Full wwPDB EM Validation Report ⓘ

Oct 8, 2022 – 01:15 PM EDT

PDB ID	:	7UEA
EMDB ID	:	EMD-26469
Title	:	Photosynthetic assembly of Chlorobaculum tepidum (RC-FMO1)
Authors	:	Puskar, R.; Truong, C.D.; Swain, K.; Li, S.; Cheng, K.-W.; Wang, T.Y.; Poh, Y.-P.; Liu, H.; Chou, T.-F.; Nannenga, B.; Chiu, P.-L.
Deposited on	:	2022-03-21
Resolution	:	3.49 Å(reported)
Based on initial model	:	6M32

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

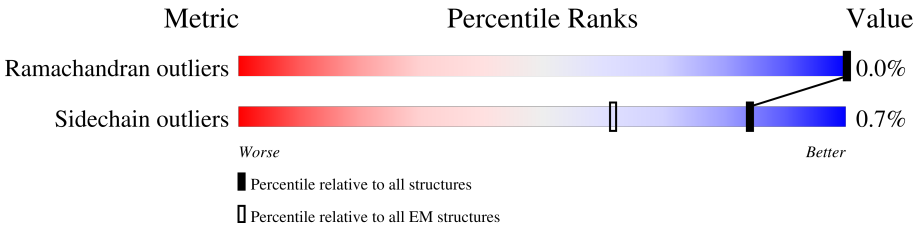
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 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	A	731	8% 88% · 12%
1	a	731	8% 86% · 13%
2	B	231	14% 48% 52%
3	C	206	35% 55% · 43%
3	c	206	24% 50% 49%
4	D	143	40% 69% · 30%
5	U	366	10% 99% ·
5	V	366	11% 98% ·
5	W	366	15% 97% · ·

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
13	G2O	A	824	X	-	-	-
13	G2O	a	801	X	-	-	-
13	G2O	a	802	X	-	-	-
13	G2O	a	805	X	-	-	-
6	GS0	A	801	X	-	-	-
6	GS0	a	804	X	-	-	-
9	F26	a	820	-	X	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 26313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem P840 reaction center, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	645	Total	C	N	O	S	0	0
			5167	3449	821	871	26		
1	a	633	Total	C	N	O	S	0	0
			5079	3398	804	852	25		

- Molecule 2 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	110	Total	C	N	O	S	0	0
			855	545	143	158	9		

- Molecule 3 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	117	Total	C	N	O	S	0	0
			916	617	142	150	7		
3	c	105	Total	C	N	O	S	0	0
			839	565	130	138	6		

- Molecule 4 is a protein called P840 reaction center 17 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			817	520	144	149	4		

- Molecule 5 is a protein called Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	364	Total	C	N	O	S	0	0
			2834	1798	503	526	7		
5	V	360	Total	C	N	O	S	0	0
			2805	1778	499	521	7		

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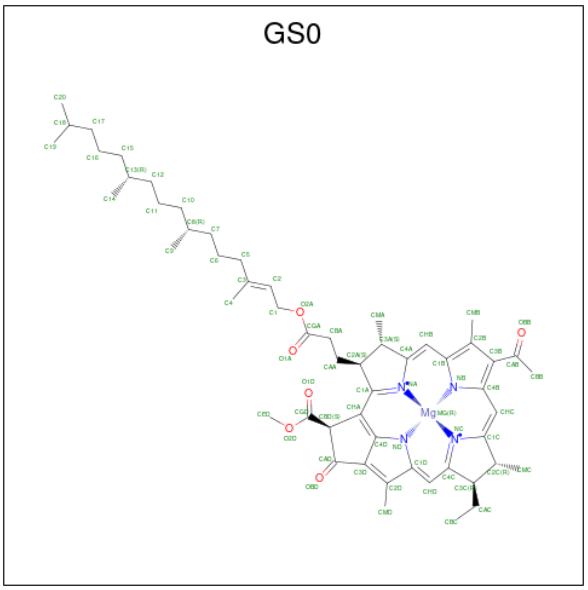
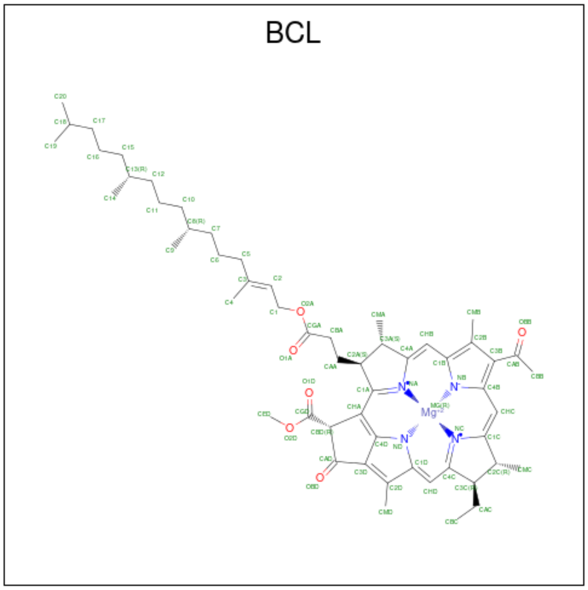
Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	359	Total	C	N	O	S	0	0
			2797	1774	497	519	7		

- Molecule 6 is Bacteriochlorophyll A isomer (three-letter code: GS0) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	A	1	Total 791	C 659	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0

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Mol	Chain	Residues	Atoms					AltConf
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	1
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0

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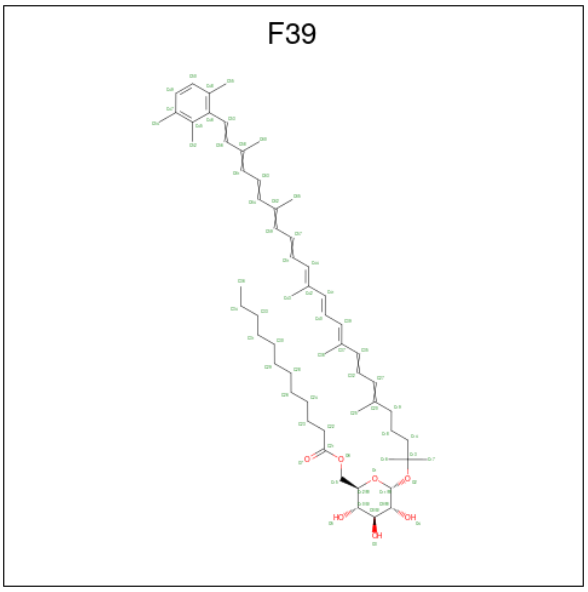
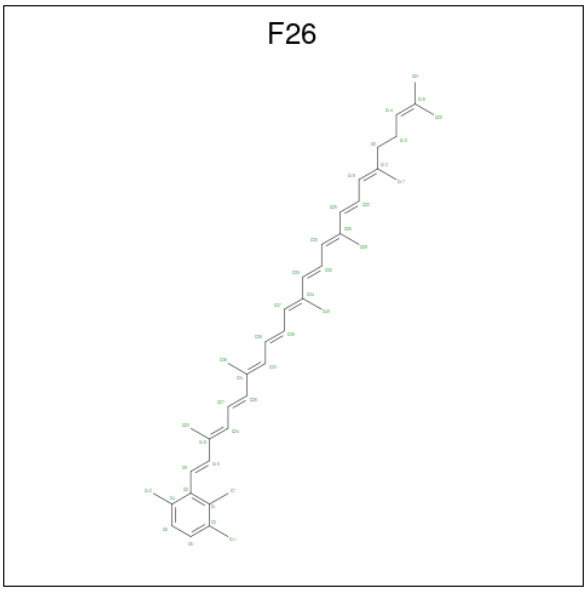
Mol	Chain	Residues	Atoms					AltConf
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	1
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	1

- Molecule 8 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(oxidan yl)oxan-2-yl]methyl dodecanoate (three-letter code: F39) (formula: $C_{58}H_{86}O_7$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 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: $C_{40}H_{52}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C 40 40	0

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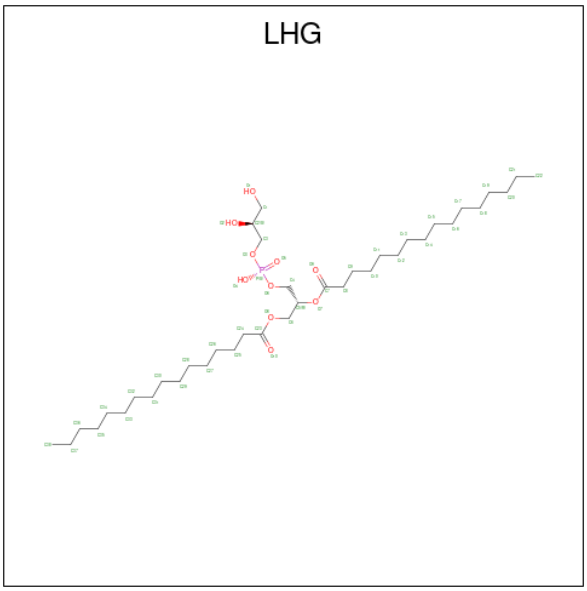
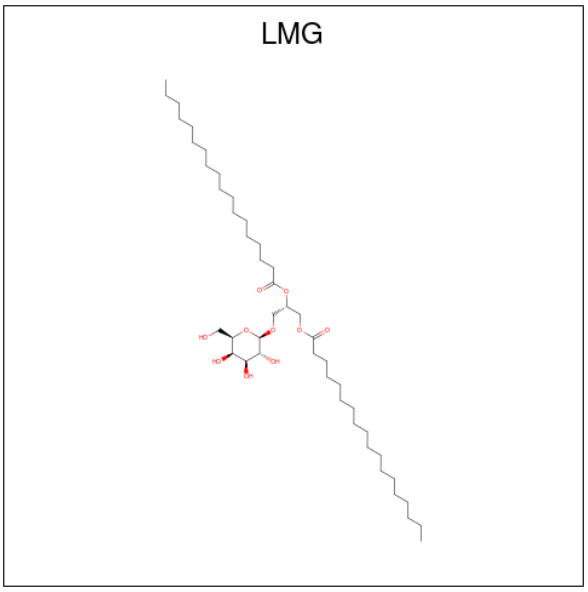
Mol	Chain	Residues	Atoms	AltConf
9	a	1	Total C 80 80	0
9	a	1	Total C 80 80	0

- Molecule 10 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O P 67 45 20 2	0
10	A	1	Total C O P 67 45 20 2	0
10	a	1	Total C O P 99 66 30 3	0
10	a	1	Total C O P 99 66 30 3	0
10	a	1	Total C O P 99 66 30 3	0
10	C	1	Total C O P 34 23 10 1	0

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

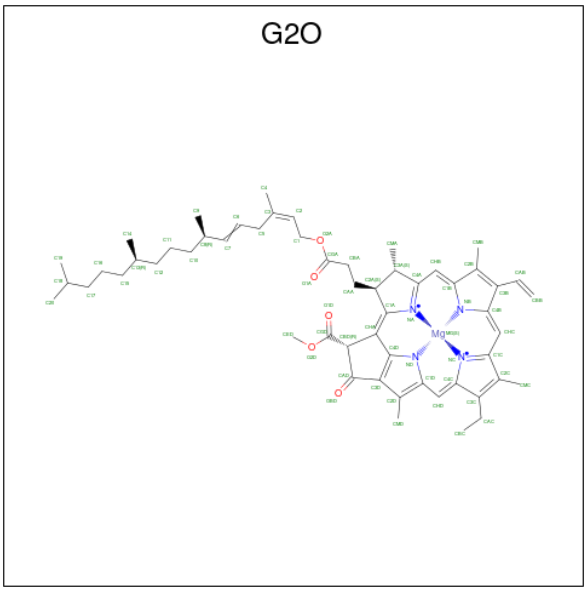


Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C O 174 124 50	0
11	A	1	Total C O 174 124 50	0
11	A	1	Total C O 174 124 50	0
11	A	1	Total C O 174 124 50	0
11	A	1	Total C O 174 124 50	0
11	a	1	Total C O 40 30 10	0
11	C	1	Total C O 35 25 10	0

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

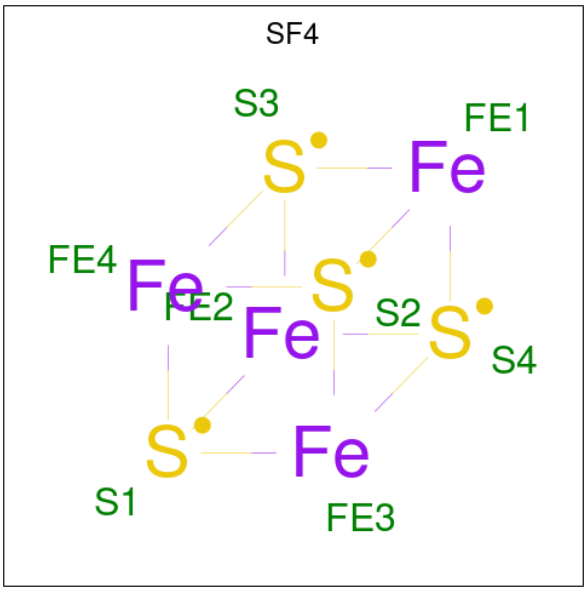
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total Ca 1 1	0
12	a	1	Total Ca 1 1	0

- Molecule 13 is Chlorophyll A ester (three-letter code: G2O) (formula: $C_{55}H_{70}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
13	a	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
13	a	1	Total	C	Mg	N	O	0
			195	165	3	12	15	

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

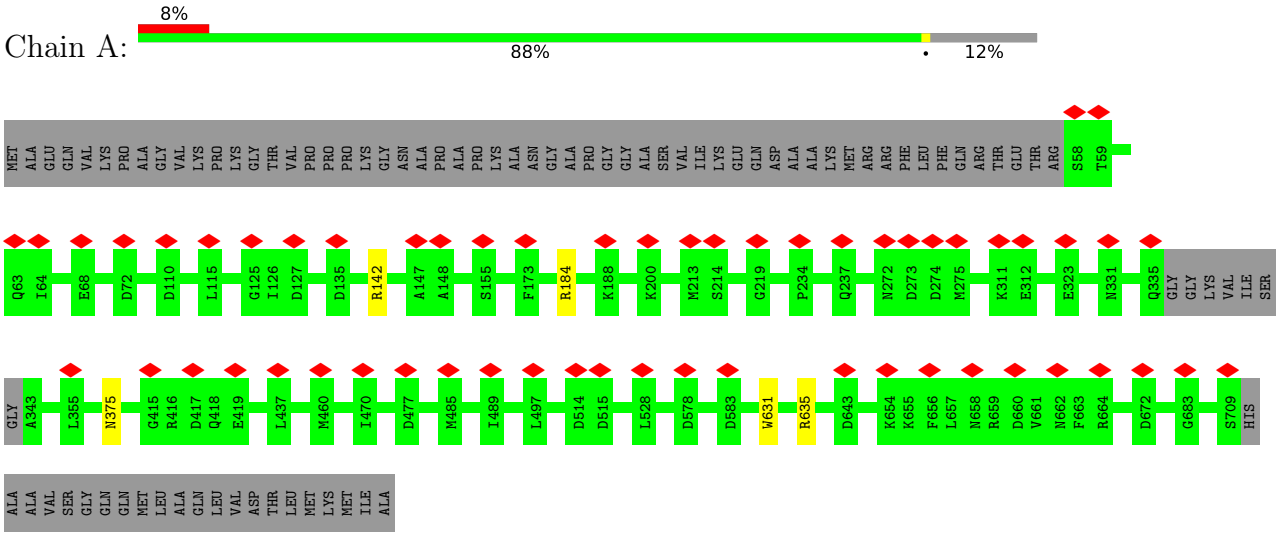


Mol	Chain	Residues	Atoms			AltConf
14	a	1	Total 8	Fe 4	S 4	0
14	B	1	Total 16	Fe 8	S 8	0
14	B	1	Total 16	Fe 8	S 8	0

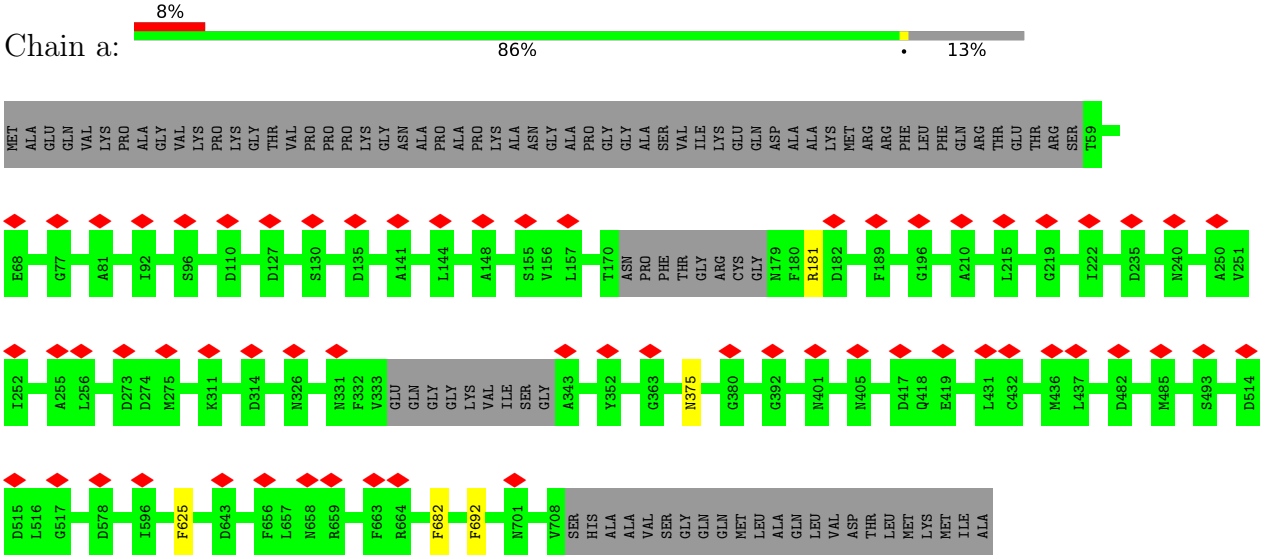
3 Residue-property plots (i)

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

• Molecule 1: Photosystem P840 reaction center, large subunit

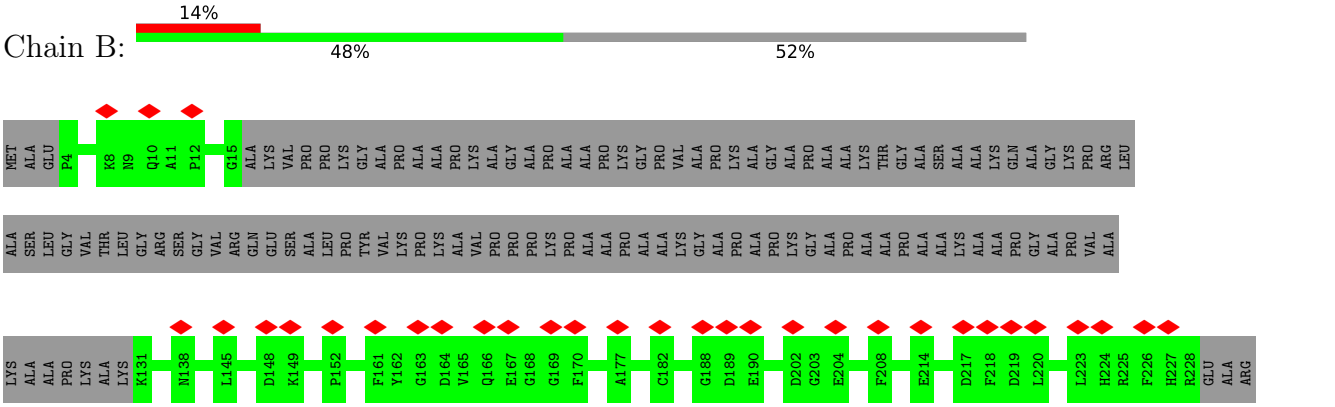


• Molecule 1: Photosystem P840 reaction center, large subunit



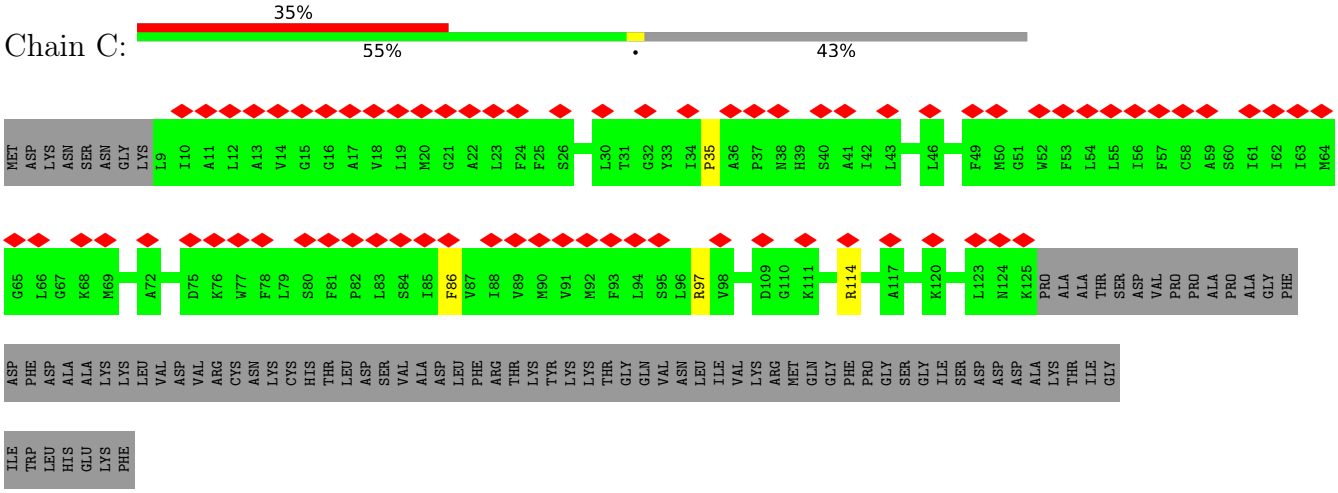
• Molecule 2: Photosystem P840 reaction center iron-sulfur protein

Chain B:



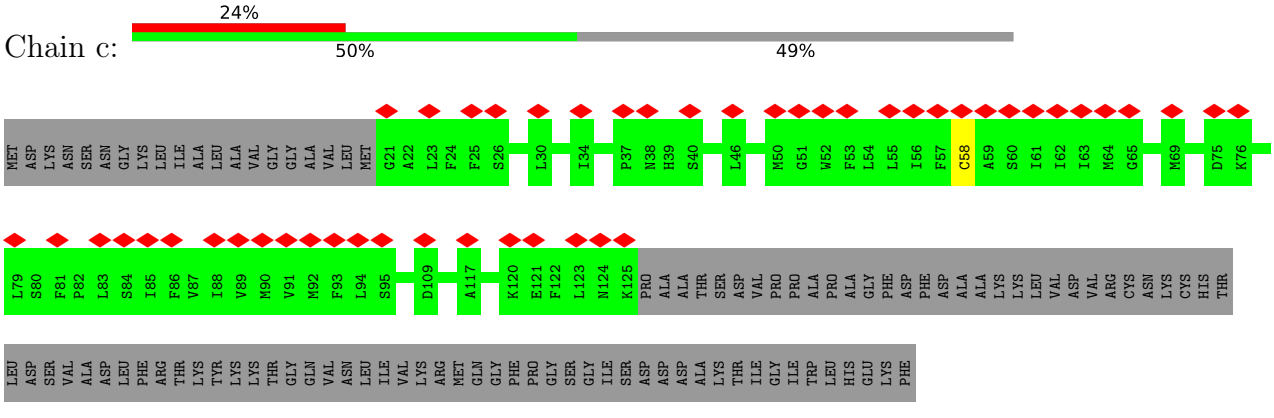
• Molecule 3: Cytochrome c

Chain C:



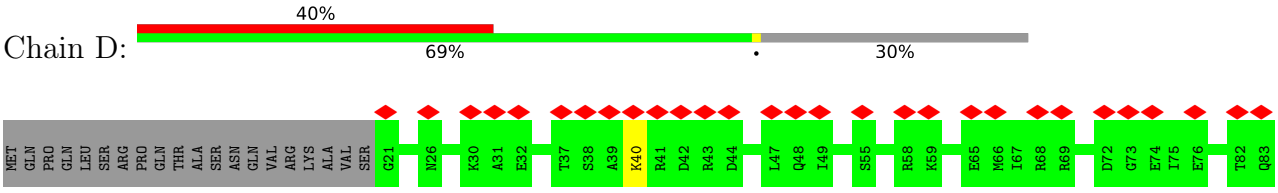
• Molecule 3: Cytochrome c

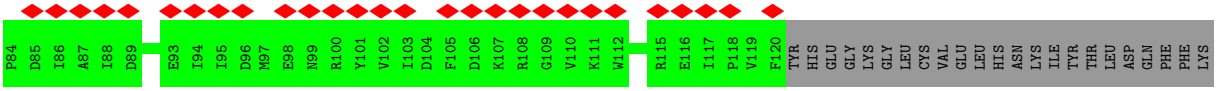
Chain c:



• Molecule 4: P840 reaction center 17 kDa protein

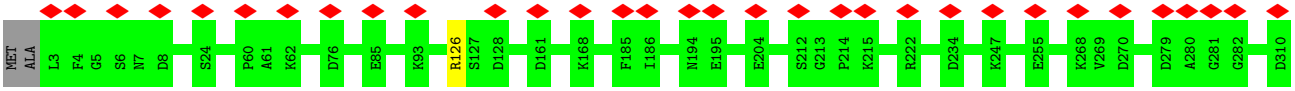
Chain D:

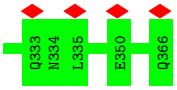




• Molecule 5: Bacteriochlorophyll a protein

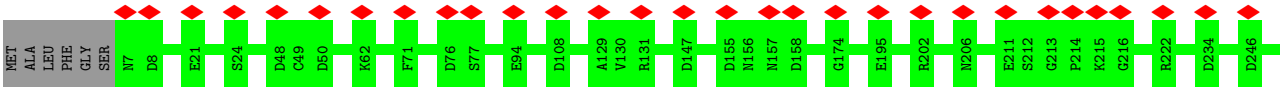
Chain U:

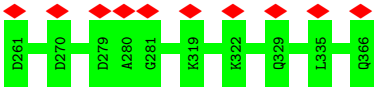




• Molecule 5: Bacteriochlorophyll a protein

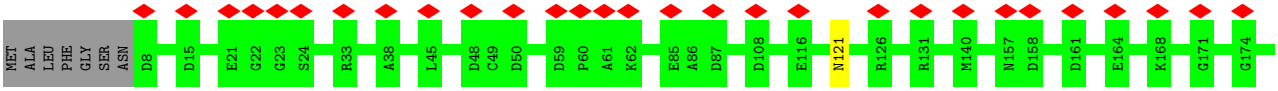
Chain V:

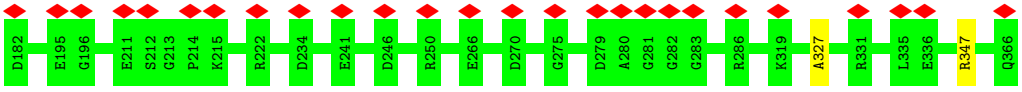




• Molecule 5: Bacteriochlorophyll a protein

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142020	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	47259	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.114	Depositor
Minimum map value	-3.718	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.352	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/5348	0.44	0/7288
1	a	0.29	0/5257	0.44	0/7164
2	B	0.30	0/878	0.49	0/1187
3	C	0.26	0/940	0.50	0/1272
3	c	0.26	0/863	0.49	0/1167
4	D	0.25	0/833	0.55	0/1122
5	U	0.29	0/2905	0.53	0/3937
5	V	0.29	0/2875	0.53	0/3897
5	W	0.29	0/2867	0.53	0/3886
All	All	0.29	0/22766	0.49	0/30920

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
4	D	0	1
5	W	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	40	LYS	Peptide
5	W	327	ALA	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	641/731 (88%)	620 (97%)	21 (3%)	0	100	100
1	a	627/731 (86%)	600 (96%)	27 (4%)	0	100	100
2	B	106/231 (46%)	99 (93%)	7 (7%)	0	100	100
3	C	115/206 (56%)	110 (96%)	4 (4%)	1 (1%)	17	56
3	c	103/206 (50%)	102 (99%)	1 (1%)	0	100	100
4	D	98/143 (68%)	84 (86%)	14 (14%)	0	100	100
5	U	362/366 (99%)	348 (96%)	14 (4%)	0	100	100
5	V	358/366 (98%)	351 (98%)	7 (2%)	0	100	100
5	W	357/366 (98%)	344 (96%)	13 (4%)	0	100	100
All	All	2767/3346 (83%)	2658 (96%)	108 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	35	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	536/599 (90%)	531 (99%)	5 (1%)	78 90
1	a	526/599 (88%)	521 (99%)	5 (1%)	76 88
2	B	93/162 (57%)	93 (100%)	0	100 100
3	C	99/173 (57%)	96 (97%)	3 (3%)	41 71
3	c	92/173 (53%)	91 (99%)	1 (1%)	73 88
4	D	89/128 (70%)	89 (100%)	0	100 100
5	U	301/302 (100%)	300 (100%)	1 (0%)	92 97
5	V	298/302 (99%)	298 (100%)	0	100 100
5	W	297/302 (98%)	295 (99%)	2 (1%)	84 93
All	All	2331/2740 (85%)	2314 (99%)	17 (1%)	84 93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	A	184	ARG
1	A	375	ASN
1	A	631	TRP
1	A	635	ARG
1	a	181	ARG
1	a	375	ASN
1	a	625	PHE
1	a	682	PHE
1	a	692	PHE
3	C	86	PHE
3	C	97	ARG
3	C	114	ARG
3	c	58	CYS
5	U	126	ARG
5	W	121	ASN
5	W	347	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	262	ASN
1	a	645	GLN
2	B	155	ASN
5	U	144	GLN

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Mol	Chain	Res	Type
5	U	146	HIS
5	V	333	GLN
5	W	121	ASN

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 77 ligands modelled in this entry, 2 are monoatomic - leaving 75 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	$\#\|Z\| > 2$
7	BCL	U	402	-	58,74,74	1.18	3 (5%)	69,115,115	1.35	9 (13%)
7	BCL	a	813	-	58,74,74	1.19	3 (5%)	69,115,115	1.44	12 (17%)
7	BCL	U	409	-	58,74,74	1.16	3 (5%)	69,115,115	1.38	10 (14%)
7	BCL	A	803	-	58,74,74	1.22	3 (5%)	69,115,115	1.39	10 (14%)
7	BCL	V	408[B]	5	38,54,74	1.41	3 (7%)	45,91,115	1.59	10 (22%)
7	BCL	W	406	-	58,74,74	1.11	2 (3%)	69,115,115	1.38	11 (15%)
9	F26	A	815	-	40,40,40	1.79	10 (25%)	46,50,50	2.10	16 (34%)
7	BCL	A	806	-	58,74,74	1.15	3 (5%)	69,115,115	1.44	9 (13%)
7	BCL	W	402	-	58,74,74	1.13	4 (6%)	69,115,115	1.50	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	LMG	A	821	-	27,27,55	1.03	0	35,35,63	1.23	5 (14%)
10	LHG	a	823	-	39,39,48	0.66	0	42,45,54	0.98	2 (4%)
7	BCL	a	815	-	58,74,74	1.20	4 (6%)	69,115,115	1.39	10 (14%)
7	BCL	U	408[B]	5	38,54,74	1.38	4 (10%)	45,91,115	1.55	9 (20%)
14	SF4	a	803	1	0,12,12	-	-	-		
10	LHG	A	816	-	25,25,48	0.83	1 (4%)	28,31,54	0.94	1 (3%)
7	BCL	a	808	-	58,74,74	1.20	2 (3%)	69,115,115	1.56	11 (15%)
7	BCL	A	811	-	58,74,74	1.16	3 (5%)	69,115,115	1.48	12 (17%)
7	BCL	a	809	-	58,74,74	1.16	4 (6%)	69,115,115	1.89	16 (23%)
7	BCL	a	812	-	58,74,74	1.16	4 (6%)	69,115,115	1.39	9 (13%)
13	G2O	a	805	-	67,73,73	4.13	39 (58%)	75,113,113	2.94	21 (28%)
9	F26	a	819	-	40,40,40	1.68	10 (25%)	46,50,50	2.22	15 (32%)
6	GS0	A	801	-	64,74,74	2.34	11 (17%)	78,115,115	2.88	30 (38%)
7	BCL	V	401	-	58,74,74	1.17	3 (5%)	69,115,115	1.51	14 (20%)
13	G2O	A	824	-	67,73,73	4.26	41 (61%)	75,113,113	3.02	22 (29%)
8	F39	a	818	-	66,66,66	2.81	21 (31%)	79,85,85	2.15	22 (27%)
7	BCL	A	804	-	58,74,74	1.15	3 (5%)	69,115,115	1.47	10 (14%)
7	BCL	U	401	-	58,74,74	1.18	4 (6%)	69,115,115	1.49	13 (18%)
7	BCL	A	813	-	57,73,74	1.17	2 (3%)	67,113,115	1.52	12 (17%)
7	BCL	A	807	-	58,74,74	1.17	3 (5%)	69,115,115	1.42	9 (13%)
13	G2O	a	801	-	67,73,73	4.14	40 (59%)	75,113,113	3.11	20 (26%)
14	SF4	B	301	2	0,12,12	-	-	-		
7	BCL	a	816	-	58,74,74	1.17	4 (6%)	69,115,115	1.37	9 (13%)
7	BCL	a	811	1	38,54,74	1.33	3 (7%)	45,91,115	1.83	11 (24%)
7	BCL	V	405	-	58,74,74	1.13	4 (6%)	69,115,115	1.42	8 (11%)
7	BCL	A	810	-	58,74,74	1.16	4 (6%)	69,115,115	1.52	11 (15%)
7	BCL	U	407	-	58,74,74	1.17	4 (6%)	69,115,115	1.37	11 (15%)
10	LHG	A	817	-	40,40,48	0.68	1 (2%)	43,46,54	1.00	2 (4%)
11	LMG	a	824	-	40,40,55	0.83	1 (2%)	48,48,63	1.18	4 (8%)
7	BCL	a	810	-	58,74,74	1.13	3 (5%)	69,115,115	1.45	12 (17%)
11	LMG	C	302	-	35,35,55	0.90	1 (2%)	43,43,63	1.16	3 (6%)
7	BCL	U	404	-	58,74,74	1.16	3 (5%)	69,115,115	1.58	14 (20%)
7	BCL	a	814	-	58,74,74	1.14	4 (6%)	69,115,115	1.56	10 (14%)
7	BCL	A	808	-	58,74,74	1.16	4 (6%)	69,115,115	1.47	11 (15%)
7	BCL	V	404	-	58,74,74	1.12	3 (5%)	69,115,115	1.42	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BCL	a	807	-	58,74,74	1.24	3 (5%)	69,115,115	1.33	8 (11%)
7	BCL	A	805	-	58,74,74	1.15	4 (6%)	69,115,115	1.62	13 (18%)
11	LMG	A	820	-	36,36,55	0.92	0	44,44,63	1.12	4 (9%)
11	LMG	A	818	-	42,42,55	0.80	0	50,50,63	1.17	5 (10%)
8	F39	A	814	-	66,66,66	2.79	20 (30%)	79,85,85	2.19	24 (30%)
7	BCL	a	817	-	58,74,74	1.15	3 (5%)	69,115,115	1.38	8 (11%)
7	BCL	V	406	-	58,74,74	1.18	3 (5%)	69,115,115	1.52	12 (17%)
7	BCL	W	401	-	58,74,74	1.19	4 (6%)	69,115,115	1.62	11 (15%)
7	BCL	U	403	-	58,74,74	1.16	3 (5%)	69,115,115	1.44	10 (14%)
6	GS0	a	804	-	64,74,74	2.39	14 (21%)	78,115,115	2.84	29 (37%)
9	F26	a	820	-	40,40,40	1.74	10 (25%)	46,50,50	2.13	15 (32%)
7	BCL	V	403	-	58,74,74	1.14	3 (5%)	69,115,115	1.47	9 (13%)
7	BCL	U	405	5	58,74,74	1.17	3 (5%)	69,115,115	1.45	10 (14%)
10	LHG	a	822	-	25,25,48	0.82	1 (4%)	28,31,54	0.95	1 (3%)
14	SF4	B	302	2	0,12,12	-	-	-		
10	LHG	a	821	-	32,32,48	0.74	1 (3%)	35,38,54	1.03	2 (5%)
11	LMG	A	822	-	30,30,55	0.96	0	38,38,63	1.28	5 (13%)
7	BCL	W	404	5	58,74,74	1.16	3 (5%)	69,115,115	1.46	13 (18%)
7	BCL	W	405	-	58,74,74	1.13	3 (5%)	69,115,115	1.56	12 (17%)
13	G2O	a	802	-	67,73,73	4.15	40 (59%)	75,113,113	3.03	20 (26%)
7	BCL	U	406	-	58,74,74	1.18	3 (5%)	69,115,115	1.41	9 (13%)
7	BCL	A	812	-	58,74,74	1.15	3 (5%)	69,115,115	1.30	9 (13%)
7	BCL	A	809	-	58,74,74	1.16	4 (6%)	69,115,115	1.41	10 (14%)
7	BCL	V	402	-	58,74,74	1.18	4 (6%)	69,115,115	1.45	12 (17%)
7	BCL	W	407[B]	5	38,54,74	1.39	3 (7%)	45,91,115	1.48	10 (22%)
7	BCL	W	403	-	58,74,74	1.12	3 (5%)	69,115,115	1.46	12 (17%)
10	LHG	C	301	-	33,33,48	0.73	1 (3%)	36,39,54	0.99	2 (5%)
7	BCL	V	407	-	58,74,74	1.13	3 (5%)	69,115,115	1.41	11 (15%)
7	BCL	a	806	-	58,74,74	1.17	3 (5%)	69,115,115	1.40	11 (15%)
11	LMG	A	819	-	39,39,55	0.83	0	47,47,63	1.13	5 (10%)
7	BCL	A	802	-	58,74,74	1.18	3 (5%)	69,115,115	1.53	12 (17%)

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
7	BCL	U	402	-	-	7/37/137/137	-
7	BCL	a	813	-	-	13/37/137/137	-
7	BCL	U	409	-	-	8/37/137/137	-
7	BCL	A	803	-	-	11/37/137/137	-
7	BCL	V	408[B]	5	-	2/13/113/137	-
7	BCL	W	406	-	-	9/37/137/137	-
9	F26	A	815	-	-	15/36/36/36	0/1/1/1
7	BCL	A	806	-	-	9/37/137/137	-
7	BCL	W	402	-	-	10/37/137/137	-
11	LMG	A	821	-	-	12/22/42/70	0/1/1/1
10	LHG	a	823	-	-	19/44/44/53	-
7	BCL	a	815	-	-	7/37/137/137	-
7	BCL	U	408[B]	5	-	4/13/113/137	-
14	SF4	a	803	1	-	-	0/6/5/5
10	LHG	A	816	-	-	12/30/30/53	-
7	BCL	A	811	-	-	7/37/137/137	-
13	G2O	a	805	-	3/3/15/22	23/39/115/115	-
7	BCL	a	808	-	-	7/37/137/137	-
7	BCL	a	809	-	-	11/37/137/137	-
7	BCL	a	812	-	-	12/37/137/137	-
9	F26	a	819	-	-	17/36/36/36	0/1/1/1
6	GS0	A	801	-	2/2/21/25	23/37/137/137	-
13	G2O	A	824	-	3/3/15/22	21/39/115/115	-
7	BCL	V	401	-	-	8/37/137/137	-
8	F39	a	818	-	-	25/58/78/78	0/2/2/2
7	BCL	A	804	-	-	8/37/137/137	-
7	BCL	U	401	-	-	7/37/137/137	-
13	G2O	a	801	-	4/4/15/22	24/39/115/115	-
7	BCL	A	807	-	-	3/37/137/137	-
7	BCL	A	813	-	-	15/36/136/137	-
14	SF4	B	301	2	-	-	0/6/5/5
7	BCL	a	816	-	-	12/37/137/137	-
7	BCL	a	811	1	-	7/13/113/137	-
7	BCL	V	405	-	-	7/37/137/137	-
7	BCL	A	810	-	-	8/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	U	407	-	-	4/37/137/137	-
10	LHG	A	817	-	-	19/45/45/53	-
11	LMG	a	824	-	-	15/35/55/70	0/1/1/1
7	BCL	a	810	-	-	11/37/137/137	-
11	LMG	C	302	-	-	16/30/50/70	0/1/1/1
7	BCL	U	404	-	-	8/37/137/137	-
7	BCL	a	814	-	-	11/37/137/137	-
7	BCL	A	808	-	-	10/37/137/137	-
7	BCL	V	404	-	-	10/37/137/137	-
7	BCL	a	807	-	-	8/37/137/137	-
7	BCL	A	805	-	-	16/37/137/137	-
11	LMG	A	820	-	-	14/31/51/70	0/1/1/1
11	LMG	A	818	-	-	20/37/57/70	0/1/1/1
8	F39	A	814	-	-	29/58/78/78	0/2/2/2
7	BCL	a	817	-	-	7/37/137/137	-
7	BCL	V	406	-	-	7/37/137/137	-
7	BCL	W	401	-	-	7/37/137/137	-
7	BCL	U	403	-	-	11/37/137/137	-
6	GS0	a	804	-	2/2/21/25	25/37/137/137	-
9	F26	a	820	-	-	26/36/36/36	0/1/1/1
7	BCL	V	403	-	-	10/37/137/137	-
7	BCL	U	405	5	-	8/37/137/137	-
10	LHG	a	822	-	-	17/30/30/53	-
14	SF4	B	302	2	-	-	0/6/5/5
10	LHG	a	821	-	-	15/37/37/53	-
11	LMG	A	822	-	-	11/24/44/70	0/1/1/1
7	BCL	W	404	5	-	10/37/137/137	-
7	BCL	W	405	-	-	9/37/137/137	-
13	G2O	a	802	-	3/3/15/22	17/39/115/115	-
7	BCL	U	406	-	-	5/37/137/137	-
7	BCL	A	812	-	-	12/37/137/137	-
7	BCL	A	809	-	-	10/37/137/137	-
7	BCL	V	402	-	-	3/37/137/137	-
7	BCL	W	407[B]	5	-	4/13/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	W	403	-	-	6/37/137/137	-
10	LHG	C	301	-	-	19/38/38/53	-
7	BCL	V	407	-	-	7/37/137/137	-
7	BCL	a	806	-	-	16/37/137/137	-
11	LMG	A	819	-	-	19/34/54/70	0/1/1/1
7	BCL	A	802	-	-	10/37/137/137	-

All (420) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	824	G2O	MG-NA	14.77	2.41	2.06
13	a	805	G2O	MG-NA	12.75	2.36	2.06
13	a	801	G2O	MG-NC	12.01	2.34	2.06
13	A	824	G2O	C1D-ND	11.50	1.45	1.35
13	a	802	G2O	MG-NC	11.41	2.33	2.06
13	a	802	G2O	C1D-ND	11.36	1.45	1.35
13	a	801	G2O	C1D-ND	11.18	1.45	1.35
13	a	805	G2O	C1D-ND	11.09	1.45	1.35
6	a	804	GS0	MG-NC	10.63	2.31	2.06
13	a	802	G2O	MG-NA	10.52	2.31	2.06
6	A	801	GS0	MG-NC	10.30	2.30	2.06
13	A	824	G2O	MG-NC	9.97	2.29	2.06
13	a	801	G2O	MG-NA	9.69	2.29	2.06
13	a	805	G2O	MG-NC	9.52	2.28	2.06
13	a	802	G2O	C4B-NB	9.40	1.49	1.37
13	a	801	G2O	C4B-NB	9.40	1.49	1.37
13	a	805	G2O	C4B-NB	9.24	1.49	1.37
13	A	824	G2O	C4B-NB	8.51	1.48	1.37
13	a	801	G2O	C3D-C4D	8.36	1.48	1.40
13	a	802	G2O	C3D-C4D	8.24	1.48	1.40
13	a	805	G2O	C3D-C4D	8.20	1.48	1.40
13	A	824	G2O	C3D-C4D	8.03	1.47	1.40
8	a	818	F39	C35-C37	7.48	1.62	1.45
8	A	814	F39	C35-C37	7.46	1.62	1.45
8	a	818	F39	C56-C58	7.18	1.61	1.45
8	A	814	F39	C56-C58	7.12	1.61	1.45
6	a	804	GS0	MG-NA	7.10	2.23	2.06
6	A	801	GS0	MG-ND	-6.97	1.92	2.05
8	a	818	F39	C64-C62	6.94	1.60	1.45
13	a	801	G2O	CAA-C2A	-6.90	1.41	1.54
13	a	801	G2O	C1A-CHA	6.85	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	814	F39	C64-C62	6.75	1.60	1.45
13	a	802	G2O	C1A-CHA	6.68	1.51	1.37
13	a	802	G2O	CAA-C2A	-6.67	1.41	1.54
13	a	805	G2O	CAA-C2A	-6.60	1.41	1.54
13	A	824	G2O	CAA-C2A	-6.59	1.41	1.54
13	a	805	G2O	C1A-CHA	6.56	1.51	1.37
6	a	804	GS0	MG-ND	-6.56	1.92	2.05
6	A	801	GS0	MG-NA	6.50	2.21	2.06
13	A	824	G2O	C1A-CHA	6.36	1.50	1.37
13	a	802	G2O	C1B-C2B	6.34	1.57	1.45
8	A	814	F39	C41-C42	6.32	1.59	1.45
13	a	801	G2O	C1B-C2B	6.32	1.57	1.45
13	a	805	G2O	C3B-C4B	6.31	1.57	1.46
13	A	824	G2O	C1B-C2B	6.31	1.57	1.45
8	a	818	F39	C41-C42	6.27	1.59	1.45
13	a	802	G2O	C3B-C4B	6.24	1.57	1.46
13	A	824	G2O	C3B-C4B	6.13	1.57	1.46
13	a	802	G2O	C4C-NC	5.97	1.46	1.37
13	a	801	G2O	C3B-C4B	5.96	1.56	1.46
13	a	801	G2O	C4C-NC	5.95	1.46	1.37
13	a	805	G2O	C4C-NC	5.95	1.46	1.37
13	a	805	G2O	C1B-C2B	5.91	1.57	1.45
8	a	818	F39	C46-C53	5.89	1.60	1.47
8	A	814	F39	C46-C53	5.67	1.60	1.47
13	A	824	G2O	C4C-NC	5.53	1.46	1.37
8	a	818	F39	C51-C44	5.43	1.60	1.43
8	A	814	F39	C51-C44	5.30	1.59	1.43
8	A	814	F39	C32-C27	5.27	1.59	1.43
8	a	818	F39	C57-C59	5.26	1.59	1.43
8	a	818	F39	C32-C27	5.26	1.59	1.43
8	a	818	F39	C63-C61	5.19	1.59	1.43
7	W	407[B]	BCL	C1B-NB	5.17	1.39	1.35
8	A	814	F39	C40-C39	5.15	1.59	1.43
8	A	814	F39	C63-C61	5.13	1.59	1.43
13	A	824	G2O	C3C-C2C	5.11	1.47	1.36
8	a	818	F39	C40-C39	5.11	1.59	1.43
7	V	408[B]	BCL	C1B-NB	5.10	1.39	1.35
7	A	802	BCL	C1B-NB	5.10	1.39	1.35
7	U	408[B]	BCL	C1B-NB	5.07	1.39	1.35
7	A	803	BCL	C1B-NB	5.05	1.39	1.35
13	A	824	G2O	CHD-C4C	5.03	1.47	1.35
7	U	405	BCL	C1B-NB	5.02	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	807	BCL	C1B-NB	5.01	1.39	1.35
13	a	802	G2O	CHD-C4C	5.00	1.47	1.35
13	A	824	G2O	CHB-C1B	5.00	1.48	1.38
13	A	824	G2O	CMA-C3A	-5.00	1.42	1.53
8	A	814	F39	C57-C59	5.00	1.58	1.43
7	A	813	BCL	C1B-NB	4.99	1.39	1.35
7	U	403	BCL	C1B-NB	4.99	1.39	1.35
7	U	409	BCL	C1B-NB	4.99	1.39	1.35
13	a	805	G2O	CHD-C4C	4.98	1.47	1.35
7	U	402	BCL	C1B-NB	4.97	1.39	1.35
7	A	806	BCL	C1B-NB	4.97	1.39	1.35
7	a	808	BCL	C1B-NB	4.95	1.39	1.35
7	a	817	BCL	C1B-NB	4.93	1.39	1.35
7	A	808	BCL	C1B-NB	4.92	1.39	1.35
7	a	816	BCL	C1B-NB	4.91	1.39	1.35
13	a	802	G2O	CHB-C1B	4.90	1.47	1.38
7	W	401	BCL	C1B-NB	4.90	1.39	1.35
7	a	806	BCL	C1B-NB	4.90	1.39	1.35
13	a	801	G2O	CHD-C4C	4.88	1.47	1.35
7	a	815	BCL	C1B-NB	4.86	1.39	1.35
7	V	402	BCL	C1B-NB	4.86	1.39	1.35
13	a	801	G2O	CMA-C3A	-4.83	1.42	1.53
13	a	802	G2O	CMA-C3A	-4.83	1.42	1.53
13	a	805	G2O	CHB-C1B	4.82	1.47	1.38
13	a	805	G2O	CMA-C3A	-4.82	1.42	1.53
7	U	407	BCL	C1B-NB	4.81	1.39	1.35
7	V	405	BCL	C1B-NB	4.81	1.39	1.35
7	a	810	BCL	C1B-NB	4.79	1.39	1.35
7	A	810	BCL	C1B-NB	4.78	1.39	1.35
7	a	812	BCL	C1B-NB	4.78	1.39	1.35
13	a	802	G2O	C3C-C2C	4.78	1.46	1.36
7	a	811	BCL	C1B-NB	4.77	1.39	1.35
8	a	818	F39	C14-C13	4.76	1.60	1.53
13	a	801	G2O	CHB-C1B	4.76	1.47	1.38
7	a	814	BCL	C1B-NB	4.75	1.39	1.35
13	a	805	G2O	C3C-C2C	4.75	1.46	1.36
7	a	809	BCL	C1B-NB	4.75	1.39	1.35
7	a	813	BCL	C1B-NB	4.74	1.39	1.35
13	a	801	G2O	C3C-C2C	4.74	1.46	1.36
7	U	404	BCL	C1B-NB	4.74	1.39	1.35
7	V	407	BCL	C1B-NB	4.74	1.39	1.35
13	a	802	G2O	C1C-C2C	4.71	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	811	BCL	C1B-NB	4.71	1.39	1.35
7	U	406	BCL	C1B-NB	4.71	1.39	1.35
7	W	406	BCL	C1B-NB	4.70	1.39	1.35
13	a	805	G2O	C1C-C2C	4.70	1.53	1.44
13	A	824	G2O	C1C-C2C	4.70	1.53	1.44
7	W	405	BCL	C1B-NB	4.68	1.39	1.35
7	A	812	BCL	C1B-NB	4.68	1.39	1.35
13	A	824	G2O	CHC-C1C	4.65	1.49	1.39
8	A	814	F39	C14-C13	4.65	1.60	1.53
7	A	809	BCL	C1B-NB	4.64	1.39	1.35
8	A	814	F39	C19-C20	4.64	1.60	1.51
7	W	404	BCL	C1B-NB	4.63	1.39	1.35
7	A	807	BCL	C1B-NB	4.61	1.39	1.35
7	V	404	BCL	C1B-NB	4.58	1.39	1.35
7	U	401	BCL	MG-NA	4.57	2.17	2.06
13	a	801	G2O	C1C-C2C	4.57	1.53	1.44
7	V	401	BCL	C1B-NB	4.55	1.39	1.35
7	A	804	BCL	C1B-NB	4.54	1.39	1.35
7	W	403	BCL	C1B-NB	4.53	1.39	1.35
7	V	406	BCL	C1B-NB	4.49	1.39	1.35
7	W	401	BCL	MG-NA	4.48	2.16	2.06
7	U	401	BCL	C1B-NB	4.46	1.39	1.35
7	W	402	BCL	C1B-NB	4.46	1.39	1.35
13	a	805	G2O	CHC-C1C	4.44	1.49	1.39
7	V	408[B]	BCL	MG-NA	4.43	2.16	2.06
7	a	812	BCL	MG-NA	4.41	2.16	2.06
7	A	804	BCL	MG-NA	4.41	2.16	2.06
7	U	406	BCL	MG-NA	4.39	2.16	2.06
7	a	815	BCL	MG-NA	4.38	2.16	2.06
7	V	403	BCL	C1B-NB	4.37	1.39	1.35
13	a	801	G2O	CBD-CGD	-4.35	1.38	1.52
13	A	824	G2O	OBD-CAD	4.34	1.28	1.22
7	V	403	BCL	MG-NA	4.34	2.16	2.06
13	a	805	G2O	OBD-CAD	4.33	1.28	1.22
13	a	802	G2O	CBD-CGD	-4.33	1.38	1.52
7	V	401	BCL	MG-NA	4.32	2.16	2.06
13	a	802	G2O	OBD-CAD	4.32	1.28	1.22
13	a	802	G2O	CHC-C1C	4.32	1.49	1.39
7	A	807	BCL	MG-NA	4.32	2.16	2.06
13	a	805	G2O	CBD-CGD	-4.31	1.38	1.52
7	W	402	BCL	MG-NA	4.31	2.16	2.06
6	a	804	GS0	O1D-CGD	-4.31	1.10	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	804	GS0	OBD-CAD	4.30	1.29	1.22
8	a	818	F39	C19-C20	4.29	1.60	1.51
7	V	406	BCL	MG-NA	4.29	2.16	2.06
7	A	805	BCL	C1B-NB	4.29	1.39	1.35
7	U	408[B]	BCL	MG-NA	4.28	2.16	2.06
7	W	404	BCL	MG-NA	4.27	2.16	2.06
7	V	402	BCL	MG-NA	4.24	2.16	2.06
6	A	801	GS0	OBD-CAD	4.24	1.29	1.22
7	U	407	BCL	MG-NA	4.23	2.16	2.06
13	A	824	G2O	CBD-CGD	-4.22	1.39	1.52
7	a	808	BCL	MG-NA	4.22	2.16	2.06
7	A	805	BCL	MG-NA	4.20	2.16	2.06
7	V	407	BCL	MG-NA	4.18	2.16	2.06
6	A	801	GS0	O1D-CGD	-4.17	1.10	1.21
7	A	808	BCL	MG-NA	4.16	2.16	2.06
7	a	816	BCL	MG-NA	4.16	2.16	2.06
7	A	803	BCL	MG-NA	4.15	2.16	2.06
7	a	807	BCL	MG-NA	4.13	2.16	2.06
7	U	403	BCL	MG-NA	4.12	2.16	2.06
6	A	801	GS0	C4D-ND	-4.11	1.32	1.37
13	a	801	G2O	CHC-C1C	4.10	1.48	1.39
7	a	806	BCL	MG-NA	4.09	2.16	2.06
7	V	404	BCL	MG-NA	4.09	2.16	2.06
13	A	824	G2O	O2D-CGD	4.09	1.43	1.33
7	W	405	BCL	MG-NA	4.09	2.16	2.06
7	a	811	BCL	MG-NA	4.08	2.16	2.06
7	U	402	BCL	MG-NA	4.07	2.15	2.06
13	a	801	G2O	O2D-CGD	4.06	1.43	1.33
7	W	403	BCL	MG-NA	4.06	2.15	2.06
7	A	811	BCL	MG-NA	4.04	2.15	2.06
13	a	805	G2O	O2D-CGD	4.04	1.43	1.33
6	a	804	GS0	C4D-ND	-4.04	1.32	1.37
7	a	813	BCL	MG-NA	4.02	2.15	2.06
13	A	824	G2O	C3B-C2B	4.02	1.45	1.37
13	a	801	G2O	C4C-C3C	4.01	1.51	1.45
7	U	404	BCL	MG-NA	4.00	2.15	2.06
7	A	813	BCL	MG-NA	3.99	2.15	2.06
7	A	812	BCL	MG-NA	3.99	2.15	2.06
7	V	405	BCL	MG-NA	3.99	2.15	2.06
13	a	801	G2O	OBD-CAD	3.98	1.27	1.22
13	a	802	G2O	O2D-CGD	3.98	1.42	1.33
7	W	406	BCL	MG-NA	3.98	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	801	G2O	C4D-CHA	3.97	1.50	1.45
7	U	405	BCL	MG-NA	3.97	2.15	2.06
13	A	824	G2O	CHB-C4A	3.96	1.50	1.39
7	A	806	BCL	MG-NA	3.95	2.15	2.06
7	A	810	BCL	MG-NA	3.94	2.15	2.06
7	W	407[B]	BCL	MG-NA	3.92	2.15	2.06
13	a	802	G2O	C4C-C3C	3.90	1.51	1.45
7	A	809	BCL	MG-NA	3.90	2.15	2.06
13	A	824	G2O	O2A-CGA	3.87	1.44	1.33
13	A	824	G2O	C4C-C3C	3.86	1.51	1.45
7	a	810	BCL	MG-NA	3.86	2.15	2.06
7	U	409	BCL	MG-NA	3.85	2.15	2.06
13	a	802	G2O	O2A-CGA	3.85	1.44	1.33
7	A	802	BCL	MG-NA	3.84	2.15	2.06
13	a	805	G2O	C4C-C3C	3.84	1.51	1.45
13	a	801	G2O	O2A-CGA	3.83	1.44	1.33
13	a	801	G2O	C3D-C2D	3.82	1.46	1.39
13	a	805	G2O	C3D-C2D	3.82	1.46	1.39
7	a	809	BCL	MG-NA	3.82	2.15	2.06
13	a	805	G2O	O2A-CGA	3.80	1.44	1.33
13	a	802	G2O	C3D-C2D	3.79	1.46	1.39
9	A	815	F26	C35-C34	3.78	1.54	1.45
13	a	802	G2O	CHB-C4A	3.77	1.49	1.39
13	a	801	G2O	C3B-C2B	3.77	1.44	1.37
13	A	824	G2O	C3D-C2D	3.76	1.46	1.39
7	a	817	BCL	MG-NA	3.72	2.15	2.06
13	a	802	G2O	C3B-C2B	3.71	1.44	1.37
13	a	805	G2O	C3B-C2B	3.70	1.44	1.37
13	a	805	G2O	CHB-C4A	3.66	1.49	1.39
13	a	802	G2O	C4D-CHA	3.66	1.49	1.45
13	a	801	G2O	CHB-C4A	3.63	1.49	1.39
7	a	814	BCL	MG-NA	3.60	2.14	2.06
9	A	815	F26	C28-C31	3.58	1.53	1.45
9	a	819	F26	C28-C31	3.53	1.53	1.45
9	a	819	F26	C15-C19	3.53	1.53	1.45
9	a	820	F26	C35-C34	3.51	1.53	1.45
9	a	820	F26	C28-C31	3.48	1.53	1.45
13	A	824	G2O	C4D-ND	3.48	1.38	1.35
13	a	801	G2O	O1D-CGD	3.44	1.29	1.21
13	A	824	G2O	O1D-CGD	3.44	1.29	1.21
13	a	805	G2O	O1D-CGD	3.43	1.29	1.21
13	A	824	G2O	C2-C3	3.42	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	802	G2O	C4D-ND	3.42	1.38	1.35
9	A	815	F26	C25-C26	3.41	1.53	1.45
13	a	802	G2O	O1D-CGD	3.41	1.29	1.21
13	a	801	G2O	C4D-ND	3.41	1.38	1.35
13	a	802	G2O	C2-C3	3.40	1.41	1.33
13	a	801	G2O	C2-C3	3.35	1.41	1.33
6	A	801	GS0	O2D-CGD	-3.35	1.25	1.33
9	a	820	F26	C15-C19	3.35	1.53	1.45
9	a	820	F26	C25-C26	3.33	1.53	1.45
6	A	801	GS0	O2D-CED	3.31	1.53	1.45
13	a	805	G2O	C2-C3	3.30	1.40	1.33
9	A	815	F26	C15-C19	3.29	1.53	1.45
13	a	805	G2O	C4D-ND	3.27	1.38	1.35
6	a	804	GS0	O2D-CED	3.26	1.53	1.45
13	a	805	G2O	C4D-CHA	3.19	1.49	1.45
9	A	815	F26	C39-C37	3.17	1.53	1.43
6	a	804	GS0	O2D-CGD	-3.13	1.25	1.33
9	A	815	F26	C32-C30	3.10	1.53	1.43
9	a	820	F26	C38-C33	3.10	1.53	1.43
6	a	804	GS0	O2A-CGA	-3.10	1.24	1.33
9	A	815	F26	C27-C24	3.07	1.53	1.43
13	A	824	G2O	C4D-CHA	3.04	1.48	1.45
9	A	815	F26	C38-C33	3.01	1.52	1.43
9	a	820	F26	C39-C37	3.00	1.52	1.43
6	A	801	GS0	C1D-C2D	-2.99	1.39	1.45
9	a	819	F26	C39-C37	2.96	1.52	1.43
6	A	801	GS0	O2A-CGA	-2.96	1.24	1.33
9	a	820	F26	C32-C30	2.95	1.52	1.43
9	a	819	F26	C25-C26	2.94	1.52	1.45
9	a	819	F26	C35-C34	2.94	1.52	1.45
9	a	820	F26	C27-C24	2.94	1.52	1.43
9	a	819	F26	C38-C33	2.94	1.52	1.43
9	A	815	F26	C22-C18	2.92	1.52	1.43
9	a	819	F26	C27-C24	2.92	1.52	1.43
6	A	801	GS0	O1A-CGA	-2.91	1.13	1.22
6	a	804	GS0	O1A-CGA	-2.85	1.14	1.22
9	a	820	F26	C22-C18	2.84	1.52	1.43
13	a	802	G2O	C5-C6	2.82	1.59	1.50
13	A	824	G2O	C5-C6	2.81	1.59	1.50
9	a	820	F26	C8-C13	2.79	1.57	1.51
13	a	805	G2O	C5-C6	2.79	1.59	1.50
13	a	801	G2O	C5-C3	2.75	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	804	GS0	C4B-NB	2.75	1.37	1.35
13	a	801	G2O	C1B-NB	2.75	1.41	1.37
13	a	801	G2O	C5-C6	2.75	1.58	1.50
13	a	805	G2O	C5-C3	2.74	1.58	1.51
13	A	824	G2O	C3A-C2A	-2.73	1.46	1.54
9	a	819	F26	C32-C30	2.72	1.51	1.43
13	A	824	G2O	C5-C3	2.69	1.58	1.51
9	A	815	F26	C8-C13	2.68	1.56	1.51
13	a	805	G2O	O1A-CGA	2.63	1.30	1.22
13	a	802	G2O	C5-C3	2.61	1.58	1.51
9	a	819	F26	C22-C18	2.59	1.51	1.43
13	a	802	G2O	O1A-CGA	2.56	1.30	1.22
8	a	818	F39	C11-C9	2.53	1.59	1.52
13	a	801	G2O	O1A-CGA	2.53	1.30	1.22
13	A	824	G2O	O1A-CGA	2.53	1.30	1.22
13	a	802	G2O	CBA-CGA	2.51	1.58	1.50
13	a	801	G2O	C3A-C2A	-2.50	1.47	1.54
13	a	805	G2O	C3A-C2A	-2.50	1.47	1.54
13	A	824	G2O	C1-C2	2.49	1.56	1.49
13	a	802	G2O	C1B-NB	2.47	1.40	1.37
13	a	802	G2O	C1-C2	2.47	1.56	1.49
13	A	824	G2O	CBA-CGA	2.47	1.57	1.50
13	a	805	G2O	CBA-CGA	2.46	1.57	1.50
9	a	819	F26	C8-C13	2.46	1.56	1.51
13	a	801	G2O	C1-C2	2.45	1.56	1.49
13	a	802	G2O	C3A-C2A	-2.44	1.47	1.54
13	a	801	G2O	CBA-CGA	2.44	1.57	1.50
8	a	818	F39	C46-C48	2.43	1.44	1.41
8	a	818	F39	O6-C21	2.42	1.40	1.33
6	a	804	GS0	C1D-C2D	-2.41	1.40	1.45
8	A	814	F39	C23-C22	2.41	1.61	1.52
13	a	805	G2O	C1-C2	2.40	1.56	1.49
6	a	804	GS0	C1B-NB	2.38	1.37	1.35
8	A	814	F39	O6-C21	2.38	1.40	1.33
13	a	805	G2O	C1B-NB	2.36	1.40	1.37
8	a	818	F39	C50-C49	2.36	1.43	1.38
13	a	801	G2O	C4-C3	2.35	1.56	1.50
7	V	402	BCL	OBD-CAD	2.35	1.25	1.22
7	U	404	BCL	OBD-CAD	2.33	1.25	1.22
8	A	814	F39	C46-C48	2.33	1.44	1.41
7	a	807	BCL	CAC-C3C	2.33	1.58	1.54
7	A	805	BCL	OBD-CAD	2.32	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	824	G2O	C4-C3	2.32	1.56	1.50
8	A	814	F39	C50-C49	2.32	1.43	1.38
7	A	805	BCL	C3B-CAB	-2.31	1.43	1.49
7	a	816	BCL	OBD-CAD	2.31	1.25	1.22
7	U	402	BCL	OBD-CAD	2.31	1.25	1.22
8	a	818	F39	C23-C22	2.30	1.60	1.52
7	A	811	BCL	OBD-CAD	2.30	1.25	1.22
13	a	805	G2O	C4-C3	2.29	1.56	1.50
7	a	809	BCL	OBD-CAD	2.29	1.25	1.22
7	U	401	BCL	OBD-CAD	2.28	1.25	1.22
7	A	812	BCL	OBD-CAD	2.28	1.25	1.22
7	U	403	BCL	OBD-CAD	2.27	1.25	1.22
7	W	405	BCL	OBD-CAD	2.26	1.25	1.22
7	V	401	BCL	OBD-CAD	2.26	1.25	1.22
8	a	818	F39	C47-C45	2.26	1.44	1.40
7	A	809	BCL	OBD-CAD	2.26	1.25	1.22
10	A	817	LHG	O7-C5	-2.24	1.41	1.46
13	A	824	G2O	MG-NB	-2.24	2.01	2.05
7	U	409	BCL	OBD-CAD	2.24	1.25	1.22
13	a	801	G2O	O2D-CED	2.24	1.50	1.45
8	a	818	F39	C38-C37	2.24	1.55	1.50
13	a	802	G2O	C4-C3	2.22	1.56	1.50
7	A	802	BCL	OBD-CAD	2.22	1.25	1.22
7	a	813	BCL	OBD-CAD	2.21	1.25	1.22
7	V	406	BCL	OBD-CAD	2.21	1.25	1.22
6	a	804	GS0	C3B-C2B	-2.21	1.35	1.39
8	A	814	F39	C11-C9	2.20	1.58	1.52
7	A	807	BCL	OBD-CAD	2.20	1.25	1.22
7	A	806	BCL	OBD-CAD	2.19	1.25	1.22
7	a	806	BCL	OBD-CAD	2.19	1.25	1.22
7	V	405	BCL	OBD-CAD	2.18	1.25	1.22
8	A	814	F39	C18-C19	2.18	1.60	1.52
7	a	815	BCL	OBD-CAD	2.18	1.25	1.22
7	A	803	BCL	OBD-CAD	2.18	1.25	1.22
7	W	401	BCL	MG-NC	2.17	2.11	2.06
13	a	805	G2O	CAA-CBA	2.17	1.59	1.52
7	U	406	BCL	OBD-CAD	2.16	1.25	1.22
8	A	814	F39	C47-C45	2.16	1.44	1.40
7	U	405	BCL	OBD-CAD	2.16	1.25	1.22
11	C	302	LMG	C4-C5	2.16	1.57	1.53
13	a	802	G2O	C7-C6	2.15	1.40	1.31
8	a	818	F39	C18-C19	2.14	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	824	LMG	O7-C8	-2.14	1.41	1.46
7	a	809	BCL	C3B-CAB	-2.14	1.43	1.49
7	a	812	BCL	C5-C3	2.14	1.55	1.51
10	A	816	LHG	P-O6	2.13	1.67	1.59
7	V	403	BCL	OBD-CAD	2.11	1.25	1.22
7	U	408[B]	BCL	MG-NC	2.11	2.11	2.06
13	A	824	G2O	CAA-CBA	2.11	1.59	1.52
8	a	818	F39	C46-C45	2.10	1.43	1.41
7	W	404	BCL	OBD-CAD	2.10	1.25	1.22
7	W	403	BCL	OBD-CAD	2.10	1.25	1.22
7	A	808	BCL	OBD-CAD	2.10	1.25	1.22
13	a	805	G2O	C7-C6	2.10	1.40	1.31
13	a	802	G2O	CAA-CBA	2.09	1.59	1.52
13	A	824	G2O	C7-C6	2.09	1.40	1.31
7	A	804	BCL	MG-NC	2.09	2.11	2.06
7	W	407[B]	BCL	OBD-CAD	2.09	1.25	1.22
7	U	407	BCL	MG-NC	2.08	2.11	2.06
7	a	815	BCL	MG-NC	2.08	2.11	2.06
13	a	801	G2O	CAA-CBA	2.08	1.59	1.52
7	A	810	BCL	OBD-CAD	2.08	1.25	1.22
7	A	810	BCL	C3B-CAB	-2.08	1.43	1.49
13	a	801	G2O	C7-C6	2.08	1.40	1.31
10	C	301	LHG	O7-C5	-2.07	1.41	1.46
7	a	810	BCL	OBD-CAD	2.07	1.25	1.22
8	A	814	F39	C38-C37	2.07	1.55	1.50
7	V	407	BCL	MG-NC	2.07	2.11	2.06
13	A	824	G2O	C1B-NB	2.07	1.40	1.37
7	W	402	BCL	OBD-CAD	2.06	1.25	1.22
7	a	814	BCL	C4B-NB	2.06	1.37	1.35
7	a	814	BCL	OBD-CAD	2.06	1.25	1.22
7	U	401	BCL	C4B-NB	2.05	1.37	1.35
7	W	401	BCL	C4B-NB	2.05	1.37	1.35
10	a	821	LHG	O7-C5	-2.05	1.41	1.46
7	V	402	BCL	C4B-NB	2.05	1.37	1.35
13	A	824	G2O	O2D-CED	2.04	1.50	1.45
7	A	808	BCL	MG-NC	2.04	2.11	2.06
7	a	817	BCL	OBD-CAD	2.04	1.25	1.22
13	a	801	G2O	CBB-CAB	2.04	1.40	1.30
7	A	809	BCL	C3B-CAB	-2.03	1.43	1.49
10	a	822	LHG	P-O6	2.03	1.67	1.59
7	a	816	BCL	C4B-NB	2.03	1.37	1.35
13	a	802	G2O	O2D-CED	2.03	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	402	BCL	C4B-NB	2.02	1.37	1.35
7	U	407	BCL	OBD-CAD	2.02	1.25	1.22
7	a	812	BCL	C4B-NB	2.02	1.37	1.35
7	U	408[B]	BCL	C3D-CAD	-2.02	1.40	1.46
13	a	805	G2O	O2D-CED	2.01	1.50	1.45
7	V	408[B]	BCL	OBD-CAD	2.01	1.25	1.22
7	a	811	BCL	MG-NC	2.01	2.11	2.06
13	A	824	G2O	CBB-CAB	2.01	1.40	1.30
13	a	802	G2O	CBB-CAB	2.01	1.40	1.30
7	V	405	BCL	CBD-CGD	-2.00	1.46	1.52
7	V	404	BCL	OBD-CAD	2.00	1.25	1.22

All (791) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	801	G2O	C1A-NA-C4A	20.39	115.87	106.71
13	a	802	G2O	C1A-NA-C4A	19.69	115.56	106.71
13	a	805	G2O	C1A-NA-C4A	17.74	114.68	106.71
13	A	824	G2O	C1A-NA-C4A	17.57	114.60	106.71
6	A	801	GS0	C4A-NA-C1A	12.63	112.38	106.71
6	a	804	GS0	C4A-NA-C1A	12.52	112.33	106.71
7	a	809	BCL	CAD-C3D-C4D	-7.98	104.02	108.47
6	a	804	GS0	C1C-NC-C4C	7.62	110.13	106.71
6	a	804	GS0	C4D-CHA-C1A	7.54	130.43	121.25
13	a	801	G2O	C5-C6-C7	-7.17	108.76	125.05
13	a	805	G2O	C5-C6-C7	-7.16	108.81	125.05
13	A	824	G2O	C5-C6-C7	-7.11	108.92	125.05
6	A	801	GS0	C4D-CHA-C1A	7.00	129.76	121.25
6	A	801	GS0	CMB-C2B-C1B	-6.85	117.94	128.46
6	A	801	GS0	C1C-NC-C4C	6.55	109.65	106.71
13	a	802	G2O	C5-C6-C7	-6.52	110.25	125.05
7	a	808	BCL	CAD-C3D-C4D	-6.50	104.84	108.47
6	a	804	GS0	CMB-C2B-C1B	-6.26	118.85	128.46
8	a	818	F39	C11-O1-C12	6.16	125.78	113.69
9	A	815	F26	C38-C33-C31	-5.97	118.79	127.31
7	a	811	BCL	CAD-C3D-C4D	-5.92	105.17	108.47
8	A	814	F39	C11-O1-C12	5.80	125.07	113.69
9	a	819	F26	C32-C30-C26	-5.77	119.07	127.31
9	a	819	F26	C38-C33-C31	-5.77	119.08	127.31
13	A	824	G2O	CMA-C3A-C4A	5.77	127.27	111.77
9	a	820	F26	C23-C19-C15	-5.61	109.24	118.08
13	a	805	G2O	CAA-C2A-C3A	5.60	128.12	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	401	BCL	C1-C2-C3	-5.59	116.37	126.04
7	A	806	BCL	CAD-C3D-C4D	-5.58	105.36	108.47
7	A	802	BCL	CAD-C3D-C4D	-5.58	105.36	108.47
7	V	406	BCL	CAD-C3D-C4D	-5.47	105.42	108.47
13	a	801	G2O	CMA-C3A-C4A	5.36	126.18	111.77
13	A	824	G2O	CHB-C4A-NA	5.36	131.03	125.08
13	a	805	G2O	CMA-C3A-C4A	5.30	126.03	111.77
13	a	802	G2O	CMA-C3A-C4A	5.29	125.99	111.77
8	A	814	F39	C57-C59-C62	-5.28	119.77	127.31
8	A	814	F39	C25-C20-C27	-5.28	108.98	122.59
7	A	803	BCL	CAD-C3D-C4D	-5.25	105.54	108.47
8	A	814	F39	C51-C44-C42	-5.24	119.83	127.31
9	a	819	F26	C23-C19-C15	-5.24	109.82	118.08
8	a	818	F39	C25-C20-C27	-5.22	109.11	122.59
13	a	802	G2O	CAA-C2A-C3A	5.21	127.04	112.78
7	A	807	BCL	CAD-C3D-C4D	-5.18	105.58	108.47
9	A	815	F26	C23-C19-C15	-5.18	109.92	118.08
13	A	824	G2O	CAA-C2A-C3A	5.14	126.85	112.78
13	A	824	G2O	C2B-C1B-NB	-5.14	106.32	110.10
6	a	804	GS0	O2D-CGD-CBD	5.11	120.34	111.27
8	A	814	F39	C40-C39-C37	-5.11	120.02	127.31
6	A	801	GS0	CAC-C3C-C2C	-5.06	101.62	114.26
6	a	804	GS0	C2A-C1A-CHA	5.00	132.60	123.86
13	a	801	G2O	CAA-C2A-C3A	4.99	126.44	112.78
8	a	818	F39	C40-C39-C37	-4.97	120.21	127.31
13	A	824	G2O	CAA-C2A-C1A	4.97	128.25	111.97
8	a	818	F39	C63-C61-C58	-4.96	120.23	127.31
7	A	805	BCL	C1C-NC-C4C	4.93	108.92	106.71
6	A	801	GS0	C2A-C1A-CHA	4.92	132.46	123.86
7	A	805	BCL	CAD-C3D-C4D	-4.91	105.73	108.47
8	A	814	F39	C63-C61-C58	-4.91	120.31	127.31
8	a	818	F39	C51-C44-C42	-4.89	120.33	127.31
7	A	811	BCL	CAD-C3D-C4D	-4.88	105.75	108.47
9	a	820	F26	C38-C33-C31	-4.88	120.34	127.31
7	a	809	BCL	C4A-NA-C1A	4.88	108.90	106.71
13	a	801	G2O	CAA-C2A-C1A	4.80	127.70	111.97
7	W	402	BCL	C4A-NA-C1A	4.78	108.86	106.71
7	A	808	BCL	CAD-C3D-C4D	-4.78	105.81	108.47
13	a	802	G2O	CAA-C2A-C1A	4.75	127.53	111.97
6	a	804	GS0	O2D-CGD-O1D	-4.75	114.56	123.84
7	a	814	BCL	CAD-C3D-C4D	-4.71	105.84	108.47
7	V	408[B]	BCL	CAD-C3D-C4D	-4.71	105.85	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	814	F39	O6-C21-C22	4.66	126.52	111.91
9	a	819	F26	C27-C24-C19	-4.65	120.67	127.31
9	a	820	F26	C27-C24-C19	-4.65	120.67	127.31
6	A	801	GS0	O2D-CGD-CBD	4.64	119.52	111.27
7	A	804	BCL	CAD-C3D-C4D	-4.62	105.89	108.47
7	V	403	BCL	C4A-NA-C1A	4.60	108.78	106.71
8	a	818	F39	C57-C59-C62	-4.60	120.75	127.31
13	a	802	G2O	CHB-C4A-NA	4.59	130.17	125.08
7	U	402	BCL	C1-C2-C3	-4.57	118.13	126.04
7	W	405	BCL	C4A-NA-C1A	4.57	108.76	106.71
9	A	815	F26	C32-C30-C26	-4.55	120.82	127.31
13	A	824	G2O	C2C-C1C-NC	-4.54	105.62	110.57
13	a	805	G2O	CAA-C2A-C1A	4.48	126.66	111.97
9	a	820	F26	C32-C30-C26	-4.46	120.94	127.31
7	V	405	BCL	C4A-NA-C1A	4.45	108.71	106.71
13	A	824	G2O	C3C-C4C-NC	-4.42	105.71	109.88
6	A	801	GS0	OBB-CAB-CBB	-4.41	110.26	120.17
7	W	403	BCL	CAD-C3D-C4D	-4.39	106.02	108.47
6	A	801	GS0	O2D-CGD-O1D	-4.39	115.25	123.84
6	A	801	GS0	CMB-C2B-C3B	4.39	132.89	124.68
7	W	402	BCL	CAD-C3D-C4D	-4.39	106.02	108.47
9	A	815	F26	C27-C24-C19	-4.35	121.11	127.31
7	A	805	BCL	C4A-NA-C1A	4.32	108.65	106.71
6	A	801	GS0	CGD-CBD-CAD	4.30	124.66	110.73
13	a	805	G2O	CHB-C4A-NA	4.30	129.85	125.08
7	A	813	BCL	CAD-C3D-C4D	-4.29	106.08	108.47
7	a	815	BCL	C4A-NA-C1A	4.27	108.62	106.71
7	U	404	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
9	A	815	F26	C39-C37-C34	-4.20	121.31	127.31
7	U	406	BCL	CAD-C3D-C4D	-4.20	106.13	108.47
6	A	801	GS0	CHA-C1A-NA	-4.18	116.82	126.40
13	a	805	G2O	C2B-C1B-NB	-4.18	107.02	110.10
8	a	818	F39	O6-C21-C22	4.17	124.99	111.91
6	a	804	GS0	OBB-CAB-CBB	-4.15	110.82	120.17
7	W	405	BCL	C1C-NC-C4C	4.15	108.57	106.71
7	U	405	BCL	CAD-C3D-C4D	-4.15	106.16	108.47
9	a	819	F26	C2-C9-C15	-4.14	119.29	128.63
7	a	807	BCL	C1C-NC-C4C	4.14	108.57	106.71
7	W	405	BCL	CAD-C3D-C4D	-4.11	106.18	108.47
7	V	407	BCL	CAD-C3D-C4D	-4.10	106.18	108.47
7	U	405	BCL	C1C-NC-C4C	4.10	108.55	106.71
7	U	403	BCL	CAD-C3D-C4D	-4.10	106.18	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	810	BCL	CAD-C3D-C4D	-4.09	106.19	108.47
7	V	404	BCL	CAD-C3D-C4D	-4.07	106.20	108.47
7	A	809	BCL	CAD-C3D-C4D	-4.05	106.21	108.47
9	a	820	F26	C2-C9-C15	-4.04	119.51	128.63
9	a	820	F26	C39-C37-C34	-4.03	121.55	127.31
7	A	812	BCL	CAD-C3D-C4D	-4.03	106.22	108.47
7	V	405	BCL	CAD-C3D-C4D	-4.03	106.22	108.47
7	V	403	BCL	CAD-C3D-C4D	-4.02	106.23	108.47
13	a	801	G2O	CHB-C4A-NA	4.02	129.54	125.08
7	U	409	BCL	CAD-C3D-C4D	-4.01	106.23	108.47
7	W	407[B]	BCL	CAD-C3D-C4D	-4.01	106.23	108.47
7	U	404	BCL	C4A-NA-C1A	4.01	108.51	106.71
7	a	806	BCL	C1-C2-C3	-4.00	119.13	126.04
7	a	813	BCL	C4A-NA-C1A	3.99	108.50	106.71
7	W	403	BCL	C4A-NA-C1A	3.97	108.49	106.71
7	a	817	BCL	CAD-C3D-C4D	-3.96	106.26	108.47
7	V	405	BCL	C1C-NC-C4C	3.96	108.49	106.71
7	a	811	BCL	C1C-NC-C4C	3.95	108.48	106.71
8	a	818	F39	C35-C37-C39	-3.94	112.89	118.94
8	A	814	F39	O6-C21-O7	-3.94	113.65	123.59
7	a	816	BCL	C4A-NA-C1A	3.94	108.48	106.71
7	a	807	BCL	CAD-C3D-C4D	-3.93	106.28	108.47
7	a	808	BCL	C4A-NA-C1A	3.93	108.47	106.71
7	W	401	BCL	CAD-C3D-C4D	-3.92	106.28	108.47
7	V	402	BCL	C4A-NA-C1A	3.92	108.47	106.71
7	a	815	BCL	CAD-C3D-C4D	-3.91	106.29	108.47
7	U	401	BCL	CAD-C3D-C4D	-3.89	106.30	108.47
7	V	401	BCL	CAD-C3D-C4D	-3.89	106.30	108.47
8	A	814	F39	C56-C58-C61	-3.89	112.98	118.94
7	A	807	BCL	C4A-NA-C1A	3.83	108.43	106.71
6	a	804	GS0	CAC-C3C-C2C	-3.83	104.68	114.26
7	a	810	BCL	CAD-C3D-C4D	-3.83	106.33	108.47
7	V	404	BCL	CMB-C2B-C1B	-3.83	122.58	128.46
7	A	805	BCL	CHA-C1A-NA	-3.83	117.63	126.40
13	a	805	G2O	CGD-CBD-CAD	3.82	123.09	110.73
7	W	401	BCL	C4A-NA-C1A	3.81	108.42	106.71
6	a	804	GS0	CMB-C2B-C3B	3.81	131.80	124.68
7	W	404	BCL	CAD-C3D-C4D	-3.81	106.35	108.47
13	a	802	G2O	C2B-C1B-NB	-3.80	107.30	110.10
7	a	808	BCL	CMB-C2B-C1B	-3.80	122.63	128.46
13	a	805	G2O	C3C-C4C-NC	-3.79	106.31	109.88
7	a	806	BCL	C4A-NA-C1A	3.78	108.41	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	402	BCL	CAD-C3D-C4D	-3.78	106.36	108.47
7	U	406	BCL	C4A-NA-C1A	3.77	108.40	106.71
7	W	403	BCL	CMB-C2B-C1B	-3.77	122.67	128.46
7	a	816	BCL	C1C-NC-C4C	3.77	108.40	106.71
6	a	804	GS0	CGD-CBD-CAD	3.76	122.93	110.73
7	a	817	BCL	C4A-NA-C1A	3.76	108.40	106.71
7	U	403	BCL	C4A-NA-C1A	3.76	108.40	106.71
7	A	813	BCL	C1C-NC-C4C	3.73	108.39	106.71
7	a	814	BCL	CMB-C2B-C1B	-3.73	122.73	128.46
7	V	404	BCL	C4A-NA-C1A	3.73	108.38	106.71
7	V	401	BCL	C4B-C3B-CAB	-3.71	119.97	127.13
7	A	806	BCL	C1C-NC-C4C	3.70	108.37	106.71
7	A	810	BCL	C1C-NC-C4C	3.69	108.37	106.71
7	a	812	BCL	CAD-C3D-C4D	-3.69	106.41	108.47
7	U	404	BCL	CAD-C3D-C4D	-3.69	106.41	108.47
7	a	810	BCL	CMB-C2B-C1B	-3.69	122.80	128.46
8	A	814	F39	C46-C53-C56	-3.68	120.33	128.63
8	A	814	F39	C41-C42-C44	-3.68	113.30	118.94
13	a	802	G2O	CGD-CBD-CAD	3.68	122.64	110.73
7	W	406	BCL	C4A-NA-C1A	3.67	108.36	106.71
7	a	812	BCL	C4A-NA-C1A	3.66	108.35	106.71
8	a	818	F39	O6-C21-O7	-3.66	114.36	123.59
13	a	801	G2O	C2B-C1B-NB	-3.66	107.41	110.10
7	W	401	BCL	C1C-NC-C4C	3.65	108.35	106.71
7	U	401	BCL	C4A-NA-C1A	3.64	108.34	106.71
7	A	804	BCL	CMB-C2B-C1B	-3.63	122.88	128.46
7	U	403	BCL	C1C-NC-C4C	3.63	108.34	106.71
8	a	818	F39	C46-C53-C56	-3.62	120.46	128.63
7	a	809	BCL	CHA-C1A-NA	-3.61	118.12	126.40
7	a	809	BCL	C1C-NC-C4C	3.61	108.33	106.71
7	V	402	BCL	C1-C2-C3	-3.60	119.82	126.04
7	A	804	BCL	C4B-C3B-CAB	-3.59	120.19	127.13
13	A	824	G2O	CGD-CBD-CAD	3.59	122.37	110.73
7	U	407	BCL	CAD-C3D-C4D	-3.58	106.47	108.47
6	A	801	GS0	CMA-C3A-C4A	-3.58	102.15	111.77
8	a	818	F39	C41-C42-C44	-3.58	113.45	118.94
7	W	401	BCL	CMB-C2B-C1B	-3.56	122.99	128.46
7	U	408[B]	BCL	CAD-C3D-C4D	-3.53	106.50	108.47
13	A	824	G2O	C2A-C3A-C4A	3.53	107.57	101.87
7	U	405	BCL	C4A-NA-C1A	3.52	108.29	106.71
7	A	810	BCL	C1-C2-C3	-3.52	119.95	126.04
7	W	405	BCL	C4-C3-C5	-3.51	109.37	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	404	BCL	C1C-NC-C4C	3.51	108.28	106.71
13	a	801	G2O	CGD-CBD-CAD	3.50	122.08	110.73
7	U	402	BCL	CAD-C3D-C4D	-3.50	106.52	108.47
7	a	814	BCL	C1C-NC-C4C	3.49	108.28	106.71
7	V	402	BCL	C1C-NC-C4C	3.49	108.27	106.71
7	A	813	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
7	A	808	BCL	C1-C2-C3	-3.48	120.03	126.04
7	U	401	BCL	C1C-NC-C4C	3.48	108.27	106.71
8	a	818	F39	C56-C58-C61	-3.48	113.61	118.94
13	A	824	G2O	O2D-CGD-O1D	-3.47	117.05	123.84
7	A	813	BCL	CHA-C1A-NA	-3.47	118.46	126.40
7	a	817	BCL	OBD-CAD-CBD	-3.46	120.94	125.89
13	a	805	G2O	C2C-C1C-NC	-3.44	106.81	110.57
7	A	809	BCL	C4A-NA-C1A	3.44	108.25	106.71
7	V	401	BCL	CMB-C2B-C1B	-3.44	123.18	128.46
7	V	403	BCL	C1C-NC-C4C	3.43	108.25	106.71
7	a	816	BCL	CAD-C3D-C4D	-3.43	106.56	108.47
7	U	408[B]	BCL	C2A-C1A-CHA	3.43	129.86	123.86
7	A	802	BCL	CMB-C2B-C1B	-3.43	123.19	128.46
7	a	814	BCL	C2A-C1A-CHA	3.42	129.84	123.86
7	a	814	BCL	CHA-C1A-NA	-3.42	118.57	126.40
7	a	813	BCL	C1C-NC-C4C	3.42	108.24	106.71
7	A	809	BCL	CMB-C2B-C1B	-3.42	123.21	128.46
7	a	810	BCL	OBD-CAD-CBD	-3.41	121.02	125.89
7	W	406	BCL	OBD-CAD-CBD	-3.41	121.03	125.89
6	a	804	GS0	CHA-C1A-NA	-3.40	118.61	126.40
7	a	810	BCL	C2A-C1A-CHA	3.39	129.79	123.86
7	A	810	BCL	CHA-C1A-NA	-3.38	118.65	126.40
7	U	406	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
7	U	401	BCL	CMB-C2B-C1B	-3.38	123.28	128.46
7	U	409	BCL	C2A-C1A-CHA	3.38	129.76	123.86
8	a	818	F39	C32-C35-C37	-3.37	116.94	126.42
7	a	807	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
9	a	819	F26	C39-C37-C34	-3.37	122.51	127.31
6	A	801	GS0	CMC-C2C-C3C	-3.36	100.25	113.83
13	a	802	G2O	C3C-C4C-NC	-3.36	106.71	109.88
7	A	802	BCL	C1C-NC-C4C	3.36	108.22	106.71
7	U	405	BCL	OBD-CAD-CBD	-3.36	121.10	125.89
7	U	402	BCL	OBD-CAD-CBD	-3.36	121.10	125.89
7	U	409	BCL	CMB-C2B-C1B	-3.35	123.31	128.46
13	a	805	G2O	CMA-C3A-C2A	3.35	127.36	113.83
7	a	811	BCL	CHA-C1A-NA	-3.35	118.73	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	407	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	a	801	G2O	CMA-C3A-C2A	3.35	127.33	113.83
7	a	806	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
7	W	401	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
7	V	403	BCL	CHA-C1A-NA	-3.34	118.75	126.40
7	a	816	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
7	V	405	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
7	V	406	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
7	U	401	BCL	CHA-C1A-NA	-3.33	118.77	126.40
7	V	401	BCL	CHA-C1A-NA	-3.32	118.78	126.40
7	A	806	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
13	a	802	G2O	CMA-C3A-C2A	3.32	127.23	113.83
7	a	813	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
7	a	811	BCL	CMB-C2B-C1B	-3.32	123.36	128.46
7	A	812	BCL	CHA-C1A-NA	-3.32	118.80	126.40
7	A	811	BCL	CMB-C2B-C1B	-3.32	123.37	128.46
6	A	801	GS0	C2D-C1D-ND	3.32	112.55	110.10
7	W	403	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
7	A	808	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
7	a	812	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
7	U	403	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
7	U	401	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
7	V	406	BCL	C4A-NA-C1A	3.31	108.19	106.71
7	W	405	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
7	V	404	BCL	OBD-CAD-CBD	-3.29	121.20	125.89
7	V	407	BCL	C4A-NA-C1A	3.29	108.18	106.71
7	U	407	BCL	OBD-CAD-CBD	-3.29	121.20	125.89
7	V	401	BCL	OBD-CAD-CBD	-3.29	121.20	125.89
7	A	809	BCL	C1C-NC-C4C	3.29	108.18	106.71
7	a	813	BCL	CMB-C2B-C1B	-3.28	123.42	128.46
6	A	801	GS0	C16-C15-C13	-3.28	105.31	115.92
7	A	811	BCL	C4A-NA-C1A	3.28	108.18	106.71
7	a	806	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
13	A	824	G2O	CBD-CHA-C1A	3.27	135.02	128.75
7	A	804	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
7	A	809	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
7	V	403	BCL	OBD-CAD-CBD	-3.26	121.23	125.89
7	A	806	BCL	C4A-NA-C1A	3.26	108.17	106.71
7	W	406	BCL	CAD-C3D-C4D	-3.26	106.65	108.47
7	V	402	BCL	OBD-CAD-CBD	-3.26	121.23	125.89
7	A	808	BCL	CMB-C2B-C1B	-3.26	123.45	128.46
7	V	404	BCL	C1C-NC-C4C	3.26	108.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	807	BCL	CHA-C1A-NA	-3.26	118.94	126.40
7	a	817	BCL	C1C-NC-C4C	3.25	108.17	106.71
7	V	406	BCL	CHA-C1A-NA	-3.25	118.95	126.40
7	A	807	BCL	CMB-C2B-C1B	-3.25	123.47	128.46
7	a	813	BCL	CAD-C3D-C4D	-3.24	106.66	108.47
7	W	404	BCL	C1-C2-C3	-3.24	120.44	126.04
7	A	805	BCL	C2A-C1A-CHA	3.24	129.52	123.86
7	A	811	BCL	OBD-CAD-CBD	-3.23	121.28	125.89
7	V	401	BCL	C4A-NA-C1A	3.23	108.16	106.71
6	a	804	GS0	C16-C15-C13	-3.23	105.47	115.92
8	A	814	F39	C35-C37-C39	-3.23	113.98	118.94
7	V	408[B]	BCL	CMB-C2B-C1B	-3.23	123.50	128.46
7	W	404	BCL	OBD-CAD-CBD	-3.23	121.28	125.89
7	U	408[B]	BCL	OBD-CAD-CBD	-3.22	121.29	125.89
7	a	811	BCL	C4A-NA-C1A	3.22	108.16	106.71
7	W	402	BCL	OBD-CAD-CBD	-3.22	121.29	125.89
7	A	812	BCL	OBD-CAD-CBD	-3.22	121.30	125.89
7	A	813	BCL	CMB-C2B-C1B	-3.21	123.53	128.46
7	V	401	BCL	C2A-C1A-CHA	3.21	129.47	123.86
7	V	408[B]	BCL	OBD-CAD-CBD	-3.20	121.32	125.89
7	U	408[B]	BCL	CMB-C2B-C1B	-3.20	123.55	128.46
7	a	809	BCL	C2A-C1A-CHA	3.20	129.45	123.86
7	U	404	BCL	OBD-CAD-CBD	-3.19	121.33	125.89
7	a	809	BCL	C5-C3-C2	-3.19	114.66	121.12
7	A	804	BCL	CHA-C1A-NA	-3.19	119.09	126.40
7	A	805	BCL	C1-C2-C3	-3.19	120.53	126.04
7	V	406	BCL	CMB-C2B-C1B	-3.18	123.57	128.46
7	A	802	BCL	C17-C16-C15	3.18	127.86	113.24
6	a	804	GS0	CMA-C3A-C4A	-3.18	103.22	111.77
7	a	814	BCL	OBD-CAD-CBD	-3.18	121.35	125.89
7	V	408[B]	BCL	CHA-C1A-NA	-3.18	119.12	126.40
7	V	403	BCL	CMB-C2B-C1B	-3.17	123.58	128.46
7	a	815	BCL	C11-C10-C8	3.17	126.18	115.92
7	a	807	BCL	CMB-C2B-C1B	-3.17	123.59	128.46
7	a	812	BCL	CMB-C2B-C1B	-3.17	123.59	128.46
7	A	803	BCL	CMB-C2B-C1B	-3.17	123.60	128.46
7	A	802	BCL	OBD-CAD-CBD	-3.17	121.37	125.89
7	a	810	BCL	C1C-NC-C4C	3.17	108.13	106.71
7	U	403	BCL	C1-C2-C3	-3.16	120.57	126.04
7	a	815	BCL	OBD-CAD-CBD	-3.16	121.38	125.89
7	a	812	BCL	CHA-C1A-NA	-3.16	119.17	126.40
7	A	810	BCL	CMB-C2B-C1B	-3.16	123.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	409	BCL	OBD-CAD-CBD	-3.15	121.39	125.89
7	W	406	BCL	C4B-C3B-CAB	-3.15	121.05	127.13
13	a	801	G2O	CHC-C4B-NB	3.15	127.35	124.45
7	A	812	BCL	CMB-C2B-C1B	-3.15	123.62	128.46
7	A	810	BCL	OBD-CAD-CBD	-3.15	121.40	125.89
8	A	814	F39	C32-C35-C37	-3.14	117.59	126.42
6	A	801	GS0	C7-C6-C5	-3.14	104.83	113.36
7	a	808	BCL	OBD-CAD-CBD	-3.14	121.41	125.89
6	a	804	GS0	C11-C10-C8	-3.14	105.78	115.92
7	A	803	BCL	OBD-CAD-CBD	-3.14	121.42	125.89
7	U	403	BCL	CHA-C1A-NA	-3.14	119.22	126.40
7	W	407[B]	BCL	OBD-CAD-CBD	-3.13	121.43	125.89
7	a	816	BCL	CMB-C2B-C1B	-3.13	123.66	128.46
7	a	807	BCL	CHA-C1A-NA	-3.12	119.25	126.40
10	a	821	LHG	O8-C23-C24	3.12	119.56	111.38
7	W	405	BCL	CHA-C1A-NA	-3.12	119.26	126.40
7	W	407[B]	BCL	CHA-C1A-NA	-3.11	119.27	126.40
7	A	803	BCL	CHA-C1A-NA	-3.11	119.28	126.40
13	A	824	G2O	CMD-C2D-C1D	-3.11	123.69	128.46
7	A	808	BCL	CHA-C1A-NA	-3.10	119.30	126.40
7	U	404	BCL	CMB-C2B-C3B	3.10	130.48	124.68
7	W	404	BCL	CMB-C2B-C1B	-3.10	123.70	128.46
7	W	401	BCL	CHA-C1A-NA	-3.09	119.32	126.40
7	U	405	BCL	CHA-C1A-NA	-3.09	119.33	126.40
7	a	809	BCL	CMB-C2B-C1B	-3.08	123.73	128.46
6	a	804	GS0	C7-C6-C5	-3.08	105.00	113.36
7	A	807	BCL	OBD-CAD-CBD	-3.07	121.50	125.89
7	U	402	BCL	CHA-C1A-NA	-3.06	119.38	126.40
7	W	407[B]	BCL	CMB-C2B-C1B	-3.06	123.76	128.46
7	a	808	BCL	CHA-C1A-NA	-3.06	119.39	126.40
7	U	402	BCL	C2A-C1A-CHA	3.06	129.21	123.86
7	A	808	BCL	C1C-NC-C4C	3.05	108.08	106.71
7	A	806	BCL	CMB-C2B-C1B	-3.05	123.77	128.46
7	W	402	BCL	C1C-NC-C4C	3.04	108.07	106.71
7	U	406	BCL	CHA-C1A-NA	-3.04	119.44	126.40
13	a	802	G2O	C2A-C3A-C4A	3.03	106.77	101.87
6	A	801	GS0	CHB-C4A-NA	-3.03	120.32	124.51
7	a	811	BCL	OBD-CAD-CBD	-3.03	121.56	125.89
7	W	402	BCL	CHA-C1A-NA	-3.03	119.46	126.40
7	U	409	BCL	CHA-C1A-NA	-3.02	119.47	126.40
7	A	805	BCL	OBD-CAD-CBD	-3.02	121.58	125.89
7	a	810	BCL	CHA-C1A-NA	-3.02	119.49	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	801	G2O	C3A-C2A-C1A	3.02	105.86	101.34
7	A	812	BCL	C1-C2-C3	-3.01	120.83	126.04
7	A	811	BCL	C2A-C1A-CHA	3.00	129.10	123.86
13	a	801	G2O	C3C-C4C-NC	-3.00	107.05	109.88
6	A	801	GS0	C3C-C2C-C1C	3.00	106.71	101.87
7	A	811	BCL	CHA-C1A-NA	-2.99	119.54	126.40
7	U	408[B]	BCL	CHA-C1A-NA	-2.99	119.55	126.40
7	V	407	BCL	CMB-C2B-C1B	-2.99	123.87	128.46
13	a	802	G2O	C2C-C1C-NC	-2.99	107.31	110.57
7	a	808	BCL	C2A-C1A-CHA	2.98	129.08	123.86
7	W	405	BCL	CMB-C2B-C1B	-2.98	123.88	128.46
7	W	402	BCL	CMB-C2B-C1B	-2.98	123.88	128.46
7	W	403	BCL	C1C-NC-C4C	2.98	108.05	106.71
13	a	805	G2O	CMD-C2D-C1D	-2.98	123.89	128.46
7	A	810	BCL	C2A-C1A-CHA	2.97	129.06	123.86
6	a	804	GS0	C2D-C1D-ND	2.97	112.29	110.10
7	V	403	BCL	C2A-C1A-CHA	2.96	129.04	123.86
7	A	809	BCL	CHA-C1A-NA	-2.96	119.61	126.40
7	V	407	BCL	CHA-C1A-NA	-2.95	119.64	126.40
7	A	809	BCL	C2A-C1A-CHA	2.95	129.02	123.86
8	A	814	F39	C25-C20-C19	2.95	120.23	115.27
6	A	801	GS0	C11-C10-C8	-2.95	106.39	115.92
7	U	402	BCL	C1C-NC-C4C	2.95	108.03	106.71
7	U	407	BCL	CHA-C1A-NA	-2.94	119.65	126.40
7	A	810	BCL	CAC-C3C-C4C	2.94	119.12	112.58
7	V	408[B]	BCL	C1C-NC-C4C	2.94	108.03	106.71
7	W	405	BCL	C2A-C1A-CHA	2.94	129.00	123.86
13	a	802	G2O	O2D-CGD-O1D	-2.94	118.09	123.84
7	a	815	BCL	CMB-C2B-C1B	-2.94	123.94	128.46
13	a	805	G2O	CBD-CHA-C1A	2.94	134.38	128.75
7	a	806	BCL	CHA-C1A-NA	-2.94	119.67	126.40
13	a	805	G2O	C2A-C3A-C4A	2.94	106.61	101.87
7	U	404	BCL	C5-C3-C2	-2.93	115.19	121.12
7	U	403	BCL	CMB-C2B-C1B	-2.93	123.97	128.46
7	a	806	BCL	CMB-C2B-C1B	-2.93	123.97	128.46
7	W	404	BCL	CHA-C1A-NA	-2.92	119.71	126.40
7	A	813	BCL	C4-C3-C5	-2.92	110.36	115.27
13	A	824	G2O	CHC-C4B-C3B	2.92	130.25	125.26
7	V	406	BCL	C2A-C1A-CHA	2.92	128.96	123.86
7	a	817	BCL	CHA-C1A-NA	-2.92	119.72	126.40
7	a	809	BCL	O2D-CGD-O1D	-2.92	118.14	123.84
7	V	402	BCL	CMB-C2B-C1B	-2.92	123.98	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	815	BCL	CHA-C1A-NA	-2.91	119.72	126.40
7	V	404	BCL	CHA-C1A-NA	-2.91	119.74	126.40
7	U	402	BCL	CMB-C2B-C1B	-2.90	124.01	128.46
7	a	809	BCL	OBD-CAD-CBD	-2.90	121.75	125.89
7	a	813	BCL	C16-C15-C13	-2.90	106.55	115.92
13	a	802	G2O	CMD-C2D-C1D	-2.89	124.02	128.46
7	W	404	BCL	C4A-NA-C1A	2.89	108.01	106.71
7	U	405	BCL	C2A-C1A-CHA	2.89	128.91	123.86
7	W	406	BCL	CMB-C2B-C1B	-2.88	124.04	128.46
7	A	803	BCL	C1C-NC-C4C	2.88	108.00	106.71
7	a	813	BCL	CHA-C1A-NA	-2.88	119.81	126.40
7	A	808	BCL	C4A-NA-C1A	2.87	108.00	106.71
7	A	813	BCL	O2A-CGA-O1A	-2.87	116.35	123.59
7	U	403	BCL	C2A-C1A-CHA	2.87	128.87	123.86
7	V	402	BCL	CHA-C1A-NA	-2.87	119.84	126.40
7	V	404	BCL	C2A-C1A-CHA	2.86	128.87	123.86
7	V	406	BCL	C1C-NC-C4C	2.86	107.99	106.71
7	A	802	BCL	CHA-C1A-NA	-2.86	119.85	126.40
13	a	801	G2O	C2A-C3A-C4A	2.86	106.49	101.87
7	W	401	BCL	C2A-C1A-CHA	2.86	128.86	123.86
7	V	405	BCL	CHA-C1A-NA	-2.86	119.86	126.40
7	W	403	BCL	CHA-C1A-NA	-2.85	119.86	126.40
7	U	407	BCL	CMB-C2B-C1B	-2.85	124.09	128.46
7	U	401	BCL	C4-C3-C5	-2.85	110.48	115.27
7	A	802	BCL	C2A-C1A-CHA	2.85	128.84	123.86
7	A	804	BCL	C2A-C1A-CHA	2.84	128.83	123.86
9	a	819	F26	C17-C13-C8	2.84	120.05	115.27
7	U	407	BCL	C4A-NA-C1A	2.84	107.98	106.71
7	A	809	BCL	C1-C2-C3	-2.83	121.14	126.04
7	W	402	BCL	C2A-C1A-CHA	2.83	128.80	123.86
7	U	406	BCL	CMB-C2B-C1B	-2.82	124.13	128.46
13	a	801	G2O	C2A-C1A-CHA	2.82	131.98	126.36
7	V	405	BCL	CMB-C2B-C1B	-2.81	124.14	128.46
13	a	801	G2O	CMD-C2D-C1D	-2.81	124.14	128.46
13	A	824	G2O	CMA-C3A-C2A	2.81	125.16	113.83
13	a	805	G2O	O2D-CGD-O1D	-2.80	118.35	123.84
7	A	808	BCL	C2A-C1A-CHA	2.80	128.76	123.86
7	W	406	BCL	CHA-C1A-NA	-2.80	120.00	126.40
7	V	403	BCL	CMD-C2D-C3D	2.79	129.91	124.68
6	a	804	GS0	C11-C12-C13	-2.79	106.89	115.92
7	a	817	BCL	CMB-C2B-C1B	-2.77	124.20	128.46
7	a	816	BCL	CHA-C1A-NA	-2.77	120.06	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	814	F39	C19-C20-C27	-2.76	113.61	121.98
7	U	404	BCL	CHA-C1A-NA	-2.76	120.07	126.40
6	A	801	GS0	O2A-CGA-O1A	-2.76	116.64	123.59
7	U	407	BCL	C1C-NC-C4C	2.76	107.94	106.71
7	V	407	BCL	C2A-C1A-CHA	2.75	128.67	123.86
7	W	403	BCL	C2A-C1A-CHA	2.75	128.66	123.86
7	A	811	BCL	C1-C2-C3	-2.75	121.29	126.04
7	a	814	BCL	O2D-CGD-O1D	-2.74	118.47	123.84
7	a	814	BCL	CMB-C2B-C3B	2.73	129.79	124.68
9	A	815	F26	C17-C13-C8	2.73	119.87	115.27
13	a	802	G2O	C3A-C2A-C1A	2.73	105.43	101.34
13	a	802	G2O	C2A-C1A-CHA	2.73	131.80	126.36
7	A	807	BCL	C2A-C1A-CHA	2.72	128.62	123.86
6	A	801	GS0	CHD-C4C-NC	-2.72	122.06	125.08
8	a	818	F39	C19-C20-C27	-2.72	113.75	121.98
10	A	816	LHG	O8-C23-C24	2.71	120.42	111.91
7	V	401	BCL	CMB-C2B-C3B	2.70	129.74	124.68
6	a	804	GS0	C4B-CHC-C1C	-2.70	124.76	130.12
9	a	819	F26	C32-C35-C34	-2.70	118.82	126.42
7	W	402	BCL	CMD-C2D-C3D	2.70	129.74	124.68
7	V	401	BCL	C4-C3-C5	-2.70	110.73	115.27
11	A	822	LMG	O6-C1-O1	-2.70	103.58	109.97
7	W	407[B]	BCL	C2A-C1A-CHA	2.70	128.57	123.86
8	a	818	F39	C25-C20-C19	2.70	119.81	115.27
9	a	820	F26	C17-C13-C8	2.70	119.81	115.27
7	a	811	BCL	C4B-C3B-CAB	-2.70	121.92	127.13
11	a	824	LMG	O6-C1-O1	-2.69	103.59	109.97
7	A	804	BCL	CMB-C2B-C3B	2.69	129.71	124.68
7	a	806	BCL	O2D-CGD-O1D	-2.68	118.59	123.84
6	A	801	GS0	CMA-C3A-C2A	-2.68	103.03	113.83
6	a	804	GS0	O2A-CGA-O1A	-2.67	116.84	123.59
7	V	404	BCL	CMB-C2B-C3B	2.67	129.68	124.68
13	a	801	G2O	CMD-C2D-C3D	2.67	129.67	124.68
7	a	810	BCL	CMB-C2B-C3B	2.67	129.67	124.68
7	a	817	BCL	C2A-C1A-CHA	2.67	128.52	123.86
9	a	820	F26	C22-C25-C26	-2.67	118.93	126.42
7	a	816	BCL	C2A-C1A-CHA	2.66	128.51	123.86
11	A	821	LMG	O6-C1-O1	-2.66	103.67	109.97
6	A	801	GS0	C11-C12-C13	-2.66	107.33	115.92
7	W	403	BCL	C4B-C3B-CAB	-2.65	122.00	127.13
7	A	809	BCL	CMD-C2D-C3D	2.65	129.64	124.68
7	a	811	BCL	C2A-C1A-CHA	2.64	128.48	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	810	BCL	C4B-C3B-CAB	-2.64	122.02	127.13
7	W	404	BCL	C2A-C1A-CHA	2.64	128.48	123.86
6	a	804	GS0	C3C-C2C-C1C	2.64	106.13	101.87
7	W	401	BCL	CMB-C2B-C3B	2.64	129.62	124.68
13	a	802	G2O	CBD-CHA-C1A	2.64	133.80	128.75
7	U	407	BCL	C4-C3-C5	-2.64	110.83	115.27
7	A	806	BCL	CHA-C1A-NA	-2.64	120.36	126.40
7	W	406	BCL	C2A-C1A-CHA	2.63	128.45	123.86
7	V	401	BCL	C1C-NC-C4C	2.62	107.89	106.71
7	U	402	BCL	C4-C3-C5	-2.62	110.86	115.27
13	a	801	G2O	O2D-CGD-O1D	-2.62	118.71	123.84
7	V	406	BCL	C4B-C3B-CAB	-2.62	122.07	127.13
7	a	808	BCL	CMB-C2B-C3B	2.62	129.57	124.68
7	U	409	BCL	CMD-C2D-C3D	2.61	129.57	124.68
7	V	407	BCL	C4B-C3B-CAB	-2.61	122.09	127.13
7	A	802	BCL	C16-C15-C13	-2.61	107.48	115.92
10	a	822	LHG	O8-C23-C24	2.61	120.09	111.91
7	U	404	BCL	C2A-C1A-CHA	2.61	128.42	123.86
7	U	405	BCL	CMB-C2B-C1B	-2.61	124.46	128.46
7	U	406	BCL	C1C-NC-C4C	2.60	107.88	106.71
7	a	806	BCL	C2A-C1A-CHA	2.60	128.41	123.86
7	U	406	BCL	C2A-C1A-CHA	2.60	128.41	123.86
7	W	401	BCL	C4B-C3B-CAB	-2.60	122.11	127.13
11	C	302	LMG	C1-C2-C3	-2.59	104.59	110.00
9	a	819	F26	C38-C39-C37	-2.59	118.16	123.47
9	a	819	F26	C22-C25-C26	-2.59	119.14	126.42
13	a	805	G2O	C3A-C2A-C1A	2.59	105.22	101.34
13	a	801	G2O	CBD-CHA-C1A	2.59	133.71	128.75
7	A	810	BCL	O2A-CGA-O1A	-2.58	117.07	123.59
7	U	403	BCL	CMD-C2D-C3D	2.58	129.51	124.68
7	W	403	BCL	CMB-C2B-C3B	2.58	129.51	124.68
7	W	405	BCL	C1-C2-C3	-2.58	121.57	126.04
7	U	401	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	A	803	BCL	C2A-C1A-CHA	2.58	128.36	123.86
13	a	801	G2O	C2C-C1C-NC	-2.58	107.76	110.57
7	W	405	BCL	C4B-C3B-CAB	-2.57	122.16	127.13
7	a	810	BCL	C4-C3-C5	-2.57	110.94	115.27
7	a	813	BCL	C2A-C1A-CHA	2.57	128.36	123.86
7	a	810	BCL	CBA-CAA-C2A	2.57	121.44	113.86
10	a	823	LHG	O8-C23-C24	2.56	119.96	111.91
7	U	404	BCL	C4B-C3B-CAB	-2.56	122.17	127.13
10	A	817	LHG	C11-C10-C9	-2.56	101.41	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	402	BCL	CMD-C2D-C3D	2.56	129.46	124.68
9	A	815	F26	C27-C28-C31	-2.55	119.24	126.42
13	A	824	G2O	CMD-C2D-C3D	2.55	129.45	124.68
10	A	817	LHG	O8-C23-C24	2.54	119.89	111.91
7	a	813	BCL	C5-C3-C2	-2.54	115.97	121.12
7	W	405	BCL	CMD-C2D-C3D	2.54	129.43	124.68
7	a	806	BCL	CMD-C2D-C3D	2.54	129.43	124.68
7	V	403	BCL	C1-C2-C3	-2.53	121.66	126.04
7	V	402	BCL	C2A-C1A-CHA	2.53	128.28	123.86
7	A	811	BCL	CAC-C3C-C4C	2.53	118.20	112.58
13	a	805	G2O	CHB-C1B-NB	2.53	126.78	124.45
7	U	407	BCL	C2A-C1A-CHA	2.53	128.28	123.86
7	a	815	BCL	C2A-C1A-CHA	2.53	128.28	123.86
7	a	809	BCL	CMD-C2D-C3D	2.53	129.40	124.68
6	a	804	GS0	CHD-C1D-ND	-2.52	122.14	124.45
11	A	822	LMG	O1-C7-C8	-2.52	104.82	110.90
11	A	820	LMG	O6-C1-O1	-2.52	104.01	109.97
9	A	815	F26	C23-C19-C24	-2.52	119.40	122.92
7	A	805	BCL	CMB-C2B-C1B	-2.51	124.60	128.46
7	A	808	BCL	CMD-C2D-C3D	2.51	129.37	124.68
7	a	809	BCL	C4B-C3B-CAB	-2.51	122.28	127.13
7	U	401	BCL	C4B-C3B-CAB	-2.51	122.28	127.13
7	A	804	BCL	CMD-C2D-C3D	2.50	129.36	124.68
7	A	807	BCL	CMD-C2D-C3D	2.50	129.36	124.68
7	A	813	BCL	C2A-C1A-CHA	2.50	128.23	123.86
7	A	812	BCL	CMD-C2D-C3D	2.50	129.35	124.68
8	a	818	F39	C38-C37-C39	-2.49	119.44	122.92
7	U	406	BCL	CMD-C2D-C3D	2.49	129.33	124.68
7	U	404	BCL	CMD-C2D-C3D	2.48	129.32	124.68
7	a	816	BCL	CMD-C2D-C3D	2.48	129.31	124.68
7	a	810	BCL	CMD-C2D-C3D	2.47	129.31	124.68
7	U	407	BCL	CMD-C2D-C3D	2.47	129.30	124.68
7	W	402	BCL	C5-C3-C2	-2.47	116.13	121.12
10	C	301	LHG	C11-C10-C9	-2.47	101.91	114.42
7	V	404	BCL	CMD-C2D-C3D	2.46	129.28	124.68
7	W	407[B]	BCL	CMD-C2D-C3D	2.46	129.28	124.68
13	a	805	G2O	CMD-C2D-C3D	2.46	129.28	124.68
7	V	405	BCL	C2A-C1A-CHA	2.46	128.16	123.86
7	U	402	BCL	CMD-C2D-C3D	2.46	129.28	124.68
7	A	805	BCL	C1-O2A-CGA	2.44	122.85	116.44
7	a	812	BCL	CMD-C2D-C3D	2.44	129.25	124.68
7	W	403	BCL	C11-C10-C8	-2.44	108.03	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	409	BCL	C1C-NC-C4C	2.44	107.80	106.71
11	A	818	LMG	O6-C1-O1	-2.44	104.20	109.97
9	A	815	F26	C36-C31-C33	-2.43	119.52	122.92
7	a	811	BCL	CMB-C2B-C3B	2.43	129.22	124.68
7	A	810	BCL	CMD-C2D-C3D	2.43	129.22	124.68
7	A	813	BCL	CMD-C2D-C3D	2.42	129.21	124.68
7	U	404	BCL	C6-C5-C3	2.42	119.80	113.45
7	A	804	BCL	C4A-NA-C1A	2.42	107.79	106.71
7	W	401	BCL	CMD-C2D-C3D	2.42	129.21	124.68
10	a	823	LHG	C11-C10-C9	-2.42	102.14	114.42
7	a	814	BCL	CMD-C2D-C3D	2.42	129.20	124.68
7	U	401	BCL	CMD-C2D-C3D	2.40	129.17	124.68
11	A	820	LMG	O2-C2-C1	-2.40	104.21	110.05
10	C	301	LHG	O8-C23-C24	2.40	119.43	111.91
13	a	802	G2O	CHC-C4B-NB	2.40	126.66	124.45
6	a	804	GS0	CHB-C4A-NA	-2.39	121.20	124.51
13	a	805	G2O	CHC-C4B-C3B	2.39	129.35	125.26
13	a	801	G2O	O2A-CGA-O1A	-2.39	117.56	123.59
7	V	406	BCL	CMD-C2D-C3D	2.39	129.14	124.68
7	a	815	BCL	C1C-NC-C4C	2.38	107.78	106.71
7	V	407	BCL	CMD-C2D-C3D	2.38	129.13	124.68
11	A	822	LMG	O3-C3-C2	-2.38	104.85	110.35
13	A	824	G2O	C3A-C2A-C1A	2.38	104.90	101.34
9	A	815	F26	C22-C25-C26	-2.38	119.74	126.42
7	A	806	BCL	C2A-C1A-CHA	2.38	128.01	123.86
7	U	408[B]	BCL	CMD-C2D-C3D	2.37	129.12	124.68
7	A	803	BCL	CMD-C2D-C3D	2.37	129.12	124.68
7	a	815	BCL	CMD-C2D-C3D	2.37	129.12	124.68
13	a	802	G2O	CMD-C2D-C3D	2.37	129.11	124.68
10	a	821	LHG	C11-C10-C9	-2.37	102.41	114.42
7	a	807	BCL	CMD-C2D-C3D	2.37	129.11	124.68
7	U	401	BCL	C1-C2-C3	-2.36	121.96	126.04
7	W	402	BCL	C1-C2-C3	-2.36	121.96	126.04
7	U	408[B]	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
7	A	805	BCL	CMD-C2D-C3D	2.36	129.10	124.68
7	a	817	BCL	CMD-C2D-C3D	2.36	129.09	124.68
7	a	813	BCL	CMD-C2D-C3D	2.36	129.09	124.68
13	a	805	G2O	C2A-C1A-CHA	2.36	131.06	126.36
11	A	819	LMG	O3-C3-C2	-2.36	104.90	110.35
7	U	404	BCL	O2A-C1-C2	-2.35	102.45	108.64
11	A	819	LMG	O6-C1-O1	-2.35	104.40	109.97
7	U	409	BCL	CMB-C2B-C3B	2.35	129.07	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	806	BCL	O2A-CGA-O1A	-2.35	117.67	123.59
7	W	404	BCL	CMD-C2D-C3D	2.34	129.06	124.68
7	U	407	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
7	U	401	BCL	CMB-C2B-C3B	2.34	129.06	124.68
7	a	808	BCL	CMD-C2D-C3D	2.34	129.05	124.68
7	U	409	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
7	A	809	BCL	CMB-C2B-C3B	2.33	129.04	124.68
7	A	811	BCL	CMD-C2D-C3D	2.33	129.04	124.68
7	a	809	BCL	CHD-C4C-NC	-2.33	122.49	125.08
7	U	405	BCL	CMD-C2D-C3D	2.32	129.03	124.68
9	A	815	F26	C32-C35-C34	-2.32	119.89	126.42
7	A	802	BCL	CMD-C2D-C3D	2.32	129.03	124.68
7	V	401	BCL	C1-C2-C3	-2.32	122.03	126.04
7	W	404	BCL	O2D-CGD-O1D	-2.32	119.30	123.84
7	U	406	BCL	C5-C3-C2	-2.32	116.42	121.12
8	A	814	F39	C9-C8-C10	-2.32	106.77	110.82
7	A	806	BCL	C1-C2-C3	-2.32	122.04	126.04
8	A	814	F39	C63-C64-C62	-2.32	119.91	126.42
7	V	408[B]	BCL	CMD-C2D-C3D	2.32	129.01	124.68
7	A	811	BCL	C1C-NC-C4C	2.32	107.75	106.71
7	W	405	BCL	CMB-C2B-C3B	2.31	129.00	124.68
7	a	812	BCL	C2A-C1A-CHA	2.30	127.89	123.86
7	a	808	BCL	C1C-NC-C4C	2.30	107.74	106.71
7	V	408[B]	BCL	C2A-C1A-CHA	2.30	127.88	123.86
7	A	803	BCL	C6-C5-C3	2.30	119.48	113.45
7	U	408[B]	BCL	CMB-C2B-C3B	2.30	128.97	124.68
11	C	302	LMG	O3-C3-C2	-2.30	105.04	110.35
8	a	818	F39	O5-C10-C12	-2.29	103.60	109.30
6	A	801	GS0	OBD-CAD-C3D	2.29	134.04	128.52
7	a	810	BCL	C4A-NA-C1A	2.29	107.74	106.71
7	a	809	BCL	OBD-CAD-C3D	2.29	131.78	127.98
7	A	810	BCL	CMB-C2B-C3B	2.29	128.96	124.68
9	A	815	F26	C20-C16-C21	2.29	119.65	114.60
7	V	406	BCL	C17-C16-C15	2.28	123.72	113.24
8	a	818	F39	C40-C41-C42	-2.28	120.02	126.42
7	V	406	BCL	CMB-C2B-C3B	2.28	128.94	124.68
7	V	408[B]	BCL	CMB-C2B-C3B	2.28	128.94	124.68
8	A	814	F39	C40-C41-C42	-2.28	120.03	126.42
11	A	819	LMG	C1-O6-C5	-2.27	109.22	113.69
9	a	820	F26	C36-C31-C33	-2.27	119.74	122.92
11	a	824	LMG	O1-C7-C8	-2.27	105.42	110.90
9	a	820	F26	C29-C26-C30	-2.27	119.74	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	302	LMG	O6-C1-O1	-2.27	104.61	109.97
11	A	818	LMG	O2-C2-C1	-2.26	104.55	110.05
7	V	405	BCL	CMD-C2D-C3D	2.26	128.91	124.68
7	A	811	BCL	C5-C3-C2	-2.26	116.55	121.12
11	a	824	LMG	O3-C3-C2	-2.26	105.13	110.35
7	a	809	BCL	C6-C7-C8	2.25	123.20	115.92
7	a	813	BCL	CMB-C2B-C3B	2.25	128.89	124.68
7	V	404	BCL	C6-C5-C3	2.25	119.36	113.45
9	a	819	F26	C36-C31-C33	-2.25	119.77	122.92
7	a	815	BCL	C1-C2-C3	-2.25	122.15	126.04
7	A	803	BCL	CMB-C2B-C3B	2.25	128.88	124.68
7	A	811	BCL	CMB-C2B-C3B	2.25	128.88	124.68
7	A	805	BCL	C6-C5-C3	2.24	119.34	113.45
7	A	802	BCL	C4-C3-C5	-2.24	111.50	115.27
9	A	815	F26	C10-C14-C16	-2.24	120.09	127.75
11	A	821	LMG	O3-C3-C2	-2.24	105.18	110.35
7	V	402	BCL	C4-C3-C5	-2.24	111.51	115.27
7	A	806	BCL	CMD-C2D-C3D	2.23	128.85	124.68
7	V	401	BCL	CMD-C2D-C3D	2.23	128.85	124.68
7	a	814	BCL	CBA-CAA-C2A	2.22	120.43	113.86
7	A	808	BCL	C4-C3-C5	-2.22	111.53	115.27
7	V	402	BCL	C4B-C3B-CAB	-2.22	122.83	127.13
7	V	407	BCL	CMB-C2B-C3B	2.22	128.84	124.68
7	W	403	BCL	O2D-CGD-O1D	-2.21	119.52	123.84
9	A	815	F26	C38-C39-C37	-2.21	118.95	123.47
8	A	814	F39	O4-C9-C11	-2.20	104.69	110.05
11	A	818	LMG	O1-C1-C2	-2.20	104.86	108.30
7	W	407[B]	BCL	C4A-NA-C1A	2.20	107.70	106.71
7	V	401	BCL	CBA-CAA-C2A	2.20	120.37	113.86
13	A	824	G2O	CHC-C1C-C2C	2.20	128.42	124.98
9	a	819	F26	C10-C14-C16	-2.20	120.22	127.75
6	A	801	GS0	CMD-C2D-C3D	2.20	132.67	127.61
9	a	820	F26	C10-C14-C16	-2.20	120.24	127.75
7	a	811	BCL	CMD-C2D-C3D	2.19	128.78	124.68
11	A	821	LMG	O2-C2-C1	-2.19	104.72	110.05
7	A	812	BCL	O2D-CGD-O1D	-2.19	119.56	123.84
7	W	404	BCL	C4-C3-C5	-2.19	111.59	115.27
7	A	805	BCL	OBB-CAB-C3B	2.19	123.87	119.99
11	A	819	LMG	O2-C2-C1	-2.18	104.74	110.05
8	a	818	F39	O4-C9-C11	-2.18	104.75	110.05
13	A	824	G2O	CHD-C4C-C3C	2.18	129.41	125.33
7	W	407[B]	BCL	CMB-C2B-C3B	2.18	128.75	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	807	BCL	CAC-C3C-C4C	2.17	117.41	112.58
7	a	816	BCL	CMB-C2B-C3B	2.17	128.74	124.68
7	A	812	BCL	C2A-C1A-CHA	2.17	127.66	123.86
9	A	815	F26	C29-C26-C30	-2.17	119.88	122.92
11	A	818	LMG	O3-C3-C2	-2.17	105.33	110.35
7	a	808	BCL	O2A-CGA-CBA	-2.17	105.10	111.91
7	a	806	BCL	C1C-NC-C4C	2.17	107.68	106.71
7	W	404	BCL	C4B-C3B-CAB	-2.17	122.94	127.13
7	W	406	BCL	CMD-C2D-C3D	2.16	128.72	124.68
7	V	402	BCL	CMB-C2B-C3B	2.16	128.72	124.68
7	W	403	BCL	CMD-C2D-C3D	2.16	128.72	124.68
7	a	809	BCL	CMB-C2B-C3B	2.16	128.72	124.68
7	a	812	BCL	CMB-C2B-C3B	2.16	128.72	124.68
13	a	802	G2O	O2A-CGA-O1A	-2.16	118.15	123.59
6	A	801	GS0	CED-O2D-CGD	-2.16	111.06	115.94
7	A	808	BCL	CMB-C2B-C3B	2.15	128.71	124.68
7	U	408[B]	BCL	CHC-C1C-NC	-2.15	121.54	124.51
11	A	822	LMG	O2-C2-C1	-2.15	104.82	110.05
9	a	820	F26	C23-C19-C24	-2.15	119.92	122.92
7	A	802	BCL	CMB-C2B-C3B	2.15	128.69	124.68
8	A	814	F39	C65-C62-C59	-2.14	119.92	122.92
7	a	809	BCL	O2D-CGD-CBD	2.14	115.07	111.27
7	W	407[B]	BCL	CHC-C1C-NC	-2.14	121.56	124.51
9	a	820	F26	C20-C16-C21	2.14	119.32	114.60
9	a	819	F26	C29-C26-C30	-2.13	119.93	122.92
7	U	407	BCL	CMB-C2B-C3B	2.13	128.67	124.68
6	a	804	GS0	C12-C11-C10	-2.13	103.44	113.24
7	a	808	BCL	OBD-CAD-C3D	2.13	131.52	127.98
13	a	805	G2O	C1-C2-C3	-2.13	122.36	126.04
9	a	819	F26	C27-C28-C31	-2.13	120.44	126.42
7	A	813	BCL	O2D-CGD-O1D	-2.12	119.69	123.84
9	a	820	F26	C32-C35-C34	-2.12	120.47	126.42
7	A	813	BCL	CMB-C2B-C3B	2.12	128.64	124.68
7	V	404	BCL	OBB-CAB-CBB	-2.11	115.42	120.17
6	a	804	GS0	C3D-C2D-C1D	-2.11	102.95	105.83
6	a	804	GS0	CMC-C2C-C3C	-2.11	105.32	113.83
8	a	818	F39	C43-C42-C44	-2.11	119.97	122.92
11	A	821	LMG	O1-C7-C8	-2.11	105.81	110.90
8	a	818	F39	C63-C64-C62	-2.11	120.50	126.42
7	a	811	BCL	OBD-CAD-C3D	2.11	131.48	127.98
7	U	401	BCL	CBA-CAA-C2A	2.10	120.07	113.86
8	A	814	F39	O5-C10-C12	-2.10	104.08	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	820	LMG	O3-C3-C2	-2.10	105.49	110.35
7	U	409	BCL	C15-C13-C12	-2.10	101.09	112.13
7	W	407[B]	BCL	C1C-NC-C4C	2.10	107.65	106.71
7	a	807	BCL	C4C-CHD-C1D	2.10	128.98	125.88
7	A	807	BCL	CMB-C2B-C3B	2.09	128.60	124.68
7	A	812	BCL	CMB-C2B-C3B	2.09	128.59	124.68
7	W	404	BCL	CMB-C2B-C3B	2.09	128.58	124.68
11	A	818	LMG	O1-C7-C8	-2.08	105.89	110.90
6	a	804	GS0	CMC-C2C-C1C	-2.08	106.20	111.77
7	a	807	BCL	CMB-C2B-C3B	2.07	128.56	124.68
7	U	404	BCL	O2D-CGD-O1D	-2.07	119.79	123.84
11	A	821	LMG	O1-C1-C2	-2.07	105.07	108.30
6	A	801	GS0	C12-C11-C10	-2.07	103.73	113.24
11	A	819	LMG	O1-C7-C8	-2.07	105.91	110.90
7	W	406	BCL	CMB-C2B-C3B	2.06	128.54	124.68
7	U	405	BCL	C1-C2-C3	-2.06	122.48	126.04
8	A	814	F39	C43-C42-C44	-2.06	120.04	122.92
7	V	401	BCL	OBB-CAB-CBB	-2.06	115.54	120.17
7	V	408[B]	BCL	C4A-NA-C1A	2.05	107.63	106.71
13	A	824	G2O	C2A-C1A-CHA	2.05	130.45	126.36
8	A	814	F39	C38-C37-C39	-2.05	120.05	122.92
11	A	820	LMG	C1-O6-C5	-2.05	109.67	113.69
7	a	812	BCL	C4-C3-C5	-2.05	111.83	115.27
6	A	801	GS0	C1D-ND-C4D	-2.05	104.88	106.33
6	a	804	GS0	OBD-CAD-C3D	2.04	133.44	128.52
6	a	804	GS0	CHD-C4C-NC	-2.04	122.81	125.08
7	W	406	BCL	C1C-NC-C4C	2.04	107.62	106.71
11	a	824	LMG	O2-C2-C1	-2.04	105.09	110.05
7	U	403	BCL	CMB-C2B-C3B	2.04	128.50	124.68
7	V	406	BCL	C5-C3-C2	-2.03	117.00	121.12
7	a	813	BCL	C1-C2-C3	-2.03	122.53	126.04
7	A	813	BCL	C16-C15-C13	2.03	122.48	115.92
7	W	406	BCL	O2D-CGD-O1D	-2.03	119.87	123.84
8	A	814	F39	C14-C18-C19	2.03	117.21	112.33
7	V	408[B]	BCL	O2D-CGD-O1D	-2.03	119.88	123.84
7	A	803	BCL	C4A-NA-C1A	2.02	107.62	106.71
7	V	407	BCL	O2A-CGA-O1A	-2.02	118.49	123.59
9	a	820	F26	C40-C34-C37	-2.02	120.09	122.92
6	A	801	GS0	CBB-CAB-C3B	2.02	126.33	120.34
7	A	804	BCL	C1-C2-C3	-2.02	122.56	126.04
7	A	805	BCL	O2D-CGD-O1D	-2.01	119.90	123.84
7	V	407	BCL	C4-C3-C5	-2.01	111.89	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	404	BCL	CAC-C3C-C4C	2.01	117.05	112.58
13	A	824	G2O	C3D-CAD-CBD	-2.01	104.96	107.61
7	U	405	BCL	OBB-CAB-C3B	2.01	123.56	119.99
11	A	822	LMG	C1-C2-C3	-2.01	105.82	110.00
7	A	802	BCL	OBB-CAB-CBB	-2.01	115.65	120.17
9	A	815	F26	C40-C34-C37	-2.00	120.12	122.92
8	a	818	F39	C60-C58-C61	-2.00	120.12	122.92
9	a	819	F26	C20-C16-C21	2.00	119.02	114.60

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	801	GS0	CBD
6	A	801	GS0	C13
6	a	804	GS0	CBD
6	a	804	GS0	C3C
13	A	824	G2O	CBD
13	A	824	G2O	C3A
13	A	824	G2O	C2A
13	a	801	G2O	C8
13	a	801	G2O	C3A
13	a	801	G2O	CBD
13	a	801	G2O	C2A
13	a	802	G2O	CBD
13	a	802	G2O	C3A
13	a	802	G2O	C2A
13	a	805	G2O	CBD
13	a	805	G2O	C3A
13	a	805	G2O	C2A

All (865) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	GS0	C1-C2-C3-C4
6	A	801	GS0	C1A-C2A-CAA-CBA
6	A	801	GS0	C3A-C2A-CAA-CBA
6	A	801	GS0	C4-C3-C5-C6
6	A	801	GS0	C2C-C3C-CAC-CBC
6	A	801	GS0	C6-C7-C8-C9
6	A	801	GS0	CBA-CGA-O2A-C1
6	A	801	GS0	O1A-CGA-O2A-C1
6	A	801	GS0	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
6	a	804	GS0	C1-C2-C3-C4
6	a	804	GS0	C1-C2-C3-C5
6	a	804	GS0	C3A-C2A-CAA-CBA
6	a	804	GS0	C2C-C3C-CAC-CBC
6	a	804	GS0	C4C-C3C-CAC-CBC
6	a	804	GS0	CBD-CGD-O2D-CED
7	A	802	BCL	C4C-C3C-CAC-CBC
7	A	802	BCL	O2A-C1-C2-C3
7	A	805	BCL	O2A-C1-C2-C3
7	A	805	BCL	C1-C2-C3-C4
7	A	805	BCL	C4-C3-C5-C6
7	A	808	BCL	CHA-CBD-CGD-O2D
7	A	808	BCL	CAD-CBD-CGD-O2D
7	A	808	BCL	C1-C2-C3-C4
7	A	809	BCL	CHA-CBD-CGD-O2D
7	A	809	BCL	C1-C2-C3-C4
7	A	811	BCL	C2C-C3C-CAC-CBC
7	A	811	BCL	C4C-C3C-CAC-CBC
7	A	811	BCL	C1-C2-C3-C4
7	A	811	BCL	C2-C3-C5-C6
7	A	812	BCL	C4C-C3C-CAC-CBC
7	A	812	BCL	CHA-CBD-CGD-O1D
7	A	812	BCL	CAD-CBD-CGD-O1D
7	A	812	BCL	CAD-CBD-CGD-O2D
7	A	812	BCL	O2A-C1-C2-C3
7	A	812	BCL	C1-C2-C3-C4
7	A	813	BCL	C1-C2-C3-C4
7	a	806	BCL	CHA-CBD-CGD-O1D
7	a	806	BCL	C1-C2-C3-C4
7	a	807	BCL	C2C-C3C-CAC-CBC
7	a	807	BCL	C4C-C3C-CAC-CBC
7	a	808	BCL	C2C-C3C-CAC-CBC
7	a	808	BCL	C4C-C3C-CAC-CBC
7	a	808	BCL	C2-C3-C5-C6
7	a	808	BCL	C4-C3-C5-C6
7	a	809	BCL	O2A-C1-C2-C3
7	a	809	BCL	C1-C2-C3-C4
7	a	809	BCL	C2-C3-C5-C6
7	a	810	BCL	CHA-CBD-CGD-O1D
7	a	810	BCL	CHA-CBD-CGD-O2D
7	a	810	BCL	C1-C2-C3-C4
7	a	811	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	a	811	BCL	C4C-C3C-CAC-CBC
7	a	812	BCL	C2A-CAA-CBA-CGA
7	a	812	BCL	C2C-C3C-CAC-CBC
7	a	812	BCL	C4C-C3C-CAC-CBC
7	a	812	BCL	CHA-CBD-CGD-O2D
7	a	812	BCL	O2A-C1-C2-C3
7	a	812	BCL	C1-C2-C3-C4
7	a	813	BCL	C2C-C3C-CAC-CBC
7	a	813	BCL	C4C-C3C-CAC-CBC
7	a	813	BCL	CHA-CBD-CGD-O2D
7	a	813	BCL	C1-C2-C3-C4
7	a	813	BCL	C2-C3-C5-C6
7	a	814	BCL	C4C-C3C-CAC-CBC
7	a	816	BCL	CHA-CBD-CGD-O2D
7	a	817	BCL	C2-C3-C5-C6
7	a	817	BCL	C4-C3-C5-C6
7	U	401	BCL	CHA-CBD-CGD-O1D
7	U	402	BCL	C1-C2-C3-C4
7	U	403	BCL	C2C-C3C-CAC-CBC
7	U	403	BCL	C4C-C3C-CAC-CBC
7	U	403	BCL	CHA-CBD-CGD-O1D
7	U	403	BCL	CAD-CBD-CGD-O2D
7	U	404	BCL	CHA-CBD-CGD-O2D
7	U	404	BCL	C4-C3-C5-C6
7	U	406	BCL	CHA-CBD-CGD-O1D
7	U	406	BCL	C1-C2-C3-C4
7	U	406	BCL	C2-C3-C5-C6
7	U	407	BCL	C1-C2-C3-C4
7	U	408[B]	BCL	CHA-CBD-CGD-O2D
7	U	409	BCL	CHA-CBD-CGD-O1D
7	U	409	BCL	CHA-CBD-CGD-O2D
7	U	409	BCL	C1-C2-C3-C4
7	V	403	BCL	C2C-C3C-CAC-CBC
7	V	403	BCL	C4C-C3C-CAC-CBC
7	V	403	BCL	C4-C3-C5-C6
7	V	404	BCL	CHA-CBD-CGD-O2D
7	V	406	BCL	CHA-CBD-CGD-O1D
7	V	406	BCL	C2-C3-C5-C6
7	V	408[B]	BCL	C2A-CAA-CBA-CGA
7	W	402	BCL	C2C-C3C-CAC-CBC
7	W	402	BCL	C4C-C3C-CAC-CBC
7	W	402	BCL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
7	W	403	BCL	C2C-C3C-CAC-CBC
7	W	403	BCL	C4C-C3C-CAC-CBC
7	W	405	BCL	CHA-CBD-CGD-O1D
7	W	405	BCL	C1-C2-C3-C4
7	W	406	BCL	C1-C2-C3-C4
8	A	814	F39	C18-C19-C20-C25
8	A	814	F39	C25-C20-C27-C32
8	A	814	F39	C32-C35-C37-C39
8	A	814	F39	C39-C40-C41-C42
8	A	814	F39	C40-C41-C42-C43
8	A	814	F39	C41-C42-C44-C51
8	A	814	F39	C43-C42-C44-C51
8	A	814	F39	C44-C51-C57-C59
8	A	814	F39	C46-C53-C56-C58
8	A	814	F39	C53-C56-C58-C60
8	A	814	F39	C56-C58-C61-C63
8	A	814	F39	C60-C58-C61-C63
8	A	814	F39	C57-C59-C62-C64
8	A	814	F39	C57-C59-C62-C65
8	A	814	F39	C58-C61-C63-C64
8	A	814	F39	C59-C62-C64-C63
8	A	814	F39	C65-C62-C64-C63
8	a	818	F39	C17-C13-C14-C18
8	a	818	F39	C19-C20-C27-C32
8	a	818	F39	C25-C20-C27-C32
8	a	818	F39	C22-C21-O6-C15
8	a	818	F39	O7-C21-O6-C15
8	a	818	F39	C38-C37-C39-C40
8	a	818	F39	C41-C42-C44-C51
8	a	818	F39	C42-C44-C51-C57
8	a	818	F39	C44-C51-C57-C59
8	a	818	F39	C53-C56-C58-C61
8	a	818	F39	C56-C58-C61-C63
8	a	818	F39	C61-C63-C64-C62
9	A	815	F26	C9-C15-C19-C23
9	A	815	F26	C23-C19-C24-C27
9	A	815	F26	C15-C19-C24-C27
9	A	815	F26	C19-C24-C27-C28
9	A	815	F26	C22-C25-C26-C29
9	A	815	F26	C22-C25-C26-C30
9	A	815	F26	C35-C34-C37-C39
9	A	815	F26	C40-C34-C37-C39

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Mol	Chain	Res	Type	Atoms
9	a	819	F26	C9-C15-C19-C24
9	a	819	F26	C23-C19-C24-C27
9	a	819	F26	C15-C19-C24-C27
9	a	819	F26	C10-C14-C16-C20
9	a	819	F26	C22-C25-C26-C29
9	a	819	F26	C22-C25-C26-C30
9	a	819	F26	C25-C26-C30-C32
9	a	819	F26	C29-C26-C30-C32
9	a	819	F26	C35-C34-C37-C39
9	a	819	F26	C40-C34-C37-C39
9	a	820	F26	C17-C13-C18-C22
9	a	820	F26	C8-C13-C18-C22
9	a	820	F26	C9-C15-C19-C24
9	a	820	F26	C15-C19-C24-C27
9	a	820	F26	C10-C14-C16-C21
9	a	820	F26	C10-C14-C16-C20
9	a	820	F26	C8-C10-C14-C16
9	a	820	F26	C22-C25-C26-C29
9	a	820	F26	C22-C25-C26-C30
9	a	820	F26	C25-C26-C30-C32
9	a	820	F26	C29-C26-C30-C32
9	a	820	F26	C28-C31-C33-C38
9	a	820	F26	C36-C31-C33-C38
9	a	820	F26	C31-C33-C38-C39
9	a	820	F26	C35-C34-C37-C39
9	a	820	F26	C40-C34-C37-C39
9	a	820	F26	C34-C37-C39-C38
10	A	816	LHG	C3-O3-P-O4
10	A	816	LHG	C3-O3-P-O5
10	A	816	LHG	C8-C7-O7-C5
10	A	817	LHG	C3-O3-P-O4
10	A	817	LHG	C3-O3-P-O5
10	A	817	LHG	C3-O3-P-O6
10	a	821	LHG	C8-C7-O7-C5
10	a	822	LHG	C3-O3-P-O4
10	a	822	LHG	C3-O3-P-O6
10	a	823	LHG	C4-O6-P-O5
10	a	823	LHG	C6-C5-O7-C7
10	C	301	LHG	C1-C2-C3-O3
10	C	301	LHG	C3-O3-P-O4
10	C	301	LHG	C3-O3-P-O5
10	C	301	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
10	C	301	LHG	O9-C7-O7-C5
10	C	301	LHG	C8-C7-O7-C5
11	A	818	LMG	C2-C1-O1-C7
11	A	818	LMG	O6-C1-O1-C7
11	A	820	LMG	O9-C10-O7-C8
11	A	820	LMG	C11-C10-O7-C8
11	A	821	LMG	C2-C1-O1-C7
11	A	821	LMG	O6-C1-O1-C7
11	A	822	LMG	O9-C10-O7-C8
11	A	822	LMG	C11-C10-O7-C8
11	a	824	LMG	O7-C8-C9-O8
11	C	302	LMG	C2-C1-O1-C7
11	C	302	LMG	O6-C1-O1-C7
11	C	302	LMG	O9-C10-O7-C8
13	A	824	G2O	C1-C2-C3-C4
13	A	824	G2O	C1-C2-C3-C5
13	A	824	G2O	C5-C6-C7-C8
13	A	824	G2O	C2B-C3B-CAB-CBB
13	A	824	G2O	C4B-C3B-CAB-CBB
13	A	824	G2O	CBD-CGD-O2D-CED
13	a	801	G2O	C1-C2-C3-C4
13	a	801	G2O	C5-C6-C7-C8
13	a	801	G2O	C11-C10-C8-C7
13	a	801	G2O	C11-C10-C8-C9
13	a	801	G2O	C1A-C2A-CAA-CBA
13	a	801	G2O	C6-C7-C8-C10
13	a	801	G2O	C6-C7-C8-C9
13	a	801	G2O	CHA-CBD-CGD-O1D
13	a	801	G2O	CBD-CGD-O2D-CED
13	a	801	G2O	O1D-CGD-O2D-CED
13	a	802	G2O	C1-C2-C3-C4
13	a	802	G2O	C5-C6-C7-C8
13	a	802	G2O	C1A-C2A-CAA-CBA
13	a	802	G2O	CHA-CBD-CGD-O2D
13	a	802	G2O	CBD-CGD-O2D-CED
13	a	805	G2O	C3-C5-C6-C7
13	a	805	G2O	C5-C6-C7-C8
13	a	805	G2O	C11-C10-C8-C9
13	a	805	G2O	C1A-C2A-CAA-CBA
13	a	805	G2O	CHA-CBD-CGD-O2D
13	a	805	G2O	CBD-CGD-O2D-CED
13	a	801	G2O	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	A	824	G2O	O1D-CGD-O2D-CED
13	a	805	G2O	O1D-CGD-O2D-CED
13	a	802	G2O	C13-C15-C16-C17
6	a	804	GS0	O1D-CGD-O2D-CED
13	a	802	G2O	O1D-CGD-O2D-CED
8	A	814	F39	O7-C21-O6-C15
10	a	822	LHG	O10-C23-O8-C6
11	A	821	LMG	O10-C28-O8-C9
13	a	801	G2O	C4C-C3C-CAC-CBC
6	A	801	GS0	O1D-CGD-O2D-CED
8	A	814	F39	C22-C21-O6-C15
9	A	815	F26	C10-C14-C16-C21
9	A	815	F26	C10-C14-C16-C20
9	a	819	F26	C10-C14-C16-C21
10	a	823	LHG	O10-C23-O8-C6
6	a	804	GS0	C15-C16-C17-C18
8	A	814	F39	O1-C12-C15-O6
13	A	824	G2O	C8-C10-C11-C12
10	A	816	LHG	O9-C7-O7-C5
10	a	821	LHG	O9-C7-O7-C5
10	a	822	LHG	O9-C7-O7-C5
10	a	823	LHG	O9-C7-O7-C5
10	a	822	LHG	C24-C23-O8-C6
11	A	821	LMG	C29-C28-O8-C9
11	C	302	LMG	C11-C10-O7-C8
13	a	805	G2O	C2C-C3C-CAC-CBC
13	a	802	G2O	C2-C3-C5-C6
7	W	402	BCL	C2-C3-C5-C6
13	A	824	G2O	C2A-CAA-CBA-CGA
10	a	823	LHG	C24-C23-O8-C6
13	A	824	G2O	CBA-CGA-O2A-C1
6	A	801	GS0	C1-C2-C3-C5
11	a	824	LMG	O10-C28-O8-C9
8	a	818	F39	C37-C39-C40-C41
9	A	815	F26	C26-C30-C32-C35
10	a	821	LHG	O2-C2-C3-O3
11	a	824	LMG	C29-C28-O8-C9
13	A	824	G2O	O1A-CGA-O2A-C1
11	A	818	LMG	O6-C5-C6-O5
11	C	302	LMG	O6-C5-C6-O5
10	a	823	LHG	C8-C7-O7-C5
13	a	801	G2O	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	A	814	F39	C10-C12-C15-O6
13	a	805	G2O	C4C-C3C-CAC-CBC
11	A	819	LMG	O9-C10-O7-C8
13	A	824	G2O	C2-C3-C5-C6
13	A	824	G2O	C4-C3-C5-C6
7	A	803	BCL	C4-C3-C5-C6
7	a	813	BCL	C4-C3-C5-C6
9	a	820	F26	C17-C13-C8-C10
6	A	801	GS0	C2-C3-C5-C6
7	A	803	BCL	C2-C3-C5-C6
7	U	404	BCL	C2-C3-C5-C6
7	V	403	BCL	C2-C3-C5-C6
9	a	820	F26	C18-C13-C8-C10
11	a	824	LMG	O6-C1-O1-C7
9	a	819	F26	C14-C10-C8-C13
9	a	820	F26	C14-C10-C8-C13
13	a	802	G2O	C2C-C3C-CAC-CBC
13	a	801	G2O	CBA-CGA-O2A-C1
10	a	822	LHG	C8-C7-O7-C5
8	a	818	F39	C51-C57-C59-C62
10	C	301	LHG	O2-C2-C3-O3
11	a	824	LMG	C2-C1-O1-C7
13	a	802	G2O	C4-C3-C5-C6
11	A	818	LMG	C4-C5-C6-O5
7	A	813	BCL	C11-C10-C8-C9
7	a	806	BCL	C6-C7-C8-C9
7	a	809	BCL	C6-C7-C8-C9
7	a	815	BCL	C6-C7-C8-C9
7	U	405	BCL	C11-C12-C13-C14
7	U	409	BCL	C6-C7-C8-C9
13	A	824	G2O	C14-C13-C15-C16
7	a	817	BCL	C2A-CAA-CBA-CGA
13	a	801	G2O	C2A-CAA-CBA-CGA
8	A	814	F39	C32-C35-C37-C38
8	a	818	F39	C40-C41-C42-C43
9	a	820	F26	C9-C15-C19-C23
9	a	820	F26	C27-C28-C31-C36
8	a	818	F39	C32-C35-C37-C39
9	A	815	F26	C9-C15-C19-C24
9	a	820	F26	C27-C28-C31-C33
10	A	817	LHG	C7-C8-C9-C10
11	A	820	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
7	A	809	BCL	C10-C11-C12-C13
6	A	801	GS0	C13-C15-C16-C17
7	A	804	BCL	C13-C15-C16-C17
7	a	806	BCL	C8-C10-C11-C12
7	a	817	BCL	C10-C11-C12-C13
7	W	405	BCL	C13-C15-C16-C17
10	a	821	LHG	C7-C8-C9-C10
11	A	818	LMG	C10-C11-C12-C13
7	W	406	BCL	C15-C16-C17-C18
7	a	814	BCL	O1D-CGD-O2D-CED
7	W	404	BCL	C8-C10-C11-C12
11	A	818	LMG	C28-C29-C30-C31
11	A	819	LMG	C28-C29-C30-C31
11	C	302	LMG	C28-C29-C30-C31
7	V	402	BCL	C8-C10-C11-C12
6	a	804	GS0	C6-C7-C8-C10
7	A	803	BCL	C11-C10-C8-C7
7	A	810	BCL	C6-C7-C8-C10
7	W	401	BCL	C6-C7-C8-C10
11	a	824	LMG	C28-C29-C30-C31
13	a	802	G2O	C2A-CAA-CBA-CGA
13	a	805	G2O	C2A-CAA-CBA-CGA
7	W	404	BCL	O1D-CGD-O2D-CED
7	A	806	BCL	C8-C10-C11-C12
13	A	824	G2O	C13-C15-C16-C17
13	a	805	G2O	C15-C16-C17-C18
11	A	819	LMG	O6-C1-O1-C7
7	a	806	BCL	C13-C15-C16-C17
8	A	814	F39	C27-C32-C35-C37
8	a	818	F39	C39-C40-C41-C42
7	A	813	BCL	C10-C11-C12-C13
7	W	404	BCL	C5-C6-C7-C8
13	a	802	G2O	C8-C10-C11-C12
11	C	302	LMG	C29-C28-O8-C9
7	A	812	BCL	C10-C11-C12-C13
10	A	816	LHG	C3-O3-P-O6
10	a	822	LHG	C4-O6-P-O3
10	C	301	LHG	C3-O3-P-O6
11	C	302	LMG	C4-C5-C6-O5
6	a	804	GS0	CBA-CGA-O2A-C1
11	A	820	LMG	C29-C28-O8-C9
6	a	804	GS0	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	a	821	LHG	C1-C2-C3-O3
6	a	804	GS0	C10-C11-C12-C13
7	a	806	BCL	C2A-CAA-CBA-CGA
7	a	809	BCL	C2A-CAA-CBA-CGA
13	a	802	G2O	C4C-C3C-CAC-CBC
8	A	814	F39	C37-C39-C40-C41
9	a	820	F26	C19-C24-C27-C28
7	A	804	BCL	O1D-CGD-O2D-CED
8	A	814	F39	C38-C37-C39-C40
8	a	818	F39	C43-C42-C44-C51
8	a	818	F39	C60-C58-C61-C63
9	A	815	F26	C29-C26-C30-C32
10	C	301	LHG	C13-C14-C15-C16
10	A	817	LHG	C25-C26-C27-C28
7	U	408[B]	BCL	O1D-CGD-O2D-CED
7	A	806	BCL	O1D-CGD-O2D-CED
11	A	818	LMG	C15-C16-C17-C18
11	a	824	LMG	C12-C13-C14-C15
10	a	823	LHG	C23-C24-C25-C26
7	V	403	BCL	O1D-CGD-O2D-CED
9	A	815	F26	C25-C26-C30-C32
11	A	819	LMG	C2-C1-O1-C7
7	V	408[B]	BCL	O1D-CGD-O2D-CED
7	W	402	BCL	O1D-CGD-O2D-CED
7	U	407	BCL	C4-C3-C5-C6
7	W	401	BCL	C4-C3-C5-C6
10	a	823	LHG	C12-C13-C14-C15
7	W	401	BCL	C2-C3-C5-C6
6	a	804	GS0	C6-C7-C8-C9
7	A	803	BCL	C14-C13-C15-C16
10	A	817	LHG	C11-C12-C13-C14
10	a	823	LHG	C11-C12-C13-C14
11	A	820	LMG	C31-C32-C33-C34
9	a	819	F26	C40-C34-C35-C32
11	A	818	LMG	C11-C12-C13-C14
10	A	817	LHG	O1-C1-C2-C3
10	a	822	LHG	O1-C1-C2-C3
8	A	814	F39	C40-C41-C42-C44
8	A	814	F39	C53-C56-C58-C61
9	a	819	F26	C37-C34-C35-C32
11	A	819	LMG	C11-C10-O7-C8
10	A	817	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	C	302	LMG	C32-C33-C34-C35
7	A	813	BCL	O1D-CGD-O2D-CED
10	A	817	LHG	C26-C27-C28-C29
11	A	818	LMG	C31-C32-C33-C34
7	A	809	BCL	C16-C17-C18-C20
11	A	822	LMG	O6-C1-O1-C7
7	U	409	BCL	C15-C16-C17-C18
10	A	817	LHG	C12-C13-C14-C15
11	A	820	LMG	C11-C12-C13-C14
11	A	819	LMG	C29-C30-C31-C32
11	A	820	LMG	C32-C33-C34-C35
7	A	803	BCL	C10-C11-C12-C13
11	A	822	LMG	C31-C32-C33-C34
7	a	808	BCL	O1D-CGD-O2D-CED
10	a	821	LHG	C12-C13-C14-C15
7	W	407[B]	BCL	O1D-CGD-O2D-CED
7	W	405	BCL	C8-C10-C11-C12
13	a	801	G2O	C15-C16-C17-C18
7	U	404	BCL	O1D-CGD-O2D-CED
11	A	818	LMG	C29-C30-C31-C32
10	a	823	LHG	C17-C18-C19-C20
11	A	822	LMG	C28-C29-C30-C31
10	C	301	LHG	C11-C10-C9-C8
7	U	402	BCL	C5-C6-C7-C8
6	a	804	GS0	O1A-CGA-O2A-C1
7	A	810	BCL	C4-C3-C5-C6
7	a	809	BCL	O1D-CGD-O2D-CED
7	A	813	BCL	C11-C10-C8-C7
7	a	807	BCL	C2-C3-C5-C6
7	U	401	BCL	C2-C3-C5-C6
7	U	403	BCL	C11-C10-C8-C7
7	V	401	BCL	C2-C3-C5-C6
7	V	405	BCL	C11-C10-C8-C7
13	A	824	G2O	C12-C13-C15-C16
6	a	804	GS0	C13-C15-C16-C17
7	a	806	BCL	O1D-CGD-O2D-CED
7	A	810	BCL	C2A-CAA-CBA-CGA
7	A	805	BCL	O1D-CGD-O2D-CED
7	W	403	BCL	O1D-CGD-O2D-CED
7	A	809	BCL	O1D-CGD-O2D-CED
7	U	405	BCL	C8-C10-C11-C12
10	A	817	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
11	C	302	LMG	C29-C30-C31-C32
11	A	821	LMG	C11-C10-O7-C8
7	a	816	BCL	C15-C16-C17-C18
11	a	824	LMG	C16-C17-C18-C19
6	a	804	GS0	C3-C5-C6-C7
7	a	817	BCL	O1D-CGD-O2D-CED
10	A	817	LHG	C13-C14-C15-C16
7	A	813	BCL	C4-C3-C5-C6
11	A	819	LMG	C37-C38-C39-C40
7	A	803	BCL	C11-C10-C8-C9
7	U	403	BCL	C11-C10-C8-C9
7	V	405	BCL	C11-C10-C8-C9
7	W	401	BCL	C6-C7-C8-C9
7	A	807	BCL	C2A-CAA-CBA-CGA
7	a	816	BCL	C10-C11-C12-C13
11	A	818	LMG	C32-C33-C34-C35
11	A	820	LMG	O10-C28-O8-C9
7	A	812	BCL	O1D-CGD-O2D-CED
6	a	804	GS0	C1A-C2A-CAA-CBA
13	A	824	G2O	C1A-C2A-CAA-CBA
10	A	816	LHG	C2-C3-O3-P
7	W	405	BCL	O1D-CGD-O2D-CED
6	A	801	GS0	C15-C16-C17-C18
10	A	816	LHG	O6-C4-C5-C6
11	A	818	LMG	C16-C17-C18-C19
7	W	405	BCL	C10-C11-C12-C13
11	A	820	LMG	C8-C9-O8-C28
10	a	823	LHG	C14-C15-C16-C17
7	A	806	BCL	C4-C3-C5-C6
7	A	802	BCL	C2C-C3C-CAC-CBC
7	A	805	BCL	C2C-C3C-CAC-CBC
7	a	814	BCL	C2C-C3C-CAC-CBC
7	V	404	BCL	C2C-C3C-CAC-CBC
7	a	811	BCL	O1D-CGD-O2D-CED
8	a	818	F39	C22-C23-C24-C26
10	a	822	LHG	C4-C5-C6-O8
10	a	823	LHG	C19-C20-C21-C22
7	A	803	BCL	O1D-CGD-O2D-CED
7	U	402	BCL	O1D-CGD-O2D-CED
7	a	810	BCL	O1A-CGA-O2A-C1
10	a	821	LHG	C13-C14-C15-C16
13	A	824	G2O	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	a	805	G2O	C6-C7-C8-C9
7	a	806	BCL	O1A-CGA-O2A-C1
10	C	301	LHG	C11-C12-C13-C14
11	A	819	LMG	C12-C13-C14-C15
7	U	409	BCL	C10-C11-C12-C13
9	a	820	F26	C23-C19-C24-C27
11	a	824	LMG	O6-C5-C6-O5
7	W	406	BCL	C4-C3-C5-C6
9	A	815	F26	C19-C15-C9-C2
10	A	817	LHG	C24-C23-O8-C6
7	V	404	BCL	C10-C11-C12-C13
10	a	822	LHG	C6-C5-O7-C7
11	A	820	LMG	C7-C8-O7-C10
7	A	809	BCL	C15-C16-C17-C18
7	W	406	BCL	O1D-CGD-O2D-CED
7	V	405	BCL	CAA-CBA-CGA-O2A
7	A	808	BCL	O1D-CGD-O2D-CED
7	A	812	BCL	C5-C6-C7-C8
11	A	822	LMG	C2-C1-O1-C7
7	A	811	BCL	O1D-CGD-O2D-CED
11	A	821	LMG	O9-C10-O7-C8
11	A	822	LMG	C33-C34-C35-C36
7	A	812	BCL	C4-C3-C5-C6
7	A	803	BCL	C6-C7-C8-C10
7	A	806	BCL	C2-C3-C5-C6
7	a	806	BCL	C6-C7-C8-C10
7	a	809	BCL	C6-C7-C8-C10
7	a	812	BCL	C2-C3-C5-C6
7	A	804	BCL	C11-C10-C8-C9
7	A	804	BCL	C11-C12-C13-C14
7	a	813	BCL	O1D-CGD-O2D-CED
7	a	814	BCL	C15-C16-C17-C18
10	A	817	LHG	C24-C25-C26-C27
10	a	822	LHG	C2-C3-O3-P
13	a	805	G2O	C3A-C2A-CAA-CBA
8	a	818	F39	C16-C13-C14-C18
10	C	301	LHG	C4-C5-C6-O8
11	A	818	LMG	C30-C31-C32-C33
10	a	823	LHG	C26-C27-C28-C29
13	a	805	G2O	C4-C3-C5-C6
7	U	401	BCL	C4-C3-C5-C6
7	V	404	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	a	814	BCL	C2A-CAA-CBA-CGA
10	a	822	LHG	O1-C1-C2-O2
7	V	405	BCL	O1D-CGD-O2D-CED
10	a	821	LHG	C11-C12-C13-C14
10	a	822	LHG	O7-C5-C6-O8
7	A	809	BCL	C16-C17-C18-C19
6	A	801	GS0	C5-C6-C7-C8
7	a	806	BCL	C10-C11-C12-C13
7	A	811	BCL	C2-C1-O2A-CGA
7	W	404	BCL	C2-C1-O2A-CGA
7	a	810	BCL	C2-C3-C5-C6
7	A	805	BCL	C6-C7-C8-C9
7	A	810	BCL	C6-C7-C8-C9
7	a	813	BCL	C11-C10-C8-C9
7	W	402	BCL	C11-C10-C8-C9
7	W	405	BCL	C11-C12-C13-C14
10	a	821	LHG	C2-C3-O3-P
10	C	301	LHG	C2-C3-O3-P
7	a	816	BCL	C2A-CAA-CBA-CGA
7	A	805	BCL	C4C-C3C-CAC-CBC
7	A	808	BCL	C4C-C3C-CAC-CBC
7	U	408[B]	BCL	C4C-C3C-CAC-CBC
7	V	404	BCL	C4C-C3C-CAC-CBC
7	a	808	BCL	C5-C6-C7-C8
11	A	818	LMG	C33-C34-C35-C36
11	a	824	LMG	C30-C31-C32-C33
7	V	407	BCL	O1D-CGD-O2D-CED
7	a	809	BCL	C8-C10-C11-C12
7	W	403	BCL	C8-C10-C11-C12
6	A	801	GS0	C6-C7-C8-C10
7	A	803	BCL	C12-C13-C15-C16
7	A	804	BCL	C11-C10-C8-C7
7	A	804	BCL	C11-C12-C13-C15
7	A	805	BCL	C6-C7-C8-C10
7	A	805	BCL	C12-C13-C15-C16
7	a	815	BCL	C6-C7-C8-C10
7	U	405	BCL	C11-C12-C13-C15
7	W	402	BCL	C11-C10-C8-C7
7	W	405	BCL	C11-C12-C13-C15
7	V	403	BCL	C1-C2-C3-C4
7	W	402	BCL	C2A-CAA-CBA-CGA
11	A	818	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
7	U	404	BCL	C10-C11-C12-C13
6	A	801	GS0	C3-C5-C6-C7
7	U	404	BCL	O1A-CGA-O2A-C1
11	A	821	LMG	C4-C5-C6-O5
7	a	807	BCL	C15-C16-C17-C18
7	A	807	BCL	CAD-CBD-CGD-O2D
7	a	807	BCL	CAD-CBD-CGD-O2D
7	a	816	BCL	CAD-CBD-CGD-O2D
7	W	403	BCL	CAD-CBD-CGD-O2D
7	W	405	BCL	CAD-CBD-CGD-O2D
7	W	406	BCL	CAD-CBD-CGD-O2D
13	a	801	G2O	CAD-CBD-CGD-O2D
13	a	805	G2O	C2B-C3B-CAB-CBB
13	a	805	G2O	CAD-CBD-CGD-O2D
10	C	301	LHG	C12-C13-C14-C15
7	A	813	BCL	C16-C17-C18-C19
11	A	818	LMG	C7-C8-C9-O8
11	A	821	LMG	O1-C7-C8-C9
11	a	824	LMG	C7-C8-C9-O8
11	C	302	LMG	C7-C8-C9-O8
10	A	816	LHG	O6-C4-C5-O7
10	a	822	LHG	O6-C4-C5-O7
6	a	804	GS0	CHA-CBD-CGD-O2D
7	A	802	BCL	CHA-CBD-CGD-O2D
7	A	807	BCL	CHA-CBD-CGD-O1D
7	A	808	BCL	CHA-CBD-CGD-O1D
7	A	811	BCL	CHA-CBD-CGD-O2D
7	A	813	BCL	CHA-CBD-CGD-O2D
7	a	809	BCL	CHA-CBD-CGD-O2D
7	a	812	BCL	CHA-CBD-CGD-O1D
7	a	814	BCL	CHA-CBD-CGD-O1D
7	a	816	BCL	CHA-CBD-CGD-O1D
7	U	401	BCL	CHA-CBD-CGD-O2D
7	U	403	BCL	CHA-CBD-CGD-O2D
7	U	406	BCL	CHA-CBD-CGD-O2D
13	A	824	G2O	CHA-CBD-CGD-O1D
7	a	817	BCL	O1A-CGA-O2A-C1
7	U	401	BCL	O1A-CGA-O2A-C1
7	V	407	BCL	O1A-CGA-O2A-C1
7	a	816	BCL	O1D-CGD-O2D-CED
11	A	821	LMG	O1-C7-C8-O7
11	C	302	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
11	C	302	LMG	O7-C8-C9-O8
8	a	818	F39	C31-C33-C34-C36
7	A	802	BCL	O1D-CGD-O2D-CED
7	a	807	BCL	C4-C3-C5-C6
7	A	805	BCL	O1A-CGA-O2A-C1
11	A	821	LMG	O6-C5-C6-O5
7	A	809	BCL	C1A-C2A-CAA-CBA
7	A	813	BCL	C8-C10-C11-C12
7	a	816	BCL	C13-C15-C16-C17
11	A	819	LMG	C11-C12-C13-C14
10	C	301	LHG	C9-C10-C11-C12
10	a	823	LHG	C4-O6-P-O3
11	a	824	LMG	C18-C19-C20-C21
7	V	405	BCL	C2-C3-C5-C6
7	a	808	BCL	O1A-CGA-O2A-C1
10	a	822	LHG	C3-O3-P-O5
10	a	822	LHG	C4-O6-P-O5
13	a	802	G2O	C11-C10-C8-C7
6	A	801	GS0	C8-C10-C11-C12
11	A	819	LMG	C29-C28-O8-C9
10	a	822	LHG	O6-C4-C5-C6
11	A	820	LMG	C12-C13-C14-C15
11	C	302	LMG	O10-C28-O8-C9
7	A	808	BCL	CAD-CBD-CGD-O1D
7	a	812	BCL	CAD-CBD-CGD-O1D
7	a	816	BCL	CAD-CBD-CGD-O1D
7	U	403	BCL	CAD-CBD-CGD-O1D
7	a	807	BCL	C10-C11-C12-C13
11	A	818	LMG	C13-C14-C15-C16
7	A	810	BCL	O1D-CGD-O2D-CED
7	A	812	BCL	C2C-C3C-CAC-CBC
7	a	814	BCL	C12-C13-C15-C16
7	U	402	BCL	C12-C13-C15-C16
7	V	403	BCL	C11-C10-C8-C7
11	a	824	LMG	C14-C15-C16-C17
7	A	802	BCL	O1A-CGA-O2A-C1
7	A	813	BCL	O1A-CGA-O2A-C1
7	A	808	BCL	O1A-CGA-O2A-C1
7	A	812	BCL	C2A-CAA-CBA-CGA
11	C	302	LMG	C12-C13-C14-C15
8	a	818	F39	O2-C13-C14-C18
10	A	816	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
11	A	820	LMG	O1-C7-C8-C9
10	C	301	LHG	O7-C5-C6-O8
11	A	820	LMG	O1-C7-C8-O7
7	a	810	BCL	O2A-C1-C2-C3
10	A	817	LHG	O1-C1-C2-O2
13	a	805	G2O	C13-C15-C16-C17
7	V	406	BCL	O1D-CGD-O2D-CED
7	a	815	BCL	C2-C3-C5-C6
13	a	801	G2O	C10-C11-C12-C13
10	C	301	LHG	C16-C17-C18-C19
11	A	820	LMG	C34-C35-C36-C37
10	A	816	LHG	C4-C5-O7-C7
11	A	819	LMG	C7-C8-O7-C10
7	U	405	BCL	C10-C11-C12-C13
11	A	818	LMG	C14-C15-C16-C17
6	A	801	GS0	C16-C17-C18-C19
7	V	404	BCL	C4-C3-C5-C6
13	a	805	G2O	C6-C7-C8-C10
10	A	816	LHG	O7-C5-C6-O8
10	A	816	LHG	C4-O6-P-O3
10	a	821	LHG	C3-O3-P-O6
10	a	821	LHG	C4-O6-P-O3
10	C	301	LHG	C4-O6-P-O3
7	a	815	BCL	O1D-CGD-O2D-CED
7	V	406	BCL	C10-C11-C12-C13
11	A	819	LMG	C7-C8-C9-O8
7	A	805	BCL	C14-C13-C15-C16
7	a	816	BCL	C11-C10-C8-C9
9	a	819	F26	C19-C24-C27-C28
11	A	819	LMG	C38-C39-C40-C41
11	A	819	LMG	C31-C32-C33-C34
7	A	802	BCL	C4-C3-C5-C6
7	A	805	BCL	C2-C3-C5-C6
7	W	406	BCL	O1A-CGA-O2A-C1
8	a	818	F39	C21-C22-C23-C24
8	A	814	F39	C20-C27-C32-C35
9	a	820	F26	C26-C30-C32-C35
11	a	824	LMG	C13-C14-C15-C16
7	a	806	BCL	C4-C3-C5-C6
7	A	805	BCL	C2-C1-O2A-CGA
7	V	404	BCL	C2-C1-O2A-CGA
11	A	818	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
7	a	810	BCL	C4-C3-C5-C6
7	U	409	BCL	C4-C3-C5-C6
7	A	809	BCL	C11-C10-C8-C9
7	a	814	BCL	C11-C10-C8-C9
7	V	401	BCL	C14-C13-C15-C16
13	a	801	G2O	C14-C13-C15-C16
6	a	804	GS0	C16-C17-C18-C20
10	a	821	LHG	C11-C10-C9-C8
7	V	401	BCL	O1D-CGD-O2D-CED
11	A	819	LMG	C32-C33-C34-C35
10	C	301	LHG	C6-C5-O7-C7
11	A	822	LMG	C9-C8-O7-C10
7	U	405	BCL	C4-C3-C5-C6
7	A	808	BCL	C1A-C2A-CAA-CBA
7	a	813	BCL	C1A-C2A-CAA-CBA
7	A	802	BCL	C6-C7-C8-C10
7	a	813	BCL	C12-C13-C15-C16
7	a	809	BCL	C5-C6-C7-C8
10	A	817	LHG	C11-C10-C9-C8
7	V	405	BCL	C8-C10-C11-C12
10	a	823	LHG	C13-C14-C15-C16
10	A	817	LHG	O6-C4-C5-O7
10	A	817	LHG	O6-C4-C5-C6
6	A	801	GS0	C16-C17-C18-C20
7	a	811	BCL	CAA-CBA-CGA-O2A
11	A	819	LMG	O7-C8-C9-O8
7	a	815	BCL	C4-C3-C5-C6
7	W	404	BCL	CAA-CBA-CGA-O2A
7	A	805	BCL	CAA-CBA-CGA-O2A
7	a	806	BCL	CAA-CBA-CGA-O2A
7	A	805	BCL	CAA-CBA-CGA-O1A
7	U	405	BCL	CAA-CBA-CGA-O1A
6	a	804	GS0	C4-C3-C5-C6
7	A	804	BCL	C4-C3-C5-C6
9	a	819	F26	C17-C13-C8-C10
7	V	406	BCL	C4C-C3C-CAC-CBC
7	W	407[B]	BCL	C4C-C3C-CAC-CBC
7	A	813	BCL	C2-C3-C5-C6
11	A	822	LMG	C8-C7-O1-C1
7	U	407	BCL	O1A-CGA-O2A-C1
7	U	405	BCL	CAA-CBA-CGA-O2A
7	a	812	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	W	407[B]	BCL	CAA-CBA-CGA-O2A
11	A	819	LMG	C30-C31-C32-C33
7	a	816	BCL	C1-C2-C3-C4
7	U	401	BCL	C1-C2-C3-C4
7	U	404	BCL	C1-C2-C3-C4
7	U	405	BCL	C1-C2-C3-C4
7	V	401	BCL	C1-C2-C3-C4
7	V	402	BCL	C1-C2-C3-C4
7	V	405	BCL	C1-C2-C3-C4
7	V	406	BCL	C1-C2-C3-C4
7	V	407	BCL	C1-C2-C3-C4
7	W	404	BCL	C1-C2-C3-C4
13	a	805	G2O	C1-C2-C3-C4
7	a	807	BCL	CAA-CBA-CGA-O2A
13	a	801	G2O	C8-C10-C11-C12
13	a	801	G2O	C4-C3-C5-C6
7	V	401	BCL	C10-C11-C12-C13
7	V	407	BCL	C4-C3-C5-C6
7	A	804	BCL	C2-C3-C5-C6
6	a	804	GS0	C14-C13-C15-C16
7	A	810	BCL	C11-C10-C8-C9
7	a	806	BCL	C11-C10-C8-C9
7	U	402	BCL	C14-C13-C15-C16
7	V	403	BCL	C11-C10-C8-C9
13	a	802	G2O	C3A-C2A-CAA-CBA
7	A	806	BCL	O1A-CGA-O2A-C1
11	A	819	LMG	O10-C28-O8-C9
7	W	402	BCL	CAA-CBA-CGA-O2A
11	A	822	LMG	O8-C28-C29-C30
6	A	801	GS0	CAD-CBD-CGD-O2D
6	a	804	GS0	CAD-CBD-CGD-O2D
7	A	803	BCL	CAD-CBD-CGD-O2D
7	A	806	BCL	CAD-CBD-CGD-O2D
7	a	814	BCL	CAD-CBD-CGD-O2D
7	V	406	BCL	CAD-CBD-CGD-O2D
7	W	402	BCL	CAD-CBD-CGD-O2D
10	a	823	LHG	C18-C19-C20-C21
7	a	809	BCL	CAA-CBA-CGA-O2A
7	U	401	BCL	CAA-CBA-CGA-O2A
11	A	821	LMG	O7-C10-C11-C12
7	W	406	BCL	C2-C3-C5-C6
9	a	819	F26	C18-C13-C8-C10

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Mol	Chain	Res	Type	Atoms
7	A	810	BCL	CAA-CBA-CGA-O2A
7	W	407[B]	BCL	CAA-CBA-CGA-O1A
10	a	823	LHG	O6-C4-C5-O7
7	W	401	BCL	CAA-CBA-CGA-O2A
7	a	817	BCL	O2A-C1-C2-C3
13	a	805	G2O	C4B-C3B-CAB-CBB
7	U	404	BCL	CAA-CBA-CGA-O2A
7	A	813	BCL	CAA-CBA-CGA-O1A
7	W	404	BCL	C3-C5-C6-C7
7	A	813	BCL	C5-C6-C7-C8
13	a	805	G2O	C2-C3-C5-C6
6	A	801	GS0	CHA-CBD-CGD-O2D
7	A	806	BCL	CHA-CBD-CGD-O1D
7	A	809	BCL	CHA-CBD-CGD-O1D
7	a	806	BCL	CHA-CBD-CGD-O2D
7	a	811	BCL	CHA-CBD-CGD-O2D
7	a	815	BCL	CHA-CBD-CGD-O2D
7	V	401	BCL	CHA-CBD-CGD-O2D
7	V	402	BCL	CHA-CBD-CGD-O2D
7	V	404	BCL	CHA-CBD-CGD-O1D
7	W	401	BCL	CHA-CBD-CGD-O2D
13	a	801	G2O	CHA-CBD-CGD-O2D
13	a	802	G2O	CHA-CBD-CGD-O1D
13	a	805	G2O	CHA-CBD-CGD-O1D
7	a	811	BCL	CAA-CBA-CGA-O1A
11	A	822	LMG	C30-C31-C32-C33
13	A	824	G2O	C6-C7-C8-C10
10	a	823	LHG	O7-C5-C6-O8
7	U	406	BCL	O1A-CGA-O2A-C1
7	a	812	BCL	O1D-CGD-O2D-CED
7	a	813	BCL	CAA-CBA-CGA-O2A
10	a	821	LHG	C14-C15-C16-C17
6	a	804	GS0	C12-C13-C15-C16
7	a	814	BCL	C11-C10-C8-C7
7	a	806	BCL	C5-C6-C7-C8
7	A	806	BCL	CAA-CBA-CGA-O2A
7	V	401	BCL	CAA-CBA-CGA-O2A
7	a	813	BCL	C14-C13-C15-C16
7	a	814	BCL	C14-C13-C15-C16
7	W	404	BCL	C14-C13-C15-C16
7	A	805	BCL	C2A-CAA-CBA-CGA
7	A	813	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
7	W	401	BCL	CAA-CBA-CGA-O1A
7	V	407	BCL	CAA-CBA-CGA-O2A
10	A	817	LHG	O10-C23-C24-C25
7	W	404	BCL	C2-C3-C5-C6
8	a	818	F39	C40-C41-C42-C44
7	a	806	BCL	C1A-C2A-CAA-CBA
7	U	408[B]	BCL	C1A-C2A-CAA-CBA
13	a	802	G2O	C11-C10-C8-C9
7	U	403	BCL	CAA-CBA-CGA-O1A
7	A	802	BCL	C2-C1-O2A-CGA
7	V	407	BCL	C2-C1-O2A-CGA
7	V	403	BCL	CAA-CBA-CGA-O1A
11	A	821	LMG	O9-C10-C11-C12
13	a	801	G2O	C16-C17-C18-C19
7	U	402	BCL	C13-C15-C16-C17
10	a	823	LHG	C3-O3-P-O5
13	A	824	G2O	C11-C10-C8-C7
13	a	805	G2O	C11-C10-C8-C7
11	A	818	LMG	C19-C20-C21-C22
6	A	801	GS0	C10-C11-C12-C13
7	a	815	BCL	C13-C15-C16-C17
7	V	401	BCL	CAA-CBA-CGA-O1A
7	U	407	BCL	CAA-CBA-CGA-O2A
11	A	819	LMG	O8-C28-C29-C30
7	a	811	BCL	C2A-CAA-CBA-CGA
7	U	402	BCL	C8-C10-C11-C12
7	A	802	BCL	CAA-CBA-CGA-O2A
7	A	810	BCL	C16-C17-C18-C20
6	a	804	GS0	CAD-CBD-CGD-O1D
7	V	403	BCL	CAA-CBA-CGA-O2A
7	W	406	BCL	C10-C11-C12-C13
7	A	803	BCL	C6-C7-C8-C9
7	a	810	BCL	C8-C10-C11-C12
11	a	824	LMG	C29-C30-C31-C32
10	a	821	LHG	O7-C7-C8-C9
7	a	810	BCL	C10-C11-C12-C13
10	a	821	LHG	C15-C16-C17-C18
7	V	404	BCL	CAA-CBA-CGA-O2A
7	U	403	BCL	O1D-CGD-O2D-CED
6	a	804	GS0	C11-C12-C13-C15
7	A	813	BCL	C3A-C2A-CAA-CBA
7	a	816	BCL	C11-C10-C8-C7

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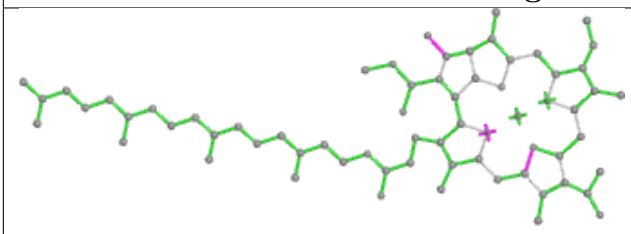
Mol	Chain	Res	Type	Atoms
7	V	404	BCL	C2-C3-C5-C6
7	V	407	BCL	C6-C7-C8-C10
7	W	404	BCL	C11-C12-C13-C15
13	a	801	G2O	C12-C13-C15-C16
7	A	806	BCL	CAA-CBA-CGA-O1A
7	a	813	BCL	CAA-CBA-CGA-O1A
7	W	406	BCL	C8-C10-C11-C12
7	a	810	BCL	CAA-CBA-CGA-O1A
7	W	403	BCL	C10-C11-C12-C13
7	a	812	BCL	C15-C16-C17-C18
7	U	403	BCL	C5-C6-C7-C8
7	U	409	BCL	C13-C15-C16-C17
7	A	808	BCL	CAA-CBA-CGA-O1A
8	A	814	F39	C29-C30-C31-C33
7	a	810	BCL	CAA-CBA-CGA-O2A
11	C	302	LMG	O8-C28-C29-C30

There are no ring outliers.

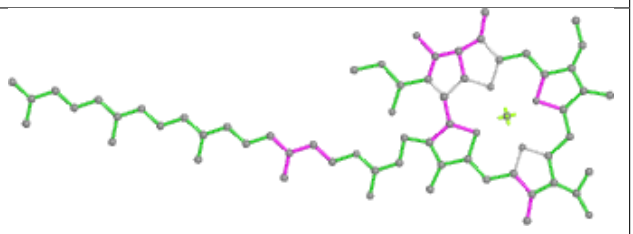
No monomer is involved in short contacts.

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.

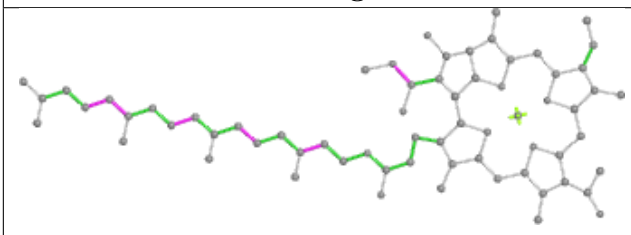
Ligand BCL U 402



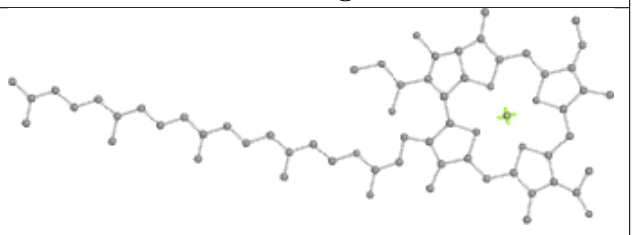
Bond lengths



Bond angles

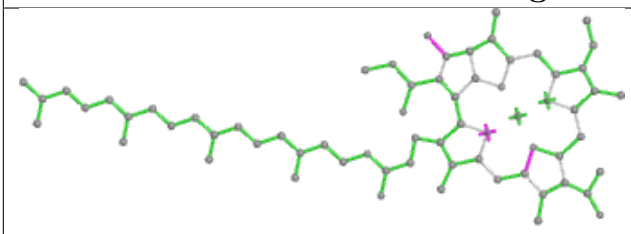


Torsions

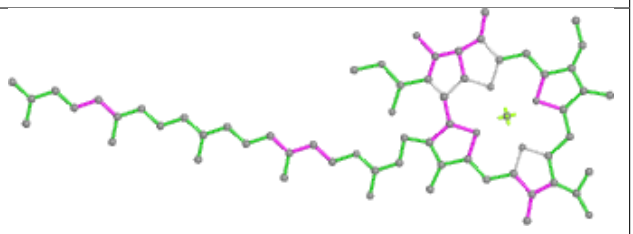


Rings

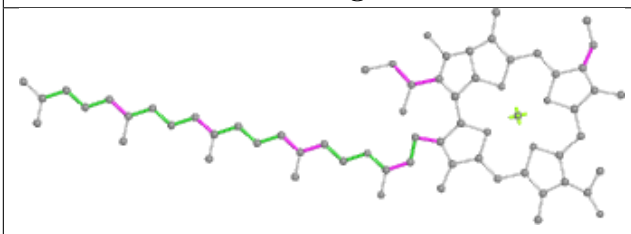
Ligand BCL a 813



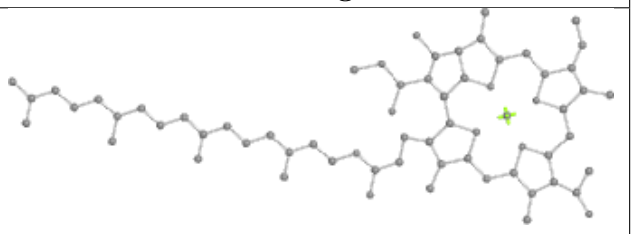
Bond lengths



Bond angles

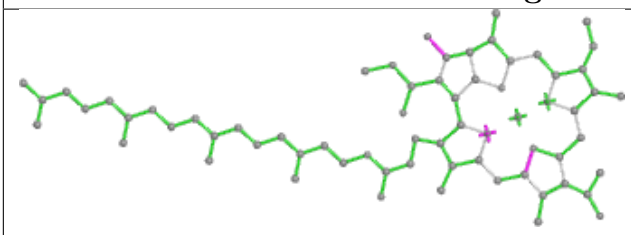


Torsions

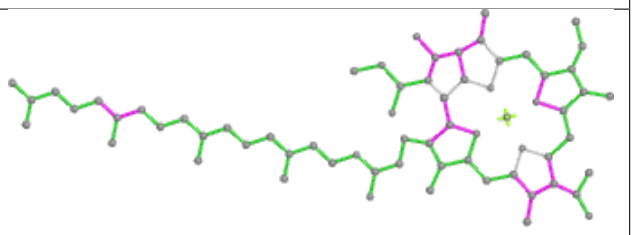


Rings

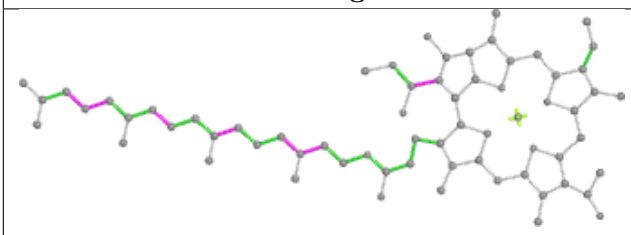
Ligand BCL U 409



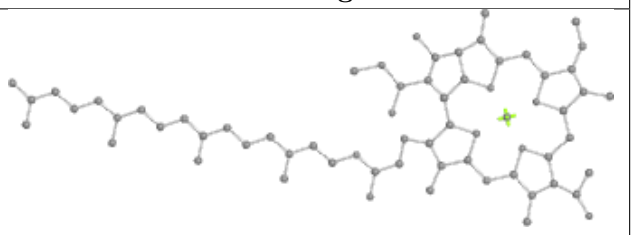
Bond lengths



Bond angles

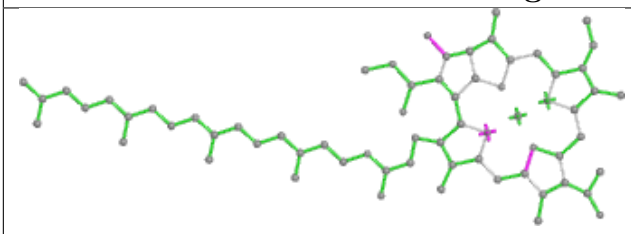


Torsions

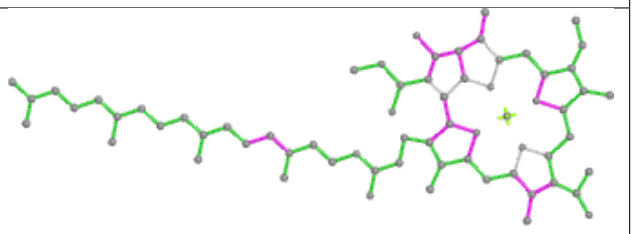


Rings

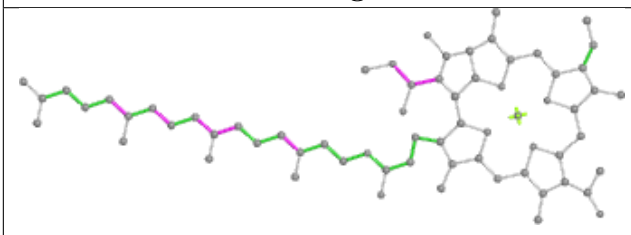
Ligand BCL A 803



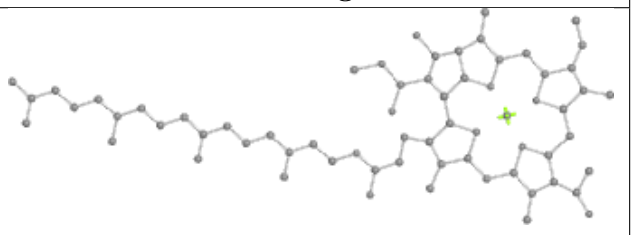
Bond lengths



Bond angles

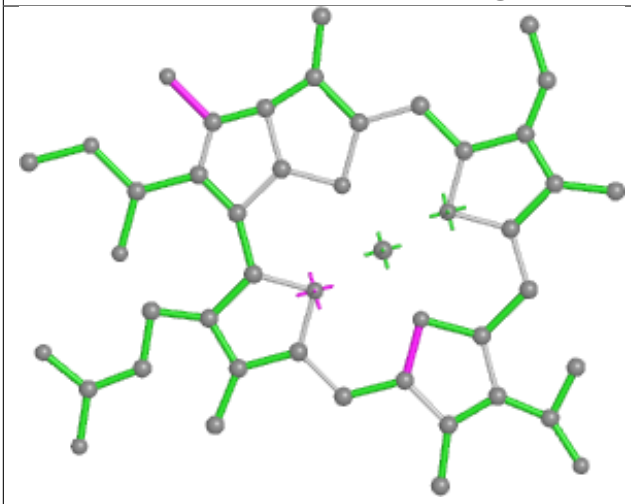


Torsions

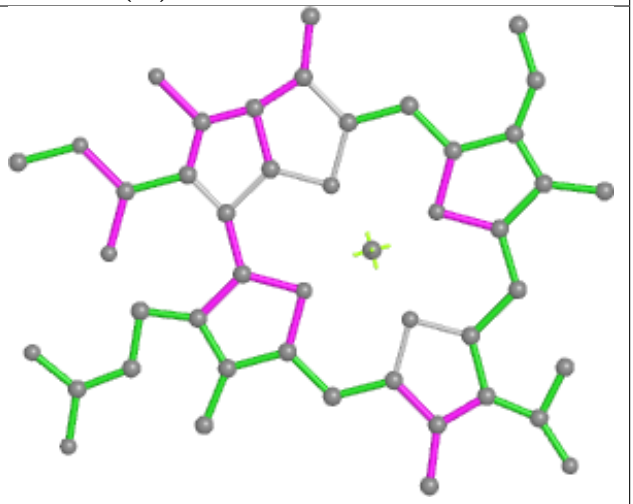


Rings

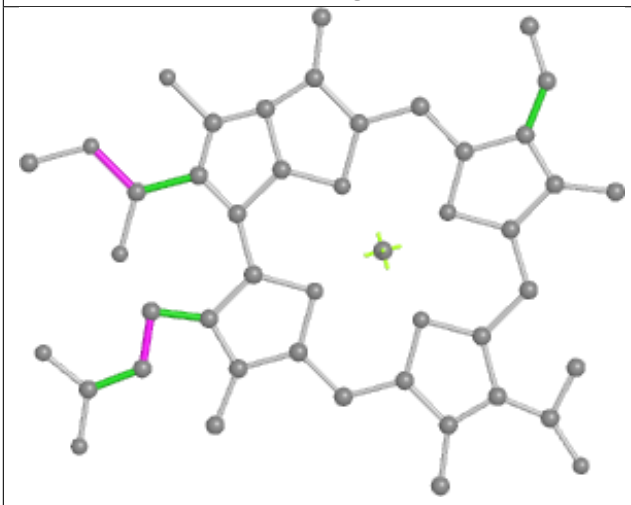
Ligand BCL V 408 (B)



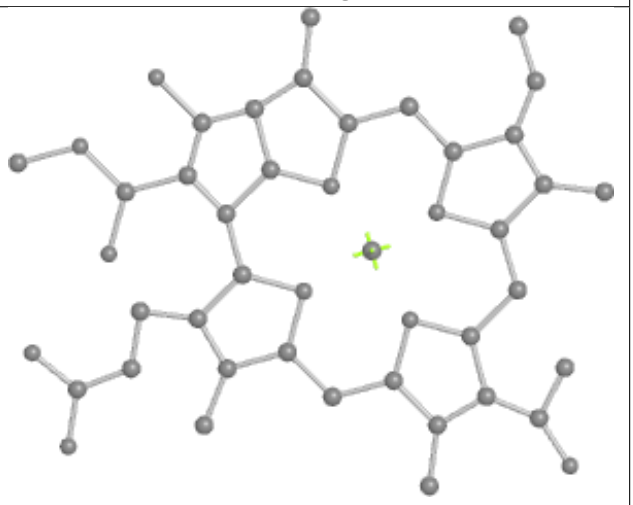
Bond lengths



Bond angles

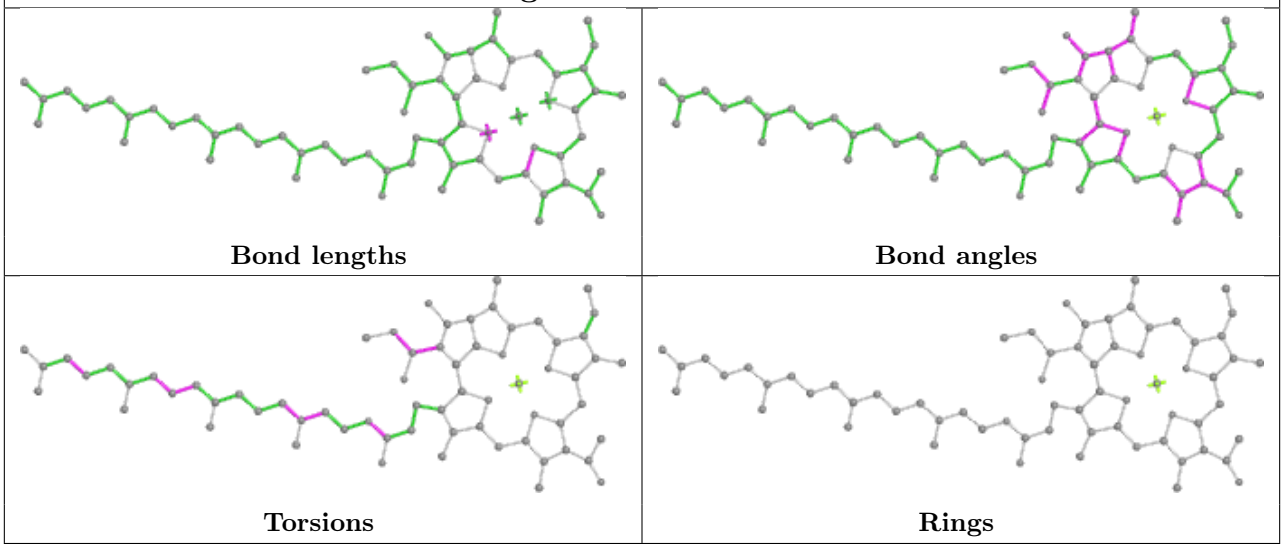


Torsions

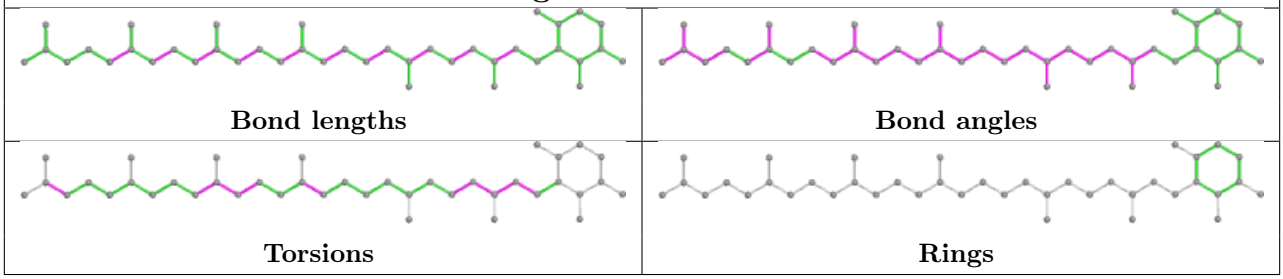


Rings

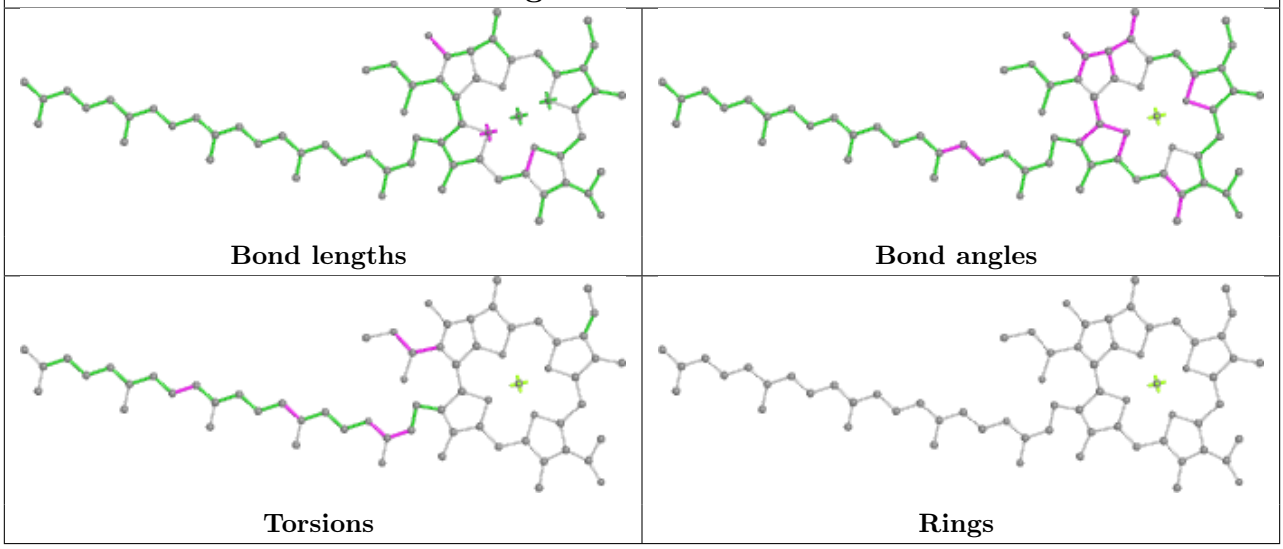
Ligand BCL W 406



Ligand F26 A 815



Ligand BCL A 806



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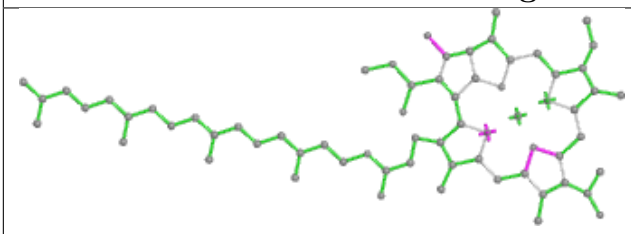
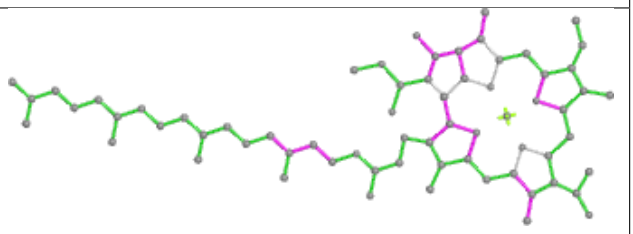
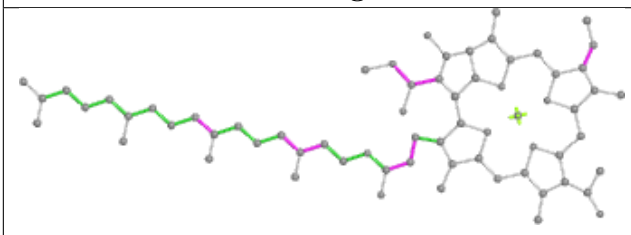


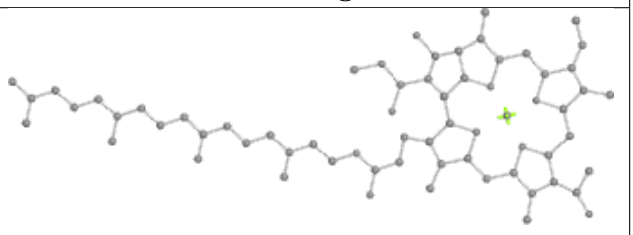
Bond lengths



Bond angles

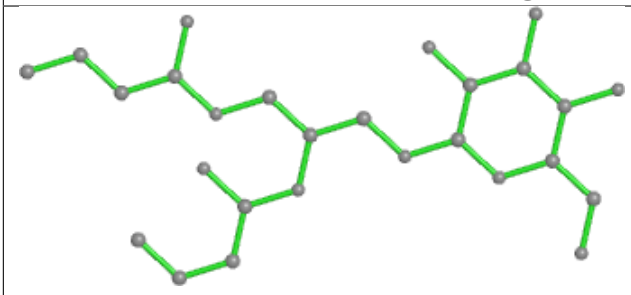


Torsions



Rings

Ligand LMG A 821



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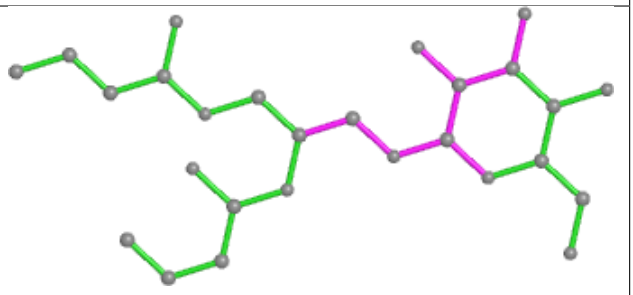
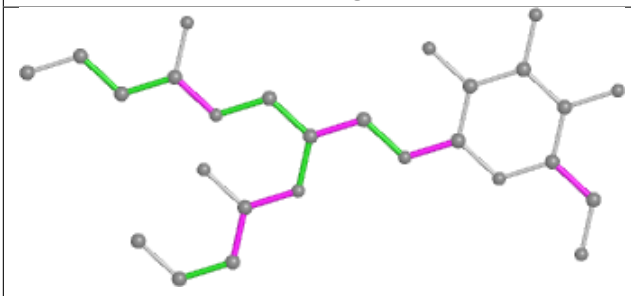


Bond angles



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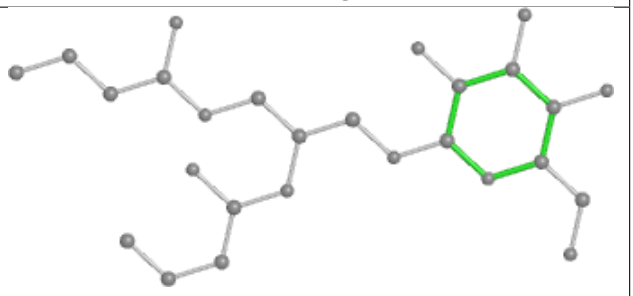
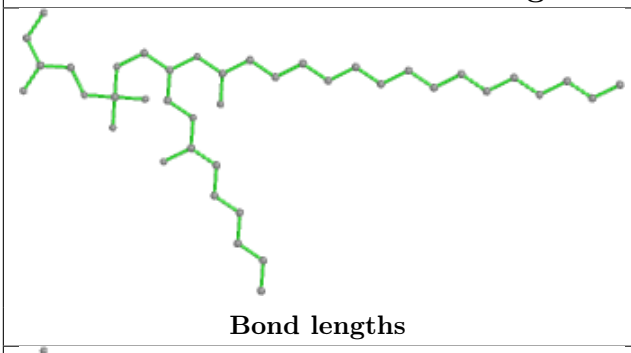


Rings

Ligand LHG a 823



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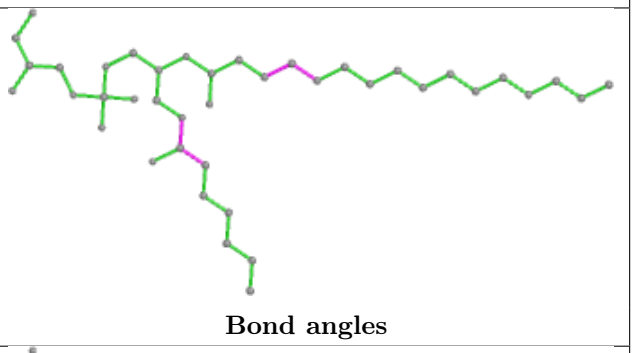
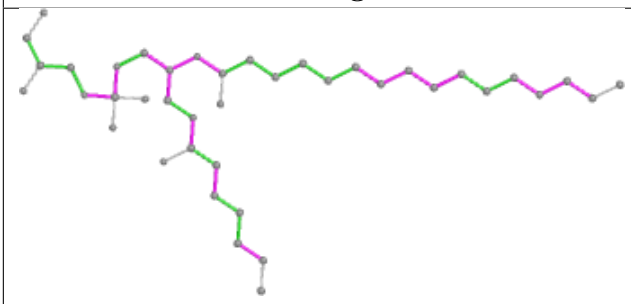
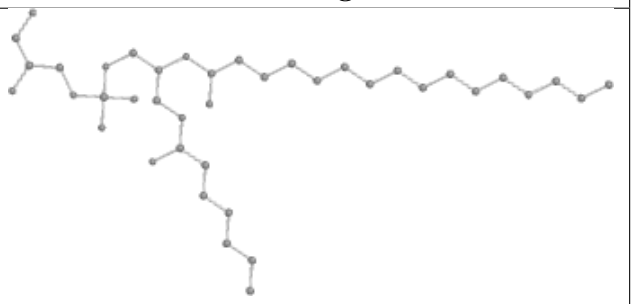


Bond angles

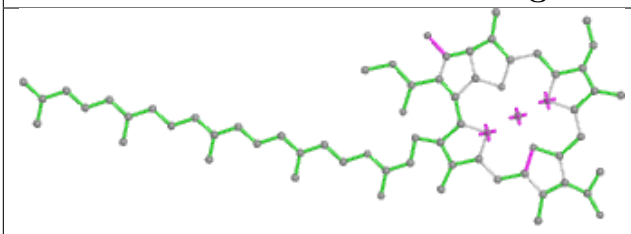


Torsions

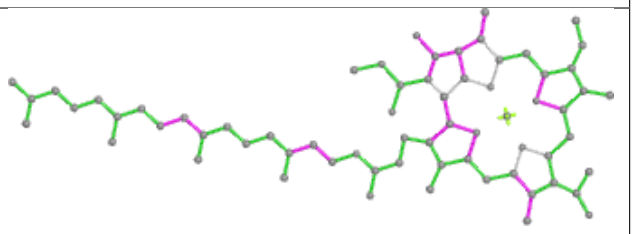


Rings

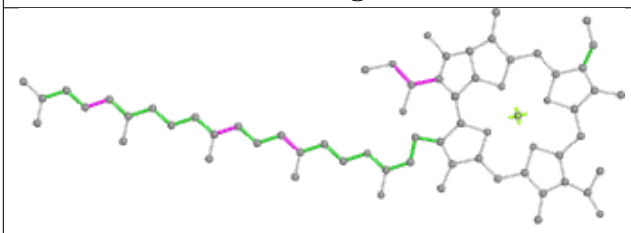
Ligand BCL a 815



Bond lengths



Bond angles



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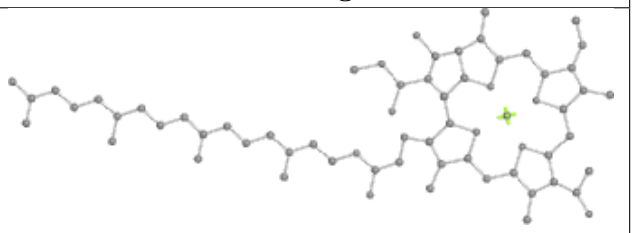
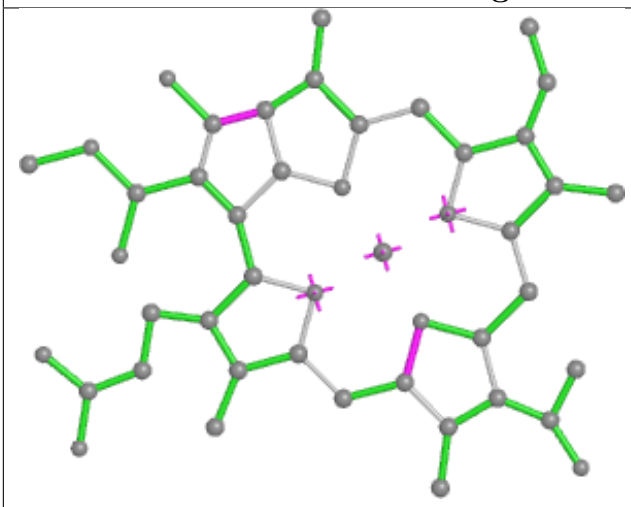
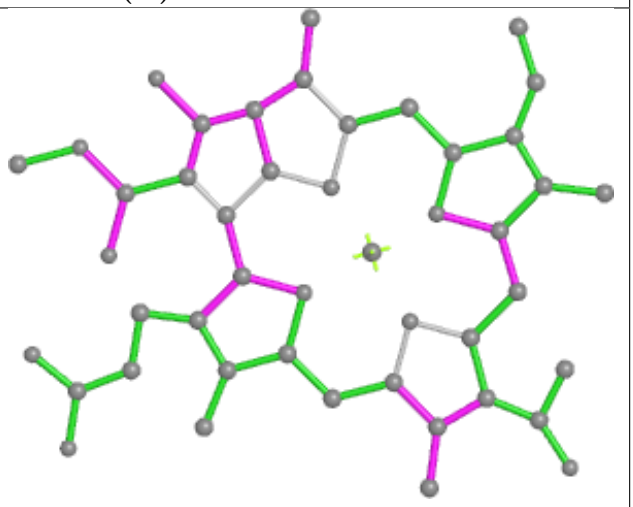


Rings

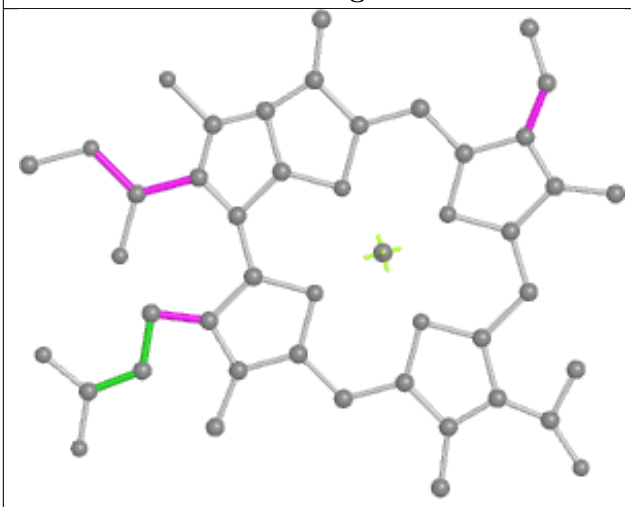
Ligand BCL U 408 (B)



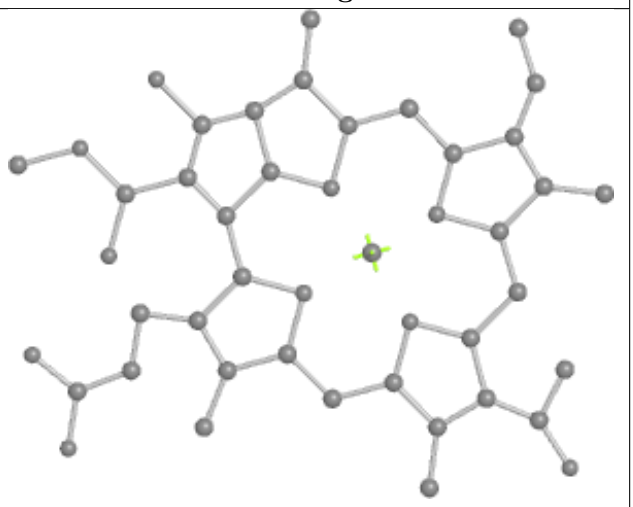
Bond lengths



Bond angles

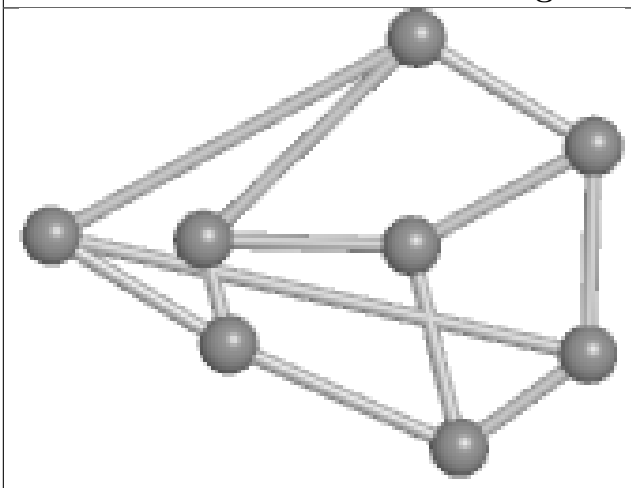


Torsions

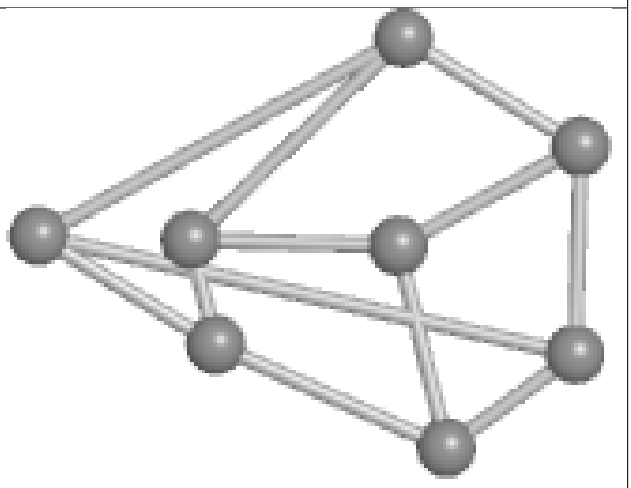


Rings

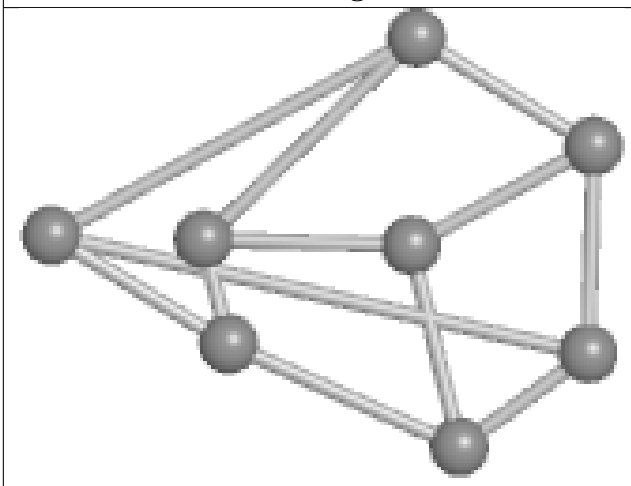
Ligand SF4 a 803



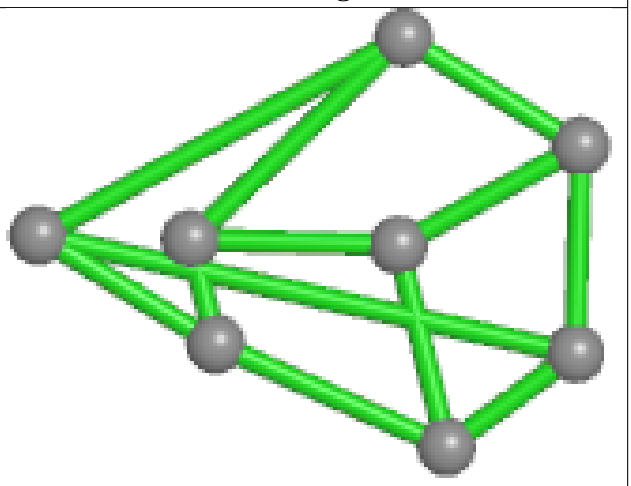
Bond lengths



Bond angles

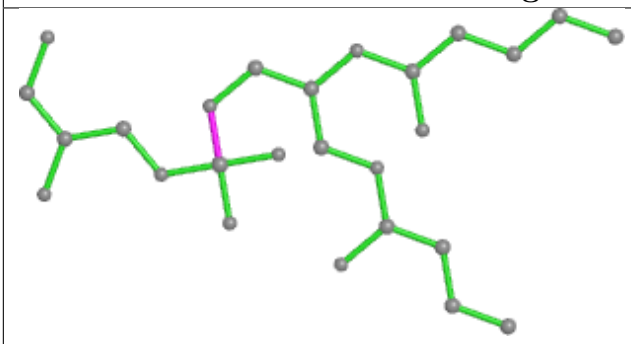


Torsions

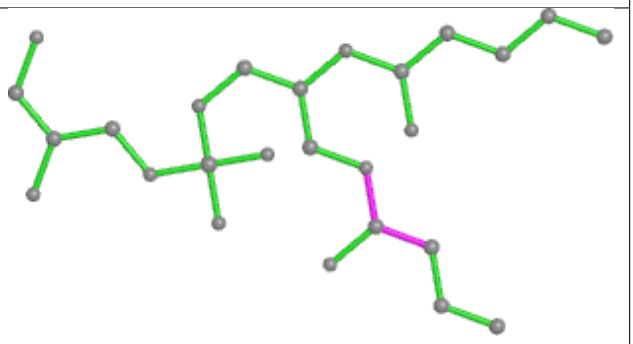


Rings

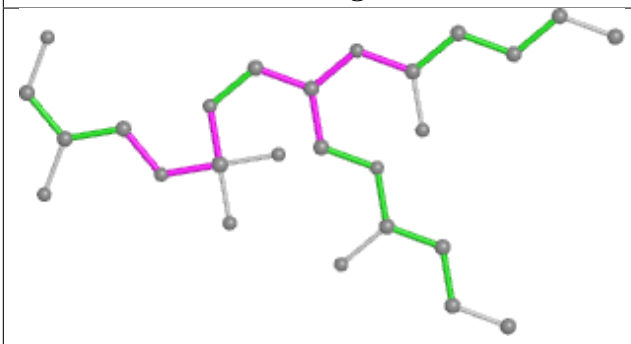
Ligand LHG A 816



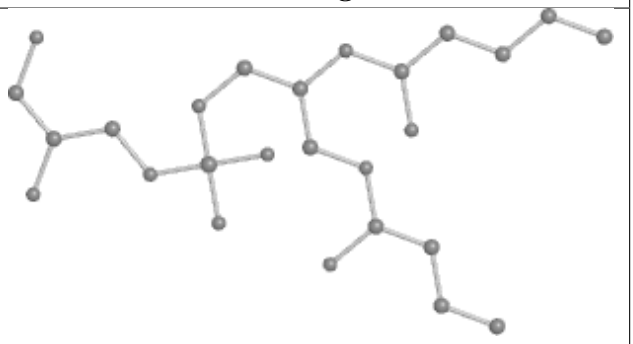
Bond lengths



Bond angles

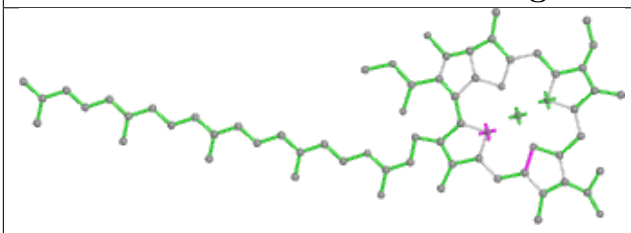


Torsions

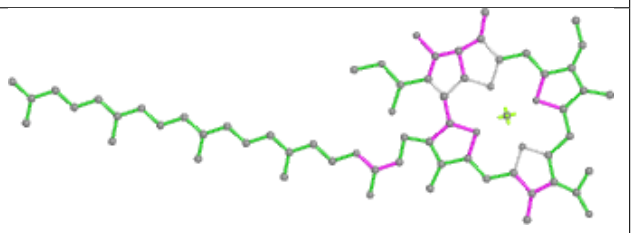


Rings

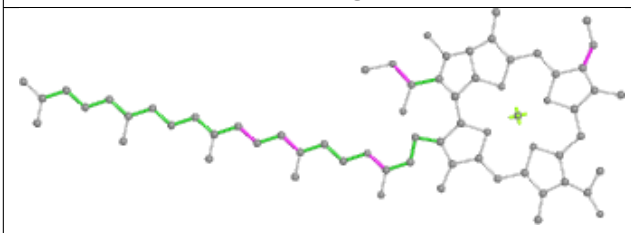
Ligand BCL a 808



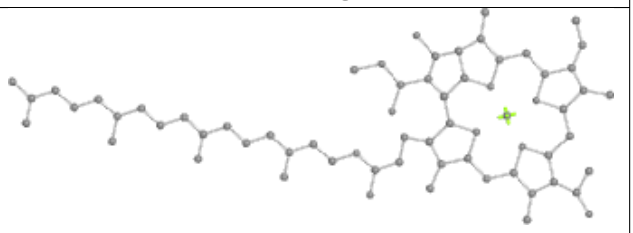
Bond lengths



Bond angles

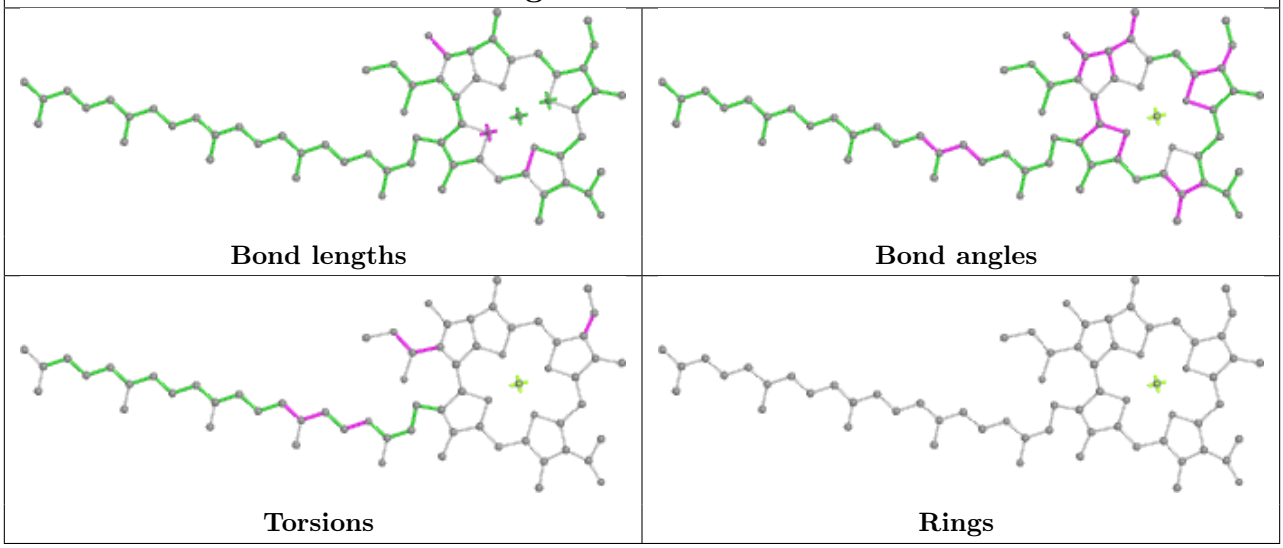


Torsions

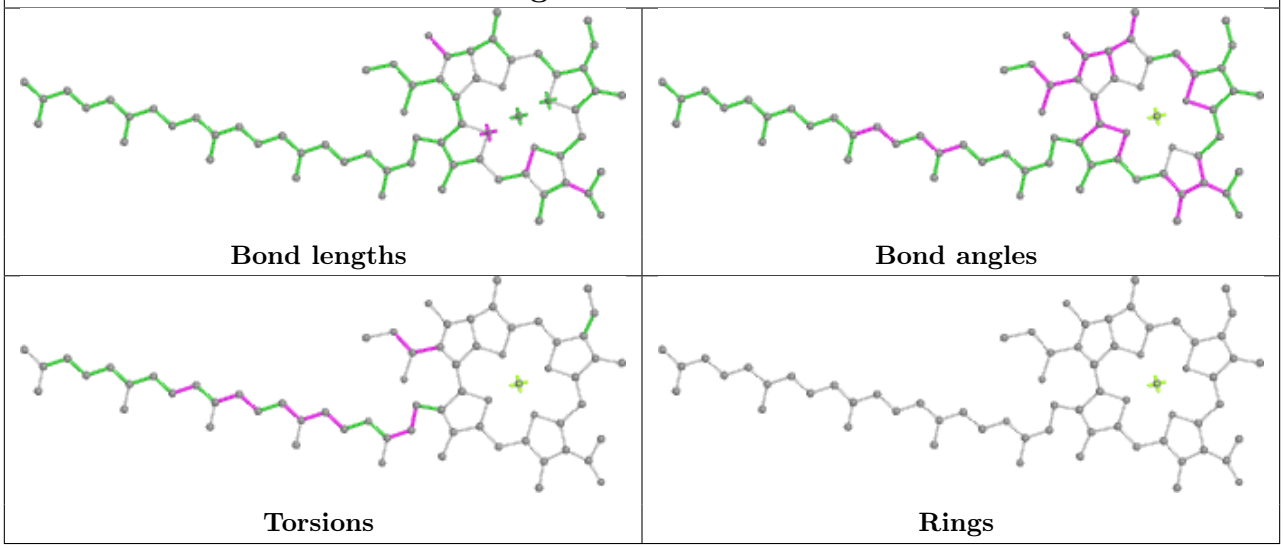


Rings

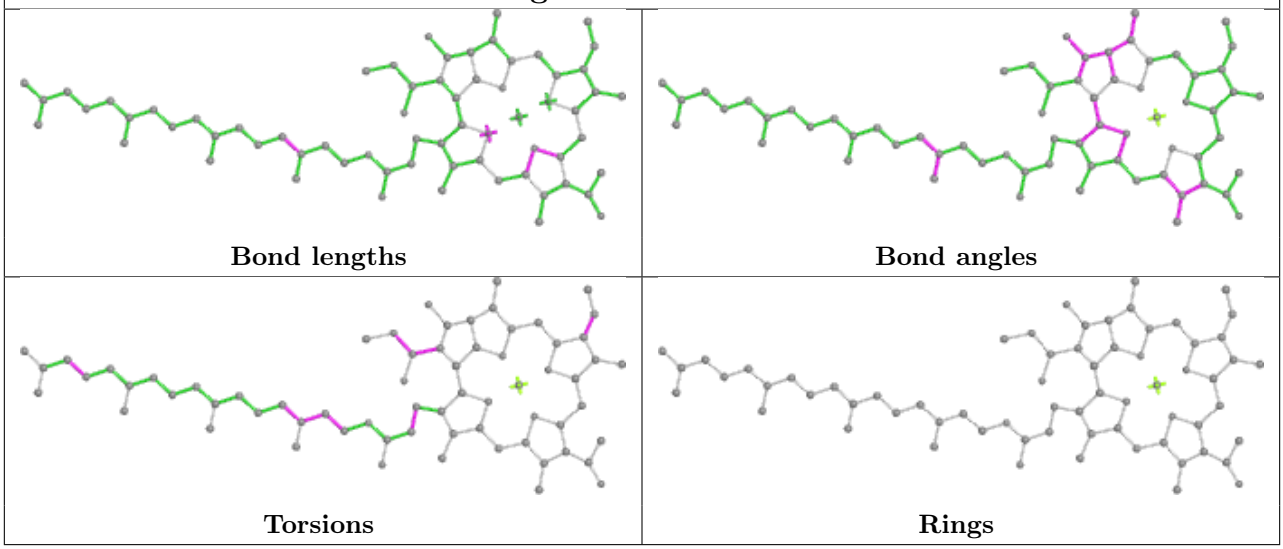
Ligand BCL A 811



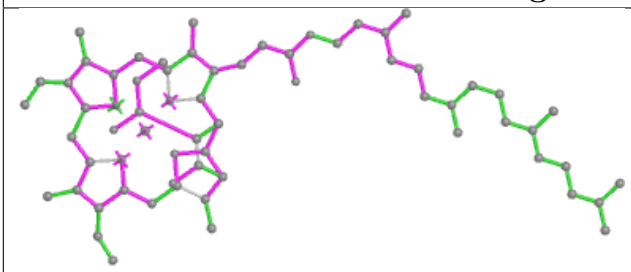
Ligand BCL a 809

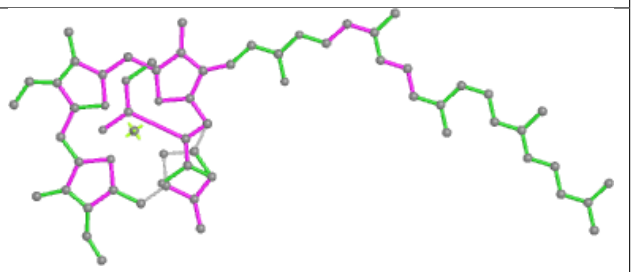


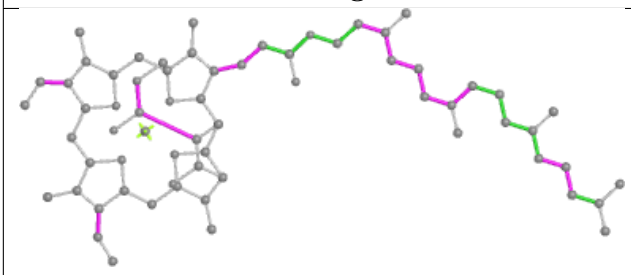
Ligand BCL a 812

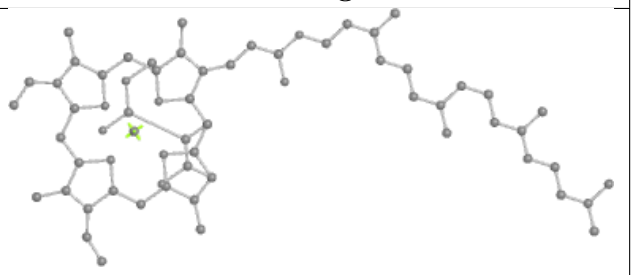


Ligand G2O a 805

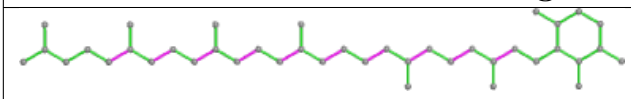

Bond lengths


Bond angles


Torsions


Rings

Ligand F26 a 819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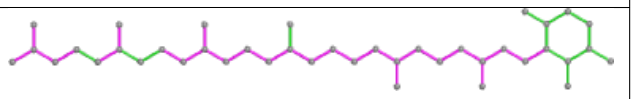
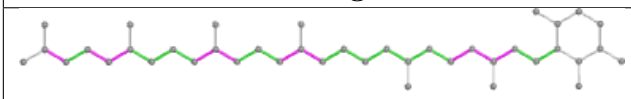

Bond angles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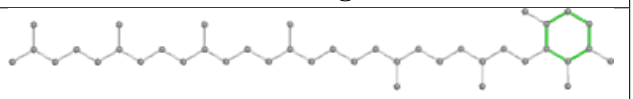
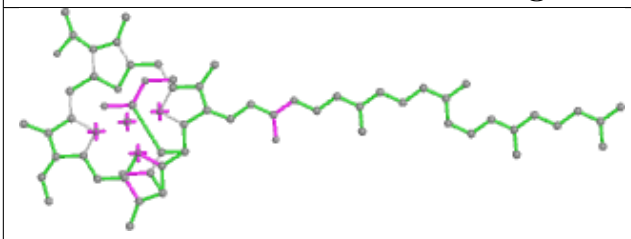

Rings

Ligand GS0 A 801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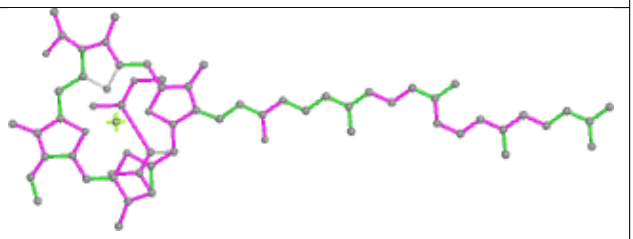
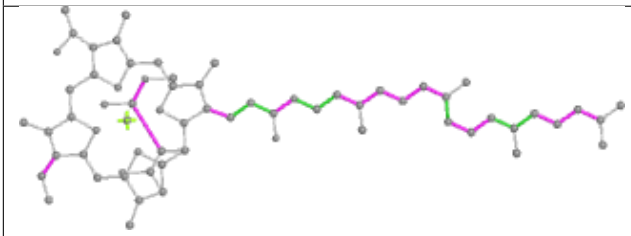

Bond angles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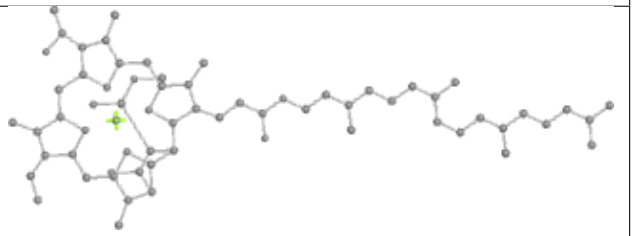
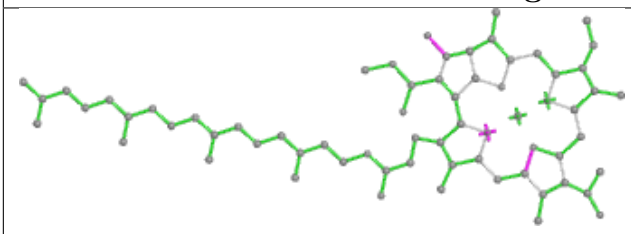
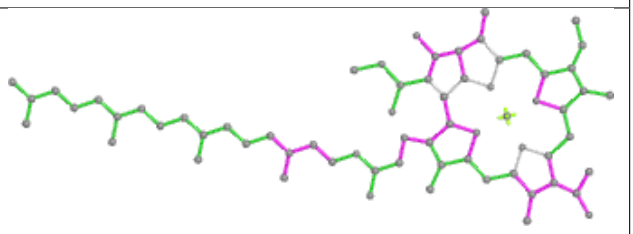

Rings

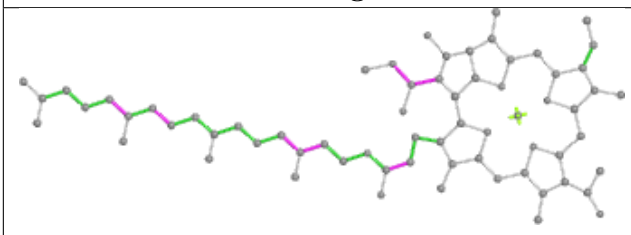
Ligand BCL V 401



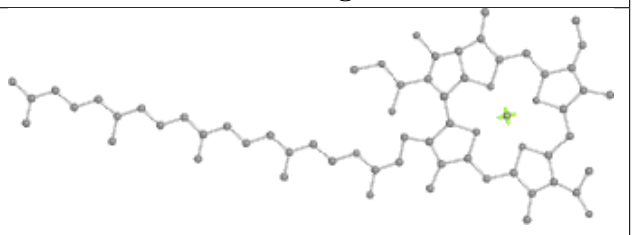
Bond lengths



Bond angles

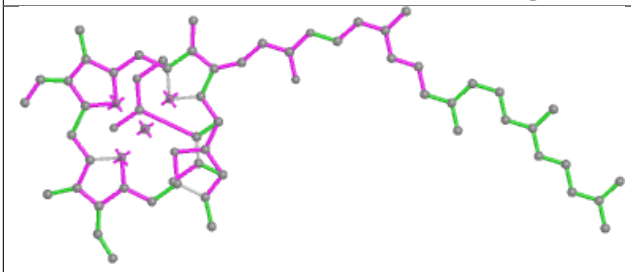


Torsions

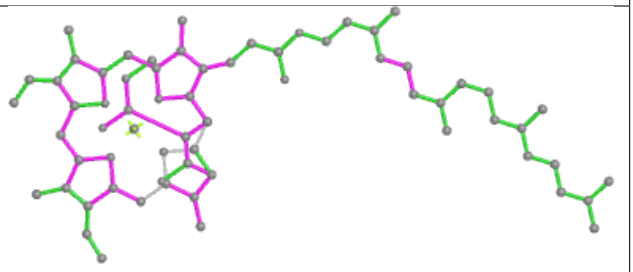


Rings

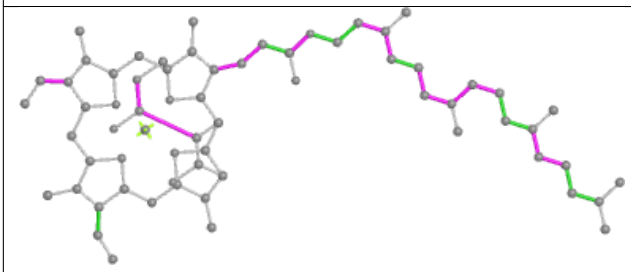
Ligand G2O A 824



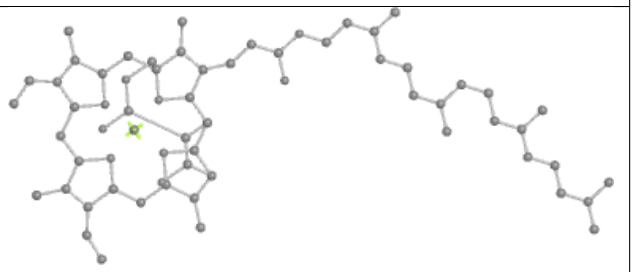
Bond lengths



Bond angles

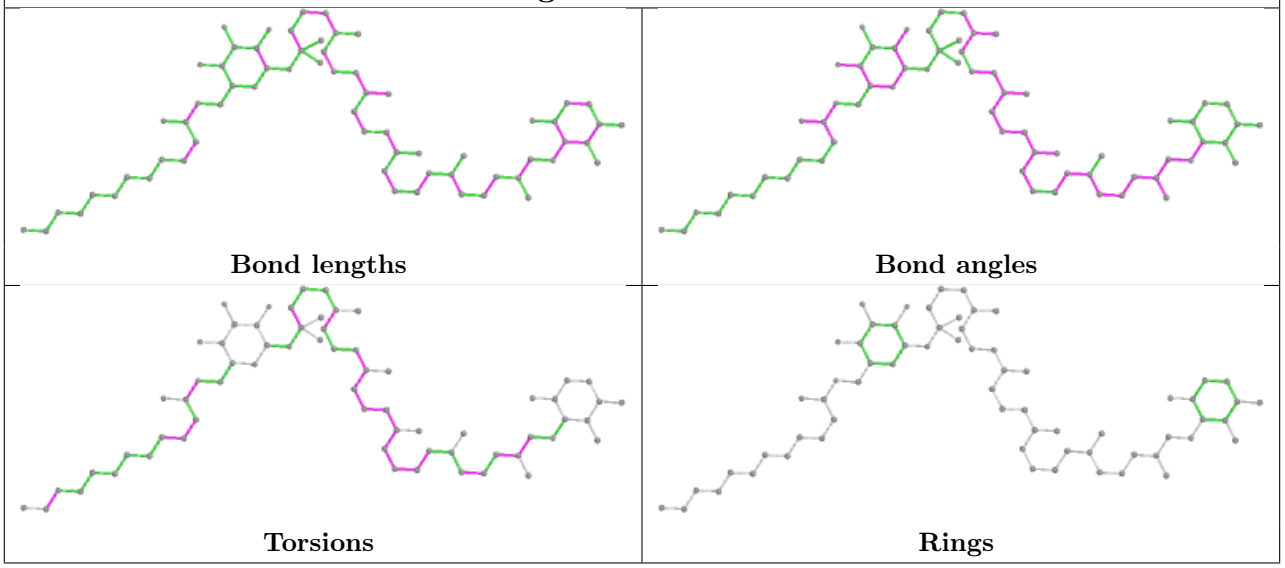


Torsions

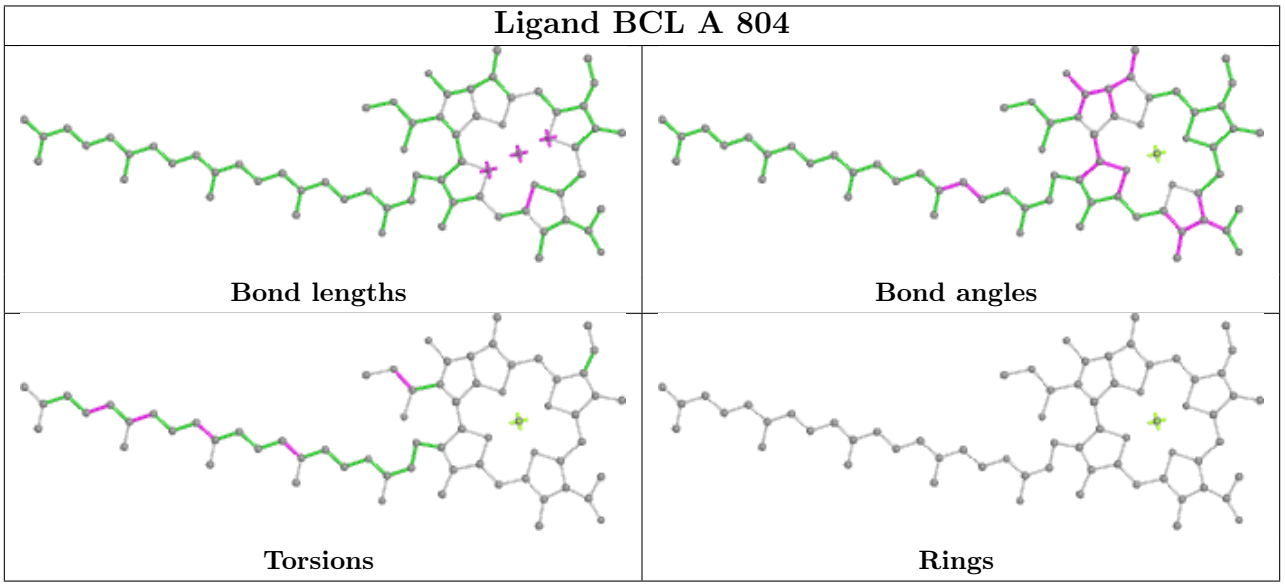


Rings

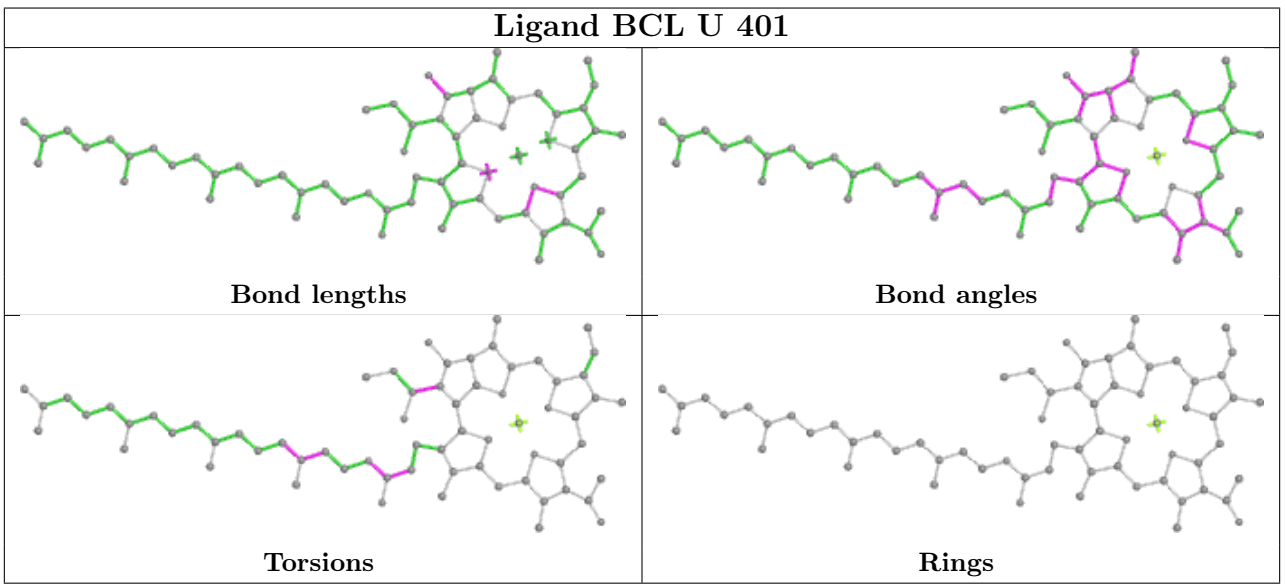
Ligand F39 a 818

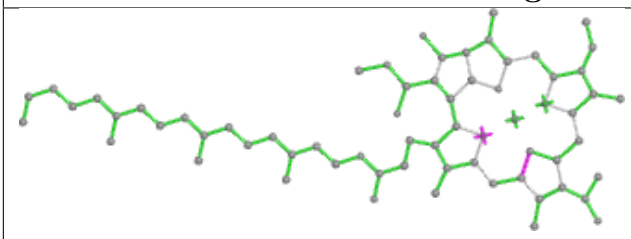
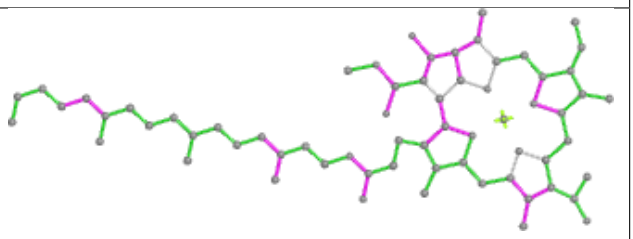
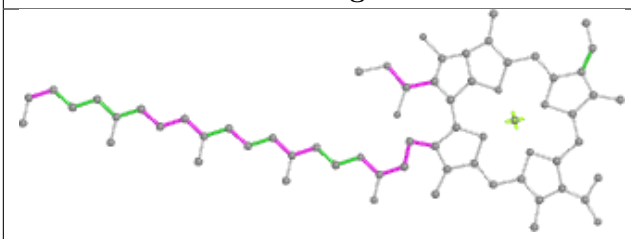
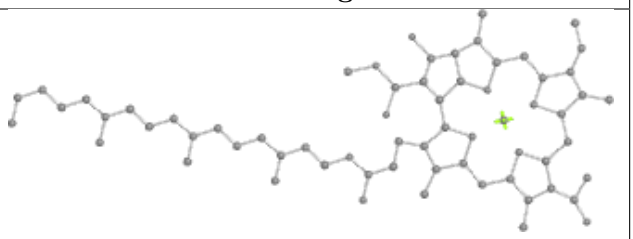


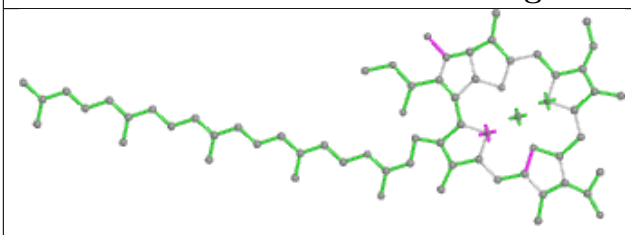
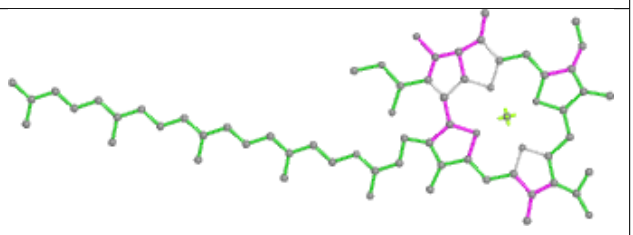
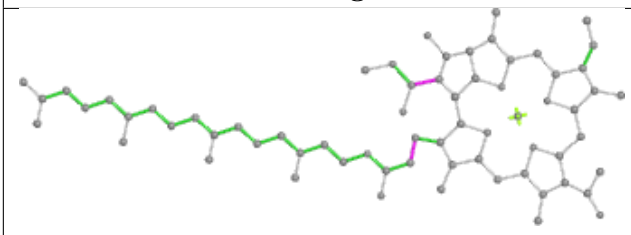
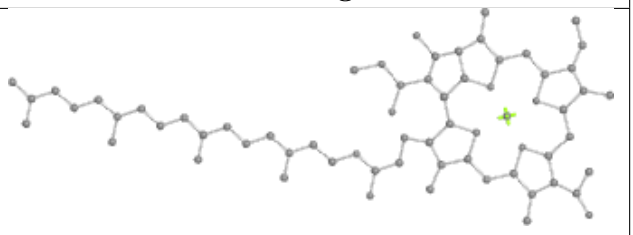
Ligand BCL A 804



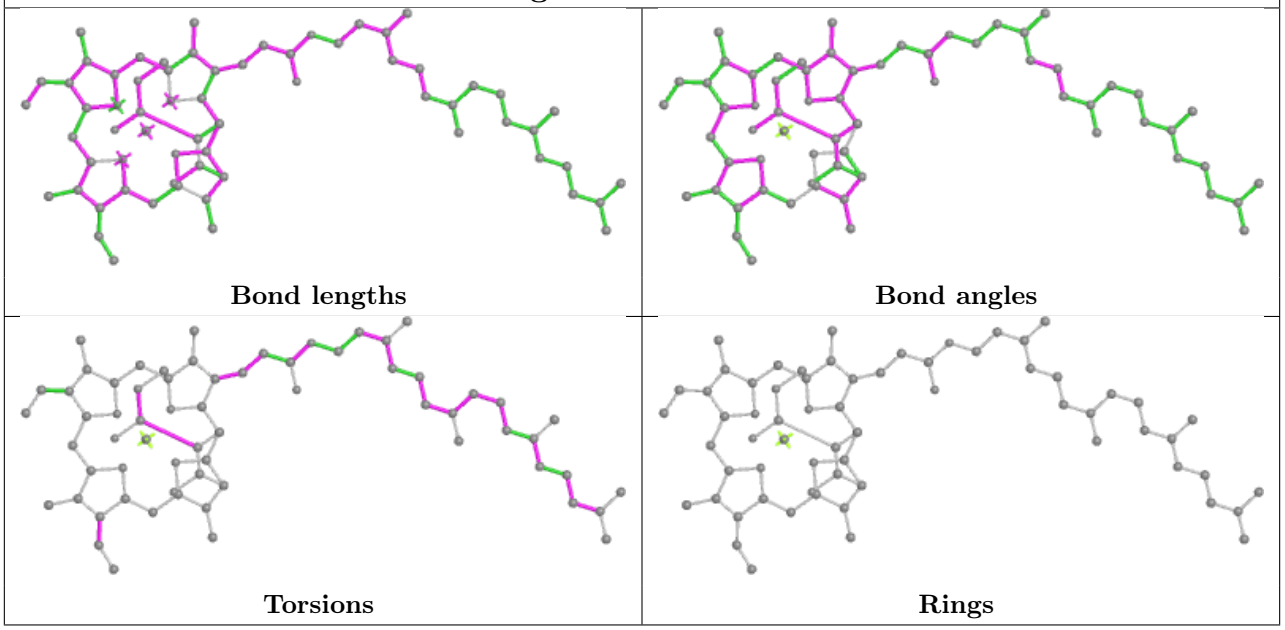
Ligand BCL U 401



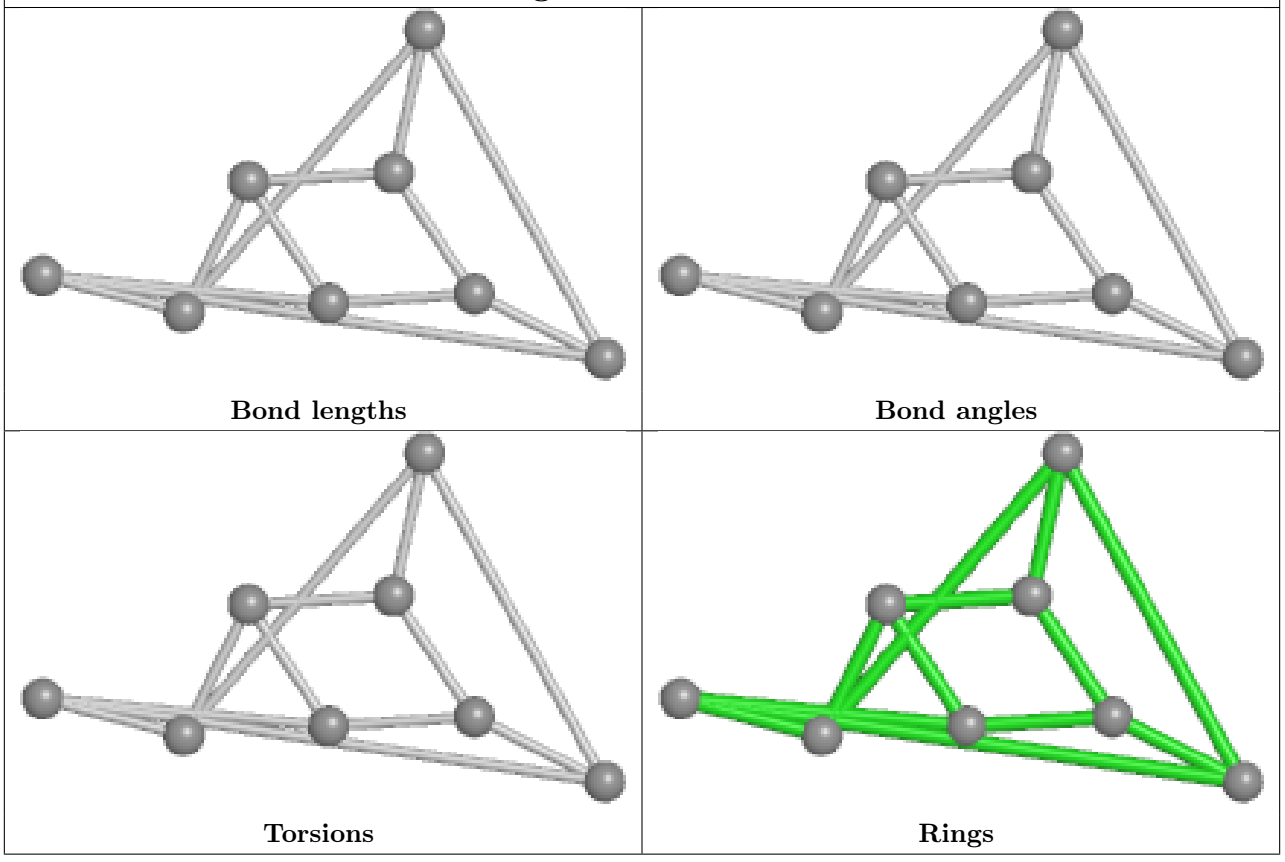
Ligand BCL A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

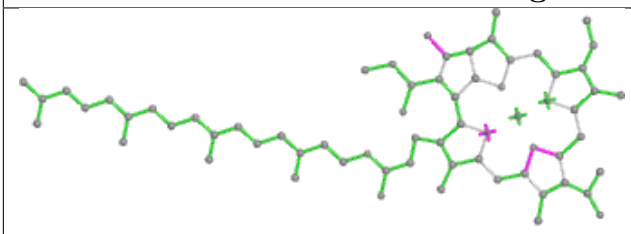
Ligand G2O a 801



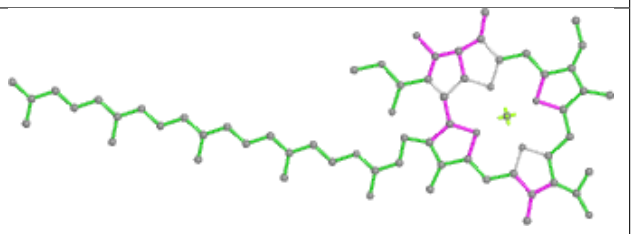
Ligand SF4 B 301



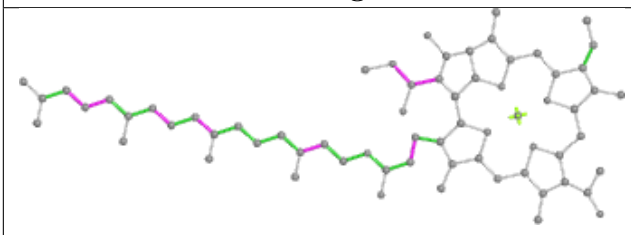
Ligand BCL a 816



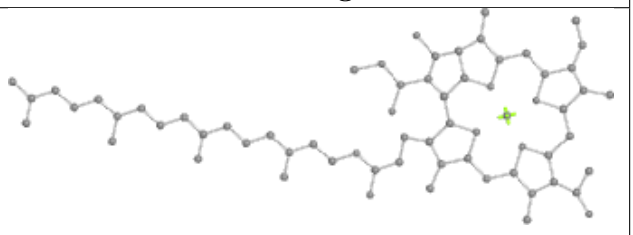
Bond lengths



Bond angles

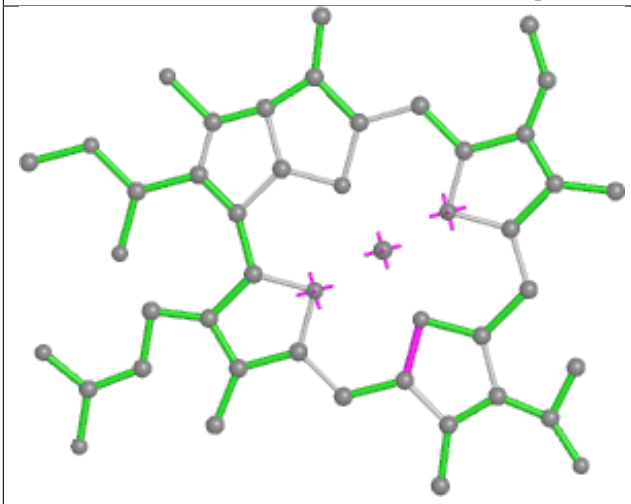


Torsions

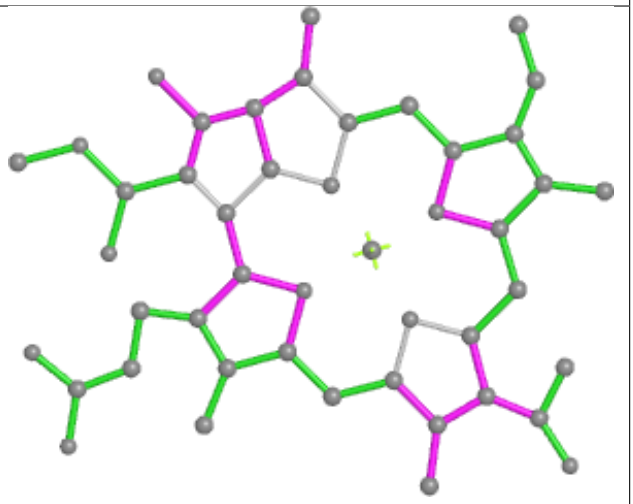


Rings

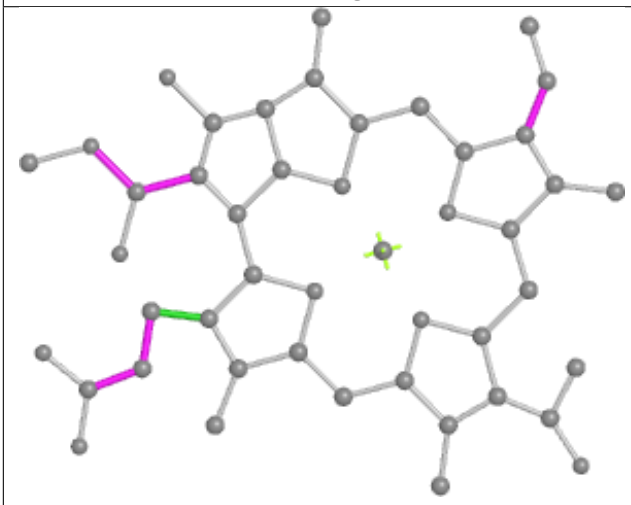
Ligand BCL a 811



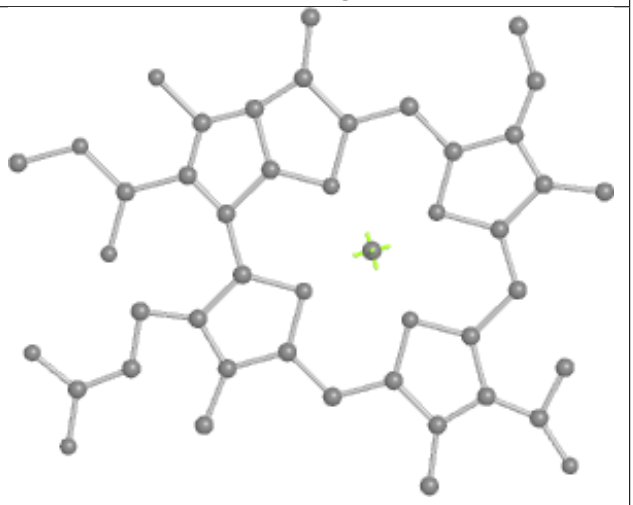
Bond lengths



Bond angles

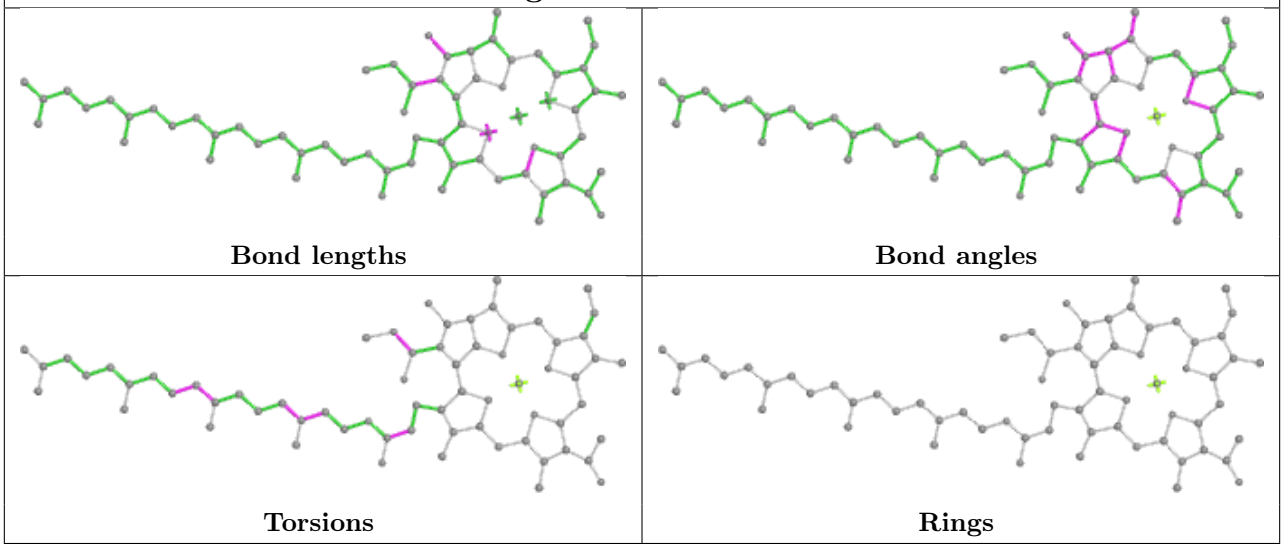


Torsions

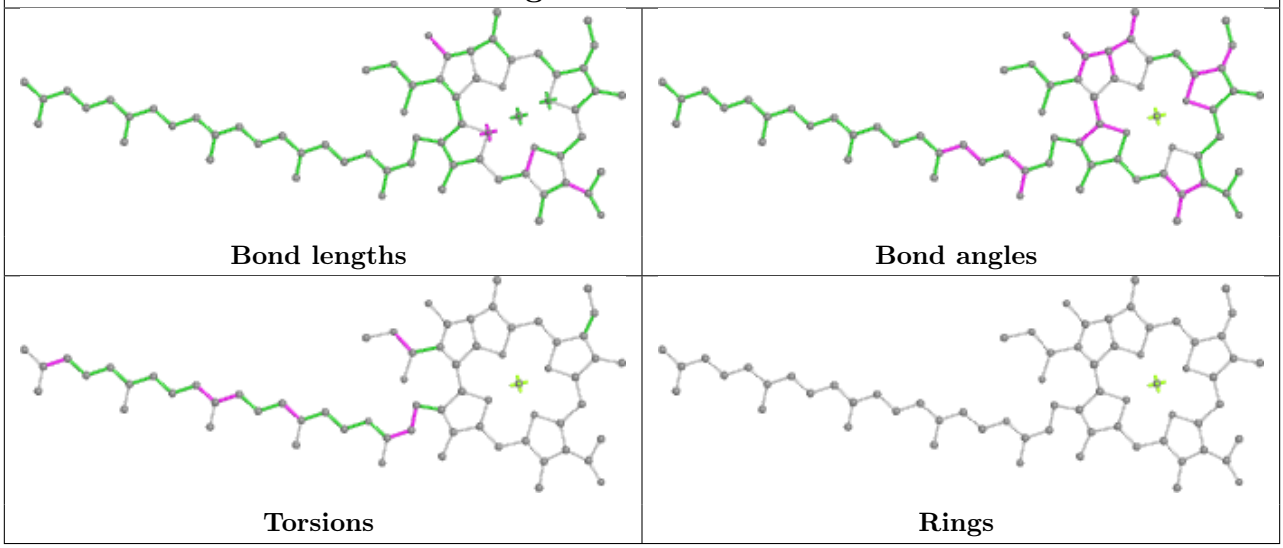


Rings

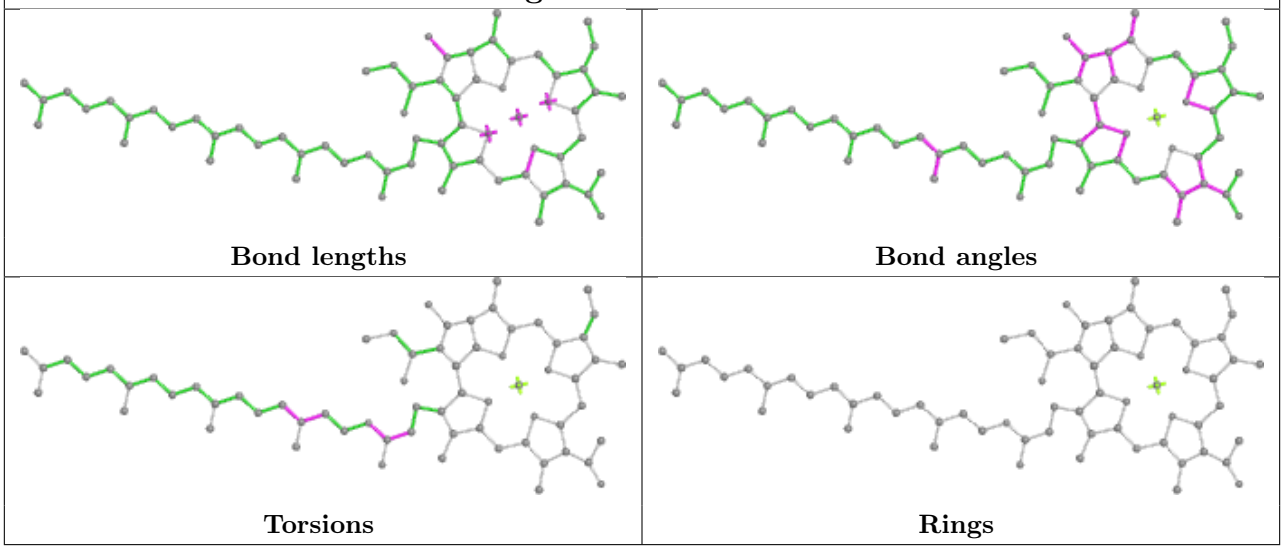
Ligand BCL V 405



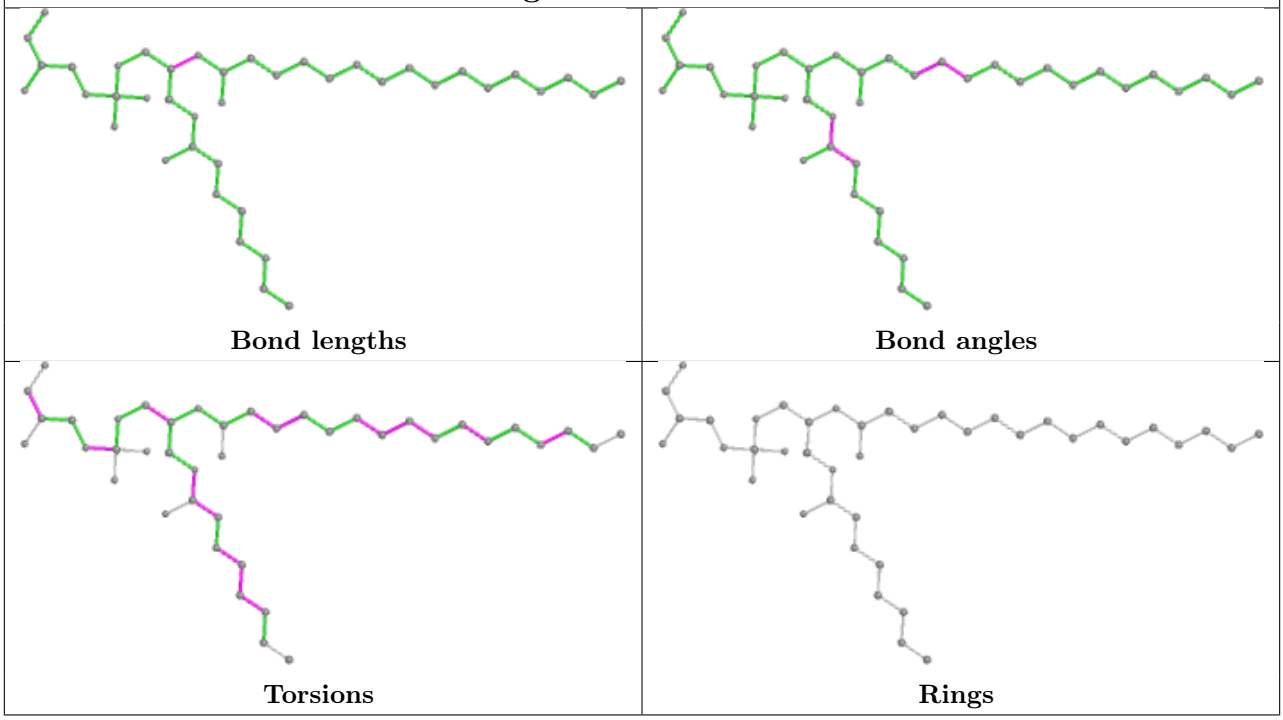
Ligand BCL A 810



Ligand BCL U 407



Ligand LHG A 817



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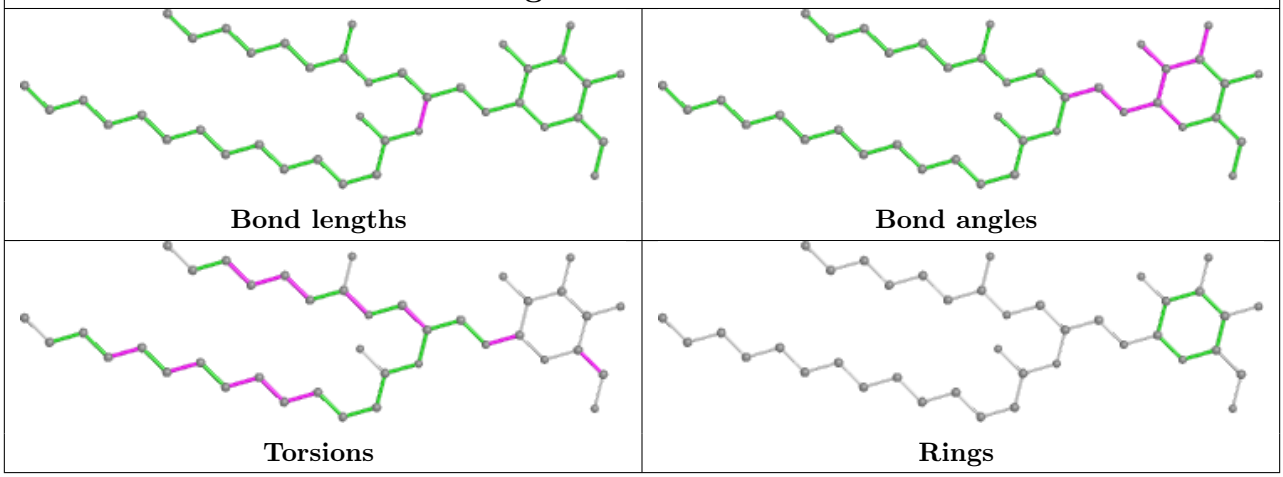
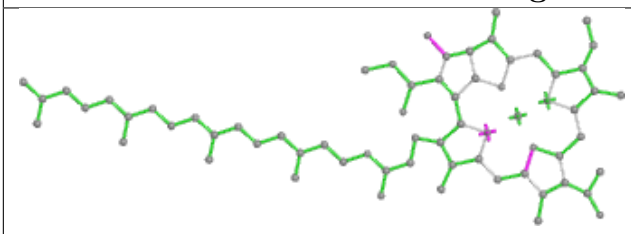
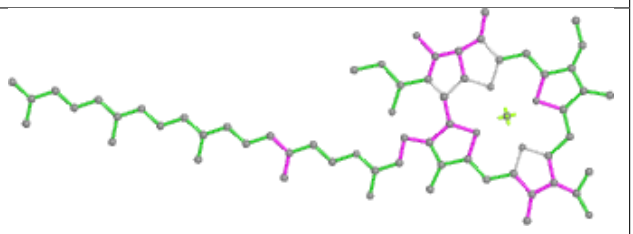


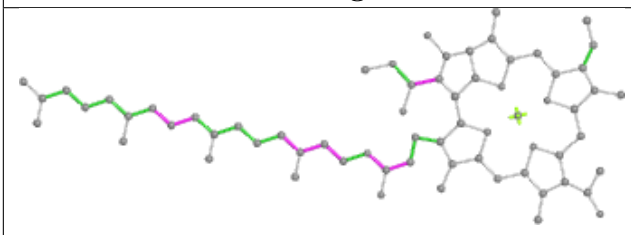
Ligand BCL a 810



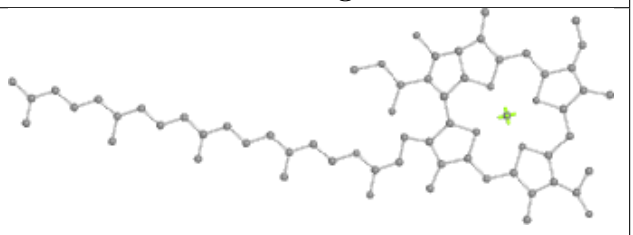
Bond lengths



Bond angles

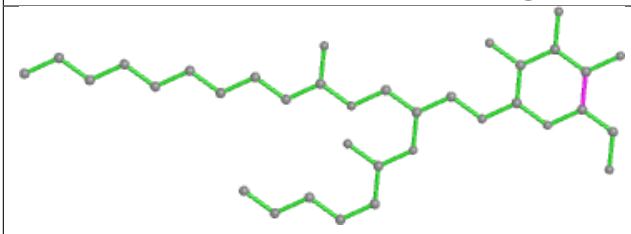


Torsions



Rings

Ligand LMG C 302



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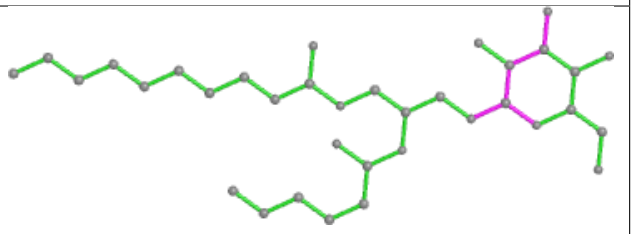
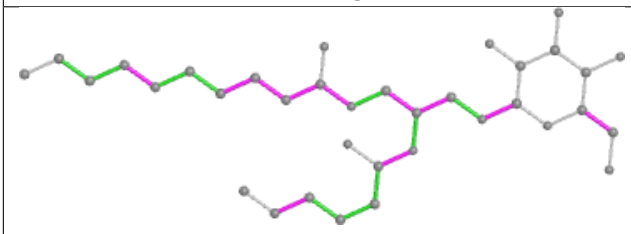
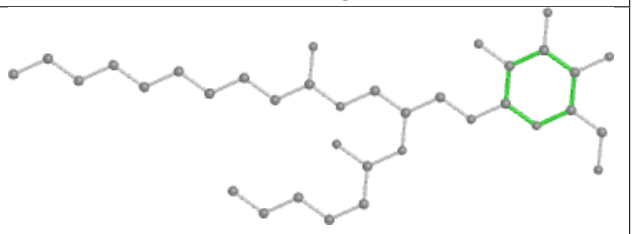


Bond angles

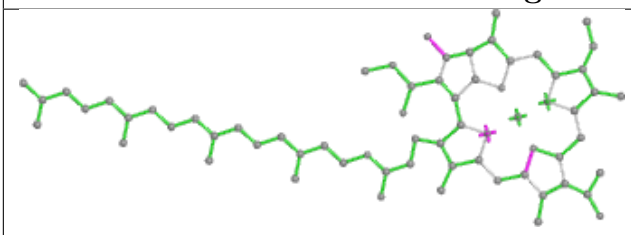


Torsions

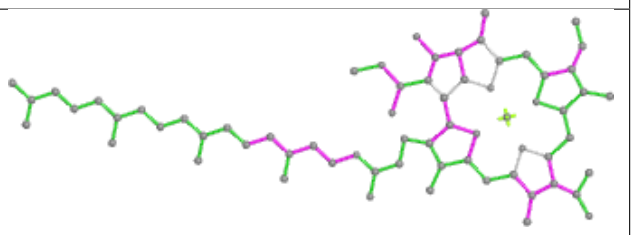


Rings

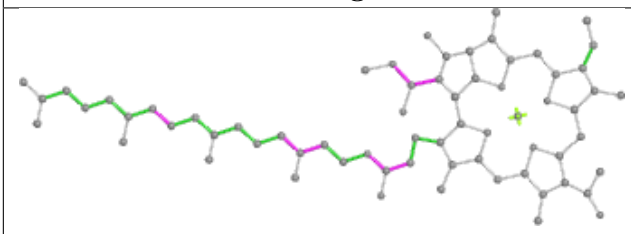
Ligand BCL U 404



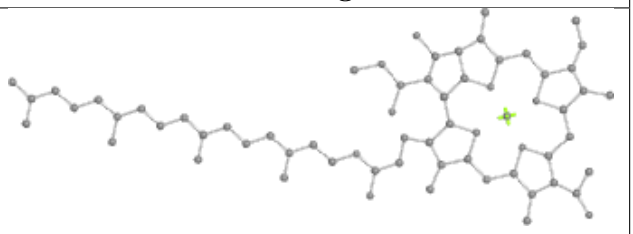
Bond lengths



Bond angles

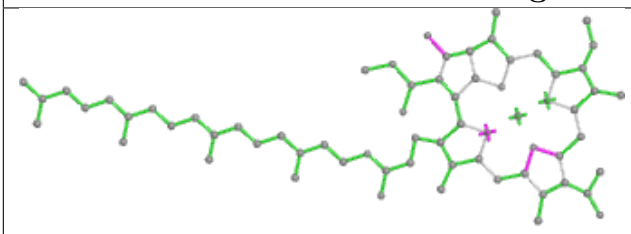


Torsions

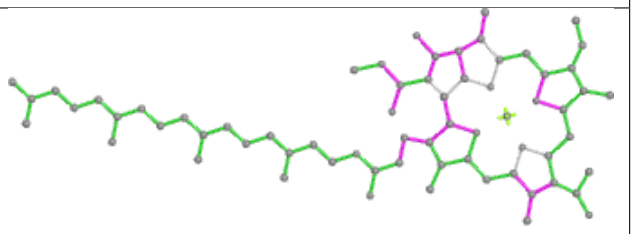


Rings

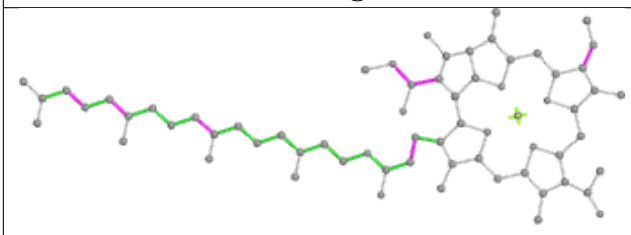
Ligand BCL a 814



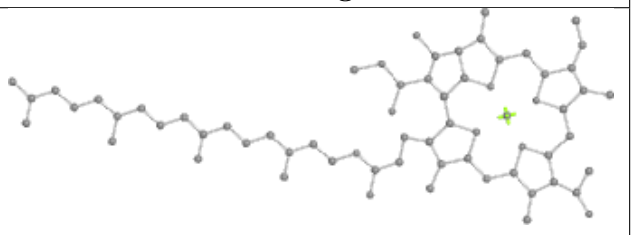
Bond lengths



Bond angles

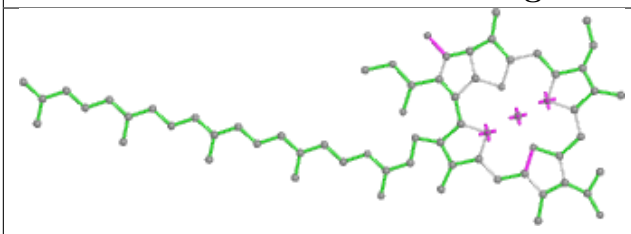


Torsions

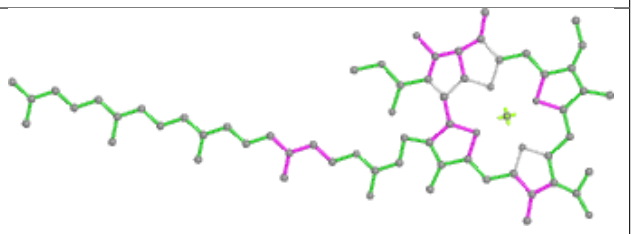


Rings

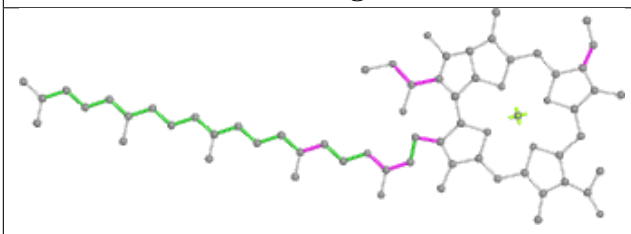
Ligand BCL A 808



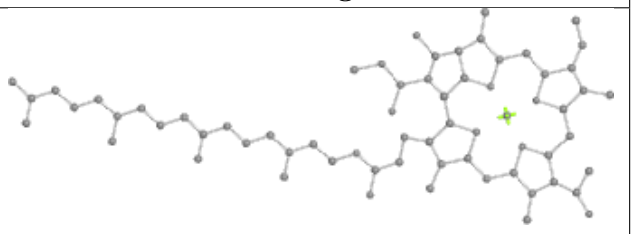
Bond lengths



Bond angles

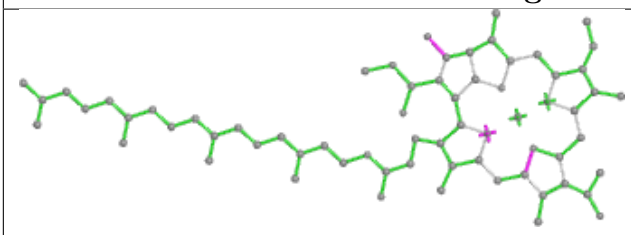


Torsions

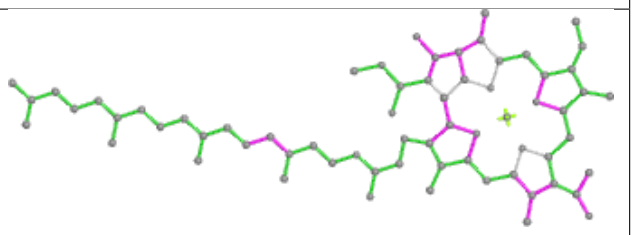


Rings

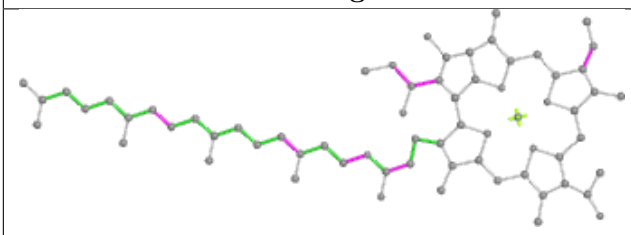
Ligand BCL V 404



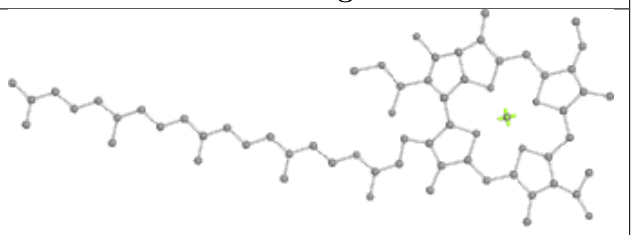
Bond lengths



Bond angles

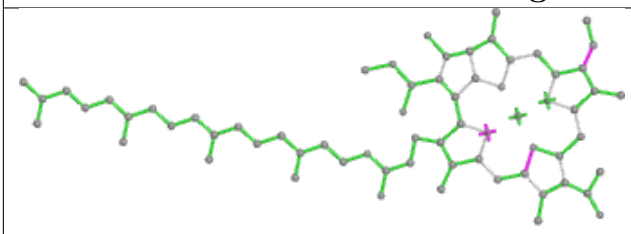


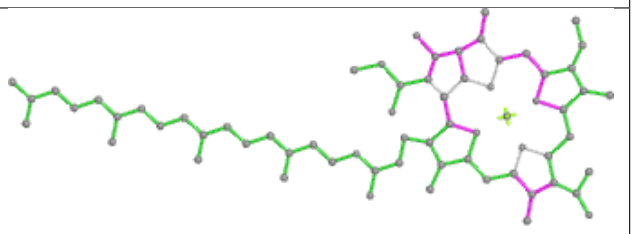
Torsions

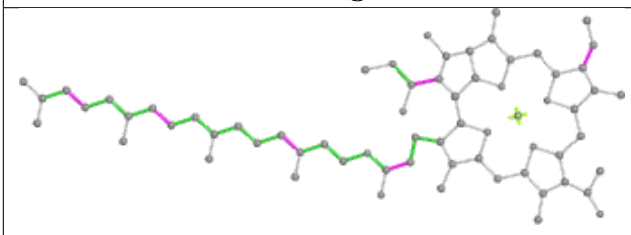


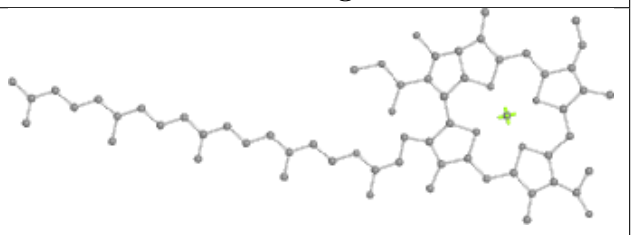
Rings

Ligand BCL a 807

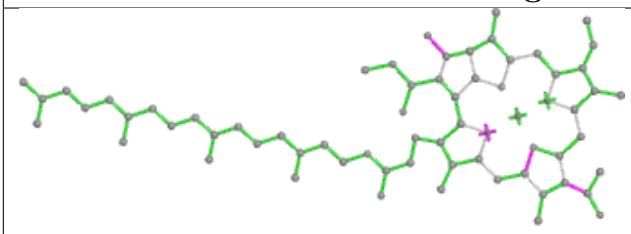

Bond lengths

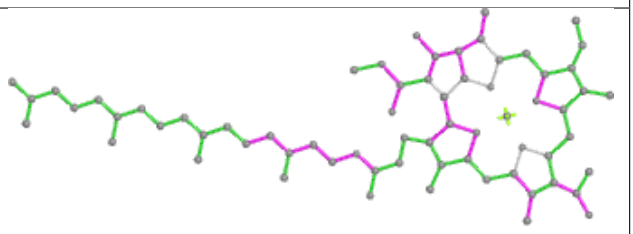

Bond angles

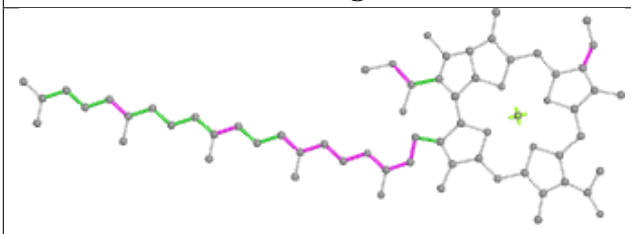

Torsions

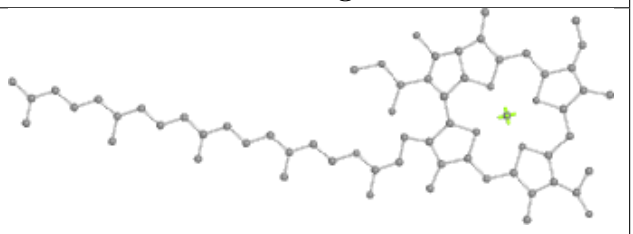

Rings

Ligand BCL A 805

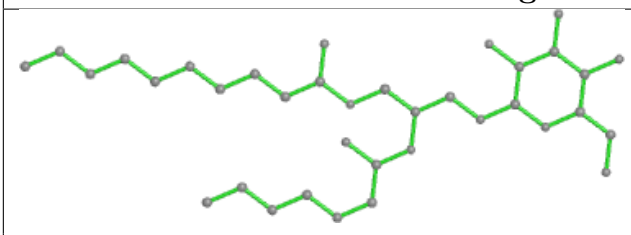

Bond lengths

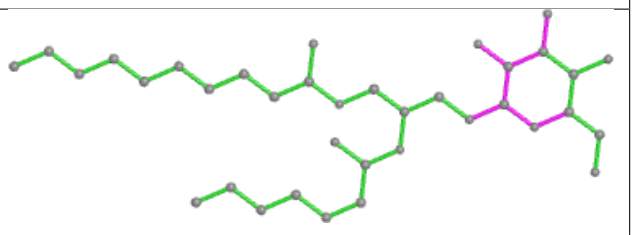

Bond angles

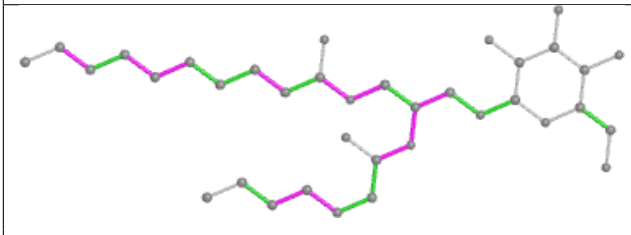

Torsions

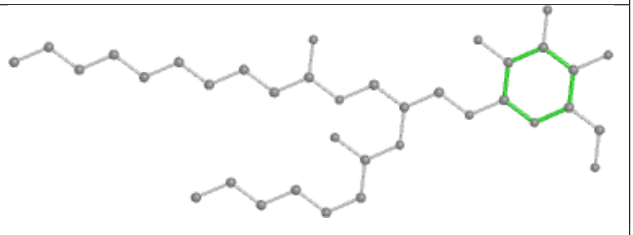

Rings

Ligand LMG A 820

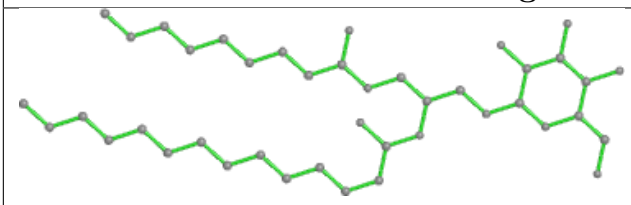

Bond lengths

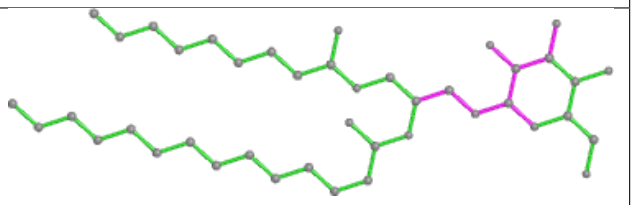

Bond angles

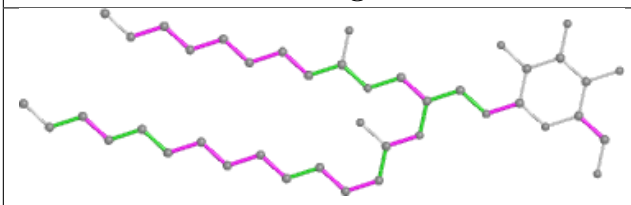

Torsions

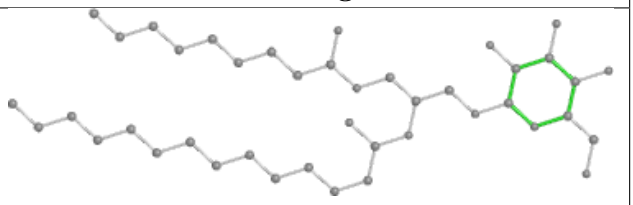

Rings

Ligand LMG A 818

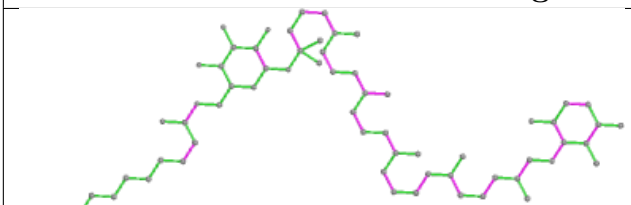

Bond lengths


Bond angles


Torsions


Rings

Ligand F39 A 814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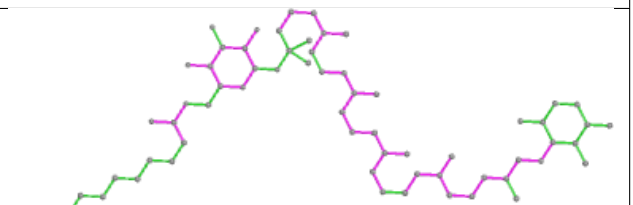
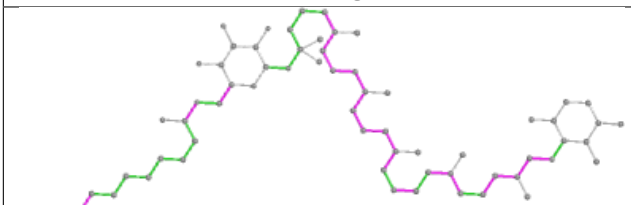
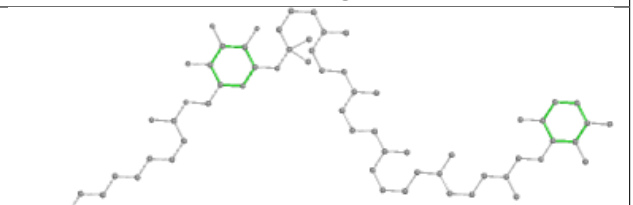
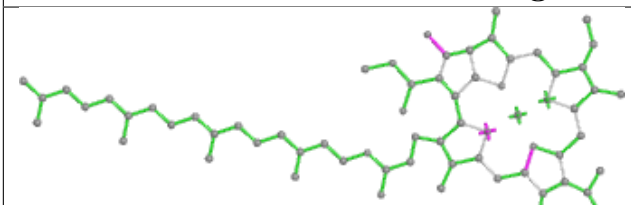

Bond angles


Torsions


Rings

Ligand BCL a 817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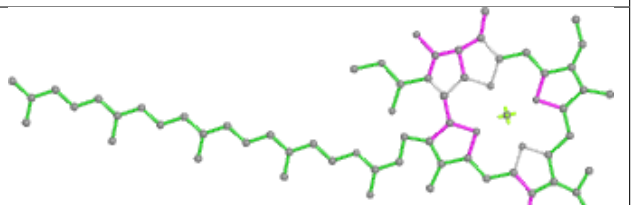
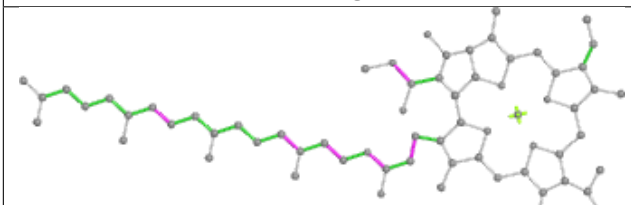
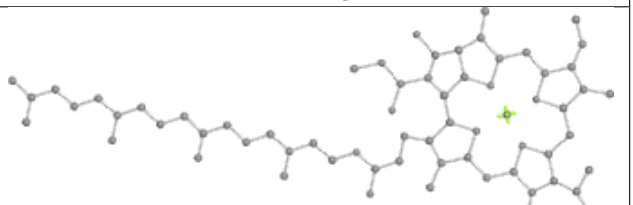
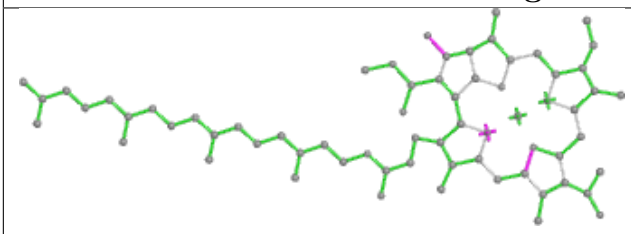

Bond angles

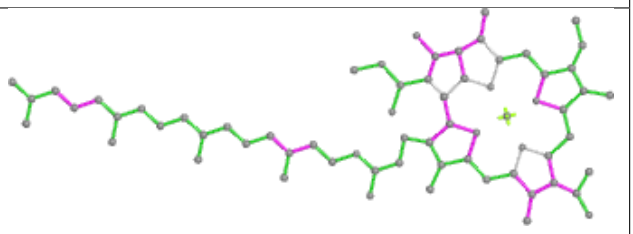

Torsions


Rings

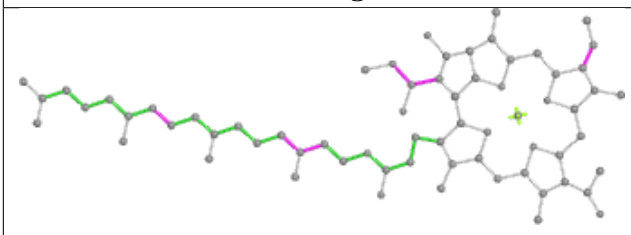
Ligand BCL V 406



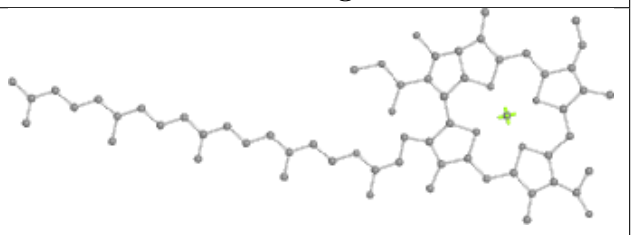
Bond lengths



Bond angles

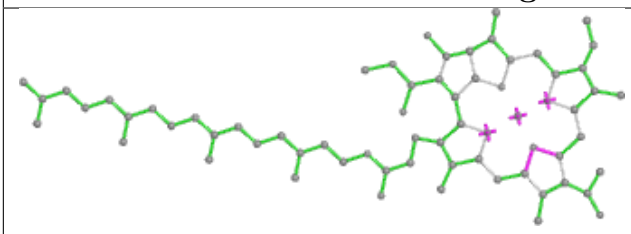


Torsions

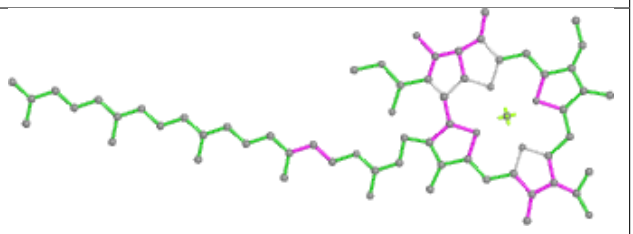


Rings

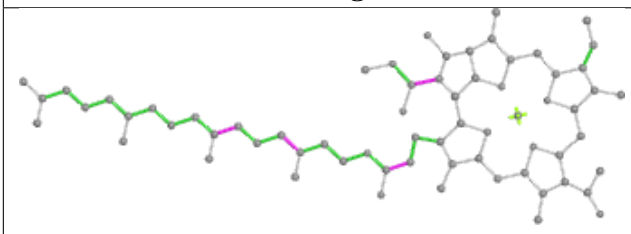
Ligand BCL W 401



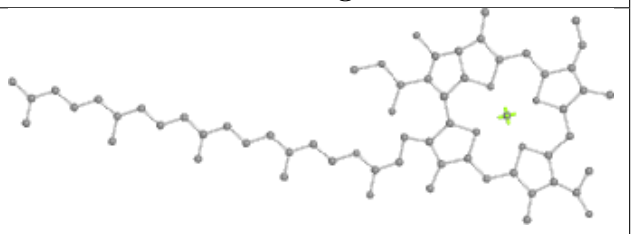
Bond lengths



Bond angles

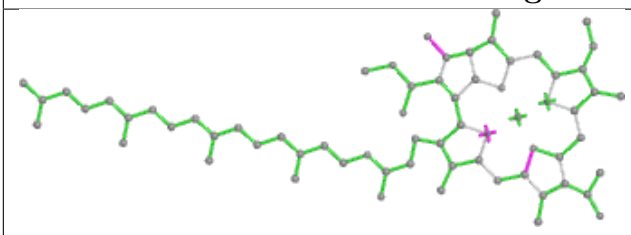


Torsions

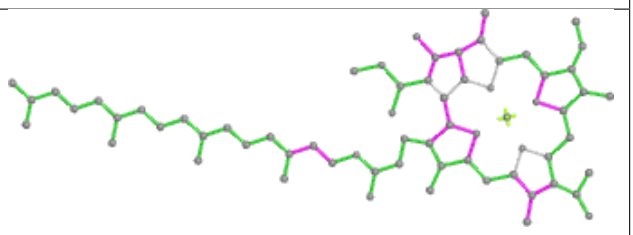


Rings

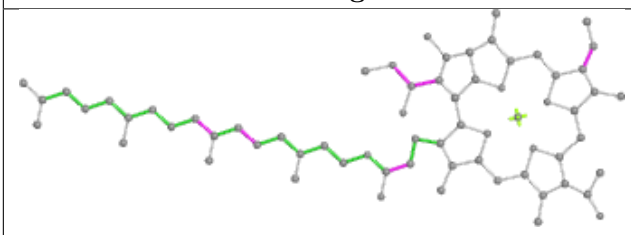
Ligand BCL U 403



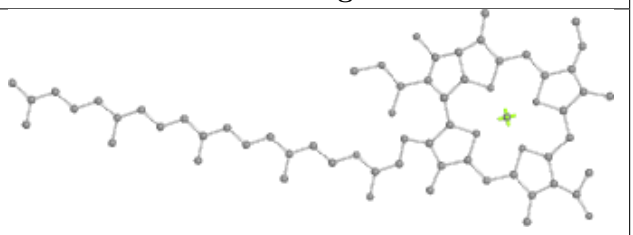
Bond lengths



Bond angles

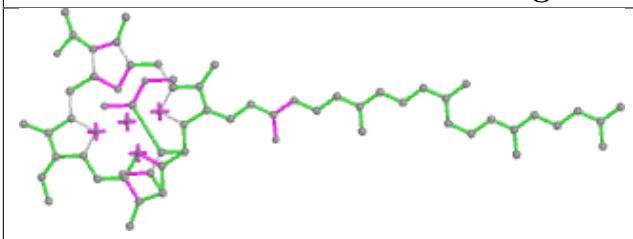


Torsions

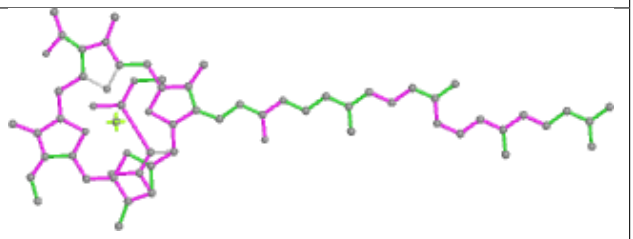


Rings

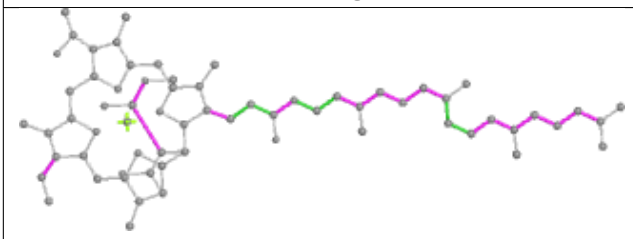
Ligand GS0 a 804



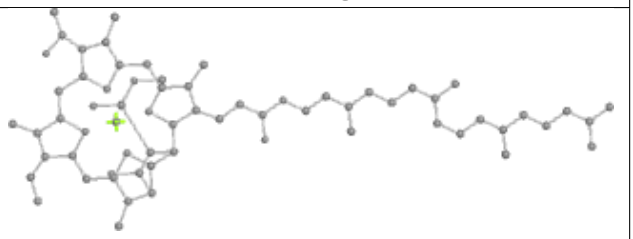
Bond lengths



Bond angles

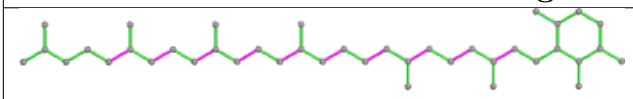


Torsions

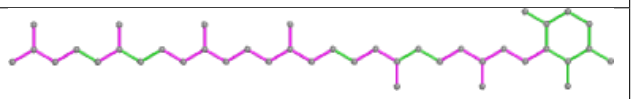


Rings

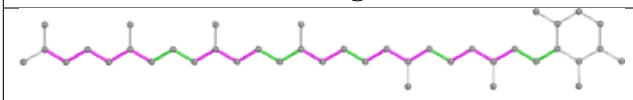
Ligand F26 a 820



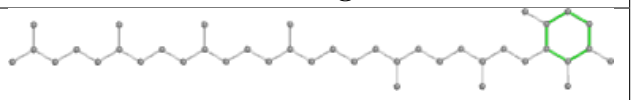
Bond lengths



Bond angles

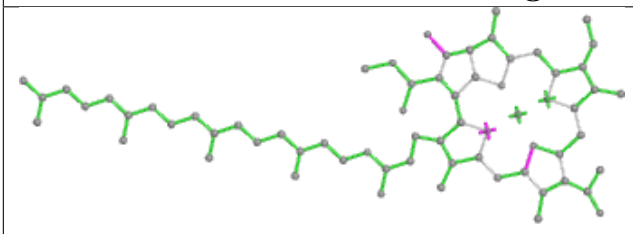


Torsions

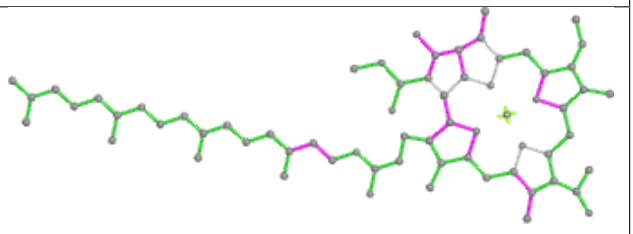


Rings

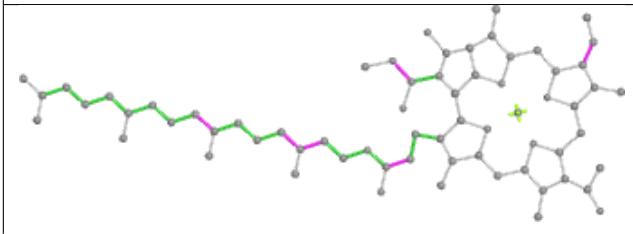
Ligand BCL V 403



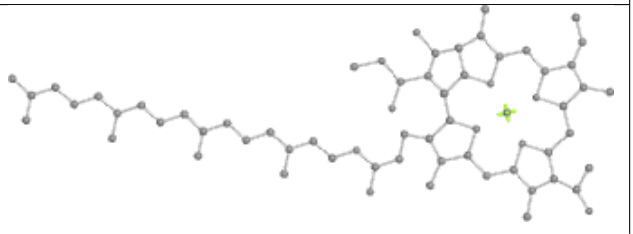
Bond lengths



Bond angles

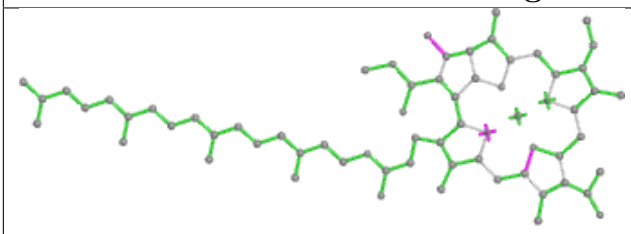


Torsions

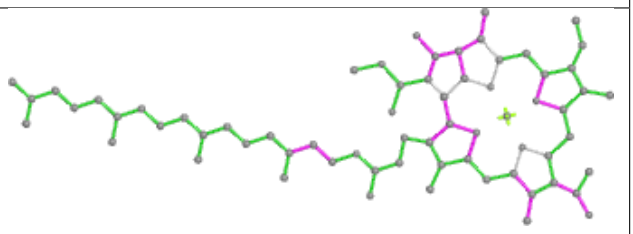


Rings

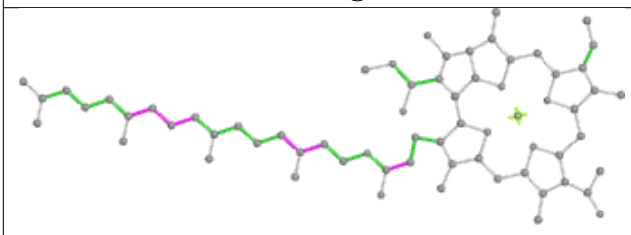
Ligand BCL U 405



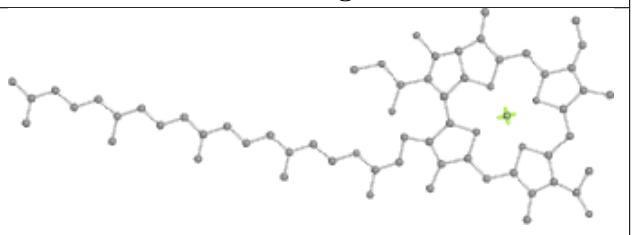
Bond lengths



Bond angles

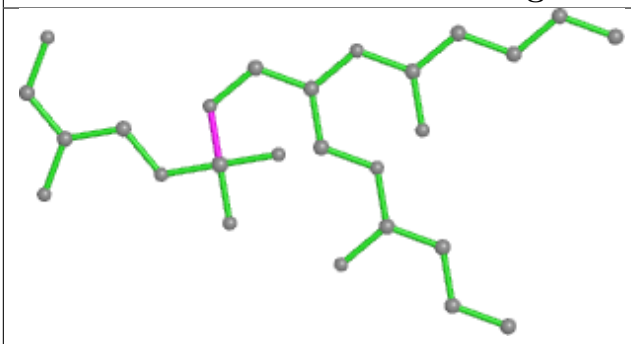


Torsions

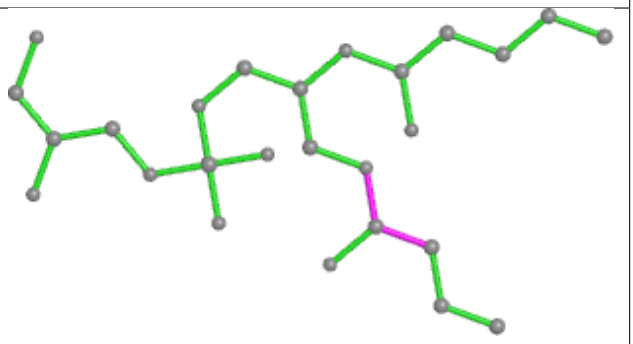


Rings

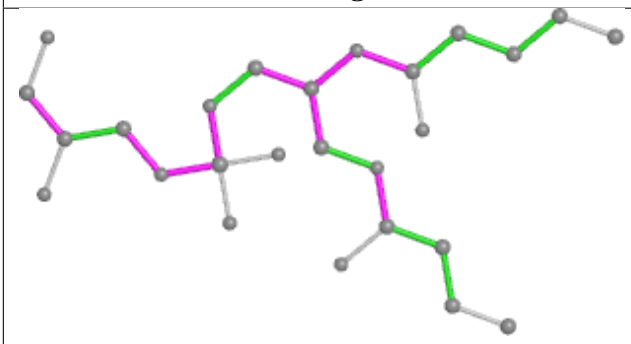
Ligand LHG a 822



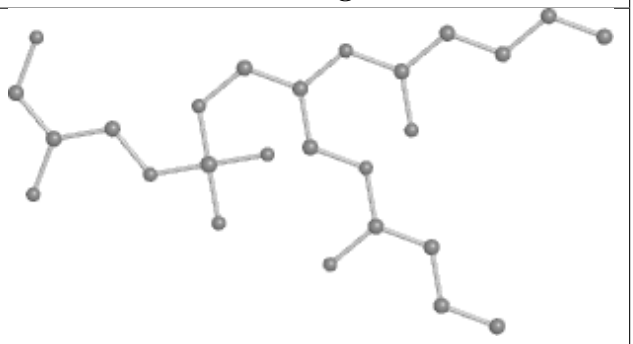
Bond lengths



Bond angles

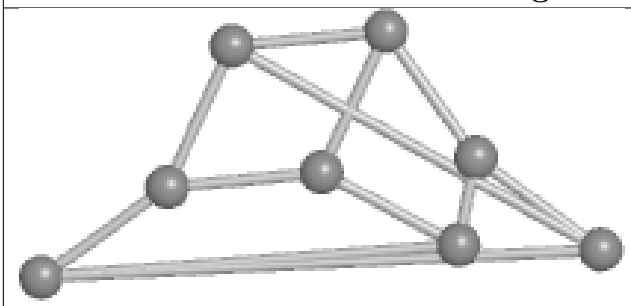


Torsions

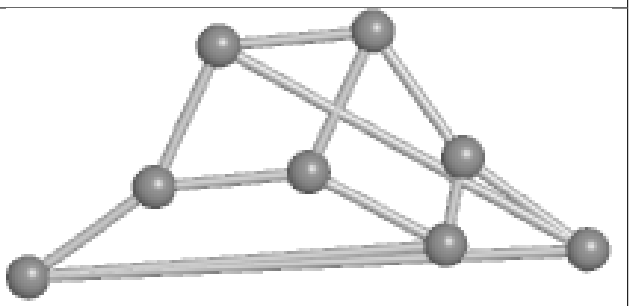


Rings

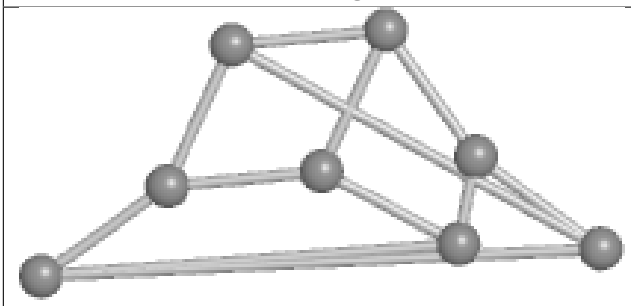
Ligand SF4 B 302



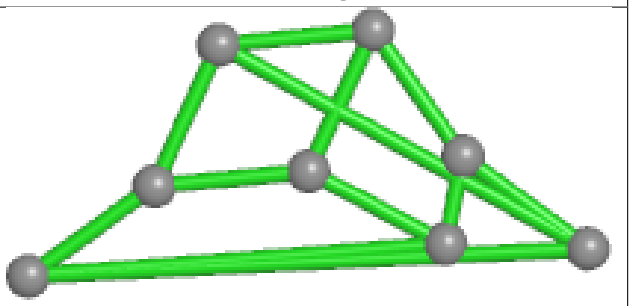
Bond lengths



Bond angles

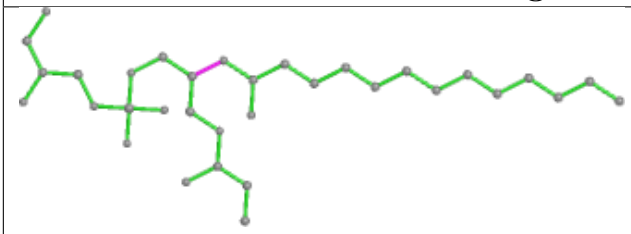


Torsions

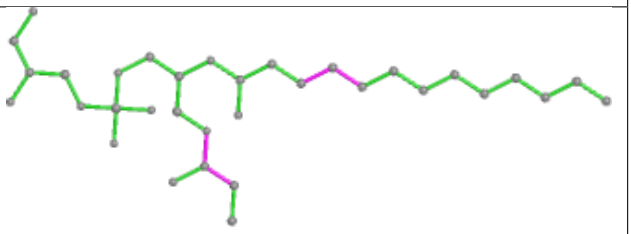


Rings

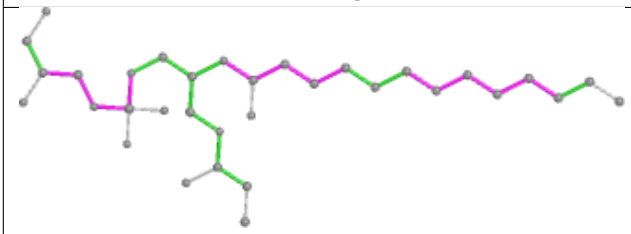
Ligand LHG a 821



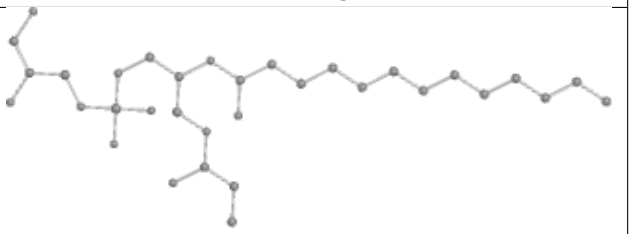
Bond lengths



Bond angles

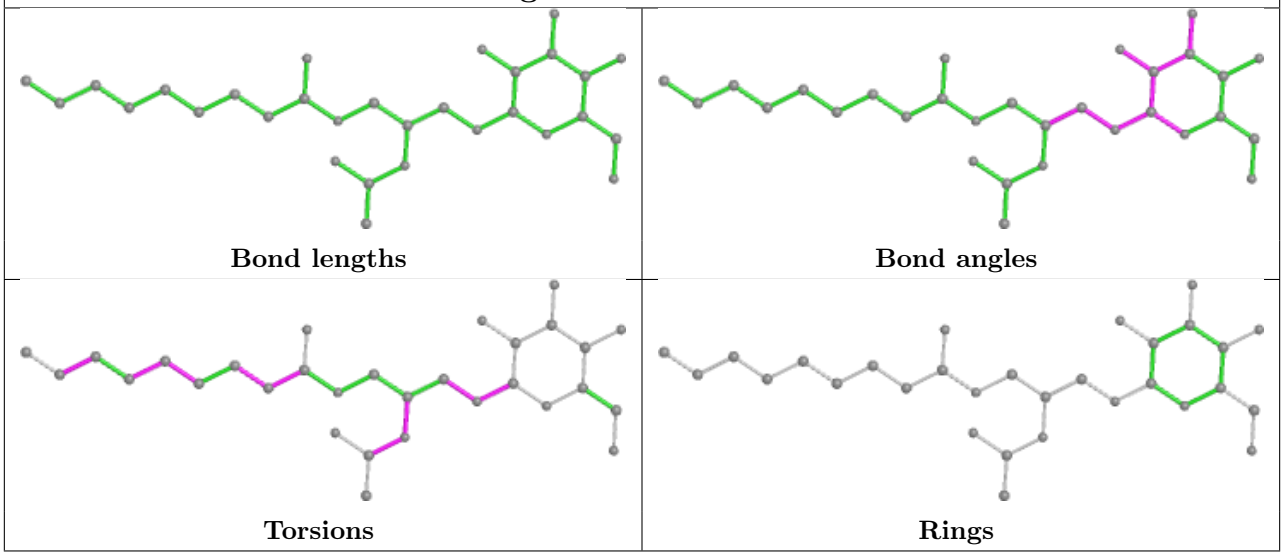


Torsions

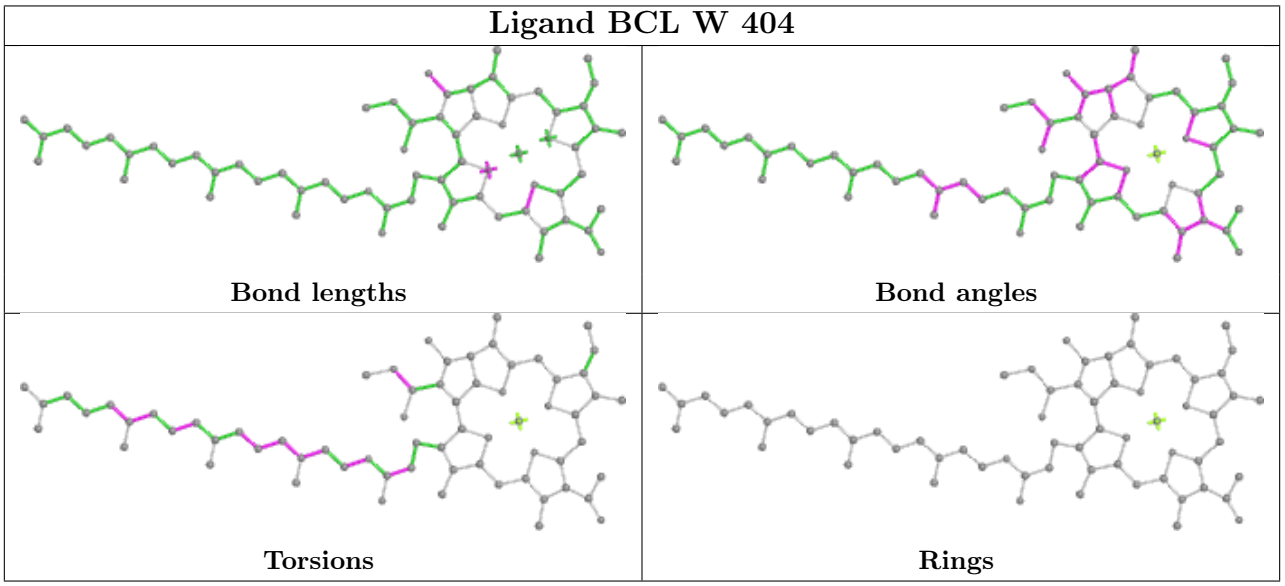


Rings

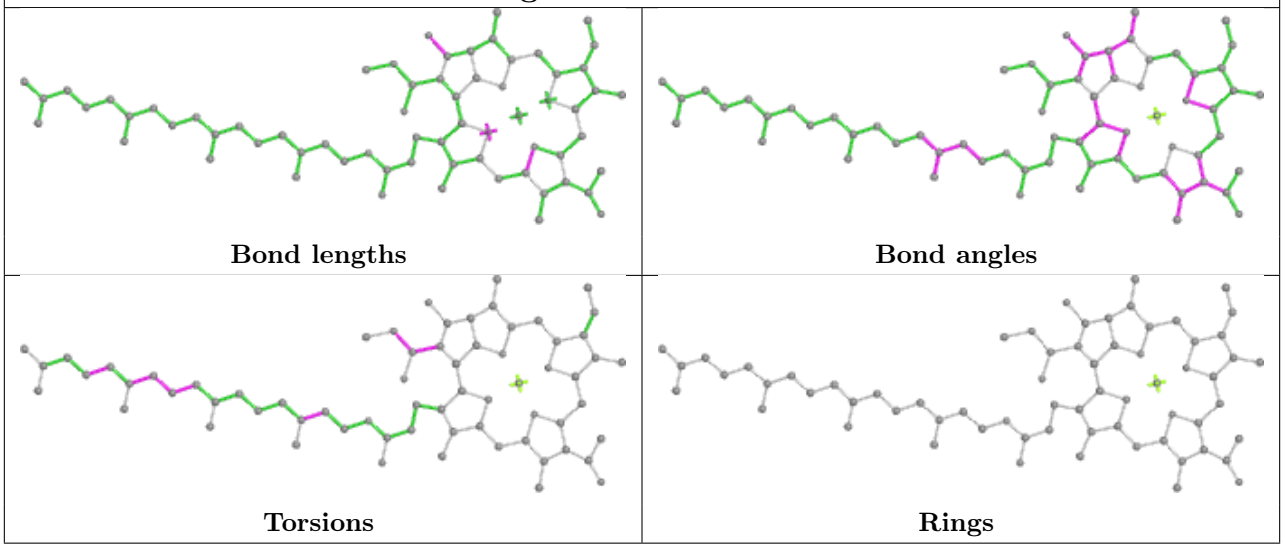
Ligand LMG A 822



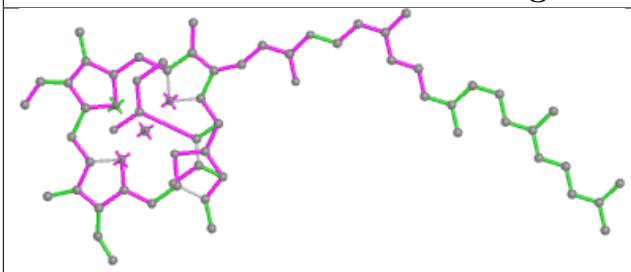
Ligand BCL W 404



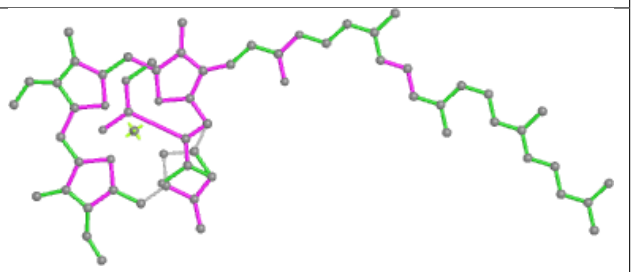
Ligand BCL W 405



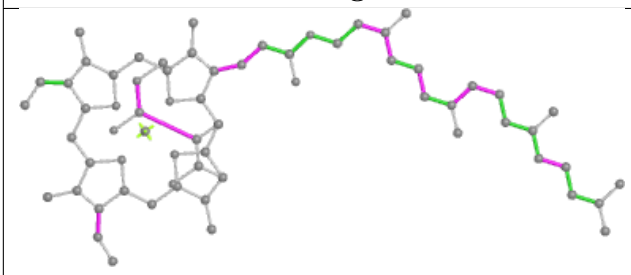
Ligand G2O a 802



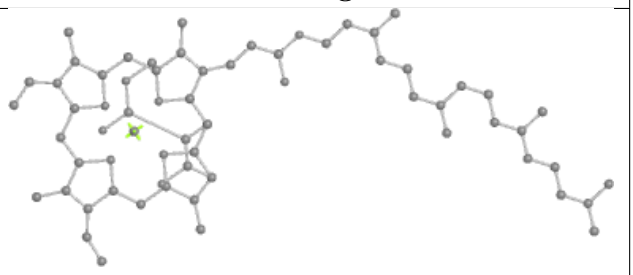
Bond lengths



Bond angles

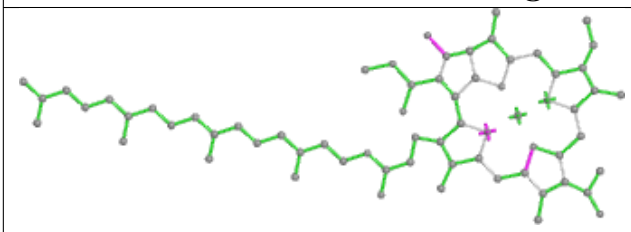


Torsions

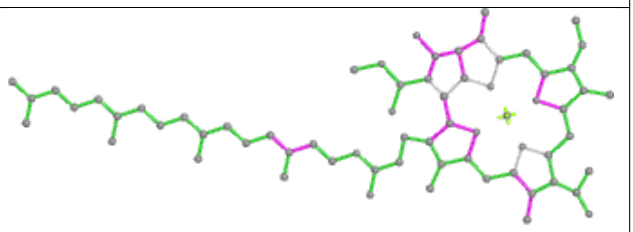


Rings

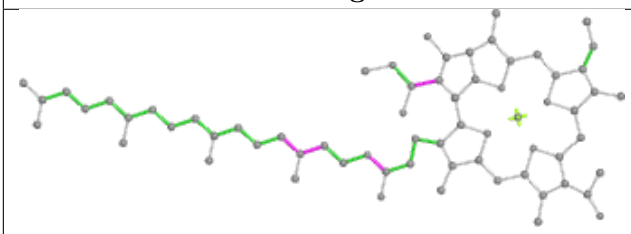
Ligand BCL U 406



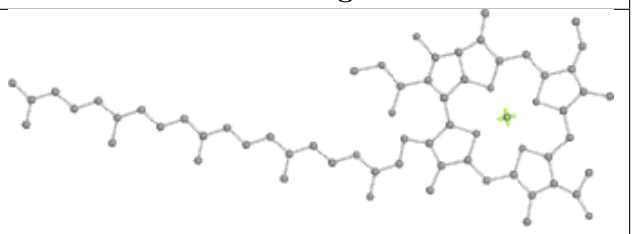
Bond lengths



Bond angles

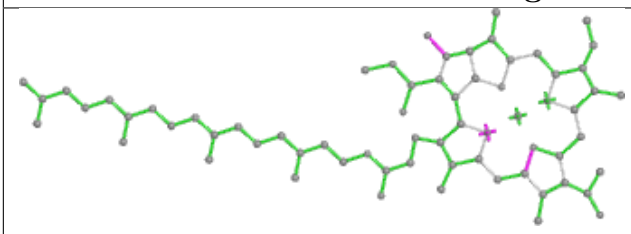


Torsions

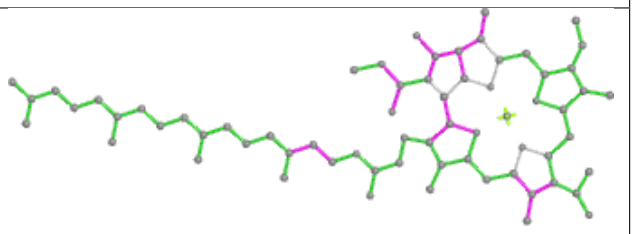


Rings

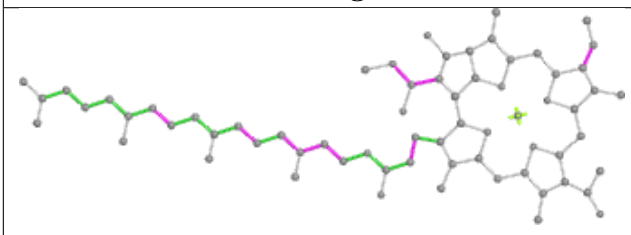
Ligand BCL A 812



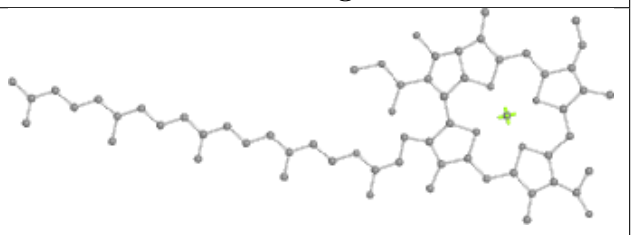
Bond lengths



Bond angles

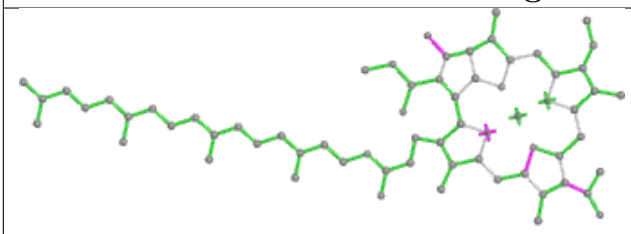


Torsions

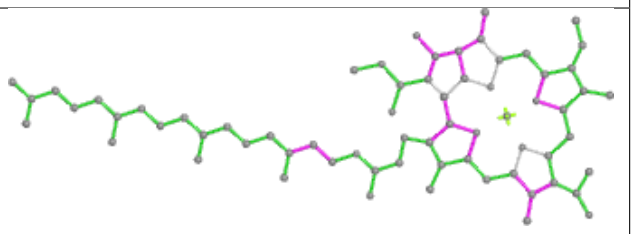


Rings

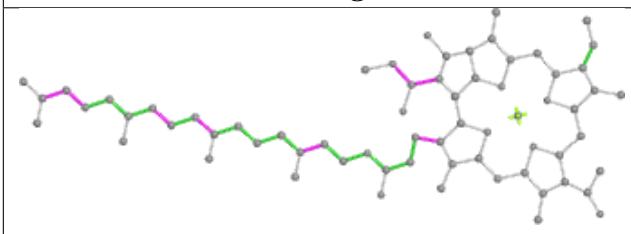
Ligand BCL A 809



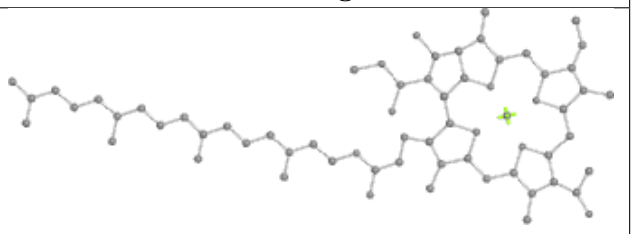
Bond lengths



Bond angles

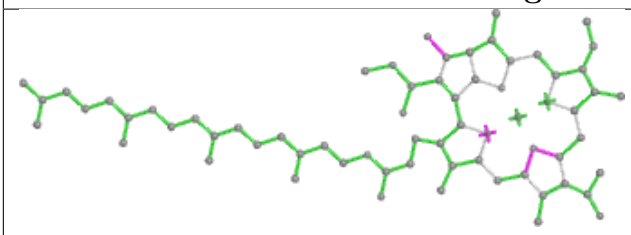


Torsions

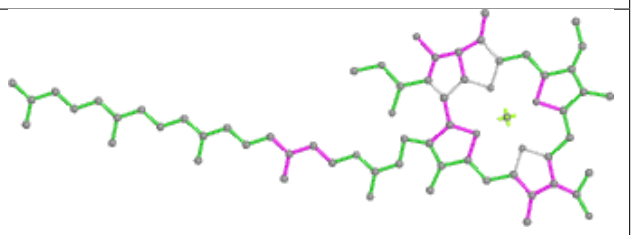


Rings

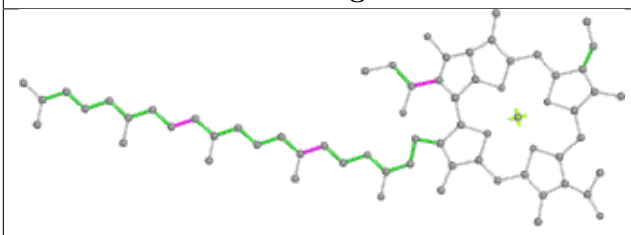
Ligand BCL V 402



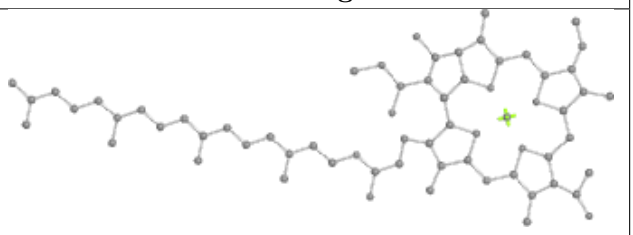
Bond lengths



Bond angles

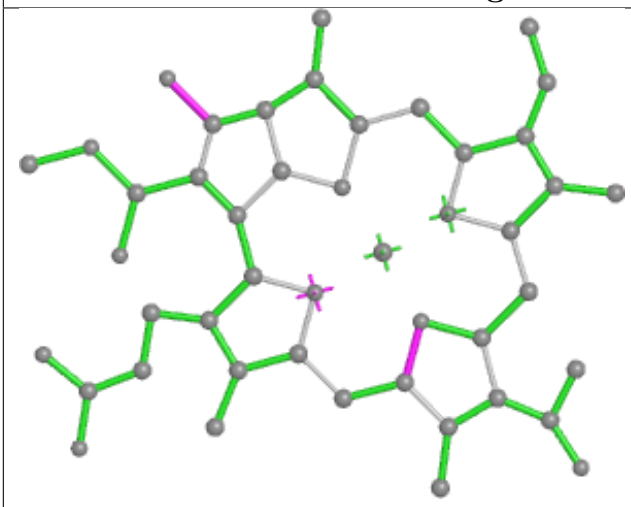


Torsions

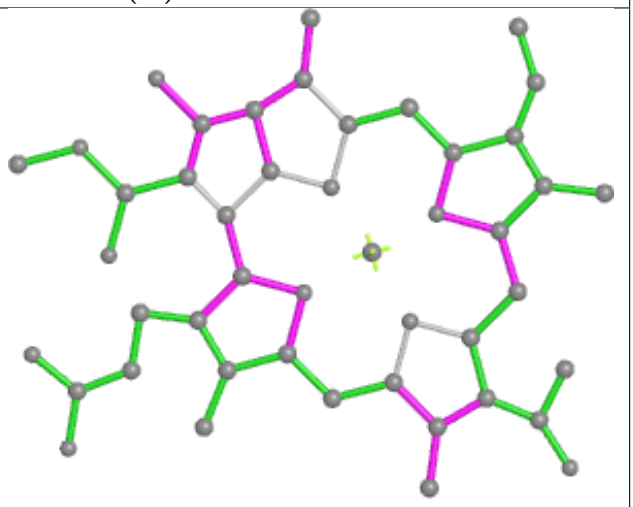


Rings

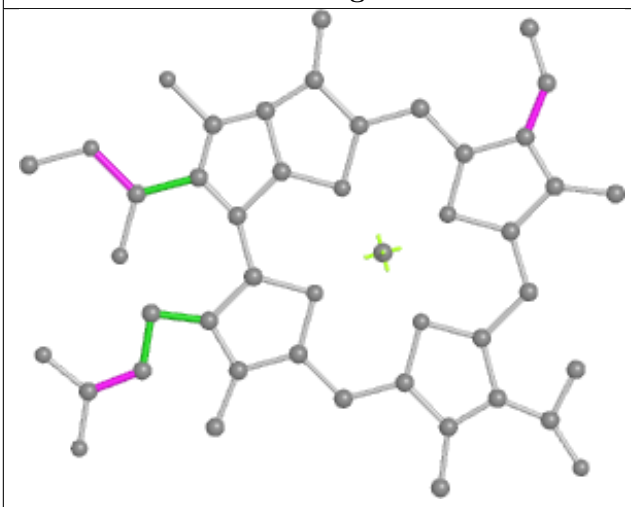
Ligand BCL W 407 (B)



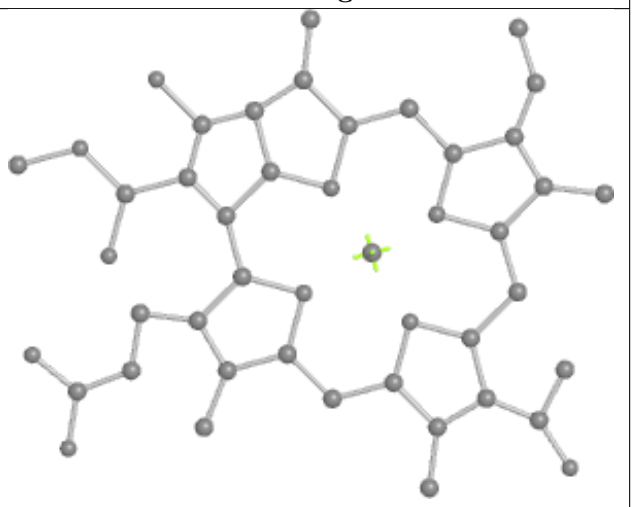
Bond lengths



Bond angles

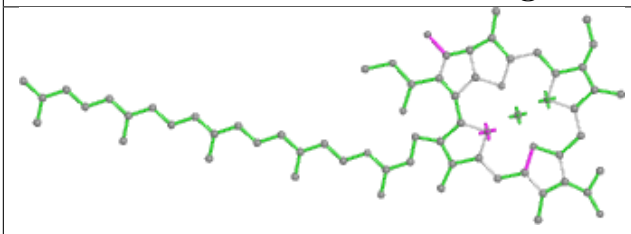


Torsions

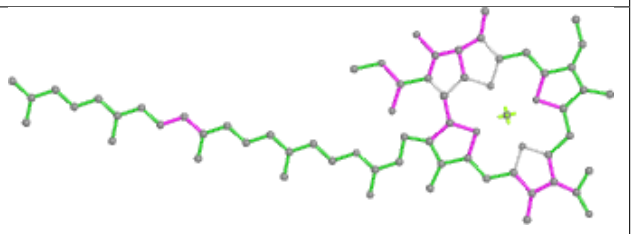


Rings

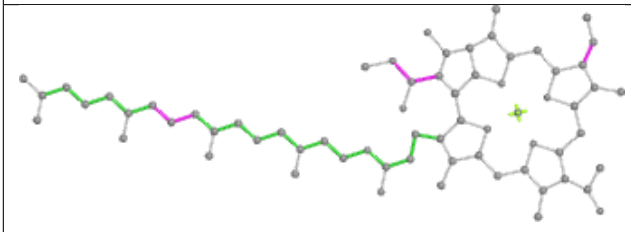
Ligand BCL W 403



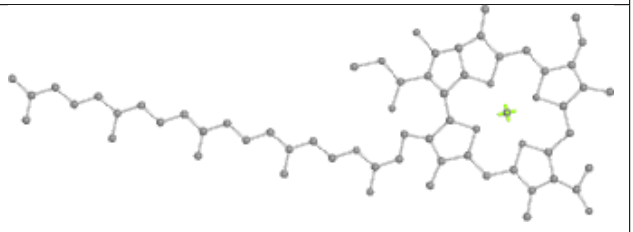
Bond lengths



Bond angles

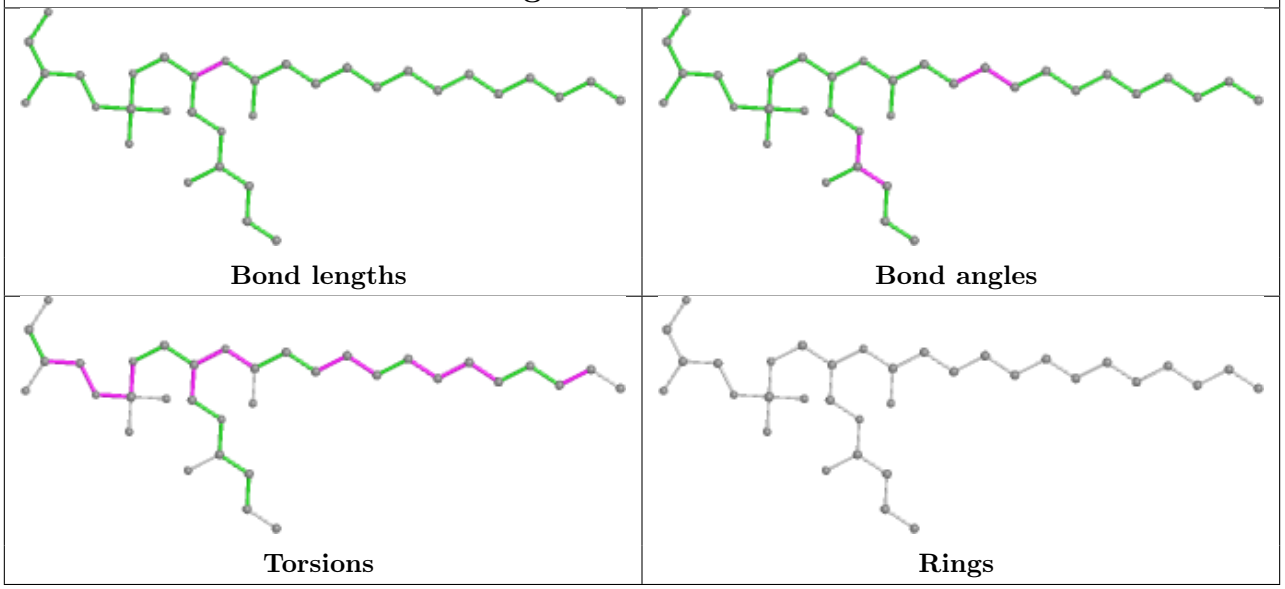


Torsions

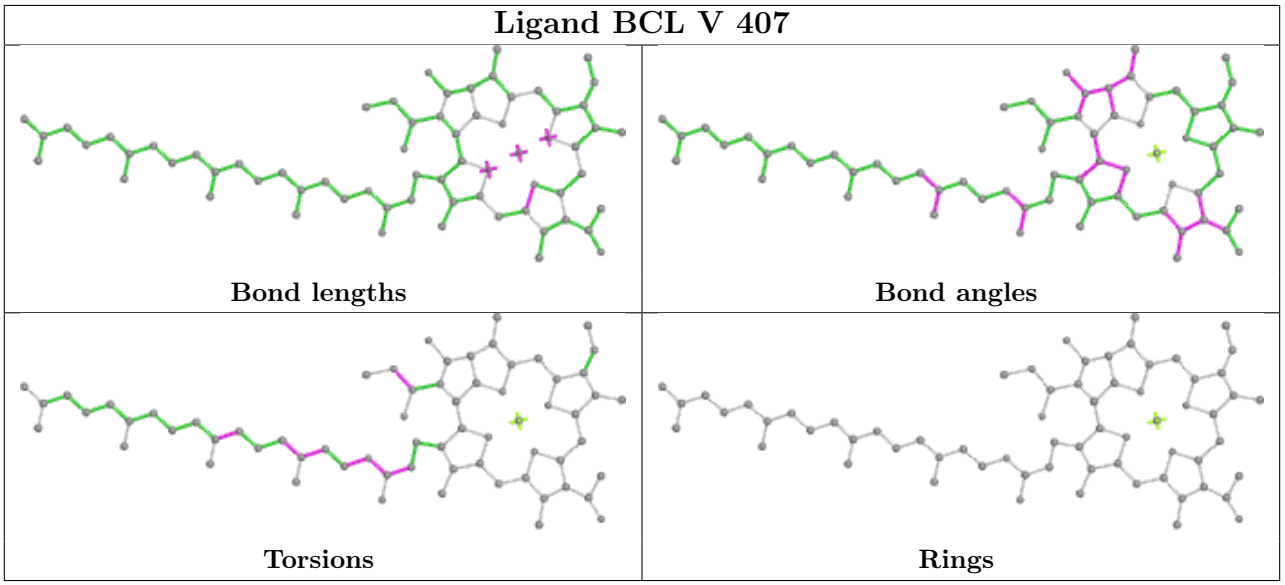


Rings

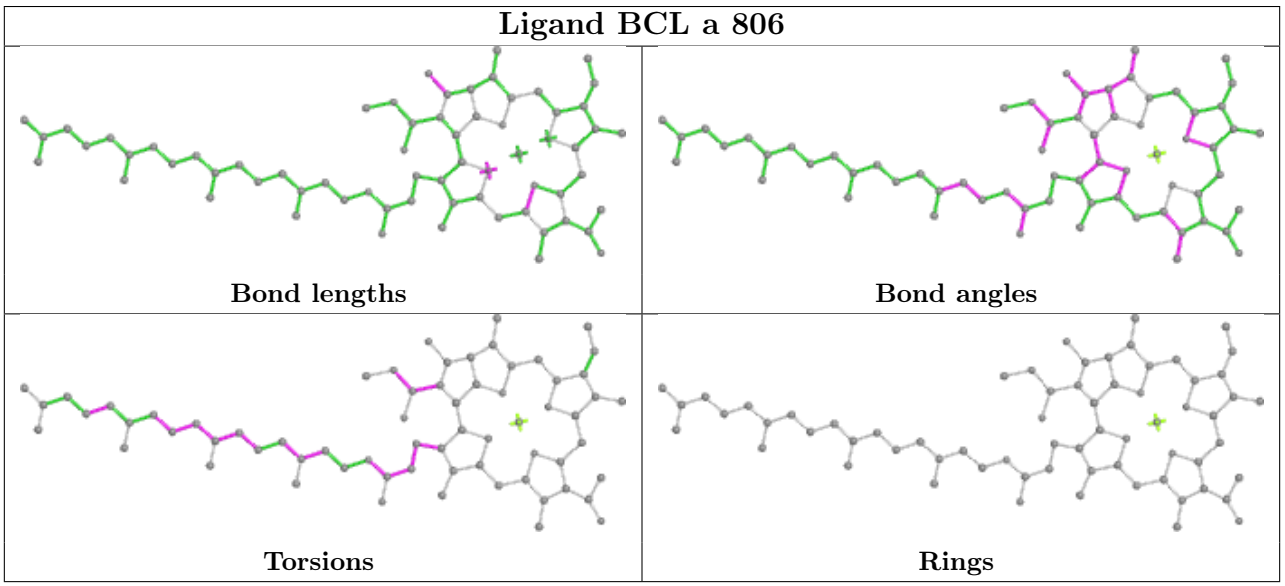
Ligand LHG C 301

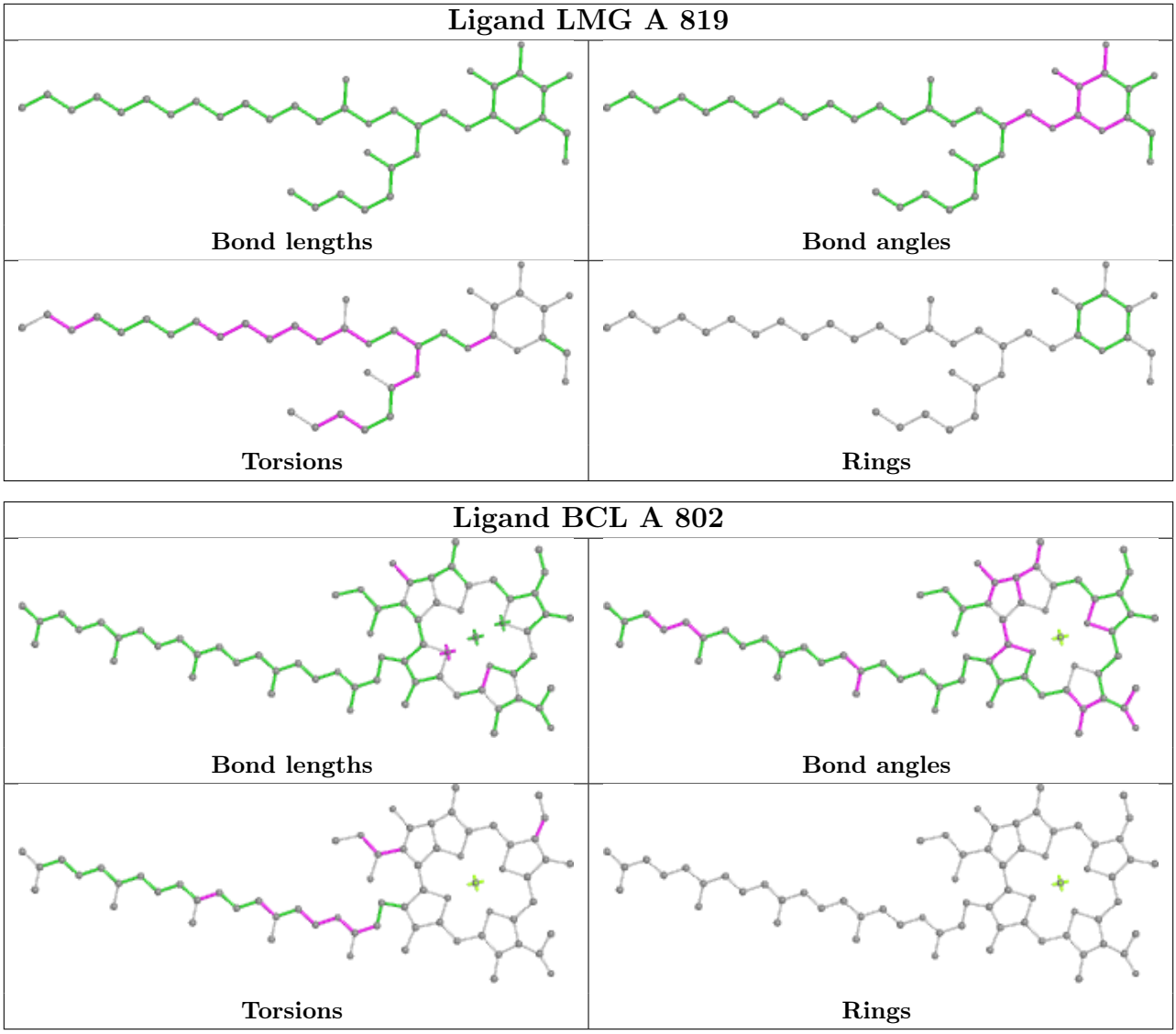


Ligand BCL V 407



Ligand BCL a 806





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

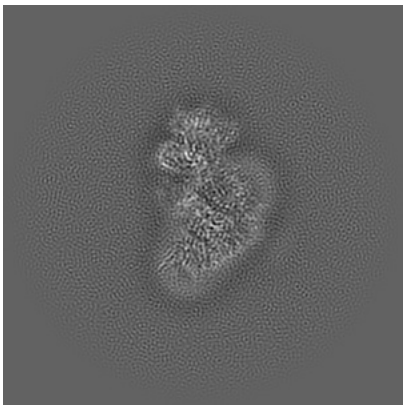
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26469. These allow visual inspection of the internal detail of the map and identification of artifacts.

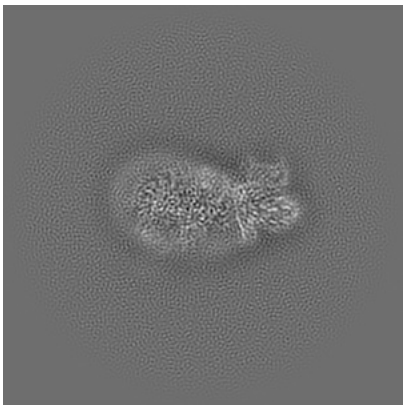
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

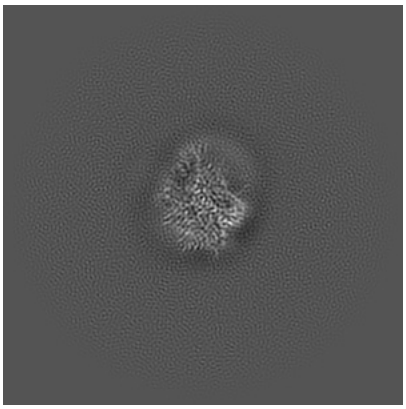
6.1.1 Primary map



X

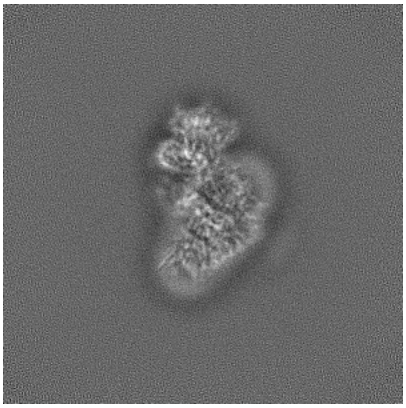


Y

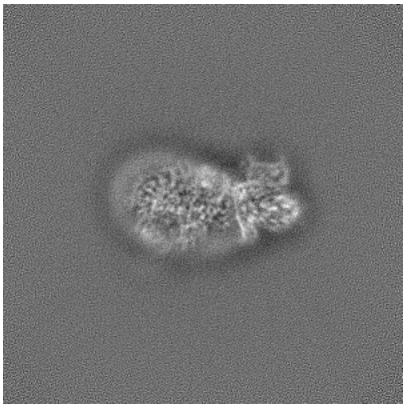


Z

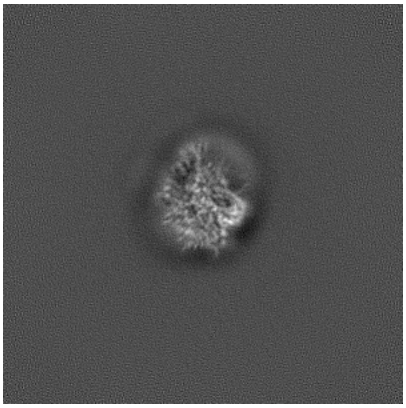
6.1.2 Raw map



X



Y

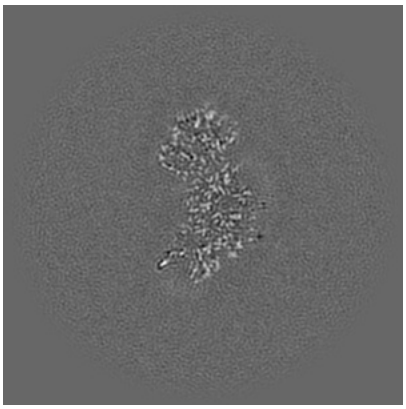


Z

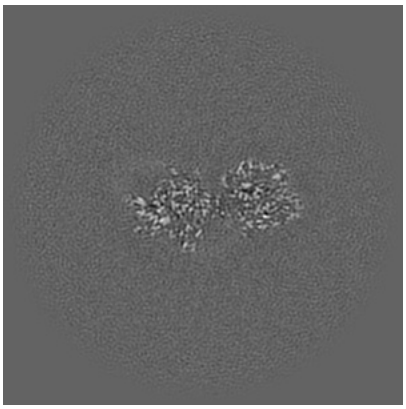
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

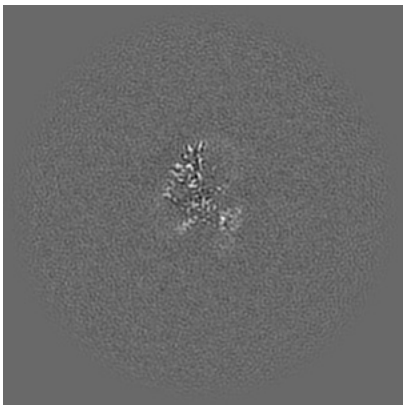
6.2.1 Primary map



X Index: 180

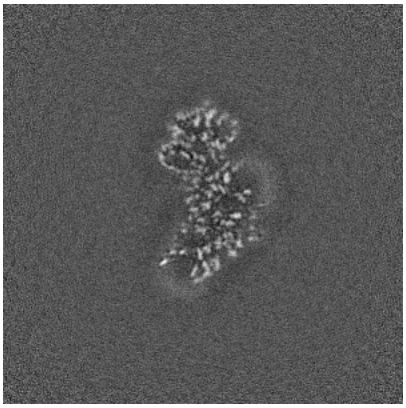


Y Index: 180

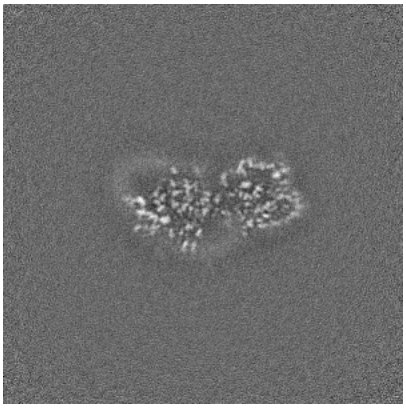


Z Index: 180

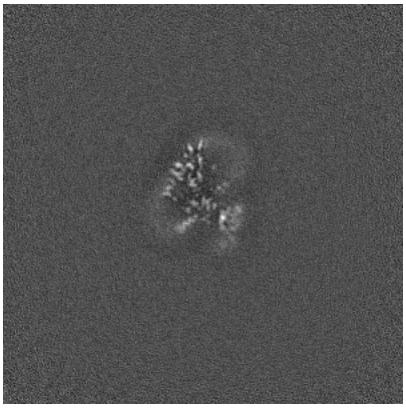
6.2.2 Raw map



X Index: 180



Y Index: 180

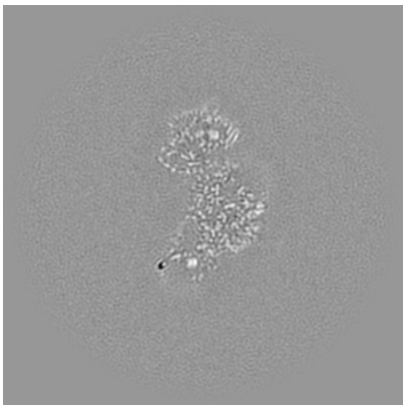


Z Index: 180

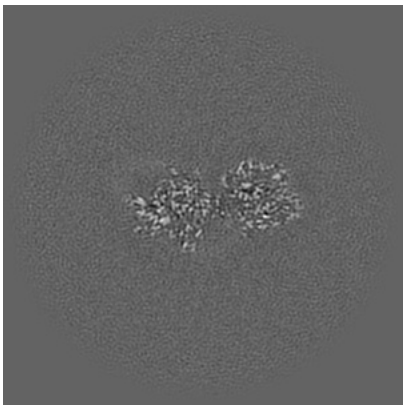
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

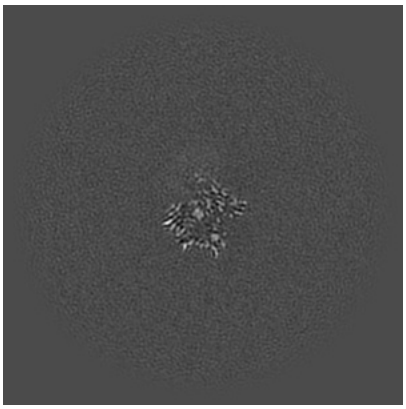
6.3.1 Primary map



X Index: 176

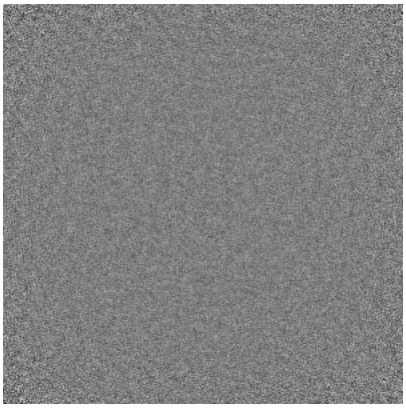


Y Index: 180

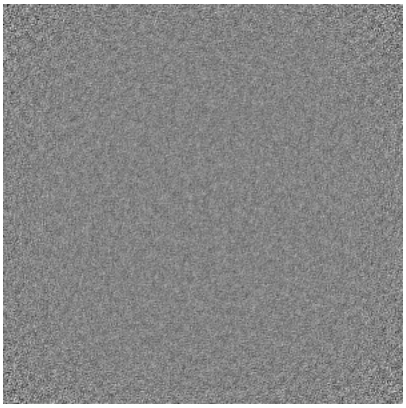


Z Index: 217

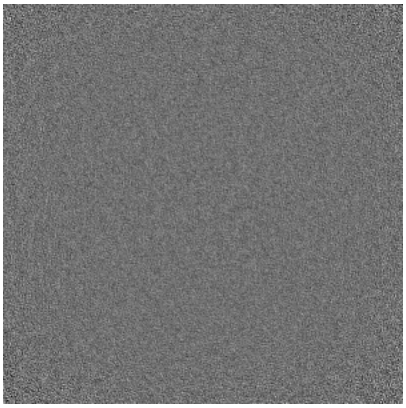
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 359

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

6.4.2 Raw map

X Y Z

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

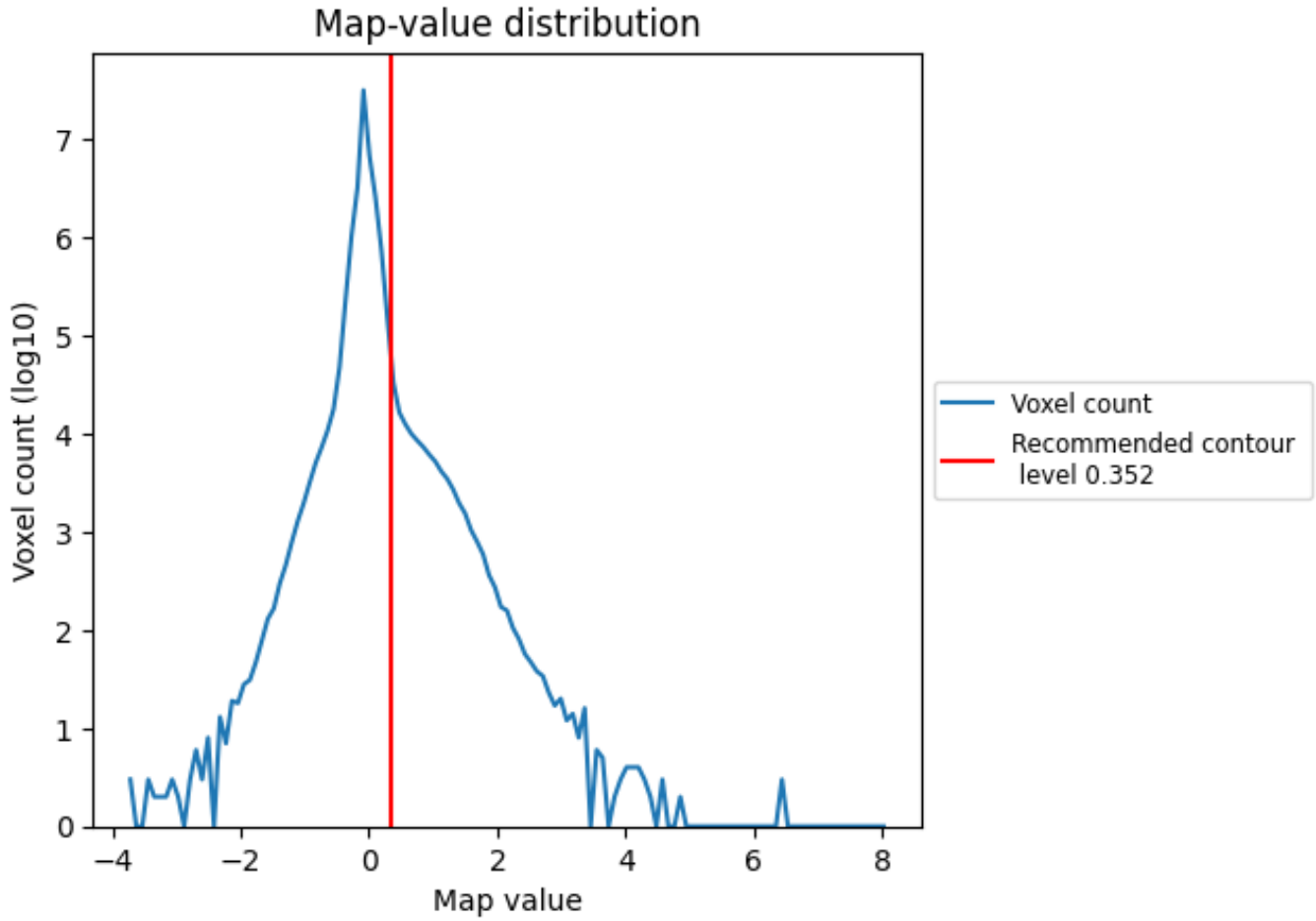
6.5 Mask visualisation (i)

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

7 Map analysis

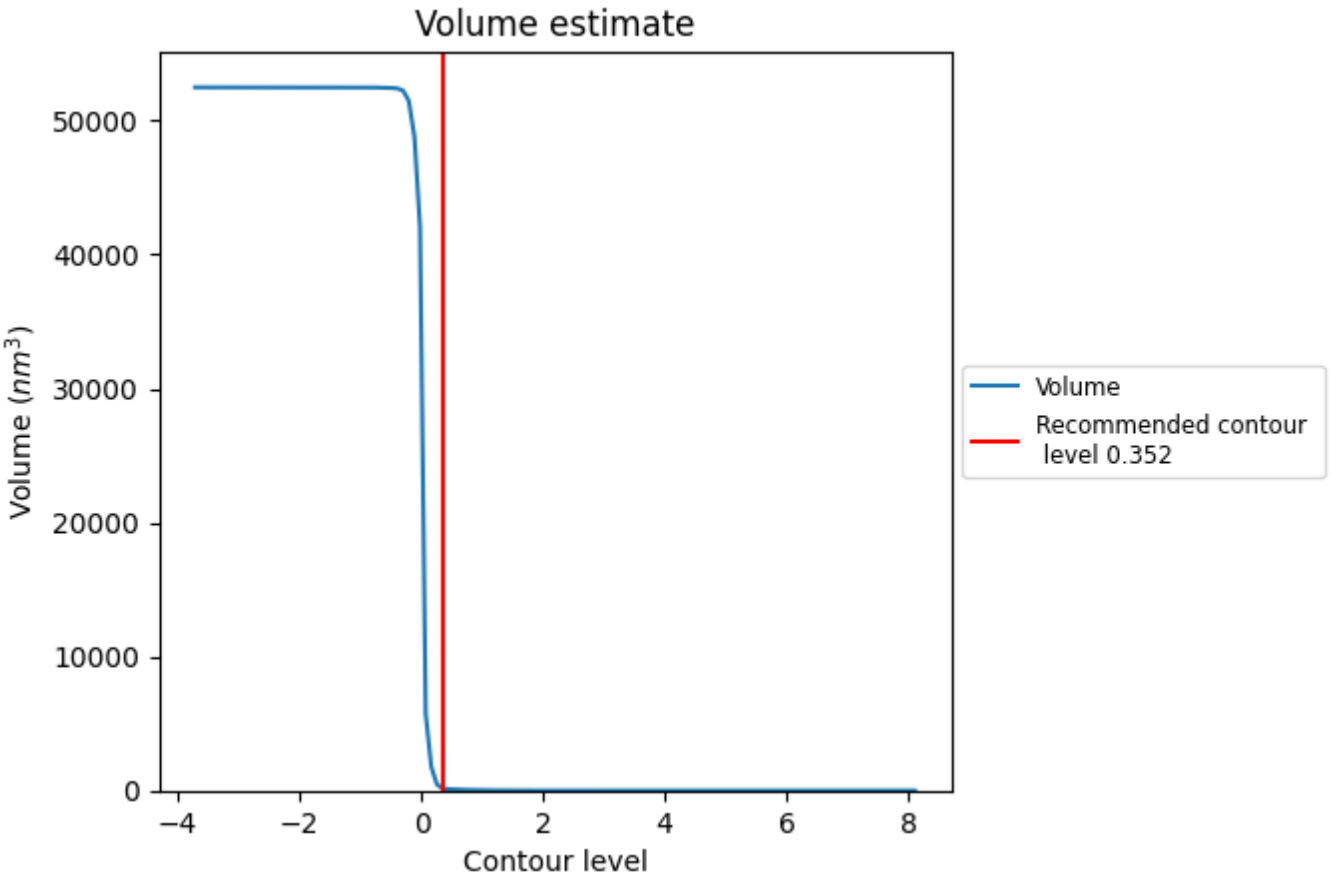
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

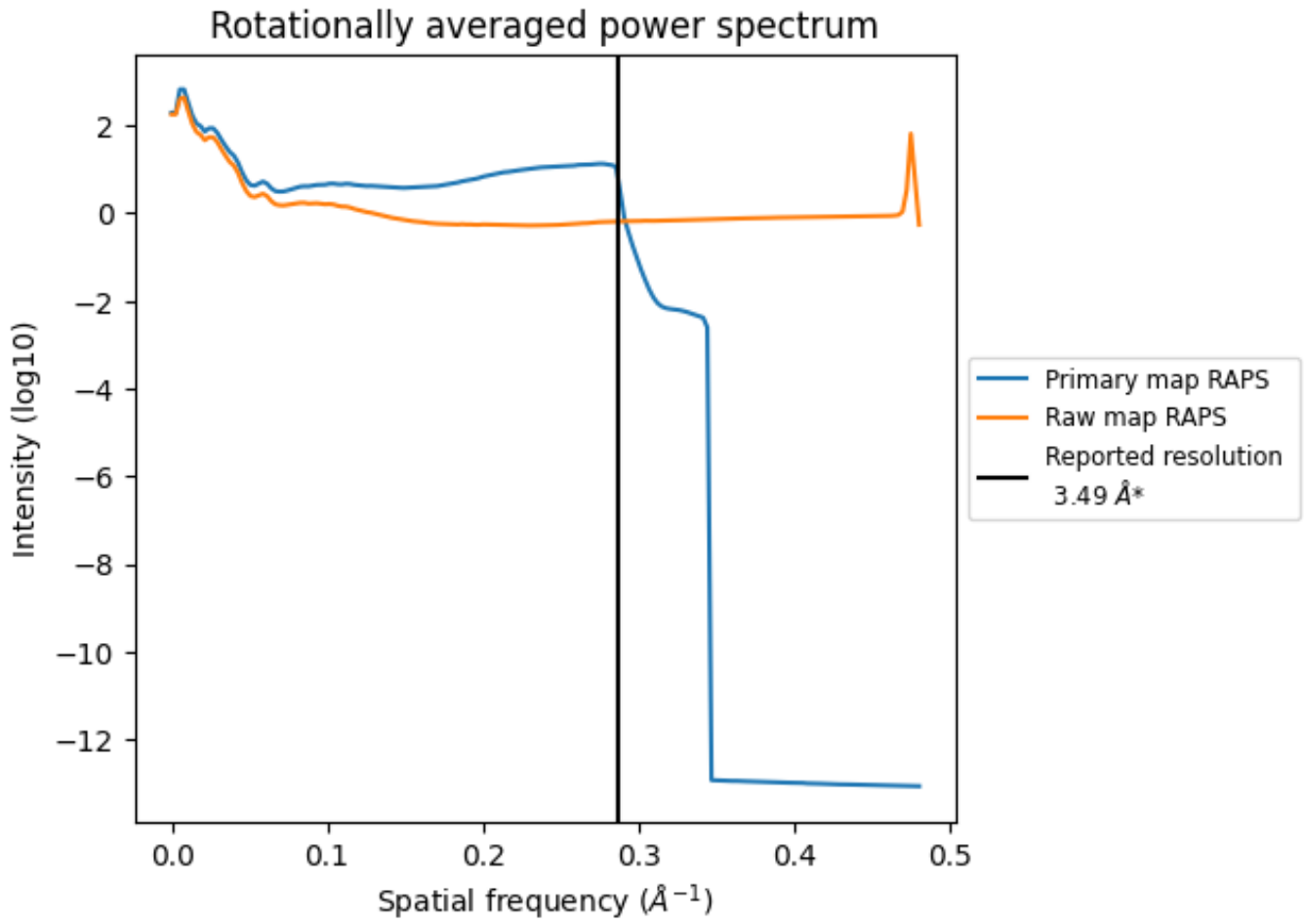
7.2 Volume estimate



The volume at the recommended contour level is 160 nm^3; this corresponds to an approximate mass of 145 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)

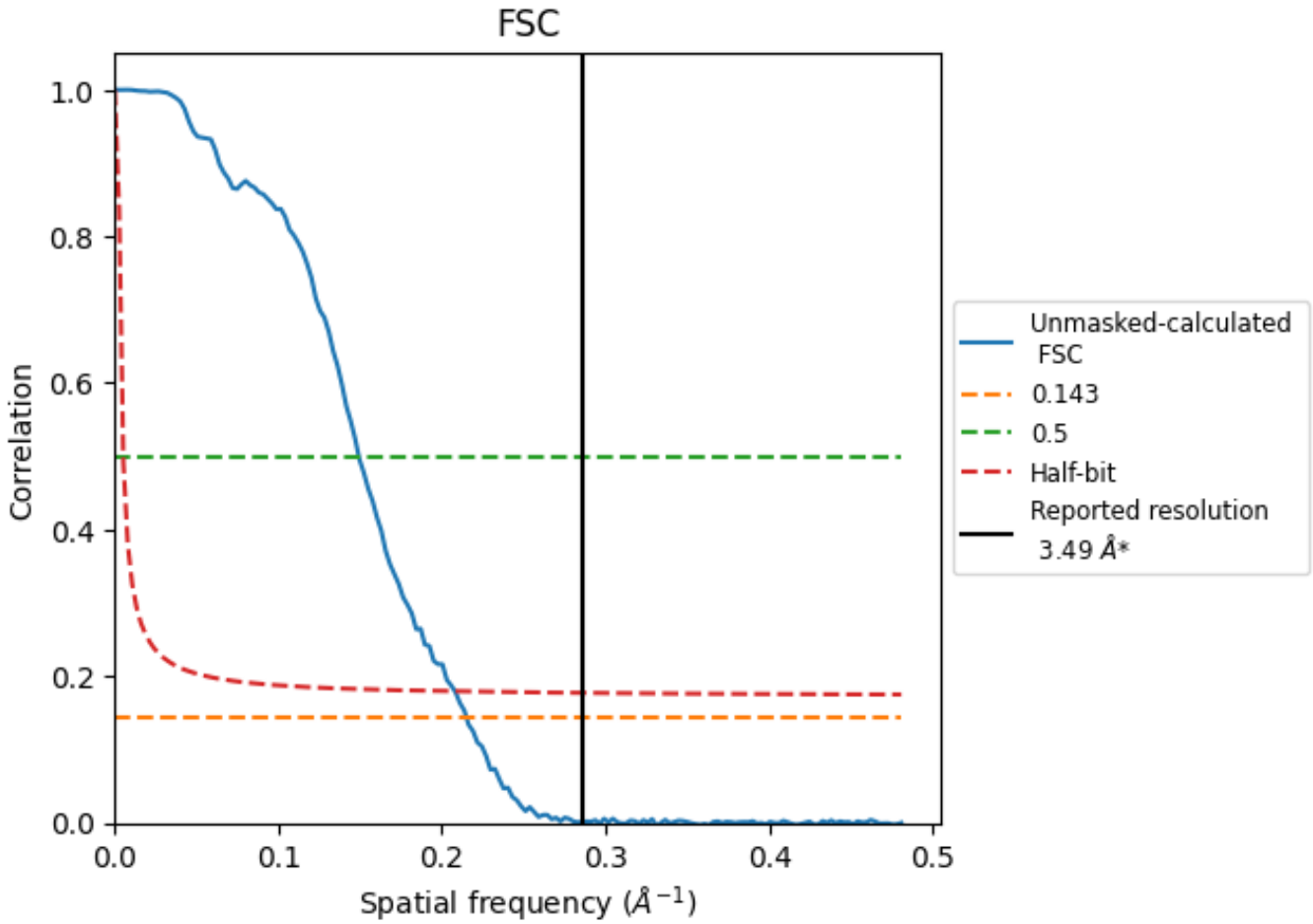


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8.2 Resolution estimates (i)

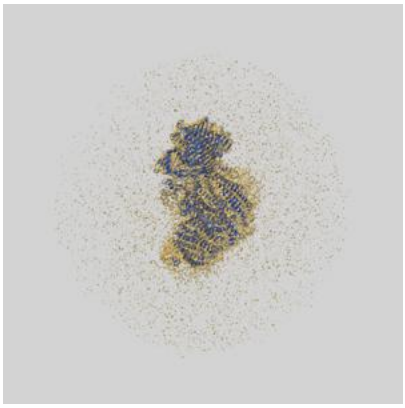
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.65	6.71	4.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.65 differs from the reported value 3.49 by more than 10 %

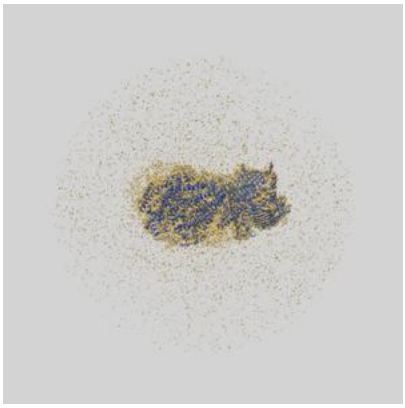
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26469 and PDB model 7UEA. Per-residue inclusion information can be found in section 3 on page 14.

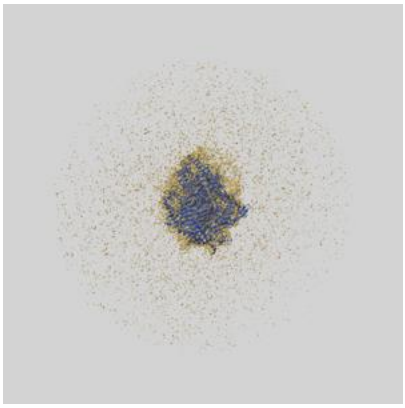
9.1 Map-model overlay



X



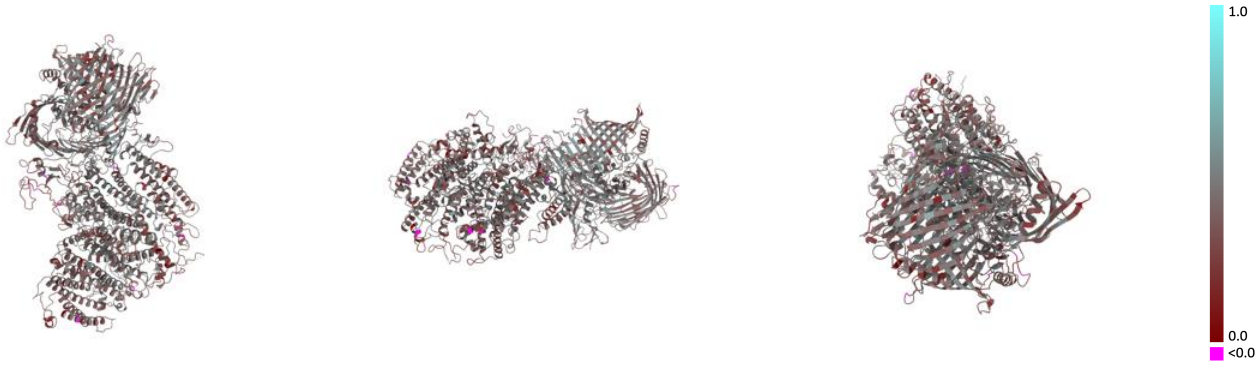
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.352 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.

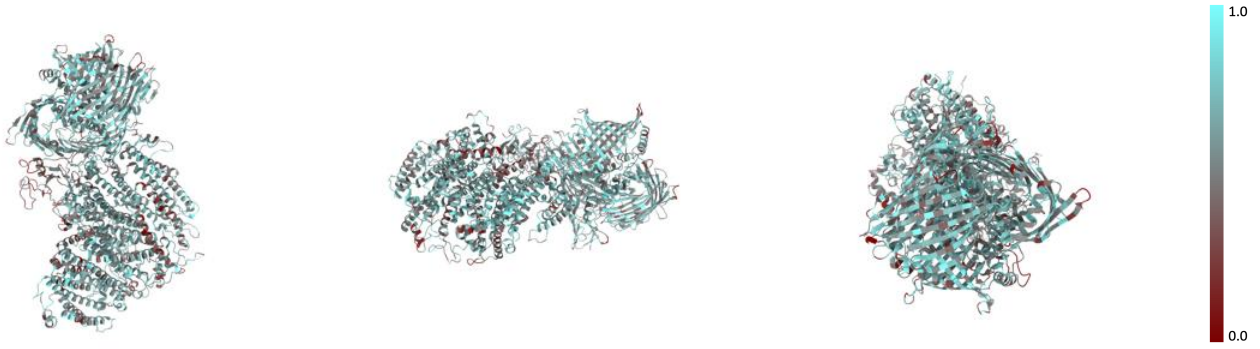
9.2 Q-score mapped to coordinate model (i)



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.

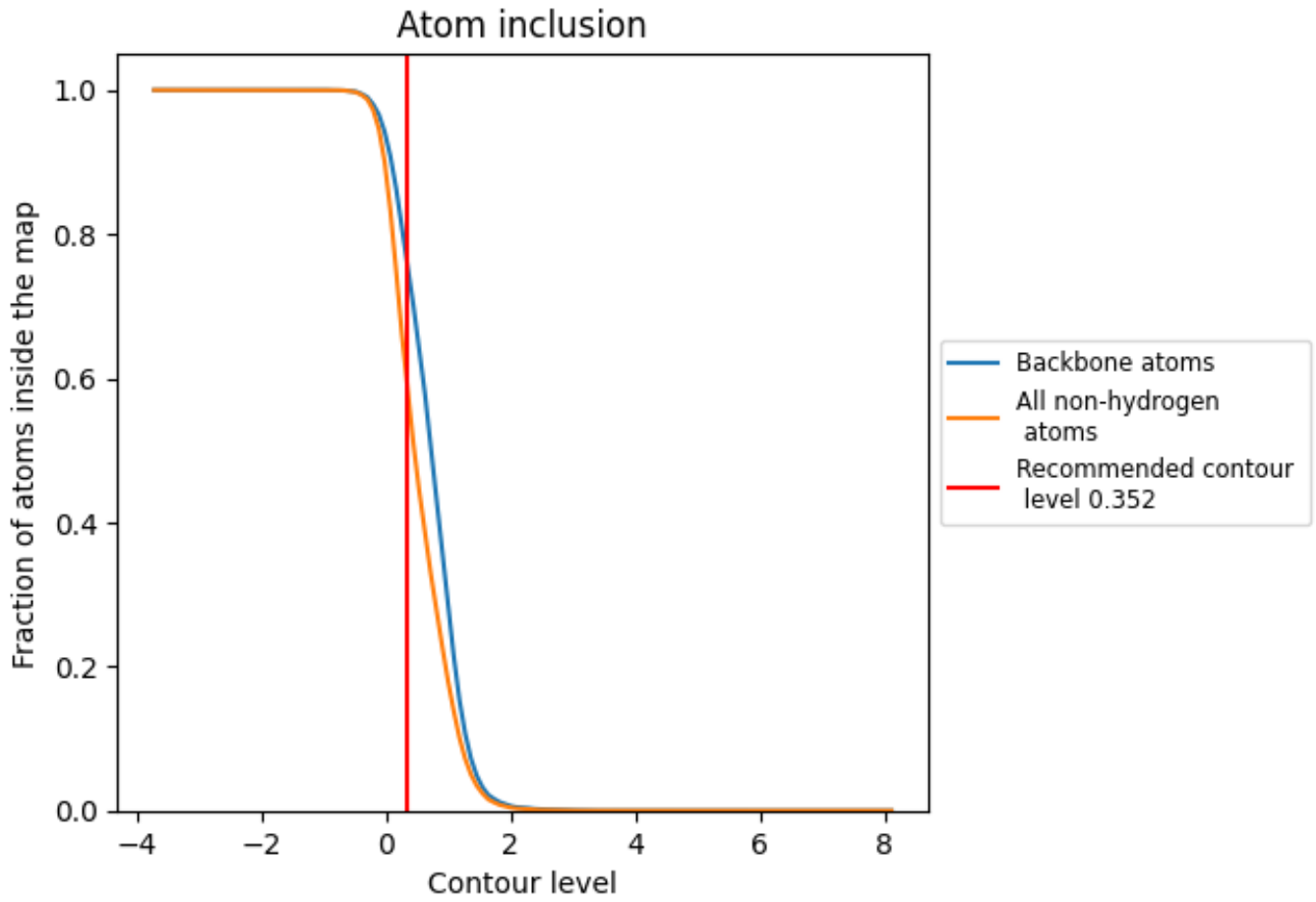
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.352).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.352) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5814	0.4060
A	0.6165	0.4250
B	0.5292	0.3720
C	0.3460	0.2920
D	0.3514	0.3080
U	0.6053	0.4160
V	0.6157	0.4350
W	0.6012	0.4070
a	0.5982	0.4080
c	0.4388	0.3370