB	2.31	1.37	1.35
7	a	801	GS0	C3D-C4D	-2.31	1.39	1.44
13	A	803	G2O	C1B-NB	-2.29	1.35	1.37
7	A	801	GS0	C3D-C4D	-2.28	1.39	1.44
5	F	378[B]	BCL	C4B-NB	2.26	1.37	1.35
13	A	803	G2O	C1A-CHA	2.26	1.42	1.37
5	F	373	BCL	C3B-C2B	-2.26	1.35	1.39
13	a	803	G2O	C1B-NB	-2.24	1.35	1.37
13	a	803	G2O	C1A-CHA	2.24	1.42	1.37
5	E	373	BCL	C3B-C2B	-2.23	1.35	1.39
5	G	378[B]	BCL	C4B-NB	2.22	1.37	1.35
5	a	812	BCL	C3B-C2B	-2.22	1.35	1.39
5	G	373	BCL	C3B-C2B	-2.21	1.35	1.39
5	A	812	BCL	C3B-C2B	-2.19	1.35	1.39
5	A	807	BCL	C3B-C2B	-2.19	1.35	1.39
5	a	807	BCL	C3B-C2B	-2.19	1.35	1.39
13	a	802	G2O	C1A-CHA	2.19	1.42	1.37
13	A	802	G2O	C1B-NB	-2.15	1.35	1.37
13	A	802	G2O	C1A-CHA	2.13	1.42	1.37
10	a	818	LHG	O7-C5	-2.13	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	818	LHG	O7-C5	-2.12	1.41	1.46
13	a	802	G2O	C1B-NB	-2.12	1.35	1.37
13	a	802	G2O	CMC-C2C	-2.10	1.46	1.50
13	A	802	G2O	CMC-C2C	-2.10	1.46	1.50
13	A	803	G2O	CMC-C2C	-2.09	1.46	1.50
5	E	377	BCL	C3B-C2B	-2.08	1.35	1.39
13	a	803	G2O	CMC-C2C	-2.08	1.46	1.50
9	A	817	F39	O6-C15	2.08	1.49	1.45
5	A	807	BCL	C3B-CAB	2.08	1.54	1.49
5	a	807	BCL	C3B-CAB	2.07	1.54	1.49
5	a	805	BCL	C3B-C2B	-2.07	1.35	1.39
5	A	805	BCL	C3B-C2B	-2.07	1.35	1.39
9	a	817	F39	O6-C15	2.06	1.49	1.45
5	E	375	BCL	C3B-C2B	-2.06	1.35	1.39
5	G	375	BCL	C3B-C2B	-2.05	1.35	1.39
7	A	801	GS0	C3D-C2D	-2.05	1.33	1.39
5	G	376	BCL	C3B-C2B	-2.04	1.35	1.39
5	A	811	BCL	C3B-C2B	-2.04	1.35	1.39
7	a	801	GS0	C3D-C2D	-2.04	1.33	1.39
5	F	375	BCL	C3B-C2B	-2.03	1.35	1.39
5	E	371	BCL	C3B-C2B	-2.03	1.35	1.39
5	E	376	BCL	C2C-C3C	-2.03	1.48	1.54
5	a	813	BCL	C2C-C3C	-2.03	1.48	1.54
5	a	813	BCL	C4B-NB	2.03	1.37	1.35
5	A	815	BCL	C2C-C3C	-2.02	1.48	1.54
5	A	813	BCL	C4B-NB	2.02	1.37	1.35
5	A	813	BCL	C2C-C3C	-2.02	1.48	1.54
11	a	819	LMG	O6-C5	-2.02	1.39	1.44
7	a	801	GS0	C3B-C2B	-2.01	1.35	1.39
11	A	819	LMG	O6-C5	-2.01	1.39	1.44
9	a	817	F39	C30-C29	2.01	1.62	1.51
9	A	817	F39	C30-C29	2.01	1.62	1.51
5	A	805	BCL	C2C-C3C	-2.01	1.48	1.54
5	G	378[B]	BCL	C3B-CAB	2.00	1.54	1.49
5	a	815	BCL	C3B-C2B	-2.00	1.35	1.39
5	E	372	BCL	C3B-CAB	2.00	1.54	1.49
5	a	811	BCL	C3B-C2B	-2.00	1.35	1.39
7	A	801	GS0	C3B-C2B	-2.00	1.35	1.39
5	a	815	BCL	C2C-C3C	-2.00	1.48	1.54
5	A	809	BCL	C3B-C2B	-2.00	1.35	1.39

All (1219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	817	F39	C57-C59-C62	-11.74	110.55	127.31
9	A	817	F39	C57-C59-C62	-11.73	110.56	127.31
9	A	817	F39	C51-C44-C42	-11.21	111.31	127.31
9	a	817	F39	C51-C44-C42	-11.20	111.33	127.31
9	A	817	F39	C40-C39-C37	-11.17	111.37	127.31
9	a	817	F39	C40-C39-C37	-11.16	111.38	127.31
9	a	817	F39	C63-C61-C58	-10.73	112.00	127.31
9	A	817	F39	C63-C61-C58	-10.68	112.06	127.31
9	A	817	F39	C65-C62-C59	-10.03	108.88	122.92
9	a	817	F39	C65-C62-C59	-9.98	108.94	122.92
9	a	817	F39	C60-C58-C61	-9.83	109.16	122.92
9	A	817	F39	C60-C58-C61	-9.79	109.21	122.92
9	a	817	F39	C38-C37-C39	-9.69	109.35	122.92
9	A	817	F39	C38-C37-C39	-9.67	109.38	122.92
9	a	817	F39	C43-C42-C44	-9.49	109.63	122.92
9	A	817	F39	C43-C42-C44	-9.46	109.67	122.92
13	A	802	G2O	C5-C6-C7	-7.13	108.86	125.05
13	a	802	G2O	C5-C6-C7	-7.12	108.87	125.05
9	A	817	F39	C46-C53-C56	-7.05	112.73	128.63
9	a	817	F39	C46-C53-C56	-7.04	112.76	128.63
9	A	817	F39	C41-C42-C44	-6.89	108.37	118.94
9	a	817	F39	C41-C42-C44	-6.87	108.39	118.94
9	a	817	F39	C64-C62-C59	-6.70	108.67	118.94
9	A	817	F39	C64-C62-C59	-6.66	108.72	118.94
13	A	803	G2O	C5-C6-C7	-6.57	110.14	125.05
13	a	803	G2O	C5-C6-C7	-6.54	110.20	125.05
5	E	378[B]	BCL	CMB-C2B-C1B	-6.38	118.66	128.46
5	G	378[B]	BCL	CMB-C2B-C1B	-6.38	118.66	128.46
5	A	811	BCL	CMB-C2B-C1B	-6.36	118.68	128.46
5	F	378[B]	BCL	CMB-C2B-C1B	-6.36	118.68	128.46
5	a	811	BCL	CMB-C2B-C1B	-6.36	118.69	128.46
5	a	809	BCL	CMB-C2B-C1B	-6.36	118.70	128.46
5	A	809	BCL	CMB-C2B-C1B	-6.35	118.71	128.46
5	A	814	BCL	CMB-C2B-C1B	-6.35	118.71	128.46
5	G	377	BCL	CMB-C2B-C1B	-6.33	118.73	128.46
5	E	377	BCL	CMB-C2B-C1B	-6.33	118.74	128.46
5	a	814	BCL	CMB-C2B-C1B	-6.33	118.74	128.46
5	G	375	BCL	CMB-C2B-C1B	-6.31	118.77	128.46
5	F	377	BCL	CMB-C2B-C1B	-6.30	118.78	128.46
5	a	815	BCL	CMB-C2B-C1B	-6.29	118.80	128.46
5	F	375	BCL	CMB-C2B-C1B	-6.28	118.81	128.46
5	E	375	BCL	CMB-C2B-C1B	-6.28	118.81	128.46
5	E	372	BCL	CMB-C2B-C1B	-6.28	118.81	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	815	BCL	CMB-C2B-C1B	-6.27	118.82	128.46
5	F	374	BCL	CMB-C2B-C1B	-6.26	118.85	128.46
5	E	374	BCL	CMB-C2B-C1B	-6.25	118.85	128.46
5	G	374	BCL	CMB-C2B-C1B	-6.25	118.86	128.46
5	F	372	BCL	CMB-C2B-C1B	-6.22	118.90	128.46
5	a	805	BCL	CMB-C2B-C1B	-6.22	118.91	128.46
5	G	376	BCL	CMB-C2B-C1B	-6.22	118.91	128.46
5	G	372	BCL	CMB-C2B-C1B	-6.21	118.92	128.46
5	G	371	BCL	CMB-C2B-C1B	-6.21	118.92	128.46
7	A	801	GS0	CMB-C2B-C1B	-6.21	118.92	128.46
5	A	805	BCL	CMB-C2B-C1B	-6.21	118.92	128.46
5	F	371	BCL	CMB-C2B-C1B	-6.20	118.93	128.46
5	E	376	BCL	CMB-C2B-C1B	-6.20	118.94	128.46
7	a	801	GS0	CMB-C2B-C1B	-6.20	118.94	128.46
5	E	371	BCL	CMB-C2B-C1B	-6.18	118.97	128.46
5	F	376	BCL	CMB-C2B-C1B	-6.17	118.99	128.46
9	a	817	F39	C56-C58-C61	-6.04	109.67	118.94
9	A	817	F39	C56-C58-C61	-6.03	109.69	118.94
5	G	373	BCL	C1C-NC-C4C	-6.01	104.00	106.71
9	a	817	F39	C35-C37-C39	-5.99	109.75	118.94
9	A	817	F39	C35-C37-C39	-5.98	109.76	118.94
5	F	373	BCL	C1C-NC-C4C	-5.95	104.03	106.71
5	E	373	BCL	C1C-NC-C4C	-5.94	104.03	106.71
5	a	807	BCL	CMB-C2B-C1B	-5.86	119.45	128.46
5	A	807	BCL	CMB-C2B-C1B	-5.81	119.53	128.46
9	a	817	F39	C65-C62-C64	-5.76	109.00	118.08
8	a	816	F26	C27-C24-C19	-5.73	119.14	127.31
8	A	816	F26	C27-C24-C19	-5.72	119.14	127.31
9	A	817	F39	C65-C62-C64	-5.71	109.09	118.08
8	a	816	F26	C38-C33-C31	-5.68	119.20	127.31
9	A	817	F39	C60-C58-C56	-5.68	109.13	118.08
9	a	817	F39	C60-C58-C56	-5.68	109.13	118.08
8	A	816	F26	C38-C33-C31	-5.66	119.23	127.31
13	A	802	G2O	C1A-NA-C4A	5.63	109.24	106.71
5	G	371	BCL	O2D-CGD-CBD	5.61	121.24	111.27
5	E	373	BCL	CMB-C2B-C1B	-5.61	119.85	128.46
5	E	371	BCL	O2D-CGD-CBD	5.61	121.23	111.27
5	F	371	BCL	O2D-CGD-CBD	5.59	121.21	111.27
5	a	812	BCL	CMB-C2B-C1B	-5.58	119.89	128.46
13	A	803	G2O	C1A-NA-C4A	5.58	109.21	106.71
5	F	373	BCL	CMB-C2B-C1B	-5.57	119.90	128.46
5	G	373	BCL	CMB-C2B-C1B	-5.57	119.90	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	812	BCL	CMB-C2B-C1B	-5.56	119.92	128.46
9	A	817	F39	C57-C51-C44	-5.55	112.10	123.47
9	a	817	F39	C57-C51-C44	-5.55	112.10	123.47
5	A	808	BCL	CMB-C2B-C1B	-5.54	119.95	128.46
5	a	808	BCL	CMB-C2B-C1B	-5.54	119.95	128.46
5	a	806	BCL	CMB-C2B-C1B	-5.53	119.97	128.46
5	A	806	BCL	CMB-C2B-C1B	-5.53	119.97	128.46
13	a	803	G2O	C1A-NA-C4A	5.51	109.18	106.71
5	A	810	BCL	CMB-C2B-C1B	-5.50	120.01	128.46
5	a	810	BCL	CMB-C2B-C1B	-5.48	120.04	128.46
13	a	802	G2O	C1A-NA-C4A	5.47	109.16	106.71
5	A	804	BCL	CMB-C2B-C1B	-5.45	120.08	128.46
5	a	804	BCL	CMB-C2B-C1B	-5.45	120.08	128.46
5	a	813	BCL	CMB-C2B-C1B	-5.44	120.10	128.46
5	A	813	BCL	CMB-C2B-C1B	-5.42	120.13	128.46
7	a	801	GS0	C1D-ND-C4D	-5.31	102.56	106.33
9	A	817	F39	C32-C35-C37	-5.25	111.67	126.42
9	a	817	F39	C32-C35-C37	-5.25	111.68	126.42
7	A	801	GS0	O2D-CGD-CBD	5.22	120.54	111.27
9	a	817	F39	C51-C57-C59	-5.22	112.79	123.47
7	a	801	GS0	O2D-CGD-CBD	5.19	120.49	111.27
9	A	817	F39	C51-C57-C59	-5.18	112.86	123.47
5	G	373	BCL	O2D-CGD-CBD	5.18	120.47	111.27
7	A	801	GS0	C1D-ND-C4D	-5.17	102.66	106.33
5	E	373	BCL	O2D-CGD-CBD	5.17	120.45	111.27
5	F	373	BCL	O2D-CGD-CBD	5.16	120.44	111.27
9	a	817	F39	C63-C64-C62	-5.15	111.95	126.42
9	A	817	F39	C63-C64-C62	-5.14	111.97	126.42
5	a	810	BCL	CAC-C3C-C2C	-5.11	101.50	114.26
5	A	810	BCL	CAC-C3C-C2C	-5.10	101.52	114.26
5	E	374	BCL	O2D-CGD-CBD	5.01	120.17	111.27
5	F	374	BCL	O2D-CGD-CBD	5.01	120.16	111.27
9	a	817	F39	C25-C20-C27	-4.99	109.72	122.59
9	A	817	F39	C25-C20-C27	-4.98	109.73	122.59
5	G	374	BCL	O2D-CGD-CBD	4.98	120.12	111.27
5	A	815	BCL	C1C-NC-C4C	-4.98	104.47	106.71
5	E	376	BCL	O2D-CGD-CBD	4.96	120.08	111.27
5	G	376	BCL	O2D-CGD-CBD	4.95	120.06	111.27
5	A	805	BCL	CAC-C3C-C2C	-4.94	101.91	114.26
5	A	810	BCL	O2D-CGD-CBD	4.94	120.05	111.27
5	a	805	BCL	CAC-C3C-C2C	-4.94	101.91	114.26
5	F	376	BCL	CAC-C3C-C2C	-4.93	101.93	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	808	BCL	O2D-CGD-CBD	4.93	120.03	111.27
7	a	801	GS0	C2D-C1D-ND	4.93	113.73	110.10
5	a	804	BCL	CAC-C3C-C2C	-4.93	101.95	114.26
5	a	810	BCL	O2D-CGD-CBD	4.93	120.02	111.27
5	G	376	BCL	CAC-C3C-C2C	-4.93	101.95	114.26
5	a	811	BCL	O2D-CGD-CBD	4.92	120.02	111.27
5	A	804	BCL	CAC-C3C-C2C	-4.92	101.97	114.26
5	a	812	BCL	O2D-CGD-CBD	4.91	119.99	111.27
5	F	376	BCL	O2D-CGD-CBD	4.91	119.99	111.27
5	E	376	BCL	CAC-C3C-C2C	-4.91	101.99	114.26
5	A	811	BCL	CAC-C3C-C2C	-4.90	102.01	114.26
5	A	811	BCL	O2D-CGD-CBD	4.90	119.98	111.27
5	a	808	BCL	O2D-CGD-CBD	4.90	119.97	111.27
5	a	811	BCL	CAC-C3C-C2C	-4.90	102.02	114.26
5	G	371	BCL	O2D-CGD-O1D	-4.89	114.27	123.84
5	E	371	BCL	O2D-CGD-O1D	-4.89	114.28	123.84
7	A	801	GS0	C2D-C1D-ND	4.89	113.70	110.10
5	F	371	BCL	O2D-CGD-O1D	-4.88	114.29	123.84
5	a	813	BCL	O2D-CGD-CBD	4.88	119.93	111.27
5	A	812	BCL	O2D-CGD-CBD	4.87	119.93	111.27
5	A	807	BCL	CAC-C3C-C2C	-4.87	102.09	114.26
5	a	814	BCL	CAC-C3C-C2C	-4.87	102.10	114.26
5	F	375	BCL	O2D-CGD-CBD	4.86	119.90	111.27
5	A	814	BCL	CAC-C3C-C2C	-4.86	102.12	114.26
5	a	815	BCL	C1C-NC-C4C	-4.86	104.52	106.71
5	E	375	BCL	O2D-CGD-CBD	4.85	119.89	111.27
5	a	807	BCL	CAC-C3C-C2C	-4.85	102.14	114.26
5	A	814	BCL	O2D-CGD-CBD	4.85	119.88	111.27
5	F	372	BCL	CAC-C3C-C2C	-4.85	102.15	114.26
5	A	813	BCL	O2D-CGD-CBD	4.85	119.88	111.27
5	G	375	BCL	O2D-CGD-CBD	4.85	119.88	111.27
5	G	372	BCL	CAC-C3C-C2C	-4.84	102.16	114.26
5	E	375	BCL	CAC-C3C-C2C	-4.84	102.17	114.26
5	a	814	BCL	O2D-CGD-CBD	4.83	119.86	111.27
5	a	809	BCL	C1C-NC-C4C	-4.83	104.54	106.71
5	E	372	BCL	CAC-C3C-C2C	-4.83	102.20	114.26
5	A	815	BCL	CAC-C3C-C2C	-4.82	102.21	114.26
5	F	375	BCL	CAC-C3C-C2C	-4.82	102.22	114.26
5	E	377	BCL	CAC-C3C-C2C	-4.81	102.23	114.26
5	A	813	BCL	CAC-C3C-C2C	-4.81	102.24	114.26
5	G	375	BCL	CAC-C3C-C2C	-4.81	102.24	114.26
5	F	377	BCL	CAC-C3C-C2C	-4.81	102.24	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	815	BCL	CAC-C3C-C2C	-4.81	102.25	114.26
5	G	374	BCL	CAC-C3C-C2C	-4.81	102.25	114.26
5	a	813	BCL	CAC-C3C-C2C	-4.81	102.25	114.26
5	a	808	BCL	CAC-C3C-C2C	-4.80	102.28	114.26
5	E	374	BCL	CAC-C3C-C2C	-4.79	102.28	114.26
5	E	371	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
5	G	377	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
5	F	374	BCL	CAC-C3C-C2C	-4.79	102.30	114.26
5	G	371	BCL	CAC-C3C-C2C	-4.79	102.30	114.26
5	A	809	BCL	C1C-NC-C4C	-4.78	104.56	106.71
5	F	371	BCL	CAC-C3C-C2C	-4.78	102.32	114.26
5	A	808	BCL	CAC-C3C-C2C	-4.77	102.35	114.26
5	A	805	BCL	O2D-CGD-CBD	4.74	119.69	111.27
5	a	804	BCL	O2D-CGD-CBD	4.74	119.68	111.27
5	a	812	BCL	CAC-C3C-C2C	-4.73	102.45	114.26
5	a	805	BCL	O2D-CGD-CBD	4.71	119.64	111.27
5	A	812	BCL	CAC-C3C-C2C	-4.71	102.50	114.26
5	A	804	BCL	O2D-CGD-CBD	4.70	119.62	111.27
5	F	372	BCL	O2D-CGD-CBD	4.69	119.60	111.27
9	A	817	F39	C43-C42-C41	-4.68	110.70	118.08
5	G	372	BCL	O2D-CGD-CBD	4.68	119.59	111.27
9	a	817	F39	C43-C42-C41	-4.68	110.70	118.08
5	A	813	BCL	C1C-NC-C4C	-4.67	104.61	106.71
5	A	815	BCL	O2D-CGD-CBD	4.66	119.54	111.27
5	E	372	BCL	O2D-CGD-CBD	4.65	119.53	111.27
5	G	377	BCL	O2D-CGD-CBD	4.65	119.53	111.27
5	a	807	BCL	O2D-CGD-CBD	4.64	119.52	111.27
7	A	801	GS0	CAC-C3C-C2C	-4.64	102.66	114.26
5	a	815	BCL	O2D-CGD-CBD	4.64	119.52	111.27
5	a	809	BCL	O2D-CGD-CBD	4.64	119.51	111.27
5	E	377	BCL	O2D-CGD-CBD	4.63	119.49	111.27
7	a	801	GS0	CAC-C3C-C2C	-4.62	102.72	114.26
5	A	807	BCL	O2D-CGD-CBD	4.62	119.47	111.27
5	F	371	BCL	C2A-C3A-C4A	-4.62	94.41	101.87
5	G	371	BCL	C2A-C3A-C4A	-4.62	94.41	101.87
5	A	809	BCL	O2D-CGD-CBD	4.61	119.46	111.27
5	A	809	BCL	CAC-C3C-C2C	-4.60	102.76	114.26
5	E	371	BCL	C2A-C3A-C4A	-4.60	94.43	101.87
5	A	806	BCL	O2D-CGD-CBD	4.60	119.45	111.27
5	a	806	BCL	O2D-CGD-CBD	4.60	119.45	111.27
5	a	809	BCL	CAC-C3C-C2C	-4.60	102.77	114.26
5	a	813	BCL	C1C-NC-C4C	-4.59	104.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	377	BCL	O2D-CGD-CBD	4.59	119.42	111.27
5	a	806	BCL	CAC-C3C-C2C	-4.54	102.92	114.26
9	A	817	F39	C40-C41-C42	-4.54	113.67	126.42
5	A	806	BCL	CAC-C3C-C2C	-4.53	102.93	114.26
9	a	817	F39	C40-C41-C42	-4.53	113.69	126.42
5	G	373	BCL	CAC-C3C-C2C	-4.51	102.98	114.26
5	F	373	BCL	CAC-C3C-C2C	-4.51	102.99	114.26
5	E	373	BCL	CAC-C3C-C2C	-4.49	103.05	114.26
5	E	377	BCL	C1C-NC-C4C	-4.47	104.70	106.71
5	F	376	BCL	C1C-NC-C4C	-4.44	104.71	106.71
9	a	817	F39	C38-C37-C35	-4.44	111.09	118.08
5	a	810	BCL	C1C-NC-C4C	-4.43	104.71	106.71
5	E	378[B]	BCL	CAC-C3C-C2C	-4.43	103.19	114.26
5	G	378[B]	BCL	CAC-C3C-C2C	-4.43	103.19	114.26
5	F	378[B]	BCL	CAC-C3C-C2C	-4.42	103.21	114.26
9	A	817	F39	C39-C40-C41	-4.42	109.42	123.22
9	a	817	F39	C39-C40-C41	-4.42	109.42	123.22
9	A	817	F39	C38-C37-C35	-4.41	111.13	118.08
5	A	810	BCL	C1C-NC-C4C	-4.41	104.72	106.71
5	a	807	BCL	O2D-CGD-O1D	-4.41	115.22	123.84
5	E	373	BCL	O2D-CGD-O1D	-4.41	115.22	123.84
5	A	807	BCL	O2D-CGD-O1D	-4.40	115.23	123.84
9	A	817	F39	C19-C20-C27	-4.40	108.65	121.98
9	a	817	F39	C19-C20-C27	-4.39	108.68	121.98
5	G	377	BCL	C1C-NC-C4C	-4.39	104.73	106.71
5	F	373	BCL	O2D-CGD-O1D	-4.39	115.26	123.84
5	G	373	BCL	O2D-CGD-O1D	-4.39	115.26	123.84
5	G	378[B]	BCL	O2D-CGD-CBD	4.38	119.05	111.27
5	E	378[B]	BCL	O2D-CGD-CBD	4.37	119.04	111.27
5	F	378[B]	BCL	O2D-CGD-CBD	4.37	119.04	111.27
7	A	801	GS0	O2D-CGD-O1D	-4.34	115.34	123.84
5	E	376	BCL	C1C-NC-C4C	-4.34	104.75	106.71
5	F	377	BCL	C1C-NC-C4C	-4.32	104.77	106.71
7	a	801	GS0	O2D-CGD-O1D	-4.29	115.44	123.84
5	G	376	BCL	C1C-NC-C4C	-4.28	104.78	106.71
8	A	816	F26	C32-C30-C26	-4.22	121.29	127.31
5	a	810	BCL	O2D-CGD-O1D	-4.22	115.59	123.84
5	F	374	BCL	O2D-CGD-O1D	-4.21	115.60	123.84
5	E	374	BCL	O2D-CGD-O1D	-4.21	115.61	123.84
5	G	377	BCL	CMB-C2B-C3B	4.21	132.55	124.68
8	a	816	F26	C32-C30-C26	-4.20	121.32	127.31
5	A	809	BCL	CMB-C2B-C3B	4.19	132.52	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	808	BCL	O2D-CGD-O1D	-4.19	115.64	123.84
5	G	375	BCL	CMB-C2B-C3B	4.19	132.52	124.68
10	A	818	LHG	O4-P-O5	4.18	132.92	112.24
5	A	810	BCL	O2D-CGD-O1D	-4.18	115.66	123.84
5	G	374	BCL	O2D-CGD-O1D	-4.18	115.66	123.84
5	F	377	BCL	CMB-C2B-C3B	4.18	132.50	124.68
5	a	809	BCL	CMB-C2B-C3B	4.18	132.50	124.68
5	A	814	BCL	CMB-C2B-C3B	4.18	132.49	124.68
10	a	818	LHG	O4-P-O5	4.18	132.88	112.24
5	A	813	BCL	O2D-CGD-O1D	-4.17	115.69	123.84
5	a	808	BCL	O2D-CGD-O1D	-4.17	115.69	123.84
5	E	375	BCL	CMB-C2B-C3B	4.17	132.47	124.68
5	a	811	BCL	CMB-C2B-C3B	4.16	132.47	124.68
5	A	811	BCL	CMB-C2B-C3B	4.16	132.46	124.68
5	F	375	BCL	CMB-C2B-C3B	4.16	132.46	124.68
5	E	377	BCL	CMB-C2B-C3B	4.15	132.45	124.68
5	a	805	BCL	C1C-NC-C4C	-4.15	104.84	106.71
5	G	375	BCL	O2D-CGD-O1D	-4.15	115.73	123.84
5	E	375	BCL	O2D-CGD-O1D	-4.14	115.74	123.84
5	a	813	BCL	O2D-CGD-O1D	-4.14	115.74	123.84
5	G	371	BCL	CMB-C2B-C3B	4.14	132.43	124.68
5	F	375	BCL	O2D-CGD-O1D	-4.14	115.74	123.84
5	a	814	BCL	CMB-C2B-C3B	4.12	132.39	124.68
5	F	371	BCL	CMB-C2B-C3B	4.12	132.38	124.68
5	A	805	BCL	C1C-NC-C4C	-4.11	104.86	106.71
5	A	811	BCL	O2D-CGD-O1D	-4.11	115.79	123.84
5	E	376	BCL	O2D-CGD-O1D	-4.11	115.80	123.84
5	a	811	BCL	O2D-CGD-O1D	-4.11	115.80	123.84
5	G	376	BCL	O2D-CGD-O1D	-4.11	115.81	123.84
5	G	374	BCL	CMB-C2B-C3B	4.11	132.36	124.68
5	F	378[B]	BCL	CMB-C2B-C3B	4.10	132.36	124.68
5	E	371	BCL	CMB-C2B-C3B	4.10	132.35	124.68
5	a	812	BCL	O2D-CGD-O1D	-4.10	115.83	123.84
5	E	377	BCL	O2D-CGD-O1D	-4.09	115.83	123.84
5	G	378[B]	BCL	CMB-C2B-C3B	4.09	132.34	124.68
5	a	815	BCL	O2D-CGD-O1D	-4.09	115.84	123.84
5	F	374	BCL	CMB-C2B-C3B	4.09	132.33	124.68
5	F	376	BCL	O2D-CGD-O1D	-4.09	115.84	123.84
5	A	814	BCL	O2D-CGD-O1D	-4.09	115.85	123.84
5	G	377	BCL	O2D-CGD-O1D	-4.09	115.85	123.84
5	A	812	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
5	A	815	BCL	O2D-CGD-O1D	-4.08	115.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	378[B]	BCL	CMB-C2B-C3B	4.08	132.31	124.68
5	E	372	BCL	CMB-C2B-C3B	4.08	132.31	124.68
5	A	815	BCL	CMB-C2B-C3B	4.08	132.31	124.68
5	a	815	BCL	CMB-C2B-C3B	4.07	132.30	124.68
5	E	374	BCL	CMB-C2B-C3B	4.07	132.29	124.68
7	A	801	GS0	CMB-C2B-C3B	4.07	132.29	124.68
5	a	814	BCL	O2D-CGD-O1D	-4.07	115.89	123.84
5	F	372	BCL	CMB-C2B-C3B	4.06	132.28	124.68
5	F	377	BCL	O2D-CGD-O1D	-4.06	115.90	123.84
5	G	372	BCL	CMB-C2B-C3B	4.06	132.27	124.68
5	a	804	BCL	O2D-CGD-O1D	-4.05	115.91	123.84
5	A	804	BCL	O2D-CGD-O1D	-4.05	115.91	123.84
5	a	805	BCL	CMB-C2B-C3B	4.05	132.25	124.68
5	E	372	BCL	C1C-NC-C4C	-4.05	104.89	106.71
7	a	801	GS0	CMB-C2B-C3B	4.05	132.25	124.68
5	G	376	BCL	CMB-C2B-C3B	4.04	132.24	124.68
5	A	805	BCL	CMB-C2B-C3B	4.04	132.23	124.68
5	E	376	BCL	CMB-C2B-C3B	4.03	132.21	124.68
5	A	809	BCL	O2D-CGD-O1D	-4.02	115.99	123.84
5	G	372	BCL	C1C-NC-C4C	-4.01	104.90	106.71
5	F	376	BCL	CMB-C2B-C3B	4.00	132.17	124.68
5	A	806	BCL	O2D-CGD-O1D	-3.99	116.03	123.84
5	a	809	BCL	O2D-CGD-O1D	-3.99	116.03	123.84
5	F	372	BCL	O2D-CGD-O1D	-3.99	116.04	123.84
5	a	806	BCL	O2D-CGD-O1D	-3.99	116.04	123.84
5	A	807	BCL	C1C-NC-C4C	-3.98	104.92	106.71
5	A	805	BCL	O2D-CGD-O1D	-3.97	116.08	123.84
5	G	372	BCL	O2D-CGD-O1D	-3.96	116.09	123.84
5	a	805	BCL	O2D-CGD-O1D	-3.96	116.10	123.84
5	E	372	BCL	O2D-CGD-O1D	-3.95	116.11	123.84
5	a	807	BCL	OBB-CAB-CBB	-3.95	111.28	120.17
5	A	807	BCL	OBB-CAB-CBB	-3.94	111.30	120.17
5	F	372	BCL	C1C-NC-C4C	-3.93	104.94	106.71
5	F	378[B]	BCL	OBB-CAB-CBB	-3.92	111.34	120.17
5	G	378[B]	BCL	OBB-CAB-CBB	-3.92	111.35	120.17
5	a	812	BCL	C1C-NC-C4C	-3.91	104.95	106.71
5	E	378[B]	BCL	OBB-CAB-CBB	-3.91	111.37	120.17
5	E	378[B]	BCL	O2D-CGD-O1D	-3.91	116.20	123.84
5	A	805	BCL	OBB-CAB-CBB	-3.90	111.39	120.17
5	a	805	BCL	OBB-CAB-CBB	-3.90	111.40	120.17
5	G	371	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
5	G	378[B]	BCL	O2D-CGD-O1D	-3.89	116.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	371	BCL	OBB-CAB-CBB	-3.88	111.44	120.17
5	G	376	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
5	F	376	BCL	OBB-CAB-CBB	-3.87	111.47	120.17
5	F	378[B]	BCL	O2D-CGD-O1D	-3.86	116.28	123.84
5	E	371	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
5	E	376	BCL	OBB-CAB-CBB	-3.85	111.51	120.17
5	F	373	BCL	C2C-C3C-C4C	-3.84	95.58	101.34
5	F	372	BCL	OBB-CAB-CBB	-3.84	111.53	120.17
5	G	372	BCL	OBB-CAB-CBB	-3.84	111.53	120.17
5	A	812	BCL	OBB-CAB-CBB	-3.84	111.53	120.17
5	G	373	BCL	C2C-C3C-C4C	-3.83	95.60	101.34
5	a	815	BCL	OBB-CAB-CBB	-3.83	111.56	120.17
9	A	817	F39	C27-C32-C35	-3.82	111.28	123.22
5	G	375	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
5	A	815	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
5	a	810	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
5	E	373	BCL	C2C-C3C-C4C	-3.82	95.62	101.34
5	A	811	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
5	G	373	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
9	a	817	F39	C27-C32-C35	-3.82	111.31	123.22
5	a	804	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
5	A	810	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
5	E	372	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
5	F	373	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
5	a	806	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
5	A	806	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
5	F	375	BCL	OBB-CAB-CBB	-3.81	111.60	120.17
5	E	375	BCL	OBB-CAB-CBB	-3.81	111.61	120.17
5	a	812	BCL	OBB-CAB-CBB	-3.80	111.62	120.17
5	E	377	BCL	OBB-CAB-CBB	-3.80	111.62	120.17
5	a	811	BCL	OBB-CAB-CBB	-3.80	111.62	120.17
5	A	812	BCL	C1C-NC-C4C	-3.80	105.00	106.71
5	A	804	BCL	OBB-CAB-CBB	-3.79	111.63	120.17
5	E	378[B]	BCL	C1C-NC-C4C	-3.79	105.00	106.71
5	E	373	BCL	OBB-CAB-CBB	-3.79	111.64	120.17
5	a	814	BCL	OBB-CAB-CBB	-3.79	111.64	120.17
5	G	377	BCL	OBB-CAB-CBB	-3.79	111.65	120.17
5	A	814	BCL	OBB-CAB-CBB	-3.78	111.66	120.17
5	F	377	BCL	OBB-CAB-CBB	-3.78	111.66	120.17
5	E	374	BCL	OBB-CAB-CBB	-3.77	111.68	120.17
5	F	374	BCL	OBB-CAB-CBB	-3.77	111.68	120.17
5	a	811	BCL	C1C-NC-C4C	-3.77	105.01	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	374	BCL	OBB-CAB-CBB	-3.77	111.69	120.17
5	A	809	BCL	OBB-CAB-CBB	-3.76	111.70	120.17
5	a	809	BCL	OBB-CAB-CBB	-3.76	111.72	120.17
11	A	819	LMG	O6-C1-O1	-3.75	101.08	109.97
11	a	819	LMG	O6-C1-O1	-3.75	101.09	109.97
7	A	801	GS0	OBB-CAB-CBB	-3.75	111.73	120.17
5	a	813	BCL	OBB-CAB-CBB	-3.75	111.73	120.17
5	G	378[B]	BCL	C1C-NC-C4C	-3.74	105.02	106.71
5	a	807	BCL	C1C-NC-C4C	-3.74	105.02	106.71
7	a	801	GS0	OBB-CAB-CBB	-3.73	111.77	120.17
5	A	813	BCL	OBB-CAB-CBB	-3.73	111.77	120.17
5	a	808	BCL	OBB-CAB-CBB	-3.70	111.84	120.17
5	G	371	BCL	C4A-NA-C1A	-3.69	105.05	106.71
5	F	378[B]	BCL	C1C-NC-C4C	-3.69	105.05	106.71
5	A	808	BCL	OBB-CAB-CBB	-3.68	111.89	120.17
5	A	811	BCL	C1C-NC-C4C	-3.67	105.06	106.71
7	a	801	GS0	CHD-C1D-ND	-3.66	121.09	124.45
9	a	817	F39	C61-C63-C64	-3.65	111.83	123.22
9	A	817	F39	C61-C63-C64	-3.63	111.88	123.22
5	F	371	BCL	C4A-NA-C1A	-3.61	105.08	106.71
7	A	801	GS0	CHD-C1D-ND	-3.59	121.15	124.45
5	E	371	BCL	C4A-NA-C1A	-3.55	105.11	106.71
9	a	817	F39	C25-C20-C19	-3.50	109.39	115.27
9	A	817	F39	C25-C20-C19	-3.50	109.39	115.27
5	A	810	BCL	CHA-C1A-NA	-3.48	118.42	126.40
5	a	810	BCL	CHA-C1A-NA	-3.47	118.44	126.40
5	a	811	BCL	C16-C15-C13	-3.44	104.79	115.92
5	A	811	BCL	C16-C15-C13	-3.44	104.81	115.92
5	E	371	BCL	C1C-NC-C4C	-3.42	105.17	106.71
5	E	376	BCL	C16-C15-C13	-3.42	104.87	115.92
5	a	815	BCL	C4B-CHC-C1C	-3.42	123.35	130.12
5	F	376	BCL	C16-C15-C13	-3.42	104.88	115.92
5	G	376	BCL	C16-C15-C13	-3.41	104.88	115.92
5	E	371	BCL	C16-C15-C13	-3.41	104.89	115.92
5	F	371	BCL	C1C-NC-C4C	-3.41	105.17	106.71
5	A	815	BCL	C4B-CHC-C1C	-3.40	123.39	130.12
5	G	371	BCL	C1C-NC-C4C	-3.40	105.18	106.71
5	G	371	BCL	C16-C15-C13	-3.39	104.95	115.92
5	F	371	BCL	C16-C15-C13	-3.39	104.96	115.92
5	a	808	BCL	CMB-C2B-C3B	3.39	131.02	124.68
5	A	808	BCL	CHA-C1A-NA	-3.37	118.69	126.40
5	a	808	BCL	CHA-C1A-NA	-3.36	118.70	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	374	BCL	C1C-NC-C4C	-3.35	105.20	106.71
5	A	812	BCL	C16-C15-C13	-3.35	105.09	115.92
5	a	812	BCL	C16-C15-C13	-3.35	105.09	115.92
5	A	808	BCL	CMB-C2B-C3B	3.35	130.94	124.68
5	G	377	BCL	C11-C10-C8	-3.34	105.14	115.92
5	F	377	BCL	C11-C10-C8	-3.33	105.15	115.92
5	a	807	BCL	CMB-C2B-C3B	3.33	130.90	124.68
5	A	807	BCL	CMB-C2B-C3B	3.32	130.89	124.68
5	A	810	BCL	CMB-C2B-C3B	3.31	130.87	124.68
5	E	377	BCL	C11-C10-C8	-3.30	105.24	115.92
5	F	371	BCL	CHA-C1A-NA	-3.29	118.86	126.40
5	a	810	BCL	CMB-C2B-C3B	3.28	130.82	124.68
5	A	811	BCL	O2A-CGA-O1A	-3.28	115.31	123.59
5	E	373	BCL	CMB-C2B-C3B	3.28	130.82	124.68
5	G	371	BCL	CHA-C1A-NA	-3.28	118.89	126.40
5	F	374	BCL	C1C-NC-C4C	-3.27	105.23	106.71
7	a	801	GS0	C16-C15-C13	-3.27	105.35	115.92
5	F	373	BCL	CMB-C2B-C3B	3.27	130.79	124.68
5	a	811	BCL	O2A-CGA-O1A	-3.27	115.34	123.59
5	F	372	BCL	CHA-C1A-NA	-3.27	118.92	126.40
5	a	812	BCL	CMB-C2B-C3B	3.27	130.79	124.68
5	G	372	BCL	CHA-C1A-NA	-3.26	118.92	126.40
5	E	375	BCL	C16-C15-C13	-3.26	105.37	115.92
7	A	801	GS0	C16-C15-C13	-3.26	105.37	115.92
5	G	373	BCL	CMB-C2B-C3B	3.26	130.78	124.68
5	E	372	BCL	CHA-C1A-NA	-3.26	118.94	126.40
5	A	804	BCL	CHA-C1A-NA	-3.25	118.95	126.40
5	F	375	BCL	C16-C15-C13	-3.25	105.41	115.92
5	E	371	BCL	CHA-C1A-NA	-3.25	118.95	126.40
5	a	806	BCL	CMB-C2B-C3B	3.25	130.76	124.68
5	A	813	BCL	CMB-C2B-C3B	3.25	130.75	124.68
8	A	816	F26	C39-C37-C34	-3.25	122.68	127.31
8	a	816	F26	C39-C37-C34	-3.24	122.68	127.31
5	G	375	BCL	C16-C15-C13	-3.24	105.44	115.92
5	E	371	BCL	C4B-CHC-C1C	-3.24	123.70	130.12
5	A	806	BCL	CMB-C2B-C3B	3.24	130.74	124.68
5	a	804	BCL	CHA-C1A-NA	-3.24	118.98	126.40
5	E	374	BCL	C4B-CHC-C1C	-3.24	123.70	130.12
5	A	812	BCL	CMB-C2B-C3B	3.24	130.74	124.68
5	G	371	BCL	C4B-CHC-C1C	-3.24	123.70	130.12
5	a	806	BCL	C1C-NC-C4C	-3.23	105.25	106.71
5	a	813	BCL	CMB-C2B-C3B	3.23	130.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	809	BCL	C4B-CHC-C1C	-3.22	123.73	130.12
5	a	809	BCL	C4B-CHC-C1C	-3.22	123.74	130.12
5	F	374	BCL	C4B-CHC-C1C	-3.22	123.75	130.12
5	G	374	BCL	C4B-CHC-C1C	-3.22	123.75	130.12
5	a	806	BCL	C16-C15-C13	-3.21	105.54	115.92
5	A	806	BCL	C16-C15-C13	-3.21	105.55	115.92
5	E	374	BCL	C16-C15-C13	-3.20	105.58	115.92
5	G	374	BCL	C16-C15-C13	-3.20	105.59	115.92
5	A	810	BCL	OBD-CAD-CBD	-3.19	121.33	125.89
5	F	371	BCL	C4B-CHC-C1C	-3.19	123.79	130.12
5	F	374	BCL	CHA-C1A-NA	-3.19	119.09	126.40
5	G	374	BCL	CHA-C1A-NA	-3.19	119.09	126.40
5	a	810	BCL	OBD-CAD-CBD	-3.19	121.34	125.89
5	E	374	BCL	CHA-C1A-NA	-3.19	119.10	126.40
5	A	806	BCL	C1C-NC-C4C	-3.19	105.27	106.71
7	a	801	GS0	CHA-C1A-NA	-3.18	119.11	126.40
5	F	374	BCL	C16-C15-C13	-3.18	105.64	115.92
5	A	810	BCL	CGD-CBD-CAD	-3.17	100.46	110.73
5	a	810	BCL	CGD-CBD-CAD	-3.17	100.47	110.73
7	A	801	GS0	CHA-C1A-NA	-3.16	119.16	126.40
7	A	801	GS0	C4B-CHC-C1C	-3.14	123.90	130.12
5	E	373	BCL	C11-C10-C8	-3.14	105.78	115.92
5	F	373	BCL	CHA-C1A-NA	-3.13	119.22	126.40
5	E	373	BCL	CHA-C1A-NA	-3.13	119.22	126.40
5	G	373	BCL	CHA-C1A-NA	-3.13	119.23	126.40
13	A	803	G2O	O2D-CGD-O1D	-3.13	117.72	123.84
5	E	376	BCL	C11-C10-C8	-3.13	105.81	115.92
5	F	376	BCL	C11-C10-C8	-3.12	105.82	115.92
5	A	809	BCL	C2C-C3C-C4C	-3.12	96.66	101.34
5	a	812	BCL	C7-C6-C5	-3.12	104.88	113.36
5	A	814	BCL	C1C-NC-C4C	-3.12	105.30	106.71
7	a	801	GS0	C4B-CHC-C1C	-3.12	123.94	130.12
5	F	373	BCL	C7-C6-C5	-3.12	104.89	113.36
5	E	373	BCL	C7-C6-C5	-3.11	104.90	113.36
5	E	374	BCL	C1C-NC-C4C	-3.11	105.31	106.71
5	F	374	BCL	O2A-CGA-O1A	-3.11	115.73	123.59
13	a	803	G2O	O2D-CGD-O1D	-3.11	117.75	123.84
5	G	378[B]	BCL	C4B-CHC-C1C	-3.11	123.95	130.12
5	G	376	BCL	C11-C10-C8	-3.11	105.86	115.92
5	A	806	BCL	C11-C10-C8	-3.11	105.88	115.92
5	F	378[B]	BCL	C4B-CHC-C1C	-3.11	123.97	130.12
5	F	373	BCL	C11-C10-C8	-3.10	105.89	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	373	BCL	C11-C10-C8	-3.10	105.89	115.92
5	G	373	BCL	C7-C6-C5	-3.10	104.93	113.36
5	E	373	BCL	C16-C15-C13	-3.10	105.90	115.92
5	a	814	BCL	C4B-CHC-C1C	-3.10	123.98	130.12
5	a	806	BCL	C11-C10-C8	-3.10	105.90	115.92
5	A	812	BCL	C7-C6-C5	-3.10	104.95	113.36
5	a	804	BCL	CMB-C2B-C3B	3.09	130.47	124.68
5	E	374	BCL	O2A-CGA-O1A	-3.09	115.79	123.59
5	A	814	BCL	C4B-CHC-C1C	-3.09	124.00	130.12
5	G	372	BCL	C16-C15-C13	-3.09	105.93	115.92
5	F	373	BCL	C16-C15-C13	-3.09	105.93	115.92
5	A	806	BCL	O2A-CGA-O1A	-3.09	115.80	123.59
5	a	806	BCL	O2A-CGA-O1A	-3.08	115.81	123.59
5	G	374	BCL	O2A-CGA-O1A	-3.08	115.82	123.59
5	a	814	BCL	C1C-NC-C4C	-3.08	105.32	106.71
5	E	377	BCL	C16-C15-C13	-3.08	105.96	115.92
5	E	372	BCL	C16-C15-C13	-3.08	105.97	115.92
5	a	809	BCL	C2C-C3C-C4C	-3.08	96.73	101.34
5	F	374	BCL	C7-C6-C5	-3.08	105.00	113.36
5	G	373	BCL	C16-C15-C13	-3.07	105.98	115.92
5	E	378[B]	BCL	C4B-CHC-C1C	-3.07	124.03	130.12
5	F	371	BCL	C2A-C1A-CHA	3.07	129.23	123.86
5	G	374	BCL	C7-C6-C5	-3.07	105.02	113.36
5	E	374	BCL	C7-C6-C5	-3.07	105.02	113.36
5	F	372	BCL	C16-C15-C13	-3.07	106.00	115.92
5	G	377	BCL	C16-C15-C13	-3.07	106.00	115.92
5	F	377	BCL	C16-C15-C13	-3.07	106.01	115.92
5	F	373	BCL	C4B-CHC-C1C	-3.06	124.05	130.12
5	G	373	BCL	C4B-CHC-C1C	-3.05	124.07	130.12
5	E	373	BCL	C4B-CHC-C1C	-3.05	124.08	130.12
5	A	814	BCL	CHA-C1A-NA	-3.05	119.42	126.40
8	a	816	F26	C38-C39-C37	-3.05	117.23	123.47
5	A	804	BCL	CMB-C2B-C3B	3.04	130.37	124.68
5	A	812	BCL	O2A-CGA-O1A	-3.04	115.91	123.59
5	a	812	BCL	O2A-CGA-O1A	-3.04	115.91	123.59
8	A	816	F26	C38-C39-C37	-3.04	117.24	123.47
5	G	371	BCL	C2A-C1A-CHA	3.04	129.17	123.86
7	A	801	GS0	C7-C6-C5	-3.04	105.12	113.36
5	a	814	BCL	CHA-C1A-NA	-3.03	119.45	126.40
7	a	801	GS0	C7-C6-C5	-3.03	105.13	113.36
5	A	805	BCL	C4B-CHC-C1C	-3.03	124.11	130.12
5	A	808	BCL	C16-C15-C13	-3.03	106.12	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	372	BCL	C11-C10-C8	-3.02	106.14	115.92
5	G	372	BCL	C7-C6-C5	-3.02	105.16	113.36
5	A	812	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
5	a	808	BCL	C16-C15-C13	-3.02	106.17	115.92
13	a	803	G2O	C1-C2-C3	-3.01	120.83	126.04
5	E	376	BCL	O2A-CGA-O1A	-3.01	115.99	123.59
5	G	376	BCL	C7-C6-C5	-3.01	105.19	113.36
5	F	372	BCL	C11-C10-C8	-3.01	106.20	115.92
5	G	372	BCL	C11-C10-C8	-3.01	106.20	115.92
5	A	809	BCL	CHA-C1A-NA	-3.00	119.52	126.40
5	a	812	BCL	C4B-CHC-C1C	-3.00	124.17	130.12
5	F	373	BCL	O2A-CGA-O1A	-3.00	116.02	123.59
5	A	806	BCL	C7-C6-C5	-3.00	105.22	113.36
5	E	371	BCL	C2A-C1A-CHA	3.00	129.10	123.86
5	E	372	BCL	C7-C6-C5	-3.00	105.22	113.36
5	F	372	BCL	C7-C6-C5	-2.99	105.23	113.36
5	F	376	BCL	O2A-CGA-O1A	-2.99	116.04	123.59
5	a	809	BCL	CHA-C1A-NA	-2.99	119.54	126.40
5	a	806	BCL	C7-C6-C5	-2.99	105.23	113.36
5	F	376	BCL	C7-C6-C5	-2.99	105.23	113.36
5	a	805	BCL	C4B-CHC-C1C	-2.99	124.20	130.12
5	E	373	BCL	O2A-CGA-O1A	-2.99	116.06	123.59
5	G	376	BCL	O2A-CGA-O1A	-2.98	116.06	123.59
5	E	376	BCL	C7-C6-C5	-2.98	105.27	113.36
13	A	803	G2O	C1-C2-C3	-2.98	120.89	126.04
5	G	371	BCL	O2A-CGA-O1A	-2.98	116.08	123.59
5	a	808	BCL	CMA-C3A-C4A	-2.97	103.79	111.77
5	G	373	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
5	E	371	BCL	O2A-CGA-O1A	-2.97	116.10	123.59
5	A	812	BCL	CHA-C1A-NA	-2.97	119.60	126.40
5	a	810	BCL	O2A-CGA-O1A	-2.96	115.92	123.30
5	A	808	BCL	CMA-C3A-C4A	-2.96	103.82	111.77
5	a	806	BCL	CHA-C1A-NA	-2.96	119.62	126.40
5	F	371	BCL	O2A-CGA-O1A	-2.96	116.13	123.59
5	A	806	BCL	CHA-C1A-NA	-2.94	119.66	126.40
5	A	806	BCL	CMC-C2C-C3C	-2.94	101.97	113.83
5	a	806	BCL	CMC-C2C-C3C	-2.94	101.97	113.83
7	a	801	GS0	C11-C10-C8	-2.94	106.42	115.92
5	a	812	BCL	CHA-C1A-NA	-2.94	119.67	126.40
5	A	810	BCL	O2A-CGA-O1A	-2.93	115.99	123.30
5	G	376	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
5	A	805	BCL	CHA-C1A-NA	-2.93	119.68	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	372	BCL	C4B-CHC-C1C	-2.93	124.32	130.12
5	A	811	BCL	C11-C10-C8	-2.93	106.45	115.92
5	F	376	BCL	C4B-CHC-C1C	-2.93	124.32	130.12
7	A	801	GS0	C11-C10-C8	-2.92	106.47	115.92
5	a	811	BCL	C11-C10-C8	-2.92	106.47	115.92
5	A	805	BCL	C7-C6-C5	-2.92	105.42	113.36
5	a	809	BCL	O2A-CGA-O1A	-2.92	116.02	123.30
5	E	371	BCL	C7-C6-C5	-2.92	105.43	113.36
5	F	371	BCL	C7-C6-C5	-2.92	105.44	113.36
5	a	805	BCL	CHA-C1A-NA	-2.92	119.72	126.40
5	a	805	BCL	C7-C6-C5	-2.91	105.44	113.36
5	a	814	BCL	O2A-CGA-O1A	-2.91	116.03	123.30
5	A	809	BCL	O2A-CGA-O1A	-2.91	116.04	123.30
5	E	376	BCL	C4B-CHC-C1C	-2.91	124.35	130.12
5	G	378[B]	BCL	O2A-CGA-O1A	-2.91	116.04	123.30
5	E	378[B]	BCL	C2C-C3C-C4C	-2.91	96.98	101.34
5	F	378[B]	BCL	O2A-CGA-O1A	-2.91	116.05	123.30
5	a	807	BCL	C4B-CHC-C1C	-2.90	124.37	130.12
5	G	371	BCL	C7-C6-C5	-2.90	105.48	113.36
5	G	378[B]	BCL	CHA-C1A-NA	-2.90	119.76	126.40
5	G	372	BCL	C4B-CHC-C1C	-2.90	124.38	130.12
5	E	378[B]	BCL	O2A-CGA-O1A	-2.89	116.09	123.30
5	F	378[B]	BCL	CHA-C1A-NA	-2.89	119.78	126.40
5	a	808	BCL	C11-C10-C8	-2.89	106.59	115.92
5	F	372	BCL	C4B-CHC-C1C	-2.88	124.41	130.12
5	A	811	BCL	CHA-C1A-NA	-2.88	119.80	126.40
5	G	378[B]	BCL	C2C-C3C-C4C	-2.88	97.02	101.34
5	E	375	BCL	C11-C10-C8	-2.88	106.61	115.92
5	A	814	BCL	O2A-CGA-O1A	-2.88	116.12	123.30
5	F	375	BCL	C11-C10-C8	-2.88	106.62	115.92
5	A	808	BCL	C11-C10-C8	-2.88	106.62	115.92
5	a	811	BCL	CHA-C1A-NA	-2.88	119.81	126.40
5	G	375	BCL	C11-C10-C8	-2.88	106.62	115.92
5	F	378[B]	BCL	C2C-C3C-C4C	-2.87	97.04	101.34
5	a	811	BCL	C7-C6-C5	-2.87	105.57	113.36
5	E	375	BCL	C7-C6-C5	-2.87	105.57	113.36
5	E	378[B]	BCL	CHA-C1A-NA	-2.86	119.84	126.40
5	F	375	BCL	C7-C6-C5	-2.86	105.59	113.36
5	A	807	BCL	C4B-CHC-C1C	-2.86	124.45	130.12
5	G	375	BCL	C7-C6-C5	-2.86	105.59	113.36
5	A	811	BCL	C7-C6-C5	-2.85	105.62	113.36
5	F	375	BCL	CHA-C1A-NA	-2.85	119.88	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	815	BCL	CMA-C3A-C4A	-2.84	104.14	111.77
5	a	815	BCL	CHA-C1A-NA	-2.83	119.91	126.40
5	G	374	BCL	C11-C10-C8	-2.83	106.77	115.92
5	G	377	BCL	CHA-C1A-NA	-2.83	119.92	126.40
5	a	815	BCL	CMA-C3A-C4A	-2.83	104.17	111.77
5	E	374	BCL	C11-C10-C8	-2.83	106.78	115.92
5	A	815	BCL	CHA-C1A-NA	-2.83	119.93	126.40
5	E	375	BCL	O2A-CGA-O1A	-2.82	116.46	123.59
5	E	375	BCL	C4B-CHC-C1C	-2.82	124.53	130.12
5	G	375	BCL	CHA-C1A-NA	-2.82	119.94	126.40
5	E	377	BCL	C7-C6-C5	-2.81	105.72	113.36
5	F	375	BCL	C4B-CHC-C1C	-2.81	124.55	130.12
5	F	375	BCL	O2A-CGA-O1A	-2.81	116.50	123.59
5	F	374	BCL	C11-C10-C8	-2.81	106.84	115.92
5	A	811	BCL	C4B-CHC-C1C	-2.80	124.57	130.12
5	E	377	BCL	CHA-C1A-NA	-2.80	119.99	126.40
5	E	375	BCL	CHA-C1A-NA	-2.80	119.99	126.40
5	F	377	BCL	CHA-C1A-NA	-2.80	119.99	126.40
5	G	375	BCL	C4B-CHC-C1C	-2.80	124.58	130.12
5	A	807	BCL	CHA-C1A-NA	-2.79	120.01	126.40
5	a	807	BCL	CHA-C1A-NA	-2.79	120.01	126.40
5	G	377	BCL	C7-C6-C5	-2.79	105.78	113.36
5	a	811	BCL	C4B-CHC-C1C	-2.79	124.59	130.12
13	a	802	G2O	O2D-CGD-O1D	-2.79	118.39	123.84
5	F	377	BCL	C7-C6-C5	-2.78	105.80	113.36
5	F	378[B]	BCL	CGD-CBD-CAD	-2.78	101.72	110.73
5	G	375	BCL	O2A-CGA-O1A	-2.78	116.57	123.59
5	A	815	BCL	CGD-CBD-CAD	-2.78	101.73	110.73
5	a	808	BCL	CMC-C2C-C3C	-2.78	102.63	113.83
7	A	801	GS0	C3D-C2D-C1D	-2.77	102.05	105.83
5	a	815	BCL	CGD-CBD-CAD	-2.77	101.75	110.73
5	F	377	BCL	C4B-CHC-C1C	-2.77	124.63	130.12
5	A	808	BCL	CMC-C2C-C3C	-2.77	102.65	113.83
5	F	377	BCL	CMC-C2C-C3C	-2.77	102.65	113.83
5	F	376	BCL	CHA-C1A-NA	-2.77	120.05	126.40
10	a	818	LHG	O8-C23-C24	2.77	120.60	111.91
5	E	377	BCL	CMC-C2C-C3C	-2.77	102.67	113.83
5	G	377	BCL	C4B-CHC-C1C	-2.77	124.64	130.12
7	a	801	GS0	C3D-C2D-C1D	-2.76	102.06	105.83
5	G	378[B]	BCL	CGD-CBD-CAD	-2.76	101.79	110.73
5	A	804	BCL	C4B-CHC-C1C	-2.76	124.65	130.12
5	A	808	BCL	C7-C6-C5	-2.76	105.86	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	818	LHG	O8-C23-C24	2.76	120.57	111.91
5	G	376	BCL	CHA-C1A-NA	-2.76	120.09	126.40
5	E	378[B]	BCL	CGD-CBD-CAD	-2.75	101.81	110.73
5	A	814	BCL	CMA-C3A-C4A	-2.75	104.37	111.77
5	a	814	BCL	CMA-C3A-C4A	-2.75	104.37	111.77
5	a	808	BCL	C7-C6-C5	-2.75	105.88	113.36
5	G	377	BCL	CMC-C2C-C3C	-2.75	102.72	113.83
7	a	801	GS0	O2A-CGA-O1A	-2.75	116.65	123.59
5	A	815	BCL	O2A-CGA-O1A	-2.75	116.44	123.30
5	E	375	BCL	CMC-C2C-C3C	-2.75	102.73	113.83
7	A	801	GS0	O2A-CGA-O1A	-2.75	116.65	123.59
5	F	376	BCL	CMC-C2C-C3C	-2.75	102.74	113.83
5	E	376	BCL	CHA-C1A-NA	-2.75	120.11	126.40
5	G	376	BCL	CMC-C2C-C3C	-2.75	102.75	113.83
13	A	802	G2O	O2D-CGD-O1D	-2.74	118.48	123.84
5	G	375	BCL	CMC-C2C-C3C	-2.74	102.78	113.83
5	E	376	BCL	CMC-C2C-C3C	-2.74	102.78	113.83
5	a	815	BCL	C2C-C3C-C4C	-2.74	97.24	101.34
5	A	804	BCL	O2A-CGA-O1A	-2.74	116.47	123.30
5	F	375	BCL	CMC-C2C-C3C	-2.74	102.79	113.83
5	a	815	BCL	O2A-CGA-O1A	-2.73	116.48	123.30
5	A	808	BCL	O2A-CGA-O1A	-2.73	116.69	123.59
5	a	808	BCL	O2A-CGA-O1A	-2.73	116.69	123.59
5	F	371	BCL	CMC-C2C-C3C	-2.73	102.81	113.83
5	a	813	BCL	CHA-C1A-NA	-2.73	120.15	126.40
5	a	804	BCL	C4B-CHC-C1C	-2.73	124.71	130.12
5	E	371	BCL	CMC-C2C-C3C	-2.73	102.82	113.83
5	E	377	BCL	C4B-CHC-C1C	-2.73	124.72	130.12
5	a	804	BCL	O2A-CGA-O1A	-2.73	116.51	123.30
5	F	377	BCL	O2A-CGA-O1A	-2.72	116.72	123.59
5	A	810	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
5	G	371	BCL	CMC-C2C-C3C	-2.72	102.86	113.83
5	A	815	BCL	C2C-C3C-C4C	-2.72	97.27	101.34
5	a	804	BCL	CMA-C3A-C4A	-2.72	104.47	111.77
5	a	810	BCL	CMA-C3A-C4A	-2.72	104.47	111.77
8	A	816	F26	C27-C28-C31	-2.71	118.79	126.42
5	G	372	BCL	C11-C12-C13	-2.71	107.16	115.92
5	a	807	BCL	O2A-CGA-O1A	-2.71	116.55	123.30
5	A	804	BCL	CMA-C3A-C4A	-2.71	104.49	111.77
5	A	813	BCL	CHA-C1A-NA	-2.71	120.19	126.40
5	E	372	BCL	C11-C12-C13	-2.71	107.17	115.92
5	E	377	BCL	O2A-CGA-O1A	-2.70	116.77	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	371	BCL	C11-C10-C8	-2.70	107.19	115.92
5	a	814	BCL	CMC-C2C-C3C	-2.70	102.93	113.83
5	G	377	BCL	O2A-CGA-O1A	-2.70	116.78	123.59
5	A	807	BCL	O2A-CGA-O1A	-2.70	116.57	123.30
5	A	814	BCL	CMC-C2C-C3C	-2.70	102.94	113.83
5	E	371	BCL	C11-C10-C8	-2.70	107.20	115.92
8	a	816	F26	C27-C28-C31	-2.70	118.84	126.42
5	A	805	BCL	O2A-CGA-O1A	-2.70	116.79	123.59
5	a	805	BCL	O2A-CGA-O1A	-2.70	116.79	123.59
5	a	808	BCL	C11-C12-C13	-2.69	107.21	115.92
5	a	805	BCL	CMA-C3A-C4A	-2.69	104.53	111.77
7	A	801	GS0	CMC-C2C-C3C	-2.69	102.97	113.83
5	A	804	BCL	CMC-C2C-C3C	-2.69	102.97	113.83
5	G	371	BCL	C11-C10-C8	-2.69	107.22	115.92
5	F	372	BCL	C11-C12-C13	-2.69	107.22	115.92
5	A	809	BCL	C4A-NA-C1A	-2.69	105.50	106.71
5	a	804	BCL	CMC-C2C-C3C	-2.69	102.97	113.83
5	a	806	BCL	CMA-C3A-C4A	-2.69	104.54	111.77
7	a	801	GS0	CMC-C2C-C3C	-2.69	102.98	113.83
5	A	806	BCL	CMA-C3A-C4A	-2.69	104.55	111.77
5	A	807	BCL	CMC-C2C-C3C	-2.69	102.99	113.83
5	a	806	BCL	C4B-CHC-C1C	-2.69	124.80	130.12
5	F	374	BCL	CMC-C2C-C3C	-2.68	103.01	113.83
13	a	802	G2O	CMD-C2D-C1D	-2.68	124.34	128.46
5	A	805	BCL	C4A-NA-C1A	-2.68	105.50	106.71
5	a	807	BCL	CMC-C2C-C3C	-2.68	103.02	113.83
5	E	375	BCL	C1C-NC-C4C	-2.68	105.50	106.71
5	E	374	BCL	CMC-C2C-C3C	-2.68	103.03	113.83
5	G	374	BCL	CMC-C2C-C3C	-2.68	103.03	113.83
13	A	802	G2O	CMD-C2D-C1D	-2.68	124.35	128.46
5	A	808	BCL	C11-C12-C13	-2.67	107.28	115.92
5	a	815	BCL	CMC-C2C-C3C	-2.67	103.05	113.83
5	A	805	BCL	CMA-C3A-C4A	-2.67	104.59	111.77
5	F	372	BCL	O2A-CGA-O1A	-2.67	116.85	123.59
5	A	813	BCL	O2A-CGA-O1A	-2.67	116.66	123.30
5	A	815	BCL	CMC-C2C-C3C	-2.66	103.09	113.83
5	G	375	BCL	CMA-C3A-C4A	-2.66	104.63	111.77
5	F	373	BCL	CMA-C3A-C4A	-2.66	104.63	111.77
5	E	373	BCL	CMA-C3A-C4A	-2.66	104.63	111.77
5	a	806	BCL	C11-C12-C13	-2.65	107.34	115.92
5	A	811	BCL	CMA-C3A-C4A	-2.65	104.65	111.77
5	a	811	BCL	CMC-C2C-C3C	-2.65	103.14	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	810	BCL	C2C-C3C-C4C	-2.65	97.37	101.34
5	A	806	BCL	C11-C12-C13	-2.65	107.36	115.92
5	E	376	BCL	CMA-C3A-C4A	-2.65	104.65	111.77
5	G	376	BCL	CMA-C3A-C4A	-2.65	104.65	111.77
5	E	375	BCL	CMA-C3A-C4A	-2.65	104.65	111.77
5	a	811	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
5	A	811	BCL	CMC-C2C-C3C	-2.65	103.15	113.83
5	A	806	BCL	C4B-CHC-C1C	-2.65	124.88	130.12
5	G	372	BCL	O2A-CGA-O1A	-2.65	116.91	123.59
5	F	376	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
5	F	375	BCL	CMA-C3A-C4A	-2.64	104.67	111.77
5	A	813	BCL	C4B-CHC-C1C	-2.64	124.88	130.12
5	G	375	BCL	C1C-NC-C4C	-2.64	105.52	106.71
5	E	372	BCL	O2A-CGA-O1A	-2.64	116.93	123.59
5	a	805	BCL	CMC-C2C-C3C	-2.64	103.18	113.83
5	A	814	BCL	C4A-NA-C1A	-2.64	105.52	106.71
5	G	373	BCL	CMA-C3A-C4A	-2.64	104.69	111.77
5	G	378[B]	BCL	CMC-C2C-C3C	-2.63	103.20	113.83
5	a	810	BCL	CMC-C2C-C3C	-2.63	103.20	113.83
5	a	813	BCL	O2A-CGA-O1A	-2.63	116.74	123.30
5	A	805	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
5	a	813	BCL	C4B-CHC-C1C	-2.63	124.91	130.12
5	A	810	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
5	F	378[B]	BCL	CMC-C2C-C3C	-2.63	103.24	113.83
5	E	377	BCL	CMA-C3A-C4A	-2.62	104.72	111.77
5	A	811	BCL	C11-C12-C13	-2.62	107.44	115.92
9	A	817	F39	O6-C21-C22	2.62	120.12	111.91
5	a	811	BCL	C11-C12-C13	-2.62	107.46	115.92
5	A	812	BCL	CMC-C2C-C3C	-2.62	103.28	113.83
5	E	378[B]	BCL	CMC-C2C-C3C	-2.62	103.28	113.83
9	a	817	F39	O6-C21-C22	2.61	120.11	111.91
5	a	812	BCL	CMC-C2C-C3C	-2.61	103.29	113.83
5	F	377	BCL	CMA-C3A-C4A	-2.61	104.76	111.77
5	a	809	BCL	C4A-NA-C1A	-2.61	105.53	106.71
5	G	377	BCL	CMA-C3A-C4A	-2.61	104.77	111.77
5	F	375	BCL	C1C-NC-C4C	-2.60	105.53	106.71
5	A	810	BCL	C2C-C3C-C4C	-2.60	97.44	101.34
5	E	372	BCL	CMA-C3A-C4A	-2.60	104.79	111.77
5	a	815	BCL	OBD-CAD-CBD	-2.60	122.19	125.89
5	G	371	BCL	CMD-C2D-C3D	2.60	129.53	124.68
5	a	808	BCL	C4B-CHC-C1C	-2.59	124.99	130.12
5	F	371	BCL	CMD-C2D-C3D	2.58	129.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	372	BCL	CMA-C3A-C4A	-2.58	104.83	111.77
5	a	814	BCL	C4A-NA-C1A	-2.58	105.55	106.71
5	F	372	BCL	CMA-C3A-C4A	-2.58	104.85	111.77
5	A	815	BCL	OBD-CAD-CBD	-2.58	122.22	125.89
5	E	371	BCL	CMD-C2D-C3D	2.58	129.50	124.68
5	A	809	BCL	CMC-C2C-C3C	-2.57	103.47	113.83
5	F	372	BCL	CMC-C2C-C3C	-2.57	103.47	113.83
5	F	378[B]	BCL	CMA-C3A-C4A	-2.57	104.88	111.77
5	a	810	BCL	C4B-CHC-C1C	-2.57	125.03	130.12
5	a	813	BCL	CMA-C3A-C4A	-2.57	104.88	111.77
5	F	372	BCL	OBD-CAD-CBD	-2.56	122.23	125.89
5	G	378[B]	BCL	CMA-C3A-C4A	-2.56	104.89	111.77
5	G	372	BCL	CMC-C2C-C3C	-2.56	103.50	113.83
5	A	808	BCL	C4B-CHC-C1C	-2.56	125.05	130.12
5	F	373	BCL	C2A-C1A-CHA	2.56	128.33	123.86
5	a	809	BCL	CMC-C2C-C3C	-2.55	103.53	113.83
5	E	372	BCL	CMC-C2C-C3C	-2.55	103.53	113.83
5	E	378[B]	BCL	CMA-C3A-C4A	-2.55	104.92	111.77
5	E	378[B]	BCL	OBD-CAD-CBD	-2.55	122.25	125.89
5	A	813	BCL	CMA-C3A-C4A	-2.55	104.93	111.77
5	G	372	BCL	OBD-CAD-CBD	-2.54	122.26	125.89
5	G	373	BCL	C2A-C1A-CHA	2.54	128.31	123.86
5	a	809	BCL	CMA-C3A-C4A	-2.54	104.94	111.77
5	G	375	BCL	C11-C12-C13	-2.54	107.71	115.92
5	E	375	BCL	C11-C12-C13	-2.54	107.71	115.92
5	A	809	BCL	CMA-C3A-C4A	-2.54	104.95	111.77
5	F	378[B]	BCL	OBD-CAD-CBD	-2.54	122.27	125.89
5	F	375	BCL	C11-C12-C13	-2.53	107.73	115.92
5	a	808	BCL	C3C-C2C-C1C	2.53	105.96	101.87
7	A	801	GS0	C11-C12-C13	-2.53	107.75	115.92
5	A	808	BCL	C3C-C2C-C1C	2.52	105.95	101.87
5	E	372	BCL	OBD-CAD-CBD	-2.52	122.29	125.89
7	a	801	GS0	C11-C12-C13	-2.52	107.76	115.92
5	A	810	BCL	C4B-CHC-C1C	-2.52	125.12	130.12
5	a	804	BCL	C2A-C3A-C4A	-2.52	97.80	101.87
5	A	813	BCL	CMC-C2C-C3C	-2.52	103.67	113.83
5	E	373	BCL	C2A-C1A-CHA	2.52	128.26	123.86
5	G	376	BCL	C11-C12-C13	-2.52	107.78	115.92
13	A	802	G2O	CMD-C2D-C3D	2.51	129.38	124.68
5	G	378[B]	BCL	OBD-CAD-CBD	-2.51	122.31	125.89
5	A	804	BCL	C2A-C3A-C4A	-2.51	97.81	101.87
5	a	804	BCL	OBD-CAD-CBD	-2.51	122.31	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	802	G2O	CMD-C2D-C3D	2.51	129.37	124.68
5	A	812	BCL	OBD-CAD-CBD	-2.51	122.31	125.89
5	a	813	BCL	CMC-C2C-C3C	-2.51	103.71	113.83
5	F	376	BCL	C11-C12-C13	-2.51	107.82	115.92
5	a	804	BCL	C1C-NC-C4C	-2.50	105.58	106.71
5	E	373	BCL	CGD-CBD-CAD	-2.50	102.63	110.73
5	E	377	BCL	C11-C12-C13	-2.50	107.83	115.92
5	G	377	BCL	C11-C12-C13	-2.50	107.83	115.92
10	a	818	LHG	C11-C10-C9	-2.50	101.73	114.42
5	G	373	BCL	CGD-CBD-CAD	-2.50	102.64	110.73
5	F	373	BCL	CGD-CBD-CAD	-2.50	102.64	110.73
13	A	803	G2O	CMD-C2D-C1D	-2.50	124.63	128.46
10	A	818	LHG	C11-C10-C9	-2.50	101.75	114.42
5	E	376	BCL	C11-C12-C13	-2.49	107.86	115.92
5	a	812	BCL	CMA-C3A-C4A	-2.49	105.08	111.77
5	E	371	BCL	CGD-CBD-CAD	-2.49	102.67	110.73
5	A	810	BCL	C4C-CHD-C1D	-2.49	122.21	125.88
5	F	377	BCL	C11-C12-C13	-2.49	107.88	115.92
5	A	812	BCL	CMA-C3A-C4A	-2.49	105.09	111.77
5	a	810	BCL	C4C-CHD-C1D	-2.49	122.21	125.88
5	a	811	BCL	C1B-CHB-C4A	-2.48	125.20	130.12
5	F	371	BCL	CGD-CBD-CAD	-2.48	102.69	110.73
5	E	374	BCL	CMA-C3A-C4A	-2.48	105.11	111.77
7	a	801	GS0	CMA-C3A-C4A	-2.48	105.11	111.77
5	G	375	BCL	C3C-C2C-C1C	2.48	105.87	101.87
5	F	373	BCL	OBD-CAD-CBD	-2.47	122.36	125.89
5	a	805	BCL	C4A-NA-C1A	-2.47	105.59	106.71
13	a	803	G2O	CMD-C2D-C1D	-2.47	124.67	128.46
5	F	374	BCL	CMA-C3A-C4A	-2.47	105.14	111.77
5	G	374	BCL	CMA-C3A-C4A	-2.47	105.14	111.77
5	G	371	BCL	CGD-CBD-CAD	-2.47	102.74	110.73
5	a	812	BCL	C4C-CHD-C1D	-2.47	122.24	125.88
5	a	812	BCL	OBD-CAD-CBD	-2.47	122.37	125.89
7	A	801	GS0	CMA-C3A-C4A	-2.46	105.15	111.77
5	a	806	BCL	C3C-C2C-C1C	2.46	105.85	101.87
5	A	804	BCL	OBD-CAD-CBD	-2.46	122.38	125.89
5	F	373	BCL	CMD-C2D-C3D	2.46	129.29	124.68
13	A	803	G2O	CHB-C4A-NA	2.46	127.81	125.08
5	A	806	BCL	C4C-CHD-C1D	-2.46	122.25	125.88
5	E	373	BCL	CMD-C2D-C3D	2.46	129.28	124.68
5	a	806	BCL	C4C-CHD-C1D	-2.46	122.26	125.88
5	a	809	BCL	OBD-CAD-CBD	-2.46	122.39	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	813	BCL	C2C-C3C-C4C	-2.45	97.67	101.34
5	G	373	BCL	CMD-C2D-C3D	2.45	129.27	124.68
5	E	375	BCL	C3C-C2C-C1C	2.45	105.83	101.87
5	A	811	BCL	C1B-CHB-C4A	-2.45	125.27	130.12
5	A	804	BCL	C1C-NC-C4C	-2.45	105.61	106.71
13	a	803	G2O	CHB-C4A-NA	2.45	127.79	125.08
5	F	375	BCL	C3C-C2C-C1C	2.44	105.82	101.87
5	G	373	BCL	OBD-CAD-CBD	-2.44	122.40	125.89
5	A	812	BCL	C4C-CHD-C1D	-2.44	122.28	125.88
5	A	806	BCL	C3C-C2C-C1C	2.44	105.81	101.87
5	A	806	BCL	CGD-CBD-CAD	-2.44	102.83	110.73
5	E	372	BCL	CGD-CBD-CAD	-2.44	102.83	110.73
5	A	807	BCL	C3D-CAD-CBD	-2.44	104.39	107.61
5	E	373	BCL	OBD-CAD-CBD	-2.44	122.42	125.89
5	F	371	BCL	C3C-C2C-C1C	2.43	105.80	101.87
5	a	812	BCL	CMD-C2D-C3D	2.43	129.23	124.68
5	G	374	BCL	C11-C12-C13	-2.43	108.06	115.92
5	A	809	BCL	OBD-CAD-CBD	-2.43	122.42	125.89
5	a	806	BCL	CGD-CBD-CAD	-2.43	102.87	110.73
5	G	376	BCL	CMD-C2D-C3D	2.43	129.22	124.68
11	A	819	LMG	O3-C3-C2	-2.42	104.75	110.35
5	E	374	BCL	C11-C12-C13	-2.42	108.09	115.92
5	G	371	BCL	C3C-C2C-C1C	2.42	105.78	101.87
5	E	374	BCL	OBD-CAD-CBD	-2.42	122.44	125.89
5	G	372	BCL	CGD-CBD-CAD	-2.42	102.89	110.73
5	F	376	BCL	CMD-C2D-C3D	2.42	129.21	124.68
5	F	374	BCL	C11-C12-C13	-2.42	108.10	115.92
5	A	812	BCL	CMD-C2D-C3D	2.42	129.20	124.68
5	a	807	BCL	C3D-CAD-CBD	-2.42	104.42	107.61
5	F	372	BCL	CGD-CBD-CAD	-2.42	102.91	110.73
5	E	375	BCL	OBD-CAD-CBD	-2.41	122.45	125.89
11	a	819	LMG	O3-C3-C2	-2.41	104.78	110.35
5	E	371	BCL	C4C-CHD-C1D	-2.40	122.33	125.88
7	a	801	GS0	C3C-C2C-C1C	2.40	105.75	101.87
5	G	377	BCL	OBD-CAD-CBD	-2.40	122.47	125.89
10	A	818	LHG	C20-C19-C18	-2.40	102.24	114.42
5	a	812	BCL	C11-C10-C8	-2.40	108.17	115.92
10	a	818	LHG	C20-C19-C18	-2.40	102.26	114.42
5	A	812	BCL	C11-C10-C8	-2.40	108.17	115.92
5	F	374	BCL	CMD-C2D-C3D	2.40	129.16	124.68
5	a	808	BCL	OBD-CAD-CBD	-2.39	122.48	125.89
5	E	376	BCL	CMD-C2D-C3D	2.39	129.15	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	808	BCL	OBD-CAD-CBD	-2.39	122.48	125.89
5	E	371	BCL	C3C-C2C-C1C	2.39	105.73	101.87
7	A	801	GS0	C3C-C2C-C1C	2.39	105.73	101.87
5	E	377	BCL	CMD-C2D-C3D	2.39	129.15	124.68
11	A	819	LMG	C6-C5-C4	-2.39	107.41	113.00
5	A	806	BCL	OBD-CAD-CBD	-2.39	122.48	125.89
5	a	814	BCL	OBD-CAD-CBD	-2.39	122.48	125.89
5	G	377	BCL	CMD-C2D-C3D	2.39	129.14	124.68
5	a	805	BCL	OBD-CAD-CBD	-2.38	122.49	125.89
5	G	375	BCL	OBD-CAD-CBD	-2.38	122.49	125.89
5	a	806	BCL	OBD-CAD-CBD	-2.38	122.49	125.89
5	a	813	BCL	C2C-C3C-C4C	-2.38	97.77	101.34
11	a	819	LMG	C6-C5-C4	-2.38	107.43	113.00
5	F	377	BCL	CMD-C2D-C3D	2.38	129.13	124.68
5	G	374	BCL	OBD-CAD-CBD	-2.38	122.50	125.89
5	F	371	BCL	C4C-CHD-C1D	-2.38	122.37	125.88
5	A	811	BCL	CMD-C2D-C3D	2.38	129.13	124.68
5	F	377	BCL	OBD-CAD-CBD	-2.38	122.50	125.89
5	F	375	BCL	OBD-CAD-CBD	-2.38	122.50	125.89
5	A	814	BCL	OBD-CAD-CBD	-2.38	122.50	125.89
5	A	811	BCL	CHC-C1C-NC	2.38	127.80	124.51
5	a	813	BCL	OBD-CAD-CBD	-2.38	122.50	125.89
5	a	811	BCL	CMD-C2D-C3D	2.37	129.12	124.68
5	E	374	BCL	CMD-C2D-C3D	2.37	129.12	124.68
13	A	802	G2O	CHB-C4A-NA	2.37	127.71	125.08
5	A	805	BCL	OBD-CAD-CBD	-2.37	122.51	125.89
5	a	812	BCL	C3D-CAD-CBD	-2.37	104.49	107.61
8	a	816	F26	C23-C19-C24	-2.37	119.61	122.92
5	G	377	BCL	C4A-NA-C1A	-2.36	105.64	106.71
8	A	816	F26	C23-C19-C24	-2.36	119.61	122.92
5	G	374	BCL	CMD-C2D-C3D	2.36	129.10	124.68
7	A	801	GS0	CBB-CAB-C3B	2.36	127.34	120.34
5	G	371	BCL	C4C-CHD-C1D	-2.36	122.40	125.88
5	a	811	BCL	CHC-C1C-NC	2.36	127.77	124.51
7	a	801	GS0	CBB-CAB-C3B	2.36	127.33	120.34
5	E	371	BCL	C11-C12-C13	-2.35	108.31	115.92
5	A	811	BCL	OBD-CAD-CBD	-2.35	122.53	125.89
5	G	371	BCL	C11-C12-C13	-2.35	108.31	115.92
5	F	374	BCL	OBD-CAD-CBD	-2.35	122.53	125.89
5	A	813	BCL	OBD-CAD-CBD	-2.35	122.53	125.89
5	A	804	BCL	C4A-NA-C1A	-2.35	105.65	106.71
5	F	371	BCL	C11-C12-C13	-2.35	108.32	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	377	BCL	C3C-C2C-C1C	2.35	105.66	101.87
5	F	373	BCL	CMC-C2C-C3C	-2.35	104.36	113.83
5	A	815	BCL	CMD-C2D-C3D	2.34	129.06	124.68
13	A	803	G2O	CMD-C2D-C3D	2.34	129.06	124.68
5	G	373	BCL	CMC-C2C-C3C	-2.34	104.38	113.83
5	A	813	BCL	CMD-C2D-C3D	2.34	129.06	124.68
5	a	813	BCL	CMD-C2D-C3D	2.34	129.06	124.68
5	E	373	BCL	CMC-C2C-C3C	-2.34	104.38	113.83
13	a	803	G2O	CMD-C2D-C3D	2.34	129.05	124.68
5	F	377	BCL	C3C-C2C-C1C	2.33	105.64	101.87
5	a	811	BCL	OBD-CAD-CBD	-2.33	122.57	125.89
5	a	804	BCL	CMD-C2D-C3D	2.33	129.03	124.68
5	E	377	BCL	C3C-C2C-C1C	2.33	105.63	101.87
5	a	815	BCL	CMD-C2D-C3D	2.33	129.03	124.68
5	F	373	BCL	C11-C12-C13	-2.32	108.42	115.92
5	A	812	BCL	C3D-CAD-CBD	-2.32	104.55	107.61
5	F	376	BCL	OBD-CAD-CBD	-2.32	122.58	125.89
5	E	377	BCL	OBD-CAD-CBD	-2.32	122.58	125.89
5	A	804	BCL	CMD-C2D-C3D	2.32	129.02	124.68
5	a	807	BCL	CMD-C2D-C3D	2.32	129.02	124.68
13	A	802	G2O	CHB-C1B-NB	2.31	126.58	124.45
5	G	373	BCL	C11-C12-C13	-2.31	108.44	115.92
5	E	373	BCL	C4C-CHD-C1D	-2.31	122.47	125.88
5	E	373	BCL	C11-C12-C13	-2.31	108.45	115.92
5	A	812	BCL	C12-C11-C10	-2.31	102.63	113.24
5	a	812	BCL	C12-C11-C10	-2.31	102.64	113.24
5	G	376	BCL	OBD-CAD-CBD	-2.30	122.60	125.89
5	F	375	BCL	CGD-CBD-CAD	-2.30	103.28	110.73
5	E	376	BCL	OBD-CAD-CBD	-2.30	122.61	125.89
5	G	376	BCL	CBB-CAB-C3B	2.29	127.15	120.34
5	G	376	BCL	C12-C11-C10	-2.29	102.70	113.24
5	G	376	BCL	CHC-C1C-NC	2.29	127.68	124.51
5	G	375	BCL	CGD-CBD-CAD	-2.29	103.31	110.73
5	E	375	BCL	CGD-CBD-CAD	-2.29	103.31	110.73
5	A	807	BCL	CMD-C2D-C3D	2.29	128.97	124.68
5	a	808	BCL	CMD-C2D-C3D	2.29	128.96	124.68
5	E	376	BCL	C12-C11-C10	-2.29	102.73	113.24
5	E	376	BCL	CBB-CAB-C3B	2.29	127.13	120.34
13	a	802	G2O	CHB-C4A-NA	2.29	127.62	125.08
8	a	816	F26	C2-C9-C15	-2.29	123.48	128.63
5	A	815	BCL	CBB-CAB-C3B	2.29	127.13	120.34
5	a	815	BCL	CBB-CAB-C3B	2.28	127.12	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	807	BCL	CHC-C1C-NC	2.28	127.67	124.51
5	a	804	BCL	C4A-NA-C1A	-2.28	105.68	106.71
5	F	376	BCL	C12-C11-C10	-2.28	102.76	113.24
5	F	376	BCL	CBB-CAB-C3B	2.28	127.11	120.34
13	A	803	G2O	CHB-C1B-NB	2.28	126.55	124.45
5	G	375	BCL	CMD-C2D-C3D	2.28	128.94	124.68
5	G	377	BCL	CBB-CAB-C3B	2.28	127.10	120.34
5	E	376	BCL	CHC-C1C-NC	2.28	127.66	124.51
5	A	808	BCL	CMD-C2D-C3D	2.28	128.94	124.68
8	A	816	F26	C2-C9-C15	-2.27	123.50	128.63
5	A	805	BCL	CBB-CAB-C3B	2.27	127.09	120.34
5	G	373	BCL	C4C-CHD-C1D	-2.27	122.53	125.88
5	a	809	BCL	CMD-C2D-C3D	2.27	128.93	124.68
5	A	805	BCL	CMD-C2D-C3D	2.27	128.93	124.68
5	F	377	BCL	CBB-CAB-C3B	2.27	127.09	120.34
5	G	378[B]	BCL	CBB-CAB-C3B	2.27	127.08	120.34
5	F	377	BCL	C4A-NA-C1A	-2.27	105.69	106.71
5	F	373	BCL	C4C-CHD-C1D	-2.27	122.53	125.88
7	a	801	GS0	CMD-C2D-C1D	2.27	128.71	124.71
5	F	375	BCL	CMD-C2D-C3D	2.27	128.92	124.68
5	G	372	BCL	CBB-CAB-C3B	2.27	127.07	120.34
5	E	375	BCL	CMD-C2D-C3D	2.26	128.91	124.68
5	F	378[B]	BCL	CBB-CAB-C3B	2.26	127.06	120.34
5	a	805	BCL	CBB-CAB-C3B	2.26	127.06	120.34
5	A	809	BCL	CMD-C2D-C3D	2.26	128.91	124.68
5	E	378[B]	BCL	CBB-CAB-C3B	2.26	127.06	120.34
7	A	801	GS0	CMD-C2D-C1D	2.26	128.70	124.71
5	E	372	BCL	CBB-CAB-C3B	2.26	127.06	120.34
5	E	377	BCL	CBB-CAB-C3B	2.26	127.05	120.34
5	E	378[B]	BCL	CMD-C2D-C3D	2.26	128.91	124.68
5	a	807	BCL	C4C-CHD-C1D	-2.26	122.55	125.88
5	A	806	BCL	C4A-NA-C1A	-2.26	105.69	106.71
5	a	806	BCL	C4A-NA-C1A	-2.26	105.69	106.71
5	a	811	BCL	C12-C11-C10	-2.26	102.87	113.24
5	F	378[B]	BCL	CMD-C2D-C3D	2.26	128.90	124.68
5	A	811	BCL	C12-C11-C10	-2.26	102.88	113.24
5	A	804	BCL	C3C-C2C-C1C	2.25	105.51	101.87
5	a	804	BCL	C3C-C2C-C1C	2.25	105.51	101.87
5	F	376	BCL	CHC-C1C-NC	2.25	127.63	124.51
5	a	809	BCL	C4C-CHD-C1D	-2.25	122.56	125.88
5	E	374	BCL	CBB-CAB-C3B	2.25	127.03	120.34
5	a	811	BCL	CBB-CAB-C3B	2.25	127.03	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	811	BCL	CBB-CAB-C3B	2.25	127.03	120.34
5	F	374	BCL	CBB-CAB-C3B	2.25	127.02	120.34
5	F	372	BCL	CBB-CAB-C3B	2.25	127.01	120.34
5	A	805	BCL	CHC-C1C-NC	2.25	127.62	124.51
5	G	377	BCL	C12-C11-C10	-2.24	102.93	113.24
13	a	803	G2O	CHB-C1B-NB	2.24	126.52	124.45
5	G	378[B]	BCL	CMD-C2D-C3D	2.24	128.87	124.68
5	F	377	BCL	C12-C11-C10	-2.24	102.94	113.24
5	G	371	BCL	CBB-CAB-C3B	2.24	126.99	120.34
5	G	374	BCL	CBB-CAB-C3B	2.24	126.99	120.34
5	A	806	BCL	CMD-C2D-C3D	2.24	128.87	124.68
5	E	377	BCL	C12-C11-C10	-2.24	102.97	113.24
5	A	809	BCL	C4C-CHD-C1D	-2.23	122.58	125.88
10	A	818	LHG	C18-C17-C16	-2.23	103.08	114.42
10	a	818	LHG	C18-C17-C16	-2.23	103.08	114.42
5	a	814	BCL	CMD-C2D-C3D	2.23	128.85	124.68
5	F	371	BCL	CBB-CAB-C3B	2.23	126.96	120.34
5	A	814	BCL	CBB-CAB-C3B	2.23	126.96	120.34
5	a	814	BCL	CBB-CAB-C3B	2.23	126.95	120.34
5	E	374	BCL	C12-C11-C10	-2.23	103.01	113.24
5	a	805	BCL	CMD-C2D-C3D	2.22	128.84	124.68
5	F	375	BCL	CBB-CAB-C3B	2.22	126.94	120.34
5	G	375	BCL	CBB-CAB-C3B	2.22	126.94	120.34
5	G	374	BCL	C12-C11-C10	-2.22	103.03	113.24
5	a	806	BCL	CMD-C2D-C3D	2.22	128.83	124.68
5	a	810	BCL	CMD-C2D-C3D	2.22	128.83	124.68
13	a	803	G2O	O2A-CGA-O1A	-2.22	117.99	123.59
13	A	803	G2O	O2A-CGA-O1A	-2.22	117.99	123.59
5	E	371	BCL	CBB-CAB-C3B	2.22	126.93	120.34
5	F	374	BCL	C12-C11-C10	-2.22	103.04	113.24
13	a	802	G2O	CHB-C1B-NB	2.22	126.49	124.45
5	a	808	BCL	CHC-C1C-NC	2.22	127.58	124.51
5	A	810	BCL	CMD-C2D-C3D	2.22	128.82	124.68
5	a	804	BCL	CGD-CBD-CAD	-2.21	103.57	110.73
5	F	371	BCL	OBD-CAD-CBD	-2.21	122.74	125.89
5	F	374	BCL	CGD-CBD-CAD	-2.21	103.58	110.73
5	A	814	BCL	CMD-C2D-C3D	2.21	128.81	124.68
5	E	372	BCL	CHC-C1C-NC	2.21	127.56	124.51
5	A	807	BCL	CHC-C1C-NC	2.21	127.56	124.51
5	A	804	BCL	CGD-CBD-CAD	-2.20	103.59	110.73
5	E	375	BCL	CBB-CAB-C3B	2.20	126.88	120.34
5	A	813	BCL	CGD-CBD-CAD	-2.20	103.60	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	813	BCL	CGD-CBD-CAD	-2.20	103.60	110.73
13	A	803	G2O	CAA-CBA-CGA	-2.20	106.82	113.25
5	E	376	BCL	C4C-CHD-C1D	-2.20	122.64	125.88
5	A	807	BCL	C4C-CHD-C1D	-2.20	122.64	125.88
13	a	803	G2O	CAA-CBA-CGA	-2.20	106.83	113.25
5	F	372	BCL	CMD-C2D-C3D	2.20	128.79	124.68
5	G	374	BCL	CGD-CBD-CAD	-2.19	103.63	110.73
5	A	812	BCL	C2A-C3A-C4A	-2.19	98.33	101.87
5	E	377	BCL	C4A-NA-C1A	-2.19	105.72	106.71
5	G	372	BCL	CHC-C1C-NC	2.19	127.54	124.51
5	E	374	BCL	CGD-CBD-CAD	-2.19	103.64	110.73
5	F	372	BCL	CHC-C1C-NC	2.19	127.54	124.51
5	a	807	BCL	C3C-C2C-C1C	2.19	105.40	101.87
5	a	805	BCL	CHC-C1C-NC	2.19	127.53	124.51
5	A	807	BCL	C3C-C2C-C1C	2.18	105.40	101.87
5	G	371	BCL	OBD-CAD-CBD	-2.18	122.78	125.89
8	A	816	F26	C23-C19-C15	2.18	121.51	118.08
5	F	376	BCL	C4C-CHD-C1D	-2.18	122.66	125.88
5	G	372	BCL	CMD-C2D-C3D	2.18	128.76	124.68
5	E	371	BCL	OBD-CAD-CBD	-2.18	122.78	125.89
5	F	372	BCL	C4C-CHD-C1D	-2.18	122.67	125.88
5	G	376	BCL	C4C-CHD-C1D	-2.18	122.67	125.88
5	a	810	BCL	C1B-CHB-C4A	-2.18	125.81	130.12
5	F	376	BCL	CGD-CBD-CAD	-2.18	103.69	110.73
5	G	372	BCL	C12-C11-C10	-2.17	103.28	113.24
5	G	376	BCL	CGD-CBD-CAD	-2.17	103.71	110.73
5	E	376	BCL	CGD-CBD-CAD	-2.17	103.72	110.73
5	F	372	BCL	C12-C11-C10	-2.16	103.30	113.24
5	A	810	BCL	C1B-CHB-C4A	-2.16	125.83	130.12
5	A	814	BCL	C3C-C2C-C1C	2.16	105.36	101.87
5	A	812	BCL	CHC-C1C-NC	2.16	127.50	124.51
5	A	811	BCL	C4C-CHD-C1D	-2.15	122.70	125.88
5	E	372	BCL	C12-C11-C10	-2.15	103.34	113.24
5	F	375	BCL	C2A-C3A-C4A	-2.15	98.39	101.87
5	a	809	BCL	C2A-C3A-C4A	-2.15	98.39	101.87
5	E	372	BCL	CMD-C2D-C3D	2.15	128.71	124.68
5	E	375	BCL	C2A-C3A-C4A	-2.15	98.39	101.87
8	a	816	F26	C23-C19-C15	2.15	121.47	118.08
5	a	812	BCL	C2A-C3A-C4A	-2.15	98.39	101.87
5	a	814	BCL	C3C-C2C-C1C	2.15	105.34	101.87
5	a	810	BCL	OBD-CAD-C3D	2.15	131.54	127.98
5	G	375	BCL	C2A-C3A-C4A	-2.15	98.40	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	811	BCL	C4C-CHD-C1D	-2.15	122.72	125.88
5	A	808	BCL	CHC-C1C-NC	2.15	127.48	124.51
5	A	809	BCL	C2A-C3A-C4A	-2.14	98.41	101.87
5	a	812	BCL	CHC-C1C-NC	2.14	127.47	124.51
5	G	372	BCL	C4C-CHD-C1D	-2.14	122.73	125.88
5	a	815	BCL	C4C-CHD-C1D	-2.13	122.73	125.88
5	A	810	BCL	OBD-CAD-C3D	2.13	131.52	127.98
5	A	804	BCL	CHC-C1C-NC	2.13	127.46	124.51
5	G	375	BCL	CHC-C1C-NC	2.13	127.45	124.51
5	a	809	BCL	CBB-CAB-C3B	2.13	126.66	120.34
5	F	375	BCL	CHC-C1C-NC	2.13	127.45	124.51
5	A	809	BCL	CBB-CAB-C3B	2.13	126.65	120.34
5	F	374	BCL	C2A-C1A-CHA	2.12	127.57	123.86
5	E	372	BCL	C4C-CHD-C1D	-2.12	122.75	125.88
5	A	805	BCL	C3C-C2C-C1C	2.12	105.29	101.87
5	A	806	BCL	C2A-C3A-C4A	-2.12	98.45	101.87
5	G	374	BCL	C2A-C1A-CHA	2.12	127.56	123.86
5	a	806	BCL	C2A-C3A-C4A	-2.11	98.46	101.87
5	A	806	BCL	C12-C11-C10	-2.11	103.55	113.24
5	a	806	BCL	C12-C11-C10	-2.11	103.56	113.24
5	E	377	BCL	C4C-CHD-C1D	-2.10	122.78	125.88
5	A	815	BCL	C4C-CHD-C1D	-2.10	122.78	125.88
5	E	375	BCL	CHC-C1C-NC	2.10	127.42	124.51
5	E	374	BCL	C2A-C1A-CHA	2.09	127.52	123.86
5	a	805	BCL	C4C-CHD-C1D	-2.09	122.79	125.88
5	G	374	BCL	C4C-CHD-C1D	-2.09	122.80	125.88
5	F	374	BCL	C4C-CHD-C1D	-2.09	122.80	125.88
5	A	805	BCL	C4C-CHD-C1D	-2.09	122.80	125.88
5	a	805	BCL	OBD-CAD-C3D	2.09	131.45	127.98
5	a	805	BCL	C3C-C2C-C1C	2.09	105.24	101.87
5	A	805	BCL	OBD-CAD-C3D	2.09	131.45	127.98
5	A	808	BCL	C1C-NC-C4C	-2.09	105.77	106.71
5	a	814	BCL	OBD-CAD-C3D	2.09	131.44	127.98
5	a	804	BCL	CHC-C1C-NC	2.08	127.39	124.51
5	A	807	BCL	CMA-C3A-C4A	-2.08	106.18	111.77
10	A	818	LHG	C27-C26-C25	-2.08	103.88	114.42
10	a	818	LHG	C27-C26-C25	-2.08	103.88	114.42
7	a	801	GS0	C4D-CHA-C1A	2.07	123.77	121.25
5	a	815	BCL	OBD-CAD-C3D	2.07	131.42	127.98
5	a	805	BCL	CGD-CBD-CAD	-2.06	104.05	110.73
5	A	805	BCL	CGD-CBD-CAD	-2.06	104.06	110.73
5	G	377	BCL	C4C-CHD-C1D	-2.06	122.84	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	807	BCL	CMA-C3A-C4A	-2.06	106.24	111.77
7	A	801	GS0	C12-C11-C10	-2.06	103.78	113.24
5	a	808	BCL	C4C-CHD-C1D	-2.06	122.85	125.88
5	F	377	BCL	C4C-CHD-C1D	-2.05	122.85	125.88
5	E	374	BCL	CHC-C1C-NC	2.05	127.35	124.51
7	a	801	GS0	C12-C11-C10	-2.05	103.80	113.24
5	A	808	BCL	C4C-CHD-C1D	-2.05	122.86	125.88
8	a	816	F26	C20-C16-C21	2.05	119.12	114.60
5	A	814	BCL	OBD-CAD-C3D	2.04	131.37	127.98
5	A	815	BCL	OBD-CAD-C3D	2.03	131.36	127.98
5	F	374	BCL	C2C-C3C-C4C	-2.03	98.29	101.34
5	F	378[B]	BCL	C2A-C1A-CHA	2.03	127.41	123.86
11	a	819	LMG	O3-C3-C4	-2.03	105.66	110.35
5	G	378[B]	BCL	C2A-C1A-CHA	2.03	127.41	123.86
8	A	816	F26	C20-C16-C21	2.03	119.08	114.60
7	A	801	GS0	C4D-CHA-C1A	2.02	123.71	121.25
5	A	812	BCL	OBD-CAD-C3D	2.02	131.34	127.98
11	A	819	LMG	O3-C3-C4	-2.02	105.67	110.35
5	E	374	BCL	C2C-C3C-C4C	-2.02	98.31	101.34
5	a	812	BCL	OBD-CAD-C3D	2.02	131.33	127.98
5	A	813	BCL	CHC-C1C-NC	2.02	127.30	124.51
5	E	374	BCL	C4C-CHD-C1D	-2.02	122.91	125.88
5	E	373	BCL	C12-C11-C10	-2.02	103.97	113.24
5	E	375	BCL	C12-C11-C10	-2.02	103.98	113.24
5	G	375	BCL	C12-C11-C10	-2.01	103.98	113.24
5	a	808	BCL	C12-C11-C10	-2.01	104.00	113.24
5	F	375	BCL	C12-C11-C10	-2.01	104.00	113.24
5	G	372	BCL	OBD-CAD-C3D	2.01	131.32	127.98
8	A	816	F26	C36-C31-C33	-2.01	120.11	122.92
5	F	375	BCL	C2A-C1A-CHA	2.01	127.37	123.86
8	A	816	F26	C40-C34-C35	2.01	121.24	118.08
5	G	374	BCL	C2C-C3C-C4C	-2.01	98.33	101.34
5	F	372	BCL	OBD-CAD-C3D	2.00	131.31	127.98
5	A	813	BCL	C2A-C3A-C4A	-2.00	98.63	101.87
5	E	373	BCL	OBD-CAD-C3D	2.00	131.31	127.98
5	A	814	BCL	C4C-CHD-C1D	-2.00	122.93	125.88
5	G	371	BCL	CHC-C1C-NC	2.00	127.28	124.51
5	E	371	BCL	C12-C11-C10	-2.00	104.04	113.24
5	F	373	BCL	OBD-CAD-C3D	2.00	131.31	127.98
5	a	813	BCL	C2A-C3A-C4A	-2.00	98.64	101.87
5	F	373	BCL	C12-C11-C10	-2.00	104.04	113.24
5	G	373	BCL	C12-C11-C10	-2.00	104.05	113.24

There are no chirality outliers.

All (785) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	371	BCL	C1A-C2A-CAA-CBA
5	E	371	BCL	C3A-C2A-CAA-CBA
5	E	371	BCL	CBD-CGD-O2D-CED
5	E	371	BCL	O1D-CGD-O2D-CED
5	E	373	BCL	C2C-C3C-CAC-CBC
5	E	373	BCL	C4C-C3C-CAC-CBC
5	E	373	BCL	C1-C2-C3-C5
5	E	373	BCL	C2-C3-C5-C6
5	E	374	BCL	C2C-C3C-CAC-CBC
5	E	374	BCL	C4C-C3C-CAC-CBC
5	E	375	BCL	C1-C2-C3-C5
5	E	376	BCL	C2-C3-C5-C6
5	E	377	BCL	C1-C2-C3-C5
5	E	378[B]	BCL	C3A-C2A-CAA-CBA
5	E	372	BCL	C2C-C3C-CAC-CBC
5	E	372	BCL	C4C-C3C-CAC-CBC
5	E	372	BCL	C1-C2-C3-C5
5	F	372	BCL	C2C-C3C-CAC-CBC
5	F	372	BCL	C4C-C3C-CAC-CBC
5	F	372	BCL	C1-C2-C3-C5
5	F	371	BCL	C1A-C2A-CAA-CBA
5	F	371	BCL	C3A-C2A-CAA-CBA
5	F	371	BCL	CBD-CGD-O2D-CED
5	F	371	BCL	O1D-CGD-O2D-CED
5	F	373	BCL	C2C-C3C-CAC-CBC
5	F	373	BCL	C4C-C3C-CAC-CBC
5	F	373	BCL	C1-C2-C3-C5
5	F	373	BCL	C2-C3-C5-C6
5	F	374	BCL	C2C-C3C-CAC-CBC
5	F	374	BCL	C4C-C3C-CAC-CBC
5	F	375	BCL	C1-C2-C3-C5
5	F	376	BCL	C2-C3-C5-C6
5	F	377	BCL	C1-C2-C3-C5
5	F	378[B]	BCL	C3A-C2A-CAA-CBA
5	G	378[B]	BCL	C3A-C2A-CAA-CBA
5	G	372	BCL	C2C-C3C-CAC-CBC
5	G	372	BCL	C4C-C3C-CAC-CBC
5	G	372	BCL	C1-C2-C3-C5
5	G	371	BCL	C1A-C2A-CAA-CBA
5	G	371	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	G	371	BCL	CBD-CGD-O2D-CED
5	G	371	BCL	O1D-CGD-O2D-CED
5	G	373	BCL	C2C-C3C-CAC-CBC
5	G	373	BCL	C4C-C3C-CAC-CBC
5	G	373	BCL	C1-C2-C3-C5
5	G	373	BCL	C2-C3-C5-C6
5	G	374	BCL	C2C-C3C-CAC-CBC
5	G	374	BCL	C4C-C3C-CAC-CBC
5	G	375	BCL	C1-C2-C3-C5
5	G	376	BCL	C2-C3-C5-C6
5	G	377	BCL	C1-C2-C3-C5
5	A	804	BCL	C2C-C3C-CAC-CBC
5	A	804	BCL	C4C-C3C-CAC-CBC
5	A	804	BCL	CHA-CBD-CGD-O1D
5	A	804	BCL	CAD-CBD-CGD-O1D
5	A	805	BCL	O2A-C1-C2-C3
5	A	806	BCL	C4C-C3C-CAC-CBC
5	A	807	BCL	C1A-C2A-CAA-CBA
5	A	807	BCL	C3A-C2A-CAA-CBA
5	A	807	BCL	C2C-C3C-CAC-CBC
5	A	808	BCL	C1-C2-C3-C4
5	A	808	BCL	C1-C2-C3-C5
5	A	810	BCL	C1A-C2A-CAA-CBA
5	A	810	BCL	C3A-C2A-CAA-CBA
5	A	810	BCL	C4C-C3C-CAC-CBC
5	A	811	BCL	C4C-C3C-CAC-CBC
5	A	811	BCL	C1-C2-C3-C5
5	A	812	BCL	C3A-C2A-CAA-CBA
5	A	812	BCL	C4C-C3C-CAC-CBC
5	A	813	BCL	C2C-C3C-CAC-CBC
5	A	813	BCL	C4C-C3C-CAC-CBC
5	A	814	BCL	CHA-CBD-CGD-O1D
5	A	814	BCL	CHA-CBD-CGD-O2D
5	A	814	BCL	CAD-CBD-CGD-O1D
5	A	814	BCL	CAD-CBD-CGD-O2D
5	A	815	BCL	C4C-C3C-CAC-CBC
5	A	815	BCL	CHA-CBD-CGD-O1D
5	A	815	BCL	CHA-CBD-CGD-O2D
5	A	815	BCL	CAD-CBD-CGD-O1D
5	A	815	BCL	CAD-CBD-CGD-O2D
5	a	804	BCL	C2C-C3C-CAC-CBC
5	a	804	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	a	804	BCL	CHA-CBD-CGD-O1D
5	a	804	BCL	CAD-CBD-CGD-O1D
5	a	805	BCL	O2A-C1-C2-C3
5	a	806	BCL	C4C-C3C-CAC-CBC
5	a	807	BCL	C1A-C2A-CAA-CBA
5	a	807	BCL	C3A-C2A-CAA-CBA
5	a	807	BCL	C2C-C3C-CAC-CBC
5	a	808	BCL	C1-C2-C3-C4
5	a	808	BCL	C1-C2-C3-C5
5	a	810	BCL	C1A-C2A-CAA-CBA
5	a	810	BCL	C3A-C2A-CAA-CBA
5	a	810	BCL	C4C-C3C-CAC-CBC
5	a	811	BCL	C4C-C3C-CAC-CBC
5	a	811	BCL	C1-C2-C3-C5
5	a	812	BCL	C3A-C2A-CAA-CBA
5	a	812	BCL	C4C-C3C-CAC-CBC
5	a	813	BCL	C2C-C3C-CAC-CBC
5	a	813	BCL	C4C-C3C-CAC-CBC
5	a	814	BCL	CHA-CBD-CGD-O1D
5	a	814	BCL	CHA-CBD-CGD-O2D
5	a	814	BCL	CAD-CBD-CGD-O1D
5	a	814	BCL	CAD-CBD-CGD-O2D
5	a	815	BCL	C4C-C3C-CAC-CBC
5	a	815	BCL	CHA-CBD-CGD-O1D
5	a	815	BCL	CHA-CBD-CGD-O2D
5	a	815	BCL	CAD-CBD-CGD-O1D
5	a	815	BCL	CAD-CBD-CGD-O2D
7	A	801	GS0	C1A-C2A-CAA-CBA
7	A	801	GS0	C3A-C2A-CAA-CBA
7	a	801	GS0	C1A-C2A-CAA-CBA
7	a	801	GS0	C3A-C2A-CAA-CBA
8	A	816	F26	C19-C15-C9-C2
8	A	816	F26	C22-C25-C26-C29
8	A	816	F26	C27-C28-C31-C36
8	A	816	F26	C37-C34-C35-C32
8	a	816	F26	C19-C15-C9-C2
8	a	816	F26	C22-C25-C26-C29
8	a	816	F26	C27-C28-C31-C36
8	a	816	F26	C37-C34-C35-C32
9	A	817	F39	O2-C13-C14-C18
9	A	817	F39	C19-C20-C27-C32
9	A	817	F39	C25-C20-C27-C32

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Mol	Chain	Res	Type	Atoms
9	A	817	F39	C22-C21-O6-C15
9	A	817	F39	O7-C21-O6-C15
9	A	817	F39	C27-C32-C35-C37
9	A	817	F39	C32-C35-C37-C39
9	A	817	F39	C38-C37-C39-C40
9	A	817	F39	C37-C39-C40-C41
9	A	817	F39	C43-C42-C44-C51
9	A	817	F39	C44-C51-C57-C59
9	A	817	F39	C46-C53-C56-C58
9	A	817	F39	C53-C56-C58-C60
9	A	817	F39	C56-C58-C61-C63
9	A	817	F39	C60-C58-C61-C63
9	A	817	F39	C57-C59-C62-C64
9	A	817	F39	C57-C59-C62-C65
9	A	817	F39	C61-C63-C64-C62
9	a	817	F39	O2-C13-C14-C18
9	a	817	F39	C19-C20-C27-C32
9	a	817	F39	C25-C20-C27-C32
9	a	817	F39	C22-C21-O6-C15
9	a	817	F39	O7-C21-O6-C15
9	a	817	F39	C27-C32-C35-C37
9	a	817	F39	C32-C35-C37-C39
9	a	817	F39	C38-C37-C39-C40
9	a	817	F39	C37-C39-C40-C41
9	a	817	F39	C43-C42-C44-C51
9	a	817	F39	C44-C51-C57-C59
9	a	817	F39	C46-C53-C56-C58
9	a	817	F39	C53-C56-C58-C60
9	a	817	F39	C56-C58-C61-C63
9	a	817	F39	C60-C58-C61-C63
9	a	817	F39	C57-C59-C62-C64
9	a	817	F39	C57-C59-C62-C65
9	a	817	F39	C61-C63-C64-C62
10	A	818	LHG	C1-C2-C3-O3
10	A	818	LHG	C3-O3-P-O5
10	A	818	LHG	C3-O3-P-O6
10	A	818	LHG	C4-O6-P-O3
10	A	818	LHG	C4-O6-P-O4
10	A	818	LHG	C4-O6-P-O5
10	a	818	LHG	C1-C2-C3-O3
10	a	818	LHG	C3-O3-P-O5
10	a	818	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
10	a	818	LHG	C4-O6-P-O3
10	a	818	LHG	C4-O6-P-O4
10	a	818	LHG	C4-O6-P-O5
11	A	819	LMG	O6-C1-O1-C7
11	A	819	LMG	C11-C10-O7-C8
11	a	819	LMG	O6-C1-O1-C7
11	a	819	LMG	C11-C10-O7-C8
13	A	802	G2O	C3-C5-C6-C7
13	A	802	G2O	C5-C6-C7-C8
13	A	802	G2O	C11-C10-C8-C7
13	A	802	G2O	C1A-C2A-CAA-CBA
13	A	802	G2O	C3A-C2A-CAA-CBA
13	A	803	G2O	C4-C3-C5-C6
13	A	803	G2O	C11-C10-C8-C7
13	A	803	G2O	C11-C10-C8-C9
13	A	803	G2O	CBD-CGD-O2D-CED
13	A	803	G2O	O1D-CGD-O2D-CED
13	a	802	G2O	C3-C5-C6-C7
13	a	802	G2O	C5-C6-C7-C8
13	a	802	G2O	C11-C10-C8-C7
13	a	802	G2O	C1A-C2A-CAA-CBA
13	a	802	G2O	C3A-C2A-CAA-CBA
13	a	803	G2O	C4-C3-C5-C6
13	a	803	G2O	C11-C10-C8-C7
13	a	803	G2O	C11-C10-C8-C9
13	a	803	G2O	CBD-CGD-O2D-CED
13	a	803	G2O	O1D-CGD-O2D-CED
9	A	817	F39	O1-C12-C15-O6
9	a	817	F39	O1-C12-C15-O6
11	A	819	LMG	O9-C10-O7-C8
11	a	819	LMG	O9-C10-O7-C8
5	E	375	BCL	C3-C5-C6-C7
5	F	375	BCL	C3-C5-C6-C7
5	G	375	BCL	C3-C5-C6-C7
9	A	817	F39	C10-C12-C15-O6
9	a	817	F39	C10-C12-C15-O6
13	A	803	G2O	C2-C3-C5-C6
13	a	803	G2O	C2-C3-C5-C6
13	A	802	G2O	C2A-CAA-CBA-CGA
13	A	803	G2O	C2A-CAA-CBA-CGA
13	a	802	G2O	C2A-CAA-CBA-CGA
13	a	803	G2O	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	A	811	BCL	C3-C5-C6-C7
5	a	811	BCL	C3-C5-C6-C7
5	A	805	BCL	C1-C2-C3-C5
5	a	805	BCL	C1-C2-C3-C5
10	A	818	LHG	O2-C2-C3-O3
10	a	818	LHG	O2-C2-C3-O3
5	A	812	BCL	C3-C5-C6-C7
5	a	812	BCL	C3-C5-C6-C7
8	A	816	F26	C14-C10-C8-C13
8	a	816	F26	C14-C10-C8-C13
9	A	817	F39	C13-C14-C18-C19
9	a	817	F39	C13-C14-C18-C19
7	A	801	GS0	C15-C16-C17-C18
7	a	801	GS0	C15-C16-C17-C18
11	A	819	LMG	C2-C1-O1-C7
11	a	819	LMG	C2-C1-O1-C7
5	A	811	BCL	C2-C3-C5-C6
5	a	811	BCL	C2-C3-C5-C6
5	A	808	BCL	C6-C7-C8-C9
5	A	812	BCL	C11-C12-C13-C14
5	a	808	BCL	C6-C7-C8-C9
5	a	812	BCL	C11-C12-C13-C14
5	E	373	BCL	C2A-CAA-CBA-CGA
5	F	373	BCL	C2A-CAA-CBA-CGA
5	G	373	BCL	C2A-CAA-CBA-CGA
9	A	817	F39	C65-C62-C64-C63
9	a	817	F39	C65-C62-C64-C63
8	A	816	F26	C22-C25-C26-C30
8	a	816	F26	C22-C25-C26-C30
9	A	817	F39	C40-C41-C42-C44
9	A	817	F39	C53-C56-C58-C61
9	a	817	F39	C40-C41-C42-C44
9	a	817	F39	C53-C56-C58-C61
5	E	372	BCL	C10-C11-C12-C13
5	F	372	BCL	C10-C11-C12-C13
5	G	372	BCL	C10-C11-C12-C13
11	A	819	LMG	C10-C11-C12-C13
11	A	819	LMG	C28-C29-C30-C31
11	a	819	LMG	C10-C11-C12-C13
11	a	819	LMG	C28-C29-C30-C31
5	E	372	BCL	C5-C6-C7-C8
5	F	372	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	G	372	BCL	C5-C6-C7-C8
10	A	818	LHG	C23-C24-C25-C26
10	a	818	LHG	C23-C24-C25-C26
9	A	817	F39	C23-C24-C26-C28
9	a	817	F39	C23-C24-C26-C28
5	A	812	BCL	C11-C12-C13-C15
5	a	812	BCL	C11-C12-C13-C15
7	A	801	GS0	C6-C7-C8-C10
7	a	801	GS0	C6-C7-C8-C10
8	A	816	F26	C19-C24-C27-C28
8	a	816	F26	C19-C24-C27-C28
9	A	817	F39	C20-C27-C32-C35
9	A	817	F39	C42-C44-C51-C57
9	a	817	F39	C20-C27-C32-C35
9	a	817	F39	C42-C44-C51-C57
5	E	372	BCL	C2A-CAA-CBA-CGA
5	F	372	BCL	C2A-CAA-CBA-CGA
5	G	372	BCL	C2A-CAA-CBA-CGA
5	A	810	BCL	C2A-CAA-CBA-CGA
5	A	815	BCL	C2A-CAA-CBA-CGA
5	a	810	BCL	C2A-CAA-CBA-CGA
5	a	815	BCL	C2A-CAA-CBA-CGA
5	A	806	BCL	C5-C6-C7-C8
5	A	806	BCL	C8-C10-C11-C12
5	a	806	BCL	C5-C6-C7-C8
13	A	803	G2O	C13-C15-C16-C17
13	a	803	G2O	C13-C15-C16-C17
5	a	806	BCL	C8-C10-C11-C12
8	A	816	F26	C18-C22-C25-C26
8	a	816	F26	C18-C22-C25-C26
5	E	371	BCL	C15-C16-C17-C18
5	F	371	BCL	C15-C16-C17-C18
5	G	371	BCL	C15-C16-C17-C18
5	A	808	BCL	C5-C6-C7-C8
5	A	812	BCL	C10-C11-C12-C13
5	a	808	BCL	C5-C6-C7-C8
5	a	812	BCL	C10-C11-C12-C13
13	A	802	G2O	C10-C11-C12-C13
13	a	802	G2O	C10-C11-C12-C13
5	E	372	BCL	C15-C16-C17-C18
5	F	372	BCL	C15-C16-C17-C18
5	G	372	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
5	E	376	BCL	O1A-CGA-O2A-C1
5	F	376	BCL	O1A-CGA-O2A-C1
5	G	376	BCL	O1A-CGA-O2A-C1
5	E	374	BCL	C10-C11-C12-C13
5	F	374	BCL	C10-C11-C12-C13
5	G	374	BCL	C10-C11-C12-C13
13	A	803	G2O	C8-C10-C11-C12
13	a	803	G2O	C8-C10-C11-C12
5	A	805	BCL	C3-C5-C6-C7
5	a	805	BCL	C3-C5-C6-C7
10	A	818	LHG	C13-C14-C15-C16
10	a	818	LHG	C13-C14-C15-C16
10	A	818	LHG	C11-C10-C9-C8
10	a	818	LHG	C11-C10-C9-C8
10	A	818	LHG	C24-C25-C26-C27
10	a	818	LHG	C24-C25-C26-C27
5	A	811	BCL	O1A-CGA-O2A-C1
5	A	812	BCL	O1A-CGA-O2A-C1
5	a	811	BCL	O1A-CGA-O2A-C1
5	A	808	BCL	C16-C17-C18-C19
5	a	808	BCL	C16-C17-C18-C19
5	E	371	BCL	C2-C3-C5-C6
5	F	371	BCL	C2-C3-C5-C6
5	G	371	BCL	C2-C3-C5-C6
5	E	374	BCL	C6-C7-C8-C9
5	F	374	BCL	C6-C7-C8-C9
5	G	374	BCL	C6-C7-C8-C9
5	A	807	BCL	C2A-CAA-CBA-CGA
5	a	807	BCL	C2A-CAA-CBA-CGA
5	a	812	BCL	O1A-CGA-O2A-C1
9	A	817	F39	C28-C29-C30-C31
9	a	817	F39	C28-C29-C30-C31
11	A	819	LMG	C32-C33-C34-C35
11	a	819	LMG	C32-C33-C34-C35
5	A	808	BCL	C16-C17-C18-C20
5	a	808	BCL	C16-C17-C18-C20
11	A	819	LMG	C15-C16-C17-C18
11	a	819	LMG	C15-C16-C17-C18
5	E	375	BCL	C8-C10-C11-C12
5	F	375	BCL	C8-C10-C11-C12
5	G	375	BCL	C8-C10-C11-C12
13	A	803	G2O	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	803	G2O	CBA-CGA-O2A-C1
5	E	372	BCL	C3A-C2A-CAA-CBA
5	F	372	BCL	C3A-C2A-CAA-CBA
5	G	372	BCL	C3A-C2A-CAA-CBA
5	A	804	BCL	C3A-C2A-CAA-CBA
5	A	808	BCL	C3A-C2A-CAA-CBA
5	a	804	BCL	C3A-C2A-CAA-CBA
5	a	808	BCL	C3A-C2A-CAA-CBA
5	E	372	BCL	C8-C10-C11-C12
5	F	372	BCL	C8-C10-C11-C12
5	G	372	BCL	C8-C10-C11-C12
5	A	806	BCL	O1A-CGA-O2A-C1
5	a	806	BCL	O1A-CGA-O2A-C1
9	A	817	F39	C24-C26-C28-C29
5	E	377	BCL	C2-C3-C5-C6
5	F	377	BCL	C2-C3-C5-C6
5	G	377	BCL	C2-C3-C5-C6
9	a	817	F39	C24-C26-C28-C29
10	A	818	LHG	C25-C26-C27-C28
10	a	818	LHG	C25-C26-C27-C28
11	A	819	LMG	C18-C19-C20-C21
11	a	819	LMG	C18-C19-C20-C21
5	E	377	BCL	C10-C11-C12-C13
5	F	377	BCL	C10-C11-C12-C13
5	G	377	BCL	C10-C11-C12-C13
5	E	371	BCL	C5-C6-C7-C8
5	F	371	BCL	C5-C6-C7-C8
5	G	371	BCL	C5-C6-C7-C8
5	A	808	BCL	C6-C7-C8-C10
5	a	808	BCL	C6-C7-C8-C10
13	A	803	G2O	O1A-CGA-O2A-C1
13	a	803	G2O	O1A-CGA-O2A-C1
5	A	808	BCL	C10-C11-C12-C13
5	a	808	BCL	C10-C11-C12-C13
9	A	817	F39	C58-C61-C63-C64
9	a	817	F39	C58-C61-C63-C64
11	A	819	LMG	C29-C28-O8-C9
11	a	819	LMG	C29-C28-O8-C9
11	A	819	LMG	C33-C34-C35-C36
11	A	819	LMG	C34-C35-C36-C37
11	a	819	LMG	C33-C34-C35-C36
13	A	802	G2O	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	a	802	G2O	C2B-C3B-CAB-CBB
11	a	819	LMG	C34-C35-C36-C37
10	A	818	LHG	C26-C27-C28-C29
10	a	818	LHG	C26-C27-C28-C29
13	A	802	G2O	C4B-C3B-CAB-CBB
13	a	802	G2O	C4B-C3B-CAB-CBB
5	A	808	BCL	C3-C5-C6-C7
5	a	808	BCL	C3-C5-C6-C7
5	E	378[B]	BCL	C1A-C2A-CAA-CBA
5	E	372	BCL	C1A-C2A-CAA-CBA
5	F	372	BCL	C1A-C2A-CAA-CBA
5	F	378[B]	BCL	C1A-C2A-CAA-CBA
5	G	378[B]	BCL	C1A-C2A-CAA-CBA
5	G	372	BCL	C1A-C2A-CAA-CBA
5	A	808	BCL	C1A-C2A-CAA-CBA
5	A	811	BCL	C1A-C2A-CAA-CBA
5	A	812	BCL	C1A-C2A-CAA-CBA
5	A	813	BCL	C1A-C2A-CAA-CBA
5	a	808	BCL	C1A-C2A-CAA-CBA
5	a	811	BCL	C1A-C2A-CAA-CBA
5	a	812	BCL	C1A-C2A-CAA-CBA
5	a	813	BCL	C1A-C2A-CAA-CBA
8	A	816	F26	C26-C30-C32-C35
8	a	816	F26	C26-C30-C32-C35
5	E	371	BCL	C4-C3-C5-C6
5	F	371	BCL	C4-C3-C5-C6
5	G	371	BCL	C4-C3-C5-C6
5	E	375	BCL	C2C-C3C-CAC-CBC
5	F	375	BCL	C2C-C3C-CAC-CBC
5	G	375	BCL	C2C-C3C-CAC-CBC
5	A	805	BCL	C2C-C3C-CAC-CBC
5	A	810	BCL	C2C-C3C-CAC-CBC
5	A	811	BCL	C2C-C3C-CAC-CBC
5	A	812	BCL	C2C-C3C-CAC-CBC
5	A	815	BCL	C2C-C3C-CAC-CBC
5	a	805	BCL	C2C-C3C-CAC-CBC
5	a	810	BCL	C2C-C3C-CAC-CBC
5	a	811	BCL	C2C-C3C-CAC-CBC
5	a	812	BCL	C2C-C3C-CAC-CBC
5	a	815	BCL	C2C-C3C-CAC-CBC
11	A	819	LMG	C16-C17-C18-C19
11	a	819	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
11	A	819	LMG	O10-C28-O8-C9
11	a	819	LMG	O10-C28-O8-C9
5	F	375	BCL	C5-C6-C7-C8
10	A	818	LHG	C29-C30-C31-C32
10	a	818	LHG	C29-C30-C31-C32
5	E	375	BCL	C5-C6-C7-C8
5	G	375	BCL	C5-C6-C7-C8
8	A	816	F26	C36-C31-C33-C38
8	a	816	F26	C36-C31-C33-C38
5	E	377	BCL	C4-C3-C5-C6
5	F	377	BCL	C4-C3-C5-C6
5	G	377	BCL	C4-C3-C5-C6
9	A	817	F39	C29-C30-C31-C33
9	a	817	F39	C29-C30-C31-C33
5	E	374	BCL	C5-C6-C7-C8
5	F	374	BCL	C5-C6-C7-C8
5	G	374	BCL	C5-C6-C7-C8
11	A	819	LMG	O6-C5-C6-O5
11	a	819	LMG	O6-C5-C6-O5
13	A	802	G2O	C6-C7-C8-C10
13	A	803	G2O	C6-C7-C8-C10
13	a	802	G2O	C6-C7-C8-C10
13	a	803	G2O	C6-C7-C8-C10
5	a	808	BCL	C8-C10-C11-C12
5	A	808	BCL	C8-C10-C11-C12
5	E	377	BCL	C11-C10-C8-C7
5	F	377	BCL	C11-C10-C8-C7
5	G	377	BCL	C11-C10-C8-C7
7	A	801	GS0	C3-C5-C6-C7
7	a	801	GS0	C3-C5-C6-C7
5	E	371	BCL	C14-C13-C15-C16
5	E	372	BCL	C11-C10-C8-C9
5	F	372	BCL	C11-C10-C8-C9
5	F	371	BCL	C14-C13-C15-C16
5	G	372	BCL	C11-C10-C8-C9
5	G	371	BCL	C14-C13-C15-C16
5	A	811	BCL	C11-C12-C13-C14
5	a	811	BCL	C11-C12-C13-C14
13	A	803	G2O	C14-C13-C15-C16
13	a	803	G2O	C14-C13-C15-C16
5	E	376	BCL	CBA-CGA-O2A-C1
5	F	376	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	G	376	BCL	CBA-CGA-O2A-C1
9	A	817	F39	C18-C19-C20-C27
9	a	817	F39	C18-C19-C20-C27
5	A	806	BCL	CBA-CGA-O2A-C1
5	a	806	BCL	CBA-CGA-O2A-C1
9	A	817	F39	C16-C13-C14-C18
9	A	817	F39	C17-C13-C14-C18
9	a	817	F39	C16-C13-C14-C18
9	a	817	F39	C17-C13-C14-C18
5	E	376	BCL	C4-C3-C5-C6
5	F	376	BCL	C4-C3-C5-C6
5	G	376	BCL	C4-C3-C5-C6
11	A	819	LMG	C17-C18-C19-C20
11	a	819	LMG	C17-C18-C19-C20
5	F	375	BCL	C16-C17-C18-C20
5	E	374	BCL	C2-C1-O2A-CGA
5	F	374	BCL	C2-C1-O2A-CGA
5	G	374	BCL	C2-C1-O2A-CGA
5	A	805	BCL	C2-C1-O2A-CGA
5	a	805	BCL	C2-C1-O2A-CGA
8	A	816	F26	C18-C13-C8-C10
8	a	816	F26	C18-C13-C8-C10
5	E	373	BCL	C11-C10-C8-C9
5	E	375	BCL	C11-C10-C8-C9
5	F	373	BCL	C11-C10-C8-C9
5	F	375	BCL	C11-C10-C8-C9
5	G	373	BCL	C11-C10-C8-C9
5	G	375	BCL	C11-C10-C8-C9
7	A	801	GS0	C6-C7-C8-C9
7	a	801	GS0	C6-C7-C8-C9
10	A	818	LHG	C15-C16-C17-C18
10	a	818	LHG	C15-C16-C17-C18
5	A	811	BCL	C5-C6-C7-C8
5	a	811	BCL	C5-C6-C7-C8
7	A	801	GS0	C10-C11-C12-C13
7	a	801	GS0	C10-C11-C12-C13
5	E	375	BCL	C16-C17-C18-C20
5	G	375	BCL	C16-C17-C18-C20
8	A	816	F26	C27-C28-C31-C33
8	a	816	F26	C27-C28-C31-C33
9	A	817	F39	C16-C13-O2-C11
9	a	817	F39	C16-C13-O2-C11

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Mol	Chain	Res	Type	Atoms
5	E	371	BCL	C12-C13-C15-C16
5	E	373	BCL	C11-C10-C8-C7
5	E	375	BCL	C11-C10-C8-C7
5	E	372	BCL	C11-C10-C8-C7
5	F	372	BCL	C11-C10-C8-C7
5	F	371	BCL	C12-C13-C15-C16
5	F	373	BCL	C11-C10-C8-C7
5	F	375	BCL	C11-C10-C8-C7
5	G	372	BCL	C11-C10-C8-C7
5	G	371	BCL	C12-C13-C15-C16
5	G	373	BCL	C11-C10-C8-C7
5	G	375	BCL	C11-C10-C8-C7
5	A	811	BCL	C11-C12-C13-C15
5	a	811	BCL	C11-C12-C13-C15
13	A	803	G2O	C12-C13-C15-C16
13	a	803	G2O	C12-C13-C15-C16
5	A	805	BCL	C1-C2-C3-C4
5	a	805	BCL	C1-C2-C3-C4
5	A	812	BCL	C8-C10-C11-C12
5	a	812	BCL	C8-C10-C11-C12
8	A	816	F26	C29-C26-C30-C32
8	a	816	F26	C29-C26-C30-C32
5	E	376	BCL	CAD-CBD-CGD-O2D
5	F	376	BCL	CAD-CBD-CGD-O2D
5	G	376	BCL	CAD-CBD-CGD-O2D
5	A	804	BCL	CAD-CBD-CGD-O2D
5	A	807	BCL	CAD-CBD-CGD-O2D
5	A	809	BCL	CAD-CBD-CGD-O2D
5	a	804	BCL	CAD-CBD-CGD-O2D
5	a	807	BCL	CAD-CBD-CGD-O2D
5	a	809	BCL	CAD-CBD-CGD-O2D
5	A	812	BCL	CBA-CGA-O2A-C1
5	a	812	BCL	CBA-CGA-O2A-C1
5	E	374	BCL	C8-C10-C11-C12
13	a	803	G2O	C15-C16-C17-C18
5	F	374	BCL	C8-C10-C11-C12
5	G	374	BCL	C8-C10-C11-C12
13	A	803	G2O	C15-C16-C17-C18
5	A	806	BCL	C16-C17-C18-C20
5	a	806	BCL	C16-C17-C18-C20
5	E	373	BCL	CHA-CBD-CGD-O1D
5	E	373	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
5	E	376	BCL	CHA-CBD-CGD-O1D
5	E	377	BCL	CHA-CBD-CGD-O1D
5	E	377	BCL	CHA-CBD-CGD-O2D
5	F	373	BCL	CHA-CBD-CGD-O1D
5	F	373	BCL	CHA-CBD-CGD-O2D
5	F	376	BCL	CHA-CBD-CGD-O1D
5	F	377	BCL	CHA-CBD-CGD-O1D
5	F	377	BCL	CHA-CBD-CGD-O2D
5	G	373	BCL	CHA-CBD-CGD-O1D
5	G	373	BCL	CHA-CBD-CGD-O2D
5	G	376	BCL	CHA-CBD-CGD-O1D
5	G	377	BCL	CHA-CBD-CGD-O1D
5	G	377	BCL	CHA-CBD-CGD-O2D
5	A	804	BCL	CHA-CBD-CGD-O2D
5	A	805	BCL	CHA-CBD-CGD-O1D
5	A	805	BCL	CHA-CBD-CGD-O2D
5	A	813	BCL	CHA-CBD-CGD-O1D
5	A	813	BCL	CHA-CBD-CGD-O2D
5	a	804	BCL	CHA-CBD-CGD-O2D
5	a	805	BCL	CHA-CBD-CGD-O1D
5	a	805	BCL	CHA-CBD-CGD-O2D
5	a	813	BCL	CHA-CBD-CGD-O1D
5	a	813	BCL	CHA-CBD-CGD-O2D
5	A	806	BCL	C3-C5-C6-C7
5	a	806	BCL	C3-C5-C6-C7
7	A	801	GS0	O1A-CGA-O2A-C1
7	a	801	GS0	O1A-CGA-O2A-C1
11	A	819	LMG	O1-C7-C8-O7
11	a	819	LMG	O1-C7-C8-O7
13	A	803	G2O	C10-C11-C12-C13
13	a	803	G2O	C10-C11-C12-C13
5	A	811	BCL	C6-C7-C8-C9
5	a	811	BCL	C6-C7-C8-C9
5	A	814	BCL	C2A-CAA-CBA-CGA
5	a	814	BCL	C2A-CAA-CBA-CGA
5	A	804	BCL	C1A-C2A-CAA-CBA
5	a	804	BCL	C1A-C2A-CAA-CBA
5	E	376	BCL	C3-C5-C6-C7
5	F	376	BCL	C3-C5-C6-C7
5	G	376	BCL	C3-C5-C6-C7
10	A	818	LHG	C2-C3-O3-P
10	a	818	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
10	A	818	LHG	C3-O3-P-O4
10	a	818	LHG	C3-O3-P-O4
7	A	801	GS0	C16-C17-C18-C20
7	a	801	GS0	C16-C17-C18-C20
5	E	373	BCL	CBA-CGA-O2A-C1
5	F	373	BCL	CBA-CGA-O2A-C1
5	G	373	BCL	CBA-CGA-O2A-C1
5	E	373	BCL	CAD-CBD-CGD-O1D
5	F	373	BCL	CAD-CBD-CGD-O1D
5	G	373	BCL	CAD-CBD-CGD-O1D
5	A	808	BCL	CAD-CBD-CGD-O1D
5	A	810	BCL	CAD-CBD-CGD-O1D
5	a	808	BCL	CAD-CBD-CGD-O1D
9	A	817	F39	C14-C13-O2-C11
9	a	817	F39	C14-C13-O2-C11
5	E	371	BCL	C11-C12-C13-C15
5	E	374	BCL	C11-C12-C13-C15
5	E	372	BCL	C11-C12-C13-C15
5	F	372	BCL	C11-C12-C13-C15
5	F	371	BCL	C11-C12-C13-C15
5	F	374	BCL	C11-C12-C13-C15
5	G	372	BCL	C11-C12-C13-C15
5	G	371	BCL	C11-C12-C13-C15
5	G	374	BCL	C11-C12-C13-C15
5	A	806	BCL	C11-C12-C13-C15
5	A	808	BCL	C2C-C3C-CAC-CBC
5	a	806	BCL	C11-C12-C13-C15
5	a	808	BCL	C2C-C3C-CAC-CBC
10	A	818	LHG	C27-C28-C29-C30
10	a	818	LHG	C27-C28-C29-C30
5	E	376	BCL	C10-C11-C12-C13
5	F	376	BCL	C10-C11-C12-C13
5	G	376	BCL	C10-C11-C12-C13
5	a	805	BCL	C5-C6-C7-C8
5	A	805	BCL	C5-C6-C7-C8
5	A	808	BCL	C15-C16-C17-C18
5	a	808	BCL	C15-C16-C17-C18
5	E	377	BCL	C11-C10-C8-C9
5	F	377	BCL	C11-C10-C8-C9
5	G	377	BCL	C11-C10-C8-C9
13	A	802	G2O	C6-C7-C8-C9
13	a	802	G2O	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
9	a	817	F39	C31-C33-C34-C36
9	A	817	F39	C31-C33-C34-C36
5	F	374	BCL	C3-C5-C6-C7
5	G	374	BCL	C3-C5-C6-C7
5	E	374	BCL	C2A-CAA-CBA-CGA
5	F	374	BCL	C2A-CAA-CBA-CGA
5	G	374	BCL	C2A-CAA-CBA-CGA
5	E	377	BCL	C2-C1-O2A-CGA
5	F	377	BCL	C2-C1-O2A-CGA
5	G	377	BCL	C2-C1-O2A-CGA
5	E	374	BCL	C3-C5-C6-C7
11	A	819	LMG	O1-C7-C8-C9
11	a	819	LMG	O1-C7-C8-C9
8	A	816	F26	C17-C13-C8-C10
8	a	816	F26	C17-C13-C8-C10
5	E	374	BCL	C11-C12-C13-C14
5	E	372	BCL	C11-C12-C13-C14
5	F	372	BCL	C11-C12-C13-C14
5	F	374	BCL	C11-C12-C13-C14
5	G	372	BCL	C11-C12-C13-C14
5	G	374	BCL	C11-C12-C13-C14
5	A	806	BCL	C11-C12-C13-C14
5	a	806	BCL	C11-C12-C13-C14
5	A	804	BCL	C2A-CAA-CBA-CGA
5	a	804	BCL	C2A-CAA-CBA-CGA
5	A	811	BCL	CBA-CGA-O2A-C1
5	a	811	BCL	CBA-CGA-O2A-C1
5	E	375	BCL	C2-C3-C5-C6
5	F	375	BCL	C2-C3-C5-C6
5	G	375	BCL	C2-C3-C5-C6
5	A	811	BCL	C2-C1-O2A-CGA
5	a	811	BCL	C2-C1-O2A-CGA
5	E	375	BCL	C16-C17-C18-C19
5	F	375	BCL	C16-C17-C18-C19
5	G	375	BCL	C16-C17-C18-C19
5	a	810	BCL	CAA-CBA-CGA-O1A
5	A	810	BCL	CAA-CBA-CGA-O1A
5	A	809	BCL	CAA-CBA-CGA-O1A
5	a	809	BCL	CAA-CBA-CGA-O1A
5	A	805	BCL	C1A-C2A-CAA-CBA
5	a	805	BCL	C1A-C2A-CAA-CBA
5	E	376	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	a	817	F39	C22-C23-C24-C26
9	A	817	F39	C22-C23-C24-C26
5	F	376	BCL	C15-C16-C17-C18
5	G	376	BCL	C15-C16-C17-C18
5	a	808	BCL	C4-C3-C5-C6
5	E	373	BCL	C2-C1-O2A-CGA
5	E	376	BCL	C2-C1-O2A-CGA
5	F	373	BCL	C2-C1-O2A-CGA
5	F	376	BCL	C2-C1-O2A-CGA
5	G	373	BCL	C2-C1-O2A-CGA
5	G	376	BCL	C2-C1-O2A-CGA
5	A	812	BCL	C13-C15-C16-C17
5	a	812	BCL	C13-C15-C16-C17
10	a	818	LHG	C32-C33-C34-C35
10	A	818	LHG	C32-C33-C34-C35
5	A	812	BCL	C2A-CAA-CBA-CGA
5	a	812	BCL	C2A-CAA-CBA-CGA
10	A	818	LHG	O1-C1-C2-C3
10	a	818	LHG	O1-C1-C2-C3
13	A	803	G2O	C5-C6-C7-C8
13	a	803	G2O	C5-C6-C7-C8
5	A	808	BCL	C4-C3-C5-C6
9	A	817	F39	C17-C13-O2-C11
9	a	817	F39	C17-C13-O2-C11
7	A	801	GS0	CAA-CBA-CGA-O2A
7	a	801	GS0	CAA-CBA-CGA-O2A
7	A	801	GS0	C4-C3-C5-C6
7	a	801	GS0	C4-C3-C5-C6
13	A	803	G2O	C6-C7-C8-C9
13	a	803	G2O	C6-C7-C8-C9
5	E	377	BCL	C1-C2-C3-C4
5	F	377	BCL	C1-C2-C3-C4
5	G	377	BCL	C1-C2-C3-C4
5	A	811	BCL	C1-C2-C3-C4
5	a	811	BCL	C1-C2-C3-C4
5	F	374	BCL	O1A-CGA-O2A-C1
5	E	374	BCL	O1A-CGA-O2A-C1
5	G	374	BCL	O1A-CGA-O2A-C1
5	E	372	BCL	C6-C7-C8-C9
5	F	372	BCL	C6-C7-C8-C9
5	G	372	BCL	C6-C7-C8-C9
5	A	806	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	A	811	BCL	C14-C13-C15-C16
5	a	806	BCL	C6-C7-C8-C9
5	a	811	BCL	C14-C13-C15-C16
5	A	812	BCL	CAD-CBD-CGD-O2D
5	a	812	BCL	CAD-CBD-CGD-O2D
5	A	805	BCL	C4-C3-C5-C6
5	a	805	BCL	C4-C3-C5-C6
5	A	809	BCL	CAA-CBA-CGA-O2A
5	a	809	BCL	CAA-CBA-CGA-O2A
5	A	804	BCL	CAA-CBA-CGA-O2A
5	a	804	BCL	CAA-CBA-CGA-O2A
5	E	376	BCL	CHA-CBD-CGD-O2D
5	F	376	BCL	CHA-CBD-CGD-O2D
5	G	376	BCL	CHA-CBD-CGD-O2D
5	A	809	BCL	CHA-CBD-CGD-O2D
5	a	809	BCL	CHA-CBD-CGD-O2D
7	A	801	GS0	CHA-CBD-CGD-O1D
7	a	801	GS0	CHA-CBD-CGD-O1D
5	A	804	BCL	CAA-CBA-CGA-O1A
5	a	804	BCL	CAA-CBA-CGA-O1A
9	a	817	F39	C18-C19-C20-C25
5	E	374	BCL	C6-C7-C8-C10
5	F	374	BCL	C6-C7-C8-C10
5	G	374	BCL	C6-C7-C8-C10
5	A	811	BCL	C12-C13-C15-C16
5	a	811	BCL	C12-C13-C15-C16
8	A	816	F26	C34-C37-C39-C38
8	a	816	F26	C34-C37-C39-C38
9	A	817	F39	C18-C19-C20-C25
5	E	373	BCL	C1A-C2A-CAA-CBA
5	F	373	BCL	C1A-C2A-CAA-CBA
5	G	373	BCL	C1A-C2A-CAA-CBA
5	E	374	BCL	CAA-CBA-CGA-O2A
5	F	374	BCL	CAA-CBA-CGA-O2A
5	G	374	BCL	CAA-CBA-CGA-O2A
5	E	377	BCL	C15-C16-C17-C18
5	F	377	BCL	C15-C16-C17-C18
5	G	377	BCL	C15-C16-C17-C18
10	a	818	LHG	C17-C18-C19-C20
5	E	375	BCL	CAD-CBD-CGD-O1D
5	E	378[B]	BCL	CAD-CBD-CGD-O1D
5	F	375	BCL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	F	378[B]	BCL	CAD-CBD-CGD-O1D
5	G	378[B]	BCL	CAD-CBD-CGD-O1D
5	G	375	BCL	CAD-CBD-CGD-O1D
5	A	805	BCL	CAD-CBD-CGD-O1D
5	a	805	BCL	CAD-CBD-CGD-O1D
5	a	810	BCL	CAD-CBD-CGD-O1D
13	A	802	G2O	CAD-CBD-CGD-O1D
13	a	802	G2O	CAD-CBD-CGD-O1D
5	A	808	BCL	C11-C10-C8-C9
5	a	808	BCL	C11-C10-C8-C9
10	A	818	LHG	C17-C18-C19-C20
5	a	810	BCL	CAA-CBA-CGA-O2A
5	E	377	BCL	C2C-C3C-CAC-CBC
5	E	372	BCL	C2-C3-C5-C6
5	F	372	BCL	C2-C3-C5-C6
5	F	377	BCL	C2C-C3C-CAC-CBC
5	G	372	BCL	C2-C3-C5-C6
5	G	377	BCL	C2C-C3C-CAC-CBC
5	A	808	BCL	C11-C10-C8-C7
5	A	811	BCL	C3A-C2A-CAA-CBA
5	a	808	BCL	C11-C10-C8-C7
5	a	811	BCL	C3A-C2A-CAA-CBA
5	A	810	BCL	CAA-CBA-CGA-O2A
11	a	819	LMG	C31-C32-C33-C34
11	A	819	LMG	C31-C32-C33-C34
5	E	371	BCL	CAA-CBA-CGA-O2A
5	E	372	BCL	C13-C15-C16-C17
5	G	371	BCL	CAA-CBA-CGA-O2A
5	F	372	BCL	C13-C15-C16-C17
5	G	372	BCL	C13-C15-C16-C17
5	F	371	BCL	CAA-CBA-CGA-O2A

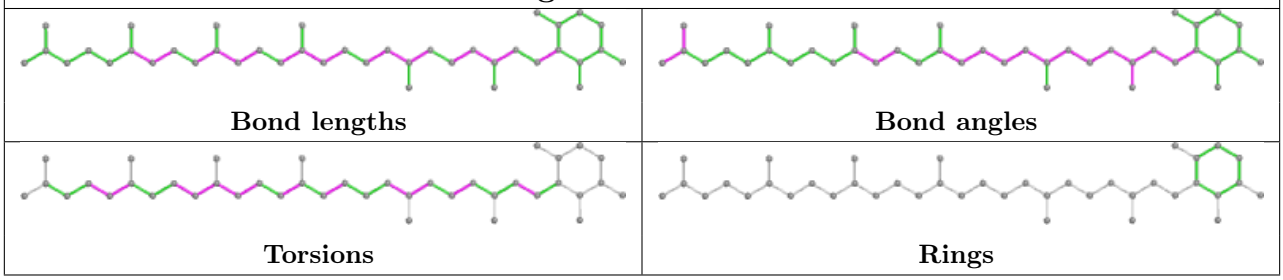
There are no ring outliers.

No monomer is involved in short contacts.

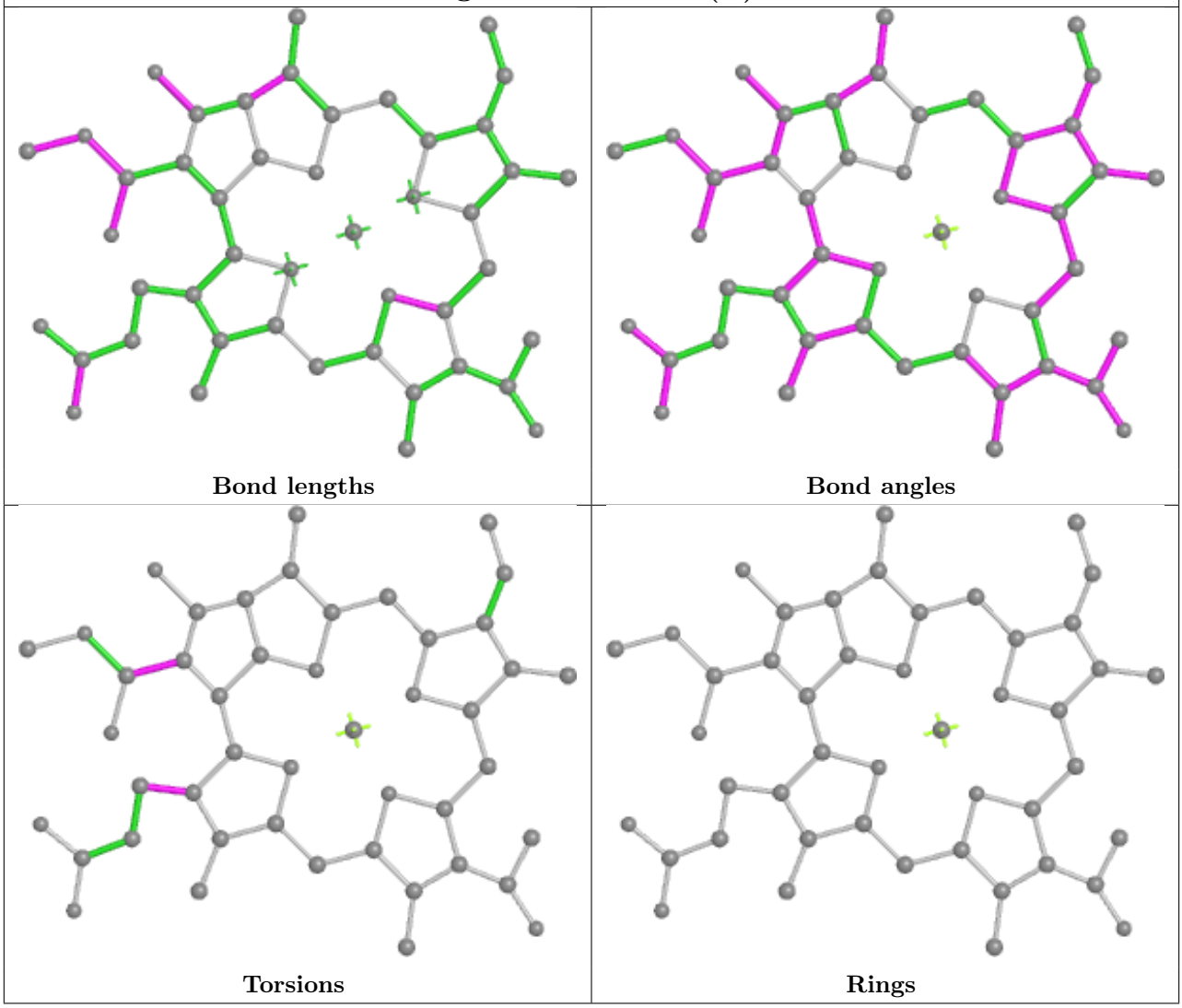
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 F26 a 816



Ligand BCL F 378 (B)



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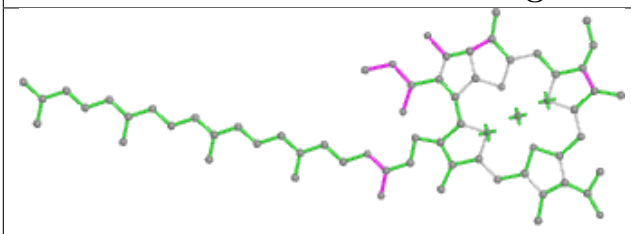
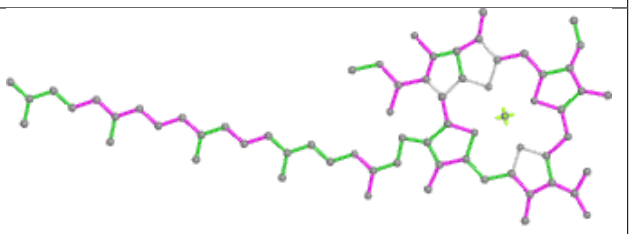
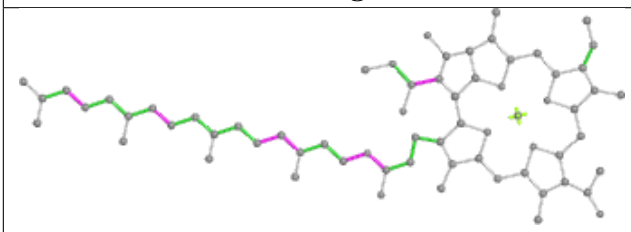
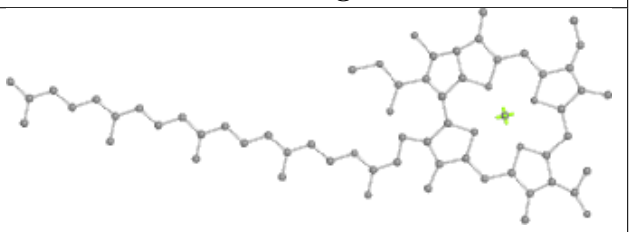
 Bond lengths	 Bond angles
 Torsions	 Rings

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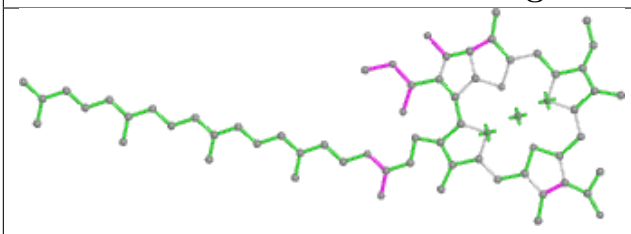
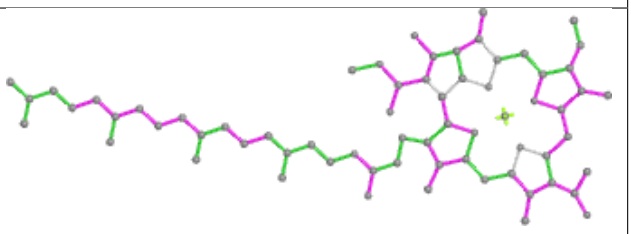
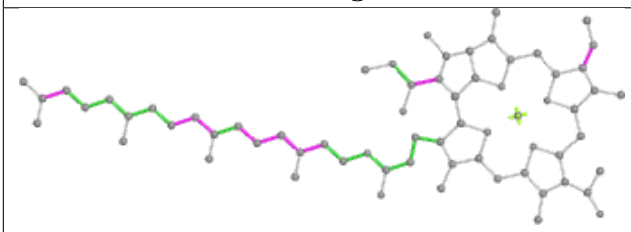
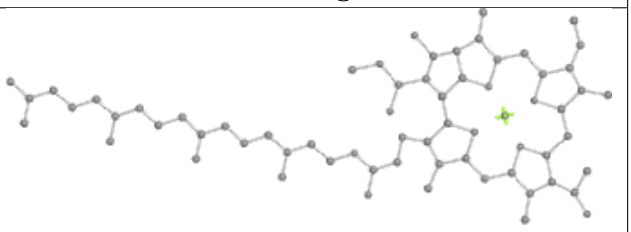
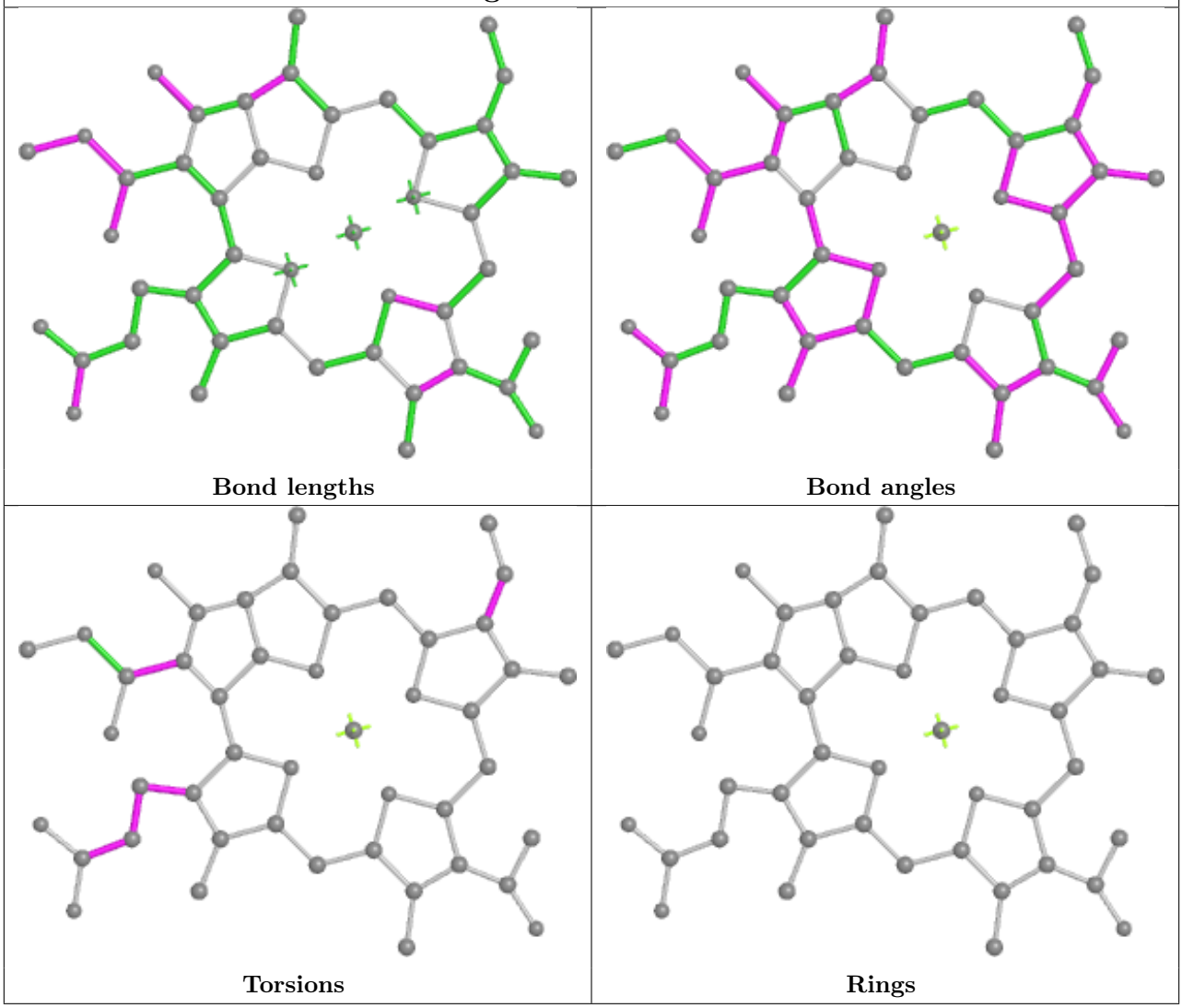
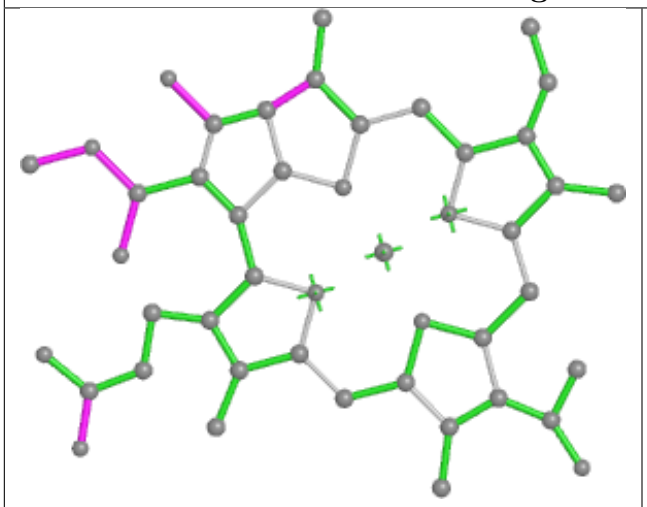
 Bond lengths	 Bond angles
 Torsions	 Rings

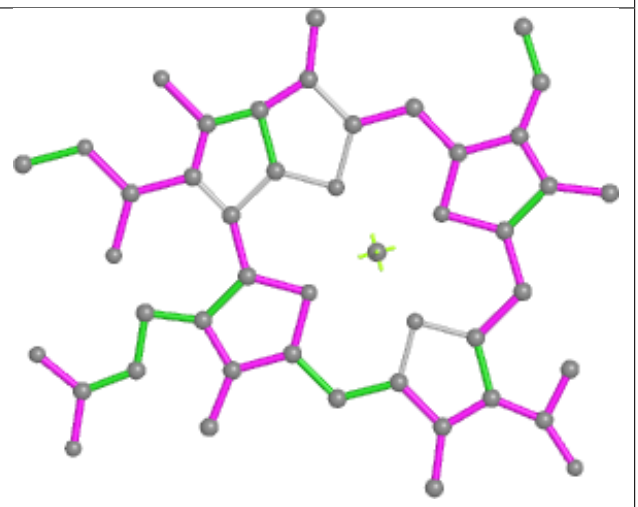
Ligand BCL A 804



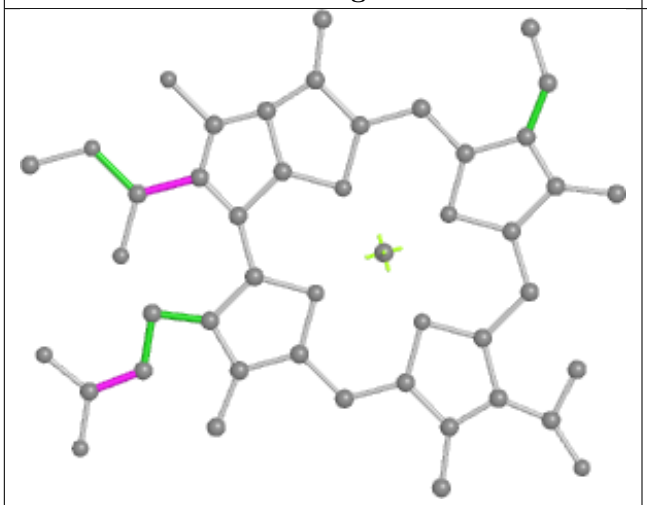
Ligand BCL a 809



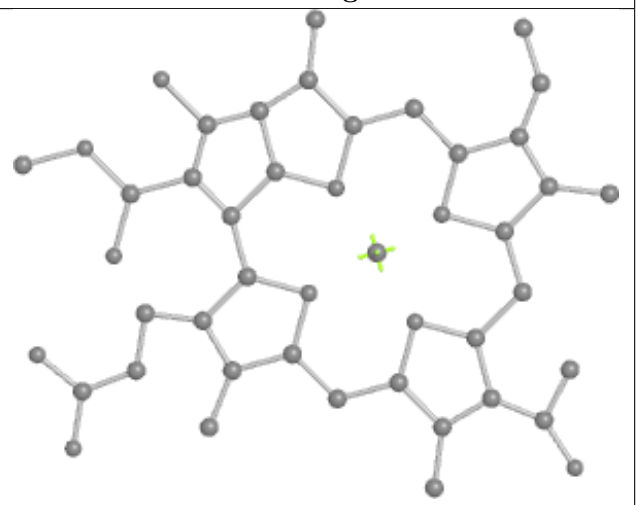
Bond lengths



Bond angles

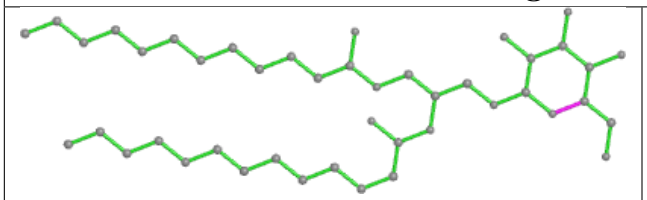


Torsions

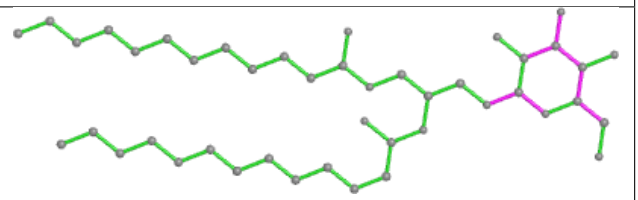


Rings

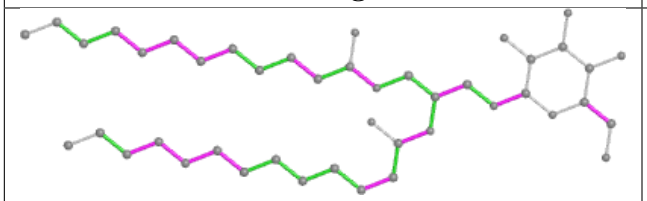
Ligand LMG a 819



Bond lengths



Bond angles



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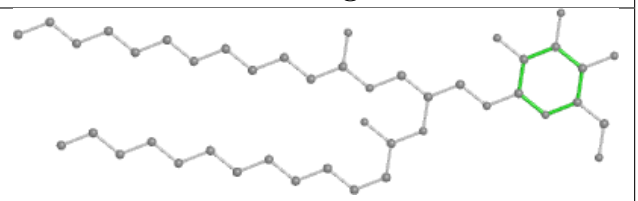
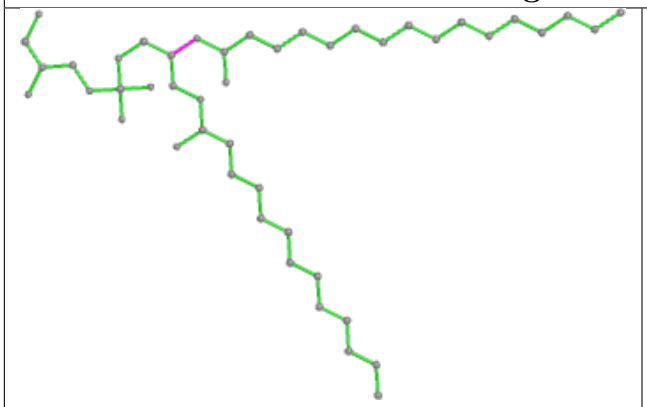
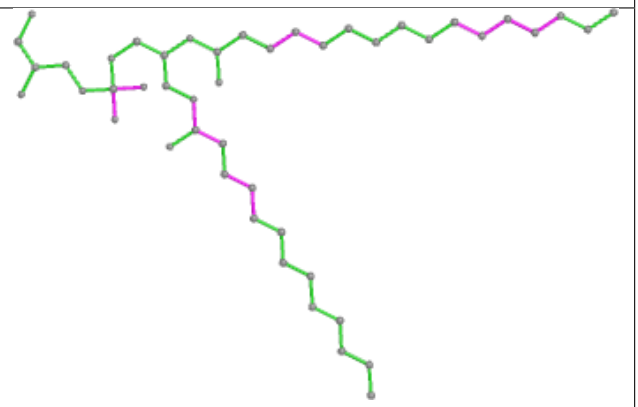


Rings

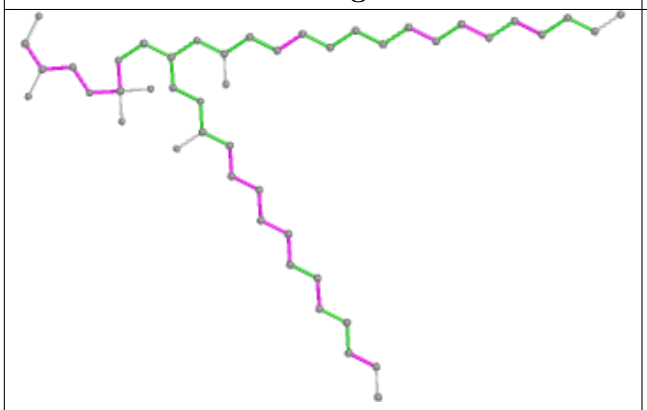
Ligand LHG A 818



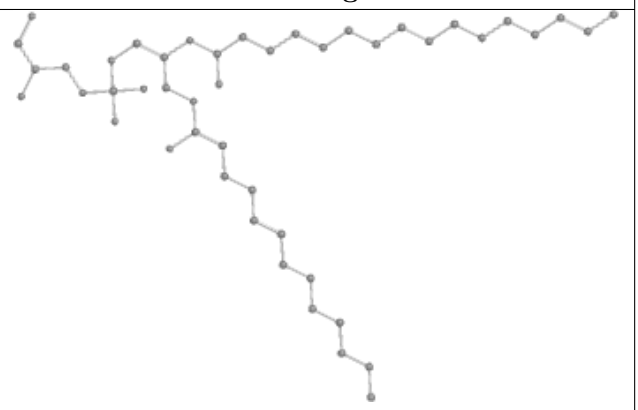
Bond lengths



Bond angles

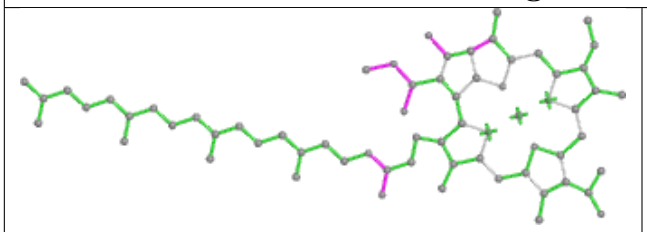


Torsions

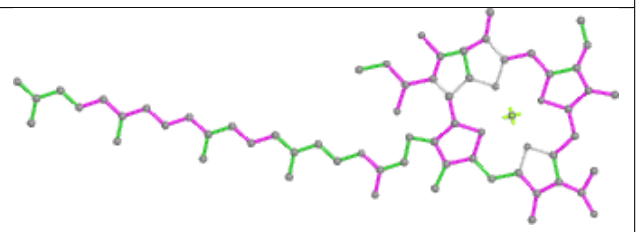


Rings

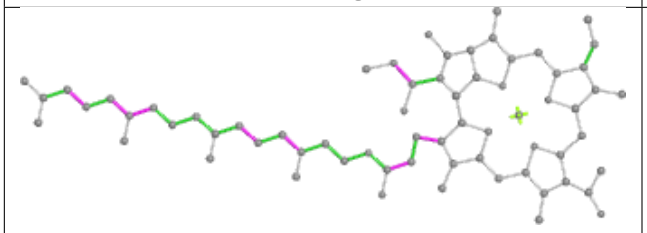
Ligand BCL G 371



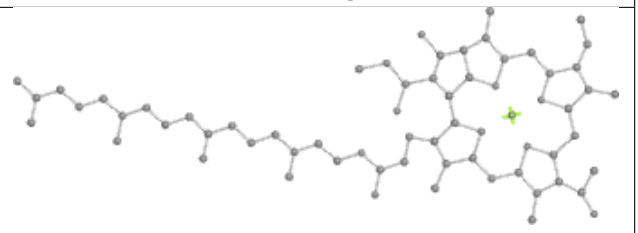
Bond lengths



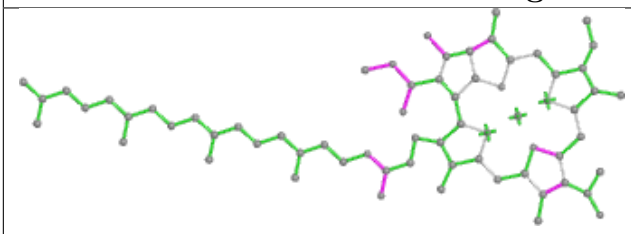
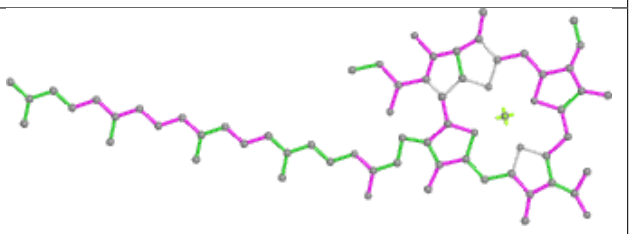
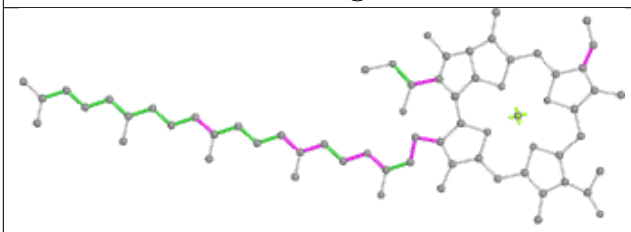
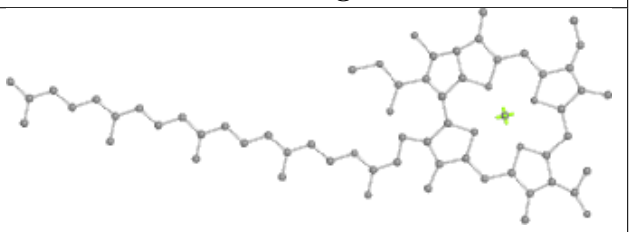
Bond angles

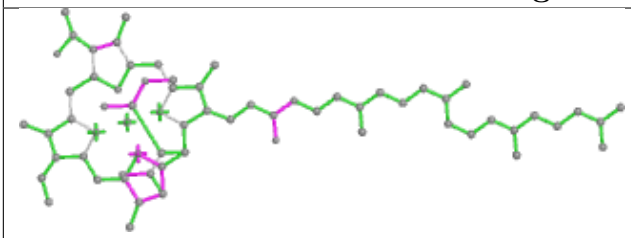
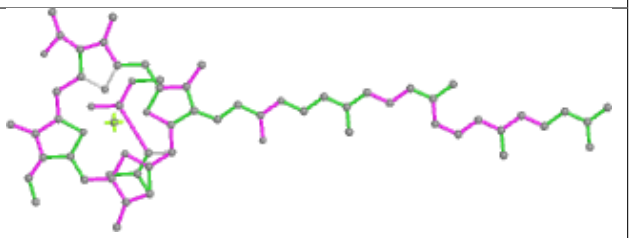
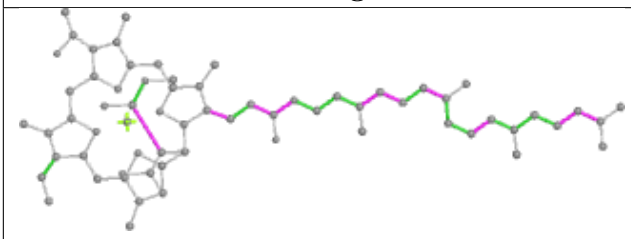
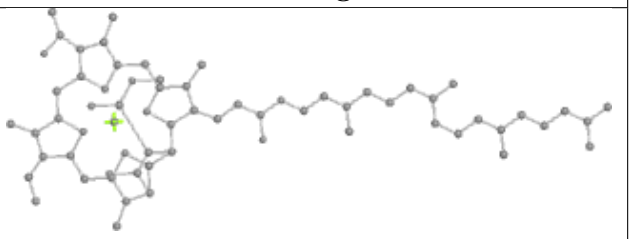


Torsions

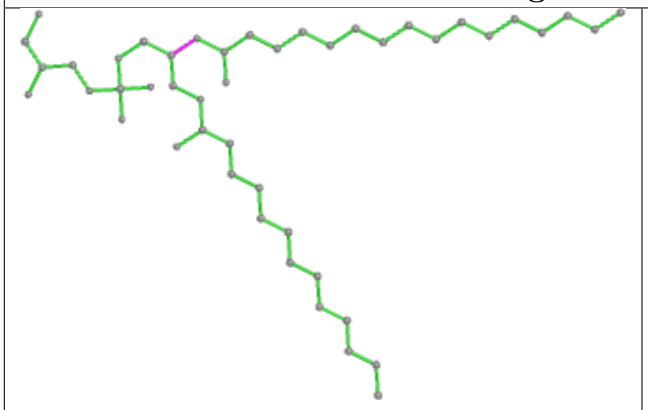


Rings

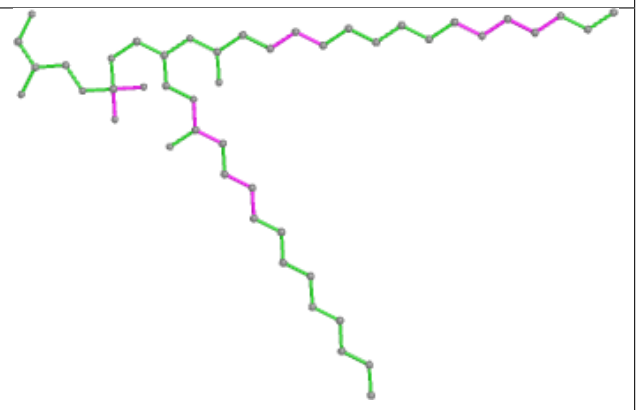
Ligand BCL E 373	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GS0 a 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

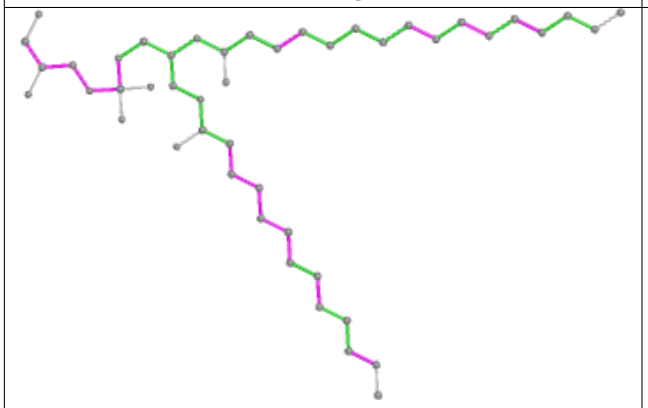
Ligand LHG a 818



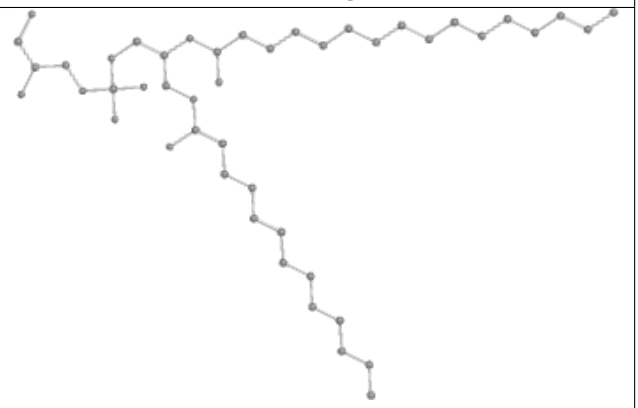
Bond lengths



Bond angles

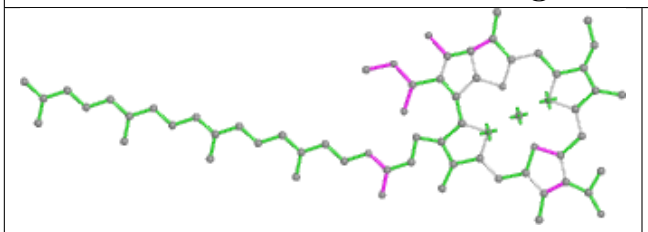


Torsions

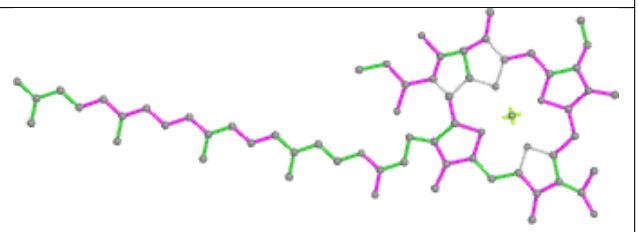


Rings

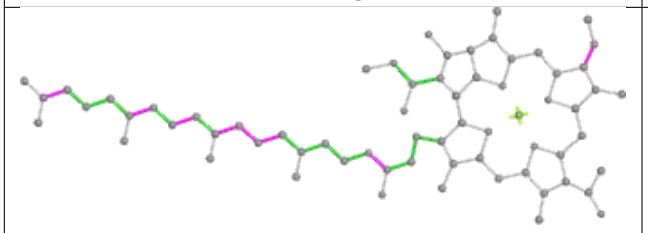
Ligand BCL a 806



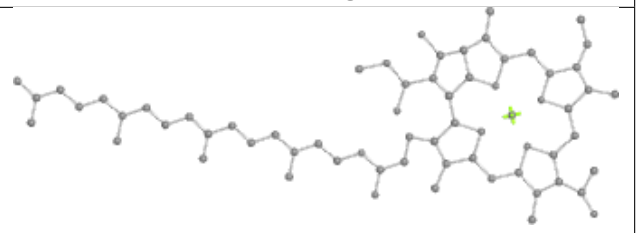
Bond lengths



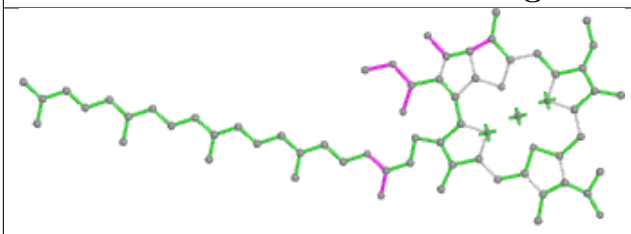
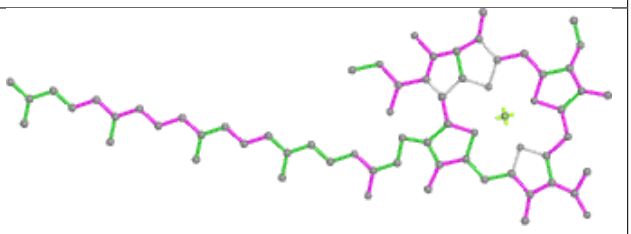
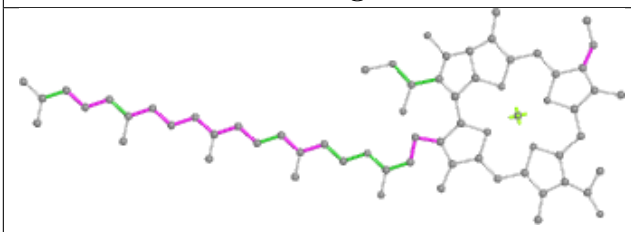
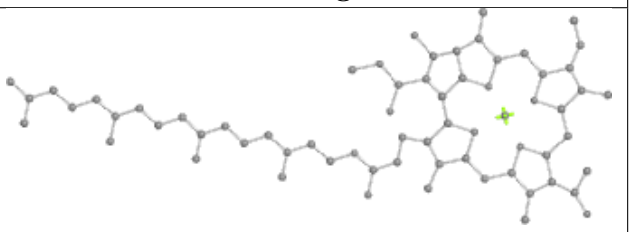
Bond angles

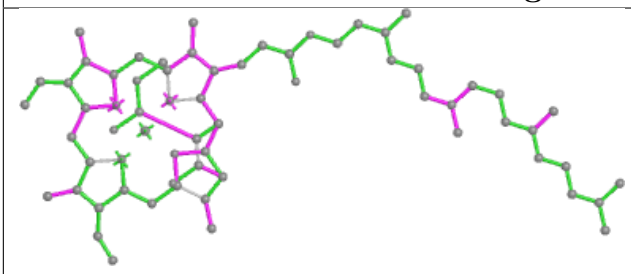
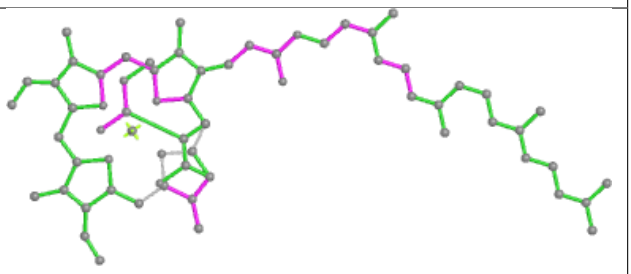
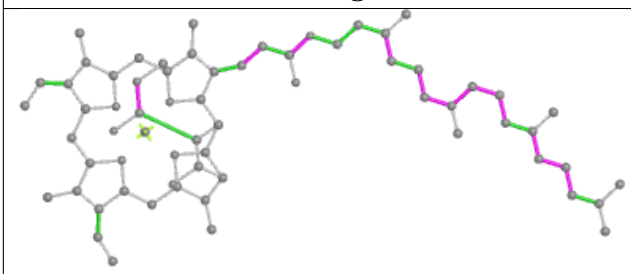
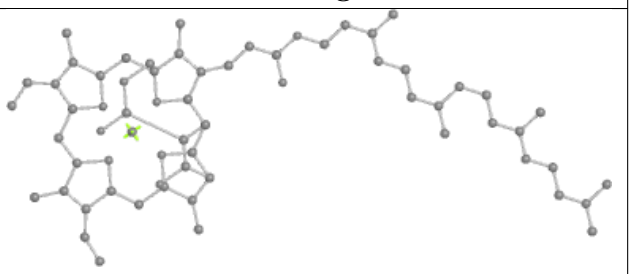


Torsions

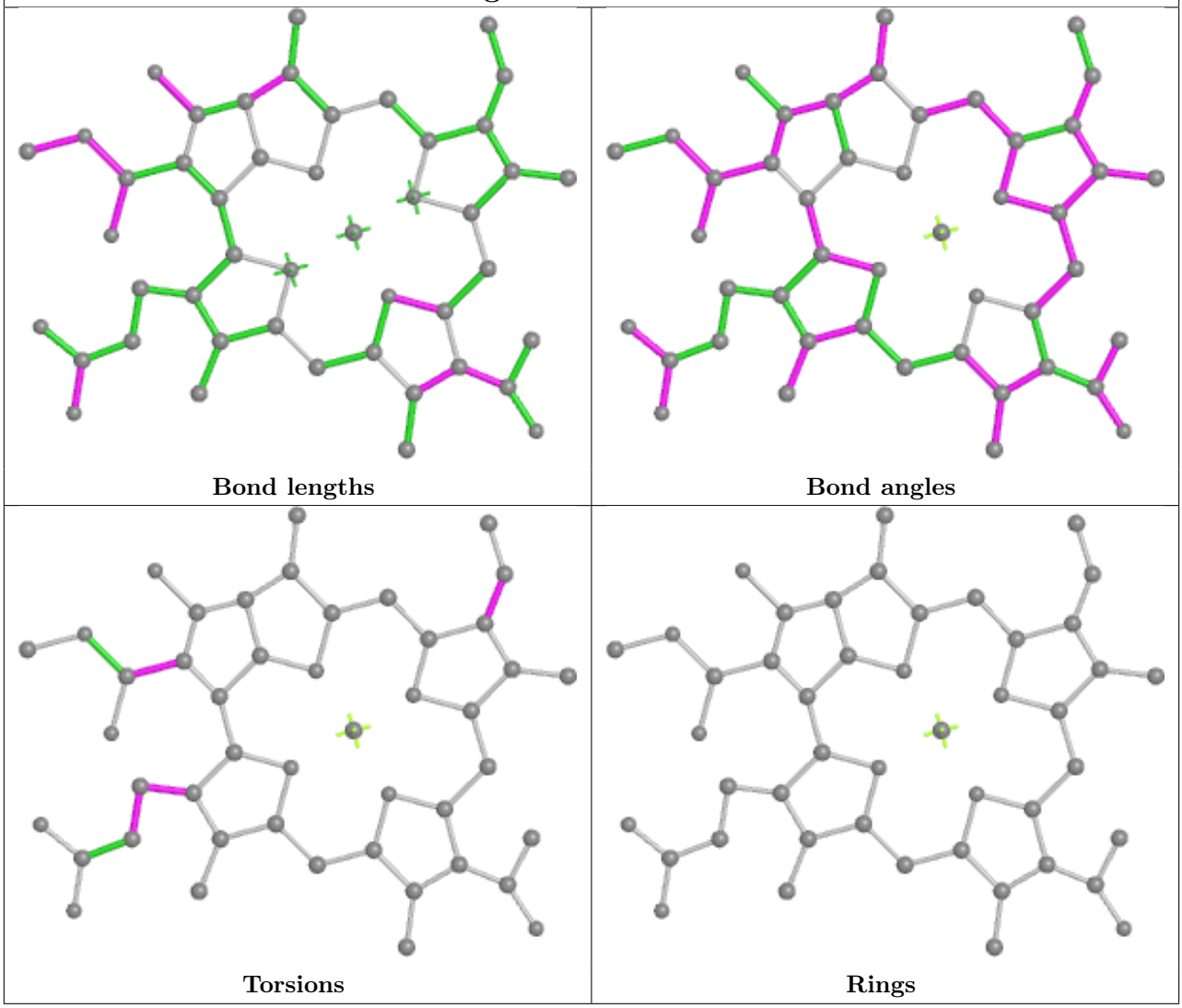


Rings

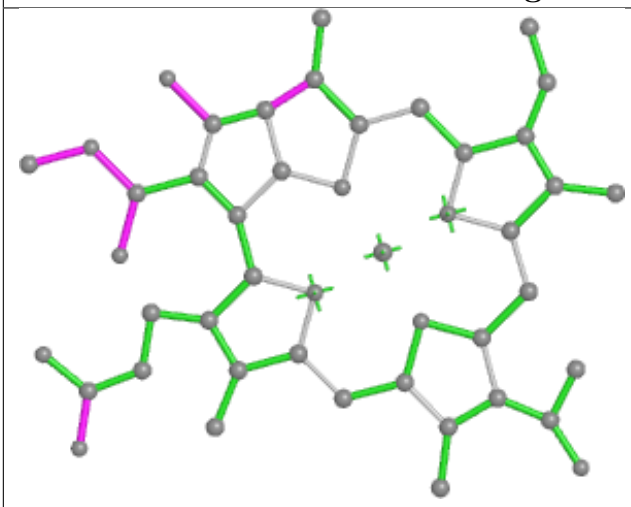
Ligand BCL G 372	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand G2O A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

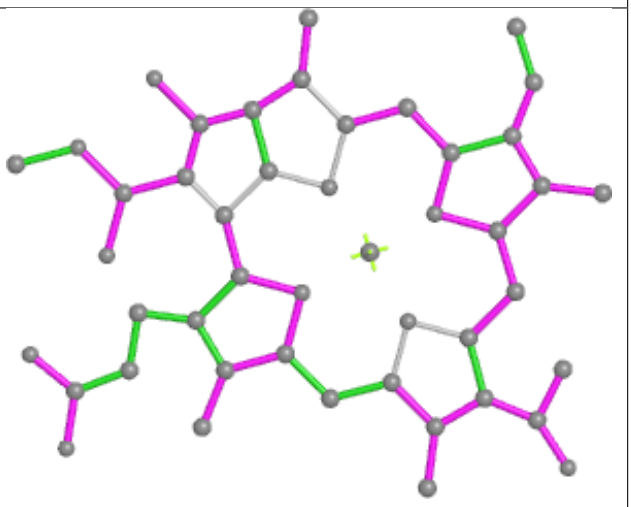
Ligand BCL A 807



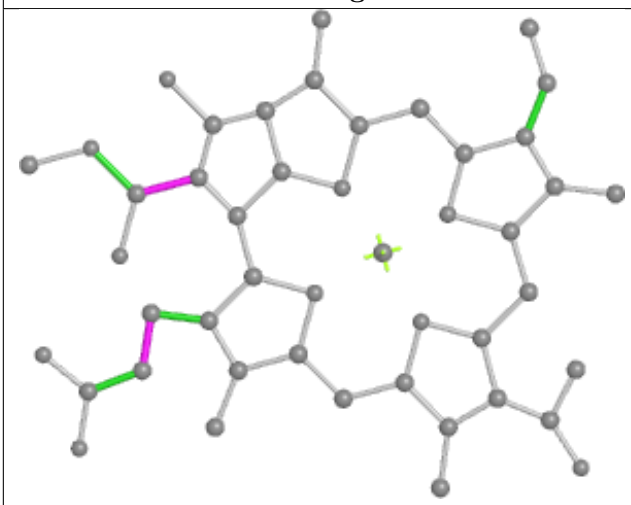
Ligand BCL A 814



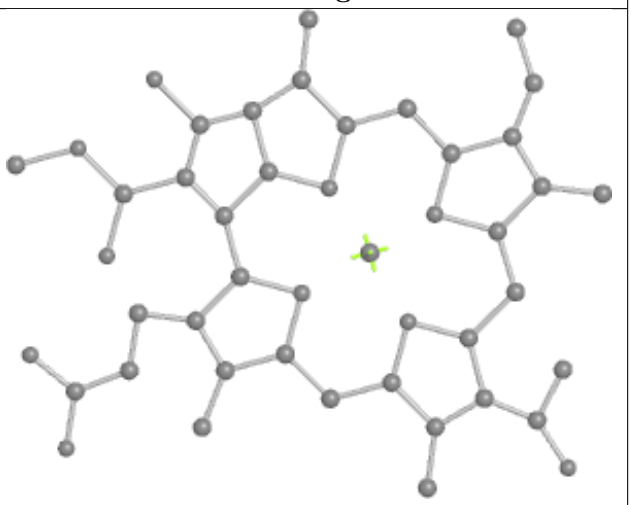
Bond lengths



Bond angles

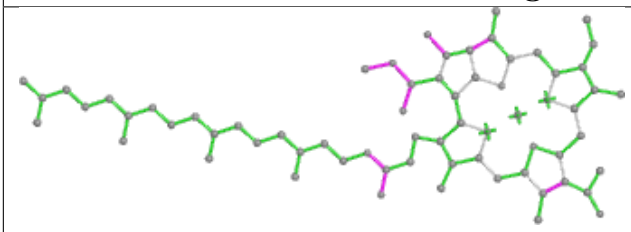


Torsions

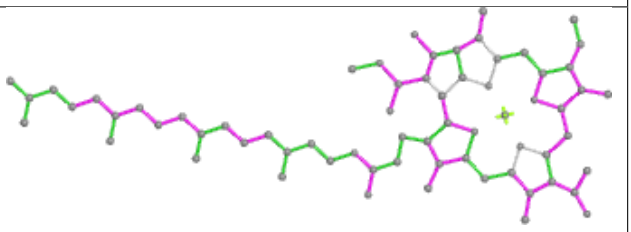


Rings

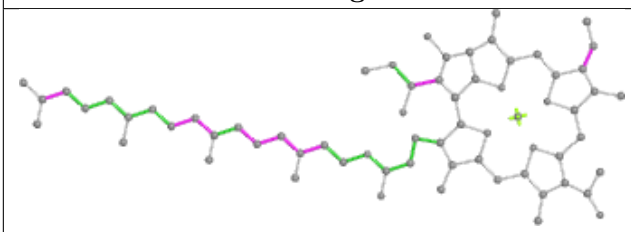
Ligand BCL G 375



Bond lengths



Bond angles



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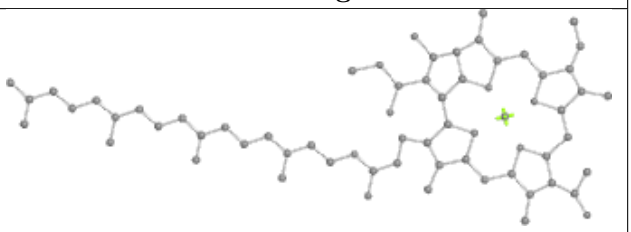
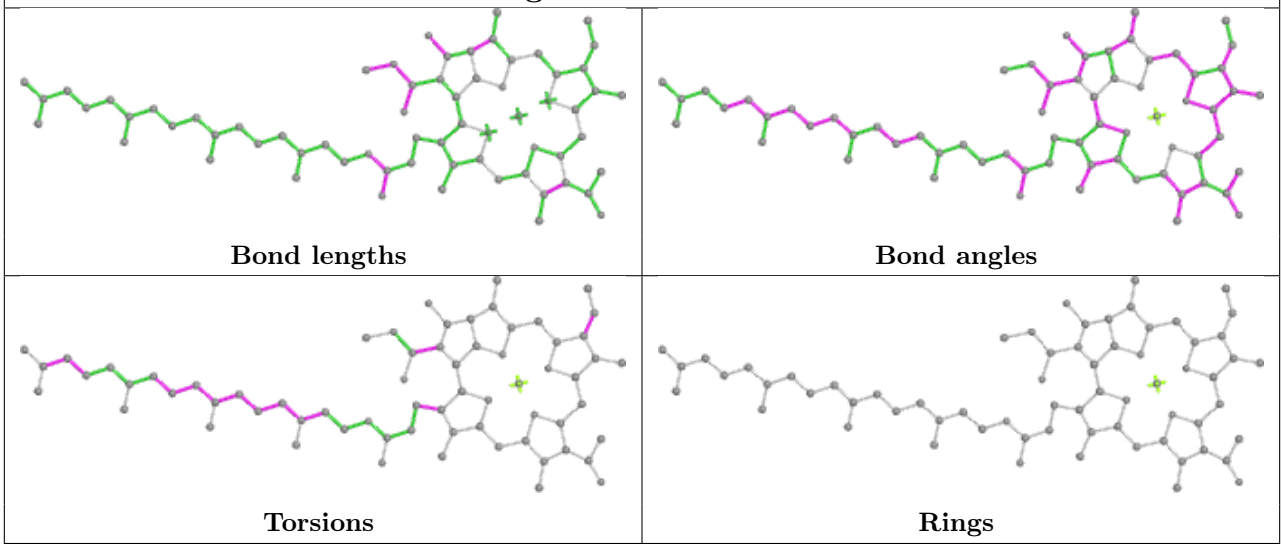
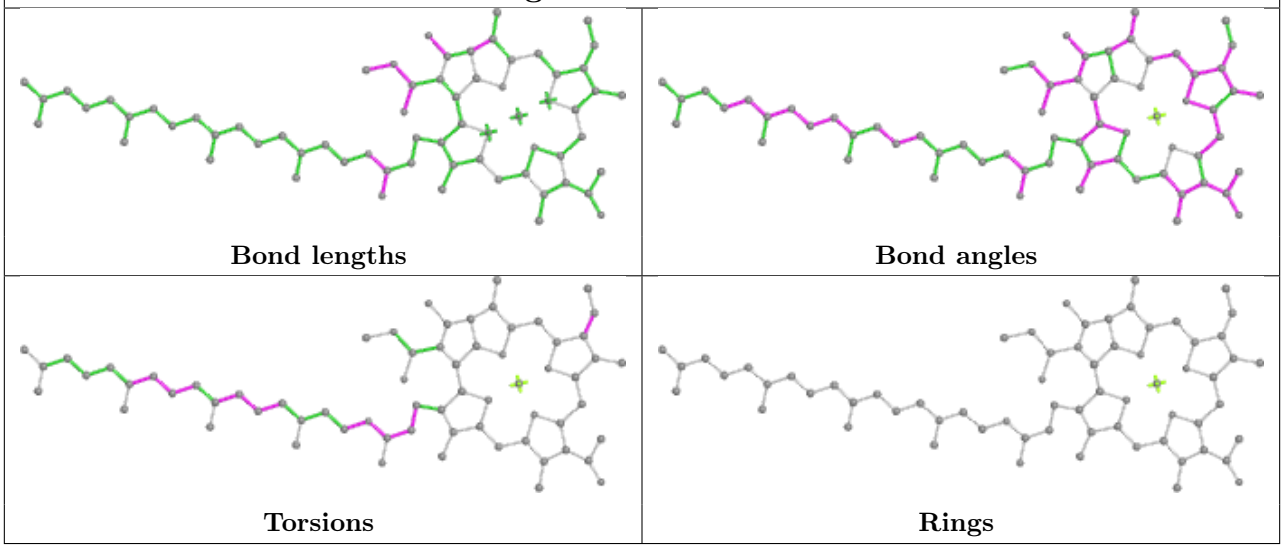


Rings

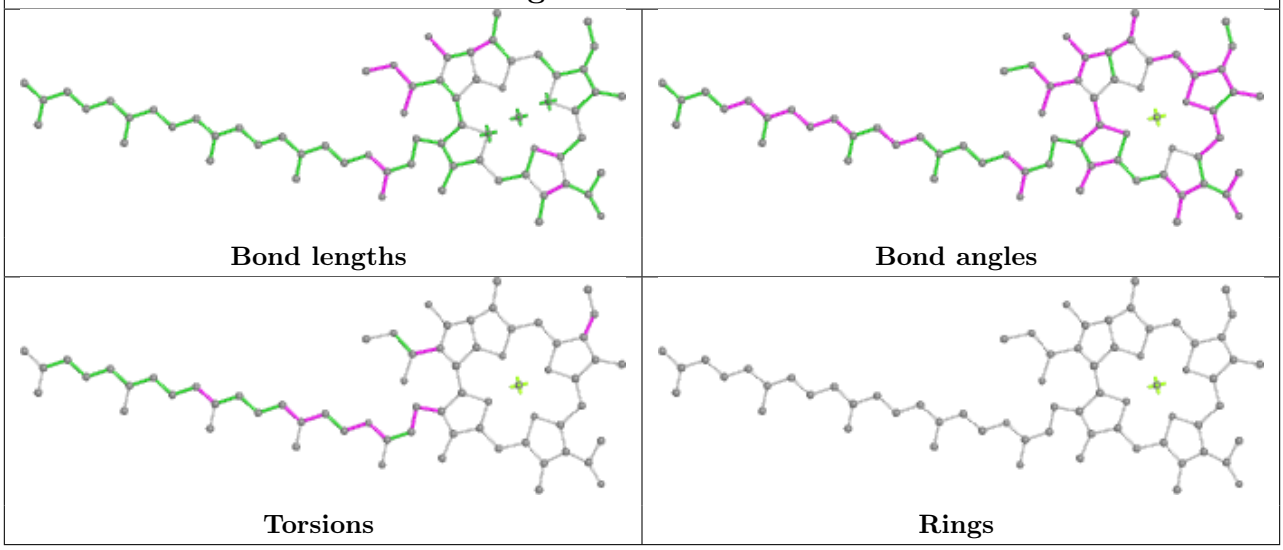
Ligand BCL A 808



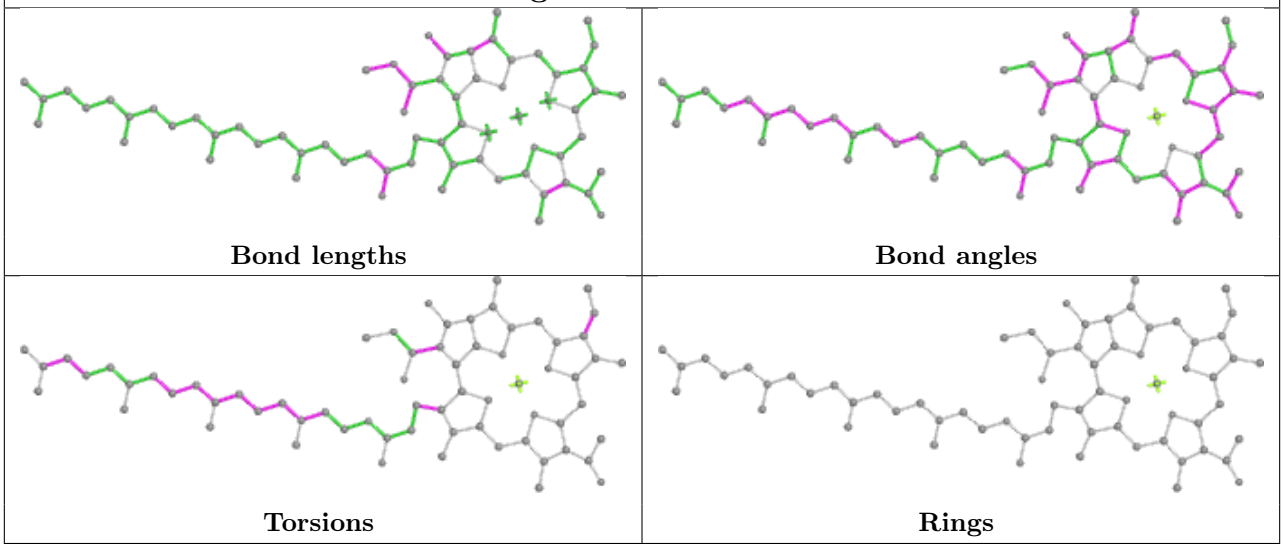
Ligand BCL G 374



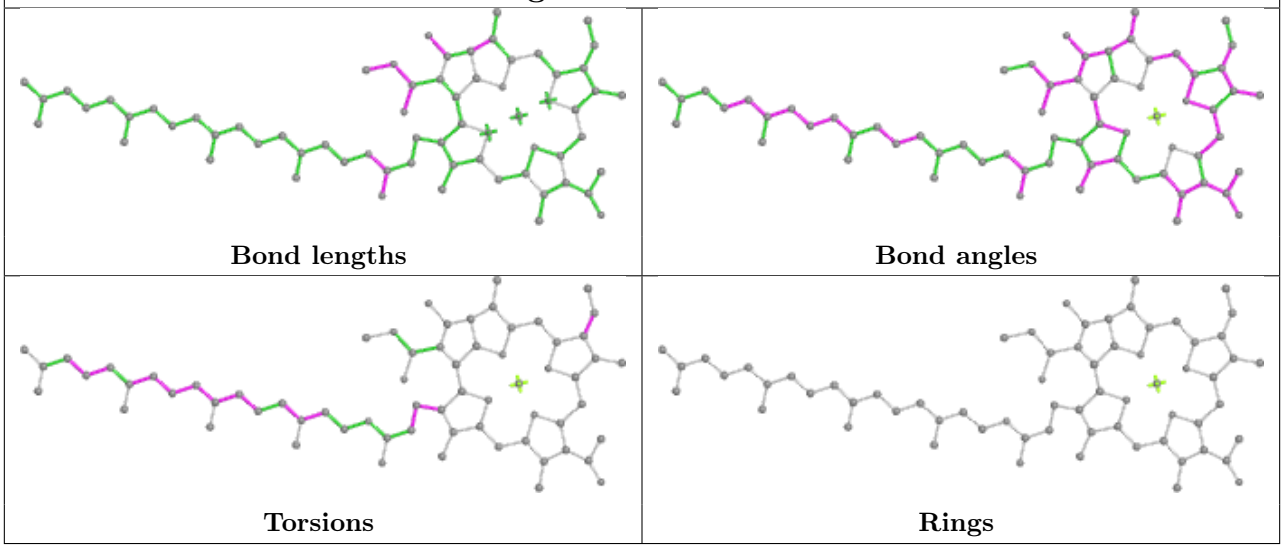
Ligand BCL F 373



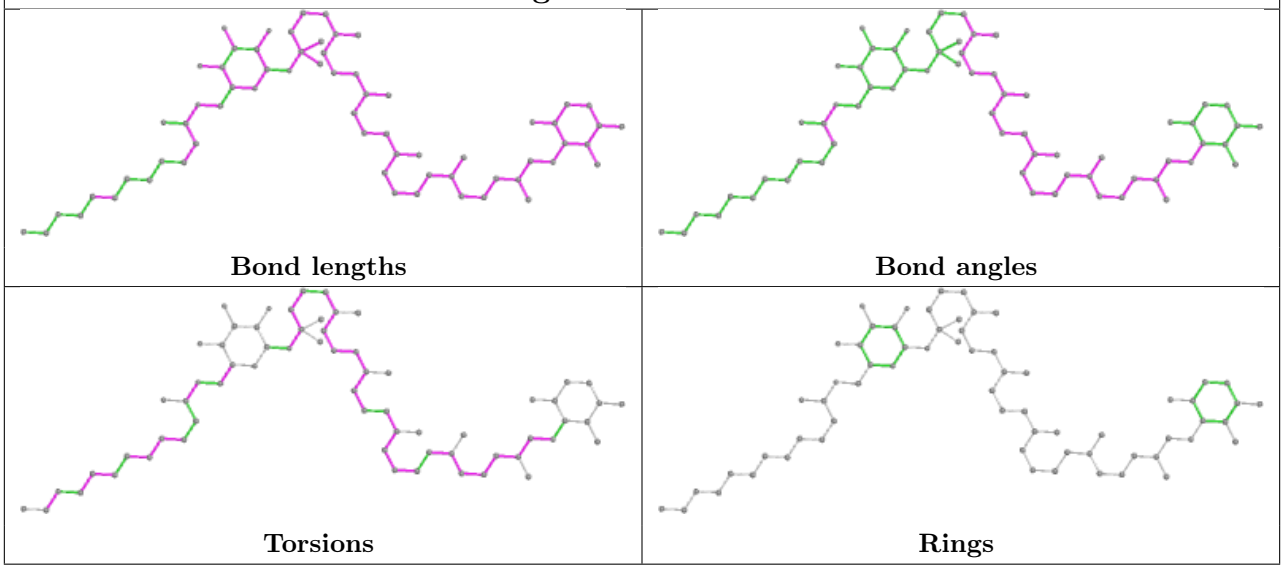
Ligand BCL a 808



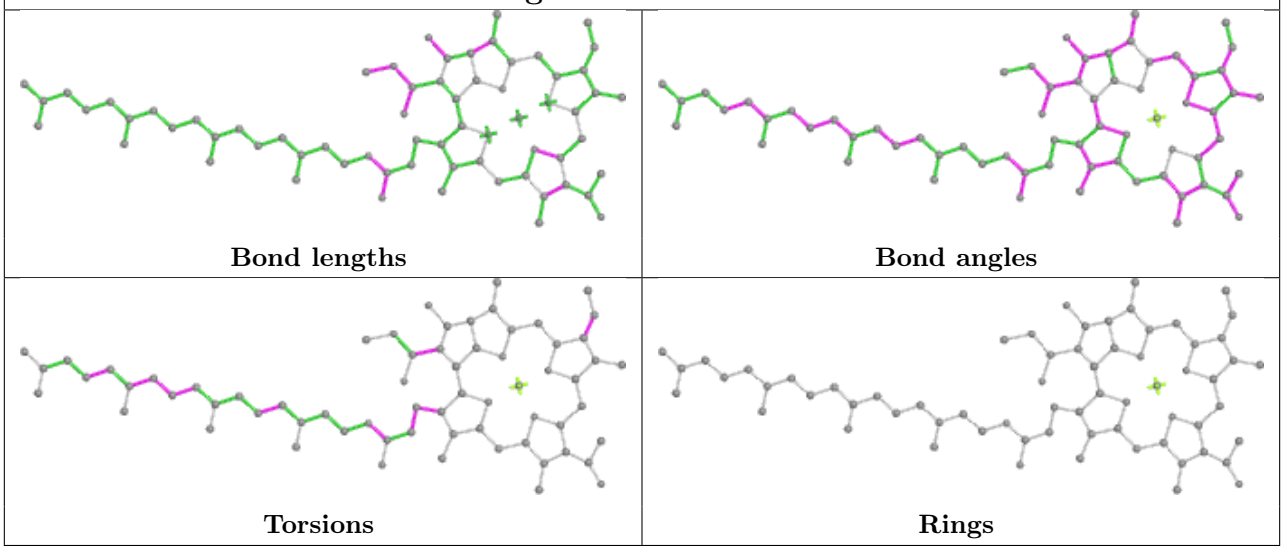
Ligand BCL F 372



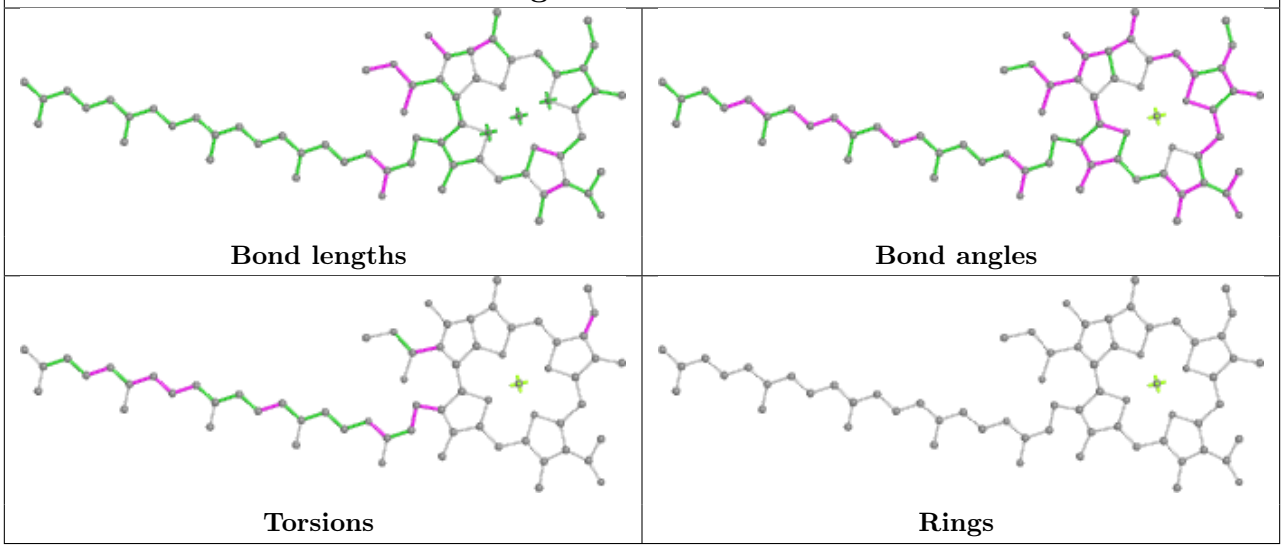
Ligand F39 A 817



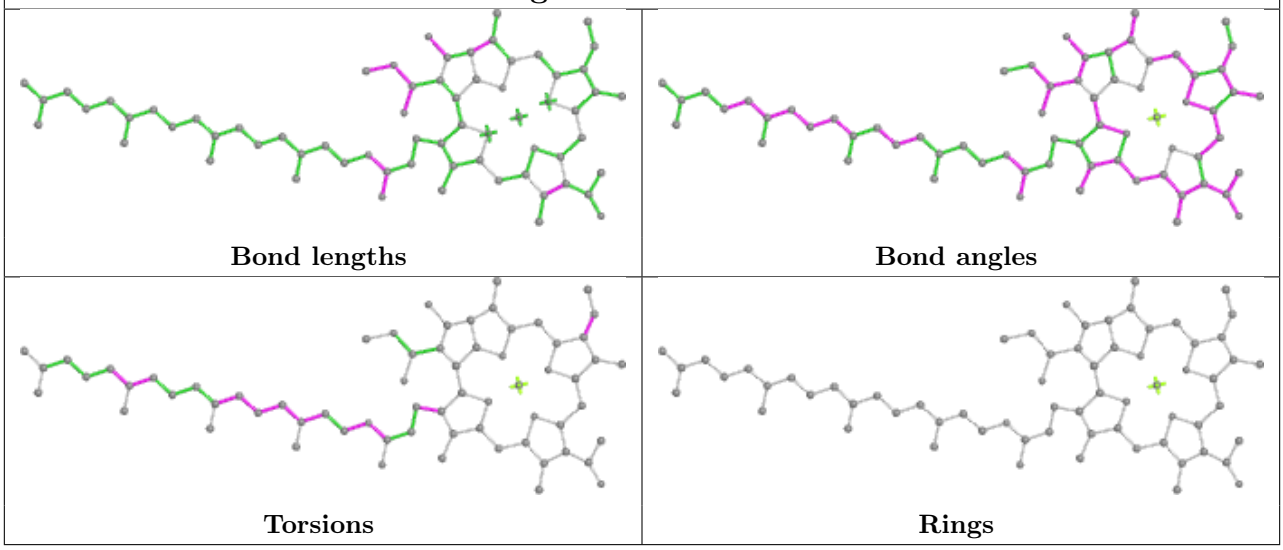
Ligand BCL A 812



Ligand BCL a 812



Ligand BCL a 811



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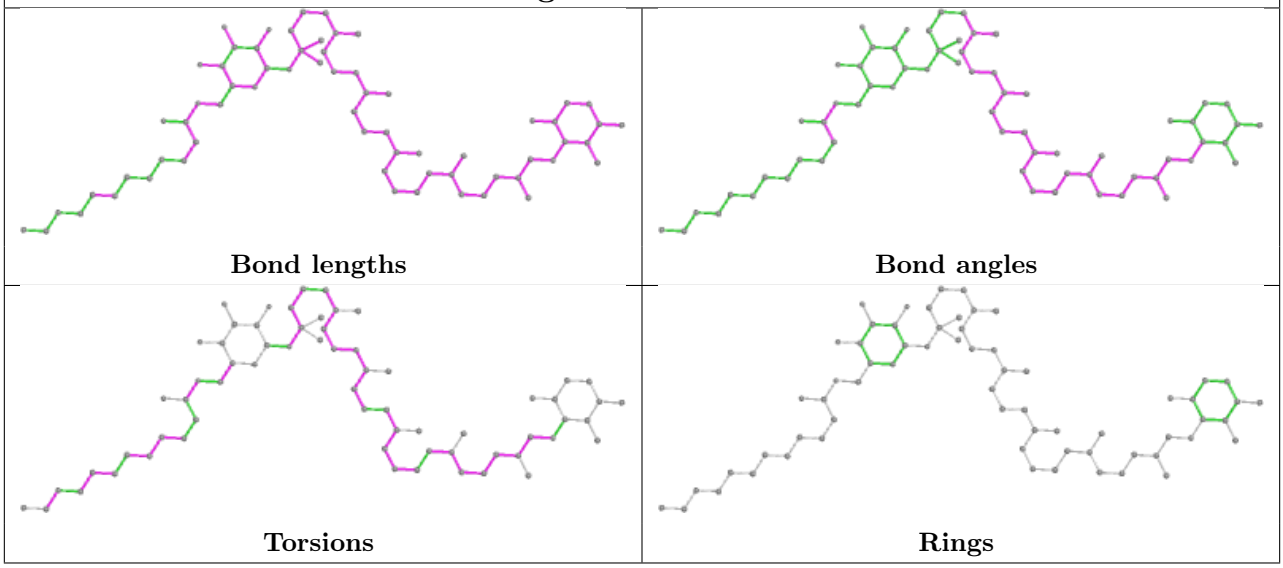
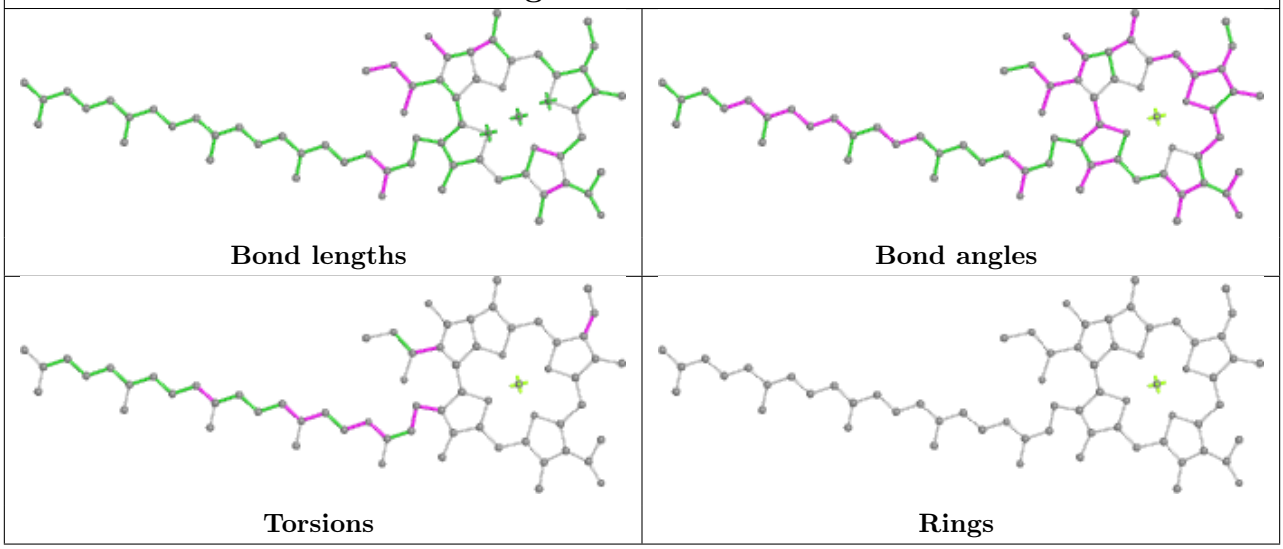
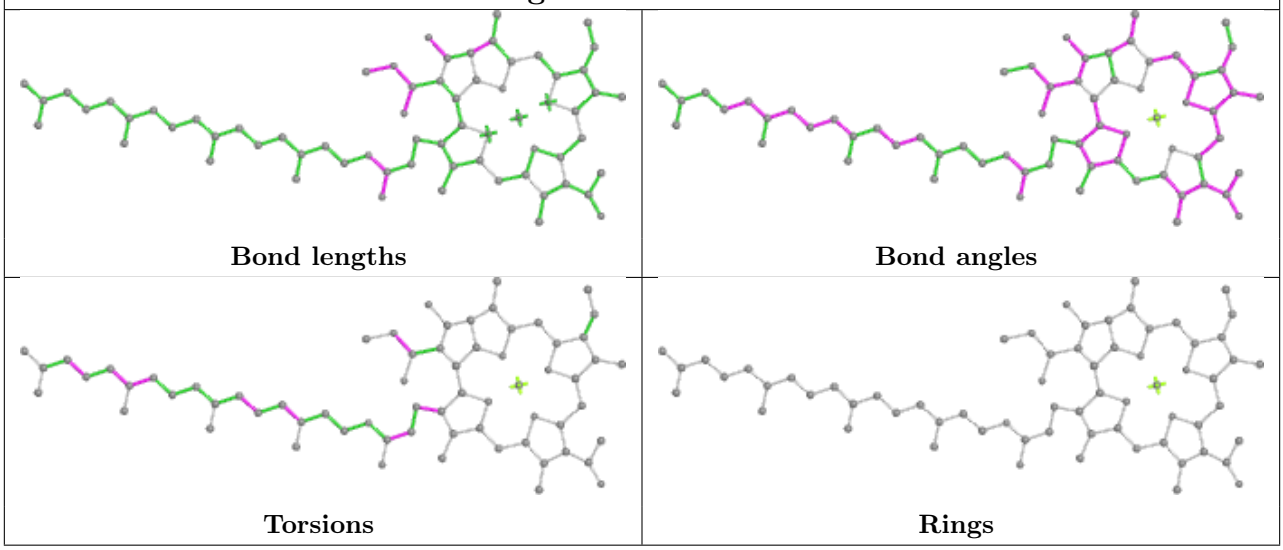


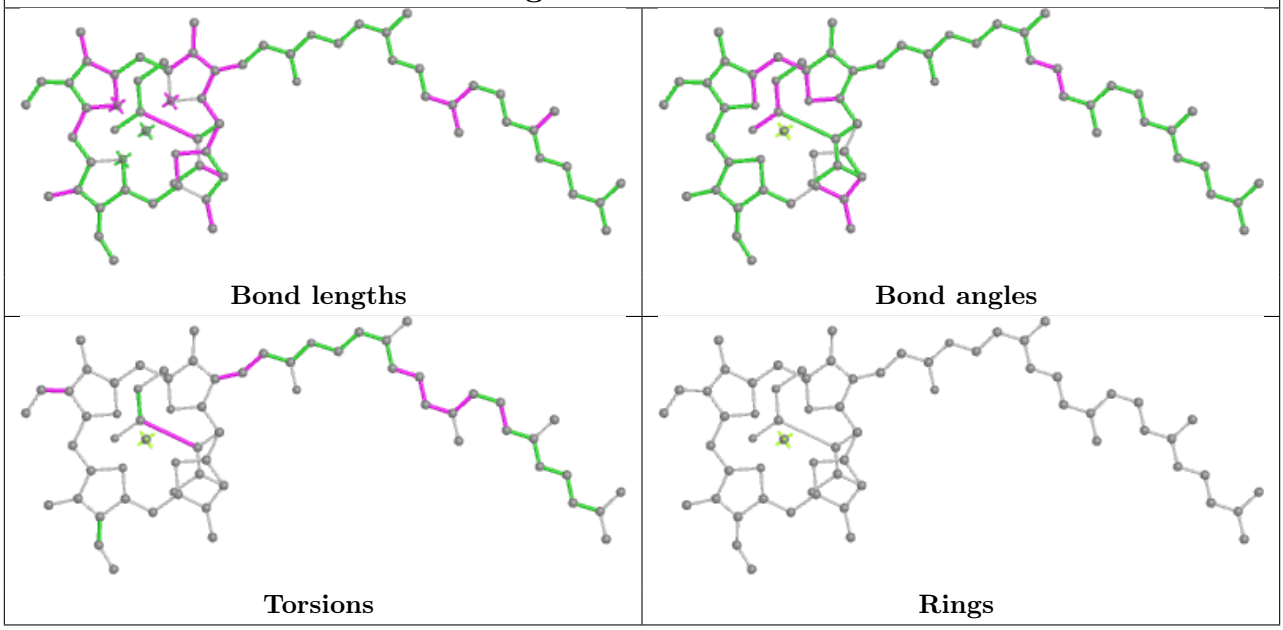
Ligand BCL G 373



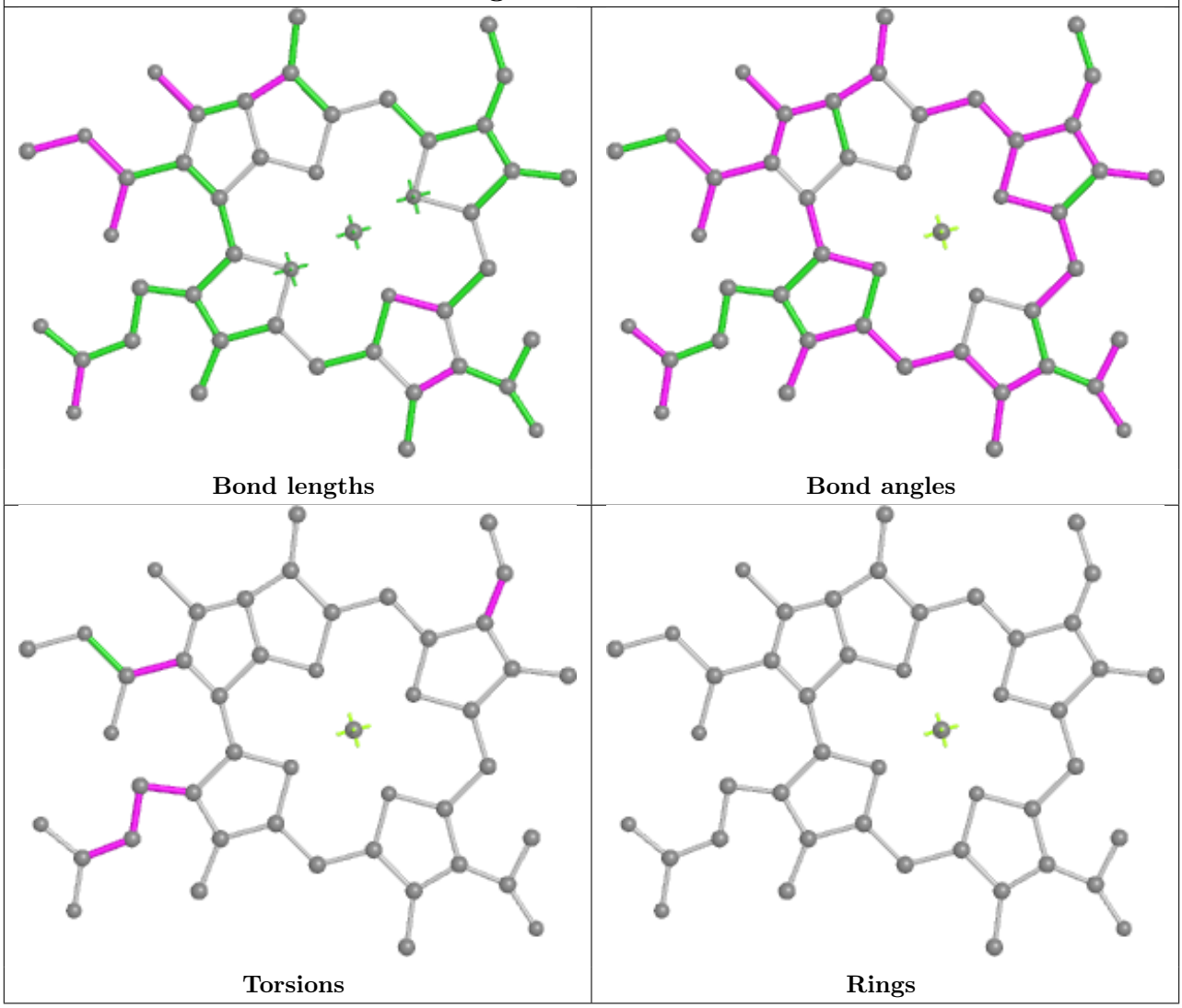
Ligand BCL F 371



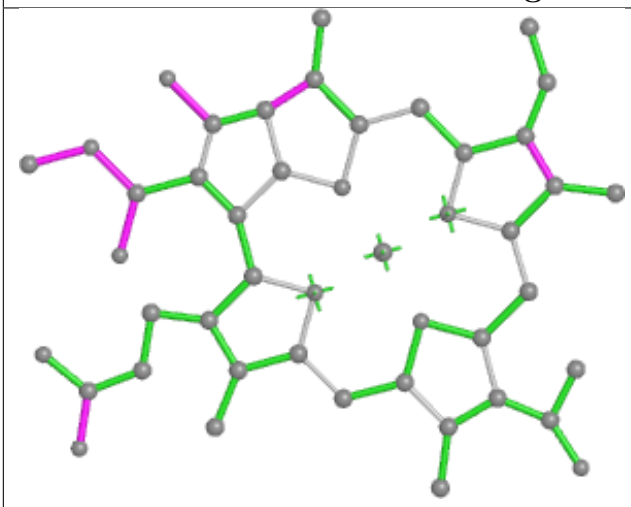
Ligand G2O A 802



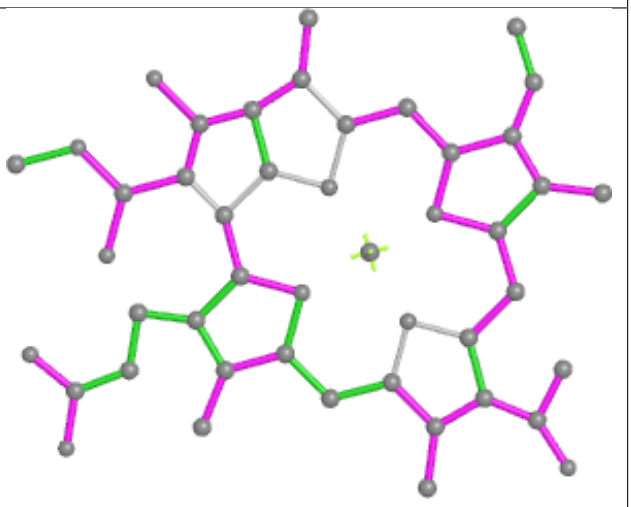
Ligand BCL a 810



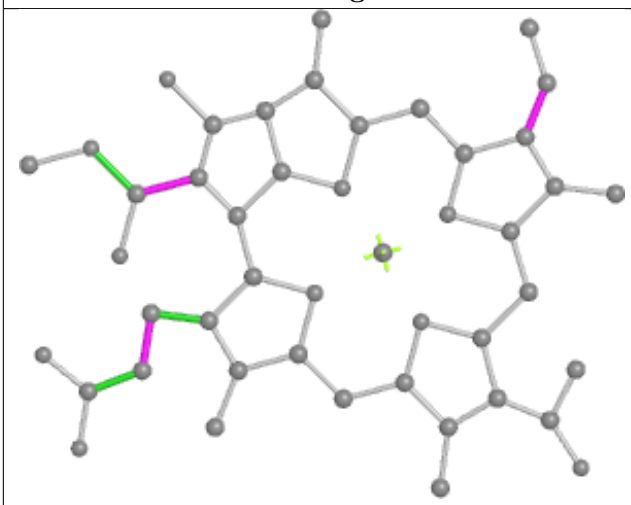
Ligand BCL A 815



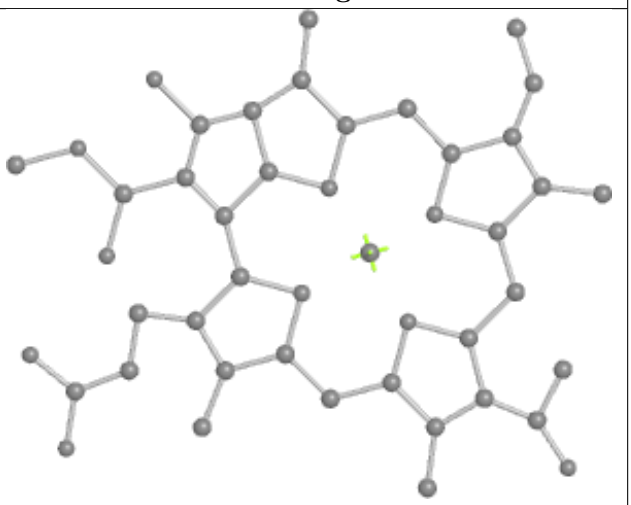
Bond lengths



Bond angles

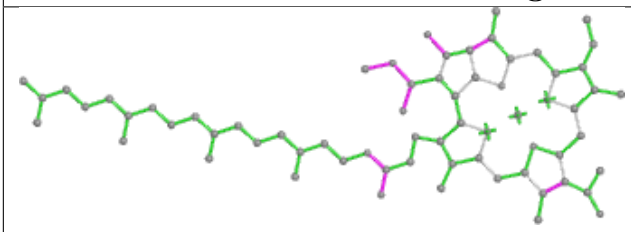


Torsions



Rings

Ligand BCL F 375



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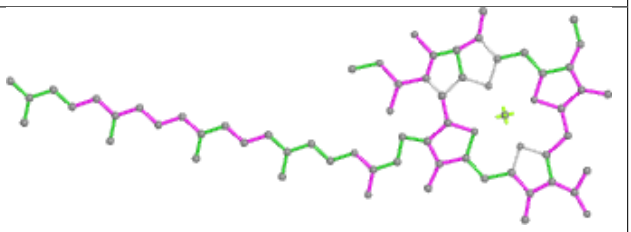
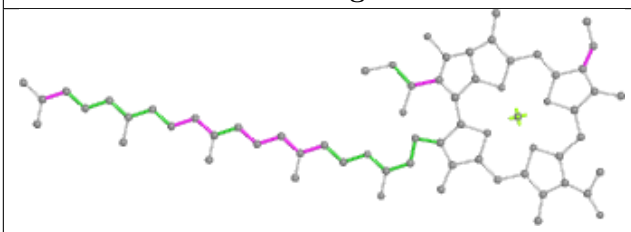
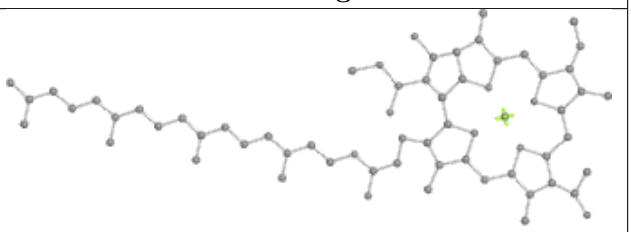


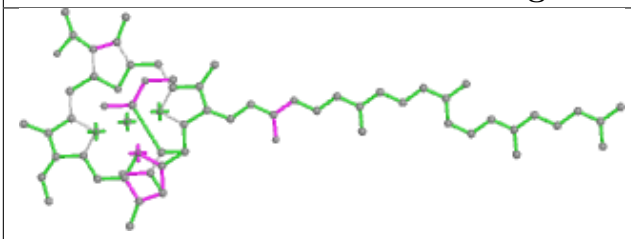
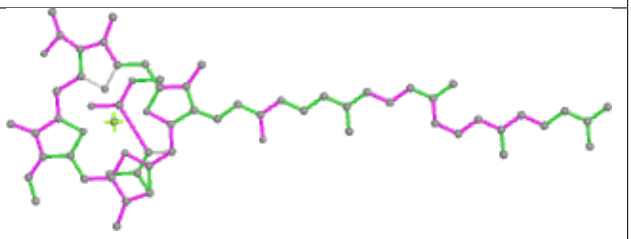
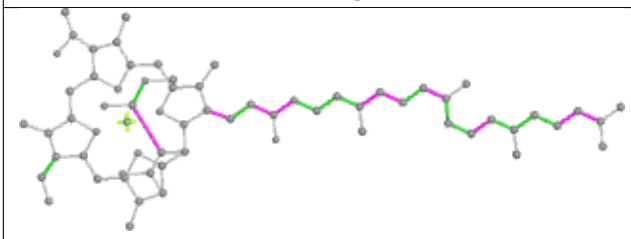
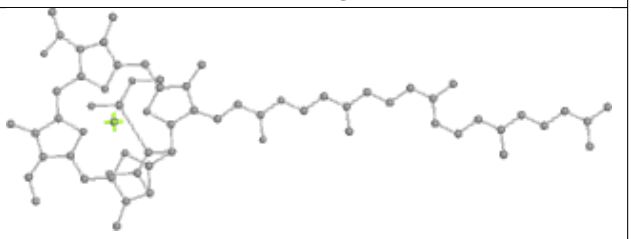
Bond angles

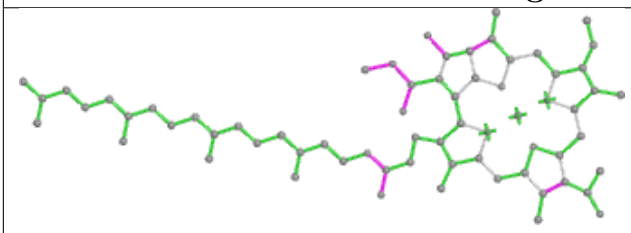
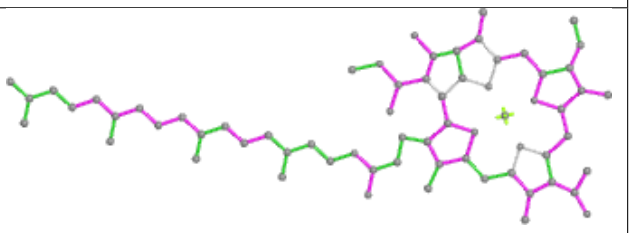
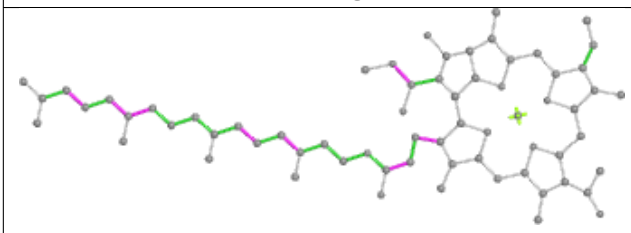
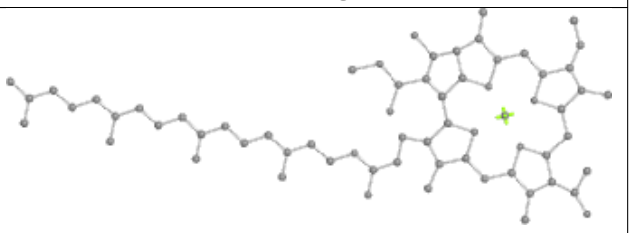


Torsions

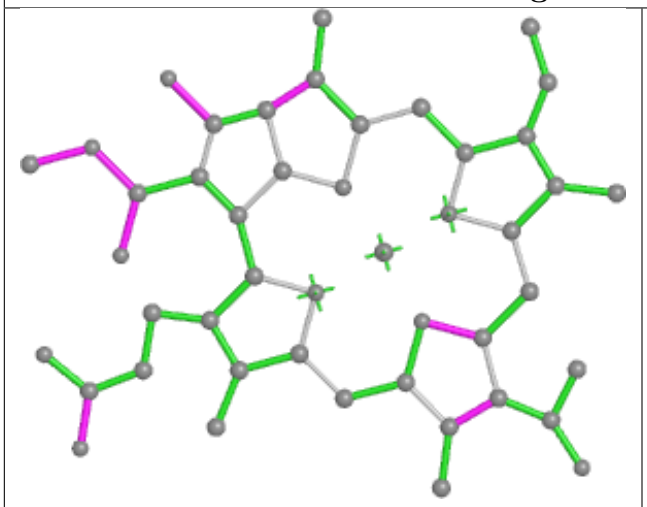


Rings

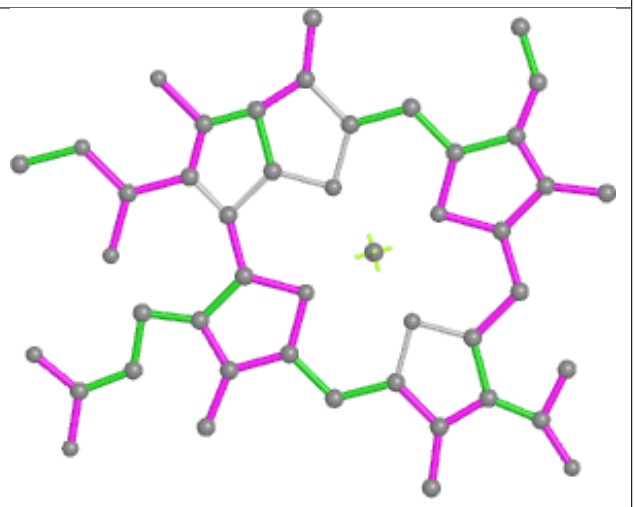
Ligand GS0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL E 371	
 Bond lengths	 Bond angles
 Torsions	 Rings

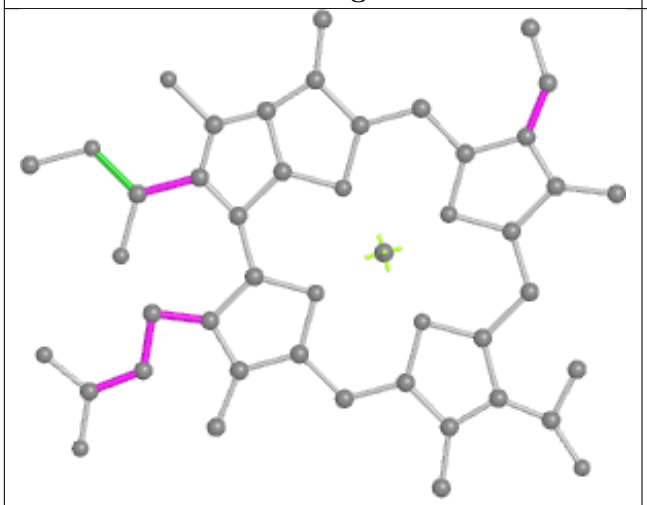
Ligand BCL a 804



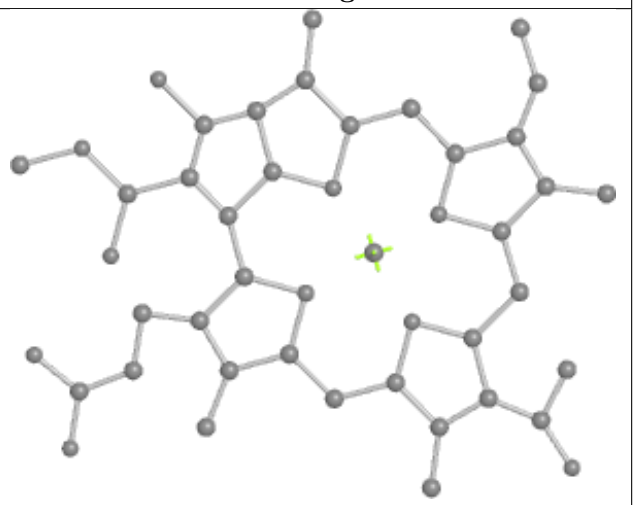
Bond lengths



Bond angles

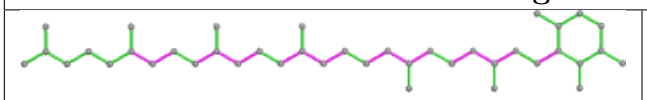


Torsions

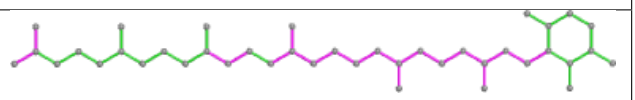


Rings

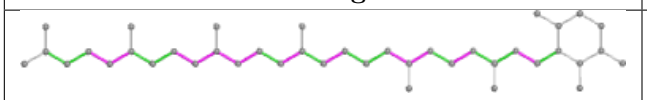
Ligand F26 A 816



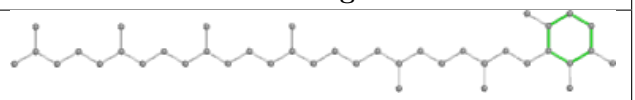
Bond lengths



Bond angles

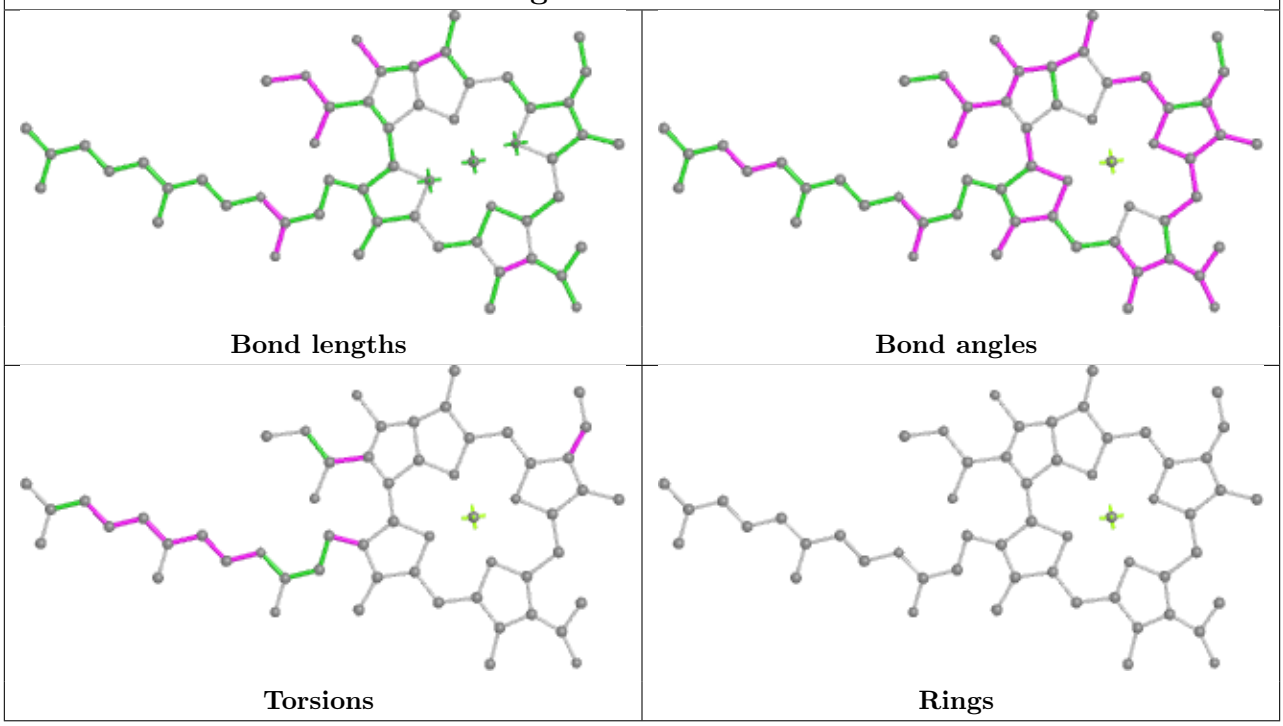


Torsions

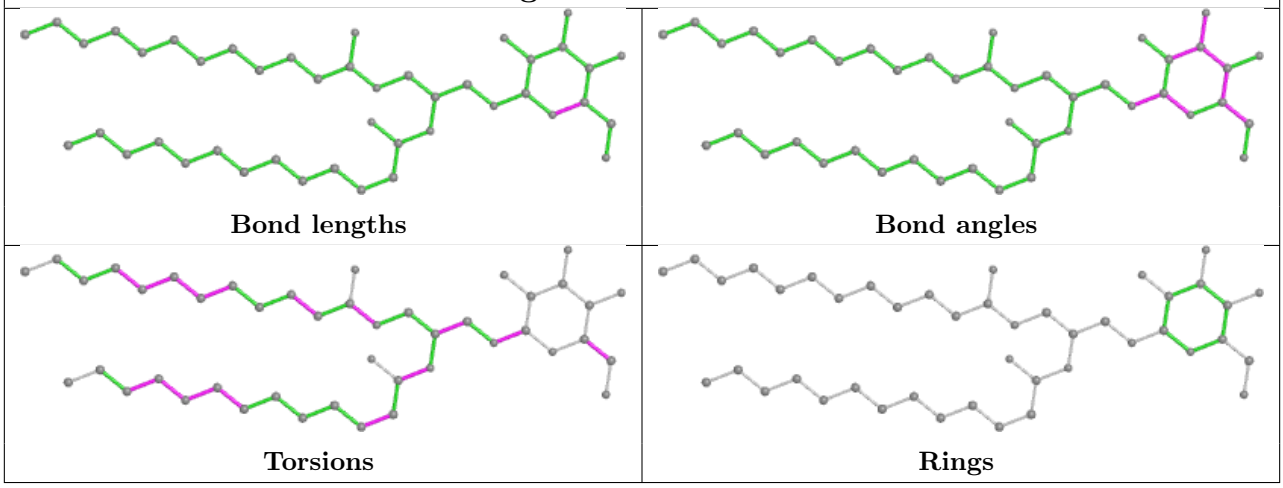


Rings

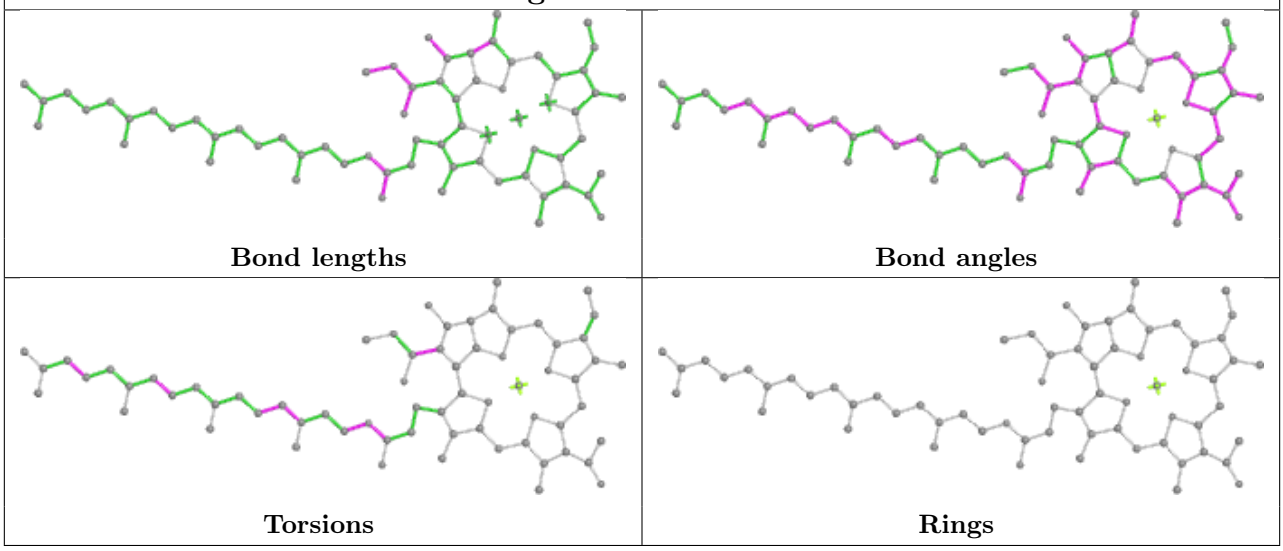
Ligand BCL a 805



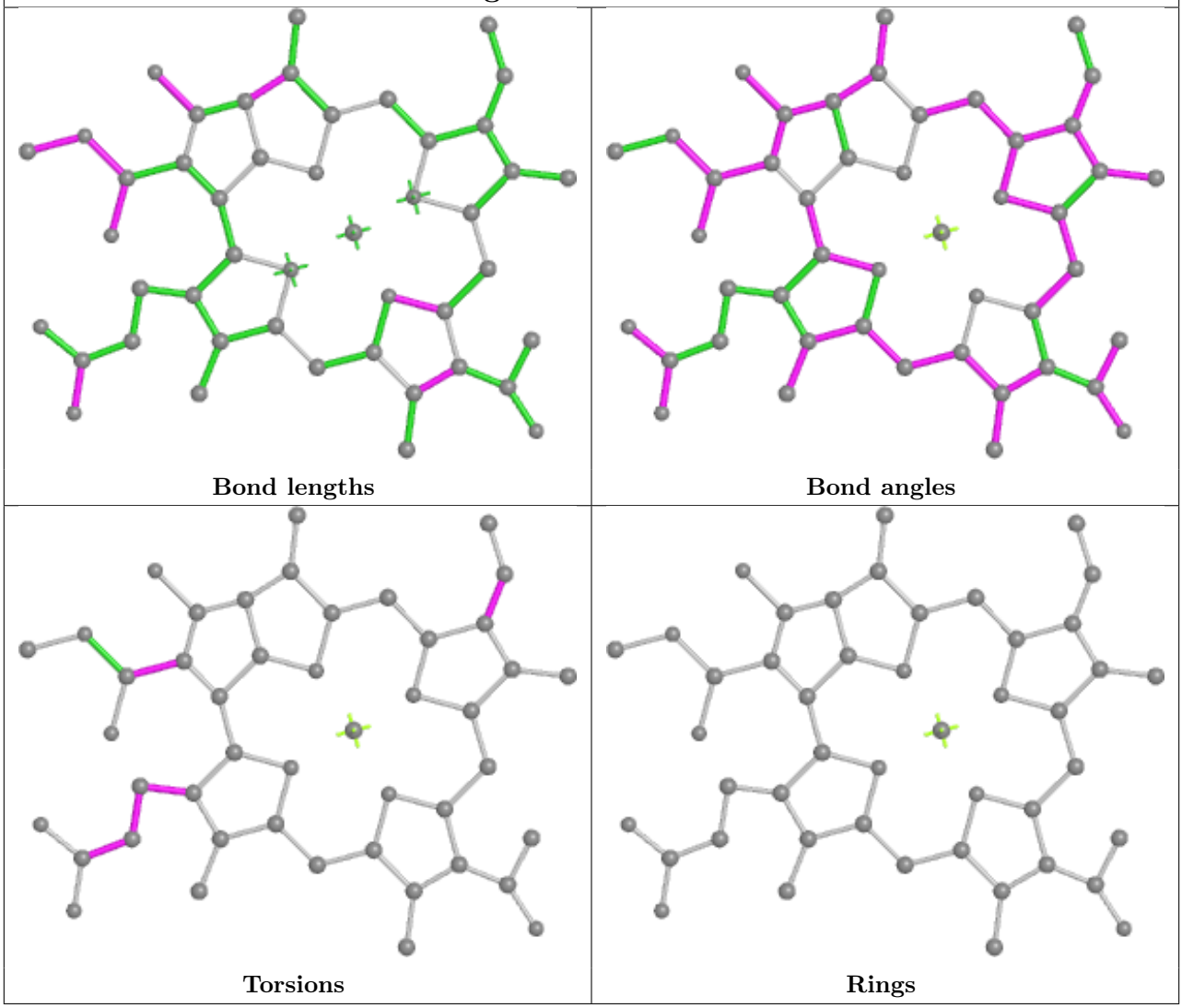
Ligand LMG A 819

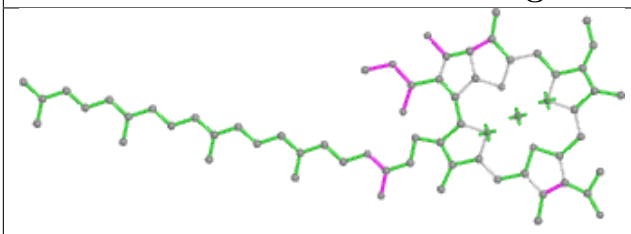
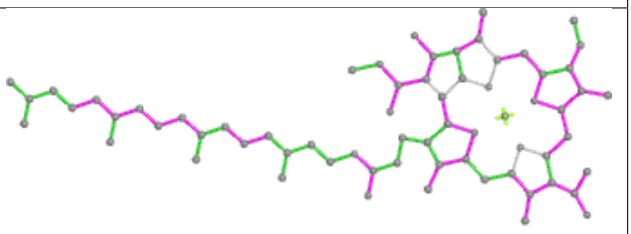
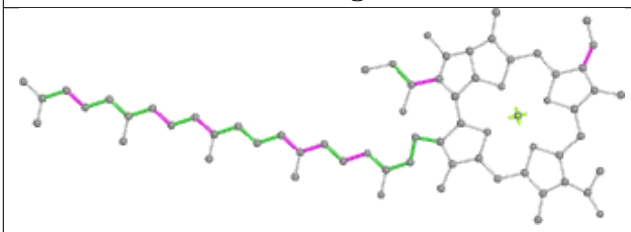
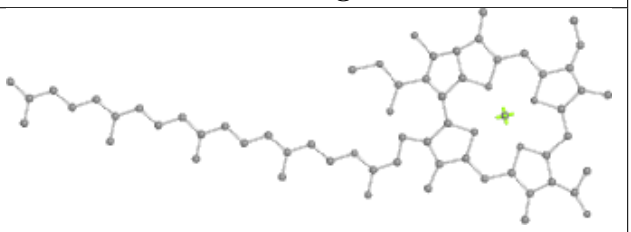


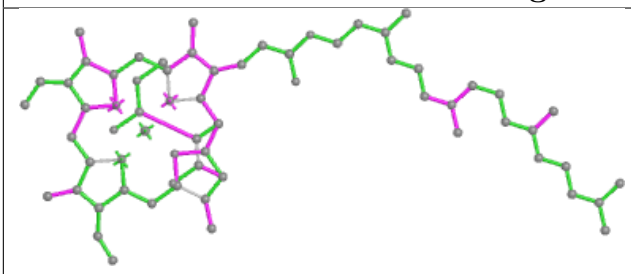
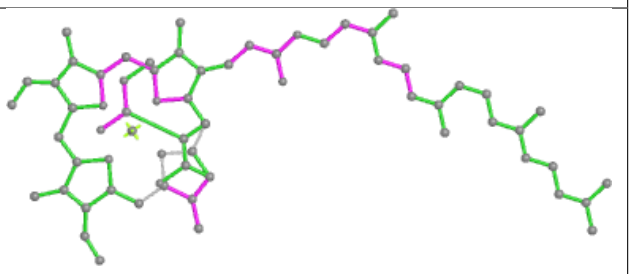
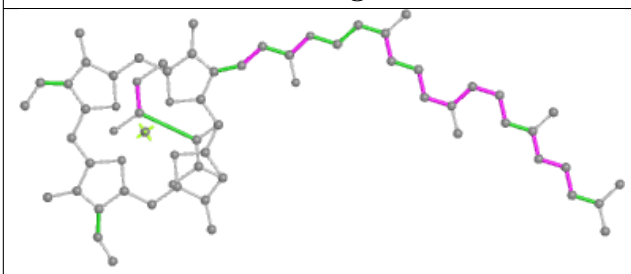
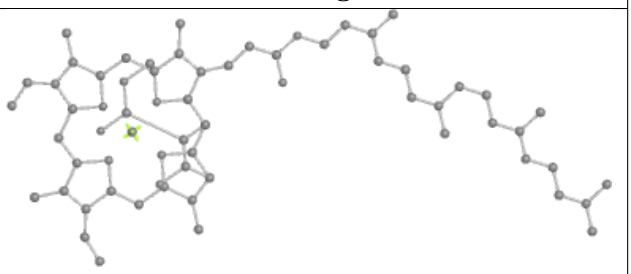
Ligand BCL F 376

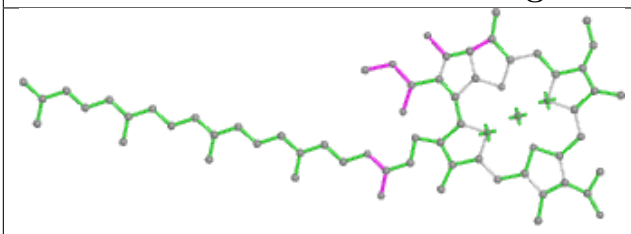
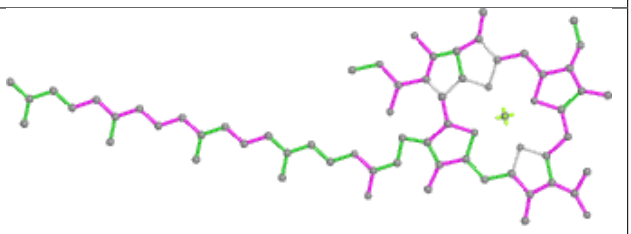
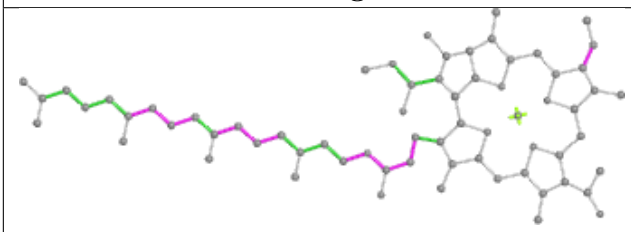
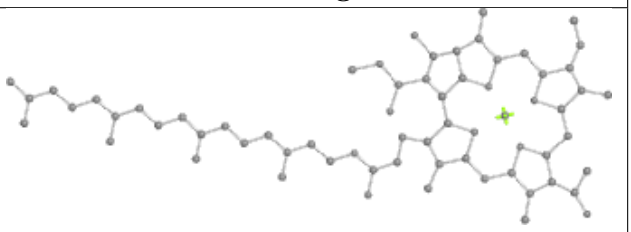


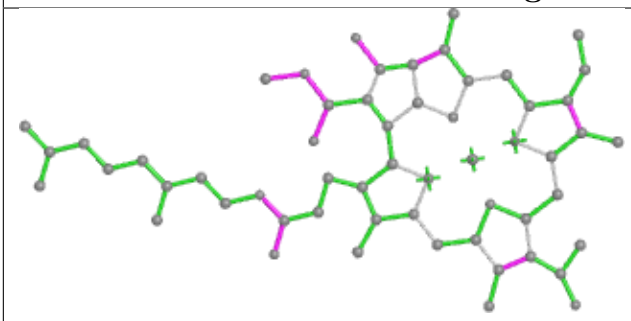
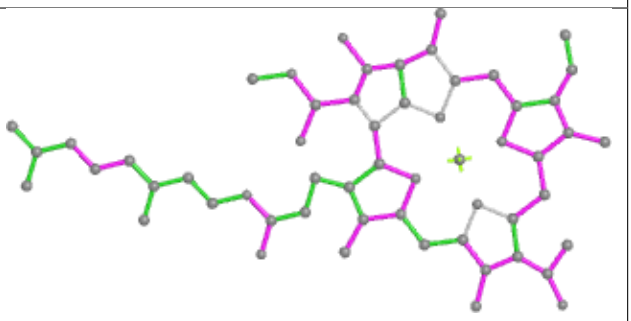
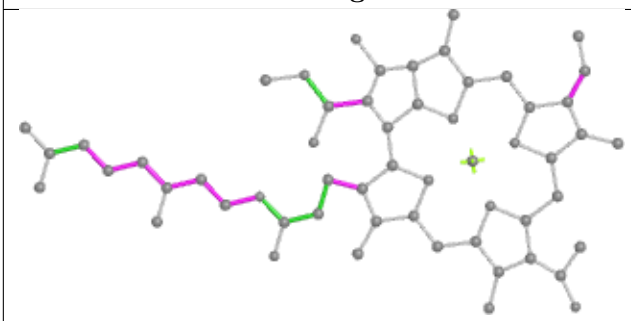
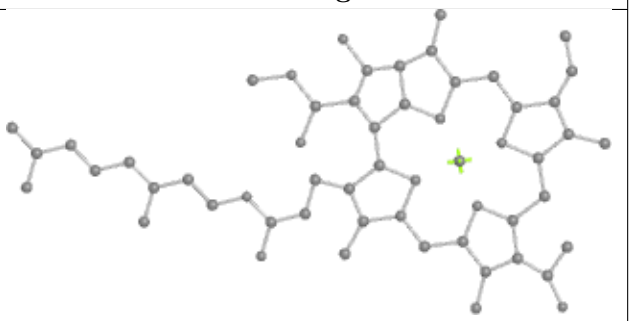
Ligand BCL A 810



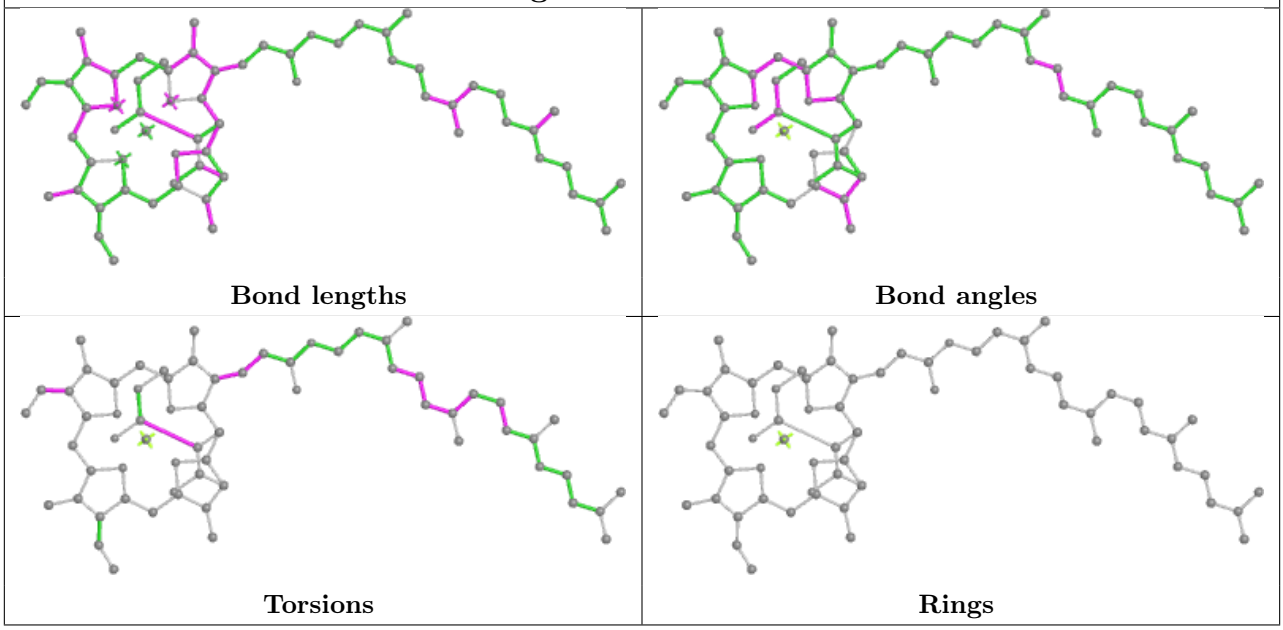
Ligand BCL E 377	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand G2O a 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

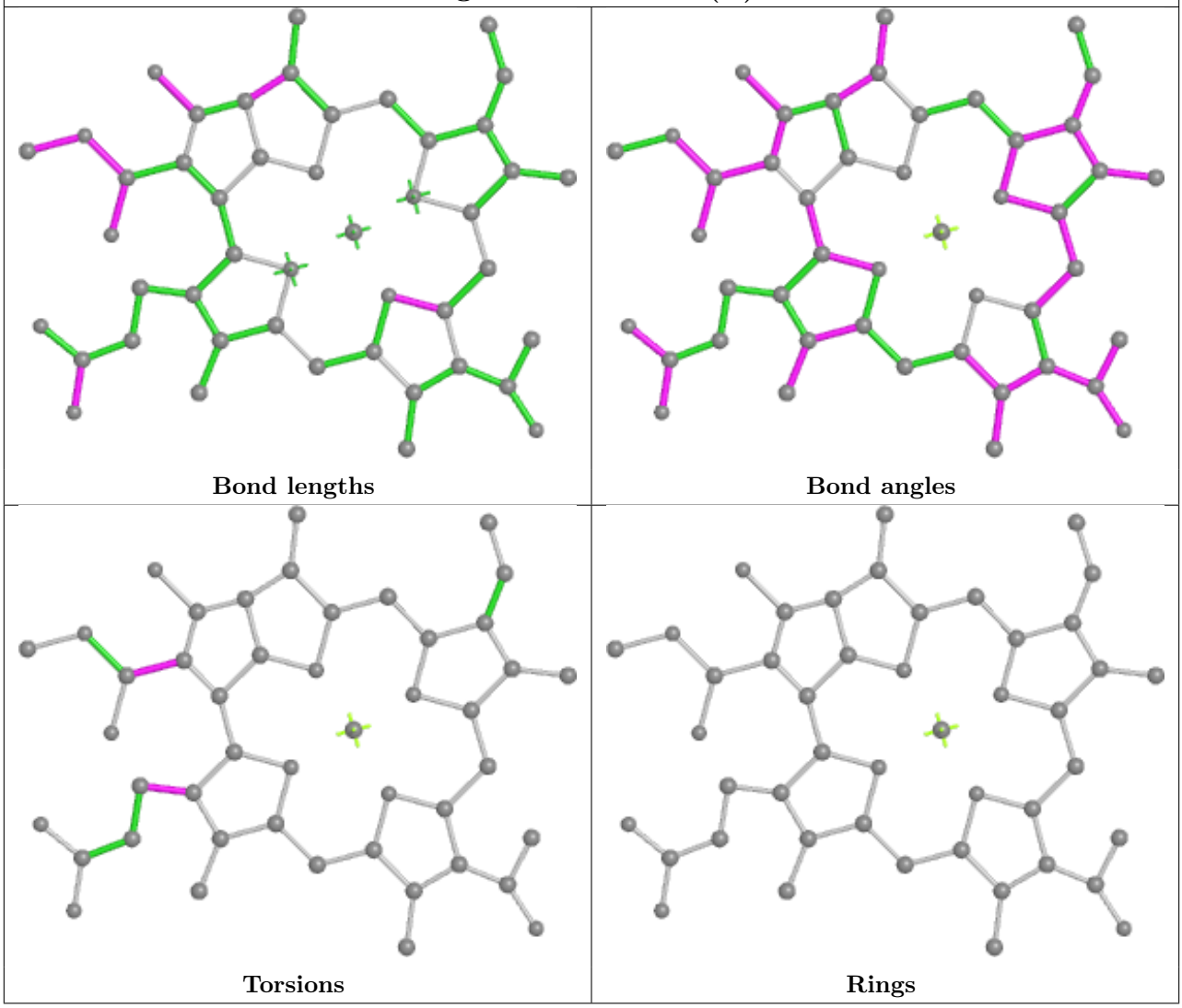
Ligand BCL E 374	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

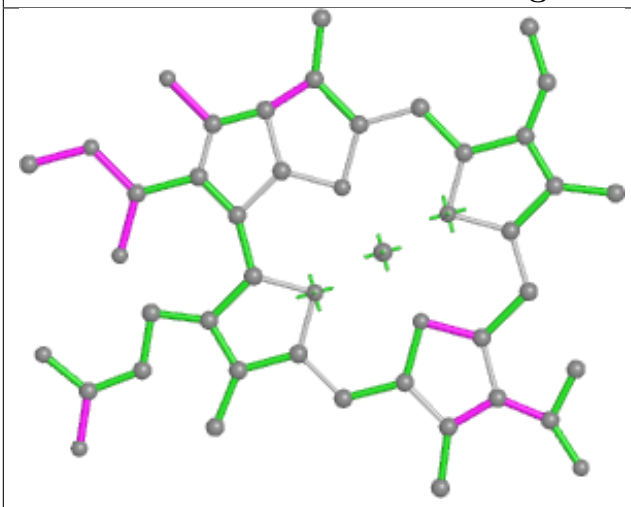
Ligand G2O a 802



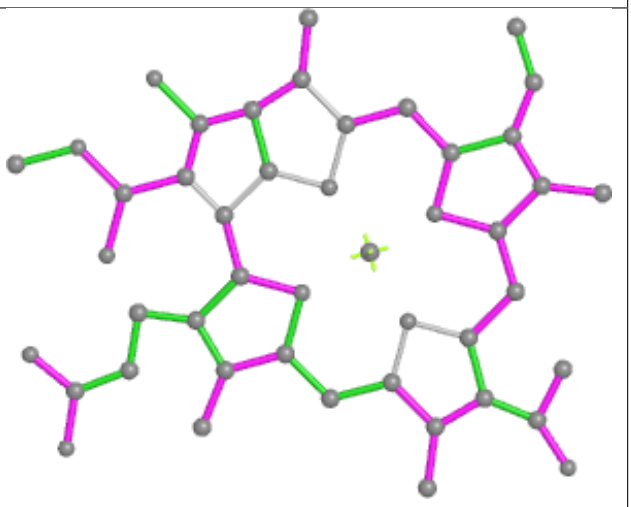
Ligand BCL E 378 (B)



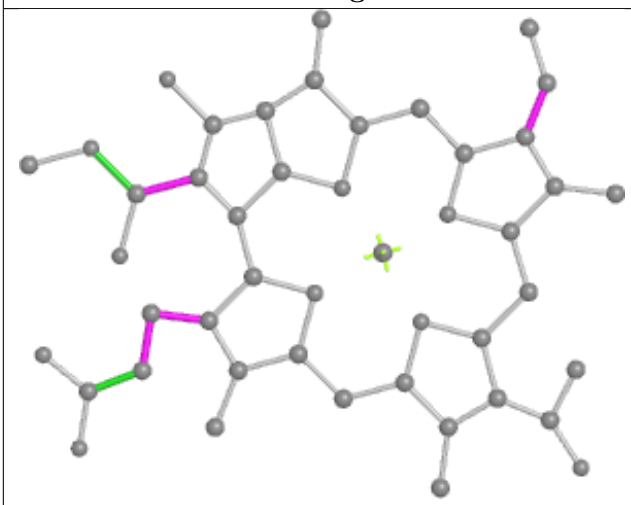
Ligand BCL a 807



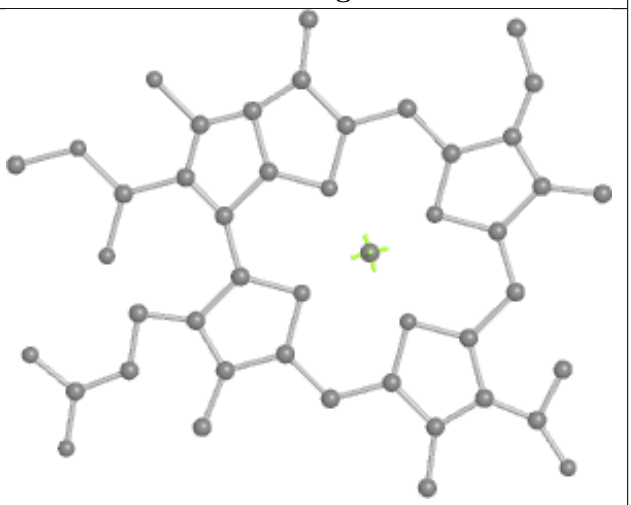
Bond lengths



Bond angles

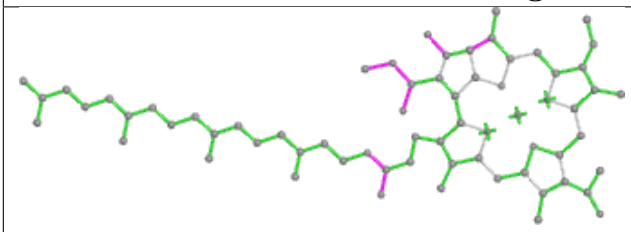


Torsions



Rings

Ligand BCL F 377



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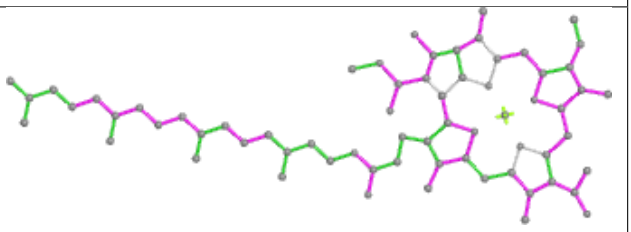
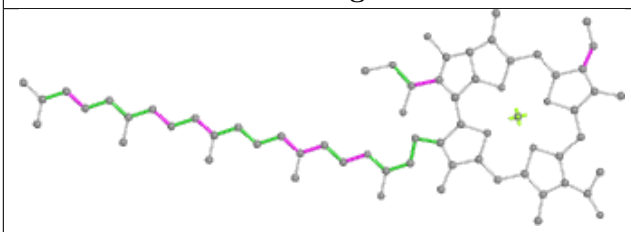
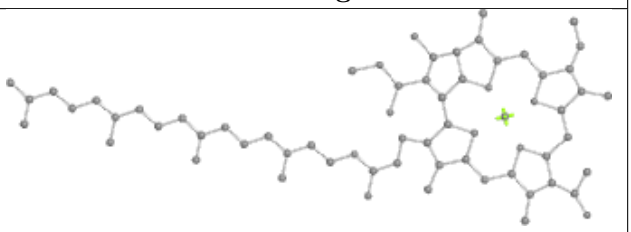


Bond angles

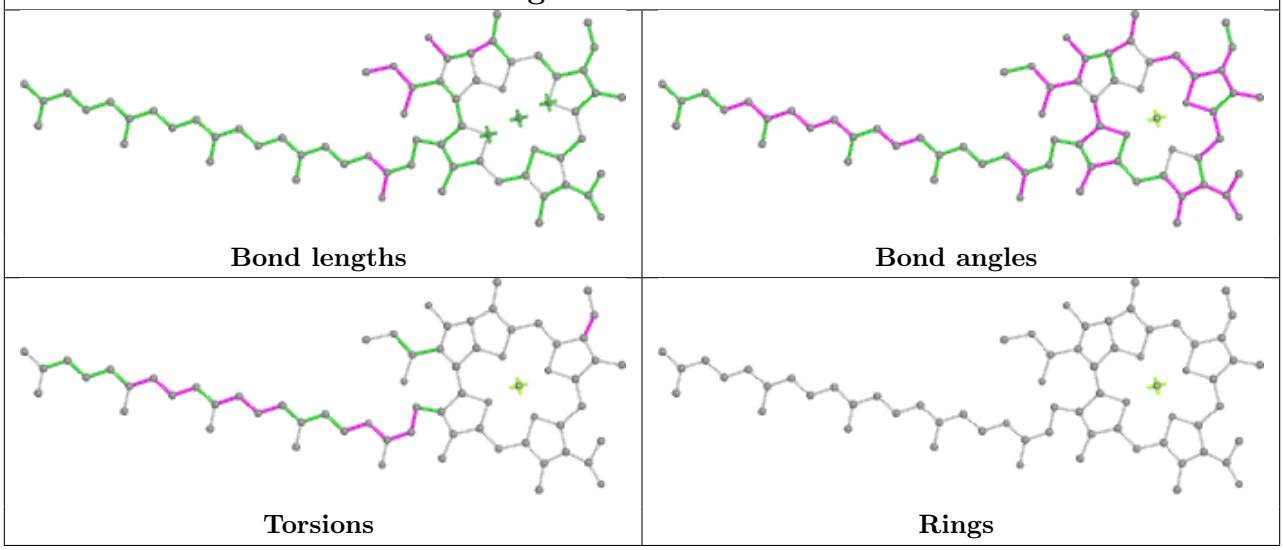


Torsions

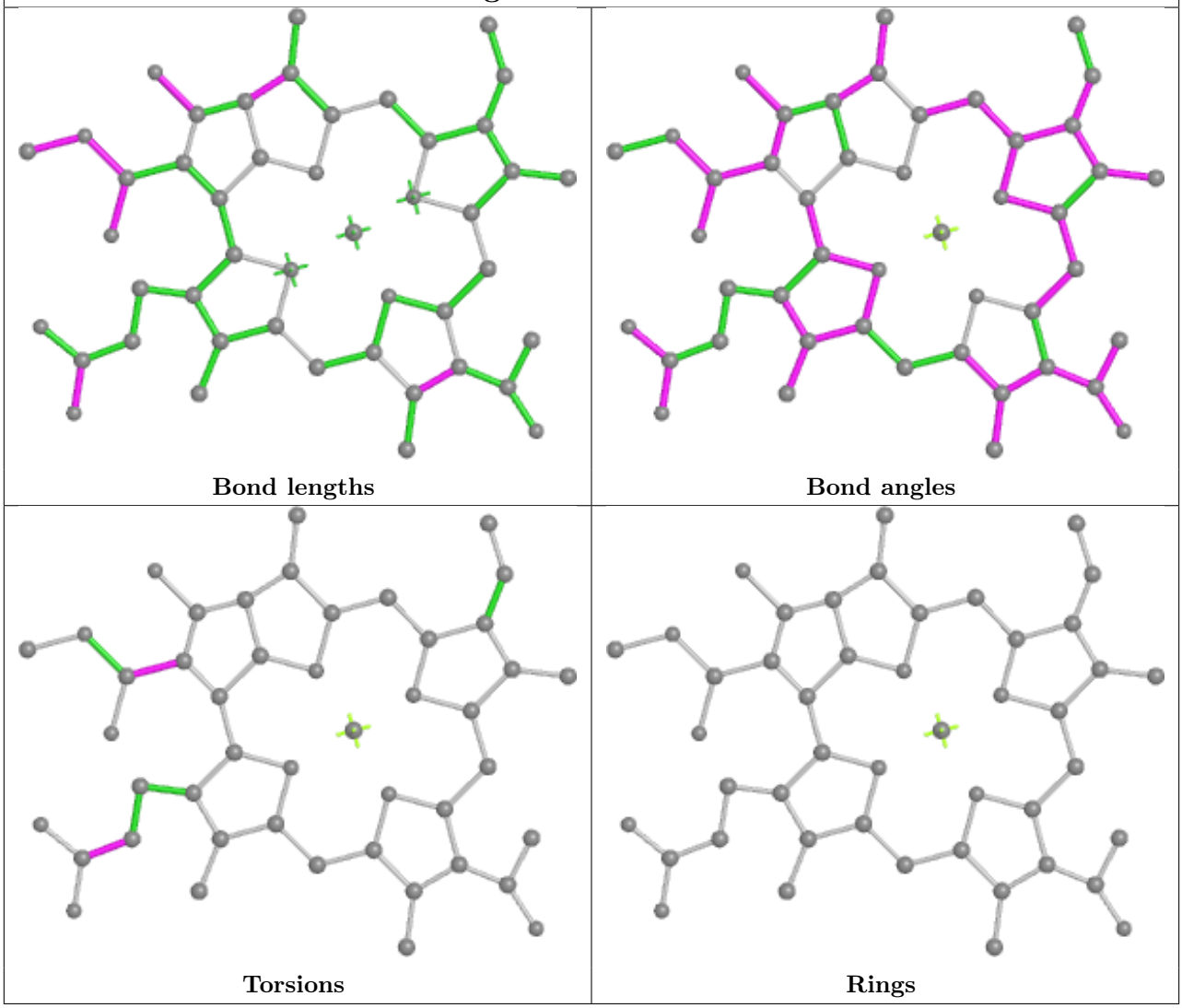


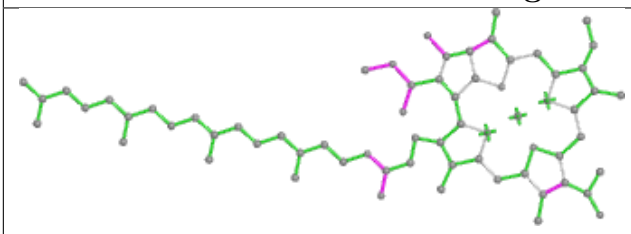
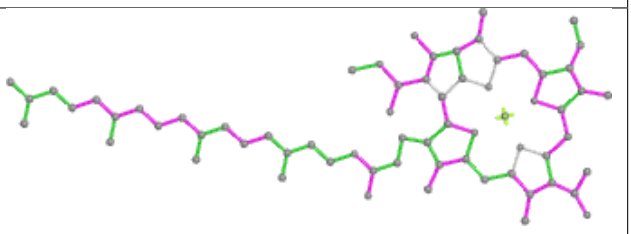
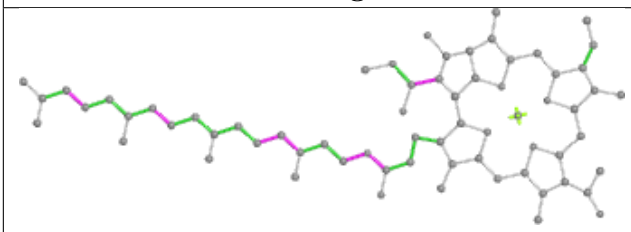
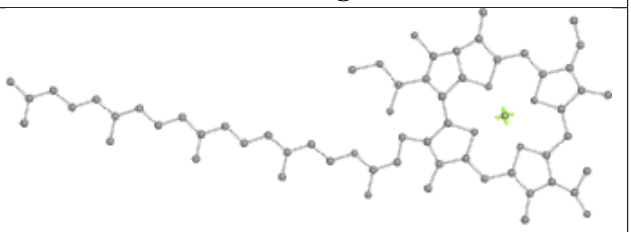
Rings

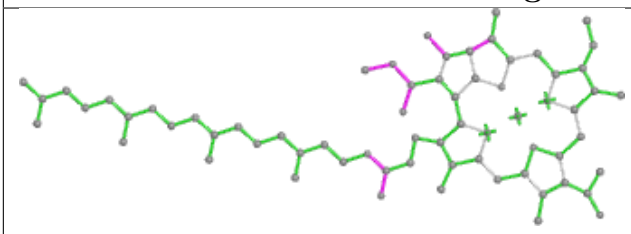
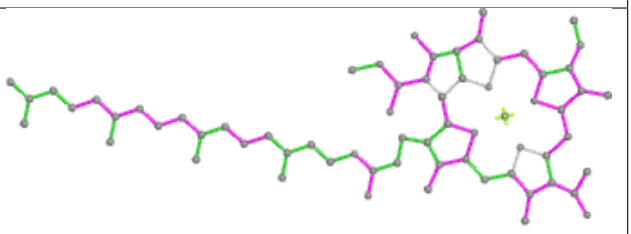
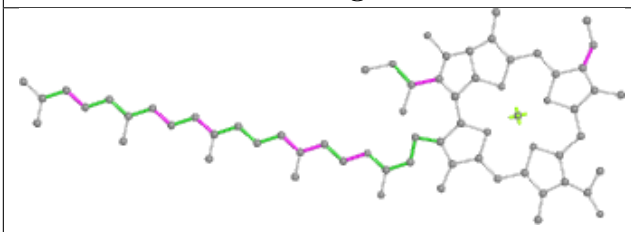
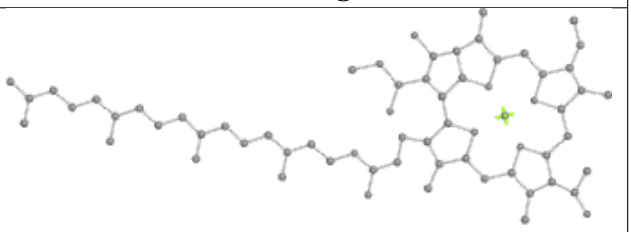
Ligand BCL F 374



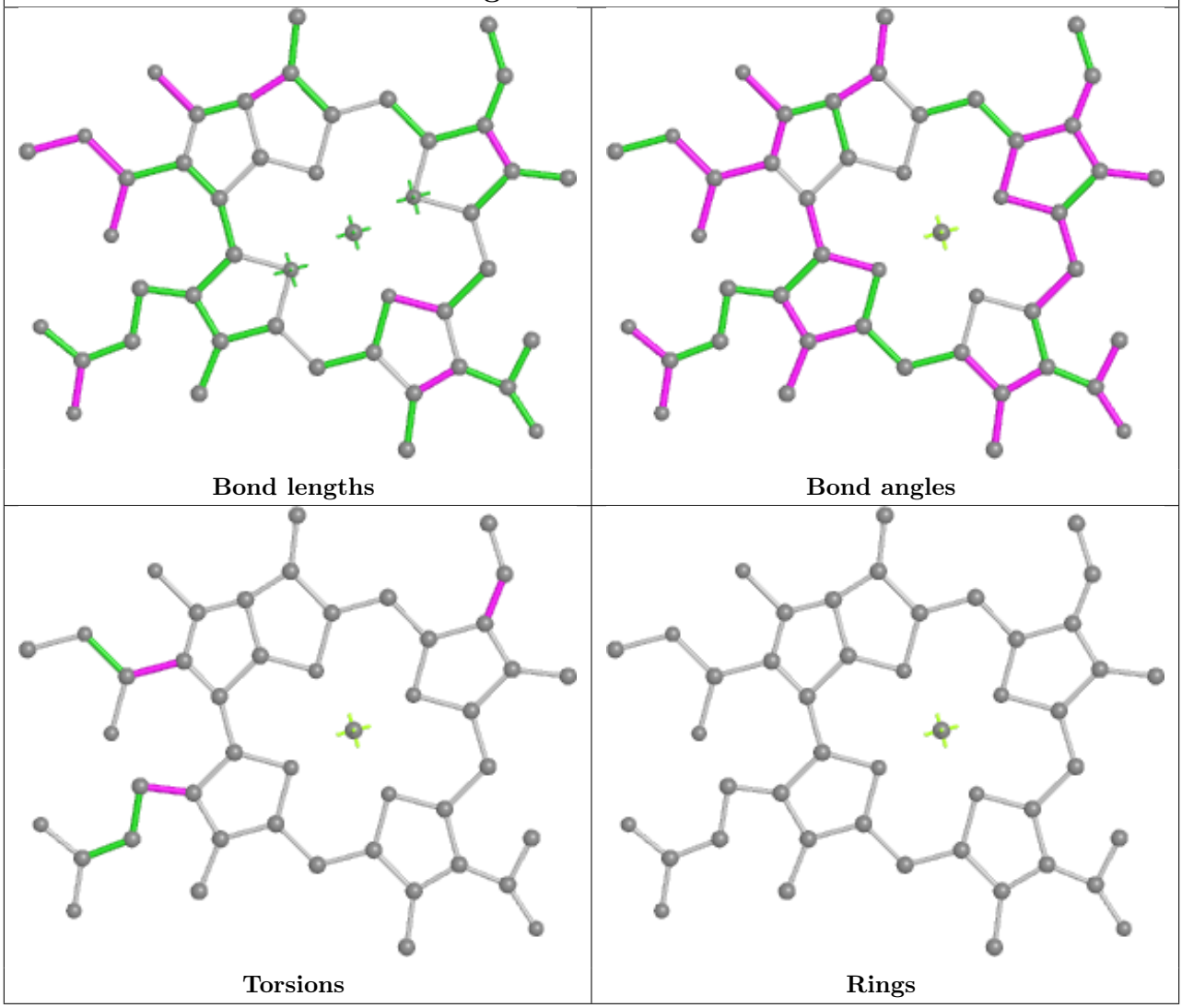
Ligand BCL A 809



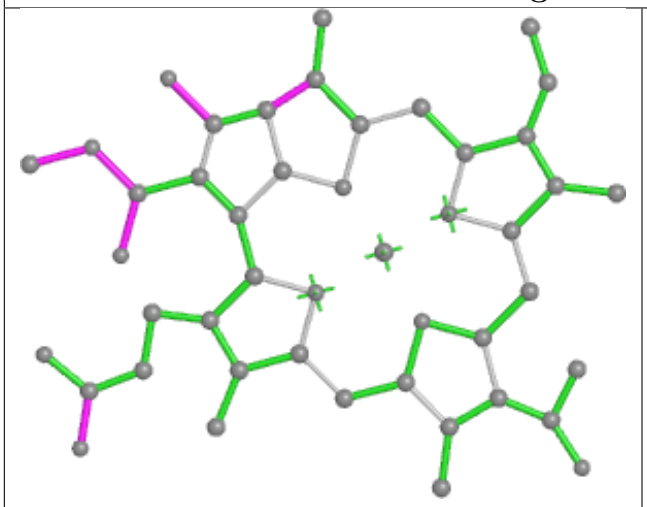
Ligand BCL G 376	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL G 377	
 Bond lengths	 Bond angles
 Torsions	 Rings

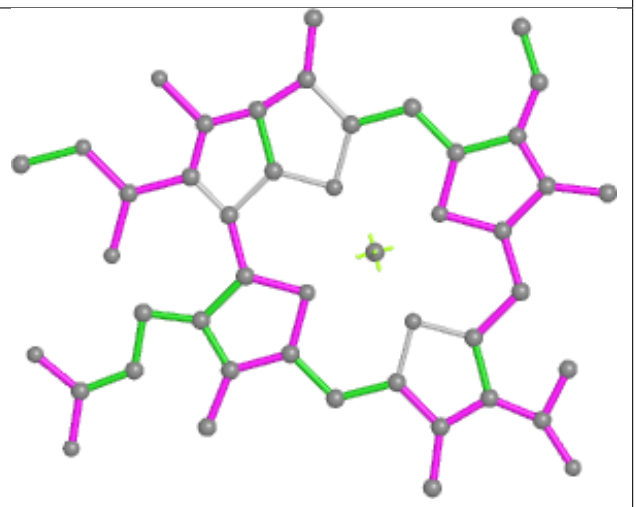
Ligand BCL A 813



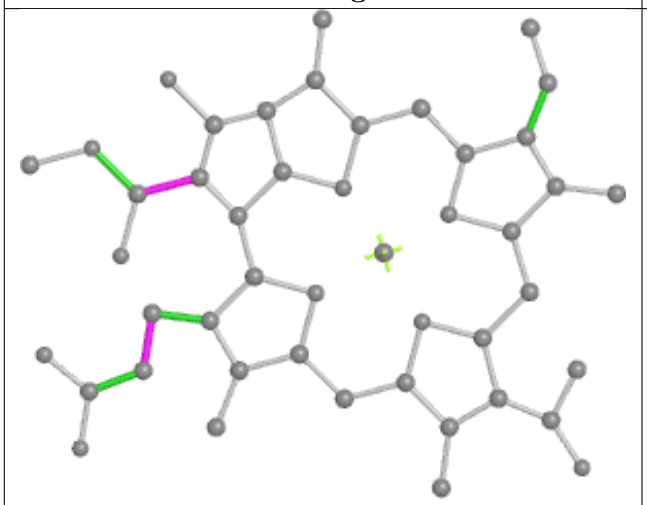
Ligand BCL a 814



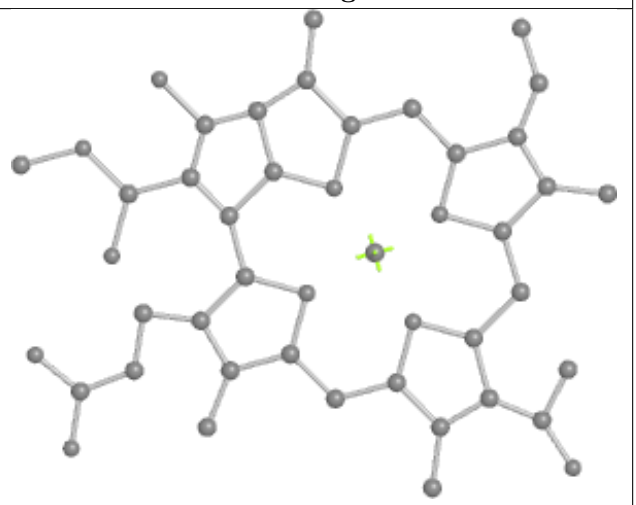
Bond lengths



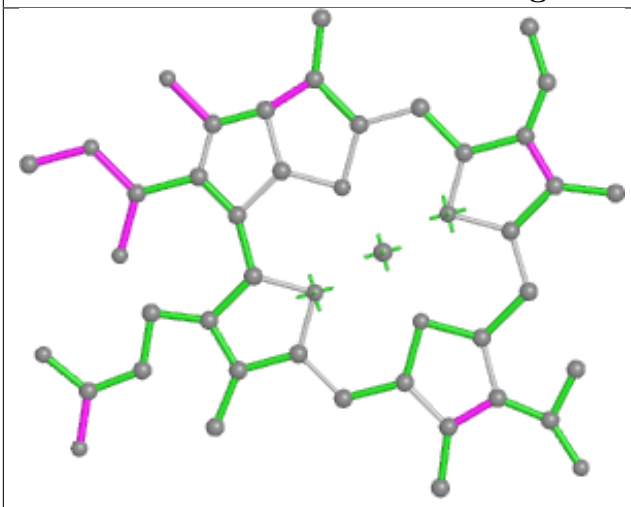
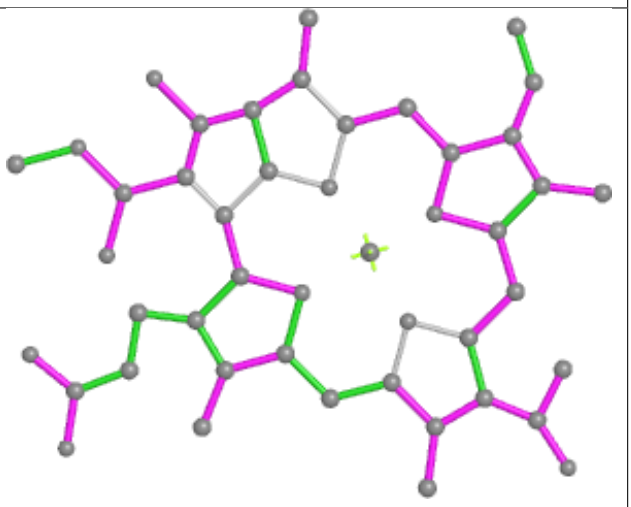
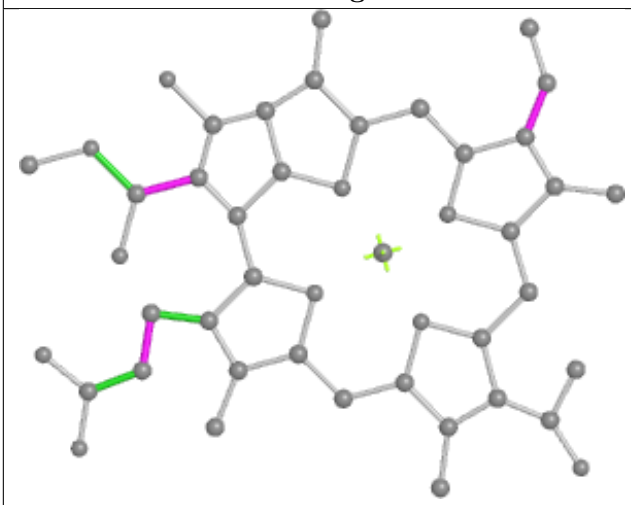
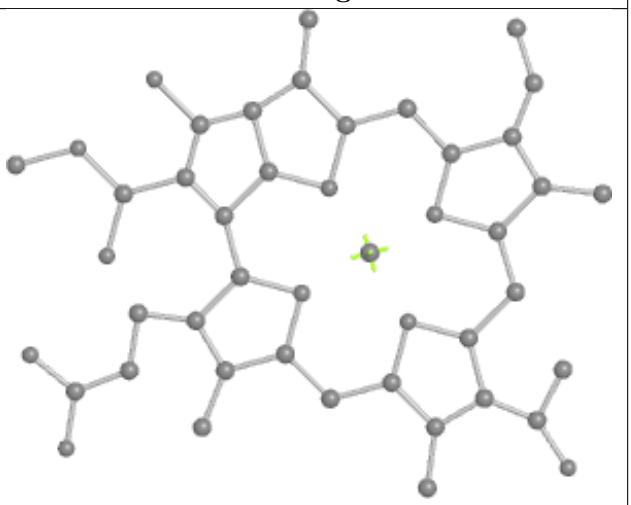
Bond angles

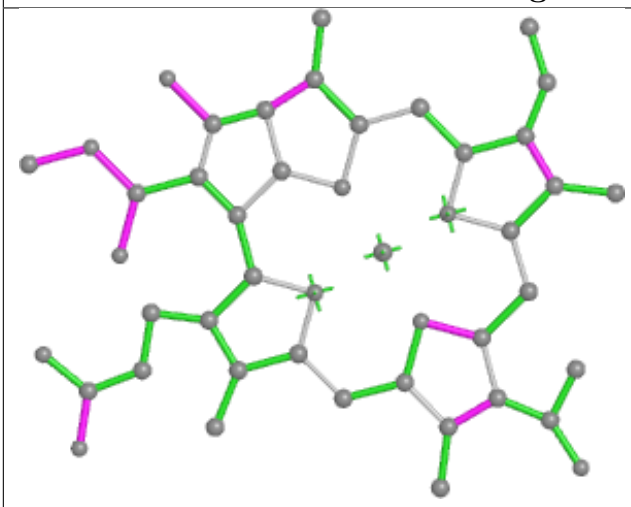
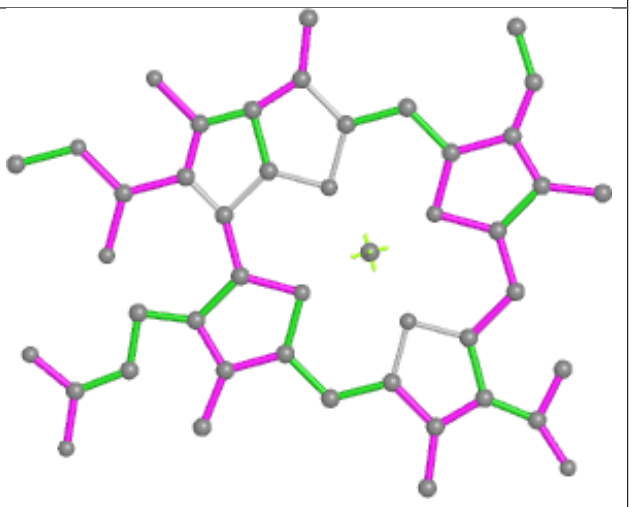
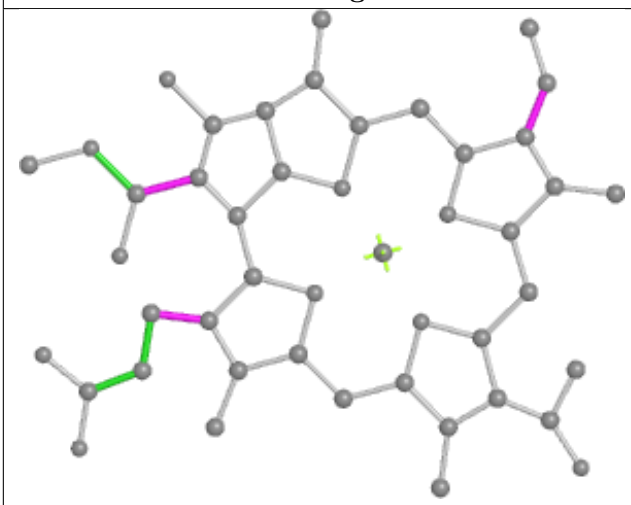
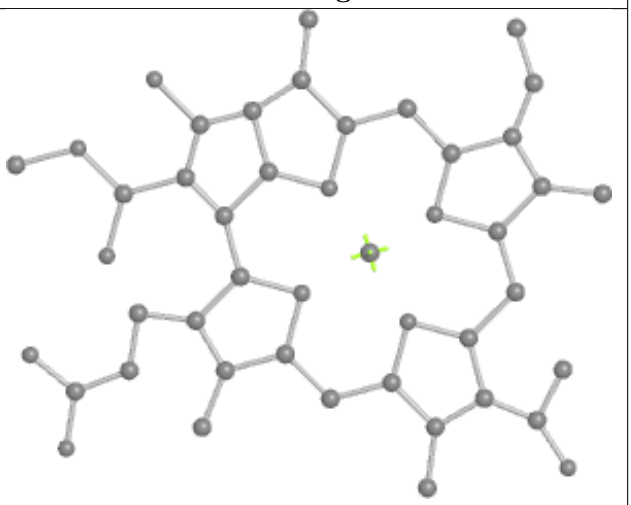


Torsions

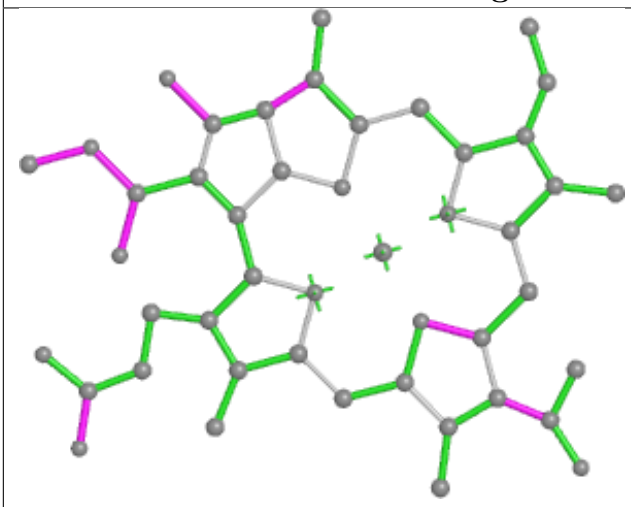


Rings

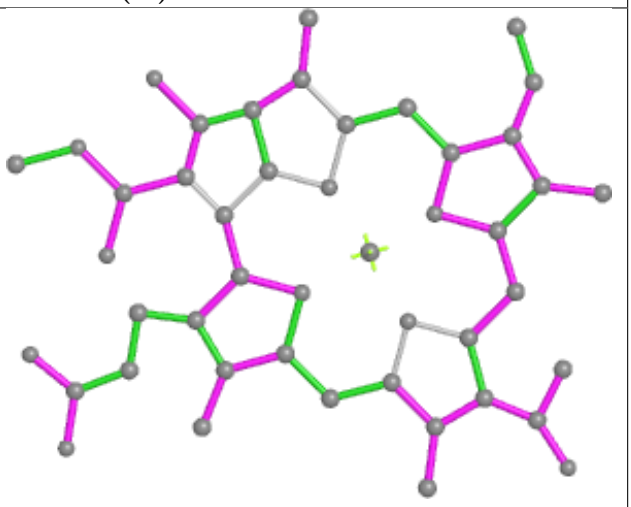
Ligand BCL a 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL a 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

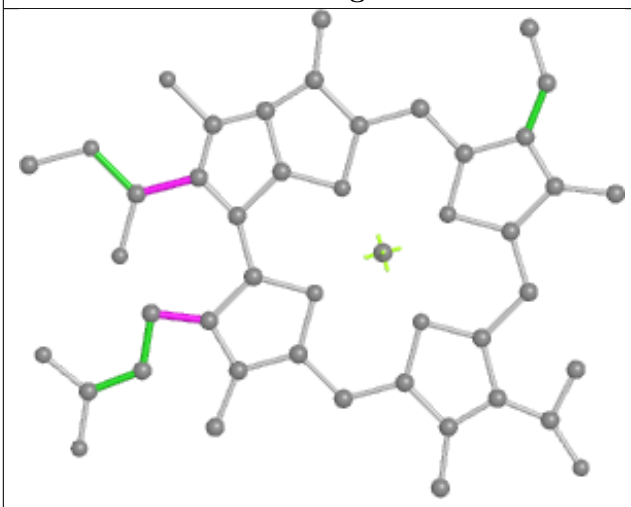
Ligand BCL G 378 (B)



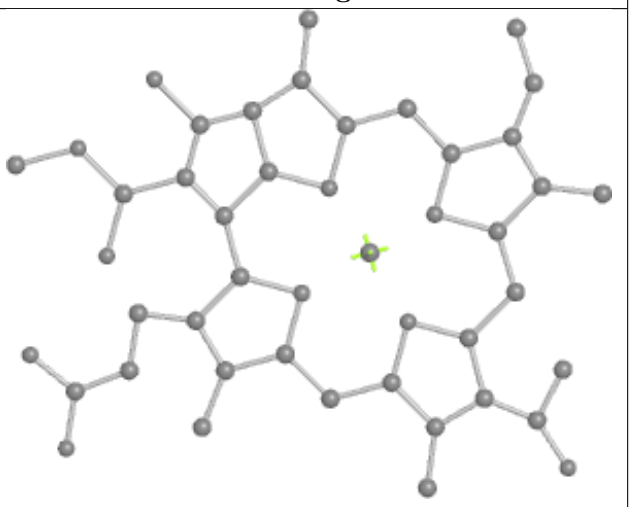
Bond lengths



Bond angles

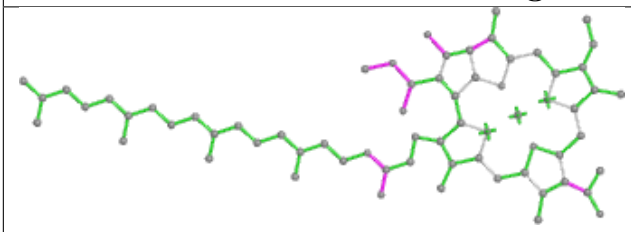


Torsions

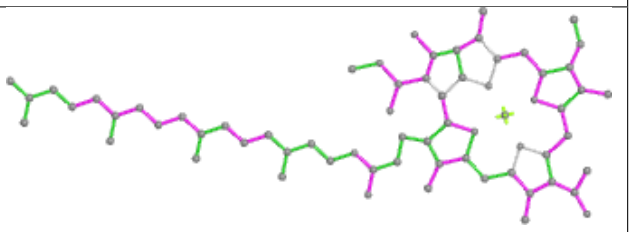


Rings

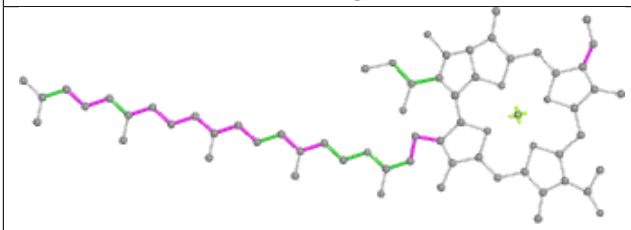
Ligand BCL E 372



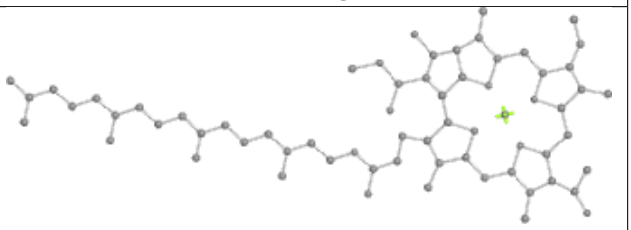
Bond lengths



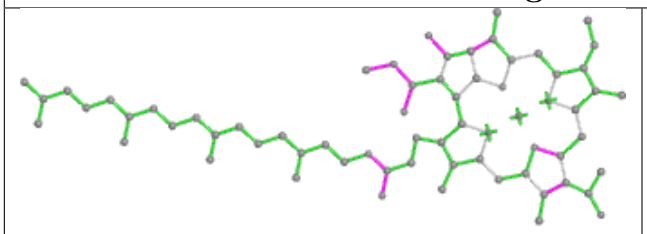
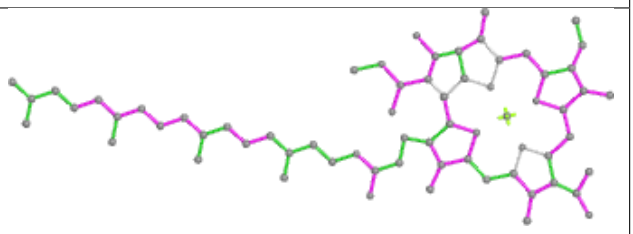
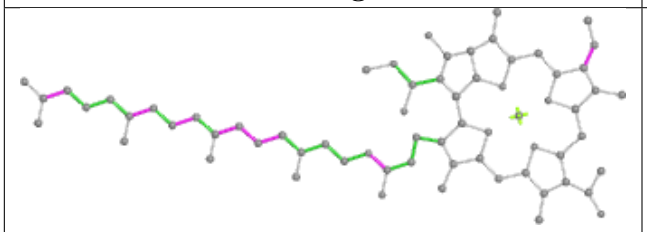
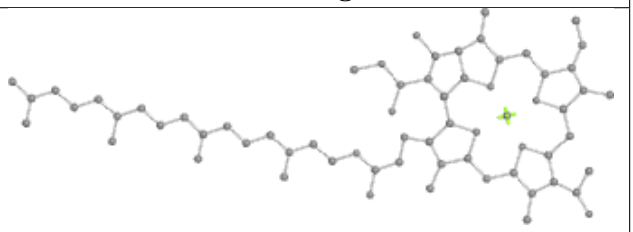
Bond angles

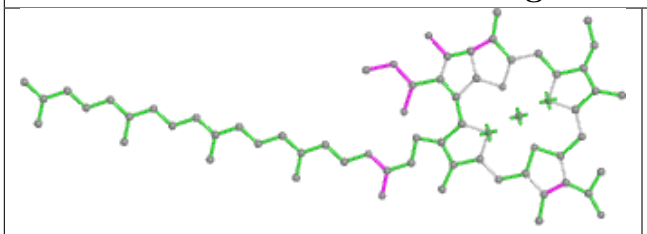
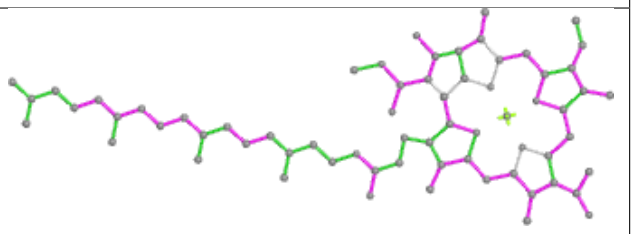
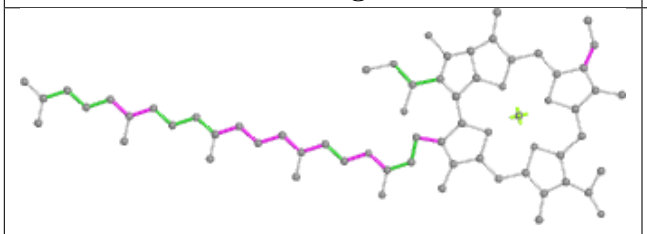
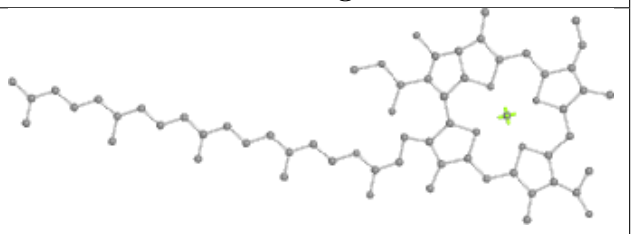


Torsions



Rings

Ligand BCL A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

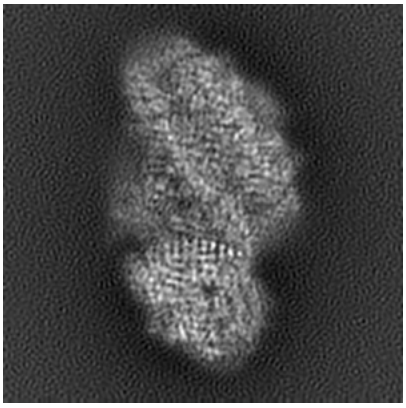
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30069. These allow visual inspection of the internal detail of the map and identification of artifacts.

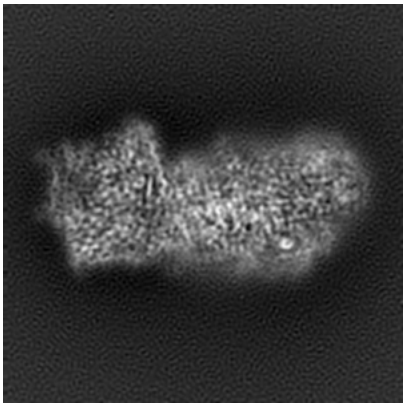
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

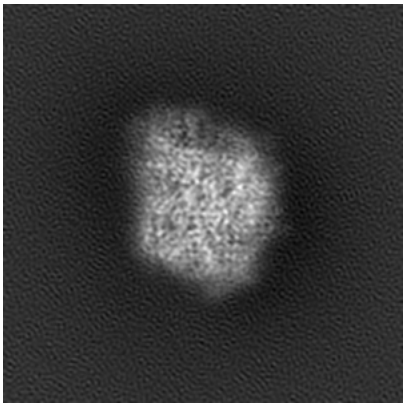
6.1.1 Primary map



X



Y

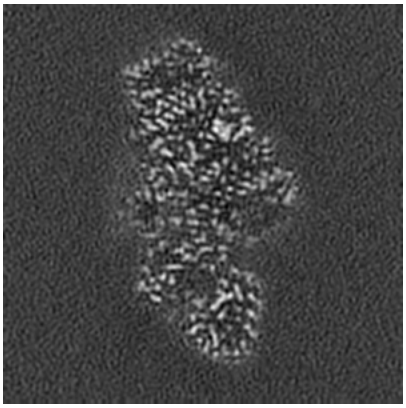


Z

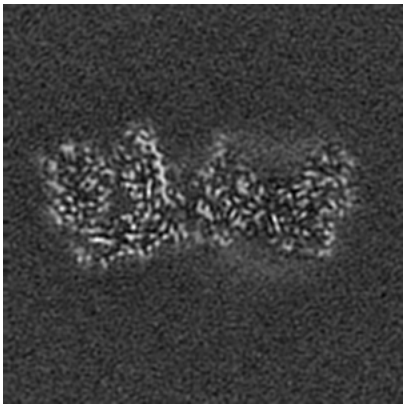
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

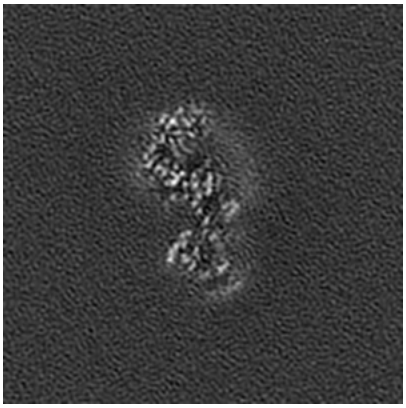
6.2.1 Primary map



X Index: 80



Y Index: 80

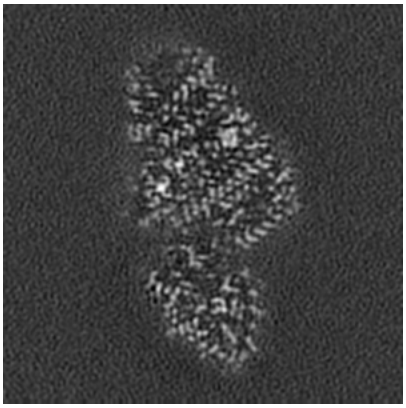


Z Index: 80

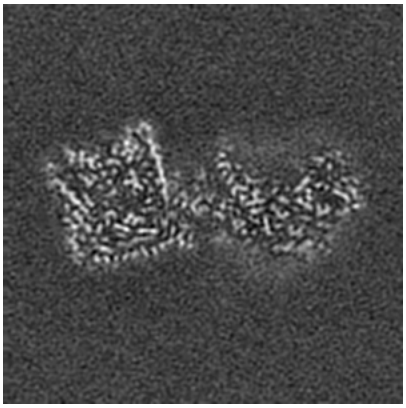
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

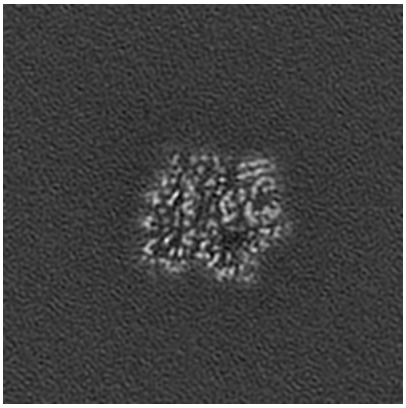
6.3.1 Primary map



X Index: 77



Y Index: 76



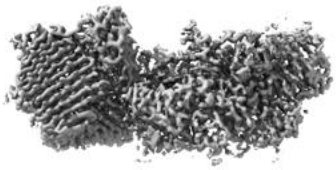
Z Index: 50

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

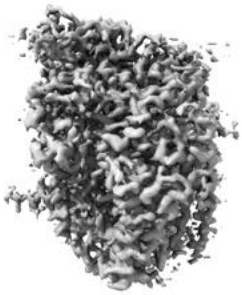
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0341. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

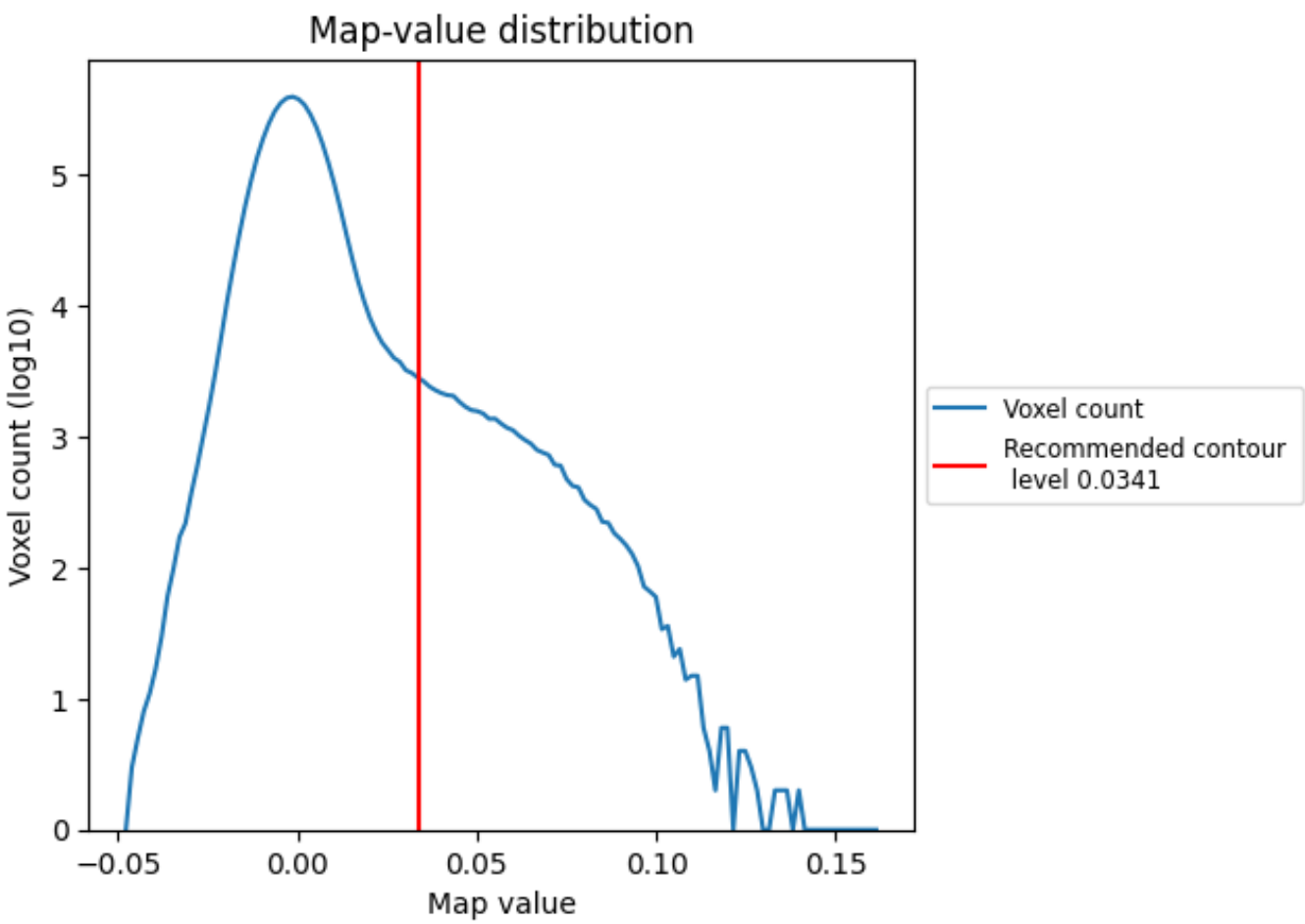
6.5 Mask visualisation (i)

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

7 Map analysis (i)

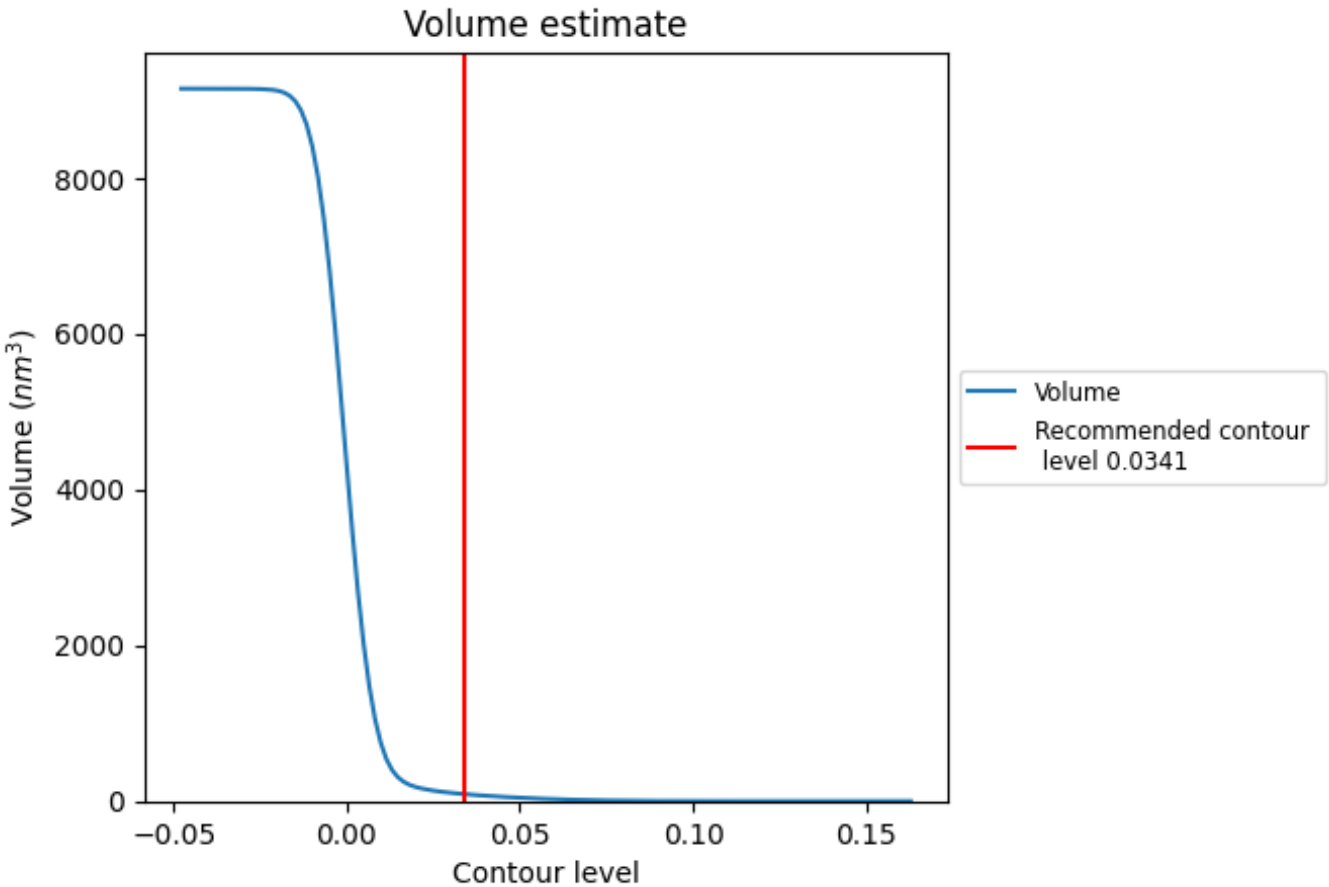
This section contains the results of statistical analysis of the map.

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.

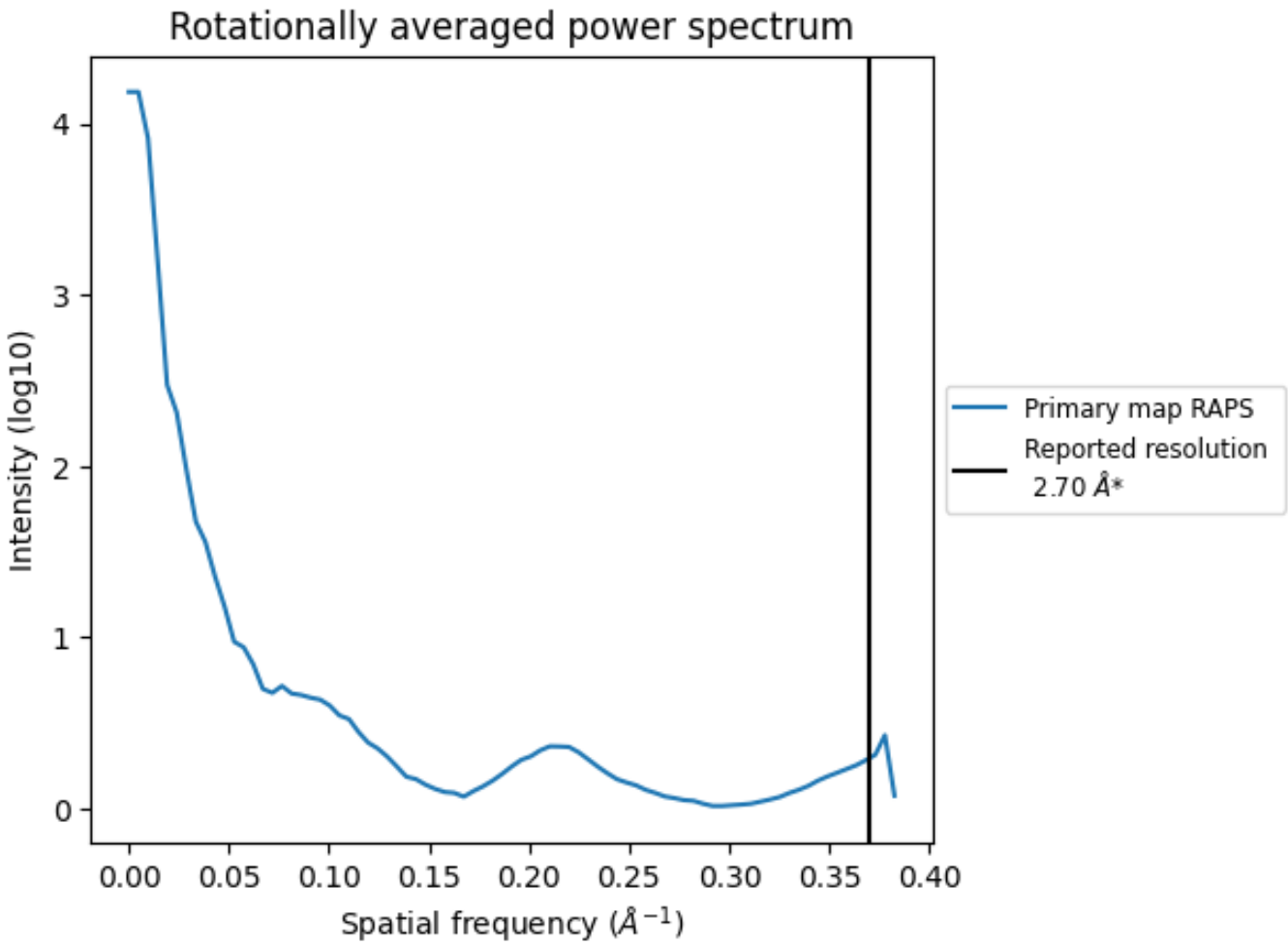
7.2 Volume estimate (i)



The volume at the recommended contour level is 90 nm^3; this corresponds to an approximate mass of 81 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 (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

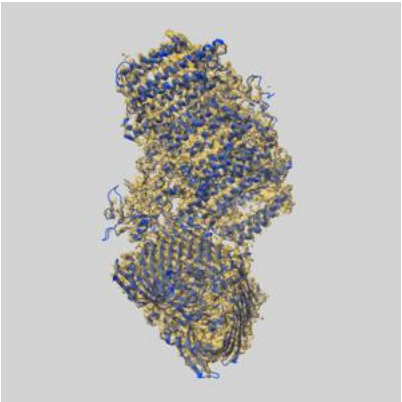
8 Fourier-Shell correlation (i)

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

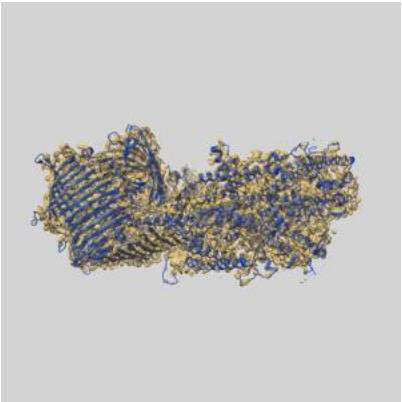
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30069 and PDB model 6M32. Per-residue inclusion information can be found in section 3 on page 13.

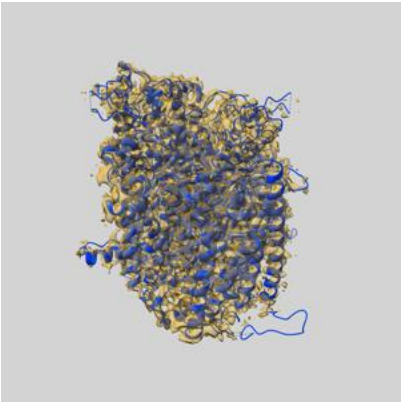
9.1 Map-model overlay (i)



X



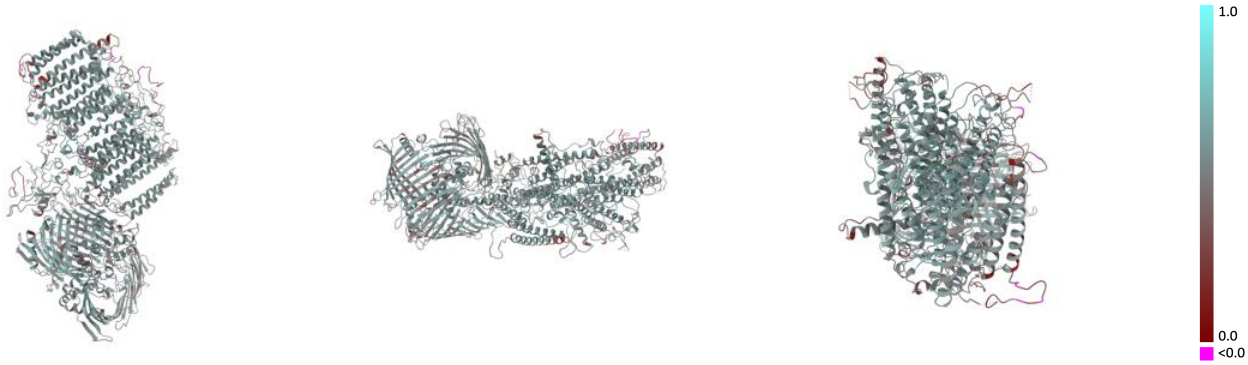
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0341 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

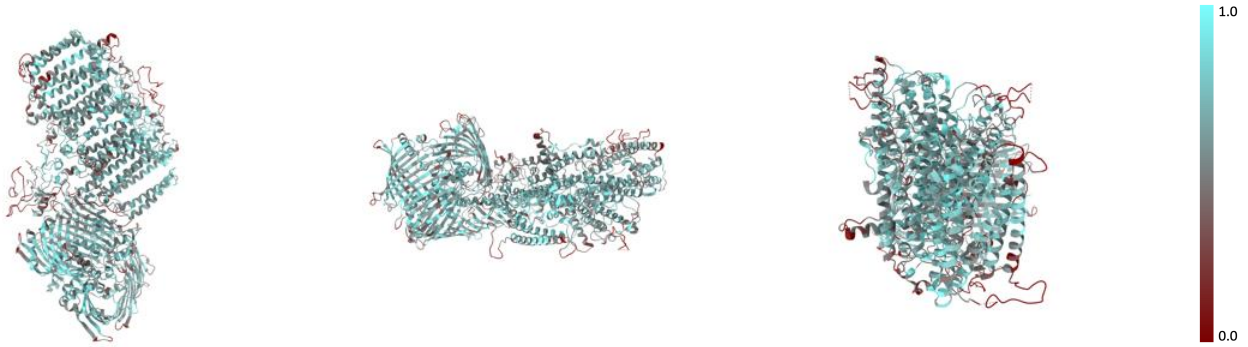
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

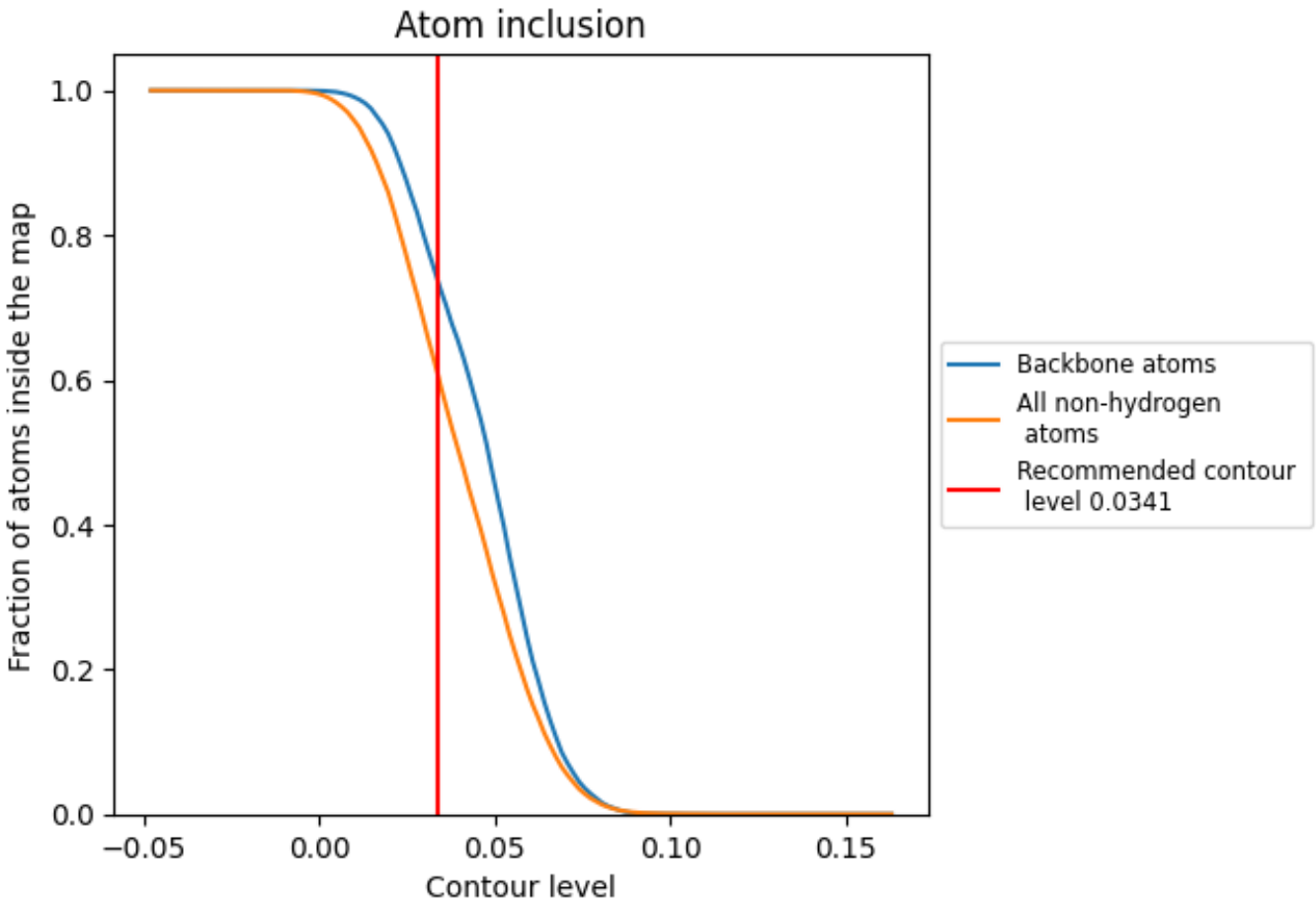
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0341).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0341) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6032	0.5250
A	0.6034	0.5350
B	0.5747	0.4900
D	0.3096	0.4350
E	0.6448	0.5350
F	0.6387	0.5260
G	0.6612	0.5420
a	0.5709	0.5150