Full wwPDB EM Validation Report ⓘ

Jun 18, 2025 – 04:26 PM JST

PDB ID	:	8GWA / pdb_00008gwa
EMDB ID	:	EMD-34307
Title	:	Structure of the intact photosynthetic light-harvesting antenna-reaction center complex from a green sulfur bacterium
Authors	:	Chen, J.H.; Zhang, X.
Deposited on	:	2022-09-16
Resolution	:	2.90 Å(reported)

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

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

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

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

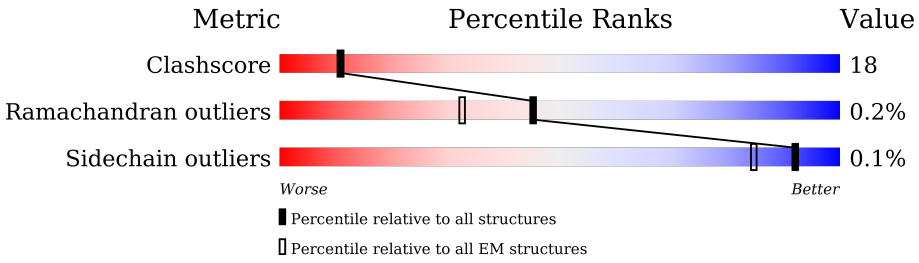
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	366	63% 36%
1	2	366	64% 33%
1	3	366	64% 34%
1	4	366	64% 34%
1	5	366	64% 33%
1	6	366	64% 34%
2	D	143	55% 43%
3	B	230	23% 22% 56%

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Mol	Chain	Length	Quality of chain
4	A	731	55% 36% 9%
4	a	731	57% 34% 9%
5	E	58	83% 16%
6	F	58	64% 22% 14%
7	C	206	40% 15% 45%
7	c	206	41% 14% 45%

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
10	SF4	B	302	-	-	X	-
13	F39	A	814	-	X	-	-
13	F39	A	815	-	X	-	-
13	F39	C	302	-	X	-	-
13	F39	a	816	-	X	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 37660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	362	Total	C	N	O	S	0	0
			2815	1783	501	524	7		
1	3	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		
1	2	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		
1	4	362	Total	C	N	O	S	0	0
			2815	1783	501	524	7		
1	6	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		
1	5	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	143	Total	C	N	O	S	0	0
			1167	741	208	212	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	102	Total	C	N	O	S	0	0
			798	510	132	147	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	667	Total	C	N	O	S	0	0
			5344	3559	858	900	27		
4	a	662	Total	C	N	O	S	0	0
			5309	3538	852	893	26		

- Molecule 5 is a protein called unkown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	57	Total	C	N	O	0	0
			285	171	57	57		

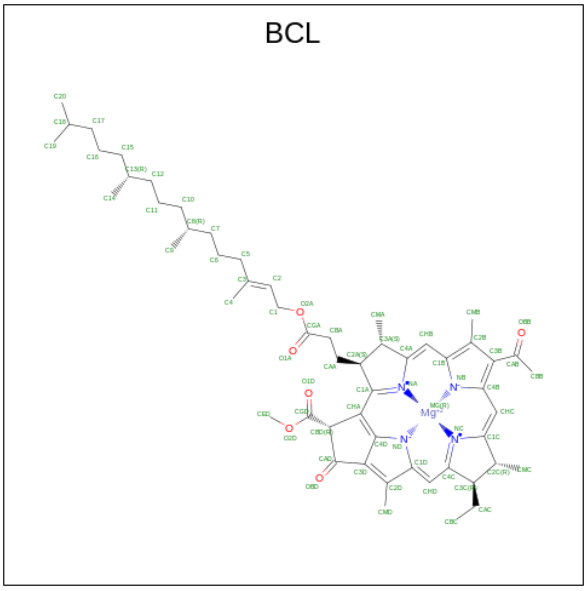
- Molecule 6 is a protein called Ric1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	50	Total	C	N	O	S	0	0
			379	253	62	61	3		

- Molecule 7 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	113	Total	C	N	O	S	0	0
			875	587	137	144	7		
7	c	113	Total	C	N	O	S	0	0
			875	587	137	144	7		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
8	2	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	a	1	Total 46	C 35	Mg 1	N 4	O 6	0
8	a	1	Total 46	C 35	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	5	1	Total 66	C 55	Mg 1	N 4	O 6	0

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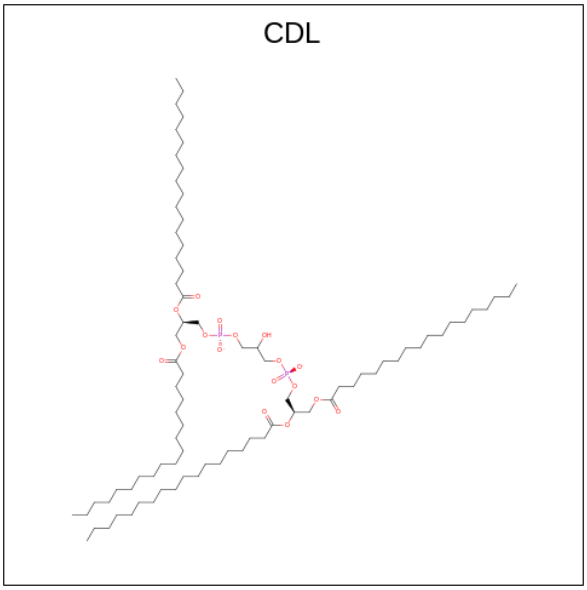
Mol	Chain	Residues	Atoms					AltConf
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	C	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 9 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	1	1	Total	C	O	P	0
			77	58	17	2	
9	a	1	Total	C	O	P	0
			70	51	17	2	
9	a	1	Total	C	O	P	0
			92	73	17	2	

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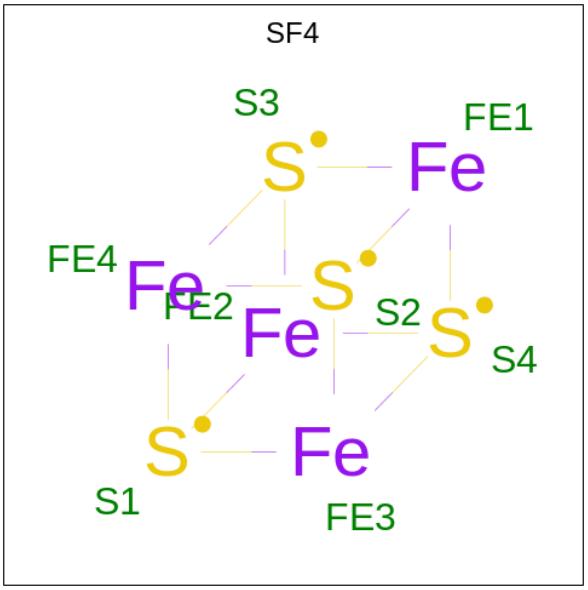
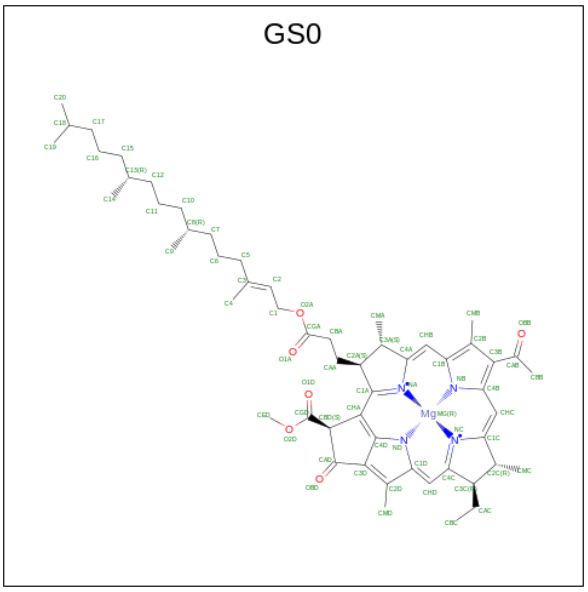
Mol	Chain	Residues	Atoms				AltConf
9	c	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



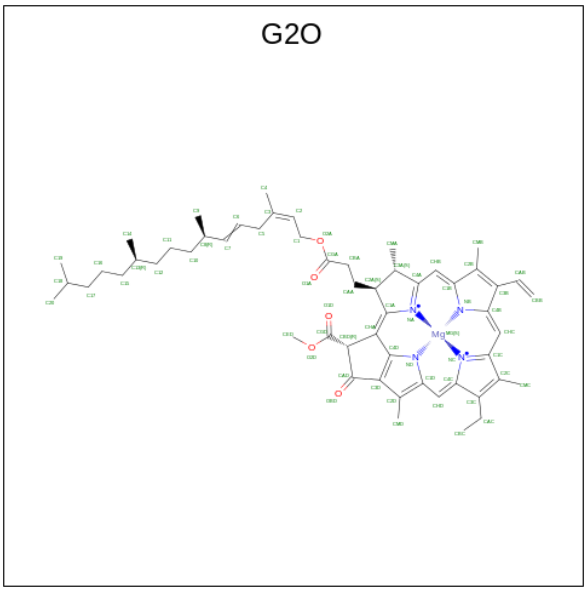
Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	
10	A	1	Total	Fe	S	0
			8	4	4	

- Molecule 11 is Bacteriochlorophyll A isomer (CCD ID: GS0) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 12 is Chlorophyll A ester (CCD ID: G2O) (formula: $C_{55}H_{70}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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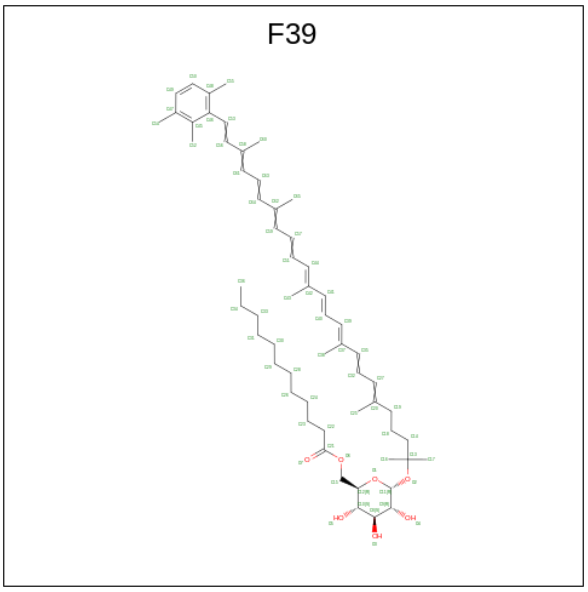
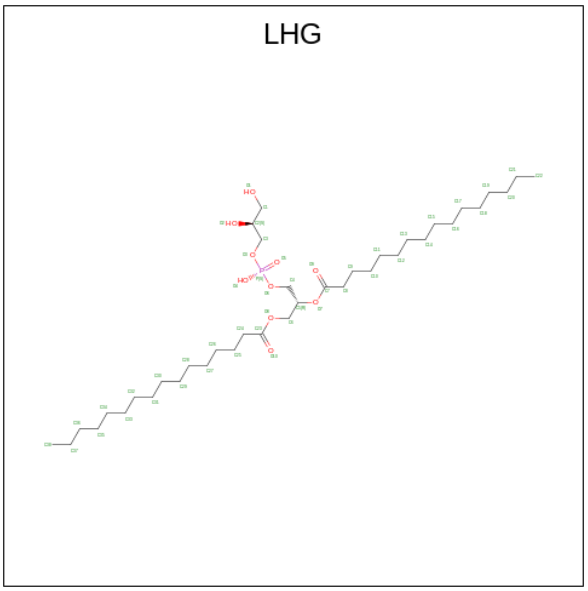
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 13 is [(2R,3S,4S,5R,6R)-6-[(10E,12E,14E)-2,6,10,14,19,23-hexamethyl-25-(2,3,6-trimethylphenyl)pentacosa-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl dodecanoate (CCD ID: F39) (formula: $C_{58}H_{86}O_7$).



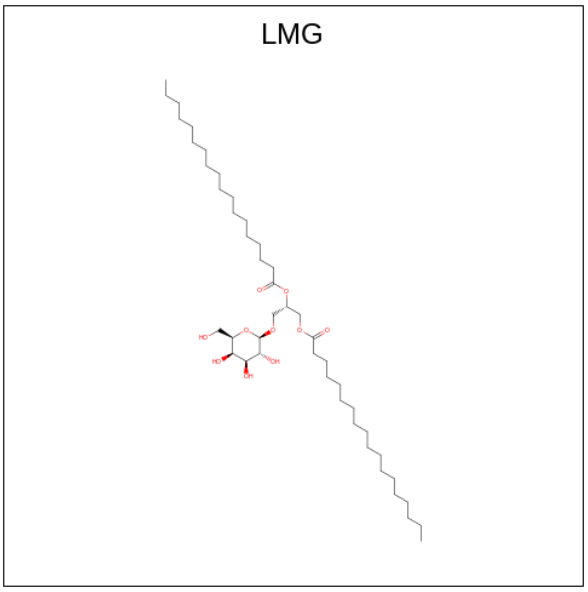
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			65	58	7	
13	A	1	Total	C	O	0
			65	58	7	
13	a	1	Total	C	O	0
			65	58	7	
13	C	1	Total	C	O	0
			65	58	7	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total 46	C 35	O 10	P 1	0
14	A	1	Total 49	C 38	O 10	P 1	0
14	A	1	Total 49	C 38	O 10	P 1	0
14	a	1	Total 46	C 35	O 10	P 1	0
14	a	1	Total 40	C 29	O 10	P 1	0
14	a	1	Total 42	C 31	O 10	P 1	0
14	E	1	Total 37	C 26	O 10	P 1	0

- Molecule 15 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

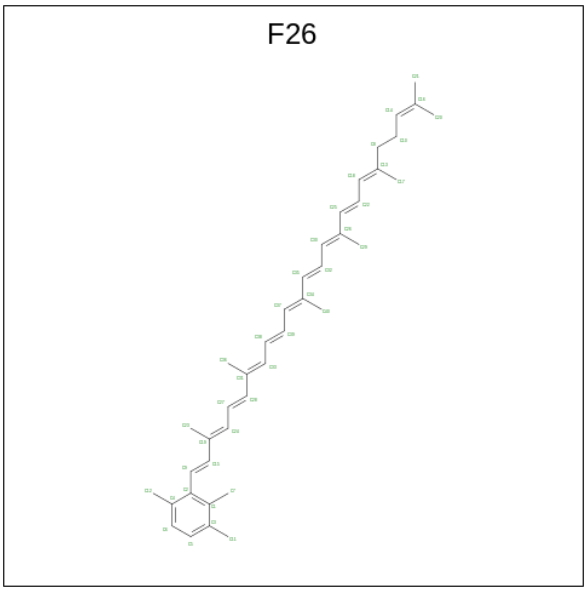


Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			44	34	10	
15	a	1	Total	C	O	0
			44	34	10	

- Molecule 16 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 17 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 (CCD ID: F26) (formula: $C_{40}H_{52}$).



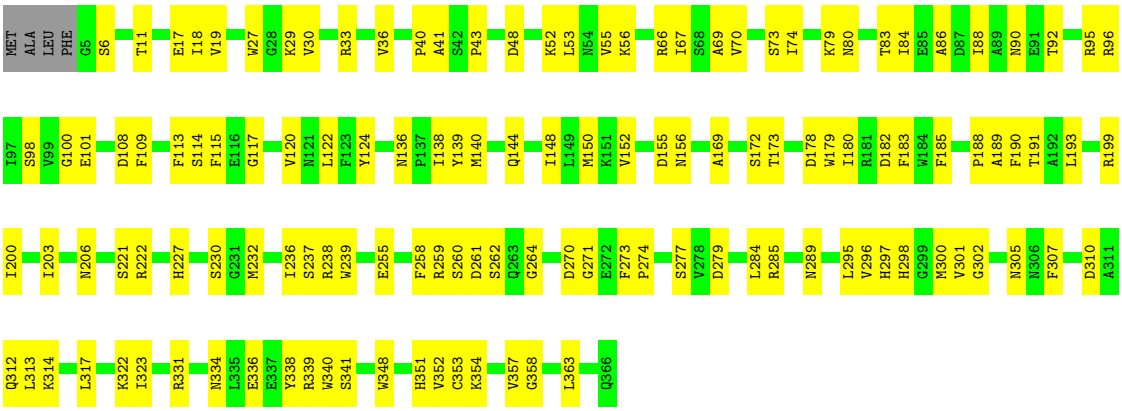
Mol	Chain	Residues	Atoms	AltConf
17	a	1	Total C 40 40	0
17	c	1	Total C 40 40	0

3 Residue-property plots (i)

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

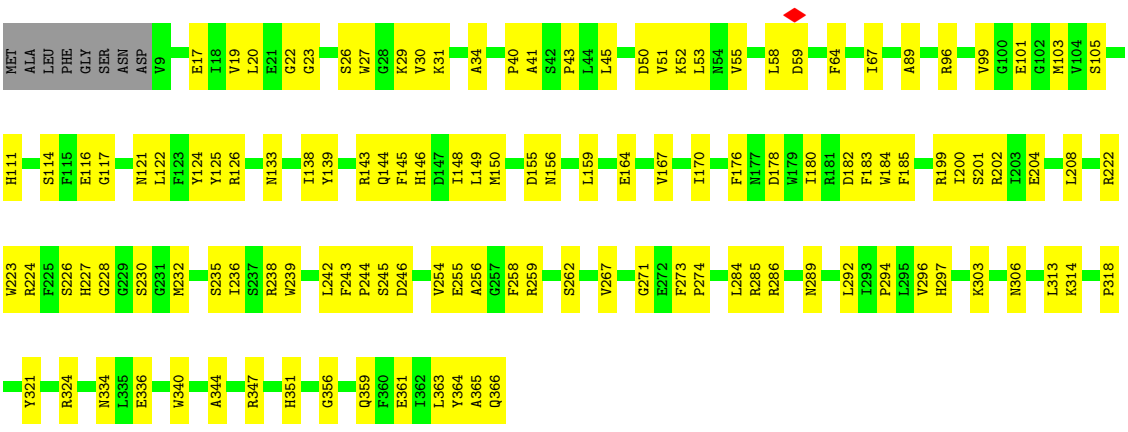
• Molecule 1: Bacteriochlorophyll a protein

Chain 1:



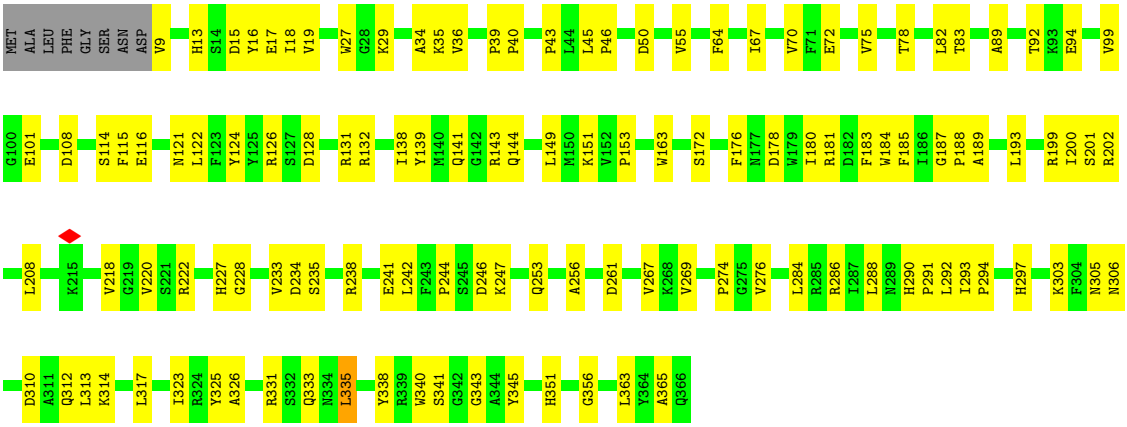
• Molecule 1: Bacteriochlorophyll a protein

Chain 3:



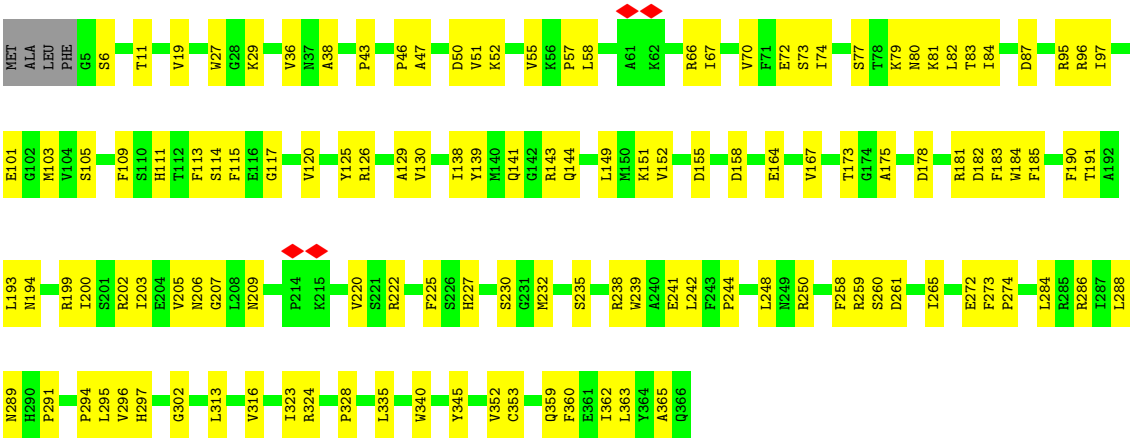
• Molecule 1: Bacteriochlorophyll a protein

Chain 2:



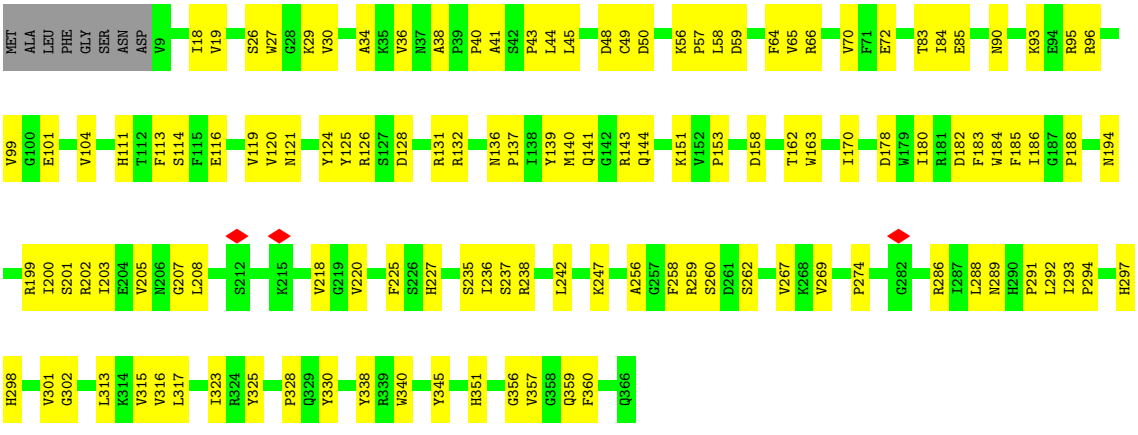
• Molecule 1: Bacteriochlorophyll a protein

Chain 4:



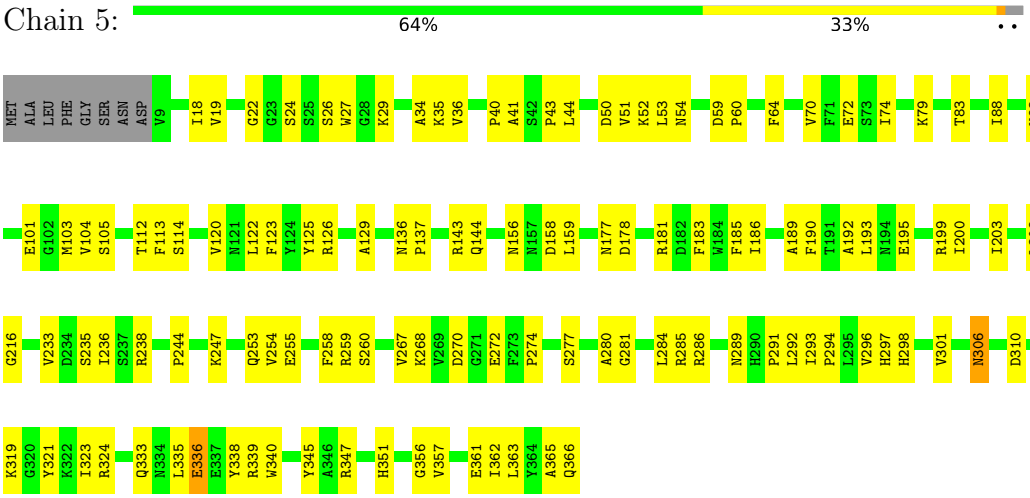
• Molecule 1: Bacteriochlorophyll a protein

Chain 6:



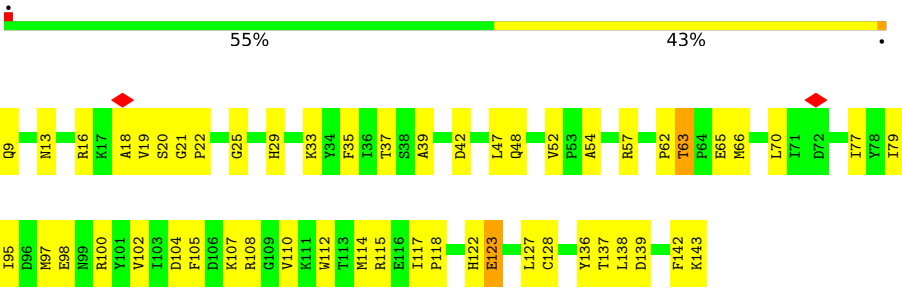
• Molecule 1: Bacteriochlorophyll a protein

Chain 5:



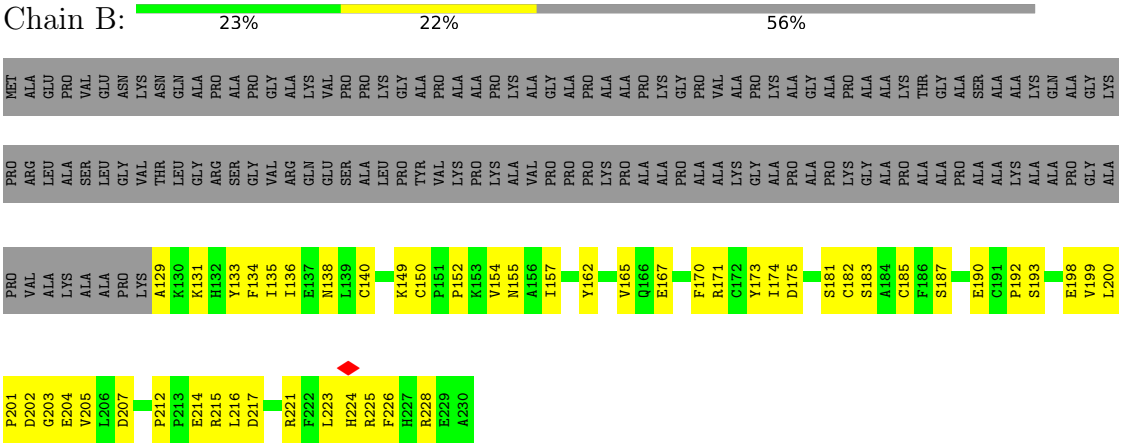
• Molecule 2: P840 reaction center 17 kDa protein

Chain D:



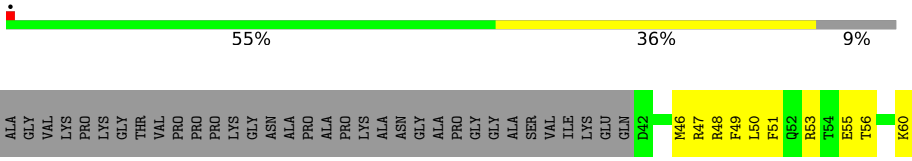
• Molecule 3: Photosystem P840 reaction center iron-sulfur protein

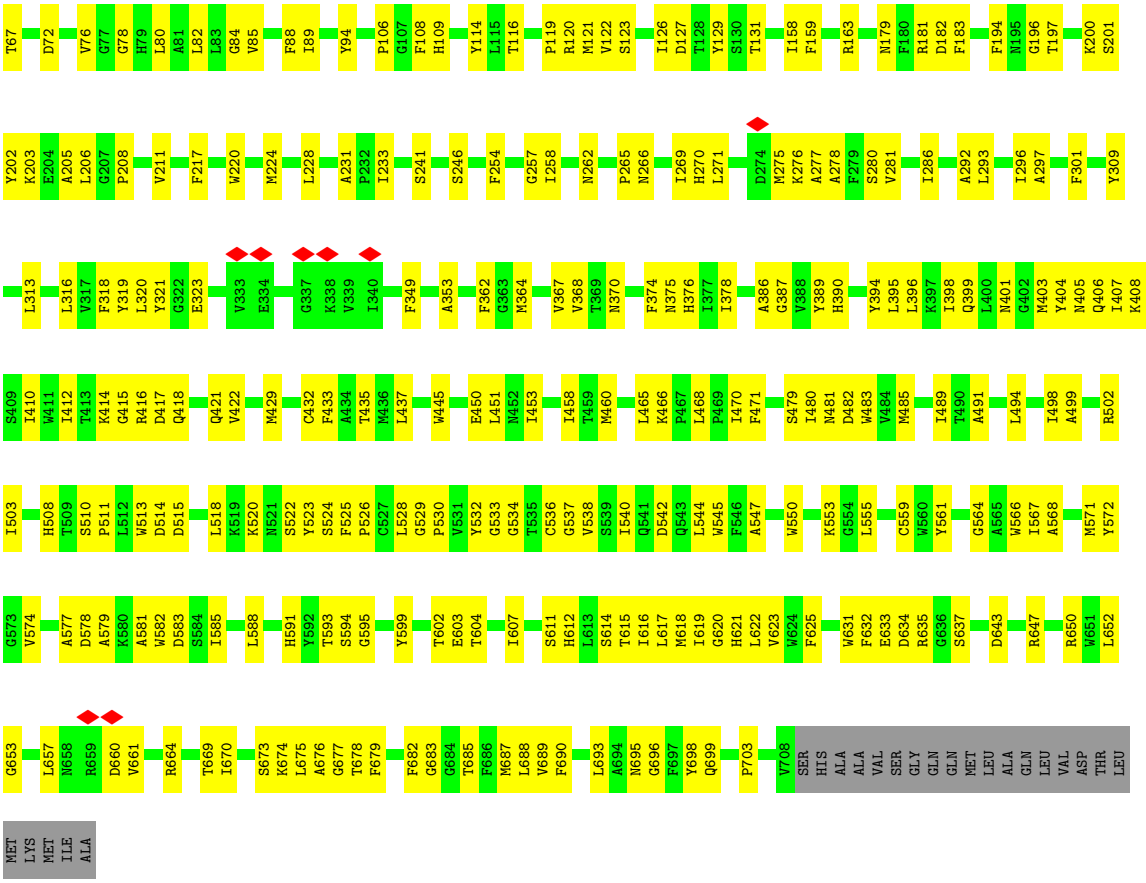
Chain B:



• Molecule 4: Photosystem P840 reaction center, large subunit

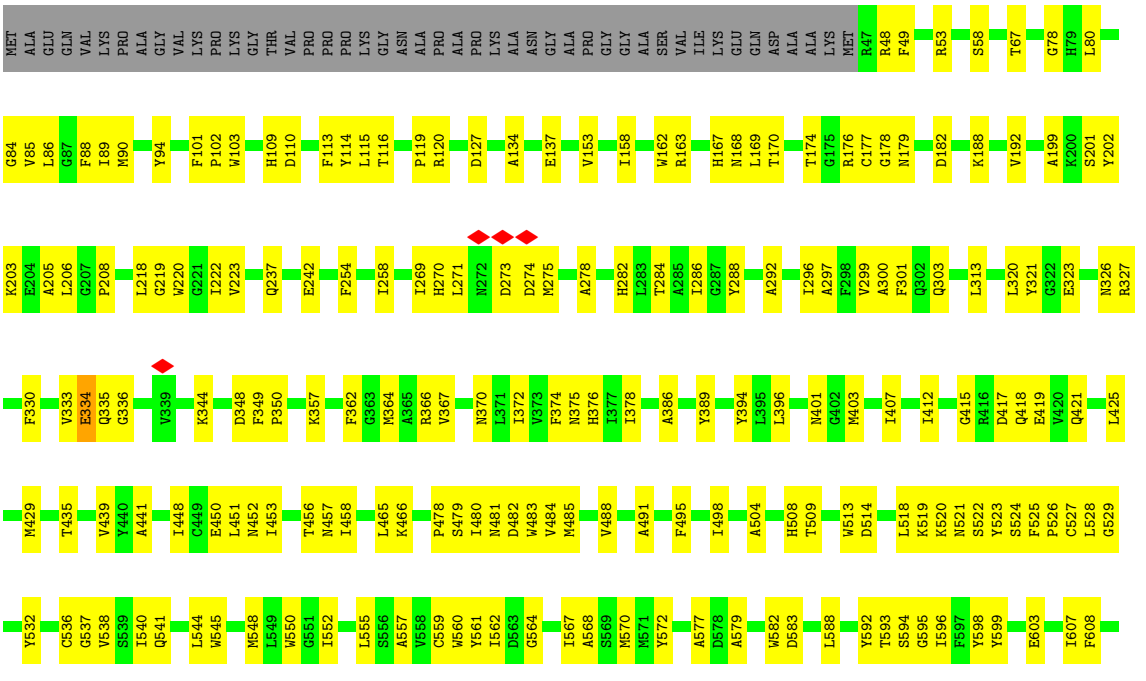
Chain A:

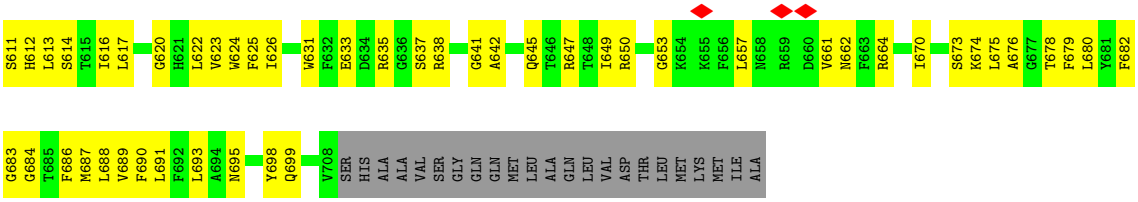




• Molecule 4: Photosystem P840 reaction center, large subunit

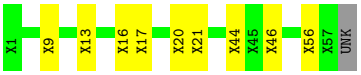
Chain a:





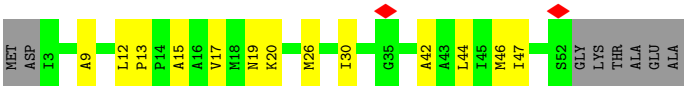
• Molecule 5: unkown protein

Chain E:



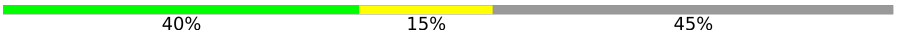
• Molecule 6: Ric1 protein

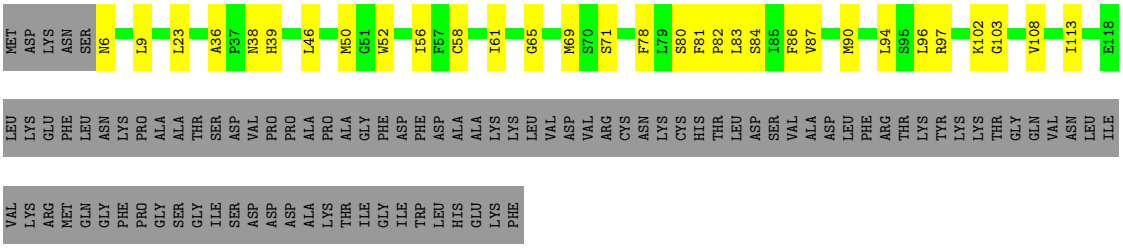
Chain F:



• Molecule 7: Cytochrome c

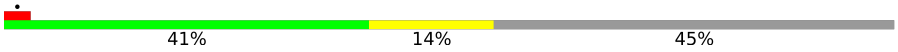
Chain C:

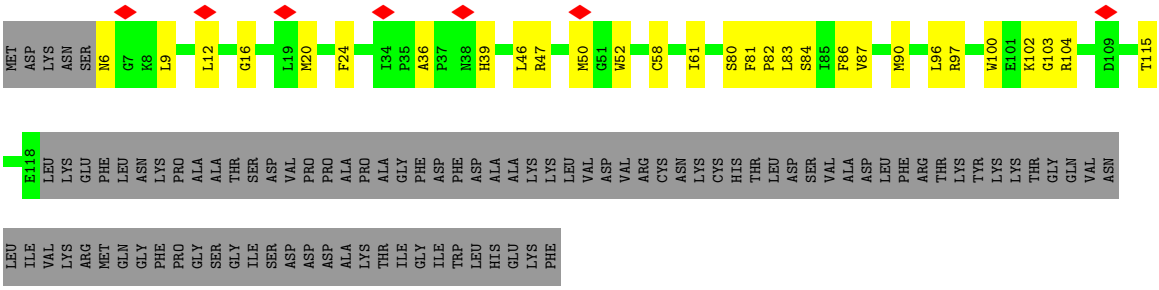




• Molecule 7: Cytochrome c

Chain c:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	227038	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	152200	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.298	Depositor
Minimum map value	-0.557	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	312.80002, 312.80002, 312.80002	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9200001, 0.9200001, 0.9200001	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.14	0/2885	0.35	0/3910
1	2	0.14	0/2859	0.33	0/3875
1	3	0.14	0/2859	0.34	0/3875
1	4	0.15	0/2885	0.37	0/3910
1	5	0.15	0/2859	0.38	0/3875
1	6	0.14	0/2859	0.35	0/3875
2	D	0.14	0/1191	0.39	0/1604
3	B	0.15	0/819	0.41	0/1106
4	A	0.15	0/5528	0.35	0/7527
4	a	0.15	0/5493	0.35	0/7481
6	F	0.12	0/386	0.38	0/525
7	C	0.14	0/898	0.37	0/1216
7	c	0.14	0/898	0.35	0/1216
All	All	0.15	0/32419	0.36	0/43995

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2815	0	2749	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2789	0	2731	105	0
1	3	2789	0	2731	109	0
1	4	2815	0	2749	101	0
1	5	2789	0	2731	112	0
1	6	2789	0	2731	115	0
2	D	1167	0	1188	62	0
3	B	798	0	752	62	0
4	A	5344	0	5236	239	0
4	a	5309	0	5202	209	0
5	E	285	0	60	5	0
6	F	379	0	418	9	0
7	C	875	0	915	27	0
7	c	875	0	915	25	0
8	1	508	0	551	59	0
8	2	554	0	586	60	0
8	3	462	0	516	57	0
8	4	620	0	660	63	0
8	5	396	0	442	48	0
8	6	508	0	551	69	0
8	A	596	0	548	42	0
8	C	46	0	35	4	0
8	F	46	0	35	3	0
8	a	596	0	547	34	0
8	c	46	0	35	6	0
9	1	77	0	103	7	0
9	a	162	0	216	12	0
9	c	70	0	82	3	0
10	A	8	0	0	0	0
10	B	16	0	0	2	0
11	A	66	0	0	4	0
11	a	66	0	0	2	0
12	A	130	0	0	3	0
12	a	130	0	0	1	0
13	A	130	0	0	0	0
13	C	65	0	0	0	0
13	a	65	0	0	1	0
14	A	144	0	211	8	0
14	E	37	0	44	1	0
14	a	128	0	172	10	0
15	A	44	0	57	4	0
15	a	44	0	57	1	0
16	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	a	1	0	0	0	0
17	a	40	0	0	0	0
17	c	40	0	0	0	0
All	All	37660	0	36556	1351	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1351) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:679:PHE:O	14:A:819:LHG:H223	1.73	0.87
4:A:553:LYS:HE2	12:A:822:G2O:NB	1.91	0.84
4:A:515:ASP:HB3	1:5:319:LYS:HG2	1.58	0.84
3:B:152:PRO:HG2	4:A:48:ARG:HB3	1.61	0.83
1:4:36:VAL:HG11	8:4:403:BCL:H3C	1.61	0.82
8:1:401:BCL:HAA1	8:1:401:BCL:HBD	1.63	0.81
8:5:401:BCL:HAA1	8:5:401:BCL:HBD	1.64	0.80
1:2:149:LEU:HD12	1:2:222:ARG:HD2	1.63	0.80
8:A:804:BCL:H43	6:F:26:MET:HE3	1.61	0.80
8:3:401:BCL:HBD	8:3:401:BCL:HAA1	1.66	0.77
1:6:121:ASN:HD21	1:6:236:ILE:HA	1.48	0.77
4:a:334:GLU:HG2	4:a:335:GLN:H	1.50	0.76
1:1:317:LEU:HD11	1:1:323:ILE:HG13	1.67	0.76
8:2:403:BCL:HAA1	8:2:403:BCL:HBD	1.69	0.75
4:a:450:GLU:OE2	4:a:582:TRP:NE1	2.16	0.75
1:6:235:SER:HA	1:6:242:LEU:HD11	1.68	0.75
1:6:317:LEU:HD11	1:6:323:ILE:HG13	1.68	0.75
1:5:123:PHE:HB2	1:5:126:ARG:HE	1.52	0.75
8:6:401:BCL:HAA1	8:6:401:BCL:HBD	1.70	0.74
3:B:221:ARG:NH2	6:F:19:ASN:O	2.20	0.74
1:4:286:ARG:HB3	1:4:363:LEU:HD23	1.70	0.74
1:4:144:GLN:NE2	1:4:235:SER:O	2.21	0.74
4:a:570:MET:HA	4:a:596:ILE:HB	1.70	0.73
1:6:186:ILE:HG21	8:6:406:BCL:H13	1.70	0.73
1:5:95:ARG:HG3	1:5:120:VAL:HG22	1.71	0.72
1:4:199:ARG:NH2	1:6:178:ASP:O	2.23	0.72
1:6:18:ILE:HB	1:6:315:VAL:HG12	1.72	0.72
4:a:603:GLU:O	4:a:695:ASN:ND2	2.22	0.71
4:a:344:LYS:HE3	4:a:350:PRO:HA	1.71	0.71
1:5:50:ASP:OD1	1:5:259:ARG:NH1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:143:ARG:HD2	1:2:228:GLY:HA3	1.71	0.71
2:D:1:MET:N	2:D:16:ARG:O	2.24	0.71
4:A:603:GLU:O	4:A:695:ASN:ND2	2.23	0.71
4:A:121:MET:HE2	8:A:805:BCL:HED3	1.73	0.70
1:3:324:ARG:HH12	1:3:365:ALA:HB3	1.55	0.70
1:5:238:ARG:HH21	8:5:404:BCL:HED2	1.57	0.70
8:4:401:BCL:HAA1	8:4:401:BCL:HBD	1.72	0.70
2:D:25:GLY:H	3:B:212:PRO:HB2	1.56	0.70
4:A:515:ASP:OD2	4:a:647:ARG:NH2	2.25	0.70
1:5:292:LEU:HD22	1:5:357:VAL:HG13	1.73	0.69
4:A:378:ILE:HG13	4:A:555:LEU:HD21	1.75	0.69
4:A:616:ILE:HG12	8:c:301:BCL:HMC3	1.74	0.69
1:3:122:LEU:HD12	8:2:402[B]:BCL:HMA2	1.74	0.69
7:c:39:HIS:HD2	7:c:47:ARG:HH22	1.37	0.69
1:1:70:VAL:HG22	1:1:83:THR:HG23	1.75	0.69
1:3:294:PRO:HG3	8:3:406:BCL:HAC1	1.75	0.69
2:D:29:HIS:NE2	3:B:207:ASP:OD2	2.25	0.68
1:3:144:GLN:NE2	1:3:235:SER:O	2.25	0.68
1:1:259:ARG:NH1	3:B:217:ASP:OD1	2.26	0.68
1:5:190:PHE:HA	1:5:193:LEU:HD12	1.75	0.68
1:2:238:ARG:HD2	8:2:406:BCL:HED3	1.76	0.68
1:2:317:LEU:HD11	1:2:323:ILE:HG13	1.74	0.68
2:D:16:ARG:NH1	4:A:514:ASP:OD1	2.25	0.68
4:a:177:CYS:SG	4:a:178:GLY:N	2.65	0.68
2:D:9:GLN:NE2	4:a:662:ASN:OD1	2.27	0.68
1:5:144:GLN:HG3	1:5:236:ILE:HG13	1.75	0.68
7:C:96:LEU:HD11	8:C:301:BCL:HAA2	1.75	0.68
4:a:269:ILE:HG21	4:a:407:ILE:HG23	1.76	0.68
4:A:269:ILE:HG21	4:A:407:ILE:HG23	1.75	0.68
4:A:206:LEU:HB2	8:A:809:BCL:HHD	1.74	0.68
1:4:72:GLU:HG2	1:4:81:LYS:HG3	1.75	0.67
1:4:183:PHE:HZ	8:4:401:BCL:H12	1.59	0.67
4:A:603:GLU:HG2	4:A:695:ASN:HD21	1.60	0.67
2:D:39:ALA:HB1	2:D:47:LEU:HD12	1.75	0.67
8:4:409:BCL:NC	8:6:406:BCL:H111	2.10	0.67
1:3:313:LEU:HB3	1:3:340:TRP:HB2	1.76	0.67
8:a:806:BCL:H11	8:a:812:BCL:H201	1.75	0.67
1:2:288:LEU:HD11	8:2:406:BCL:HBA1	1.77	0.67
4:A:321:TYR:HB3	8:c:301:BCL:HMA2	1.77	0.67
1:3:143:ARG:NH2	1:3:226:SER:OG	2.26	0.67
4:a:218:LEU:O	4:a:222:ILE:HD12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:95:ARG:HG3	1:1:120:VAL:HG22	1.77	0.66
4:a:366:ARG:NH1	4:a:562:ILE:O	2.28	0.66
1:4:82:LEU:HD13	8:4:407:BCL:H191	1.77	0.66
4:A:206:LEU:HB2	8:A:809:BCL:CHD	2.26	0.66
2:D:70:LEU:HD22	2:D:77:ILE:HD13	1.78	0.66
1:4:288:LEU:HD21	8:4:405:BCL:HBA2	1.77	0.66
8:2:404:BCL:H42	8:2:406:BCL:H151	1.78	0.66
3:B:224:HIS:HA	3:B:228:ARG:HG2	1.78	0.66
1:1:144:GLN:HG3	1:1:236:ILE:HG12	1.78	0.66
4:a:163:ARG:HH11	8:a:807:BCL:HED2	1.61	0.66
8:4:405:BCL:H193	8:4:407:BCL:H203	1.77	0.66
4:A:201:SER:HB2	4:A:271:LEU:HD12	1.78	0.65
4:A:450:GLU:OE2	4:A:582:TRP:NE1	2.27	0.65
4:a:364:MET:HA	4:a:367:VAL:HB	1.75	0.65
1:1:305:ASN:HD21	1:2:351:HIS:HB2	1.61	0.65
1:6:119:VAL:HG11	1:6:144:GLN:HE21	1.60	0.65
2:D:87:ALA:HB2	2:D:143:LYS:HD3	1.78	0.65
3:B:171:ARG:NH2	1:5:366:GLN:O	2.30	0.65
8:6:401:BCL:HBB2	8:6:401:BCL:H93	1.78	0.65
1:2:128:ASP:OD1	1:2:131:ARG:NH1	2.30	0.65
4:A:67:THR:HB	4:A:275:MET:HB3	1.78	0.65
1:1:11:THR:HG21	9:1:409:CDL:HA21	1.78	0.65
1:4:284:LEU:HA	1:4:365:ALA:HB2	1.79	0.65
1:5:70:VAL:HG13	1:5:83:THR:HG22	1.77	0.65
2:D:104:ASP:HB3	2:D:107:LYS:HA	1.79	0.65
4:A:683:GLY:O	4:A:687:MET:HG3	1.97	0.65
4:a:203:LYS:H	4:a:271:LEU:HD11	1.60	0.65
4:a:509:THR:OG1	4:a:514:ASP:OD1	2.12	0.64
1:2:256:ALA:HB2	1:2:269:VAL:HG23	1.78	0.64
4:A:529:GLY:HA2	4:a:529:GLY:HA2	1.80	0.64
4:a:452:ASN:ND2	4:a:456:THR:O	2.30	0.64
4:a:679:PHE:HE1	8:a:813:BCL:HBC1	1.61	0.64
1:1:310:ASP:O	3:B:225:ARG:NH2	2.28	0.64
4:a:201:SER:HB2	4:a:271:LEU:HD12	1.77	0.64
1:6:96:ARG:HG2	8:6:405:BCL:HED2	1.80	0.64
8:6:408:BCL:H12	8:5:401:BCL:H12	1.80	0.64
8:1:406:BCL:H111	8:2:401:BCL:NC	2.12	0.64
2:D:112:TRP:NE1	3:B:175:ASP:OD1	2.31	0.64
1:1:33:ARG:NH1	1:1:270:ASP:OD2	2.31	0.64
1:3:96:ARG:NH2	1:3:239:TRP:O	2.31	0.64
2:D:20:SER:OG	3:B:217:ASP:OD2	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:811:BCL:H143	8:A:811:BCL:HAC2	1.79	0.64
1:4:250:ARG:NH2	1:4:272:GLU:OE2	2.30	0.64
8:6:408:BCL:HAC1	8:5:406:BCL:H52	1.80	0.64
1:4:50:ASP:OD2	1:4:52:LYS:NZ	2.29	0.63
4:a:335:GLN:HG3	4:a:336:GLY:H	1.63	0.63
3:B:133:TYR:HH	3:B:183:SER:HG	1.35	0.63
1:1:148:ILE:HG12	8:1:405:BCL:HMA1	1.80	0.63
1:3:50:ASP:OD1	1:3:259:ARG:NH1	2.26	0.63
4:a:481:ASN:HA	4:a:568:ALA:HB2	1.79	0.63
1:1:279:ASP:OD1	1:1:285:ARG:NH1	2.31	0.63
3:B:131:LYS:HB3	3:B:201:PRO:HD3	1.81	0.63
4:a:617:LEU:HA	4:a:688:LEU:HD22	1.79	0.63
4:a:690:PHE:HB2	8:a:811:BCL:H42	1.80	0.63
1:6:19:VAL:HG12	1:6:316:VAL:HB	1.80	0.63
1:1:96:ARG:HB2	1:1:239:TRP:HZ2	1.64	0.63
4:a:199:ALA:HB3	8:a:808:BCL:H2C	1.81	0.63
14:E:101:LHG:HC81	7:C:9:LEU:HB3	1.81	0.63
4:A:633:GLU:HB2	4:a:674:LYS:HE2	1.80	0.63
1:1:169:ALA:O	1:1:173:THR:OG1	2.17	0.62
1:3:55:VAL:HG22	1:3:67:ILE:HG13	1.81	0.62
1:4:184:TRP:HE1	8:4:406:BCL:HBB1	1.64	0.62
7:c:87:VAL:HA	7:c:90:MET:HG3	1.80	0.62
1:3:344:ALA:HA	1:3:347:ARG:HD3	1.79	0.62
2:D:9:GLN:OE1	4:a:664:ARG:NH2	2.31	0.62
4:A:203:LYS:H	4:A:271:LEU:HD11	1.64	0.62
3:B:199:VAL:HG12	3:B:205:VAL:HG22	1.80	0.62
2:D:136:TYR:HB3	2:D:142:PHE:HB2	1.81	0.62
1:6:18:ILE:HG12	1:6:30:VAL:HG22	1.81	0.62
1:5:313:LEU:HB3	1:5:340:TRP:HB2	1.80	0.62
4:A:203:LYS:HB3	4:A:271:LEU:HD21	1.80	0.62
8:4:401:BCL:HBB2	8:4:401:BCL:H93	1.80	0.62
1:6:125:TYR:O	1:6:126:ARG:NE	2.31	0.62
1:6:90:ASN:HD21	1:6:96:ARG:HH21	1.48	0.62
1:3:232:MET:HA	1:3:292:LEU:HD23	1.81	0.62
1:2:99:VAL:HG23	1:2:116:GLU:HG2	1.82	0.62
1:2:331:ARG:NH2	1:2:341:SER:O	2.33	0.62
4:a:564:GLY:HA3	4:a:699:GLN:HG3	1.80	0.62
2:D:22:PRO:HG2	4:A:418:GLN:HE21	1.65	0.61
1:6:95:ARG:HA	1:6:120:VAL:HA	1.81	0.61
1:3:180:ILE:O	1:3:184:TRP:HB2	2.00	0.61
7:C:97:ARG:NH1	7:C:102:LYS:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:MET:HE3	1:5:281:GLY:HA3	1.83	0.61
4:a:386:ALA:HB2	8:a:813:BCL:HMC3	1.83	0.61
1:6:36:VAL:HG12	1:6:38:ALA:H	1.65	0.61
2:D:118:PRO:HB2	1:5:24:SER:HB3	1.83	0.61
4:a:465:LEU:HB3	4:a:480:ILE:HD13	1.81	0.61
1:6:294:PRO:HG3	8:6:406:BCL:HAC1	1.82	0.61
4:a:616:ILE:HG12	8:C:301:BCL:HMC3	1.82	0.61
1:5:294:PRO:HG3	8:5:406:BCL:HAC1	1.83	0.61
1:3:238:ARG:HH22	1:3:289:ASN:HB2	1.66	0.61
4:A:66:ASP:OD1	4:A:276:LYS:NZ	2.33	0.61
4:A:622:LEU:HA	4:A:625:PHE:CE1	2.36	0.61
1:1:108:ASP:OD1	1:1:109:PHE:N	2.33	0.61
1:3:121:ASN:HD21	1:3:236:ILE:HA	1.65	0.61
4:a:48:ARG:HH12	1:4:261:ASP:HB3	1.66	0.60
1:4:164:GLU:HA	1:4:167:VAL:HG22	1.83	0.60
1:1:188:PRO:HB2	8:1:406:BCL:HBA1	1.83	0.60
4:A:482:ASP:OD1	4:A:561:TYR:OH	2.19	0.60
1:2:286:ARG:HB3	1:2:363:LEU:HD23	1.82	0.60
6:F:12:LEU:HD23	6:F:15:ALA:HB2	1.83	0.60
8:6:408:BCL:NC	8:5:406:BCL:H111	2.15	0.60
4:A:415:GLY:O	4:A:421:GLN:NE2	2.29	0.60
4:a:415:GLY:O	4:a:421:GLN:NE2	2.33	0.60
1:2:34:ALA:HB3	1:2:267:VAL:HB	1.82	0.60
4:a:321:TYR:HB3	8:C:301:BCL:HMA2	1.83	0.60
1:4:143:ARG:NH2	1:6:182:ASP:OD2	2.35	0.60
1:6:70:VAL:HG22	1:6:83:THR:HG22	1.84	0.60
1:4:238:ARG:NH1	1:4:289:ASN:OD1	2.35	0.60
1:6:50:ASP:HB2	1:6:72:GLU:HB2	1.82	0.60
2:D:42:ASP:OD2	2:D:48:GLN:NE2	2.34	0.60
2:D:122:HIS:O	2:D:123:GLU:HB2	2.01	0.60
8:4:410[B]:BCL:HMA2	1:5:122:LEU:HD12	1.84	0.60
1:5:53:LEU:HB3	8:5:405:BCL:H203	1.82	0.60
4:a:670:ILE:HG22	4:a:674:LYS:HE3	1.84	0.60
1:1:348:TRP:NE1	1:1:358:GLY:O	2.28	0.60
4:a:559:CYS:SG	4:a:689:VAL:HG13	2.41	0.60
7:C:80:SER:HA	7:C:83:LEU:HB2	1.84	0.60
1:6:34:ALA:HB3	1:6:267:VAL:HB	1.84	0.59
1:4:96:ARG:HB2	1:4:239:TRP:HZ2	1.67	0.59
1:1:144:GLN:OE1	1:1:227:HIS:NE2	2.36	0.59
4:A:407:ILE:HG21	4:A:412:ILE:HD12	1.83	0.59
4:A:451:LEU:HB3	4:a:611:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:617:LEU:HA	4:A:688:LEU:HD22	1.84	0.59
1:6:238:ARG:NH1	1:6:289:ASN:O	2.26	0.59
1:5:34:ALA:HB3	1:5:267:VAL:HB	1.83	0.59
4:A:78:GLY:HA3	8:A:803:BCL:HBA2	1.84	0.59
1:3:256:ALA:HB3	8:3:404:BCL:H92	1.84	0.59
2:D:108:ARG:NH2	3:B:155:ASN:O	2.35	0.59
8:4:402:BCL:HAC1	8:4:407:BCL:H52	1.83	0.59
1:4:19:VAL:HG22	1:4:316:VAL:HB	1.83	0.59
1:6:132:ARG:NH1	1:5:158:ASP:OD2	2.25	0.59
1:5:41:ALA:HB3	1:5:301:VAL:HG23	1.84	0.59
1:5:74:ILE:HG12	1:5:79:LYS:HG2	1.85	0.59
1:3:306:ASN:OD1	1:2:306:ASN:ND2	2.35	0.59
4:A:386:ALA:O	4:A:390:HIS:ND1	2.35	0.59
3:B:133:TYR:HA	3:B:198:GLU:HA	1.84	0.59
1:1:188:PRO:HG3	8:1:406:BCL:H2	1.84	0.58
1:3:143:ARG:HH22	1:3:201:SER:HB3	1.67	0.58
1:3:297:HIS:HE1	8:3:406:BCL:NB	1.96	0.58
4:A:669:THR:O	4:A:673:SER:N	2.23	0.58
1:4:324:ARG:HH12	1:4:365:ALA:HB3	1.67	0.58
7:c:9:LEU:HD22	9:c:303:CDL:H711	1.84	0.58
1:3:180:ILE:HD11	8:3:401:BCL:H192	1.84	0.58
1:2:325:TYR:HE2	4:A:406:GLN:HE22	1.50	0.58
4:a:116:THR:HG23	4:a:372:ILE:HG12	1.85	0.58
1:6:58:LEU:HD13	1:6:64:PHE:HB3	1.84	0.58
4:A:49:PHE:O	4:A:53:ARG:NH2	2.36	0.58
4:a:116:THR:HG21	8:a:811:BCL:HMA2	1.85	0.58
1:1:238:ARG:NH1	1:1:289:ASN:O	2.36	0.58
4:a:622:LEU:HA	4:a:625:PHE:CE1	2.38	0.58
7:c:20:MET:HE2	7:c:24:PHE:HE2	1.68	0.58
3:B:167:GLU:OE1	1:5:333:GLN:NE2	2.36	0.58
1:4:46:PRO:HB3	1:4:261:ASP:HA	1.85	0.58
1:5:35:LYS:NZ	5:E:56:UNK:O	2.36	0.58
4:a:206:LEU:HB2	8:a:810:BCL:HHD	1.86	0.58
1:5:144:GLN:NE2	1:5:235:SER:O	2.37	0.58
1:1:260:SER:O	3:B:215:ARG:NH2	2.36	0.58
3:B:165:VAL:HG22	4:a:525:PHE:HB2	1.85	0.58
4:a:84:GLY:HA3	4:a:158:ILE:HG13	1.85	0.58
1:5:253:GLN:NE2	1:5:255:GLU:OE2	2.37	0.58
1:3:180:ILE:O	1:3:184:TRP:CB	2.52	0.58
4:a:483:TRP:HE1	8:a:814:BCL:C1D	2.16	0.58
8:4:409:BCL:HAA1	8:6:406:BCL:H142	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:264:GLY:HA3	4:A:408:LYS:HG3	1.86	0.57
4:a:94:TYR:OH	8:a:806:BCL:O1D	2.21	0.57
1:5:181:ARG:NH1	1:5:200:ILE:O	2.37	0.57
4:A:607:ILE:HG13	4:A:695:ASN:HD22	1.69	0.57
1:6:128:ASP:OD1	1:6:131:ARG:NH2	2.37	0.57
8:6:403:BCL:H72	8:6:404:BCL:H52	1.86	0.57
1:3:321:TYR:HD1	1:3:366:GLN:HB3	1.70	0.57
1:1:313:LEU:HB3	1:1:340:TRP:HB2	1.86	0.57
1:6:141:GLN:NE2	1:5:183:PHE:O	2.37	0.57
4:a:401:ASN:HD21	4:a:403:MET:HE2	1.68	0.57
1:5:51:VAL:HG21	8:5:403:BCL:H152	1.86	0.57
4:A:396:LEU:HD23	4:A:523:TYR:HB3	1.85	0.57
4:A:84:GLY:HA3	4:A:158:ILE:HG13	1.86	0.57
1:1:74:ILE:HG12	1:1:79:LYS:HG2	1.86	0.57
2:D:62:PRO:O	2:D:66:MET:HB2	2.05	0.57
4:A:508:HIS:ND1	4:A:520:LYS:O	2.38	0.57
1:6:99:VAL:HG23	1:6:116:GLU:HG2	1.86	0.57
1:1:259:ARG:NH1	3:B:216:LEU:O	2.37	0.57
1:3:17:GLU:HB3	1:3:31:LYS:HG3	1.86	0.57
4:A:571:MET:HE3	4:a:614:SER:HB3	1.87	0.57
1:6:90:ASN:OD1	1:6:96:ARG:NE	2.37	0.57
1:5:335:LEU:O	1:5:336:GLU:HB2	2.04	0.57
1:4:27:TRP:HA	1:4:274:PRO:HA	1.86	0.56
1:1:88:ILE:HG12	1:1:98:SER:HB2	1.86	0.56
8:1:406:BCL:H71	1:2:139:TYR:HE2	1.70	0.56
1:3:150:MET:HE2	1:3:223:TRP:NE1	2.19	0.56
8:3:407:BCL:H192	8:2:403:BCL:HMC3	1.87	0.56
2:D:13:ASN:ND2	1:5:22:GLY:O	2.38	0.56
9:a:822:CDL:H172	9:a:822:CDL:H382	1.86	0.56
3:B:215:ARG:HD3	4:A:405:ASN:HB3	1.87	0.56
4:a:286:ILE:HG21	8:a:804:BCL:HBC3	1.86	0.56
1:5:268:LYS:NZ	1:5:270:ASP:OD1	2.38	0.56
4:A:485:MET:HA	4:A:567:ILE:HD11	1.86	0.56
8:5:402:BCL:H42	8:5:404:BCL:H151	1.87	0.56
5:E:17:UNK:O	5:E:21:UNK:N	2.38	0.56
1:2:153:PRO:HA	1:2:218:VAL:HA	1.87	0.56
8:4:409:BCL:H141	1:6:84:ILE:HG21	1.88	0.56
8:4:409:BCL:H3A	8:6:401:BCL:OBD	2.05	0.56
1:3:27:TRP:HA	1:3:274:PRO:HA	1.86	0.56
4:A:410:ILE:O	4:A:414:LYS:HG2	2.06	0.56
4:a:78:GLY:HA2	7:C:78:PHE:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:806:BCL:HBB3	8:a:808:BCL:H101	1.88	0.56
1:5:306:ASN:O	1:5:306:ASN:ND2	2.34	0.56
4:A:489:ILE:HD12	15:A:817:LMG:H181	1.87	0.56
1:1:180:ILE:HG21	1:1:203:ILE:HG12	1.88	0.56
8:3:407:BCL:H72	8:2:403:BCL:HAC1	1.87	0.56
1:2:15:ASP:OD1	4:A:181:ARG:NH2	2.34	0.56
7:C:38:ASN:O	7:C:39:HIS:ND1	2.38	0.56
4:a:110:ASP:HB3	4:a:115:LEU:HD11	1.87	0.56
4:A:293:LEU:HD11	8:A:805:BCL:H141	1.87	0.56
1:3:199:ARG:NH2	1:2:178:ASP:O	2.39	0.55
1:4:38:ALA:HA	1:5:347:ARG:HD3	1.87	0.55
1:6:297:HIS:HE1	8:6:406:BCL:NB	2.02	0.55
1:1:331:ARG:HE	1:1:341:SER:HB3	1.69	0.55
1:5:333:GLN:HG2	1:5:335:LEU:H	1.71	0.55
4:A:483:TRP:HE1	8:F:101:BCL:C1D	2.19	0.55
8:1:401:BCL:OBD	8:2:401:BCL:H3A	2.07	0.55
4:A:670:ILE:HA	4:A:673:SER:HB2	1.88	0.55
4:A:674:LYS:HE2	4:a:633:GLU:HB2	1.89	0.55
4:a:676:ALA:HB1	14:a:821:LHG:HC91	1.89	0.55
1:1:323:ILE:HD12	1:1:338:TYR:CG	2.42	0.55
4:A:399:GLN:HG2	4:A:404:TYR:CG	2.41	0.55
4:a:120:ARG:NH2	4:a:242:GLU:OE2	2.35	0.55
1:2:284:LEU:HD12	1:2:365:ALA:HB2	1.89	0.55
1:6:328:PRO:HD2	1:6:360:PHE:HD1	1.70	0.55
4:A:682:PHE:HD2	8:A:810:BCL:H121	1.71	0.55
4:a:508:HIS:ND1	4:a:520:LYS:O	2.39	0.55
9:a:820:CDL:H731	9:a:820:CDL:H511	1.89	0.55
1:1:17:GLU:HB2	3:B:223:LEU:HD23	1.87	0.55
1:2:143:ARG:HH22	1:2:201:SER:HB3	1.70	0.55
4:A:254:PHE:O	4:A:258:ILE:HG12	2.06	0.55
6:F:44:LEU:HA	6:F:47:ILE:HG22	1.88	0.55
3:B:167:GLU:OE2	1:5:338:TYR:OH	2.20	0.55
4:a:170:THR:HA	4:a:177:CYS:HA	1.89	0.55
4:a:675:LEU:HD21	9:a:820:CDL:H142	1.87	0.55
1:2:19:VAL:HB	1:2:29:LYS:HB2	1.88	0.55
4:A:109:HIS:NE2	7:c:103:GLY:O	2.40	0.55
4:A:594:SER:OG	4:A:602:THR:OG1	2.25	0.55
4:A:620:GLY:HA3	4:A:688:LEU:HD21	1.90	0.55
4:a:174:THR:HG21	4:a:176:ARG:NH1	2.22	0.55
8:a:812:BCL:HAC2	8:a:812:BCL:H143	1.89	0.55
4:A:520:LYS:HG2	4:A:525:PHE:HZ	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:564:GLY:HA3	4:A:699:GLN:HG3	1.87	0.54
8:1:401:BCL:H203	8:1:401:BCL:HBC1	1.88	0.54
9:1:409:CDL:H111	9:1:409:CDL:H521	1.88	0.54
1:2:178:ASP:HB3	1:2:202:ARG:HG2	1.88	0.54
2:D:127:LEU:HB3	2:D:138:LEU:HD12	1.89	0.54
4:A:131:THR:HG22	7:c:115:THR:HG21	1.88	0.54
8:A:805:BCL:HMD3	8:A:811:BCL:H152	1.89	0.54
1:5:189:ALA:HB1	8:5:406:BCL:HMB3	1.90	0.54
1:5:339:ARG:HH22	7:C:71:SER:HB2	1.72	0.54
1:1:138:ILE:HG21	1:3:43:PRO:HB2	1.89	0.54
8:1:408:BCL:H3A	8:3:401:BCL:OBD	2.06	0.54
4:A:690:PHE:HB2	8:A:810:BCL:H42	1.88	0.54
8:4:401:BCL:OBD	8:4:402:BCL:H3A	2.07	0.54
1:6:45:LEU:HD13	1:6:262:SER:HA	1.90	0.54
1:2:75:VAL:O	1:2:78:THR:HG22	2.07	0.54
4:a:163:ARG:HD3	4:a:168:ASN:OD1	2.07	0.54
2:D:83:GLN:HG3	2:D:85:ASP:H	1.73	0.54
4:A:55:GLU:HG3	4:A:526:PRO:HD3	1.89	0.54
4:a:653:GLY:HA2	4:a:657:LEU:HB2	1.89	0.54
8:1:406:BCL:H41	8:2:401:BCL:HBC1	1.90	0.54
1:2:193:LEU:HD21	1:2:200:ILE:HG12	1.89	0.54
4:A:82:LEU:HD11	8:A:803:BCL:HBD	1.89	0.54
4:A:159:PHE:CZ	4:A:163:ARG:HD2	2.42	0.54
4:a:485:MET:SD	4:a:561:TYR:HB2	2.47	0.54
4:a:607:ILE:HG13	4:a:695:ASN:HD22	1.72	0.54
4:a:617:LEU:HD11	11:a:802:GS0:CHD	2.38	0.54
1:4:185:PHE:CZ	1:4:200:ILE:HG13	2.42	0.54
2:D:82:THR:HB	2:D:114:MET:HG3	1.89	0.54
9:a:822:CDL:H211	9:a:822:CDL:H441	1.90	0.54
4:a:254:PHE:O	4:a:258:ILE:HG12	2.08	0.54
1:4:205:VAL:HG12	1:4:207:GLY:H	1.73	0.54
4:A:270:HIS:HB3	4:A:278:ALA:HB2	1.90	0.53
4:a:620:GLY:HA3	4:a:688:LEU:HD21	1.89	0.53
1:4:141:GLN:HG2	1:6:183:PHE:HA	1.90	0.53
1:6:188:PRO:HB2	8:6:406:BCL:HBA1	1.90	0.53
4:a:333:VAL:O	4:a:335:GLN:N	2.40	0.53
7:C:81:PHE:HB3	7:C:82:PRO:HD3	1.91	0.53
4:a:109:HIS:NE2	7:C:103:GLY:O	2.34	0.53
4:a:334:GLU:HG2	4:a:335:GLN:N	2.21	0.53
1:6:143:ARG:HH12	1:6:201:SER:HB3	1.72	0.53
1:6:186:ILE:HG22	8:6:402:BCL:H92	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:313:LEU:HD21	1:6:315:VAL:HG13	1.90	0.53
4:a:485:MET:HA	4:a:567:ILE:HD11	1.90	0.53
1:4:96:ARG:HG2	8:4:406:BCL:HED2	1.90	0.53
1:5:340:TRP:HB3	1:5:345:TYR:CG	2.44	0.53
4:A:398:ILE:HB	4:A:403:MET:HB3	1.90	0.53
4:A:545:TRP:CG	4:A:678:THR:HG1	2.25	0.53
1:3:170:ILE:HD13	1:3:208:LEU:HD22	1.89	0.53
4:a:162:TRP:CZ2	1:4:6:SER:HB3	2.44	0.53
4:a:520:LYS:HG2	4:a:525:PHE:CZ	2.44	0.53
1:4:291:PRO:HB2	1:4:294:PRO:HG2	1.91	0.53
1:5:27:TRP:HA	1:5:274:PRO:HA	1.91	0.53
1:1:84:ILE:HG21	8:2:401:BCL:H141	1.91	0.53
1:1:300:MET:HE2	8:1:406:BCL:HBA2	1.91	0.53
2:D:33:LYS:HE2	2:D:35:PHE:CZ	2.43	0.53
4:A:395:LEU:HD12	4:A:398:ILE:HD11	1.91	0.53
4:A:510:SER:O	4:A:514:ASP:N	2.33	0.53
4:a:49:PHE:O	4:a:53:ARG:HG2	2.09	0.53
1:2:294:PRO:HG3	8:2:408:BCL:HAC1	1.90	0.53
4:A:422:VAL:HG22	4:A:511:PRO:HG3	1.91	0.53
4:A:502:ARG:HH22	4:a:637:SER:HA	1.72	0.53
4:a:466:LYS:HG2	4:a:479:SER:HA	1.90	0.53
4:a:518:LEU:HD22	4:a:528:LEU:HD13	1.91	0.53
1:6:188:PRO:HG3	8:6:406:BCL:H2	1.91	0.53
1:3:184:TRP:CD1	8:3:401:BCL:H193	2.44	0.53
8:3:407:BCL:HAC1	8:2:408:BCL:H52	1.91	0.53
1:2:184:TRP:CZ3	1:2:200:ILE:HG21	2.44	0.53
7:C:65:GLY:O	7:C:69:MET:HG2	2.09	0.53
1:3:52:LYS:HD3	1:3:255:GLU:HG3	1.91	0.52
3:B:135:ILE:HG13	3:B:174:ILE:HG13	1.91	0.52
4:A:545:TRP:CE3	4:A:678:THR:HG21	2.45	0.52
4:A:679:PHE:HB3	14:A:819:LHG:H141	1.91	0.52
1:2:126:ARG:HE	1:2:131:ARG:HH21	1.57	0.52
4:a:526:PRO:HG3	4:a:670:ILE:HB	1.90	0.52
4:a:688:LEU:HA	4:a:691:LEU:HG	1.90	0.52
8:4:402:BCL:H171	8:4:406:BCL:HMB2	1.90	0.52
8:4:405:BCL:H203	8:4:406:BCL:H52	1.91	0.52
1:3:303:LYS:HD2	1:2:303:LYS:HD2	1.91	0.52
2:D:37:THR:HG21	2:D:52:VAL:HB	1.90	0.52
3:B:182:CYS:N	10:B:302:SF4:S2	2.78	0.52
3:B:192:PRO:HG3	4:A:528:LEU:HD22	1.91	0.52
9:a:822:CDL:H422	9:a:822:CDL:H191	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:359:GLN:HB3	1:6:45:LEU:HB2	1.90	0.52
1:6:203:ILE:HG22	1:6:225:PHE:HB3	1.92	0.52
1:5:93:LYS:NZ	1:5:126:ARG:HH12	2.07	0.52
1:3:34:ALA:HB3	1:3:267:VAL:HB	1.91	0.52
1:3:321:TYR:CD1	1:3:366:GLN:HB3	2.44	0.52
4:A:414:LYS:HB2	8:A:804:BCL:H11	1.91	0.52
4:a:206:LEU:HB2	8:a:810:BCL:CHD	2.39	0.52
4:a:572:TYR:HB3	4:a:595:GLY:N	2.24	0.52
5:E:44:UNK:O	5:E:46:UNK:N	2.42	0.52
14:A:816:LHG:H302	15:A:817:LMG:H182	1.92	0.52
1:4:51:VAL:HG21	8:4:404:BCL:H152	1.92	0.52
1:6:269:VAL:HG21	8:6:403:BCL:H52	1.90	0.52
1:6:313:LEU:HB3	1:6:340:TRP:HB2	1.91	0.52
8:5:403:BCL:HBB2	8:5:404:BCL:H51	1.91	0.52
1:1:183:PHE:HA	1:2:141:GLN:HG2	1.90	0.52
8:5:403:BCL:H72	8:5:404:BCL:H41	1.91	0.52
1:6:151:LYS:HG2	1:6:220:VAL:HG13	1.92	0.52
1:6:359:GLN:OE1	1:5:44:LEU:HA	2.10	0.52
1:1:96:ARG:HB2	1:1:239:TRP:CZ2	2.44	0.52
1:1:122:LEU:HD12	8:1:407[B]:BCL:HMA2	1.91	0.52
1:3:185:PHE:CE2	1:3:200:ILE:HG13	2.45	0.52
1:2:13:HIS:HB2	1:2:35:LYS:HB2	1.93	0.52
1:2:181:ARG:NH1	1:2:200:ILE:O	2.43	0.52
1:2:297:HIS:HE1	8:2:408:BCL:NB	2.02	0.52
4:A:292:ALA:O	4:A:296:ILE:HG12	2.10	0.52
4:a:376:HIS:HE1	8:a:812:BCL:NA	2.07	0.52
1:5:19:VAL:HB	1:5:29:LYS:HB2	1.92	0.52
1:1:295:LEU:HD22	1:1:352:VAL:HB	1.92	0.51
4:A:523:TYR:HB2	4:A:540:ILE:HD11	1.93	0.51
4:A:532:TYR:HB3	1:5:335:LEU:HD11	1.92	0.51
4:a:174:THR:HG21	4:a:176:ARG:HH11	1.74	0.51
1:4:178:ASP:HB2	1:4:181:ARG:HH21	1.74	0.51
1:6:66:ARG:HH22	1:6:85:GLU:HG3	1.74	0.51
1:6:298:HIS:O	1:6:302:GLY:N	2.43	0.51
1:1:312:GLN:NE2	1:1:339:ARG:HD3	2.26	0.51
1:6:57:PRO:HA	1:6:65:VAL:HA	1.91	0.51
8:5:401:BCL:HAA1	8:5:401:BCL:CBD	2.38	0.51
1:1:172:SER:OG	8:2:409[B]:BCL:O1A	2.21	0.51
9:1:409:CDL:HA61	4:A:265:PRO:HB3	1.93	0.51
1:3:103:MET:HE1	1:3:105:SER:HB3	1.93	0.51
1:3:318:PRO:HD2	1:3:321:TYR:HD2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:152:PRO:HB3	4:A:47:ARG:HB3	1.92	0.51
4:A:466:LYS:HG2	4:A:479:SER:HA	1.91	0.51
4:A:513:TRP:CH2	4:A:538:VAL:HG21	2.46	0.51
8:4:409:BCL:H2	8:6:406:BCL:H141	1.93	0.51
1:6:170:ILE:HD12	1:6:208:LEU:HD11	1.92	0.51
1:3:64:PHE:HA	1:3:89:ALA:HB2	1.92	0.51
4:A:386:ALA:HB2	8:A:812:BCL:HMC3	1.92	0.51
8:6:408:BCL:H171	8:5:405:BCL:HMB2	1.91	0.51
2:D:80:LEU:HD11	3:B:205:VAL:HG11	1.93	0.51
14:a:817:LHG:HC62	15:a:818:LMG:HC8	1.93	0.51
1:1:6:SER:HB3	4:A:262:ASN:HA	1.91	0.51
4:A:603:GLU:HG2	4:A:695:ASN:ND2	2.26	0.51
1:6:18:ILE:HD11	8:6:403:BCL:HAA1	1.93	0.51
1:6:180:ILE:O	1:6:184:TRP:CB	2.59	0.51
6:F:9:ALA:HA	6:F:13:PRO:HA	1.93	0.51
1:3:143:ARG:HD2	1:3:228:GLY:HA3	1.93	0.51
8:3:407:BCL:H3A	8:2:403:BCL:OBD	2.10	0.51
4:A:163:ARG:NE	8:A:806:BCL:HED2	2.26	0.51
4:A:465:LEU:HB3	4:A:480:ILE:HD13	1.93	0.51
4:a:88:PHE:HB3	7:C:86:PHE:CZ	2.46	0.51
1:4:43:PRO:HD2	8:4:402:BCL:HMD2	1.93	0.51
7:c:81:PHE:HB3	7:c:82:PRO:HD3	1.91	0.51
1:3:111:HIS:HB3	1:3:159:LEU:HD21	1.92	0.51
1:3:144:GLN:OE1	1:3:227:HIS:NE2	2.43	0.51
1:2:333:GLN:NE2	1:2:335:LEU:O	2.44	0.51
4:A:503:ILE:HA	4:A:540:ILE:HG22	1.92	0.51
1:6:111:HIS:O	1:6:111:HIS:ND1	2.44	0.51
1:6:185:PHE:CZ	1:6:200:ILE:HG13	2.45	0.51
1:5:306:ASN:HD22	1:5:306:ASN:C	2.13	0.51
1:1:19:VAL:HB	1:1:29:LYS:HB2	1.92	0.51
1:5:88:ILE:HG12	1:5:98:SER:HB2	1.92	0.51
8:1:403:BCL:HBB2	8:1:404:BCL:H51	1.92	0.50
4:a:624:TRP:HB2	4:a:684:GLY:HA3	1.93	0.50
8:6:405:BCL:H2A	8:6:405:BCL:O2D	2.11	0.50
8:5:402:BCL:H13	8:5:404:BCL:H191	1.93	0.50
5:E:16:UNK:O	5:E:20:UNK:N	2.44	0.50
7:c:96:LEU:HG	8:c:301:BCL:HAA2	1.93	0.50
1:3:139:TYR:HE1	1:3:292:LEU:HD21	1.76	0.50
2:D:3:PRO:O	4:a:650:ARG:NH2	2.42	0.50
2:D:18:ALA:O	2:D:21:GLY:N	2.43	0.50
2:D:54:ALA:HB1	3:B:207:ASP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:108:PHE:CE1	7:c:97:ARG:HB2	2.46	0.50
4:a:284:THR:HG23	8:a:805:BCL:HMC3	1.93	0.50
1:6:56:LYS:O	1:6:66:ARG:N	2.44	0.50
1:6:144:GLN:HE22	8:6:405:BCL:C1D	2.24	0.50
1:5:50:ASP:N	1:5:72:GLU:O	2.37	0.50
1:1:73:SER:O	1:1:80:ASN:N	2.43	0.50
1:3:22:GLY:HA2	1:3:321:TYR:CE2	2.47	0.50
4:a:357:LYS:HD3	4:a:362:PHE:CD2	2.47	0.50
1:6:313:LEU:HB2	1:6:345:TYR:OH	2.11	0.50
1:5:52:LYS:NZ	1:5:54:ASN:OD1	2.41	0.50
1:1:41:ALA:HB3	1:1:301:VAL:HG23	1.93	0.50
8:3:407:BCL:H191	1:2:115:PHE:HB3	1.92	0.50
3:B:225:ARG:HG3	3:B:226:PHE:CD2	2.47	0.50
1:4:141:GLN:HE22	1:6:186:ILE:HD12	1.75	0.50
1:1:113:PHE:HB3	1:1:152:VAL:HG22	1.93	0.50
1:3:20:LEU:HD13	1:3:364:TYR:CZ	2.47	0.50
1:3:23:GLY:N	1:3:321:TYR:OH	2.37	0.50
1:2:234:ASP:OD2	1:2:292:LEU:N	2.45	0.50
4:A:581:ALA:HB1	4:a:330:PHE:HZ	1.75	0.50
4:a:326:ASN:ND2	4:a:349:PHE:O	2.32	0.50
1:6:41:ALA:HB3	1:6:301:VAL:HG23	1.93	0.50
8:3:407:BCL:H12	8:2:403:BCL:H12	1.94	0.50
1:2:288:LEU:HD12	8:2:406:BCL:HED2	1.94	0.50
2:D:108:ARG:HH22	3:B:155:ASN:HB3	1.77	0.50
1:4:323:ILE:HD11	1:4:362:ILE:HG23	1.94	0.50
14:a:817:LHG:H251	14:a:817:LHG:H122	1.94	0.50
1:4:191:THR:HG23	1:5:195:GLU:HA	1.93	0.50
8:4:404:BCL:HBD	8:4:404:BCL:O1A	2.12	0.50
1:6:101:GLU:HG2	1:6:114:SER:HB3	1.93	0.50
1:1:74:ILE:HD12	3:B:216:LEU:HG	1.94	0.50
8:1:402:BCL:H42	8:1:404:BCL:H151	1.93	0.50
4:A:653:GLY:HA3	4:A:661:VAL:HG21	1.94	0.50
4:a:649:ILE:HG22	4:a:661:VAL:HG11	1.94	0.50
8:5:401:BCL:H41	8:5:401:BCL:HAC2	1.93	0.50
1:3:53:LEU:HB2	1:3:254:VAL:HB	1.94	0.50
1:3:144:GLN:HG3	1:3:236:ILE:HG12	1.93	0.50
1:3:164:GLU:HA	1:3:167:VAL:HG12	1.94	0.50
1:3:347:ARG:NH2	1:2:9:VAL:HB	2.26	0.50
4:A:635:ARG:N	4:a:536:CYS:HB2	2.25	0.50
1:5:280:ALA:N	1:5:284:LEU:O	2.41	0.50
3:B:167:GLU:OE2	1:5:323:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:437:LEU:HD11	7:C:56:ILE:HG23	1.92	0.49
4:A:602:THR:C	4:A:604:THR:H	2.20	0.49
4:a:638:ARG:NH2	4:a:673:SER:OG	2.39	0.49
1:6:323:ILE:HD12	1:6:338:TYR:CG	2.47	0.49
1:1:150:MET:HG2	1:1:221:SER:HB2	1.93	0.49
4:A:88:PHE:HB3	7:c:86:PHE:CE1	2.47	0.49
1:6:313:LEU:HD12	8:6:403:BCL:OBD	2.11	0.49
1:2:183:PHE:HZ	8:2:403:BCL:H12	1.76	0.49
1:2:227:HIS:NE2	8:2:407:BCL:H3C	2.27	0.49
1:5:36:VAL:HG11	8:5:402:BCL:H3C	1.94	0.49
1:1:297:HIS:HB3	8:1:406:BCL:C4D	2.42	0.49
8:2:403:BCL:HAA1	8:2:403:BCL:CBD	2.37	0.49
4:a:588:LEU:HD13	4:a:592:TYR:HE2	1.78	0.49
4:a:623:VAL:HG13	4:a:680:LEU:HD23	1.95	0.49
7:C:52:TRP:O	7:C:56:ILE:HG13	2.13	0.49
8:1:408:BCL:H12	8:3:401:BCL:H11	1.94	0.49
1:3:30:VAL:O	1:3:271:GLY:N	2.44	0.49
4:a:282:HIS:O	4:a:286:ILE:HG12	2.13	0.49
1:5:192:ALA:HA	1:5:195:GLU:HG2	1.94	0.49
4:a:202:TYR:HA	4:a:205:ALA:HB3	1.95	0.49
9:a:822:CDL:H372	9:a:822:CDL:H202	1.93	0.49
1:6:140:MET:HB2	1:6:237:SER:HA	1.93	0.49
1:3:19:VAL:HB	1:3:29:LYS:HB2	1.95	0.49
4:A:532:TYR:O	4:a:635:ARG:NH1	2.45	0.49
4:a:80:LEU:HD21	8:a:807:BCL:HMC3	1.93	0.49
1:1:53:LEU:HD21	8:1:405:BCL:H61	1.95	0.49
1:2:180:ILE:HD11	8:2:403:BCL:H192	1.95	0.49
1:2:246:ASP:OD1	1:2:247:LYS:N	2.45	0.49
4:A:313:LEU:HD23	4:A:316:LEU:HD12	1.94	0.49
4:A:389:TYR:CG	4:A:544:LEU:HD22	2.47	0.49
4:a:120:ARG:HB2	8:a:809:BCL:HBB3	1.95	0.49
1:4:151:LYS:HG2	1:4:220:VAL:HG22	1.95	0.49
1:4:178:ASP:HB3	1:4:202:ARG:HG2	1.95	0.49
8:4:409:BCL:H12	8:6:401:BCL:H12	1.95	0.49
8:4:409:BCL:H43	8:6:401:BCL:H43	1.93	0.49
8:4:409:BCL:C1C	8:6:406:BCL:H111	2.43	0.49
8:6:401:BCL:H41	8:6:401:BCL:H201	1.94	0.49
1:3:124:TYR:CD2	1:2:183:PHE:HB2	2.47	0.49
1:3:246:ASP:OD1	1:3:246:ASP:N	2.44	0.49
2:D:105:PHE:HB3	4:a:519:LYS:HG3	1.94	0.49
1:6:40:PRO:HA	8:6:402:BCL:HMD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:117:GLY:HA3	8:1:405:BCL:HMA2	1.94	0.49
8:1:402:BCL:HAA1	8:1:406:BCL:OBD	2.13	0.49
8:1:408:BCL:NC	8:3:406:BCL:H111	2.27	0.49
1:3:258:PHE:HD1	8:3:403:BCL:H141	1.77	0.49
1:3:286:ARG:HB3	1:3:363:LEU:HD23	1.95	0.49
1:2:18:ILE:N	1:2:314:LYS:O	2.46	0.49
1:2:241:GLU:HG2	8:2:406:BCL:HED1	1.94	0.49
2:D:79:ILE:HB	2:D:117:ILE:HG13	1.95	0.49
8:A:806:BCL:HBC1	8:A:807:BCL:H111	1.95	0.49
1:4:209:ASN:OD1	1:4:222:ARG:NH1	2.26	0.49
8:1:407[B]:BCL:HAC1	8:3:401:BCL:H61	1.95	0.48
8:1:408:BCL:H192	8:3:401:BCL:HMC1	1.95	0.48
1:4:57:PRO:HG3	1:4:248:LEU:HG	1.94	0.48
1:4:203:ILE:HG22	1:4:225:PHE:HB3	1.94	0.48
1:6:137:PRO:HB2	1:6:140:MET:HE2	1.94	0.48
1:1:312:GLN:HE21	1:1:339:ARG:HD3	1.77	0.48
2:D:105:PHE:HE2	4:a:521:ASN:HD22	1.61	0.48
4:A:122:VAL:HG21	4:A:129:TYR:CE1	2.48	0.48
4:A:511:PRO:HB2	4:a:647:ARG:CZ	2.43	0.48
4:a:119:PRO:HG3	4:a:313:LEU:HD11	1.94	0.48
4:a:370:ASN:HB3	4:a:693:LEU:HD22	1.95	0.48
4:a:450:GLU:O	4:a:577:ALA:HB3	2.13	0.48
1:4:138:ILE:HG13	1:6:43:PRO:HB2	1.95	0.48
8:6:408:BCL:H3A	8:5:401:BCL:OBD	2.13	0.48
1:1:48:ASP:HB3	3:B:216:LEU:HB2	1.95	0.48
4:A:276:LYS:HB3	4:A:394:TYR:HB2	1.94	0.48
1:4:101:GLU:HA	1:4:114:SER:HA	1.96	0.48
8:6:408:BCL:H192	8:5:401:BCL:HMC1	1.96	0.48
4:A:349:PHE:HB3	4:A:353:ALA:HB3	1.94	0.48
1:1:40:PRO:HA	8:1:402:BCL:HMD2	1.95	0.48
1:1:277:SER:HG	1:1:285:ARG:HH21	1.60	0.48
1:3:232:MET:HG3	1:2:187:GLY:HA2	1.96	0.48
1:2:101:GLU:HA	1:2:114:SER:HA	1.96	0.48
2:D:115:ARG:HH12	1:5:284:LEU:HG	1.78	0.48
3:B:200:LEU:N	3:B:204:GLU:O	2.24	0.48
4:A:206:LEU:HB2	8:A:809:BCL:C1D	2.32	0.48
4:a:687:MET:HE3	8:C:301:BCL:HAC2	1.95	0.48
1:1:56:LYS:HE3	1:1:66:ARG:HG2	1.95	0.48
1:1:124:TYR:CD1	1:3:183:PHE:HB2	2.47	0.48
1:2:313:LEU:HB3	1:2:340:TRP:HB2	1.95	0.48
4:A:60:LYS:O	4:A:63:GLN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:169:LEU:O	4:a:178:GLY:N	2.47	0.48
1:4:55:VAL:HG22	1:4:67:ILE:HG13	1.96	0.48
1:4:297:HIS:HB3	8:4:407:BCL:CHA	2.44	0.48
1:6:93:LYS:HA	1:6:93:LYS:HD2	1.72	0.48
1:1:314:LYS:HE3	3:B:224:HIS:ND1	2.28	0.48
8:2:405:BCL:H72	8:2:406:BCL:H41	1.96	0.48
4:a:85:VAL:O	4:a:89:ILE:HG12	2.14	0.48
1:4:193:LEU:HD21	1:4:200:ILE:HG12	1.95	0.48
1:6:178:ASP:HB3	1:6:202:ARG:HG3	1.95	0.48
4:a:113:PHE:CD1	8:a:811:BCL:HBD	2.48	0.48
1:4:302:GLY:HA2	8:4:403:BCL:HAC1	1.94	0.48
8:1:401:BCL:HAC1	8:2:401:BCL:H102	1.96	0.48
1:3:149:LEU:HD12	1:3:222:ARG:HE	1.78	0.48
1:3:297:HIS:HB3	8:3:406:BCL:C4D	2.44	0.48
8:3:407:BCL:H142	1:2:82:LEU:HD11	1.94	0.48
2:D:1:MET:HE1	4:A:422:VAL:HG21	1.96	0.48
4:a:219:GLY:O	4:a:223:VAL:HG23	2.14	0.48
4:a:348:ASP:HA	7:C:108:VAL:HB	1.96	0.48
8:4:402:BCL:HED2	1:5:137:PRO:HB3	1.96	0.48
1:6:194:ASN:O	1:6:194:ASN:ND2	2.45	0.48
1:5:254:VAL:HG21	8:5:405:BCL:H162	1.95	0.48
1:1:96:ARG:HG2	8:1:405:BCL:HED2	1.95	0.48
1:1:206:ASN:HD22	1:1:222:ARG:HG3	1.79	0.48
1:3:143:ARG:NH2	1:3:201:SER:HB3	2.29	0.48
1:2:17:GLU:HA	1:2:314:LYS:HB2	1.95	0.48
4:a:299:VAL:O	4:a:303:GLN:NE2	2.41	0.48
1:4:273:PHE:HB3	8:4:406:BCL:H192	1.95	0.48
1:3:138:ILE:HG21	1:2:43:PRO:HB2	1.96	0.47
1:2:184:TRP:HE1	8:2:407:BCL:HBB1	1.79	0.47
4:A:429:MET:HG3	4:A:498:ILE:HG12	1.95	0.47
4:A:612:HIS:CE1	4:A:616:ILE:HD11	2.49	0.47
14:a:819:LHG:O2	7:C:6:ASN:N	2.47	0.47
1:5:298:HIS:CE1	8:5:402:BCL:NC	2.82	0.47
1:1:27:TRP:HA	1:1:274:PRO:HA	1.96	0.47
1:1:232:MET:HE2	1:1:296:VAL:HG11	1.94	0.47
1:1:259:ARG:NH2	4:A:405:ASN:O	2.47	0.47
1:6:163:TRP:CH2	1:6:208:LEU:HB3	2.49	0.47
1:5:213:GLY:N	1:5:216:GLY:O	2.43	0.47
1:5:351:HIS:CD2	1:5:356:GLY:HA3	2.49	0.47
1:3:117:GLY:HA3	8:3:405:BCL:HMA2	1.96	0.47
1:3:155:ASP:H	1:3:159:LEU:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:407:BCL:H202	8:3:407:BCL:H162	1.74	0.47
1:2:276:VAL:HA	1:2:288:LEU:HD22	1.95	0.47
4:A:553:LYS:HE2	12:A:822:G2O:C4B	2.44	0.47
4:a:67:THR:HB	4:a:275:MET:HB3	1.97	0.47
8:a:807:BCL:HBC1	8:a:808:BCL:H112	1.96	0.47
1:5:59:ASP:OD1	1:5:64:PHE:HB2	2.13	0.47
1:5:101:GLU:HA	1:5:114:SER:HA	1.95	0.47
8:5:401:BCL:H112	8:5:401:BCL:H72	1.59	0.47
7:c:97:ARG:NH1	7:c:102:LYS:O	2.47	0.47
3:B:193:SER:HB3	4:A:518:LEU:HD23	1.96	0.47
4:A:94:TYR:CE1	4:A:121:MET:HE3	2.49	0.47
4:A:650:ARG:HA	4:A:661:VAL:HB	1.95	0.47
1:4:115:PHE:HB3	8:4:402:BCL:H191	1.96	0.47
8:6:406:BCL:H151	8:6:406:BCL:H112	1.62	0.47
8:5:402:BCL:HAA1	8:5:406:BCL:OBD	2.14	0.47
8:3:402:BCL:H112	8:3:406:BCL:HMB2	1.95	0.47
1:2:188:PRO:HG3	8:2:408:BCL:H2	1.96	0.47
4:A:370:ASN:HB3	4:A:693:LEU:HD22	1.96	0.47
4:a:682:PHE:HD2	8:a:811:BCL:H121	1.80	0.47
1:4:206:ASN:HB2	1:4:222:ARG:HB3	1.96	0.47
1:4:232:MET:SD	1:4:296:VAL:HG21	2.55	0.47
1:4:258:PHE:HD2	8:4:404:BCL:H141	1.80	0.47
1:6:184:TRP:NE1	8:6:401:BCL:H202	2.29	0.47
1:6:256:ALA:HB3	8:6:404:BCL:H92	1.95	0.47
3:B:200:LEU:HB2	3:B:204:GLU:HB2	1.96	0.47
4:A:566:TRP:CZ3	4:A:588:LEU:HD21	2.50	0.47
8:A:807:BCL:H121	8:A:807:BCL:H162	1.85	0.47
4:a:378:ILE:HG13	4:a:555:LEU:HD21	1.97	0.47
1:4:84:ILE:HD11	8:4:402:BCL:H143	1.96	0.47
1:4:141:GLN:NE2	1:6:186:ILE:HD12	2.30	0.47
1:6:330:TYR:HB3	1:6:340:TRP:CZ2	2.49	0.47
1:5:185:PHE:CG	1:5:193:LEU:HD11	2.48	0.47
1:1:108:ASP:CG	1:2:132:ARG:HE	2.22	0.47
9:1:409:CDL:H201	8:A:809:BCL:HED2	1.97	0.47
8:3:407:BCL:H141	8:3:407:BCL:H161	1.67	0.47
1:2:290:HIS:CD2	8:2:405:BCL:NA	2.83	0.47
2:D:37:THR:HB	3:B:203:GLY:O	2.15	0.47
4:A:220:TRP:O	4:A:224:MET:HG2	2.15	0.47
4:A:643:ASP:O	4:A:647:ARG:HG3	2.15	0.47
4:a:484:VAL:HG11	4:a:568:ALA:HA	1.95	0.47
1:4:182:ASP:OD2	1:5:143:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:184:TRP:CD1	8:4:401:BCL:H202	2.50	0.47
1:6:48:ASP:HB3	1:6:259:ARG:NH2	2.30	0.47
1:5:238:ARG:NH1	1:5:289:ASN:O	2.43	0.47
1:5:244:PRO:HD2	8:5:404:BCL:C2B	2.44	0.47
1:5:258:PHE:HD2	8:5:403:BCL:H141	1.79	0.47
1:3:359:GLN:HB3	1:2:45:LEU:HB2	1.96	0.47
1:2:343:GLY:HA2	4:A:271:LEU:HB3	1.97	0.47
14:A:816:LHG:H322	15:A:817:LMG:H202	1.97	0.47
1:4:238:ARG:NH2	1:4:241:GLU:OE2	2.47	0.47
4:a:205:ALA:HA	4:a:208:PRO:HG2	1.96	0.47
4:a:626:ILE:HG22	4:a:680:LEU:HD13	1.97	0.47
1:6:297:HIS:HB3	8:6:406:BCL:C4D	2.44	0.47
1:1:351:HIS:CD2	1:1:358:GLY:H	2.33	0.47
1:1:357:VAL:HG12	1:1:357:VAL:O	2.15	0.47
8:3:403:BCL:HBB2	8:3:404:BCL:H51	1.96	0.47
2:D:25:GLY:HA3	3:B:214:GLU:OE2	2.15	0.47
2:D:128:CYS:HA	2:D:137:THR:HA	1.97	0.47
4:a:115:LEU:HD13	4:a:364:MET:SD	2.55	0.47
4:a:162:TRP:HZ2	1:4:6:SER:HB3	1.80	0.47
4:a:435:THR:HG22	4:a:491:ALA:HB2	1.97	0.47
1:2:297:HIS:HB3	8:2:408:BCL:C4D	2.46	0.46
2:D:123:GLU:OE1	1:5:60:PRO:HG2	2.15	0.46
4:a:297:ALA:HB1	4:a:301:PHE:CE2	2.49	0.46
1:4:138:ILE:HG12	1:6:44:LEU:HG	1.97	0.46
1:4:353:CYS:HA	8:4:404:BCL:HBC3	1.97	0.46
1:5:103:MET:HE1	1:5:105:SER:HB3	1.95	0.46
8:1:406:BCL:H142	8:2:401:BCL:HAA1	1.97	0.46
1:3:146:HIS:HB3	1:3:148:ILE:HD11	1.98	0.46
4:A:320:LEU:HB2	4:A:323:GLU:HG3	1.96	0.46
4:A:635:ARG:H	4:a:536:CYS:HB2	1.79	0.46
4:a:527:CYS:HB3	4:a:536:CYS:HA	1.97	0.46
4:a:642:ALA:HA	4:a:645:GLN:HG3	1.96	0.46
8:4:409:BCL:H102	8:6:401:BCL:HAC1	1.97	0.46
1:5:323:ILE:HD11	1:5:362:ILE:HG23	1.97	0.46
1:1:183:PHE:HZ	8:1:401:BCL:H12	1.80	0.46
1:3:347:ARG:HB3	1:2:39:PRO:HD3	1.97	0.46
8:3:406:BCL:H13	8:3:406:BCL:H101	1.78	0.46
4:a:167:HIS:ND1	1:4:11:THR:HG21	2.31	0.46
1:4:29:LYS:HG2	1:4:272:GLU:OE1	2.15	0.46
1:4:297:HIS:HE1	8:4:407:BCL:C4B	2.29	0.46
1:3:59:ASP:OD1	1:3:64:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:96:ARG:HH12	1:3:242:LEU:HD11	1.80	0.46
1:3:148:ILE:HG13	8:3:405:BCL:HMA1	1.96	0.46
8:3:404:BCL:H102	8:3:404:BCL:H62	1.63	0.46
2:D:115:ARG:HH22	1:5:365:ALA:HB1	1.81	0.46
1:6:186:ILE:HG21	8:6:406:BCL:H101	1.96	0.46
1:6:288:LEU:HD11	8:6:404:BCL:HBA1	1.97	0.46
1:5:185:PHE:CZ	1:5:200:ILE:HG13	2.50	0.46
4:A:675:LEU:HD11	14:A:818:LHG:H142	1.97	0.46
1:1:115:PHE:HB3	8:2:401:BCL:H191	1.97	0.46
1:3:26:SER:HA	1:3:285:ARG:HH22	1.81	0.46
1:3:101:GLU:HA	1:3:114:SER:HA	1.98	0.46
1:2:121:ASN:HB2	1:2:144:GLN:HG2	1.98	0.46
1:4:184:TRP:HE1	8:4:406:BCL:CBB	2.28	0.46
2:D:47:LEU:HD21	2:D:139:ASP:HA	1.96	0.46
12:A:802:G2O:C2D	4:a:550:TRP:HZ2	2.28	0.46
4:a:389:TYR:CG	4:a:544:LEU:HD22	2.51	0.46
9:a:822:CDL:H612	9:a:822:CDL:H212	1.98	0.46
1:5:208:LEU:HD11	8:5:401:BCL:H142	1.98	0.46
8:3:405:BCL:H61	8:3:405:BCL:H41	1.67	0.46
4:A:179:ASN:O	4:A:183:PHE:HB3	2.16	0.46
4:A:513:TRP:CZ2	4:A:538:VAL:HG21	2.51	0.46
4:A:595:GLY:O	4:A:599:TYR:HB2	2.16	0.46
4:A:685:THR:OG1	11:A:801:GS0:O1D	2.26	0.46
4:a:418:GLN:H	4:a:421:GLN:HG3	1.80	0.46
1:5:40:PRO:HG3	1:5:260:SER:OG	2.16	0.46
6:F:42:ALA:O	6:F:46:MET:HG2	2.15	0.46
1:3:156:ASN:HB2	1:3:159:LEU:HG	1.98	0.46
2:D:128:CYS:HB3	2:D:137:THR:HG22	1.98	0.46
4:A:375:ASN:HB2	8:A:810:BCL:CHB	2.46	0.46
4:a:572:TYR:HA	4:a:579:ALA:HB1	1.98	0.46
1:4:297:HIS:HE1	8:4:407:BCL:NB	2.08	0.46
1:1:297:HIS:HE1	8:1:406:BCL:NB	2.07	0.46
8:3:407:BCL:H62	8:3:407:BCL:H41	1.70	0.46
1:2:193:LEU:HD11	1:2:200:ILE:HD11	1.96	0.46
1:2:286:ARG:HH22	2:D:57:ARG:HH22	1.64	0.46
4:A:395:LEU:O	4:A:399:GLN:HG3	2.16	0.46
4:A:522:SER:C	4:A:524:SER:H	2.24	0.46
8:4:401:BCL:H201	8:4:401:BCL:H41	1.98	0.46
1:6:153:PRO:HA	1:6:218:VAL:HA	1.98	0.46
1:6:258:PHE:HD2	8:6:403:BCL:H141	1.81	0.46
8:5:402:BCL:H142	8:5:402:BCL:H111	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:84:SER:HA	7:c:87:VAL:HG12	1.96	0.46
1:3:297:HIS:HE1	8:3:406:BCL:C4B	2.28	0.45
4:A:194:PHE:CZ	4:A:208:PRO:HA	2.51	0.45
4:A:399:GLN:HA	4:A:404:TYR:HB2	1.99	0.45
4:A:683:GLY:HA2	8:A:810:BCL:H101	1.98	0.45
4:a:612:HIS:CE1	4:a:616:ILE:HD11	2.51	0.45
8:a:811:BCL:H43	8:a:811:BCL:C3B	2.47	0.45
8:4:409:BCL:H202	8:4:409:BCL:H162	1.75	0.45
1:1:307:PHE:CE1	1:1:354:LYS:HE2	2.51	0.45
1:3:232:MET:CE	1:3:296:VAL:HG11	2.47	0.45
1:2:297:HIS:HE1	8:2:408:BCL:C4B	2.29	0.45
1:2:340:TRP:HB3	1:2:345:TYR:CG	2.51	0.45
8:A:811:BCL:H61	8:A:811:BCL:H101	1.65	0.45
4:a:86:LEU:HD21	8:a:812:BCL:H122	1.98	0.45
4:a:520:LYS:HG2	4:a:525:PHE:HZ	1.81	0.45
4:a:595:GLY:O	4:a:599:TYR:HB2	2.16	0.45
4:a:641:GLY:O	4:a:645:GLN:HG3	2.17	0.45
4:a:661:VAL:HG12	4:a:661:VAL:O	2.16	0.45
8:4:406:BCL:H61	8:4:406:BCL:H41	1.59	0.45
8:3:401:BCL:HAA1	8:3:401:BCL:CBD	2.39	0.45
8:3:405:BCL:O2D	8:3:405:BCL:H2A	2.16	0.45
2:D:47:LEU:HD23	2:D:47:LEU:H	1.82	0.45
2:D:88:ILE:HB	2:D:90:MET:HE2	1.98	0.45
3:B:165:VAL:HG12	3:B:170:PHE:HB3	1.98	0.45
4:A:536:CYS:HB2	4:a:635:ARG:N	2.31	0.45
4:A:622:LEU:HA	4:A:625:PHE:HE1	1.81	0.45
4:A:660:ASP:OD1	4:A:660:ASP:N	2.50	0.45
8:4:401:BCL:H112	8:4:401:BCL:H72	1.65	0.45
1:3:254:VAL:HG11	8:3:404:BCL:H72	1.99	0.45
1:2:36:VAL:HG11	8:2:404:BCL:H3C	1.97	0.45
3:B:170:PHE:CZ	4:A:530:PRO:HD2	2.51	0.45
4:A:286:ILE:HG21	8:A:803:BCL:HBC3	1.99	0.45
4:a:101:PHE:O	4:a:103:TRP:N	2.49	0.45
4:a:288:TYR:OH	8:a:805:BCL:OBB	2.31	0.45
4:a:683:GLY:O	4:a:687:MET:HG3	2.17	0.45
1:4:340:TRP:HB3	1:4:345:TYR:CG	2.51	0.45
1:6:242:LEU:O	8:6:404:BCL:NB	2.48	0.45
8:6:406:BCL:H161	8:6:406:BCL:H192	1.66	0.45
1:5:18:ILE:HD11	8:5:403:BCL:HAA1	1.98	0.45
8:5:402:BCL:H161	8:5:404:BCL:H201	1.97	0.45
7:c:58:CYS:HA	7:c:61:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:178:ASP:HB3	1:3:202:ARG:HD2	1.98	0.45
4:A:376:HIS:HE1	8:A:811:BCL:NA	2.11	0.45
4:A:485:MET:SD	4:A:561:TYR:HB2	2.57	0.45
4:A:614:SER:O	4:A:618:MET:HG3	2.16	0.45
4:a:572:TYR:OH	4:a:583:ASP:OD1	2.34	0.45
1:4:184:TRP:HZ3	1:4:200:ILE:HG21	1.81	0.45
1:6:162:THR:HG21	8:6:401:BCL:H3A	1.99	0.45
1:6:292:LEU:HD22	1:6:357:VAL:HB	1.98	0.45
8:6:402:BCL:HAA1	8:6:406:BCL:OBD	2.16	0.45
1:5:297:HIS:HE1	8:5:406:BCL:C4B	2.29	0.45
7:c:46:LEU:O	7:c:50:MET:HG2	2.16	0.45
1:2:92:THR:HG23	1:2:94:GLU:H	1.81	0.45
2:D:114:MET:HE3	3:B:134:PHE:HB3	1.98	0.45
8:A:805:BCL:H101	8:A:805:BCL:H61	1.56	0.45
8:6:402:BCL:H201	8:6:404:BCL:HBC1	1.98	0.45
1:5:136:ASN:OD1	1:5:289:ASN:ND2	2.45	0.45
1:1:182:ASP:OD1	1:2:199:ARG:HD3	2.16	0.45
1:1:273:PHE:HB3	8:1:405:BCL:H192	1.99	0.45
8:1:405:BCL:H61	8:1:405:BCL:H102	1.65	0.45
1:3:125:TYR:O	1:3:126:ARG:NE	2.37	0.45
2:D:98:GLU:HB2	2:D:110:VAL:HG13	1.99	0.45
4:A:582:TRP:HA	4:A:585:ILE:HG22	1.98	0.45
4:a:109:HIS:HB2	4:a:321:TYR:CZ	2.51	0.45
4:a:374:PHE:O	4:a:378:ILE:HG22	2.17	0.45
1:4:313:LEU:HB3	1:4:340:TRP:HB2	1.98	0.45
1:6:19:VAL:HG22	1:6:29:LYS:HB2	1.99	0.45
1:6:59:ASP:OD1	1:6:59:ASP:N	2.49	0.45
1:6:235:SER:HB2	8:6:405:BCL:HHD	1.98	0.45
1:3:121:ASN:ND2	1:3:236:ILE:HA	2.31	0.45
1:3:133:ASN:ND2	1:2:108:ASP:OD1	2.33	0.45
3:B:140:CYS:O	3:B:171:ARG:NH1	2.50	0.45
4:A:48:ARG:HG2	4:A:48:ARG:O	2.16	0.45
1:5:244:PRO:HB3	1:5:247:LYS:NZ	2.31	0.45
1:1:258:PHE:HD2	8:1:403:BCL:H141	1.81	0.45
8:3:403:BCL:H2C	8:3:403:BCL:H92	1.99	0.45
1:2:351:HIS:NE2	1:2:356:GLY:HA3	2.32	0.45
4:A:49:PHE:CZ	4:A:664:ARG:HB2	2.52	0.45
4:A:432:CYS:HB2	4:A:494:LEU:HB3	1.99	0.45
4:a:495:PHE:HA	4:a:498:ILE:HD12	1.98	0.45
8:6:402:BCL:HMB3	8:6:403:BCL:H41	1.99	0.45
1:5:104:VAL:HG23	1:5:113:PHE:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:404:BCL:H62	8:1:404:BCL:H102	1.71	0.45
4:A:80:LEU:HD21	8:A:806:BCL:HMC3	1.99	0.45
4:A:574:VAL:O	4:A:579:ALA:HB3	2.17	0.45
4:A:687:MET:HG2	8:A:810:BCL:H61	1.99	0.45
9:a:820:CDL:H551	9:a:820:CDL:H582	1.53	0.45
1:4:129:ALA:N	1:6:158:ASP:OD2	2.50	0.45
1:6:104:VAL:HG23	1:6:113:PHE:HE1	1.82	0.45
1:6:328:PRO:HD2	1:6:360:PHE:CD1	2.52	0.45
9:1:409:CDL:H182	8:A:809:BCL:HMA3	1.99	0.44
2:D:95:ILE:HG12	2:D:110:VAL:HG12	1.98	0.44
3:B:136:ILE:HG22	3:B:138:ASN:H	1.82	0.44
3:B:157:ILE:HA	3:B:173:TYR:O	2.17	0.44
4:A:545:TRP:HB3	4:A:631:TRP:HH2	1.82	0.44
4:A:688:LEU:HB2	11:A:801:GS0:CBD	2.48	0.44
8:a:806:BCL:HBB3	8:a:808:BCL:H91	1.99	0.44
14:a:819:LHG:H111	14:a:819:LHG:HC81	1.71	0.44
1:4:297:HIS:HB3	8:4:407:BCL:C4D	2.48	0.44
8:6:408:BCL:H202	8:6:408:BCL:H162	1.77	0.44
1:1:36:VAL:HG11	8:1:402:BCL:H3C	1.97	0.44
1:1:298:HIS:HA	1:1:301:VAL:HG12	1.99	0.44
8:3:406:BCL:H192	8:3:406:BCL:H161	1.68	0.44
2:D:115:ARG:NH2	3:B:138:ASN:OD1	2.23	0.44
4:A:364:MET:HA	4:A:367:VAL:HB	1.98	0.44
4:A:619:ILE:HD12	8:c:301:BCL:HMC2	1.98	0.44
4:a:522:SER:C	4:a:524:SER:H	2.24	0.44
4:a:545:TRP:CE3	4:a:678:THR:HG21	2.52	0.44
1:5:26:SER:HA	1:5:285:ARG:HH22	1.81	0.44
7:C:90:MET:O	7:C:94:LEU:HG	2.17	0.44
9:1:409:CDL:HA22	4:A:266:ASN:O	2.17	0.44
1:3:17:GLU:HG3	1:3:314:LYS:HD2	1.99	0.44
8:3:407:BCL:C4C	8:2:408:BCL:H111	2.46	0.44
4:A:182:ASP:OD1	4:A:200:LYS:NZ	2.51	0.44
4:A:280:SER:HB2	4:A:387:GLY:O	2.17	0.44
4:A:537:GLY:O	4:a:637:SER:HB2	2.17	0.44
1:5:339:ARG:NH2	7:C:71:SER:HB2	2.32	0.44
8:5:401:BCL:HBC2	8:5:401:BCL:H2C	1.62	0.44
8:5:405:BCL:H61	8:5:405:BCL:H102	1.78	0.44
1:1:43:PRO:HB2	1:2:138:ILE:HG21	1.99	0.44
8:3:401:BCL:H152	8:3:401:BCL:H18	1.64	0.44
1:6:351:HIS:CD2	1:6:356:GLY:HA3	2.52	0.44
8:6:403:BCL:H162	8:6:403:BCL:H192	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:284:LEU:HG	1:1:363:LEU:HD23	1.98	0.44
1:2:40:PRO:HA	8:2:404:BCL:HMD2	1.98	0.44
4:A:106:PRO:HB3	7:c:104:ARG:H	1.83	0.44
4:A:217:PHE:O	4:A:246:SER:OG	2.36	0.44
4:A:631:TRP:HE1	4:A:677:GLY:C	2.25	0.44
4:a:179:ASN:HB3	4:a:182:ASP:O	2.17	0.44
4:a:688:LEU:HB2	11:a:802:GS0:CBD	2.48	0.44
1:4:173:THR:HG22	1:4:175:ALA:H	1.82	0.44
1:5:177:ASN:ND2	1:5:203:ILE:O	2.51	0.44
1:5:185:PHE:CE2	1:5:200:ILE:HG13	2.53	0.44
1:5:321:TYR:CD1	1:5:366:GLN:HB3	2.53	0.44
5:E:9:UNK:O	5:E:13:UNK:N	2.50	0.44
7:c:12:LEU:O	7:c:16:GLY:N	2.36	0.44
1:1:353:CYS:SG	8:1:402:BCL:HBB3	2.58	0.44
1:3:45:LEU:HD13	1:3:262:SER:HA	2.00	0.44
8:2:407:BCL:H2C	8:2:407:BCL:HBC3	1.82	0.44
2:D:25:GLY:N	3:B:212:PRO:HB2	2.26	0.44
2:D:63:THR:HG22	2:D:65:GLU:H	1.83	0.44
2:D:100:ARG:HB3	4:a:53:ARG:HH12	1.83	0.44
3:B:202:ASP:OD1	3:B:202:ASP:N	2.48	0.44
4:A:450:GLU:CD	4:A:582:TRP:HE1	2.20	0.44
8:A:810:BCL:HED2	8:A:811:BCL:HBA2	2.00	0.44
4:a:58:SER:O	4:a:58:SER:OG	2.31	0.44
1:4:155:ASP:OD1	1:4:155:ASP:N	2.51	0.44
1:6:49:CYS:O	1:6:259:ARG:NH2	2.51	0.44
8:6:401:BCL:HAA1	8:6:401:BCL:CBD	2.39	0.44
7:C:84:SER:HA	7:C:87:VAL:HG12	2.00	0.44
8:1:401:BCL:H112	8:1:401:BCL:H72	1.69	0.44
1:2:55:VAL:HG22	1:2:67:ILE:HG13	1.99	0.44
4:A:270:HIS:HD1	4:A:277:ALA:HB1	1.83	0.44
4:A:550:TRP:HZ2	12:a:803:G2O:C2D	2.30	0.44
14:a:819:LHG:H112	14:a:819:LHG:H142	1.77	0.44
1:4:194:ASN:O	1:4:194:ASN:ND2	2.50	0.44
8:4:404:BCL:H52	8:4:405:BCL:H41	1.99	0.44
1:6:136:ASN:HB2	1:6:286:ARG:HH12	1.83	0.44
1:6:139:TYR:HB2	1:5:186:ILE:HD11	2.00	0.44
1:5:40:PRO:HA	8:5:402:BCL:HMD2	1.99	0.44
1:1:185:PHE:CD2	1:1:193:LEU:HD11	2.53	0.44
4:A:116:THR:HA	4:A:368:VAL:HG13	2.00	0.44
4:a:300:ALA:HA	4:a:303:GLN:HG2	2.00	0.44
4:a:450:GLU:CD	4:a:582:TRP:HE1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:613:LEU:HD22	4:a:691:LEU:HD22	2.00	0.44
1:4:125:TYR:HE2	1:4:130:VAL:HG21	1.83	0.44
8:4:403:BCL:HAA1	8:4:407:BCL:OBD	2.18	0.44
1:5:310:ASP:OD1	1:5:310:ASP:N	2.51	0.44
1:3:58:LEU:HD21	1:3:64:PHE:HB3	1.99	0.44
8:3:403:BCL:O1A	8:3:403:BCL:HBD	2.18	0.44
8:2:404:BCL:H61	8:2:404:BCL:H102	1.79	0.44
3:B:157:ILE:HG12	3:B:174:ILE:HG12	2.00	0.44
4:A:374:PHE:O	4:A:378:ILE:HG22	2.17	0.44
4:a:448:ILE:HG23	4:a:453:ILE:HB	1.99	0.44
1:4:313:LEU:HB2	1:4:345:TYR:OH	2.18	0.44
8:4:402:BCL:H91	8:4:402:BCL:H112	1.74	0.44
8:4:406:BCL:O2D	8:4:406:BCL:H2A	2.17	0.44
1:6:258:PHE:CE1	8:6:402:BCL:HED2	2.53	0.44
8:6:402:BCL:H42	8:6:404:BCL:H151	2.00	0.44
8:6:403:BCL:H11	8:6:403:BCL:HBA2	1.64	0.44
1:1:30:VAL:O	1:1:271:GLY:N	2.51	0.43
1:1:185:PHE:CE2	1:1:200:ILE:HG13	2.52	0.43
1:3:351:HIS:O	1:3:356:GLY:N	2.42	0.43
8:3:402:BCL:H61	8:3:402:BCL:H41	1.91	0.43
4:a:114:TYR:OH	4:a:127:ASP:OD2	2.26	0.43
1:6:180:ILE:O	1:6:184:TRP:HB3	2.18	0.43
1:1:86:ALA:HA	1:1:100:GLY:HA3	1.99	0.43
1:1:312:GLN:OE1	3:B:225:ARG:HD3	2.19	0.43
1:3:22:GLY:HA2	1:3:321:TYR:HE2	1.81	0.43
1:3:145:PHE:HZ	8:2:402[B]:BCL:HED3	1.82	0.43
1:5:18:ILE:HB	1:5:315:VAL:HG22	2.00	0.43
7:C:58:CYS:HA	7:C:61:ILE:HG12	2.00	0.43
8:1:406:BCL:H111	8:2:401:BCL:C4C	2.48	0.43
9:1:409:CDL:H201	8:A:805:BCL:H191	2.00	0.43
1:3:53:LEU:HD22	8:3:405:BCL:H162	2.00	0.43
4:A:109:HIS:HB2	4:A:321:TYR:CZ	2.54	0.43
4:A:319:TYR:HB2	7:c:104:ARG:NH1	2.33	0.43
4:A:485:MET:HE3	4:A:489:ILE:HG12	2.00	0.43
4:A:577:ALA:O	4:a:327:ARG:HD2	2.19	0.43
4:A:637:SER:HB2	4:a:537:GLY:O	2.18	0.43
4:a:101:PHE:HE2	7:C:97:ARG:HE	1.66	0.43
4:a:370:ASN:ND2	4:a:562:ILE:O	2.47	0.43
1:4:178:ASP:HB2	1:4:181:ARG:NH2	2.33	0.43
1:6:40:PRO:HG3	1:6:260:SER:OG	2.18	0.43
8:6:401:BCL:H72	8:6:401:BCL:H112	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5:401:BCL:H192	8:5:401:BCL:H161	1.75	0.43
7:c:80:SER:HA	7:c:83:LEU:HB2	1.99	0.43
4:A:468:LEU:HB2	4:A:471:PHE:HD2	1.83	0.43
4:A:657:LEU:HD22	9:c:303:CDL:H121	2.00	0.43
4:a:86:LEU:O	4:a:90:MET:HG2	2.18	0.43
1:6:27:TRP:HA	1:6:274:PRO:HA	1.99	0.43
8:6:408:BCL:HBD	1:5:186:ILE:HD11	2.00	0.43
1:5:178:ASP:HB2	1:5:181:ARG:HH21	1.83	0.43
1:2:176:PHE:CZ	1:2:180:ILE:HD13	2.54	0.43
1:2:267:VAL:HG22	8:2:404:BCL:HMA2	2.01	0.43
4:a:374:PHE:CZ	4:a:555:LEU:HG	2.53	0.43
8:4:403:BCL:H61	8:4:403:BCL:H41	1.87	0.43
8:4:410[B]:BCL:H3A	8:4:410[B]:BCL:HBA2	1.54	0.43
8:6:402:BCL:H192	8:6:402:BCL:H162	1.70	0.43
1:2:238:ARG:HG3	1:2:238:ARG:O	2.17	0.43
2:D:102:VAL:HG22	3:B:162:TYR:HB3	1.99	0.43
4:A:270:HIS:CE1	4:A:281:VAL:HG21	2.54	0.43
4:A:536:CYS:HB2	4:a:635:ARG:H	1.84	0.43
4:A:617:LEU:HD11	11:A:801:GS0:CHD	2.48	0.43
4:a:603:GLU:HG2	4:a:695:ASN:HD21	1.81	0.43
1:4:144:GLN:HB2	1:4:227:HIS:CD2	2.54	0.43
1:6:143:ARG:NH1	1:6:201:SER:HB3	2.33	0.43
1:6:180:ILE:HG21	1:6:203:ILE:HG12	2.00	0.43
1:6:297:HIS:HE1	8:6:406:BCL:C4B	2.30	0.43
8:6:408:BCL:HMD2	1:5:43:PRO:HG2	2.01	0.43
1:5:324:ARG:HG3	1:5:363:LEU:HD23	2.00	0.43
7:c:36:ALA:HB3	7:c:39:HIS:ND1	2.34	0.43
1:3:167:VAL:HA	1:3:170:ILE:HG12	1.99	0.43
8:2:408:BCL:H161	8:2:408:BCL:H192	1.57	0.43
2:D:102:VAL:HG22	3:B:162:TYR:CB	2.48	0.43
4:A:120:ARG:HB2	8:A:808:BCL:HBB3	2.00	0.43
4:A:231:ALA:O	4:A:233:ILE:HD12	2.18	0.43
8:A:806:BCL:HMC2	8:A:807:BCL:HMA1	2.01	0.43
4:a:67:THR:HG23	8:a:813:BCL:HMA1	2.00	0.43
4:a:504:ALA:HB2	8:a:805:BCL:HHB	1.99	0.43
8:4:403:BCL:H112	8:4:407:BCL:HMB2	2.00	0.43
8:4:406:BCL:HBC3	8:4:406:BCL:H2C	1.84	0.43
1:6:36:VAL:HG11	8:6:402:BCL:H3C	2.00	0.43
4:A:205:ALA:HA	4:A:208:PRO:HG2	2.01	0.43
4:A:395:LEU:HD11	4:A:404:TYR:HE1	1.83	0.43
4:A:571:MET:HB3	4:A:574:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:478:PRO:HA	4:a:482:ASP:OD2	2.19	0.43
7:c:6:ASN:N	9:c:303:CDL:OB4	2.52	0.43
1:3:99:VAL:HG22	1:3:116:GLU:HG2	2.00	0.43
1:3:184:TRP:NE1	8:3:401:BCL:H202	2.34	0.43
8:3:402:BCL:H13	8:3:404:BCL:H191	2.00	0.43
1:2:184:TRP:HZ3	1:2:200:ILE:HG21	1.84	0.43
1:2:323:ILE:HG21	1:2:326:ALA:HB2	2.00	0.43
2:D:7:ARG:HH11	4:a:664:ARG:HD3	1.83	0.43
4:A:297:ALA:HB1	4:A:301:PHE:CE2	2.54	0.43
4:A:390:HIS:HE1	8:A:812:BCL:NC	2.16	0.43
4:A:445:TRP:NE1	4:A:460:MET:O	2.48	0.43
4:A:603:GLU:HG3	4:A:698:TYR:HD2	1.83	0.43
4:A:621:HIS:CD2	11:A:801:GS0:NB	2.86	0.43
8:A:811:BCL:H111	8:A:811:BCL:H142	1.66	0.43
1:4:70:VAL:HG13	1:4:83:THR:HG22	2.01	0.43
1:4:103:MET:HE1	1:4:105:SER:HB3	2.00	0.43
8:4:401:BCL:HAA1	8:4:401:BCL:CBD	2.39	0.43
8:F:101:BCL:H2C	8:F:101:BCL:HBC3	1.75	0.43
1:1:140:MET:HB3	1:1:237:SER:HB2	2.01	0.43
1:2:325:TYR:HD2	4:A:401:ASN:O	2.01	0.43
8:2:407:BCL:H41	8:2:407:BCL:H61	1.48	0.43
4:a:401:ASN:OD1	4:a:403:MET:HG2	2.18	0.43
4:a:485:MET:HE1	4:a:557:ALA:C	2.44	0.43
1:4:113:PHE:HB3	1:4:152:VAL:HG22	2.01	0.43
8:6:408:BCL:C4C	8:5:406:BCL:H111	2.49	0.43
6:F:19:ASN:HB2	6:F:20:LYS:HE2	2.01	0.43
7:c:102:LYS:HE3	7:c:102:LYS:HB3	1.86	0.43
1:1:178:ASP:OD2	1:1:179:TRP:N	2.52	0.42
1:1:190:PHE:CZ	1:2:199:ARG:HD2	2.55	0.42
1:2:46:PRO:HB3	1:2:261:ASP:HA	2.01	0.42
1:2:163:TRP:CH2	1:2:208:LEU:HB3	2.53	0.42
1:2:244:PRO:HD2	8:2:406:BCL:C2B	2.49	0.42
4:A:481:ASN:HA	4:A:568:ALA:HB2	2.00	0.42
4:A:530:PRO:HA	4:A:534:GLY:HA2	2.01	0.42
4:A:611:SER:OG	4:a:451:LEU:HB3	2.18	0.42
4:a:320:LEU:HB2	4:a:323:GLU:HG3	2.01	0.42
4:a:425:LEU:HG	4:a:429:MET:HE3	2.00	0.42
4:a:441:ALA:HB3	7:c:52:TRP:NE1	2.34	0.42
4:a:555:LEU:HD23	4:a:686:PHE:CZ	2.54	0.42
4:a:560:TRP:HZ3	4:a:596:ILE:HG23	1.84	0.42
4:a:622:LEU:HA	4:a:625:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:814:BCL:H2C	8:a:814:BCL:HBC3	1.80	0.42
1:4:74:ILE:HD13	1:4:79:LYS:HA	2.01	0.42
1:5:313:LEU:HB2	1:5:345:TYR:OH	2.19	0.42
7:c:96:LEU:HD13	7:c:100:TRP:HB2	2.00	0.42
1:1:84:ILE:HD11	8:1:405:BCL:H43	2.01	0.42
8:1:401:BCL:H52	8:1:401:BCL:H18	2.01	0.42
1:2:9:VAL:HG13	4:A:197:THR:HG22	2.00	0.42
4:A:123:SER:HA	4:A:309:TYR:CE1	2.54	0.42
4:a:90:MET:HE1	8:a:812:BCL:HBA1	2.00	0.42
4:a:594:SER:HB2	4:a:598:TYR:HB3	2.01	0.42
1:4:66:ARG:NE	1:4:87:ASP:OD2	2.49	0.42
1:4:185:PHE:HZ	1:4:200:ILE:HG13	1.83	0.42
1:5:324:ARG:HG2	1:5:363:LEU:O	2.18	0.42
6:F:17:VAL:HG11	6:F:46:MET:SD	2.59	0.42
8:1:406:BCL:H192	8:1:406:BCL:H161	1.70	0.42
8:3:405:BCL:H61	8:3:405:BCL:H102	1.86	0.42
8:3:406:BCL:H122	8:3:406:BCL:H162	1.79	0.42
1:2:312:GLN:HA	1:2:340:TRP:O	2.19	0.42
4:A:499:ALA:HB3	4:A:547:ALA:HB2	2.01	0.42
4:a:407:ILE:HG21	4:a:412:ILE:HG13	2.01	0.42
4:a:513:TRP:CZ2	4:a:538:VAL:HG21	2.54	0.42
1:6:199:ARG:HD2	1:5:190:PHE:CZ	2.54	0.42
1:1:139:TYR:CZ	1:3:43:PRO:HG3	2.55	0.42
1:3:347:ARG:HH22	1:2:9:VAL:HB	1.84	0.42
8:3:404:BCL:H61	8:3:404:BCL:H2	1.78	0.42
1:2:16:TYR:CD1	8:2:405:BCL:H12	2.55	0.42
8:2:406:BCL:H193	8:2:408:BCL:H203	2.02	0.42
2:D:80:LEU:O	2:D:83:GLN:N	2.51	0.42
3:B:150:CYS:HA	10:B:302:SF4:S4	2.59	0.42
4:A:46:MET:HG3	4:A:664:ARG:HH21	1.83	0.42
4:A:72:ASP:O	4:A:76:VAL:HG23	2.19	0.42
4:a:417:ASP:C	4:a:419:GLU:H	2.28	0.42
8:4:410[B]:BCL:C4B	1:5:125:TYR:HA	2.49	0.42
8:1:405:BCL:HMB1	8:2:401:BCL:H203	2.00	0.42
1:3:204:GLU:HB3	1:3:224:ARG:HG2	2.01	0.42
1:2:325:TYR:HE2	4:A:406:GLN:NE2	2.17	0.42
4:A:220:TRP:CH2	8:A:805:BCL:H3A	2.55	0.42
1:4:190:PHE:CZ	1:5:199:ARG:HD2	2.55	0.42
1:6:144:GLN:HB2	1:6:236:ILE:HG12	2.01	0.42
1:1:52:LYS:HG3	1:1:255:GLU:HG3	2.01	0.42
1:3:273:PHE:HB3	8:3:405:BCL:H192	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:402:BCL:HAA1	8:3:406:BCL:OBD	2.20	0.42
1:2:27:TRP:HA	1:2:274:PRO:HA	2.01	0.42
1:2:39:PRO:HD2	1:2:305:ASN:ND2	2.34	0.42
2:D:100:ARG:HG2	1:4:77:SER:OG	2.19	0.42
3:B:152:PRO:HG3	4:A:51:PHE:HD2	1.83	0.42
3:B:165:VAL:CG2	4:a:525:PHE:HB2	2.50	0.42
4:A:458:ILE:HB	4:A:578:ASP:HB3	2.02	0.42
4:A:696:GLY:HA3	4:A:698:TYR:CZ	2.54	0.42
4:a:375:ASN:HB2	8:a:811:BCL:CHB	2.50	0.42
4:a:457:ASN:OD1	4:a:458:ILE:N	2.53	0.42
1:4:295:LEU:HD22	1:4:352:VAL:HB	2.00	0.42
8:5:406:BCL:H192	8:5:406:BCL:H161	1.61	0.42
1:1:144:GLN:HE21	1:1:239:TRP:CD1	2.38	0.42
1:1:183:PHE:HB2	1:2:124:TYR:CD2	2.55	0.42
1:1:261:ASP:OD2	1:1:262:SER:N	2.46	0.42
4:A:559:CYS:SG	4:A:689:VAL:HG13	2.60	0.42
4:a:134:ALA:O	4:a:137:GLU:HB2	2.20	0.42
4:a:396:LEU:HD23	4:a:523:TYR:HB3	2.02	0.42
8:a:811:BCL:H92	8:a:811:BCL:H61	1.86	0.42
1:4:95:ARG:NH1	1:4:97:ILE:HG22	2.35	0.42
8:4:401:BCL:HBD	8:4:401:BCL:HED2	1.87	0.42
8:6:401:BCL:H3A	8:6:401:BCL:HBA2	1.75	0.42
1:5:319:LYS:HD2	1:5:336:GLU:OE2	2.19	0.42
8:5:404:BCL:H193	8:5:406:BCL:H203	2.01	0.42
1:1:199:ARG:NH1	1:3:182:ASP:OD2	2.52	0.42
8:1:402:BCL:C4B	8:1:403:BCL:HBC1	2.50	0.42
8:1:408:BCL:H141	8:1:408:BCL:H161	1.82	0.42
1:3:51:VAL:HG21	8:3:403:BCL:H152	2.02	0.42
1:3:96:ARG:HG3	1:3:239:TRP:CZ2	2.55	0.42
1:2:70:VAL:HG13	1:2:83:THR:HG22	2.02	0.42
3:B:149:LYS:HE2	3:B:185:CYS:HA	2.02	0.42
4:A:119:PRO:HG3	4:A:313:LEU:HD11	2.02	0.42
9:a:822:CDL:H372	9:a:822:CDL:H222	2.01	0.42
1:4:242:LEU:C	1:4:244:PRO:HD3	2.44	0.42
1:5:306:ASN:ND2	1:5:306:ASN:C	2.77	0.42
1:5:315:VAL:HB	1:5:340:TRP:HZ3	1.84	0.42
8:5:401:BCL:H112	8:5:401:BCL:H152	1.74	0.42
6:F:26:MET:O	6:F:30:ILE:HG12	2.20	0.42
1:1:334:ASN:C	1:1:336:GLU:H	2.27	0.42
1:3:40:PRO:HA	8:3:402:BCL:HMD2	2.00	0.42
4:A:114:TYR:OH	4:A:127:ASP:OD2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:395:LEU:HA	4:A:398:ILE:HG12	2.01	0.42
4:A:623:VAL:HG11	14:A:819:LHG:H211	2.01	0.42
4:a:335:GLN:HG3	4:a:336:GLY:N	2.32	0.42
4:a:439:VAL:HG21	4:a:488:VAL:HG23	2.02	0.42
4:a:593:THR:HG22	4:a:698:TYR:O	2.20	0.42
1:4:139:TYR:HB2	1:6:186:ILE:HD11	2.02	0.42
1:4:259:ARG:O	1:4:265:ILE:HA	2.20	0.42
1:4:328:PRO:HD2	1:4:360:PHE:CD1	2.55	0.42
8:4:409:BCL:H192	8:6:401:BCL:HMC1	2.02	0.42
1:6:313:LEU:HD22	1:6:340:TRP:CE3	2.54	0.42
1:1:90:ASN:OD1	1:1:96:ARG:NE	2.37	0.42
1:1:227:HIS:CD2	8:1:405:BCL:HMC3	2.55	0.42
8:1:405:BCL:H2A	8:1:405:BCL:O2D	2.19	0.42
1:3:41:ALA:N	8:3:402:BCL:OBD	2.51	0.42
1:3:244:PRO:HD2	8:3:404:BCL:C2B	2.50	0.42
1:2:172:SER:OG	8:2:402[B]:BCL:O1A	2.29	0.42
8:2:405:BCL:H192	8:2:405:BCL:H162	1.80	0.42
4:A:404:TYR:CE2	4:A:416:ARG:HG3	2.55	0.42
4:A:591:HIS:HB2	4:A:703:PRO:HA	2.01	0.42
4:a:560:TRP:CD1	4:a:560:TRP:N	2.88	0.42
4:a:560:TRP:CZ3	4:a:596:ILE:HG23	2.54	0.42
1:1:136:ASN:OD1	1:1:289:ASN:ND2	2.50	0.41
1:1:185:PHE:CZ	1:1:200:ILE:HG13	2.55	0.41
1:2:323:ILE:HD12	1:2:338:TYR:CG	2.55	0.41
3:B:138:ASN:ND2	1:5:366:GLN:HE21	2.18	0.41
4:A:319:TYR:HB2	7:c:104:ARG:HH12	1.85	0.41
4:A:362:PHE:O	4:A:364:MET:N	2.53	0.41
4:A:414:LYS:HB3	8:A:804:BCL:H42	2.02	0.41
4:A:435:THR:HG22	4:A:491:ALA:HB2	2.01	0.41
4:A:574:VAL:HG23	4:a:608:PHE:HB3	2.02	0.41
4:A:687:MET:CE	8:c:301:BCL:HMC1	2.50	0.41
8:5:402:BCL:H192	8:5:402:BCL:H162	1.83	0.41
8:5:406:BCL:H122	8:5:406:BCL:H162	1.81	0.41
7:C:80:SER:H	7:C:83:LEU:HD12	1.85	0.41
1:1:53:LEU:HD23	8:1:405:BCL:H203	2.02	0.41
1:3:159:LEU:HD23	1:3:159:LEU:HA	1.80	0.41
1:3:170:ILE:HG22	1:3:176:PHE:CD2	2.55	0.41
1:3:318:PRO:HD2	1:3:321:TYR:CD2	2.53	0.41
4:A:615:THR:O	4:A:619:ILE:HG13	2.20	0.41
8:5:406:BCL:H101	8:5:406:BCL:H13	1.85	0.41
8:1:402:BCL:H142	8:1:402:BCL:H111	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:359:GLN:HE21	1:3:361:GLU:HB3	1.84	0.41
1:2:64:PHE:HD1	1:2:89:ALA:HB2	1.84	0.41
1:2:185:PHE:CE2	1:2:200:ILE:HG13	2.55	0.41
8:2:404:BCL:H61	8:2:406:BCL:H192	2.02	0.41
3:B:154:VAL:HG23	3:B:154:VAL:O	2.20	0.41
14:a:821:LHG:H362	14:a:821:LHG:H332	1.92	0.41
1:6:180:ILE:O	1:6:184:TRP:HB2	2.20	0.41
1:5:297:HIS:HB3	8:5:406:BCL:CHA	2.50	0.41
1:1:18:ILE:HD11	8:1:403:BCL:HAA1	2.03	0.41
8:1:402:BCL:HAA2	8:1:402:BCL:CGD	2.50	0.41
1:3:230:SER:HB2	1:2:185:PHE:O	2.21	0.41
1:2:122:LEU:HB2	8:2:409[B]:BCL:HED2	2.02	0.41
4:A:121:MET:SD	4:A:126:ILE:HD12	2.60	0.41
4:A:572:TYR:HB3	4:A:595:GLY:N	2.35	0.41
4:a:523:TYR:HB2	4:a:540:ILE:HG12	2.02	0.41
4:a:679:PHE:CE2	9:a:820:CDL:H141	2.55	0.41
1:1:92:THR:HG23	1:1:95:ARG:H	1.85	0.41
1:2:291:PRO:HB2	1:2:294:PRO:HD2	2.03	0.41
8:2:403:BCL:HBD	8:2:403:BCL:HED2	1.85	0.41
8:2:408:BCL:H162	8:2:408:BCL:H122	1.88	0.41
4:a:188:LYS:O	4:a:192:VAL:HG23	2.21	0.41
1:4:73:SER:HB3	1:4:80:ASN:HB2	2.02	0.41
8:4:403:BCL:H42	8:4:405:BCL:H151	2.02	0.41
1:6:325:TYR:O	1:6:325:TYR:CD1	2.74	0.41
7:C:46:LEU:O	7:C:50:MET:HG2	2.20	0.41
7:C:113:ILE:HG13	7:C:113:ILE:O	2.21	0.41
1:1:322:LYS:HE3	1:1:322:LYS:HB2	1.73	0.41
8:1:401:BCL:H112	8:1:401:BCL:H152	1.64	0.41
8:1:402:BCL:HAA2	8:1:402:BCL:O1D	2.21	0.41
8:1:408:BCL:H171	8:3:401:BCL:HBC3	2.02	0.41
1:3:59:ASP:OD1	1:3:59:ASP:N	2.52	0.41
8:2:405:BCL:HBD	8:2:405:BCL:O1A	2.20	0.41
4:A:433:PHE:CD1	14:a:821:LHG:H331	2.55	0.41
4:a:220:TRP:CD1	8:a:806:BCL:H43	2.56	0.41
4:a:540:ILE:HG13	4:a:541:GLN:N	2.35	0.41
8:6:401:BCL:H112	8:6:401:BCL:H152	1.89	0.41
8:6:403:BCL:H72	8:6:404:BCL:H41	2.03	0.41
1:1:191:THR:HG22	1:1:300:MET:HE1	2.03	0.41
8:3:403:BCL:H92	8:3:403:BCL:H62	1.91	0.41
3:B:190:GLU:OE2	4:A:56:THR:HA	2.20	0.41
4:A:593:THR:HG22	4:A:698:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:513:TRP:CH2	4:a:538:VAL:HG21	2.56	0.41
14:a:821:LHG:H382	14:a:821:LHG:H352	1.90	0.41
1:4:58:LEU:HD23	1:4:58:LEU:HA	1.94	0.41
1:5:293:ILE:HA	1:5:296:VAL:HG22	2.02	0.41
1:1:55:VAL:HG22	1:1:67:ILE:HG13	2.02	0.41
1:1:230:SER:HB2	1:3:185:PHE:O	2.20	0.41
1:3:185:PHE:CZ	1:3:200:ILE:HG13	2.55	0.41
8:2:404:BCL:H162	8:2:404:BCL:H192	1.81	0.41
2:D:6:SER:HA	4:a:647:ARG:NH1	2.36	0.41
2:D:83:GLN:NE2	2:D:85:ASP:OD1	2.53	0.41
4:A:50:LEU:HD12	4:a:532:TYR:HB3	2.02	0.41
4:A:224:MET:SD	4:A:228:LEU:HD12	2.61	0.41
4:A:676:ALA:HB1	14:A:819:LHG:HC91	2.02	0.41
1:4:47:ALA:HB3	1:4:260:SER:HB3	2.03	0.41
1:4:117:GLY:HA3	8:4:406:BCL:HMA2	2.03	0.41
8:4:402:BCL:H161	8:4:402:BCL:H141	1.85	0.41
8:4:402:BCL:H202	8:4:402:BCL:H162	1.81	0.41
1:6:57:PRO:HA	1:6:65:VAL:HG12	2.02	0.41
1:5:185:PHE:CD2	1:5:193:LEU:HD11	2.56	0.41
1:5:253:GLN:O	1:5:272:GLU:N	2.53	0.41
1:1:189:ALA:HA	8:1:406:BCL:HHB	2.03	0.41
8:1:401:BCL:H121	8:1:401:BCL:H8	1.86	0.41
8:1:401:BCL:H2C	8:1:401:BCL:HBC2	1.65	0.41
8:1:403:BCL:H92	8:1:403:BCL:H2C	2.03	0.41
8:1:408:BCL:H91	8:1:408:BCL:H112	1.83	0.41
8:2:401:BCL:H62	8:2:401:BCL:H41	1.48	0.41
2:D:86:ILE:HG12	2:D:90:MET:HG2	2.03	0.41
3:B:183:SER:O	3:B:187:SER:OG	2.27	0.41
4:A:85:VAL:O	4:A:89:ILE:HG23	2.21	0.41
4:A:241:SER:OG	8:A:808:BCL:HHD	2.21	0.41
4:A:542:ASP:OD1	4:A:674:LYS:HD3	2.21	0.41
4:A:622:LEU:HD12	4:A:625:PHE:CE1	2.56	0.41
4:A:632:PHE:CD1	4:a:631:TRP:HB3	2.56	0.41
4:a:88:PHE:HB3	7:C:86:PHE:CE1	2.55	0.41
4:a:153:VAL:HG11	8:a:806:BCL:HBB2	2.01	0.41
8:a:811:BCL:H62	8:a:811:BCL:H41	1.59	0.41
1:4:115:PHE:HA	1:4:149:LEU:O	2.21	0.41
1:6:205:VAL:HG12	1:6:207:GLY:H	1.85	0.41
1:6:238:ARG:O	1:6:242:LEU:HG	2.21	0.41
8:6:405:BCL:HBC3	8:6:405:BCL:H2C	1.86	0.41
8:6:408:BCL:H72	8:5:401:BCL:HMD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:235:SER:HB2	8:5:405:BCL:HHD	2.02	0.41
1:5:286:ARG:NE	1:5:361:GLU:OE1	2.52	0.41
1:5:297:HIS:CE1	8:5:406:BCL:C4B	3.03	0.41
8:5:402:BCL:C4B	8:5:403:BCL:HBC1	2.50	0.41
7:C:36:ALA:HB3	7:C:39:HIS:CG	2.55	0.41
8:1:408:BCL:H162	8:1:408:BCL:H202	1.76	0.41
4:A:211:VAL:HG23	4:A:257:GLY:HA3	2.03	0.41
4:A:451:LEU:HB2	4:A:453:ILE:HG12	2.02	0.41
4:A:470:ILE:HG13	4:A:471:PHE:CD2	2.56	0.41
4:A:533:GLY:O	4:a:670:ILE:HG13	2.21	0.41
4:A:561:TYR:CE2	15:A:817:LMG:HC61	2.56	0.41
4:A:583:ASP:HA	4:A:588:LEU:HB2	2.02	0.41
8:A:809:BCL:CBB	8:A:809:BCL:HHC	2.51	0.41
4:a:237:GLN:OE1	13:a:816:F39:O5	2.39	0.41
9:a:822:CDL:H542	9:a:822:CDL:H171	2.03	0.41
8:4:405:BCL:H102	8:4:405:BCL:H62	1.80	0.41
8:6:403:BCL:H92	8:6:403:BCL:H62	1.82	0.41
1:5:26:SER:HB2	1:5:277:SER:O	2.21	0.41
1:5:156:ASN:HB2	1:5:159:LEU:HD23	2.02	0.41
1:1:155:ASP:OD1	1:1:156:ASN:N	2.54	0.40
1:3:238:ARG:NH2	1:3:289:ASN:O	2.54	0.40
1:3:243:PHE:CE2	1:3:245:SER:HB2	2.57	0.40
1:2:184:TRP:NE1	8:2:407:BCL:HBB1	2.36	0.40
1:2:189:ALA:HA	8:2:408:BCL:HHB	2.03	0.40
3:B:129:ALA:HB3	3:B:181:SER:HB2	2.02	0.40
4:A:318:PHE:CE1	4:A:364:MET:HG2	2.56	0.40
4:A:395:LEU:HD11	4:A:404:TYR:CE1	2.56	0.40
4:A:632:PHE:O	4:A:634:ASP:N	2.53	0.40
8:A:804:BCL:H92	8:A:804:BCL:H62	1.88	0.40
4:a:101:PHE:HE2	7:C:97:ARG:NE	2.20	0.40
1:4:95:ARG:HG3	1:4:120:VAL:HG22	2.03	0.40
1:4:126:ARG:HB2	8:4:408[B]:BCL:HMB2	2.03	0.40
1:6:26:SER:OG	1:6:247:LYS:HD3	2.21	0.40
1:6:293:ILE:HD13	1:6:293:ILE:HA	1.93	0.40
8:F:101:BCL:HBC1	7:C:23:LEU:HG	2.03	0.40
7:c:20:MET:HE2	7:c:24:PHE:CE2	2.54	0.40
1:1:69:ALA:HB3	1:1:84:ILE:HG12	2.02	0.40
8:1:403:BCL:H192	8:1:403:BCL:H162	1.84	0.40
8:3:401:BCL:HBD	8:3:401:BCL:HED2	1.87	0.40
1:2:233:VAL:HA	1:2:293:ILE:HD11	2.03	0.40
8:2:404:BCL:HAA1	8:2:408:BCL:OBD	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:194:PHE:O	4:A:196:GLY:N	2.54	0.40
4:A:203:LYS:H	4:A:271:LEU:CD1	2.32	0.40
4:A:652:LEU:HD23	4:A:652:LEU:HA	1.92	0.40
14:a:821:LHG:HC92	14:a:821:LHG:H121	1.77	0.40
9:a:822:CDL:H182	9:a:822:CDL:H562	2.02	0.40
1:4:109:PHE:HE1	1:4:111:HIS:HD2	1.68	0.40
1:6:313:LEU:HB2	1:6:345:TYR:CZ	2.56	0.40
8:6:403:BCL:H161	8:6:403:BCL:H122	1.81	0.40
8:6:404:BCL:H202	8:6:406:BCL:H201	2.03	0.40
1:5:103:MET:HA	1:5:112:THR:HA	2.02	0.40
1:5:291:PRO:O	1:5:294:PRO:HD2	2.21	0.40
1:1:101:GLU:HA	1:1:114:SER:HA	2.02	0.40
1:1:314:LYS:HD3	3:B:224:HIS:HB2	2.04	0.40
2:D:19:VAL:HG22	4:A:417:ASP:O	2.21	0.40
4:A:202:TYR:HB3	8:A:809:BCL:HBC2	2.04	0.40
14:A:818:LHG:H272	14:A:818:LHG:H301	1.78	0.40
4:a:270:HIS:HB3	4:a:278:ALA:HB2	2.03	0.40
4:a:292:ALA:O	4:a:296:ILE:HG12	2.22	0.40
1:4:158:ASP:OD2	1:5:129:ALA:N	2.39	0.40
1:6:124:TYR:CD2	1:5:183:PHE:HB2	2.56	0.40
1:6:199:ARG:O	1:6:227:HIS:HA	2.21	0.40
8:6:408:BCL:H111	8:6:408:BCL:H142	1.89	0.40
8:5:404:BCL:H122	8:5:404:BCL:H161	1.81	0.40
8:5:406:BCL:H151	8:5:406:BCL:H112	1.92	0.40
1:1:298:HIS:O	1:1:302:GLY:N	2.53	0.40
1:3:284:LEU:HD11	1:3:363:LEU:HB3	2.04	0.40
8:3:405:BCL:HBC3	8:3:405:BCL:H2C	1.84	0.40
1:2:310:ASP:HB3	4:A:200:LYS:HD2	2.03	0.40
8:2:403:BCL:H72	8:2:403:BCL:H112	1.65	0.40
8:2:409[B]:BCL:HBC3	8:2:409[B]:BCL:H2C	1.78	0.40
4:A:116:THR:HG21	8:A:810:BCL:H3A	2.02	0.40
4:A:320:LEU:HD22	8:c:301:BCL:HED3	2.03	0.40
4:a:548:MET:O	4:a:552:ILE:HG13	2.22	0.40
1:4:185:PHE:CE2	1:4:200:ILE:HG13	2.56	0.40
1:4:230:SER:HB2	1:6:185:PHE:O	2.21	0.40
8:1:408:BCL:H92	8:3:402:BCL:H101	2.04	0.40
1:3:334:ASN:C	1:3:336:GLU:H	2.30	0.40
1:2:50:ASP:N	1:2:72:GLU:O	2.36	0.40
1:2:151:LYS:HG2	1:2:220:VAL:HG13	2.03	0.40
1:2:235:SER:HA	1:2:242:LEU:CD2	2.50	0.40
8:A:810:BCL:H62	8:A:810:BCL:H41	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:811:BCL:HBA2	8:A:811:BCL:H3A	1.88	0.40
4:a:273:ASP:HB3	4:a:394:TYR:CE1	2.57	0.40
4:a:274:ASP:OD1	4:a:274:ASP:N	2.54	0.40
8:4:403:BCL:H111	8:4:403:BCL:H142	1.82	0.40
8:4:403:BCL:H141	8:4:403:BCL:H162	1.96	0.40
1:6:291:PRO:O	1:6:294:PRO:HD2	2.22	0.40
1:6:315:VAL:HG22	1:6:340:TRP:HZ3	1.86	0.40
8:6:402:BCL:H162	8:6:402:BCL:H141	1.85	0.40
1:5:233:VAL:HA	1:5:293:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	360/366 (98%)	349 (97%)	11 (3%)	0	100 100
1	2	356/366 (97%)	343 (96%)	12 (3%)	1 (0%)	37 66
1	3	356/366 (97%)	347 (98%)	9 (2%)	0	100 100
1	4	360/366 (98%)	346 (96%)	13 (4%)	1 (0%)	37 66
1	5	356/366 (97%)	349 (98%)	6 (2%)	1 (0%)	37 66
1	6	356/366 (97%)	349 (98%)	7 (2%)	0	100 100
2	D	141/143 (99%)	123 (87%)	16 (11%)	2 (1%)	9 31
3	B	100/230 (44%)	84 (84%)	16 (16%)	0	100 100
4	A	665/731 (91%)	607 (91%)	58 (9%)	0	100 100
4	a	660/731 (90%)	601 (91%)	57 (9%)	2 (0%)	37 66
6	F	48/58 (83%)	45 (94%)	3 (6%)	0	100 100
7	C	111/206 (54%)	101 (91%)	10 (9%)	0	100 100
7	c	111/206 (54%)	103 (93%)	8 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3980/4501 (88%)	3747 (94%)	226 (6%)	7 (0%)	45 73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	123	GLU
4	a	334	GLU
1	5	336	GLU
1	4	335	LEU
1	2	335	LEU
2	D	63	THR
4	a	102	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	299/302 (99%)	299 (100%)	0	100 100
1	2	296/302 (98%)	295 (100%)	1 (0%)	91 97
1	3	296/302 (98%)	296 (100%)	0	100 100
1	4	299/302 (99%)	299 (100%)	0	100 100
1	5	296/302 (98%)	295 (100%)	1 (0%)	91 97
1	6	296/302 (98%)	296 (100%)	0	100 100
2	D	128/128 (100%)	128 (100%)	0	100 100
3	B	86/161 (53%)	86 (100%)	0	100 100
4	A	553/599 (92%)	553 (100%)	0	100 100
4	a	550/599 (92%)	550 (100%)	0	100 100
6	F	40/45 (89%)	40 (100%)	0	100 100
7	C	94/173 (54%)	94 (100%)	0	100 100
7	c	94/173 (54%)	94 (100%)	0	100 100
All	All	3327/3690 (90%)	3325 (100%)	2 (0%)	92 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	253	GLN
1	5	306	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	194	ASN
1	1	263	GLN
1	1	305	ASN
1	1	308	ASN
1	3	37	ASN
1	3	133	ASN
1	3	136	ASN
1	3	194	ASN
1	2	54	ASN
1	2	144	GLN
1	2	156	ASN
1	2	177	ASN
1	2	194	ASN
1	2	306	ASN
2	D	48	GLN
4	A	406	GLN
4	A	418	GLN
4	A	541	GLN
4	A	695	ASN
4	a	99	GLN
4	a	695	ASN
1	4	37	ASN
1	4	194	ASN
1	6	13	HIS
1	6	54	ASN
1	6	80	ASN
1	6	121	ASN
1	6	144	GLN
1	6	194	ASN
1	6	308	ASN
1	5	194	ASN
1	5	198	GLN
1	5	253	GLN
1	5	366	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 103 ligands modelled in this entry, 2 are monoatomic - leaving 101 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BCL	4	408[B]	1	44,54,74	1.97	12 (27%)	54,91,115	2.42	21 (38%)
11	GS0	a	802	4	64,74,74	1.73	10 (15%)	78,115,115	2.31	28 (35%)
8	BCL	a	805	-	54,64,74	1.84	12 (22%)	66,103,115	2.38	24 (36%)
8	BCL	4	406	1	64,74,74	1.70	13 (20%)	78,115,115	2.34	28 (35%)
8	BCL	3	403	1	64,74,74	1.72	12 (18%)	78,115,115	2.23	26 (33%)
8	BCL	5	405	1	64,74,74	1.70	11 (17%)	78,115,115	2.30	27 (34%)
8	BCL	c	301	4	44,54,74	1.97	11 (25%)	54,91,115	2.61	21 (38%)
15	LMG	a	818	-	44,44,55	0.79	0	52,52,63	1.37	4 (7%)
8	BCL	6	401	1	64,74,74	1.72	12 (18%)	78,115,115	2.44	30 (38%)
12	G2O	A	822	4	67,73,73	2.39	23 (34%)	75,113,113	1.51	9 (12%)
8	BCL	5	402	1	64,74,74	1.73	13 (20%)	78,115,115	2.26	23 (29%)
8	BCL	a	804	4	44,54,74	1.98	11 (25%)	54,91,115	2.39	20 (37%)
8	BCL	2	407	1	64,74,74	1.71	13 (20%)	78,115,115	2.34	29 (37%)
8	BCL	a	814	4	44,54,74	1.97	11 (25%)	54,91,115	2.63	23 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	F	101	4	44,54,74	1.98	10 (22%)	54,91,115	2.63	23 (42%)
8	BCL	2	408	1	64,74,74	1.70	12 (18%)	78,115,115	2.27	26 (33%)
8	BCL	a	810	4	44,54,74	1.94	10 (22%)	54,91,115	2.67	23 (42%)
8	BCL	3	401	1	64,74,74	1.72	11 (17%)	78,115,115	2.49	30 (38%)
14	LHG	A	819	-	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
8	BCL	4	401	1	64,74,74	1.72	12 (18%)	78,115,115	2.46	28 (35%)
8	BCL	2	404	1	64,74,74	1.73	13 (20%)	78,115,115	2.22	25 (32%)
8	BCL	a	811	4	64,74,74	1.70	13 (20%)	78,115,115	2.39	29 (37%)
8	BCL	6	402	1	64,74,74	1.73	13 (20%)	78,115,115	2.24	23 (29%)
12	G2O	a	803	-	67,73,73	2.41	24 (35%)	75,113,113	1.49	9 (12%)
8	BCL	6	407[B]	1	44,54,74	1.97	11 (25%)	54,91,115	2.40	22 (40%)
14	LHG	a	819	-	39,39,48	0.68	1 (2%)	42,45,54	1.25	4 (9%)
8	BCL	6	405	1	64,74,74	1.70	11 (17%)	78,115,115	2.31	26 (33%)
8	BCL	5	403	1	64,74,74	1.71	12 (18%)	78,115,115	2.28	29 (37%)
8	BCL	6	408	-	64,74,74	1.71	12 (18%)	78,115,115	2.26	27 (34%)
14	LHG	a	821	-	41,41,48	0.65	0	44,47,54	1.20	4 (9%)
8	BCL	4	404	1	64,74,74	1.71	12 (18%)	78,115,115	2.24	27 (34%)
8	BCL	1	404	-	64,74,74	1.70	11 (17%)	78,115,115	2.29	30 (38%)
8	BCL	A	812	4	44,54,74	2.00	12 (27%)	54,91,115	2.62	22 (40%)
8	BCL	1	406	1	64,74,74	1.70	11 (17%)	78,115,115	2.26	26 (33%)
8	BCL	2	403	1	64,74,74	1.72	12 (18%)	78,115,115	2.43	28 (35%)
8	BCL	4	410[B]	1	44,54,74	1.98	12 (27%)	54,91,115	2.43	21 (38%)
8	BCL	A	805	-	64,74,74	1.72	14 (21%)	78,115,115	2.27	26 (33%)
8	BCL	1	408	-	64,74,74	1.71	11 (17%)	78,115,115	2.25	27 (34%)
17	F26	c	302	-	40,40,40	2.00	15 (37%)	46,50,50	2.15	9 (19%)
14	LHG	A	816	-	45,45,48	0.64	2 (4%)	48,51,54	1.26	6 (12%)
8	BCL	2	405	1	64,74,74	1.71	12 (18%)	78,115,115	2.27	27 (34%)
8	BCL	4	402	-	64,74,74	1.72	13 (20%)	78,115,115	2.24	26 (33%)
8	BCL	5	404	1	64,74,74	1.70	11 (17%)	78,115,115	2.26	28 (35%)
9	CDL	c	303	-	69,69,99	1.04	8 (11%)	75,81,111	1.14	4 (5%)
13	F39	A	814	-	66,66,66	8.14	55 (83%)	79,85,85	4.10	29 (36%)
8	BCL	4	409	-	64,74,74	1.72	11 (17%)	78,115,115	2.26	27 (34%)
8	BCL	A	806	-	44,54,74	2.01	12 (27%)	54,91,115	2.57	20 (37%)
8	BCL	A	809	4	44,54,74	1.93	9 (20%)	54,91,115	2.71	21 (38%)
13	F39	a	816	-	66,66,66	8.12	57 (86%)	79,85,85	4.15	29 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	F26	a	815	-	40,40,40	2.00	15 (37%)	46,50,50	1.98	11 (23%)
8	BCL	a	806	9	64,74,74	1.72	14 (21%)	78,115,115	2.29	26 (33%)
8	BCL	4	403	1	64,74,74	1.73	13 (20%)	78,115,115	2.22	25 (32%)
8	BCL	A	803	4	44,54,74	1.98	11 (25%)	54,91,115	2.45	22 (40%)
12	G2O	a	801	4	67,73,73	2.40	24 (35%)	75,113,113	1.47	9 (12%)
8	BCL	1	402	1	64,74,74	1.73	12 (18%)	78,115,115	2.29	23 (29%)
13	F39	A	815	-	66,66,66	8.15	58 (87%)	79,85,85	4.10	29 (36%)
8	BCL	a	807	-	44,54,74	2.01	10 (22%)	54,91,115	2.67	22 (40%)
8	BCL	1	405	1	64,74,74	1.70	12 (18%)	78,115,115	2.33	28 (35%)
8	BCL	3	402	1	64,74,74	1.73	13 (20%)	78,115,115	2.19	25 (32%)
8	BCL	3	407	-	64,74,74	1.72	11 (17%)	78,115,115	2.23	26 (33%)
8	BCL	4	405	-	64,74,74	1.71	12 (18%)	78,115,115	2.26	30 (38%)
8	BCL	2	401	-	64,74,74	1.72	11 (17%)	78,115,115	2.25	26 (33%)
8	BCL	A	808	4	44,54,74	1.97	10 (22%)	54,91,115	2.59	23 (42%)
8	BCL	A	807	4	64,74,74	1.70	12 (18%)	78,115,115	2.28	28 (35%)
9	CDL	a	820	-	69,69,99	1.04	8 (11%)	75,81,111	1.16	4 (5%)
8	BCL	A	810	4	64,74,74	1.71	12 (18%)	78,115,115	2.33	30 (38%)
8	BCL	2	409[B]	1	44,54,74	1.98	12 (27%)	54,91,115	2.41	21 (38%)
8	BCL	2	402[B]	1	44,54,74	1.98	11 (25%)	54,91,115	2.43	22 (40%)
10	SF4	A	821	4	0,12,12	-	-	-		
8	BCL	6	403	1	64,74,74	1.71	13 (20%)	78,115,115	2.29	28 (35%)
14	LHG	E	101	-	36,36,48	0.70	0	39,42,54	1.26	4 (10%)
8	BCL	3	404	-	64,74,74	1.70	11 (17%)	78,115,115	2.30	30 (38%)
8	BCL	1	401	1	64,74,74	1.72	11 (17%)	78,115,115	2.45	29 (37%)
8	BCL	6	404	1	64,74,74	1.70	11 (17%)	78,115,115	2.28	25 (32%)
11	GS0	A	801	4	64,74,74	1.71	10 (15%)	78,115,115	2.28	28 (35%)
8	BCL	6	406	1	64,74,74	1.70	12 (18%)	78,115,115	2.27	24 (30%)
9	CDL	1	409	-	76,76,99	0.99	8 (10%)	82,88,111	1.14	4 (4%)
8	BCL	5	401	1	64,74,74	1.72	12 (18%)	78,115,115	2.49	29 (37%)
8	BCL	5	406	1	64,74,74	1.71	12 (18%)	78,115,115	2.31	27 (34%)
8	BCL	A	804	-	54,64,74	1.85	12 (22%)	66,103,115	2.34	23 (34%)
8	BCL	a	812	4	64,74,74	1.72	13 (20%)	78,115,115	2.31	26 (33%)
12	G2O	A	802	-	67,73,73	2.43	24 (35%)	75,113,113	1.43	9 (12%)
8	BCL	2	406	1	64,74,74	1.70	11 (17%)	78,115,115	2.25	26 (33%)
8	BCL	a	808	4	64,74,74	1.71	12 (18%)	78,115,115	2.21	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	4	407	1	64,74,74	1.71	13 (20%)	78,115,115	2.25	25 (32%)
9	CDL	a	822	8	91,91,99	0.91	8 (8%)	97,103,111	1.09	4 (4%)
10	SF4	B	301	3	0,12,12	-	-	-		
8	BCL	a	809	4	44,54,74	1.98	11 (25%)	54,91,115	2.60	22 (40%)
15	LMG	A	817	-	44,44,55	0.78	0	52,52,63	1.35	3 (5%)
13	F39	C	302	-	66,66,66	8.14	59 (89%)	79,85,85	4.03	29 (36%)
14	LHG	a	817	-	45,45,48	0.64	1 (2%)	48,51,54	1.27	6 (12%)
8	BCL	A	813	-	44,54,74	1.98	12 (27%)	54,91,115	2.62	23 (42%)
14	LHG	A	818	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
8	BCL	3	405	1	64,74,74	1.70	11 (17%)	78,115,115	2.44	29 (37%)
8	BCL	A	811	4	64,74,74	1.72	13 (20%)	78,115,115	2.24	25 (32%)
10	SF4	B	302	3	0,12,12	-	-	-		
8	BCL	3	406	1	64,74,74	1.70	11 (17%)	78,115,115	2.27	28 (35%)
8	BCL	1	407[B]	1	44,54,74	1.97	11 (25%)	54,91,115	2.39	21 (38%)
8	BCL	a	813	4	44,54,74	1.97	11 (25%)	54,91,115	2.65	25 (46%)
8	BCL	C	301	4	44,54,74	1.97	11 (25%)	54,91,115	2.56	22 (40%)
8	BCL	1	403	1	64,74,74	1.71	12 (18%)	78,115,115	2.26	25 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	4	408[B]	1	-	5/13/113/137	-
11	GS0	a	802	4	-	11/37/137/137	-
8	BCL	a	805	-	-	11/25/125/137	-
8	BCL	4	406	1	-	13/37/137/137	-
8	BCL	3	403	1	-	18/37/137/137	-
8	BCL	5	405	1	-	11/37/137/137	-
8	BCL	c	301	4	-	5/13/113/137	-
15	LMG	a	818	-	-	19/39/59/70	0/1/1/1
8	BCL	6	401	1	-	13/37/137/137	-
12	G2O	A	822	4	-	16/39/115/115	-
8	BCL	5	402	1	-	11/37/137/137	-
8	BCL	a	804	4	-	9/13/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	2	407	1	-	7/37/137/137	-
8	BCL	a	814	4	-	2/13/113/137	-
8	BCL	F	101	4	-	2/13/113/137	-
8	BCL	2	408	1	-	13/37/137/137	-
8	BCL	a	810	4	-	5/13/113/137	-
8	BCL	3	401	1	-	12/37/137/137	-
14	LHG	A	819	-	-	30/53/53/53	-
8	BCL	4	401	1	-	12/37/137/137	-
8	BCL	2	404	1	-	16/37/137/137	-
8	BCL	a	811	4	-	19/37/137/137	-
8	BCL	6	402	1	-	17/37/137/137	-
12	G2O	a	803	-	-	16/39/115/115	-
8	BCL	6	407[B]	1	-	5/13/113/137	-
14	LHG	a	819	-	-	19/44/44/53	-
8	BCL	6	405	1	-	14/37/137/137	-
8	BCL	5	403	1	-	14/37/137/137	-
8	BCL	6	408	-	-	11/37/137/137	-
14	LHG	a	821	-	-	26/46/46/53	-
8	BCL	4	404	1	-	17/37/137/137	-
8	BCL	1	404	-	-	10/37/137/137	-
8	BCL	A	812	4	-	4/13/113/137	-
8	BCL	1	406	1	-	14/37/137/137	-
8	BCL	2	403	1	-	10/37/137/137	-
8	BCL	4	410[B]	1	-	7/13/113/137	-
8	BCL	A	805	-	-	11/37/137/137	-
8	BCL	1	408	-	-	15/37/137/137	-
17	F26	c	302	-	-	23/36/36/36	0/1/1/1
14	LHG	A	816	-	-	23/50/50/53	-
8	BCL	2	405	1	-	16/37/137/137	-
8	BCL	4	402	-	-	13/37/137/137	-
8	BCL	5	404	1	-	11/37/137/137	-
9	CDL	c	303	-	-	31/80/80/110	-
13	F39	A	814	-	-	39/58/78/78	0/2/2/2
8	BCL	4	409	-	-	14/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	A	806	-	-	4/13/113/137	-
8	BCL	A	809	4	-	7/13/113/137	-
13	F39	a	816	-	-	38/58/78/78	0/2/2/2
17	F26	a	815	-	-	21/36/36/36	0/1/1/1
8	BCL	a	806	9	-	16/37/137/137	-
8	BCL	4	403	1	-	18/37/137/137	-
8	BCL	A	803	4	-	3/13/113/137	-
12	G2O	a	801	4	-	18/39/115/115	-
8	BCL	1	402	1	-	10/37/137/137	-
13	F39	A	815	-	-	41/58/78/78	0/2/2/2
8	BCL	a	807	-	-	4/13/113/137	-
8	BCL	1	405	1	-	9/37/137/137	-
8	BCL	3	402	1	-	12/37/137/137	-
8	BCL	3	407	-	-	15/37/137/137	-
8	BCL	4	405	-	-	14/37/137/137	-
8	BCL	2	401	-	-	21/37/137/137	-
8	BCL	A	808	4	-	2/13/113/137	-
8	BCL	A	807	4	-	19/37/137/137	-
9	CDL	a	820	-	-	40/80/80/110	-
8	BCL	A	810	4	-	15/37/137/137	-
8	BCL	2	409[B]	1	-	1/13/113/137	-
8	BCL	2	402[B]	1	-	7/13/113/137	-
10	SF4	A	821	4	-	-	0/6/5/5
8	BCL	6	403	1	-	16/37/137/137	-
14	LHG	E	101	-	-	16/41/41/53	-
8	BCL	3	404	-	-	16/37/137/137	-
8	BCL	1	401	1	-	12/37/137/137	-
8	BCL	6	404	1	-	12/37/137/137	-
11	GS0	A	801	4	-	10/37/137/137	-
8	BCL	6	406	1	-	11/37/137/137	-
9	CDL	1	409	-	-	47/87/87/110	-
8	BCL	5	401	1	-	12/37/137/137	-
8	BCL	5	406	1	-	14/37/137/137	-
8	BCL	A	804	-	-	12/25/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	a	812	4	-	16/37/137/137	-
12	G2O	A	802	-	-	21/39/115/115	-
8	BCL	2	406	1	-	15/37/137/137	-
8	BCL	a	808	4	-	24/37/137/137	-
8	BCL	4	407	1	-	13/37/137/137	-
9	CDL	a	822	8	-	49/102/102/110	-
10	SF4	B	301	3	-	-	0/6/5/5
8	BCL	a	809	4	-	3/13/113/137	-
15	LMG	A	817	-	-	19/39/59/70	0/1/1/1
13	F39	C	302	-	-	42/58/78/78	0/2/2/2
14	LHG	a	817	-	-	20/50/50/53	-
8	BCL	A	813	-	-	3/13/113/137	-
14	LHG	A	818	-	-	24/53/53/53	-
8	BCL	3	405	1	-	11/37/137/137	-
8	BCL	A	811	4	-	11/37/137/137	-
10	SF4	B	302	3	-	-	0/6/5/5
8	BCL	3	406	1	-	11/37/137/137	-
8	BCL	1	407[B]	1	-	6/13/113/137	-
8	BCL	a	813	4	-	5/13/113/137	-
8	BCL	C	301	4	-	5/13/113/137	-
8	BCL	1	403	1	-	16/37/137/137	-

All (1267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	815	F39	C27-C20	27.42	1.62	1.34
13	A	814	F39	C27-C20	27.38	1.62	1.34
13	a	816	F39	C27-C20	27.27	1.62	1.34
13	C	302	F39	C27-C20	27.06	1.62	1.34
13	A	815	F39	C39-C37	22.67	1.65	1.35
13	C	302	F39	C39-C37	22.67	1.65	1.35
13	A	814	F39	C39-C37	22.65	1.65	1.35
13	a	816	F39	C39-C37	22.54	1.65	1.35
13	A	815	F39	C44-C42	20.46	1.62	1.35
13	A	814	F39	C44-C42	20.35	1.62	1.35
13	C	302	F39	C44-C42	20.28	1.62	1.35
13	a	816	F39	C44-C42	20.28	1.62	1.35
13	C	302	F39	C59-C62	20.14	1.62	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	814	F39	C61-C58	20.10	1.62	1.35
13	a	816	F39	C59-C62	19.99	1.62	1.35
13	A	815	F39	C61-C58	19.97	1.62	1.35
13	C	302	F39	C61-C58	19.92	1.62	1.35
13	a	816	F39	C61-C58	19.91	1.62	1.35
13	A	814	F39	C59-C62	19.89	1.62	1.35
13	A	815	F39	C59-C62	19.87	1.62	1.35
13	C	302	F39	C40-C41	12.08	1.65	1.34
13	A	814	F39	C40-C41	12.07	1.65	1.34
13	A	815	F39	C40-C41	12.03	1.65	1.34
13	a	816	F39	C40-C41	12.01	1.65	1.34
13	A	815	F39	C32-C35	12.00	1.65	1.34
13	a	816	F39	C32-C35	11.97	1.65	1.34
13	C	302	F39	C32-C35	11.89	1.65	1.34
13	A	814	F39	C32-C35	11.89	1.65	1.34
13	A	815	F39	C56-C53	11.70	1.63	1.33
13	C	302	F39	C56-C53	11.68	1.63	1.33
13	A	814	F39	C56-C53	11.64	1.63	1.33
13	C	302	F39	C63-C64	11.63	1.64	1.34
13	a	816	F39	C56-C53	11.56	1.63	1.33
13	A	814	F39	C63-C64	11.53	1.64	1.34
13	a	816	F39	C63-C64	11.52	1.64	1.34
13	A	815	F39	C63-C64	11.50	1.64	1.34
13	C	302	F39	C57-C51	10.88	1.64	1.36
13	A	814	F39	C57-C51	10.85	1.64	1.36
13	A	815	F39	C57-C51	10.85	1.64	1.36
13	a	816	F39	C57-C51	10.82	1.64	1.36
13	A	815	F39	C35-C37	8.99	1.65	1.45
13	C	302	F39	C35-C37	8.96	1.65	1.45
13	a	816	F39	C35-C37	8.93	1.65	1.45
13	A	814	F39	C35-C37	8.90	1.65	1.45
13	A	815	F39	C14-C13	8.81	1.66	1.53
13	A	814	F39	C14-C13	8.79	1.66	1.53
13	C	302	F39	C14-C13	8.67	1.66	1.53
13	a	816	F39	C14-C13	8.66	1.66	1.53
13	C	302	F39	C64-C62	8.06	1.63	1.45
13	C	302	F39	C41-C42	7.97	1.63	1.45
13	A	815	F39	C64-C62	7.95	1.63	1.45
13	A	814	F39	C64-C62	7.91	1.62	1.45
13	A	815	F39	C41-C42	7.91	1.62	1.45
13	a	816	F39	C64-C62	7.90	1.62	1.45
12	A	802	G2O	CMA-C3A	-7.89	1.36	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	822	G2O	CMA-C3A	-7.88	1.36	1.53
13	a	816	F39	C41-C42	7.86	1.62	1.45
12	a	803	G2O	CMA-C3A	-7.84	1.36	1.53
13	A	814	F39	C41-C42	7.83	1.62	1.45
12	a	801	G2O	CMA-C3A	-7.81	1.36	1.53
13	A	815	F39	C56-C58	7.67	1.62	1.45
13	a	816	F39	C56-C58	7.63	1.62	1.45
13	C	302	F39	C56-C58	7.63	1.62	1.45
13	A	814	F39	C56-C58	7.58	1.62	1.45
13	A	815	F39	C46-C53	7.39	1.64	1.47
13	A	814	F39	C46-C53	7.35	1.63	1.47
13	a	816	F39	C46-C53	7.34	1.63	1.47
13	C	302	F39	C46-C53	7.33	1.63	1.47
13	C	302	F39	C51-C44	7.08	1.65	1.43
13	A	815	F39	C51-C44	7.00	1.65	1.43
13	a	816	F39	C51-C44	6.98	1.65	1.43
13	A	814	F39	C51-C44	6.98	1.65	1.43
13	a	816	F39	C40-C39	6.97	1.65	1.43
13	A	815	F39	C40-C39	6.94	1.64	1.43
13	A	814	F39	C40-C39	6.94	1.64	1.43
13	C	302	F39	C40-C39	6.94	1.64	1.43
13	C	302	F39	C57-C59	6.91	1.64	1.43
13	a	816	F39	C57-C59	6.89	1.64	1.43
13	A	814	F39	C57-C59	6.86	1.64	1.43
13	C	302	F39	C63-C61	6.85	1.64	1.43
13	A	815	F39	C57-C59	6.84	1.64	1.43
13	A	815	F39	C32-C27	6.84	1.64	1.43
13	A	814	F39	C32-C27	6.83	1.64	1.43
13	a	816	F39	C32-C27	6.80	1.64	1.43
13	C	302	F39	C32-C27	6.80	1.64	1.43
13	A	814	F39	C63-C61	6.76	1.64	1.43
13	A	815	F39	C63-C61	6.74	1.64	1.43
13	a	816	F39	C63-C61	6.73	1.64	1.43
12	A	802	G2O	CBD-CGD	-6.18	1.33	1.52
11	a	802	GS0	MG-ND	-6.18	1.93	2.05
12	a	803	G2O	CBD-CGD	-6.14	1.33	1.52
12	a	801	G2O	CBD-CGD	-6.13	1.33	1.52
12	A	822	G2O	CBD-CGD	-6.13	1.33	1.52
11	A	801	GS0	MG-ND	-6.05	1.93	2.05
13	A	814	F39	C19-C20	5.87	1.63	1.51
13	A	815	F39	C19-C20	5.85	1.63	1.51
13	a	816	F39	C19-C20	5.83	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	410[B]	BCL	MG-ND	-5.81	1.94	2.05
8	2	409[B]	BCL	MG-ND	-5.78	1.94	2.05
8	1	402	BCL	MG-ND	-5.78	1.94	2.05
8	4	408[B]	BCL	MG-ND	-5.78	1.94	2.05
13	C	302	F39	C19-C20	5.77	1.63	1.51
8	1	407[B]	BCL	MG-ND	-5.75	1.94	2.05
8	2	402[B]	BCL	MG-ND	-5.73	1.94	2.05
8	3	407	BCL	MG-ND	-5.72	1.94	2.05
8	3	402	BCL	MG-ND	-5.70	1.94	2.05
8	2	404	BCL	MG-ND	-5.70	1.94	2.05
8	6	407[B]	BCL	MG-ND	-5.69	1.94	2.05
8	2	401	BCL	MG-ND	-5.69	1.94	2.05
8	A	813	BCL	MG-ND	-5.68	1.94	2.05
8	6	402	BCL	MG-ND	-5.67	1.94	2.05
8	4	402	BCL	MG-ND	-5.66	1.94	2.05
8	1	408	BCL	MG-ND	-5.66	1.94	2.05
8	6	403	BCL	MG-ND	-5.66	1.94	2.05
8	4	403	BCL	MG-ND	-5.64	1.94	2.05
8	F	101	BCL	MG-ND	-5.64	1.94	2.05
8	A	807	BCL	MG-ND	-5.63	1.94	2.05
8	4	404	BCL	MG-ND	-5.63	1.94	2.05
8	4	409	BCL	MG-ND	-5.63	1.94	2.05
8	2	403	BCL	MG-ND	-5.62	1.94	2.05
8	6	408	BCL	MG-ND	-5.62	1.94	2.05
8	6	401	BCL	MG-ND	-5.61	1.94	2.05
8	4	401	BCL	MG-ND	-5.61	1.94	2.05
8	C	301	BCL	MG-ND	-5.60	1.94	2.05
8	6	404	BCL	MG-ND	-5.60	1.94	2.05
8	5	403	BCL	MG-ND	-5.59	1.94	2.05
8	3	403	BCL	MG-ND	-5.58	1.94	2.05
8	2	405	BCL	MG-ND	-5.57	1.94	2.05
8	2	408	BCL	MG-ND	-5.57	1.94	2.05
8	1	403	BCL	MG-ND	-5.57	1.94	2.05
8	A	806	BCL	MG-ND	-5.57	1.94	2.05
8	a	806	BCL	MG-ND	-5.56	1.94	2.05
8	4	407	BCL	MG-ND	-5.56	1.94	2.05
8	5	401	BCL	MG-ND	-5.55	1.94	2.05
8	6	406	BCL	MG-ND	-5.55	1.94	2.05
8	4	405	BCL	MG-ND	-5.54	1.94	2.05
8	4	406	BCL	MG-ND	-5.54	1.94	2.05
8	a	808	BCL	MG-ND	-5.53	1.94	2.05
8	c	301	BCL	MG-ND	-5.53	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	406	BCL	MG-ND	-5.53	1.94	2.05
8	5	405	BCL	MG-ND	-5.52	1.94	2.05
8	5	402	BCL	MG-ND	-5.52	1.94	2.05
13	C	302	F39	O6-C21	5.52	1.49	1.33
8	A	804	BCL	MG-ND	-5.52	1.94	2.05
8	1	401	BCL	MG-ND	-5.51	1.94	2.05
8	5	404	BCL	MG-ND	-5.51	1.94	2.05
13	A	815	F39	O6-C21	5.51	1.49	1.33
8	A	808	BCL	MG-ND	-5.51	1.94	2.05
8	3	406	BCL	MG-ND	-5.51	1.94	2.05
8	a	805	BCL	MG-ND	-5.51	1.94	2.05
13	a	816	F39	O6-C21	5.50	1.49	1.33
8	a	814	BCL	MG-ND	-5.50	1.94	2.05
8	A	810	BCL	MG-ND	-5.50	1.94	2.05
8	a	804	BCL	MG-ND	-5.49	1.94	2.05
8	a	809	BCL	MG-ND	-5.49	1.94	2.05
8	2	407	BCL	MG-ND	-5.48	1.94	2.05
8	A	803	BCL	MG-ND	-5.48	1.94	2.05
8	6	405	BCL	MG-ND	-5.47	1.94	2.05
8	A	805	BCL	MG-ND	-5.47	1.94	2.05
8	a	813	BCL	MG-ND	-5.46	1.95	2.05
13	a	816	F39	O1-C11	5.46	1.55	1.41
8	3	404	BCL	MG-ND	-5.45	1.95	2.05
8	a	812	BCL	MG-ND	-5.45	1.95	2.05
8	1	406	BCL	MG-ND	-5.45	1.95	2.05
8	a	807	BCL	MG-ND	-5.45	1.95	2.05
8	1	404	BCL	MG-ND	-5.45	1.95	2.05
8	A	811	BCL	MG-ND	-5.45	1.95	2.05
13	A	814	F39	O6-C21	5.44	1.49	1.33
8	3	401	BCL	MG-ND	-5.43	1.95	2.05
8	a	811	BCL	MG-ND	-5.43	1.95	2.05
8	1	405	BCL	MG-ND	-5.43	1.95	2.05
8	A	812	BCL	MG-ND	-5.42	1.95	2.05
13	A	814	F39	O1-C11	5.41	1.55	1.41
13	C	302	F39	C54-C47	5.39	1.61	1.51
13	A	815	F39	C54-C47	5.39	1.61	1.51
13	A	815	F39	O2-C13	5.37	1.54	1.46
8	5	406	BCL	MG-ND	-5.37	1.95	2.05
8	A	809	BCL	MG-ND	-5.35	1.95	2.05
13	a	816	F39	C54-C47	5.31	1.61	1.51
8	3	405	BCL	MG-ND	-5.31	1.95	2.05
13	A	814	F39	O2-C13	5.30	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	814	F39	C54-C47	5.26	1.61	1.51
13	C	302	F39	O1-C11	5.26	1.55	1.41
8	a	810	BCL	MG-ND	-5.25	1.95	2.05
13	a	816	F39	O2-C13	5.24	1.54	1.46
13	A	814	F39	C55-C48	5.24	1.61	1.51
13	A	815	F39	O1-C11	5.21	1.55	1.41
13	C	302	F39	C55-C48	5.19	1.61	1.51
13	a	816	F39	C55-C48	5.19	1.61	1.51
13	C	302	F39	O2-C13	5.18	1.54	1.46
13	A	815	F39	C55-C48	5.10	1.61	1.51
13	A	814	F39	O1-C12	5.05	1.56	1.44
12	a	801	G2O	C2A-C1A	-5.05	1.40	1.52
13	a	816	F39	O1-C12	5.04	1.56	1.44
13	A	814	F39	C38-C37	5.00	1.61	1.50
13	A	815	F39	C38-C37	4.99	1.61	1.50
13	a	816	F39	C38-C37	4.97	1.61	1.50
12	a	803	G2O	C2A-C1A	-4.94	1.41	1.52
13	C	302	F39	C38-C37	4.93	1.61	1.50
12	A	822	G2O	C2A-C1A	-4.92	1.41	1.52
12	A	822	G2O	C3A-C2A	-4.88	1.40	1.54
12	A	802	G2O	C3A-C2A	-4.87	1.40	1.54
12	a	803	G2O	C3A-C2A	-4.87	1.40	1.54
13	C	302	F39	O1-C12	4.85	1.56	1.44
8	3	405	BCL	OBD-CAD	4.85	1.30	1.22
8	6	405	BCL	OBD-CAD	4.83	1.30	1.22
13	A	815	F39	O1-C12	4.82	1.56	1.44
8	4	405	BCL	OBD-CAD	4.82	1.30	1.22
8	6	402	BCL	OBD-CAD	4.81	1.30	1.22
8	3	403	BCL	OBD-CAD	4.80	1.30	1.22
8	6	404	BCL	OBD-CAD	4.79	1.30	1.22
8	a	804	BCL	OBD-CAD	4.79	1.30	1.22
8	1	405	BCL	OBD-CAD	4.78	1.30	1.22
8	a	809	BCL	OBD-CAD	4.77	1.30	1.22
8	6	407[B]	BCL	OBD-CAD	4.77	1.30	1.22
8	a	811	BCL	OBD-CAD	4.77	1.30	1.22
8	2	406	BCL	OBD-CAD	4.77	1.30	1.22
8	A	806	BCL	OBD-CAD	4.77	1.30	1.22
8	1	408	BCL	OBD-CAD	4.77	1.30	1.22
13	C	302	F39	C50-C49	4.76	1.47	1.38
8	1	403	BCL	OBD-CAD	4.76	1.30	1.22
8	1	404	BCL	OBD-CAD	4.76	1.30	1.22
8	A	813	BCL	OBD-CAD	4.76	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	802	G2O	C2A-C1A	-4.76	1.41	1.52
8	c	301	BCL	OBD-CAD	4.75	1.30	1.22
8	5	405	BCL	OBD-CAD	4.75	1.30	1.22
8	2	407	BCL	OBD-CAD	4.75	1.30	1.22
8	a	812	BCL	OBD-CAD	4.75	1.30	1.22
8	3	404	BCL	OBD-CAD	4.75	1.30	1.22
8	5	404	BCL	OBD-CAD	4.74	1.30	1.22
8	a	808	BCL	OBD-CAD	4.74	1.30	1.22
8	4	403	BCL	OBD-CAD	4.74	1.30	1.22
8	5	403	BCL	OBD-CAD	4.74	1.30	1.22
8	5	401	BCL	OBD-CAD	4.74	1.30	1.22
8	4	404	BCL	OBD-CAD	4.73	1.30	1.22
8	A	803	BCL	OBD-CAD	4.73	1.30	1.22
8	2	405	BCL	OBD-CAD	4.73	1.30	1.22
8	4	406	BCL	OBD-CAD	4.72	1.30	1.22
8	6	408	BCL	OBD-CAD	4.72	1.30	1.22
8	3	407	BCL	OBD-CAD	4.72	1.30	1.22
12	a	801	G2O	C3A-C2A	-4.71	1.41	1.54
8	1	402	BCL	OBD-CAD	4.71	1.30	1.22
8	A	808	BCL	OBD-CAD	4.71	1.30	1.22
8	2	402[B]	BCL	OBD-CAD	4.71	1.30	1.22
13	A	814	F39	C50-C49	4.71	1.47	1.38
8	A	810	BCL	OBD-CAD	4.71	1.30	1.22
13	A	815	F39	C50-C49	4.71	1.47	1.38
8	A	812	BCL	OBD-CAD	4.70	1.30	1.22
8	A	811	BCL	OBD-CAD	4.70	1.30	1.22
8	F	101	BCL	OBD-CAD	4.70	1.30	1.22
8	A	807	BCL	OBD-CAD	4.70	1.30	1.22
8	4	409	BCL	OBD-CAD	4.69	1.30	1.22
8	2	401	BCL	OBD-CAD	4.69	1.30	1.22
8	3	402	BCL	OBD-CAD	4.69	1.30	1.22
12	A	802	G2O	MG-NB	-4.69	1.96	2.05
8	2	403	BCL	OBD-CAD	4.69	1.30	1.22
8	5	402	BCL	OBD-CAD	4.68	1.30	1.22
8	3	406	BCL	OBD-CAD	4.68	1.30	1.22
8	2	404	BCL	OBD-CAD	4.68	1.30	1.22
8	a	805	BCL	OBD-CAD	4.68	1.30	1.22
13	a	816	F39	C50-C49	4.67	1.47	1.38
12	A	802	G2O	C1D-ND	4.67	1.39	1.35
8	4	407	BCL	OBD-CAD	4.66	1.30	1.22
8	1	401	BCL	OBD-CAD	4.66	1.30	1.22
8	A	804	BCL	OBD-CAD	4.65	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	814	BCL	OBD-CAD	4.64	1.30	1.22
8	3	401	BCL	OBD-CAD	4.64	1.30	1.22
8	2	409[B]	BCL	OBD-CAD	4.64	1.30	1.22
8	4	402	BCL	OBD-CAD	4.64	1.30	1.22
8	6	406	BCL	OBD-CAD	4.64	1.30	1.22
8	1	406	BCL	OBD-CAD	4.63	1.30	1.22
8	4	410[B]	BCL	OBD-CAD	4.63	1.30	1.22
8	a	806	BCL	OBD-CAD	4.63	1.30	1.22
8	4	401	BCL	OBD-CAD	4.63	1.30	1.22
8	4	409	BCL	C4D-ND	-4.63	1.31	1.37
8	5	406	BCL	OBD-CAD	4.62	1.30	1.22
8	C	301	BCL	OBD-CAD	4.62	1.30	1.22
13	A	815	F39	C46-C45	4.62	1.47	1.41
8	2	408	BCL	OBD-CAD	4.61	1.30	1.22
8	A	805	BCL	OBD-CAD	4.61	1.30	1.22
8	6	401	BCL	OBD-CAD	4.61	1.30	1.22
8	4	408[B]	BCL	OBD-CAD	4.61	1.30	1.22
8	a	807	BCL	C4D-ND	-4.59	1.31	1.37
13	A	815	F39	O3-C8	4.58	1.53	1.43
8	1	407[B]	BCL	OBD-CAD	4.57	1.30	1.22
8	a	813	BCL	OBD-CAD	4.57	1.30	1.22
12	a	801	G2O	MG-NB	-4.57	1.96	2.05
13	a	816	F39	C52-C45	4.57	1.61	1.51
13	A	814	F39	O3-C8	4.56	1.53	1.43
8	6	403	BCL	OBD-CAD	4.56	1.30	1.22
13	A	814	F39	C52-C45	4.56	1.61	1.51
12	A	822	G2O	MG-NB	-4.55	1.96	2.05
13	C	302	F39	C52-C45	4.54	1.61	1.51
12	a	803	G2O	MG-NB	-4.54	1.96	2.05
13	A	814	F39	C46-C45	4.54	1.47	1.41
8	a	807	BCL	OBD-CAD	4.54	1.30	1.22
11	a	802	GS0	OBD-CAD	4.54	1.30	1.22
13	A	815	F39	C52-C45	4.54	1.61	1.51
13	C	302	F39	O3-C8	4.53	1.53	1.43
12	a	803	G2O	C1D-ND	4.53	1.39	1.35
13	a	816	F39	C46-C45	4.52	1.47	1.41
13	C	302	F39	C46-C48	4.51	1.47	1.41
13	a	816	F39	O3-C8	4.50	1.53	1.43
13	C	302	F39	C46-C45	4.48	1.47	1.41
13	A	814	F39	C46-C48	4.46	1.47	1.41
11	A	801	GS0	OBD-CAD	4.46	1.30	1.22
8	C	301	BCL	C4D-ND	-4.43	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	401	BCL	C4D-ND	-4.41	1.31	1.37
8	A	806	BCL	C4D-ND	-4.40	1.31	1.37
13	A	815	F39	C46-C48	4.39	1.47	1.41
12	a	801	G2O	C1D-ND	4.39	1.39	1.35
8	4	402	BCL	C4D-ND	-4.38	1.31	1.37
8	6	408	BCL	C4D-ND	-4.38	1.31	1.37
8	A	809	BCL	C4D-ND	-4.38	1.31	1.37
11	A	801	GS0	C4D-ND	-4.34	1.31	1.37
11	a	802	GS0	C4D-ND	-4.34	1.31	1.37
13	a	816	F39	C46-C48	4.34	1.47	1.41
8	a	810	BCL	C4D-ND	-4.33	1.31	1.37
8	2	403	BCL	C4D-ND	-4.31	1.31	1.37
8	3	407	BCL	C4D-ND	-4.31	1.31	1.37
8	2	409[B]	BCL	C4D-ND	-4.31	1.31	1.37
8	6	403	BCL	C4D-ND	-4.29	1.31	1.37
8	1	408	BCL	C4D-ND	-4.27	1.31	1.37
12	A	822	G2O	C1D-ND	4.27	1.39	1.35
8	4	401	BCL	C4D-ND	-4.26	1.31	1.37
8	3	401	BCL	C4D-ND	-4.25	1.31	1.37
8	6	401	BCL	C4D-ND	-4.24	1.31	1.37
8	2	405	BCL	C4D-ND	-4.24	1.31	1.37
8	a	809	BCL	C4D-ND	-4.24	1.31	1.37
8	2	407	BCL	C4D-ND	-4.23	1.31	1.37
8	a	806	BCL	C4D-ND	-4.23	1.31	1.37
8	1	407[B]	BCL	C4D-ND	-4.23	1.31	1.37
8	1	401	BCL	C4D-ND	-4.22	1.31	1.37
8	5	405	BCL	C4D-ND	-4.20	1.31	1.37
8	1	402	BCL	C4D-ND	-4.20	1.31	1.37
8	4	406	BCL	C4D-ND	-4.20	1.31	1.37
13	A	815	F39	C22-C21	4.19	1.63	1.50
13	a	816	F39	C22-C21	4.19	1.63	1.50
12	a	801	G2O	C4B-NB	4.17	1.42	1.37
8	4	407	BCL	C4D-ND	-4.17	1.32	1.37
8	1	403	BCL	C4D-ND	-4.17	1.32	1.37
13	C	302	F39	C60-C58	4.16	1.59	1.50
8	1	405	BCL	C4D-ND	-4.16	1.32	1.37
13	a	816	F39	C60-C58	4.16	1.59	1.50
13	A	814	F39	C22-C21	4.16	1.62	1.50
8	1	406	BCL	C4D-ND	-4.15	1.32	1.37
13	A	814	F39	C60-C58	4.15	1.59	1.50
8	A	808	BCL	C4D-ND	-4.15	1.32	1.37
8	c	301	BCL	C4D-ND	-4.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	408[B]	BCL	C4D-ND	-4.14	1.32	1.37
8	4	403	BCL	C4D-ND	-4.14	1.32	1.37
12	A	822	G2O	C4B-NB	4.14	1.42	1.37
8	4	404	BCL	C4D-ND	-4.14	1.32	1.37
13	A	815	F39	C60-C58	4.14	1.59	1.50
8	A	811	BCL	C4D-ND	-4.14	1.32	1.37
8	6	405	BCL	C4D-ND	-4.13	1.32	1.37
8	6	406	BCL	C4D-ND	-4.13	1.32	1.37
8	a	808	BCL	C4D-ND	-4.13	1.32	1.37
8	2	406	BCL	C4D-ND	-4.13	1.32	1.37
8	4	410[B]	BCL	C4D-ND	-4.13	1.32	1.37
17	c	302	F26	C30-C26	-4.12	1.30	1.35
13	C	302	F39	C22-C21	4.12	1.62	1.50
8	2	408	BCL	C4D-ND	-4.12	1.32	1.37
8	A	805	BCL	C4D-ND	-4.12	1.32	1.37
8	6	402	BCL	C4D-ND	-4.12	1.32	1.37
8	5	406	BCL	C4D-ND	-4.11	1.32	1.37
8	2	402[B]	BCL	C4D-ND	-4.11	1.32	1.37
8	a	814	BCL	C4D-ND	-4.11	1.32	1.37
8	A	804	BCL	C4D-ND	-4.11	1.32	1.37
8	3	406	BCL	C4D-ND	-4.11	1.32	1.37
13	C	302	F39	C17-C13	4.11	1.61	1.52
17	a	815	F26	C30-C26	-4.10	1.30	1.35
8	6	407[B]	BCL	C4D-ND	-4.10	1.32	1.37
13	C	302	F39	C65-C62	4.10	1.59	1.50
8	A	812	BCL	C4D-ND	-4.10	1.32	1.37
8	4	405	BCL	C4D-ND	-4.10	1.32	1.37
8	2	404	BCL	C4D-ND	-4.09	1.32	1.37
8	F	101	BCL	C4D-ND	-4.09	1.32	1.37
8	a	813	BCL	C4D-ND	-4.09	1.32	1.37
8	A	810	BCL	C4D-ND	-4.08	1.32	1.37
8	5	404	BCL	C4D-ND	-4.08	1.32	1.37
8	3	402	BCL	C4D-ND	-4.08	1.32	1.37
13	a	816	F39	C17-C13	4.08	1.61	1.52
8	A	809	BCL	O1D-CGD	-4.07	1.11	1.21
8	5	401	BCL	O1D-CGD	-4.07	1.11	1.21
8	A	803	BCL	C4D-ND	-4.07	1.32	1.37
13	A	815	F39	C17-C13	4.07	1.61	1.52
8	5	402	BCL	C4D-ND	-4.07	1.32	1.37
8	a	804	BCL	C4D-ND	-4.06	1.32	1.37
8	5	403	BCL	C4D-ND	-4.06	1.32	1.37
8	a	805	BCL	C4D-ND	-4.06	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	5	401	BCL	C4D-ND	-4.06	1.32	1.37
12	A	802	G2O	C10-C8	-4.05	1.41	1.54
8	a	812	BCL	C4D-ND	-4.05	1.32	1.37
8	3	403	BCL	C4D-ND	-4.04	1.32	1.37
8	A	807	BCL	C4D-ND	-4.03	1.32	1.37
8	1	404	BCL	C4D-ND	-4.03	1.32	1.37
8	3	404	BCL	C4D-ND	-4.03	1.32	1.37
13	A	814	F39	C17-C13	4.03	1.61	1.52
8	1	401	BCL	O1D-CGD	-4.02	1.11	1.21
8	2	404	BCL	O1D-CGD	-4.02	1.11	1.21
8	4	404	BCL	O1D-CGD	-4.01	1.11	1.21
8	1	402	BCL	O1D-CGD	-4.01	1.11	1.21
8	A	810	BCL	O1D-CGD	-4.01	1.11	1.21
8	2	407	BCL	O1D-CGD	-4.01	1.11	1.21
12	a	803	G2O	C4B-NB	4.01	1.42	1.37
8	a	812	BCL	O1D-CGD	-4.01	1.11	1.21
8	6	402	BCL	O1D-CGD	-4.00	1.11	1.21
8	1	405	BCL	O1D-CGD	-4.00	1.11	1.21
8	6	406	BCL	O1D-CGD	-4.00	1.11	1.21
8	4	406	BCL	O1D-CGD	-4.00	1.11	1.21
8	3	407	BCL	O1D-CGD	-4.00	1.11	1.21
8	2	403	BCL	O1D-CGD	-4.00	1.11	1.21
8	4	405	BCL	O1D-CGD	-4.00	1.11	1.21
8	3	405	BCL	C4D-ND	-4.00	1.32	1.37
8	6	401	BCL	O1D-CGD	-4.00	1.11	1.21
8	a	809	BCL	O1D-CGD	-3.99	1.11	1.21
8	3	403	BCL	O1D-CGD	-3.99	1.11	1.21
8	C	301	BCL	O1D-CGD	-3.99	1.11	1.21
8	6	405	BCL	O1D-CGD	-3.99	1.11	1.21
8	a	811	BCL	O1D-CGD	-3.99	1.11	1.21
8	6	408	BCL	O1D-CGD	-3.99	1.11	1.21
8	1	406	BCL	O1D-CGD	-3.99	1.11	1.21
8	6	407[B]	BCL	O1D-CGD	-3.98	1.11	1.21
8	a	806	BCL	O1D-CGD	-3.98	1.11	1.21
8	a	814	BCL	O1D-CGD	-3.98	1.11	1.21
8	4	401	BCL	O1D-CGD	-3.98	1.11	1.21
12	a	801	G2O	C10-C8	-3.98	1.42	1.54
8	2	401	BCL	O1D-CGD	-3.98	1.11	1.21
8	a	805	BCL	O1D-CGD	-3.98	1.11	1.21
8	3	401	BCL	O1D-CGD	-3.98	1.11	1.21
8	A	805	BCL	O1D-CGD	-3.98	1.11	1.21
8	A	812	BCL	O1D-CGD	-3.98	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	5	404	BCL	O1D-CGD	-3.98	1.11	1.21
8	1	403	BCL	O1D-CGD	-3.98	1.11	1.21
8	A	811	BCL	O1D-CGD	-3.98	1.11	1.21
8	1	407[B]	BCL	O1D-CGD	-3.97	1.11	1.21
8	a	810	BCL	O1D-CGD	-3.97	1.11	1.21
8	3	402	BCL	O1D-CGD	-3.97	1.11	1.21
8	4	407	BCL	O1D-CGD	-3.97	1.11	1.21
8	6	404	BCL	C4D-ND	-3.97	1.32	1.37
11	A	801	GS0	O1D-CGD	-3.97	1.11	1.21
8	A	806	BCL	O1D-CGD	-3.97	1.11	1.21
8	6	404	BCL	O1D-CGD	-3.97	1.11	1.21
8	c	301	BCL	O1D-CGD	-3.97	1.11	1.21
8	6	403	BCL	O1D-CGD	-3.97	1.11	1.21
8	2	402[B]	BCL	O1D-CGD	-3.96	1.11	1.21
8	5	405	BCL	O1D-CGD	-3.96	1.11	1.21
8	2	406	BCL	O1D-CGD	-3.96	1.11	1.21
12	a	803	G2O	C10-C8	-3.96	1.42	1.54
8	A	808	BCL	O1D-CGD	-3.96	1.11	1.21
8	4	409	BCL	O1D-CGD	-3.96	1.11	1.21
8	a	808	BCL	O1D-CGD	-3.96	1.11	1.21
8	5	406	BCL	O1D-CGD	-3.96	1.11	1.21
8	A	804	BCL	O1D-CGD	-3.96	1.11	1.21
8	5	402	BCL	O1D-CGD	-3.96	1.11	1.21
8	3	405	BCL	O1D-CGD	-3.96	1.11	1.21
8	4	410[B]	BCL	O1D-CGD	-3.96	1.11	1.21
8	A	807	BCL	O1D-CGD	-3.96	1.11	1.21
8	4	403	BCL	O1D-CGD	-3.95	1.11	1.21
8	a	811	BCL	C4D-ND	-3.95	1.32	1.37
8	4	408[B]	BCL	O1D-CGD	-3.95	1.11	1.21
8	3	406	BCL	O1D-CGD	-3.95	1.11	1.21
8	a	804	BCL	O1D-CGD	-3.95	1.11	1.21
8	5	403	BCL	O1D-CGD	-3.95	1.11	1.21
8	1	404	BCL	O1D-CGD	-3.94	1.11	1.21
8	4	402	BCL	O1D-CGD	-3.94	1.11	1.21
8	A	803	BCL	O1D-CGD	-3.94	1.11	1.21
8	1	408	BCL	O1D-CGD	-3.94	1.11	1.21
8	2	405	BCL	O1D-CGD	-3.94	1.11	1.21
11	a	802	GS0	O1D-CGD	-3.94	1.11	1.21
8	a	810	BCL	OBD-CAD	3.93	1.29	1.22
8	F	101	BCL	O1D-CGD	-3.93	1.11	1.21
8	2	408	BCL	O1D-CGD	-3.93	1.11	1.21
8	2	409[B]	BCL	O1D-CGD	-3.93	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	404	BCL	O1D-CGD	-3.93	1.11	1.21
17	c	302	F26	C37-C34	-3.93	1.30	1.35
8	a	813	BCL	O1D-CGD	-3.93	1.11	1.21
13	A	815	F39	C16-C13	3.92	1.61	1.52
12	A	802	G2O	C4B-NB	3.91	1.42	1.37
8	A	813	BCL	O1D-CGD	-3.91	1.11	1.21
13	A	814	F39	C16-C13	3.90	1.61	1.52
12	A	822	G2O	C10-C8	-3.88	1.42	1.54
8	A	813	BCL	C4D-ND	-3.88	1.32	1.37
13	A	815	F39	C18-C19	3.87	1.66	1.52
13	A	814	F39	C18-C19	3.87	1.66	1.52
13	a	816	F39	C16-C13	3.87	1.61	1.52
13	a	816	F39	C18-C19	3.86	1.66	1.52
13	A	815	F39	C65-C62	3.85	1.58	1.50
13	a	816	F39	C14-C18	3.85	1.66	1.52
13	C	302	F39	C14-C18	3.84	1.66	1.52
13	A	814	F39	C14-C18	3.84	1.66	1.52
8	A	809	BCL	OBD-CAD	3.83	1.29	1.22
13	C	302	F39	C16-C13	3.82	1.61	1.52
13	A	814	F39	C65-C62	3.82	1.58	1.50
13	C	302	F39	C18-C19	3.82	1.66	1.52
13	A	815	F39	C14-C18	3.82	1.66	1.52
13	A	815	F39	C10-C12	3.82	1.61	1.53
17	a	815	F26	C37-C34	-3.80	1.30	1.35
13	a	816	F39	C10-C12	3.78	1.61	1.53
13	a	816	F39	C65-C62	3.78	1.58	1.50
12	A	802	G2O	CHC-C4B	-3.77	1.31	1.38
13	A	814	F39	O5-C10	3.76	1.51	1.43
13	A	814	F39	C10-C12	3.74	1.60	1.53
8	a	807	BCL	O1D-CGD	-3.74	1.11	1.21
13	C	302	F39	O5-C10	3.72	1.51	1.43
13	C	302	F39	C10-C12	3.72	1.60	1.53
13	a	816	F39	O5-C10	3.70	1.51	1.43
13	A	815	F39	C43-C42	3.69	1.58	1.50
13	A	815	F39	O5-C10	3.68	1.51	1.43
13	a	816	F39	C43-C42	3.68	1.58	1.50
12	a	803	G2O	CHC-C4B	-3.65	1.31	1.38
12	a	801	G2O	CHC-C4B	-3.64	1.31	1.38
13	C	302	F39	C43-C42	3.63	1.58	1.50
12	A	802	G2O	C14-C13	-3.60	1.41	1.52
13	A	814	F39	C43-C42	3.60	1.58	1.50
12	A	822	G2O	CHC-C4B	-3.60	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	802	G2O	C4D-CHA	-3.59	1.40	1.45
13	A	815	F39	C47-C45	3.56	1.47	1.40
12	a	803	G2O	C14-C13	-3.56	1.41	1.52
12	A	802	G2O	C9-C8	-3.55	1.41	1.53
8	A	812	BCL	O2D-CED	3.53	1.53	1.45
13	C	302	F39	C47-C45	3.52	1.47	1.40
12	a	803	G2O	C4D-CHA	-3.52	1.40	1.45
12	A	822	G2O	C14-C13	-3.51	1.41	1.52
13	A	814	F39	C47-C45	3.50	1.47	1.40
12	a	801	G2O	C14-C13	-3.50	1.41	1.52
8	3	404	BCL	O2D-CED	3.49	1.53	1.45
8	A	811	BCL	O2D-CED	3.49	1.53	1.45
12	A	822	G2O	C4D-CHA	-3.49	1.40	1.45
11	a	802	GS0	O2D-CED	3.48	1.53	1.45
12	a	803	G2O	C9-C8	-3.48	1.41	1.53
8	4	404	BCL	O2D-CED	3.48	1.53	1.45
13	a	816	F39	C47-C45	3.48	1.47	1.40
8	6	406	BCL	O2D-CED	3.48	1.53	1.45
12	a	801	G2O	C9-C8	-3.48	1.41	1.53
8	6	403	BCL	O2D-CED	3.46	1.53	1.45
8	A	813	BCL	O2D-CED	3.46	1.53	1.45
8	6	404	BCL	O2D-CED	3.46	1.53	1.45
8	1	403	BCL	O2D-CED	3.46	1.53	1.45
11	A	801	GS0	O2D-CED	3.46	1.53	1.45
12	a	801	G2O	C4D-ND	-3.45	1.32	1.35
12	A	822	G2O	C9-C8	-3.45	1.41	1.53
12	a	801	G2O	C4D-CHA	-3.45	1.40	1.45
8	a	807	BCL	O2D-CED	3.45	1.53	1.45
8	c	301	BCL	O2D-CED	3.45	1.53	1.45
8	1	404	BCL	O2D-CED	3.45	1.53	1.45
8	a	812	BCL	O2D-CED	3.44	1.53	1.45
8	1	406	BCL	O2D-CED	3.44	1.53	1.45
8	5	406	BCL	O2D-CED	3.44	1.53	1.45
8	2	408	BCL	O2D-CED	3.44	1.53	1.45
8	3	403	BCL	O2D-CED	3.44	1.53	1.45
8	4	407	BCL	O2D-CED	3.43	1.53	1.45
8	2	404	BCL	O2D-CED	3.43	1.53	1.45
8	a	813	BCL	O2D-CED	3.43	1.53	1.45
8	4	401	BCL	O2D-CED	3.42	1.53	1.45
8	4	408[B]	BCL	O2D-CED	3.42	1.53	1.45
8	3	401	BCL	O2D-CED	3.42	1.53	1.45
13	A	815	F39	C50-C48	3.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	810	BCL	O2D-CED	3.41	1.53	1.45
13	A	814	F39	C50-C48	3.41	1.47	1.39
8	6	407[B]	BCL	O2D-CED	3.41	1.53	1.45
8	3	406	BCL	O2D-CED	3.41	1.53	1.45
8	5	403	BCL	O2D-CED	3.41	1.53	1.45
8	5	404	BCL	O2D-CED	3.41	1.53	1.45
8	a	804	BCL	O2D-CED	3.40	1.53	1.45
8	F	101	BCL	O2D-CED	3.40	1.53	1.45
8	A	809	BCL	O2D-CED	3.40	1.53	1.45
8	4	402	BCL	O2D-CED	3.40	1.53	1.45
13	C	302	F39	C50-C48	3.39	1.47	1.39
8	2	405	BCL	O2D-CED	3.39	1.53	1.45
8	C	301	BCL	O2D-CED	3.39	1.53	1.45
8	5	405	BCL	O2D-CED	3.39	1.53	1.45
13	a	816	F39	C50-C48	3.39	1.47	1.39
8	3	407	BCL	O2D-CED	3.39	1.53	1.45
8	4	410[B]	BCL	O2D-CED	3.38	1.53	1.45
8	6	401	BCL	O2D-CED	3.38	1.53	1.45
8	A	810	BCL	O2D-CED	3.38	1.53	1.45
8	a	811	BCL	O2D-CED	3.38	1.53	1.45
8	2	403	BCL	O2D-CED	3.37	1.53	1.45
8	A	807	BCL	O2D-CED	3.37	1.53	1.45
17	c	302	F26	C24-C19	-3.37	1.31	1.35
8	2	409[B]	BCL	O2D-CED	3.37	1.53	1.45
8	4	405	BCL	O2D-CED	3.37	1.53	1.45
8	a	814	BCL	O2D-CED	3.37	1.53	1.45
8	a	808	BCL	O2D-CED	3.37	1.53	1.45
8	3	402	BCL	O2D-CED	3.36	1.53	1.45
8	1	408	BCL	O2D-CED	3.36	1.53	1.45
8	1	401	BCL	O2D-CED	3.36	1.53	1.45
8	5	402	BCL	O2D-CED	3.35	1.53	1.45
12	A	802	G2O	C4D-ND	-3.35	1.32	1.35
13	a	816	F39	C49-C47	3.35	1.47	1.39
8	6	402	BCL	O2D-CED	3.35	1.53	1.45
8	2	401	BCL	O2D-CED	3.35	1.53	1.45
8	A	805	BCL	O2D-CED	3.34	1.53	1.45
8	a	809	BCL	O2D-CED	3.34	1.53	1.45
8	1	405	BCL	O2D-CED	3.34	1.53	1.45
13	A	815	F39	C49-C47	3.34	1.46	1.39
8	A	808	BCL	O2D-CED	3.34	1.53	1.45
8	3	405	BCL	O2D-CED	3.33	1.53	1.45
13	C	302	F39	C49-C47	3.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	407[B]	BCL	O2D-CED	3.33	1.53	1.45
8	1	402	BCL	O2D-CED	3.33	1.53	1.45
8	4	403	BCL	O2D-CED	3.33	1.53	1.45
12	A	802	G2O	C3A-C4A	-3.32	1.41	1.51
8	A	803	BCL	O2D-CED	3.32	1.53	1.45
8	A	806	BCL	O2D-CED	3.32	1.53	1.45
8	a	806	BCL	O2D-CED	3.32	1.53	1.45
8	6	408	BCL	O2D-CED	3.31	1.53	1.45
8	A	804	BCL	O2D-CED	3.31	1.53	1.45
8	2	402[B]	BCL	O2D-CED	3.30	1.53	1.45
8	5	401	BCL	O2D-CED	3.30	1.53	1.45
8	2	407	BCL	O2D-CED	3.29	1.53	1.45
12	a	803	G2O	C4D-ND	-3.28	1.32	1.35
12	a	803	G2O	C3A-C4A	-3.28	1.41	1.51
12	A	822	G2O	C4D-ND	-3.28	1.32	1.35
12	A	822	G2O	C3A-C4A	-3.27	1.41	1.51
12	a	801	G2O	C3A-C4A	-3.26	1.41	1.51
8	a	805	BCL	O2D-CED	3.26	1.53	1.45
8	4	406	BCL	O2D-CED	3.26	1.53	1.45
13	A	814	F39	C49-C47	3.25	1.46	1.39
17	a	815	F26	C15-C19	3.25	1.52	1.45
8	2	406	BCL	O2D-CED	3.25	1.52	1.45
8	4	409	BCL	O2D-CED	3.23	1.52	1.45
8	a	807	BCL	O2D-CGD	-3.19	1.25	1.33
17	a	815	F26	C24-C19	-3.18	1.31	1.35
17	c	302	F26	C33-C31	-3.18	1.31	1.35
13	A	815	F39	O4-C9	3.18	1.50	1.43
8	6	405	BCL	O2D-CED	3.18	1.52	1.45
13	A	814	F39	O4-C9	3.17	1.50	1.43
13	C	302	F39	O4-C9	3.16	1.50	1.43
17	c	302	F26	C15-C19	3.16	1.52	1.45
13	a	816	F39	O4-C9	3.14	1.50	1.43
17	a	815	F26	C33-C31	-3.13	1.31	1.35
13	a	816	F39	C25-C20	3.09	1.58	1.50
8	6	405	BCL	O2A-CGA	-3.06	1.24	1.33
8	5	403	BCL	O2A-CGA	-3.06	1.24	1.33
8	3	403	BCL	O2A-CGA	-3.04	1.24	1.33
13	A	815	F39	C25-C20	3.04	1.58	1.50
8	2	401	BCL	O2A-CGA	-3.04	1.24	1.33
13	C	302	F39	C25-C20	3.04	1.58	1.50
8	1	405	BCL	O2A-CGA	-3.04	1.24	1.33
8	1	401	BCL	O2A-CGA	-3.03	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	5	406	BCL	O2A-CGA	-3.03	1.24	1.33
11	A	801	GS0	O2A-CGA	-3.03	1.24	1.33
8	2	407	BCL	O2A-CGA	-3.03	1.24	1.33
13	A	814	F39	C25-C20	3.03	1.58	1.50
8	2	406	BCL	O2A-CGA	-3.02	1.24	1.33
17	a	815	F26	C28-C31	3.02	1.52	1.45
8	3	401	BCL	O2A-CGA	-3.02	1.24	1.33
8	4	405	BCL	O2A-CGA	-3.02	1.24	1.33
8	4	404	BCL	O2A-CGA	-3.02	1.24	1.33
8	a	812	BCL	O2A-CGA	-3.02	1.24	1.33
8	A	810	BCL	O2A-CGA	-3.01	1.24	1.33
8	4	409	BCL	O2A-CGA	-3.01	1.24	1.33
8	4	403	BCL	O2A-CGA	-3.01	1.24	1.33
8	6	404	BCL	O2A-CGA	-3.01	1.24	1.33
8	a	806	BCL	O2A-CGA	-3.00	1.24	1.33
8	5	405	BCL	O2A-CGA	-3.00	1.24	1.33
8	5	401	BCL	O2A-CGA	-3.00	1.24	1.33
8	5	402	BCL	O2A-CGA	-3.00	1.24	1.33
8	A	803	BCL	O2D-CGD	-3.00	1.25	1.33
8	1	408	BCL	O2A-CGA	-2.99	1.24	1.33
8	2	403	BCL	O2A-CGA	-2.99	1.24	1.33
8	4	406	BCL	O2A-CGA	-2.99	1.24	1.33
8	1	402	BCL	O2D-CGD	-2.99	1.25	1.33
8	3	402	BCL	O2A-CGA	-2.98	1.24	1.33
8	a	811	BCL	O2A-CGA	-2.98	1.24	1.33
8	2	404	BCL	O2A-CGA	-2.98	1.24	1.33
8	6	401	BCL	O2A-CGA	-2.98	1.24	1.33
8	6	408	BCL	O2A-CGA	-2.98	1.24	1.33
8	3	404	BCL	O2A-CGA	-2.98	1.24	1.33
8	5	402	BCL	C4B-NB	2.98	1.37	1.35
8	1	402	BCL	O2A-CGA	-2.98	1.24	1.33
8	4	409	BCL	O2D-CGD	-2.98	1.25	1.33
8	3	405	BCL	O2A-CGA	-2.98	1.24	1.33
8	A	811	BCL	O2A-CGA	-2.98	1.24	1.33
8	6	403	BCL	O2A-CGA	-2.98	1.24	1.33
8	5	401	BCL	O2D-CGD	-2.98	1.25	1.33
8	1	403	BCL	O2A-CGA	-2.97	1.24	1.33
8	4	401	BCL	O2A-CGA	-2.97	1.24	1.33
8	4	402	BCL	O2A-CGA	-2.97	1.24	1.33
8	a	805	BCL	O2A-CGA	-2.97	1.24	1.33
8	A	805	BCL	O2A-CGA	-2.96	1.24	1.33
8	A	807	BCL	O2A-CGA	-2.96	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	808	BCL	O2A-CGA	-2.96	1.24	1.33
8	3	407	BCL	O2A-CGA	-2.95	1.24	1.33
8	4	405	BCL	O2D-CGD	-2.95	1.26	1.33
8	2	405	BCL	O2A-CGA	-2.95	1.24	1.33
8	4	407	BCL	O2A-CGA	-2.95	1.24	1.33
8	6	405	BCL	O2D-CGD	-2.95	1.26	1.33
8	4	403	BCL	O2D-CGD	-2.95	1.26	1.33
11	a	802	GS0	O2D-CGD	-2.95	1.26	1.33
8	6	402	BCL	O2A-CGA	-2.95	1.24	1.33
11	a	802	GS0	O2A-CGA	-2.95	1.24	1.33
8	3	401	BCL	O2D-CGD	-2.94	1.26	1.33
11	A	801	GS0	O2D-CGD	-2.94	1.26	1.33
8	C	301	BCL	O2D-CGD	-2.94	1.26	1.33
8	1	404	BCL	O2A-CGA	-2.94	1.24	1.33
8	1	406	BCL	O2A-CGA	-2.94	1.24	1.33
8	1	401	BCL	O2D-CGD	-2.93	1.26	1.33
17	a	815	F26	C39-C37	2.93	1.52	1.43
8	A	810	BCL	O2D-CGD	-2.93	1.26	1.33
8	2	403	BCL	O2D-CGD	-2.93	1.26	1.33
8	4	401	BCL	O2D-CGD	-2.93	1.26	1.33
8	6	401	BCL	O2D-CGD	-2.92	1.26	1.33
8	5	404	BCL	O2A-CGA	-2.92	1.24	1.33
8	F	101	BCL	O2D-CGD	-2.92	1.26	1.33
8	6	402	BCL	O2D-CGD	-2.92	1.26	1.33
8	3	402	BCL	O2D-CGD	-2.92	1.26	1.33
8	6	406	BCL	O2A-CGA	-2.92	1.24	1.33
8	3	405	BCL	O2D-CGD	-2.91	1.26	1.33
8	2	408	BCL	O2A-CGA	-2.91	1.24	1.33
11	a	802	GS0	C1D-C2D	-2.91	1.39	1.45
17	c	302	F26	C22-C18	2.91	1.52	1.43
8	2	404	BCL	O2D-CGD	-2.91	1.26	1.33
8	a	806	BCL	O2D-CGD	-2.91	1.26	1.33
8	3	406	BCL	O2A-CGA	-2.90	1.24	1.33
8	2	401	BCL	O2D-CGD	-2.90	1.26	1.33
8	a	808	BCL	O2D-CGD	-2.90	1.26	1.33
8	4	406	BCL	O2D-CGD	-2.90	1.26	1.33
8	1	408	BCL	O2D-CGD	-2.90	1.26	1.33
8	A	806	BCL	O2D-CGD	-2.90	1.26	1.33
8	a	814	BCL	O2D-CGD	-2.90	1.26	1.33
13	a	816	F39	C23-C22	2.90	1.62	1.52
8	2	406	BCL	O2D-CGD	-2.90	1.26	1.33
8	3	405	BCL	O1A-CGA	-2.90	1.13	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	5	405	BCL	O2D-CGD	-2.90	1.26	1.33
8	A	807	BCL	O2D-CGD	-2.89	1.26	1.33
8	3	407	BCL	O2D-CGD	-2.89	1.26	1.33
8	6	408	BCL	O2D-CGD	-2.89	1.26	1.33
8	A	805	BCL	O2D-CGD	-2.89	1.26	1.33
8	a	813	BCL	O2D-CGD	-2.89	1.26	1.33
8	5	406	BCL	O2D-CGD	-2.89	1.26	1.33
13	A	815	F39	C23-C22	2.89	1.62	1.52
8	1	405	BCL	O2D-CGD	-2.89	1.26	1.33
8	2	407	BCL	O2D-CGD	-2.89	1.26	1.33
8	a	809	BCL	O2D-CGD	-2.89	1.26	1.33
17	c	302	F26	C39-C37	2.89	1.52	1.43
8	a	811	BCL	O2D-CGD	-2.88	1.26	1.33
8	5	402	BCL	O2D-CGD	-2.88	1.26	1.33
13	A	814	F39	C23-C22	2.88	1.62	1.52
8	c	301	BCL	O2D-CGD	-2.88	1.26	1.33
8	3	403	BCL	O2D-CGD	-2.88	1.26	1.33
8	a	805	BCL	O2D-CGD	-2.88	1.26	1.33
8	1	407[B]	BCL	O2D-CGD	-2.87	1.26	1.33
8	2	402[B]	BCL	O2D-CGD	-2.87	1.26	1.33
8	5	404	BCL	O2D-CGD	-2.87	1.26	1.33
17	c	302	F26	C28-C31	2.87	1.52	1.45
13	C	302	F39	C23-C22	2.87	1.62	1.52
8	a	804	BCL	O2D-CGD	-2.87	1.26	1.33
17	a	815	F26	C38-C33	2.87	1.52	1.43
8	1	406	BCL	O2D-CGD	-2.87	1.26	1.33
8	A	804	BCL	O2A-CGA	-2.87	1.24	1.33
8	2	408	BCL	O2D-CGD	-2.87	1.26	1.33
8	A	813	BCL	O2D-CGD	-2.86	1.26	1.33
8	4	407	BCL	O2D-CGD	-2.86	1.26	1.33
8	6	407[B]	BCL	O2D-CGD	-2.86	1.26	1.33
8	3	404	BCL	O2D-CGD	-2.86	1.26	1.33
8	4	402	BCL	O2D-CGD	-2.86	1.26	1.33
8	A	812	BCL	O2D-CGD	-2.86	1.26	1.33
8	4	408[B]	BCL	O2D-CGD	-2.86	1.26	1.33
12	a	803	G2O	C8-C7	-2.86	1.42	1.51
8	2	405	BCL	O2D-CGD	-2.86	1.26	1.33
8	2	409[B]	BCL	O2D-CGD	-2.86	1.26	1.33
8	A	808	BCL	O2D-CGD	-2.86	1.26	1.33
8	3	406	BCL	O2D-CGD	-2.85	1.26	1.33
8	5	406	BCL	O1A-CGA	-2.85	1.14	1.22
8	3	406	BCL	O1A-CGA	-2.85	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	806	BCL	C4B-NB	2.85	1.37	1.35
8	5	403	BCL	O2D-CGD	-2.85	1.26	1.33
8	4	410[B]	BCL	O2D-CGD	-2.85	1.26	1.33
8	a	810	BCL	O2D-CGD	-2.85	1.26	1.33
8	A	804	BCL	O2D-CGD	-2.85	1.26	1.33
8	A	811	BCL	O2D-CGD	-2.85	1.26	1.33
12	a	803	G2O	C3D-CAD	-2.84	1.41	1.47
8	1	404	BCL	O2D-CGD	-2.84	1.26	1.33
8	1	403	BCL	O2D-CGD	-2.84	1.26	1.33
12	A	802	G2O	C8-C7	-2.84	1.42	1.51
8	a	812	BCL	C4B-NB	2.83	1.37	1.35
8	4	404	BCL	O2D-CGD	-2.83	1.26	1.33
8	2	404	BCL	O1A-CGA	-2.83	1.14	1.22
8	6	404	BCL	O2D-CGD	-2.83	1.26	1.33
8	6	402	BCL	O1A-CGA	-2.83	1.14	1.22
12	A	802	G2O	C3D-CAD	-2.83	1.41	1.47
8	6	405	BCL	O1A-CGA	-2.83	1.14	1.22
8	6	406	BCL	O2D-CGD	-2.83	1.26	1.33
8	2	401	BCL	O1A-CGA	-2.82	1.14	1.22
17	c	302	F26	C38-C33	2.82	1.52	1.43
8	4	403	BCL	O1A-CGA	-2.82	1.14	1.22
8	3	403	BCL	O1A-CGA	-2.82	1.14	1.22
8	1	401	BCL	O1A-CGA	-2.82	1.14	1.22
8	1	402	BCL	O1A-CGA	-2.82	1.14	1.22
17	a	815	F26	C22-C18	2.81	1.52	1.43
8	A	811	BCL	O1A-CGA	-2.81	1.14	1.22
8	a	806	BCL	O1A-CGA	-2.81	1.14	1.22
8	5	403	BCL	O1A-CGA	-2.80	1.14	1.22
8	2	405	BCL	O1A-CGA	-2.80	1.14	1.22
8	6	403	BCL	O1A-CGA	-2.80	1.14	1.22
11	a	802	GS0	O1A-CGA	-2.80	1.14	1.22
8	6	403	BCL	O2D-CGD	-2.80	1.26	1.33
8	A	811	BCL	C4B-NB	2.80	1.37	1.35
13	C	302	F39	C11-C9	2.80	1.60	1.52
8	4	406	BCL	O1A-CGA	-2.80	1.14	1.22
8	a	808	BCL	O1A-CGA	-2.80	1.14	1.22
8	5	405	BCL	O1A-CGA	-2.80	1.14	1.22
8	5	402	BCL	O1A-CGA	-2.80	1.14	1.22
8	A	809	BCL	O2D-CGD	-2.80	1.26	1.33
8	a	812	BCL	O1A-CGA	-2.79	1.14	1.22
8	1	405	BCL	O1A-CGA	-2.79	1.14	1.22
8	A	807	BCL	O1A-CGA	-2.79	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	5	404	BCL	O1A-CGA	-2.79	1.14	1.22
8	3	401	BCL	O1A-CGA	-2.79	1.14	1.22
11	A	801	GS0	O1A-CGA	-2.79	1.14	1.22
12	A	822	G2O	C8-C7	-2.79	1.42	1.51
17	c	302	F26	C32-C30	2.79	1.52	1.43
8	A	804	BCL	O1A-CGA	-2.79	1.14	1.22
8	a	810	BCL	C4B-NB	2.79	1.37	1.35
8	1	403	BCL	O1A-CGA	-2.79	1.14	1.22
12	a	801	G2O	C8-C7	-2.79	1.42	1.51
8	4	404	BCL	O1A-CGA	-2.78	1.14	1.22
8	a	812	BCL	O2D-CGD	-2.78	1.26	1.33
8	1	406	BCL	O1A-CGA	-2.78	1.14	1.22
8	3	402	BCL	O1A-CGA	-2.78	1.14	1.22
13	A	814	F39	C11-C9	2.78	1.60	1.52
8	4	409	BCL	O1A-CGA	-2.78	1.14	1.22
8	4	403	BCL	C4B-NB	2.78	1.37	1.35
17	a	815	F26	C32-C30	2.78	1.52	1.43
8	A	810	BCL	O1A-CGA	-2.78	1.14	1.22
8	1	404	BCL	O1A-CGA	-2.78	1.14	1.22
8	2	403	BCL	O1A-CGA	-2.78	1.14	1.22
8	5	401	BCL	O1A-CGA	-2.78	1.14	1.22
8	4	405	BCL	O1A-CGA	-2.78	1.14	1.22
8	6	401	BCL	O1A-CGA	-2.78	1.14	1.22
8	4	402	BCL	O1A-CGA	-2.77	1.14	1.22
8	a	807	BCL	C4B-NB	2.77	1.37	1.35
8	a	811	BCL	O1A-CGA	-2.77	1.14	1.22
8	4	401	BCL	O1A-CGA	-2.77	1.14	1.22
13	a	816	F39	C11-C9	2.77	1.60	1.52
8	3	402	BCL	C4B-NB	2.77	1.37	1.35
8	6	408	BCL	O1A-CGA	-2.77	1.14	1.22
8	1	402	BCL	C4B-NB	2.77	1.37	1.35
8	3	404	BCL	O1A-CGA	-2.77	1.14	1.22
8	2	407	BCL	O1A-CGA	-2.77	1.14	1.22
8	2	406	BCL	O1A-CGA	-2.76	1.14	1.22
8	6	404	BCL	O1A-CGA	-2.76	1.14	1.22
8	A	812	BCL	C4B-NB	2.76	1.37	1.35
8	1	408	BCL	O1A-CGA	-2.76	1.14	1.22
8	a	805	BCL	O1A-CGA	-2.76	1.14	1.22
8	4	407	BCL	O1A-CGA	-2.76	1.14	1.22
8	2	408	BCL	O1A-CGA	-2.76	1.14	1.22
8	A	805	BCL	O1A-CGA	-2.76	1.14	1.22
17	a	815	F26	C27-C24	2.76	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	6	406	BCL	O1A-CGA	-2.76	1.14	1.22
8	2	404	BCL	C4B-NB	2.73	1.37	1.35
8	3	407	BCL	O1A-CGA	-2.73	1.14	1.22
17	a	815	F26	C18-C13	-2.72	1.31	1.34
12	A	802	G2O	MG-NA	2.72	2.12	2.06
8	A	805	BCL	C4B-NB	2.72	1.37	1.35
8	a	806	BCL	C4B-NB	2.71	1.37	1.35
8	6	402	BCL	C4B-NB	2.70	1.37	1.35
8	A	813	BCL	C4B-NB	2.69	1.37	1.35
13	A	815	F39	C11-C9	2.69	1.60	1.52
12	a	803	G2O	MG-NA	2.68	2.12	2.06
17	c	302	F26	C18-C13	-2.67	1.31	1.34
8	A	803	BCL	C4B-NB	2.66	1.37	1.35
12	A	822	G2O	C3D-CAD	-2.65	1.42	1.47
9	a	820	CDL	OA6-CA4	-2.65	1.40	1.46
17	c	302	F26	C27-C24	2.64	1.51	1.43
12	a	801	G2O	MG-NA	2.64	2.12	2.06
17	c	302	F26	C35-C34	2.64	1.51	1.45
17	a	815	F26	C35-C34	2.64	1.51	1.45
8	a	804	BCL	C4B-NB	2.61	1.37	1.35
12	a	801	G2O	C3D-CAD	-2.60	1.42	1.47
12	A	802	G2O	CMD-C2D	-2.59	1.46	1.51
12	A	822	G2O	MG-NA	2.59	2.12	2.06
8	A	809	BCL	C4B-NB	2.59	1.37	1.35
12	a	803	G2O	CMD-C2D	-2.59	1.46	1.51
8	1	402	BCL	C1D-C2D	-2.58	1.40	1.45
17	c	302	F26	C25-C26	2.56	1.51	1.45
9	1	409	CDL	OB6-CB4	-2.55	1.40	1.46
9	c	303	CDL	OA6-CA4	-2.54	1.40	1.46
12	a	803	G2O	C1B-C2B	2.53	1.50	1.45
12	A	802	G2O	CMB-C2B	-2.53	1.45	1.50
8	6	402	BCL	C1D-C2D	-2.52	1.40	1.45
9	c	303	CDL	OB6-CB4	-2.52	1.40	1.46
12	a	801	G2O	C1B-C2B	2.51	1.50	1.45
8	a	808	BCL	C4B-NB	2.50	1.37	1.35
8	F	101	BCL	C1D-C2D	-2.49	1.40	1.45
9	a	822	CDL	OB6-CB4	-2.49	1.40	1.46
9	a	820	CDL	OB6-CB4	-2.49	1.40	1.46
17	a	815	F26	C2-C9	2.48	1.53	1.47
8	5	406	BCL	C4B-NB	2.48	1.37	1.35
8	5	402	BCL	C1D-C2D	-2.47	1.40	1.45
12	A	822	G2O	C1B-C2B	2.47	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	813	BCL	C4B-NB	2.46	1.37	1.35
8	1	404	BCL	C4B-NB	2.46	1.37	1.35
8	4	410[B]	BCL	C1D-C2D	-2.45	1.40	1.45
17	a	815	F26	C25-C26	2.45	1.51	1.45
12	A	802	G2O	C1B-C2B	2.45	1.50	1.45
9	1	409	CDL	OA8-CA7	2.44	1.40	1.33
8	2	404	BCL	C1D-C2D	-2.44	1.40	1.45
8	5	401	BCL	C1D-C2D	-2.44	1.40	1.45
9	c	303	CDL	OB8-CB7	2.44	1.40	1.33
9	a	822	CDL	OA8-CA7	2.43	1.40	1.33
12	A	822	G2O	CMD-C2D	-2.43	1.46	1.51
11	A	801	GS0	C1D-C2D	-2.43	1.40	1.45
8	A	803	BCL	O1A-CGA	-2.42	1.14	1.22
8	a	814	BCL	C4B-NB	2.42	1.37	1.35
12	A	822	G2O	CMB-C2B	-2.41	1.45	1.50
8	a	810	BCL	O1A-CGA	-2.41	1.14	1.22
8	2	402[B]	BCL	C1D-C2D	-2.41	1.40	1.45
8	A	804	BCL	C1D-C2D	-2.41	1.40	1.45
8	F	101	BCL	C4B-NB	2.40	1.37	1.35
9	a	820	CDL	OB8-CB7	2.40	1.40	1.33
12	a	801	G2O	CMB-C2B	-2.40	1.45	1.50
12	a	801	G2O	CMD-C2D	-2.40	1.46	1.51
8	5	405	BCL	C1D-C2D	-2.40	1.40	1.45
8	4	403	BCL	C1D-C2D	-2.40	1.40	1.45
9	a	822	CDL	OB8-CB7	2.40	1.40	1.33
8	6	403	BCL	C1D-C2D	-2.39	1.40	1.45
8	2	407	BCL	C4B-NB	2.39	1.37	1.35
8	1	407[B]	BCL	O1A-CGA	-2.39	1.14	1.22
8	a	813	BCL	O1A-CGA	-2.39	1.14	1.22
8	6	401	BCL	C1D-C2D	-2.39	1.40	1.45
8	a	812	BCL	C3B-C2B	-2.39	1.35	1.39
8	3	402	BCL	C1D-C2D	-2.39	1.40	1.45
8	2	409[B]	BCL	O1A-CGA	-2.38	1.14	1.22
8	a	809	BCL	O1A-CGA	-2.38	1.14	1.22
8	A	809	BCL	O1A-CGA	-2.38	1.14	1.22
17	c	302	F26	C2-C9	2.38	1.53	1.47
8	2	402[B]	BCL	O1A-CGA	-2.38	1.14	1.22
12	a	803	G2O	CMB-C2B	-2.38	1.45	1.50
8	4	401	BCL	C1D-C2D	-2.38	1.40	1.45
8	4	410[B]	BCL	O1A-CGA	-2.38	1.14	1.22
8	A	813	BCL	O1A-CGA	-2.37	1.14	1.22
8	A	812	BCL	C3B-C2B	-2.37	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	820	CDL	OA8-CA7	2.37	1.40	1.33
8	A	807	BCL	C4B-NB	2.37	1.37	1.35
8	2	406	BCL	C4B-NB	2.37	1.37	1.35
8	C	301	BCL	O1A-CGA	-2.37	1.14	1.22
8	a	814	BCL	O1A-CGA	-2.37	1.14	1.22
9	c	303	CDL	OA8-CA7	2.37	1.40	1.33
8	2	409[B]	BCL	C1D-C2D	-2.36	1.40	1.45
12	A	802	G2O	C1A-CHA	2.36	1.42	1.37
8	a	807	BCL	O1A-CGA	-2.36	1.14	1.22
8	A	806	BCL	O1A-CGA	-2.36	1.14	1.22
8	6	407[B]	BCL	O1A-CGA	-2.36	1.14	1.22
9	1	409	CDL	OB8-CB7	2.36	1.40	1.33
8	4	407	BCL	C4B-NB	2.36	1.37	1.35
8	A	805	BCL	C1D-C2D	-2.36	1.40	1.45
8	1	407[B]	BCL	C1D-C2D	-2.36	1.40	1.45
8	A	812	BCL	O1A-CGA	-2.36	1.14	1.22
8	4	408[B]	BCL	O1A-CGA	-2.35	1.14	1.22
8	A	813	BCL	C1D-C2D	-2.35	1.40	1.45
8	6	406	BCL	C4B-NB	2.35	1.37	1.35
8	a	804	BCL	O1A-CGA	-2.35	1.14	1.22
8	1	403	BCL	C1D-C2D	-2.35	1.40	1.45
8	A	808	BCL	O1A-CGA	-2.35	1.14	1.22
8	a	813	BCL	C3B-C2B	-2.35	1.35	1.39
8	C	301	BCL	C1D-C2D	-2.34	1.40	1.45
8	2	408	BCL	C4B-NB	2.34	1.37	1.35
8	2	405	BCL	C1D-C2D	-2.34	1.40	1.45
8	4	404	BCL	C1D-C2D	-2.34	1.40	1.45
8	3	401	BCL	C1D-C2D	-2.34	1.40	1.45
8	4	408[B]	BCL	C1D-C2D	-2.34	1.40	1.45
8	3	403	BCL	C4B-NB	2.33	1.37	1.35
12	a	803	G2O	C1A-CHA	2.33	1.42	1.37
8	3	406	BCL	C4B-NB	2.33	1.37	1.35
8	F	101	BCL	O1A-CGA	-2.33	1.14	1.22
8	c	301	BCL	O1A-CGA	-2.33	1.14	1.22
8	5	405	BCL	C4B-NB	2.33	1.37	1.35
8	2	402[B]	BCL	C4B-NB	2.32	1.37	1.35
9	1	409	CDL	OA6-CA5	2.32	1.40	1.34
12	a	801	G2O	C3B-C4B	2.32	1.50	1.46
8	5	403	BCL	C1D-C2D	-2.32	1.40	1.45
8	A	810	BCL	C1D-C2D	-2.31	1.40	1.45
8	1	405	BCL	C1D-C2D	-2.31	1.40	1.45
8	a	805	BCL	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	404	BCL	C1D-C2D	-2.31	1.40	1.45
8	4	402	BCL	C4B-NB	2.30	1.37	1.35
8	a	811	BCL	C1D-C2D	-2.30	1.40	1.45
8	5	404	BCL	C1D-C2D	-2.30	1.40	1.45
8	4	410[B]	BCL	C4B-NB	2.30	1.37	1.35
8	1	401	BCL	C1D-C2D	-2.30	1.40	1.45
8	1	406	BCL	C4B-NB	2.30	1.37	1.35
8	3	404	BCL	C4B-NB	2.30	1.37	1.35
8	2	403	BCL	C1D-C2D	-2.29	1.40	1.45
8	6	405	BCL	C1D-C2D	-2.29	1.40	1.45
8	1	403	BCL	C4B-NB	2.29	1.37	1.35
8	2	406	BCL	C1D-C2D	-2.29	1.40	1.45
8	A	811	BCL	C1D-C2D	-2.29	1.40	1.45
8	2	407	BCL	C1D-C2D	-2.29	1.40	1.45
8	a	804	BCL	C1D-C2D	-2.29	1.40	1.45
8	6	407[B]	BCL	C1D-C2D	-2.28	1.40	1.45
9	1	409	CDL	OA6-CA4	-2.28	1.40	1.46
8	4	405	BCL	C4B-NB	2.28	1.37	1.35
12	A	822	G2O	C1A-CHA	2.28	1.42	1.37
8	A	808	BCL	C1D-C2D	-2.28	1.40	1.45
8	5	406	BCL	C1D-C2D	-2.28	1.40	1.45
8	A	803	BCL	C3B-C2B	-2.28	1.35	1.39
8	A	812	BCL	C1D-C2D	-2.27	1.40	1.45
8	6	408	BCL	C4B-NB	2.27	1.37	1.35
9	a	822	CDL	OA6-CA5	2.27	1.40	1.34
8	a	812	BCL	C1D-C2D	-2.27	1.40	1.45
8	a	806	BCL	C3B-C2B	-2.27	1.35	1.39
8	3	403	BCL	C1D-C2D	-2.27	1.40	1.45
8	4	407	BCL	C1D-C2D	-2.27	1.40	1.45
8	a	806	BCL	C1D-C2D	-2.27	1.40	1.45
8	c	301	BCL	C1D-C2D	-2.26	1.40	1.45
8	6	404	BCL	C1D-C2D	-2.26	1.40	1.45
8	4	405	BCL	C1D-C2D	-2.26	1.40	1.45
8	a	808	BCL	C1D-C2D	-2.26	1.40	1.45
8	4	402	BCL	C1D-C2D	-2.26	1.40	1.45
8	3	406	BCL	C1D-C2D	-2.26	1.40	1.45
8	1	406	BCL	C1D-C2D	-2.25	1.40	1.45
8	a	805	BCL	C4B-NB	2.25	1.37	1.35
8	4	408[B]	BCL	C4B-NB	2.25	1.37	1.35
8	a	814	BCL	C1D-C2D	-2.25	1.40	1.45
8	3	407	BCL	C1D-C2D	-2.25	1.40	1.45
9	a	822	CDL	OA6-CA4	-2.25	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	810	BCL	C3B-C2B	-2.24	1.35	1.39
8	A	811	BCL	C3B-C2B	-2.24	1.35	1.39
8	A	806	BCL	C1D-C2D	-2.24	1.40	1.45
8	a	809	BCL	C1D-C2D	-2.24	1.40	1.45
8	A	810	BCL	C4B-NB	2.24	1.37	1.35
8	5	403	BCL	C4B-NB	2.24	1.37	1.35
8	4	404	BCL	C4B-NB	2.24	1.37	1.35
8	4	409	BCL	C3D-C4D	-2.23	1.39	1.44
8	2	405	BCL	C4B-NB	2.23	1.37	1.35
8	a	809	BCL	C4B-NB	2.23	1.37	1.35
8	a	804	BCL	C3B-C2B	-2.23	1.35	1.39
8	1	404	BCL	C1D-C2D	-2.23	1.40	1.45
8	4	406	BCL	C1D-C2D	-2.23	1.40	1.45
8	a	808	BCL	C3B-C2B	-2.23	1.35	1.39
8	6	403	BCL	C4B-NB	2.22	1.37	1.35
8	2	409[B]	BCL	C3D-C4D	-2.22	1.39	1.44
12	a	801	G2O	C1A-CHA	2.22	1.42	1.37
8	A	808	BCL	C4B-NB	2.22	1.37	1.35
8	A	803	BCL	C1D-C2D	-2.22	1.40	1.45
8	5	401	BCL	C4B-NB	2.22	1.37	1.35
8	1	408	BCL	C1D-C2D	-2.21	1.41	1.45
8	3	405	BCL	C1D-C2D	-2.21	1.41	1.45
8	2	408	BCL	C1D-C2D	-2.21	1.41	1.45
8	2	409[B]	BCL	C4B-NB	2.21	1.37	1.35
8	A	804	BCL	C4B-NB	2.21	1.37	1.35
8	A	805	BCL	C3B-C2B	-2.21	1.35	1.39
8	2	402[B]	BCL	C3D-C4D	-2.21	1.39	1.44
9	1	409	CDL	OB8-CB6	-2.20	1.40	1.45
8	2	401	BCL	C1D-C2D	-2.20	1.41	1.45
8	6	406	BCL	C1D-C2D	-2.20	1.41	1.45
8	3	401	BCL	C4B-NB	2.20	1.37	1.35
8	1	405	BCL	C4B-NB	2.20	1.37	1.35
13	C	302	F39	O6-C15	2.20	1.50	1.45
8	A	807	BCL	C3B-C2B	-2.20	1.35	1.39
8	1	408	BCL	C4B-NB	2.20	1.37	1.35
8	a	811	BCL	C4B-NB	2.19	1.37	1.35
8	2	401	BCL	C3D-C4D	-2.19	1.39	1.44
13	a	816	F39	O6-C15	2.19	1.50	1.45
8	a	813	BCL	C1D-C2D	-2.19	1.41	1.45
8	2	404	BCL	C3B-C2B	-2.19	1.35	1.39
8	4	410[B]	BCL	C3D-C4D	-2.19	1.39	1.44
8	A	809	BCL	C3B-C2B	-2.19	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	401	BCL	C4B-NB	2.19	1.37	1.35
9	c	303	CDL	OA6-CA5	2.18	1.40	1.34
8	4	402	BCL	C3D-C4D	-2.18	1.39	1.44
13	A	815	F39	O6-C15	2.18	1.50	1.45
8	6	408	BCL	C1D-C2D	-2.18	1.41	1.45
9	c	303	CDL	OB8-CB6	-2.17	1.40	1.45
8	5	402	BCL	C3B-C2B	-2.17	1.35	1.39
8	4	408[B]	BCL	C3D-C4D	-2.17	1.39	1.44
9	c	303	CDL	OB6-CB5	2.17	1.40	1.34
8	3	407	BCL	C3D-C4D	-2.17	1.39	1.44
8	a	806	BCL	C3D-C4D	-2.17	1.39	1.44
8	a	806	BCL	C3D-C2D	-2.17	1.33	1.39
8	1	406	BCL	C3D-C4D	-2.17	1.39	1.44
8	1	407[B]	BCL	C3D-C4D	-2.16	1.39	1.44
8	1	408	BCL	C3D-C4D	-2.16	1.39	1.44
12	A	822	G2O	C3B-C4B	2.16	1.50	1.46
8	a	807	BCL	C3B-C2B	-2.16	1.35	1.39
8	4	403	BCL	C3B-C2B	-2.16	1.35	1.39
8	6	408	BCL	C3D-C4D	-2.16	1.39	1.44
8	A	805	BCL	C3D-C2D	-2.16	1.33	1.39
8	a	809	BCL	C3D-C4D	-2.16	1.39	1.44
12	A	802	G2O	C1B-NB	-2.16	1.35	1.37
9	a	822	CDL	OB8-CB6	-2.16	1.40	1.45
8	4	407	BCL	C3D-C4D	-2.16	1.39	1.44
8	3	407	BCL	C4B-NB	2.15	1.37	1.35
8	A	813	BCL	C3B-CAB	2.15	1.54	1.49
8	A	805	BCL	C3D-C4D	-2.15	1.39	1.44
8	a	805	BCL	C3D-C4D	-2.15	1.39	1.44
12	A	822	G2O	CMC-C2C	-2.15	1.46	1.50
8	A	807	BCL	C1D-C2D	-2.15	1.41	1.45
8	3	405	BCL	C4B-NB	2.15	1.37	1.35
8	A	806	BCL	C3D-C4D	-2.15	1.39	1.44
8	A	806	BCL	C3B-C2B	-2.14	1.35	1.39
9	a	820	CDL	OB6-CB5	2.14	1.40	1.34
8	6	407[B]	BCL	C3D-C4D	-2.14	1.39	1.44
8	A	803	BCL	C3D-C4D	-2.14	1.39	1.44
8	6	401	BCL	C4B-NB	2.14	1.37	1.35
12	a	803	G2O	C1B-NB	-2.14	1.35	1.37
8	C	301	BCL	C3B-C2B	-2.14	1.35	1.39
8	5	406	BCL	C3D-C4D	-2.14	1.39	1.44
8	6	407[B]	BCL	C4B-NB	2.14	1.37	1.35
9	c	303	CDL	OA8-CA6	-2.14	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	6	406	BCL	C3D-C4D	-2.14	1.39	1.44
8	1	402	BCL	C3B-C2B	-2.13	1.35	1.39
8	A	812	BCL	C3D-C4D	-2.13	1.39	1.44
8	c	301	BCL	C3D-C4D	-2.13	1.39	1.44
9	a	822	CDL	OB6-CB5	2.13	1.40	1.34
8	5	404	BCL	C4B-NB	2.13	1.37	1.35
8	6	402	BCL	C3B-C2B	-2.13	1.35	1.39
8	A	804	BCL	C3D-C4D	-2.13	1.39	1.44
8	4	406	BCL	C4B-NB	2.13	1.37	1.35
8	A	813	BCL	C3D-C2D	-2.13	1.33	1.39
8	4	406	BCL	C3D-C4D	-2.13	1.39	1.44
8	A	807	BCL	C3D-C4D	-2.12	1.39	1.44
8	1	401	BCL	C4B-NB	2.12	1.37	1.35
8	6	405	BCL	C4B-NB	2.12	1.37	1.35
8	6	403	BCL	C3D-C4D	-2.12	1.39	1.44
12	a	801	G2O	CMC-C2C	-2.12	1.46	1.50
9	a	820	CDL	OA6-CA5	2.12	1.40	1.34
8	2	401	BCL	C4B-NB	2.12	1.37	1.35
8	2	408	BCL	C3D-C4D	-2.12	1.39	1.44
9	1	409	CDL	OA8-CA6	-2.12	1.40	1.45
8	3	406	BCL	C3D-C4D	-2.12	1.39	1.44
8	4	409	BCL	C4B-NB	2.11	1.37	1.35
8	a	804	BCL	C3D-C4D	-2.11	1.39	1.44
8	a	808	BCL	C3D-C4D	-2.11	1.39	1.44
13	A	814	F39	O6-C15	2.11	1.50	1.45
8	a	810	BCL	C3B-CAB	2.11	1.54	1.49
14	a	819	LHG	O7-C5	-2.11	1.41	1.46
8	1	405	BCL	C3D-C4D	-2.11	1.39	1.44
8	4	410[B]	BCL	C3D-C2D	-2.10	1.33	1.39
9	1	409	CDL	OB6-CB5	2.10	1.40	1.34
11	a	802	GS0	C3B-C2B	-2.10	1.35	1.39
8	4	409	BCL	C1D-C2D	-2.10	1.41	1.45
9	a	822	CDL	OA8-CA6	-2.10	1.40	1.45
8	6	404	BCL	C4B-NB	2.10	1.37	1.35
8	3	405	BCL	C3B-C2B	-2.10	1.35	1.39
8	A	808	BCL	C3D-C4D	-2.10	1.39	1.44
8	3	402	BCL	C3B-C2B	-2.10	1.35	1.39
8	2	403	BCL	C4B-NB	2.10	1.37	1.35
8	4	405	BCL	C3D-C4D	-2.10	1.39	1.44
8	5	406	BCL	C3D-C2D	-2.09	1.33	1.39
8	2	402[B]	BCL	C3D-C2D	-2.09	1.33	1.39
9	a	820	CDL	OB8-CB6	-2.09	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	407	BCL	C3D-C4D	-2.09	1.39	1.44
8	a	814	BCL	C3B-CAB	2.09	1.54	1.49
8	a	814	BCL	C3D-C4D	-2.09	1.39	1.44
8	6	405	BCL	C3D-C4D	-2.09	1.39	1.44
8	C	301	BCL	C3D-C4D	-2.09	1.39	1.44
8	2	404	BCL	C3B-CAB	2.09	1.54	1.49
8	1	407[B]	BCL	C4B-NB	2.09	1.37	1.35
8	A	813	BCL	C3D-C4D	-2.08	1.39	1.44
8	a	813	BCL	C3D-C4D	-2.08	1.39	1.44
8	A	805	BCL	C3B-CAB	2.08	1.54	1.49
8	F	101	BCL	C3B-CAB	2.07	1.54	1.49
8	4	403	BCL	C3D-C4D	-2.07	1.39	1.44
8	4	404	BCL	C3D-C4D	-2.07	1.39	1.44
8	3	403	BCL	C3D-C4D	-2.07	1.39	1.44
14	A	816	LHG	O7-C5	-2.07	1.41	1.46
14	A	818	LHG	O7-C5	-2.07	1.41	1.46
13	A	815	F39	C29-C28	2.07	1.63	1.51
13	a	816	F39	C30-C29	2.07	1.63	1.51
8	5	402	BCL	C3B-CAB	2.07	1.54	1.49
8	1	404	BCL	C3D-C4D	-2.07	1.39	1.44
8	6	401	BCL	C3D-C4D	-2.07	1.39	1.44
8	1	405	BCL	C3B-C2B	-2.07	1.35	1.39
8	5	404	BCL	C3D-C4D	-2.07	1.39	1.44
8	4	401	BCL	C3B-CAB	2.06	1.54	1.49
8	6	402	BCL	C3B-CAB	2.06	1.54	1.49
8	a	807	BCL	C3B-CAB	2.06	1.54	1.49
14	a	817	LHG	O7-C5	-2.06	1.41	1.46
13	A	815	F39	C30-C29	2.06	1.63	1.51
8	3	403	BCL	C3B-CAB	2.06	1.54	1.49
8	2	409[B]	BCL	C3B-CAB	2.06	1.54	1.49
13	C	302	F39	C29-C28	2.06	1.63	1.51
8	5	403	BCL	C3D-C4D	-2.05	1.39	1.44
8	6	407[B]	BCL	C3B-CAB	2.05	1.54	1.49
8	5	405	BCL	C3D-C4D	-2.05	1.39	1.44
8	2	407	BCL	C3D-C2D	-2.05	1.33	1.39
8	5	401	BCL	C3D-C2D	-2.05	1.33	1.39
9	a	820	CDL	OA8-CA6	-2.05	1.40	1.45
12	A	802	G2O	CMC-C2C	-2.05	1.46	1.50
8	1	403	BCL	C3D-C4D	-2.05	1.39	1.44
8	6	403	BCL	C3B-CAB	2.05	1.54	1.49
8	A	811	BCL	C3B-CAB	2.05	1.54	1.49
8	6	401	BCL	C3D-C2D	-2.05	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	406	BCL	C3D-C4D	-2.05	1.39	1.44
12	a	801	G2O	C1B-NB	-2.04	1.35	1.37
8	2	409[B]	BCL	C3D-C2D	-2.04	1.33	1.39
12	a	803	G2O	CMC-C2C	-2.04	1.46	1.50
8	5	401	BCL	C3B-CAB	2.04	1.54	1.49
13	C	302	F39	C30-C29	2.04	1.63	1.51
8	6	402	BCL	C3D-C4D	-2.04	1.39	1.44
8	3	402	BCL	C3D-C4D	-2.04	1.39	1.44
8	2	407	BCL	C3B-C2B	-2.04	1.35	1.39
8	A	804	BCL	C3D-C2D	-2.04	1.33	1.39
8	4	410[B]	BCL	C3B-CAB	2.04	1.54	1.49
8	3	401	BCL	C3B-CAB	2.04	1.54	1.49
8	2	405	BCL	C3D-C4D	-2.04	1.39	1.44
8	2	404	BCL	C3D-C4D	-2.04	1.39	1.44
13	C	302	F39	C26-C24	2.04	1.63	1.51
8	4	408[B]	BCL	C3D-C2D	-2.04	1.33	1.39
8	3	402	BCL	C3B-CAB	2.04	1.54	1.49
11	A	801	GS0	C3D-C4D	-2.04	1.39	1.44
8	6	404	BCL	C3D-C4D	-2.03	1.39	1.44
8	c	301	BCL	C4B-NB	2.03	1.37	1.35
13	C	302	F39	C28-C26	2.03	1.63	1.51
8	2	403	BCL	C3D-C4D	-2.03	1.39	1.44
13	A	814	F39	C29-C28	2.03	1.63	1.51
8	1	401	BCL	C3D-C2D	-2.03	1.33	1.39
13	A	815	F39	C28-C26	2.03	1.63	1.51
13	A	815	F39	C33-C31	2.03	1.63	1.51
8	4	403	BCL	C3B-CAB	2.03	1.54	1.49
8	2	405	BCL	C3B-CAB	2.03	1.54	1.49
13	a	816	F39	C29-C28	2.03	1.63	1.51
13	a	816	F39	C33-C31	2.03	1.63	1.51
13	a	816	F39	C26-C24	2.03	1.63	1.51
8	a	811	BCL	C3D-C2D	-2.03	1.33	1.39
8	1	402	BCL	C3B-CAB	2.03	1.54	1.49
8	A	811	BCL	C3D-C4D	-2.02	1.39	1.44
8	4	404	BCL	C3B-CAB	2.02	1.54	1.49
8	a	805	BCL	C3D-C2D	-2.02	1.33	1.39
13	A	815	F39	C26-C24	2.02	1.62	1.51
8	1	407[B]	BCL	C3B-CAB	2.02	1.54	1.49
8	4	406	BCL	C3D-C2D	-2.02	1.33	1.39
8	4	402	BCL	C3B-CAB	2.02	1.54	1.49
13	C	302	F39	C9-C8	2.02	1.57	1.52
8	2	403	BCL	C3D-C2D	-2.02	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	806	BCL	C3B-CAB	2.02	1.54	1.49
8	a	811	BCL	C3D-C4D	-2.02	1.39	1.44
8	C	301	BCL	C4B-NB	2.02	1.37	1.35
8	4	407	BCL	C3B-CAB	2.02	1.54	1.49
8	a	812	BCL	C3D-C4D	-2.02	1.39	1.44
8	1	403	BCL	C3B-CAB	2.02	1.54	1.49
8	5	402	BCL	C3D-C2D	-2.02	1.33	1.39
8	3	404	BCL	C3D-C4D	-2.02	1.39	1.44
14	A	816	LHG	P-O6	2.02	1.67	1.59
8	6	403	BCL	C3D-C2D	-2.02	1.33	1.39
8	6	408	BCL	C3B-CAB	2.01	1.54	1.49
8	a	811	BCL	C3B-C2B	-2.01	1.35	1.39
12	A	802	G2O	C4C-NC	2.01	1.40	1.37
8	6	406	BCL	C3B-CAB	2.01	1.54	1.49
8	a	809	BCL	C3D-C2D	-2.01	1.33	1.39
13	C	302	F39	C31-C30	2.01	1.62	1.51
13	a	816	F39	C28-C26	2.01	1.62	1.51
13	C	302	F39	C33-C31	2.01	1.62	1.51
13	A	815	F39	C31-C30	2.01	1.62	1.51
8	A	812	BCL	C3D-C2D	-2.01	1.33	1.39
8	A	810	BCL	C3B-C2B	-2.01	1.35	1.39
8	4	401	BCL	C3D-C4D	-2.01	1.39	1.44
12	a	803	G2O	CHD-C4C	2.01	1.40	1.35
8	4	406	BCL	C3B-C2B	-2.01	1.35	1.39
13	A	814	F39	C26-C24	2.01	1.62	1.51
8	4	408[B]	BCL	C3B-CAB	2.01	1.54	1.49
8	c	301	BCL	C3D-C2D	-2.01	1.33	1.39
8	2	408	BCL	C3B-CAB	2.01	1.54	1.49
8	5	403	BCL	C3B-CAB	2.01	1.54	1.49
8	4	405	BCL	C3D-C2D	-2.01	1.33	1.39
13	A	814	F39	C30-C29	2.01	1.62	1.51
8	A	810	BCL	C3D-C4D	-2.00	1.39	1.44
8	a	812	BCL	C3B-CAB	2.00	1.54	1.49
8	A	806	BCL	C3D-C2D	-2.00	1.33	1.39
8	4	402	BCL	C3D-C2D	-2.00	1.33	1.39
8	4	407	BCL	C3D-C2D	-2.00	1.33	1.39

All (2140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	816	F39	C40-C39-C37	-10.90	111.76	127.31
13	a	816	F39	C51-C44-C42	-10.79	111.92	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	814	F39	C57-C59-C62	-10.71	112.02	127.31
13	a	816	F39	C63-C61-C58	-10.63	112.14	127.31
13	A	815	F39	C40-C39-C37	-10.50	112.32	127.31
13	A	814	F39	C51-C44-C42	-10.49	112.34	127.31
13	A	815	F39	C57-C59-C62	-10.46	112.38	127.31
13	A	814	F39	C63-C61-C58	-10.38	112.50	127.31
13	A	815	F39	C63-C61-C58	-10.34	112.56	127.31
13	C	302	F39	C57-C59-C62	-10.27	112.65	127.31
13	C	302	F39	C40-C39-C37	-10.21	112.73	127.31
13	A	814	F39	C40-C39-C37	-10.07	112.94	127.31
13	A	815	F39	C51-C44-C42	-10.02	113.01	127.31
13	a	816	F39	C57-C59-C62	-10.02	113.02	127.31
13	C	302	F39	C63-C61-C58	-9.98	113.07	127.31
13	C	302	F39	C51-C44-C42	-9.90	113.18	127.31
13	A	814	F39	C43-C42-C44	-9.72	109.31	122.92
13	a	816	F39	C65-C62-C59	-9.65	109.41	122.92
13	a	816	F39	C43-C42-C44	-9.65	109.41	122.92
13	C	302	F39	C43-C42-C44	-9.63	109.44	122.92
13	A	815	F39	C60-C58-C61	-9.61	109.46	122.92
13	A	814	F39	C60-C58-C61	-9.59	109.49	122.92
13	A	815	F39	C65-C62-C59	-9.57	109.51	122.92
13	a	816	F39	C60-C58-C61	-9.55	109.54	122.92
13	A	814	F39	C65-C62-C59	-9.45	109.69	122.92
13	C	302	F39	C65-C62-C59	-9.29	109.90	122.92
13	A	815	F39	C43-C42-C44	-9.23	110.00	122.92
13	C	302	F39	C60-C58-C61	-9.16	110.09	122.92
13	A	815	F39	C38-C37-C39	-8.51	111.01	122.92
13	a	816	F39	C38-C37-C39	-8.40	111.16	122.92
13	C	302	F39	C38-C37-C39	-8.19	111.45	122.92
13	A	814	F39	C38-C37-C39	-7.78	112.03	122.92
13	C	302	F39	C46-C53-C56	-7.25	112.27	128.63
13	A	815	F39	C46-C53-C56	-7.19	112.42	128.63
8	A	813	BCL	CMB-C2B-C1B	-7.16	117.47	128.46
17	c	302	F26	C27-C24-C19	-7.14	117.11	127.31
13	a	816	F39	C46-C53-C56	-7.10	112.63	128.63
8	a	807	BCL	C1D-ND-C4D	-6.88	101.45	106.33
13	A	814	F39	C46-C53-C56	-6.79	113.32	128.63
8	3	405	BCL	C1C-NC-C4C	-6.69	103.70	106.71
8	3	405	BCL	C1D-ND-C4D	-6.65	101.61	106.33
8	a	805	BCL	C1D-ND-C4D	-6.62	101.63	106.33
8	5	406	BCL	C1D-ND-C4D	-6.61	101.64	106.33
8	A	812	BCL	C1D-ND-C4D	-6.60	101.65	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	815	F39	C64-C62-C59	-6.59	108.82	118.94
8	a	809	BCL	CMB-C2B-C1B	-6.59	118.34	128.46
8	A	809	BCL	C2D-C1D-ND	6.58	114.95	110.10
8	A	805	BCL	C1D-ND-C4D	-6.58	101.66	106.33
8	a	811	BCL	CMB-C2B-C1B	-6.58	118.35	128.46
8	4	406	BCL	CMB-C2B-C1B	-6.56	118.39	128.46
8	5	405	BCL	C1D-ND-C4D	-6.55	101.68	106.33
8	2	407	BCL	CMB-C2B-C1B	-6.53	118.43	128.46
8	A	808	BCL	C1D-ND-C4D	-6.51	101.71	106.33
8	2	407	BCL	C1D-ND-C4D	-6.49	101.72	106.33
8	2	406	BCL	CMB-C2B-C1B	-6.48	118.50	128.46
8	A	810	BCL	C1D-ND-C4D	-6.46	101.74	106.33
8	1	405	BCL	CMB-C2B-C1B	-6.46	118.53	128.46
8	a	809	BCL	C1D-ND-C4D	-6.46	101.75	106.33
8	1	406	BCL	C1D-ND-C4D	-6.45	101.75	106.33
8	3	401	BCL	C1D-ND-C4D	-6.45	101.75	106.33
8	A	808	BCL	CMB-C2B-C1B	-6.45	118.55	128.46
13	a	816	F39	C56-C58-C61	-6.44	109.06	118.94
8	1	404	BCL	CMB-C2B-C1B	-6.44	118.57	128.46
8	a	811	BCL	C1D-ND-C4D	-6.42	101.78	106.33
8	5	405	BCL	CMB-C2B-C1B	-6.42	118.60	128.46
8	a	806	BCL	C1D-ND-C4D	-6.41	101.78	106.33
8	A	811	BCL	C1D-ND-C4D	-6.40	101.79	106.33
8	6	404	BCL	CMB-C2B-C1B	-6.39	118.64	128.46
8	3	401	BCL	CMB-C2B-C1B	-6.38	118.66	128.46
12	A	802	G2O	C5-C6-C7	-6.38	110.57	125.05
8	1	405	BCL	C1D-ND-C4D	-6.38	101.80	106.33
8	a	804	BCL	C1D-ND-C4D	-6.37	101.81	106.33
8	5	402	BCL	C1D-ND-C4D	-6.36	101.82	106.33
8	4	408[B]	BCL	CMB-C2B-C1B	-6.36	118.69	128.46
8	6	408	BCL	CMB-C2B-C1B	-6.36	118.69	128.46
8	2	409[B]	BCL	CMB-C2B-C1B	-6.36	118.69	128.46
8	A	809	BCL	C1C-NC-C4C	-6.35	103.85	106.71
8	1	407[B]	BCL	CMB-C2B-C1B	-6.35	118.71	128.46
8	4	409	BCL	C1D-ND-C4D	-6.34	101.83	106.33
12	A	822	G2O	C5-C6-C7	-6.34	110.65	125.05
8	A	806	BCL	C1D-ND-C4D	-6.34	101.83	106.33
8	3	404	BCL	CMB-C2B-C1B	-6.34	118.72	128.46
8	2	402[B]	BCL	CMB-C2B-C1B	-6.34	118.72	128.46
13	C	302	F39	C56-C58-C61	-6.33	109.23	118.94
8	4	410[B]	BCL	CMB-C2B-C1B	-6.32	118.75	128.46
8	A	810	BCL	CMB-C2B-C1B	-6.31	118.77	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	406	BCL	CMB-C2B-C1B	-6.31	118.77	128.46
8	2	408	BCL	CMB-C2B-C1B	-6.30	118.78	128.46
8	a	814	BCL	CMB-C2B-C1B	-6.30	118.78	128.46
8	1	408	BCL	CMB-C2B-C1B	-6.30	118.79	128.46
8	6	406	BCL	CMB-C2B-C1B	-6.29	118.79	128.46
8	2	403	BCL	C1D-ND-C4D	-6.29	101.87	106.33
8	6	405	BCL	CMB-C2B-C1B	-6.28	118.81	128.46
8	C	301	BCL	CMB-C2B-C1B	-6.27	118.82	128.46
8	3	407	BCL	CMB-C2B-C1B	-6.27	118.83	128.46
8	6	405	BCL	C1D-ND-C4D	-6.27	101.88	106.33
8	a	812	BCL	C1D-ND-C4D	-6.27	101.88	106.33
8	6	401	BCL	C1D-ND-C4D	-6.26	101.89	106.33
8	A	804	BCL	C1D-ND-C4D	-6.26	101.89	106.33
8	6	407[B]	BCL	CMB-C2B-C1B	-6.26	118.85	128.46
12	a	803	G2O	C5-C6-C7	-6.25	110.86	125.05
8	1	404	BCL	C1D-ND-C4D	-6.25	101.90	106.33
8	5	404	BCL	CMB-C2B-C1B	-6.25	118.86	128.46
8	1	406	BCL	CMB-C2B-C1B	-6.24	118.87	128.46
8	5	401	BCL	C1D-ND-C4D	-6.24	101.90	106.33
8	a	810	BCL	C2D-C1D-ND	6.23	114.70	110.10
8	a	810	BCL	C1D-ND-C4D	-6.23	101.91	106.33
8	4	405	BCL	CMB-C2B-C1B	-6.23	118.89	128.46
8	a	805	BCL	CMB-C2B-C1B	-6.23	118.89	128.46
8	4	407	BCL	C1D-ND-C4D	-6.22	101.92	106.33
8	4	407	BCL	CMB-C2B-C1B	-6.22	118.90	128.46
8	3	404	BCL	C1D-ND-C4D	-6.22	101.92	106.33
8	6	403	BCL	CMB-C2B-C1B	-6.22	118.91	128.46
13	A	814	F39	C56-C58-C61	-6.22	109.40	118.94
8	4	402	BCL	C1D-ND-C4D	-6.21	101.92	106.33
8	c	301	BCL	CMB-C2B-C1B	-6.21	118.92	128.46
8	A	803	BCL	C1D-ND-C4D	-6.21	101.93	106.33
8	6	408	BCL	C1D-ND-C4D	-6.20	101.93	106.33
8	c	301	BCL	C1D-ND-C4D	-6.20	101.93	106.33
8	2	405	BCL	CMB-C2B-C1B	-6.20	118.94	128.46
8	2	403	BCL	CMB-C2B-C1B	-6.20	118.94	128.46
8	C	301	BCL	C1D-ND-C4D	-6.19	101.94	106.33
8	2	401	BCL	CMB-C2B-C1B	-6.19	118.95	128.46
13	A	814	F39	C64-C62-C59	-6.18	109.45	118.94
8	a	813	BCL	C1D-ND-C4D	-6.18	101.94	106.33
8	2	401	BCL	C1D-ND-C4D	-6.18	101.94	106.33
8	a	814	BCL	C1D-ND-C4D	-6.18	101.94	106.33
8	1	403	BCL	C1D-ND-C4D	-6.18	101.95	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	804	BCL	CMB-C2B-C1B	-6.18	118.97	128.46
8	F	101	BCL	CMB-C2B-C1B	-6.18	118.97	128.46
8	1	401	BCL	C1D-ND-C4D	-6.17	101.95	106.33
8	4	402	BCL	CMB-C2B-C1B	-6.17	118.99	128.46
8	1	408	BCL	C1D-ND-C4D	-6.16	101.96	106.33
8	1	403	BCL	CMB-C2B-C1B	-6.16	119.00	128.46
8	a	808	BCL	C1D-ND-C4D	-6.15	101.97	106.33
8	4	404	BCL	CMB-C2B-C1B	-6.15	119.02	128.46
8	2	406	BCL	C1D-ND-C4D	-6.13	101.98	106.33
8	6	401	BCL	CMB-C2B-C1B	-6.13	119.04	128.46
11	a	802	GS0	CMB-C2B-C1B	-6.13	119.05	128.46
8	4	401	BCL	CMB-C2B-C1B	-6.12	119.05	128.46
8	3	403	BCL	C1D-ND-C4D	-6.12	101.98	106.33
8	4	406	BCL	C1D-ND-C4D	-6.12	101.99	106.33
8	6	406	BCL	C1D-ND-C4D	-6.12	101.99	106.33
8	4	401	BCL	C1D-ND-C4D	-6.12	101.99	106.33
8	5	401	BCL	CMB-C2B-C1B	-6.12	119.06	128.46
8	4	409	BCL	CMB-C2B-C1B	-6.12	119.06	128.46
13	a	816	F39	C41-C42-C44	-6.11	109.57	118.94
8	1	401	BCL	CMB-C2B-C1B	-6.11	119.08	128.46
8	2	408	BCL	C1D-ND-C4D	-6.11	102.00	106.33
8	5	403	BCL	CMB-C2B-C1B	-6.10	119.09	128.46
13	C	302	F39	C64-C62-C59	-6.09	109.60	118.94
8	1	402	BCL	C1C-NC-C4C	-6.06	103.98	106.71
8	F	101	BCL	C1D-ND-C4D	-6.05	102.03	106.33
8	6	403	BCL	C1D-ND-C4D	-6.05	102.04	106.33
8	3	405	BCL	CMB-C2B-C1B	-6.04	119.17	128.46
13	A	815	F39	C41-C42-C44	-6.03	109.68	118.94
13	A	814	F39	C41-C42-C44	-6.03	109.69	118.94
8	5	404	BCL	C1D-ND-C4D	-6.03	102.05	106.33
13	A	815	F39	C56-C58-C61	-6.03	109.69	118.94
8	4	404	BCL	C1D-ND-C4D	-6.02	102.06	106.33
11	A	801	GS0	CMB-C2B-C1B	-6.01	119.22	128.46
8	3	406	BCL	C1D-ND-C4D	-6.01	102.06	106.33
8	5	403	BCL	C1D-ND-C4D	-6.00	102.07	106.33
11	a	802	GS0	C2D-C1D-ND	6.00	114.52	110.10
8	4	405	BCL	C1D-ND-C4D	-5.99	102.08	106.33
8	A	809	BCL	C1D-ND-C4D	-5.99	102.08	106.33
13	A	814	F39	C43-C42-C41	-5.99	108.65	118.08
8	a	807	BCL	CMB-C2B-C1B	-5.98	119.28	128.46
8	5	406	BCL	CMB-C2B-C1B	-5.97	119.29	128.46
8	1	402	BCL	C1D-ND-C4D	-5.96	102.10	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	405	BCL	C2D-C1D-ND	5.95	114.49	110.10
8	A	806	BCL	CMB-C2B-C1B	-5.93	119.34	128.46
8	3	403	BCL	CMB-C2B-C1B	-5.93	119.35	128.46
8	a	813	BCL	C1C-NC-C4C	-5.92	104.05	106.71
17	a	815	F26	C27-C24-C19	-5.91	118.87	127.31
8	6	404	BCL	C1D-ND-C4D	-5.90	102.14	106.33
8	2	405	BCL	C1D-ND-C4D	-5.90	102.15	106.33
8	3	401	BCL	C2D-C1D-ND	5.89	114.44	110.10
8	2	402[B]	BCL	C1D-ND-C4D	-5.88	102.16	106.33
8	4	403	BCL	C1D-ND-C4D	-5.88	102.16	106.33
8	5	402	BCL	C2D-C1D-ND	5.88	114.43	110.10
8	A	807	BCL	C1D-ND-C4D	-5.88	102.16	106.33
8	3	407	BCL	C1D-ND-C4D	-5.87	102.16	106.33
8	1	402	BCL	C2D-C1D-ND	5.87	114.43	110.10
8	5	405	BCL	C2D-C1D-ND	5.86	114.42	110.10
8	a	812	BCL	CMB-C2B-C1B	-5.84	119.49	128.46
13	a	816	F39	C64-C62-C59	-5.83	109.99	118.94
8	5	401	BCL	C2D-C1D-ND	5.82	114.39	110.10
8	6	402	BCL	C1D-ND-C4D	-5.82	102.20	106.33
8	5	401	BCL	O2D-CGD-CBD	5.81	121.59	111.27
8	2	404	BCL	C1D-ND-C4D	-5.80	102.22	106.33
8	a	807	BCL	C2D-C1D-ND	5.78	114.36	110.10
13	C	302	F39	C43-C42-C41	-5.78	108.97	118.08
12	a	801	G2O	C5-C6-C7	-5.75	112.00	125.05
8	6	402	BCL	C1C-NC-C4C	-5.72	104.13	106.71
8	4	401	BCL	C2D-C1D-ND	5.71	114.31	110.10
8	4	408[B]	BCL	C1D-ND-C4D	-5.71	102.28	106.33
8	1	401	BCL	O2D-CGD-CBD	5.70	121.39	111.27
8	A	808	BCL	C2D-C1D-ND	5.69	114.30	110.10
8	A	811	BCL	CMB-C2B-C1B	-5.69	119.72	128.46
8	5	406	BCL	C2D-C1D-ND	5.68	114.29	110.10
12	a	803	G2O	C1A-NA-C4A	5.67	109.25	106.71
8	A	807	BCL	CMB-C2B-C1B	-5.65	119.79	128.46
8	4	401	BCL	O2D-CGD-CBD	5.64	121.30	111.27
8	A	810	BCL	C2D-C1D-ND	5.64	114.26	110.10
8	1	405	BCL	C2D-C1D-ND	5.64	114.26	110.10
8	C	301	BCL	C2D-C1D-ND	5.64	114.26	110.10
8	A	811	BCL	C2D-C1D-ND	5.63	114.25	110.10
8	F	101	BCL	C2D-C1D-ND	5.63	114.25	110.10
8	3	402	BCL	C1D-ND-C4D	-5.62	102.34	106.33
8	6	407[B]	BCL	C1D-ND-C4D	-5.62	102.34	106.33
8	A	812	BCL	C2D-C1D-ND	5.61	114.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	6	402	BCL	CMB-C2B-C1B	-5.61	119.84	128.46
8	6	401	BCL	C2D-C1D-ND	5.61	114.24	110.10
8	2	409[B]	BCL	C1D-ND-C4D	-5.61	102.35	106.33
8	1	401	BCL	C2D-C1D-ND	5.60	114.23	110.10
13	a	816	F39	C51-C57-C59	-5.60	112.01	123.47
8	3	401	BCL	O2D-CGD-CBD	5.59	121.21	111.27
8	2	407	BCL	C2D-C1D-ND	5.59	114.22	110.10
8	6	401	BCL	O2D-CGD-CBD	5.58	121.19	111.27
13	a	816	F39	C65-C62-C64	-5.58	109.29	118.08
8	4	403	BCL	CMB-C2B-C1B	-5.58	119.89	128.46
8	4	410[B]	BCL	C1D-ND-C4D	-5.57	102.38	106.33
13	A	815	F39	C57-C51-C44	-5.56	112.08	123.47
8	a	812	BCL	C2D-C1D-ND	5.56	114.20	110.10
8	6	403	BCL	C2D-C1D-ND	5.56	114.20	110.10
8	A	805	BCL	C2D-C1D-ND	5.56	114.20	110.10
8	a	808	BCL	CMB-C2B-C1B	-5.56	119.92	128.46
13	A	815	F39	C43-C42-C41	-5.56	109.32	118.08
8	1	403	BCL	C2D-C1D-ND	5.55	114.20	110.10
8	2	403	BCL	O2D-CGD-CBD	5.55	121.12	111.27
8	a	806	BCL	CMB-C2B-C1B	-5.54	119.95	128.46
8	F	101	BCL	C1C-NC-C4C	-5.54	104.22	106.71
8	A	805	BCL	CMB-C2B-C1B	-5.53	119.96	128.46
8	a	805	BCL	C2D-C1D-ND	5.53	114.18	110.10
8	6	402	BCL	C2D-C1D-ND	5.53	114.18	110.10
8	a	810	BCL	CMB-C2B-C1B	-5.53	119.96	128.46
8	2	403	BCL	C2D-C1D-ND	5.53	114.18	110.10
8	a	813	BCL	CMB-C2B-C1B	-5.53	119.96	128.46
8	3	404	BCL	C2D-C1D-ND	5.52	114.17	110.10
8	a	809	BCL	C2D-C1D-ND	5.51	114.16	110.10
8	5	402	BCL	C1C-NC-C4C	-5.50	104.23	106.71
8	a	811	BCL	C2D-C1D-ND	5.50	114.16	110.10
8	A	812	BCL	CMB-C2B-C1B	-5.49	120.02	128.46
8	1	407[B]	BCL	C1D-ND-C4D	-5.49	102.44	106.33
8	1	406	BCL	C2D-C1D-ND	5.49	114.15	110.10
13	A	814	F39	C60-C58-C56	-5.48	109.44	118.08
8	A	812	BCL	C1C-NC-C4C	-5.48	104.24	106.71
13	a	816	F39	C43-C42-C41	-5.48	109.45	118.08
12	a	801	G2O	C1A-NA-C4A	5.47	109.17	106.71
8	a	804	BCL	C2D-C1D-ND	5.47	114.13	110.10
13	A	815	F39	C60-C58-C56	-5.46	109.47	118.08
8	A	803	BCL	CMB-C2B-C1B	-5.46	120.08	128.46
13	A	814	F39	C57-C51-C44	-5.45	112.30	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	a	815	F26	C38-C33-C31	-5.45	119.53	127.31
8	2	406	BCL	C2D-C1D-ND	5.45	114.12	110.10
8	1	402	BCL	CMB-C2B-C1B	-5.45	120.09	128.46
11	a	802	GS0	O2D-CGD-CBD	5.45	120.94	111.27
8	3	402	BCL	CMB-C2B-C1B	-5.45	120.09	128.46
13	A	814	F39	C65-C62-C64	-5.44	109.50	118.08
8	A	806	BCL	C2D-C1D-ND	5.43	114.11	110.10
13	C	302	F39	C41-C42-C44	-5.43	110.61	118.94
8	6	405	BCL	C2D-C1D-ND	5.43	114.11	110.10
13	C	302	F39	C32-C35-C37	-5.42	111.18	126.42
8	a	806	BCL	C2D-C1D-ND	5.42	114.10	110.10
8	5	402	BCL	CMB-C2B-C1B	-5.41	120.16	128.46
8	2	405	BCL	C2D-C1D-ND	5.40	114.09	110.10
12	A	822	G2O	C1A-NA-C4A	5.40	109.14	106.71
8	A	804	BCL	C2D-C1D-ND	5.40	114.08	110.10
13	C	302	F39	C60-C58-C56	-5.39	109.59	118.08
8	2	404	BCL	CMB-C2B-C1B	-5.38	120.20	128.46
8	5	403	BCL	C2D-C1D-ND	5.37	114.06	110.10
8	1	404	BCL	C2D-C1D-ND	5.37	114.06	110.10
8	A	809	BCL	CMB-C2B-C1B	-5.37	120.21	128.46
8	a	813	BCL	C2D-C1D-ND	5.37	114.06	110.10
8	a	814	BCL	C2D-C1D-ND	5.37	114.06	110.10
8	3	401	BCL	C4A-NA-C1A	-5.37	104.29	106.71
8	a	804	BCL	CMB-C2B-C1B	-5.37	120.21	128.46
13	a	816	F39	C57-C51-C44	-5.36	112.48	123.47
8	4	403	BCL	C2D-C1D-ND	5.36	114.06	110.10
8	a	808	BCL	C2D-C1D-ND	5.36	114.05	110.10
8	4	407	BCL	C2D-C1D-ND	5.35	114.05	110.10
13	C	302	F39	C25-C20-C27	-5.35	108.78	122.59
8	4	404	BCL	C2D-C1D-ND	5.35	114.05	110.10
8	6	406	BCL	C2D-C1D-ND	5.34	114.04	110.10
8	6	404	BCL	O2D-CGD-CBD	5.33	120.74	111.27
13	A	814	F39	C51-C57-C59	-5.33	112.56	123.47
8	3	403	BCL	C2D-C1D-ND	5.33	114.03	110.10
8	A	813	BCL	C1C-NC-C4C	-5.32	104.31	106.71
8	2	408	BCL	C2D-C1D-ND	5.31	114.02	110.10
8	A	813	BCL	C1D-ND-C4D	-5.31	102.56	106.33
13	C	302	F39	C57-C51-C44	-5.30	112.61	123.47
8	5	404	BCL	C2D-C1D-ND	5.29	114.00	110.10
8	2	404	BCL	C2D-C1D-ND	5.29	114.00	110.10
8	4	409	BCL	C2D-C1D-ND	5.29	114.00	110.10
8	6	404	BCL	C2D-C1D-ND	5.27	113.99	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	801	GS0	C2D-C1D-ND	5.27	113.99	110.10
8	c	301	BCL	C2D-C1D-ND	5.27	113.98	110.10
8	3	406	BCL	C2D-C1D-ND	5.25	113.98	110.10
8	A	803	BCL	C2D-C1D-ND	5.25	113.97	110.10
8	A	806	BCL	C1C-NC-C4C	-5.25	104.35	106.71
13	A	815	F39	C51-C57-C59	-5.24	112.73	123.47
8	A	812	BCL	O2D-CGD-CBD	5.24	120.59	111.27
8	4	406	BCL	C2D-C1D-ND	5.24	113.97	110.10
13	A	814	F39	C25-C20-C27	-5.23	109.09	122.59
13	a	816	F39	C63-C64-C62	-5.23	111.74	126.42
8	3	404	BCL	O2D-CGD-CBD	5.20	120.51	111.27
8	4	401	BCL	C4A-NA-C1A	-5.20	104.37	106.71
13	A	815	F39	C65-C62-C64	-5.19	109.91	118.08
13	a	816	F39	C60-C58-C56	-5.19	109.91	118.08
8	a	811	BCL	C1C-NC-C4C	-5.18	104.38	106.71
8	1	408	BCL	C2D-C1D-ND	5.18	113.92	110.10
8	6	408	BCL	C2D-C1D-ND	5.18	113.92	110.10
17	c	302	F26	C38-C33-C31	-5.18	119.92	127.31
8	a	810	BCL	C1C-NC-C4C	-5.18	104.38	106.71
13	A	814	F39	C35-C37-C39	-5.17	111.00	118.94
13	a	816	F39	C32-C35-C37	-5.17	111.89	126.42
8	3	402	BCL	C2D-C1D-ND	5.17	113.91	110.10
8	2	401	BCL	C2D-C1D-ND	5.16	113.91	110.10
8	4	405	BCL	C2D-C1D-ND	5.15	113.90	110.10
8	4	402	BCL	C2D-C1D-ND	5.13	113.88	110.10
8	A	809	BCL	CHD-C1D-ND	-5.12	119.75	124.45
12	A	802	G2O	C1A-NA-C4A	5.12	109.01	106.71
11	A	801	GS0	O2D-CGD-CBD	5.11	120.36	111.27
11	A	801	GS0	C1D-ND-C4D	-5.11	102.70	106.33
13	A	814	F39	C63-C64-C62	-5.10	112.08	126.42
8	3	402	BCL	C1C-NC-C4C	-5.10	104.41	106.71
13	A	814	F39	C32-C35-C37	-5.09	112.12	126.42
13	C	302	F39	C40-C41-C42	-5.09	112.12	126.42
8	A	807	BCL	C2D-C1D-ND	5.09	113.86	110.10
8	a	807	BCL	CAC-C3C-C2C	-5.09	101.55	114.26
13	a	816	F39	C25-C20-C27	-5.07	109.51	122.59
8	1	401	BCL	O2D-CGD-O1D	-5.07	113.94	123.84
8	c	301	BCL	O2D-CGD-CBD	5.06	120.26	111.27
8	5	401	BCL	O2D-CGD-O1D	-5.05	113.97	123.84
13	A	815	F39	C40-C41-C42	-5.05	112.24	126.42
8	5	401	BCL	C2A-C3A-C4A	-5.03	93.75	101.87
11	a	802	GS0	C1D-ND-C4D	-5.03	102.77	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	402[B]	BCL	C2D-C1D-ND	5.02	113.81	110.10
8	4	408[B]	BCL	C2D-C1D-ND	5.02	113.80	110.10
8	4	401	BCL	O2D-CGD-O1D	-5.02	114.02	123.84
8	6	407[B]	BCL	C2D-C1D-ND	5.01	113.80	110.10
8	5	401	BCL	C4A-NA-C1A	-5.01	104.45	106.71
13	A	815	F39	C25-C20-C27	-5.01	109.67	122.59
8	3	407	BCL	C2D-C1D-ND	5.00	113.79	110.10
8	a	810	BCL	CAC-C3C-C2C	-5.00	101.77	114.26
8	2	403	BCL	C4A-NA-C1A	-5.00	104.46	106.71
13	a	816	F39	C40-C41-C42	-5.00	112.38	126.42
8	1	407[B]	BCL	C2D-C1D-ND	4.99	113.78	110.10
8	6	401	BCL	O2D-CGD-O1D	-4.98	114.10	123.84
8	2	403	BCL	O2D-CGD-O1D	-4.97	114.11	123.84
8	1	404	BCL	CAC-C3C-C2C	-4.97	101.85	114.26
8	A	809	BCL	CAC-C3C-C2C	-4.96	101.87	114.26
8	1	401	BCL	C4A-NA-C1A	-4.95	104.48	106.71
8	3	401	BCL	O2D-CGD-O1D	-4.95	114.16	123.84
8	6	401	BCL	C4A-NA-C1A	-4.95	104.48	106.71
13	A	815	F39	C32-C35-C37	-4.95	112.52	126.42
8	1	402	BCL	O2D-CGD-CBD	4.94	120.05	111.27
13	C	302	F39	C51-C57-C59	-4.94	113.36	123.47
13	A	815	F39	C35-C37-C39	-4.92	111.39	118.94
8	5	406	BCL	C1C-NC-C4C	-4.92	104.49	106.71
8	5	406	BCL	O2D-CGD-CBD	4.92	120.01	111.27
8	F	101	BCL	O2D-CGD-CBD	4.91	120.00	111.27
11	a	802	GS0	CAC-C3C-C2C	-4.91	101.99	114.26
8	3	406	BCL	CAC-C3C-C2C	-4.90	102.00	114.26
8	6	405	BCL	C1C-NC-C4C	-4.90	104.50	106.71
8	c	301	BCL	C1C-NC-C4C	-4.90	104.50	106.71
8	5	404	BCL	O2D-CGD-CBD	4.89	119.96	111.27
8	a	812	BCL	O2D-CGD-CBD	4.89	119.96	111.27
8	2	409[B]	BCL	C2D-C1D-ND	4.88	113.70	110.10
8	6	403	BCL	CAC-C3C-C2C	-4.87	102.09	114.26
8	1	403	BCL	O2D-CGD-CBD	4.86	119.91	111.27
8	a	814	BCL	C1C-NC-C4C	-4.86	104.52	106.71
8	4	410[B]	BCL	C2D-C1D-ND	4.86	113.68	110.10
8	A	811	BCL	O2D-CGD-CBD	4.86	119.90	111.27
8	6	404	BCL	CAC-C3C-C2C	-4.86	102.13	114.26
8	2	408	BCL	O2D-CGD-CBD	4.86	119.90	111.27
8	2	403	BCL	CAC-C3C-C2C	-4.85	102.13	114.26
8	A	808	BCL	CAC-C3C-C2C	-4.85	102.14	114.26
8	6	406	BCL	O2D-CGD-CBD	4.85	119.89	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	813	BCL	O2D-CGD-CBD	4.85	119.88	111.27
13	C	302	F39	C63-C64-C62	-4.84	112.81	126.42
8	5	403	BCL	O2D-CGD-CBD	4.84	119.88	111.27
8	c	301	BCL	CAC-C3C-C2C	-4.84	102.16	114.26
8	a	805	BCL	CAC-C3C-C2C	-4.84	102.17	114.26
8	3	407	BCL	O2D-CGD-CBD	4.84	119.87	111.27
8	5	404	BCL	CAC-C3C-C2C	-4.83	102.18	114.26
8	A	810	BCL	CAC-C3C-C2C	-4.83	102.19	114.26
8	1	401	BCL	CAC-C3C-C2C	-4.83	102.20	114.26
8	2	404	BCL	C1C-NC-C4C	-4.83	104.54	106.71
8	4	406	BCL	C1C-NC-C4C	-4.82	104.54	106.71
8	A	804	BCL	CAC-C3C-C2C	-4.82	102.21	114.26
8	1	403	BCL	CAC-C3C-C2C	-4.82	102.21	114.26
8	4	404	BCL	CAC-C3C-C2C	-4.82	102.21	114.26
8	a	808	BCL	O2D-CGD-CBD	4.82	119.83	111.27
13	a	816	F39	C35-C37-C39	-4.82	111.55	118.94
8	2	405	BCL	O2D-CGD-CBD	4.81	119.82	111.27
8	A	810	BCL	O2D-CGD-CBD	4.80	119.80	111.27
8	3	404	BCL	CAC-C3C-C2C	-4.80	102.26	114.26
8	2	401	BCL	CAC-C3C-C2C	-4.80	102.27	114.26
8	a	811	BCL	O2D-CGD-CBD	4.79	119.78	111.27
8	a	811	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
8	4	405	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
8	4	409	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
8	3	401	BCL	CAC-C3C-C2C	-4.78	102.31	114.26
8	6	406	BCL	CAC-C3C-C2C	-4.78	102.31	114.26
8	6	401	BCL	CAC-C3C-C2C	-4.78	102.31	114.26
8	2	406	BCL	CAC-C3C-C2C	-4.78	102.32	114.26
8	6	408	BCL	CAC-C3C-C2C	-4.78	102.32	114.26
8	3	406	BCL	O2D-CGD-CBD	4.78	119.76	111.27
8	1	408	BCL	CAC-C3C-C2C	-4.77	102.33	114.26
8	4	402	BCL	CAC-C3C-C2C	-4.77	102.34	114.26
8	A	807	BCL	O2D-CGD-CBD	4.77	119.75	111.27
8	4	404	BCL	O2D-CGD-CBD	4.77	119.74	111.27
11	A	801	GS0	CAC-C3C-C2C	-4.77	102.34	114.26
8	2	405	BCL	CAC-C3C-C2C	-4.77	102.35	114.26
8	1	404	BCL	O2D-CGD-CBD	4.76	119.72	111.27
13	C	302	F39	C65-C62-C64	-4.76	110.58	118.08
8	A	813	BCL	C2D-C1D-ND	4.75	113.61	110.10
8	3	407	BCL	CAC-C3C-C2C	-4.75	102.38	114.26
8	A	813	BCL	CAC-C3C-C2C	-4.74	102.42	114.26
8	4	408[B]	BCL	O2D-CGD-CBD	4.74	119.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	404	BCL	O2D-CGD-CBD	4.73	119.68	111.27
8	2	408	BCL	CAC-C3C-C2C	-4.73	102.44	114.26
8	a	813	BCL	CAC-C3C-C2C	-4.73	102.45	114.26
8	a	808	BCL	CAC-C3C-C2C	-4.72	102.47	114.26
8	3	403	BCL	O2D-CGD-CBD	4.71	119.64	111.27
8	A	807	BCL	CAC-C3C-C2C	-4.71	102.48	114.26
8	a	807	BCL	C1C-NC-C4C	-4.71	104.59	106.71
8	a	806	BCL	O2D-CGD-CBD	4.71	119.64	111.27
8	A	812	BCL	CAC-C3C-C2C	-4.71	102.49	114.26
8	A	806	BCL	CAC-C3C-C2C	-4.71	102.49	114.26
8	4	405	BCL	O2D-CGD-CBD	4.71	119.64	111.27
8	1	401	BCL	C2A-C3A-C4A	-4.71	94.26	101.87
8	3	403	BCL	CAC-C3C-C2C	-4.70	102.50	114.26
13	A	814	F39	C40-C41-C42	-4.70	113.20	126.42
8	F	101	BCL	CAC-C3C-C2C	-4.70	102.52	114.26
8	A	803	BCL	CAC-C3C-C2C	-4.69	102.53	114.26
8	a	812	BCL	CAC-C3C-C2C	-4.69	102.53	114.26
8	4	407	BCL	O2D-CGD-CBD	4.69	119.61	111.27
8	a	814	BCL	O2D-CGD-CBD	4.69	119.60	111.27
8	1	406	BCL	CAC-C3C-C2C	-4.68	102.56	114.26
8	3	405	BCL	CAC-C3C-C2C	-4.68	102.56	114.26
13	C	302	F39	C35-C37-C39	-4.68	111.77	118.94
8	6	403	BCL	O2D-CGD-CBD	4.67	119.57	111.27
8	a	810	BCL	CHD-C1D-ND	-4.67	120.17	124.45
8	1	406	BCL	O2D-CGD-CBD	4.66	119.55	111.27
13	A	815	F39	C63-C64-C62	-4.65	113.35	126.42
8	a	810	BCL	O2D-CGD-CBD	4.65	119.52	111.27
8	2	404	BCL	CAC-C3C-C2C	-4.64	102.66	114.26
8	4	407	BCL	CAC-C3C-C2C	-4.64	102.67	114.26
8	C	301	BCL	O2D-CGD-CBD	4.64	119.51	111.27
8	6	405	BCL	CAC-C3C-C2C	-4.63	102.68	114.26
8	a	814	BCL	CAC-C3C-C2C	-4.63	102.69	114.26
8	a	806	BCL	CAC-C3C-C2C	-4.63	102.69	114.26
8	5	403	BCL	CAC-C3C-C2C	-4.63	102.70	114.26
8	A	806	BCL	O2D-CGD-CBD	4.61	119.47	111.27
8	5	402	BCL	O2D-CGD-CBD	4.61	119.46	111.27
8	4	406	BCL	CAC-C3C-C2C	-4.61	102.74	114.26
8	a	804	BCL	O2D-CGD-CBD	4.60	119.45	111.27
8	a	809	BCL	C4A-NA-C1A	-4.60	104.64	106.71
8	5	406	BCL	CAC-C3C-C2C	-4.60	102.77	114.26
8	5	401	BCL	CAC-C3C-C2C	-4.59	102.79	114.26
13	C	302	F39	C38-C37-C35	-4.59	110.85	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	803	BCL	O2D-CGD-CBD	4.57	119.39	111.27
8	3	402	BCL	O2D-CGD-CBD	4.57	119.39	111.27
8	a	809	BCL	CAC-C3C-C2C	-4.56	102.86	114.26
8	1	405	BCL	CAC-C3C-C2C	-4.55	102.89	114.26
8	4	403	BCL	O2D-CGD-CBD	4.55	119.36	111.27
8	A	813	BCL	CMB-C2B-C3B	4.54	133.18	124.68
8	A	805	BCL	CAC-C3C-C2C	-4.54	102.92	114.26
8	A	808	BCL	O2D-CGD-CBD	4.51	119.29	111.27
8	5	405	BCL	O2D-CGD-CBD	4.51	119.29	111.27
8	1	408	BCL	O2D-CGD-CBD	4.51	119.28	111.27
8	4	402	BCL	O2D-CGD-CBD	4.51	119.28	111.27
8	4	403	BCL	C1C-NC-C4C	-4.51	104.68	106.71
8	1	405	BCL	O2D-CGD-CBD	4.50	119.27	111.27
8	4	406	BCL	CHD-C1D-ND	-4.50	120.32	124.45
8	4	401	BCL	CAC-C3C-C2C	-4.49	103.04	114.26
8	6	402	BCL	CAC-C3C-C2C	-4.49	103.04	114.26
8	A	809	BCL	O2D-CGD-CBD	4.48	119.23	111.27
11	A	801	GS0	CHD-C1D-ND	-4.47	120.34	124.45
8	1	407[B]	BCL	CAC-C3C-C2C	-4.47	103.09	114.26
8	2	407	BCL	CAC-C3C-C2C	-4.46	103.11	114.26
8	3	405	BCL	CHD-C1D-ND	-4.46	120.35	124.45
8	4	410[B]	BCL	O2D-CGD-CBD	4.46	119.19	111.27
8	3	401	BCL	C2A-C3A-C4A	-4.46	94.67	101.87
8	a	807	BCL	O2D-CGD-CBD	4.45	119.18	111.27
8	A	804	BCL	O2D-CGD-CBD	4.45	119.17	111.27
8	6	407[B]	BCL	CAC-C3C-C2C	-4.44	103.16	114.26
8	4	401	BCL	C2A-C3A-C4A	-4.44	94.70	101.87
8	4	408[B]	BCL	CAC-C3C-C2C	-4.43	103.18	114.26
13	a	816	F39	C38-C37-C35	-4.43	111.09	118.08
8	A	805	BCL	O2D-CGD-CBD	4.43	119.14	111.27
8	a	811	BCL	CMB-C2B-C3B	4.42	132.94	124.68
8	A	812	BCL	O2D-CGD-O1D	-4.41	115.21	123.84
13	A	815	F39	C38-C37-C35	-4.41	111.14	118.08
8	4	406	BCL	CMB-C2B-C3B	4.40	132.91	124.68
8	4	403	BCL	CAC-C3C-C2C	-4.40	103.28	114.26
8	2	409[B]	BCL	CAC-C3C-C2C	-4.39	103.30	114.26
8	6	404	BCL	O2D-CGD-O1D	-4.37	115.29	123.84
8	2	402[B]	BCL	CAC-C3C-C2C	-4.37	103.34	114.26
8	6	402	BCL	O2D-CGD-CBD	4.36	119.02	111.27
8	1	405	BCL	CHD-C1D-ND	-4.36	120.45	124.45
8	5	402	BCL	CAC-C3C-C2C	-4.36	103.38	114.26
8	4	410[B]	BCL	CAC-C3C-C2C	-4.36	103.38	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	809	BCL	CMB-C2B-C3B	4.35	132.82	124.68
8	3	402	BCL	CAC-C3C-C2C	-4.35	103.38	114.26
8	5	403	BCL	C1C-NC-C4C	-4.34	104.75	106.71
9	a	820	CDL	OA6-CA5-C11	4.34	120.86	111.50
8	2	407	BCL	CHD-C1D-ND	-4.34	120.46	124.45
8	6	407[B]	BCL	O2D-CGD-CBD	4.34	118.98	111.27
8	6	406	BCL	C1C-NC-C4C	-4.34	104.75	106.71
8	3	405	BCL	O2D-CGD-CBD	4.34	118.98	111.27
8	4	406	BCL	O2D-CGD-CBD	4.32	118.95	111.27
8	6	408	BCL	O2D-CGD-CBD	4.32	118.95	111.27
11	a	802	GS0	O2D-CGD-O1D	-4.32	115.38	123.84
8	2	407	BCL	O2D-CGD-CBD	4.31	118.93	111.27
8	1	407[B]	BCL	O2D-CGD-CBD	4.31	118.93	111.27
8	a	804	BCL	CAC-C3C-C2C	-4.30	103.50	114.26
8	A	813	BCL	O2D-CGD-CBD	4.30	118.92	111.27
8	C	301	BCL	CMB-C2B-C3B	4.30	132.72	124.68
13	A	814	F39	C38-C37-C35	-4.30	111.30	118.08
8	3	404	BCL	O2D-CGD-O1D	-4.29	115.44	123.84
8	a	806	BCL	CHD-C1D-ND	-4.29	120.51	124.45
8	2	409[B]	BCL	O2D-CGD-CBD	4.28	118.88	111.27
8	a	812	BCL	CHD-C1D-ND	-4.28	120.52	124.45
8	2	401	BCL	O2D-CGD-CBD	4.28	118.88	111.27
8	2	406	BCL	O2D-CGD-CBD	4.28	118.88	111.27
8	1	405	BCL	CMB-C2B-C3B	4.28	132.69	124.68
8	a	812	BCL	C1C-NC-C4C	-4.28	104.78	106.71
8	a	809	BCL	O2D-CGD-CBD	4.28	118.87	111.27
8	2	404	BCL	O2D-CGD-O1D	-4.27	115.48	123.84
8	6	404	BCL	CMB-C2B-C3B	4.27	132.66	124.68
8	c	301	BCL	CHD-C1D-ND	-4.26	120.54	124.45
8	1	404	BCL	CMB-C2B-C3B	4.26	132.65	124.68
8	2	407	BCL	CMB-C2B-C3B	4.26	132.65	124.68
8	6	403	BCL	CHD-C1D-ND	-4.26	120.54	124.45
8	2	403	BCL	C2A-C3A-C4A	-4.26	94.99	101.87
8	2	406	BCL	CMB-C2B-C3B	4.25	132.64	124.68
8	a	807	BCL	CHD-C1D-ND	-4.25	120.55	124.45
8	A	808	BCL	CMB-C2B-C3B	4.25	132.63	124.68
8	A	811	BCL	CAC-C3C-C2C	-4.25	103.65	114.26
13	C	302	F39	C19-C20-C27	-4.24	109.15	121.98
8	a	807	BCL	O2D-CGD-O1D	-4.23	115.56	123.84
8	6	405	BCL	CHD-C1D-ND	-4.23	120.56	124.45
14	A	819	LHG	O4-P-O5	4.23	133.15	112.24
8	3	401	BCL	C1C-NC-C4C	-4.23	104.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	401	BCL	CMB-C2B-C3B	4.22	132.57	124.68
8	2	402[B]	BCL	O2D-CGD-CBD	4.21	118.76	111.27
8	4	409	BCL	O2D-CGD-CBD	4.21	118.75	111.27
8	6	402	BCL	O2D-CGD-O1D	-4.21	115.60	123.84
8	c	301	BCL	O2D-CGD-O1D	-4.21	115.62	123.84
8	3	404	BCL	CMB-C2B-C3B	4.20	132.54	124.68
8	5	405	BCL	CMB-C2B-C3B	4.20	132.54	124.68
11	A	801	GS0	O2D-CGD-O1D	-4.20	115.63	123.84
8	3	406	BCL	C1C-NC-C4C	-4.19	104.82	106.71
8	6	408	BCL	CMB-C2B-C3B	4.19	132.51	124.68
14	a	817	LHG	O4-P-O5	4.18	132.92	112.24
14	a	821	LHG	O4-P-O5	4.18	132.91	112.24
8	2	405	BCL	CHD-C1D-ND	-4.18	120.62	124.45
14	E	101	LHG	O4-P-O5	4.17	132.87	112.24
14	A	818	LHG	O4-P-O5	4.17	132.86	112.24
8	1	402	BCL	O2D-CGD-O1D	-4.17	115.69	123.84
8	c	301	BCL	CMB-C2B-C3B	4.17	132.47	124.68
8	C	301	BCL	CHD-C1D-ND	-4.16	120.63	124.45
8	a	813	BCL	O2D-CGD-O1D	-4.16	115.70	123.84
8	5	404	BCL	CMB-C2B-C3B	4.16	132.47	124.68
14	a	819	LHG	O4-P-O5	4.16	132.80	112.24
8	6	405	BCL	CMB-C2B-C3B	4.16	132.45	124.68
8	4	403	BCL	O2D-CGD-O1D	-4.15	115.72	123.84
8	A	805	BCL	C1C-NC-C4C	-4.15	104.84	106.71
8	1	403	BCL	O2D-CGD-O1D	-4.15	115.73	123.84
8	A	810	BCL	CMB-C2B-C3B	4.15	132.44	124.68
8	2	408	BCL	O2D-CGD-O1D	-4.15	115.73	123.84
8	4	405	BCL	O2D-CGD-O1D	-4.15	115.73	123.84
8	5	404	BCL	O2D-CGD-O1D	-4.15	115.73	123.84
8	5	403	BCL	O2D-CGD-O1D	-4.14	115.74	123.84
8	6	405	BCL	O2D-CGD-CBD	4.14	118.63	111.27
8	a	812	BCL	O2D-CGD-O1D	-4.14	115.74	123.84
8	A	809	BCL	O2D-CGD-O1D	-4.14	115.75	123.84
8	A	811	BCL	O2D-CGD-O1D	-4.13	115.76	123.84
14	A	816	LHG	O4-P-O5	4.13	132.65	112.24
8	1	402	BCL	CAC-C3C-C2C	-4.13	103.94	114.26
8	4	407	BCL	C1C-NC-C4C	-4.13	104.85	106.71
8	A	807	BCL	O2D-CGD-O1D	-4.13	115.77	123.84
8	1	407[B]	BCL	CMB-C2B-C3B	4.12	132.39	124.68
8	4	405	BCL	CMB-C2B-C3B	4.12	132.39	124.68
8	a	805	BCL	CMB-C2B-C3B	4.12	132.39	124.68
8	A	811	BCL	CHD-C1D-ND	-4.12	120.67	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	5	406	BCL	O2D-CGD-O1D	-4.12	115.79	123.84
8	F	101	BCL	O2D-CGD-O1D	-4.12	115.79	123.84
8	2	403	BCL	CMB-C2B-C3B	4.11	132.38	124.68
8	1	408	BCL	CMB-C2B-C3B	4.11	132.38	124.68
8	3	402	BCL	O2D-CGD-O1D	-4.11	115.80	123.84
8	2	402[B]	BCL	CMB-C2B-C3B	4.11	132.37	124.68
8	6	406	BCL	O2D-CGD-O1D	-4.11	115.80	123.84
8	C	301	BCL	O2D-CGD-O1D	-4.11	115.81	123.84
8	5	405	BCL	CHD-C1D-ND	-4.10	120.68	124.45
9	1	409	CDL	OA6-CA5-C11	4.10	120.34	111.50
8	2	405	BCL	O2D-CGD-O1D	-4.10	115.82	123.84
9	a	820	CDL	OB6-CB5-C51	4.10	120.34	111.50
8	1	403	BCL	CHD-C1D-ND	-4.10	120.69	124.45
8	a	814	BCL	CMB-C2B-C3B	4.10	132.34	124.68
8	A	810	BCL	O2D-CGD-O1D	-4.09	115.83	123.84
8	A	808	BCL	CHD-C1D-ND	-4.09	120.69	124.45
8	a	808	BCL	O2D-CGD-O1D	-4.09	115.84	123.84
8	2	409[B]	BCL	CMB-C2B-C3B	4.09	132.33	124.68
8	3	407	BCL	CMB-C2B-C3B	4.09	132.33	124.68
8	5	402	BCL	O2D-CGD-O1D	-4.09	115.84	123.84
8	6	401	BCL	CMB-C2B-C3B	4.09	132.32	124.68
8	3	406	BCL	O2D-CGD-O1D	-4.08	115.85	123.84
8	a	804	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
13	a	816	F39	C19-C20-C27	-4.08	109.64	121.98
8	a	811	BCL	O2D-CGD-O1D	-4.07	115.88	123.84
8	4	401	BCL	CMB-C2B-C3B	4.07	132.30	124.68
8	3	406	BCL	CMB-C2B-C3B	4.07	132.30	124.68
8	4	408[B]	BCL	CMB-C2B-C3B	4.07	132.29	124.68
8	5	405	BCL	CAC-C3C-C2C	-4.07	104.09	114.26
8	3	403	BCL	O2D-CGD-O1D	-4.07	115.89	123.84
8	a	814	BCL	O2D-CGD-O1D	-4.06	115.89	123.84
8	4	409	BCL	CHD-C1D-ND	-4.06	120.72	124.45
8	4	410[B]	BCL	CMB-C2B-C3B	4.06	132.28	124.68
8	4	408[B]	BCL	O2D-CGD-O1D	-4.06	115.90	123.84
8	2	408	BCL	CMB-C2B-C3B	4.06	132.27	124.68
9	c	303	CDL	OB6-CB5-C51	4.06	120.25	111.50
8	A	805	BCL	CHD-C1D-ND	-4.05	120.73	124.45
13	A	814	F39	C19-C20-C27	-4.05	109.72	121.98
8	1	404	BCL	O2D-CGD-O1D	-4.05	115.92	123.84
9	1	409	CDL	OB6-CB5-C51	4.05	120.23	111.50
8	1	401	BCL	CMB-C2B-C3B	4.05	132.25	124.68
8	A	809	BCL	C3D-C2D-C1D	-4.04	100.31	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	4	402	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
8	4	407	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
8	4	404	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
8	1	406	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
8	A	813	BCL	OBB-CAB-CBB	-4.04	111.09	120.17
8	6	407[B]	BCL	CMB-C2B-C3B	4.03	132.22	124.68
8	C	301	BCL	CAC-C3C-C2C	-4.03	104.19	114.26
13	A	815	F39	C19-C20-C27	-4.03	109.78	121.98
8	a	806	BCL	O2D-CGD-O1D	-4.03	115.96	123.84
8	6	403	BCL	O2D-CGD-O1D	-4.03	115.97	123.84
8	5	405	BCL	O2D-CGD-O1D	-4.02	115.97	123.84
8	3	407	BCL	O2D-CGD-O1D	-4.02	115.97	123.84
8	A	804	BCL	CMB-C2B-C3B	4.02	132.20	124.68
8	2	401	BCL	CMB-C2B-C3B	4.02	132.20	124.68
8	4	410[B]	BCL	O2D-CGD-O1D	-4.02	115.98	123.84
8	1	406	BCL	CMB-C2B-C3B	4.02	132.19	124.68
8	a	809	BCL	CHD-C1D-ND	-4.02	120.76	124.45
8	a	813	BCL	CHD-C1D-ND	-4.01	120.77	124.45
8	4	407	BCL	CMB-C2B-C3B	4.01	132.19	124.68
8	6	406	BCL	CMB-C2B-C3B	4.01	132.19	124.68
17	a	815	F26	C32-C30-C26	-4.01	121.59	127.31
8	a	807	BCL	OBB-CAB-CBB	-4.01	111.16	120.17
8	3	405	BCL	CMB-C2B-C3B	4.00	132.17	124.68
8	5	401	BCL	CMB-C2B-C3B	4.00	132.17	124.68
8	6	401	BCL	OBB-CAB-CBB	-4.00	111.16	120.17
8	2	405	BCL	CMB-C2B-C3B	4.00	132.17	124.68
8	A	807	BCL	CHD-C1D-ND	-4.00	120.78	124.45
8	a	810	BCL	O2D-CGD-O1D	-4.00	116.02	123.84
11	A	801	GS0	CMB-C2B-C3B	3.99	132.15	124.68
8	A	808	BCL	O2D-CGD-O1D	-3.99	116.03	123.84
8	a	805	BCL	O2D-CGD-CBD	3.99	118.36	111.27
8	A	804	BCL	O2D-CGD-O1D	-3.99	116.04	123.84
8	1	405	BCL	C1C-NC-C4C	-3.99	104.91	106.71
8	2	408	BCL	C1C-NC-C4C	-3.99	104.91	106.71
9	a	822	CDL	OA6-CA5-C11	3.98	120.07	111.50
8	1	405	BCL	O2D-CGD-O1D	-3.98	116.07	123.84
8	1	408	BCL	O2D-CGD-O1D	-3.97	116.08	123.84
8	5	403	BCL	CHD-C1D-ND	-3.97	120.81	124.45
8	6	404	BCL	C1C-NC-C4C	-3.96	104.92	106.71
8	5	401	BCL	OBB-CAB-CBB	-3.96	111.25	120.17
8	3	403	BCL	OBB-CAB-CBB	-3.96	111.26	120.17
8	A	804	BCL	OBB-CAB-CBB	-3.96	111.26	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	4	409	BCL	CMB-C2B-C3B	3.95	132.07	124.68
9	a	822	CDL	OB6-CB5-C51	3.95	120.02	111.50
8	6	403	BCL	CMB-C2B-C3B	3.95	132.07	124.68
8	4	402	BCL	CMB-C2B-C3B	3.95	132.07	124.68
8	a	809	BCL	O2D-CGD-O1D	-3.95	116.12	123.84
8	4	401	BCL	OBB-CAB-CBB	-3.95	111.29	120.17
8	A	803	BCL	O2D-CGD-O1D	-3.94	116.12	123.84
8	A	806	BCL	O2D-CGD-O1D	-3.94	116.13	123.84
8	C	301	BCL	C4D-CHA-C1A	3.94	126.05	121.25
11	a	802	GS0	CHD-C1D-ND	-3.94	120.83	124.45
8	1	401	BCL	OBB-CAB-CBB	-3.94	111.31	120.17
11	a	802	GS0	OBB-CAB-CBB	-3.94	111.31	120.17
8	A	813	BCL	O2D-CGD-O1D	-3.93	116.14	123.84
17	c	302	F26	C32-C30-C26	-3.93	121.69	127.31
8	4	404	BCL	CHD-C1D-ND	-3.92	120.85	124.45
8	2	407	BCL	O2D-CGD-O1D	-3.92	116.18	123.84
8	a	805	BCL	OBB-CAB-CBB	-3.91	111.36	120.17
8	F	101	BCL	OBB-CAB-CBB	-3.91	111.36	120.17
8	a	814	BCL	OBB-CAB-CBB	-3.91	111.36	120.17
8	2	406	BCL	O2D-CGD-O1D	-3.91	116.19	123.84
8	2	401	BCL	O2D-CGD-O1D	-3.91	116.19	123.84
8	1	403	BCL	CMB-C2B-C3B	3.91	131.99	124.68
8	5	406	BCL	CHD-C1D-ND	-3.91	120.86	124.45
8	3	401	BCL	OBB-CAB-CBB	-3.91	111.38	120.17
15	A	817	LMG	O6-C1-O1	-3.90	100.73	109.97
8	2	403	BCL	OBB-CAB-CBB	-3.90	111.39	120.17
8	4	404	BCL	CMB-C2B-C3B	3.90	131.98	124.68
8	1	407[B]	BCL	O2D-CGD-O1D	-3.90	116.21	123.84
8	A	808	BCL	C4A-NA-C1A	-3.90	104.95	106.71
8	6	407[B]	BCL	O2D-CGD-O1D	-3.89	116.23	123.84
8	6	408	BCL	O2D-CGD-O1D	-3.89	116.23	123.84
8	A	810	BCL	CHD-C1D-ND	-3.89	120.88	124.45
8	6	403	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
8	A	805	BCL	O2D-CGD-O1D	-3.89	116.24	123.84
8	2	409[B]	BCL	O2D-CGD-O1D	-3.89	116.24	123.84
8	1	403	BCL	OBB-CAB-CBB	-3.88	111.44	120.17
8	5	406	BCL	OBB-CAB-CBB	-3.87	111.45	120.17
8	5	403	BCL	CMB-C2B-C3B	3.87	131.92	124.68
8	5	403	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
8	4	410[B]	BCL	C1C-NC-C4C	-3.87	104.97	106.71
8	4	402	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
8	1	408	BCL	OBB-CAB-CBB	-3.87	111.46	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	806	BCL	OBB-CAB-CBB	-3.87	111.47	120.17
8	4	402	BCL	C1C-NC-C4C	-3.87	104.97	106.71
8	a	814	BCL	CHD-C1D-ND	-3.86	120.90	124.45
8	4	406	BCL	O2D-CGD-O1D	-3.86	116.29	123.84
8	2	408	BCL	CHD-C1D-ND	-3.86	120.91	124.45
8	2	402[B]	BCL	O2D-CGD-O1D	-3.86	116.30	123.84
8	2	405	BCL	C1C-NC-C4C	-3.86	104.97	106.71
9	c	303	CDL	OA6-CA5-C11	3.86	119.81	111.50
8	6	406	BCL	OBB-CAB-CBB	-3.86	111.49	120.17
8	1	407[B]	BCL	CHD-C1D-ND	-3.85	120.91	124.45
8	4	408[B]	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
8	6	408	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
8	4	409	BCL	O2D-CGD-O1D	-3.85	116.31	123.84
8	1	406	BCL	CHD-C1D-ND	-3.84	120.92	124.45
8	6	401	BCL	C2A-C3A-C4A	-3.84	95.66	101.87
8	F	101	BCL	CMB-C2B-C3B	3.84	131.87	124.68
8	4	409	BCL	OBB-CAB-CBB	-3.84	111.54	120.17
8	a	808	BCL	CHD-C1D-ND	-3.83	120.93	124.45
8	1	406	BCL	OBB-CAB-CBB	-3.83	111.54	120.17
8	2	401	BCL	CHD-C1D-ND	-3.83	120.93	124.45
8	3	404	BCL	C1C-NC-C4C	-3.83	104.98	106.71
8	4	407	BCL	OBB-CAB-CBB	-3.83	111.56	120.17
8	a	805	BCL	CHD-C1D-ND	-3.82	120.94	124.45
8	2	405	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
15	a	818	LMG	O6-C1-O1	-3.82	100.92	109.97
8	2	401	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
8	2	404	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
8	a	805	BCL	O2D-CGD-O1D	-3.82	116.37	123.84
8	4	404	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
8	2	408	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
8	3	404	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
8	a	806	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
8	6	406	BCL	CHD-C1D-ND	-3.81	120.95	124.45
8	1	408	BCL	CHD-C1D-ND	-3.81	120.95	124.45
8	A	805	BCL	OBB-CAB-CBB	-3.81	111.60	120.17
17	c	302	F26	C23-C19-C24	-3.81	117.59	122.92
8	6	407[B]	BCL	CHD-C1D-ND	-3.80	120.96	124.45
8	F	101	BCL	C4A-NA-C1A	-3.80	105.00	106.71
8	c	301	BCL	OBB-CAB-CBB	-3.80	111.62	120.17
8	A	807	BCL	OBB-CAB-CBB	-3.80	111.62	120.17
17	c	302	F26	C39-C37-C34	-3.79	121.89	127.31
8	6	405	BCL	O2D-CGD-O1D	-3.79	116.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	406	BCL	CHD-C1D-ND	-3.79	120.97	124.45
8	2	409[B]	BCL	OBB-CAB-CBB	-3.79	111.63	120.17
8	1	404	BCL	OBB-CAB-CBB	-3.79	111.64	120.17
8	4	407	BCL	CHD-C1D-ND	-3.79	120.97	124.45
8	A	811	BCL	OBB-CAB-CBB	-3.79	111.64	120.17
8	5	404	BCL	OBB-CAB-CBB	-3.79	111.64	120.17
8	6	407[B]	BCL	OBB-CAB-CBB	-3.79	111.65	120.17
8	6	404	BCL	CHD-C1D-ND	-3.79	120.97	124.45
8	A	810	BCL	OBB-CAB-CBB	-3.78	111.65	120.17
8	a	812	BCL	OBB-CAB-CBB	-3.78	111.66	120.17
8	5	406	BCL	CMB-C2B-C3B	3.78	131.75	124.68
8	1	402	BCL	OBB-CAB-CBB	-3.78	111.66	120.17
8	1	401	BCL	CHD-C1D-ND	-3.78	120.98	124.45
8	a	808	BCL	OBB-CAB-CBB	-3.78	111.66	120.17
8	A	803	BCL	C4A-NA-C1A	-3.78	105.01	106.71
11	A	801	GS0	OBB-CAB-CBB	-3.78	111.67	120.17
8	4	410[B]	BCL	OBB-CAB-CBB	-3.78	111.67	120.17
8	6	402	BCL	OBB-CAB-CBB	-3.77	111.68	120.17
8	4	405	BCL	OBB-CAB-CBB	-3.77	111.68	120.17
8	A	812	BCL	CHD-C1D-ND	-3.77	120.99	124.45
8	2	402[B]	BCL	OBB-CAB-CBB	-3.77	111.69	120.17
8	a	811	BCL	OBB-CAB-CBB	-3.77	111.69	120.17
8	a	810	BCL	OBB-CAB-CBB	-3.77	111.69	120.17
8	4	408[B]	BCL	CHD-C1D-ND	-3.76	121.00	124.45
8	a	807	BCL	C4D-CHA-C1A	3.76	125.83	121.25
8	4	402	BCL	CHD-C1D-ND	-3.76	121.00	124.45
8	a	811	BCL	C4A-NA-C1A	-3.76	105.02	106.71
8	A	812	BCL	OBB-CAB-CBB	-3.76	111.71	120.17
8	4	401	BCL	CHD-C1D-ND	-3.76	121.00	124.45
8	3	406	BCL	OBB-CAB-CBB	-3.75	111.72	120.17
8	a	813	BCL	OBB-CAB-CBB	-3.75	111.72	120.17
8	a	810	BCL	C3D-C2D-C1D	-3.75	100.71	105.83
8	5	402	BCL	OBB-CAB-CBB	-3.75	111.73	120.17
8	2	406	BCL	OBB-CAB-CBB	-3.75	111.73	120.17
8	4	403	BCL	OBB-CAB-CBB	-3.75	111.73	120.17
8	3	402	BCL	OBB-CAB-CBB	-3.74	111.74	120.17
13	A	815	F39	C61-C63-C64	-3.74	111.53	123.22
8	1	407[B]	BCL	OBB-CAB-CBB	-3.74	111.75	120.17
8	3	403	BCL	CHD-C1D-ND	-3.74	121.02	124.45
8	3	407	BCL	CHD-C1D-ND	-3.74	121.02	124.45
8	5	401	BCL	CHD-C1D-ND	-3.73	121.02	124.45
8	3	407	BCL	OBB-CAB-CBB	-3.73	111.77	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	403	BCL	CHD-C1D-ND	-3.73	121.03	124.45
8	3	405	BCL	O2D-CGD-O1D	-3.73	116.55	123.84
8	A	803	BCL	CHD-C1D-ND	-3.73	121.03	124.45
8	6	401	BCL	CHD-C1D-ND	-3.72	121.03	124.45
8	6	404	BCL	OBB-CAB-CBB	-3.72	111.79	120.17
8	A	808	BCL	OBB-CAB-CBB	-3.72	111.80	120.17
8	a	804	BCL	OBB-CAB-CBB	-3.72	111.80	120.17
8	C	301	BCL	OBB-CAB-CBB	-3.71	111.81	120.17
8	2	407	BCL	C1C-NC-C4C	-3.70	105.04	106.71
8	a	814	BCL	C4A-NA-C1A	-3.69	105.05	106.71
8	5	401	BCL	C1C-NC-C4C	-3.69	105.05	106.71
8	A	803	BCL	OBB-CAB-CBB	-3.69	111.86	120.17
8	A	809	BCL	OBB-CAB-CBB	-3.69	111.87	120.17
11	a	802	GS0	CMB-C2B-C3B	3.69	131.58	124.68
8	A	812	BCL	C4A-NA-C1A	-3.68	105.05	106.71
8	3	401	BCL	CHD-C1D-ND	-3.68	121.07	124.45
8	a	812	BCL	C16-C15-C13	-3.67	104.05	115.92
8	A	806	BCL	C4A-NA-C1A	-3.67	105.06	106.71
8	6	403	BCL	C1C-NC-C4C	-3.66	105.06	106.71
8	a	809	BCL	OBB-CAB-CBB	-3.66	111.94	120.17
8	A	813	BCL	CHD-C1D-ND	-3.65	121.10	124.45
8	6	408	BCL	CHD-C1D-ND	-3.64	121.11	124.45
8	3	403	BCL	CMB-C2B-C3B	3.64	131.49	124.68
8	a	811	BCL	CHD-C1D-ND	-3.63	121.12	124.45
13	a	816	F39	C27-C32-C35	-3.62	111.91	123.22
8	6	401	BCL	C1C-NC-C4C	-3.61	105.08	106.71
8	2	407	BCL	C4D-CHA-C1A	3.61	125.64	121.25
8	2	409[B]	BCL	C1C-NC-C4C	-3.60	105.09	106.71
8	1	405	BCL	OBB-CAB-CBB	-3.60	112.07	120.17
11	a	802	GS0	C7-C6-C5	-3.59	103.61	113.36
8	2	407	BCL	OBB-CAB-CBB	-3.59	112.09	120.17
8	a	804	BCL	CHD-C1D-ND	-3.59	121.16	124.45
8	5	402	BCL	C2C-C3C-C4C	-3.58	95.97	101.34
8	A	807	BCL	C4A-NA-C1A	-3.58	105.10	106.71
8	5	405	BCL	OBB-CAB-CBB	-3.58	112.12	120.17
11	A	801	GS0	C7-C6-C5	-3.58	103.65	113.36
8	2	409[B]	BCL	CHD-C1D-ND	-3.57	121.17	124.45
8	6	405	BCL	OBB-CAB-CBB	-3.56	112.15	120.17
8	3	407	BCL	C1C-NC-C4C	-3.56	105.10	106.71
8	A	804	BCL	CHD-C1D-ND	-3.56	121.19	124.45
8	c	301	BCL	C4D-CHA-C1A	3.55	125.57	121.25
8	3	403	BCL	C1C-NC-C4C	-3.55	105.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	406	BCL	C1C-NC-C4C	-3.54	105.12	106.71
13	A	814	F39	C61-C63-C64	-3.53	112.19	123.22
13	A	815	F39	C25-C20-C19	-3.52	109.36	115.27
8	A	806	BCL	CHD-C1D-ND	-3.51	121.23	124.45
8	3	404	BCL	C16-C15-C13	-3.51	104.58	115.92
13	C	302	F39	C39-C40-C41	-3.50	112.30	123.22
13	a	816	F39	C61-C63-C64	-3.50	112.30	123.22
8	5	405	BCL	C1C-NC-C4C	-3.50	105.13	106.71
17	a	815	F26	C23-C19-C24	-3.49	118.04	122.92
8	4	406	BCL	OBB-CAB-CBB	-3.49	112.33	120.17
8	5	404	BCL	CHD-C1D-ND	-3.48	121.25	124.45
8	2	403	BCL	CHA-C1A-NA	-3.48	118.43	126.40
8	2	402[B]	BCL	CHD-C1D-ND	-3.48	121.26	124.45
8	C	301	BCL	C1C-NC-C4C	-3.47	105.14	106.71
8	2	406	BCL	CHD-C1D-ND	-3.47	121.27	124.45
13	C	302	F39	C25-C20-C19	-3.46	109.44	115.27
8	5	401	BCL	C2A-C1A-CHA	3.46	129.91	123.86
13	a	816	F39	C39-C40-C41	-3.46	112.43	123.22
8	A	811	BCL	C4A-NA-C1A	-3.46	105.15	106.71
8	a	813	BCL	C4A-NA-C1A	-3.46	105.15	106.71
8	2	403	BCL	C4B-CHC-C1C	-3.45	123.28	130.12
8	4	409	BCL	CHA-C1A-NA	-3.45	118.50	126.40
8	F	101	BCL	CHA-C1A-NA	-3.45	118.50	126.40
8	1	404	BCL	CHD-C1D-ND	-3.44	121.29	124.45
8	A	809	BCL	CHA-C1A-NA	-3.44	118.53	126.40
8	A	810	BCL	C1C-NC-C4C	-3.44	105.16	106.71
8	1	402	BCL	C2C-C3C-C4C	-3.43	96.20	101.34
8	A	810	BCL	C16-C15-C13	-3.43	104.84	115.92
8	3	404	BCL	CHD-C1D-ND	-3.43	121.31	124.45
8	A	806	BCL	CMB-C2B-C3B	3.43	131.09	124.68
8	5	404	BCL	C16-C15-C13	-3.42	104.85	115.92
8	a	813	BCL	C4B-CHC-C1C	-3.42	123.33	130.12
8	a	807	BCL	CMB-C2B-C3B	3.42	131.07	124.68
8	1	401	BCL	C4B-CHC-C1C	-3.41	123.36	130.12
8	A	813	BCL	C2A-C3A-C4A	-3.41	96.36	101.87
8	A	807	BCL	C16-C15-C13	-3.41	104.90	115.92
8	4	405	BCL	CHD-C1D-ND	-3.41	121.32	124.45
8	3	405	BCL	C4A-NA-C1A	-3.39	105.18	106.71
8	2	408	BCL	C11-C10-C8	-3.39	104.97	115.92
13	A	815	F39	C39-C40-C41	-3.39	112.64	123.22
8	1	404	BCL	C1C-NC-C4C	-3.38	105.19	106.71
8	4	404	BCL	C1C-NC-C4C	-3.38	105.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	4	401	BCL	C16-C15-C13	-3.38	104.99	115.92
8	6	405	BCL	C4D-CHA-C1A	3.38	125.36	121.25
8	4	407	BCL	C11-C10-C8	-3.37	105.02	115.92
8	6	401	BCL	CHA-C1A-NA	-3.37	118.68	126.40
8	4	405	BCL	C16-C15-C13	-3.37	105.03	115.92
8	a	812	BCL	CMB-C2B-C3B	3.37	130.98	124.68
8	1	405	BCL	C16-C15-C13	-3.36	105.06	115.92
8	6	402	BCL	C16-C15-C13	-3.36	105.07	115.92
11	a	802	GS0	CMA-C3A-C4A	-3.36	102.75	111.77
8	4	401	BCL	C4D-CHA-C1A	3.35	125.33	121.25
8	a	810	BCL	CHA-C1A-NA	-3.35	118.72	126.40
8	4	401	BCL	CHA-C1A-NA	-3.35	118.72	126.40
8	3	401	BCL	CHA-C1A-NA	-3.35	118.73	126.40
8	A	813	BCL	CHA-C1A-NA	-3.34	118.74	126.40
8	2	406	BCL	C4D-CHA-C1A	3.34	125.32	121.25
8	A	804	BCL	C1C-NC-C4C	-3.33	105.21	106.71
8	2	404	BCL	C16-C15-C13	-3.33	105.14	115.92
8	4	410[B]	BCL	CHD-C1D-ND	-3.33	121.39	124.45
8	3	405	BCL	OBB-CAB-CBB	-3.33	112.68	120.17
8	1	401	BCL	C1C-NC-C4C	-3.33	105.21	106.71
8	1	401	BCL	CHA-C1A-NA	-3.33	118.78	126.40
8	6	404	BCL	C16-C15-C13	-3.33	105.16	115.92
8	5	405	BCL	C16-C15-C13	-3.33	105.17	115.92
8	a	812	BCL	C4B-CHC-C1C	-3.32	123.54	130.12
13	A	814	F39	C25-C20-C19	-3.32	109.68	115.27
8	3	402	BCL	C2C-C3C-C4C	-3.32	96.36	101.34
8	a	813	BCL	CMB-C2B-C3B	3.32	130.88	124.68
8	2	402[B]	BCL	C1C-NC-C4C	-3.32	105.22	106.71
8	3	407	BCL	CHA-C1A-NA	-3.32	118.81	126.40
8	a	805	BCL	C1C-NC-C4C	-3.31	105.22	106.71
11	a	802	GS0	C16-C15-C13	-3.31	105.21	115.92
13	A	814	F39	C39-C40-C41	-3.31	112.89	123.22
13	A	815	F39	C27-C32-C35	-3.31	112.89	123.22
8	6	406	BCL	C11-C10-C8	-3.31	105.23	115.92
8	1	402	BCL	C16-C15-C13	-3.31	105.23	115.92
8	1	402	BCL	CHA-C1A-NA	-3.31	118.83	126.40
8	6	402	BCL	CMB-C2B-C3B	3.30	130.86	124.68
8	2	407	BCL	O2A-CGA-O1A	-3.30	115.26	123.59
8	A	806	BCL	C4D-CHA-C1A	3.30	125.27	121.25
8	4	401	BCL	C4B-CHC-C1C	-3.30	123.58	130.12
8	1	404	BCL	C7-C6-C5	-3.30	104.41	113.36
8	4	407	BCL	C4B-CHC-C1C	-3.29	123.60	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	816	F39	C25-C20-C19	-3.29	109.74	115.27
13	A	814	F39	C27-C32-C35	-3.29	112.95	123.22
8	F	101	BCL	CHD-C1D-ND	-3.29	121.43	124.45
8	4	403	BCL	CMB-C2B-C3B	3.29	130.83	124.68
8	6	408	BCL	C16-C15-C13	-3.29	105.30	115.92
8	4	404	BCL	C4D-CHA-C1A	3.29	125.25	121.25
12	A	822	G2O	CMD-C2D-C1D	-3.28	123.42	128.46
8	4	403	BCL	O2A-CGA-O1A	-3.28	115.31	123.59
8	A	811	BCL	CMB-C2B-C3B	3.28	130.82	124.68
8	a	807	BCL	CMA-C3A-C4A	-3.28	102.95	111.77
8	a	813	BCL	CMA-C3A-C4A	-3.28	102.96	111.77
8	a	810	BCL	CMB-C2B-C3B	3.28	130.81	124.68
8	4	403	BCL	CHA-C1A-NA	-3.28	118.89	126.40
8	4	410[B]	BCL	C4B-CHC-C1C	-3.28	123.63	130.12
8	2	403	BCL	C1C-NC-C4C	-3.27	105.23	106.71
8	A	807	BCL	CMB-C2B-C3B	3.27	130.80	124.68
8	1	404	BCL	C16-C15-C13	-3.27	105.35	115.92
8	2	404	BCL	CHA-C1A-NA	-3.27	118.91	126.40
8	A	805	BCL	CMB-C2B-C3B	3.27	130.79	124.68
8	2	406	BCL	C16-C15-C13	-3.27	105.36	115.92
11	A	801	GS0	C4D-CHA-C1A	3.26	125.22	121.25
8	A	812	BCL	CMB-C2B-C3B	3.26	130.78	124.68
8	6	408	BCL	C1C-NC-C4C	-3.26	105.24	106.71
8	A	811	BCL	C4B-CHC-C1C	-3.26	123.66	130.12
8	5	405	BCL	C4D-CHA-C1A	3.26	125.21	121.25
8	a	805	BCL	C4A-NA-C1A	-3.26	105.24	106.71
8	a	806	BCL	CMB-C2B-C3B	3.25	130.77	124.68
8	a	806	BCL	C4A-NA-C1A	-3.25	105.24	106.71
8	a	811	BCL	C16-C15-C13	-3.25	105.41	115.92
12	A	822	G2O	C1-C2-C3	-3.25	120.42	126.04
8	4	403	BCL	CHD-C1D-ND	-3.25	121.47	124.45
8	2	404	BCL	CHD-C1D-ND	-3.25	121.47	124.45
8	4	403	BCL	C16-C15-C13	-3.25	105.42	115.92
8	A	803	BCL	CMB-C2B-C3B	3.24	130.75	124.68
8	A	807	BCL	C2A-C3A-C4A	-3.24	96.63	101.87
8	6	401	BCL	C16-C15-C13	-3.24	105.45	115.92
8	6	401	BCL	C4B-CHC-C1C	-3.24	123.71	130.12
8	5	402	BCL	CHA-C1A-NA	-3.24	118.99	126.40
8	2	404	BCL	O2A-CGA-O1A	-3.24	115.42	123.59
8	a	808	BCL	CMB-C2B-C3B	3.24	130.73	124.68
8	5	401	BCL	C16-C15-C13	-3.23	105.47	115.92
8	6	404	BCL	C7-C6-C5	-3.23	104.58	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	801	G2O	C1-C2-C3	-3.23	120.45	126.04
8	4	406	BCL	C16-C15-C13	-3.23	105.47	115.92
8	2	406	BCL	CHA-C1A-NA	-3.23	119.00	126.40
8	a	809	BCL	C4B-CHC-C1C	-3.23	123.72	130.12
11	A	801	GS0	CMA-C3A-C4A	-3.23	103.10	111.77
8	2	401	BCL	C1C-NC-C4C	-3.23	105.26	106.71
8	4	405	BCL	C1C-NC-C4C	-3.23	105.26	106.71
8	5	402	BCL	O2A-CGA-O1A	-3.22	115.46	123.59
8	A	807	BCL	C1C-NC-C4C	-3.22	105.26	106.71
8	4	401	BCL	C1C-NC-C4C	-3.22	105.26	106.71
8	6	402	BCL	C11-C10-C8	-3.22	105.51	115.92
8	5	401	BCL	C4B-CHC-C1C	-3.22	123.74	130.12
8	a	814	BCL	C4D-CHA-C1A	3.22	125.17	121.25
8	5	406	BCL	C11-C10-C8	-3.22	105.51	115.92
8	1	402	BCL	CGD-CBD-CAD	-3.22	100.31	110.73
8	2	403	BCL	C16-C15-C13	-3.22	105.52	115.92
8	3	405	BCL	C16-C15-C13	-3.22	105.52	115.92
8	6	405	BCL	C16-C15-C13	-3.22	105.52	115.92
8	a	806	BCL	C16-C15-C13	-3.21	105.53	115.92
8	2	403	BCL	C4D-CHA-C1A	3.21	125.16	121.25
8	2	405	BCL	C4D-CHA-C1A	3.21	125.16	121.25
8	2	408	BCL	C16-C15-C13	-3.21	105.53	115.92
8	3	406	BCL	C4B-CHC-C1C	-3.21	123.76	130.12
8	3	402	BCL	CHA-C1A-NA	-3.21	119.05	126.40
8	a	808	BCL	C4D-CHA-C1A	3.21	125.16	121.25
8	4	405	BCL	C7-C6-C5	-3.21	104.65	113.36
8	a	810	BCL	CGD-CBD-CAD	-3.20	100.36	110.73
8	A	809	BCL	CGD-CBD-CAD	-3.20	100.36	110.73
8	5	402	BCL	CMB-C2B-C3B	3.20	130.67	124.68
8	1	408	BCL	C1C-NC-C4C	-3.20	105.27	106.71
8	5	401	BCL	CHA-C1A-NA	-3.20	119.07	126.40
13	C	302	F39	C61-C63-C64	-3.20	113.24	123.22
8	2	405	BCL	C16-C15-C13	-3.20	105.58	115.92
13	C	302	F39	C27-C32-C35	-3.20	113.24	123.22
8	1	402	BCL	CMB-C2B-C3B	3.19	130.65	124.68
8	1	405	BCL	C4D-CHA-C1A	3.19	125.13	121.25
8	5	402	BCL	C16-C15-C13	-3.19	105.60	115.92
8	5	404	BCL	C7-C6-C5	-3.19	104.70	113.36
11	A	801	GS0	C16-C15-C13	-3.18	105.63	115.92
8	6	402	BCL	O2A-CGA-O1A	-3.18	115.56	123.59
8	3	401	BCL	C4B-CHC-C1C	-3.18	123.82	130.12
8	4	403	BCL	C11-C10-C8	-3.18	105.64	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	811	BCL	C4D-CHA-C1A	3.18	125.12	121.25
8	4	406	BCL	C4D-CHA-C1A	3.18	125.11	121.25
8	C	301	BCL	CHA-C1A-NA	-3.17	119.13	126.40
8	A	809	BCL	CMB-C2B-C3B	3.17	130.62	124.68
8	a	804	BCL	CMB-C2B-C3B	3.17	130.61	124.68
8	A	805	BCL	C16-C15-C13	-3.17	105.67	115.92
8	4	409	BCL	C16-C15-C13	-3.17	105.67	115.92
8	2	407	BCL	C4A-NA-C1A	-3.17	105.28	106.71
8	3	401	BCL	C4D-CHA-C1A	3.17	125.11	121.25
8	a	806	BCL	C1C-NC-C4C	-3.17	105.28	106.71
8	6	401	BCL	C4D-CHA-C1A	3.17	125.10	121.25
8	5	403	BCL	C4D-CHA-C1A	3.17	125.10	121.25
8	6	402	BCL	C2C-C3C-C4C	-3.16	96.60	101.34
8	3	403	BCL	C4B-CHC-C1C	-3.16	123.85	130.12
8	2	407	BCL	C16-C15-C13	-3.16	105.71	115.92
8	2	401	BCL	CHA-C1A-NA	-3.16	119.17	126.40
8	2	406	BCL	C7-C6-C5	-3.16	104.78	113.36
8	3	402	BCL	CMB-C2B-C3B	3.15	130.58	124.68
8	6	402	BCL	CHA-C1A-NA	-3.15	119.18	126.40
8	4	402	BCL	CHA-C1A-NA	-3.15	119.18	126.40
8	3	406	BCL	C16-C15-C13	-3.15	105.73	115.92
8	1	406	BCL	C11-C10-C8	-3.15	105.74	115.92
8	5	406	BCL	C4B-CHC-C1C	-3.15	123.88	130.12
8	2	401	BCL	C16-C15-C13	-3.15	105.74	115.92
8	a	811	BCL	O2A-CGA-O1A	-3.15	115.65	123.59
8	1	401	BCL	C16-C15-C13	-3.15	105.75	115.92
8	3	406	BCL	C11-C10-C8	-3.14	105.76	115.92
8	3	402	BCL	CHD-C1D-ND	-3.14	121.57	124.45
8	5	405	BCL	C11-C10-C8	-3.14	105.77	115.92
8	A	807	BCL	C11-C10-C8	-3.14	105.77	115.92
8	5	403	BCL	C7-C6-C5	-3.13	104.84	113.36
8	1	408	BCL	CHA-C1A-NA	-3.13	119.23	126.40
8	A	808	BCL	C4B-CHC-C1C	-3.12	123.93	130.12
8	1	402	BCL	O2A-CGA-O1A	-3.12	115.71	123.59
12	a	801	G2O	O2D-CGD-O1D	-3.12	117.73	123.84
8	1	407[B]	BCL	C4B-CHC-C1C	-3.12	123.94	130.12
8	2	407	BCL	CHA-C1A-NA	-3.12	119.25	126.40
8	a	805	BCL	C4D-CHA-C1A	3.12	125.04	121.25
8	5	402	BCL	C11-C10-C8	-3.12	105.84	115.92
11	a	802	GS0	C3D-C2D-C1D	-3.11	101.58	105.83
8	c	301	BCL	CMA-C3A-C4A	-3.11	103.41	111.77
8	6	405	BCL	C11-C10-C8	-3.11	105.86	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	806	BCL	C4D-CHA-C1A	3.11	125.03	121.25
8	a	813	BCL	C1B-CHB-C4A	-3.11	123.96	130.12
8	A	806	BCL	CHA-C1A-NA	-3.11	119.28	126.40
8	2	404	BCL	C11-C10-C8	-3.11	105.87	115.92
8	1	402	BCL	CHD-C1D-ND	-3.11	121.60	124.45
8	a	814	BCL	CHA-C1A-NA	-3.10	119.29	126.40
8	4	404	BCL	C16-C15-C13	-3.10	105.89	115.92
8	A	811	BCL	C7-C6-C5	-3.10	104.94	113.36
8	1	405	BCL	C11-C10-C8	-3.10	105.89	115.92
8	6	405	BCL	CHA-C1A-NA	-3.10	119.30	126.40
8	2	407	BCL	C11-C10-C8	-3.10	105.90	115.92
8	2	407	BCL	C4B-CHC-C1C	-3.10	123.98	130.12
8	3	407	BCL	C11-C10-C8	-3.10	105.90	115.92
8	2	409[B]	BCL	C4B-CHC-C1C	-3.09	123.99	130.12
8	6	408	BCL	CHA-C1A-NA	-3.09	119.32	126.40
8	1	405	BCL	O2A-CGA-O1A	-3.09	115.79	123.59
12	A	822	G2O	O2D-CGD-O1D	-3.09	117.80	123.84
8	2	408	BCL	C4B-CHC-C1C	-3.09	124.01	130.12
8	1	408	BCL	C16-C15-C13	-3.08	105.95	115.92
8	4	402	BCL	C4B-CHC-C1C	-3.08	124.01	130.12
8	3	405	BCL	CMA-C3A-C4A	-3.08	103.49	111.77
8	2	404	BCL	C4D-CHA-C1A	3.08	125.00	121.25
8	5	406	BCL	C16-C15-C13	-3.08	105.97	115.92
8	4	406	BCL	O2A-CGA-O1A	-3.08	115.82	123.59
8	6	406	BCL	C4B-CHC-C1C	-3.08	124.02	130.12
8	a	807	BCL	CHA-C1A-NA	-3.08	119.36	126.40
8	6	403	BCL	C16-C15-C13	-3.07	105.98	115.92
8	1	406	BCL	C4B-CHC-C1C	-3.07	124.03	130.12
8	3	402	BCL	C4B-CHC-C1C	-3.07	124.03	130.12
8	F	101	BCL	C4D-CHA-C1A	3.07	124.98	121.25
8	6	408	BCL	C4B-CHC-C1C	-3.06	124.05	130.12
8	4	406	BCL	C11-C10-C8	-3.06	106.02	115.92
8	C	301	BCL	C4B-CHC-C1C	-3.06	124.05	130.12
8	1	402	BCL	C4B-CHC-C1C	-3.06	124.06	130.12
8	a	808	BCL	C16-C15-C13	-3.06	106.03	115.92
8	a	808	BCL	CMA-C3A-C4A	-3.06	103.55	111.77
8	4	403	BCL	CGD-CBD-CAD	-3.06	100.83	110.73
8	1	402	BCL	C3D-C2D-C1D	-3.06	101.66	105.83
8	A	813	BCL	CMD-C2D-C1D	3.06	130.10	124.71
8	3	402	BCL	C11-C10-C8	-3.06	106.04	115.92
8	a	804	BCL	O2A-CGA-O1A	-3.05	115.69	123.30
8	4	402	BCL	C11-C10-C8	-3.05	106.05	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	404	BCL	CMB-C2B-C3B	3.05	130.39	124.68
8	A	804	BCL	C4B-CHC-C1C	-3.05	124.07	130.12
8	3	405	BCL	O2A-CGA-O1A	-3.05	115.89	123.59
8	4	407	BCL	C16-C15-C13	-3.05	106.06	115.92
8	A	805	BCL	O2A-CGA-O1A	-3.05	115.90	123.59
8	A	810	BCL	O2A-CGA-O1A	-3.05	115.90	123.59
8	6	404	BCL	C4D-CHA-C1A	3.05	124.95	121.25
8	1	402	BCL	C11-C10-C8	-3.05	106.08	115.92
8	1	403	BCL	C1C-NC-C4C	-3.05	105.34	106.71
8	4	410[B]	BCL	CHA-C1A-NA	-3.04	119.43	126.40
8	2	405	BCL	C4B-CHC-C1C	-3.04	124.09	130.12
8	2	409[B]	BCL	CHA-C1A-NA	-3.04	119.43	126.40
8	A	813	BCL	C4B-CHC-C1C	-3.04	124.09	130.12
8	6	408	BCL	C11-C10-C8	-3.04	106.09	115.92
12	a	801	G2O	CMD-C2D-C1D	-3.04	123.80	128.46
8	3	404	BCL	CHA-C1A-NA	-3.03	119.45	126.40
8	3	401	BCL	C3D-C2D-C1D	-3.03	101.70	105.83
8	6	402	BCL	CHD-C1D-ND	-3.03	121.67	124.45
8	a	812	BCL	O2A-CGA-O1A	-3.03	115.95	123.59
8	A	807	BCL	CMA-C3A-C4A	-3.03	103.64	111.77
8	c	301	BCL	CHA-C1A-NA	-3.03	119.47	126.40
8	1	406	BCL	C16-C15-C13	-3.03	106.14	115.92
8	6	403	BCL	C4D-CHA-C1A	3.02	124.93	121.25
8	2	401	BCL	C4B-CHC-C1C	-3.02	124.13	130.12
8	4	408[B]	BCL	C1C-NC-C4C	-3.02	105.35	106.71
8	1	403	BCL	C4D-CHA-C1A	3.02	124.93	121.25
8	6	407[B]	BCL	C4B-CHC-C1C	-3.02	124.13	130.12
8	5	403	BCL	CHA-C1A-NA	-3.02	119.48	126.40
8	a	812	BCL	C2A-C3A-C4A	-3.02	96.99	101.87
8	1	408	BCL	C4B-CHC-C1C	-3.02	124.13	130.12
8	A	812	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
8	1	401	BCL	C4D-CHA-C1A	3.02	124.92	121.25
8	a	808	BCL	CHA-C1A-NA	-3.02	119.48	126.40
8	a	812	BCL	C4A-NA-C1A	-3.02	105.35	106.71
8	3	404	BCL	C4D-CHA-C1A	3.02	124.92	121.25
8	F	101	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
8	a	811	BCL	C11-C10-C8	-3.01	106.18	115.92
8	c	301	BCL	C4B-CHC-C1C	-3.01	124.15	130.12
8	4	401	BCL	C7-C6-C5	-3.01	105.18	113.36
8	4	401	BCL	C3D-C2D-C1D	-3.01	101.72	105.83
8	3	405	BCL	C11-C10-C8	-3.01	106.19	115.92
8	6	402	BCL	C4B-CHC-C1C	-3.01	124.16	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	5	402	BCL	CGD-CBD-CAD	-3.01	100.99	110.73
11	a	802	GS0	CHA-C1A-NA	-3.01	119.51	126.40
8	4	402	BCL	C16-C15-C13	-3.01	106.20	115.92
8	5	406	BCL	C4D-CHA-C1A	3.01	124.91	121.25
8	3	407	BCL	C16-C15-C13	-3.00	106.21	115.92
8	3	407	BCL	C4B-CHC-C1C	-3.00	124.17	130.12
8	A	811	BCL	C2A-C3A-C4A	-3.00	97.02	101.87
8	A	807	BCL	CHA-C1A-NA	-3.00	119.52	126.40
8	a	812	BCL	CMA-C3A-C4A	-3.00	103.70	111.77
8	2	402[B]	BCL	CHA-C1A-NA	-3.00	119.53	126.40
8	4	405	BCL	CHA-C1A-NA	-3.00	119.54	126.40
8	5	405	BCL	CHA-C1A-NA	-3.00	119.54	126.40
8	1	408	BCL	C11-C10-C8	-3.00	106.23	115.92
8	3	403	BCL	C16-C15-C13	-3.00	106.24	115.92
8	a	805	BCL	C7-C6-C5	-2.99	105.23	113.36
8	2	401	BCL	O2A-CGA-O1A	-2.99	116.04	123.59
8	A	807	BCL	C4D-CHA-C1A	2.99	124.89	121.25
8	a	805	BCL	CHA-C1A-NA	-2.99	119.55	126.40
8	4	403	BCL	C2C-C3C-C4C	-2.99	96.86	101.34
8	5	401	BCL	C3D-C2D-C1D	-2.99	101.75	105.83
11	A	801	GS0	CHA-C1A-NA	-2.99	119.55	126.40
12	A	822	G2O	CMD-C2D-C3D	2.99	130.26	124.68
8	1	407[B]	BCL	CHA-C1A-NA	-2.98	119.56	126.40
8	3	403	BCL	C11-C10-C8	-2.98	106.28	115.92
8	a	807	BCL	C3D-C2D-C1D	-2.98	101.77	105.83
8	6	403	BCL	C3D-C2D-C1D	-2.98	101.77	105.83
8	A	810	BCL	C4A-NA-C1A	-2.98	105.37	106.71
8	2	402[B]	BCL	C4B-CHC-C1C	-2.98	124.22	130.12
8	A	805	BCL	C4D-CHA-C1A	2.98	124.87	121.25
8	4	404	BCL	C7-C6-C5	-2.98	105.28	113.36
8	4	403	BCL	C4B-CHC-C1C	-2.97	124.23	130.12
8	A	811	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
8	4	408[B]	BCL	CHA-C1A-NA	-2.97	119.59	126.40
8	a	806	BCL	C11-C10-C8	-2.97	106.32	115.92
8	5	405	BCL	C4B-CHC-C1C	-2.97	124.24	130.12
8	a	809	BCL	C4D-CHA-C1A	2.97	124.86	121.25
8	2	406	BCL	C4B-CHC-C1C	-2.96	124.25	130.12
8	4	406	BCL	C1B-CHB-C4A	-2.96	124.25	130.12
8	a	813	BCL	C2A-C3A-C4A	-2.96	97.08	101.87
8	2	406	BCL	C1C-NC-C4C	-2.96	105.37	106.71
8	a	811	BCL	CHA-C1A-NA	-2.96	119.62	126.40
8	A	805	BCL	CHA-C1A-NA	-2.96	119.63	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	5	402	BCL	C3D-C2D-C1D	-2.95	101.80	105.83
8	A	813	BCL	C2A-C1A-CHA	2.95	129.03	123.86
8	3	405	BCL	C1B-CHB-C4A	-2.95	124.27	130.12
8	4	409	BCL	C7-C6-C5	-2.95	105.35	113.36
8	a	814	BCL	O2A-CGA-O1A	-2.95	115.95	123.30
8	4	404	BCL	C11-C10-C8	-2.95	106.40	115.92
8	5	405	BCL	O2A-CGA-O1A	-2.94	116.16	123.59
8	2	405	BCL	C11-C10-C8	-2.94	106.40	115.92
8	A	808	BCL	C4D-CHA-C1A	2.94	124.83	121.25
8	a	806	BCL	CHA-C1A-NA	-2.94	119.66	126.40
8	6	404	BCL	C4B-CHC-C1C	-2.94	124.29	130.12
8	C	301	BCL	C3D-C2D-C1D	-2.94	101.82	105.83
8	5	405	BCL	C7-C6-C5	-2.94	105.37	113.36
8	4	409	BCL	C4B-CHC-C1C	-2.94	124.29	130.12
8	4	409	BCL	C11-C10-C8	-2.94	106.41	115.92
8	1	401	BCL	C3D-C2D-C1D	-2.94	101.82	105.83
8	5	403	BCL	C4B-CHC-C1C	-2.94	124.30	130.12
8	A	810	BCL	CHA-C1A-NA	-2.94	119.67	126.40
8	1	403	BCL	C16-C15-C13	-2.94	106.43	115.92
8	4	405	BCL	C11-C10-C8	-2.94	106.43	115.92
8	1	403	BCL	C11-C10-C8	-2.93	106.44	115.92
8	4	406	BCL	CHA-C1A-NA	-2.93	119.68	126.40
8	4	403	BCL	C4D-CHA-C1A	2.93	124.82	121.25
8	6	403	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
8	3	405	BCL	C3D-C2D-C1D	-2.93	101.83	105.83
8	1	403	BCL	C7-C6-C5	-2.93	105.40	113.36
8	1	405	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
8	a	805	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
8	6	407[B]	BCL	CHA-C1A-NA	-2.93	119.69	126.40
8	6	406	BCL	O2A-CGA-O1A	-2.93	116.20	123.59
8	6	401	BCL	C3D-C2D-C1D	-2.93	101.83	105.83
8	a	808	BCL	C7-C6-C5	-2.93	105.41	113.36
8	2	405	BCL	C7-C6-C5	-2.93	105.41	113.36
8	5	404	BCL	C4D-CHA-C1A	2.92	124.81	121.25
8	4	405	BCL	C4B-CHC-C1C	-2.92	124.33	130.12
8	a	806	BCL	O2A-CGA-O1A	-2.92	116.21	123.59
8	6	405	BCL	C7-C6-C5	-2.92	105.43	113.36
8	A	806	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
8	3	405	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
8	a	814	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
8	1	403	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
8	A	807	BCL	C7-C6-C5	-2.92	105.44	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	404	BCL	C4B-CHC-C1C	-2.91	124.35	130.12
17	a	815	F26	C38-C39-C37	-2.91	117.51	123.47
8	4	410[B]	BCL	CGD-CBD-CAD	-2.91	101.30	110.73
8	a	809	BCL	O2A-CGA-O1A	-2.91	116.04	123.30
8	A	803	BCL	CHA-C1A-NA	-2.91	119.73	126.40
8	A	804	BCL	CHA-C1A-NA	-2.91	119.73	126.40
8	a	810	BCL	CMD-C2D-C1D	2.91	129.84	124.71
8	5	406	BCL	CHA-C1A-NA	-2.91	119.74	126.40
8	A	809	BCL	C4D-CHA-C1A	2.91	124.78	121.25
8	5	403	BCL	C16-C15-C13	-2.90	106.53	115.92
8	3	405	BCL	CHA-C1A-NA	-2.90	119.75	126.40
8	a	804	BCL	C4B-CHC-C1C	-2.90	124.37	130.12
8	a	809	BCL	C1C-NC-C4C	-2.90	105.40	106.71
8	2	404	BCL	C4B-CHC-C1C	-2.90	124.38	130.12
8	3	401	BCL	O2A-CGA-O1A	-2.90	116.28	123.59
8	1	405	BCL	CHA-C1A-NA	-2.90	119.76	126.40
8	3	404	BCL	C4B-CHC-C1C	-2.90	124.38	130.12
8	1	404	BCL	O2A-CGA-O1A	-2.90	116.28	123.59
8	A	808	BCL	CHA-C1A-NA	-2.90	119.77	126.40
8	6	406	BCL	C11-C12-C13	-2.90	106.56	115.92
8	a	806	BCL	C7-C6-C5	-2.89	105.50	113.36
8	a	809	BCL	CHA-C1A-NA	-2.89	119.77	126.40
8	1	406	BCL	C7-C6-C5	-2.89	105.50	113.36
8	2	401	BCL	C11-C10-C8	-2.89	106.57	115.92
8	2	408	BCL	CHA-C1A-NA	-2.89	119.77	126.40
8	4	408[B]	BCL	C4B-CHC-C1C	-2.89	124.39	130.12
8	6	404	BCL	CHA-C1A-NA	-2.89	119.77	126.40
8	6	402	BCL	C4D-CHA-C1A	2.89	124.77	121.25
8	6	403	BCL	C7-C6-C5	-2.89	105.51	113.36
8	A	805	BCL	CMD-C2D-C1D	2.89	129.81	124.71
17	c	302	F26	C27-C28-C31	-2.89	118.30	126.42
8	5	404	BCL	CHA-C1A-NA	-2.89	119.78	126.40
8	3	405	BCL	C7-C6-C5	-2.89	105.51	113.36
8	A	811	BCL	CHA-C1A-NA	-2.89	119.79	126.40
8	A	809	BCL	O2A-CGA-O1A	-2.89	116.11	123.30
11	A	801	GS0	C3D-C2D-C1D	-2.88	101.89	105.83
8	5	404	BCL	C4B-CHC-C1C	-2.88	124.41	130.12
8	2	401	BCL	C4D-CHA-C1A	2.88	124.75	121.25
8	5	402	BCL	CHD-C1D-ND	-2.88	121.81	124.45
8	5	406	BCL	O2A-CGA-O1A	-2.88	116.33	123.59
8	A	804	BCL	C4D-CHA-C1A	2.88	124.75	121.25
8	4	406	BCL	C7-C6-C5	-2.88	105.54	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	408	BCL	C7-C6-C5	-2.88	105.54	113.36
17	a	815	F26	C39-C37-C34	-2.88	123.20	127.31
8	5	406	BCL	C3D-C2D-C1D	-2.88	101.90	105.83
8	C	301	BCL	CMA-C3A-C4A	-2.88	104.04	111.77
8	2	403	BCL	C3D-C2D-C1D	-2.87	101.91	105.83
8	A	806	BCL	C3D-C2D-C1D	-2.87	101.91	105.83
8	A	811	BCL	C16-C15-C13	-2.87	106.63	115.92
8	a	810	BCL	C4D-CHA-C1A	2.87	124.75	121.25
8	6	402	BCL	C3D-C2D-C1D	-2.87	101.91	105.83
8	a	811	BCL	C7-C6-C5	-2.87	105.56	113.36
8	a	808	BCL	C4B-CHC-C1C	-2.87	124.43	130.12
8	4	409	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
8	2	405	BCL	O2A-CGA-O1A	-2.87	116.35	123.59
8	5	402	BCL	C4B-CHC-C1C	-2.87	124.44	130.12
8	3	405	BCL	C4D-CHA-C1A	2.87	124.74	121.25
8	3	406	BCL	CHA-C1A-NA	-2.86	119.84	126.40
8	1	404	BCL	C11-C10-C8	-2.86	106.66	115.92
8	4	402	BCL	C7-C6-C5	-2.86	105.58	113.36
8	6	402	BCL	CGD-CBD-CAD	-2.86	101.46	110.73
11	A	801	GS0	O2A-CGA-O1A	-2.86	116.37	123.59
11	a	802	GS0	O2A-CGA-O1A	-2.86	116.37	123.59
8	a	812	BCL	CHA-C1A-NA	-2.86	119.85	126.40
8	C	301	BCL	O2A-CGA-O1A	-2.86	116.17	123.30
8	4	407	BCL	CHA-C1A-NA	-2.86	119.85	126.40
8	3	403	BCL	CHA-C1A-NA	-2.86	119.85	126.40
8	A	808	BCL	O2A-CGA-O1A	-2.86	116.17	123.30
8	2	407	BCL	C7-C6-C5	-2.86	105.60	113.36
8	1	404	BCL	CHA-C1A-NA	-2.86	119.86	126.40
8	5	405	BCL	C3D-C2D-C1D	-2.86	101.93	105.83
8	A	812	BCL	CMA-C3A-C4A	-2.86	104.09	111.77
8	1	406	BCL	CHA-C1A-NA	-2.86	119.86	126.40
8	4	403	BCL	C7-C6-C5	-2.85	105.61	113.36
8	a	807	BCL	O2A-CGA-O1A	-2.85	116.18	123.30
8	2	408	BCL	C7-C6-C5	-2.85	105.61	113.36
8	4	403	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
8	1	405	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
8	4	409	BCL	C4D-CHA-C1A	2.85	124.72	121.25
8	3	406	BCL	C7-C6-C5	-2.85	105.61	113.36
8	A	808	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
8	A	806	BCL	CMC-C2C-C3C	-2.85	102.33	113.83
8	1	402	BCL	C4D-CHA-C1A	2.85	124.72	121.25
8	6	403	BCL	CHA-C1A-NA	-2.85	119.88	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	811	BCL	CMA-C3A-C4A	-2.85	104.12	111.77
8	2	405	BCL	CHA-C1A-NA	-2.85	119.88	126.40
8	4	406	BCL	C4B-CHC-C1C	-2.84	124.48	130.12
8	1	402	BCL	C7-C6-C5	-2.84	105.64	113.36
8	a	809	BCL	C3D-C2D-C1D	-2.84	101.95	105.83
8	4	408[B]	BCL	O2A-CGA-O1A	-2.84	116.21	123.30
8	3	401	BCL	C16-C15-C13	-2.84	106.73	115.92
8	3	402	BCL	O2A-CGA-O1A	-2.84	116.42	123.59
8	A	810	BCL	C4B-CHC-C1C	-2.84	124.49	130.12
8	2	406	BCL	C11-C10-C8	-2.84	106.74	115.92
8	6	406	BCL	CHA-C1A-NA	-2.84	119.90	126.40
8	3	402	BCL	CGD-CBD-CAD	-2.84	101.54	110.73
8	A	810	BCL	C4D-CHA-C1A	2.84	124.70	121.25
8	6	403	BCL	C11-C10-C8	-2.83	106.76	115.92
8	A	810	BCL	C11-C10-C8	-2.83	106.77	115.92
8	6	407[B]	BCL	O2A-CGA-O1A	-2.83	116.25	123.30
8	5	404	BCL	C1C-NC-C4C	-2.83	105.43	106.71
8	2	405	BCL	C3D-C2D-C1D	-2.83	101.97	105.83
8	3	404	BCL	C7-C6-C5	-2.83	105.68	113.36
8	4	404	BCL	C4B-CHC-C1C	-2.83	124.52	130.12
8	3	402	BCL	C4D-CHA-C1A	2.83	124.69	121.25
8	6	401	BCL	O2A-CGA-O1A	-2.83	116.46	123.59
8	3	403	BCL	C7-C6-C5	-2.82	105.69	113.36
8	2	407	BCL	C3D-C2D-C1D	-2.82	101.98	105.83
8	1	406	BCL	C11-C12-C13	-2.82	106.79	115.92
8	a	806	BCL	CMD-C2D-C1D	2.82	129.69	124.71
8	6	405	BCL	C4B-CHC-C1C	-2.82	124.53	130.12
8	5	404	BCL	C11-C10-C8	-2.82	106.80	115.92
8	2	408	BCL	O2A-CGA-O1A	-2.82	116.47	123.59
8	a	804	BCL	CMA-C3A-C4A	-2.82	104.19	111.77
8	2	402[B]	BCL	CGD-CBD-CAD	-2.82	101.60	110.73
8	2	406	BCL	C3D-C2D-C1D	-2.82	101.98	105.83
8	A	811	BCL	C3D-C2D-C1D	-2.82	101.98	105.83
8	4	409	BCL	CMC-C2C-C3C	-2.82	102.46	113.83
8	A	804	BCL	C7-C6-C5	-2.82	105.71	113.36
8	4	404	BCL	CHA-C1A-NA	-2.82	119.95	126.40
8	1	403	BCL	C3D-C2D-C1D	-2.82	101.99	105.83
8	4	406	BCL	CMA-C3A-C4A	-2.81	104.21	111.77
8	2	404	BCL	C2C-C3C-C4C	-2.81	97.13	101.34
8	6	403	BCL	O2A-CGA-O1A	-2.81	116.50	123.59
8	3	404	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
12	a	803	G2O	O2D-CGD-O1D	-2.81	118.35	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	811	BCL	C4B-CHC-C1C	-2.81	124.56	130.12
8	6	401	BCL	C7-C6-C5	-2.81	105.74	113.36
8	4	405	BCL	O2A-CGA-O1A	-2.81	116.51	123.59
14	A	816	LHG	O8-C23-C24	2.81	120.71	111.91
8	6	406	BCL	C16-C15-C13	-2.81	106.85	115.92
14	a	821	LHG	O8-C23-C24	2.80	120.71	111.91
8	a	806	BCL	C3D-C2D-C1D	-2.80	102.00	105.83
8	a	806	BCL	C4B-CHC-C1C	-2.80	124.57	130.12
8	A	812	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
8	2	409[B]	BCL	CGD-CBD-CAD	-2.80	101.66	110.73
8	2	401	BCL	C7-C6-C5	-2.80	105.76	113.36
8	5	401	BCL	C11-C12-C13	-2.80	106.87	115.92
8	5	406	BCL	CMC-C2C-C3C	-2.80	102.54	113.83
8	4	407	BCL	C7-C6-C5	-2.80	105.76	113.36
8	a	806	BCL	C11-C12-C13	-2.80	106.88	115.92
8	a	805	BCL	CMC-C2C-C3C	-2.80	102.55	113.83
8	5	403	BCL	C3D-C2D-C1D	-2.80	102.02	105.83
8	A	813	BCL	O2A-CGA-O1A	-2.79	116.33	123.30
8	a	812	BCL	C4D-CHA-C1A	2.79	124.65	121.25
8	A	812	BCL	O2A-CGA-O1A	-2.79	116.34	123.30
8	6	405	BCL	O2A-CGA-O1A	-2.79	116.54	123.59
8	A	810	BCL	C3D-C2D-C1D	-2.79	102.02	105.83
11	a	802	GS0	CMC-C2C-C3C	-2.79	102.56	113.83
8	3	403	BCL	C4D-CHA-C1A	2.79	124.65	121.25
8	1	403	BCL	CHA-C1A-NA	-2.79	120.01	126.40
8	3	407	BCL	C7-C6-C5	-2.79	105.78	113.36
8	A	805	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
8	F	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
8	5	402	BCL	C4D-CHA-C1A	2.79	124.64	121.25
8	5	401	BCL	O2A-CGA-O1A	-2.79	116.55	123.59
8	a	811	BCL	C11-C12-C13	-2.79	106.91	115.92
8	a	807	BCL	C4B-CHC-C1C	-2.79	124.60	130.12
8	A	812	BCL	CHA-C1A-NA	-2.79	120.02	126.40
8	5	405	BCL	CMC-C2C-C3C	-2.79	102.59	113.83
8	4	404	BCL	O2A-CGA-O1A	-2.78	116.56	123.59
8	2	403	BCL	O2A-CGA-O1A	-2.78	116.57	123.59
14	A	819	LHG	O8-C23-C24	2.78	120.63	111.91
8	3	402	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	a	808	BCL	C11-C10-C8	-2.78	106.94	115.92
8	A	805	BCL	CMC-C2C-C3C	-2.78	102.62	113.83
14	a	819	LHG	O8-C23-C24	2.78	120.63	111.91
8	3	402	BCL	C16-C15-C13	-2.78	106.94	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	812	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	a	813	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
11	a	802	GS0	C4D-CHA-C1A	2.77	124.62	121.25
8	5	403	BCL	O2A-CGA-O1A	-2.77	116.59	123.59
8	1	406	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	a	804	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	A	803	BCL	O2A-CGA-O1A	-2.77	116.39	123.30
8	2	404	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	6	406	BCL	C7-C6-C5	-2.77	105.84	113.36
8	1	408	BCL	C2A-C1A-CHA	2.77	128.70	123.86
8	a	814	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	6	406	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
11	a	802	GS0	C11-C10-C8	-2.77	106.97	115.92
8	A	807	BCL	C4B-CHC-C1C	-2.77	124.64	130.12
8	6	408	BCL	C4D-CHA-C1A	2.77	124.61	121.25
8	3	406	BCL	O2A-CGA-O1A	-2.76	116.61	123.59
8	1	401	BCL	C2A-C1A-CHA	2.76	128.69	123.86
8	5	404	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
8	a	813	BCL	CHA-C1A-NA	-2.76	120.07	126.40
8	5	401	BCL	C4D-CHA-C1A	2.76	124.61	121.25
8	4	407	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
8	A	807	BCL	CMC-C2C-C3C	-2.76	102.71	113.83
8	A	803	BCL	C4B-CHC-C1C	-2.76	124.66	130.12
8	a	807	BCL	CMD-C2D-C1D	2.76	129.57	124.71
8	2	408	BCL	C3D-C2D-C1D	-2.75	102.07	105.83
8	6	404	BCL	C3D-C2D-C1D	-2.75	102.07	105.83
8	1	401	BCL	O2A-CGA-O1A	-2.75	116.64	123.59
8	2	404	BCL	C7-C6-C5	-2.75	105.89	113.36
8	4	410[B]	BCL	O2A-CGA-O1A	-2.75	116.44	123.30
8	a	808	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	A	809	BCL	CMD-C2D-C1D	2.75	129.56	124.71
8	a	804	BCL	CHA-C1A-NA	-2.75	120.10	126.40
8	3	404	BCL	C11-C10-C8	-2.75	107.03	115.92
8	1	404	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	3	403	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	A	806	BCL	O2A-CGA-O1A	-2.75	116.45	123.30
8	1	407[B]	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	3	406	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
11	A	801	GS0	C11-C10-C8	-2.74	107.05	115.92
8	2	402[B]	BCL	CMA-C3A-C4A	-2.74	104.40	111.77
8	1	405	BCL	CMA-C3A-C4A	-2.74	104.40	111.77
8	4	409	BCL	O2A-CGA-O1A	-2.74	116.67	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	4	405	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	3	406	BCL	C11-C12-C13	-2.74	107.06	115.92
11	A	801	GS0	C1C-NC-C4C	-2.74	105.48	106.71
11	a	802	GS0	C1C-NC-C4C	-2.74	105.48	106.71
8	2	401	BCL	C3D-C2D-C1D	-2.74	102.10	105.83
8	a	813	BCL	O2A-CGA-O1A	-2.74	116.48	123.30
8	5	401	BCL	C1B-CHB-C4A	-2.73	124.70	130.12
8	4	406	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
8	6	408	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
8	6	406	BCL	C4D-CHA-C1A	2.73	124.57	121.25
8	6	404	BCL	C11-C10-C8	-2.73	107.09	115.92
8	4	409	BCL	C11-C12-C13	-2.73	107.10	115.92
13	C	302	F39	O6-C21-C22	2.73	120.46	111.91
8	6	405	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	2	404	BCL	CGD-CBD-CAD	-2.72	101.91	110.73
8	a	805	BCL	C3D-C2D-C1D	-2.72	102.11	105.83
12	a	801	G2O	CMD-C2D-C3D	2.72	129.77	124.68
8	a	810	BCL	C4B-CHC-C1C	-2.72	124.73	130.12
8	6	408	BCL	C7-C6-C5	-2.72	105.97	113.36
8	3	403	BCL	O2A-CGA-O1A	-2.72	116.73	123.59
8	4	407	BCL	O2A-CGA-O1A	-2.72	116.73	123.59
8	a	808	BCL	O2A-CGA-O1A	-2.72	116.73	123.59
8	A	803	BCL	C2A-C3A-C4A	-2.72	97.48	101.87
8	5	405	BCL	CMA-C3A-C4A	-2.72	104.47	111.77
8	1	408	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
8	4	404	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
8	4	407	BCL	CMC-C2C-C3C	-2.72	102.88	113.83
8	c	301	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
8	A	810	BCL	C7-C6-C5	-2.71	105.99	113.36
13	a	816	F39	O6-C21-C22	2.71	120.43	111.91
8	2	409[B]	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
8	5	404	BCL	C11-C12-C13	-2.71	107.16	115.92
8	3	406	BCL	CMC-C2C-C3C	-2.71	102.89	113.83
8	1	406	BCL	O2A-CGA-O1A	-2.71	116.75	123.59
8	6	407[B]	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
8	4	402	BCL	O2A-CGA-O1A	-2.71	116.75	123.59
8	a	812	BCL	C7-C6-C5	-2.71	106.00	113.36
8	2	402[B]	BCL	O2A-CGA-O1A	-2.71	116.55	123.30
8	2	407	BCL	CMA-C3A-C4A	-2.71	104.50	111.77
8	a	806	BCL	CMC-C2C-C3C	-2.71	102.91	113.83
8	c	301	BCL	O2A-CGA-O1A	-2.71	116.56	123.30
8	6	407[B]	BCL	C1C-NC-C4C	-2.70	105.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	804	BCL	O2A-CGA-O1A	-2.70	116.77	123.59
8	1	404	BCL	CMC-C2C-C3C	-2.70	102.93	113.83
8	3	401	BCL	CMC-C2C-C3C	-2.70	102.94	113.83
17	c	302	F26	C38-C39-C37	-2.69	117.95	123.47
8	3	404	BCL	CMC-C2C-C3C	-2.69	102.96	113.83
8	4	408[B]	BCL	C3D-C2D-C1D	-2.69	102.15	105.83
14	a	817	LHG	O8-C23-C24	2.69	120.36	111.91
8	2	406	BCL	O2A-CGA-O1A	-2.69	116.80	123.59
8	3	402	BCL	C7-C6-C5	-2.69	106.05	113.36
8	4	401	BCL	CMC-C2C-C3C	-2.69	102.97	113.83
11	a	802	GS0	C2A-C3A-C4A	-2.69	97.53	101.87
8	A	804	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
8	3	407	BCL	O2A-CGA-O1A	-2.69	116.81	123.59
8	6	408	BCL	C2A-C1A-CHA	2.69	128.56	123.86
8	4	401	BCL	O2A-CGA-O1A	-2.69	116.81	123.59
8	a	811	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
8	2	408	BCL	CMC-C2C-C3C	-2.69	102.99	113.83
8	1	401	BCL	C11-C10-C8	-2.68	107.25	115.92
8	A	807	BCL	O2A-CGA-O1A	-2.68	116.82	123.59
8	2	406	BCL	CMC-C2C-C3C	-2.68	103.01	113.83
8	4	402	BCL	C3D-C2D-C1D	-2.68	102.17	105.83
8	4	405	BCL	C4D-CHA-C1A	2.68	124.51	121.25
8	4	401	BCL	C11-C10-C8	-2.68	107.25	115.92
8	4	408[B]	BCL	CMC-C2C-C3C	-2.68	103.02	113.83
14	A	818	LHG	O8-C23-C24	2.68	120.31	111.91
13	A	814	F39	O6-C21-C22	2.67	120.30	111.91
8	1	406	BCL	CMC-C2C-C3C	-2.67	103.04	113.83
8	A	803	BCL	C3D-C2D-C1D	-2.67	102.18	105.83
8	A	807	BCL	C3D-C2D-C1D	-2.67	102.18	105.83
8	A	805	BCL	C4A-NA-C1A	-2.67	105.50	106.71
12	A	802	G2O	O2D-CGD-O1D	-2.67	118.61	123.84
8	a	810	BCL	O2A-CGA-O1A	-2.67	116.64	123.30
8	1	403	BCL	O2A-CGA-O1A	-2.67	116.85	123.59
8	A	803	BCL	CMC-C2C-C3C	-2.67	103.05	113.83
8	6	402	BCL	C7-C6-C5	-2.67	106.10	113.36
8	5	406	BCL	CMD-C2D-C1D	2.67	129.42	124.71
8	F	101	BCL	CMC-C2C-C3C	-2.67	103.05	113.83
11	A	801	GS0	C4B-CHC-C1C	-2.67	124.83	130.12
8	4	410[B]	BCL	CMA-C3A-C4A	-2.67	104.60	111.77
8	A	805	BCL	C4B-CHC-C1C	-2.67	124.83	130.12
8	3	407	BCL	C3D-C2D-C1D	-2.67	102.19	105.83
8	A	809	BCL	C2C-C3C-C4C	-2.67	97.34	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	808	BCL	C11-C12-C13	-2.67	107.30	115.92
8	a	808	BCL	CMC-C2C-C3C	-2.67	103.07	113.83
8	a	814	BCL	CMC-C2C-C3C	-2.67	103.07	113.83
8	A	808	BCL	CMC-C2C-C3C	-2.66	103.09	113.83
8	F	101	BCL	O2A-CGA-O1A	-2.66	116.66	123.30
9	a	820	CDL	OB8-CB7-C71	2.66	120.26	111.91
8	a	811	BCL	CMC-C2C-C3C	-2.66	103.10	113.83
8	5	406	BCL	C7-C6-C5	-2.66	106.14	113.36
13	A	815	F39	O6-C21-C22	2.66	120.24	111.91
14	E	101	LHG	O8-C23-C24	2.66	120.24	111.91
8	2	407	BCL	CMC-C2C-C3C	-2.65	103.12	113.83
8	2	409[B]	BCL	O2A-CGA-O1A	-2.65	116.68	123.30
8	A	803	BCL	C2A-C1A-CHA	2.65	128.50	123.86
11	A	801	GS0	CMC-C2C-C3C	-2.65	103.12	113.83
8	6	403	BCL	CMC-C2C-C3C	-2.65	103.13	113.83
11	a	802	GS0	C4B-CHC-C1C	-2.65	124.86	130.12
8	A	807	BCL	C2A-C1A-CHA	2.65	128.50	123.86
8	5	403	BCL	C11-C10-C8	-2.65	107.36	115.92
8	1	408	BCL	C4D-CHA-C1A	2.65	124.47	121.25
8	a	810	BCL	CMC-C2C-C3C	-2.65	103.14	113.83
8	3	401	BCL	C11-C10-C8	-2.65	107.36	115.92
8	A	804	BCL	C4A-NA-C1A	-2.64	105.52	106.71
8	1	407[B]	BCL	CGD-CBD-CAD	-2.64	102.17	110.73
8	3	401	BCL	C7-C6-C5	-2.64	106.18	113.36
8	2	409[B]	BCL	C2C-C3C-C4C	-2.64	97.38	101.34
8	4	402	BCL	C11-C12-C13	-2.64	107.38	115.92
9	a	822	CDL	OA8-CA7-C31	2.64	120.20	111.91
8	A	804	BCL	CMC-C2C-C3C	-2.64	103.17	113.83
8	5	401	BCL	C7-C6-C5	-2.64	106.19	113.36
8	6	406	BCL	CMC-C2C-C3C	-2.64	103.18	113.83
8	1	404	BCL	C4D-CHA-C1A	2.64	124.46	121.25
8	1	408	BCL	CMC-C2C-C3C	-2.64	103.19	113.83
8	6	401	BCL	C11-C12-C13	-2.64	107.40	115.92
8	2	405	BCL	CMC-C2C-C3C	-2.63	103.20	113.83
8	5	404	BCL	O2A-CGA-O1A	-2.63	116.94	123.59
8	2	403	BCL	CMC-C2C-C3C	-2.63	103.20	113.83
8	A	810	BCL	CMC-C2C-C3C	-2.63	103.20	113.83
8	1	408	BCL	O2A-CGA-O1A	-2.63	116.95	123.59
8	4	410[B]	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
8	3	406	BCL	CMA-C3A-C4A	-2.63	104.70	111.77
8	2	402[B]	BCL	CMC-C2C-C3C	-2.63	103.22	113.83
17	a	815	F26	C2-C9-C15	-2.63	122.70	128.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	4	404	BCL	CMC-C2C-C3C	-2.63	103.22	113.83
8	6	404	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
8	1	403	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
8	4	410[B]	BCL	C2C-C3C-C4C	-2.63	97.40	101.34
8	5	406	BCL	C11-C12-C13	-2.63	107.43	115.92
8	3	407	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
8	2	403	BCL	C11-C10-C8	-2.63	107.43	115.92
8	1	405	BCL	C7-C6-C5	-2.62	106.23	113.36
9	1	409	CDL	OA8-CA7-C31	2.62	120.14	111.91
17	a	815	F26	C27-C28-C31	-2.62	119.05	126.42
8	1	405	BCL	CMC-C2C-C3C	-2.62	103.26	113.83
8	2	402[B]	BCL	C3D-C2D-C1D	-2.62	102.26	105.83
8	1	407[B]	BCL	CMA-C3A-C4A	-2.62	104.74	111.77
8	5	401	BCL	CMC-C2C-C3C	-2.61	103.29	113.83
8	3	404	BCL	O2A-CGA-O1A	-2.61	117.00	123.59
14	A	818	LHG	C11-C10-C9	-2.61	101.18	114.42
8	4	407	BCL	C4D-CHA-C1A	2.61	124.42	121.25
8	2	401	BCL	C2A-C1A-CHA	2.61	128.42	123.86
8	2	401	BCL	CMC-C2C-C3C	-2.61	103.30	113.83
8	4	406	BCL	CMD-C2D-C1D	2.61	129.31	124.71
8	4	402	BCL	CMC-C2C-C3C	-2.61	103.31	113.83
8	2	403	BCL	C7-C6-C5	-2.61	106.28	113.36
8	1	401	BCL	C7-C6-C5	-2.60	106.29	113.36
8	1	407[B]	BCL	CMC-C2C-C3C	-2.60	103.34	113.83
8	6	405	BCL	C1B-CHB-C4A	-2.60	124.97	130.12
8	a	811	BCL	C4D-CHA-C1A	2.60	124.41	121.25
8	6	407[B]	BCL	CMC-C2C-C3C	-2.60	103.35	113.83
8	a	814	BCL	CMA-C3A-C4A	-2.60	104.79	111.77
8	5	403	BCL	C2C-C3C-C4C	-2.60	97.45	101.34
12	A	822	G2O	CHB-C4A-NA	2.60	127.96	125.08
8	a	811	BCL	C2A-C3A-C4A	-2.59	97.68	101.87
8	4	405	BCL	C11-C12-C13	-2.59	107.53	115.92
8	a	804	BCL	CMC-C2C-C3C	-2.59	103.36	113.83
11	a	802	GS0	C3C-C2C-C1C	2.59	106.06	101.87
8	2	408	BCL	CMA-C3A-C4A	-2.59	104.81	111.77
8	2	409[B]	BCL	CMC-C2C-C3C	-2.59	103.38	113.83
8	6	408	BCL	O2A-CGA-O1A	-2.59	117.06	123.59
8	6	406	BCL	CMA-C3A-C4A	-2.59	104.81	111.77
8	3	404	BCL	C11-C12-C13	-2.59	107.55	115.92
8	a	809	BCL	CMC-C2C-C3C	-2.59	103.39	113.83
8	6	408	BCL	CMC-C2C-C3C	-2.59	103.39	113.83
8	a	804	BCL	C4D-CHA-C1A	2.59	124.40	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	407	BCL	C4D-CHA-C1A	2.59	124.40	121.25
9	1	409	CDL	OB8-CB7-C71	2.59	120.02	111.91
8	4	406	BCL	CMC-C2C-C3C	-2.59	103.40	113.83
8	3	405	BCL	C3C-C2C-C1C	2.58	106.04	101.87
8	4	410[B]	BCL	C3D-C2D-C1D	-2.58	102.31	105.83
12	a	803	G2O	CHB-C4A-NA	2.58	127.94	125.08
8	A	808	BCL	CMA-C3A-C4A	-2.58	104.84	111.77
8	F	101	BCL	CMA-C3A-C4A	-2.58	104.85	111.77
8	2	403	BCL	C11-C12-C13	-2.58	107.59	115.92
8	6	407[B]	BCL	CGD-CBD-CAD	-2.58	102.39	110.73
8	1	407[B]	BCL	O2A-CGA-O1A	-2.58	116.88	123.30
8	A	805	BCL	C7-C6-C5	-2.57	106.37	113.36
8	5	401	BCL	C11-C10-C8	-2.57	107.61	115.92
8	A	813	BCL	C3D-C2D-C1D	-2.57	102.32	105.83
8	a	805	BCL	O2A-CGA-O1A	-2.57	117.10	123.59
8	A	809	BCL	CMC-C2C-C3C	-2.57	103.46	113.83
8	6	405	BCL	CMC-C2C-C3C	-2.57	103.46	113.83
8	2	404	BCL	CMC-C2C-C3C	-2.57	103.47	113.83
8	a	813	BCL	C2C-C3C-C4C	-2.57	97.49	101.34
8	2	408	BCL	C11-C12-C13	-2.57	107.62	115.92
8	6	402	BCL	CMA-C3A-C4A	-2.57	104.88	111.77
8	2	402[B]	BCL	CMD-C2D-C1D	2.57	129.23	124.71
8	A	811	BCL	CMC-C2C-C3C	-2.57	103.48	113.83
12	A	802	G2O	CHB-C4A-NA	2.56	127.92	125.08
9	c	303	CDL	OA8-CA7-C31	2.56	119.95	111.91
9	a	820	CDL	OA8-CA7-C31	2.56	119.94	111.91
8	A	809	BCL	C4B-CHC-C1C	-2.56	125.05	130.12
8	4	401	BCL	C11-C12-C13	-2.56	107.65	115.92
8	6	401	BCL	C11-C10-C8	-2.56	107.65	115.92
8	5	404	BCL	CMC-C2C-C3C	-2.56	103.51	113.83
8	5	402	BCL	C7-C6-C5	-2.56	106.42	113.36
8	6	404	BCL	C11-C12-C13	-2.56	107.66	115.92
8	1	401	BCL	CMC-C2C-C3C	-2.56	103.52	113.83
8	A	808	BCL	C1C-NC-C4C	-2.56	105.56	106.71
8	A	812	BCL	CMC-C2C-C3C	-2.55	103.52	113.83
8	a	810	BCL	CMA-C3A-C4A	-2.55	104.91	111.77
9	c	303	CDL	OB8-CB7-C71	2.55	119.92	111.91
8	6	402	BCL	C11-C12-C13	-2.55	107.67	115.92
8	3	407	BCL	CMA-C3A-C4A	-2.55	104.91	111.77
8	6	401	BCL	CMC-C2C-C3C	-2.55	103.54	113.83
8	a	809	BCL	CMA-C3A-C4A	-2.55	104.92	111.77
8	4	402	BCL	C4D-CHA-C1A	2.55	124.35	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	4	407	BCL	C11-C12-C13	-2.55	107.69	115.92
8	1	403	BCL	CMA-C3A-C4A	-2.54	104.93	111.77
8	3	403	BCL	CMC-C2C-C3C	-2.54	103.56	113.83
8	2	407	BCL	CMD-C2D-C1D	2.54	129.20	124.71
14	a	821	LHG	C11-C10-C9	-2.54	101.51	114.42
8	2	405	BCL	C11-C12-C13	-2.54	107.70	115.92
8	4	405	BCL	CMC-C2C-C3C	-2.54	103.57	113.83
8	A	805	BCL	CMA-C3A-C4A	-2.54	104.94	111.77
8	1	402	BCL	CMC-C2C-C3C	-2.54	103.58	113.83
8	A	811	BCL	C1C-NC-C4C	-2.54	105.56	106.71
8	3	407	BCL	C11-C12-C13	-2.54	107.71	115.92
8	A	813	BCL	CMC-C2C-C3C	-2.54	103.58	113.83
15	A	817	LMG	O3-C3-C2	-2.54	104.48	110.35
8	4	403	BCL	C11-C12-C13	-2.54	107.72	115.92
8	a	811	BCL	C1B-CHB-C4A	-2.54	125.09	130.12
9	a	822	CDL	OB8-CB7-C71	2.54	119.87	111.91
8	c	301	BCL	CMD-C2D-C1D	2.53	129.17	124.71
8	A	803	BCL	CMA-C3A-C4A	-2.53	104.97	111.77
8	5	402	BCL	CMC-C2C-C3C	-2.53	103.62	113.83
8	a	807	BCL	CMC-C2C-C3C	-2.53	103.62	113.83
8	6	404	BCL	O2A-CGA-O1A	-2.53	117.21	123.59
8	1	402	BCL	CMA-C3A-C4A	-2.53	104.98	111.77
8	3	405	BCL	CMC-C2C-C3C	-2.53	103.63	113.83
8	6	402	BCL	CMC-C2C-C3C	-2.53	103.63	113.83
14	a	817	LHG	C11-C10-C9	-2.53	101.59	114.42
8	6	405	BCL	C11-C12-C13	-2.53	107.75	115.92
8	6	403	BCL	CMD-C2D-C1D	2.52	129.16	124.71
8	6	403	BCL	CMA-C3A-C4A	-2.52	104.99	111.77
8	2	409[B]	BCL	CMD-C2D-C1D	2.52	129.16	124.71
8	A	811	BCL	CMA-C3A-C4A	-2.52	104.99	111.77
8	A	809	BCL	CMA-C3A-C4A	-2.52	105.00	111.77
8	1	404	BCL	CMA-C3A-C4A	-2.52	105.00	111.77
8	A	810	BCL	C11-C12-C13	-2.52	107.77	115.92
8	6	407[B]	BCL	CMA-C3A-C4A	-2.52	105.00	111.77
8	1	406	BCL	CMA-C3A-C4A	-2.52	105.01	111.77
8	4	403	BCL	CMC-C2C-C3C	-2.52	103.68	113.83
8	5	405	BCL	C3C-C2C-C1C	2.51	105.93	101.87
8	4	410[B]	BCL	CMD-C2D-C1D	2.51	129.14	124.71
8	4	409	BCL	CMD-C2D-C1D	2.51	129.14	124.71
8	2	406	BCL	C11-C12-C13	-2.51	107.81	115.92
8	a	805	BCL	CMA-C3A-C4A	-2.51	105.03	111.77
8	A	803	BCL	C3C-C2C-C1C	2.51	105.92	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	401	BCL	C1B-CHB-C4A	-2.51	125.15	130.12
8	a	813	BCL	CMD-C2D-C1D	2.51	129.13	124.71
8	A	805	BCL	C11-C12-C13	-2.51	107.82	115.92
14	E	101	LHG	C11-C10-C9	-2.51	101.71	114.42
8	a	806	BCL	CMA-C3A-C4A	-2.51	105.04	111.77
8	a	810	BCL	C1B-CHB-C4A	-2.50	125.16	130.12
8	4	408[B]	BCL	CMD-C2D-C1D	2.50	129.12	124.71
8	4	401	BCL	C1B-CHB-C4A	-2.50	125.16	130.12
8	4	405	BCL	CMA-C3A-C4A	-2.50	105.05	111.77
8	6	408	BCL	CMA-C3A-C4A	-2.50	105.05	111.77
8	A	812	BCL	C1B-CHB-C4A	-2.50	125.16	130.12
8	A	808	BCL	C2A-C3A-C4A	-2.50	97.83	101.87
8	2	401	BCL	CMA-C3A-C4A	-2.50	105.06	111.77
8	F	101	BCL	C2C-C3C-C4C	-2.50	97.60	101.34
8	1	405	BCL	CMD-C2D-C1D	2.49	129.10	124.71
15	a	818	LMG	C3-C4-C5	-2.49	105.80	110.24
8	3	405	BCL	CMD-C2D-C1D	2.49	129.10	124.71
8	2	404	BCL	C11-C12-C13	-2.49	107.88	115.92
8	5	403	BCL	CMC-C2C-C3C	-2.49	103.80	113.83
15	a	818	LMG	O3-C3-C2	-2.48	104.60	110.35
12	a	803	G2O	C1-C2-C3	-2.48	121.75	126.04
8	A	805	BCL	C11-C10-C8	-2.48	107.89	115.92
8	2	401	BCL	C11-C12-C13	-2.48	107.89	115.92
8	4	401	BCL	C3C-C2C-C1C	2.48	105.88	101.87
8	4	404	BCL	CMA-C3A-C4A	-2.48	105.11	111.77
8	2	406	BCL	CMA-C3A-C4A	-2.48	105.11	111.77
8	1	404	BCL	C11-C12-C13	-2.48	107.90	115.92
14	A	819	LHG	C20-C19-C18	-2.48	101.85	114.42
8	3	406	BCL	C4D-CHA-C1A	2.47	124.26	121.25
8	1	407[B]	BCL	CMD-C2D-C1D	2.47	129.07	124.71
8	a	809	BCL	CMD-C2D-C1D	2.47	129.07	124.71
8	a	804	BCL	C3C-C2C-C1C	2.47	105.86	101.87
8	6	405	BCL	CMA-C3A-C4A	-2.47	105.13	111.77
8	3	404	BCL	CMA-C3A-C4A	-2.47	105.13	111.77
8	4	402	BCL	CMA-C3A-C4A	-2.47	105.14	111.77
8	A	806	BCL	CMD-C2D-C1D	2.46	129.06	124.71
8	a	810	BCL	C2C-C3C-C4C	-2.46	97.65	101.34
8	5	401	BCL	CMD-C2D-C1D	2.46	129.05	124.71
11	A	801	GS0	C2A-C3A-C4A	-2.46	97.89	101.87
8	3	401	BCL	C2A-C1A-CHA	2.46	128.16	123.86
8	3	402	BCL	CMC-C2C-C3C	-2.46	103.91	113.83
8	4	404	BCL	C11-C12-C13	-2.46	107.97	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	6	404	BCL	CMA-C3A-C4A	-2.46	105.17	111.77
8	1	408	BCL	C11-C12-C13	-2.46	107.98	115.92
11	a	802	GS0	C11-C12-C13	-2.46	107.98	115.92
8	a	808	BCL	CMD-C2D-C1D	2.45	129.04	124.71
8	4	407	BCL	CMD-C2D-C1D	2.45	129.03	124.71
8	a	805	BCL	CMD-C2D-C1D	2.45	129.03	124.71
8	5	406	BCL	CGD-CBD-CAD	-2.45	102.80	110.73
8	1	405	BCL	C1B-CHB-C4A	-2.45	125.27	130.12
8	a	814	BCL	C2C-C3C-C4C	-2.45	97.67	101.34
8	6	403	BCL	C11-C12-C13	-2.45	108.00	115.92
8	1	403	BCL	C11-C12-C13	-2.45	108.01	115.92
8	4	408[B]	BCL	CMA-C3A-C4A	-2.45	105.20	111.77
8	6	401	BCL	CMD-C2D-C1D	2.45	129.03	124.71
8	5	405	BCL	C11-C12-C13	-2.45	108.01	115.92
8	5	406	BCL	CBB-CAB-C3B	2.45	127.60	120.34
14	A	819	LHG	C11-C10-C9	-2.44	102.02	114.42
8	A	812	BCL	C4D-CHA-C1A	2.44	124.22	121.25
8	1	404	BCL	C4A-NA-C1A	-2.44	105.61	106.71
8	1	405	BCL	C4A-NA-C1A	-2.44	105.61	106.71
8	1	408	BCL	CMA-C3A-C4A	-2.44	105.22	111.77
8	A	803	BCL	CMD-C2D-C1D	2.44	129.01	124.71
8	1	406	BCL	C4D-CHA-C1A	2.44	124.22	121.25
8	4	407	BCL	CMA-C3A-C4A	-2.44	105.22	111.77
8	5	404	BCL	CMA-C3A-C4A	-2.44	105.23	111.77
8	c	301	BCL	C1B-CHB-C4A	-2.44	125.29	130.12
8	1	401	BCL	C11-C12-C13	-2.43	108.05	115.92
8	6	407[B]	BCL	CMD-C2D-C1D	2.43	129.00	124.71
8	4	406	BCL	C11-C12-C13	-2.43	108.07	115.92
8	3	405	BCL	C11-C12-C13	-2.43	108.08	115.92
8	4	409	BCL	CMA-C3A-C4A	-2.43	105.25	111.77
8	2	407	BCL	C11-C12-C13	-2.42	108.09	115.92
8	5	403	BCL	C11-C12-C13	-2.42	108.09	115.92
8	A	807	BCL	CMD-C2D-C1D	2.42	128.98	124.71
8	a	810	BCL	C4A-NA-C1A	-2.42	105.62	106.71
8	2	403	BCL	CMD-C2D-C1D	2.42	128.98	124.71
8	A	810	BCL	CMA-C3A-C4A	-2.42	105.27	111.77
8	6	408	BCL	C11-C12-C13	-2.42	108.10	115.92
8	A	810	BCL	C3C-C2C-C1C	2.42	105.77	101.87
8	4	405	BCL	CMD-C2D-C1D	2.42	128.97	124.71
8	1	405	BCL	C11-C12-C13	-2.42	108.11	115.92
8	a	812	BCL	CMC-C2C-C3C	-2.42	104.08	113.83
14	a	817	LHG	C20-C19-C18	-2.42	102.16	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	801	G2O	CHB-C4A-NA	2.41	127.76	125.08
8	2	405	BCL	CMA-C3A-C4A	-2.41	105.29	111.77
11	A	801	GS0	C4A-NA-C1A	-2.41	105.62	106.71
8	2	406	BCL	CMD-C2D-C1D	2.41	128.96	124.71
8	3	403	BCL	C11-C12-C13	-2.41	108.14	115.92
8	2	409[B]	BCL	CMA-C3A-C4A	-2.41	105.31	111.77
14	A	816	LHG	C11-C10-C9	-2.41	102.21	114.42
8	a	808	BCL	C3C-C2C-C1C	2.41	105.75	101.87
8	A	813	BCL	C4D-CHA-C1A	2.41	124.18	121.25
8	a	804	BCL	CMD-C2D-C1D	2.40	128.95	124.71
12	A	822	G2O	O2A-CGA-O1A	-2.40	117.53	123.59
8	A	807	BCL	C3C-C2C-C1C	2.40	105.75	101.87
8	3	404	BCL	CMD-C2D-C1D	2.40	128.94	124.71
8	4	403	BCL	CMA-C3A-C4A	-2.40	105.33	111.77
8	1	401	BCL	CMD-C2D-C1D	2.39	128.93	124.71
8	2	403	BCL	C3C-C2C-C1C	2.39	105.73	101.87
8	5	404	BCL	CMD-C2D-C1D	2.39	128.93	124.71
8	5	406	BCL	C3C-C4C-CHD	-2.39	118.29	123.39
8	A	804	BCL	CMA-C3A-C4A	-2.39	105.36	111.77
8	A	805	BCL	CGD-CBD-CAD	-2.39	103.00	110.73
8	3	401	BCL	CMD-C2D-C1D	2.39	128.92	124.71
14	a	819	LHG	C11-C10-C9	-2.39	102.31	114.42
8	6	401	BCL	C3C-C2C-C1C	2.39	105.72	101.87
8	a	814	BCL	CMD-C2D-C1D	2.38	128.92	124.71
11	a	802	GS0	CBB-CAB-C3B	2.38	127.42	120.34
8	4	410[B]	BCL	C4D-CHA-C1A	2.38	124.15	121.25
8	3	402	BCL	CMA-C3A-C4A	-2.38	105.38	111.77
8	3	404	BCL	C4A-NA-C1A	-2.38	105.64	106.71
8	2	402[B]	BCL	C4D-CHA-C1A	2.38	124.14	121.25
8	4	401	BCL	CMD-C2D-C1D	2.38	128.90	124.71
8	1	406	BCL	CMD-C2D-C1D	2.37	128.90	124.71
8	6	404	BCL	CMD-C2D-C1D	2.37	128.90	124.71
11	A	801	GS0	CBB-CAB-C3B	2.37	127.38	120.34
11	A	801	GS0	CGD-CBD-CAD	-2.37	103.07	110.73
12	A	802	G2O	CHB-C1B-NB	2.36	126.63	124.45
8	3	402	BCL	C11-C12-C13	-2.36	108.28	115.92
8	a	812	BCL	C1B-CHB-C4A	-2.36	125.43	130.12
8	3	406	BCL	CMD-C2D-C1D	2.36	128.88	124.71
8	a	806	BCL	C2A-C3A-C4A	-2.36	98.05	101.87
8	4	405	BCL	C4A-NA-C1A	-2.36	105.64	106.71
8	1	408	BCL	CMD-C2D-C1D	2.36	128.88	124.71
8	6	405	BCL	CMD-C2D-C1D	2.36	128.88	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	812	BCL	CMD-C2D-C1D	2.36	128.87	124.71
8	1	404	BCL	CMD-C2D-C1D	2.36	128.87	124.71
8	A	812	BCL	C2A-C3A-C4A	-2.36	98.06	101.87
8	3	401	BCL	C11-C12-C13	-2.36	108.30	115.92
8	5	404	BCL	C3C-C2C-C1C	2.36	105.67	101.87
8	5	403	BCL	C1B-CHB-C4A	-2.35	125.45	130.12
8	A	811	BCL	C11-C10-C8	-2.35	108.31	115.92
8	2	408	BCL	CMD-C2D-C1D	2.35	128.86	124.71
8	6	408	BCL	CMD-C2D-C1D	2.35	128.86	124.71
8	A	804	BCL	CMD-C2D-C1D	2.35	128.86	124.71
8	4	409	BCL	C3C-C2C-C1C	2.35	105.67	101.87
8	2	408	BCL	C4D-CHA-C1A	2.35	124.11	121.25
8	a	812	BCL	C11-C10-C8	-2.35	108.32	115.92
8	4	403	BCL	CMD-C2D-C1D	2.35	128.85	124.71
8	2	405	BCL	C2C-C3C-C4C	-2.35	97.83	101.34
8	4	406	BCL	C3C-C2C-C1C	2.35	105.66	101.87
8	5	401	BCL	C3C-C2C-C1C	2.34	105.66	101.87
8	a	811	BCL	CMD-C2D-C1D	2.34	128.84	124.71
8	6	405	BCL	C3C-C2C-C1C	2.34	105.65	101.87
8	4	402	BCL	CMD-C2D-C1D	2.34	128.83	124.71
8	5	402	BCL	CMA-C3A-C4A	-2.33	105.50	111.77
8	A	810	BCL	C12-C11-C10	-2.33	102.52	113.24
8	C	301	BCL	CMD-C2D-C1D	2.33	128.82	124.71
8	F	101	BCL	CBB-CAB-C3B	2.33	127.26	120.34
8	4	402	BCL	C2A-C1A-CHA	2.33	127.93	123.86
8	2	401	BCL	CMD-C2D-C1D	2.33	128.82	124.71
8	A	807	BCL	C11-C12-C13	-2.33	108.39	115.92
8	1	407[B]	BCL	C1C-NC-C4C	-2.33	105.66	106.71
8	6	406	BCL	CMD-C2D-C1D	2.33	128.82	124.71
8	5	404	BCL	CGD-CBD-CAD	-2.33	103.19	110.73
8	1	402	BCL	C11-C12-C13	-2.33	108.39	115.92
8	3	407	BCL	CMD-C2D-C1D	2.33	128.81	124.71
8	1	406	BCL	C3C-C2C-C1C	2.33	105.63	101.87
8	F	101	BCL	CGD-CBD-CAD	-2.33	103.20	110.73
11	A	801	GS0	C11-C12-C13	-2.33	108.40	115.92
8	5	405	BCL	CMD-C2D-C1D	2.33	128.81	124.71
8	6	401	BCL	C1B-CHB-C4A	-2.33	125.51	130.12
8	a	814	BCL	C2A-C3A-C4A	-2.32	98.11	101.87
8	A	808	BCL	C3C-C2C-C1C	2.32	105.62	101.87
8	a	805	BCL	C3C-C2C-C1C	2.32	105.62	101.87
8	3	404	BCL	C2A-C3A-C4A	-2.32	98.12	101.87
8	1	401	BCL	C1B-CHB-C4A	-2.32	125.52	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	402	BCL	C2A-C1A-CHA	2.32	127.91	123.86
14	A	816	LHG	C20-C19-C18	-2.32	102.67	114.42
8	5	402	BCL	C11-C12-C13	-2.32	108.44	115.92
8	A	808	BCL	CMD-C2D-C1D	2.32	128.79	124.71
8	A	810	BCL	C1B-CHB-C4A	-2.31	125.53	130.12
8	3	403	BCL	CBB-CAB-C3B	2.31	127.20	120.34
8	3	403	BCL	CMA-C3A-C4A	-2.31	105.56	111.77
8	A	810	BCL	CMD-C2D-C1D	2.31	128.78	124.71
8	c	301	BCL	C3C-C2C-C1C	2.31	105.60	101.87
8	2	408	BCL	C3C-C2C-C1C	2.30	105.59	101.87
8	4	408[B]	BCL	CBB-CAB-C3B	2.30	127.18	120.34
8	6	407[B]	BCL	C2C-C3C-C4C	-2.30	97.89	101.34
8	6	406	BCL	CBB-CAB-C3B	2.30	127.17	120.34
8	a	805	BCL	CBB-CAB-C3B	2.30	127.16	120.34
8	a	814	BCL	CBB-CAB-C3B	2.30	127.16	120.34
8	4	407	BCL	C3C-C2C-C1C	2.30	105.58	101.87
12	a	803	G2O	O2A-CGA-O1A	-2.29	117.81	123.59
8	2	402[B]	BCL	C2C-C3C-C4C	-2.29	97.91	101.34
8	a	808	BCL	C1C-NC-C4C	-2.29	105.68	106.71
8	2	405	BCL	CMD-C2D-C1D	2.29	128.75	124.71
8	A	811	BCL	CMD-C2D-C1D	2.29	128.75	124.71
14	A	818	LHG	C20-C19-C18	-2.29	102.80	114.42
8	A	805	BCL	C12-C11-C10	-2.29	102.72	113.24
8	1	401	BCL	C3C-C2C-C1C	2.29	105.57	101.87
8	5	403	BCL	CMD-C2D-C1D	2.29	128.75	124.71
8	5	403	BCL	C2A-C3A-C4A	-2.29	98.17	101.87
8	1	401	BCL	CGD-CBD-CAD	-2.29	103.33	110.73
8	4	407	BCL	CBB-CAB-C3B	2.29	127.12	120.34
8	3	403	BCL	CMD-C2D-C1D	2.28	128.74	124.71
11	a	802	GS0	CHB-C4A-NA	-2.28	121.36	124.51
8	1	404	BCL	C2A-C3A-C4A	-2.28	98.18	101.87
14	a	821	LHG	C27-C26-C25	-2.28	102.84	114.42
8	5	403	BCL	CMA-C3A-C4A	-2.28	105.64	111.77
8	a	807	BCL	C2A-C1A-CHA	2.28	127.84	123.86
14	A	818	LHG	C27-C26-C25	-2.28	102.86	114.42
8	4	408[B]	BCL	C2C-C3C-C4C	-2.28	97.93	101.34
8	C	301	BCL	CBB-CAB-C3B	2.27	127.09	120.34
8	A	803	BCL	C4D-CHA-C1A	2.27	124.01	121.25
8	4	410[B]	BCL	CBB-CAB-C3B	2.27	127.08	120.34
8	a	811	BCL	C2C-C3C-C4C	-2.27	97.94	101.34
8	4	409	BCL	C2A-C1A-CHA	2.27	127.83	123.86
8	5	403	BCL	CBB-CAB-C3B	2.27	127.08	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	405	BCL	C3C-C2C-C1C	2.27	105.54	101.87
8	1	405	BCL	CHC-C1C-NC	2.27	127.65	124.51
8	6	407[B]	BCL	C4D-CHA-C1A	2.27	124.01	121.25
8	1	403	BCL	CBB-CAB-C3B	2.27	127.07	120.34
8	3	407	BCL	CGD-CBD-CAD	-2.27	103.40	110.73
8	2	408	BCL	CBB-CAB-C3B	2.26	127.06	120.34
8	2	407	BCL	C2A-C3A-C4A	-2.26	98.21	101.87
12	a	803	G2O	CMD-C2D-C1D	-2.26	124.99	128.46
15	A	817	LMG	O1-C1-C2	-2.26	104.77	108.30
8	3	406	BCL	CBB-CAB-C3B	2.26	127.05	120.34
8	A	804	BCL	CBB-CAB-C3B	2.26	127.05	120.34
8	4	402	BCL	CBB-CAB-C3B	2.26	127.04	120.34
8	6	403	BCL	CBB-CAB-C3B	2.26	127.04	120.34
8	A	806	BCL	CMA-C3A-C4A	-2.26	105.71	111.77
8	1	406	BCL	CBB-CAB-C3B	2.26	127.04	120.34
8	5	401	BCL	CBB-CAB-C3B	2.26	127.04	120.34
8	A	809	BCL	C1B-CHB-C4A	-2.25	125.65	130.12
8	4	401	BCL	CBB-CAB-C3B	2.25	127.03	120.34
8	2	409[B]	BCL	CBB-CAB-C3B	2.25	127.01	120.34
8	C	301	BCL	C3C-C2C-C1C	2.25	105.50	101.87
8	5	405	BCL	C1B-CHB-C4A	-2.25	125.67	130.12
8	a	812	BCL	CMD-C2D-C1D	2.24	128.67	124.71
8	4	406	BCL	C12-C11-C10	-2.24	102.93	113.24
8	4	405	BCL	CGD-CBD-CAD	-2.24	103.47	110.73
8	a	813	BCL	CMC-C2C-C3C	-2.24	104.78	113.83
14	A	819	LHG	C27-C26-C25	-2.24	103.05	114.42
8	c	301	BCL	CMC-C2C-C3C	-2.24	104.79	113.83
8	1	405	BCL	C12-C11-C10	-2.24	102.95	113.24
8	1	403	BCL	CMD-C2D-C1D	2.24	128.66	124.71
14	a	819	LHG	C27-C26-C25	-2.24	103.07	114.42
8	3	405	BCL	C2A-C3A-C4A	-2.24	98.26	101.87
8	6	407[B]	BCL	CBB-CAB-C3B	2.24	126.98	120.34
8	2	401	BCL	C12-C11-C10	-2.24	102.96	113.24
8	1	407[B]	BCL	CBB-CAB-C3B	2.24	126.98	120.34
8	5	401	BCL	CGD-CBD-CAD	-2.24	103.49	110.73
8	6	401	BCL	CBB-CAB-C3B	2.23	126.97	120.34
8	1	407[B]	BCL	C2A-C1A-CHA	2.23	127.76	123.86
8	1	408	BCL	CBB-CAB-C3B	2.23	126.97	120.34
8	3	401	BCL	CBB-CAB-C3B	2.23	126.97	120.34
8	4	405	BCL	C2A-C3A-C4A	-2.23	98.27	101.87
8	2	403	BCL	C2A-C1A-CHA	2.23	127.76	123.86
11	A	801	GS0	C3C-C2C-C1C	2.23	105.47	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	813	BCL	C1B-CHB-C4A	-2.23	125.70	130.12
12	a	803	G2O	CMD-C2D-C3D	2.23	128.84	124.68
8	4	404	BCL	CBB-CAB-C3B	2.22	126.94	120.34
14	a	817	LHG	C18-C17-C16	-2.22	103.14	114.42
8	1	401	BCL	CBB-CAB-C3B	2.22	126.93	120.34
8	A	810	BCL	C2A-C3A-C4A	-2.22	98.28	101.87
8	3	406	BCL	C3C-C2C-C1C	2.22	105.45	101.87
8	2	402[B]	BCL	CBB-CAB-C3B	2.22	126.93	120.34
11	A	801	GS0	CHB-C4A-NA	-2.22	121.44	124.51
14	A	819	LHG	C18-C17-C16	-2.22	103.17	114.42
8	2	407	BCL	C12-C11-C10	-2.22	103.05	113.24
8	4	409	BCL	CBB-CAB-C3B	2.22	126.92	120.34
8	3	406	BCL	CGD-CBD-CAD	-2.22	103.56	110.73
8	2	405	BCL	CBB-CAB-C3B	2.21	126.92	120.34
8	6	408	BCL	CBB-CAB-C3B	2.21	126.92	120.34
8	2	403	BCL	CBB-CAB-C3B	2.21	126.91	120.34
8	5	406	BCL	C3C-C2C-C1C	2.21	105.44	101.87
8	a	809	BCL	C3C-C2C-C1C	2.21	105.43	101.87
8	1	408	BCL	C2A-C3A-C4A	-2.21	98.31	101.87
8	4	406	BCL	C4A-NA-C1A	-2.20	105.72	106.71
8	2	401	BCL	C2A-C3A-C4A	-2.20	98.31	101.87
8	3	405	BCL	C12-C11-C10	-2.20	103.11	113.24
8	3	402	BCL	CMD-C2D-C1D	2.20	128.59	124.71
8	2	404	BCL	CMA-C3A-C4A	-2.20	105.86	111.77
8	5	404	BCL	C2A-C3A-C4A	-2.20	98.31	101.87
8	A	813	BCL	C4A-NA-C1A	-2.20	105.72	106.71
8	6	406	BCL	C3C-C2C-C1C	2.20	105.42	101.87
12	A	802	G2O	CMD-C2D-C1D	-2.20	125.09	128.46
8	a	805	BCL	C2A-C3A-C4A	-2.20	98.32	101.87
8	1	404	BCL	CHC-C1C-NC	2.19	127.55	124.51
12	a	801	G2O	O2A-CGA-O1A	-2.19	118.06	123.59
8	4	405	BCL	CHC-C1C-NC	2.19	127.54	124.51
8	3	405	BCL	CHC-C1C-NC	2.19	127.54	124.51
8	3	404	BCL	CGD-CBD-CAD	-2.19	103.64	110.73
8	5	403	BCL	C12-C11-C10	-2.19	103.17	113.24
8	6	403	BCL	C1D-CHD-C4C	-2.19	121.34	126.62
8	4	409	BCL	C12-C11-C10	-2.19	103.18	113.24
8	a	804	BCL	C1C-NC-C4C	-2.19	105.72	106.71
8	6	405	BCL	C12-C11-C10	-2.19	103.19	113.24
8	4	406	BCL	CHC-C1C-NC	2.19	127.54	124.51
8	4	408[B]	BCL	CGD-CBD-CAD	-2.19	103.65	110.73
8	F	101	BCL	CHC-C1C-NC	2.19	127.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	818	LHG	C18-C17-C16	-2.18	103.33	114.42
14	a	817	LHG	C27-C26-C25	-2.18	103.34	114.42
8	6	404	BCL	CGD-CBD-CAD	-2.18	103.66	110.73
8	A	804	BCL	C3C-C2C-C1C	2.18	105.38	101.87
8	4	402	BCL	CGD-CBD-CAD	-2.17	103.69	110.73
8	5	403	BCL	CHC-C1C-NC	2.17	127.52	124.51
8	3	401	BCL	C3C-C2C-C1C	2.17	105.38	101.87
8	a	804	BCL	CGD-CBD-CAD	-2.17	103.70	110.73
8	3	404	BCL	CBB-CAB-C3B	2.17	126.79	120.34
8	C	301	BCL	C1B-CHB-C4A	-2.17	125.82	130.12
8	4	401	BCL	C2A-C1A-CHA	2.16	127.64	123.86
8	2	407	BCL	C3C-C2C-C1C	2.16	105.36	101.87
8	5	404	BCL	CHC-C1C-NC	2.16	127.50	124.51
8	c	301	BCL	CBB-CAB-C3B	2.16	126.76	120.34
8	6	408	BCL	C2A-C3A-C4A	-2.16	98.38	101.87
11	a	802	GS0	C2A-C1A-CHA	2.16	127.64	123.86
8	a	806	BCL	C12-C11-C10	-2.16	103.32	113.24
8	a	812	BCL	CHC-C1C-NC	2.16	127.50	124.51
8	4	407	BCL	CGD-CBD-CAD	-2.16	103.75	110.73
8	A	805	BCL	C2A-C3A-C4A	-2.16	98.39	101.87
8	1	404	BCL	CBB-CAB-C3B	2.16	126.74	120.34
8	a	813	BCL	C2A-C1A-CHA	2.15	127.63	123.86
8	5	405	BCL	C12-C11-C10	-2.15	103.34	113.24
12	a	803	G2O	CHB-C1B-NB	2.15	126.43	124.45
8	1	403	BCL	CHC-C1C-NC	2.15	127.49	124.51
8	3	401	BCL	CGD-CBD-CAD	-2.15	103.77	110.73
8	A	806	BCL	C2C-C3C-C4C	-2.15	98.12	101.34
8	2	407	BCL	C1B-CHB-C4A	-2.15	125.86	130.12
8	3	407	BCL	CBB-CAB-C3B	2.15	126.72	120.34
8	C	301	BCL	CMC-C2C-C3C	-2.15	105.16	113.83
8	2	406	BCL	CHC-C1C-NC	2.15	127.48	124.51
8	a	808	BCL	CGD-CBD-CAD	-2.15	103.78	110.73
8	a	812	BCL	C12-C11-C10	-2.15	103.38	113.24
8	a	813	BCL	CHB-C4A-NA	-2.14	121.55	124.51
8	6	408	BCL	C4A-NA-C1A	-2.14	105.74	106.71
8	4	402	BCL	C12-C11-C10	-2.14	103.40	113.24
8	4	405	BCL	C1B-CHB-C4A	-2.14	125.88	130.12
8	2	404	BCL	CMD-C2D-C1D	2.14	128.48	124.71
8	4	405	BCL	CBB-CAB-C3B	2.14	126.69	120.34
14	A	816	LHG	C18-C17-C16	-2.13	103.59	114.42
12	A	802	G2O	O2A-CGA-O1A	-2.13	118.21	123.59
8	a	805	BCL	C1B-CHB-C4A	-2.13	125.89	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	810	BCL	C1-C2-C3	-2.13	122.36	126.04
8	5	404	BCL	CBB-CAB-C3B	2.13	126.67	120.34
8	A	810	BCL	CBB-CAB-C3B	2.13	126.67	120.34
17	c	302	F26	C12-C4-C6	-2.13	116.15	120.31
8	6	401	BCL	C2A-C1A-CHA	2.13	127.58	123.86
17	a	815	F26	C36-C31-C33	-2.13	119.94	122.92
8	3	405	BCL	C1D-CHD-C4C	-2.13	121.49	126.62
8	1	404	BCL	C1B-CHB-C4A	-2.13	125.91	130.12
8	a	813	BCL	CHC-C1C-NC	2.13	127.45	124.51
8	4	401	BCL	CHB-C4A-NA	-2.12	121.57	124.51
8	2	406	BCL	CBB-CAB-C3B	2.12	126.64	120.34
8	A	813	BCL	CHC-C1C-NC	2.12	127.45	124.51
17	c	302	F26	C40-C34-C35	2.12	121.42	118.08
8	5	406	BCL	CMA-C3A-C4A	-2.12	106.07	111.77
8	6	405	BCL	CHC-C1C-NC	2.12	127.44	124.51
14	E	101	LHG	C27-C26-C25	-2.12	103.66	114.42
8	2	406	BCL	C3C-C2C-C1C	2.12	105.29	101.87
8	2	403	BCL	C1B-CHB-C4A	-2.12	125.92	130.12
8	a	809	BCL	C1B-CHB-C4A	-2.12	125.92	130.12
8	a	806	BCL	CGD-CBD-CAD	-2.12	103.88	110.73
12	a	801	G2O	CHB-C1B-NB	2.12	126.40	124.45
8	3	401	BCL	CHB-C4A-NA	-2.11	121.59	124.51
12	A	802	G2O	CMD-C2D-C3D	2.11	128.63	124.68
8	4	404	BCL	CMD-C2D-C1D	2.11	128.44	124.71
8	2	401	BCL	CBB-CAB-C3B	2.11	126.61	120.34
8	3	407	BCL	C2A-C3A-C4A	-2.11	98.46	101.87
8	2	402[B]	BCL	C2A-C1A-CHA	2.11	127.55	123.86
8	a	807	BCL	CHC-C1C-NC	2.11	127.43	124.51
8	3	407	BCL	C12-C11-C10	-2.11	103.55	113.24
8	4	406	BCL	C2A-C3A-C4A	-2.11	98.47	101.87
11	a	802	GS0	C1D-CHD-C4C	-2.11	121.54	126.62
8	3	403	BCL	CHC-C1C-NC	2.11	127.42	124.51
8	3	403	BCL	C2C-C3C-C4C	-2.10	98.19	101.34
8	a	807	BCL	C1B-CHB-C4A	-2.10	125.95	130.12
15	a	818	LMG	O1-C1-C2	-2.10	105.02	108.30
8	a	811	BCL	C12-C11-C10	-2.10	103.58	113.24
12	A	822	G2O	CHB-C1B-NB	2.10	126.39	124.45
8	a	813	BCL	C4D-CHA-C1A	2.10	123.81	121.25
8	a	811	BCL	CBB-CAB-C3B	2.10	126.57	120.34
8	a	807	BCL	C4A-NA-C1A	-2.10	105.76	106.71
8	3	403	BCL	C12-C11-C10	-2.10	103.61	113.24
8	3	404	BCL	C1B-CHB-C4A	-2.09	125.97	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	811	BCL	CHC-C1C-NC	2.09	127.40	124.51
8	2	407	BCL	CHC-C1C-NC	2.09	127.40	124.51
8	A	808	BCL	C1B-CHB-C4A	-2.09	125.99	130.12
8	6	404	BCL	CBB-CAB-C3B	2.08	126.53	120.34
8	3	406	BCL	C2A-C1A-CHA	2.08	127.50	123.86
8	4	405	BCL	C12-C11-C10	-2.08	103.67	113.24
8	A	803	BCL	C1B-CHB-C4A	-2.08	126.00	130.12
8	1	408	BCL	CGD-CBD-CAD	-2.08	104.00	110.73
8	3	406	BCL	C12-C11-C10	-2.08	103.69	113.24
8	6	403	BCL	C12-C11-C10	-2.08	103.69	113.24
8	5	406	BCL	C12-C11-C10	-2.08	103.69	113.24
8	4	405	BCL	C3C-C2C-C1C	2.08	105.22	101.87
8	A	807	BCL	C3A-C2A-C1A	-2.08	98.23	101.34
8	4	404	BCL	C1B-CHB-C4A	-2.07	126.01	130.12
8	6	401	BCL	CGD-CBD-CAD	-2.07	104.02	110.73
8	3	406	BCL	C3C-C4C-CHD	-2.07	118.96	123.39
8	5	405	BCL	CBB-CAB-C3B	2.07	126.49	120.34
8	A	811	BCL	C1B-CHB-C4A	-2.07	126.02	130.12
8	A	811	BCL	C3C-C2C-C1C	2.07	105.21	101.87
11	A	801	GS0	C1D-CHD-C4C	-2.07	121.63	126.62
8	6	403	BCL	C2A-C3A-C4A	-2.07	98.53	101.87
8	2	407	BCL	CBB-CAB-C3B	2.07	126.48	120.34
8	A	804	BCL	C2A-C3A-C4A	-2.06	98.53	101.87
8	1	405	BCL	CBB-CAB-C3B	2.06	126.47	120.34
8	C	301	BCL	C1D-CHD-C4C	-2.06	121.65	126.62
8	4	403	BCL	C2A-C1A-CHA	2.06	127.46	123.86
8	3	404	BCL	C3C-C2C-C1C	2.06	105.20	101.87
8	4	408[B]	BCL	C4D-CHA-C1A	2.06	123.76	121.25
8	1	404	BCL	CGD-CBD-CAD	-2.06	104.06	110.73
8	A	810	BCL	CHC-C1C-NC	2.06	127.36	124.51
8	a	810	BCL	C3C-C2C-C1C	2.06	105.19	101.87
8	A	807	BCL	C12-C11-C10	-2.06	103.79	113.24
8	2	409[B]	BCL	C2A-C1A-CHA	2.05	127.45	123.86
8	2	405	BCL	C12-C11-C10	-2.05	103.80	113.24
8	4	409	BCL	C4A-NA-C1A	-2.05	105.78	106.71
8	1	406	BCL	C12-C11-C10	-2.05	103.81	113.24
8	A	808	BCL	CBB-CAB-C3B	2.05	126.43	120.34
11	a	802	GS0	C4A-NA-C1A	-2.05	105.78	106.71
14	A	816	LHG	C27-C26-C25	-2.05	104.02	114.42
8	5	403	BCL	C2A-C1A-CHA	2.05	127.44	123.86
8	1	404	BCL	C1-C2-C3	-2.05	122.50	126.04
8	4	404	BCL	C3C-C2C-C1C	2.05	105.17	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	6	404	BCL	C12-C11-C10	-2.05	103.84	113.24
8	2	405	BCL	C2A-C1A-CHA	2.04	127.43	123.86
17	a	815	F26	C40-C34-C35	2.04	121.29	118.08
8	A	813	BCL	CMA-C3A-C4A	-2.04	106.29	111.77
8	5	401	BCL	CHB-C4A-NA	-2.04	121.69	124.51
8	2	408	BCL	CGD-CBD-CAD	-2.04	104.13	110.73
8	a	809	BCL	C2A-C3A-C4A	-2.04	98.58	101.87
8	4	409	BCL	CHC-C1C-NC	2.04	127.33	124.51
8	2	405	BCL	C1D-CHD-C4C	-2.03	121.71	126.62
8	6	407[B]	BCL	C2A-C1A-CHA	2.03	127.42	123.86
8	4	404	BCL	C12-C11-C10	-2.03	103.90	113.24
8	1	401	BCL	C1-O2A-CGA	2.03	121.78	116.44
8	1	408	BCL	C12-C11-C10	-2.03	103.91	113.24
8	1	406	BCL	C3C-C4C-CHD	-2.03	119.06	123.39
8	5	404	BCL	C4A-NA-C1A	-2.03	105.79	106.71
8	3	401	BCL	C12-C11-C10	-2.02	103.94	113.24
8	A	812	BCL	C2C-C3C-C4C	-2.02	98.31	101.34
8	6	401	BCL	CHB-C4A-NA	-2.02	121.72	124.51
8	1	403	BCL	C12-C11-C10	-2.02	103.95	113.24
8	2	403	BCL	CGD-CBD-CAD	-2.02	104.19	110.73
8	1	404	BCL	C12-C11-C10	-2.02	103.95	113.24
8	6	401	BCL	CHC-C1C-NC	2.02	127.31	124.51
8	4	404	BCL	C2A-C1A-CHA	2.02	127.39	123.86
8	2	406	BCL	C12-C11-C10	-2.02	103.95	113.24
8	6	403	BCL	C2A-C1A-CHA	2.02	127.39	123.86
8	2	408	BCL	C12-C11-C10	-2.01	103.98	113.24
8	a	814	BCL	C1B-CHB-C4A	-2.01	126.13	130.12
8	3	404	BCL	CHC-C1C-NC	2.01	127.30	124.51
12	A	802	G2O	O1D-CGD-CBD	2.01	128.60	124.48
8	F	101	BCL	CMD-C2D-C1D	2.01	128.26	124.71
8	1	407[B]	BCL	C4D-CHA-C1A	2.01	123.70	121.25
17	a	815	F26	C23-C19-C15	2.01	121.24	118.08
8	6	403	BCL	C1B-CHB-C4A	-2.01	126.14	130.12
8	3	404	BCL	C1-O2A-CGA	2.01	121.71	116.44
8	a	808	BCL	C2A-C3A-C4A	-2.00	98.63	101.87
8	5	405	BCL	CHC-C1C-NC	2.00	127.28	124.51
8	6	408	BCL	C12-C11-C10	-2.00	104.04	113.24
8	2	404	BCL	CHC-C1C-NC	2.00	127.28	124.51

There are no chirality outliers.

All (1467) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1	401	BCL	C1A-C2A-CAA-CBA
8	1	401	BCL	C3A-C2A-CAA-CBA
8	1	401	BCL	CBD-CGD-O2D-CED
8	1	401	BCL	O1D-CGD-O2D-CED
8	1	402	BCL	C2C-C3C-CAC-CBC
8	1	402	BCL	C4C-C3C-CAC-CBC
8	1	403	BCL	C2C-C3C-CAC-CBC
8	1	403	BCL	C4C-C3C-CAC-CBC
8	1	404	BCL	C2C-C3C-CAC-CBC
8	1	404	BCL	C4C-C3C-CAC-CBC
8	1	406	BCL	C1-C2-C3-C5
8	1	407[B]	BCL	C3A-C2A-CAA-CBA
8	1	407[B]	BCL	C4C-C3C-CAC-CBC
8	1	408	BCL	C4C-C3C-CAC-CBC
8	1	408	BCL	C4-C3-C5-C6
8	3	401	BCL	C1A-C2A-CAA-CBA
8	3	401	BCL	C3A-C2A-CAA-CBA
8	3	401	BCL	CBD-CGD-O2D-CED
8	3	401	BCL	O1D-CGD-O2D-CED
8	3	402	BCL	C2C-C3C-CAC-CBC
8	3	402	BCL	C4C-C3C-CAC-CBC
8	3	402	BCL	C2-C3-C5-C6
8	3	403	BCL	C2C-C3C-CAC-CBC
8	3	403	BCL	C4C-C3C-CAC-CBC
8	3	403	BCL	CHA-CBD-CGD-O1D
8	3	404	BCL	C2C-C3C-CAC-CBC
8	3	404	BCL	C4C-C3C-CAC-CBC
8	3	404	BCL	CHA-CBD-CGD-O1D
8	3	404	BCL	CHA-CBD-CGD-O2D
8	3	404	BCL	C1-C2-C3-C5
8	3	405	BCL	C2-C3-C5-C6
8	3	406	BCL	C2C-C3C-CAC-CBC
8	3	407	BCL	C2C-C3C-CAC-CBC
8	3	407	BCL	C4C-C3C-CAC-CBC
8	2	401	BCL	C2C-C3C-CAC-CBC
8	2	401	BCL	C4C-C3C-CAC-CBC
8	2	402[B]	BCL	CHA-CBD-CGD-O1D
8	2	402[B]	BCL	CHA-CBD-CGD-O2D
8	2	402[B]	BCL	CAD-CBD-CGD-O1D
8	2	403	BCL	C1A-C2A-CAA-CBA
8	2	403	BCL	C3A-C2A-CAA-CBA
8	2	403	BCL	CBD-CGD-O2D-CED
8	2	403	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	2	404	BCL	C2C-C3C-CAC-CBC
8	2	404	BCL	C4C-C3C-CAC-CBC
8	2	404	BCL	C1-C2-C3-C5
8	2	404	BCL	C2-C3-C5-C6
8	2	405	BCL	C4C-C3C-CAC-CBC
8	2	405	BCL	C6-C7-C8-C9
8	2	406	BCL	C2C-C3C-CAC-CBC
8	2	406	BCL	C4C-C3C-CAC-CBC
8	2	406	BCL	C1-C2-C3-C5
8	2	407	BCL	C4-C3-C5-C6
8	2	408	BCL	C1-C2-C3-C5
8	A	804	BCL	CHA-CBD-CGD-O1D
8	A	804	BCL	CHA-CBD-CGD-O2D
8	A	804	BCL	C1-C2-C3-C4
8	A	804	BCL	C1-C2-C3-C5
8	A	804	BCL	C4-C3-C5-C6
8	A	805	BCL	C2C-C3C-CAC-CBC
8	A	805	BCL	C4C-C3C-CAC-CBC
8	A	806	BCL	C2C-C3C-CAC-CBC
8	A	806	BCL	C4C-C3C-CAC-CBC
8	A	807	BCL	C4C-C3C-CAC-CBC
8	A	807	BCL	C1-C2-C3-C4
8	A	807	BCL	C1-C2-C3-C5
8	A	809	BCL	C4C-C3C-CAC-CBC
8	A	809	BCL	CHA-CBD-CGD-O1D
8	A	809	BCL	CHA-CBD-CGD-O2D
8	A	809	BCL	CAD-CBD-CGD-O1D
8	A	809	BCL	CAD-CBD-CGD-O2D
8	A	810	BCL	C2C-C3C-CAC-CBC
8	A	810	BCL	C4C-C3C-CAC-CBC
8	A	810	BCL	C2-C3-C5-C6
8	A	811	BCL	C3A-C2A-CAA-CBA
8	A	812	BCL	C2C-C3C-CAC-CBC
8	A	812	BCL	C4C-C3C-CAC-CBC
8	A	813	BCL	C2C-C3C-CAC-CBC
8	A	813	BCL	C4C-C3C-CAC-CBC
8	a	804	BCL	C1A-C2A-CAA-CBA
8	a	804	BCL	C3A-C2A-CAA-CBA
8	a	804	BCL	CHA-CBD-CGD-O1D
8	a	804	BCL	CHA-CBD-CGD-O2D
8	a	804	BCL	CAD-CBD-CGD-O1D
8	a	804	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	a	805	BCL	CHA-CBD-CGD-O1D
8	a	805	BCL	CHA-CBD-CGD-O2D
8	a	806	BCL	C2C-C3C-CAC-CBC
8	a	806	BCL	C4C-C3C-CAC-CBC
8	a	808	BCL	C2C-C3C-CAC-CBC
8	a	808	BCL	C4C-C3C-CAC-CBC
8	a	810	BCL	C4C-C3C-CAC-CBC
8	a	811	BCL	C1A-C2A-CAA-CBA
8	a	811	BCL	C2C-C3C-CAC-CBC
8	a	811	BCL	C4C-C3C-CAC-CBC
8	a	811	BCL	CHA-CBD-CGD-O1D
8	a	811	BCL	CHA-CBD-CGD-O2D
8	a	811	BCL	C1-C2-C3-C5
8	a	811	BCL	C2-C3-C5-C6
8	a	812	BCL	C3A-C2A-CAA-CBA
8	a	812	BCL	C2C-C3C-CAC-CBC
8	a	813	BCL	C1A-C2A-CAA-CBA
8	a	813	BCL	C2C-C3C-CAC-CBC
8	a	813	BCL	C4C-C3C-CAC-CBC
8	4	401	BCL	C1A-C2A-CAA-CBA
8	4	401	BCL	C3A-C2A-CAA-CBA
8	4	401	BCL	C2C-C3C-CAC-CBC
8	4	401	BCL	C4C-C3C-CAC-CBC
8	4	401	BCL	CBD-CGD-O2D-CED
8	4	401	BCL	O1D-CGD-O2D-CED
8	4	402	BCL	C4C-C3C-CAC-CBC
8	4	402	BCL	C2-C3-C5-C6
8	4	403	BCL	C2C-C3C-CAC-CBC
8	4	403	BCL	C4C-C3C-CAC-CBC
8	4	404	BCL	C2C-C3C-CAC-CBC
8	4	404	BCL	C4C-C3C-CAC-CBC
8	4	404	BCL	C6-C7-C8-C9
8	4	405	BCL	C1-C2-C3-C5
8	4	406	BCL	C2-C3-C5-C6
8	4	407	BCL	C2C-C3C-CAC-CBC
8	4	407	BCL	C4C-C3C-CAC-CBC
8	4	409	BCL	C2C-C3C-CAC-CBC
8	4	409	BCL	C6-C7-C8-C9
8	4	410[B]	BCL	C3A-C2A-CAA-CBA
8	6	401	BCL	C1A-C2A-CAA-CBA
8	6	401	BCL	C3A-C2A-CAA-CBA
8	6	401	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	6	401	BCL	O1D-CGD-O2D-CED
8	6	401	BCL	C1-C2-C3-C5
8	6	402	BCL	C2C-C3C-CAC-CBC
8	6	402	BCL	C4C-C3C-CAC-CBC
8	6	402	BCL	CHA-CBD-CGD-O1D
8	6	402	BCL	CHA-CBD-CGD-O2D
8	6	402	BCL	CAD-CBD-CGD-O1D
8	6	402	BCL	C1-C2-C3-C5
8	6	402	BCL	C4-C3-C5-C6
8	6	403	BCL	CBA-CGA-O2A-C1
8	6	403	BCL	C4C-C3C-CAC-CBC
8	6	403	BCL	CHA-CBD-CGD-O1D
8	6	403	BCL	CHA-CBD-CGD-O2D
8	6	404	BCL	C2C-C3C-CAC-CBC
8	6	404	BCL	C4C-C3C-CAC-CBC
8	6	406	BCL	C1-C2-C3-C5
8	6	408	BCL	C2C-C3C-CAC-CBC
8	6	408	BCL	C4C-C3C-CAC-CBC
8	5	401	BCL	C1A-C2A-CAA-CBA
8	5	401	BCL	C3A-C2A-CAA-CBA
8	5	401	BCL	C4C-C3C-CAC-CBC
8	5	401	BCL	CBD-CGD-O2D-CED
8	5	401	BCL	O1D-CGD-O2D-CED
8	5	402	BCL	C2C-C3C-CAC-CBC
8	5	402	BCL	C4C-C3C-CAC-CBC
8	5	402	BCL	C2-C3-C5-C6
8	5	403	BCL	C2C-C3C-CAC-CBC
8	5	403	BCL	C4C-C3C-CAC-CBC
8	5	404	BCL	CHA-CBD-CGD-O1D
8	5	404	BCL	CHA-CBD-CGD-O2D
8	5	404	BCL	C1-C2-C3-C5
8	5	405	BCL	C1A-C2A-CAA-CBA
8	5	405	BCL	C3A-C2A-CAA-CBA
8	5	406	BCL	C2C-C3C-CAC-CBC
8	C	301	BCL	C1A-C2A-CAA-CBA
8	C	301	BCL	C3A-C2A-CAA-CBA
8	C	301	BCL	C2C-C3C-CAC-CBC
8	C	301	BCL	C4C-C3C-CAC-CBC
8	c	301	BCL	C4C-C3C-CAC-CBC
9	1	409	CDL	CA2-C1-CB2-OB2
9	1	409	CDL	CA2-OA2-PA1-OA4
9	1	409	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
9	1	409	CDL	C11-CA5-OA6-CA4
9	1	409	CDL	C51-CB5-OB6-CB4
9	a	820	CDL	CA3-OA5-PA1-OA3
9	a	820	CDL	C11-CA5-OA6-CA4
9	a	820	CDL	CB3-OB5-PB2-OB3
9	a	822	CDL	CB2-C1-CA2-OA2
9	a	822	CDL	OA7-CA5-OA6-CA4
9	c	303	CDL	CA3-OA5-PA1-OA3
11	A	801	GS0	C3A-C2A-CAA-CBA
11	a	802	GS0	C3A-C2A-CAA-CBA
12	A	802	G2O	C2-C3-C5-C6
12	A	802	G2O	C4-C3-C5-C6
12	A	802	G2O	C5-C6-C7-C8
12	A	802	G2O	CBD-CGD-O2D-CED
12	A	802	G2O	O1D-CGD-O2D-CED
12	A	822	G2O	C2-C3-C5-C6
12	A	822	G2O	C4-C3-C5-C6
12	A	822	G2O	C5-C6-C7-C8
12	A	822	G2O	C11-C10-C8-C9
12	A	822	G2O	C3A-C2A-CAA-CBA
12	a	801	G2O	C5-C6-C7-C8
12	a	801	G2O	C11-C10-C8-C9
12	a	801	G2O	C3A-C2A-CAA-CBA
12	a	803	G2O	C5-C6-C7-C8
12	a	803	G2O	C11-C10-C8-C7
12	a	803	G2O	C11-C10-C8-C9
12	a	803	G2O	C6-C7-C8-C10
12	a	803	G2O	C6-C7-C8-C9
12	a	803	G2O	CBD-CGD-O2D-CED
13	A	814	F39	C16-C13-C14-C18
13	A	814	F39	C17-C13-C14-C18
13	A	814	F39	O2-C13-C14-C18
13	A	814	F39	C14-C13-O2-C11
13	A	814	F39	C17-C13-O2-C11
13	A	814	F39	C18-C19-C20-C25
13	A	814	F39	C19-C20-C27-C32
13	A	814	F39	C25-C20-C27-C32
13	A	814	F39	C27-C32-C35-C37
13	A	814	F39	C35-C37-C39-C40
13	A	814	F39	C39-C40-C41-C42
13	A	814	F39	C41-C42-C44-C51
13	A	814	F39	C44-C51-C57-C59

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Mol	Chain	Res	Type	Atoms
13	A	814	F39	C46-C53-C56-C58
13	A	814	F39	C60-C58-C61-C63
13	A	814	F39	C57-C59-C62-C65
13	A	814	F39	C59-C62-C64-C63
13	A	815	F39	C16-C13-C14-C18
13	A	815	F39	C17-C13-C14-C18
13	A	815	F39	C14-C13-O2-C11
13	A	815	F39	C17-C13-O2-C11
13	A	815	F39	C18-C19-C20-C25
13	A	815	F39	C19-C20-C27-C32
13	A	815	F39	C25-C20-C27-C32
13	A	815	F39	C20-C27-C32-C35
13	A	815	F39	C35-C37-C39-C40
13	A	815	F39	C37-C39-C40-C41
13	A	815	F39	C40-C41-C42-C43
13	A	815	F39	C40-C41-C42-C44
13	A	815	F39	C41-C42-C44-C51
13	A	815	F39	C60-C58-C61-C63
13	A	815	F39	C57-C59-C62-C64
13	A	815	F39	C57-C59-C62-C65
13	A	815	F39	C59-C62-C64-C63
13	a	816	F39	C14-C13-O2-C11
13	a	816	F39	C17-C13-O2-C11
13	a	816	F39	C18-C19-C20-C27
13	a	816	F39	C19-C20-C27-C32
13	a	816	F39	C25-C20-C27-C32
13	a	816	F39	C27-C32-C35-C37
13	a	816	F39	C32-C35-C37-C38
13	a	816	F39	C38-C37-C39-C40
13	a	816	F39	C39-C40-C41-C42
13	a	816	F39	C40-C41-C42-C43
13	a	816	F39	C43-C42-C44-C51
13	a	816	F39	C44-C51-C57-C59
13	a	816	F39	C53-C56-C58-C61
13	a	816	F39	C56-C58-C61-C63
13	a	816	F39	C60-C58-C61-C63
13	a	816	F39	C57-C59-C62-C65
13	a	816	F39	C58-C61-C63-C64
13	a	816	F39	C61-C63-C64-C62
13	C	302	F39	C16-C13-C14-C18
13	C	302	F39	C17-C13-C14-C18
13	C	302	F39	C19-C20-C27-C32

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Mol	Chain	Res	Type	Atoms
13	C	302	F39	C25-C20-C27-C32
13	C	302	F39	C20-C27-C32-C35
13	C	302	F39	C32-C35-C37-C38
13	C	302	F39	C32-C35-C37-C39
13	C	302	F39	C35-C37-C39-C40
13	C	302	F39	C40-C41-C42-C43
13	C	302	F39	C41-C42-C44-C51
13	C	302	F39	C46-C53-C56-C58
13	C	302	F39	C53-C56-C58-C60
13	C	302	F39	C56-C58-C61-C63
13	C	302	F39	C57-C59-C62-C64
13	C	302	F39	C59-C62-C64-C63
13	C	302	F39	C61-C63-C64-C62
14	A	816	LHG	C1-C2-C3-O3
14	A	816	LHG	O2-C2-C3-O3
14	A	816	LHG	C3-O3-P-O5
14	A	816	LHG	C4-O6-P-O5
14	A	818	LHG	O2-C2-C3-O3
14	A	818	LHG	C3-O3-P-O6
14	A	818	LHG	C4-O6-P-O5
14	A	818	LHG	C8-C7-O7-C5
14	A	819	LHG	C4-O6-P-O5
14	a	817	LHG	O2-C2-C3-O3
14	a	817	LHG	C3-O3-P-O5
14	a	817	LHG	C4-O6-P-O5
14	a	819	LHG	C3-O3-P-O4
14	a	819	LHG	C8-C7-O7-C5
14	a	821	LHG	C4-O6-P-O5
14	E	101	LHG	C4-O6-P-O5
15	A	817	LMG	C11-C10-O7-C8
15	a	818	LMG	C11-C10-O7-C8
17	a	815	F26	C17-C13-C18-C22
17	a	815	F26	C8-C13-C18-C22
17	a	815	F26	C23-C19-C24-C27
17	a	815	F26	C15-C19-C24-C27
17	a	815	F26	C22-C25-C26-C29
17	a	815	F26	C24-C27-C28-C31
17	a	815	F26	C30-C32-C35-C34
17	a	815	F26	C37-C34-C35-C32
17	a	815	F26	C40-C34-C35-C32
17	c	302	F26	C9-C15-C19-C23
17	c	302	F26	C23-C19-C24-C27

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Mol	Chain	Res	Type	Atoms
17	c	302	F26	C15-C19-C24-C27
17	c	302	F26	C19-C15-C9-C2
17	c	302	F26	C19-C24-C27-C28
17	c	302	F26	C22-C25-C26-C29
17	c	302	F26	C29-C26-C30-C32
17	c	302	F26	C24-C27-C28-C31
17	c	302	F26	C27-C28-C31-C36
17	c	302	F26	C37-C34-C35-C32
12	a	801	G2O	CBD-CGD-O2D-CED
8	1	403	BCL	O1A-CGA-O2A-C1
8	4	404	BCL	O1A-CGA-O2A-C1
8	6	403	BCL	O1A-CGA-O2A-C1
9	a	822	CDL	OA9-CA7-OA8-CA6
9	a	822	CDL	OB9-CB7-OB8-CB6
13	A	814	F39	O7-C21-O6-C15
12	a	803	G2O	O1D-CGD-O2D-CED
9	a	822	CDL	C31-CA7-OA8-CA6
13	A	814	F39	C22-C21-O6-C15
8	a	808	BCL	O1A-CGA-O2A-C1
8	6	405	BCL	O1A-CGA-O2A-C1
13	C	302	F39	O7-C21-O6-C15
14	a	819	LHG	O10-C23-O8-C6
13	a	816	F39	O1-C12-C15-O6
13	C	302	F39	O1-C12-C15-O6
9	1	409	CDL	OA7-CA5-OA6-CA4
9	1	409	CDL	OB7-CB5-OB6-CB4
14	A	818	LHG	O9-C7-O7-C5
14	a	819	LHG	O9-C7-O7-C5
15	A	817	LMG	O9-C10-O7-C8
15	a	818	LMG	O9-C10-O7-C8
8	1	408	BCL	C3-C5-C6-C7
8	3	404	BCL	C3-C5-C6-C7
8	A	810	BCL	C3-C5-C6-C7
8	a	812	BCL	C3-C5-C6-C7
8	6	408	BCL	C3-C5-C6-C7
8	1	403	BCL	CBA-CGA-O2A-C1
8	2	405	BCL	CBA-CGA-O2A-C1
8	a	808	BCL	CBA-CGA-O2A-C1
8	6	405	BCL	CBA-CGA-O2A-C1
8	5	403	BCL	CBA-CGA-O2A-C1
9	a	822	CDL	C71-CB7-OB8-CB6
14	a	819	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
9	a	822	CDL	C11-CA5-OA6-CA4
13	C	302	F39	C10-C12-C15-O6
8	2	401	BCL	C4-C3-C5-C6
8	2	404	BCL	C4-C3-C5-C6
8	4	402	BCL	C4-C3-C5-C6
8	5	402	BCL	C4-C3-C5-C6
8	1	403	BCL	C2-C3-C5-C6
8	2	401	BCL	C2-C3-C5-C6
17	a	815	F26	C18-C13-C8-C10
8	1	403	BCL	C2A-CAA-CBA-CGA
8	a	807	BCL	C2A-CAA-CBA-CGA
8	4	410[B]	BCL	C2A-CAA-CBA-CGA
8	6	403	BCL	C2A-CAA-CBA-CGA
8	5	406	BCL	C2A-CAA-CBA-CGA
12	A	822	G2O	C2A-CAA-CBA-CGA
12	a	801	G2O	C2A-CAA-CBA-CGA
8	2	405	BCL	O1A-CGA-O2A-C1
13	a	816	F39	C28-C29-C30-C31
8	A	804	BCL	C3-C5-C6-C7
8	a	811	BCL	C3-C5-C6-C7
8	4	404	BCL	C3-C5-C6-C7
8	3	403	BCL	CBA-CGA-O2A-C1
8	4	404	BCL	CBA-CGA-O2A-C1
9	1	409	CDL	C71-CB7-OB8-CB6
9	c	303	CDL	C31-CA7-OA8-CA6
12	A	802	G2O	CBA-CGA-O2A-C1
13	C	302	F39	C22-C21-O6-C15
14	A	819	LHG	C24-C23-O8-C6
14	a	821	LHG	C24-C23-O8-C6
12	a	801	G2O	O1D-CGD-O2D-CED
17	c	302	F26	C10-C14-C16-C20
9	a	820	CDL	OA7-CA5-OA6-CA4
8	5	403	BCL	O1A-CGA-O2A-C1
9	1	409	CDL	OB9-CB7-OB8-CB6
9	c	303	CDL	OA9-CA7-OA8-CA6
12	A	802	G2O	O1A-CGA-O2A-C1
14	A	819	LHG	O10-C23-O8-C6
14	a	821	LHG	O10-C23-O8-C6
13	A	814	F39	C37-C39-C40-C41
13	C	302	F39	C37-C39-C40-C41
9	1	409	CDL	O1-C1-CB2-OB2
9	a	822	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
14	a	821	LHG	O2-C2-C3-O3
8	1	403	BCL	C3-C5-C6-C7
8	2	405	BCL	C3-C5-C6-C7
13	C	302	F39	C14-C18-C19-C20
13	a	816	F39	C10-C12-C15-O6
9	1	409	CDL	C31-CA7-OA8-CA6
12	a	801	G2O	CBA-CGA-O2A-C1
9	1	409	CDL	OA9-CA7-OA8-CA6
14	A	819	LHG	C8-C7-O7-C5
8	1	405	BCL	CBA-CGA-O2A-C1
15	A	817	LMG	O6-C5-C6-O5
8	3	403	BCL	O1A-CGA-O2A-C1
12	a	803	G2O	C2-C3-C5-C6
12	a	803	G2O	C4-C3-C5-C6
8	3	407	BCL	C4-C3-C5-C6
17	a	815	F26	C17-C13-C8-C10
8	3	407	BCL	C2-C3-C5-C6
8	2	407	BCL	C2-C3-C5-C6
8	A	804	BCL	C2-C3-C5-C6
8	6	402	BCL	C2-C3-C5-C6
8	2	405	BCL	C2A-CAA-CBA-CGA
8	a	808	BCL	C2A-CAA-CBA-CGA
15	a	818	LMG	O6-C5-C6-O5
8	a	812	BCL	O1A-CGA-O2A-C1
11	A	801	GS0	O1A-CGA-O2A-C1
12	a	801	G2O	O1A-CGA-O2A-C1
17	a	815	F26	C14-C10-C8-C13
17	c	302	F26	C14-C10-C8-C13
8	a	812	BCL	CBA-CGA-O2A-C1
9	a	820	CDL	C71-CB7-OB8-CB6
9	a	820	CDL	CB2-C1-CA2-OA2
14	A	818	LHG	C1-C2-C3-O3
14	a	821	LHG	C1-C2-C3-O3
9	a	820	CDL	OB9-CB7-OB8-CB6
11	A	801	GS0	CBA-CGA-O2A-C1
15	a	818	LMG	C29-C28-O8-C9
8	a	812	BCL	C10-C11-C12-C13
13	A	814	F39	C42-C44-C51-C57
13	A	814	F39	C51-C57-C59-C62
9	c	303	CDL	CA5-C11-C12-C13
8	1	403	BCL	C10-C11-C12-C13
8	a	806	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	a	815	F26	C10-C14-C16-C21
9	a	822	CDL	C11-C12-C13-C14
14	a	821	LHG	C28-C29-C30-C31
14	A	819	LHG	C27-C28-C29-C30
8	2	405	BCL	C10-C11-C12-C13
8	a	806	BCL	C13-C15-C16-C17
8	6	406	BCL	C5-C6-C7-C8
9	a	820	CDL	CA5-C11-C12-C13
14	A	818	LHG	C7-C8-C9-C10
13	A	815	F39	C23-C24-C26-C28
8	A	805	BCL	O1A-CGA-O2A-C1
8	A	811	BCL	O1A-CGA-O2A-C1
8	1	403	BCL	C6-C7-C8-C9
8	3	403	BCL	C6-C7-C8-C9
8	a	811	BCL	C6-C7-C8-C9
8	a	812	BCL	C11-C12-C13-C14
8	6	403	BCL	C6-C7-C8-C9
12	a	801	G2O	C11-C12-C13-C14
8	3	407	BCL	C2A-CAA-CBA-CGA
8	a	804	BCL	C2A-CAA-CBA-CGA
12	A	802	G2O	C2A-CAA-CBA-CGA
13	A	814	F39	C65-C62-C64-C63
17	a	815	F26	C27-C28-C31-C36
13	A	814	F39	C40-C41-C42-C44
13	A	814	F39	C53-C56-C58-C61
13	A	815	F39	C32-C35-C37-C39
13	A	815	F39	C53-C56-C58-C61
13	a	816	F39	C40-C41-C42-C44
13	a	816	F39	C59-C62-C64-C63
17	c	302	F26	C27-C28-C31-C33
14	A	819	LHG	O9-C7-O7-C5
9	a	822	CDL	CA7-C31-C32-C33
14	A	816	LHG	C23-C24-C25-C26
8	A	810	BCL	O1A-CGA-O2A-C1
15	a	818	LMG	O10-C28-O8-C9
8	1	408	BCL	C15-C16-C17-C18
8	2	401	BCL	C8-C10-C11-C12
8	A	805	BCL	C5-C6-C7-C8
8	a	806	BCL	C8-C10-C11-C12
8	4	405	BCL	C15-C16-C17-C18
9	a	822	CDL	C74-C75-C76-C77
15	a	818	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
13	a	816	F39	C14-C18-C19-C20
8	a	806	BCL	CBA-CGA-O2A-C1
13	A	815	F39	C22-C21-O6-C15
8	a	811	BCL	C5-C6-C7-C8
8	6	403	BCL	C5-C6-C7-C8
8	5	405	BCL	C13-C15-C16-C17
14	a	817	LHG	C23-C24-C25-C26
8	A	811	BCL	C15-C16-C17-C18
8	4	409	BCL	C5-C6-C7-C8
8	6	408	BCL	C15-C16-C17-C18
8	5	404	BCL	C15-C16-C17-C18
12	A	802	G2O	C8-C10-C11-C12
12	A	802	G2O	C10-C11-C12-C13
17	c	302	F26	C10-C14-C16-C21
14	A	819	LHG	O1-C1-C2-O2
14	a	819	LHG	O1-C1-C2-O2
9	1	409	CDL	CA5-C11-C12-C13
9	1	409	CDL	CB7-C71-C72-C73
9	a	820	CDL	CB7-C71-C72-C73
9	a	822	CDL	CB7-C71-C72-C73
13	A	814	F39	C21-C22-C23-C24
14	A	819	LHG	C23-C24-C25-C26
14	a	821	LHG	C23-C24-C25-C26
8	2	401	BCL	C15-C16-C17-C18
8	2	406	BCL	C5-C6-C7-C8
8	4	409	BCL	C8-C10-C11-C12
14	a	821	LHG	C7-C8-C9-C10
14	E	101	LHG	C23-C24-C25-C26
15	A	817	LMG	C10-C11-C12-C13
13	a	816	F39	C23-C24-C26-C28
8	3	407	BCL	C15-C16-C17-C18
8	2	405	BCL	C8-C10-C11-C12
8	a	808	BCL	C5-C6-C7-C8
8	a	812	BCL	C13-C15-C16-C17
8	1	401	BCL	C12-C13-C15-C16
8	2	401	BCL	O1A-CGA-O2A-C1
13	C	302	F39	C58-C61-C63-C64
17	c	302	F26	C26-C30-C32-C35
8	3	402	BCL	C2A-CAA-CBA-CGA
8	5	402	BCL	C2A-CAA-CBA-CGA
12	a	803	G2O	C2A-CAA-CBA-CGA
8	3	404	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	4	407	BCL	C15-C16-C17-C18
8	6	404	BCL	C5-C6-C7-C8
12	A	802	G2O	C13-C15-C16-C17
12	A	822	G2O	C15-C16-C17-C18
12	a	803	G2O	C15-C16-C17-C18
8	6	408	BCL	C8-C10-C11-C12
9	c	303	CDL	CB7-C71-C72-C73
15	a	818	LMG	C10-C11-C12-C13
13	C	302	F39	C27-C32-C35-C37
9	a	820	CDL	O1-C1-CA2-OA2
14	a	819	LHG	O2-C2-C3-O3
8	1	404	BCL	C5-C6-C7-C8
8	A	807	BCL	C15-C16-C17-C18
12	a	803	G2O	C8-C10-C11-C12
13	A	815	F39	O7-C21-O6-C15
14	A	818	LHG	C23-C24-C25-C26
14	a	817	LHG	C7-C8-C9-C10
15	A	817	LMG	C4-C5-C6-O5
8	2	408	BCL	C15-C16-C17-C18
8	a	806	BCL	C15-C16-C17-C18
8	a	808	BCL	C15-C16-C17-C18
8	4	404	BCL	C10-C11-C12-C13
8	6	403	BCL	C10-C11-C12-C13
8	5	403	BCL	C10-C11-C12-C13
13	A	815	F39	C26-C28-C29-C30
9	a	822	CDL	C51-CB5-OB6-CB4
11	a	802	GS0	C15-C16-C17-C18
9	a	822	CDL	CA2-OA2-PA1-OA5
14	A	818	LHG	C4-O6-P-O3
14	A	819	LHG	C3-O3-P-O6
14	a	817	LHG	C3-O3-P-O6
14	a	817	LHG	C4-O6-P-O3
14	a	819	LHG	C3-O3-P-O6
14	a	821	LHG	C4-O6-P-O3
15	A	817	LMG	C28-C29-C30-C31
8	A	805	BCL	CBA-CGA-O2A-C1
8	1	401	BCL	C15-C16-C17-C18
12	a	801	G2O	C10-C11-C12-C13
15	a	818	LMG	C28-C29-C30-C31
9	a	822	CDL	CA2-C1-CB2-OB2
14	a	817	LHG	C1-C2-C3-O3
9	a	822	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
8	3	403	BCL	C5-C6-C7-C8
8	3	406	BCL	C2A-CAA-CBA-CGA
8	4	404	BCL	C2A-CAA-CBA-CGA
8	5	403	BCL	C2A-CAA-CBA-CGA
8	A	807	BCL	C16-C17-C18-C20
8	A	810	BCL	CBA-CGA-O2A-C1
8	A	811	BCL	CBA-CGA-O2A-C1
13	A	814	F39	C58-C61-C63-C64
13	A	815	F39	C42-C44-C51-C57
13	A	815	F39	C51-C57-C59-C62
17	a	815	F26	C19-C24-C27-C28
9	1	409	CDL	C11-C12-C13-C14
13	a	816	F39	C30-C31-C33-C34
9	a	820	CDL	C51-CB5-OB6-CB4
14	a	821	LHG	C8-C7-O7-C5
8	6	405	BCL	C13-C15-C16-C17
13	A	814	F39	C43-C42-C44-C51
13	C	302	F39	C60-C58-C61-C63
17	a	815	F26	C40-C34-C37-C39
9	1	409	CDL	C20-C21-C22-C23
9	1	409	CDL	C22-C23-C24-C25
9	c	303	CDL	C16-C17-C18-C19
9	c	303	CDL	C53-C54-C55-C56
13	a	816	F39	C26-C28-C29-C30
13	C	302	F39	C23-C24-C26-C28
14	A	819	LHG	C25-C26-C27-C28
9	a	822	CDL	C63-C64-C65-C66
14	a	821	LHG	C24-C25-C26-C27
14	a	821	LHG	O9-C7-O7-C5
12	A	822	G2O	CBD-CGD-O2D-CED
9	a	822	CDL	C15-C16-C17-C18
8	1	405	BCL	O1A-CGA-O2A-C1
14	a	821	LHG	C32-C33-C34-C35
9	a	820	CDL	O1-C1-CB2-OB2
9	a	822	CDL	O1-C1-CA2-OA2
9	c	303	CDL	O1-C1-CB2-OB2
14	A	819	LHG	O2-C2-C3-O3
14	A	818	LHG	C27-C28-C29-C30
13	a	816	F39	C35-C37-C39-C40
13	a	816	F39	C57-C59-C62-C64
9	a	820	CDL	C16-C17-C18-C19
13	A	814	F39	C23-C24-C26-C28

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Mol	Chain	Res	Type	Atoms
14	A	816	LHG	C24-C25-C26-C27
15	A	817	LMG	C33-C34-C35-C36
8	4	403	BCL	C16-C17-C18-C20
8	4	405	BCL	C16-C17-C18-C19
9	1	409	CDL	C72-C73-C74-C75
9	c	303	CDL	C52-C53-C54-C55
9	c	303	CDL	C72-C73-C74-C75
15	a	818	LMG	C32-C33-C34-C35
15	a	818	LMG	C34-C35-C36-C37
8	1	401	BCL	C14-C13-C15-C16
8	2	406	BCL	C14-C13-C15-C16
8	A	810	BCL	C14-C13-C15-C16
8	a	808	BCL	C6-C7-C8-C9
9	a	822	CDL	C51-C52-C53-C54
13	A	815	F39	C28-C29-C30-C31
14	A	818	LHG	C33-C34-C35-C36
15	A	817	LMG	C34-C35-C36-C37
15	a	818	LMG	C33-C34-C35-C36
9	a	822	CDL	C19-C20-C21-C22
9	a	822	CDL	C56-C57-C58-C59
14	A	816	LHG	C11-C12-C13-C14
14	A	819	LHG	O1-C1-C2-C3
14	a	817	LHG	O1-C1-C2-C3
14	a	819	LHG	O1-C1-C2-C3
13	A	814	F39	C32-C35-C37-C39
13	C	302	F39	C53-C56-C58-C61
17	a	815	F26	C27-C28-C31-C33
17	c	302	F26	C9-C15-C19-C24
17	c	302	F26	C22-C25-C26-C30
9	a	820	CDL	OB7-CB5-OB6-CB4
8	A	807	BCL	C5-C6-C7-C8
11	A	801	GS0	C15-C16-C17-C18
9	a	822	CDL	C72-C73-C74-C75
14	E	101	LHG	C10-C11-C12-C13
15	A	817	LMG	C32-C33-C34-C35
13	a	816	F39	C46-C53-C56-C58
9	1	409	CDL	CA7-C31-C32-C33
9	1	409	CDL	C58-C59-C60-C61
9	a	822	CDL	C77-C78-C79-C80
13	A	814	F39	C24-C26-C28-C29
13	A	814	F39	C26-C28-C29-C30
14	E	101	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
8	A	807	BCL	C16-C17-C18-C19
8	a	805	BCL	C6-C7-C8-C10
8	4	405	BCL	C16-C17-C18-C20
8	5	404	BCL	C16-C17-C18-C19
8	5	404	BCL	C16-C17-C18-C20
9	a	820	CDL	C52-C53-C54-C55
14	A	816	LHG	C12-C13-C14-C15
14	A	819	LHG	C32-C33-C34-C35
14	a	817	LHG	C25-C26-C27-C28
9	1	409	CDL	C51-C52-C53-C54
8	6	406	BCL	C10-C11-C12-C13
12	a	801	G2O	C13-C15-C16-C17
8	3	401	BCL	CBA-CGA-O2A-C1
9	1	409	CDL	C17-C18-C19-C20
8	3	407	BCL	C3A-C2A-CAA-CBA
8	A	807	BCL	C3A-C2A-CAA-CBA
8	a	808	BCL	C3A-C2A-CAA-CBA
8	a	805	BCL	C5-C6-C7-C8
13	C	302	F39	C13-C14-C18-C19
9	a	822	CDL	C58-C59-C60-C61
9	a	822	CDL	C76-C77-C78-C79
14	A	818	LHG	C28-C29-C30-C31
14	E	101	LHG	C25-C26-C27-C28
13	C	302	F39	C22-C23-C24-C26
14	A	816	LHG	C10-C11-C12-C13
8	6	402	BCL	C5-C6-C7-C8
8	6	401	BCL	C4-C3-C5-C6
8	1	401	BCL	C2-C3-C5-C6
8	3	404	BCL	C2-C3-C5-C6
8	2	403	BCL	C2-C3-C5-C6
14	A	816	LHG	C14-C15-C16-C17
8	2	401	BCL	C1-C2-C3-C5
14	a	817	LHG	O1-C1-C2-O2
13	C	302	F39	C29-C30-C31-C33
14	A	819	LHG	C15-C16-C17-C18
8	4	406	BCL	O1A-CGA-O2A-C1
8	3	404	BCL	C16-C17-C18-C20
8	4	403	BCL	C16-C17-C18-C19
8	2	401	BCL	C3-C5-C6-C7
11	A	801	GS0	C10-C11-C12-C13
14	a	819	LHG	C1-C2-C3-O3
9	1	409	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	C	302	F39	C26-C28-C29-C30
8	3	403	BCL	C10-C11-C12-C13
8	a	811	BCL	C8-C10-C11-C12
9	1	409	CDL	C15-C16-C17-C18
9	c	303	CDL	C54-C55-C56-C57
14	A	819	LHG	C7-C8-C9-C10
8	6	405	BCL	C3-C5-C6-C7
14	a	819	LHG	C24-C25-C26-C27
14	a	821	LHG	C27-C28-C29-C30
8	4	409	BCL	C15-C16-C17-C18
8	5	403	BCL	C15-C16-C17-C18
8	3	402	BCL	C4-C3-C5-C6
8	1	403	BCL	C6-C7-C8-C10
8	1	406	BCL	C2-C3-C5-C6
8	3	401	BCL	C2-C3-C5-C6
8	3	406	BCL	C2-C3-C5-C6
8	2	406	BCL	C12-C13-C15-C16
8	A	810	BCL	C12-C13-C15-C16
8	a	811	BCL	C12-C13-C15-C16
8	4	401	BCL	C2-C3-C5-C6
8	6	401	BCL	C2-C3-C5-C6
8	6	401	BCL	C12-C13-C15-C16
12	A	802	G2O	C12-C13-C15-C16
8	4	402	BCL	C3-C5-C6-C7
14	A	818	LHG	C11-C10-C9-C8
8	1	408	BCL	C8-C10-C11-C12
8	3	404	BCL	C16-C17-C18-C19
8	a	805	BCL	C6-C7-C8-C9
9	a	822	CDL	CB5-C51-C52-C53
8	3	403	BCL	C2A-CAA-CBA-CGA
8	c	301	BCL	C2A-CAA-CBA-CGA
8	4	402	BCL	C15-C16-C17-C18
8	4	409	BCL	C10-C11-C12-C13
12	A	822	G2O	C13-C15-C16-C17
14	A	816	LHG	C27-C28-C29-C30
8	3	404	BCL	C5-C6-C7-C8
8	6	405	BCL	C15-C16-C17-C18
11	a	802	GS0	C10-C11-C12-C13
14	a	819	LHG	C28-C29-C30-C31
15	A	817	LMG	C29-C28-O8-C9
9	a	822	CDL	C75-C76-C77-C78
9	c	303	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
14	A	818	LHG	C24-C25-C26-C27
15	A	817	LMG	C12-C13-C14-C15
9	1	409	CDL	OA5-CA3-CA4-OA6
9	a	822	CDL	C73-C74-C75-C76
13	C	302	F39	C44-C51-C57-C59
8	3	401	BCL	C15-C16-C17-C18
14	a	817	LHG	C11-C10-C9-C8
15	A	817	LMG	C2-C1-O1-C7
8	2	401	BCL	CBA-CGA-O2A-C1
8	6	404	BCL	C16-C17-C18-C20
9	a	820	CDL	C57-C58-C59-C60
14	a	817	LHG	C11-C12-C13-C14
15	a	818	LMG	C15-C16-C17-C18
8	5	401	BCL	C14-C13-C15-C16
8	5	406	BCL	C11-C10-C8-C9
9	1	409	CDL	C60-C61-C62-C63
8	5	403	BCL	C3-C5-C6-C7
9	c	303	CDL	C11-C12-C13-C14
9	a	822	CDL	C16-C17-C18-C19
14	A	819	LHG	C10-C11-C12-C13
8	1	403	BCL	C1A-C2A-CAA-CBA
8	1	407[B]	BCL	C1A-C2A-CAA-CBA
8	3	407	BCL	C1A-C2A-CAA-CBA
8	A	806	BCL	C1A-C2A-CAA-CBA
8	A	807	BCL	C1A-C2A-CAA-CBA
8	A	810	BCL	C1A-C2A-CAA-CBA
8	A	811	BCL	C1A-C2A-CAA-CBA
8	A	812	BCL	C1A-C2A-CAA-CBA
8	a	808	BCL	C1A-C2A-CAA-CBA
8	a	810	BCL	C1A-C2A-CAA-CBA
8	a	812	BCL	C1A-C2A-CAA-CBA
8	4	410[B]	BCL	C1A-C2A-CAA-CBA
8	6	403	BCL	C1A-C2A-CAA-CBA
8	6	405	BCL	C1A-C2A-CAA-CBA
8	5	403	BCL	C1A-C2A-CAA-CBA
11	A	801	GS0	C1A-C2A-CAA-CBA
11	a	802	GS0	C1A-C2A-CAA-CBA
12	A	822	G2O	C1A-C2A-CAA-CBA
12	a	801	G2O	C1A-C2A-CAA-CBA
8	5	405	BCL	C16-C17-C18-C20
9	1	409	CDL	C13-C14-C15-C16
14	a	817	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
13	A	814	F39	C20-C27-C32-C35
17	a	815	F26	C26-C30-C32-C35
17	c	302	F26	C31-C33-C38-C39
9	a	820	CDL	CA3-OA5-PA1-OA2
9	a	820	CDL	CB3-OB5-PB2-OB2
14	A	816	LHG	C4-O6-P-O3
8	A	811	BCL	C3-C5-C6-C7
8	6	403	BCL	C3-C5-C6-C7
8	2	408	BCL	C5-C6-C7-C8
8	5	404	BCL	C5-C6-C7-C8
9	1	409	CDL	OA5-CA3-CA4-CA6
9	c	303	CDL	OA5-CA3-CA4-CA6
14	A	819	LHG	O6-C4-C5-C6
13	A	815	F39	C24-C26-C28-C29
9	a	822	CDL	C13-C14-C15-C16
9	a	822	CDL	C20-C21-C22-C23
15	a	818	LMG	C14-C15-C16-C17
14	A	819	LHG	C26-C27-C28-C29
9	a	820	CDL	CB5-C51-C52-C53
8	4	407	BCL	C4-C3-C5-C6
8	1	406	BCL	C2C-C3C-CAC-CBC
8	1	408	BCL	C2C-C3C-CAC-CBC
8	2	405	BCL	C2C-C3C-CAC-CBC
8	2	408	BCL	C2C-C3C-CAC-CBC
8	A	807	BCL	C2C-C3C-CAC-CBC
8	A	809	BCL	C2C-C3C-CAC-CBC
8	a	807	BCL	C2C-C3C-CAC-CBC
8	a	810	BCL	C2C-C3C-CAC-CBC
8	4	402	BCL	C2C-C3C-CAC-CBC
8	6	403	BCL	C2C-C3C-CAC-CBC
8	c	301	BCL	C2C-C3C-CAC-CBC
11	a	802	GS0	C2C-C3C-CAC-CBC
14	A	816	LHG	C26-C27-C28-C29
8	a	811	BCL	O1A-CGA-O2A-C1
14	a	819	LHG	C27-C28-C29-C30
9	1	409	CDL	CB3-CB4-CB6-OB8
9	a	820	CDL	CB3-CB4-CB6-OB8
14	a	817	LHG	C26-C27-C28-C29
14	E	101	LHG	C4-C5-C6-O8
8	a	812	BCL	C8-C10-C11-C12
9	a	820	CDL	C15-C16-C17-C18
9	a	820	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
9	a	822	CDL	C14-C15-C16-C17
14	a	821	LHG	C29-C30-C31-C32
12	a	801	G2O	C15-C16-C17-C18
8	1	404	BCL	C4-C3-C5-C6
8	1	406	BCL	C4-C3-C5-C6
8	2	403	BCL	C4-C3-C5-C6
9	a	822	CDL	CA5-C11-C12-C13
9	a	820	CDL	C58-C59-C60-C61
13	A	814	F39	C28-C29-C30-C31
9	a	822	CDL	CA6-CA4-OA6-CA5
14	A	819	LHG	C6-C5-O7-C7
8	4	402	BCL	C2-C1-O2A-CGA
14	A	818	LHG	C30-C31-C32-C33
8	2	406	BCL	C3-C5-C6-C7
9	1	409	CDL	C52-C53-C54-C55
14	A	819	LHG	C30-C31-C32-C33
15	A	817	LMG	O10-C28-O8-C9
13	C	302	F39	C21-C22-C23-C24
14	A	818	LHG	C17-C18-C19-C20
14	A	818	LHG	C29-C30-C31-C32
15	a	818	LMG	C18-C19-C20-C21
8	4	405	BCL	C5-C6-C7-C8
15	a	818	LMG	C2-C1-O1-C7
17	c	302	F26	C28-C31-C33-C38
9	1	409	CDL	OA6-CA4-CA6-OA8
8	5	406	BCL	C15-C16-C17-C18
13	A	815	F39	C21-C22-C23-C24
8	4	401	BCL	C4-C3-C5-C6
9	c	303	CDL	C74-C75-C76-C77
8	1	406	BCL	C11-C10-C8-C7
8	3	402	BCL	C11-C10-C8-C7
8	3	404	BCL	C11-C10-C8-C7
8	2	401	BCL	C12-C13-C15-C16
8	2	403	BCL	C12-C13-C15-C16
8	2	404	BCL	C11-C10-C8-C7
8	a	808	BCL	C11-C12-C13-C15
8	a	812	BCL	C11-C12-C13-C15
8	4	404	BCL	C6-C7-C8-C10
8	4	407	BCL	C2-C3-C5-C6
8	4	407	BCL	C11-C10-C8-C7
8	4	409	BCL	C6-C7-C8-C10
8	4	409	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
8	5	401	BCL	C12-C13-C15-C16
8	5	403	BCL	C11-C12-C13-C15
8	5	406	BCL	C11-C10-C8-C7
11	A	801	GS0	C12-C13-C15-C16
12	a	801	G2O	C12-C13-C15-C16
8	1	406	BCL	C11-C10-C8-C9
8	3	402	BCL	C11-C10-C8-C9
8	3	403	BCL	C11-C12-C13-C14
8	3	404	BCL	C11-C10-C8-C9
8	2	401	BCL	C11-C12-C13-C14
8	2	401	BCL	C14-C13-C15-C16
8	2	403	BCL	C14-C13-C15-C16
8	2	408	BCL	C11-C10-C8-C9
8	A	805	BCL	C11-C12-C13-C14
8	4	407	BCL	C11-C10-C8-C9
8	5	402	BCL	C11-C10-C8-C9
12	A	802	G2O	C14-C13-C15-C16
12	a	801	G2O	C14-C13-C15-C16
8	3	402	BCL	CBA-CGA-O2A-C1
8	5	406	BCL	CBA-CGA-O2A-C1
8	a	808	BCL	C13-C15-C16-C17
8	4	402	BCL	C2A-CAA-CBA-CGA
8	5	402	BCL	O1A-CGA-O2A-C1
13	A	814	F39	C40-C41-C42-C43
13	A	815	F39	C53-C56-C58-C60
13	a	816	F39	C65-C62-C64-C63
8	1	408	BCL	C16-C17-C18-C19
8	2	407	BCL	C16-C17-C18-C19
8	6	404	BCL	C16-C17-C18-C19
13	C	302	F39	C40-C41-C42-C44
17	a	815	F26	C9-C15-C19-C24
14	A	819	LHG	C1-C2-C3-O3
8	3	406	BCL	CBA-CGA-O2A-C1
12	a	803	G2O	CBA-CGA-O2A-C1
9	c	303	CDL	C58-C59-C60-C61
9	a	820	CDL	C12-C13-C14-C15
9	1	409	CDL	C56-C57-C58-C59
14	a	817	LHG	C29-C30-C31-C32
12	A	822	G2O	C10-C11-C12-C13
8	6	404	BCL	C1-C2-C3-C5
8	5	405	BCL	C1-C2-C3-C5
8	3	406	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	A	810	BCL	C4-C3-C5-C6
8	a	808	BCL	C4-C3-C5-C6
8	4	406	BCL	C4-C3-C5-C6
8	6	404	BCL	C4-C3-C5-C6
8	5	404	BCL	C4-C3-C5-C6
8	1	402	BCL	C2-C3-C5-C6
8	1	408	BCL	C2-C3-C5-C6
8	2	408	BCL	C2-C3-C5-C6
8	A	807	BCL	C2-C3-C5-C6
8	5	406	BCL	C2-C3-C5-C6
17	c	302	F26	C18-C13-C8-C10
8	2	401	BCL	C13-C15-C16-C17
8	5	405	BCL	C16-C17-C18-C19
9	a	820	CDL	C55-C56-C57-C58
8	2	402[B]	BCL	C3A-C2A-CAA-CBA
8	A	806	BCL	C3A-C2A-CAA-CBA
8	a	807	BCL	C3A-C2A-CAA-CBA
8	a	813	BCL	C3A-C2A-CAA-CBA
8	1	406	BCL	C15-C16-C17-C18
8	a	806	BCL	C5-C6-C7-C8
13	a	816	F39	C31-C33-C34-C36
8	1	408	BCL	C16-C17-C18-C20
8	a	805	BCL	CBA-CGA-O2A-C1
9	1	409	CDL	C62-C63-C64-C65
8	6	403	BCL	C15-C16-C17-C18
9	a	822	CDL	CB3-CB4-CB6-OB8
14	A	816	LHG	C11-C10-C9-C8
8	a	805	BCL	O2A-C1-C2-C3
8	a	806	BCL	C3-C5-C6-C7
8	6	406	BCL	C15-C16-C17-C18
8	a	811	BCL	C4-C3-C5-C6
8	4	405	BCL	C4-C3-C5-C6
9	1	409	CDL	C12-C13-C14-C15
8	4	407	BCL	C5-C6-C7-C8
9	c	303	CDL	CA3-OA5-PA1-OA2
14	E	101	LHG	C3-O3-P-O6
8	2	407	BCL	C3-C5-C6-C7
8	A	805	BCL	C3-C5-C6-C7
8	3	405	BCL	C2A-CAA-CBA-CGA
9	1	409	CDL	C57-C58-C59-C60
9	a	820	CDL	OB5-CB3-CB4-OB6
9	c	303	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
12	A	822	G2O	CBA-CGA-O2A-C1
8	3	407	BCL	C16-C17-C18-C20
8	4	409	BCL	C16-C17-C18-C20
14	A	819	LHG	C17-C18-C19-C20
9	1	409	CDL	OB6-CB4-CB6-OB8
9	a	820	CDL	OB6-CB4-CB6-OB8
14	A	818	LHG	O7-C5-C6-O8
14	a	819	LHG	O7-C5-C6-O8
14	E	101	LHG	O7-C5-C6-O8
12	A	822	G2O	O1D-CGD-O2D-CED
8	6	405	BCL	C16-C17-C18-C19
9	a	822	CDL	C44-C45-C46-C47
14	E	101	LHG	C1-C2-C3-O3
8	A	807	BCL	C4-C3-C5-C6
8	3	406	BCL	C2-C1-O2A-CGA
8	2	403	BCL	C2-C1-O2A-CGA
8	a	811	BCL	C2-C1-O2A-CGA
8	4	401	BCL	C2-C1-O2A-CGA
8	5	403	BCL	C2-C1-O2A-CGA
12	A	802	G2O	C15-C16-C17-C18
8	1	402	BCL	C11-C10-C8-C9
8	A	810	BCL	C6-C7-C8-C9
8	a	806	BCL	C11-C12-C13-C14
8	4	401	BCL	C14-C13-C15-C16
8	4	403	BCL	C11-C10-C8-C9
8	6	408	BCL	C6-C7-C8-C9
14	a	819	LHG	C13-C14-C15-C16
8	A	811	BCL	C2A-CAA-CBA-CGA
8	6	402	BCL	C2A-CAA-CBA-CGA
9	a	822	CDL	C40-C41-C42-C43
9	a	822	CDL	C61-C62-C63-C64
9	c	303	CDL	C71-CB7-OB8-CB6
8	2	402[B]	BCL	C4C-C3C-CAC-CBC
8	4	408[B]	BCL	C4C-C3C-CAC-CBC
8	4	410[B]	BCL	C4C-C3C-CAC-CBC
8	6	407[B]	BCL	C4C-C3C-CAC-CBC
9	c	303	CDL	C31-C32-C33-C34
8	2	407	BCL	C16-C17-C18-C20
13	A	814	F39	C16-C13-O2-C11
13	A	815	F39	C16-C13-O2-C11
13	a	816	F39	C16-C13-O2-C11
9	a	820	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	a	820	CDL	OA5-CA3-CA4-CA6
9	a	822	CDL	OA5-CA3-CA4-CA6
9	c	303	CDL	OB5-CB3-CB4-CB6
14	E	101	LHG	O6-C4-C5-C6
8	1	402	BCL	C11-C10-C8-C7
8	3	403	BCL	C6-C7-C8-C10
8	3	403	BCL	C11-C12-C13-C15
8	2	405	BCL	C6-C7-C8-C10
8	2	408	BCL	C11-C10-C8-C7
8	A	805	BCL	C11-C12-C13-C15
8	A	810	BCL	C11-C12-C13-C15
8	a	806	BCL	C12-C13-C15-C16
8	a	811	BCL	C6-C7-C8-C10
8	4	403	BCL	C11-C10-C8-C7
8	4	404	BCL	C11-C12-C13-C15
8	6	403	BCL	C11-C12-C13-C15
8	5	402	BCL	C11-C10-C8-C7
11	a	802	GS0	C12-C13-C15-C16
13	C	302	F39	C28-C29-C30-C31
8	1	406	BCL	C1-C2-C3-C4
13	C	302	F39	C42-C44-C51-C57
8	a	812	BCL	C16-C17-C18-C20
8	6	405	BCL	C16-C17-C18-C20
8	1	404	BCL	C15-C16-C17-C18
13	A	814	F39	C38-C37-C39-C40
13	A	815	F39	C38-C37-C39-C40
14	A	816	LHG	C13-C14-C15-C16
8	3	407	BCL	C16-C17-C18-C19
8	4	406	BCL	CBA-CGA-O2A-C1
8	3	404	BCL	CAA-CBA-CGA-O2A
9	1	409	CDL	C31-C32-C33-C34
15	A	817	LMG	C16-C17-C18-C19
8	1	406	BCL	CAD-CBD-CGD-O2D
8	3	405	BCL	CAD-CBD-CGD-O2D
8	3	406	BCL	CAD-CBD-CGD-O2D
8	2	402[B]	BCL	CAD-CBD-CGD-O2D
8	2	407	BCL	CAD-CBD-CGD-O2D
8	A	811	BCL	CAD-CBD-CGD-O2D
8	A	813	BCL	CAD-CBD-CGD-O2D
8	4	406	BCL	CAD-CBD-CGD-O2D
8	6	402	BCL	CAD-CBD-CGD-O2D
8	5	405	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	5	406	BCL	CAD-CBD-CGD-O2D
8	C	301	BCL	CAD-CBD-CGD-O2D
12	A	802	G2O	C2B-C3B-CAB-CBB
17	c	302	F26	C17-C13-C18-C22
14	A	816	LHG	C25-C26-C27-C28
14	a	821	LHG	C31-C32-C33-C34
8	3	404	BCL	C8-C10-C11-C12
15	a	818	LMG	C30-C31-C32-C33
14	E	101	LHG	C2-C3-O3-P
15	A	817	LMG	O1-C7-C8-C9
15	a	818	LMG	O1-C7-C8-C9
9	c	303	CDL	OB9-CB7-OB8-CB6
12	A	822	G2O	O1A-CGA-O2A-C1
9	a	820	CDL	OA5-CA3-CA4-OA6
14	A	819	LHG	O6-C4-C5-O7
14	E	101	LHG	O6-C4-C5-O7
14	a	821	LHG	C30-C31-C32-C33
8	A	804	BCL	C6-C7-C8-C9
8	1	405	BCL	CHA-CBD-CGD-O1D
8	1	407[B]	BCL	CHA-CBD-CGD-O1D
8	1	407[B]	BCL	CHA-CBD-CGD-O2D
8	3	403	BCL	CHA-CBD-CGD-O2D
8	3	405	BCL	CHA-CBD-CGD-O1D
8	2	404	BCL	CHA-CBD-CGD-O1D
8	2	404	BCL	CHA-CBD-CGD-O2D
8	2	406	BCL	CHA-CBD-CGD-O1D
8	2	406	BCL	CHA-CBD-CGD-O2D
8	a	808	BCL	CHA-CBD-CGD-O1D
8	a	808	BCL	CHA-CBD-CGD-O2D
8	4	403	BCL	CHA-CBD-CGD-O1D
8	4	405	BCL	CHA-CBD-CGD-O1D
8	4	405	BCL	CHA-CBD-CGD-O2D
8	4	406	BCL	CHA-CBD-CGD-O1D
8	4	408[B]	BCL	CHA-CBD-CGD-O1D
8	4	408[B]	BCL	CHA-CBD-CGD-O2D
8	4	410[B]	BCL	CHA-CBD-CGD-O1D
8	6	405	BCL	CHA-CBD-CGD-O1D
8	6	405	BCL	CHA-CBD-CGD-O2D
8	1	408	BCL	O1A-CGA-O2A-C1
8	4	405	BCL	O1A-CGA-O2A-C1
12	a	803	G2O	O1A-CGA-O2A-C1
14	A	816	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
8	4	403	BCL	C1-C2-C3-C5
8	3	403	BCL	C3-C5-C6-C7
8	3	401	BCL	C4-C3-C5-C6
8	6	408	BCL	C13-C15-C16-C17
8	A	810	BCL	C11-C12-C13-C14
8	4	404	BCL	C11-C12-C13-C14
8	6	401	BCL	C14-C13-C15-C16
8	6	403	BCL	C11-C12-C13-C14
8	a	812	BCL	C2A-CAA-CBA-CGA
13	A	814	F39	C53-C56-C58-C60
13	C	302	F39	C65-C62-C64-C63
13	C	302	F39	C24-C26-C28-C29
8	a	805	BCL	C1A-C2A-CAA-CBA
8	1	406	BCL	C16-C17-C18-C19
8	2	408	BCL	C16-C17-C18-C19
9	1	409	CDL	C21-C22-C23-C24
8	6	408	BCL	C2-C1-O2A-CGA
13	a	816	F39	C42-C44-C51-C57
13	C	302	F39	C51-C57-C59-C62
9	a	820	CDL	CA2-OA2-PA1-OA5
9	c	303	CDL	C56-C57-C58-C59
9	1	409	CDL	C1-CB2-OB2-PB2
9	c	303	CDL	C1-CA2-OA2-PA1
8	4	403	BCL	C2-C3-C5-C6
9	1	409	CDL	CA2-OA2-PA1-OA3
9	a	820	CDL	CA2-OA2-PA1-OA3
9	a	820	CDL	CA2-OA2-PA1-OA4
9	a	820	CDL	CB3-OB5-PB2-OB4
9	a	822	CDL	CA2-OA2-PA1-OA4
12	A	822	G2O	C11-C10-C8-C7
12	a	801	G2O	C11-C10-C8-C7
14	A	816	LHG	C4-O6-P-O4
14	A	818	LHG	C3-O3-P-O5
14	A	819	LHG	C3-O3-P-O5
14	a	817	LHG	C3-O3-P-O4
14	a	817	LHG	C4-O6-P-O4
14	E	101	LHG	C3-O3-P-O4
8	1	406	BCL	C16-C17-C18-C20
8	3	405	BCL	C16-C17-C18-C19
8	3	405	BCL	C16-C17-C18-C20
9	a	822	CDL	C32-C33-C34-C35
8	1	404	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
8	a	808	BCL	C3-C5-C6-C7
13	A	814	F39	C14-C18-C19-C20
8	5	402	BCL	C10-C11-C12-C13
8	1	404	BCL	CAD-CBD-CGD-O1D
8	1	407[B]	BCL	CAD-CBD-CGD-O1D
8	3	402	BCL	CAD-CBD-CGD-O1D
8	2	404	BCL	CAD-CBD-CGD-O1D
8	2	409[B]	BCL	CAD-CBD-CGD-O1D
8	4	403	BCL	CAD-CBD-CGD-O1D
8	4	408[B]	BCL	CAD-CBD-CGD-O1D
8	4	410[B]	BCL	CAD-CBD-CGD-O1D
8	6	407[B]	BCL	CAD-CBD-CGD-O1D
8	c	301	BCL	CAD-CBD-CGD-O1D
12	A	822	G2O	CAD-CBD-CGD-O1D
12	a	801	G2O	CAD-CBD-CGD-O1D
8	4	405	BCL	CAA-CBA-CGA-O2A
8	4	406	BCL	C16-C17-C18-C20
8	3	401	BCL	C11-C12-C13-C15
8	3	403	BCL	C11-C10-C8-C7
8	2	401	BCL	C11-C12-C13-C15
8	A	804	BCL	C2C-C3C-CAC-CBC
8	a	805	BCL	C2C-C3C-CAC-CBC
8	a	806	BCL	C11-C12-C13-C15
8	4	401	BCL	C12-C13-C15-C16
8	4	404	BCL	C2-C3-C5-C6
8	4	406	BCL	C11-C10-C8-C7
8	6	402	BCL	C11-C10-C8-C7
8	6	403	BCL	C6-C7-C8-C10
8	6	406	BCL	C2C-C3C-CAC-CBC
9	a	822	CDL	OA5-CA3-CA4-OA6
12	a	801	G2O	C11-C12-C13-C15
13	a	816	F39	C13-C14-C18-C19
14	A	816	LHG	C9-C10-C11-C12
8	1	402	BCL	C2A-CAA-CBA-CGA
8	2	408	BCL	C16-C17-C18-C20
8	a	808	BCL	C16-C17-C18-C20
13	A	815	F39	O2-C13-C14-C18
13	C	302	F39	O2-C13-C14-C18
14	A	818	LHG	C4-C5-C6-O8
14	a	819	LHG	C4-C5-C6-O8
9	a	822	CDL	OA6-CA4-CA6-OA8
9	a	822	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
15	A	817	LMG	O1-C7-C8-O7
15	a	818	LMG	O1-C7-C8-O7
14	E	101	LHG	C9-C10-C11-C12
8	2	404	BCL	O1A-CGA-O2A-C1
8	6	406	BCL	C13-C15-C16-C17
13	a	816	F39	C29-C30-C31-C33
14	A	816	LHG	C2-C3-O3-P
8	4	403	BCL	C8-C10-C11-C12
17	c	302	F26	C17-C13-C8-C10
8	2	405	BCL	C2-C3-C5-C6
8	2	403	BCL	C15-C16-C17-C18
8	2	401	BCL	C6-C7-C8-C9
8	2	404	BCL	C11-C10-C8-C9
8	a	808	BCL	C11-C12-C13-C14
8	a	811	BCL	C14-C13-C15-C16
8	4	406	BCL	C11-C10-C8-C9
8	4	409	BCL	C14-C13-C15-C16
8	5	403	BCL	C11-C12-C13-C14
11	A	801	GS0	C14-C13-C15-C16
8	3	401	BCL	O1A-CGA-O2A-C1
8	3	406	BCL	O1A-CGA-O2A-C1
13	A	815	F39	C58-C61-C63-C64
13	A	815	F39	C65-C62-C64-C63
8	3	403	BCL	C8-C10-C11-C12
8	4	407	BCL	C8-C10-C11-C12
8	A	811	BCL	C10-C11-C12-C13
8	6	404	BCL	C15-C16-C17-C18
9	1	409	CDL	CA6-CA4-OA6-CA5
14	a	821	LHG	C6-C5-O7-C7
9	a	820	CDL	OB5-CB3-CB4-CB6
8	6	407[B]	BCL	C2A-CAA-CBA-CGA
8	1	408	BCL	C2-C1-O2A-CGA
8	3	405	BCL	C2-C1-O2A-CGA
8	A	810	BCL	C2-C1-O2A-CGA
8	4	409	BCL	C2-C1-O2A-CGA
12	a	803	G2O	C2-C1-O2A-CGA
14	a	817	LHG	C2-C3-O3-P
9	a	820	CDL	C13-C14-C15-C16
9	c	303	CDL	OA5-CA3-CA4-OA6
8	1	405	BCL	C16-C17-C18-C20
8	A	810	BCL	C5-C6-C7-C8
8	A	804	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
11	a	802	GS0	O1A-CGA-O2A-C1
8	4	404	BCL	C15-C16-C17-C18
15	A	817	LMG	C30-C31-C32-C33
9	1	409	CDL	CA3-OA5-PA1-OA2
14	A	819	LHG	C4-O6-P-O3
14	a	821	LHG	C3-O3-P-O6
9	a	822	CDL	C39-C40-C41-C42
8	2	401	BCL	C10-C11-C12-C13
8	2	406	BCL	C4-C3-C5-C6
8	3	403	BCL	C11-C10-C8-C9
8	6	402	BCL	C11-C10-C8-C9
11	a	802	GS0	C14-C13-C15-C16
8	3	401	BCL	C16-C17-C18-C19
8	3	403	BCL	C16-C17-C18-C19
8	4	406	BCL	C16-C17-C18-C19
8	1	402	BCL	C15-C16-C17-C18
8	2	405	BCL	C5-C6-C7-C8
8	5	401	BCL	C15-C16-C17-C18
8	1	404	BCL	C16-C17-C18-C20
8	2	406	BCL	C16-C17-C18-C20
8	A	807	BCL	C13-C15-C16-C17
9	1	409	CDL	C24-C25-C26-C27
8	4	403	BCL	O1A-CGA-O2A-C1
9	a	820	CDL	C56-C57-C58-C59
8	3	406	BCL	C15-C16-C17-C18
17	a	815	F26	C31-C33-C38-C39
15	a	818	LMG	C16-C17-C18-C19
9	c	303	CDL	C75-C76-C77-C78
8	A	803	BCL	CAA-CBA-CGA-O1A
17	c	302	F26	C18-C22-C25-C26
8	2	404	BCL	C3-C5-C6-C7
8	5	404	BCL	C3-C5-C6-C7
12	a	803	G2O	C13-C15-C16-C17
14	A	816	LHG	C15-C16-C17-C18
8	2	404	BCL	C2-C1-O2A-CGA
8	A	805	BCL	C2-C1-O2A-CGA
8	A	807	BCL	C2-C1-O2A-CGA
8	a	808	BCL	C2-C1-O2A-CGA
8	4	404	BCL	C2-C1-O2A-CGA
14	A	818	LHG	C15-C16-C17-C18
8	6	408	BCL	C16-C17-C18-C20
14	A	819	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
14	a	821	LHG	O7-C5-C6-O8
14	A	819	LHG	C33-C34-C35-C36
8	1	408	BCL	C3A-C2A-CAA-CBA
8	4	409	BCL	C16-C17-C18-C19
14	A	819	LHG	C29-C30-C31-C32
8	a	808	BCL	C2-C3-C5-C6
8	6	406	BCL	C2-C3-C5-C6
9	a	820	CDL	C74-C75-C76-C77
8	5	404	BCL	CAA-CBA-CGA-O2A
8	A	811	BCL	C11-C10-C8-C9
8	A	811	BCL	C11-C12-C13-C14
9	c	303	CDL	CA2-C1-CB2-OB2
9	c	303	CDL	OA7-CA5-OA6-CA4
8	5	406	BCL	C16-C17-C18-C19
8	3	407	BCL	CBA-CGA-O2A-C1
8	4	406	BCL	C3-C5-C6-C7
8	A	803	BCL	CAA-CBA-CGA-O2A
8	1	401	BCL	C4-C3-C5-C6
8	1	408	BCL	C1A-C2A-CAA-CBA
8	2	402[B]	BCL	C1A-C2A-CAA-CBA
8	a	807	BCL	C1A-C2A-CAA-CBA
8	4	404	BCL	C1A-C2A-CAA-CBA
8	6	407[B]	BCL	C1A-C2A-CAA-CBA
8	1	401	BCL	C11-C12-C13-C15
8	1	403	BCL	C11-C12-C13-C15
8	3	404	BCL	C6-C7-C8-C10
8	2	401	BCL	C11-C10-C8-C7
8	2	405	BCL	C11-C12-C13-C15
8	A	805	BCL	C6-C7-C8-C10
8	4	409	BCL	C11-C10-C8-C7
8	5	405	BCL	C11-C10-C8-C7
9	a	822	CDL	C35-C36-C37-C38
8	2	404	BCL	C2A-CAA-CBA-CGA
8	4	403	BCL	C2A-CAA-CBA-CGA
14	A	818	LHG	O6-C4-C5-O7
14	A	818	LHG	O8-C23-C24-C25
8	a	804	BCL	CAA-CBA-CGA-O1A
9	a	820	CDL	C73-C74-C75-C76
8	1	408	BCL	CBA-CGA-O2A-C1
8	1	405	BCL	C16-C17-C18-C19
8	A	808	BCL	CAA-CBA-CGA-O2A
8	A	804	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	C	302	F39	C18-C19-C20-C27
8	a	809	BCL	CAA-CBA-CGA-O2A
8	3	407	BCL	C13-C15-C16-C17
8	1	404	BCL	O1A-CGA-O2A-C1
9	a	820	CDL	CA2-C1-CB2-OB2
8	a	804	BCL	CAA-CBA-CGA-O2A
8	2	408	BCL	C4-C3-C5-C6
8	1	406	BCL	C2-C1-O2A-CGA
8	2	408	BCL	C2-C1-O2A-CGA
8	a	805	BCL	C2-C1-O2A-CGA
8	6	401	BCL	C2-C1-O2A-CGA
8	6	406	BCL	C2-C1-O2A-CGA
8	5	405	BCL	C2-C1-O2A-CGA
8	1	404	BCL	C2-C3-C5-C6
8	A	804	BCL	O1A-CGA-O2A-C1
8	a	809	BCL	CAA-CBA-CGA-O1A
14	a	821	LHG	C25-C26-C27-C28
8	a	806	BCL	C14-C13-C15-C16
8	6	404	BCL	CAA-CBA-CGA-O2A
14	A	818	LHG	C11-C12-C13-C14
14	a	819	LHG	C12-C13-C14-C15
8	4	401	BCL	C16-C17-C18-C19
8	a	805	BCL	O1A-CGA-O2A-C1
9	1	409	CDL	CA3-CA4-CA6-OA8
8	a	812	BCL	C4-C3-C5-C6
8	6	405	BCL	C4-C3-C5-C6
8	5	406	BCL	C4-C3-C5-C6
8	1	401	BCL	C4C-C3C-CAC-CBC
8	a	814	BCL	C4C-C3C-CAC-CBC
8	5	406	BCL	C4C-C3C-CAC-CBC
8	A	808	BCL	CAA-CBA-CGA-O1A
9	c	303	CDL	C11-CA5-OA6-CA4
14	a	821	LHG	O6-C4-C5-O7
8	a	810	BCL	C2A-CAA-CBA-CGA
8	4	402	BCL	C10-C11-C12-C13
13	A	815	F39	C14-C18-C19-C20
8	2	401	BCL	C5-C6-C7-C8
8	6	406	BCL	C4-C3-C5-C6
8	2	407	BCL	C12-C13-C15-C16
8	5	404	BCL	C2-C3-C5-C6
8	4	402	BCL	C5-C6-C7-C8
8	2	404	BCL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
8	2	406	BCL	C1-C2-C3-C4
8	2	408	BCL	C1-C2-C3-C4
8	a	808	BCL	C1-C2-C3-C4
8	a	811	BCL	C1-C2-C3-C4
8	4	407	BCL	C1-C2-C3-C4
8	6	401	BCL	C1-C2-C3-C4
8	6	402	BCL	C1-C2-C3-C4
8	6	406	BCL	C1-C2-C3-C4
8	5	401	BCL	CAA-CBA-CGA-O2A
15	A	817	LMG	C18-C19-C20-C21
8	6	402	BCL	C15-C16-C17-C18
13	C	302	F39	C43-C42-C44-C51
8	1	406	BCL	C13-C15-C16-C17
8	4	402	BCL	C8-C10-C11-C12
8	4	403	BCL	C13-C15-C16-C17
8	5	401	BCL	C1-C2-C3-C5
17	a	815	F26	C19-C15-C9-C2
8	6	404	BCL	C2-C3-C5-C6
8	1	403	BCL	C11-C12-C13-C14
8	2	405	BCL	C11-C12-C13-C14
8	2	406	BCL	C6-C7-C8-C9
8	6	405	BCL	C11-C10-C8-C9
8	5	405	BCL	C11-C10-C8-C9
8	a	811	BCL	C3A-C2A-CAA-CBA
8	6	407[B]	BCL	C3A-C2A-CAA-CBA
13	A	815	F39	C13-C14-C18-C19
8	1	405	BCL	CAD-CBD-CGD-O2D
8	A	803	BCL	CAD-CBD-CGD-O2D
8	A	807	BCL	CAD-CBD-CGD-O2D
8	A	812	BCL	CAD-CBD-CGD-O2D
8	a	809	BCL	CAD-CBD-CGD-O2D
8	4	407	BCL	CAD-CBD-CGD-O2D
8	6	405	BCL	CAD-CBD-CGD-O2D
8	F	101	BCL	CAD-CBD-CGD-O2D
14	A	816	LHG	C30-C31-C32-C33
8	4	406	BCL	C15-C16-C17-C18
8	A	807	BCL	C10-C11-C12-C13
8	3	402	BCL	C2-C1-O2A-CGA
12	A	802	G2O	C2-C1-O2A-CGA
8	a	814	BCL	CAA-CBA-CGA-O2A
8	a	808	BCL	C16-C17-C18-C19
12	A	802	G2O	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	815	F39	C29-C30-C31-C33
9	a	822	CDL	CA3-CA4-CA6-OA8
12	A	802	G2O	C3-C5-C6-C7
14	A	819	LHG	C4-C5-C6-O8
14	a	821	LHG	C4-C5-C6-O8
8	A	807	BCL	O2A-C1-C2-C3
12	A	802	G2O	C4B-C3B-CAB-CBB
8	6	406	BCL	C16-C17-C18-C19
14	E	101	LHG	O2-C2-C3-O3
8	1	403	BCL	CHA-CBD-CGD-O1D
8	1	403	BCL	CHA-CBD-CGD-O2D
8	1	405	BCL	CHA-CBD-CGD-O2D
8	3	405	BCL	CHA-CBD-CGD-O2D
8	3	407	BCL	CHA-CBD-CGD-O1D
8	3	407	BCL	CHA-CBD-CGD-O2D
8	2	405	BCL	CHA-CBD-CGD-O1D
8	2	405	BCL	CHA-CBD-CGD-O2D
8	a	812	BCL	CHA-CBD-CGD-O1D
8	a	813	BCL	CHA-CBD-CGD-O2D
8	4	403	BCL	CHA-CBD-CGD-O2D
8	4	404	BCL	CHA-CBD-CGD-O1D
8	4	404	BCL	CHA-CBD-CGD-O2D
8	4	406	BCL	CHA-CBD-CGD-O2D
8	4	410[B]	BCL	CHA-CBD-CGD-O2D
8	6	404	BCL	CHA-CBD-CGD-O1D
8	5	403	BCL	CHA-CBD-CGD-O1D
8	5	403	BCL	CHA-CBD-CGD-O2D
8	5	405	BCL	CHA-CBD-CGD-O1D
8	5	406	BCL	CHA-CBD-CGD-O2D
11	A	801	GS0	CHA-CBD-CGD-O2D
8	4	405	BCL	C2-C3-C5-C6
14	a	821	LHG	O6-C4-C5-C6
12	A	802	G2O	C16-C17-C18-C20
8	2	406	BCL	CAA-CBA-CGA-O2A
14	A	816	LHG	C29-C30-C31-C32
8	3	402	BCL	O1A-CGA-O2A-C1
15	A	817	LMG	C19-C20-C21-C22
8	3	406	BCL	C11-C10-C8-C7
8	a	806	BCL	C11-C10-C8-C7
8	6	408	BCL	C2-C3-C5-C6
8	a	812	BCL	C16-C17-C18-C19
8	5	406	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	A	815	F39	O6-C21-C22-C23
8	3	405	BCL	C11-C10-C8-C9
8	3	406	BCL	C11-C10-C8-C9
8	2	401	BCL	C11-C10-C8-C9
8	a	806	BCL	C11-C10-C8-C9
8	4	409	BCL	C11-C10-C8-C9
8	4	405	BCL	C8-C10-C11-C12
14	a	819	LHG	C23-C24-C25-C26
9	a	822	CDL	C54-C55-C56-C57
8	6	401	BCL	C15-C16-C17-C18
9	1	409	CDL	C23-C24-C25-C26
8	6	402	BCL	CAA-CBA-CGA-O1A
8	4	402	BCL	C1A-C2A-CAA-CBA
8	4	405	BCL	C1A-C2A-CAA-CBA
8	c	301	BCL	C1A-C2A-CAA-CBA
12	A	802	G2O	CAA-CBA-CGA-O1A
8	2	406	BCL	C8-C10-C11-C12
8	4	407	BCL	O1A-CGA-O2A-C1
8	4	403	BCL	CAA-CBA-CGA-O1A
8	a	806	BCL	C10-C11-C12-C13
8	4	407	BCL	C2A-CAA-CBA-CGA
8	1	403	BCL	C1-C2-C3-C5
8	5	406	BCL	C1-C2-C3-C5
8	2	401	BCL	C16-C17-C18-C20
13	A	815	F39	O7-C21-C22-C23
8	2	408	BCL	C8-C10-C11-C12
9	1	409	CDL	CB2-OB2-PB2-OB3
9	c	303	CDL	CA2-OA2-PA1-OA3
14	a	821	LHG	C3-O3-P-O5
8	1	402	BCL	CAA-CBA-CGA-O1A
14	a	819	LHG	O6-C4-C5-C6
8	2	404	BCL	CAA-CBA-CGA-O1A
8	5	402	BCL	CAA-CBA-CGA-O1A
8	1	401	BCL	CAA-CBA-CGA-O2A
8	6	402	BCL	CAA-CBA-CGA-O2A
8	3	402	BCL	C10-C11-C12-C13
8	F	101	BCL	CAA-CBA-CGA-O2A
8	4	403	BCL	CAA-CBA-CGA-O2A
8	1	402	BCL	CAD-CBD-CGD-O1D
8	1	408	BCL	CAD-CBD-CGD-O1D
8	a	810	BCL	CAD-CBD-CGD-O1D
8	4	402	BCL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	5	402	BCL	CAD-CBD-CGD-O1D
11	a	802	GS0	CAD-CBD-CGD-O1D
8	6	408	BCL	C5-C6-C7-C8
8	1	405	BCL	C11-C10-C8-C9
8	A	807	BCL	C11-C10-C8-C9
14	a	821	LHG	O1-C1-C2-O2
8	4	408[B]	BCL	CAA-CBA-CGA-O2A
8	5	401	BCL	CAA-CBA-CGA-O1A
13	A	815	F39	C31-C33-C34-C36
14	a	817	LHG	C10-C11-C12-C13
9	1	409	CDL	C73-C74-C75-C76
8	1	402	BCL	CAA-CBA-CGA-O2A
8	3	405	BCL	C4-C3-C5-C6
11	a	802	GS0	C4-C3-C5-C6
8	4	405	BCL	C10-C11-C12-C13
8	1	405	BCL	C11-C10-C8-C7
8	3	405	BCL	C11-C10-C8-C7
8	A	807	BCL	C11-C10-C8-C7
8	a	808	BCL	C6-C7-C8-C10
8	6	405	BCL	C11-C10-C8-C7
11	a	802	GS0	CAA-CBA-CGA-O2A
13	a	816	F39	C32-C35-C37-C39
13	a	816	F39	C37-C39-C40-C41
11	A	801	GS0	CAA-CBA-CGA-O2A
8	A	805	BCL	C8-C10-C11-C12
8	5	401	BCL	C8-C10-C11-C12
13	A	815	F39	C22-C23-C24-C26
8	1	406	BCL	C10-C11-C12-C13
8	4	403	BCL	C10-C11-C12-C13
9	c	303	CDL	C52-C51-CB5-OB6
14	A	819	LHG	C28-C29-C30-C31
8	a	808	BCL	C10-C11-C12-C13
14	E	101	LHG	C26-C27-C28-C29
8	6	401	BCL	C8-C10-C11-C12
8	6	404	BCL	C8-C10-C11-C12
8	3	401	BCL	CAA-CBA-CGA-O2A
8	3	407	BCL	CAA-CBA-CGA-O2A
8	A	809	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

91 monomers are involved in 461 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	4	408[B]	BCL	1	0
11	a	802	GS0	2	0
8	a	805	BCL	3	0
8	4	406	BCL	10	0
8	3	403	BCL	6	0
8	5	405	BCL	5	0
8	c	301	BCL	6	0
15	a	818	LMG	1	0
8	6	401	BCL	14	0
12	A	822	G2O	2	0
8	5	402	BCL	10	0
8	a	804	BCL	1	0
8	2	407	BCL	5	0
8	a	814	BCL	2	0
8	F	101	BCL	3	0
8	2	408	BCL	12	0
8	a	810	BCL	2	0
8	3	401	BCL	12	0
14	A	819	LHG	4	0
8	4	401	BCL	9	0
8	2	404	BCL	8	0
8	a	811	BCL	8	0
8	6	402	BCL	10	0
12	a	803	G2O	1	0
14	a	819	LHG	3	0
8	6	405	BCL	5	0
8	5	403	BCL	6	0
8	6	408	BCL	12	0
14	a	821	LHG	5	0
8	4	404	BCL	5	0
8	1	404	BCL	3	0
8	A	812	BCL	2	0
8	1	406	BCL	13	0
8	2	403	BCL	10	0
8	4	410[B]	BCL	3	0
8	A	805	BCL	6	0
8	1	408	BCL	9	0
14	A	816	LHG	2	0
8	2	405	BCL	5	0
8	4	402	BCL	10	0
8	5	404	BCL	9	0
9	c	303	CDL	3	0
8	4	409	BCL	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	806	BCL	4	0
8	A	809	BCL	7	0
13	a	816	F39	1	0
8	a	806	BCL	6	0
8	4	403	BCL	8	0
8	A	803	BCL	3	0
8	1	402	BCL	9	0
8	a	807	BCL	3	0
8	1	405	BCL	11	0
8	3	402	BCL	7	0
8	3	407	BCL	11	0
8	4	405	BCL	6	0
8	2	401	BCL	10	0
8	A	808	BCL	2	0
8	A	807	BCL	3	0
9	a	820	CDL	4	0
8	A	810	BCL	8	0
8	2	409[B]	BCL	3	0
8	2	402[B]	BCL	3	0
8	6	403	BCL	11	0
14	E	101	LHG	1	0
8	3	404	BCL	7	0
8	1	401	BCL	10	0
8	6	404	BCL	8	0
11	A	801	GS0	4	0
8	6	406	BCL	16	0
9	1	409	CDL	7	0
8	5	401	BCL	12	0
8	5	406	BCL	14	0
8	A	804	BCL	4	0
8	a	812	BCL	5	0
12	A	802	G2O	1	0
8	2	406	BCL	9	0
8	a	808	BCL	4	0
8	4	407	BCL	9	0
9	a	822	CDL	8	0
8	a	809	BCL	1	0
15	A	817	LMG	4	0
14	a	817	LHG	2	0
14	A	818	LHG	2	0
8	3	405	BCL	8	0
8	A	811	BCL	7	0

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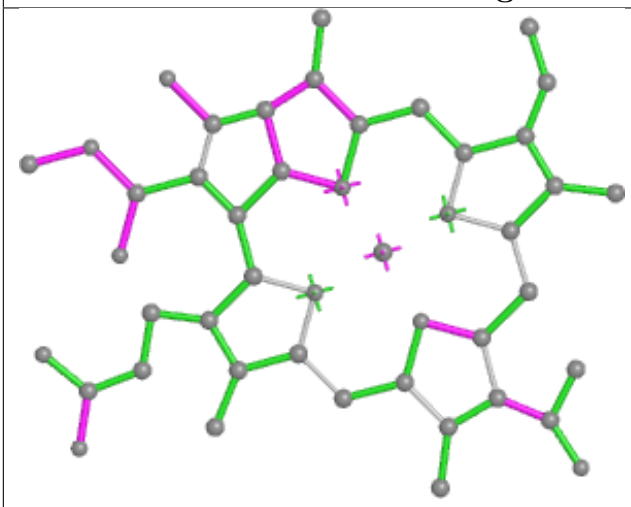
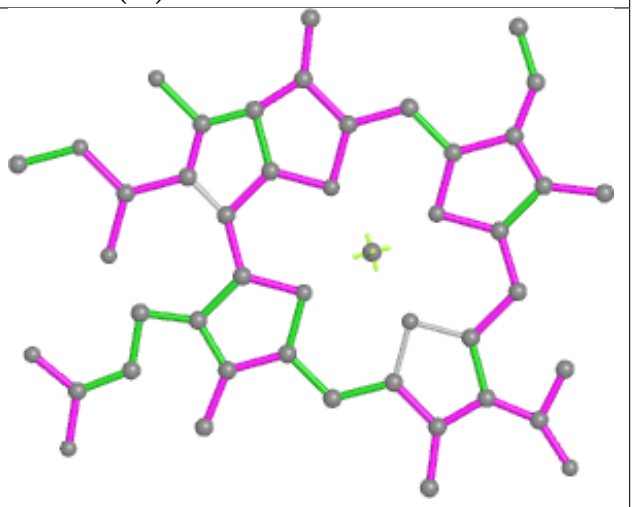
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	302	SF4	2	0
8	3	406	BCL	10	0
8	1	407[B]	BCL	2	0
8	a	813	BCL	3	0
8	C	301	BCL	4	0
8	1	403	BCL	6	0

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

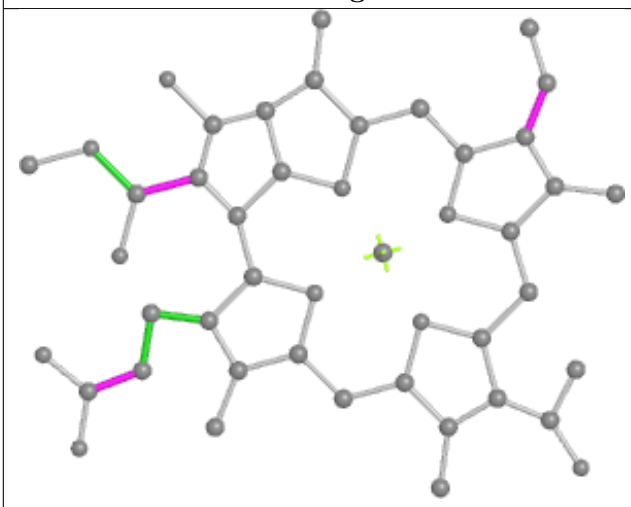
Ligand BCL 4 408 (B)



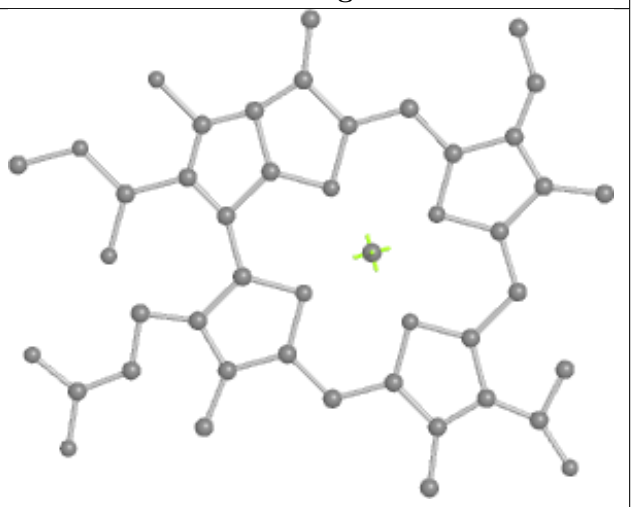
Bond lengths



Bond angles

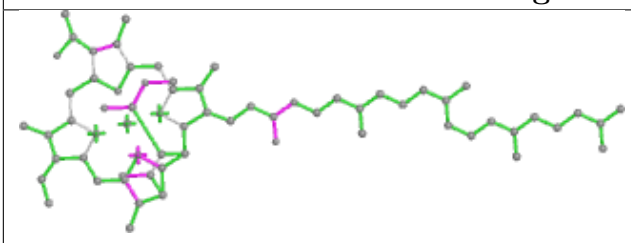


Torsions

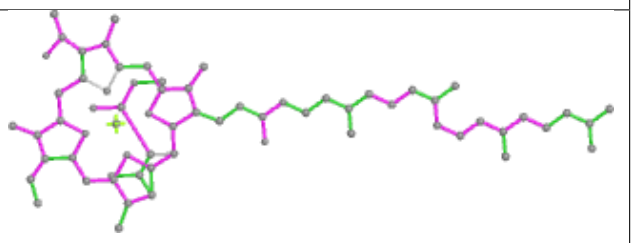


Rings

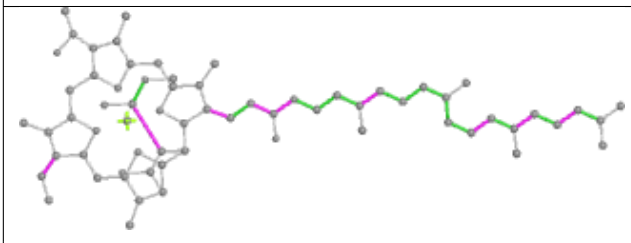
Ligand GS0 a 802



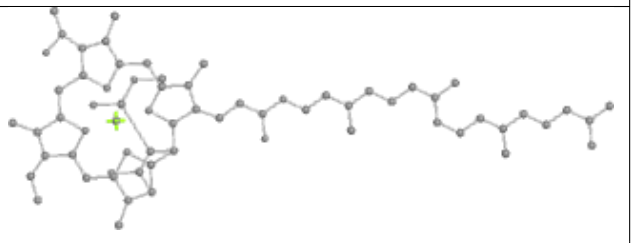
Bond lengths



Bond angles

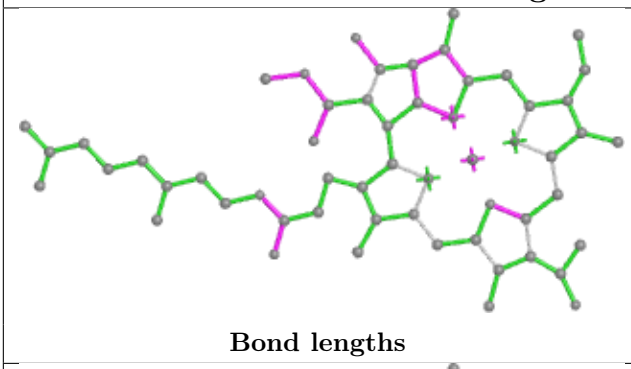


Torsions

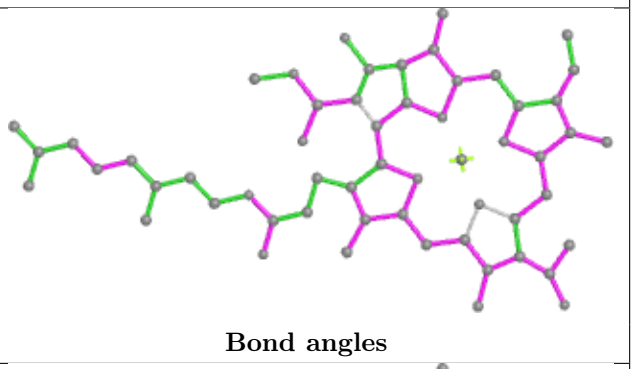


Rings

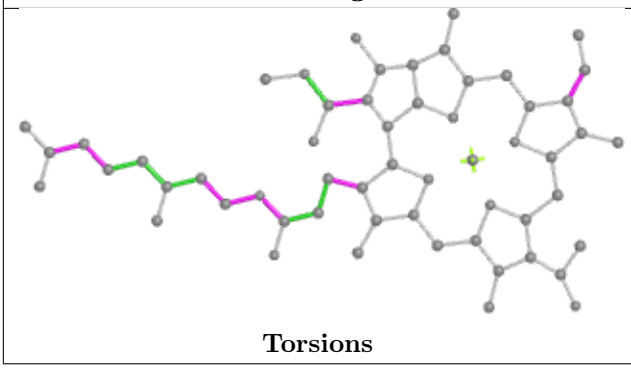
Ligand BCL a 805



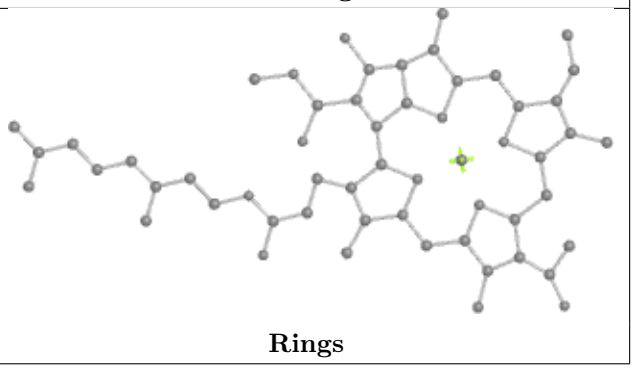
Bond lengths



Bond angles

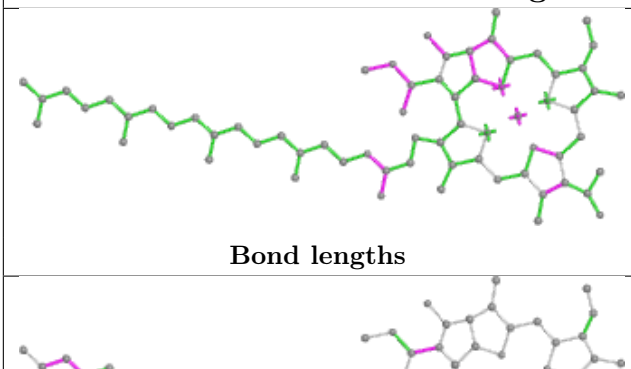


Torsions

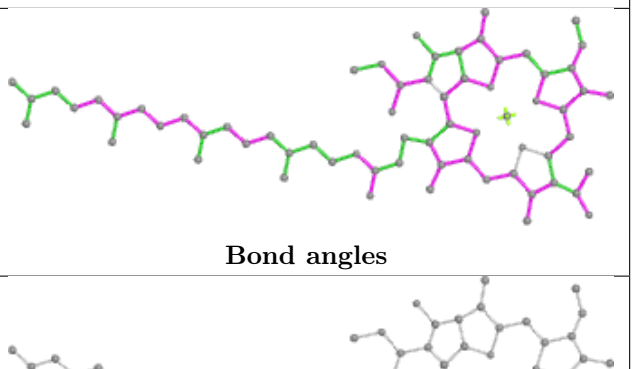


Rings

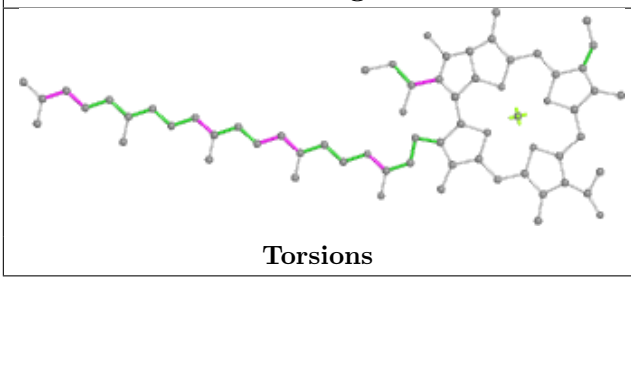
Ligand BCL 4 406



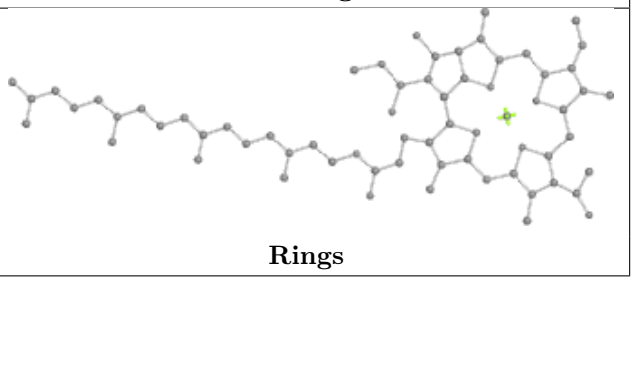
Bond lengths



Bond angles

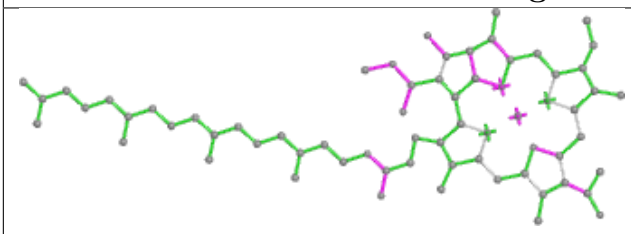


Torsions

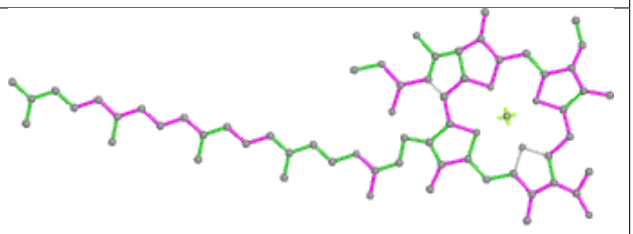


Rings

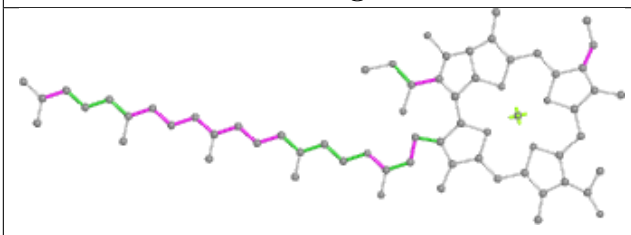
Ligand BCL 3 403



Bond lengths



Bond angles



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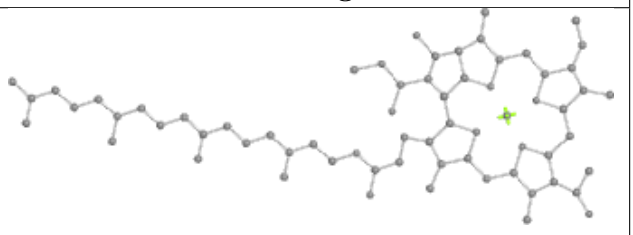
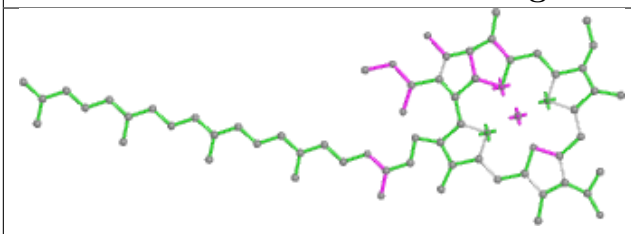


Rings

Ligand BCL 5 405



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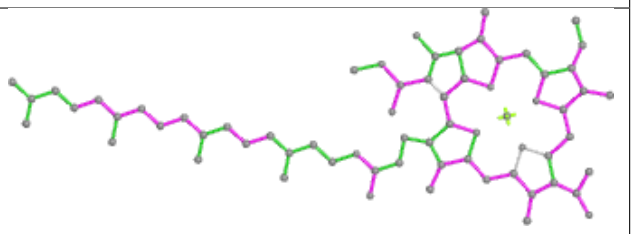
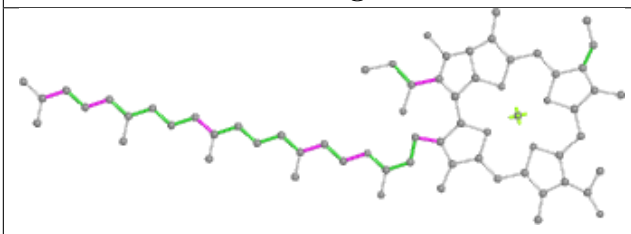


Bond angles



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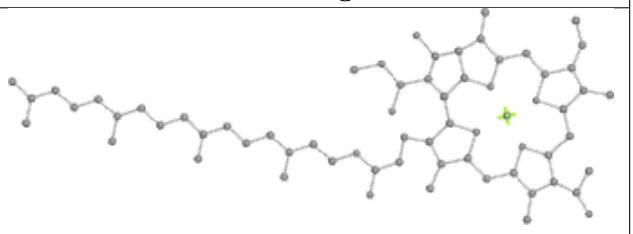
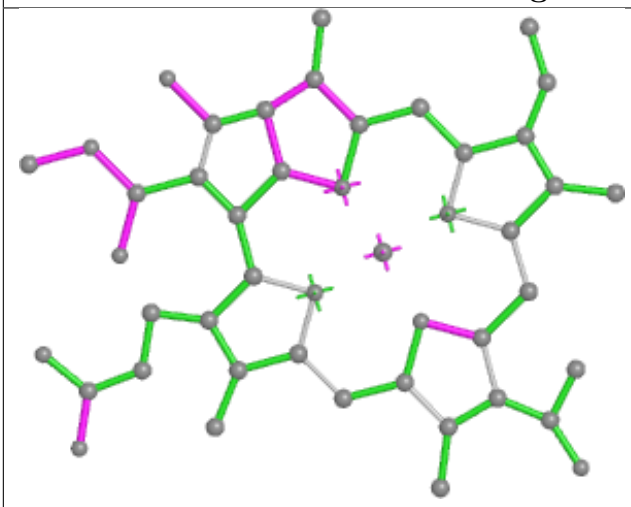
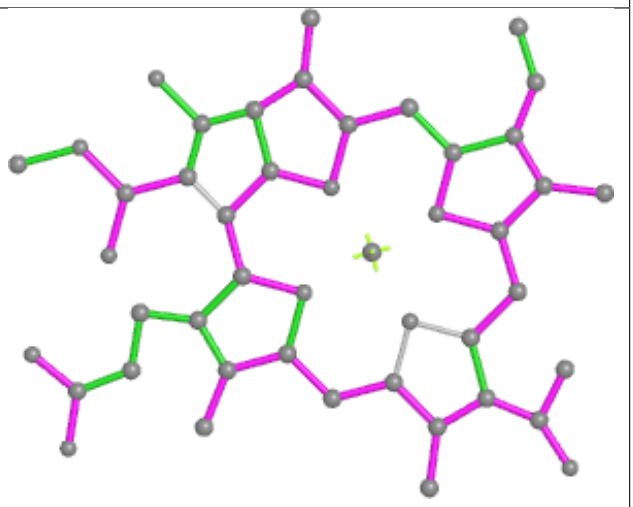


Rings

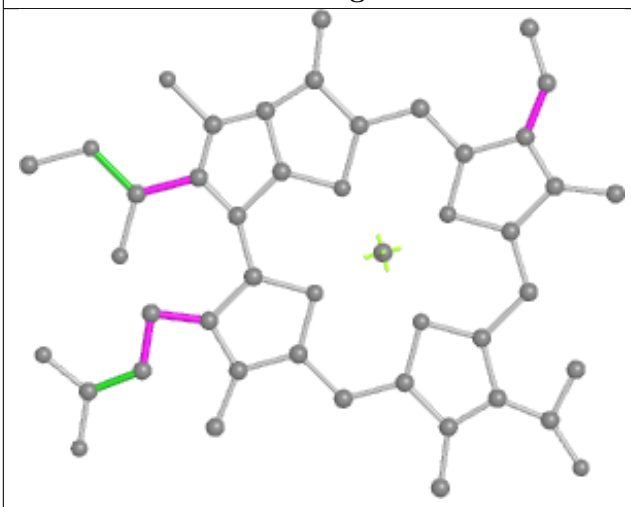
Ligand BCL c 301



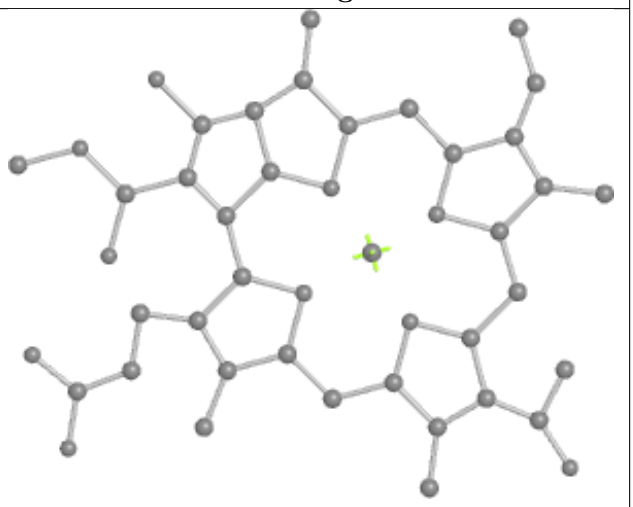
Bond lengths



Bond angles

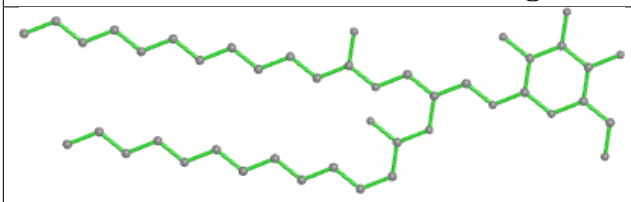


Torsions

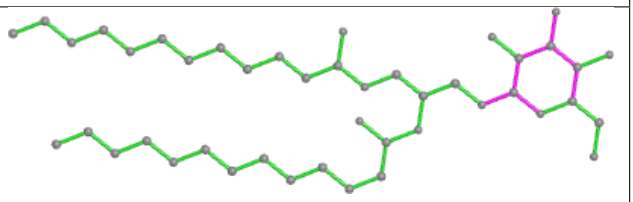


Rings

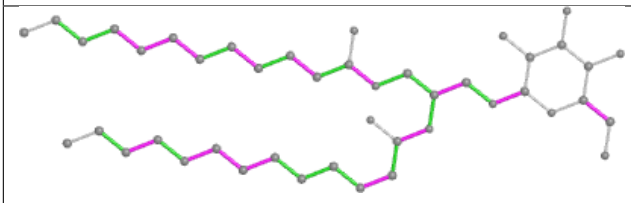
Ligand LMG a 818



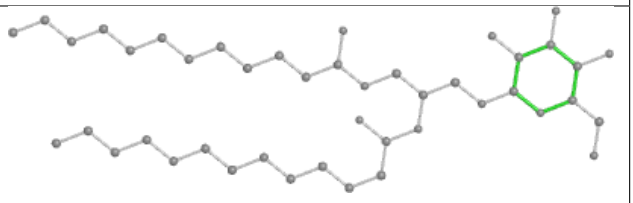
Bond lengths



Bond angles

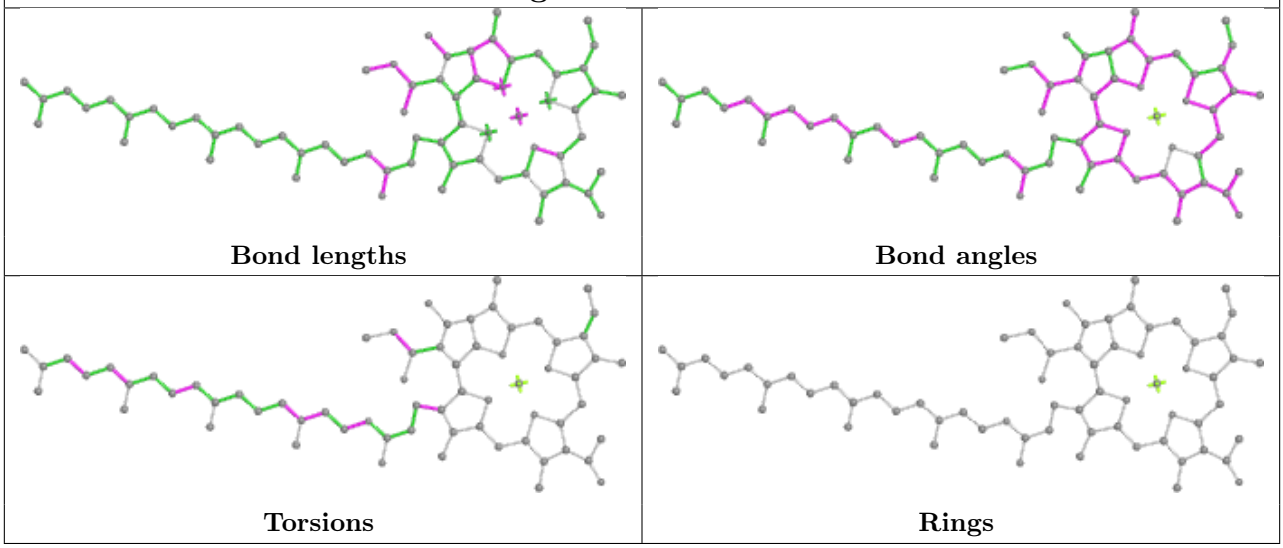


Torsions

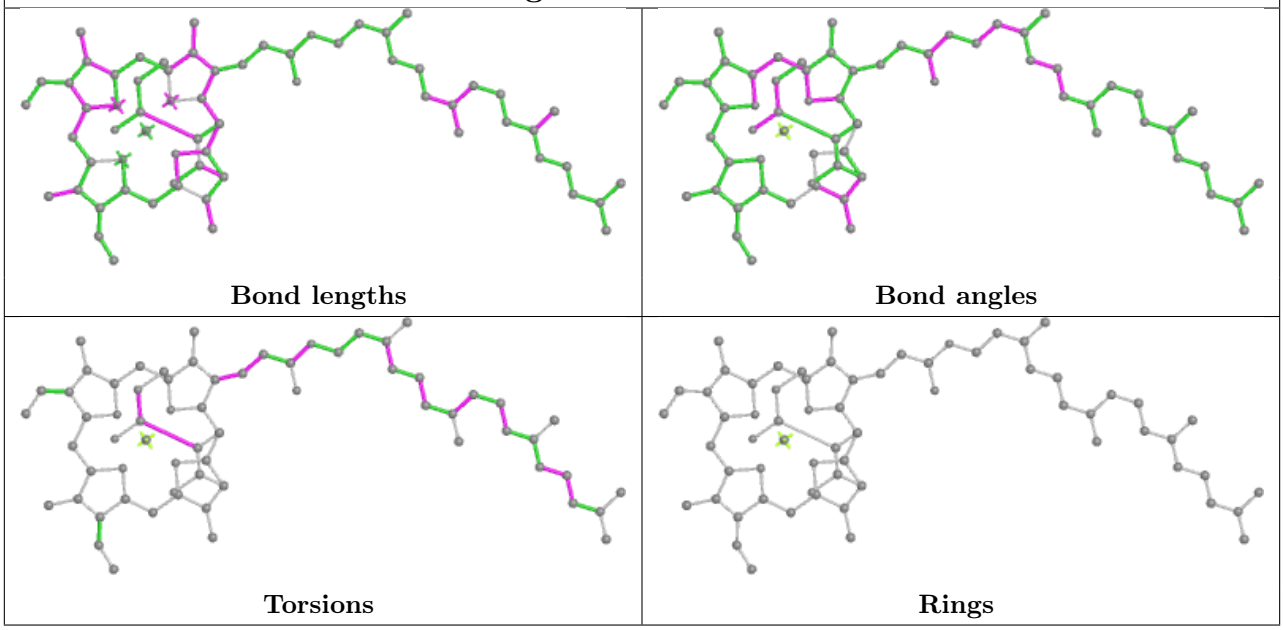


Rings

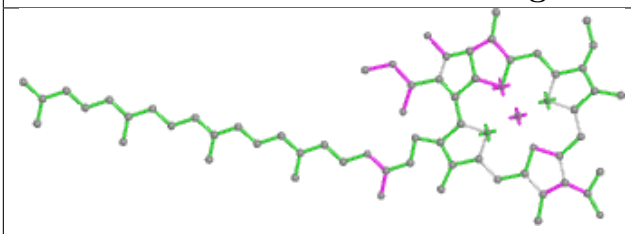
Ligand BCL 6 401



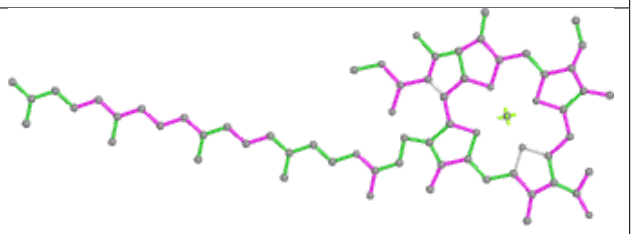
Ligand G2O A 822



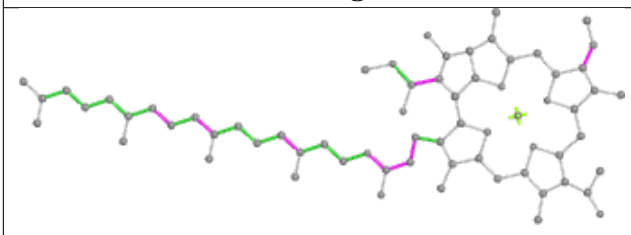
Ligand BCL 5 402



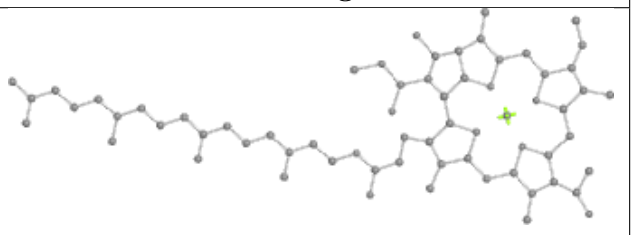
Bond lengths



Bond angles

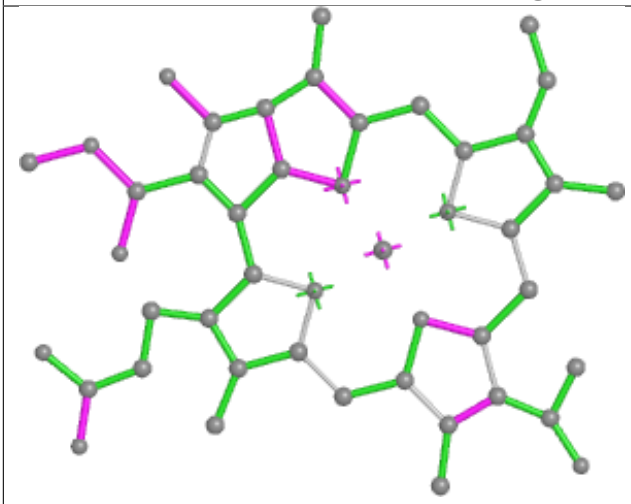


Torsions

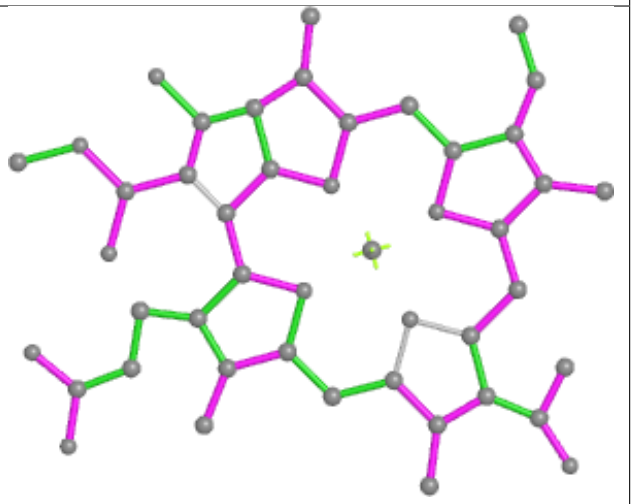


Rings

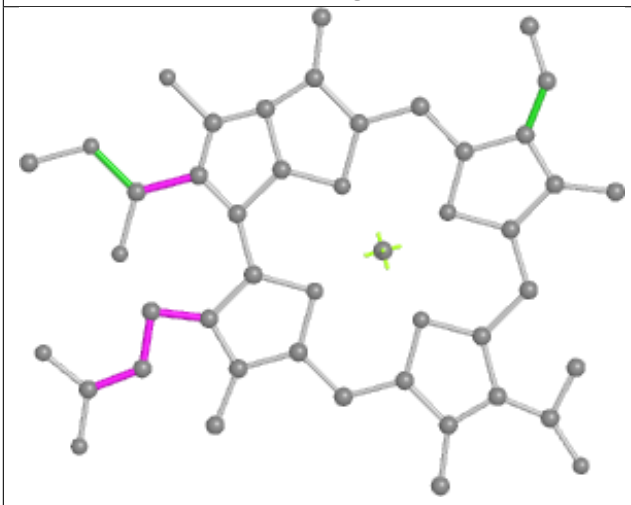
Ligand BCL a 804



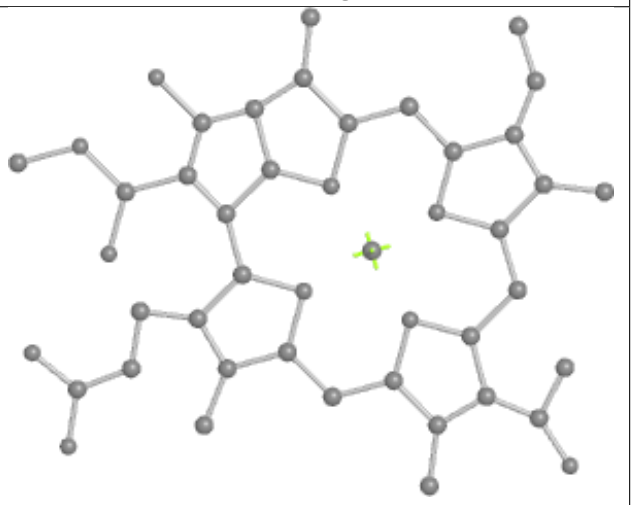
Bond lengths



Bond angles

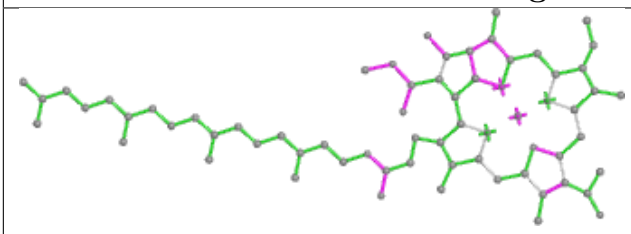


Torsions

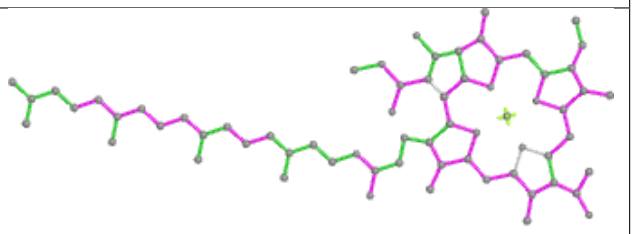


Rings

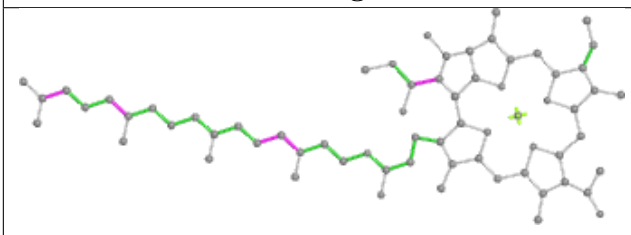
Ligand BCL 2 407



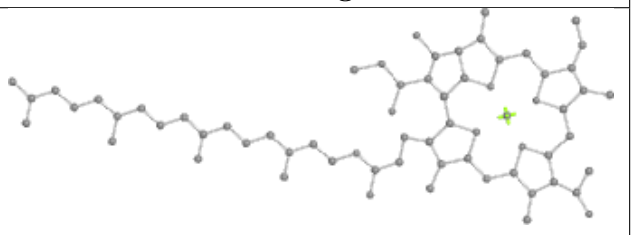
Bond lengths



Bond angles

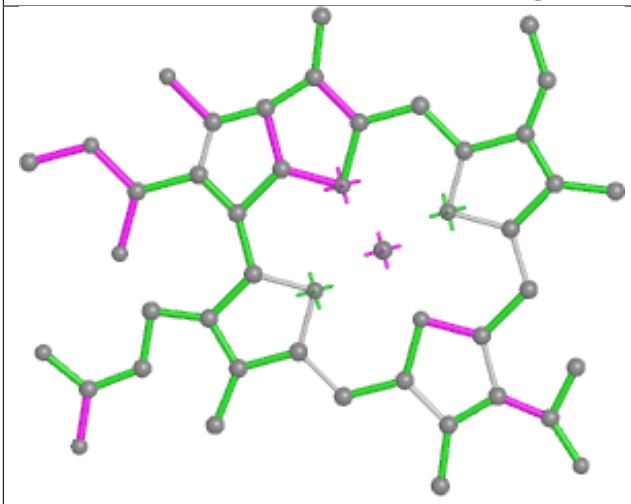


Torsions

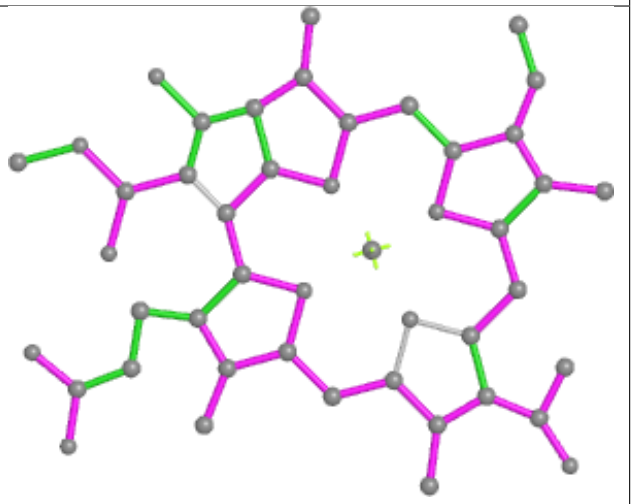


Rings

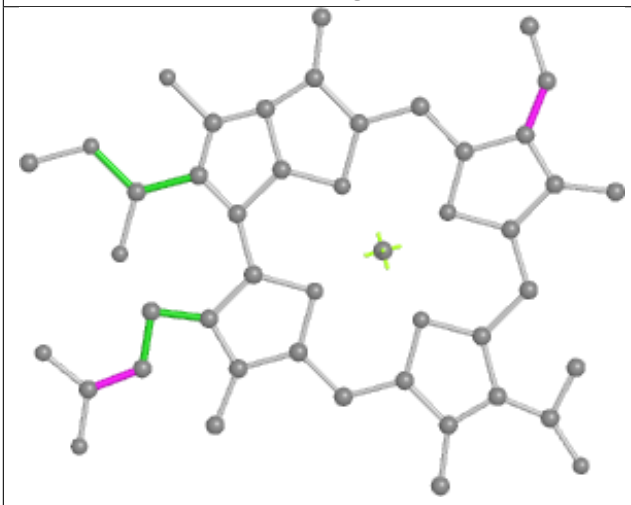
Ligand BCL a 814



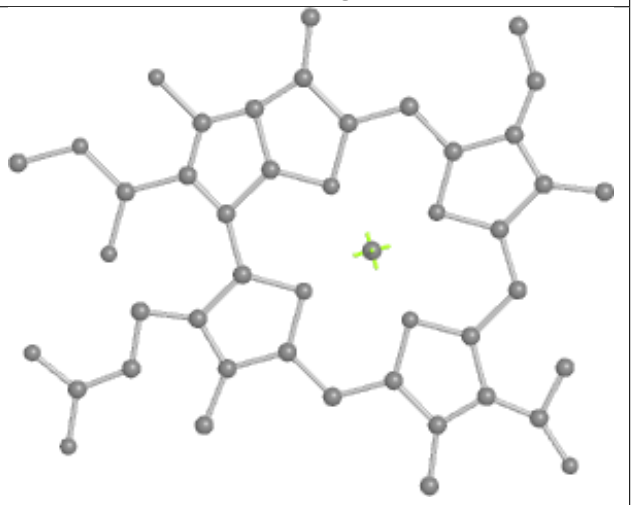
Bond lengths



Bond angles

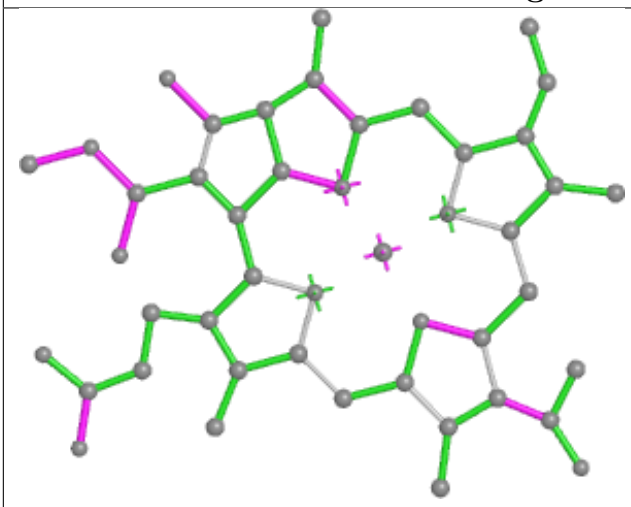


Torsions

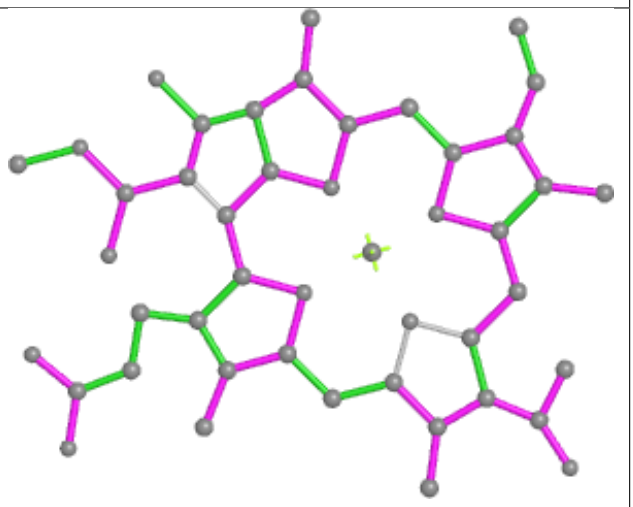


Rings

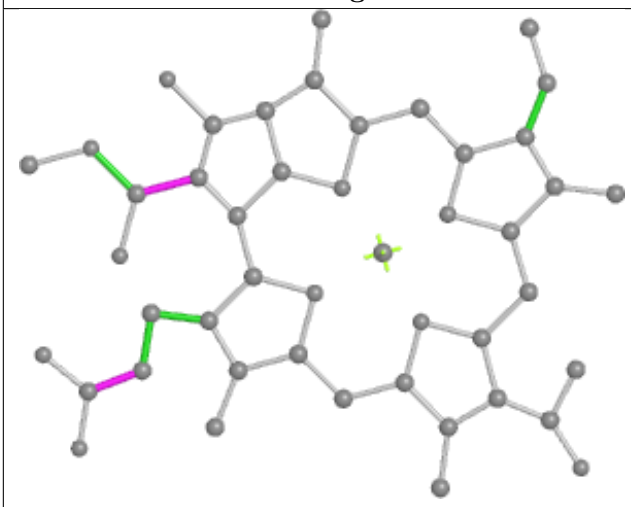
Ligand BCL F 101



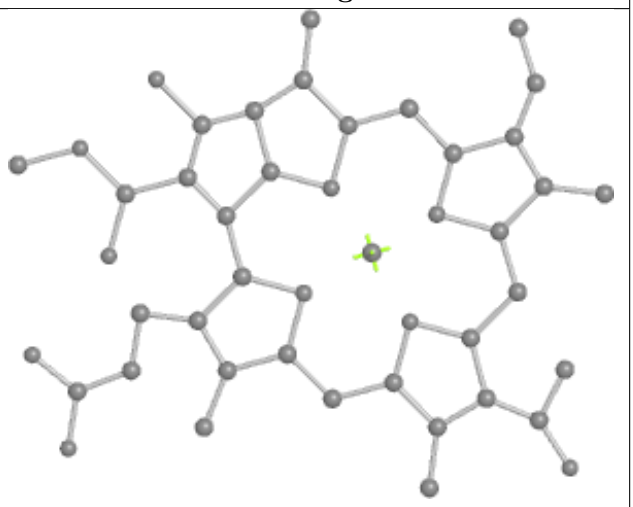
Bond lengths



Bond angles

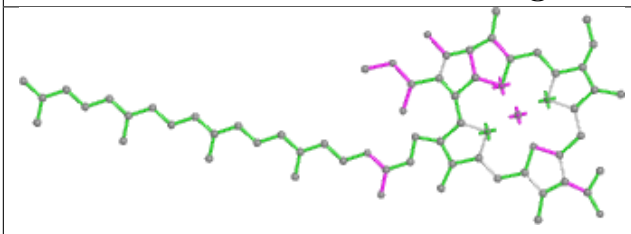


Torsions

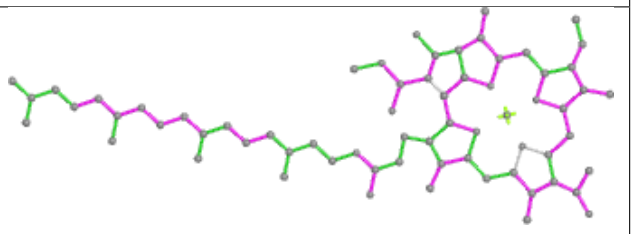


Rings

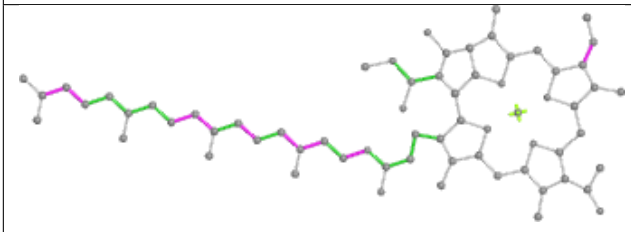
Ligand BCL 2 408



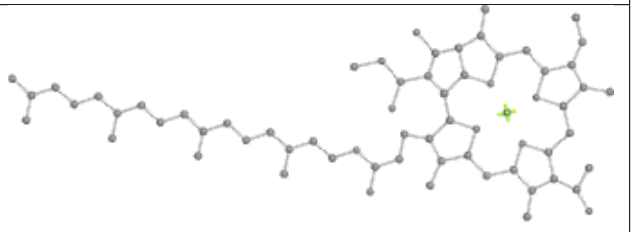
Bond lengths



Bond angles

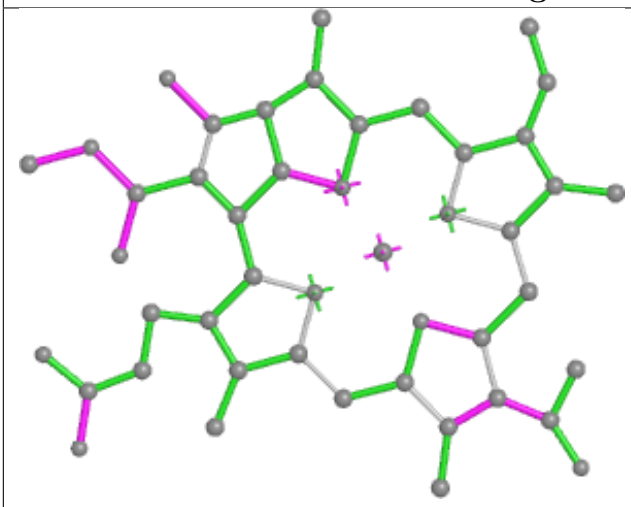


Torsions

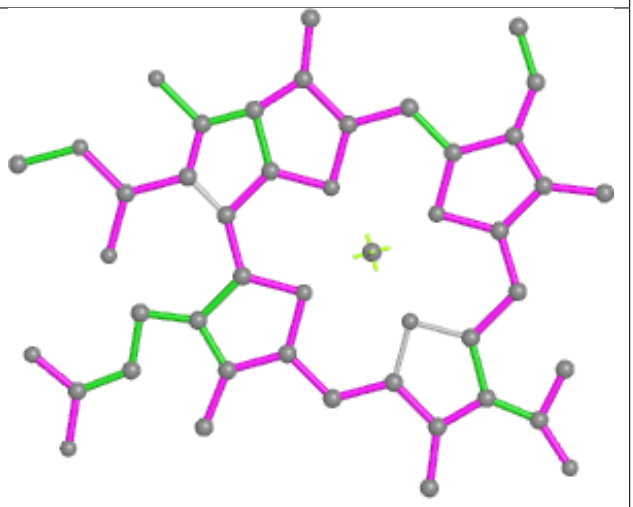


Rings

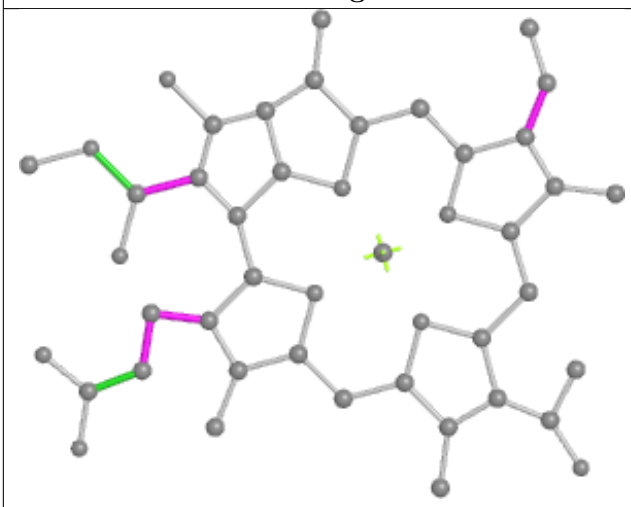
Ligand BCL a 810



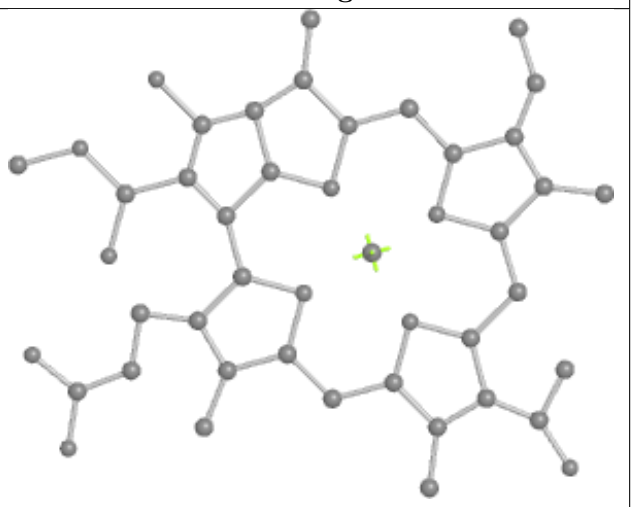
Bond lengths



Bond angles

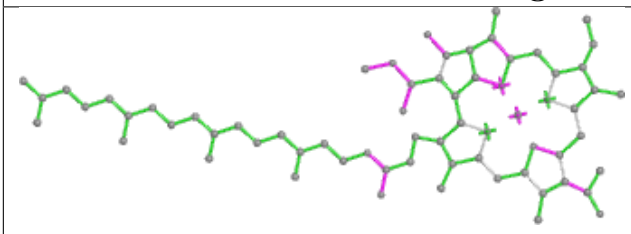


Torsions

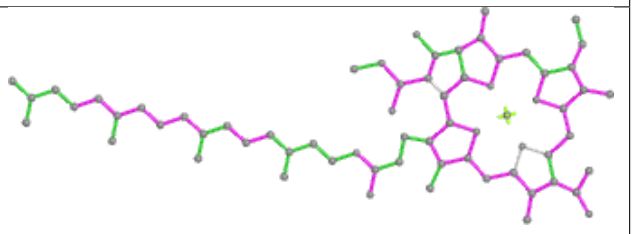


Rings

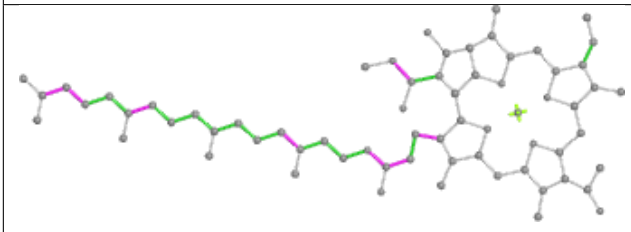
Ligand BCL 3 401



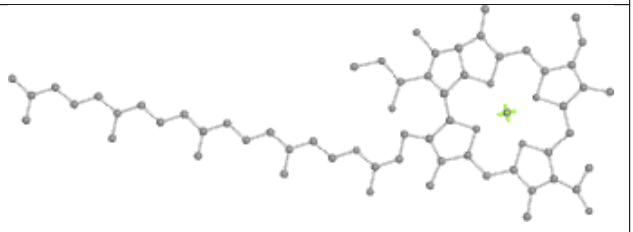
Bond lengths



Bond angles

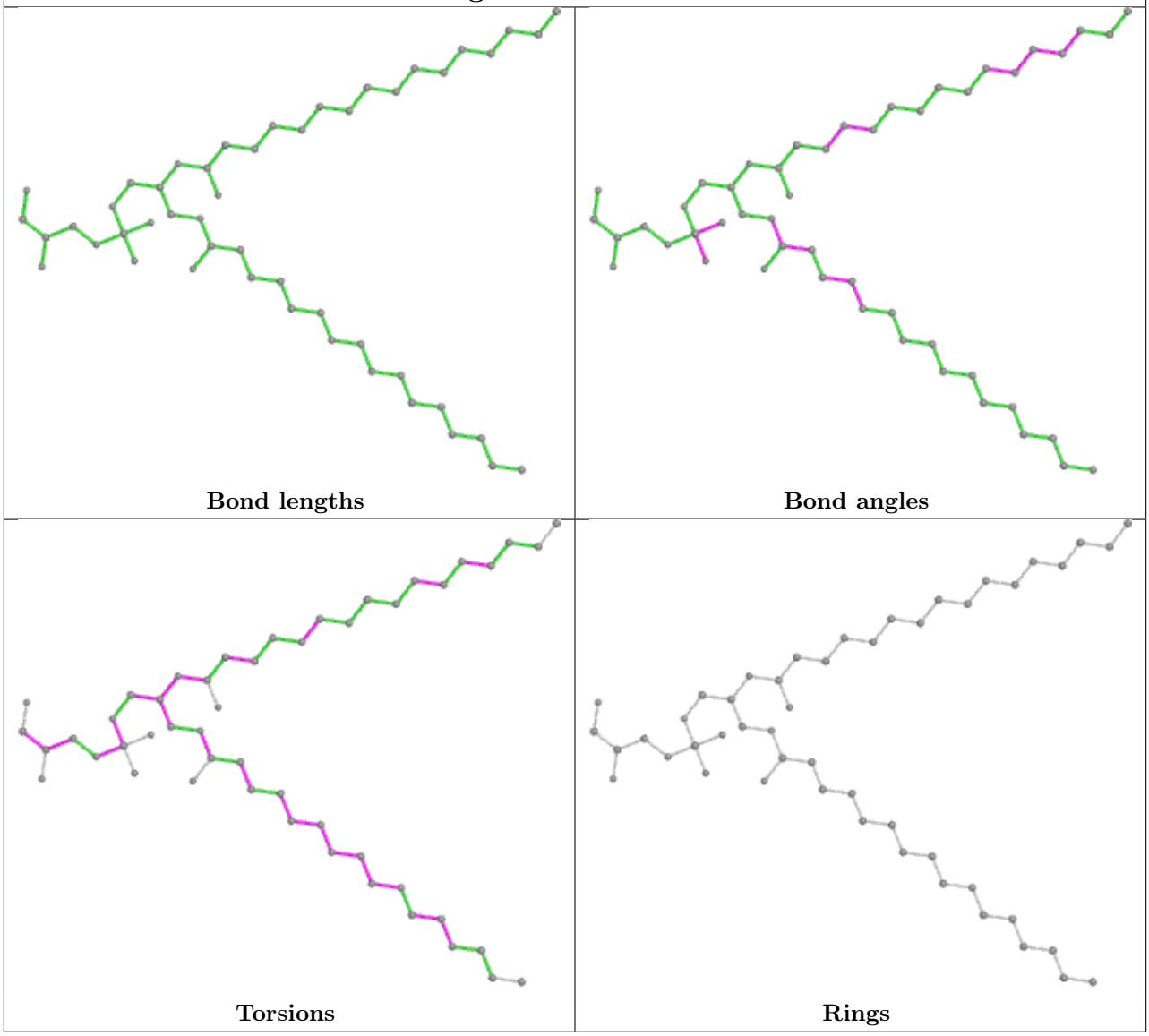


Torsions

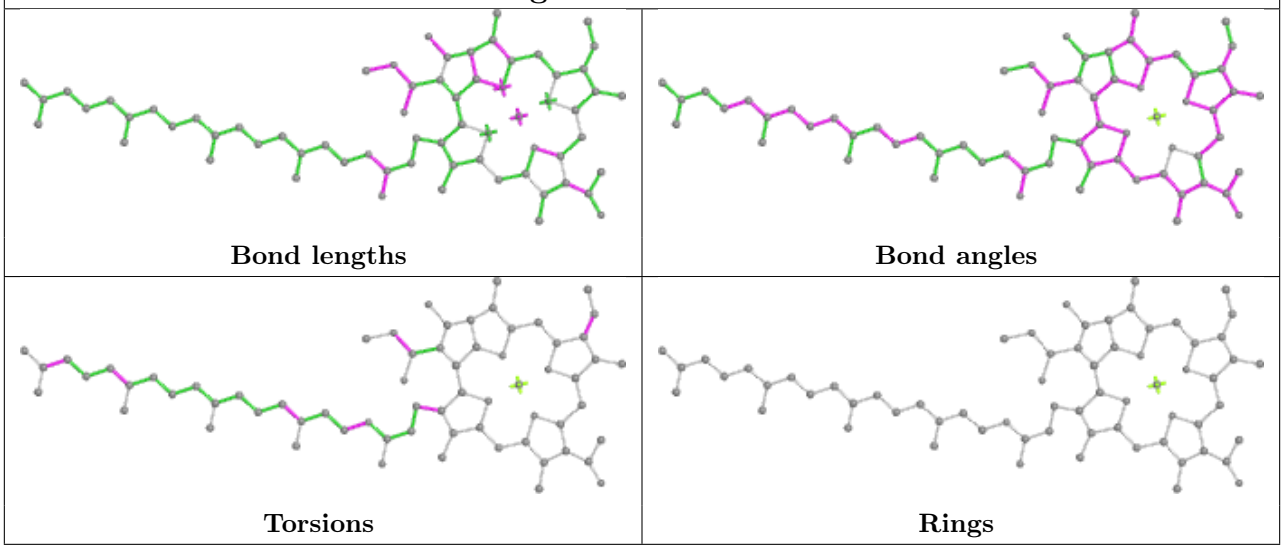


Rings

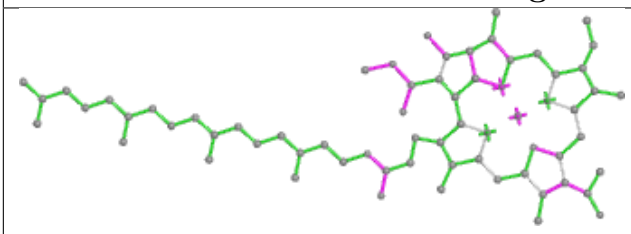
Ligand LHG A 819



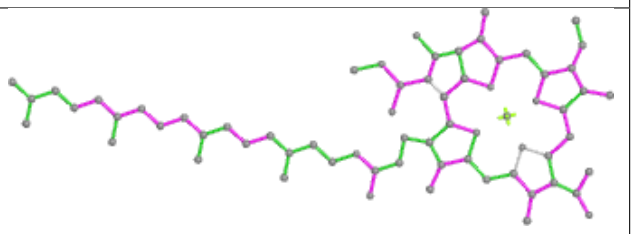
Ligand BCL 4 401



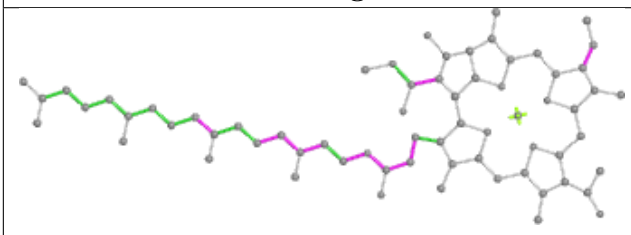
Ligand BCL 2 404



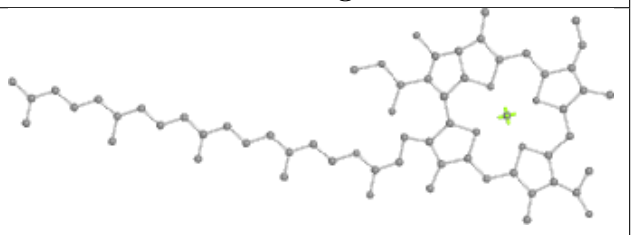
Bond lengths



Bond angles

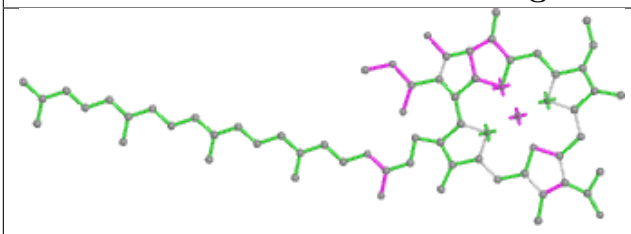


Torsions

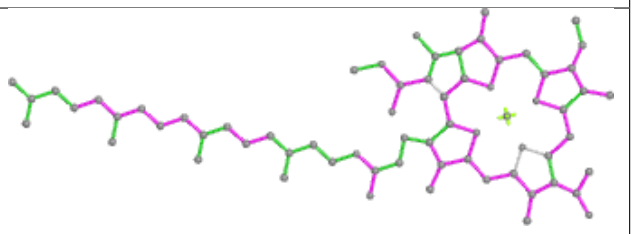


Rings

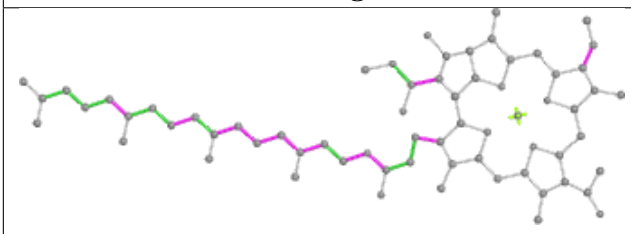
Ligand BCL a 811



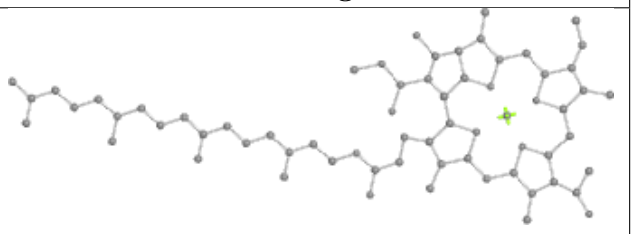
Bond lengths



Bond angles

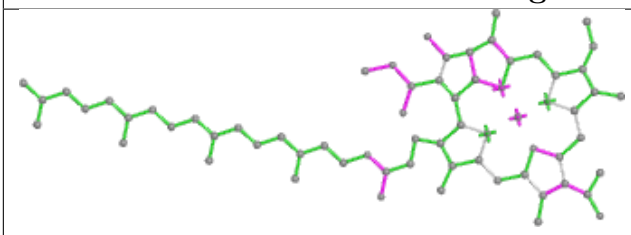


Torsions

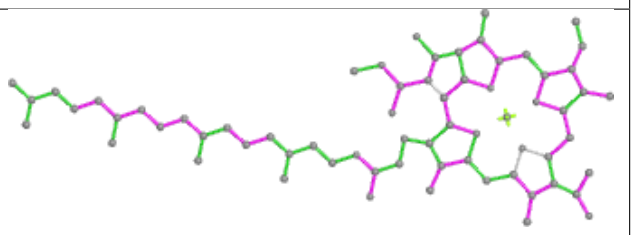


Rings

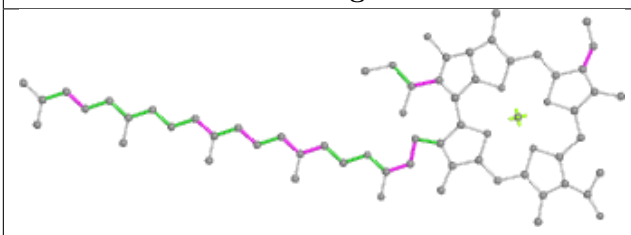
Ligand BCL 6 402



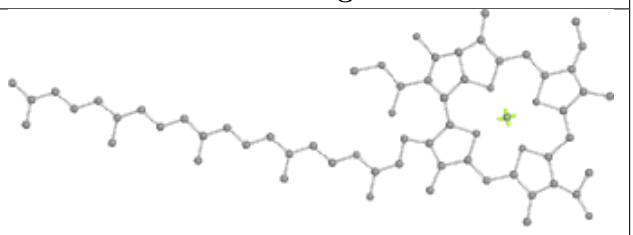
Bond lengths



Bond angles

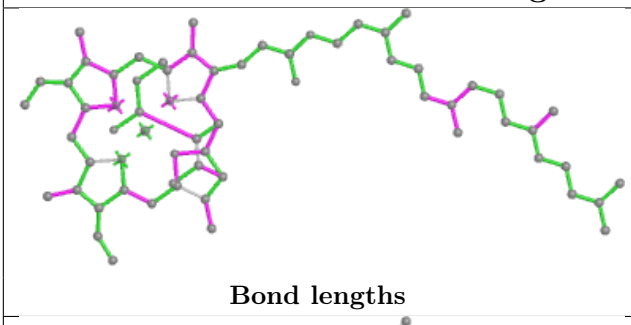


Torsions

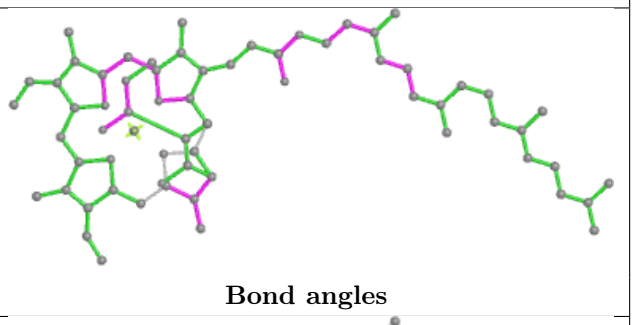


Rings

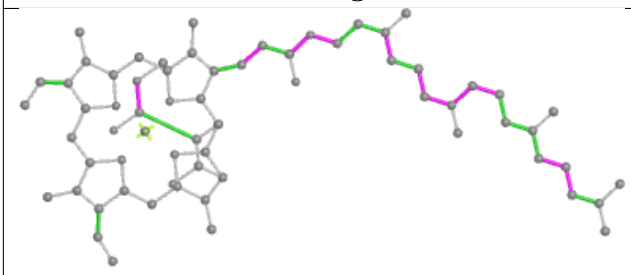
Ligand G2O a 803



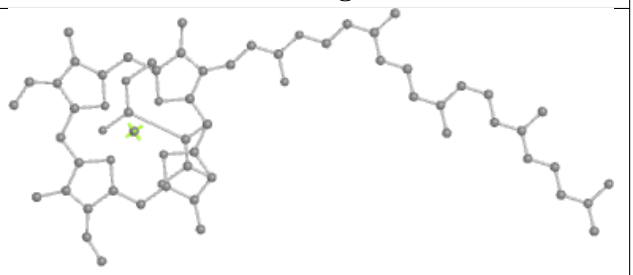
Bond lengths



Bond angles

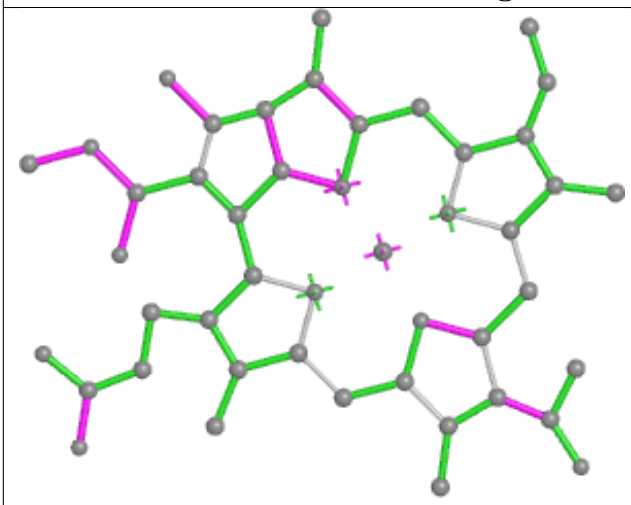


Torsions



Rings

Ligand BCL 6 407 (B)



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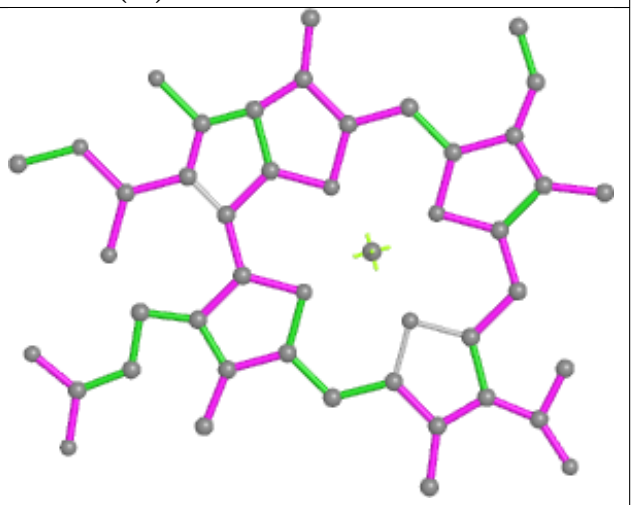
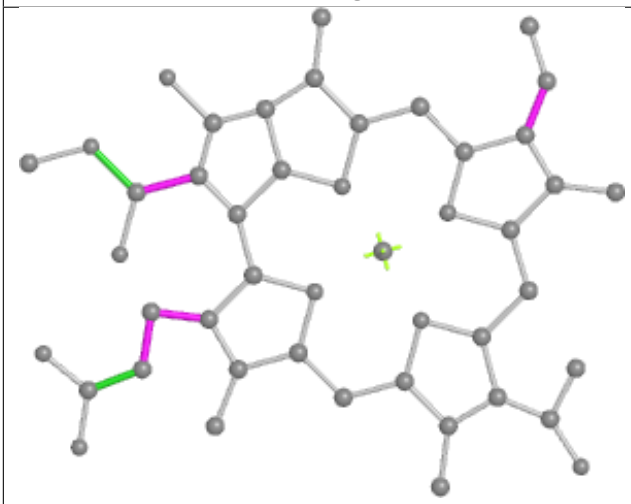
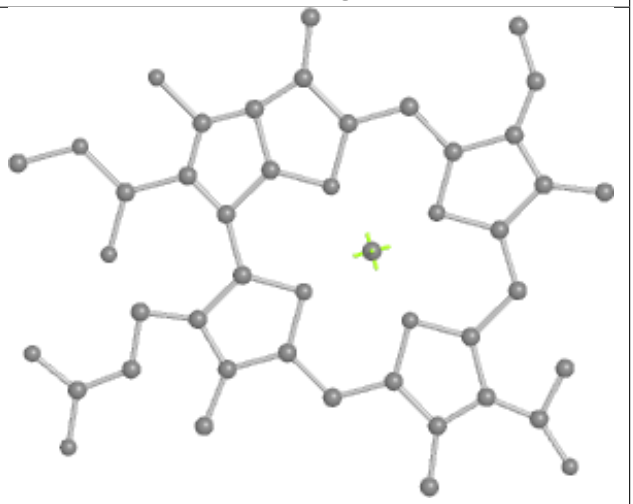


Bond angles

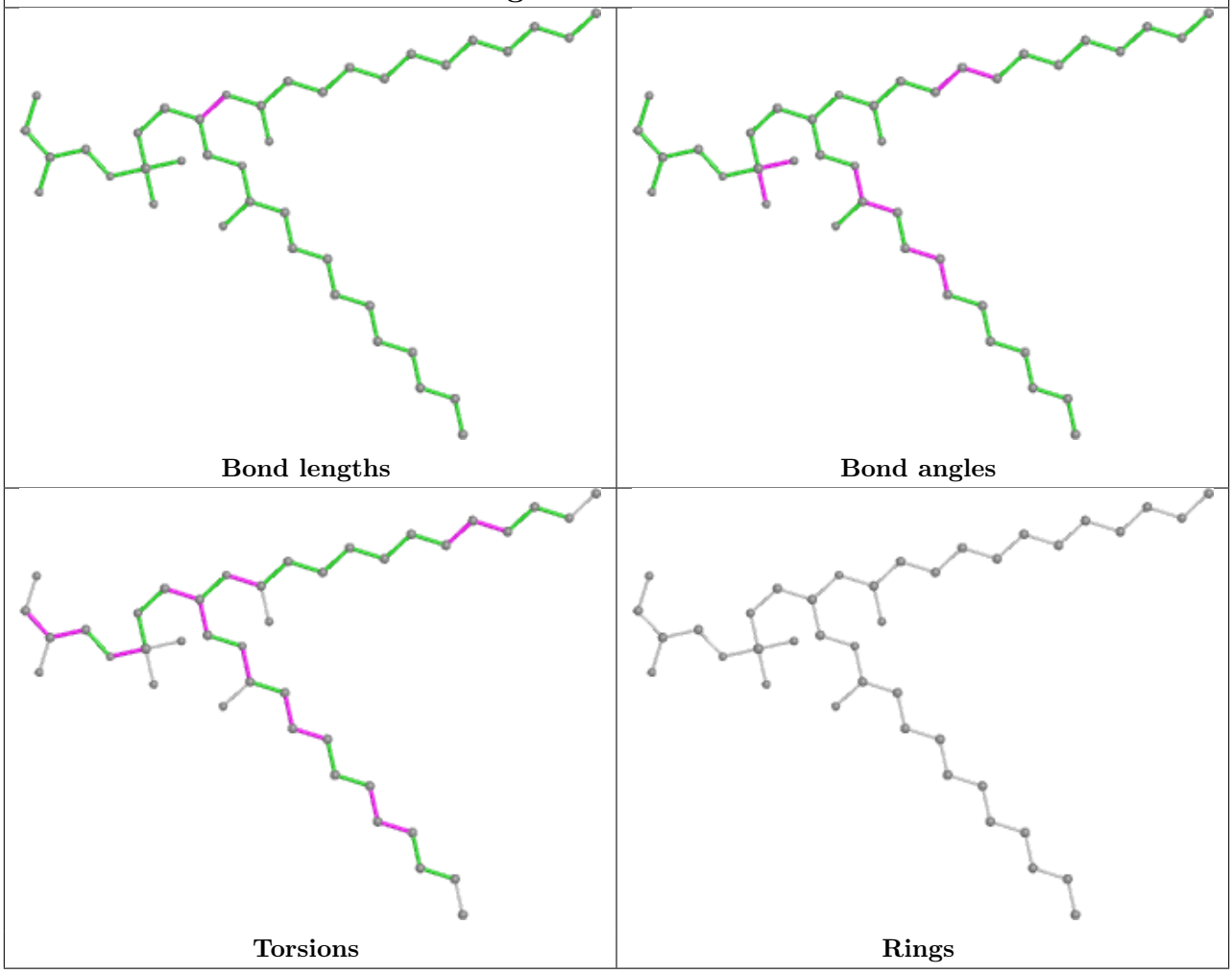


Torsions

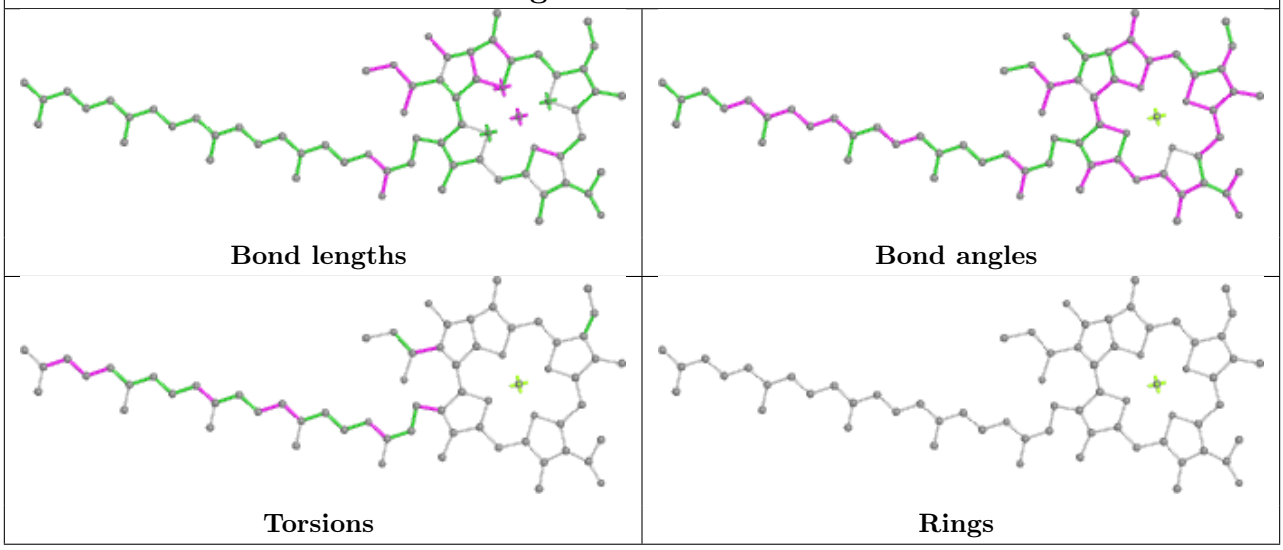


Rings

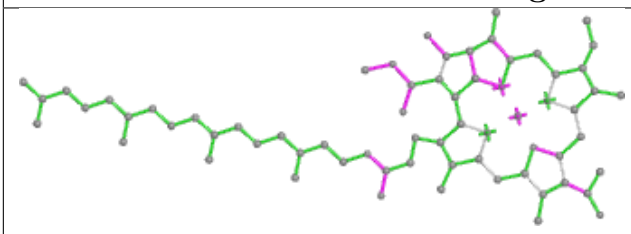
Ligand LHG a 819



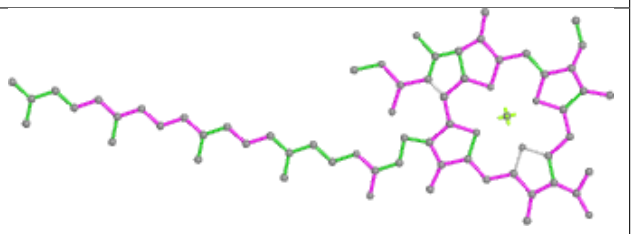
Ligand BCL 6 405



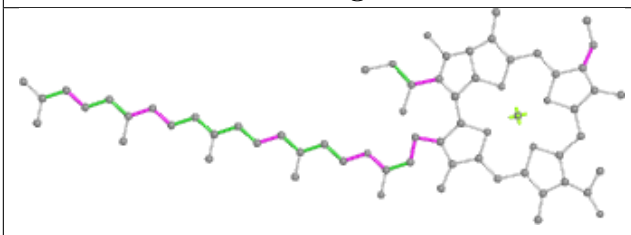
Ligand BCL 5 403



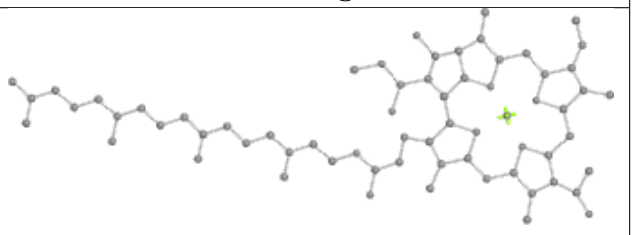
Bond lengths



Bond angles

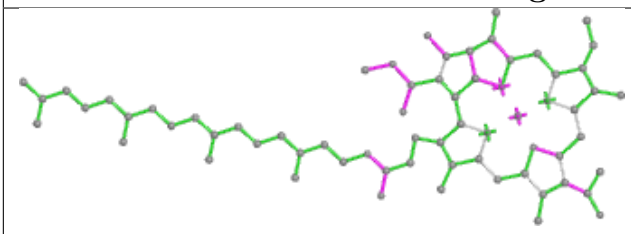


Torsions

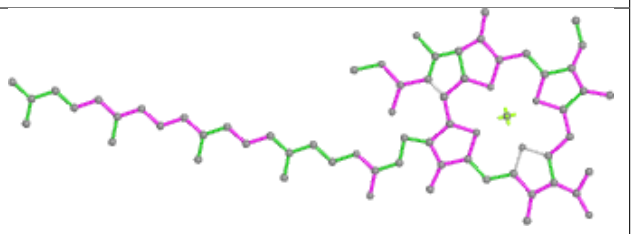


Rings

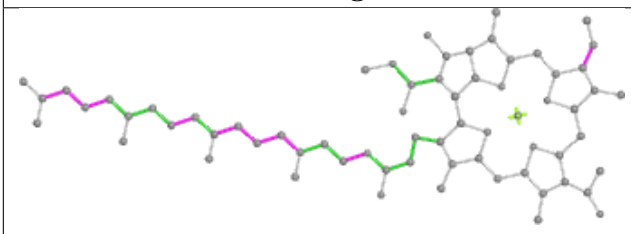
Ligand BCL 6 408



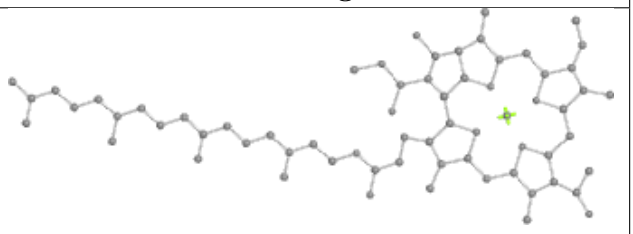
Bond lengths



Bond angles

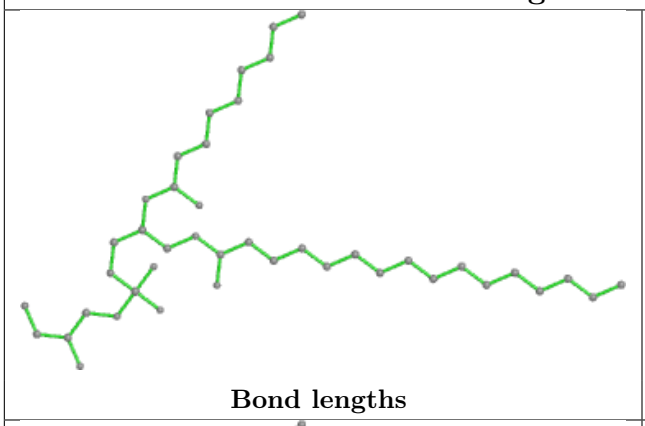


Torsions

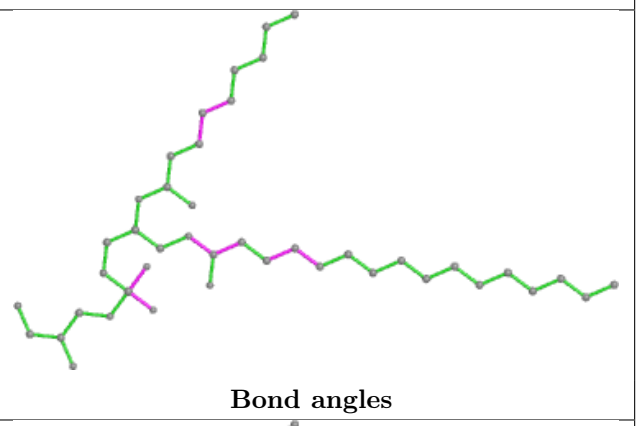


Rings

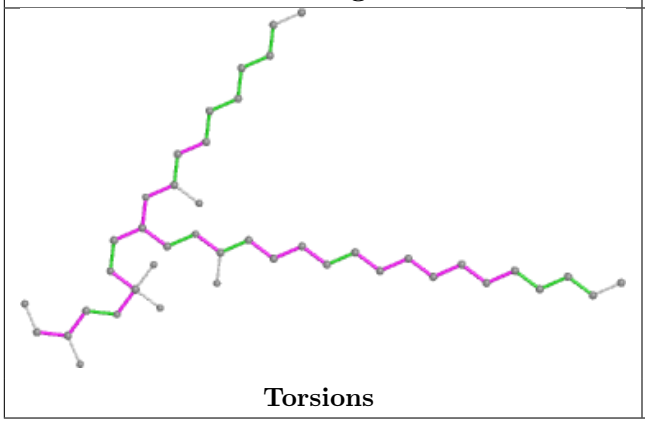
Ligand LHG a 821



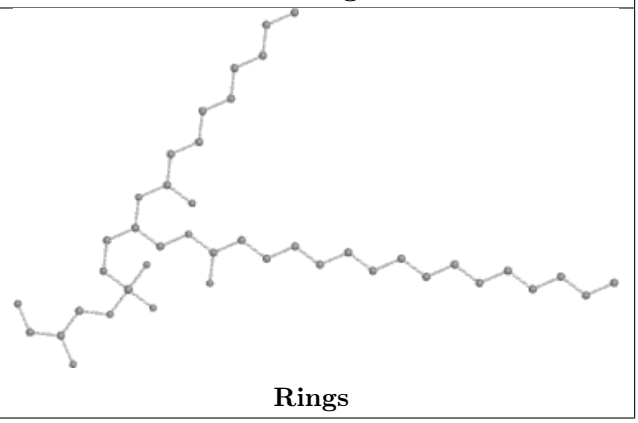
Bond lengths



Bond angles

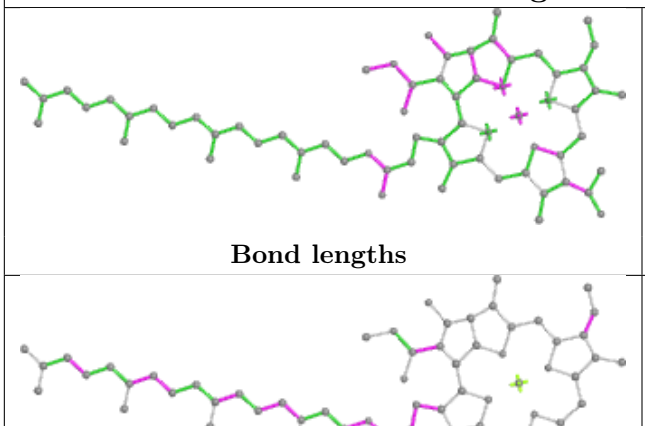


Torsions

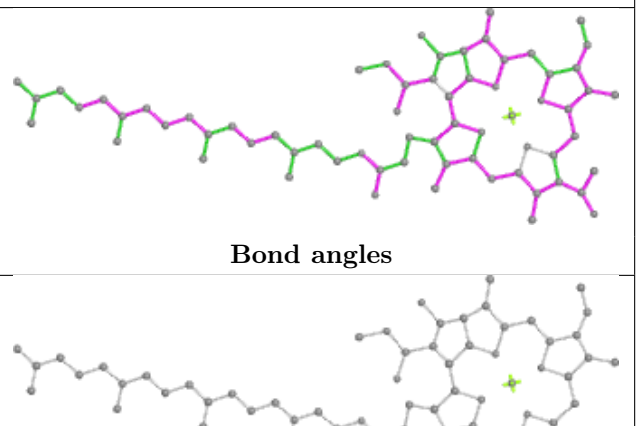


Rings

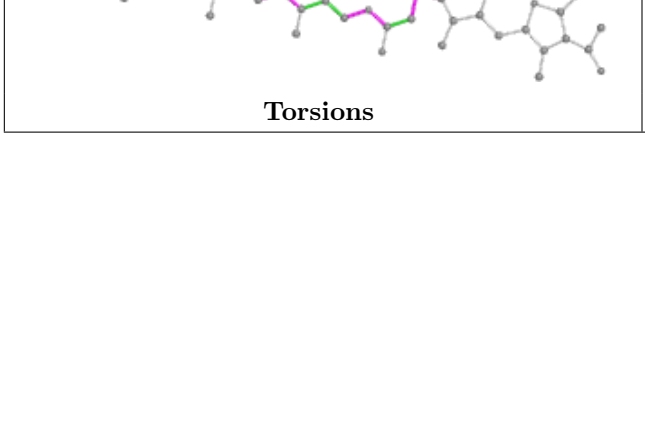
Ligand BCL 4 404



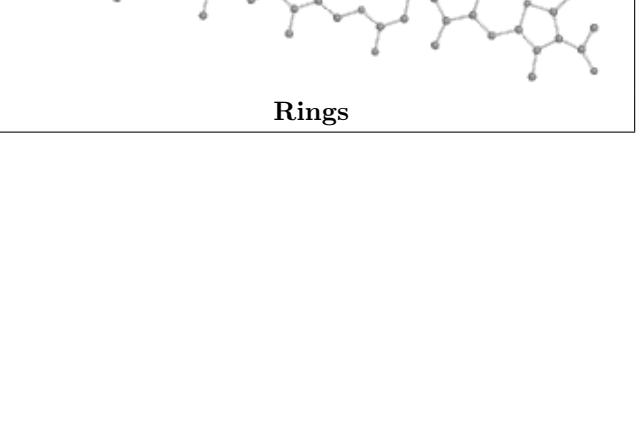
Bond lengths



Bond angles

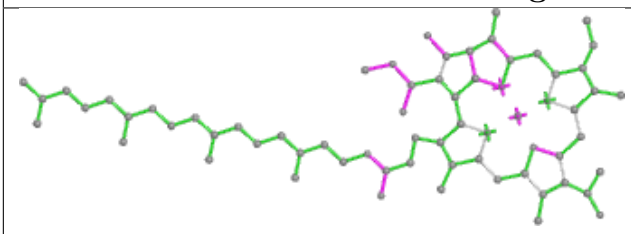


Torsions

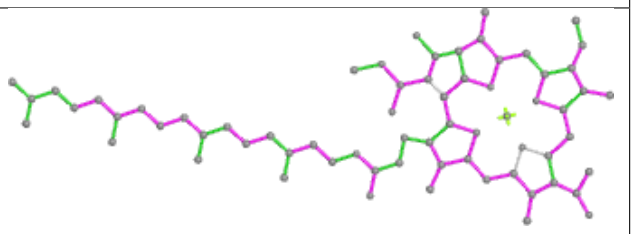


Rings

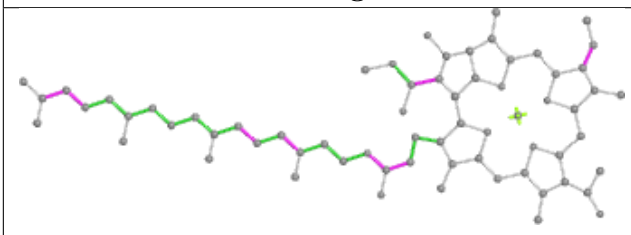
Ligand BCL 1 404



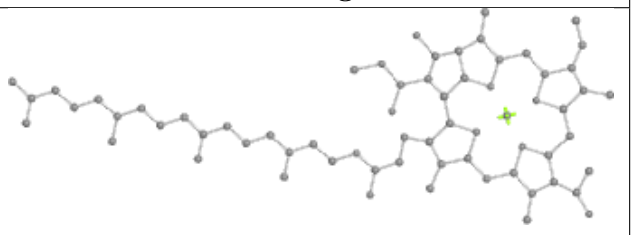
Bond lengths



Bond angles

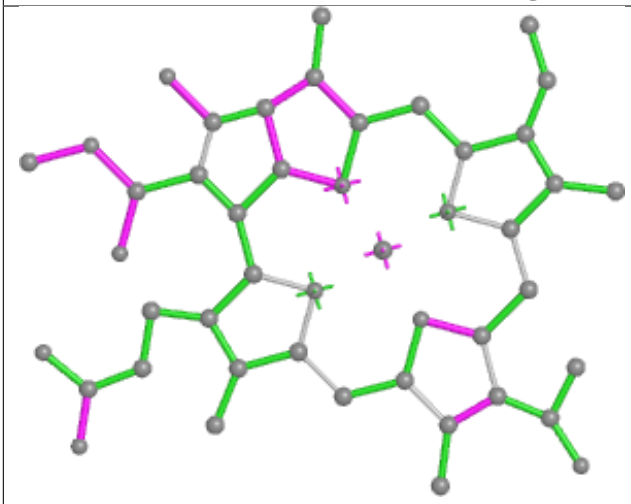


Torsions

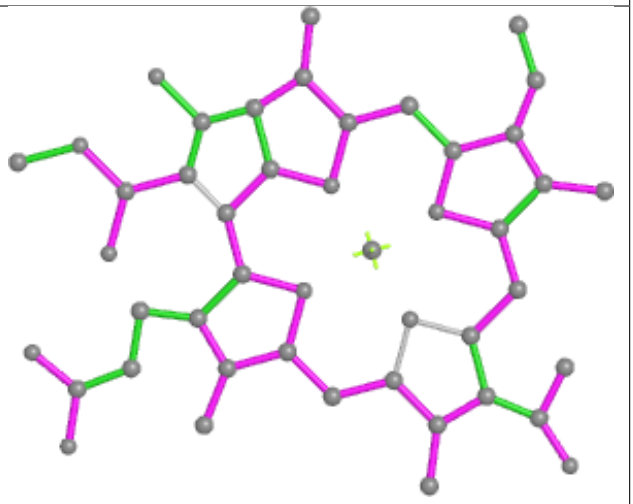


Rings

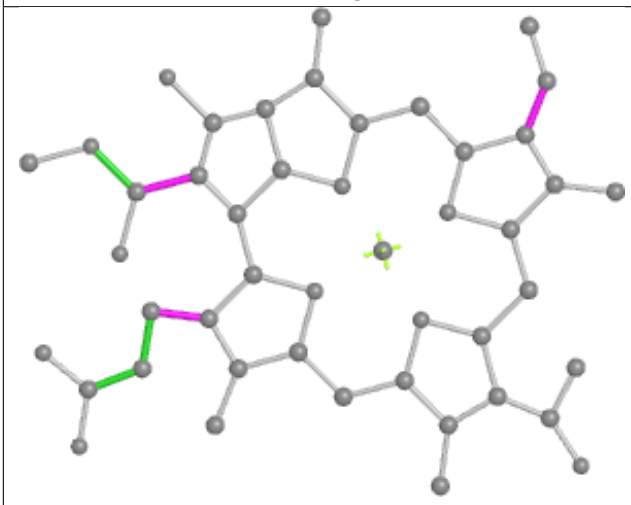
Ligand BCL A 812



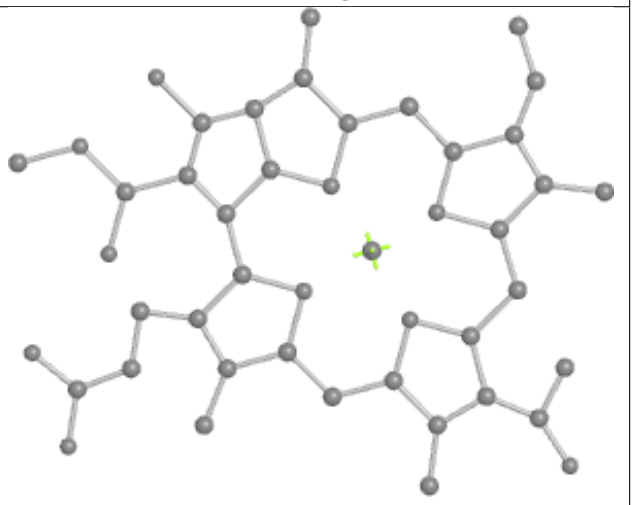
Bond lengths



Bond angles

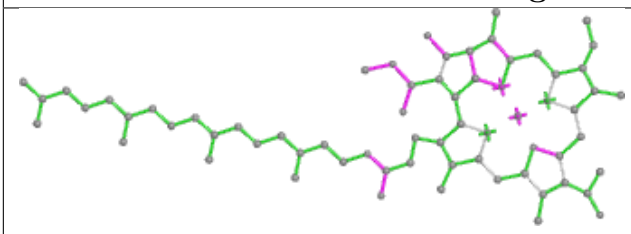


Torsions

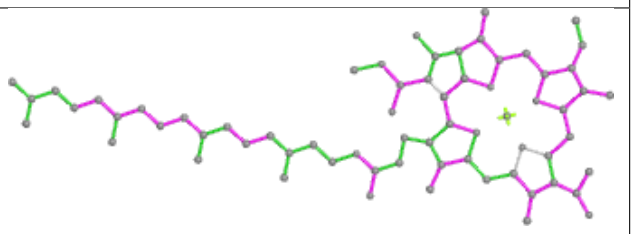


Rings

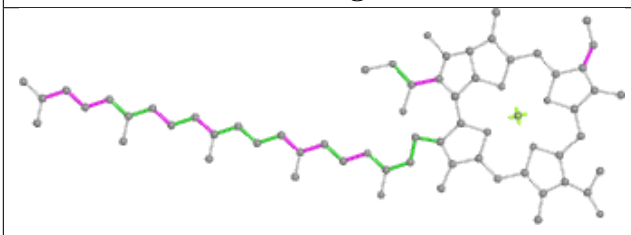
Ligand BCL 1 406



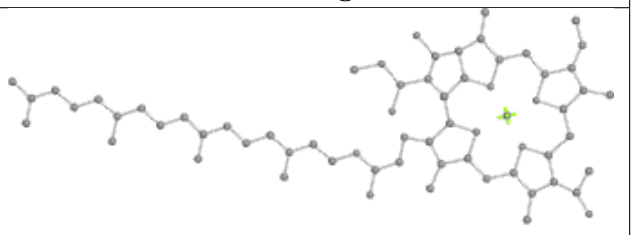
Bond lengths



Bond angles

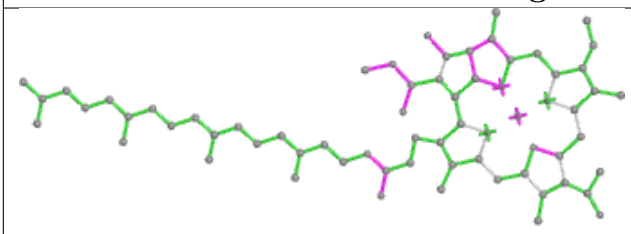


Torsions

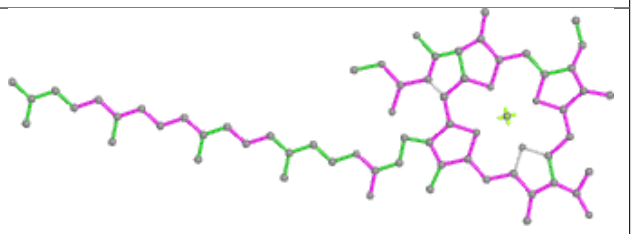


Rings

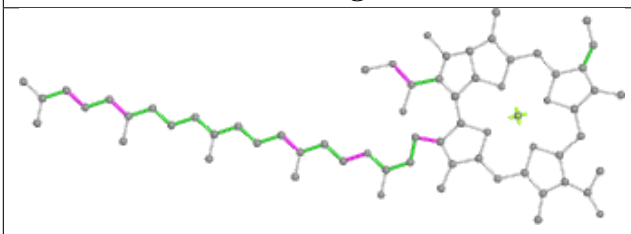
Ligand BCL 2 403



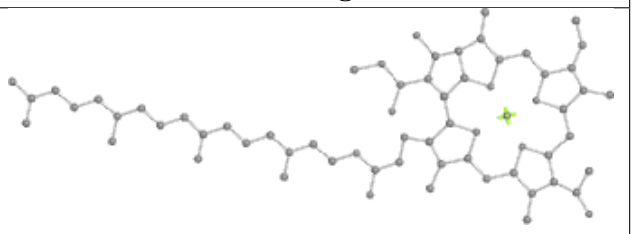
Bond lengths



Bond angles

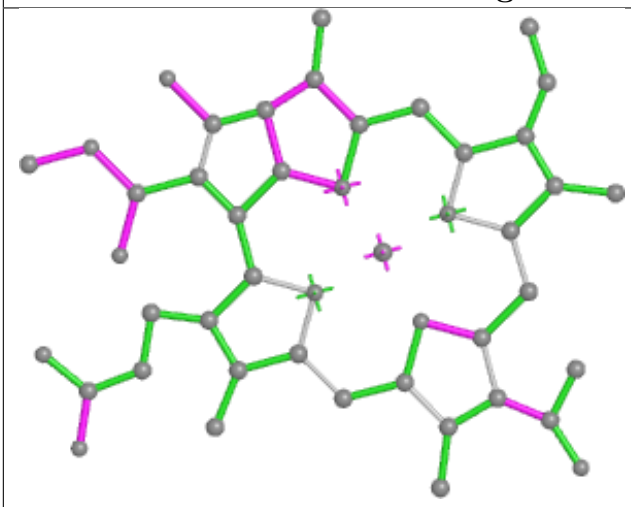


Torsions

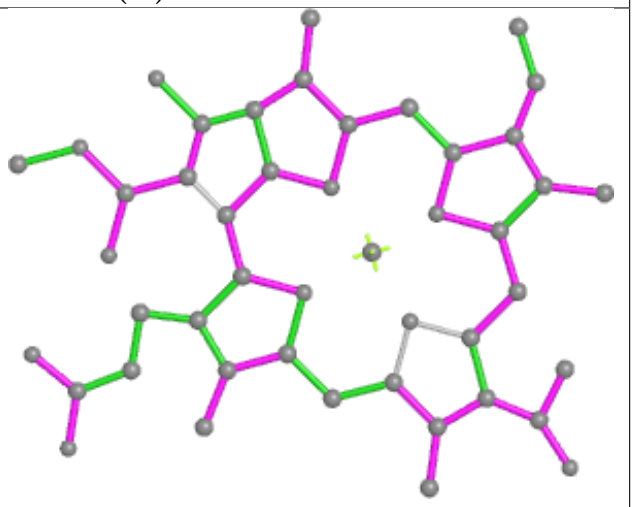


Rings

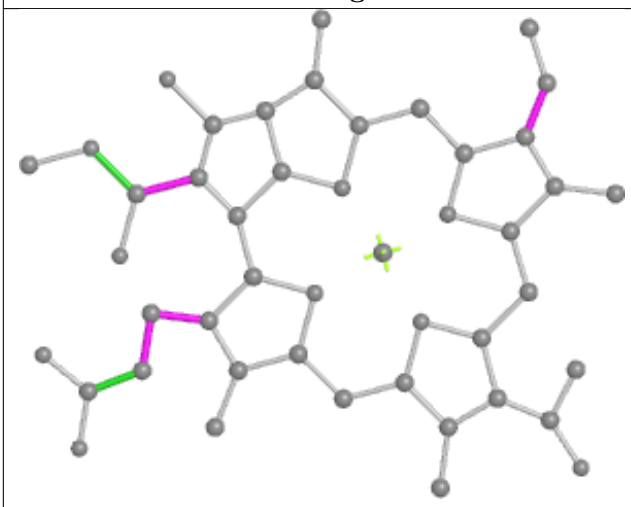
Ligand BCL 4 410 (B)



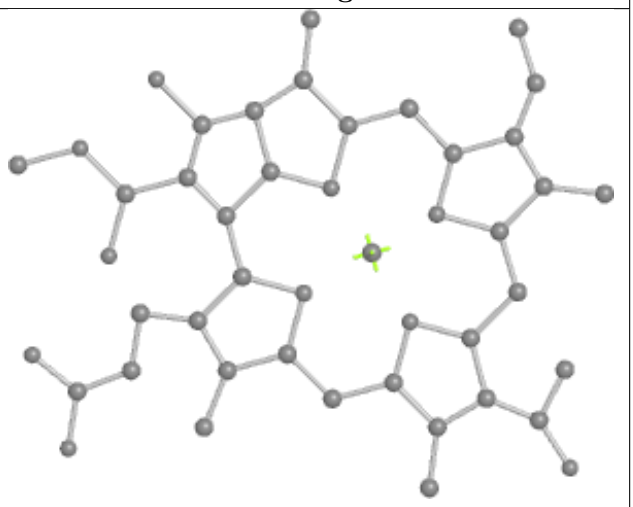
Bond lengths



Bond angles

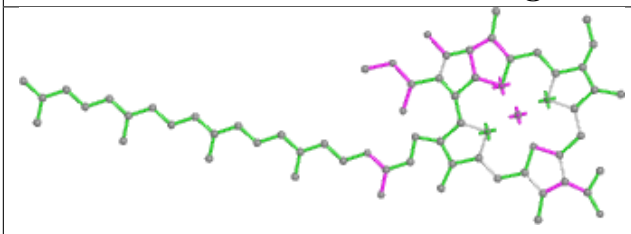


Torsions

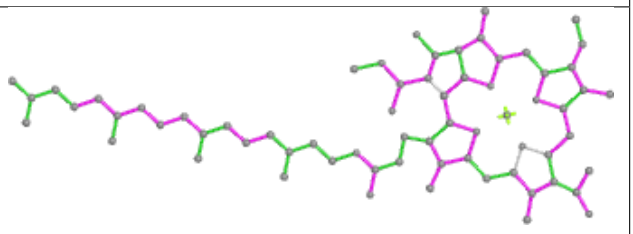


Rings

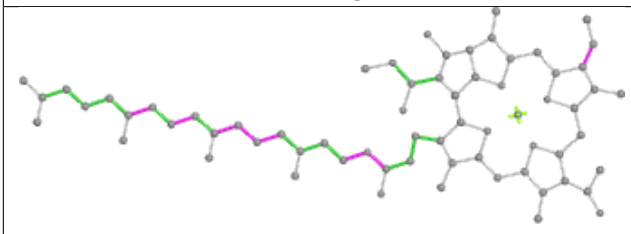
Ligand BCL A 805



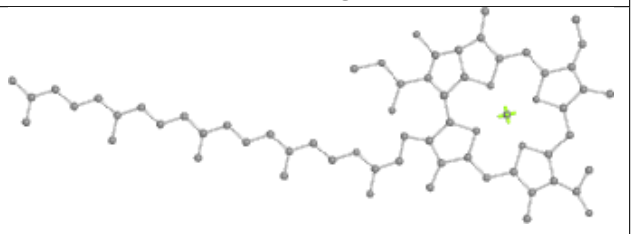
Bond lengths



Bond angles

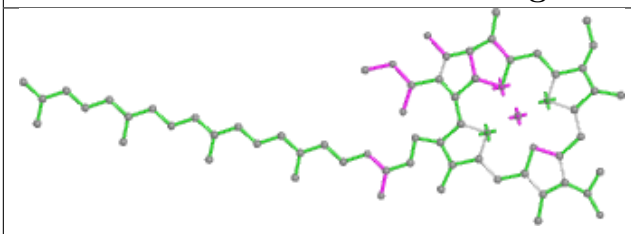


Torsions

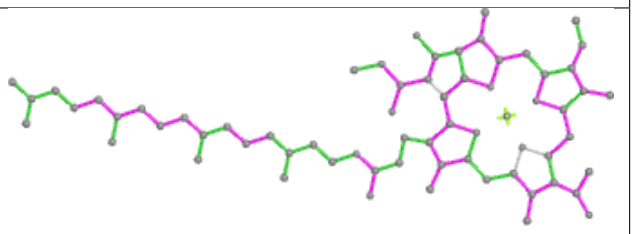


Rings

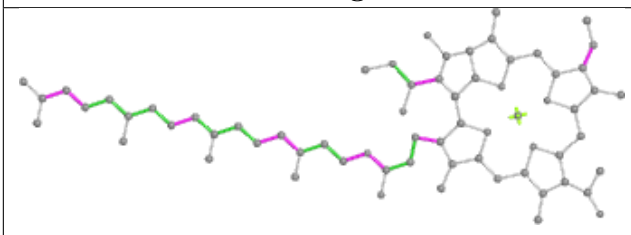
Ligand BCL 1 408



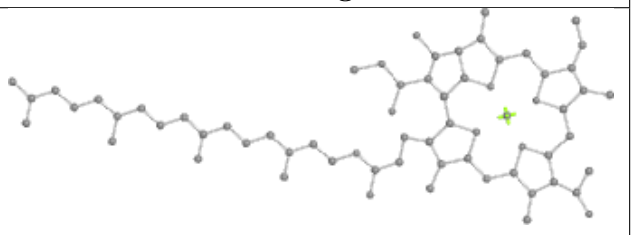
Bond lengths



Bond angles

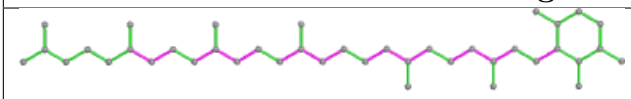


Torsions

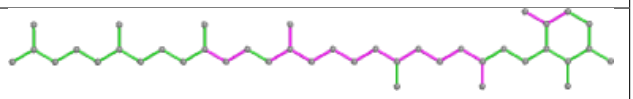


Rings

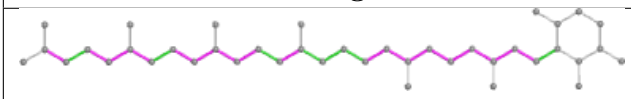
Ligand F26 c 302



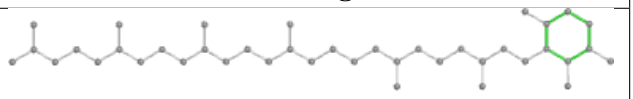
Bond lengths



Bond angles

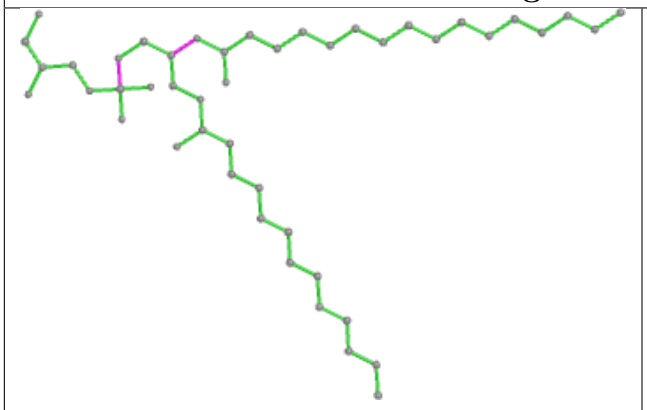


Torsions

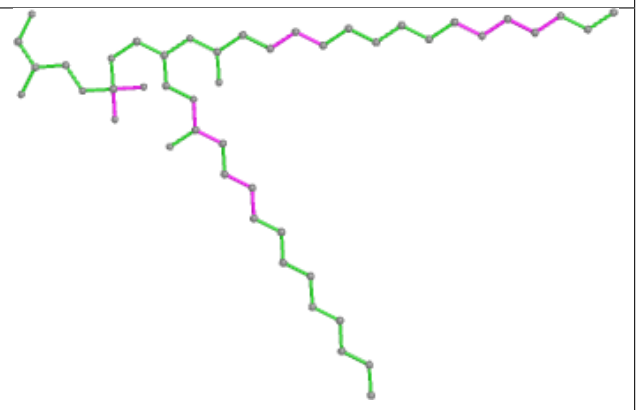


Rings

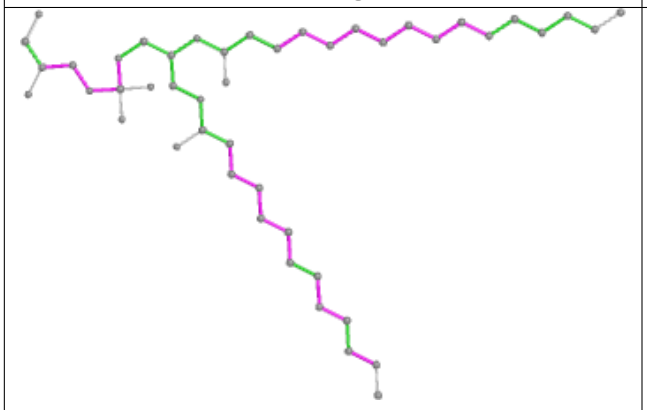
Ligand LHG A 816



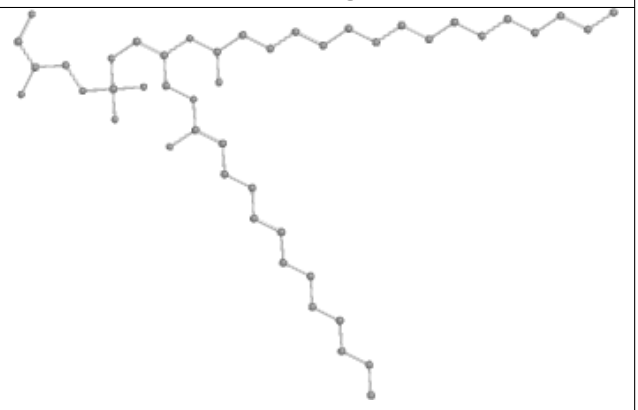
Bond lengths



Bond angles

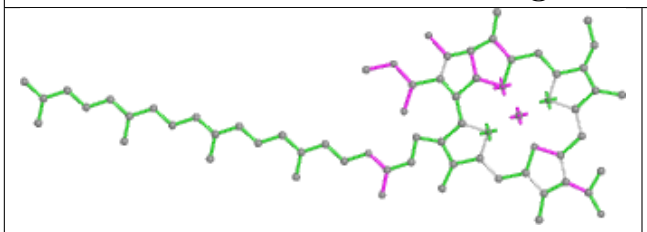


Torsions

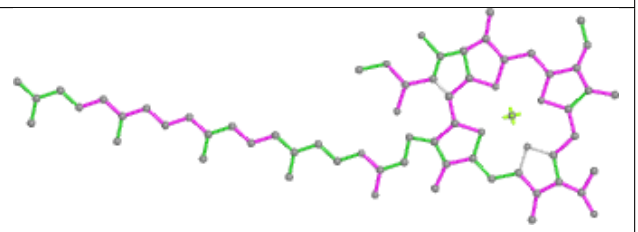


Rings

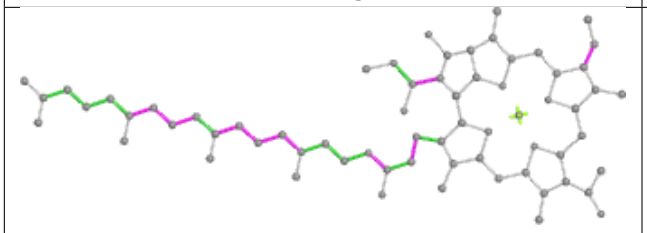
Ligand BCL 2 405



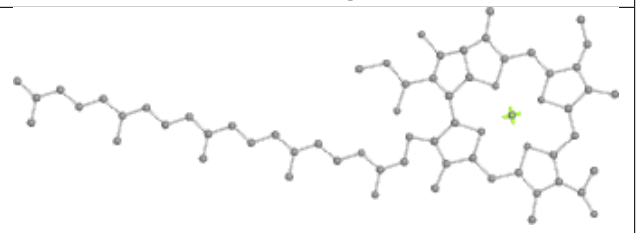
Bond lengths



Bond angles

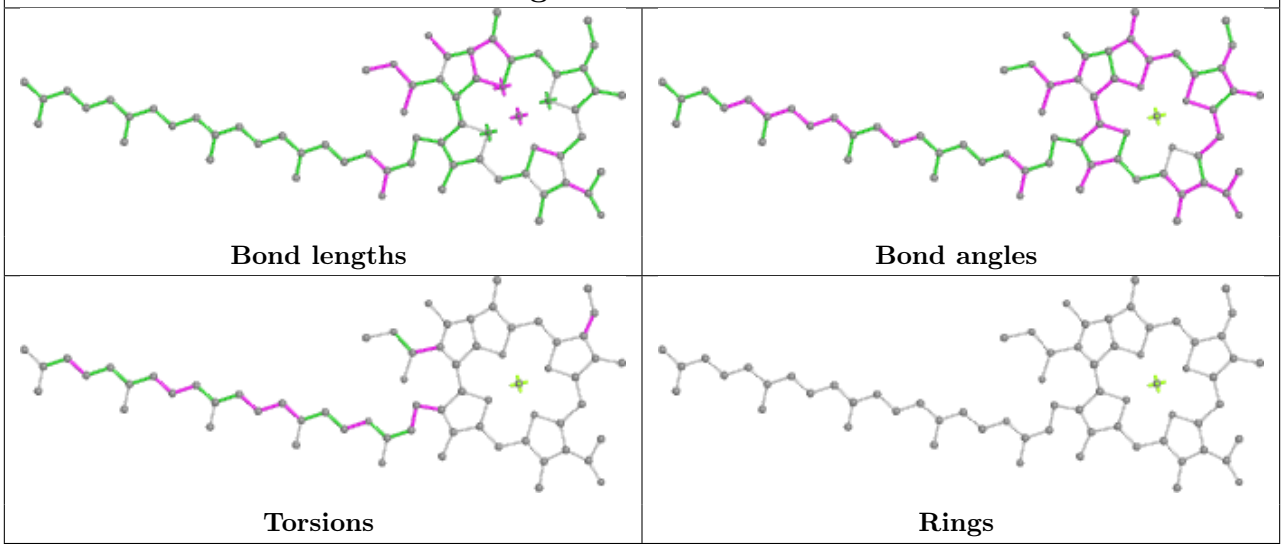


Torsions

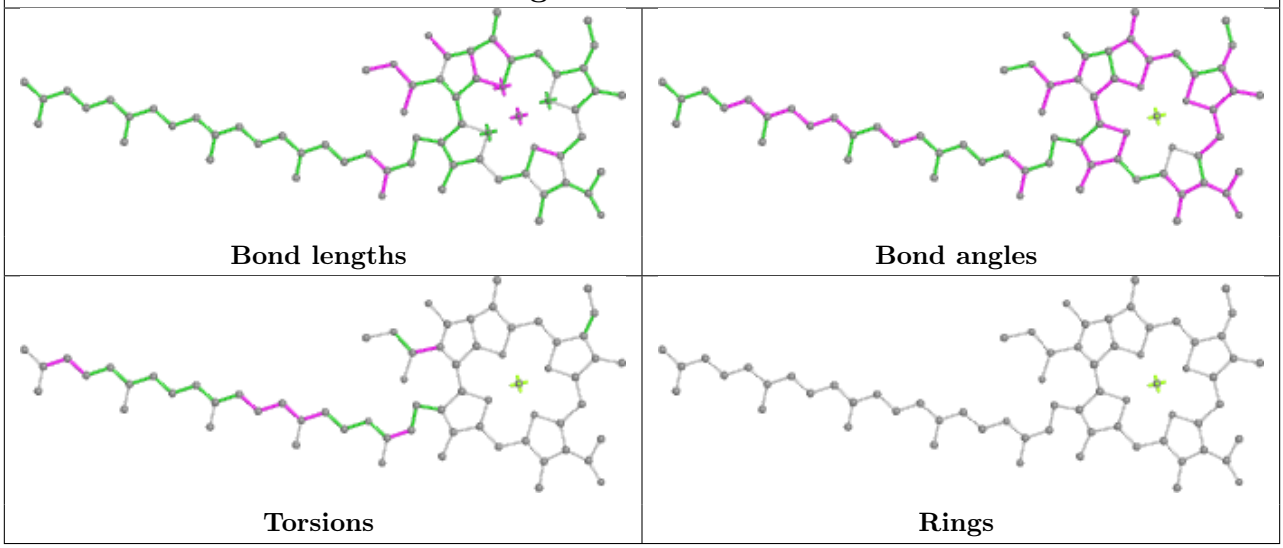


Rings

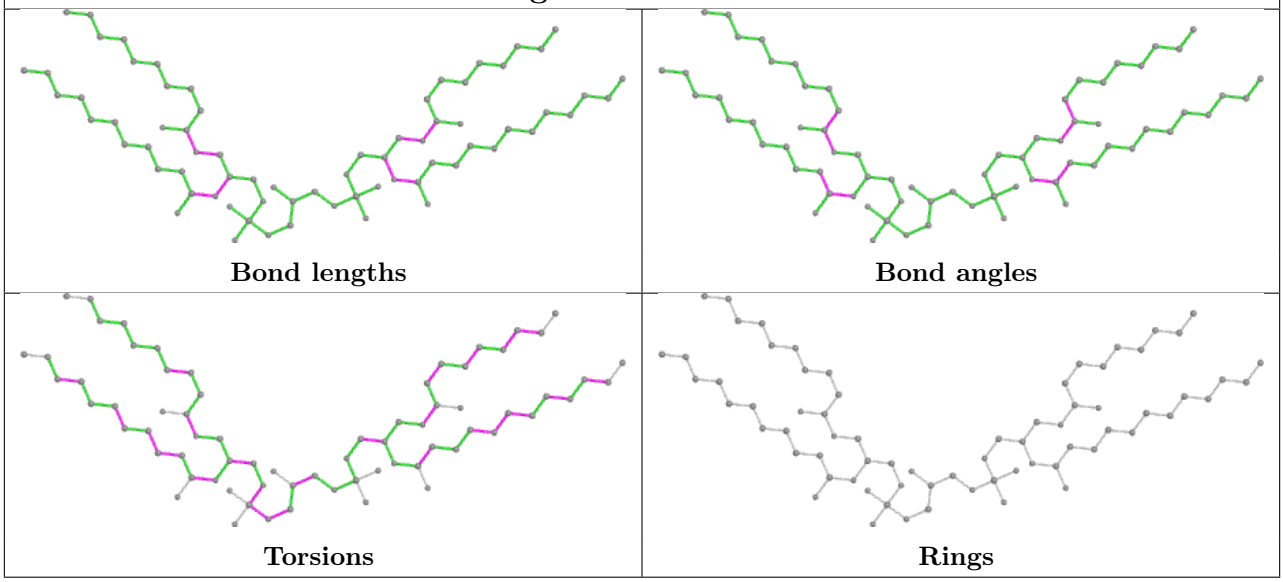
Ligand BCL 4 402



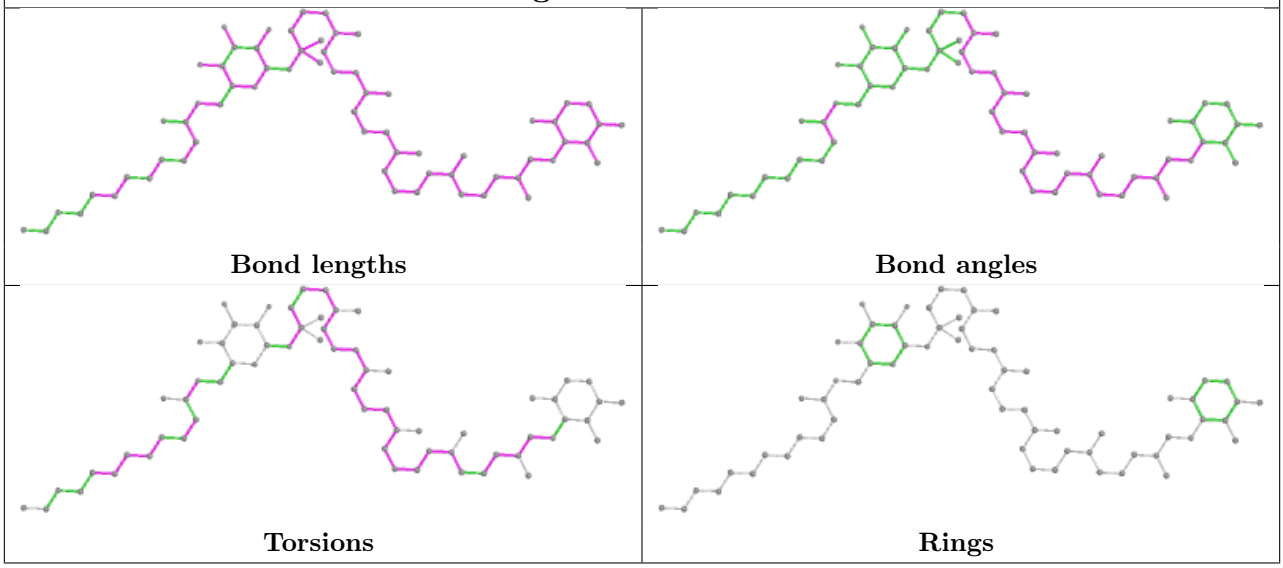
Ligand BCL 5 404



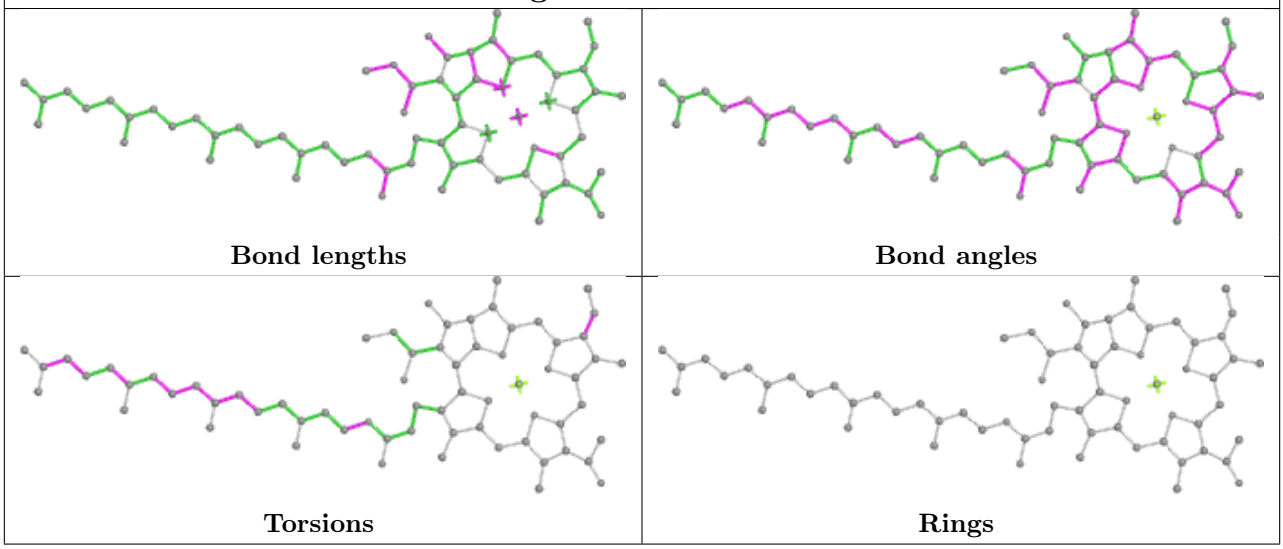
Ligand CDL c 303



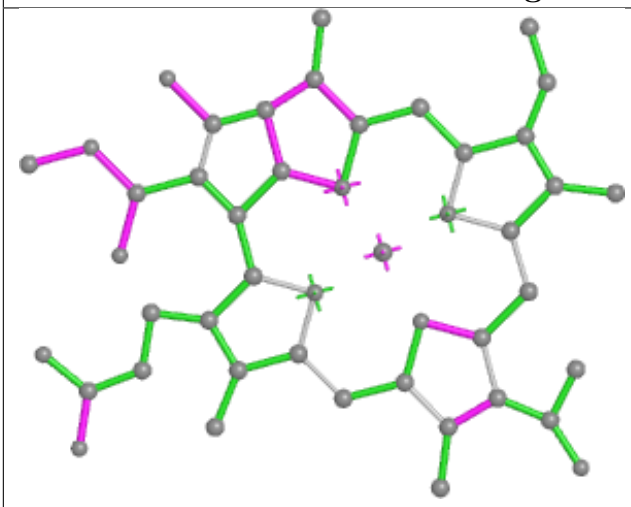
Ligand F39 A 814



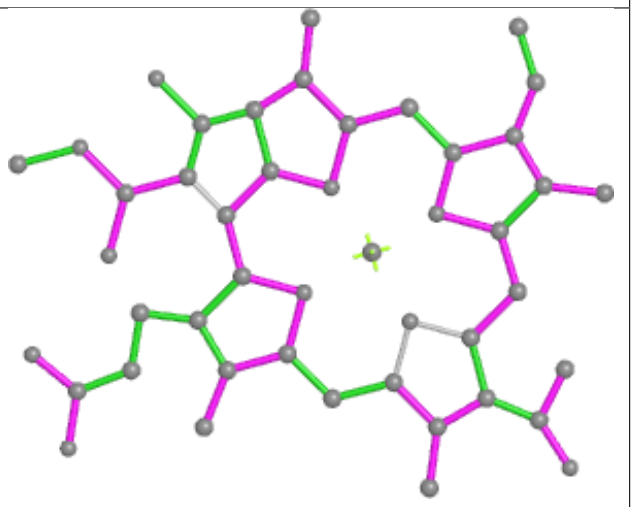
Ligand BCL 4 409



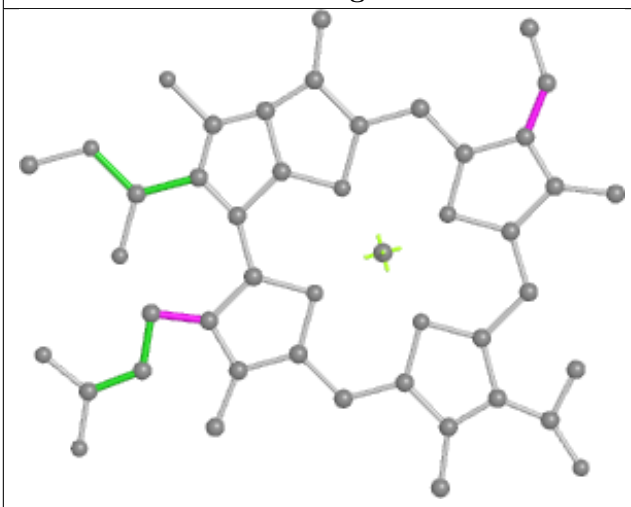
Ligand BCL A 806



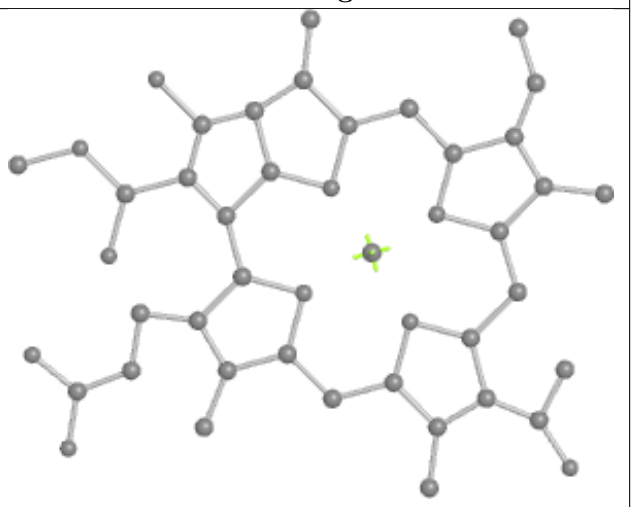
Bond lengths



Bond angles

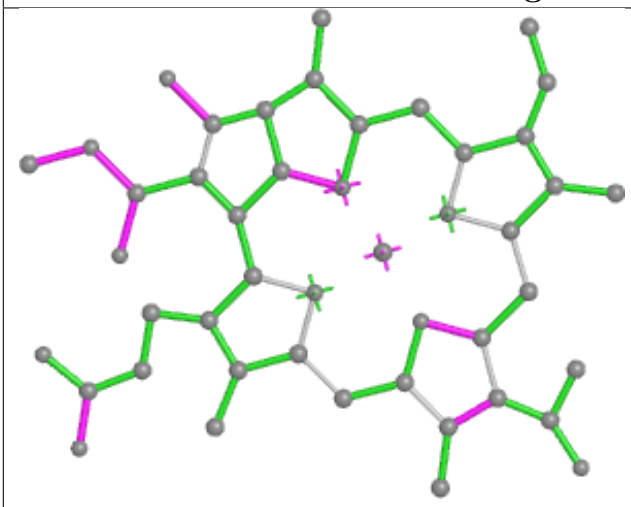


Torsions

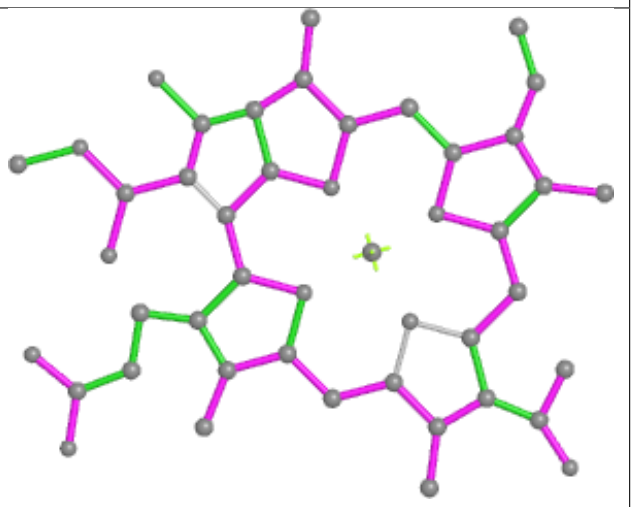


Rings

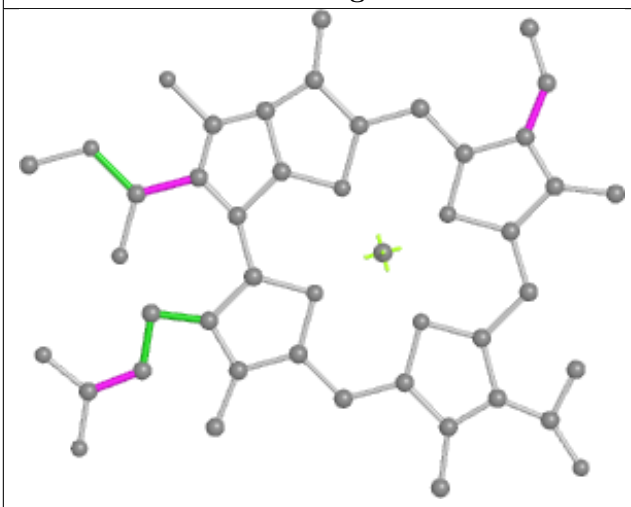
Ligand BCL A 809



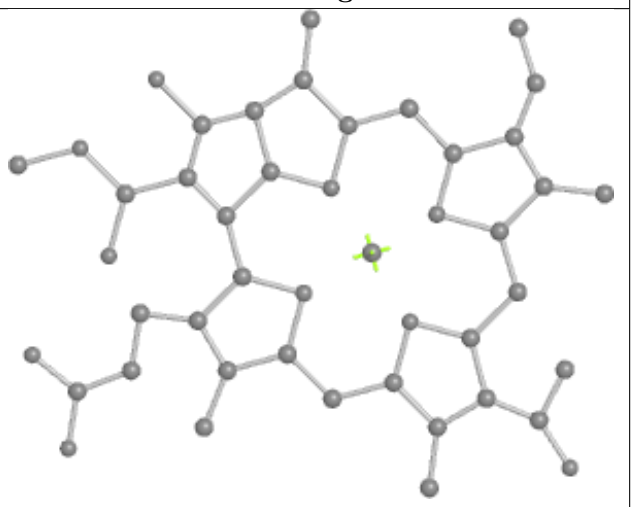
Bond lengths



Bond angles

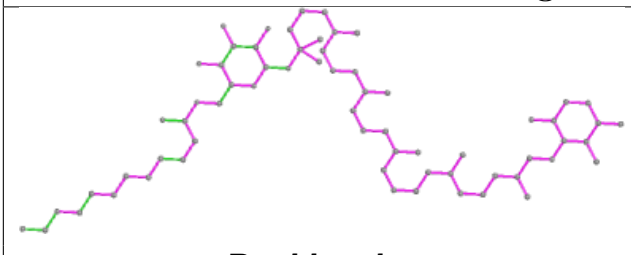


Torsions

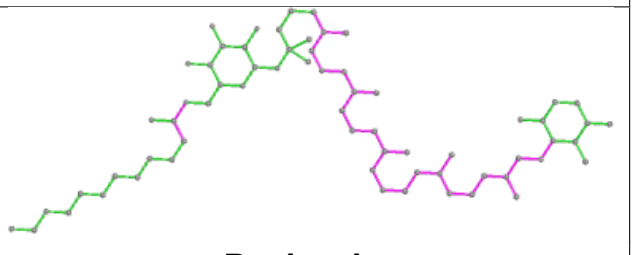


Rings

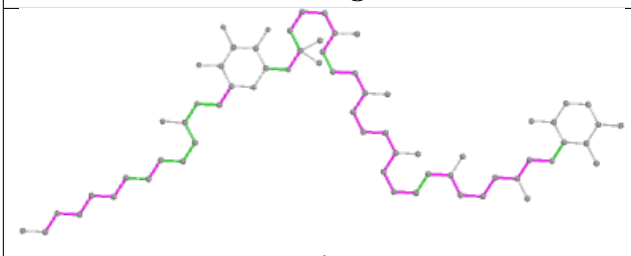
Ligand F39 a 816



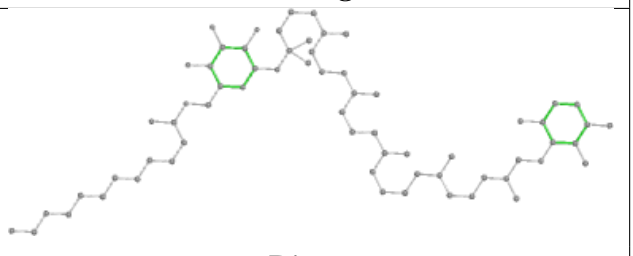
Bond lengths



Bond angles

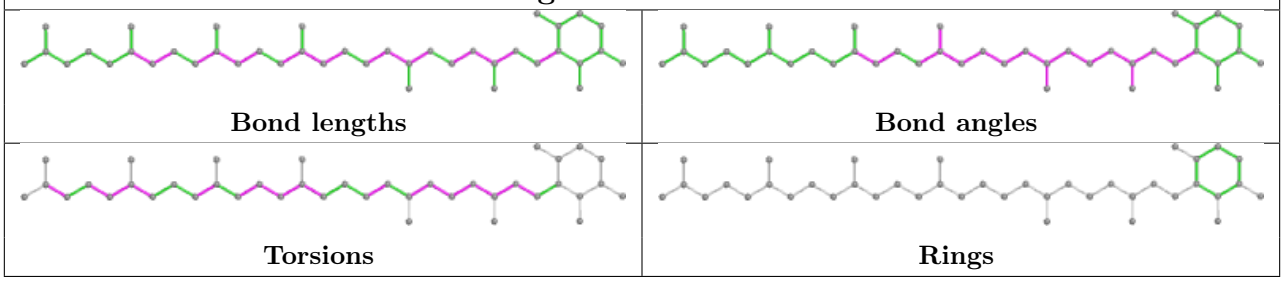


Torsions

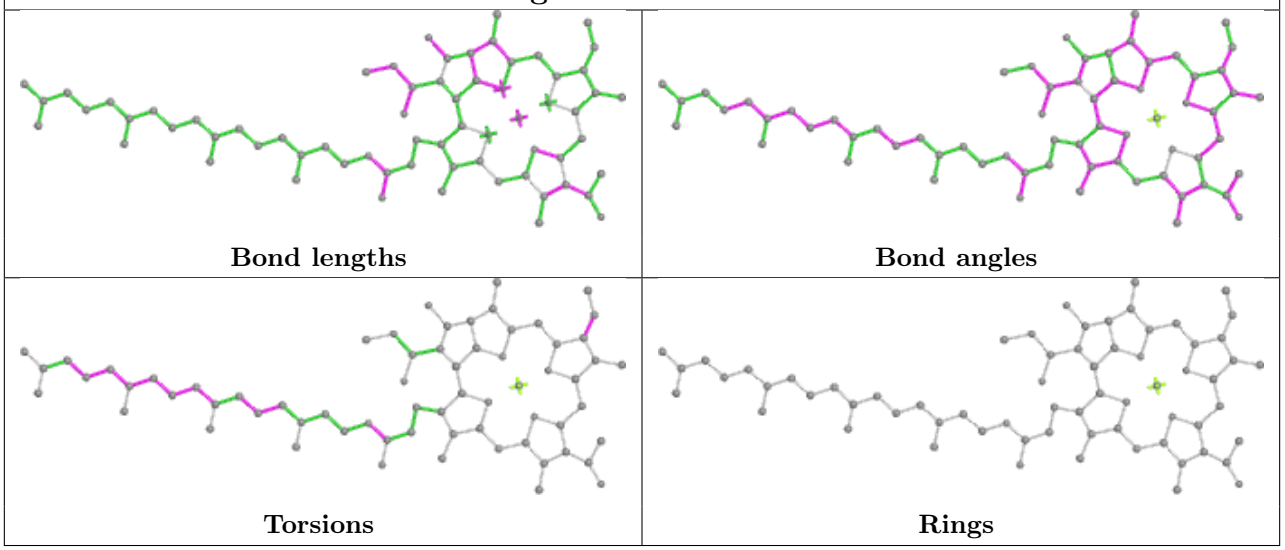


Rings

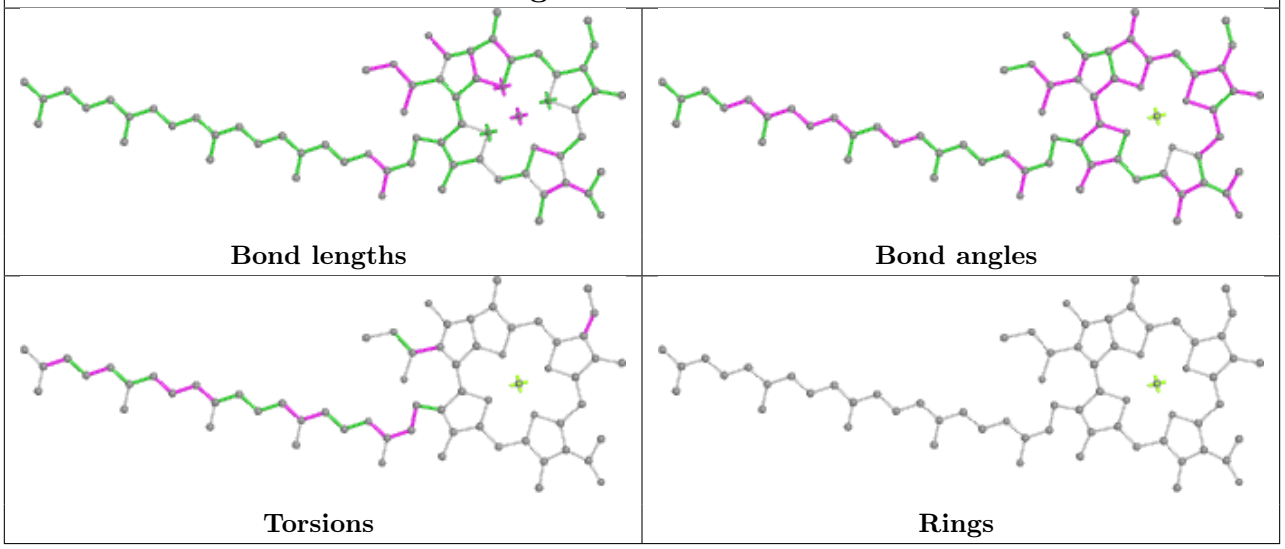
Ligand F26 a 815



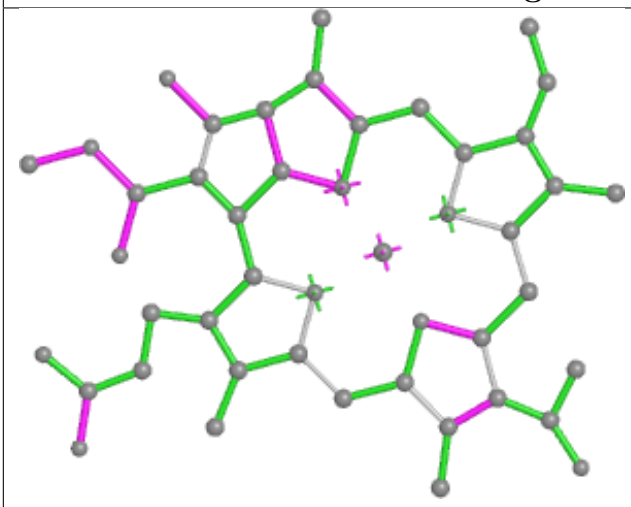
Ligand BCL a 806



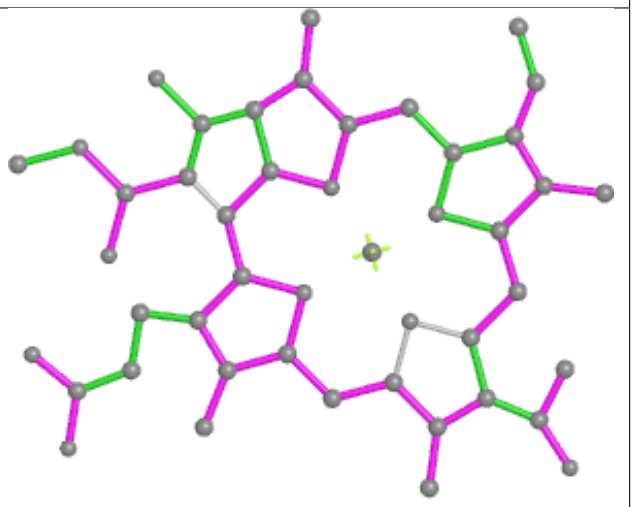
Ligand BCL 4 403



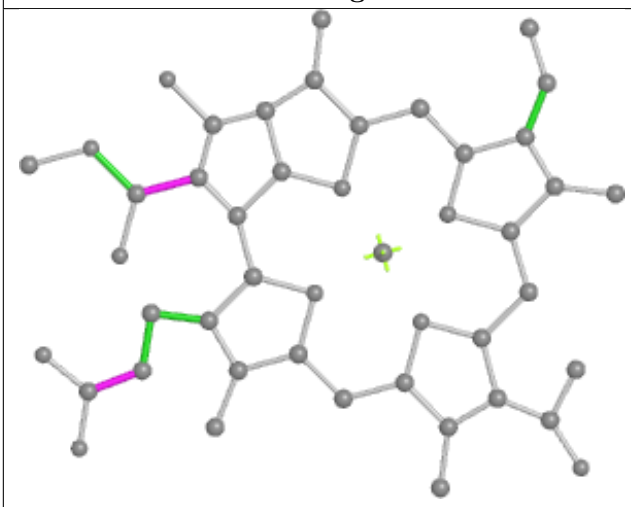
Ligand BCL A 803



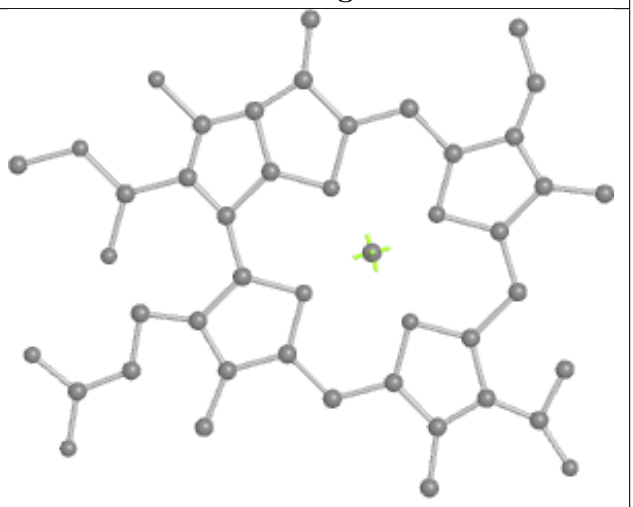
Bond lengths



Bond angles

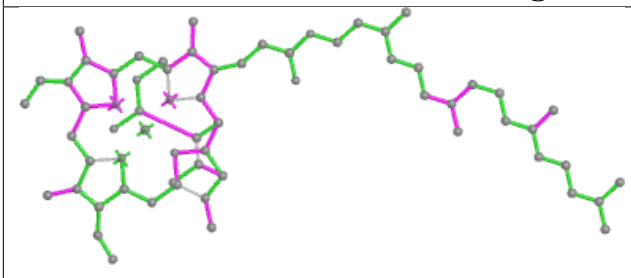


Torsions

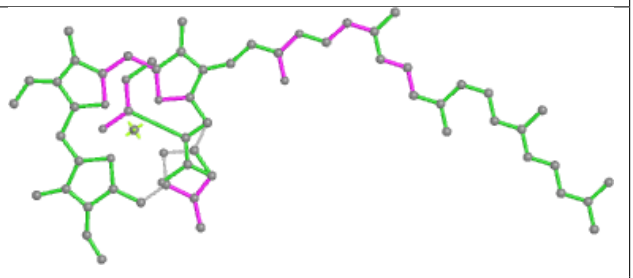


Rings

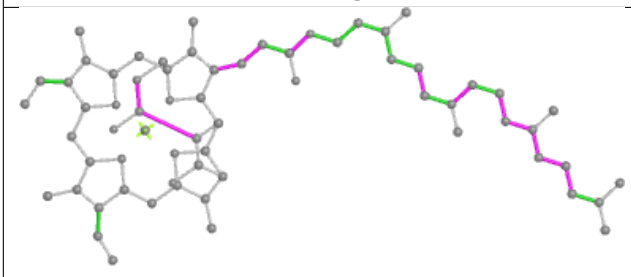
Ligand G2O a 801



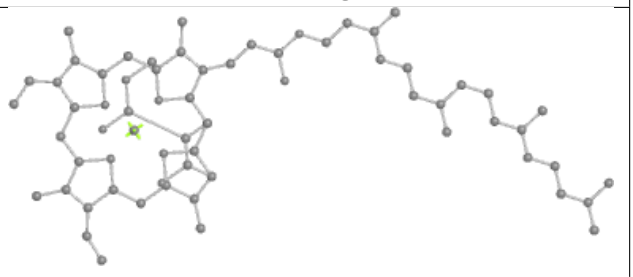
Bond lengths



Bond angles

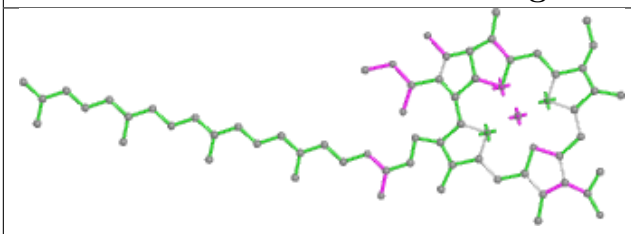


Torsions



Rings

Ligand BCL 1 402



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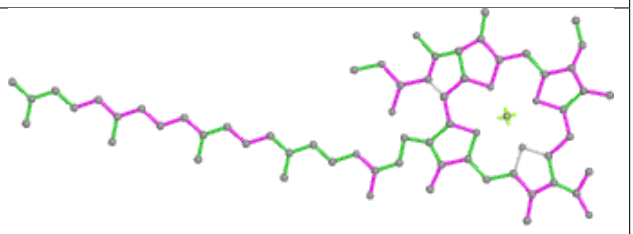
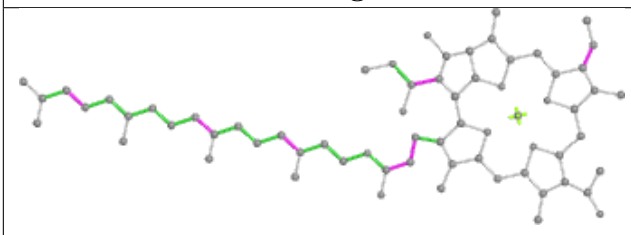
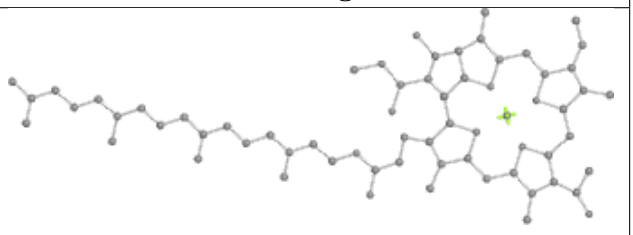


Bond angles

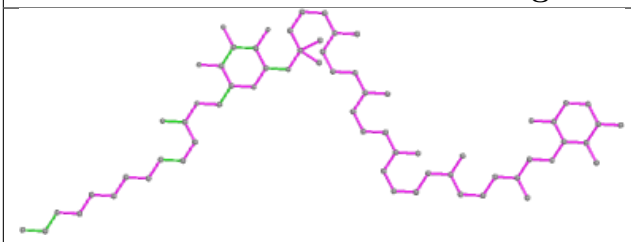


Torsions

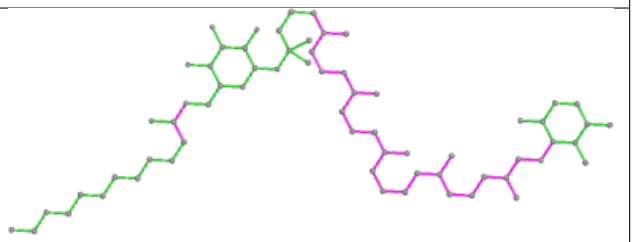


Rings

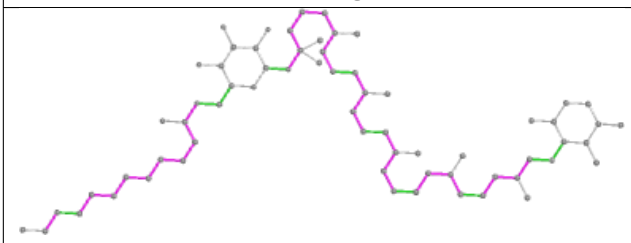
Ligand F39 A 815



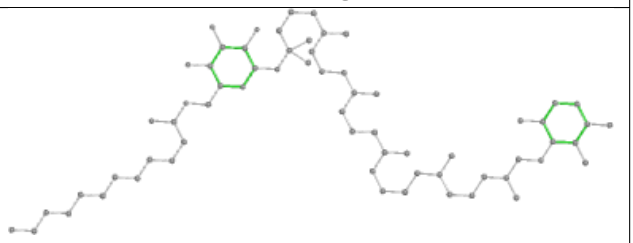
Bond lengths



Bond angles

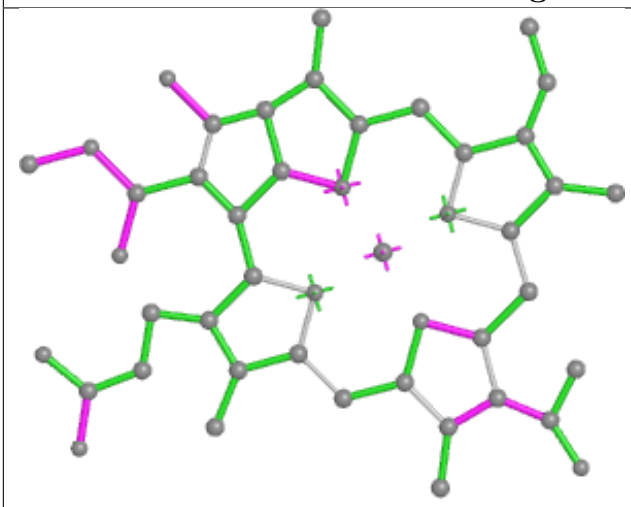


Torsions

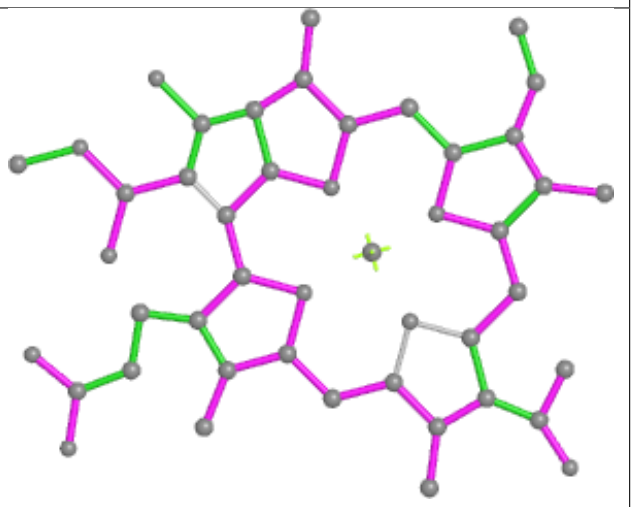


Rings

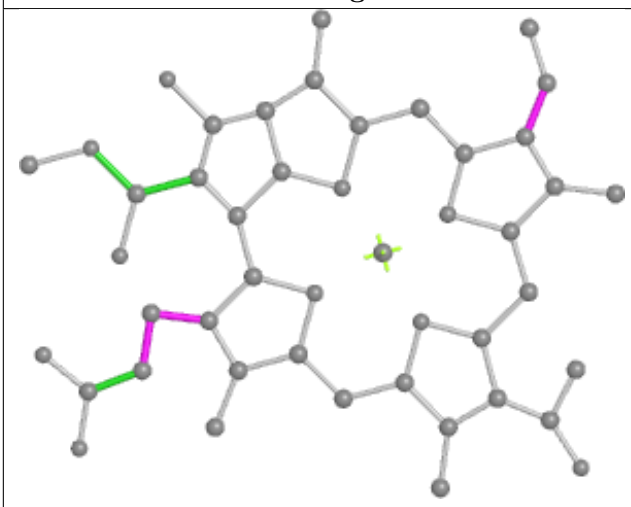
Ligand BCL a 807



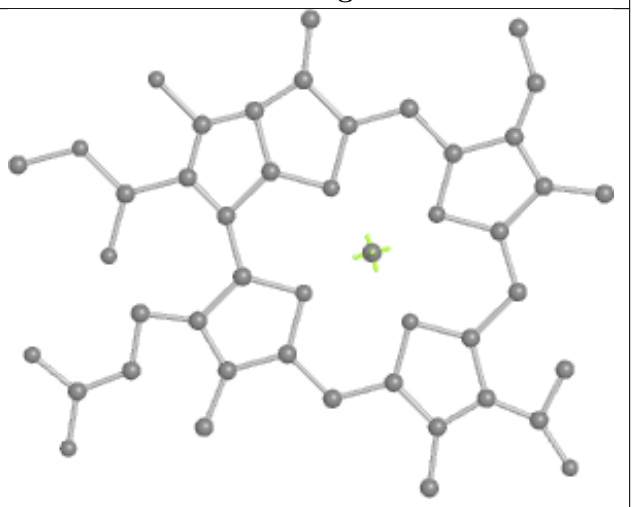
Bond lengths



Bond angles

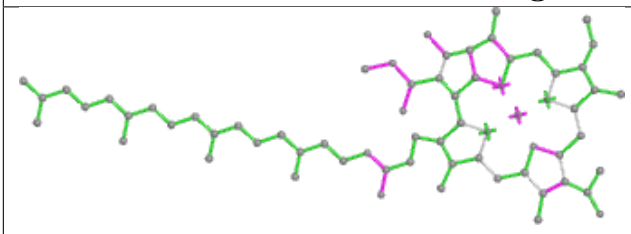


Torsions

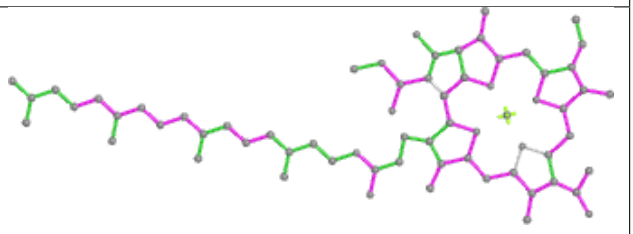


Rings

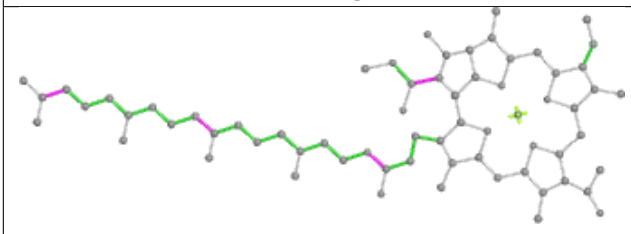
Ligand BCL 1 405



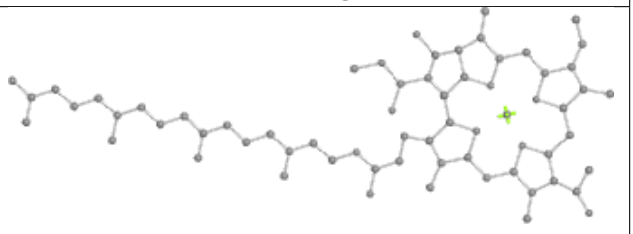
Bond lengths



Bond angles

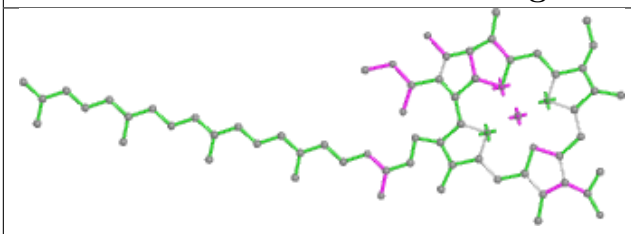


Torsions

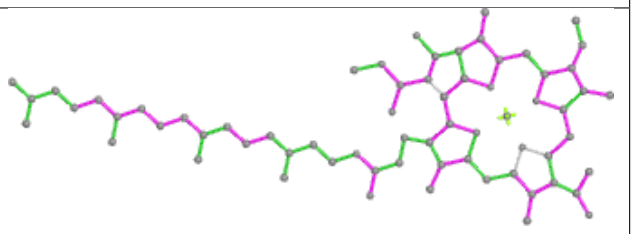


Rings

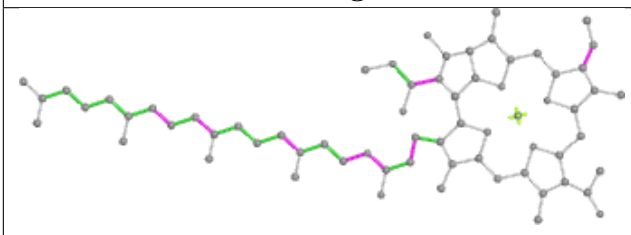
Ligand BCL 3 402



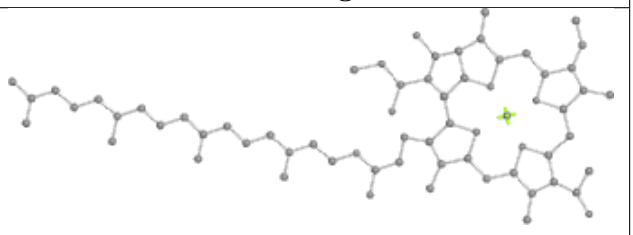
Bond lengths



Bond angles

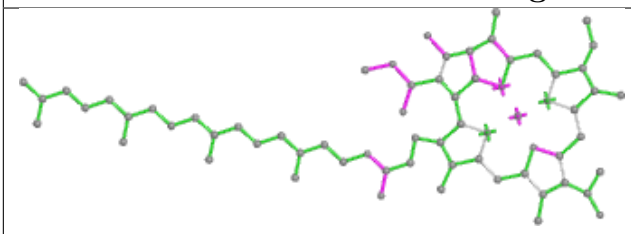


Torsions

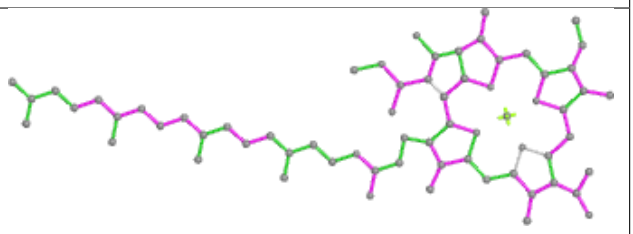


Rings

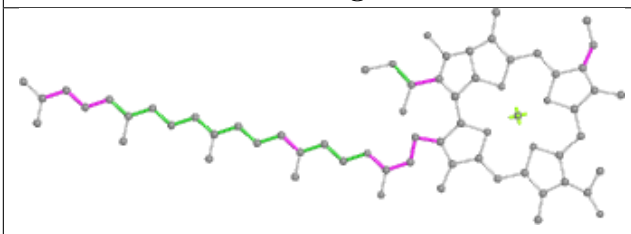
Ligand BCL 3 407



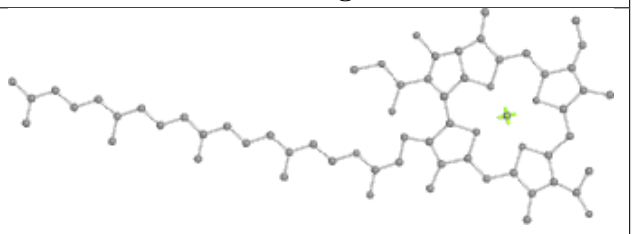
Bond lengths



Bond angles

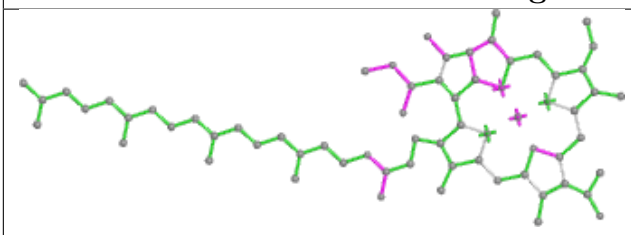


Torsions

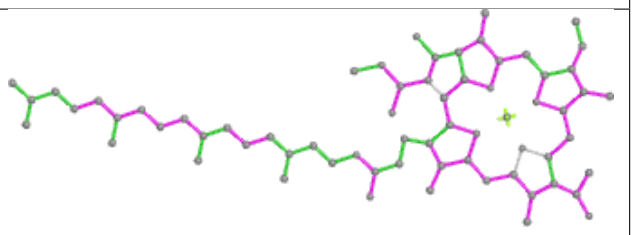


Rings

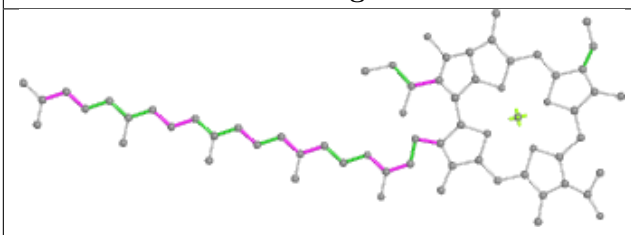
Ligand BCL 4 405



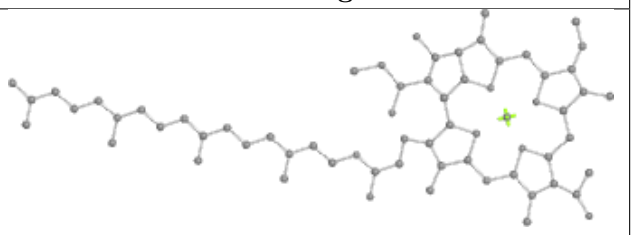
Bond lengths



Bond angles

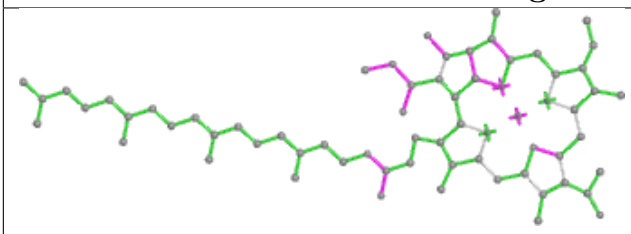


Torsions

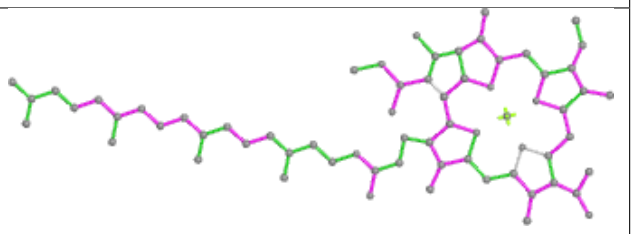


Rings

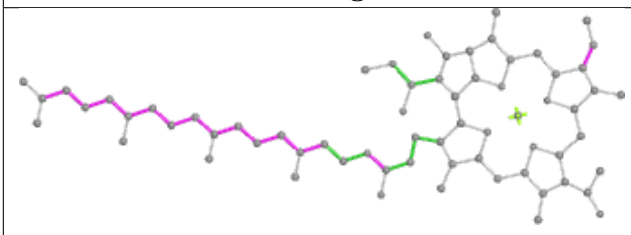
Ligand BCL 2 401



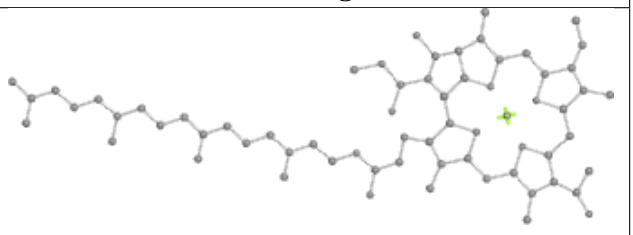
Bond lengths



Bond angles

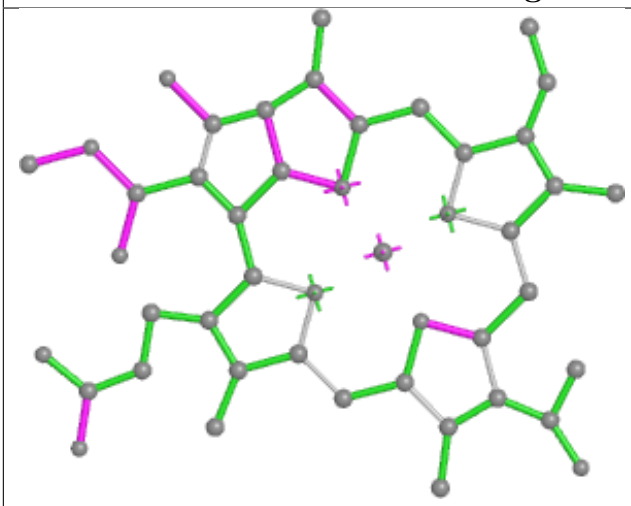


Torsions

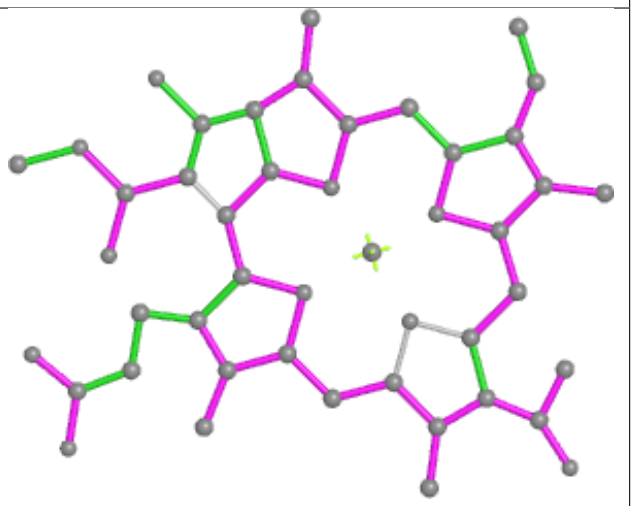


Rings

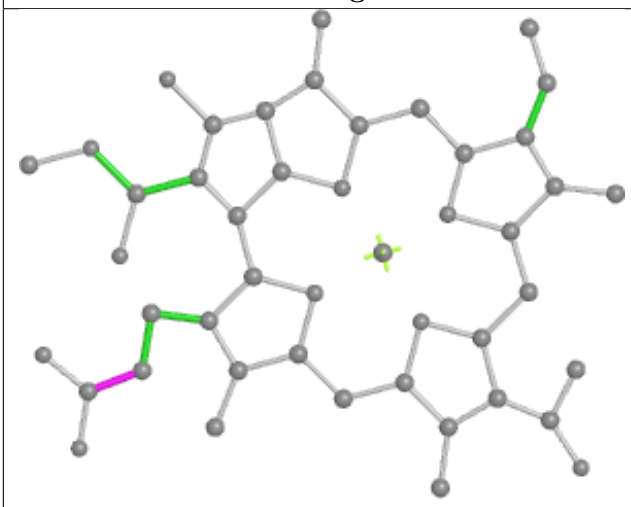
Ligand BCL A 808



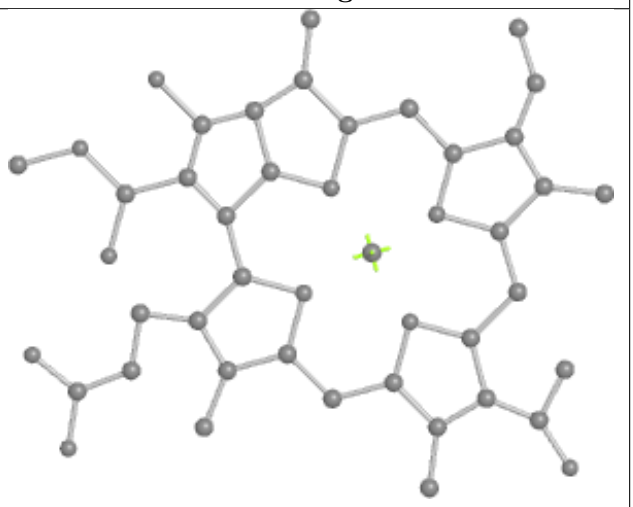
Bond lengths



Bond angles

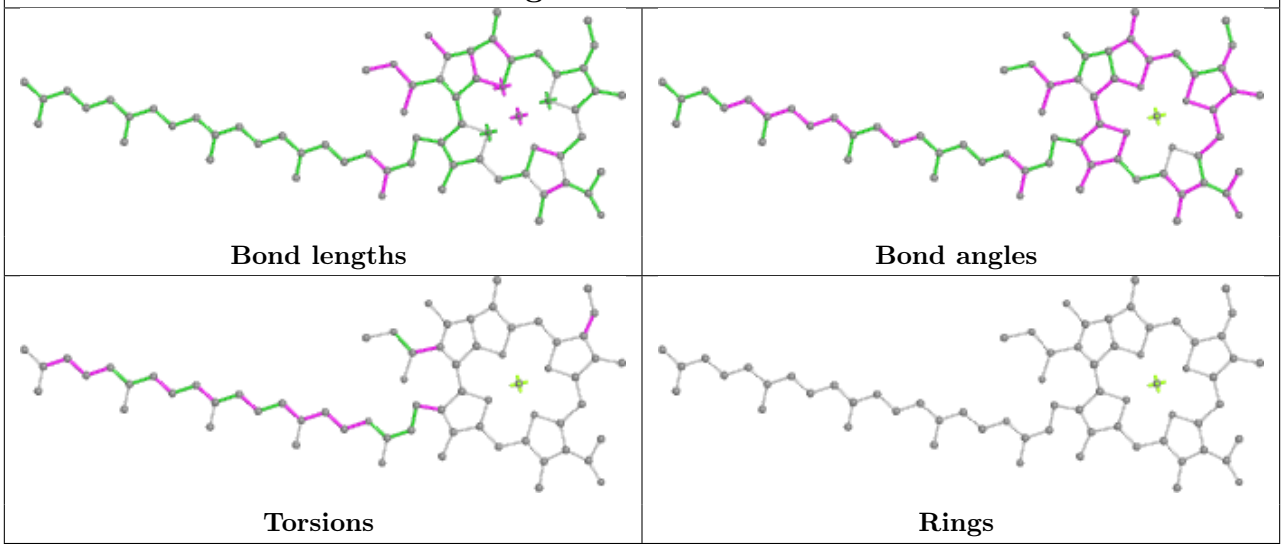


Torsions

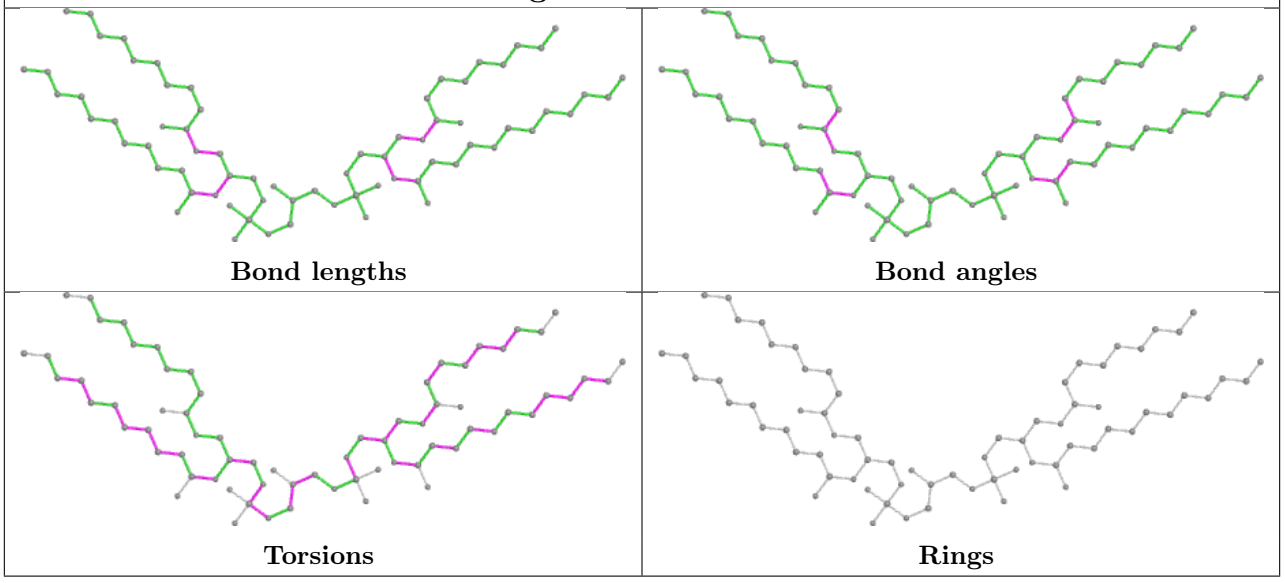


Rings

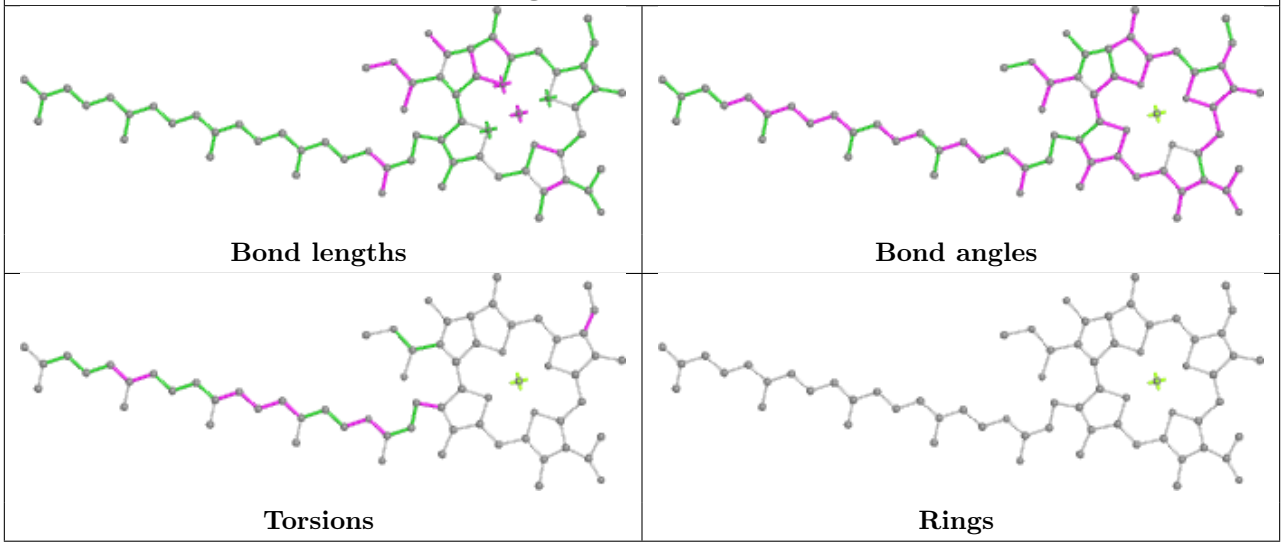
Ligand BCL A 807



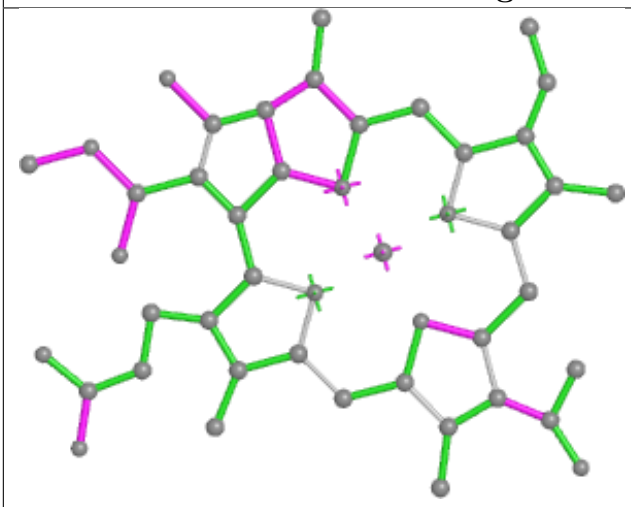
Ligand CDL a 820



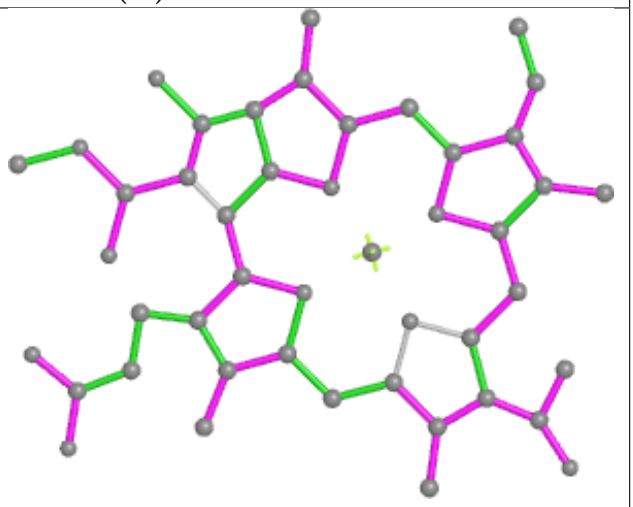
Ligand BCL A 810



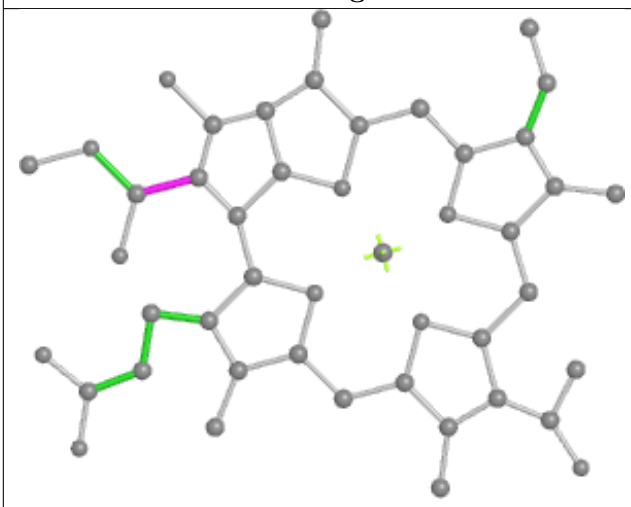
Ligand BCL 2 409 (B)



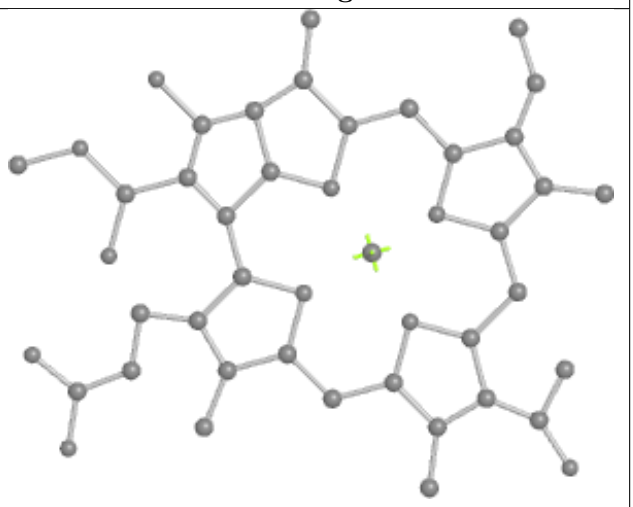
Bond lengths



Bond angles

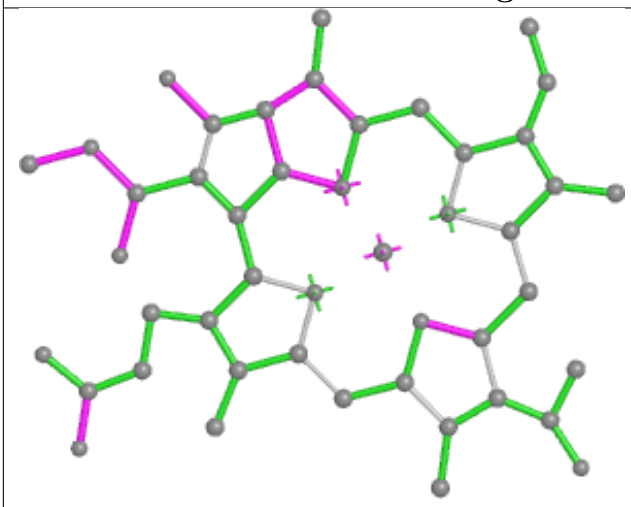


Torsions

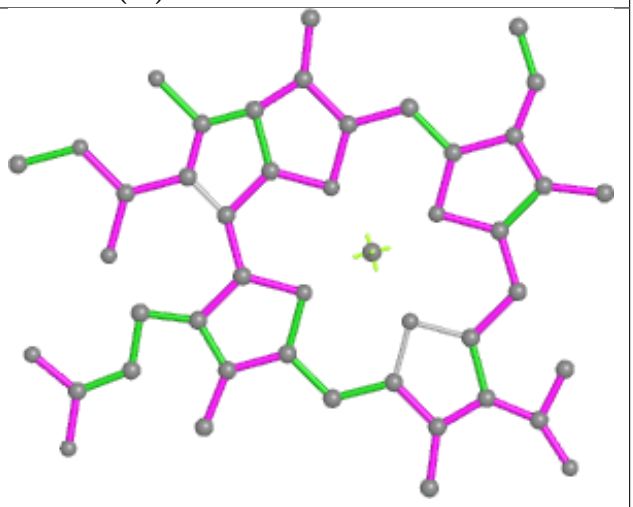


Rings

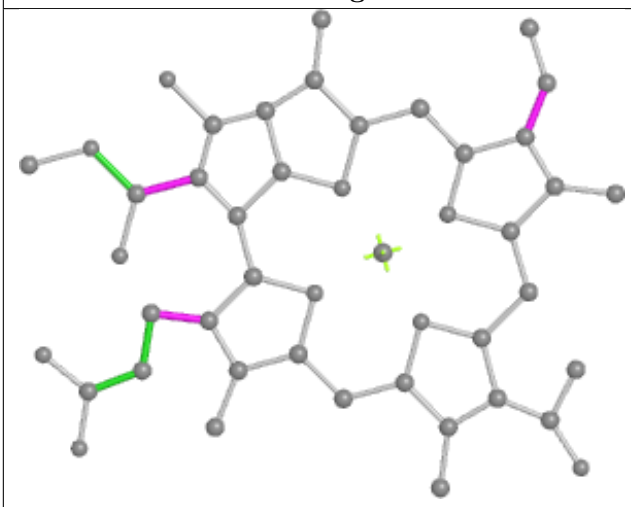
Ligand BCL 2 402 (B)



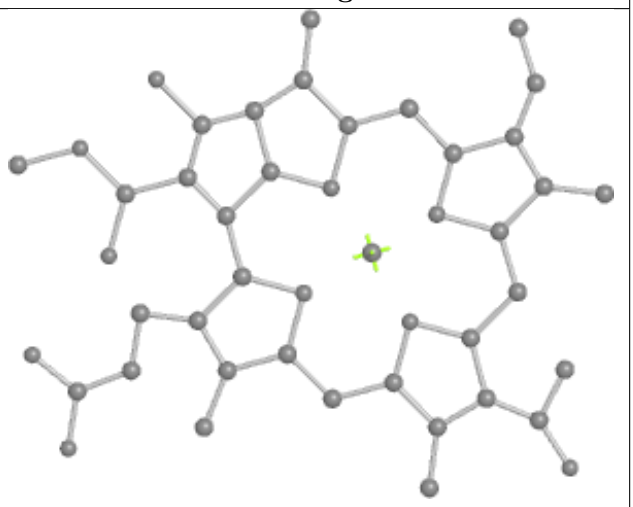
Bond lengths



Bond angles

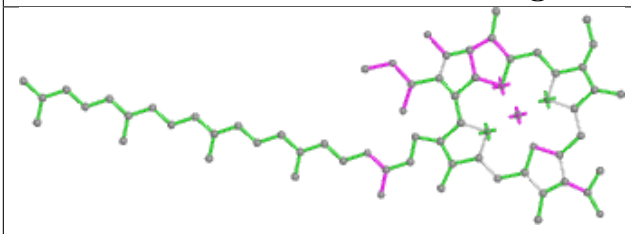


Torsions



Rings

Ligand BCL 6 403



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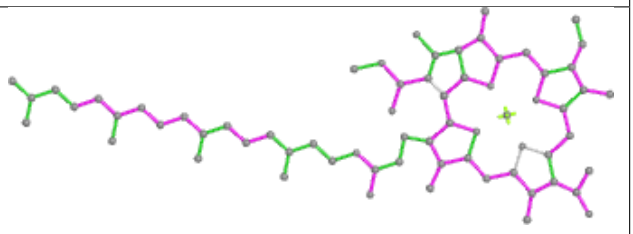
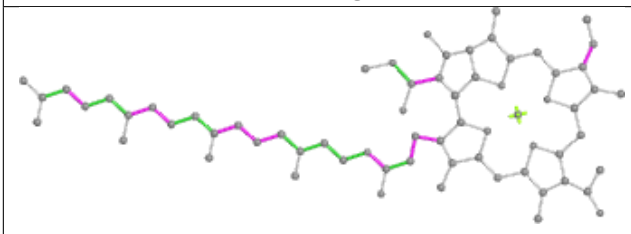
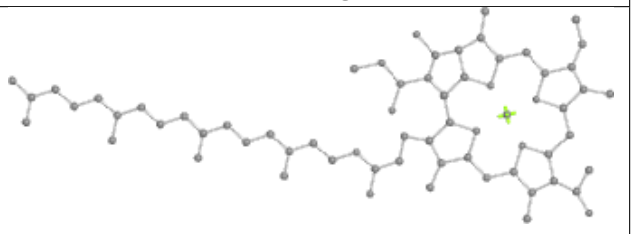


Bond angles

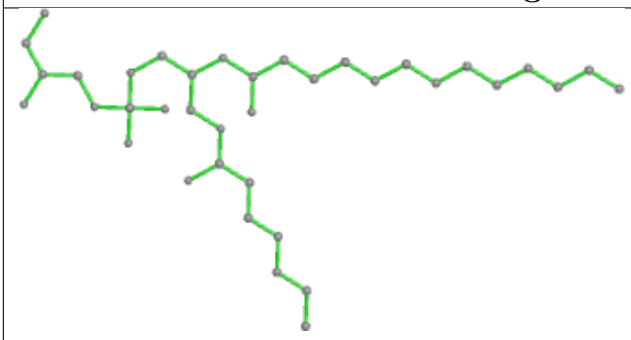


Torsions

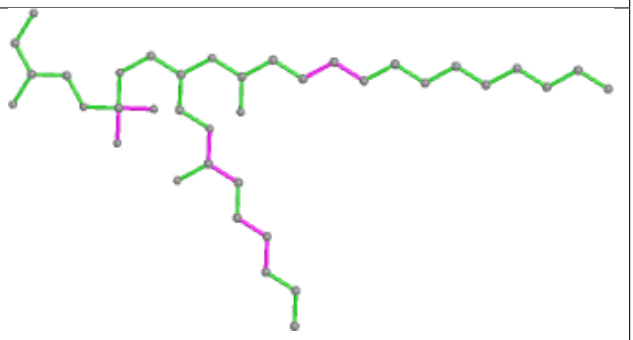


Rings

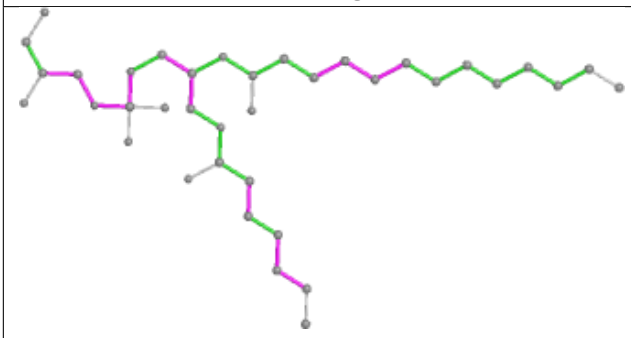
Ligand LHG E 101



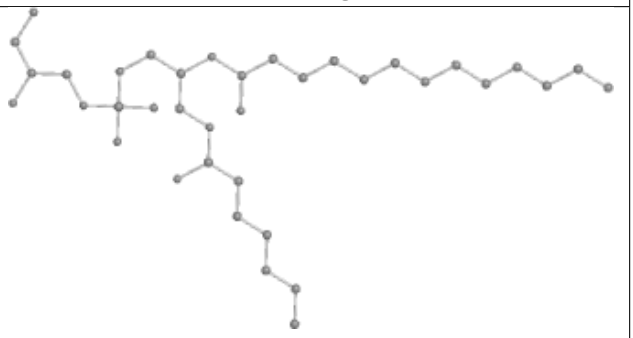
Bond lengths



Bond angles

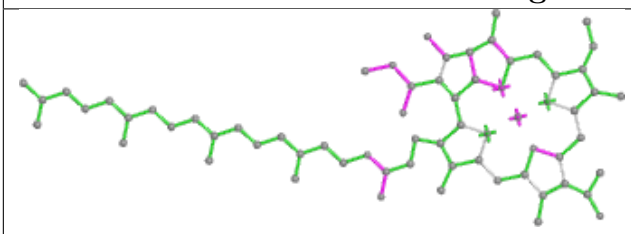


Torsions

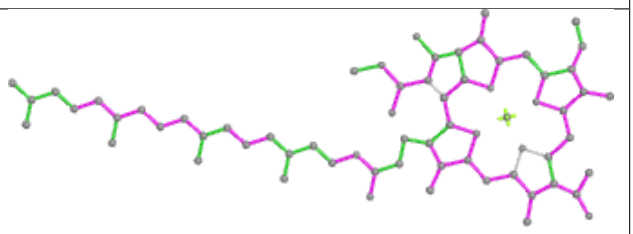


Rings

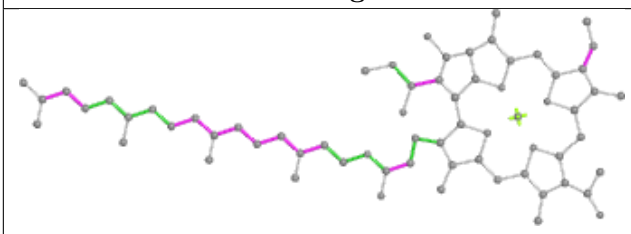
Ligand BCL 3 404



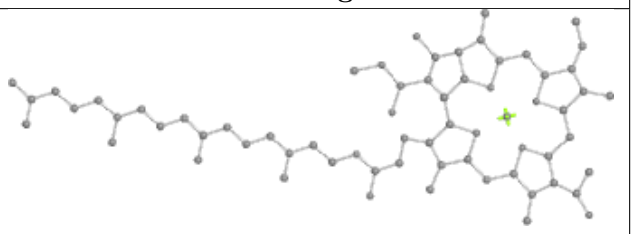
Bond lengths



Bond angles

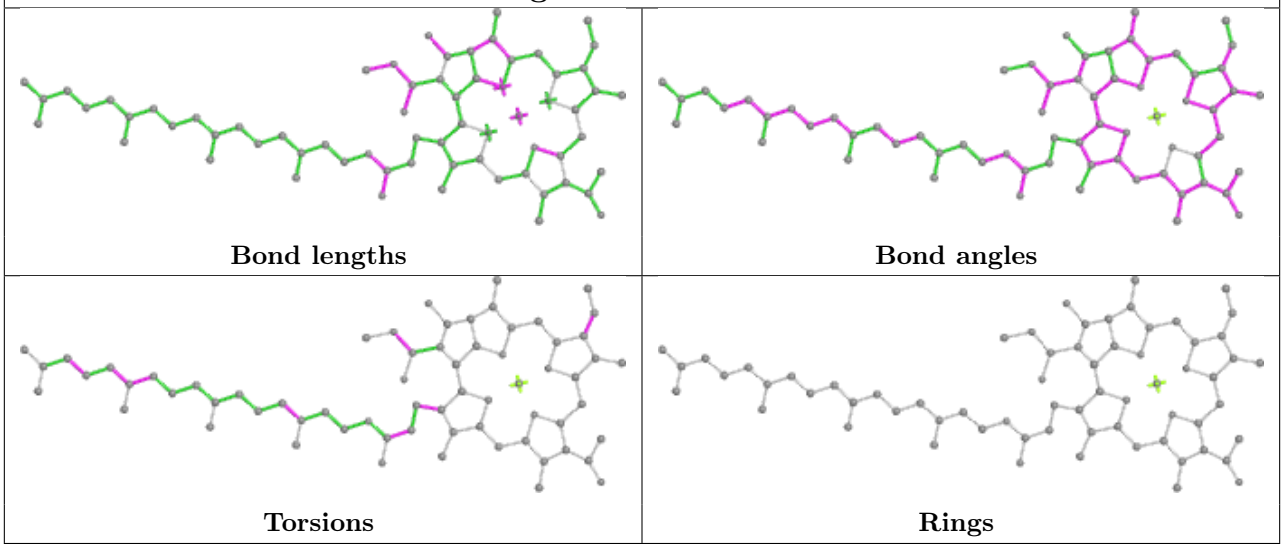


Torsions

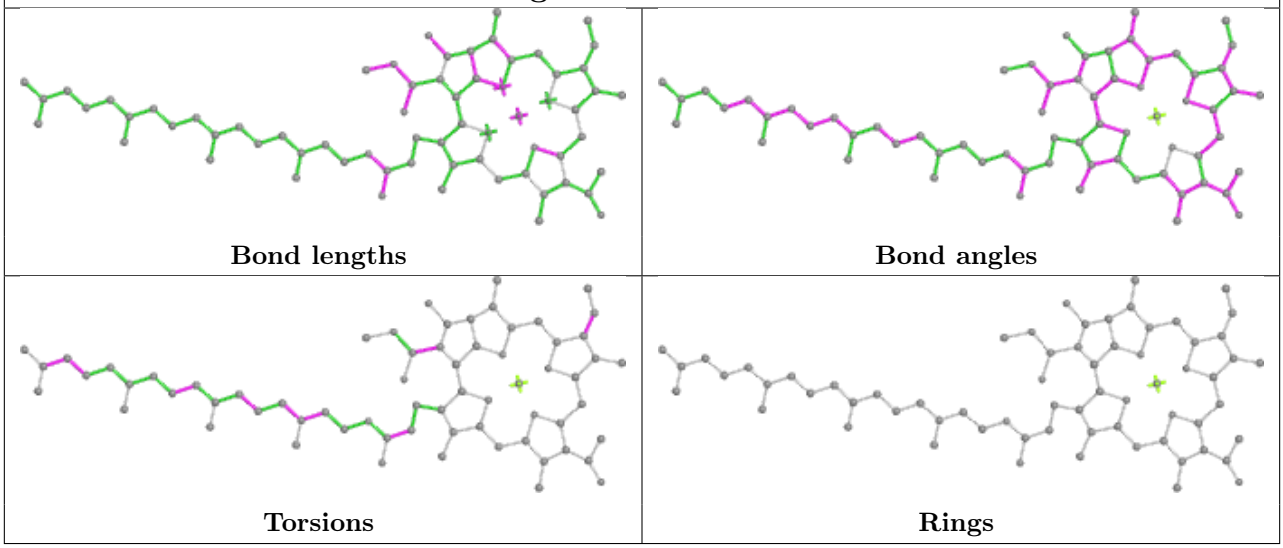


Rings

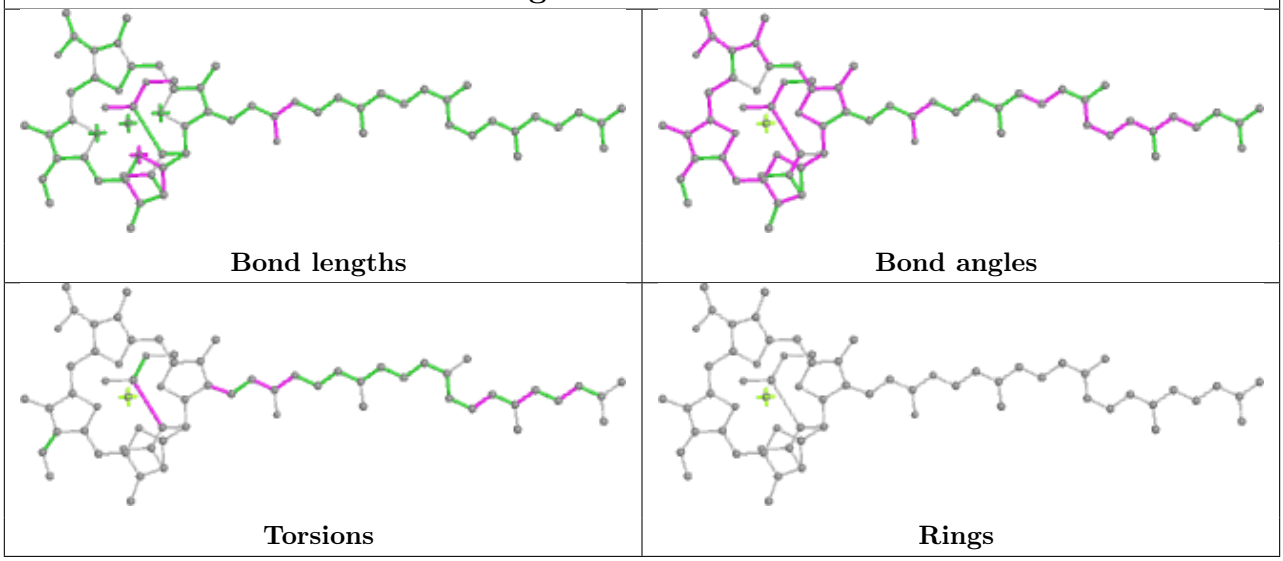
Ligand BCL 1 401



Ligand BCL 6 404



Ligand GS0 A 801



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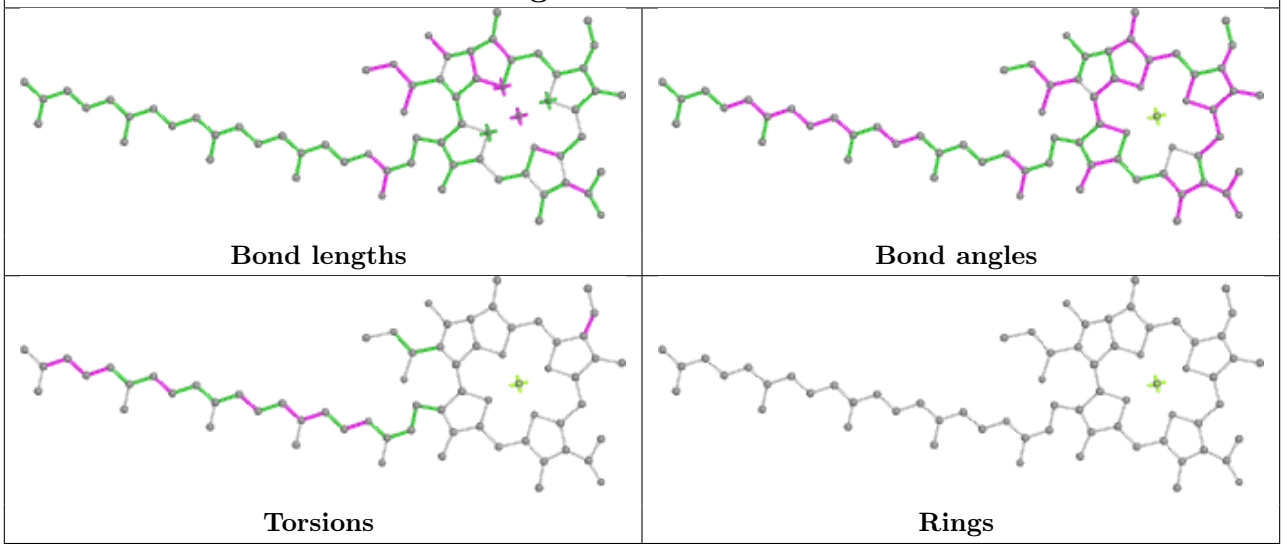
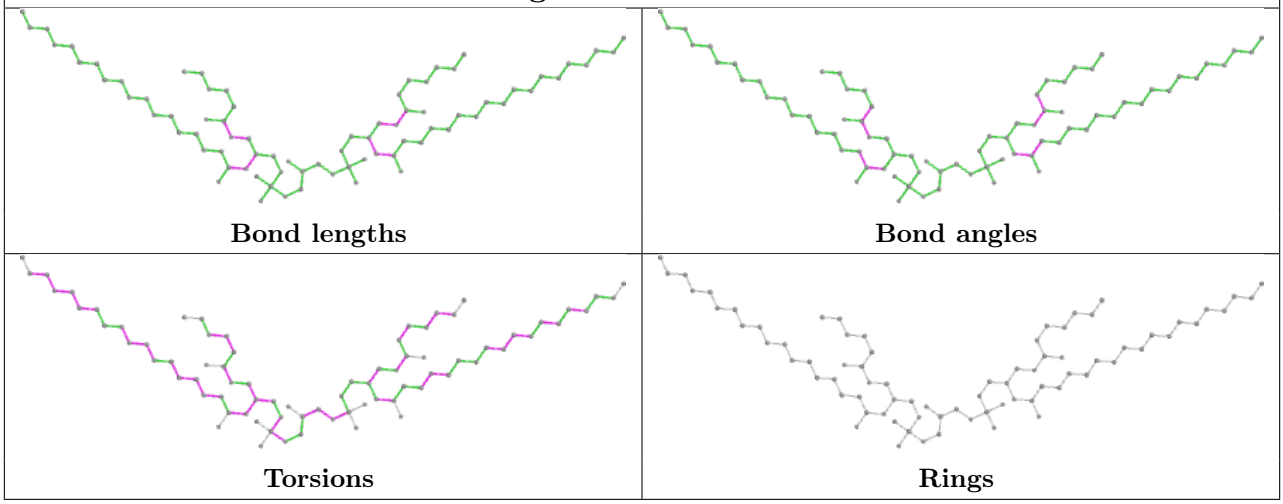


Ligand CDL 1 409



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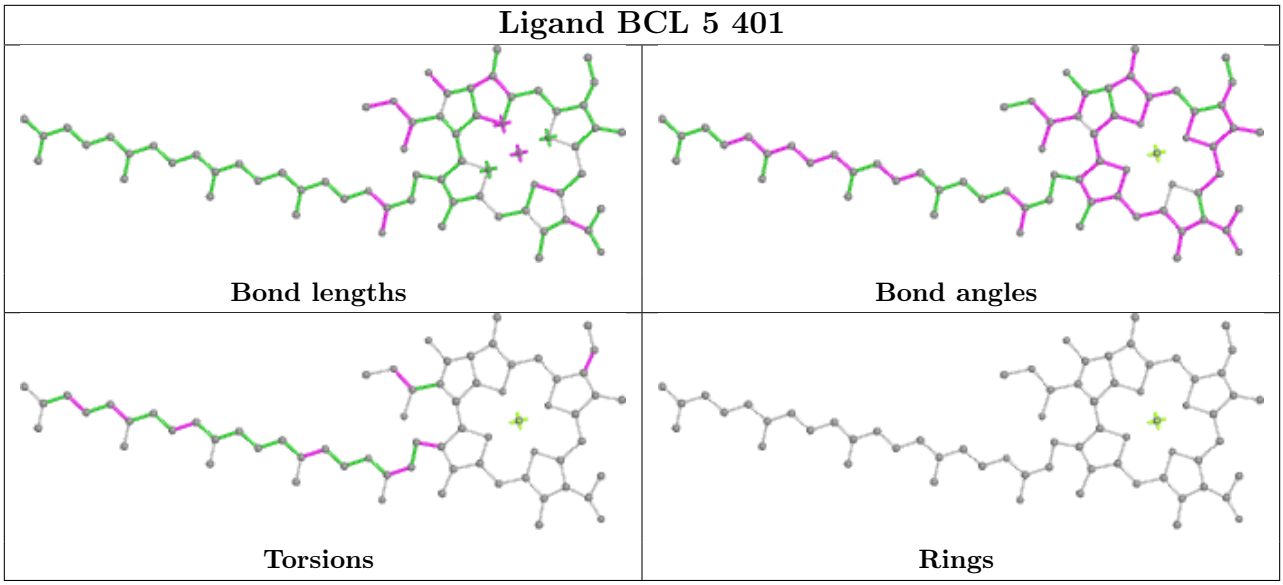

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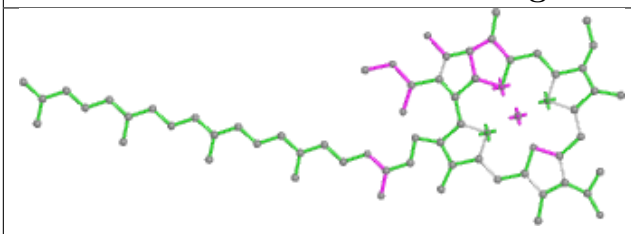
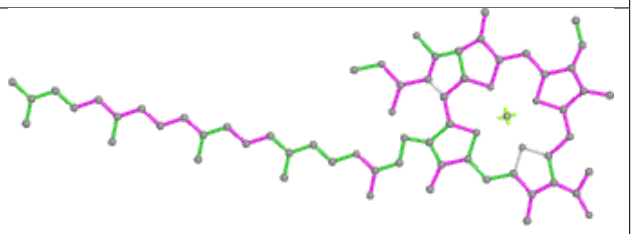
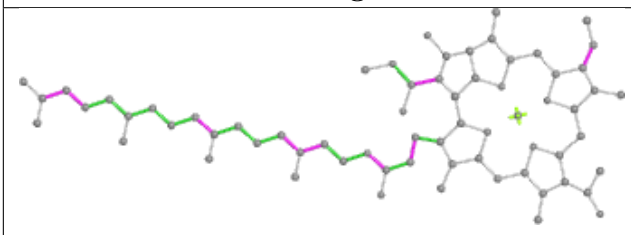


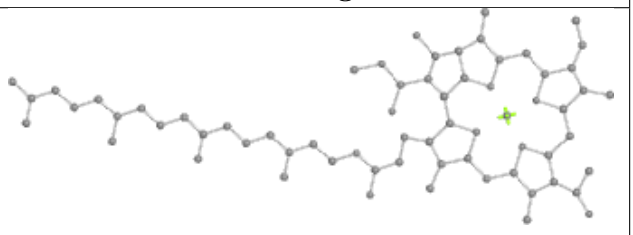
Bond lengths



Bond angles

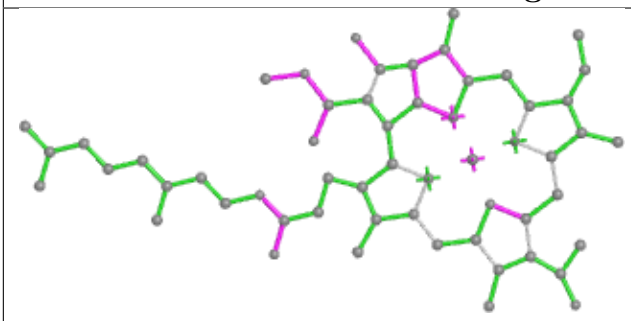


Torsions

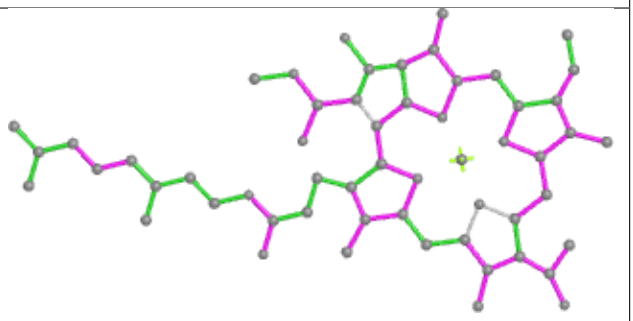


Rings

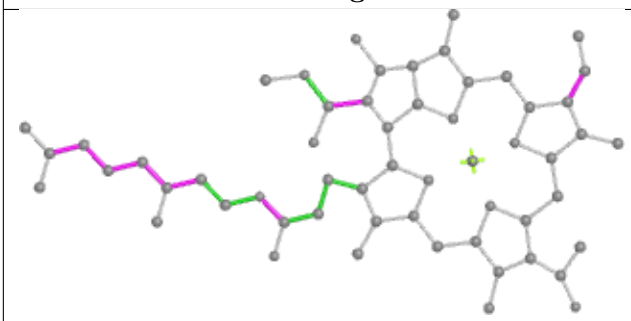
Ligand BCL A 804



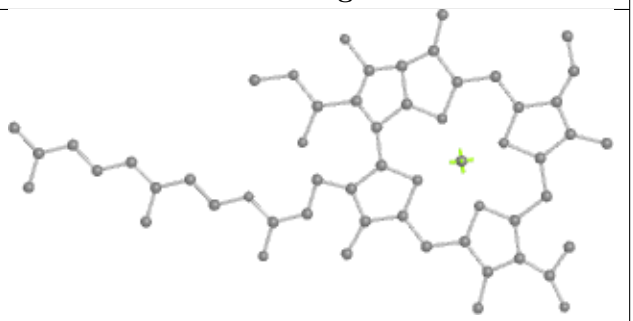
Bond lengths



Bond angles

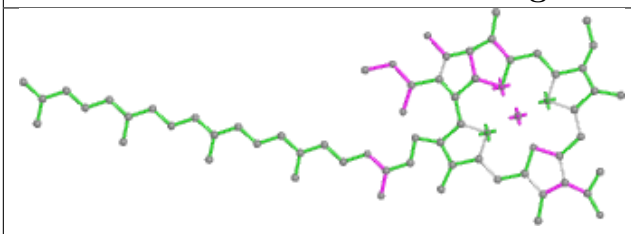


Torsions

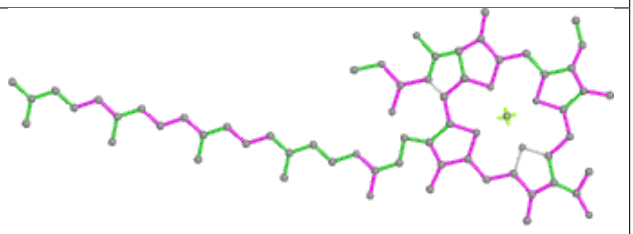


Rings

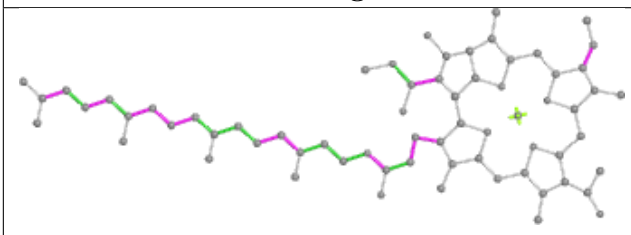
Ligand BCL a 812



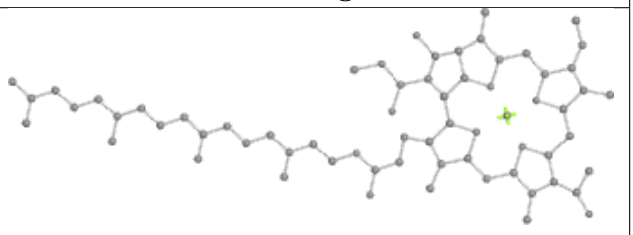
Bond lengths



Bond angles

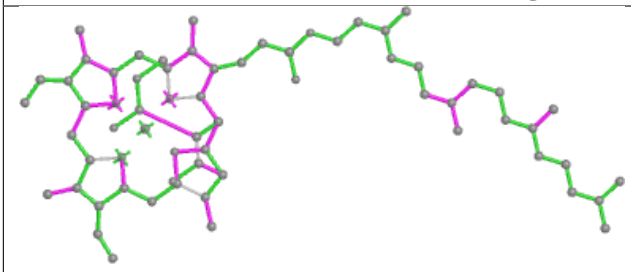


Torsions

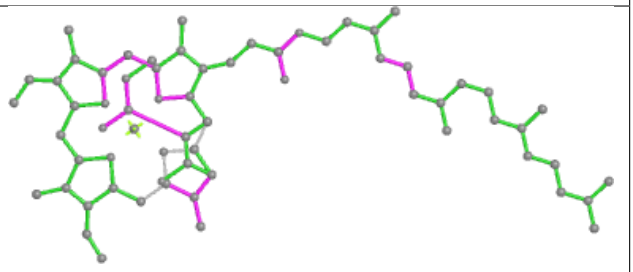


Rings

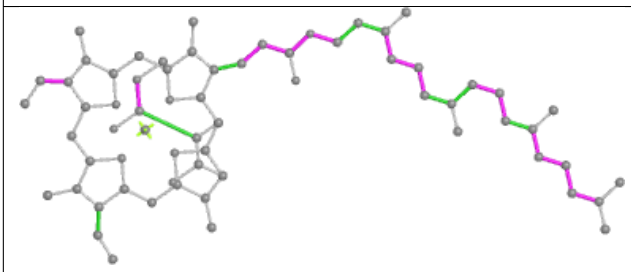
Ligand G2O A 802



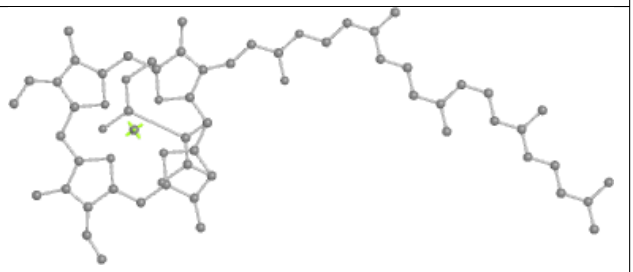
Bond lengths



Bond angles

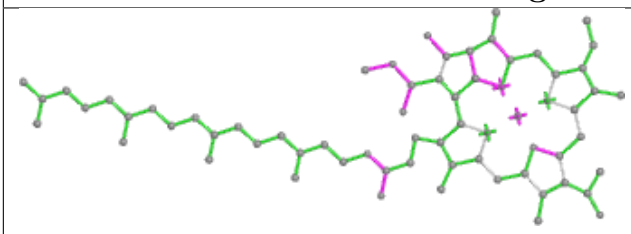


Torsions

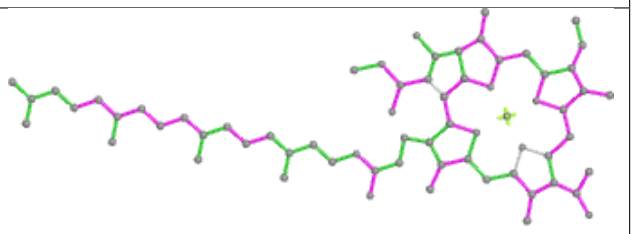


Rings

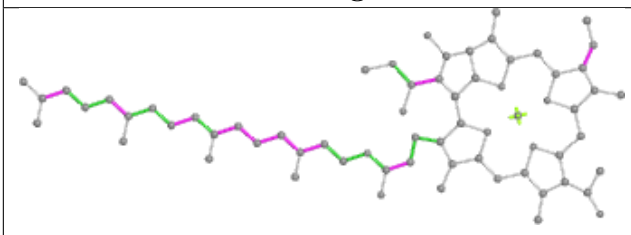
Ligand BCL 2 406



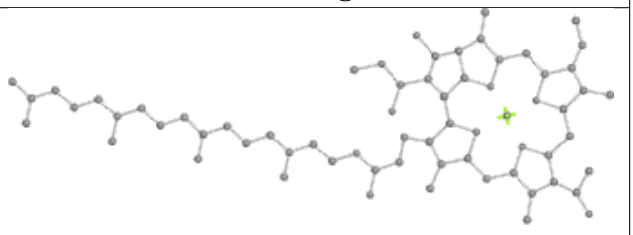
Bond lengths



Bond angles

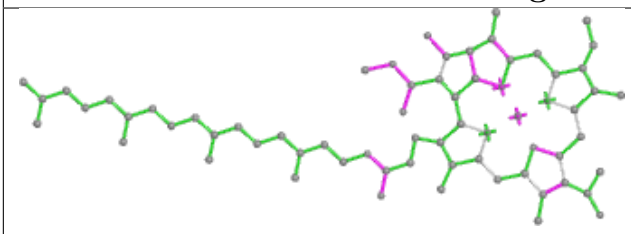


Torsions

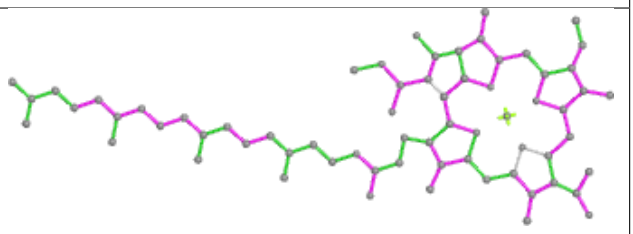


Rings

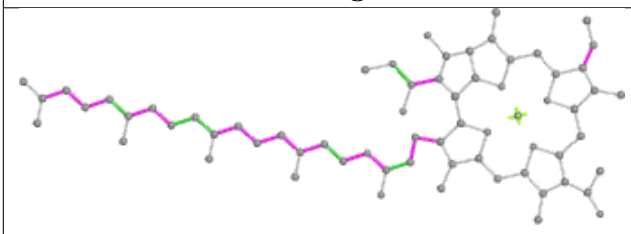
Ligand BCL a 808



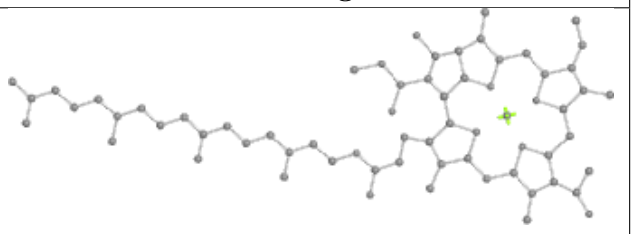
Bond lengths



Bond angles

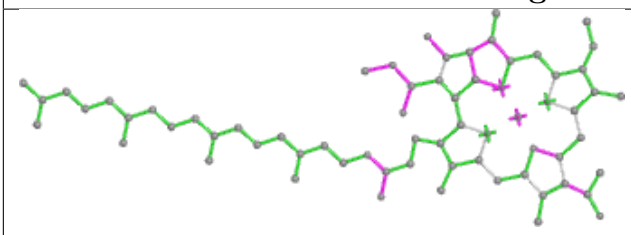


Torsions

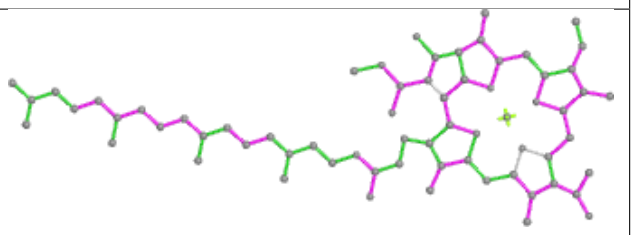


Rings

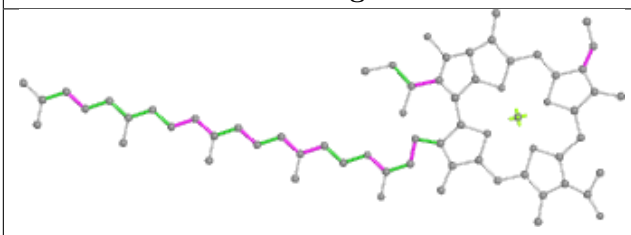
Ligand BCL 4 407



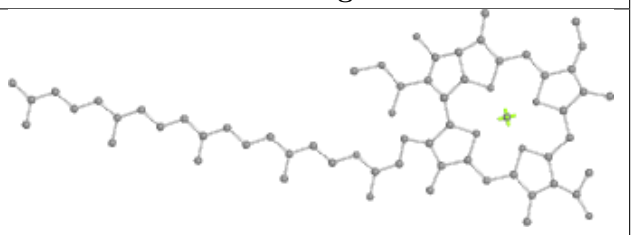
Bond lengths



Bond angles

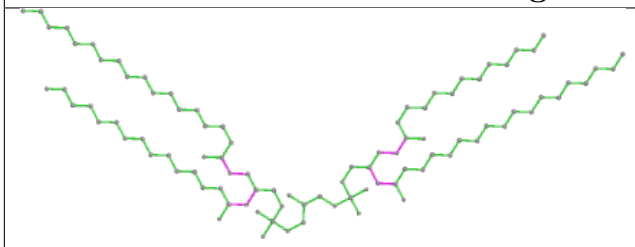


Torsions

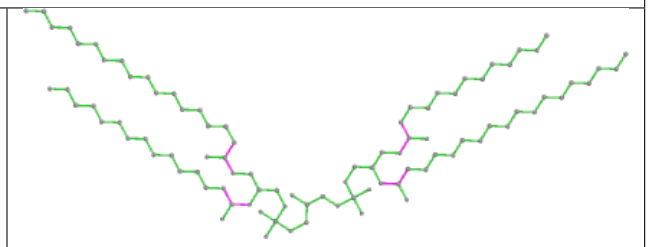


Rings

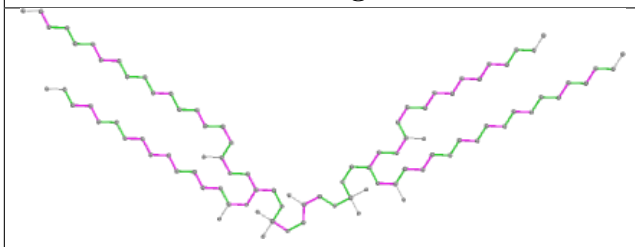
Ligand CDL a 822



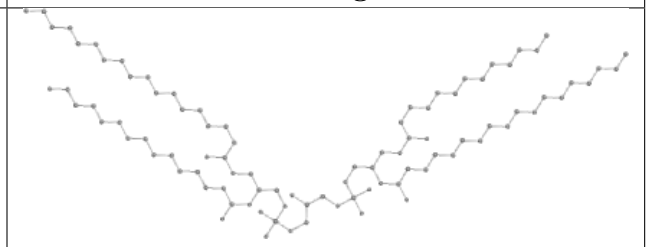
Bond lengths



Bond angles

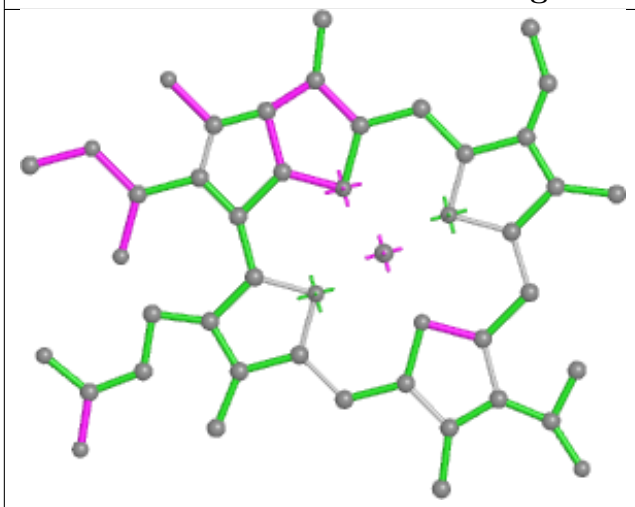


Torsions

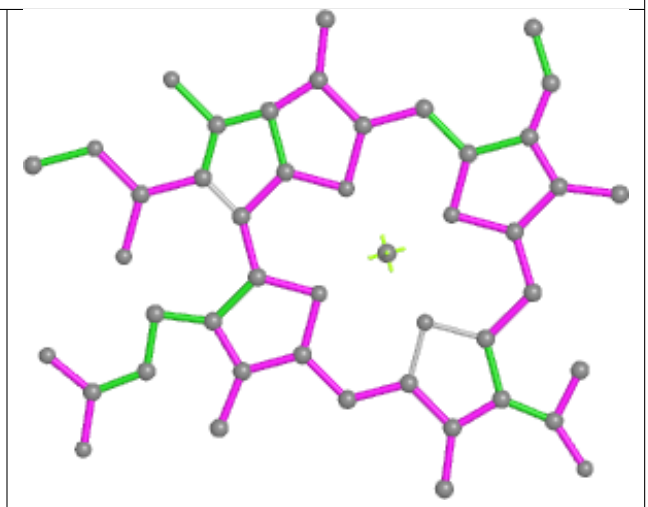


Rings

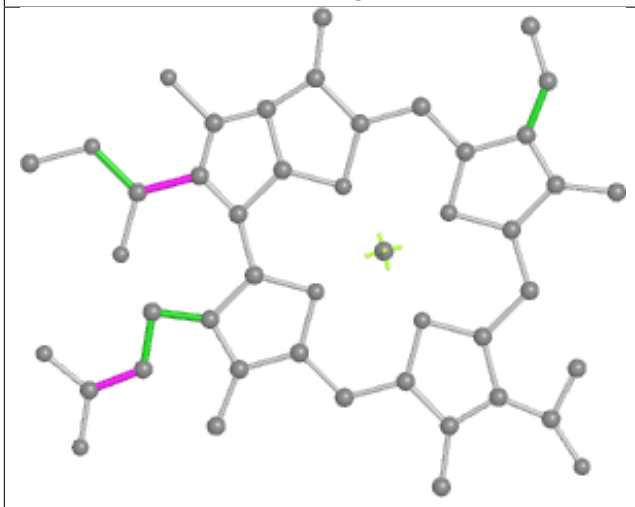
Ligand BCL a 809



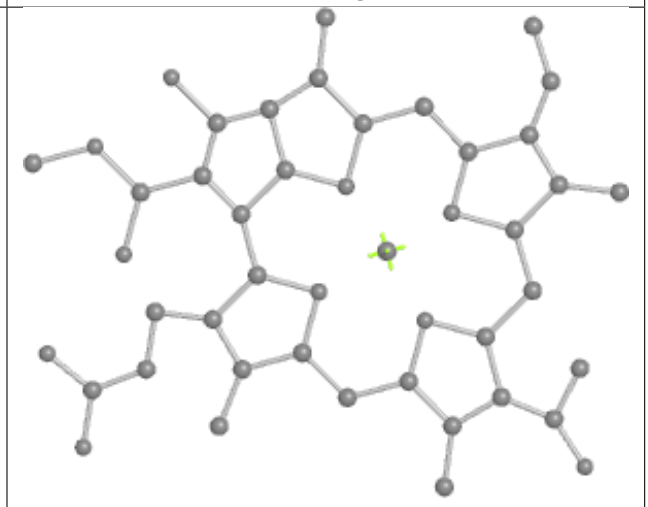
Bond lengths



Bond angles

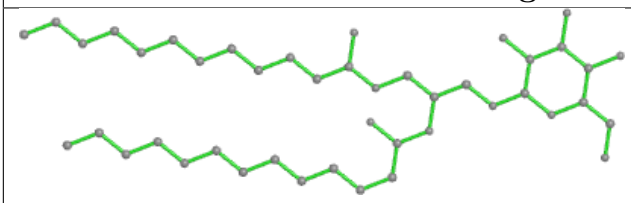


Torsions

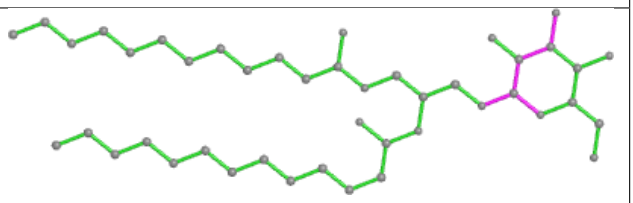


Rings

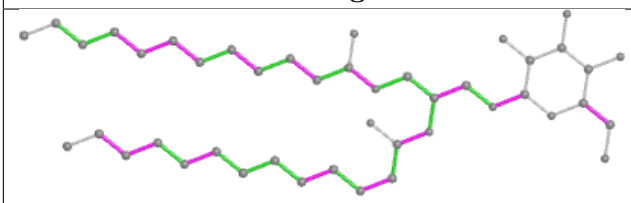
Ligand LMG A 817



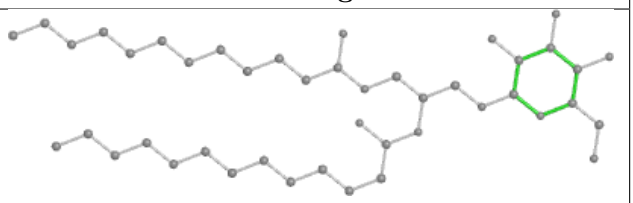
Bond lengths



Bond angles

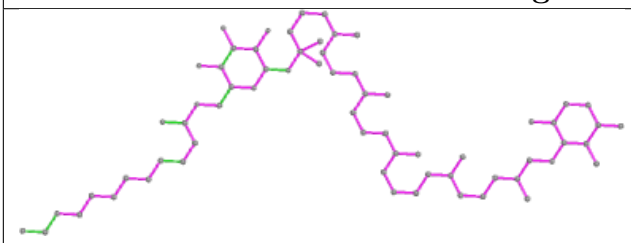


Torsions

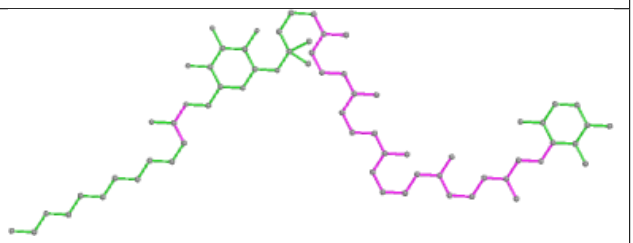


Rings

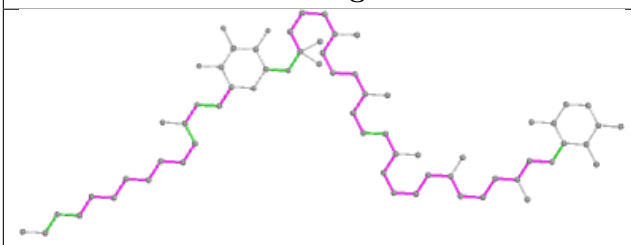
Ligand F39 C 302



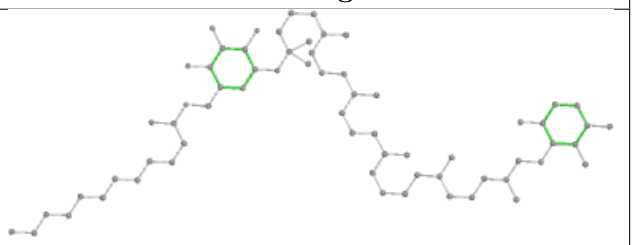
Bond lengths



Bond angles

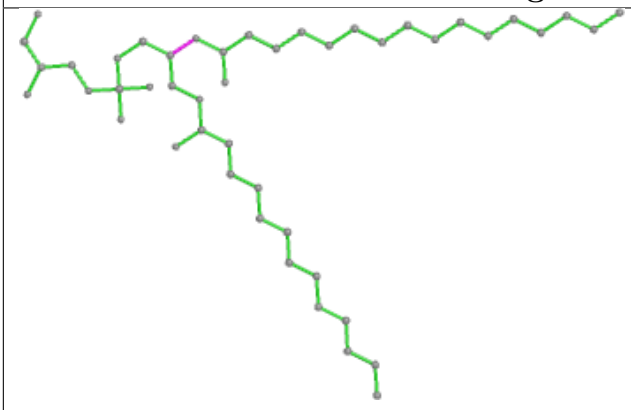


Torsions

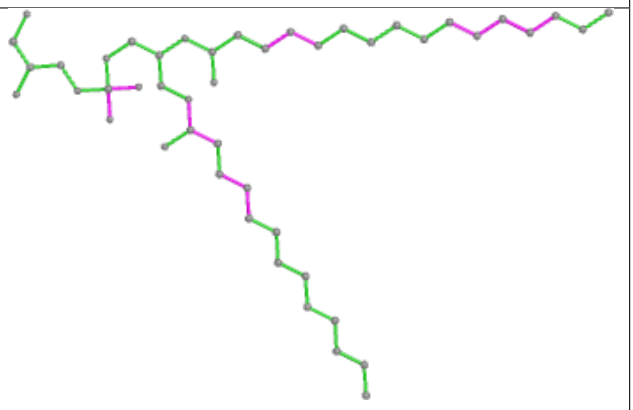


Rings

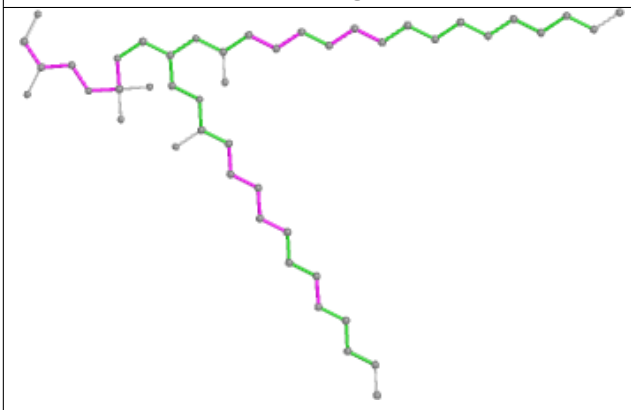
Ligand LHG a 817



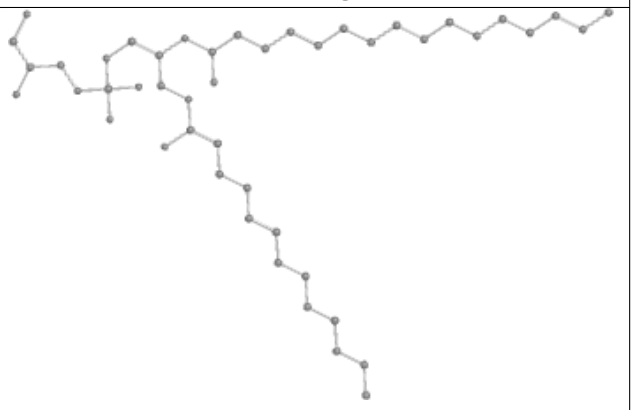
Bond lengths



Bond angles

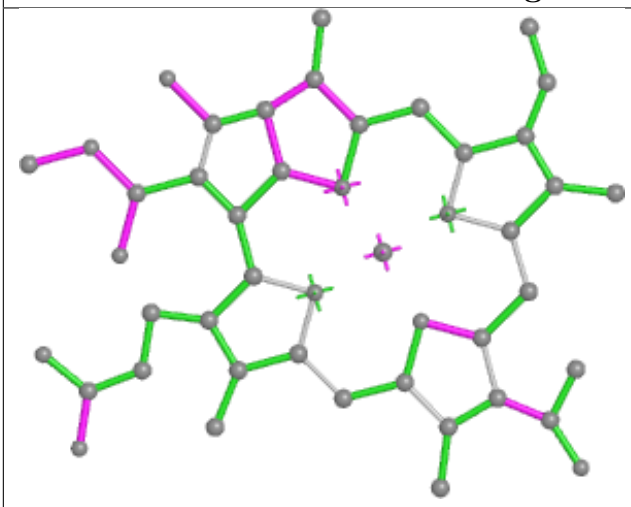


Torsions

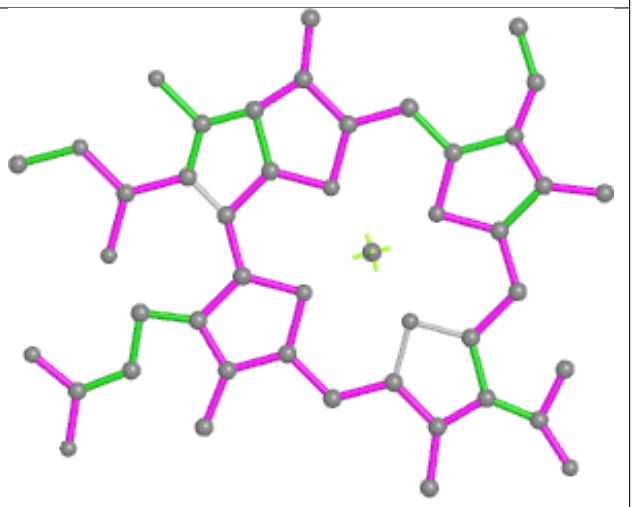


Rings

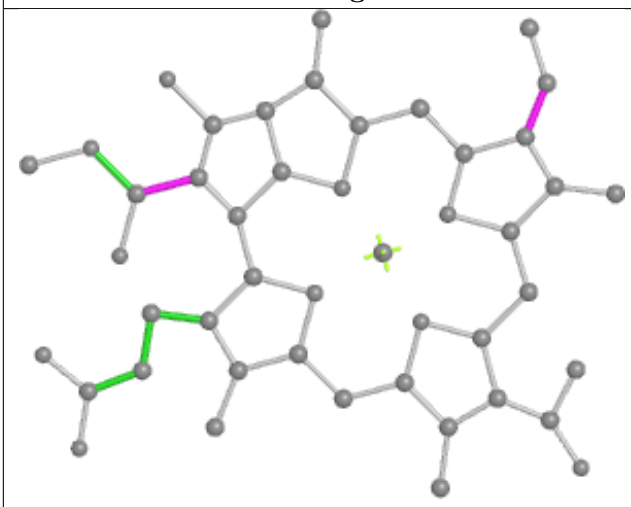
Ligand BCL A 813



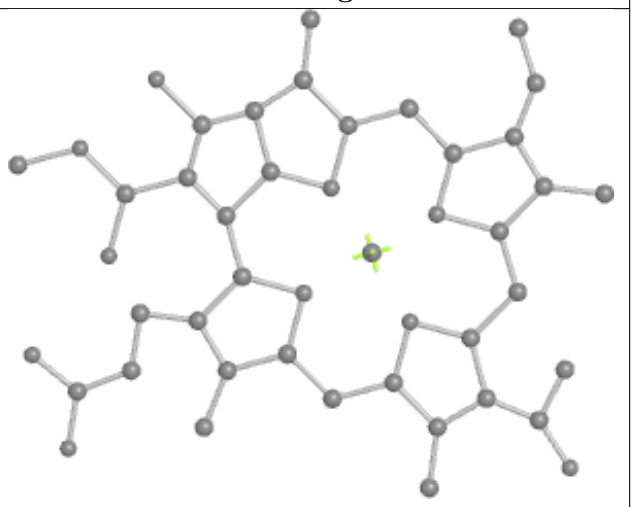
Bond lengths



Bond angles

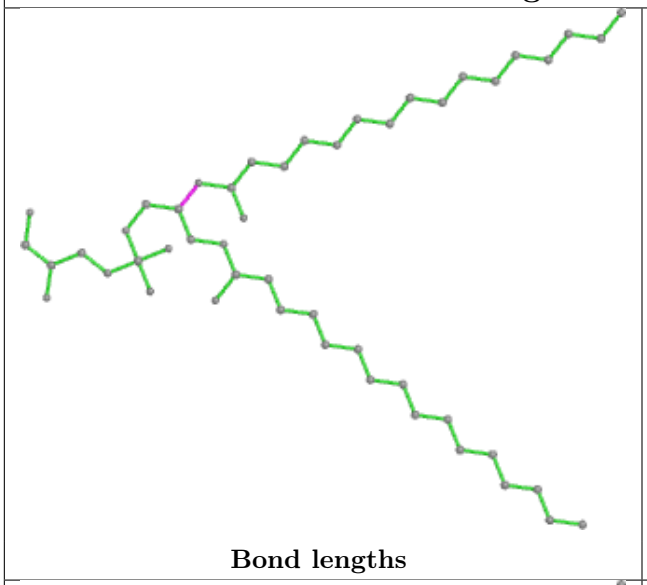


Torsions

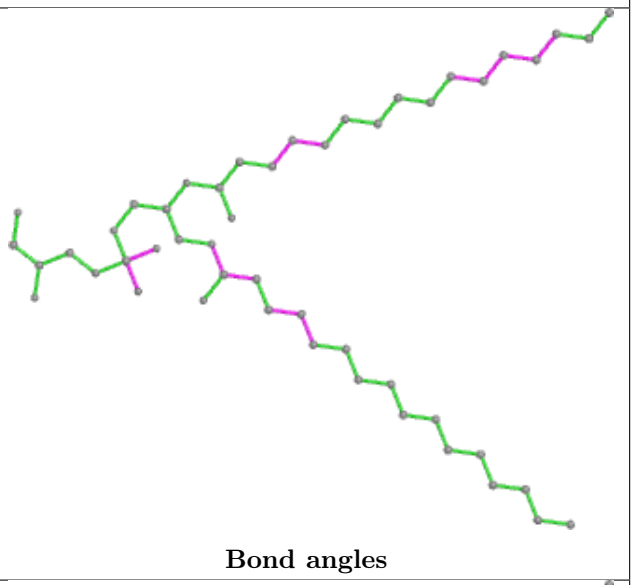


Rings

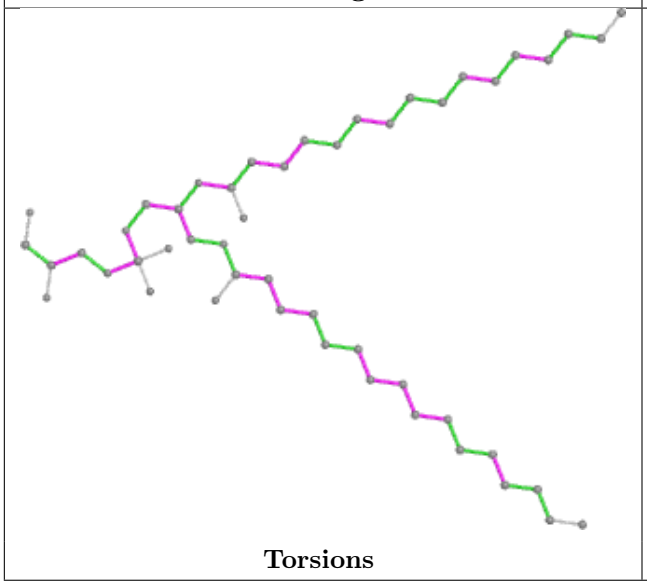
Ligand LHG A 818



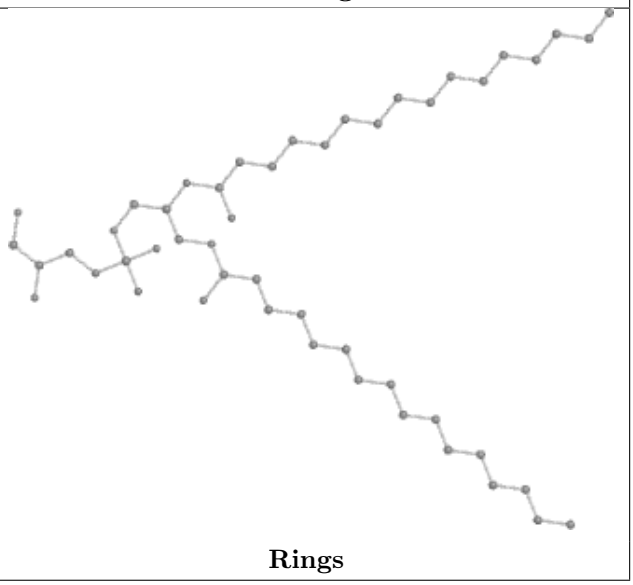
Bond lengths



Bond angles

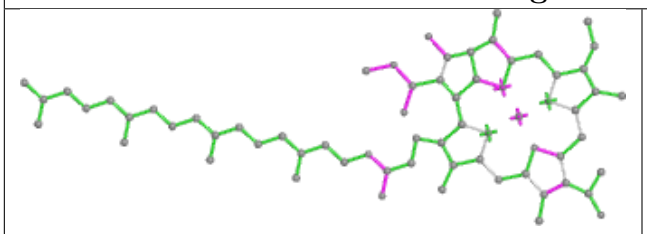


Torsions

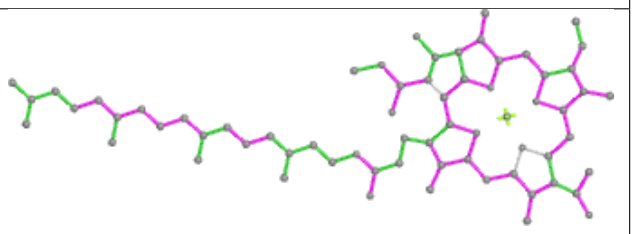


Rings

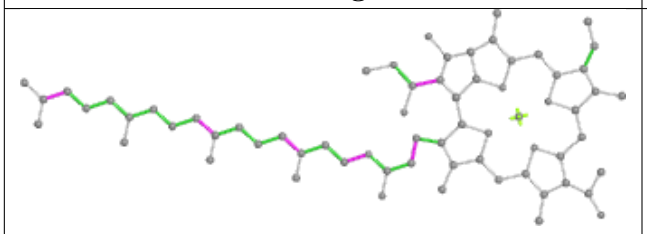
Ligand BCL 3 405



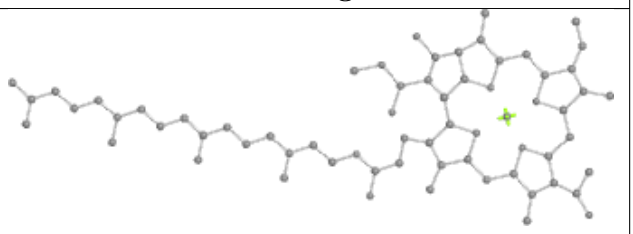
Bond lengths



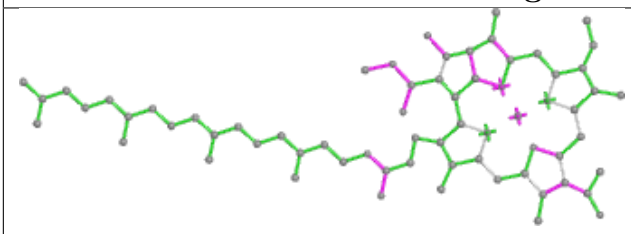
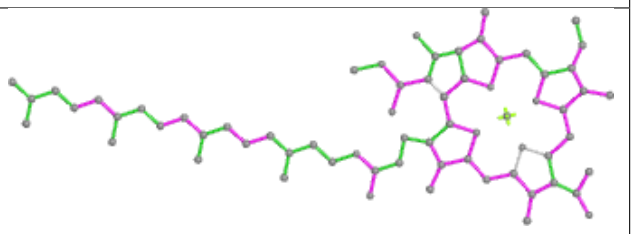
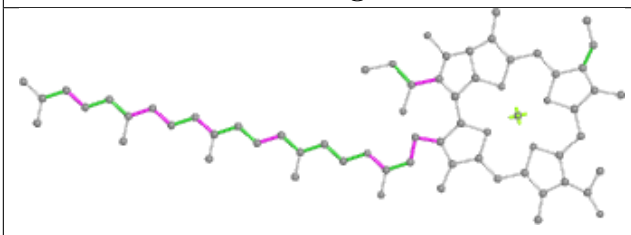
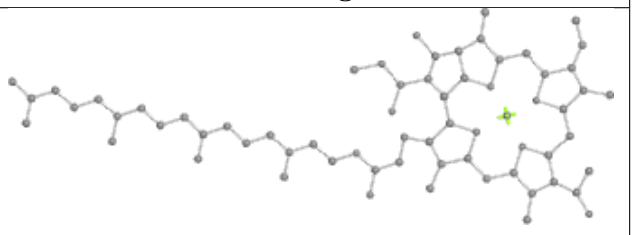
Bond angles

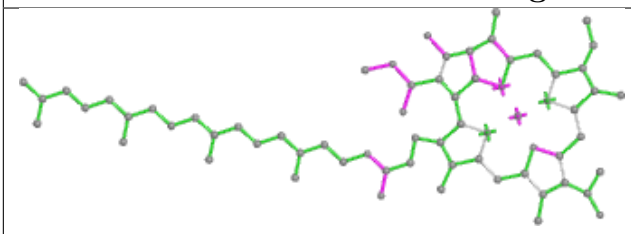
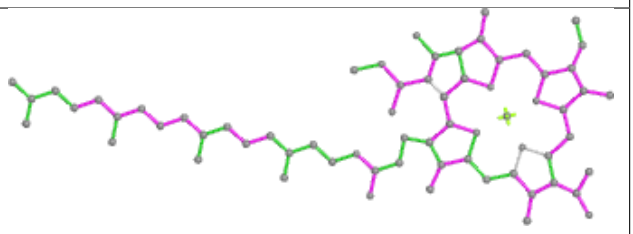
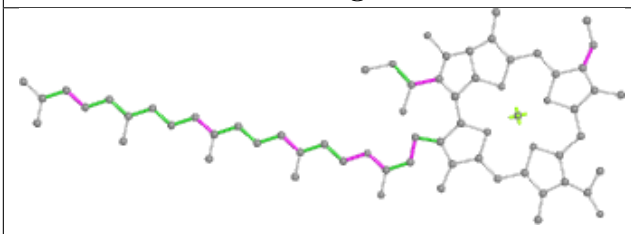
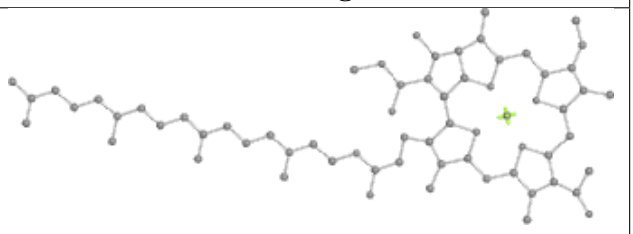


Torsions

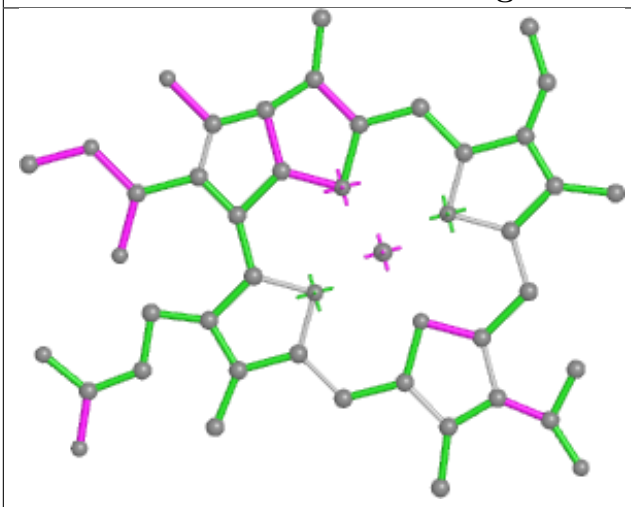


Rings

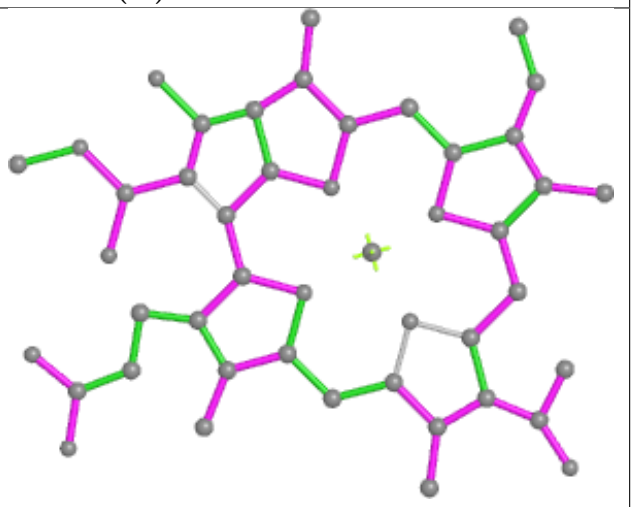
Ligand BCL A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 3 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

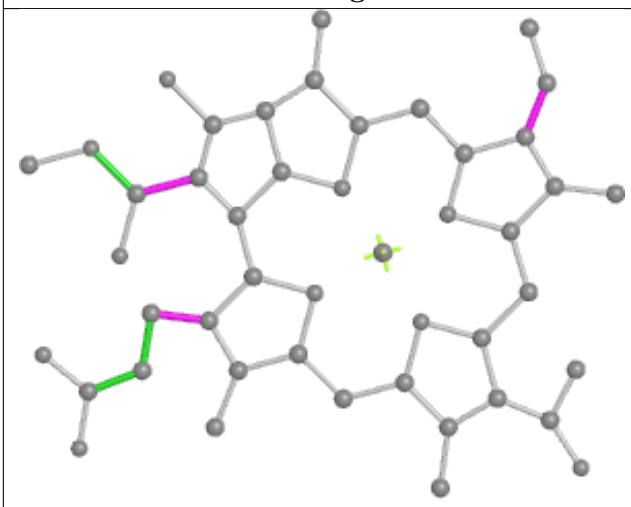
Ligand BCL 1 407 (B)



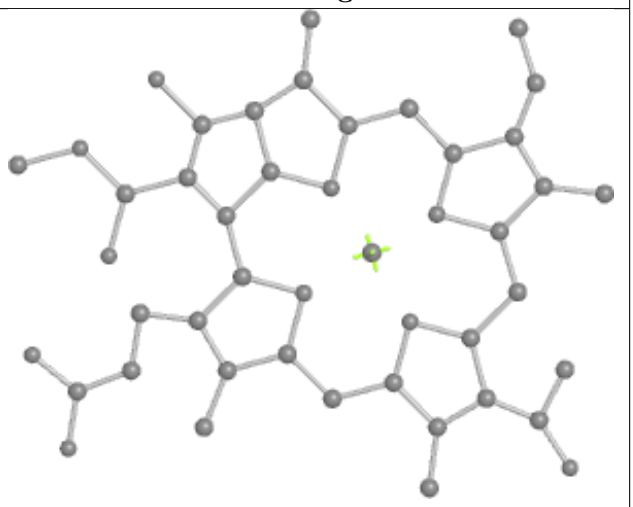
Bond lengths



Bond angles

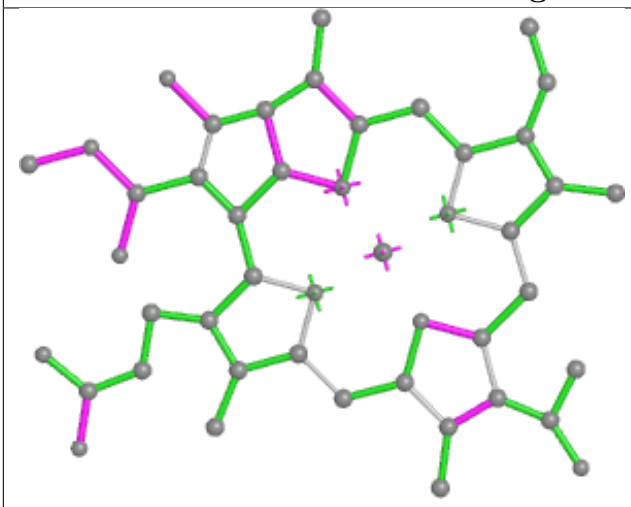


Torsions

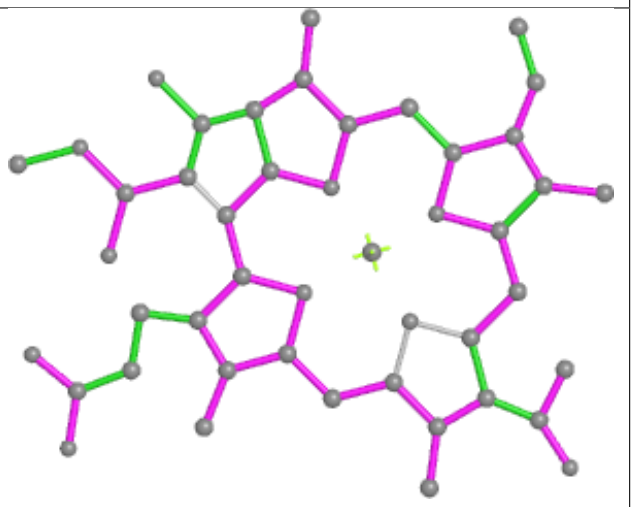


Rings

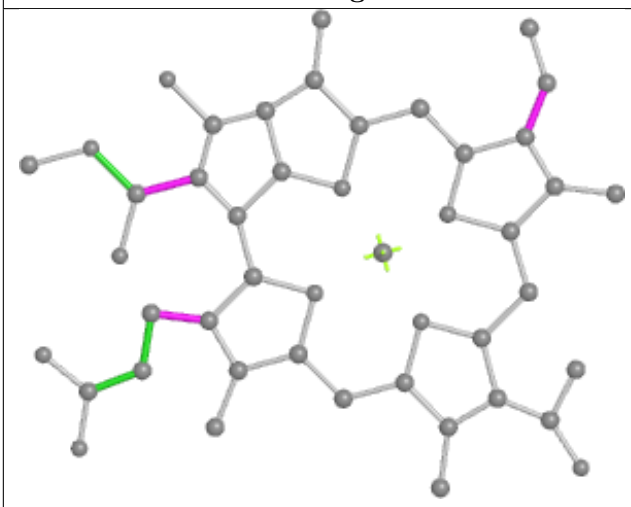
Ligand BCL a 813



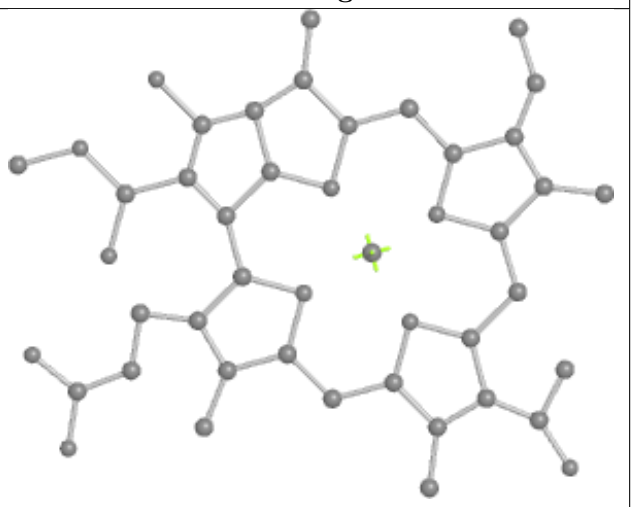
Bond lengths



Bond angles

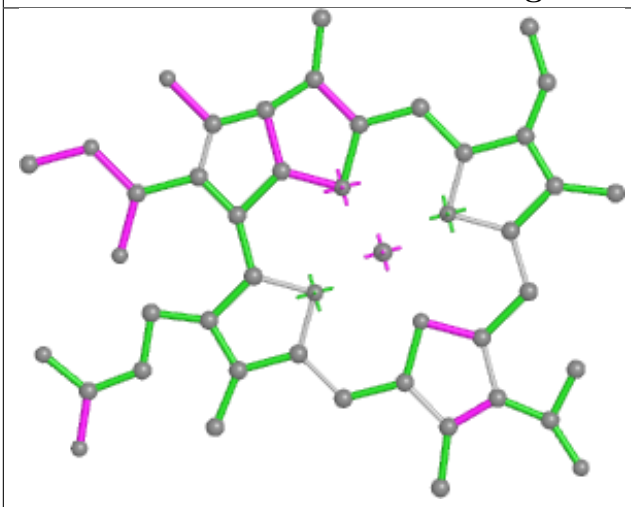


Torsions

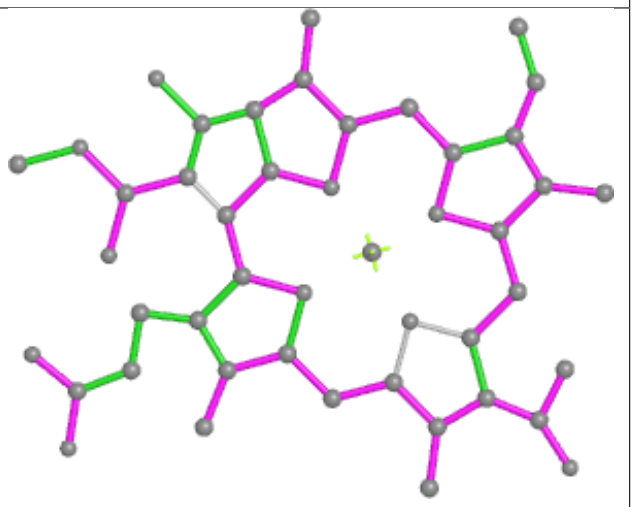


Rings

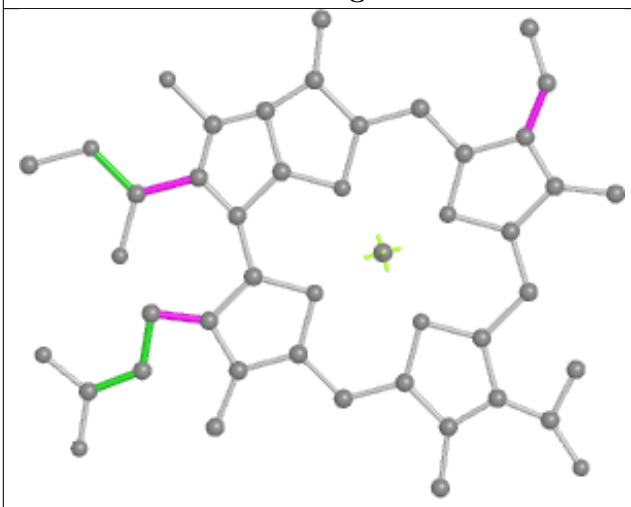
Ligand BCL C 301



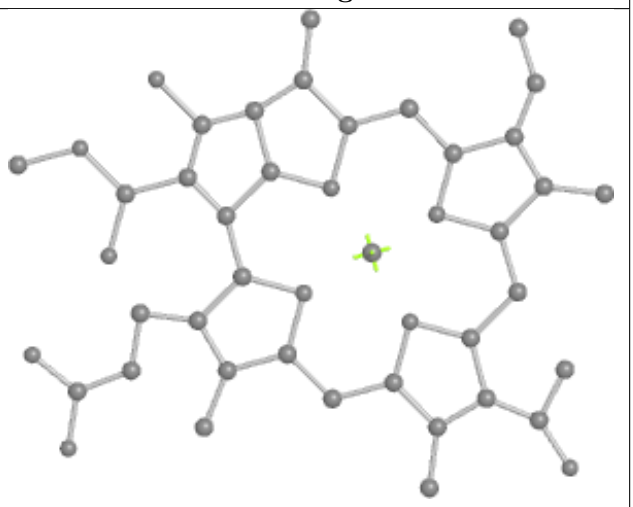
Bond lengths



Bond angles

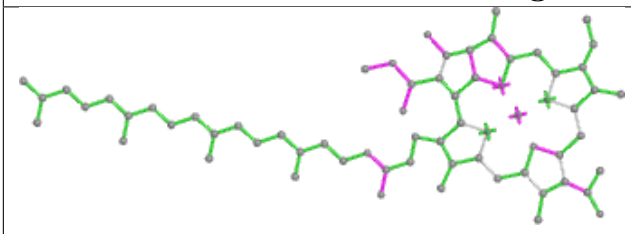


Torsions

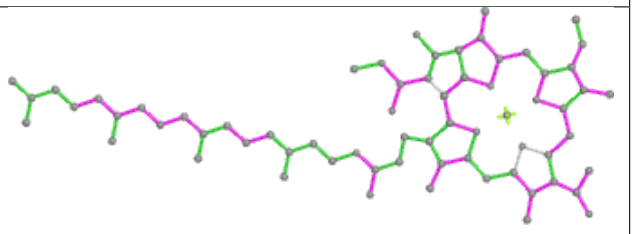


Rings

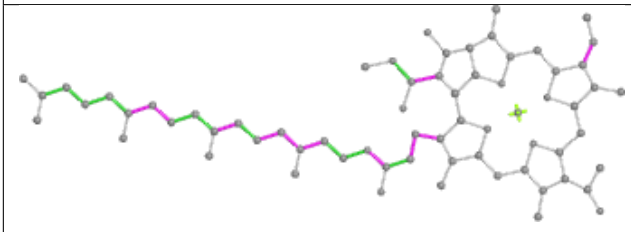
Ligand BCL 1 403



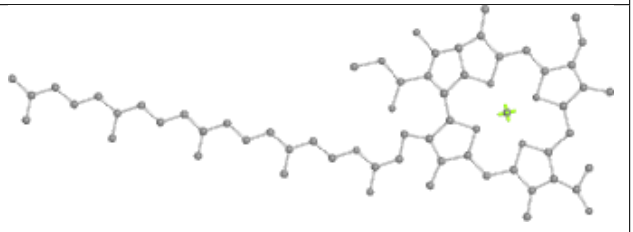
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

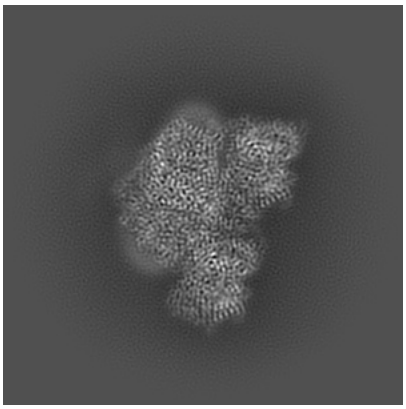
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34307. These allow visual inspection of the internal detail of the map and identification of artifacts.

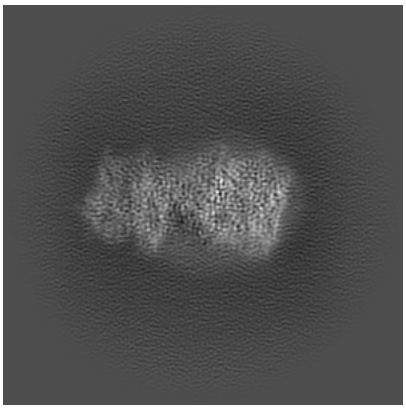
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

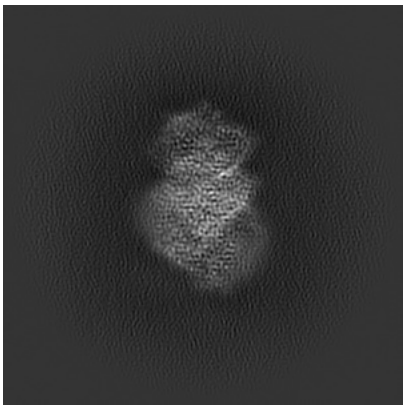
6.1.1 Primary map



X

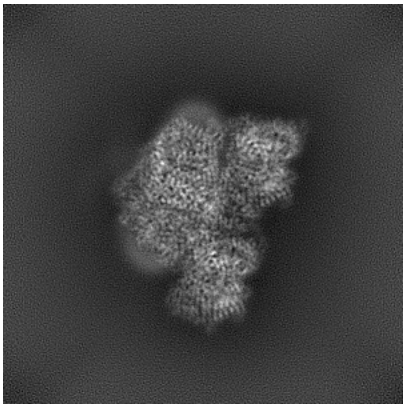


Y

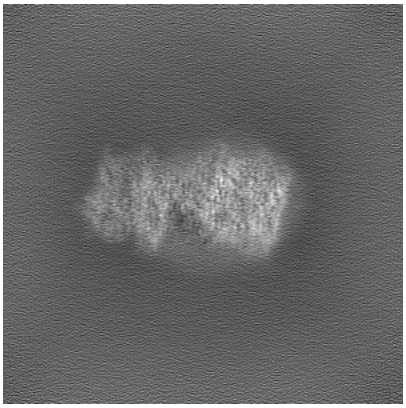


Z

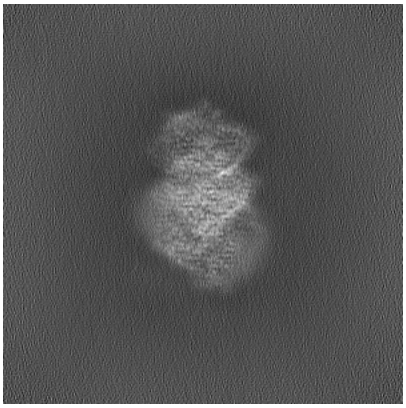
6.1.2 Raw map



X



Y

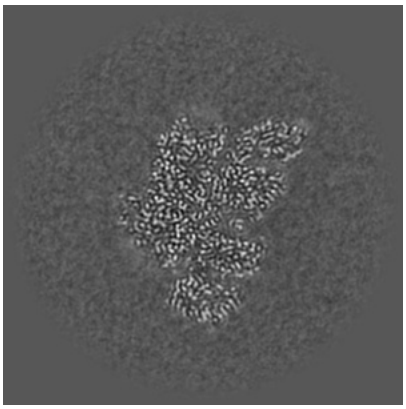


Z

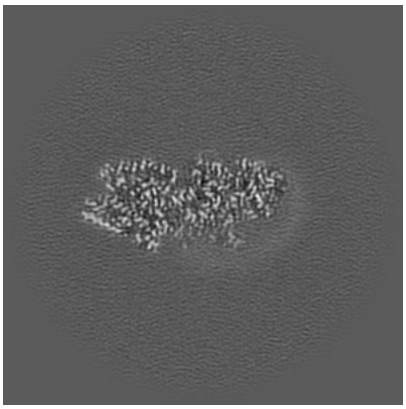
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

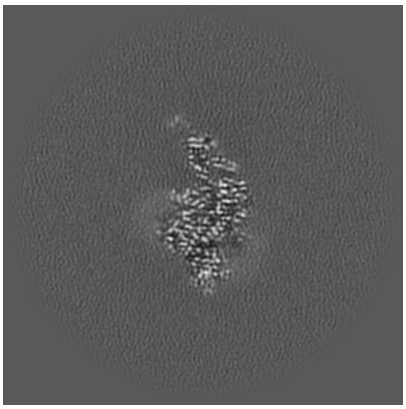
6.2.1 Primary map



X Index: 170

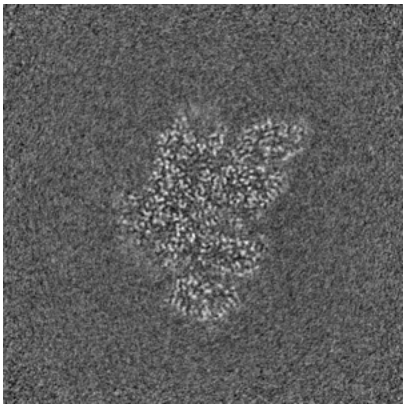


Y Index: 170

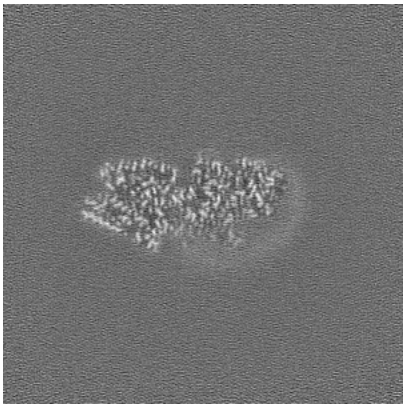


Z Index: 170

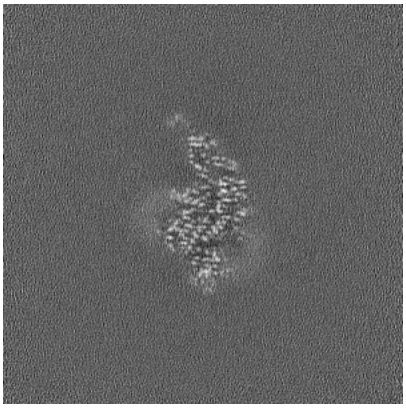
6.2.2 Raw map



X Index: 170



Y Index: 170

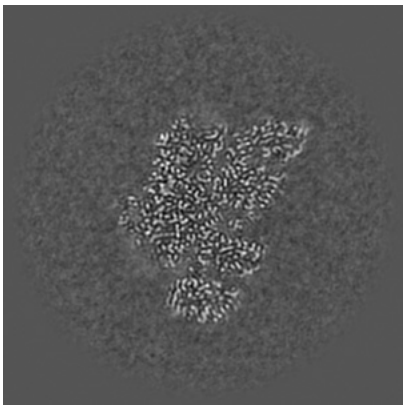


Z Index: 170

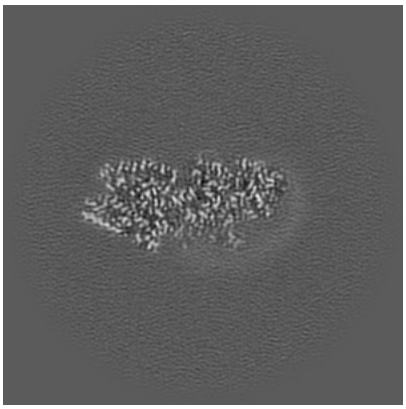
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

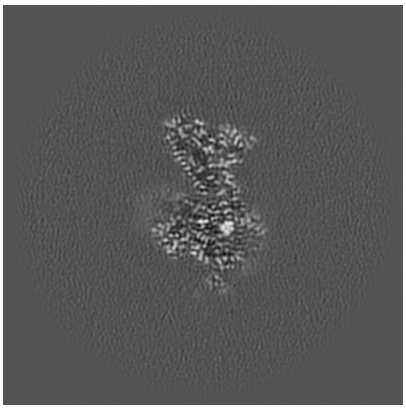
6.3.1 Primary map



X Index: 171

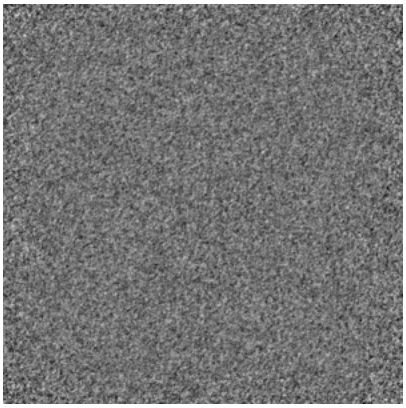


Y Index: 170

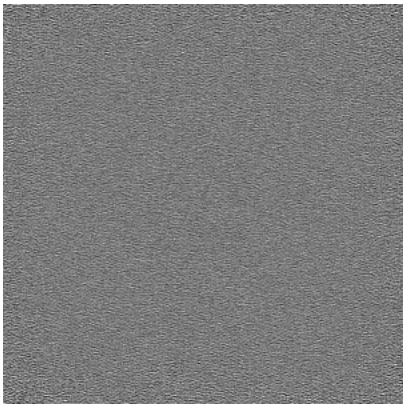


Z Index: 185

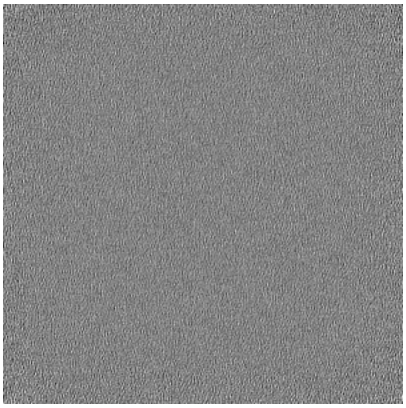
6.3.2 Raw map



X Index: 0



Y Index: 0

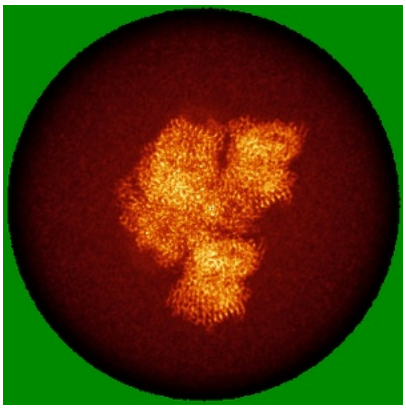


Z Index: 0

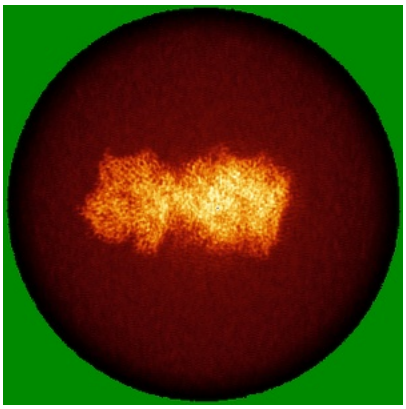
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

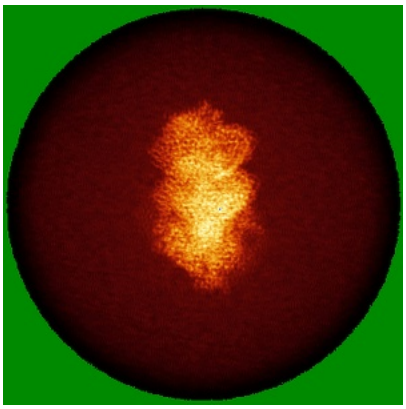
6.4.1 Primary map



X

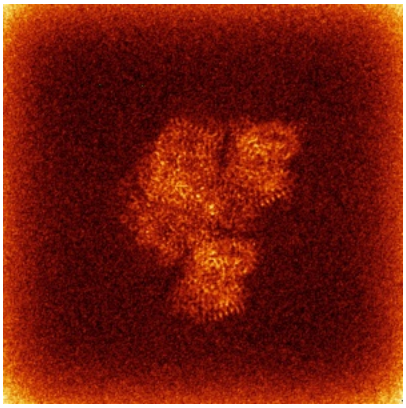


Y

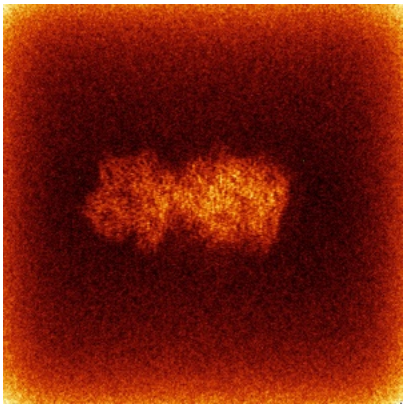


Z

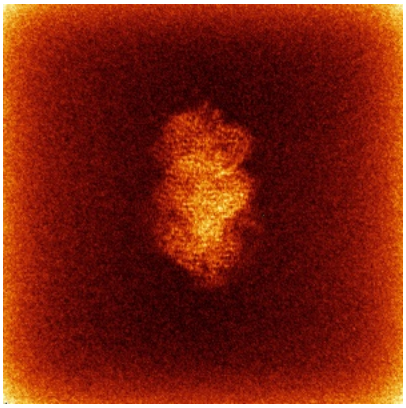
6.4.2 Raw map



X



Y

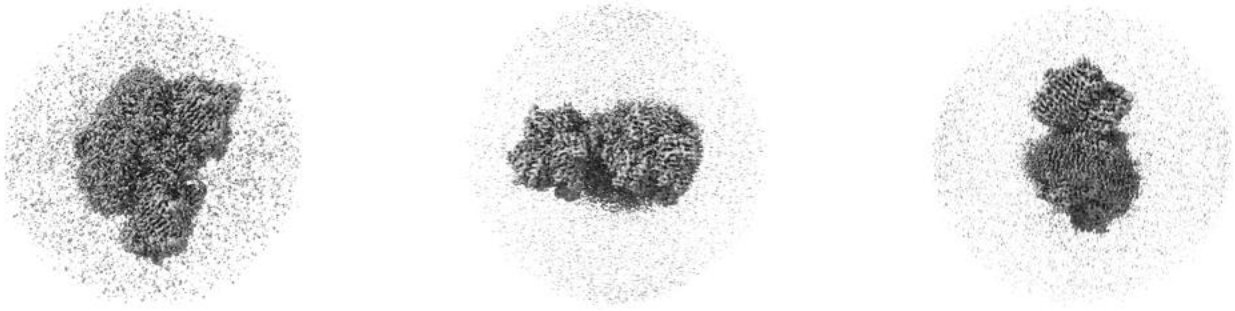


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

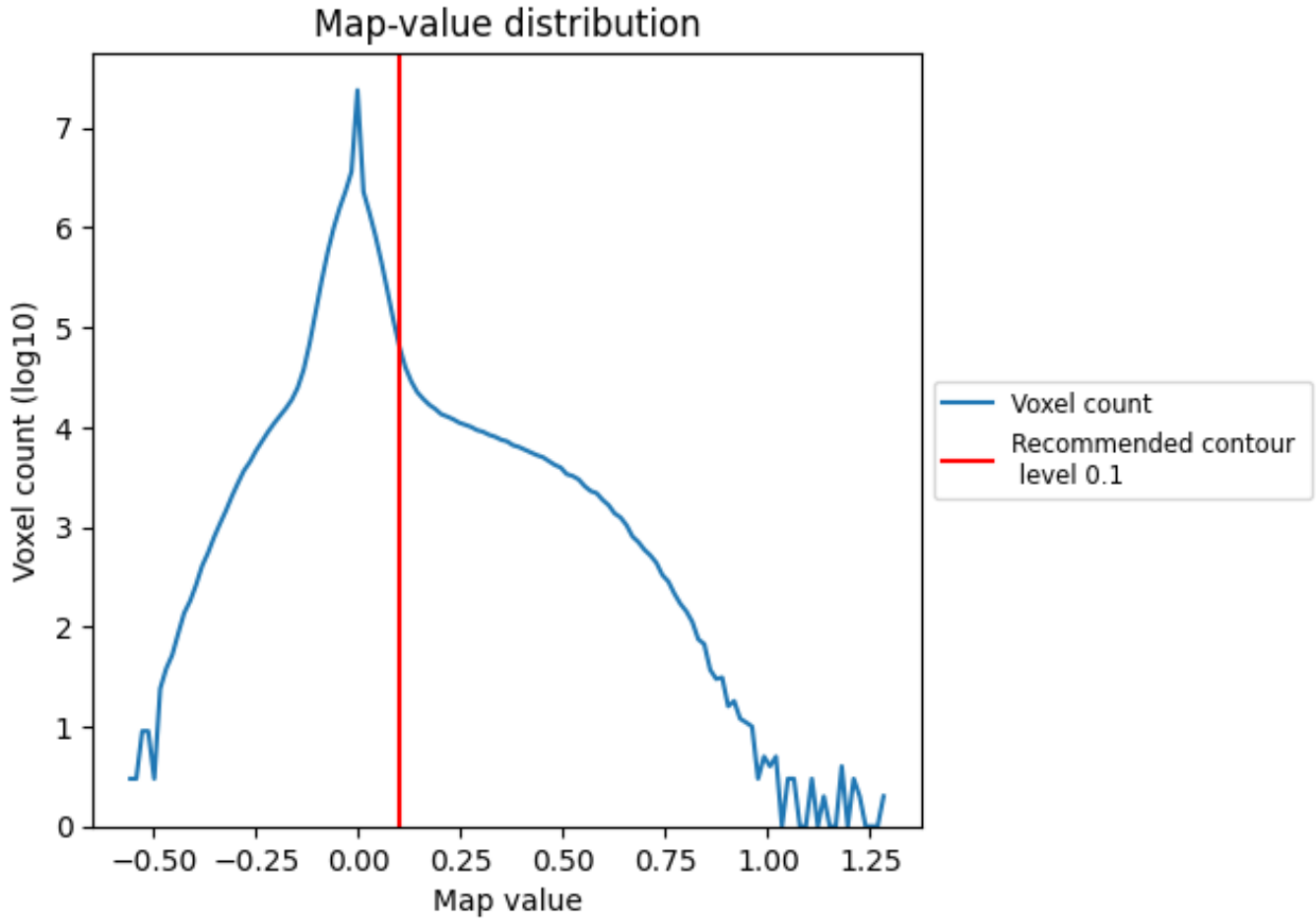
6.6 Mask visualisation (i)

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

7 Map analysis

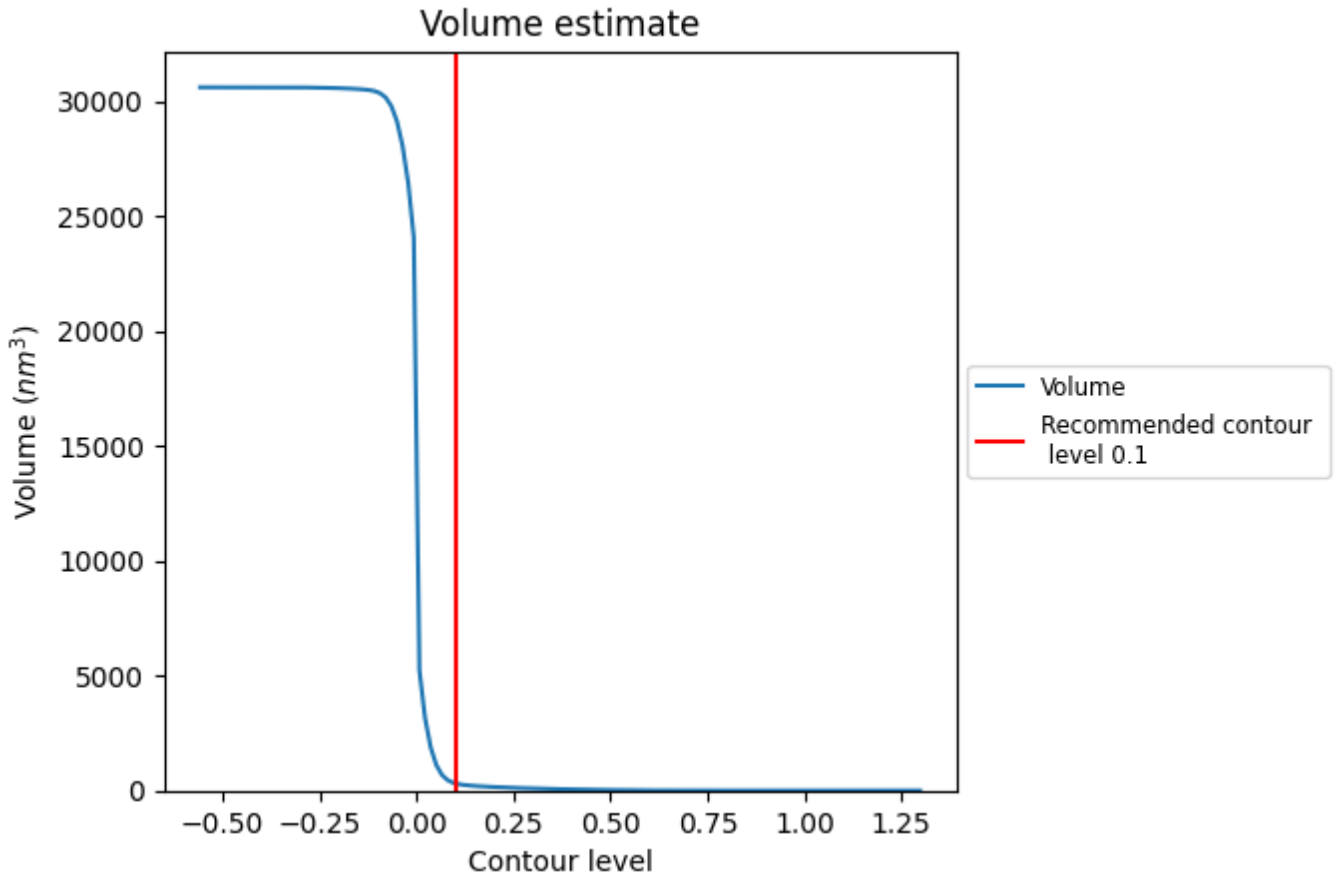
This section contains the results of statistical analysis of the map.

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.

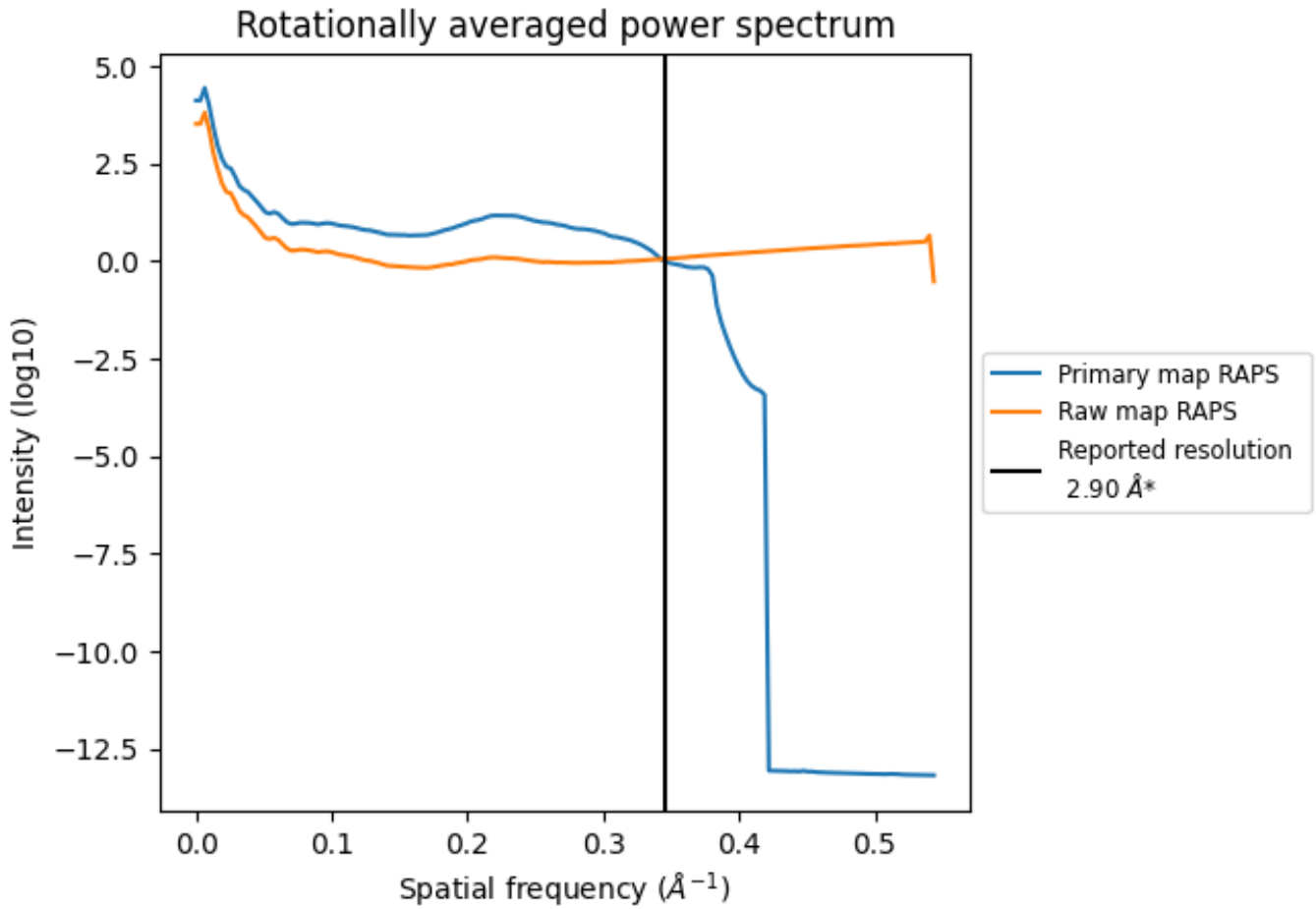
7.2 Volume estimate



The volume at the recommended contour level is 318 nm^3; this corresponds to an approximate mass of 287 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)

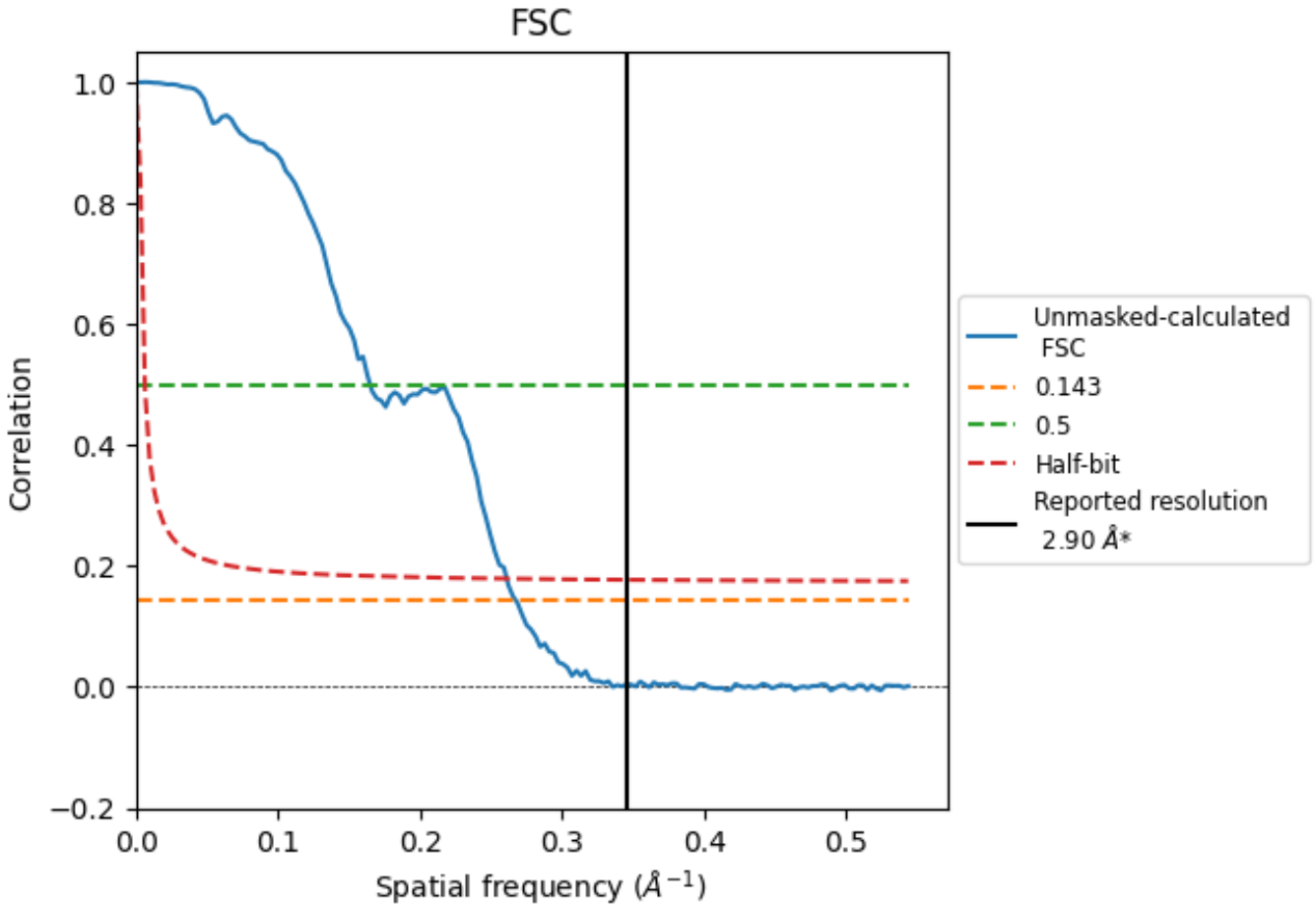


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	6.06	3.83

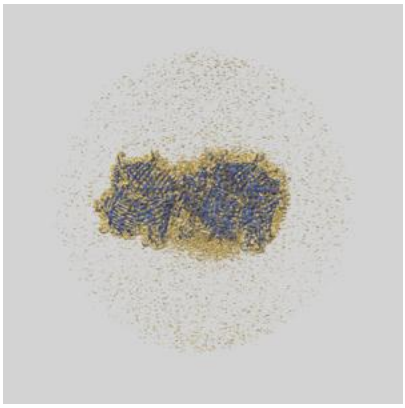
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 2.9 by more than 10 %

9 Map-model fit

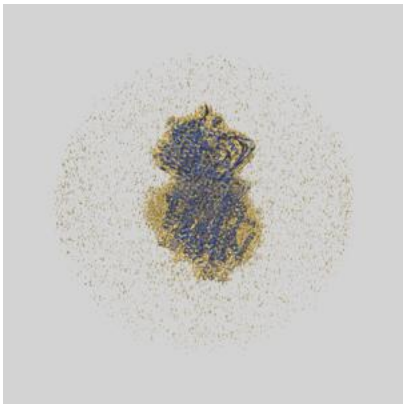
This section contains information regarding the fit between EMDB map EMD-34307 and PDB model 8GWA. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay

X



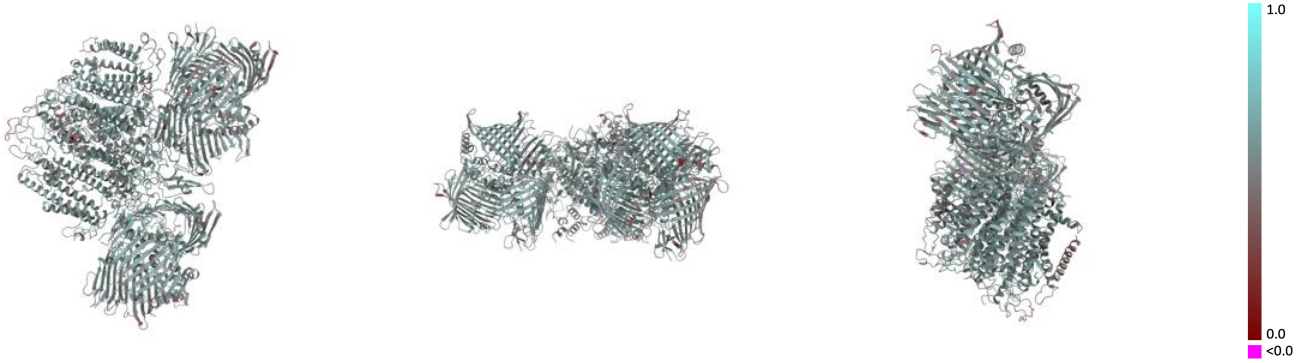
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

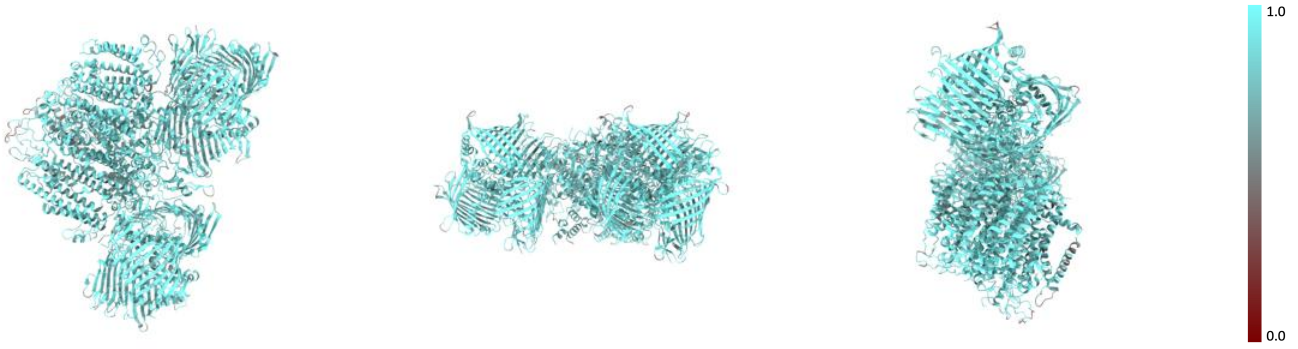
9.2 Q-score mapped to coordinate model (i)



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.

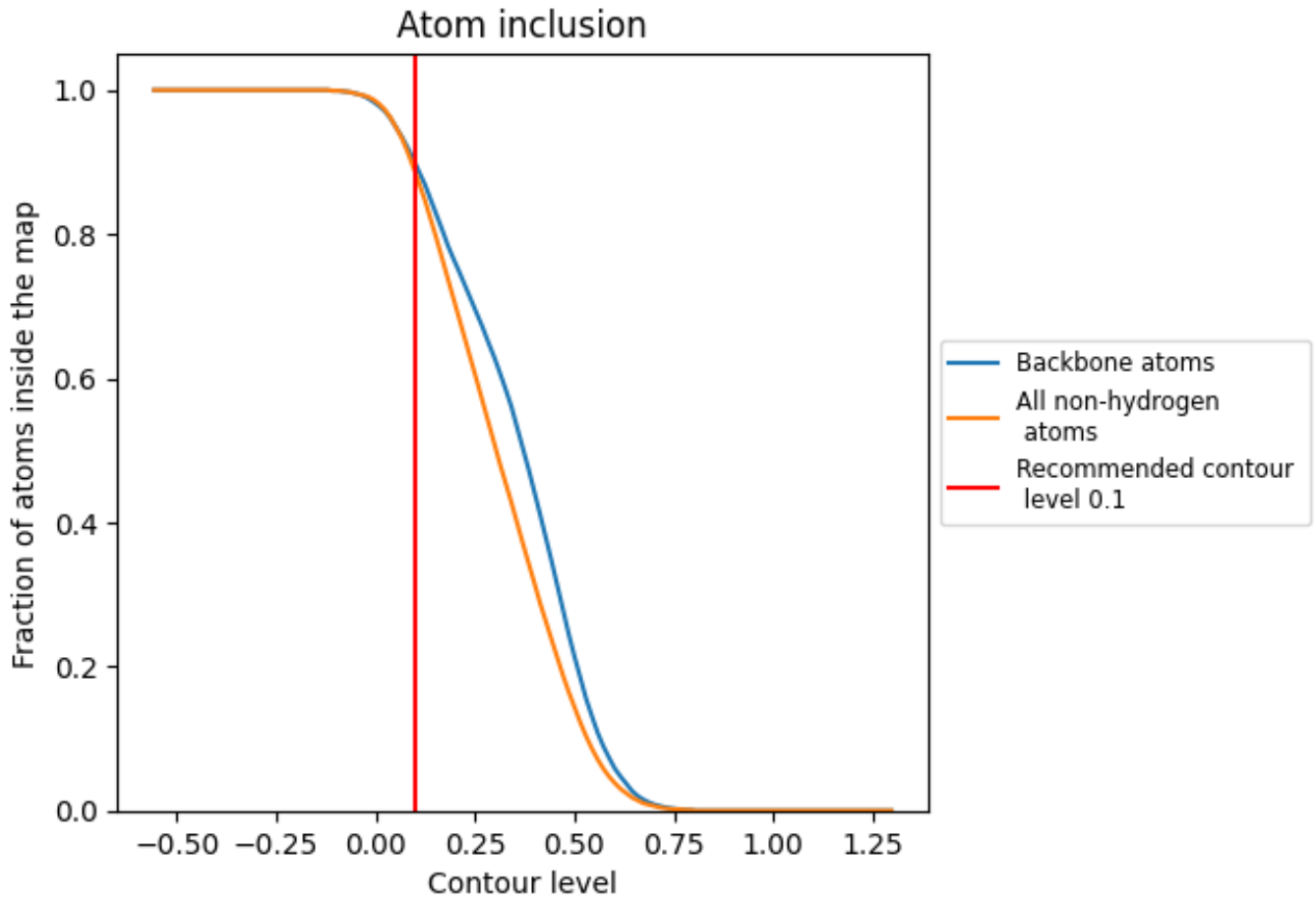
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8850	0.5410
1	0.9110	0.5550
2	0.8980	0.5550
3	0.8900	0.5330
4	0.8750	0.5370
5	0.8850	0.5500
6	0.8910	0.5270
A	0.8900	0.5480
B	0.8960	0.5320
C	0.8730	0.5320
D	0.8610	0.5330
E	0.8630	0.5060
F	0.7900	0.4990
a	0.8970	0.5480
c	0.7470	0.4760