Full wwPDB EM Validation Report

Apr 28, 2024 – 12:45 AM JST

PDB ID	:	8WDU
EMDB ID	:	EMD-37465
Title	:	Photosynthetic LH1-RC complex from the purple sulfur bacterium Allochromatium vinosum purified by sucrose density
Authors	:	Tani, K.; Kanno, R.; Harada, A.; Kobayashi, A.; Minamino, A.; Nakamura, N.; Ji, X.-C.; Purba, E.R.; Hall, M.; Yu, L.-J.; Madigan, M.T.; Mizoguchi, A.; Iwasaki, K.; Humbel, B.M.; Kimura, Y.; Wang-Otomo, Z.-Y.
Deposited on	:	2023-09-16
Resolution	:	2.24 Å(reported)
Based on initial model	:	7VRJ

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

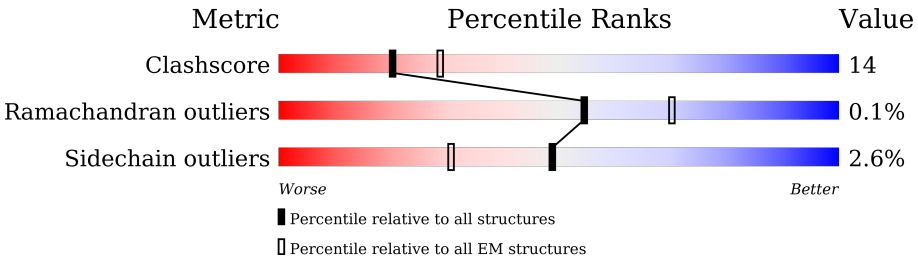
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.24 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	C	383	67% 14% 19%
2	L	278	80% 19%
3	M	325	81% 17%
4	H	259	82% 18%
5	1	44	9% 66% 32%
5	5	44	66% 27%
5	7	44	59% 36% 5%

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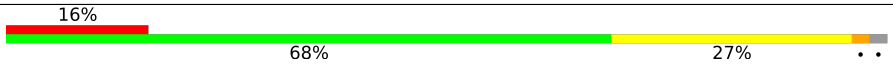
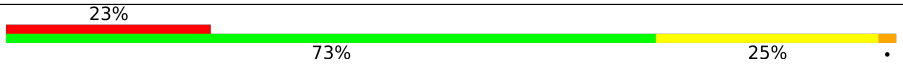
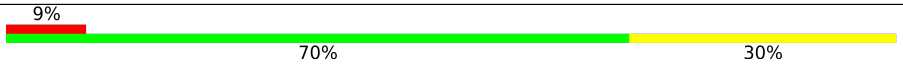
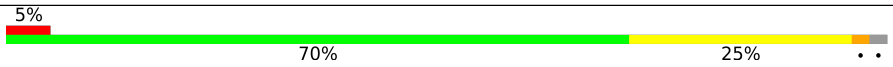
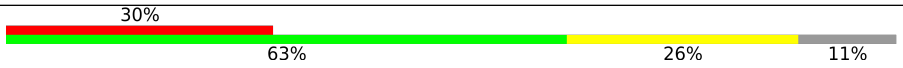
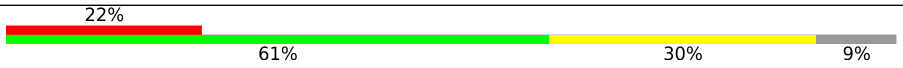
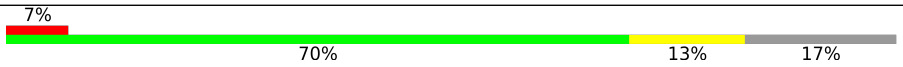
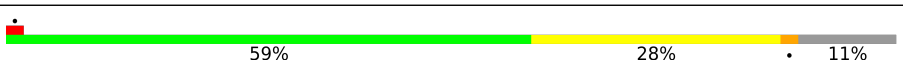
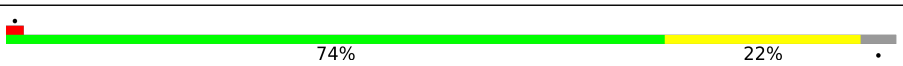
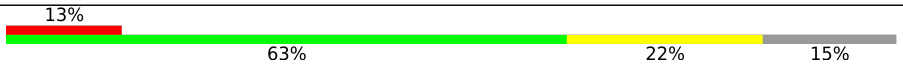
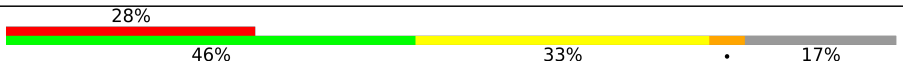
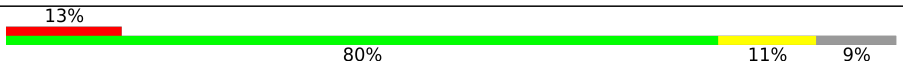
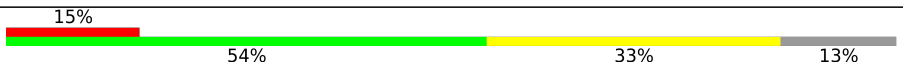
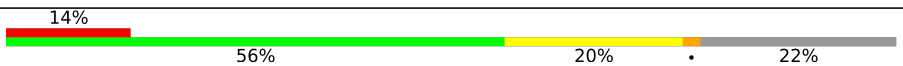
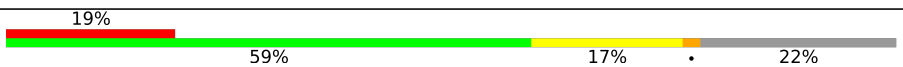
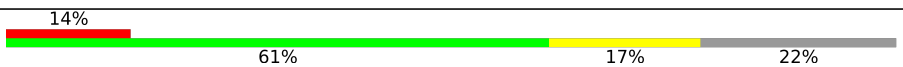
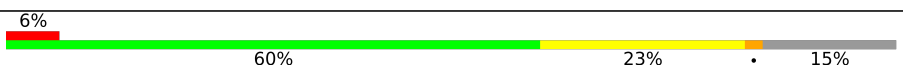
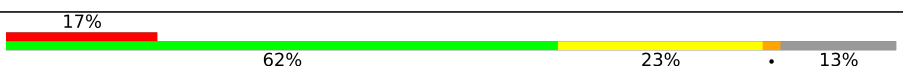
Mol	Chain	Length	Quality of chain
5	9	44	
5	A	44	
5	I	44	
5	K	44	
5	O	44	
5	Q	44	
6	0	46	
6	2	46	
6	4	46	
6	6	46	
6	8	46	
6	B	46	
6	J	46	
6	N	46	
6	P	46	
6	R	46	
7	D	64	
7	F	64	
7	S	64	
7	U	64	
7	W	64	
7	Y	64	
8	E	47	
8	G	47	
8	T	47	

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Mol	Chain	Length	Quality of chain
8	V	47	15% 53% 32% 15%
8	X	47	21% 53% 34% 13%
8	Z	47	21% 51% 36% 13%
9	3	66	12% 77% 17% 5%

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 26274 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	311	Total	C	N	O	S	0	0
			2429	1535	418	460	16		

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	277	Total	C	N	O	S	0	0
			2210	1489	354	357	10		

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	318	Total	C	N	O	S	0	0
			2533	1702	405	414	12		

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	259	Total	C	N	O	S	1	0
			1993	1281	339	366	7		

- Molecule 5 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	I	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	K	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	O	44	Total	C	N	O	S	0	0
			366	251	59	55	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	1	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	5	43	Total	C	N	O	S	0	0
			355	245	57	52	1		
5	7	42	Total	C	N	O	S	1	0
			359	251	56	51	1		
5	9	43	Total	C	N	O	S	0	0
			359	248	58	52	1		

- Molecule 6 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	44	Total	C	N	O	S	0	0
			359	238	58	61	2		
6	J	39	Total	C	N	O	S	0	0
			324	219	52	52	1		
6	N	38	Total	C	N	O	S	0	0
			320	217	51	51	1		
6	P	42	Total	C	N	O	S	0	0
			345	231	55	57	2		
6	R	40	Total	C	N	O	S	0	0
			331	223	53	54	1		
6	2	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	4	42	Total	C	N	O	S	0	0
			345	231	55	57	2		
6	6	38	Total	C	N	O	S	0	0
			320	217	51	51	1		
6	8	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	0	43	Total	C	N	O	S	0	0
			351	234	56	59	2		

- Molecule 7 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	49	Total	C	N	O	S	0	0
			397	270	62	64	1		
7	F	49	Total	C	N	O	S	0	0
			397	270	62	64	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	50	Total	C	N	O	S	0	0
			402	273	63	65	1		
7	U	50	Total	C	N	O	S	1	0
			407	277	63	65	2		
7	W	50	Total	C	N	O	S	0	0
			402	273	63	65	1		
7	Y	59	Total	C	N	O	S	0	0
			470	317	76	76	1		

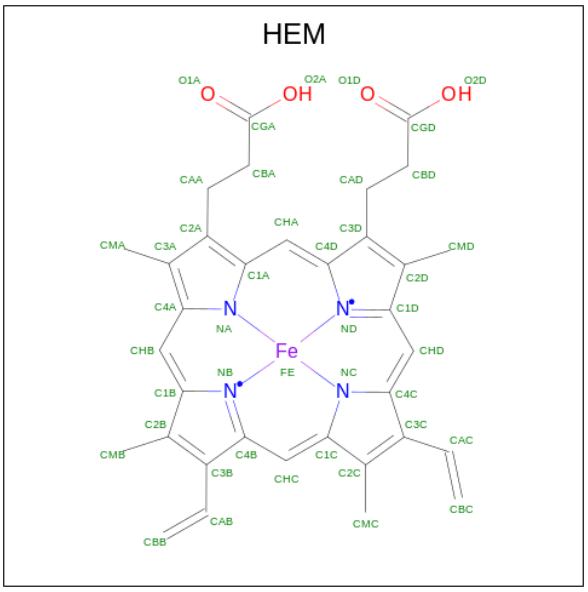
- Molecule 8 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	41	Total	C	N	O	S	0	0
			343	231	53	56	3		
8	G	40	Total	C	N	O	S	0	0
			335	226	52	55	2		
8	T	41	Total	C	N	O	S	0	0
			343	231	53	56	3		
8	V	40	Total	C	N	O	S	0	0
			335	226	52	55	2		
8	X	41	Total	C	N	O	S	0	0
			343	231	53	56	3		
8	Z	41	Total	C	N	O	S	0	0
			343	231	53	56	3		

- Molecule 9 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	63	Total	C	N	O	S	0	0
			498	337	78	80	3		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

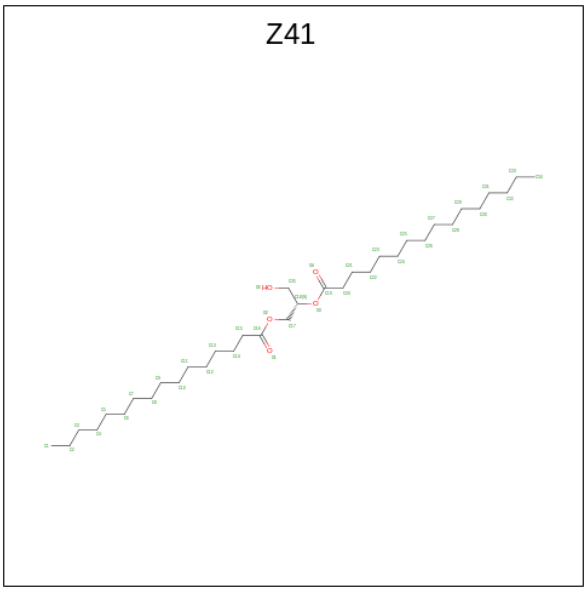


Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

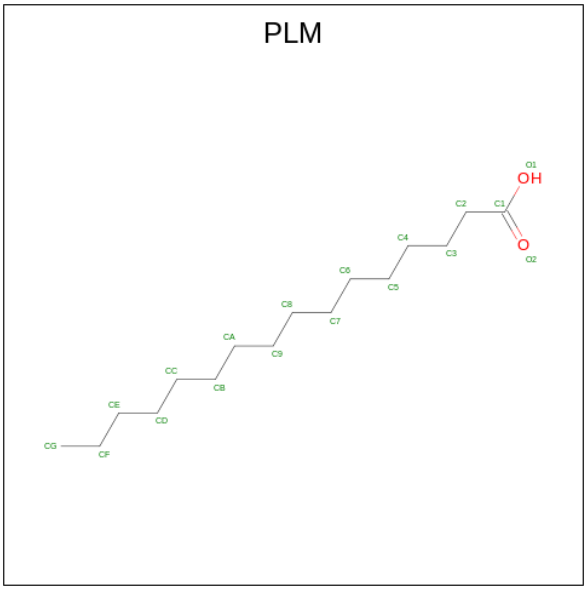
Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	Mg	0
			1	1	

- Molecule 12 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (three-letter code: Z41) (formula: $C_{35}H_{68}O_5$).



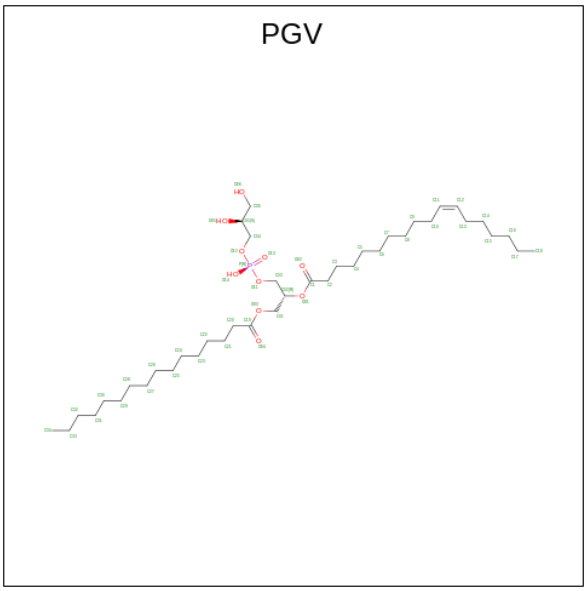
Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			35	31	4	

- Molecule 13 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



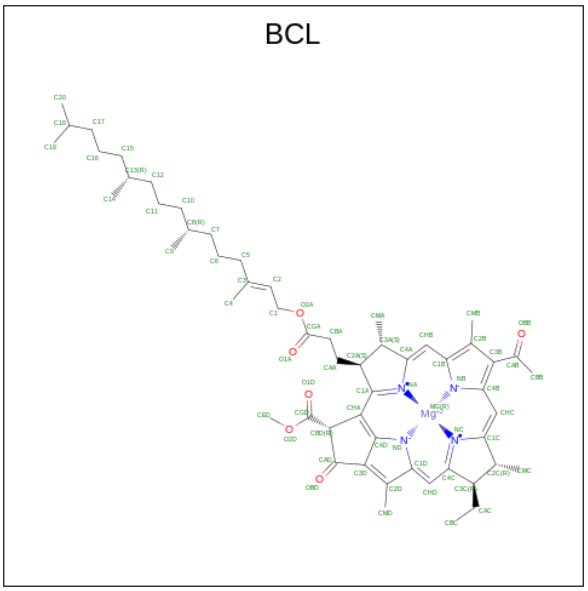
Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			12	11	1	

- Molecule 14 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total 31	C 20	O 10	P 1	0
14	L	1	Total 29	C 18	O 10	P 1	0
14	L	1	Total 35	C 24	O 10	P 1	0
14	L	1	Total 37	C 26	O 10	P 1	0
14	M	1	Total 27	C 18	O 8	P 1	0
14	H	1	Total 36	C 25	O 10	P 1	0
14	A	1	Total 39	C 28	O 10	P 1	0
14	A	1	Total 33	C 22	O 10	P 1	0
14	F	1	Total 31	C 22	O 8	P 1	0
14	Q	1	Total 24	C 15	O 8	P 1	0
14	1	1	Total 27	C 18	O 8	P 1	0

- Molecule 15 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
15	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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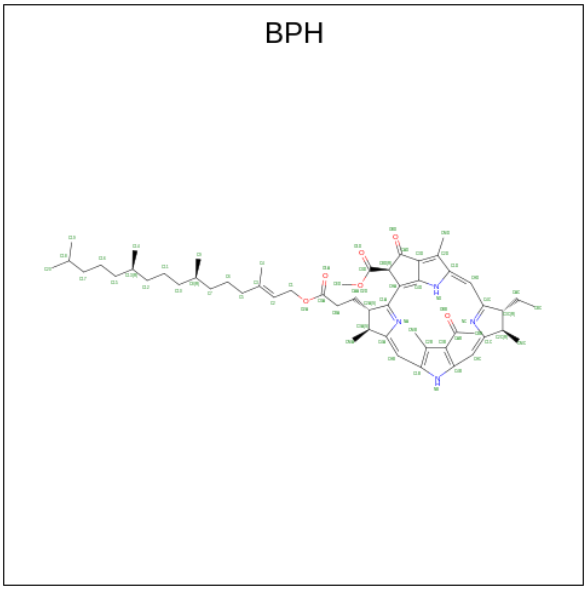
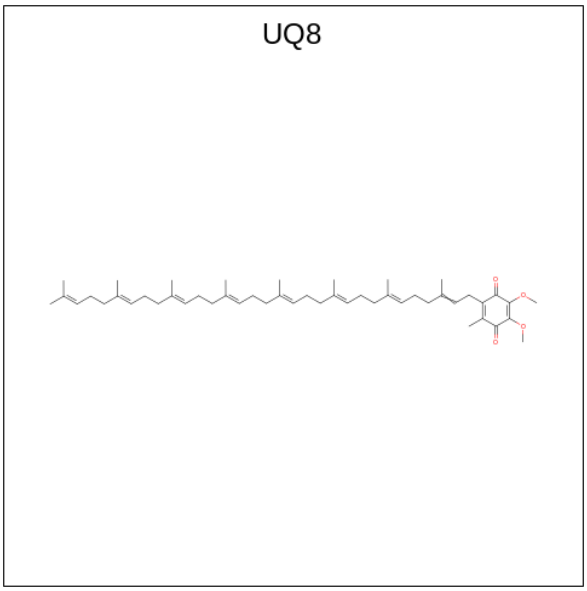
Mol	Chain	Residues	Atoms					AltConf
15	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 16 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



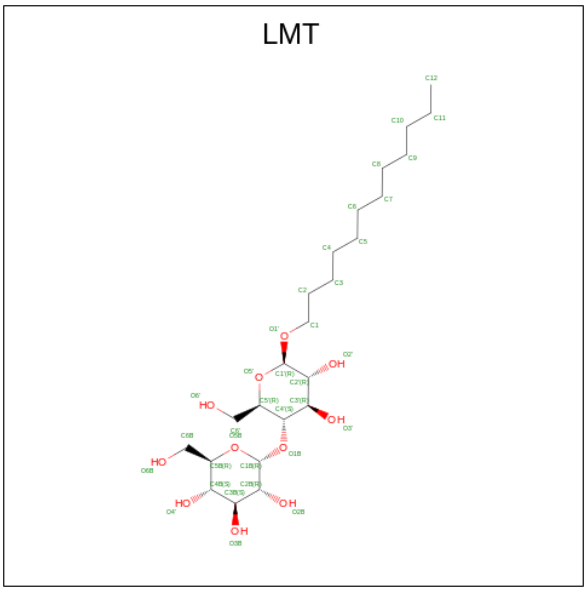
Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total	C	N	O	0
			65	55	4	6	
16	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 17 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



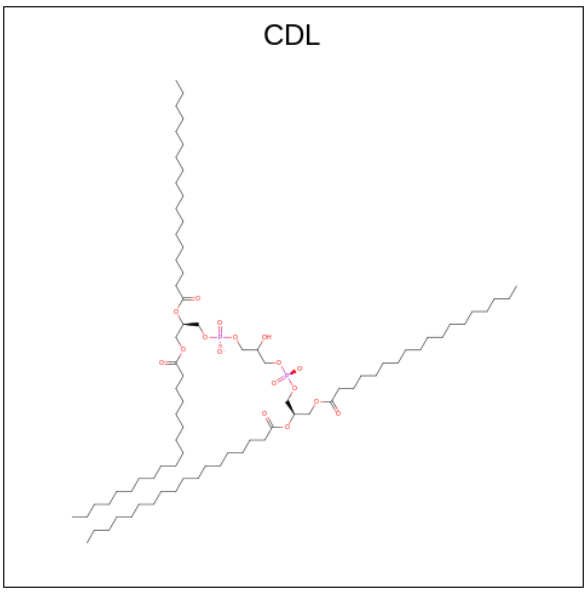
Mol	Chain	Residues	Atoms			AltConf
17	L	1	Total	C	O	0
			33	29	4	
17	L	1	Total	C	O	0
			53	49	4	
17	L	1	Total	C	O	0
			53	49	4	

- Molecule 18 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
18	L	1	Total	C	O	0
			35	24	11	
18	M	1	Total	C	O	0
			35	24	11	
18	M	1	Total	C	O	0
			24	13	11	
18	H	1	Total	C	O	0
			35	24	11	
18	B	1	Total	C	O	0
			35	24	11	
18	E	1	Total	C	O	0
			35	24	11	
18	G	1	Total	C	O	0
			35	24	11	
18	J	1	Total	C	O	0
			35	24	11	
18	J	1	Total	C	O	0
			35	24	11	
18	P	1	Total	C	O	0
			35	24	11	
18	P	1	Total	C	O	0
			35	24	11	
18	R	1	Total	C	O	0
			35	24	11	
18	S	1	Total	C	O	0
			26	15	11	
18	T	1	Total	C	O	0
			35	24	11	
18	X	1	Total	C	O	0
			35	24	11	
18	Z	1	Total	C	O	0
			35	24	11	
18	2	1	Total	C	O	0
			35	24	11	
18	4	1	Total	C	O	0
			35	24	11	
18	4	1	Total	C	O	0
			35	24	11	
18	5	1	Total	C	O	0
			31	20	11	
18	8	1	Total	C	O	0
			35	24	11	
18	8	1	Total	C	O	0
			35	24	11	

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

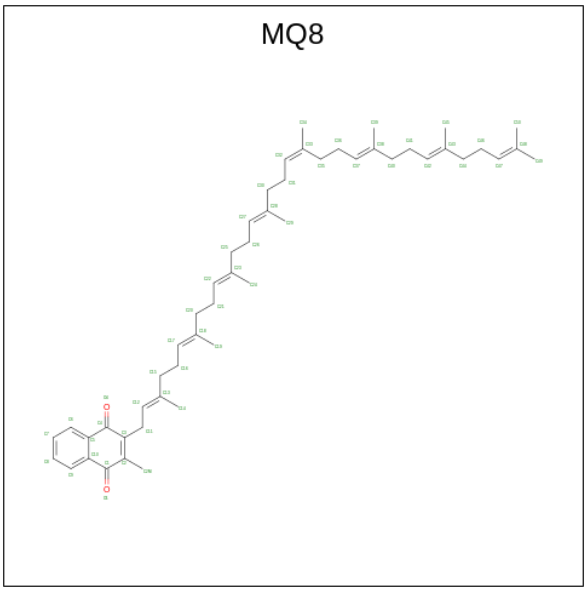


Mol	Chain	Residues	Atoms				AltConf
19	L	1	Total	C	O	P	0
			80	61	17	2	
19	M	1	Total	C	O	P	0
			39	21	16	2	
19	M	1	Total	C	O	P	0
			95	76	17	2	
19	H	1	Total	C	O	P	0
			79	60	17	2	
19	D	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 20 is FE (III) ION (three-letter code: FE) (formula: Fe).

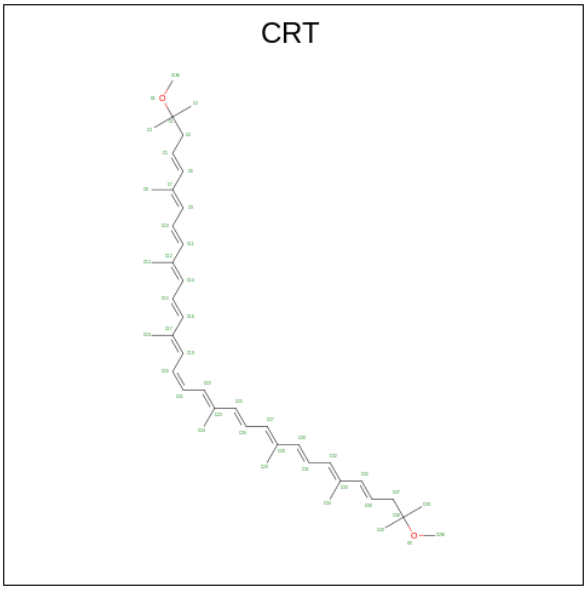
Mol	Chain	Residues	Atoms		AltConf
20	M	1	Total	Fe	0
			1	1	

- Molecule 21 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total	C	O	0
			53	51	2	

- Molecule 22 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			AltConf
22	M	1	Total	C	O	0
			44	42	2	
22	B	1	Total	C	O	0
			44	42	2	
22	E	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms	AltConf
22	G	1	Total C O 44 42 2	0
22	J	1	Total C O 44 42 2	0
22	N	1	Total C O 44 42 2	0
22	P	1	Total C O 44 42 2	0
22	R	1	Total C O 44 42 2	0
22	T	1	Total C O 44 42 2	0
22	V	1	Total C O 44 42 2	0
22	Y	1	Total C O 44 42 2	0
22	Z	1	Total C O 44 42 2	0
22	2	1	Total C O 44 42 2	0
22	4	1	Total C O 44 42 2	0
22	6	1	Total C O 44 42 2	0
22	9	1	Total C O 44 42 2	0
22	0	1	Total C O 44 42 2	0

- Molecule 23 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
23	D	1	Total Ca 1 1	0
23	F	1	Total Ca 1 1	0
23	S	1	Total Ca 1 1	0
23	U	1	Total Ca 1 1	0
23	W	1	Total Ca 1 1	0

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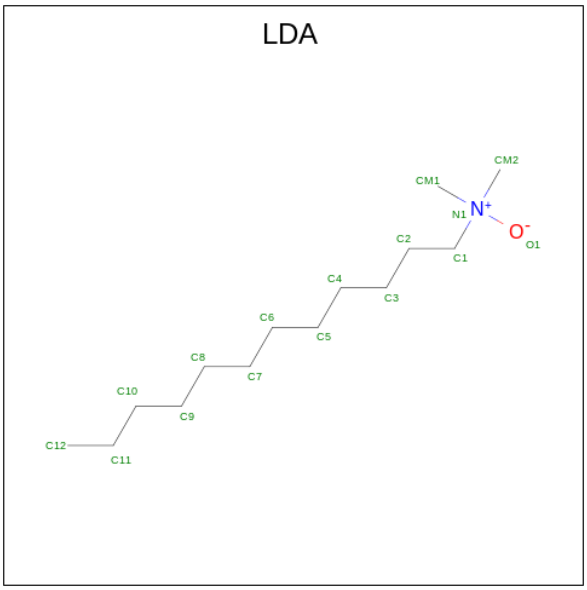
Mol	Chain	Residues	Atoms	AltConf
23	Y	1	Total Ca 1 1	0

- Molecule 24 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	AltConf
24	K	1	Total C N O 16 14 1 1	0
24	O	1	Total C N O 16 14 1 1	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	AltConf
25	C	119	Total O 119 119	0
25	L	50	Total O 50 50	0
25	M	77	Total O 77 77	0
25	H	19	Total O 19 19	0
25	A	2	Total O 2 2	0
25	B	1	Total O 1 1	0

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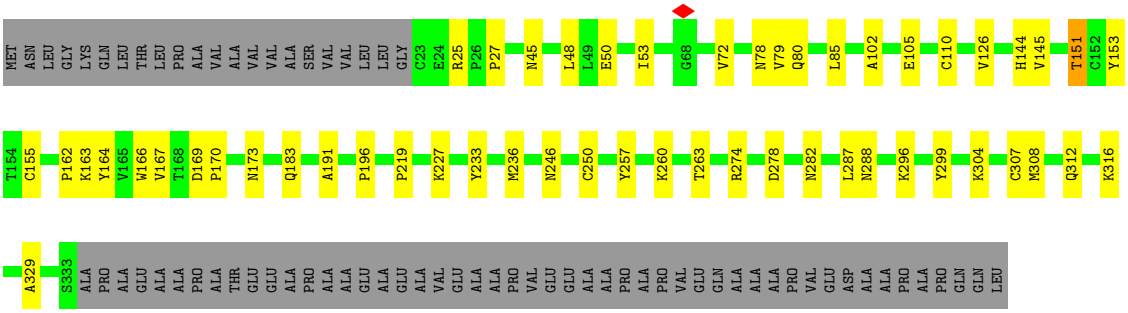
Mol	Chain	Residues	Atoms	AltConf
25	D	4	Total O 4 4	0
25	E	2	Total O 2 2	0
25	F	2	Total O 2 2	0
25	I	2	Total O 2 2	0
25	K	1	Total O 1 1	0
25	O	1	Total O 1 1	0
25	P	1	Total O 1 1	0
25	Q	2	Total O 2 2	0
25	R	1	Total O 1 1	0
25	S	5	Total O 5 5	0
25	T	3	Total O 3 3	0
25	U	10	Total O 10 10	0
25	V	3	Total O 3 3	0
25	W	7	Total O 7 7	0
25	X	1	Total O 1 1	0
25	Y	5	Total O 5 5	0
25	1	1	Total O 1 1	0
25	3	10	Total O 10 10	0
25	7	1	Total O 1 1	0
25	9	4	Total O 4 4	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.

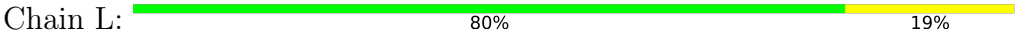
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

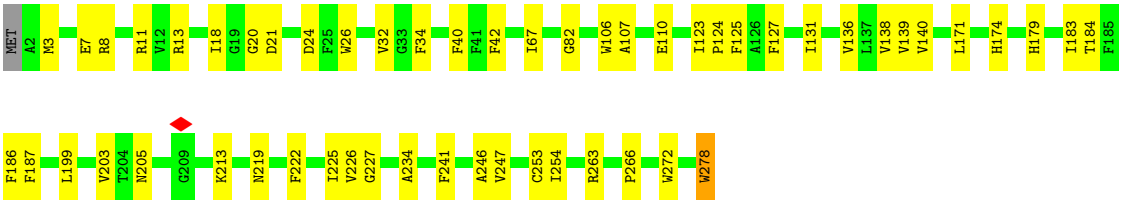
Chain C:



• Molecule 2: Reaction center protein L chain

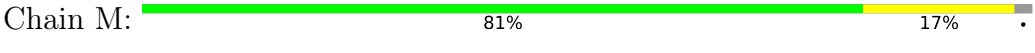
Chain L:

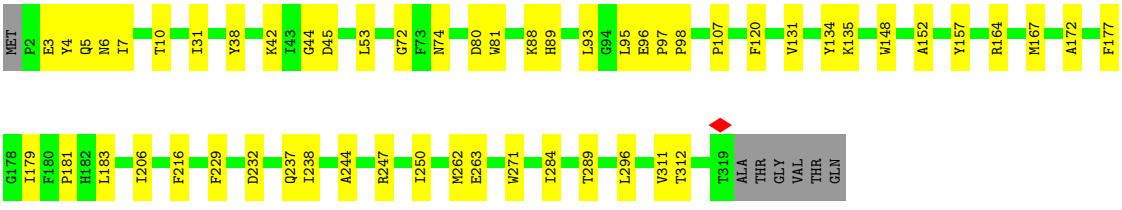




• Molecule 3: Reaction center protein M chain

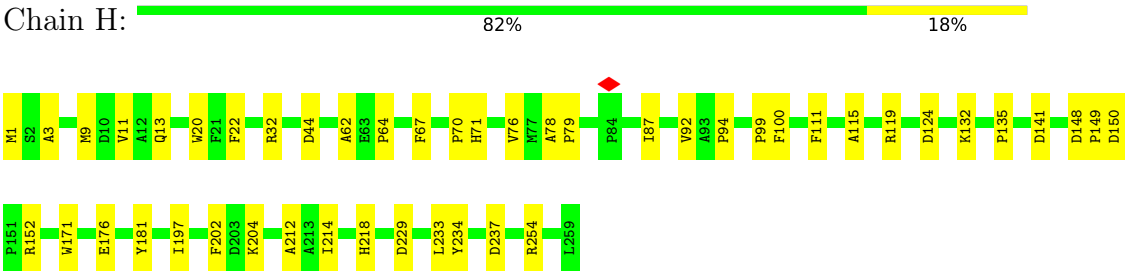
Chain M:





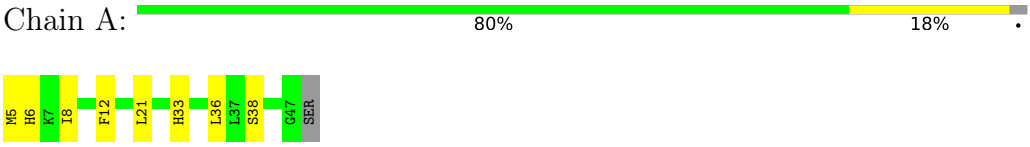
• Molecule 4: Photosynthetic reaction center H subunit

Chain H:



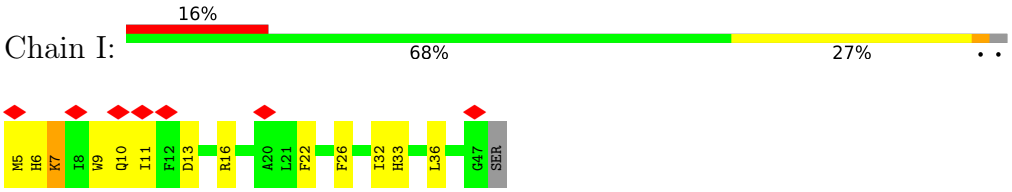
• Molecule 5: Antenna complex alpha/beta subunit

Chain A:



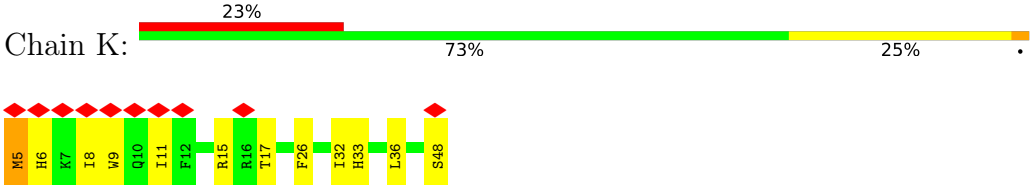
• Molecule 5: Antenna complex alpha/beta subunit

Chain I:



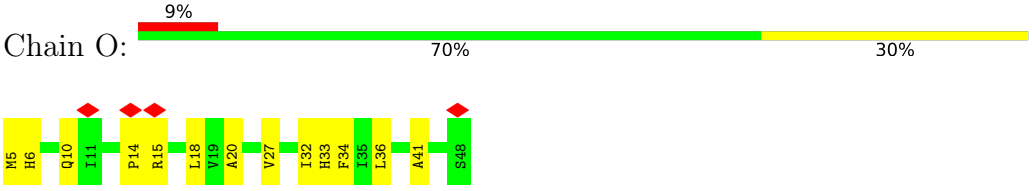
• Molecule 5: Antenna complex alpha/beta subunit

Chain K:



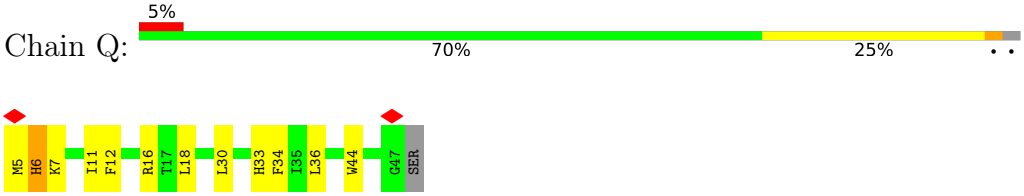
• Molecule 5: Antenna complex alpha/beta subunit

Chain O:



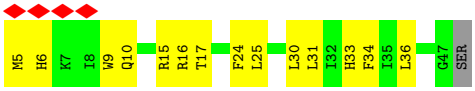
• Molecule 5: Antenna complex alpha/beta subunit

Chain Q:



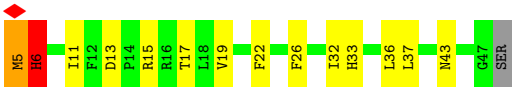
• Molecule 5: Antenna complex alpha/beta subunit

Chain 1:



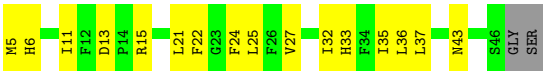
• Molecule 5: Antenna complex alpha/beta subunit

Chain 5:



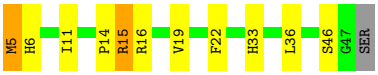
• Molecule 5: Antenna complex alpha/beta subunit

Chain 7:



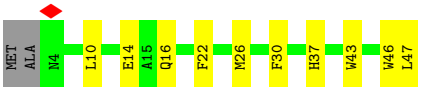
• Molecule 5: Antenna complex alpha/beta subunit

Chain 9:



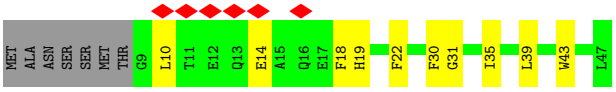
• Molecule 6: Antenna complex alpha/beta subunit

Chain B:



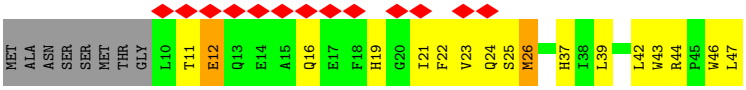
• Molecule 6: Antenna complex alpha/beta subunit

Chain J:



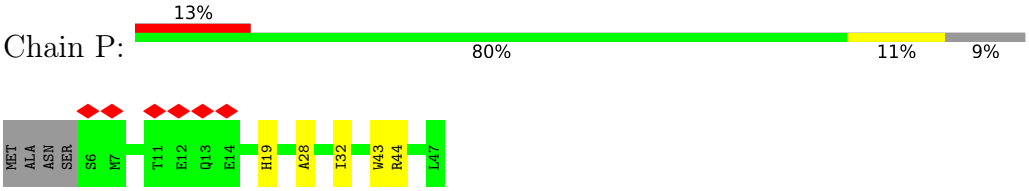
• Molecule 6: Antenna complex alpha/beta subunit

Chain N:



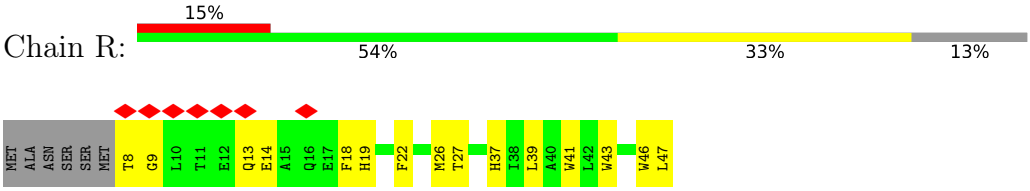
• Molecule 6: Antenna complex alpha/beta subunit

Chain P:



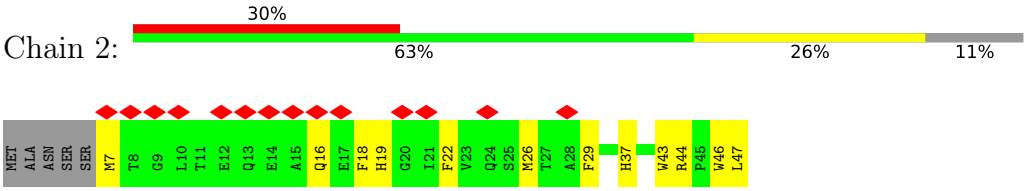
• Molecule 6: Antenna complex alpha/beta subunit

Chain R:



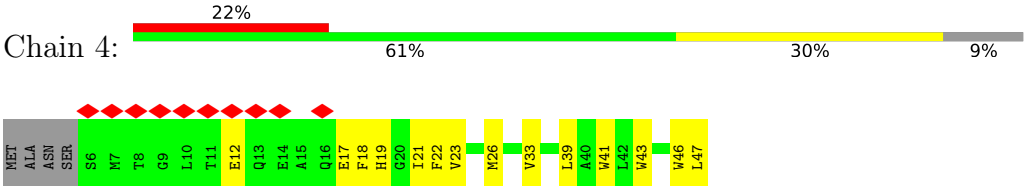
• Molecule 6: Antenna complex alpha/beta subunit

Chain 2:



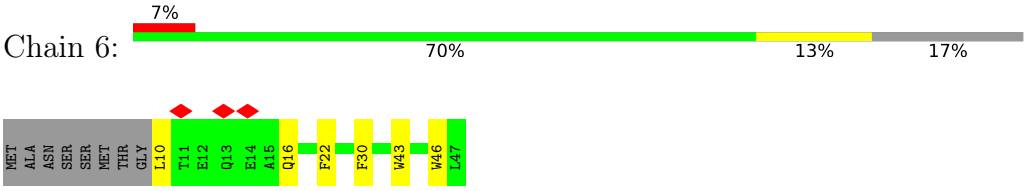
• Molecule 6: Antenna complex alpha/beta subunit

Chain 4:



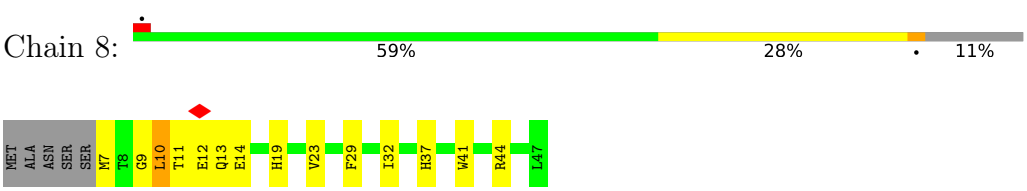
• Molecule 6: Antenna complex alpha/beta subunit

Chain 6:



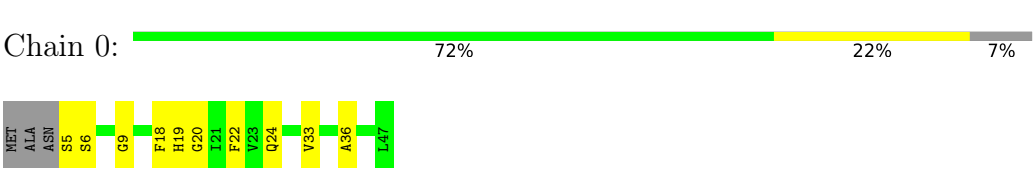
• Molecule 6: Antenna complex alpha/beta subunit

Chain 8:



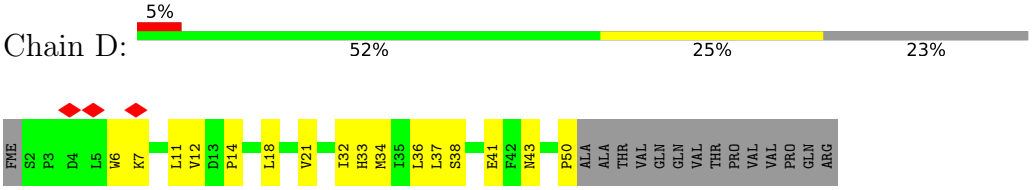
• Molecule 6: Antenna complex alpha/beta subunit

Chain 0:



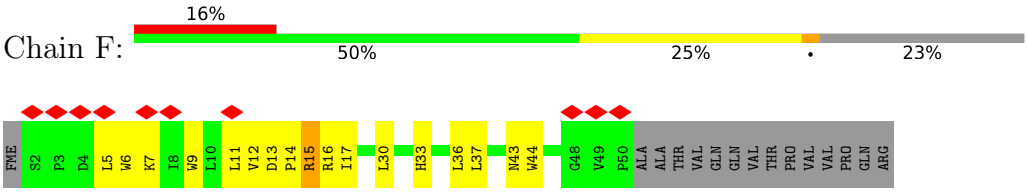
• Molecule 7: Antenna complex alpha/beta subunit

Chain D:



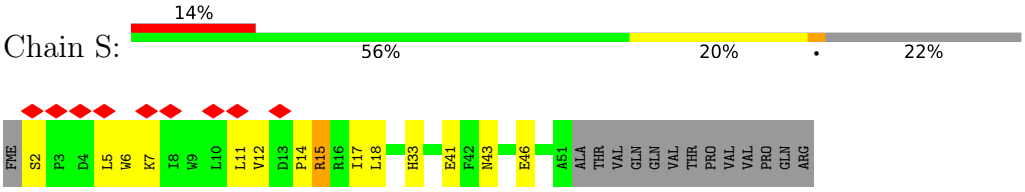
• Molecule 7: Antenna complex alpha/beta subunit

Chain F:



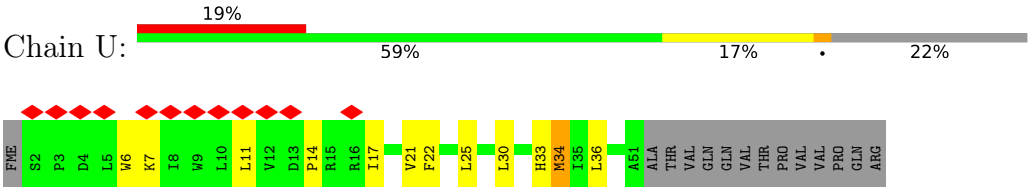
• Molecule 7: Antenna complex alpha/beta subunit

Chain S:



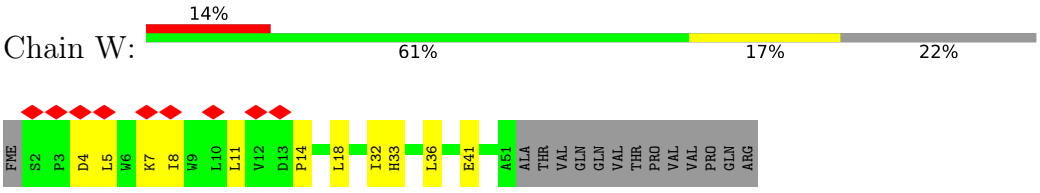
• Molecule 7: Antenna complex alpha/beta subunit

Chain U:



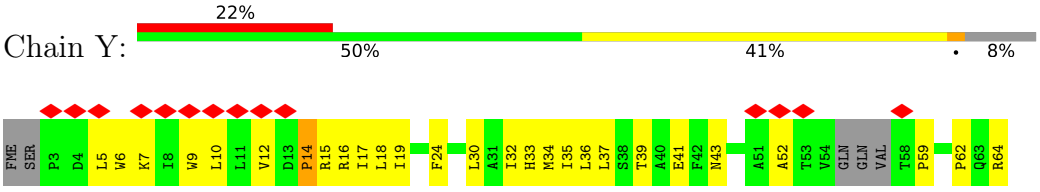
• Molecule 7: Antenna complex alpha/beta subunit

Chain W:



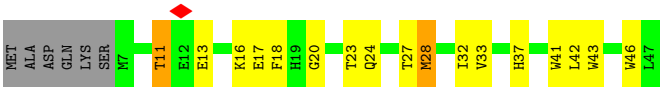
• Molecule 7: Antenna complex alpha/beta subunit

Chain Y:

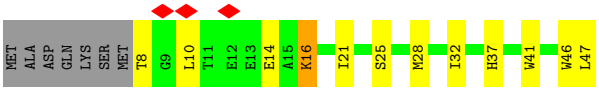


• Molecule 8: Antenna complex alpha/beta subunit

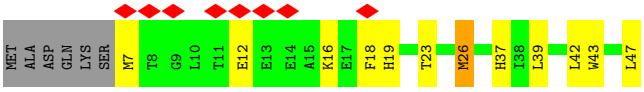
Chain E:



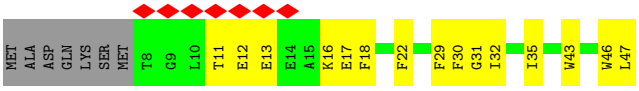
• Molecule 8: Antenna complex alpha/beta subunit



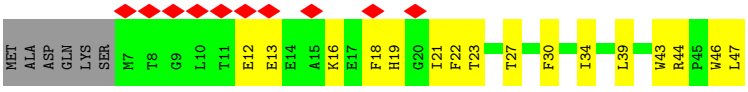
• Molecule 8: Antenna complex alpha/beta subunit



• Molecule 8: Antenna complex alpha/beta subunit

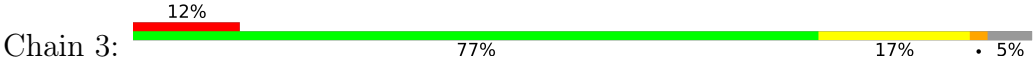


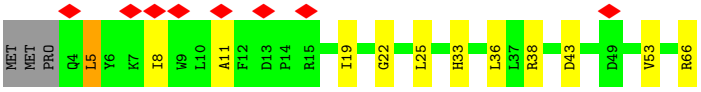
• Molecule 8: Antenna complex alpha/beta subunit



• Molecule 8: Antenna complex alpha/beta subunit

• Molecule 9: Antenna complex alpha/beta subunit





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252230	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	290.88, 290.88, 290.88	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.606, 0.606, 0.606	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, FME, FE, BPH, CDL, HEM, CA, LDA, UQ8, MQ8, BCL, CRT, PLM, MG, Z41, LMT

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	C	0.29	0/2502	0.47	0/3426
2	L	0.29	0/2295	0.45	0/3135
3	M	0.28	0/2632	0.45	0/3601
4	H	0.28	0/2039	0.49	0/2776
5	1	0.25	0/362	0.46	0/492
5	5	0.25	0/358	0.41	0/488
5	7	0.28	0/366	0.45	0/499
5	9	0.27	0/362	0.44	0/492
5	A	0.27	0/362	0.40	0/492
5	I	0.27	0/362	0.44	0/492
5	K	0.25	0/369	0.44	0/500
5	O	0.27	0/369	0.42	0/500
5	Q	0.26	0/362	0.41	0/492
6	0	0.25	0/363	0.39	0/493
6	2	0.24	0/351	0.43	0/477
6	4	0.24	0/357	0.38	0/485
6	6	0.23	0/332	0.35	0/452
6	8	0.25	0/351	0.39	0/477
6	B	0.23	0/371	0.38	0/504
6	J	0.26	0/336	0.39	0/457
6	N	0.24	0/332	0.39	0/452
6	P	0.24	0/357	0.35	0/485
6	R	0.25	0/343	0.41	0/467
7	D	0.25	0/409	0.46	0/561
7	F	0.25	0/409	0.49	0/561
7	S	0.24	0/414	0.46	0/568
7	U	0.24	0/422	0.44	0/578
7	W	0.22	0/414	0.44	0/568
7	Y	0.47	1/483 (0.2%)	0.87	3/663 (0.5%)
8	E	0.26	0/355	0.42	0/480
8	G	0.25	0/347	0.39	0/470
8	T	0.25	0/355	0.41	0/480

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
8	V	0.24	0/347	0.39	0/470
8	X	0.25	0/355	0.39	0/480
8	Z	0.25	0/355	0.42	0/480
9	3	0.30	0/515	0.55	0/700
All	All	0.27	1/21413 (0.0%)	0.46	3/29193 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	59	PRO	CG-CD	-8.08	1.24	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	59	PRO	N-CD-CG	-12.55	84.37	103.20
7	Y	59	PRO	CA-CB-CG	-9.03	86.85	104.00
7	Y	14	PRO	CA-N-CD	-5.20	104.23	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	C	2429	0	2327	55	0
2	L	2210	0	2166	48	0
3	M	2533	0	2490	49	0
4	H	1993	0	1994	35	0
5	1	359	0	371	10	0
5	5	355	0	360	15	0
5	7	359	0	366	19	0
5	9	359	0	371	10	0
5	A	359	0	371	8	0
5	I	359	0	371	14	0
5	K	366	0	376	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	366	0	376	14	0
5	Q	359	0	371	16	0
6	0	351	0	339	10	0
6	2	339	0	329	15	0
6	4	345	0	334	13	0
6	6	320	0	310	5	0
6	8	339	0	329	13	0
6	B	359	0	345	11	0
6	J	324	0	313	10	0
6	N	320	0	310	18	0
6	P	345	0	334	4	0
6	R	331	0	320	16	0
7	D	397	0	413	15	0
7	F	397	0	413	16	0
7	S	402	0	418	12	0
7	U	407	0	427	13	0
7	W	402	0	418	13	0
7	Y	470	0	494	27	0
8	E	343	0	336	16	0
8	G	335	0	327	11	0
8	T	343	0	336	11	0
8	V	335	0	327	13	0
8	X	343	0	336	16	0
8	Z	343	0	336	13	0
9	3	498	0	505	16	0
10	C	172	0	120	21	0
11	C	1	0	0	0	0
12	C	35	0	0	0	0
13	C	12	0	18	2	0
14	1	27	0	25	5	0
14	A	72	0	87	7	0
14	C	31	0	32	2	0
14	F	31	0	35	0	0
14	H	36	0	42	3	0
14	L	101	0	115	13	0
14	M	27	0	27	3	0
14	Q	24	0	21	1	0
15	0	66	0	74	8	0
15	1	66	0	74	11	0
15	2	66	0	74	9	0
15	3	66	0	74	9	0
15	4	66	0	74	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	5	66	0	74	7	0
15	6	66	0	74	7	0
15	7	61	0	61	8	0
15	8	66	0	74	11	0
15	9	66	0	74	5	0
15	A	66	0	74	5	0
15	B	66	0	74	9	0
15	D	66	0	74	4	0
15	E	66	0	74	10	0
15	F	66	0	74	1	0
15	G	66	0	74	9	0
15	I	66	0	74	6	0
15	J	66	0	74	6	0
15	K	66	0	74	8	0
15	L	132	0	148	8	0
15	M	132	0	148	5	0
15	N	66	0	74	10	0
15	O	66	0	74	2	0
15	P	66	0	74	4	0
15	Q	66	0	74	5	0
15	R	66	0	74	6	0
15	S	66	0	74	5	0
15	T	66	0	74	4	0
15	U	66	0	74	6	0
15	V	66	0	74	6	0
15	W	66	0	74	2	0
15	X	66	0	74	5	0
15	Y	66	0	74	4	0
15	Z	66	0	74	6	0
16	L	65	0	76	6	0
16	M	65	0	76	6	0
17	L	139	0	187	24	0
18	2	35	0	46	4	0
18	4	70	0	92	8	0
18	5	31	0	35	1	0
18	8	70	0	92	3	0
18	B	35	0	46	3	0
18	E	35	0	46	2	0
18	G	35	0	46	1	0
18	H	35	0	46	3	0
18	J	70	0	92	4	0
18	L	35	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	M	59	0	67	3	0
18	P	70	0	92	4	0
18	R	35	0	46	4	0
18	S	26	0	25	3	0
18	T	35	0	46	3	0
18	X	35	0	46	3	0
18	Z	35	0	46	2	0
19	D	58	0	60	0	0
19	H	79	0	105	2	0
19	L	80	0	110	7	0
19	M	134	0	168	9	0
20	M	1	0	0	0	0
21	M	53	0	72	8	0
22	0	44	0	60	8	0
22	2	44	0	60	11	0
22	4	44	0	60	10	0
22	6	44	0	60	5	0
22	9	44	0	60	6	0
22	B	44	0	60	6	0
22	E	44	0	60	7	0
22	G	44	0	60	5	0
22	J	44	0	60	9	0
22	M	44	0	60	5	0
22	N	44	0	60	9	0
22	P	44	0	60	3	0
22	R	44	0	60	4	0
22	T	44	0	60	8	0
22	V	44	0	60	9	0
22	Y	44	0	60	6	0
22	Z	44	0	60	7	0
23	D	1	0	0	0	0
23	F	1	0	0	0	0
23	S	1	0	0	0	0
23	U	1	0	0	0	0
23	W	1	0	0	0	0
23	Y	1	0	0	0	0
24	K	16	0	31	0	0
24	O	16	0	31	1	0
25	1	1	0	0	0	0
25	3	10	0	0	0	0
25	7	1	0	0	0	0
25	9	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	119	0	0	1	0
25	D	4	0	0	0	0
25	E	2	0	0	0	0
25	F	2	0	0	0	0
25	H	19	0	0	0	0
25	I	2	0	0	0	0
25	K	1	0	0	0	0
25	L	50	0	0	0	0
25	M	77	0	0	4	0
25	O	1	0	0	0	0
25	P	1	0	0	0	0
25	Q	2	0	0	0	0
25	R	1	0	0	0	0
25	S	5	0	0	0	0
25	T	3	0	0	0	0
25	U	10	0	0	0	0
25	V	3	0	0	0	0
25	W	7	0	0	0	0
25	X	1	0	0	0	0
25	Y	5	0	0	0	0
All	All	26274	0	26723	718	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 14.

All (718) 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)
1:C:155:CYS:SG	10:C:402:HEM:HAC	1.60	1.42
1:C:155:CYS:SG	10:C:402:HEM:CAC	2.09	1.41
1:C:250:CYS:SG	10:C:403:HEM:HAC	1.62	1.39
1:C:110:CYS:SG	10:C:401:HEM:HAC	1.71	1.30
1:C:155:CYS:HG	10:C:402:HEM:CAC	1.43	1.29
1:C:250:CYS:SG	10:C:403:HEM:CAC	2.19	1.29
1:C:110:CYS:SG	10:C:401:HEM:CAC	2.23	1.27
3:M:96:GLU:OE1	25:M:501:HOH:O	1.77	1.02
3:M:96:GLU:OE2	25:M:502:HOH:O	1.81	0.97
1:C:250:CYS:HG	10:C:403:HEM:HAC	1.11	0.94
3:M:72:GLY:HA3	22:M:406:CRT:H6	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:CYS:SG	10:C:402:HEM:C3C	2.73	0.80
22:N:102:CRT:H35	15:O:502:BCL:HMB2	1.64	0.79
7:W:7:LYS:HG2	22:Z:103:CRT:H41	1.66	0.77
7:S:7:LYS:HB3	22:V:102:CRT:H23	1.67	0.77
18:R:103:LMT:H52	8:T:39:LEU:HB3	1.68	0.75
2:L:219:ASN:HD21	4:H:176:GLU:HG2	1.51	0.75
1:C:151:THR:HG22	1:C:153:TYR:H	1.54	0.72
8:X:43:TRP:HB2	18:X:101:LMT:H22	1.72	0.71
5:5:36:LEU:HD11	15:6:101:BCL:HHD	1.72	0.70
15:0:101:BCL:H43	15:0:101:BCL:H3A	1.73	0.70
7:Y:7:LYS:HD3	22:2:103:CRT:H32A	1.74	0.70
8:Z:21:ILE:HA	8:Z:24:GLN:HG2	1.74	0.70
9:3:11:ALA:HB1	5:5:15:ARG:HG3	1.74	0.70
1:C:307:CYS:O	25:C:501:HOH:O	2.09	0.69
18:4:104:LMT:H22	6:6:43:TRP:HB2	1.73	0.69
22:2:103:CRT:H35	15:3:101:BCL:HMB2	1.74	0.69
1:C:110:CYS:CB	10:C:401:HEM:HAC	2.23	0.69
5:Q:33:HIS:CE1	15:R:101:BCL:HMD1	2.29	0.68
17:L:304:UQ8:H1MB	5:9:22:PHE:HB2	1.76	0.68
8:Z:18:PHE:HB2	22:Z:103:CRT:H23	1.76	0.67
5:5:22:PHE:HB3	15:5:102:BCL:H51	1.75	0.67
5:9:33:HIS:CE1	15:0:101:BCL:HMD1	2.29	0.67
5:A:33:HIS:CE1	15:B:102:BCL:HMD1	2.28	0.67
7:U:33:HIS:CE1	15:V:101:BCL:HMD1	2.29	0.67
15:1:402:BCL:H92	6:2:29:PHE:HB2	1.75	0.67
5:I:33:HIS:CE1	15:J:102:BCL:HMD1	2.30	0.66
5:1:36:LEU:HD11	15:2:102:BCL:HHD	1.77	0.66
9:3:22:GLY:HA3	15:3:101:BCL:H151	1.77	0.66
7:S:33:HIS:CE1	15:T:101:BCL:HMD1	2.31	0.66
3:M:5:GLN:HB2	19:M:407:CDL:HA32	1.77	0.66
5:Q:6:HIS:HA	6:R:19:HIS:CD2	2.31	0.66
7:D:33:HIS:CE1	15:E:102:BCL:HMD1	2.31	0.66
5:I:10:GLN:NE2	6:J:10:LEU:O	2.29	0.66
5:K:6:HIS:HA	6:N:19:HIS:ND1	2.10	0.66
2:L:174:HIS:HB3	3:M:183:LEU:HD13	1.78	0.66
18:P:104:LMT:H42	6:R:39:LEU:HB3	1.78	0.65
15:U:101:BCL:H102	8:V:29:PHE:HB2	1.78	0.65
3:M:98:PRO:HB3	3:M:107:PRO:HG3	1.78	0.65
8:V:30:PHE:CE2	15:V:101:BCL:H11	2.31	0.65
5:7:11:ILE:HD11	22:0:102:CRT:H23	1.79	0.65
7:W:33:HIS:CE1	15:X:102:BCL:HMD1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:33:HIS:CE1	15:P:102:BCL:HMD1	2.31	0.65
21:M:405:MQ8:H491	14:A:503:PGV:H221	1.79	0.65
7:D:11:LEU:HD11	22:G:103:CRT:H23	1.78	0.65
8:G:21:ILE:O	8:G:25:SER:OG	2.14	0.65
5:I:13:ASP:HB3	5:I:16:ARG:HD3	1.79	0.65
5:1:33:HIS:CE1	15:2:102:BCL:HMD1	2.33	0.64
2:L:7:GLU:HG3	3:M:250:ILE:HG12	1.80	0.64
17:L:304:UQ8:H4M	5:7:21:LEU:HB2	1.80	0.64
1:C:110:CYS:SG	10:C:401:HEM:CBC	2.84	0.64
8:X:23:THR:O	8:X:27:THR:OG1	2.16	0.64
5:I:36:LEU:HD11	15:J:102:BCL:HHD	1.80	0.64
5:I:7:LYS:HG3	22:N:102:CRT:H41	1.80	0.63
7:F:36:LEU:HD11	15:G:102:BCL:HHD	1.80	0.63
22:T:102:CRT:H35	15:U:101:BCL:HMB2	1.78	0.63
3:M:167:MET:HE3	3:M:289:THR:HG21	1.81	0.63
6:J:43:TRP:HB2	18:J:101:LMT:H12	1.79	0.63
5:5:33:HIS:CE1	15:6:101:BCL:HMD1	2.33	0.63
5:Q:11:ILE:HD11	22:T:102:CRT:H82	1.79	0.63
9:3:36:LEU:HD11	15:4:102:BCL:HHD	1.79	0.63
4:H:64:PRO:HA	4:H:79:PRO:HD2	1.80	0.63
6:8:19:HIS:O	6:8:23:VAL:HG23	1.99	0.63
18:T:103:LMT:H31	8:V:43:TRP:HB2	1.80	0.62
9:3:33:HIS:CE1	15:4:102:BCL:HMD1	2.34	0.62
13:C:407:PLM:H61	14:L:305:PGV:H42	1.80	0.62
2:L:8:ARG:HG2	4:H:87:ILE:HG21	1.80	0.62
16:L:302:BPH:HHC	16:L:302:BPH:HBB3	1.82	0.62
22:N:102:CRT:H393	5:O:33:HIS:HB3	1.82	0.62
5:7:33:HIS:CE1	15:8:102:BCL:HMD1	2.35	0.62
5:K:33:HIS:CE1	15:N:101:BCL:HMD1	2.35	0.61
1:C:110:CYS:HG	10:C:401:HEM:HAC	1.62	0.61
14:L:310:PGV:O13	18:S:101:LMT:O3'	2.16	0.61
6:R:13:GLN:HE21	6:R:14:GLU:HG3	1.66	0.61
9:3:8:ILE:H	9:3:8:ILE:HD12	1.66	0.61
6:0:20:GLY:O	6:0:24:GLN:HG3	2.00	0.61
22:E:103:CRT:H35	15:F:502:BCL:HMB2	1.83	0.60
1:C:236:MET:HB3	10:C:403:HEM:C4B	2.36	0.60
7:Y:33:HIS:CE1	15:Z:102:BCL:HMD1	2.37	0.60
14:L:305:PGV:H32	14:1:401:PGV:H51	1.84	0.60
8:T:47:LEU:HD12	15:T:101:BCL:H172	1.83	0.60
15:M:402:BCL:H61	21:M:405:MQ8:H243	1.83	0.60
16:M:404:BPH:HHC	16:M:404:BPH:HBB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:6:HIS:H	5:1:6:HIS:CD2	2.20	0.60
2:L:107:ALA:HB1	19:L:311:CDL:H782	1.85	0.59
1:C:27:PRO:HD3	9:3:38:ARG:HG3	1.84	0.59
4:H:78:ALA:HB3	4:H:79:PRO:HD3	1.83	0.59
6:R:13:GLN:NE2	6:R:14:GLU:HG3	2.17	0.59
7:F:33:HIS:CE1	15:G:102:BCL:HMD1	2.38	0.59
5:A:38:SER:O	14:A:501:PGV:O06	2.21	0.59
22:Z:103:CRT:H372	5:1:33:HIS:CG	2.37	0.58
6:8:10:LEU:HD13	6:8:14:GLU:HB2	1.85	0.58
18:L:307:LMT:H1'	5:7:43:ASN:HD21	1.67	0.58
3:M:157:TYR:CZ	22:M:406:CRT:H293	2.37	0.58
2:L:21:ASP:O	5:9:15:ARG:NH1	2.22	0.58
1:C:288:ASN:O	1:C:296:LYS:NZ	2.35	0.58
2:L:13:ARG:HD3	4:H:92:VAL:HG11	1.86	0.58
15:N:101:BCL:H91	15:N:101:BCL:H143	1.86	0.58
8:Z:43:TRP:HB2	18:Z:101:LMT:H12	1.86	0.58
4:H:67:PHE:HB2	4:H:76:VAL:HG22	1.84	0.57
8:E:18:PHE:HB2	22:E:103:CRT:H21A	1.85	0.57
5:O:36:LEU:HD11	15:P:102:BCL:HHD	1.86	0.57
16:L:302:BPH:H171	14:A:501:PGV:H332	1.85	0.57
7:Y:36:LEU:HD11	15:Z:102:BCL:HHD	1.85	0.57
8:T:19:HIS:O	8:T:23:THR:HG23	2.04	0.57
22:M:406:CRT:H393	5:O:34:PHE:HD2	1.69	0.57
22:4:103:CRT:H32	22:4:103:CRT:H291	1.86	0.57
7:Y:35:ILE:HD13	22:Z:103:CRT:H2M3	1.86	0.57
6:2:43:TRP:HB2	18:2:101:LMT:H22	1.85	0.57
8:G:10:LEU:HG	8:G:14:GLU:HG3	1.87	0.57
8:V:22:PHE:CD2	22:V:102:CRT:H14	2.40	0.57
1:C:45:ASN:HB3	1:C:48:LEU:HB2	1.87	0.57
16:M:404:BPH:H192	18:S:101:LMT:H12	1.85	0.57
22:4:103:CRT:H371	15:5:102:BCL:HMB2	1.87	0.57
15:2:102:BCL:HBB1	18:4:101:LMT:H62	1.86	0.56
5:Q:36:LEU:HD11	15:R:101:BCL:HHD	1.86	0.56
15:8:102:BCL:HMB1	18:8:103:LMT:H102	1.87	0.56
4:H:100:PHE:HB2	4:H:111:PHE:CZ	2.41	0.56
22:G:103:CRT:H35	15:I:101:BCL:HMB2	1.87	0.56
3:M:95:LEU:HB3	3:M:177:PHE:HB2	1.88	0.56
16:M:404:BPH:HBC3	16:M:404:BPH:HHD	1.88	0.56
7:W:8:ILE:HA	22:Z:103:CRT:H83	1.88	0.56
7:W:36:LEU:HD11	15:X:102:BCL:HHD	1.87	0.56
5:5:43:ASN:HD21	18:5:101:LMT:H6E	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:18:PHE:HB2	22:J:103:CRT:H32A	1.88	0.55
7:Y:9:TRP:HZ3	8:Z:19:HIS:CD2	2.24	0.55
5:7:25:LEU:HB3	15:7:101:BCL:H12	1.88	0.55
15:L:301:BCL:H202	21:M:405:MQ8:H292	1.87	0.55
4:H:11:VAL:HG21	18:H:303:LMT:H31	1.87	0.55
6:B:43:TRP:HB2	18:B:101:LMT:H12	1.87	0.55
6:0:33:VAL:HG11	15:0:101:BCL:HBA2	1.87	0.55
8:Z:30:PHE:O	8:Z:34:ILE:HD12	2.06	0.55
8:E:18:PHE:HA	22:E:103:CRT:H6	1.88	0.55
6:R:18:PHE:HA	22:R:102:CRT:H6	1.88	0.55
1:C:246:ASN:HA	2:L:171:LEU:HD21	1.89	0.55
2:L:26:TRP:HZ3	4:H:99:PRO:HB3	1.73	0.54
17:L:304:UQ8:H1M	5:9:19:VAL:HA	1.90	0.54
3:M:3:GLU:O	3:M:5:GLN:NE2	2.39	0.54
15:U:101:BCL:H161	8:V:32:ILE:HD11	1.88	0.54
5:I:9:TRP:HE1	6:J:19:HIS:HB2	1.72	0.54
22:T:102:CRT:H372	7:U:33:HIS:CG	2.42	0.54
7:U:11:LEU:HD21	22:Y:101:CRT:H1M1	1.88	0.54
7:D:12:VAL:HG12	7:F:15:ARG:HG2	1.90	0.54
7:Y:30:LEU:O	7:Y:34:MET:HG2	2.08	0.54
1:C:110:CYS:CB	10:C:401:HEM:CAC	2.84	0.54
7:W:41:GLU:O	8:X:44:ARG:NH1	2.40	0.54
1:C:167:VAL:HG22	7:Y:62:PRO:HD2	1.89	0.54
2:L:32:VAL:HG13	21:M:405:MQ8:H453	1.89	0.54
3:M:206:ILE:HD13	15:M:402:BCL:HMD1	1.89	0.54
3:M:148:TRP:HE1	19:M:409:CDL:H332	1.73	0.54
3:M:271:TRP:CH2	19:M:409:CDL:H541	2.43	0.54
5:K:6:HIS:HB3	6:N:16:GLN:HE22	1.72	0.54
8:V:18:PHE:HD1	22:V:102:CRT:H6	1.73	0.54
7:Y:5:LEU:HD13	15:1:402:BCL:H171	1.89	0.54
4:H:70:PRO:HB2	4:H:71:HIS:CD2	2.43	0.54
22:V:102:CRT:H35	15:W:101:BCL:HHB	1.89	0.54
15:7:101:BCL:H141	6:8:32:ILE:HG21	1.89	0.53
22:B:103:CRT:H23	5:9:11:ILE:HD11	1.90	0.53
5:Q:11:ILE:O	7:S:15:ARG:NE	2.42	0.53
22:9:101:CRT:H35	15:9:102:BCL:HMB2	1.90	0.53
4:H:44:ASP:OD1	14:A:503:PGV:O05	2.15	0.53
6:2:37:HIS:CG	15:2:102:BCL:H8	2.44	0.53
2:L:227:GLY:HA3	14:L:310:PGV:H221	1.90	0.53
6:J:10:LEU:HG	6:J:14:GLU:HG3	1.90	0.53
7:Y:37:LEU:O	7:Y:43:ASN:ND2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:10:THR:HG21	4:H:202:PHE:HB2	1.91	0.53
18:R:103:LMT:H2'	8:T:43:TRP:HD1	1.74	0.53
7:S:11:LEU:HD21	7:U:14:PRO:HB2	1.90	0.53
15:1:402:BCL:H122	15:1:402:BCL:H192	1.89	0.53
5:7:36:LEU:HD11	15:8:102:BCL:HHD	1.91	0.53
17:L:304:UQ8:H40B	17:L:304:UQ8:H16A	1.90	0.53
2:L:187:PHE:HB3	16:M:404:BPH:HBB2	1.90	0.52
6:J:22:PHE:CD2	22:J:103:CRT:H14	2.44	0.52
5:K:11:ILE:HB	5:O:15:ARG:HH21	1.73	0.52
4:H:13:GLN:NE2	14:H:301:PGV:O13	2.41	0.52
7:U:22:PHE:HA	15:U:101:BCL:H41	1.91	0.52
6:4:43:TRP:HA	18:4:101:LMT:H6D	1.92	0.52
1:C:278:ASP:OD1	1:C:282:ASN:ND2	2.40	0.52
8:X:13:GLU:HA	8:X:16:LYS:NZ	2.24	0.52
6:6:30:PHE:CE2	15:6:101:BCL:H11	2.45	0.52
8:E:20:GLY:O	8:E:24:GLN:HG3	2.10	0.52
1:C:250:CYS:SG	10:C:403:HEM:C3C	2.99	0.52
7:Y:9:TRP:CD1	7:Y:14:PRO:HB3	2.45	0.52
3:M:53:LEU:O	5:Q:16:ARG:NH1	2.42	0.52
6:N:11:THR:OG1	6:N:12:GLU:N	2.43	0.52
4:H:67:PHE:HE2	4:H:78:ALA:HB2	1.76	0.51
15:B:102:BCL:H43	15:B:102:BCL:H3A	1.93	0.51
6:R:46:TRP:CD1	6:R:47:LEU:HG	2.45	0.51
15:L:308:BCL:H171	3:M:179:ILE:HD11	1.91	0.51
5:K:36:LEU:HD11	15:N:101:BCL:HHD	1.92	0.51
15:2:102:BCL:H162	18:4:101:LMT:H21	1.93	0.51
5:5:5:FME:HCN	22:9:101:CRT:H21A	1.93	0.51
3:M:31:ILE:HB	18:S:101:LMT:H3B	1.92	0.51
4:H:94:PRO:HB2	6:0:9:GLY:HA3	1.92	0.51
5:5:11:ILE:HG23	5:7:15:ARG:HE	1.76	0.51
6:4:22:PHE:HA	22:4:103:CRT:H14	1.93	0.51
5:A:36:LEU:HD11	15:B:102:BCL:HHD	1.93	0.51
2:L:138:VAL:HG23	2:L:139:VAL:HG23	1.92	0.51
6:N:22:PHE:CD2	22:N:102:CRT:H14	2.46	0.51
7:U:25:LEU:HB2	15:U:101:BCL:H43	1.93	0.51
22:V:102:CRT:H372	7:W:33:HIS:CG	2.46	0.51
6:2:43:TRP:HD1	18:2:101:LMT:H2'	1.75	0.51
2:L:40:PHE:HB2	21:M:405:MQ8:H392	1.93	0.51
5:K:11:ILE:HB	5:O:15:ARG:HE	1.76	0.51
8:Z:46:TRP:CD2	15:Z:102:BCL:H2C	2.45	0.51
1:C:110:CYS:HB2	10:C:401:HEM:C3C	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:302:BPH:HHC	16:L:302:BPH:CBB	2.40	0.50
4:H:70:PRO:HB2	4:H:71:HIS:HD2	1.76	0.50
8:E:33:VAL:HG11	15:E:102:BCL:HAA1	1.92	0.50
8:E:46:TRP:HZ2	15:E:102:BCL:H121	1.76	0.50
7:D:18:LEU:HA	7:D:21:VAL:HG12	1.94	0.50
6:N:46:TRP:CE2	15:N:101:BCL:H2C	2.47	0.50
15:4:102:BCL:HMA2	22:4:103:CRT:H30	1.93	0.50
2:L:179:HIS:CE1	2:L:183:ILE:HD11	2.46	0.50
15:4:102:BCL:O1A	22:4:103:CRT:H25	2.10	0.50
5:O:41:ALA:O	6:P:44:ARG:NH1	2.36	0.50
5:7:13:ASP:OD2	5:7:15:ARG:HG2	2.10	0.50
14:M:408:PGV:H202	5:O:20:ALA:HA	1.93	0.50
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.93	0.50
7:S:2:SER:HB3	7:S:5:LEU:HG	1.94	0.50
7:U:6:TRP:HH2	8:V:12:GLU:HG3	1.77	0.50
2:L:136:VAL:HA	2:L:140:VAL:HB	1.93	0.50
2:L:18:ILE:HD11	19:L:311:CDL:H672	1.94	0.50
7:W:11:LEU:HB3	7:Y:15:ARG:HB2	1.94	0.50
8:X:19:HIS:O	8:X:23:THR:OG1	2.21	0.50
3:M:271:TRP:HH2	19:M:409:CDL:H541	1.77	0.49
6:R:22:PHE:CD2	22:R:102:CRT:H14	2.47	0.49
8:X:21:ILE:H	8:X:21:ILE:HD12	1.76	0.49
22:9:101:CRT:H82	22:9:101:CRT:H42	1.94	0.49
6:0:5:SER:OG	6:0:6:SER:N	2.45	0.49
5:1:15:ARG:HH11	5:1:15:ARG:HG2	1.77	0.49
22:6:102:CRT:H372	5:7:33:HIS:CD2	2.48	0.49
6:0:18:PHE:HB2	22:0:102:CRT:H21A	1.94	0.49
7:Y:10:LEU:HB2	22:2:103:CRT:H1M1	1.95	0.49
8:G:37:HIS:CG	15:G:102:BCL:H8	2.47	0.49
7:Y:5:LEU:HD22	15:1:402:BCL:H193	1.95	0.49
2:L:225:ILE:HG22	2:L:226:VAL:HG13	1.94	0.49
6:B:26:MET:HG3	22:B:103:CRT:C19	2.43	0.49
7:F:12:VAL:HG22	7:F:17:ILE:HD11	1.95	0.49
22:J:103:CRT:H342	15:K:102:BCL:HBA2	1.94	0.49
8:X:39:LEU:HB3	18:X:101:LMT:H62	1.93	0.49
6:2:46:TRP:CD2	15:2:102:BCL:H2C	2.48	0.49
5:7:22[B]:PHE:CD1	15:7:101:BCL:H41	2.48	0.49
14:L:305:PGV:H211	14:1:401:PGV:H42	1.95	0.49
8:E:42:LEU:O	18:E:101:LMT:O3'	2.30	0.49
7:U:17:ILE:O	7:U:21:VAL:HG12	2.12	0.49
1:C:173:ASN:O	3:M:80:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:403:BCL:HAA2	15:M:403:BCL:HBD	1.95	0.49
6:4:39:LEU:HB3	18:4:101:LMT:H22	1.95	0.49
1:C:85:LEU:HD11	1:C:329:ALA:HB2	1.95	0.49
8:X:43:TRP:O	18:X:101:LMT:O3'	2.28	0.49
3:M:164:ARG:HD2	3:M:284:ILE:HG23	1.95	0.49
7:U:36:LEU:HD11	15:V:101:BCL:HHD	1.95	0.49
1:C:169:ASP:OD2	7:Y:64:ARG:NE	2.40	0.48
17:L:304:UQ8:H4MB	15:9:102:BCL:H112	1.95	0.48
5:9:36:LEU:HD11	15:0:101:BCL:HHD	1.93	0.48
1:C:308:MET:HA	1:C:312:GLN:H	1.78	0.48
18:L:307:LMT:H122	18:L:307:LMT:H62	1.95	0.48
9:3:19:ILE:HA	15:3:101:BCL:H152	1.95	0.48
8:G:37:HIS:CD2	15:G:102:BCL:H8	2.47	0.48
15:1:402:BCL:H61	15:1:402:BCL:H101	1.55	0.48
2:L:3:MET:HG2	2:L:11:ARG:CZ	2.43	0.48
15:K:102:BCL:H193	6:N:25:SER:HA	1.94	0.48
18:T:103:LMT:O3'	18:T:103:LMT:O2B	2.26	0.48
16:M:404:BPH:H142	16:M:404:BPH:H8	1.94	0.48
6:J:39:LEU:HB3	18:J:101:LMT:H42	1.95	0.48
8:V:18:PHE:CD1	22:V:102:CRT:H6	2.48	0.48
1:C:53:ILE:HG22	9:3:53:VAL:HG21	1.96	0.48
15:G:102:BCL:H141	15:G:102:BCL:H161	1.67	0.48
4:H:9:MET:HA	4:H:13:GLN:OE1	2.13	0.48
5:A:6:HIS:CD2	6:B:16:GLN:HG2	2.48	0.48
8:G:46:TRP:CE2	15:G:102:BCL:H2C	2.49	0.48
15:R:101:BCL:H91	15:R:101:BCL:H111	1.71	0.48
5:5:32:ILE:HD12	15:6:101:BCL:O1D	2.14	0.48
18:8:103:LMT:H91	6:0:36:ALA:HB1	1.95	0.48
14:A:503:PGV:H202	5:9:16:ARG:CZ	2.44	0.48
18:T:103:LMT:H2'	8:V:43:TRP:HD1	1.79	0.48
2:L:199:LEU:HD22	2:L:222:PHE:CE2	2.49	0.48
4:H:149:PRO:HG3	4:H:204:LYS:HG2	1.95	0.48
8:G:28:MET:O	8:G:32:ILE:HG13	2.14	0.48
15:Y:102:BCL:H112	15:Y:102:BCL:H72	1.53	0.48
16:L:302:BPH:HED1	21:M:405:MQ8:H211	1.96	0.48
15:M:403:BCL:H141	16:M:404:BPH:H4C2	1.96	0.48
6:R:46:TRP:CE2	15:R:101:BCL:H2C	2.49	0.48
2:L:205:ASN:HB3	19:M:409:CDL:HB21	1.96	0.47
6:P:43:TRP:HB2	18:P:101:LMT:H12	1.95	0.47
18:P:104:LMT:H31	6:R:43:TRP:HB2	1.95	0.47
6:4:19:HIS:O	6:4:23:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:6:TRP:CD2	8:T:16:LYS:HG2	2.48	0.47
9:3:8:ILE:HD12	9:3:8:ILE:N	2.29	0.47
9:3:25:LEU:HB3	15:3:101:BCL:H12	1.96	0.47
17:L:303:UQ8:H16	17:L:303:UQ8:H12	1.59	0.47
4:H:20:TRP:NE1	14:H:301:PGV:H211	2.29	0.47
5:I:16:ARG:HH22	5:K:15:ARG:CZ	2.27	0.47
6:4:41:TRP:HH2	6:4:47:LEU:HB2	1.79	0.47
17:L:304:UQ8:H12	17:L:304:UQ8:H16	1.68	0.47
4:H:197:ILE:HD11	4:H:202:PHE:HE2	1.79	0.47
22:G:103:CRT:H371	15:I:101:BCL:C2B	2.45	0.47
1:C:260:LYS:HE3	1:C:260:LYS:HB3	1.68	0.47
4:H:135:PRO:HG3	4:H:171:TRP:CE2	2.49	0.47
4:H:141:ASP:OD1	4:H:141:ASP:N	2.37	0.47
5:A:21:LEU:HD11	22:B:103:CRT:H243	1.96	0.47
6:N:46:TRP:CD2	15:N:101:BCL:H2C	2.50	0.47
5:O:32:ILE:HD12	15:P:102:BCL:O1D	2.13	0.47
8:T:12:GLU:O	8:T:16:LYS:HG3	2.14	0.47
2:L:247:VAL:HG21	16:L:302:BPH:HBC3	1.96	0.47
15:A:502:BCL:HMB2	22:0:102:CRT:H35	1.97	0.47
7:D:6:TRP:CH2	7:D:7:LYS:HD3	2.50	0.47
14:C:408:PGV:H211	5:1:31:LEU:HD22	1.97	0.47
2:L:82:GLY:HA2	18:L:307:LMT:H21	1.97	0.47
7:D:36:LEU:HD11	15:E:102:BCL:HHD	1.97	0.47
7:F:9:TRP:HZ3	7:F:17:ILE:HG13	1.80	0.47
6:J:30:PHE:CE1	15:J:102:BCL:H11	2.49	0.47
15:Y:102:BCL:H101	15:Y:102:BCL:H13	1.55	0.47
6:N:46:TRP:CZ3	15:N:101:BCL:HAC2	2.50	0.47
5:7:6:HIS:NE2	6:8:12:GLU:OE2	2.37	0.47
5:I:6:HIS:HA	6:J:19:HIS:CG	2.49	0.47
6:N:43:TRP:CE2	6:N:44:ARG:HG3	2.50	0.47
5:I:26:PHE:HA	15:I:101:BCL:H11	1.96	0.47
7:Y:9:TRP:CZ3	8:Z:19:HIS:CD2	3.02	0.47
6:2:47:LEU:HD13	18:4:101:LMT:H32	1.97	0.47
2:L:241:PHE:HB2	19:L:311:CDL:H412	1.97	0.46
3:M:247:ARG:NH2	4:H:115:ALA:O	2.47	0.46
7:D:37:LEU:O	7:D:43:ASN:ND2	2.47	0.46
8:E:17:GLU:HG2	22:E:103:CRT:H41	1.97	0.46
22:J:103:CRT:H35	15:K:102:BCL:HMB2	1.97	0.46
15:N:101:BCL:H141	15:N:101:BCL:H162	1.70	0.46
18:P:104:LMT:H5B	18:P:104:LMT:H6E	1.97	0.46
5:Q:11:ILE:HG13	5:Q:12:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:MET:O	1:C:308:MET:HG3	2.14	0.46
17:L:303:UQ8:H22	17:L:303:UQ8:H25	1.66	0.46
6:B:10:LEU:HD23	6:B:14:GLU:HB3	1.96	0.46
7:Y:15:ARG:O	7:Y:19:ILE:HG12	2.15	0.46
2:L:34:PHE:CZ	17:L:304:UQ8:H42A	2.50	0.46
7:S:41:GLU:OE2	7:S:41:GLU:N	2.48	0.46
15:2:102:BCL:H62	15:2:102:BCL:H41	1.69	0.46
6:4:17:GLU:O	6:4:21:ILE:HG13	2.16	0.46
6:2:19:HIS:O	6:2:19:HIS:ND1	2.44	0.46
1:C:78:ASN:HD21	1:C:80:GLN:HE21	1.63	0.46
6:N:19:HIS:HD2	6:N:19:HIS:O	1.97	0.46
5:Q:16:ARG:HE	14:Q:101:PGV:H02	1.80	0.46
15:Q:102:BCL:H61	15:Q:102:BCL:H41	1.59	0.46
15:S:102:BCL:H93	15:S:102:BCL:H61	1.73	0.46
8:Z:31:GLY:O	8:Z:35:ILE:HG13	2.16	0.46
6:8:7:MET:HG3	6:8:9:GLY:H	1.80	0.46
5:K:9:TRP:HZ3	5:K:17:THR:HG21	1.80	0.46
15:7:101:BCL:HMD1	6:8:37:HIS:CE1	2.50	0.46
15:G:102:BCL:H61	15:G:102:BCL:H2	1.61	0.46
5:O:6:HIS:HA	6:P:19:HIS:ND1	2.31	0.46
8:V:46:TRP:CD1	8:V:47:LEU:HG	2.51	0.46
7:F:13:ASP:OD2	7:F:15:ARG:N	2.47	0.46
22:J:103:CRT:H343	5:K:26:PHE:CE1	2.51	0.46
3:M:4:TYR:CZ	3:M:6:ASN:HA	2.50	0.46
15:D:102:BCL:H203	8:E:32:ILE:HD12	1.98	0.46
15:I:101:BCL:H62	15:I:101:BCL:H41	1.63	0.46
7:W:14:PRO:HB3	8:X:18:PHE:CZ	2.51	0.46
7:Y:12:VAL:HB	7:Y:17:ILE:HD11	1.98	0.46
6:2:18:PHE:HD2	22:2:103:CRT:C6	2.29	0.46
5:5:37:LEU:O	5:5:43:ASN:ND2	2.48	0.46
2:L:184:THR:HG22	17:L:303:UQ8:H25A	1.97	0.45
19:H:302:CDL:OA6	14:A:503:PGV:H21	2.16	0.45
8:G:47:LEU:HD13	18:J:101:LMT:H32	1.97	0.45
5:K:5:FME:O	5:K:8:ILE:HG12	2.16	0.45
6:P:28:ALA:O	6:P:32:ILE:HD12	2.16	0.45
7:S:12:VAL:HB	7:S:17:ILE:HD13	1.98	0.45
6:8:37:HIS:CG	15:8:102:BCL:H91	2.51	0.45
5:Q:7:LYS:HB2	5:Q:7:LYS:HE2	1.77	0.45
7:Y:14:PRO:O	7:Y:18:LEU:HD12	2.16	0.45
22:2:103:CRT:H372	9:3:33:HIS:CD2	2.51	0.45
8:E:11:THR:OG1	8:E:13:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:12:VAL:CG2	7:F:17:ILE:HD11	2.46	0.45
4:H:124:ASP:HB2	4:H:233:LEU:HD21	1.98	0.45
15:D:102:BCL:HMD1	8:E:37:HIS:CE1	2.52	0.45
15:N:101:BCL:HMB2	15:N:101:BCL:H62	1.98	0.45
18:2:101:LMT:H5B	18:2:101:LMT:H6E	1.98	0.45
4:H:32:ARG:HG2	4:H:62:ALA:HB2	1.99	0.45
4:H:214:ILE:HB	4:H:218:HIS:HB2	1.98	0.45
8:E:23:THR:O	8:E:27:THR:HG23	2.16	0.45
15:E:102:BCL:H161	15:E:102:BCL:H141	1.67	0.45
7:Y:14:PRO:HG2	22:Z:103:CRT:H1M1	1.98	0.45
8:Z:46:TRP:CE2	15:Z:102:BCL:H2C	2.52	0.45
1:C:227:LYS:NZ	3:M:97:PRO:O	2.48	0.45
1:C:316:LYS:HG2	10:C:404:HEM:HAD2	1.98	0.45
15:A:502:BCL:HAC2	15:A:502:BCL:HHD	1.73	0.45
15:S:102:BCL:HMD1	8:T:37:HIS:CE1	2.52	0.45
8:T:18:PHE:HB2	22:T:102:CRT:H1M2	1.98	0.45
6:0:22:PHE:CD2	22:0:102:CRT:H14	2.52	0.45
15:L:308:BCL:HBB2	15:L:308:BCL:HMB1	1.99	0.45
3:M:237:GLN:HB2	3:M:262:MET:HG2	1.99	0.45
18:B:101:LMT:H62	18:B:101:LMT:H91	1.78	0.45
7:W:14:PRO:HB3	8:X:18:PHE:CE1	2.52	0.45
5:I:32:ILE:HD12	15:J:102:BCL:O1D	2.16	0.45
15:O:502:BCL:H91	15:O:502:BCL:H112	1.67	0.45
3:M:42:LYS:HE2	3:M:42:LYS:HB2	1.77	0.45
15:D:102:BCL:HBC2	8:E:43:TRP:CZ3	2.51	0.45
15:I:101:BCL:H143	15:I:101:BCL:H111	1.78	0.45
22:P:103:CRT:H372	5:Q:33:HIS:CD2	2.52	0.45
6:R:8:THR:OG1	6:R:9:GLY:N	2.49	0.45
7:S:14:PRO:HB3	8:T:18:PHE:CZ	2.51	0.45
5:5:13:ASP:O	5:5:17:THR:OG1	2.26	0.45
6:8:11:THR:C	6:8:13:GLN:H	2.19	0.45
2:L:272:TRP:CE2	17:L:309:UQ8:H4MA	2.52	0.44
7:Y:9:TRP:CE2	8:Z:18:PHE:HE1	2.35	0.44
3:M:284:ILE:HD13	3:M:284:ILE:HA	1.81	0.44
6:R:41:TRP:CZ2	15:R:101:BCL:H202	2.52	0.44
5:5:11:ILE:HG23	5:7:15:ARG:NE	2.31	0.44
15:5:102:BCL:H62	15:5:102:BCL:H93	1.72	0.44
5:7:35:ILE:HD13	22:9:101:CRT:H391	1.98	0.44
15:B:102:BCL:CHB	15:B:102:BCL:H71	2.48	0.44
15:B:102:BCL:HBA2	15:B:102:BCL:HED3	1.98	0.44
15:0:101:BCL:H3A	15:0:101:BCL:HBA1	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:0:101:BCL:H62	15:0:101:BCL:H41	1.73	0.44
2:L:234:ALA:HB2	3:M:44:GLY:HA2	1.99	0.44
3:M:74:ASN:ND2	25:M:510:HOH:O	2.50	0.44
5:I:22:PHE:HE1	22:J:103:CRT:H182	1.82	0.44
1:C:163:LYS:HE3	1:C:163:LYS:HB2	1.73	0.44
2:L:127:PHE:CE2	2:L:131:ILE:HD11	2.51	0.44
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.99	0.44
19:M:409:CDL:H202	19:M:409:CDL:H171	1.89	0.44
7:F:6:TRP:CD2	8:G:16:LYS:HD2	2.53	0.44
7:F:37:LEU:O	7:F:43:ASN:ND2	2.43	0.44
8:G:41:TRP:CE2	15:G:102:BCL:H192	2.52	0.44
6:2:46:TRP:CD1	6:2:47:LEU:HG	2.53	0.44
15:2:102:BCL:H91	15:2:102:BCL:H111	1.78	0.44
15:3:101:BCL:HHD	15:3:101:BCL:HAC2	1.75	0.44
2:L:40:PHE:HD1	21:M:405:MQ8:H362	1.82	0.44
2:L:110:GLU:HB3	2:L:124:PRO:HG3	1.99	0.44
2:L:241:PHE:HB2	19:L:311:CDL:H382	1.99	0.44
19:H:302:CDL:H821	19:H:302:CDL:H852	1.73	0.44
15:1:402:BCL:H62	15:1:402:BCL:H41	1.79	0.44
15:5:102:BCL:H192	15:5:102:BCL:H161	1.79	0.44
2:L:183:ILE:HD13	15:L:308:BCL:HMD1	1.99	0.44
3:M:38:TYR:OH	4:H:148:ASP:OD1	2.25	0.44
5:A:12:PHE:HZ	7:D:18:LEU:HB2	1.82	0.44
7:F:7:LYS:HB3	22:J:103:CRT:H41	1.99	0.44
6:N:19:HIS:HD2	6:N:23:VAL:HG23	1.82	0.44
6:R:47:LEU:HD13	18:R:103:LMT:H41	2.00	0.44
7:Y:32:ILE:HD12	15:Z:102:BCL:O1D	2.17	0.44
22:6:102:CRT:H35	15:7:101:BCL:HMB2	2.00	0.44
14:C:408:PGV:H52	22:2:103:CRT:H401	1.99	0.44
15:D:102:BCL:H192	15:D:102:BCL:H162	1.83	0.44
15:Q:102:BCL:HMD1	6:R:37:HIS:CE1	2.52	0.44
7:S:43:ASN:CG	7:S:46:GLU:HG2	2.38	0.44
5:K:6:HIS:HB3	6:N:16:GLN:NE2	2.32	0.44
6:N:19:HIS:CD2	6:N:23:VAL:HG23	2.53	0.44
22:T:102:CRT:H15	22:T:102:CRT:H131	1.87	0.44
15:V:101:BCL:H93	15:V:101:BCL:H62	1.75	0.44
1:C:102:ALA:HB1	1:C:105:GLU:HB2	1.99	0.43
2:L:42:PHE:CE1	17:L:304:UQ8:H18	2.53	0.43
14:L:306:PGV:H22	7:D:34:MET:HB3	1.99	0.43
22:Y:101:CRT:H291	15:Y:102:BCL:H11	2.00	0.43
5:1:9:TRP:HZ3	5:1:17:THR:HG21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:22:PHE:CD2	22:2:103:CRT:H11	2.52	0.43
15:6:101:BCL:H61	15:6:101:BCL:H93	1.65	0.43
5:7:32:ILE:HG12	22:9:101:CRT:H403	2.00	0.43
15:0:101:BCL:H61	15:0:101:BCL:H101	1.89	0.43
2:L:203:VAL:HG13	2:L:213:LYS:HB2	1.99	0.43
5:K:32:ILE:HD12	15:N:101:BCL:O1D	2.18	0.43
8:V:31:GLY:O	8:V:35:ILE:HD12	2.19	0.43
6:2:18:PHE:O	6:2:22:PHE:HB2	2.17	0.43
15:5:102:BCL:HAC2	15:5:102:BCL:HHD	1.80	0.43
1:C:162:PRO:HD2	10:C:402:HEM:HBD2	2.00	0.43
19:L:311:CDL:H611	19:L:311:CDL:H582	1.79	0.43
15:A:502:BCL:HMD1	6:B:37:HIS:CE1	2.54	0.43
22:B:103:CRT:H20	22:B:103:CRT:H181	1.90	0.43
15:1:402:BCL:HMD1	6:2:37:HIS:CE1	2.54	0.43
22:4:103:CRT:H343	5:5:26:PHE:CD1	2.54	0.43
1:C:50:GLU:OE1	9:3:53:VAL:HG12	2.18	0.43
17:L:304:UQ8:H7	17:L:304:UQ8:H10	1.68	0.43
19:M:409:CDL:H522	19:M:409:CDL:H552	1.63	0.43
15:2:102:BCL:H93	15:2:102:BCL:H61	1.70	0.43
5:9:5:FME:O	6:0:19:HIS:NE2	2.52	0.43
1:C:144:HIS:HE1	10:C:404:HEM:C1C	2.37	0.43
14:L:305:PGV:H41	14:1:401:PGV:H72	2.00	0.43
14:L:310:PGV:H272	14:L:310:PGV:H242	1.68	0.43
15:A:502:BCL:HBC3	15:A:502:BCL:H2C	1.86	0.43
15:P:102:BCL:H93	15:P:102:BCL:H111	1.72	0.43
15:Q:102:BCL:HBC2	6:R:43:TRP:CZ3	2.53	0.43
5:7:37:LEU:O	5:7:43:ASN:ND2	2.47	0.43
1:C:25:ARG:NH2	9:3:43:ASP:OD2	2.52	0.43
1:C:145:VAL:O	10:C:404:HEM:HBD2	2.19	0.43
1:C:126:VAL:HG13	1:C:287:LEU:HD13	2.00	0.43
2:L:186:PHE:CD2	2:L:246:ALA:HB1	2.54	0.43
18:M:411:LMT:O3'	18:M:411:LMT:O2B	2.28	0.43
22:E:103:CRT:H26	22:E:103:CRT:H241	1.89	0.43
15:G:102:BCL:H93	15:G:102:BCL:H62	1.71	0.43
6:J:31:GLY:O	6:J:35:ILE:HG13	2.18	0.43
6:N:21:ILE:HA	6:N:24:GLN:OE1	2.19	0.43
8:Z:12:GLU:O	8:Z:16:LYS:HG2	2.19	0.43
6:4:33:VAL:HG11	15:4:102:BCL:HAA1	2.01	0.43
1:C:151:THR:HG22	1:C:153:TYR:N	2.26	0.43
3:M:134:TYR:CZ	14:M:408:PGV:H21	2.53	0.43
3:M:232:ASP:N	3:M:232:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:28:MET:O	8:E:32:ILE:HG13	2.18	0.43
22:R:102:CRT:H20	22:R:102:CRT:H181	1.88	0.43
18:R:103:LMT:H6E	8:T:42:LEU:O	2.19	0.43
22:T:102:CRT:H20	22:T:102:CRT:H181	1.85	0.43
15:X:102:BCL:H61	15:X:102:BCL:H2	1.63	0.43
7:Y:30:LEU:HD23	22:Y:101:CRT:H36	2.01	0.43
15:1:402:BCL:H122	15:1:402:BCL:H161	1.82	0.43
6:4:23:VAL:HA	6:4:26:MET:HB2	1.99	0.43
5:9:33:HIS:CD2	22:9:101:CRT:H372	2.53	0.43
17:L:304:UQ8:H40	17:L:304:UQ8:H37	1.57	0.43
14:A:501:PGV:H031	7:D:37:LEU:HB3	2.00	0.43
15:S:102:BCL:H193	15:S:102:BCL:H161	1.88	0.43
7:Y:35:ILE:HG12	14:1:401:PGV:H22	2.01	0.43
6:2:26:MET:HG3	22:2:103:CRT:C19	2.48	0.43
7:D:32:ILE:HD12	15:E:102:BCL:O1D	2.19	0.43
5:Q:6:HIS:HA	6:R:19:HIS:HD2	1.83	0.43
6:6:22:PHE:CD1	22:6:102:CRT:H14	2.54	0.43
6:8:41:TRP:CZ2	15:8:102:BCL:H202	2.54	0.43
1:C:170:PRO:HB3	1:C:299:TYR:HE1	1.83	0.42
6:B:46:TRP:CE2	15:B:102:BCL:H2C	2.54	0.42
5:Q:18:LEU:HD23	5:Q:18:LEU:HA	1.85	0.42
14:L:310:PGV:H291	14:L:310:PGV:H322	1.83	0.42
7:F:13:ASP:O	7:F:17:ILE:HG12	2.18	0.42
22:G:103:CRT:H372	5:I:33:HIS:CD2	2.54	0.42
5:I:11:ILE:HG12	22:N:102:CRT:H1M1	2.00	0.42
15:J:102:BCL:H91	15:J:102:BCL:H111	1.73	0.42
22:Y:101:CRT:H10	22:Y:101:CRT:H81	1.78	0.42
1:C:263:THR:HA	3:M:311:VAL:HG22	2.01	0.42
19:L:311:CDL:H362	3:M:7:ILE:HD12	2.00	0.42
3:M:238:ILE:HG12	3:M:263:GLU:HB2	2.00	0.42
4:H:150:ASP:OD2	4:H:152:ARG:NH2	2.49	0.42
6:B:46:TRP:CD2	15:B:102:BCL:H2C	2.53	0.42
5:5:19:VAL:HA	15:5:102:BCL:H151	2.01	0.42
15:8:102:BCL:HBB2	18:8:103:LMT:H81	2.00	0.42
13:C:407:PLM:H21	14:L:305:PGV:H031	2.01	0.42
17:L:304:UQ8:H7A	15:9:102:BCL:H72	2.02	0.42
22:G:103:CRT:H20	22:G:103:CRT:H181	1.91	0.42
5:Q:7:LYS:HB3	22:T:102:CRT:H41	2.02	0.42
15:S:102:BCL:H143	15:S:102:BCL:H111	1.91	0.42
22:T:102:CRT:H393	7:U:30:LEU:HD23	2.02	0.42
15:V:101:BCL:O1A	22:V:102:CRT:H25	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:24:PHE:O	5:7:27:VAL:HG12	2.19	0.42
6:0:22:PHE:HA	22:0:102:CRT:H11	2.01	0.42
1:C:250:CYS:SG	10:C:403:HEM:CBC	2.98	0.42
2:L:183:ILE:HG12	15:L:301:BCL:HMB3	2.01	0.42
2:L:278:TRP:CG	3:M:88:LYS:HB2	2.54	0.42
15:L:301:BCL:H2	16:L:302:BPH:HBB3	2.02	0.42
17:L:304:UQ8:H3MB	15:9:102:BCL:H142	2.00	0.42
3:M:131:VAL:HG12	3:M:135:LYS:HD2	2.02	0.42
22:M:406:CRT:H2M3	5:Q:34:PHE:CE1	2.54	0.42
6:B:22:PHE:CD2	22:B:103:CRT:H14	2.55	0.42
5:Q:44:TRP:CD2	15:Q:102:BCL:H2C	2.54	0.42
6:4:18:PHE:HB2	22:4:103:CRT:H21A	2.02	0.42
17:L:309:UQ8:H22	17:L:309:UQ8:H25	1.79	0.42
15:B:102:BCL:H93	15:B:102:BCL:H61	1.81	0.42
15:K:102:BCL:H143	15:K:102:BCL:H111	1.80	0.42
15:N:101:BCL:H91	15:N:101:BCL:H111	1.65	0.42
7:S:15:ARG:HE	7:S:15:ARG:HB2	1.75	0.42
8:X:47:LEU:HD13	18:Z:101:LMT:H32	2.00	0.42
9:3:8:ILE:H	9:3:8:ILE:CD1	2.31	0.42
5:5:11:ILE:O	5:7:15:ARG:NH2	2.53	0.42
2:L:20:GLY:O	2:L:24:ASP:HB2	2.20	0.42
4:H:135:PRO:HG3	4:H:171:TRP:CZ2	2.54	0.42
15:J:102:BCL:H93	15:J:102:BCL:H61	1.67	0.42
22:N:102:CRT:H20	22:N:102:CRT:H181	1.79	0.42
5:O:14:PRO:O	5:O:18:LEU:HB2	2.20	0.42
15:R:101:BCL:H141	15:R:101:BCL:H161	1.80	0.42
7:W:41:GLU:OE2	7:Y:52:ALA:HA	2.19	0.42
22:4:103:CRT:H36	22:4:103:CRT:H341	1.82	0.42
5:9:14:PRO:HB3	6:0:18:PHE:CZ	2.55	0.42
2:L:125:PHE:HA	19:L:311:CDL:H752	2.02	0.42
4:H:212:ALA:O	4:H:254:ARG:NH2	2.47	0.42
22:J:103:CRT:H10	22:J:103:CRT:H81	1.86	0.42
15:T:101:BCL:H102	15:T:101:BCL:C1B	2.49	0.42
15:W:101:BCL:H143	15:W:101:BCL:H111	1.88	0.42
8:Z:47:LEU:HD23	8:Z:47:LEU:HA	1.90	0.42
22:4:103:CRT:H10	22:4:103:CRT:H81	1.87	0.42
15:8:102:BCL:H111	15:8:102:BCL:H142	1.83	0.42
22:P:103:CRT:H35	15:Q:102:BCL:HMB2	2.02	0.42
15:T:101:BCL:H192	15:T:101:BCL:H162	1.79	0.42
8:V:11:THR:OG1	8:V:13:GLU:HG3	2.20	0.42
5:1:24:PHE:CD2	5:1:25:LEU:HD23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:101:BCL:HBB2	15:3:101:BCL:HMB1	2.02	0.42
6:4:46:TRP:CD2	15:4:102:BCL:H2C	2.55	0.42
1:C:166:TRP:CZ2	1:C:304:LYS:HD2	2.55	0.42
1:C:307:CYS:O	1:C:308:MET:HB3	2.20	0.42
2:L:254:ILE:HD12	2:L:254:ILE:HA	1.90	0.42
3:M:152:ALA:HA	19:M:409:CDL:H191	2.02	0.42
6:B:30:PHE:CE1	15:B:102:BCL:H11	2.55	0.42
6:B:43:TRP:HB2	18:B:101:LMT:H31	2.02	0.42
22:Z:103:CRT:H35	15:1:402:BCL:CHB	2.49	0.42
15:3:101:BCL:C1D	15:4:102:BCL:HMD2	2.50	0.42
15:4:102:BCL:H92	15:4:102:BCL:H61	1.81	0.42
5:7:25:LEU:HB2	15:7:101:BCL:H43	2.00	0.42
1:C:227:LYS:HG3	3:M:172:ALA:HB1	2.01	0.41
17:L:309:UQ8:H42	17:L:309:UQ8:H46	1.75	0.41
6:N:46:TRP:CD1	6:N:47:LEU:HG	2.55	0.41
8:X:12:GLU:H	8:X:12:GLU:HG2	1.66	0.41
15:3:101:BCL:HBC3	15:3:101:BCL:H2C	1.89	0.41
2:L:3:MET:HB3	2:L:7:GLU:HB3	2.02	0.41
3:M:81:TRP:O	7:U:34[A]:MET:HB3	2.21	0.41
5:A:8:ILE:HD13	22:E:103:CRT:H10	2.02	0.41
6:B:47:LEU:O	7:D:50:PRO:HD3	2.20	0.41
7:S:18:LEU:HD23	7:S:18:LEU:HA	1.91	0.41
18:4:104:LMT:H1B	18:4:104:LMT:H3'	1.71	0.41
6:6:46:TRP:CE2	15:6:101:BCL:H2C	2.55	0.41
15:9:102:BCL:HAC2	15:9:102:BCL:HHD	1.81	0.41
22:0:102:CRT:H20	22:0:102:CRT:H181	1.92	0.41
14:M:408:PGV:H241	5:O:27:VAL:HG21	2.02	0.41
8:E:41:TRP:CZ2	15:E:102:BCL:H18	2.54	0.41
7:W:32:ILE:HD12	15:X:102:BCL:O1D	2.19	0.41
5:1:9:TRP:CD1	6:2:18:PHE:HD1	2.38	0.41
5:1:30:LEU:HD12	5:1:34:PHE:CE2	2.55	0.41
15:7:101:BCL:C1D	15:8:102:BCL:HMD2	2.50	0.41
6:8:37:HIS:CD2	15:8:102:BCL:H91	2.54	0.41
15:0:101:BCL:H192	15:0:101:BCL:H161	1.69	0.41
1:C:163:LYS:HG2	1:C:164:TYR:CE2	2.55	0.41
18:J:104:LMT:H62	15:K:102:BCL:H3C	2.03	0.41
15:K:102:BCL:H61	15:K:102:BCL:H102	1.49	0.41
22:N:102:CRT:H10	22:N:102:CRT:H81	1.82	0.41
22:P:103:CRT:H20	22:P:103:CRT:H181	1.82	0.41
15:U:101:BCL:HBC3	15:U:101:BCL:HHD	2.01	0.41
22:V:102:CRT:H26	22:V:102:CRT:H241	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:22:PHE:HA	22:Y:101:CRT:H14	2.02	0.41
6:4:41:TRP:CH2	6:4:47:LEU:HB2	2.54	0.41
3:M:89:HIS:O	3:M:93:LEU:HG	2.20	0.41
19:M:409:CDL:H822	4:H:22:PHE:HB2	2.01	0.41
22:B:103:CRT:H10	22:B:103:CRT:H81	1.92	0.41
8:X:30:PHE:O	8:X:34:ILE:HD12	2.21	0.41
8:X:46:TRP:CE2	15:X:102:BCL:H2C	2.56	0.41
22:6:102:CRT:H20	22:6:102:CRT:H181	1.84	0.41
6:8:41:TRP:CZ3	15:8:102:BCL:H172	2.56	0.41
22:0:102:CRT:H15	22:0:102:CRT:H131	1.95	0.41
17:L:304:UQ8:H46	17:L:304:UQ8:H42	1.78	0.41
15:L:308:BCL:HED1	3:M:179:ILE:HG23	2.03	0.41
22:M:406:CRT:H393	5:O:34:PHE:CD2	2.53	0.41
7:F:5:LEU:HD13	15:I:101:BCL:H193	2.03	0.41
7:W:18:LEU:HD23	7:W:18:LEU:HA	1.84	0.41
22:2:103:CRT:H181	22:2:103:CRT:H20	1.80	0.41
9:3:5:LEU:HB3	6:4:19:HIS:CE1	2.56	0.41
6:4:43:TRP:HB2	18:4:101:LMT:H12	2.02	0.41
1:C:257:TYR:OH	3:M:296:LEU:HD21	2.20	0.41
18:M:410:LMT:H71	18:M:410:LMT:H101	1.84	0.41
4:H:3:ALA:HB2	18:H:303:LMT:H6E	2.02	0.41
4:H:64:PRO:HA	4:H:79:PRO:CD	2.50	0.41
8:V:46:TRP:CE2	15:V:101:BCL:H2C	2.55	0.41
9:3:5:LEU:HD13	9:3:8:ILE:HD13	2.03	0.41
15:5:102:BCL:C1D	15:6:101:BCL:HMD2	2.51	0.41
2:L:272:TRP:CD1	17:L:309:UQ8:H4MA	2.56	0.41
17:L:303:UQ8:H21A	17:L:303:UQ8:H17	1.71	0.41
15:E:102:BCL:HBB2	18:G:101:LMT:H111	2.02	0.41
22:V:102:CRT:H20	22:V:102:CRT:H181	1.85	0.41
8:Z:47:LEU:HD13	18:2:101:LMT:H41	2.03	0.41
5:7:32:ILE:HD12	15:8:102:BCL:O1D	2.21	0.41
6:8:11:THR:O	6:8:13:GLN:N	2.52	0.41
1:C:219:PRO:HG2	18:H:303:LMT:H6D	2.02	0.41
15:A:502:BCL:H151	15:A:502:BCL:H18	1.89	0.41
18:E:101:LMT:H1B	18:E:101:LMT:H3'	1.84	0.41
15:E:102:BCL:H92	15:E:102:BCL:H62	1.87	0.41
7:F:37:LEU:HG	7:F:44:TRP:CH2	2.56	0.41
22:J:103:CRT:H20	22:J:103:CRT:H181	1.86	0.41
15:K:102:BCL:HMD1	6:N:37:HIS:CE1	2.55	0.41
6:N:26:MET:HG3	22:N:102:CRT:C19	2.51	0.41
7:Y:9:TRP:HD1	7:Y:14:PRO:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:35:ILE:O	7:Y:39:THR:HG23	2.20	0.41
15:Y:102:BCL:HMB1	15:Y:102:BCL:HBB3	2.01	0.41
15:1:402:BCL:HAC2	15:1:402:BCL:HHD	1.85	0.41
22:2:103:CRT:H10	22:2:103:CRT:H81	1.94	0.41
2:L:106:TRP:HH2	21:M:405:MQ8:H301	1.85	0.41
17:L:309:UQ8:H35A	17:L:309:UQ8:H37	1.71	0.41
7:D:6:TRP:CZ2	7:D:7:LYS:HD3	2.56	0.41
7:D:14:PRO:HB3	8:E:18:PHE:CZ	2.56	0.41
7:F:14:PRO:HG2	8:G:10:LEU:HD22	2.03	0.41
8:T:26:MET:HE3	8:T:26:MET:HB3	1.95	0.41
7:Y:35:ILE:HG13	14:1:401:PGV:H52	2.03	0.41
15:Z:102:BCL:H162	15:Z:102:BCL:H192	1.81	0.41
1:C:183:GLN:HB3	1:C:196:PRO:HA	2.03	0.40
14:L:306:PGV:H042	7:D:38:SER:HB3	2.03	0.40
14:L:306:PGV:H202	14:H:301:PGV:H062	2.02	0.40
8:G:8:THR:O	8:G:8:THR:OG1	2.32	0.40
6:N:39:LEU:HD23	6:N:42:LEU:HD12	2.03	0.40
15:S:102:BCL:HAC2	15:S:102:BCL:HHD	1.85	0.40
2:L:67:ILE:HG12	14:L:306:PGV:H201	2.03	0.40
5:A:33:HIS:CG	22:0:102:CRT:H372	2.56	0.40
8:E:46:TRP:CE2	15:E:102:BCL:H2C	2.56	0.40
5:I:7:LYS:CG	22:N:102:CRT:H41	2.49	0.40
3:M:296:LEU:HD23	3:M:296:LEU:HA	1.92	0.40
7:F:17:ILE:HG12	7:F:17:ILE:H	1.62	0.40
15:K:102:BCL:HBA1	15:K:102:BCL:H3A	1.81	0.40
6:R:26:MET:HG3	22:R:102:CRT:C19	2.51	0.40
22:4:103:CRT:H31	22:4:103:CRT:H35	1.66	0.40
15:L:301:BCL:H162	15:L:301:BCL:H141	1.85	0.40
17:L:304:UQ8:H27A	17:L:304:UQ8:H30	1.58	0.40
3:M:181:PRO:HB3	25:M:502:HOH:O	2.22	0.40
15:M:402:BCL:H162	15:M:402:BCL:H192	1.86	0.40
22:E:103:CRT:H36	7:F:30:LEU:HD23	2.03	0.40
5:O:34:PHE:HD1	24:O:501:LDA:H111	1.87	0.40
8:X:12:GLU:O	8:X:16:LYS:HG3	2.22	0.40
15:1:402:BCL:H93	15:1:402:BCL:H111	1.81	0.40
6:2:22:PHE:CD2	22:2:103:CRT:H14	2.57	0.40
5:5:6:HIS:CE1	6:6:16:GLN:HA	2.56	0.40
15:7:101:BCL:H93	6:8:29:PHE:HB2	2.03	0.40
1:C:72:VAL:HG11	1:C:79:VAL:HG11	2.03	0.40
1:C:191:ALA:O	2:L:266:PRO:HB2	2.21	0.40
2:L:42:PHE:HE2	17:L:304:UQ8:H37	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:123:ILE:HB	2:L:124:PRO:HD3	2.03	0.40
3:M:81:TRP:O	7:U:34[B]:MET:HB3	2.21	0.40
3:M:120:PHE:HE2	5:Q:30:LEU:HD13	1.86	0.40
3:M:167:MET:O	18:M:410:LMT:H3'	2.22	0.40
4:H:119:ARG:O	4:H:234:TYR:HB2	2.22	0.40
7:U:7:LYS:HE2	7:U:7:LYS:HB3	1.87	0.40
7:W:5:LEU:HD12	7:W:5:LEU:HA	1.92	0.40
22:Y:101:CRT:H181	22:Y:101:CRT:H20	1.84	0.40
15:3:101:BCL:H62	15:3:101:BCL:H41	1.54	0.40
22:6:102:CRT:H5	22:6:102:CRT:H23	1.82	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	C	309/383 (81%)	297 (96%)	12 (4%)	0	100	100
2	L	275/278 (99%)	268 (98%)	7 (2%)	0	100	100
3	M	316/325 (97%)	311 (98%)	5 (2%)	0	100	100
4	H	258/259 (100%)	254 (98%)	4 (2%)	0	100	100
5	1	41/44 (93%)	41 (100%)	0	0	100	100
5	5	41/44 (93%)	40 (98%)	0	1 (2%)	6	2
5	7	41/44 (93%)	41 (100%)	0	0	100	100
5	9	41/44 (93%)	40 (98%)	0	1 (2%)	6	2
5	A	41/44 (93%)	41 (100%)	0	0	100	100
5	I	41/44 (93%)	39 (95%)	2 (5%)	0	100	100
5	K	42/44 (96%)	42 (100%)	0	0	100	100
5	O	42/44 (96%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Q	41/44 (93%)	39 (95%)	1 (2%)	1 (2%)	6	2
6	0	41/46 (89%)	41 (100%)	0	0	100	100
6	2	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
6	4	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
6	6	36/46 (78%)	36 (100%)	0	0	100	100
6	8	39/46 (85%)	37 (95%)	2 (5%)	0	100	100
6	B	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
6	J	37/46 (80%)	37 (100%)	0	0	100	100
6	N	36/46 (78%)	36 (100%)	0	0	100	100
6	P	40/46 (87%)	40 (100%)	0	0	100	100
6	R	38/46 (83%)	37 (97%)	1 (3%)	0	100	100
7	D	47/64 (73%)	47 (100%)	0	0	100	100
7	F	47/64 (73%)	47 (100%)	0	0	100	100
7	S	48/64 (75%)	47 (98%)	1 (2%)	0	100	100
7	U	49/64 (77%)	49 (100%)	0	0	100	100
7	W	48/64 (75%)	48 (100%)	0	0	100	100
7	Y	55/64 (86%)	52 (94%)	3 (6%)	0	100	100
8	E	39/47 (83%)	39 (100%)	0	0	100	100
8	G	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
8	T	39/47 (83%)	39 (100%)	0	0	100	100
8	V	38/47 (81%)	38 (100%)	0	0	100	100
8	X	39/47 (83%)	39 (100%)	0	0	100	100
8	Z	39/47 (83%)	39 (100%)	0	0	100	100
9	3	61/66 (92%)	60 (98%)	1 (2%)	0	100	100
All	All	2504/2833 (88%)	2458 (98%)	43 (2%)	3 (0%)	54	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Q	6	HIS
5	9	6	HIS
5	5	6	HIS

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	C	265/311 (85%)	262 (99%)	3 (1%)	73 80
2	L	223/224 (100%)	220 (99%)	3 (1%)	69 76
3	M	252/257 (98%)	249 (99%)	3 (1%)	71 78
4	H	206/206 (100%)	203 (98%)	3 (2%)	65 72
5	1	37/38 (97%)	35 (95%)	2 (5%)	22 20
5	5	36/38 (95%)	35 (97%)	1 (3%)	43 49
5	7	37/38 (97%)	37 (100%)	0	100 100
5	9	37/38 (97%)	35 (95%)	2 (5%)	22 20
5	A	37/38 (97%)	37 (100%)	0	100 100
5	I	37/38 (97%)	36 (97%)	1 (3%)	44 51
5	K	38/38 (100%)	37 (97%)	1 (3%)	46 52
5	O	38/38 (100%)	37 (97%)	1 (3%)	46 52
5	Q	37/38 (97%)	37 (100%)	0	100 100
6	0	36/38 (95%)	36 (100%)	0	100 100
6	2	34/38 (90%)	31 (91%)	3 (9%)	10 6
6	4	35/38 (92%)	34 (97%)	1 (3%)	42 48
6	6	32/38 (84%)	31 (97%)	1 (3%)	40 46
6	8	34/38 (90%)	32 (94%)	2 (6%)	19 17
6	B	37/38 (97%)	37 (100%)	0	100 100
6	J	32/38 (84%)	32 (100%)	0	100 100
6	N	32/38 (84%)	30 (94%)	2 (6%)	18 15
6	P	35/38 (92%)	35 (100%)	0	100 100
6	R	33/38 (87%)	32 (97%)	1 (3%)	41 47
7	D	43/55 (78%)	42 (98%)	1 (2%)	50 57
7	F	43/55 (78%)	40 (93%)	3 (7%)	15 12
7	S	43/55 (78%)	42 (98%)	1 (2%)	50 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	U	44/55 (80%)	42 (96%)	2 (4%)	27 29
7	W	43/55 (78%)	42 (98%)	1 (2%)	50 57
7	Y	51/55 (93%)	47 (92%)	4 (8%)	12 9
8	E	35/40 (88%)	32 (91%)	3 (9%)	10 7
8	G	34/40 (85%)	33 (97%)	1 (3%)	42 48
8	T	35/40 (88%)	33 (94%)	2 (6%)	20 19
8	V	34/40 (85%)	32 (94%)	2 (6%)	19 17
8	X	35/40 (88%)	35 (100%)	0	100 100
8	Z	35/40 (88%)	31 (89%)	4 (11%)	5 3
9	3	49/52 (94%)	47 (96%)	2 (4%)	30 33
All	All	2144/2342 (92%)	2088 (97%)	56 (3%)	49 52

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	151	THR
1	C	233	TYR
1	C	274	ARG
2	L	253	CYS
2	L	263	ARG
2	L	278	TRP
3	M	45	ASP
3	M	216	PHE
3	M	312	THR
4	H	132	LYS
4	H	229	ASP
4	H	237	ASP
7	D	41	GLU
8	E	11	THR
8	E	16	LYS
8	E	28	MET
7	F	11	LEU
7	F	15	ARG
7	F	16	ARG
8	G	16	LYS
5	I	7	LYS
5	K	48	SER
6	N	12	GLU

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Mol	Chain	Res	Type
6	N	26	MET
5	O	10	GLN
6	R	27	THR
7	S	15	ARG
8	T	7	MET
8	T	26	MET
7	U	34[A]	MET
7	U	34[B]	MET
8	V	16	LYS
8	V	17	GLU
7	W	4	ASP
7	Y	6	TRP
7	Y	16	ARG
7	Y	24	PHE
7	Y	41	GLU
8	Z	7	MET
8	Z	11	THR
8	Z	17	GLU
8	Z	26	MET
5	1	10	GLN
5	1	16	ARG
6	2	7	MET
6	2	16	GLN
6	2	44	ARG
9	3	5	LEU
9	3	66	ARG
6	4	12	GLU
5	5	6	HIS
6	6	10	LEU
6	8	10	LEU
6	8	44	ARG
5	9	15	ARG
5	9	46	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	78	ASN
1	C	206	GLN
2	L	207	GLN
2	L	219	ASN
4	H	71	HIS

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Mol	Chain	Res	Type
4	H	103	ASN
4	H	192	ASN
5	A	6	HIS
6	B	4	ASN
5	I	10	GLN
6	J	24	GLN
5	K	6	HIS
6	N	16	GLN
6	N	19	HIS
5	O	10	GLN
6	P	13	GLN
6	R	13	GLN
6	R	19	HIS
5	1	6	HIS
6	2	16	GLN
5	5	6	HIS
5	7	10	GLN
6	0	24	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
5	FME	A	5	5	8,9,10	0.50	0	7,9,11	1.12	1 (14%)
4	FME	H	1	4	8,9,10	0.49	0	7,9,11	1.04	1 (14%)
5	FME	Q	5	5	8,9,10	0.53	0	7,9,11	1.00	1 (14%)
5	FME	5	5	5	8,9,10	0.52	0	7,9,11	0.95	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FME	1	5	5	8,9,10	0.52	0	7,9,11	0.83	1 (14%)
5	FME	7	5	5	8,9,10	0.48	0	7,9,11	1.18	1 (14%)
5	FME	9	5	5	8,9,10	0.49	0	7,9,11	0.99	1 (14%)
5	FME	K	5	5	8,9,10	0.50	0	7,9,11	0.92	1 (14%)
5	FME	I	5	5	8,9,10	0.50	0	7,9,11	1.10	1 (14%)
5	FME	O	5	5	8,9,10	0.52	0	7,9,11	1.02	1 (14%)

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
5	FME	A	5	5	-	0/7/9/11	-
4	FME	H	1	4	-	0/7/9/11	-
5	FME	Q	5	5	-	2/7/9/11	-
5	FME	5	5	5	-	3/7/9/11	-
5	FME	1	5	5	-	2/7/9/11	-
5	FME	7	5	5	-	1/7/9/11	-
5	FME	9	5	5	-	0/7/9/11	-
5	FME	K	5	5	-	3/7/9/11	-
5	FME	I	5	5	-	3/7/9/11	-
5	FME	O	5	5	-	0/7/9/11	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	7	5	FME	O-C-CA	-2.74	117.59	124.78
5	I	5	FME	O-C-CA	-2.68	117.74	124.78
5	A	5	FME	O-C-CA	-2.68	117.76	124.78
5	9	5	FME	O-C-CA	-2.50	118.22	124.78
5	O	5	FME	O-C-CA	-2.48	118.27	124.78
5	Q	5	FME	O-C-CA	-2.45	118.36	124.78
4	H	1	FME	O-C-CA	-2.42	118.45	124.78
5	K	5	FME	O-C-CA	-2.39	118.52	124.78
5	5	5	FME	O-C-CA	-2.34	118.65	124.78
5	1	5	FME	O-C-CA	-2.16	119.11	124.78

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	5	FME	O-C-CA-CB
5	I	5	FME	CA-CB-CG-SD
5	K	5	FME	O1-CN-N-CA
5	K	5	FME	CB-CA-N-CN
5	Q	5	FME	O1-CN-N-CA
5	Q	5	FME	CB-CA-N-CN
5	1	5	FME	O1-CN-N-CA
5	5	5	FME	O1-CN-N-CA
5	5	5	FME	N-CA-CB-CG
5	5	5	FME	C-CA-CB-CG
5	K	5	FME	N-CA-CB-CG
5	7	5	FME	C-CA-CB-CG
5	1	5	FME	N-CA-CB-CG
5	I	5	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	5	FME	1	0
5	9	5	FME	1	0
5	K	5	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 113 ligands modelled in this entry, 8 are monoatomic - leaving 105 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CRT	E	103	-	41,43,43	0.73	0	50,54,54	1.82	14 (28%)
15	BCL	Q	102	-	64,74,74	1.68	12 (18%)	78,115,115	2.33	18 (23%)
15	BCL	N	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.25	20 (25%)
17	UQ8	L	303	-	33,33,53	1.46	2 (6%)	40,43,67	1.67	9 (22%)
22	CRT	B	103	-	41,43,43	0.71	0	50,54,54	1.69	15 (30%)
15	BCL	O	502	-	64,74,74	1.68	12 (18%)	78,115,115	2.31	21 (26%)
15	BCL	U	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.33	18 (23%)
22	CRT	Y	101	-	41,43,43	0.70	0	50,54,54	1.61	9 (18%)
18	LMT	B	101	-	36,36,36	0.42	0	47,47,47	0.75	1 (2%)
24	LDA	O	501	-	12,15,15	2.12	1 (8%)	14,17,17	0.50	0
14	PGV	L	305	-	28,28,50	1.23	2 (7%)	31,34,56	1.31	4 (12%)
18	LMT	P	104	-	36,36,36	0.38	0	47,47,47	0.68	1 (2%)
18	LMT	2	101	-	36,36,36	0.40	0	47,47,47	0.89	2 (4%)
19	CDL	D	101	-	57,57,99	1.11	4 (7%)	63,69,111	1.14	3 (4%)
16	BPH	L	302	-	51,70,70	0.53	0	52,101,101	0.66	1 (1%)
22	CRT	4	103	-	41,43,43	0.70	0	50,54,54	1.89	13 (26%)
15	BCL	B	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.19	21 (26%)
18	LMT	8	101	-	36,36,36	0.39	0	47,47,47	0.76	1 (2%)
18	LMT	P	101	-	36,36,36	0.38	0	47,47,47	0.73	1 (2%)
14	PGV	C	408	-	30,30,50	1.17	2 (6%)	33,36,56	1.09	2 (6%)
15	BCL	3	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.29	22 (28%)
18	LMT	H	303	-	36,36,36	0.43	0	47,47,47	0.78	1 (2%)
13	PLM	C	407	1	11,11,17	0.39	0	10,10,17	0.45	0
18	LMT	T	103	-	36,36,36	0.42	0	47,47,47	0.83	1 (2%)
14	PGV	A	503	-	32,32,50	1.14	2 (6%)	35,38,56	1.17	4 (11%)
15	BCL	E	102	-	64,74,74	1.67	11 (17%)	78,115,115	2.19	20 (25%)
15	BCL	G	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.21	21 (26%)
15	BCL	4	102	-	64,74,74	1.68	12 (18%)	78,115,115	2.19	20 (25%)
18	LMT	J	104	-	36,36,36	0.38	0	47,47,47	0.69	1 (2%)
21	MQ8	M	405	-	54,54,54	1.34	2 (3%)	66,69,69	1.57	15 (22%)
14	PGV	Q	101	-	23,23,50	1.40	2 (8%)	27,28,56	1.27	3 (11%)
22	CRT	Z	103	-	41,43,43	0.71	0	50,54,54	1.75	9 (18%)
15	BCL	P	102	-	64,74,74	1.66	12 (18%)	78,115,115	2.21	22 (28%)
15	BCL	R	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.10	21 (26%)
15	BCL	L	301	-	64,74,74	1.65	12 (18%)	78,115,115	2.18	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CRT	V	102	-	41,43,43	0.70	0	50,54,54	2.20	19 (38%)
10	HEM	C	402	1	41,50,50	1.31	5 (12%)	45,82,82	1.83	11 (24%)
15	BCL	9	102	-	64,74,74	1.68	12 (18%)	78,115,115	2.29	20 (25%)
18	LMT	4	104	-	36,36,36	0.41	0	47,47,47	0.79	1 (2%)
22	CRT	0	102	-	41,43,43	0.73	0	50,54,54	1.74	16 (32%)
15	BCL	7	101	-	59,69,74	1.74	13 (22%)	72,109,115	2.31	20 (27%)
14	PGV	L	310	-	36,36,50	1.07	2 (5%)	39,42,56	1.13	3 (7%)
10	HEM	C	401	1	41,50,50	1.32	3 (7%)	45,82,82	1.91	10 (22%)
10	HEM	C	404	1	41,50,50	1.33	3 (7%)	45,82,82	1.77	8 (17%)
22	CRT	P	103	-	41,43,43	0.71	0	50,54,54	3.62	15 (30%)
15	BCL	M	402	-	64,74,74	1.69	13 (20%)	78,115,115	2.23	21 (26%)
18	LMT	Z	101	-	36,36,36	0.39	0	47,47,47	0.90	2 (4%)
24	LDA	K	101	-	12,15,15	2.10	1 (8%)	14,17,17	0.53	0
19	CDL	L	311	-	79,79,99	1.07	4 (5%)	85,91,111	1.11	5 (5%)
15	BCL	S	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.28	19 (24%)
19	CDL	M	407	-	38,38,99	1.30	3 (7%)	43,49,111	1.25	5 (11%)
15	BCL	0	101	-	64,74,74	1.66	11 (17%)	78,115,115	2.18	20 (25%)
19	CDL	M	409	-	94,94,99	0.94	4 (4%)	100,106,111	1.08	7 (7%)
14	PGV	F	501	-	30,30,50	1.22	2 (6%)	34,35,56	1.34	4 (11%)
22	CRT	M	406	-	41,43,43	0.68	0	50,54,54	2.28	12 (24%)
22	CRT	G	103	-	41,43,43	0.71	0	50,54,54	1.43	8 (16%)
15	BCL	Z	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.24	20 (25%)
18	LMT	G	101	-	36,36,36	0.44	0	47,47,47	0.82	1 (2%)
15	BCL	8	102	-	64,74,74	1.66	11 (17%)	78,115,115	2.18	21 (26%)
22	CRT	9	101	-	41,43,43	0.71	0	50,54,54	1.70	12 (24%)
22	CRT	J	103	-	41,43,43	0.73	0	50,54,54	3.80	14 (28%)
14	PGV	M	408	-	26,26,50	1.28	2 (7%)	30,31,56	1.35	5 (16%)
18	LMT	X	101	-	36,36,36	0.45	0	47,47,47	0.85	2 (4%)
12	Z41	C	406	-	34,34,39	0.28	0	36,36,41	0.30	0
14	PGV	L	306	-	34,34,50	1.09	2 (5%)	37,40,56	1.05	2 (5%)
15	BCL	F	502	-	64,74,74	1.70	14 (21%)	78,115,115	2.28	19 (24%)
15	BCL	W	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.27	20 (25%)
14	PGV	A	501	-	38,38,50	1.02	2 (5%)	41,44,56	1.19	3 (7%)
15	BCL	X	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.22	21 (26%)
15	BCL	V	101	-	64,74,74	1.67	13 (20%)	78,115,115	2.22	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	PGV	H	301	-	35,35,50	1.09	2 (5%)	38,41,56	1.39	4 (10%)
15	BCL	Y	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.31	21 (26%)
18	LMT	5	101	-	32,32,36	0.41	0	43,43,47	1.30	5 (11%)
18	LMT	M	411	-	25,25,36	0.48	0	36,36,47	0.84	1 (2%)
18	LMT	E	101	-	36,36,36	0.39	0	47,47,47	0.73	1 (2%)
22	CRT	2	103	-	41,43,43	0.74	0	50,54,54	2.07	10 (20%)
22	CRT	R	102	-	41,43,43	0.69	0	50,54,54	1.61	12 (24%)
15	BCL	1	402	-	64,74,74	1.70	14 (21%)	78,115,115	2.28	19 (24%)
17	UQ8	L	309	-	53,53,53	1.24	2 (3%)	64,67,67	1.55	14 (21%)
15	BCL	5	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.31	20 (25%)
18	LMT	M	410	-	36,36,36	0.41	0	47,47,47	0.78	1 (2%)
15	BCL	A	502	-	64,74,74	1.69	13 (20%)	78,115,115	2.25	19 (24%)
18	LMT	J	101	-	36,36,36	0.41	0	47,47,47	0.71	0
15	BCL	K	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.34	22 (28%)
15	BCL	6	101	-	64,74,74	1.68	13 (20%)	78,115,115	2.25	19 (24%)
18	LMT	S	101	-	27,27,36	0.59	0	37,38,47	1.33	4 (10%)
10	HEM	C	403	1	41,50,50	1.34	5 (12%)	45,82,82	1.81	10 (22%)
15	BCL	I	101	-	64,74,74	1.70	14 (21%)	78,115,115	2.29	19 (24%)
18	LMT	4	101	-	36,36,36	0.40	0	47,47,47	0.75	1 (2%)
16	BPH	M	404	-	51,70,70	0.50	0	52,101,101	0.69	1 (1%)
19	CDL	H	302	-	78,78,99	1.02	4 (5%)	84,90,111	1.06	5 (5%)
22	CRT	6	102	-	41,43,43	0.67	0	50,54,54	1.70	13 (26%)
14	PGV	1	401	-	26,26,50	1.24	2 (7%)	29,31,56	1.23	4 (13%)
15	BCL	T	101	-	64,74,74	1.67	11 (17%)	78,115,115	2.16	21 (26%)
17	UQ8	L	304	-	53,53,53	1.20	2 (3%)	64,67,67	1.83	19 (29%)
15	BCL	2	102	-	64,74,74	1.69	11 (17%)	78,115,115	2.17	22 (28%)
18	LMT	L	307	-	36,36,36	0.39	0	47,47,47	0.79	1 (2%)
15	BCL	J	102	-	64,74,74	1.69	14 (21%)	78,115,115	2.18	20 (25%)
22	CRT	N	102	-	41,43,43	0.73	0	50,54,54	1.82	14 (28%)
15	BCL	D	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.25	22 (28%)
15	BCL	L	308	-	64,74,74	1.70	12 (18%)	78,115,115	2.23	20 (25%)
18	LMT	R	103	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
18	LMT	8	103	-	36,36,36	0.43	0	47,47,47	0.87	1 (2%)
22	CRT	T	102	-	41,43,43	0.70	0	50,54,54	1.79	14 (28%)
15	BCL	M	403	-	64,74,74	1.69	14 (21%)	78,115,115	2.36	23 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CRT	E	103	-	-	6/51/51/51	-
15	BCL	Q	102	-	-	17/37/137/137	-
15	BCL	N	101	-	-	16/37/137/137	-
17	UQ8	L	303	-	-	2/27/51/75	0/1/1/1
22	CRT	B	103	-	-	4/51/51/51	-
15	BCL	O	502	-	-	16/37/137/137	-
15	BCL	U	101	-	-	21/37/137/137	-
22	CRT	Y	101	-	-	3/51/51/51	-
18	LMT	B	101	-	-	6/21/61/61	0/2/2/2
24	LDA	O	501	-	-	2/13/13/13	-
14	PGV	L	305	-	-	12/33/33/55	-
18	LMT	P	104	-	-	1/21/61/61	0/2/2/2
18	LMT	2	101	-	-	4/21/61/61	0/2/2/2
19	CDL	D	101	-	-	27/67/67/110	-
16	BPH	L	302	-	-	5/37/105/105	0/5/6/6
22	CRT	4	103	-	-	5/51/51/51	-
15	BCL	B	102	-	-	11/37/137/137	-
18	LMT	8	101	-	-	4/21/61/61	0/2/2/2
18	LMT	P	101	-	-	5/21/61/61	0/2/2/2
14	PGV	C	408	-	-	9/35/35/55	-
15	BCL	3	101	-	-	11/37/137/137	-
18	LMT	H	303	-	-	4/21/61/61	0/2/2/2
13	PLM	C	407	1	-	1/8/9/15	-
18	LMT	T	103	-	-	10/21/61/61	0/2/2/2
14	PGV	A	503	-	-	15/37/37/55	-
15	BCL	E	102	-	-	16/37/137/137	-
15	BCL	G	102	-	-	17/37/137/137	-
15	BCL	4	102	-	-	15/37/137/137	-
18	LMT	J	104	-	-	4/21/61/61	0/2/2/2
21	MQ8	M	405	-	-	4/47/67/67	0/2/2/2
14	PGV	Q	101	-	-	9/25/25/55	-
22	CRT	Z	103	-	-	13/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCL	P	102	-	-	15/37/137/137	-
15	BCL	R	101	-	-	14/37/137/137	-
15	BCL	L	301	-	-	9/37/137/137	-
22	CRT	V	102	-	-	5/51/51/51	-
10	HEM	C	402	1	-	5/12/54/54	-
15	BCL	9	102	-	-	12/37/137/137	-
18	LMT	4	104	-	-	3/21/61/61	0/2/2/2
22	CRT	0	102	-	-	2/51/51/51	-
15	BCL	7	101	-	-	13/31/131/137	-
14	PGV	L	310	-	-	19/41/41/55	-
10	HEM	C	401	1	-	4/12/54/54	-
10	HEM	C	404	1	-	4/12/54/54	-
22	CRT	P	103	-	-	7/51/51/51	-
15	BCL	M	402	-	-	6/37/137/137	-
18	LMT	Z	101	-	-	4/21/61/61	0/2/2/2
24	LDA	K	101	-	-	2/13/13/13	-
19	CDL	L	311	-	-	27/89/89/110	-
15	BCL	S	102	-	-	12/37/137/137	-
19	CDL	M	407	-	-	17/48/48/110	-
15	BCL	0	101	-	-	17/37/137/137	-
19	CDL	M	409	-	-	31/105/105/110	-
14	PGV	F	501	-	-	11/32/32/55	-
22	CRT	M	406	-	-	8/51/51/51	-
22	CRT	G	103	-	-	9/51/51/51	-
15	BCL	Z	102	-	-	15/37/137/137	-
18	LMT	G	101	-	-	4/21/61/61	0/2/2/2
15	BCL	8	102	-	-	16/37/137/137	-
22	CRT	9	101	-	-	3/51/51/51	-
22	CRT	J	103	-	-	10/51/51/51	-
14	PGV	M	408	-	-	9/28/28/55	-
18	LMT	X	101	-	-	5/21/61/61	0/2/2/2
12	Z41	C	406	-	-	6/35/35/41	-
14	PGV	L	306	-	-	8/39/39/55	-
15	BCL	F	502	-	-	19/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCL	W	101	-	-	16/37/137/137	-
14	PGV	A	501	-	-	12/43/43/55	-
15	BCL	X	102	-	-	15/37/137/137	-
15	BCL	V	101	-	-	19/37/137/137	-
14	PGV	H	301	-	-	12/40/40/55	-
15	BCL	Y	102	-	-	15/37/137/137	-
18	LMT	5	101	-	-	6/17/57/61	0/2/2/2
18	LMT	M	411	-	-	3/10/50/61	0/2/2/2
18	LMT	E	101	-	-	6/21/61/61	0/2/2/2
22	CRT	2	103	-	-	7/51/51/51	-
22	CRT	R	102	-	-	1/51/51/51	-
15	BCL	1	402	-	-	11/37/137/137	-
17	UQ8	L	309	-	-	15/51/75/75	0/1/1/1
15	BCL	5	102	-	-	17/37/137/137	-
18	LMT	M	410	-	-	4/21/61/61	0/2/2/2
15	BCL	A	502	-	-	13/37/137/137	-
18	LMT	J	101	-	-	2/21/61/61	0/2/2/2
15	BCL	K	102	-	-	11/37/137/137	-
15	BCL	6	101	-	-	20/37/137/137	-
18	LMT	S	101	-	-	3/12/52/61	0/2/2/2
10	HEM	C	403	1	-	2/12/54/54	-
15	BCL	I	101	-	-	15/37/137/137	-
18	LMT	4	101	-	-	5/21/61/61	0/2/2/2
16	BPH	M	404	-	-	9/37/105/105	0/5/6/6
19	CDL	H	302	-	-	26/89/89/110	-
22	CRT	6	102	-	-	8/51/51/51	-
14	PGV	1	401	-	-	10/30/30/55	-
15	BCL	T	101	-	-	16/37/137/137	-
17	UQ8	L	304	-	-	7/51/75/75	0/1/1/1
15	BCL	2	102	-	-	15/37/137/137	-
18	LMT	L	307	-	-	7/21/61/61	0/2/2/2
15	BCL	J	102	-	-	18/37/137/137	-
22	CRT	N	102	-	-	9/51/51/51	-
15	BCL	D	102	-	-	14/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCL	L	308	-	-	12/37/137/137	-
18	LMT	R	103	-	-	6/21/61/61	0/2/2/2
18	LMT	8	103	-	-	4/21/61/61	0/2/2/2
22	CRT	T	102	-	-	9/51/51/51	-
15	BCL	M	403	-	-	7/37/137/137	-

All (519) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	M	405	MQ8	C3-C2	8.05	1.49	1.35
17	L	309	UQ8	C6-C1	7.69	1.49	1.35
17	L	304	UQ8	C6-C1	7.49	1.48	1.35
17	L	303	UQ8	C6-C1	7.43	1.48	1.35
24	O	501	LDA	O1-N1	-7.31	1.25	1.42
24	K	101	LDA	O1-N1	-7.24	1.25	1.42
15	L	301	BCL	O2D-CGD	5.22	1.45	1.33
15	T	101	BCL	O2D-CGD	5.14	1.45	1.33
15	2	102	BCL	O2D-CGD	5.10	1.45	1.33
15	0	101	BCL	O2D-CGD	5.09	1.45	1.33
15	B	102	BCL	O2D-CGD	5.09	1.45	1.33
15	3	101	BCL	O2D-CGD	5.08	1.45	1.33
15	1	402	BCL	O2D-CGD	5.08	1.45	1.33
15	R	101	BCL	O2D-CGD	5.08	1.45	1.33
15	I	101	BCL	O2D-CGD	5.07	1.45	1.33
15	M	403	BCL	C3B-C2B	5.07	1.48	1.39
15	X	102	BCL	O2D-CGD	5.07	1.45	1.33
15	6	101	BCL	O2D-CGD	5.06	1.45	1.33
15	W	101	BCL	O2D-CGD	5.05	1.45	1.33
15	J	102	BCL	O2D-CGD	5.05	1.45	1.33
15	O	502	BCL	O2D-CGD	5.05	1.45	1.33
15	V	101	BCL	O2D-CGD	5.04	1.45	1.33
15	8	102	BCL	O2D-CGD	5.04	1.45	1.33
15	U	101	BCL	O2D-CGD	5.03	1.45	1.33
15	D	102	BCL	O2D-CGD	5.03	1.45	1.33
15	F	502	BCL	O2D-CGD	5.02	1.45	1.33
15	A	502	BCL	O2D-CGD	5.02	1.45	1.33
15	7	101	BCL	O2D-CGD	5.02	1.45	1.33
15	9	102	BCL	O2D-CGD	5.00	1.45	1.33
15	4	102	BCL	O2D-CGD	5.00	1.45	1.33
15	5	102	BCL	O2D-CGD	5.00	1.45	1.33
15	M	402	BCL	O2D-CGD	4.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	102	BCL	O2D-CGD	4.98	1.45	1.33
15	G	102	BCL	O2D-CGD	4.98	1.45	1.33
15	S	102	BCL	O2D-CGD	4.98	1.45	1.33
15	Z	102	BCL	C3B-C2B	4.97	1.48	1.39
15	E	102	BCL	O2D-CGD	4.96	1.45	1.33
15	Z	102	BCL	O2D-CGD	4.96	1.45	1.33
15	N	101	BCL	O2D-CGD	4.95	1.45	1.33
19	L	311	CDL	OA6-CA5	4.94	1.46	1.35
15	X	102	BCL	C3B-C2B	4.93	1.48	1.39
15	K	102	BCL	O2D-CGD	4.93	1.45	1.33
15	G	102	BCL	C3B-C2B	4.93	1.48	1.39
15	B	102	BCL	C3B-C2B	4.93	1.48	1.39
15	M	403	BCL	O2D-CGD	4.92	1.45	1.33
15	P	102	BCL	O2D-CGD	4.92	1.45	1.33
15	M	402	BCL	C3B-C2B	4.92	1.48	1.39
15	Y	102	BCL	O2D-CGD	4.90	1.45	1.33
15	R	101	BCL	C3B-C2B	4.90	1.48	1.39
15	K	102	BCL	C3B-C2B	4.90	1.48	1.39
15	N	101	BCL	C3B-C2B	4.89	1.48	1.39
15	1	402	BCL	C3B-C2B	4.89	1.48	1.39
15	2	102	BCL	C3B-C2B	4.89	1.48	1.39
15	L	301	BCL	C3B-C2B	4.88	1.48	1.39
15	S	102	BCL	C3B-C2B	4.85	1.48	1.39
15	6	101	BCL	C3B-C2B	4.85	1.48	1.39
15	V	101	BCL	C3B-C2B	4.85	1.48	1.39
15	Q	102	BCL	C3B-C2B	4.85	1.48	1.39
15	A	502	BCL	C3B-C2B	4.84	1.48	1.39
15	9	102	BCL	C3B-C2B	4.83	1.48	1.39
15	O	502	BCL	C3B-C2B	4.82	1.48	1.39
15	E	102	BCL	C3B-C2B	4.82	1.48	1.39
15	I	101	BCL	C3B-C2B	4.82	1.48	1.39
15	F	502	BCL	C3B-C2B	4.82	1.48	1.39
21	M	405	MQ8	C10-C5	4.81	1.48	1.40
15	U	101	BCL	C3B-C2B	4.81	1.48	1.39
15	W	101	BCL	C3B-C2B	4.81	1.48	1.39
15	T	101	BCL	C3B-C2B	4.80	1.48	1.39
15	P	102	BCL	C3B-C2B	4.80	1.48	1.39
15	J	102	BCL	C3B-C2B	4.79	1.48	1.39
15	L	308	BCL	C3D-C4D	-4.79	1.33	1.44
15	5	102	BCL	C3B-C2B	4.76	1.48	1.39
15	L	308	BCL	C3B-C2B	4.76	1.48	1.39
15	0	101	BCL	C3B-C2B	4.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	102	BCL	C3B-C2B	4.72	1.47	1.39
15	4	102	BCL	C3B-C2B	4.71	1.47	1.39
15	M	403	BCL	C3D-C4D	-4.71	1.33	1.44
15	Y	102	BCL	C3B-C2B	4.71	1.47	1.39
15	7	101	BCL	C3B-C2B	4.70	1.47	1.39
15	9	102	BCL	C3D-C4D	-4.70	1.33	1.44
15	3	101	BCL	C3B-C2B	4.70	1.47	1.39
15	8	102	BCL	C3B-C2B	4.69	1.47	1.39
15	I	101	BCL	C3D-C4D	-4.68	1.33	1.44
15	U	101	BCL	C3D-C4D	-4.68	1.33	1.44
15	L	308	BCL	O2D-CGD	4.67	1.44	1.33
15	K	102	BCL	C3D-C4D	-4.67	1.33	1.44
15	Y	102	BCL	C3D-C4D	-4.65	1.33	1.44
15	M	402	BCL	C3D-C4D	-4.64	1.33	1.44
15	S	102	BCL	C3D-C4D	-4.61	1.33	1.44
15	4	102	BCL	C3D-C4D	-4.61	1.33	1.44
15	L	301	BCL	C3D-C4D	-4.60	1.33	1.44
15	3	101	BCL	C3D-C4D	-4.59	1.33	1.44
15	B	102	BCL	C3D-C4D	-4.59	1.33	1.44
15	2	102	BCL	C3D-C4D	-4.59	1.33	1.44
15	1	402	BCL	C3D-C4D	-4.59	1.33	1.44
15	7	101	BCL	C3D-C4D	-4.59	1.33	1.44
15	O	502	BCL	C3D-C4D	-4.58	1.33	1.44
15	F	502	BCL	C3D-C4D	-4.57	1.33	1.44
15	A	502	BCL	C3D-C4D	-4.56	1.33	1.44
15	Q	102	BCL	C3D-C4D	-4.56	1.33	1.44
15	5	102	BCL	C3D-C4D	-4.56	1.33	1.44
15	W	101	BCL	C3D-C4D	-4.54	1.33	1.44
15	R	101	BCL	C3D-C4D	-4.54	1.33	1.44
15	6	101	BCL	C3D-C4D	-4.54	1.33	1.44
15	E	102	BCL	C3D-C4D	-4.54	1.33	1.44
15	D	102	BCL	C3D-C4D	-4.53	1.33	1.44
15	T	101	BCL	C3D-C4D	-4.53	1.33	1.44
15	Z	102	BCL	C3D-C4D	-4.53	1.33	1.44
15	J	102	BCL	C3D-C4D	-4.52	1.34	1.44
15	8	102	BCL	C3D-C4D	-4.52	1.34	1.44
15	G	102	BCL	C3D-C4D	-4.49	1.34	1.44
15	V	101	BCL	C3D-C4D	-4.49	1.34	1.44
15	P	102	BCL	C3D-C4D	-4.48	1.34	1.44
15	X	102	BCL	C3D-C4D	-4.48	1.34	1.44
15	0	101	BCL	C3D-C4D	-4.48	1.34	1.44
15	N	101	BCL	C3D-C4D	-4.48	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	102	BCL	O2A-CGA	4.37	1.46	1.33
15	M	402	BCL	O2A-CGA	4.37	1.46	1.33
14	L	305	PGV	O03-C19	4.36	1.46	1.33
15	9	102	BCL	O2A-CGA	4.34	1.46	1.33
15	W	101	BCL	O2A-CGA	4.33	1.46	1.33
15	O	502	BCL	O2A-CGA	4.32	1.46	1.33
14	M	408	PGV	O03-C19	4.30	1.45	1.33
14	Q	101	PGV	O03-C19	4.30	1.45	1.33
19	D	101	CDL	OB8-CB7	4.30	1.45	1.33
14	Q	101	PGV	O01-C1	4.30	1.46	1.34
14	F	501	PGV	O03-C19	4.30	1.45	1.33
19	M	407	CDL	OA8-CA7	4.29	1.45	1.33
15	1	402	BCL	O2A-CGA	4.28	1.45	1.33
14	H	301	PGV	O03-C19	4.28	1.45	1.33
15	D	102	BCL	O2A-CGA	4.27	1.45	1.33
15	K	102	BCL	O2A-CGA	4.27	1.45	1.33
15	F	502	BCL	O2A-CGA	4.27	1.45	1.33
19	M	407	CDL	OA6-CA5	4.26	1.46	1.34
15	Z	102	BCL	O2A-CGA	4.25	1.45	1.33
15	S	102	BCL	O2A-CGA	4.25	1.45	1.33
15	N	101	BCL	O2A-CGA	4.24	1.45	1.33
15	E	102	BCL	O2A-CGA	4.24	1.45	1.33
19	M	409	CDL	OA8-CA7	4.24	1.45	1.33
14	L	310	PGV	O03-C19	4.24	1.45	1.33
15	6	101	BCL	O2A-CGA	4.24	1.45	1.33
19	L	311	CDL	OB8-CB7	4.23	1.45	1.33
15	T	101	BCL	O2A-CGA	4.23	1.45	1.33
15	X	102	BCL	O2A-CGA	4.23	1.45	1.33
15	G	102	BCL	O2A-CGA	4.22	1.45	1.33
19	M	409	CDL	OA6-CA5	4.21	1.46	1.34
14	A	503	PGV	O03-C19	4.21	1.45	1.33
15	A	502	BCL	O2A-CGA	4.21	1.45	1.33
15	R	101	BCL	O2A-CGA	4.21	1.45	1.33
14	C	408	PGV	O03-C19	4.20	1.45	1.33
15	L	308	BCL	O2A-CGA	4.19	1.45	1.33
14	L	306	PGV	O03-C19	4.18	1.45	1.33
15	B	102	BCL	O2A-CGA	4.18	1.45	1.33
15	3	101	BCL	O2A-CGA	4.18	1.45	1.33
15	V	101	BCL	O2A-CGA	4.18	1.45	1.33
15	2	102	BCL	O2A-CGA	4.17	1.45	1.33
19	L	311	CDL	OA8-CA7	4.17	1.45	1.33
15	L	301	BCL	O2A-CGA	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	102	BCL	O2A-CGA	4.16	1.45	1.33
19	D	101	CDL	OA6-CA5	4.15	1.46	1.34
14	F	501	PGV	O01-C1	4.15	1.46	1.34
15	U	101	BCL	O2A-CGA	4.15	1.45	1.33
15	Y	102	BCL	O2A-CGA	4.15	1.45	1.33
14	A	501	PGV	O01-C1	4.14	1.46	1.34
14	1	401	PGV	O03-C19	4.13	1.45	1.33
19	H	302	CDL	OA6-CA5	4.13	1.46	1.34
15	P	102	BCL	O2A-CGA	4.13	1.45	1.33
19	M	407	CDL	OB6-CB5	4.13	1.45	1.34
15	M	403	BCL	O2A-CGA	4.13	1.45	1.33
19	L	311	CDL	OB6-CB5	4.11	1.45	1.34
15	8	102	BCL	O2A-CGA	4.11	1.45	1.33
19	H	302	CDL	OA8-CA7	4.11	1.45	1.33
15	Q	102	BCL	O2A-CGA	4.10	1.45	1.33
15	0	101	BCL	O2A-CGA	4.09	1.45	1.33
15	7	101	BCL	O2A-CGA	4.09	1.45	1.33
14	L	305	PGV	O01-C1	4.08	1.45	1.34
14	C	408	PGV	O01-C1	4.07	1.45	1.34
19	M	409	CDL	OB8-CB7	4.07	1.45	1.33
14	1	401	PGV	O01-C1	4.06	1.45	1.34
19	H	302	CDL	OB8-CB7	4.05	1.45	1.33
15	I	101	BCL	O2A-CGA	4.04	1.45	1.33
14	A	503	PGV	O01-C1	4.04	1.45	1.34
14	L	306	PGV	O01-C1	4.04	1.45	1.34
14	L	310	PGV	O01-C1	4.03	1.45	1.34
15	5	102	BCL	O2A-CGA	4.03	1.45	1.33
19	H	302	CDL	OB6-CB5	4.01	1.45	1.34
14	H	301	PGV	O01-C1	4.01	1.45	1.34
19	M	409	CDL	OB6-CB5	4.00	1.45	1.34
19	D	101	CDL	OB6-CB5	3.99	1.45	1.34
14	A	501	PGV	O03-C19	3.93	1.44	1.33
14	M	408	PGV	O01-C1	3.90	1.45	1.34
10	C	403	HEM	C1B-NB	-3.66	1.34	1.40
15	W	101	BCL	CHD-C1D	3.65	1.45	1.38
15	J	102	BCL	OBD-CAD	3.63	1.28	1.22
15	U	101	BCL	CHD-C1D	3.60	1.45	1.38
15	R	101	BCL	OBD-CAD	3.59	1.28	1.22
15	G	102	BCL	OBD-CAD	3.59	1.28	1.22
15	7	101	BCL	CHD-C1D	3.58	1.45	1.38
15	2	102	BCL	OBD-CAD	3.58	1.28	1.22
15	X	102	BCL	OBD-CAD	3.58	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	101	BCL	CHD-C1D	3.58	1.45	1.38
15	5	102	BCL	OBD-CAD	3.57	1.28	1.22
15	I	101	BCL	OBD-CAD	3.57	1.28	1.22
10	C	404	HEM	C1B-NB	-3.57	1.34	1.40
15	1	402	BCL	CHD-C1D	3.57	1.45	1.38
15	3	101	BCL	CHD-C1D	3.57	1.45	1.38
15	Z	102	BCL	OBD-CAD	3.56	1.28	1.22
15	F	502	BCL	CHD-C1D	3.55	1.45	1.38
15	Q	102	BCL	OBD-CAD	3.55	1.28	1.22
15	W	101	BCL	OBD-CAD	3.55	1.28	1.22
15	3	101	BCL	OBD-CAD	3.52	1.28	1.22
15	4	102	BCL	OBD-CAD	3.52	1.28	1.22
15	M	403	BCL	CHD-C1D	3.52	1.45	1.38
15	S	102	BCL	CHD-C1D	3.51	1.45	1.38
15	U	101	BCL	OBD-CAD	3.51	1.28	1.22
15	0	101	BCL	OBD-CAD	3.51	1.28	1.22
15	D	102	BCL	CHD-C1D	3.50	1.45	1.38
15	F	502	BCL	OBD-CAD	3.50	1.28	1.22
15	Y	102	BCL	OBD-CAD	3.49	1.28	1.22
15	8	102	BCL	OBD-CAD	3.49	1.28	1.22
15	V	101	BCL	OBD-CAD	3.48	1.28	1.22
15	A	502	BCL	OBD-CAD	3.48	1.28	1.22
15	6	101	BCL	OBD-CAD	3.48	1.28	1.22
15	1	402	BCL	OBD-CAD	3.47	1.28	1.22
15	Q	102	BCL	CHD-C1D	3.47	1.45	1.38
15	N	101	BCL	OBD-CAD	3.47	1.28	1.22
15	L	308	BCL	C1D-ND	-3.46	1.33	1.37
15	K	102	BCL	OBD-CAD	3.46	1.28	1.22
15	P	102	BCL	OBD-CAD	3.45	1.28	1.22
15	B	102	BCL	OBD-CAD	3.44	1.28	1.22
15	D	102	BCL	OBD-CAD	3.44	1.28	1.22
15	T	101	BCL	OBD-CAD	3.43	1.28	1.22
15	M	402	BCL	CHD-C1D	3.43	1.45	1.38
15	9	102	BCL	CHD-C1D	3.43	1.45	1.38
15	A	502	BCL	CHD-C1D	3.41	1.45	1.38
15	K	102	BCL	CHD-C1D	3.41	1.45	1.38
15	5	102	BCL	CHD-C1D	3.40	1.45	1.38
15	8	102	BCL	CHD-C1D	3.40	1.45	1.38
15	Y	102	BCL	CHD-C1D	3.39	1.45	1.38
15	L	308	BCL	OBD-CAD	3.39	1.28	1.22
15	9	102	BCL	OBD-CAD	3.39	1.28	1.22
15	O	502	BCL	CHD-C1D	3.38	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	301	BCL	CHD-C1D	3.38	1.44	1.38
15	J	102	BCL	CHD-C1D	3.38	1.44	1.38
15	O	502	BCL	OBD-CAD	3.38	1.28	1.22
10	C	401	HEM	C1B-NB	-3.38	1.34	1.40
15	L	308	BCL	CHD-C1D	3.37	1.44	1.38
15	E	102	BCL	OBD-CAD	3.37	1.28	1.22
15	2	102	BCL	C1D-ND	-3.36	1.33	1.37
10	C	402	HEM	C1B-NB	-3.34	1.34	1.40
15	S	102	BCL	OBD-CAD	3.33	1.28	1.22
15	R	101	BCL	CHD-C1D	3.31	1.44	1.38
10	C	403	HEM	C4D-ND	-3.31	1.34	1.40
15	L	301	BCL	OBD-CAD	3.31	1.28	1.22
15	G	102	BCL	CHD-C1D	3.31	1.44	1.38
15	0	101	BCL	CHD-C1D	3.31	1.44	1.38
15	T	101	BCL	CHD-C1D	3.30	1.44	1.38
15	B	102	BCL	CHD-C1D	3.30	1.44	1.38
15	M	402	BCL	OBD-CAD	3.29	1.28	1.22
15	7	101	BCL	OBD-CAD	3.29	1.28	1.22
15	B	102	BCL	C1D-ND	-3.28	1.33	1.37
15	X	102	BCL	C1D-ND	-3.28	1.33	1.37
15	Z	102	BCL	CHD-C1D	3.28	1.44	1.38
15	P	102	BCL	C1D-ND	-3.28	1.33	1.37
15	6	101	BCL	CHD-C1D	3.26	1.44	1.38
15	4	102	BCL	CHD-C1D	3.26	1.44	1.38
15	M	402	BCL	C1D-ND	-3.25	1.33	1.37
17	L	309	UQ8	C4-C3	3.25	1.49	1.36
15	T	101	BCL	C1D-ND	-3.25	1.33	1.37
10	C	404	HEM	C4D-ND	-3.25	1.34	1.40
15	N	101	BCL	CHD-C1D	3.23	1.44	1.38
15	2	102	BCL	CHD-C1D	3.23	1.44	1.38
10	C	401	HEM	C4D-ND	-3.22	1.34	1.40
15	E	102	BCL	CHD-C1D	3.22	1.44	1.38
15	G	102	BCL	C1D-ND	-3.21	1.33	1.37
15	J	102	BCL	C1D-ND	-3.21	1.33	1.37
15	V	101	BCL	C1D-ND	-3.20	1.33	1.37
15	R	101	BCL	C1D-ND	-3.20	1.33	1.37
15	P	102	BCL	CHD-C1D	3.17	1.44	1.38
10	C	402	HEM	C4D-ND	-3.17	1.34	1.40
15	X	102	BCL	CHD-C1D	3.17	1.44	1.38
15	N	101	BCL	C1D-ND	-3.11	1.34	1.37
17	L	304	UQ8	C4-C3	3.11	1.49	1.36
15	M	402	BCL	C3D-C2D	3.09	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	0	101	BCL	C1D-ND	-3.09	1.34	1.37
15	L	308	BCL	C3D-C2D	3.08	1.47	1.39
15	4	102	BCL	C1D-ND	-3.08	1.34	1.37
15	E	102	BCL	C1D-ND	-3.08	1.34	1.37
15	M	403	BCL	OBD-CAD	3.07	1.27	1.22
15	Z	102	BCL	C1D-ND	-3.07	1.34	1.37
15	V	101	BCL	CHD-C1D	3.06	1.44	1.38
15	D	102	BCL	C3D-C2D	3.06	1.47	1.39
15	8	102	BCL	C1D-ND	-3.05	1.34	1.37
17	L	303	UQ8	C4-C3	3.03	1.48	1.36
15	6	101	BCL	C1D-ND	-3.01	1.34	1.37
15	W	101	BCL	C3D-C2D	3.00	1.47	1.39
15	G	102	BCL	C3D-C2D	2.99	1.47	1.39
15	O	502	BCL	C3D-C2D	2.99	1.47	1.39
15	7	101	BCL	C3D-C2D	2.99	1.47	1.39
15	A	502	BCL	C3D-C2D	2.98	1.47	1.39
15	S	102	BCL	C3D-C2D	2.98	1.47	1.39
15	J	102	BCL	C3D-C2D	2.97	1.47	1.39
15	P	102	BCL	C3D-C2D	2.97	1.47	1.39
15	X	102	BCL	C3D-C2D	2.97	1.47	1.39
15	4	102	BCL	C3D-C2D	2.97	1.47	1.39
15	E	102	BCL	C3D-C2D	2.96	1.47	1.39
10	C	404	HEM	FE-NB	2.96	2.11	1.96
15	O	502	BCL	C1D-ND	-2.95	1.34	1.37
15	R	101	BCL	C3D-C2D	2.95	1.47	1.39
15	I	101	BCL	C3D-C2D	2.95	1.47	1.39
15	N	101	BCL	C3D-C2D	2.94	1.47	1.39
10	C	403	HEM	FE-NB	2.94	2.11	1.96
15	8	102	BCL	C3D-C2D	2.94	1.47	1.39
15	5	102	BCL	C3D-C2D	2.94	1.47	1.39
15	Q	102	BCL	C3D-C2D	2.93	1.47	1.39
15	K	102	BCL	C3D-C2D	2.93	1.47	1.39
15	6	101	BCL	C3D-C2D	2.92	1.47	1.39
10	C	402	HEM	FE-NB	2.92	2.11	1.96
15	T	101	BCL	C3D-C2D	2.92	1.47	1.39
15	1	402	BCL	C3D-C2D	2.91	1.47	1.39
15	V	101	BCL	C3D-C2D	2.90	1.47	1.39
15	U	101	BCL	C3D-C2D	2.89	1.47	1.39
15	3	101	BCL	C3D-C2D	2.89	1.47	1.39
15	2	102	BCL	C3D-C2D	2.88	1.47	1.39
15	Y	102	BCL	C3D-C2D	2.88	1.47	1.39
15	0	101	BCL	C3D-C2D	2.88	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	102	BCL	C3D-C2D	2.87	1.47	1.39
15	M	403	BCL	C3D-C2D	2.87	1.47	1.39
15	M	403	BCL	C1D-ND	-2.87	1.34	1.37
15	F	502	BCL	C3D-C2D	2.87	1.46	1.39
15	9	102	BCL	C3D-C2D	2.86	1.46	1.39
10	C	401	HEM	FE-NB	2.85	2.11	1.96
15	L	301	BCL	C1D-ND	-2.85	1.34	1.37
15	F	502	BCL	CHD-C4C	2.84	1.47	1.39
15	A	502	BCL	C1D-ND	-2.83	1.34	1.37
15	D	102	BCL	C1D-ND	-2.82	1.34	1.37
15	I	101	BCL	C1D-ND	-2.82	1.34	1.37
15	F	502	BCL	C1D-ND	-2.81	1.34	1.37
15	1	402	BCL	C1D-ND	-2.80	1.34	1.37
15	L	301	BCL	C3D-C2D	2.78	1.46	1.39
15	I	101	BCL	CHD-C4C	2.78	1.47	1.39
15	U	101	BCL	CHD-C4C	2.78	1.47	1.39
15	W	101	BCL	C1D-ND	-2.76	1.34	1.37
15	Z	102	BCL	C3D-C2D	2.76	1.46	1.39
15	7	101	BCL	C1D-ND	-2.76	1.34	1.37
15	F	502	BCL	C1D-C2D	2.76	1.50	1.45
15	1	402	BCL	CHD-C4C	2.76	1.47	1.39
15	5	102	BCL	C1D-ND	-2.75	1.34	1.37
15	S	102	BCL	C1D-ND	-2.75	1.34	1.37
15	Q	102	BCL	CHD-C4C	2.74	1.47	1.39
15	K	102	BCL	C1D-ND	-2.74	1.34	1.37
15	U	101	BCL	C1D-C2D	2.73	1.50	1.45
15	Y	102	BCL	C1D-ND	-2.73	1.34	1.37
15	Q	102	BCL	C1D-ND	-2.72	1.34	1.37
15	3	101	BCL	CHD-C4C	2.71	1.46	1.39
15	W	101	BCL	CHD-C4C	2.71	1.46	1.39
15	K	102	BCL	CHD-C4C	2.70	1.46	1.39
15	I	101	BCL	C1D-C2D	2.70	1.50	1.45
15	Y	102	BCL	CHD-C4C	2.70	1.46	1.39
15	5	102	BCL	CHD-C4C	2.70	1.46	1.39
15	U	101	BCL	C1D-ND	-2.69	1.34	1.37
15	O	502	BCL	CHD-C4C	2.68	1.46	1.39
15	Q	102	BCL	C1D-C2D	2.68	1.50	1.45
15	9	102	BCL	CHD-C4C	2.68	1.46	1.39
15	M	403	BCL	C1D-C2D	2.67	1.50	1.45
15	7	101	BCL	CHD-C4C	2.67	1.46	1.39
15	L	308	BCL	MG-NA	-2.67	1.99	2.06
15	S	102	BCL	CHD-C4C	2.67	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	502	BCL	C1D-C2D	2.65	1.50	1.45
15	1	402	BCL	C1D-C2D	2.64	1.50	1.45
15	D	102	BCL	CHD-C4C	2.64	1.46	1.39
15	A	502	BCL	CHD-C4C	2.63	1.46	1.39
15	L	308	BCL	CHD-C4C	2.62	1.46	1.39
15	W	101	BCL	C1D-C2D	2.62	1.50	1.45
15	D	102	BCL	C1D-C2D	2.62	1.50	1.45
15	9	102	BCL	C1D-ND	-2.61	1.34	1.37
15	K	102	BCL	C1D-C2D	2.60	1.50	1.45
15	M	403	BCL	CHD-C4C	2.59	1.46	1.39
15	3	101	BCL	C1D-C2D	2.58	1.50	1.45
15	5	102	BCL	C1D-C2D	2.57	1.50	1.45
15	Y	102	BCL	C1D-C2D	2.57	1.50	1.45
15	S	102	BCL	C1D-C2D	2.55	1.50	1.45
15	3	101	BCL	C1D-ND	-2.54	1.34	1.37
15	M	402	BCL	CHD-C4C	2.53	1.46	1.39
15	5	102	BCL	MG-NA	-2.53	2.00	2.06
15	Z	102	BCL	CHD-C4C	2.51	1.46	1.39
15	N	101	BCL	CHD-C4C	2.51	1.46	1.39
15	G	102	BCL	CHD-C4C	2.50	1.46	1.39
15	9	102	BCL	C1D-C2D	2.49	1.50	1.45
15	K	102	BCL	MG-NA	-2.48	2.00	2.06
15	4	102	BCL	CHD-C4C	2.47	1.46	1.39
15	A	502	BCL	C1D-C2D	2.47	1.50	1.45
15	7	101	BCL	C1D-C2D	2.46	1.50	1.45
19	D	101	CDL	OA8-CA7	2.45	1.45	1.33
15	8	102	BCL	CHD-C4C	2.45	1.46	1.39
15	L	301	BCL	CHD-C4C	2.44	1.46	1.39
15	6	101	BCL	CHD-C4C	2.44	1.46	1.39
15	2	102	BCL	CHD-C4C	2.44	1.46	1.39
15	R	101	BCL	CHD-C4C	2.44	1.46	1.39
15	J	102	BCL	CHD-C4C	2.43	1.46	1.39
15	L	308	BCL	C1D-C2D	2.43	1.50	1.45
15	Y	102	BCL	MG-NA	-2.42	2.00	2.06
15	B	102	BCL	CHD-C4C	2.41	1.46	1.39
15	3	101	BCL	MG-NA	-2.41	2.00	2.06
15	E	102	BCL	CHD-C4C	2.40	1.46	1.39
15	L	308	BCL	C1B-CHB	2.39	1.47	1.41
15	P	102	BCL	CHD-C4C	2.39	1.45	1.39
15	0	101	BCL	CHD-C4C	2.38	1.45	1.39
15	M	402	BCL	MG-NA	-2.38	2.00	2.06
15	X	102	BCL	CHD-C4C	2.37	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	101	BCL	CHD-C4C	2.34	1.45	1.39
15	O	502	BCL	C1B-CHB	2.34	1.47	1.41
15	T	101	BCL	CHD-C4C	2.32	1.45	1.39
15	I	101	BCL	MG-NA	-2.32	2.00	2.06
15	I	101	BCL	MG-NC	-2.32	2.00	2.06
15	M	402	BCL	C1D-C2D	2.31	1.49	1.45
15	K	102	BCL	C1B-CHB	2.29	1.47	1.41
15	X	102	BCL	MG-NA	-2.29	2.00	2.06
15	2	102	BCL	MG-NA	-2.28	2.00	2.06
15	1	402	BCL	MG-NA	-2.28	2.00	2.06
15	F	502	BCL	MG-NA	-2.26	2.00	2.06
15	E	102	BCL	C1B-CHB	2.24	1.47	1.41
15	O	502	BCL	MG-NA	-2.24	2.00	2.06
15	L	301	BCL	C1D-C2D	2.23	1.49	1.45
15	A	502	BCL	C1B-CHB	2.23	1.47	1.41
15	M	402	BCL	C1B-CHB	2.23	1.47	1.41
15	S	102	BCL	MG-NA	-2.23	2.01	2.06
15	A	502	BCL	MG-NA	-2.22	2.01	2.06
15	3	101	BCL	C1B-CHB	2.22	1.47	1.41
15	P	102	BCL	C1B-CHB	2.22	1.47	1.41
15	Y	102	BCL	MG-NC	-2.22	2.01	2.06
15	6	101	BCL	C1D-C2D	2.22	1.49	1.45
15	R	101	BCL	C1B-CHB	2.22	1.47	1.41
15	S	102	BCL	C1B-CHB	2.22	1.47	1.41
15	1	402	BCL	C1B-CHB	2.21	1.47	1.41
15	Z	102	BCL	C1D-C2D	2.21	1.49	1.45
15	7	101	BCL	MG-NA	-2.21	2.01	2.06
15	B	102	BCL	C1B-CHB	2.21	1.47	1.41
15	W	101	BCL	MG-NA	-2.20	2.01	2.06
15	N	101	BCL	C1D-C2D	2.20	1.49	1.45
15	L	301	BCL	C1B-CHB	2.19	1.47	1.41
15	Y	102	BCL	C1B-CHB	2.19	1.47	1.41
15	G	102	BCL	C1D-C2D	2.19	1.49	1.45
15	5	102	BCL	C1B-CHB	2.18	1.47	1.41
15	M	403	BCL	MG-NA	-2.18	2.01	2.06
15	6	101	BCL	MG-NA	-2.18	2.01	2.06
15	7	101	BCL	MG-NC	-2.18	2.01	2.06
15	6	101	BCL	C1B-CHB	2.18	1.47	1.41
15	X	102	BCL	C1B-CHB	2.18	1.47	1.41
15	N	101	BCL	MG-NA	-2.17	2.01	2.06
15	G	102	BCL	C1B-CHB	2.17	1.47	1.41
15	T	101	BCL	C1B-CHB	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	0	101	BCL	C1B-CHB	2.17	1.47	1.41
15	G	102	BCL	MG-NA	-2.17	2.01	2.06
15	F	502	BCL	C1B-CHB	2.17	1.47	1.41
15	J	102	BCL	MG-NA	-2.17	2.01	2.06
15	D	102	BCL	MG-NA	-2.17	2.01	2.06
15	4	102	BCL	MG-NA	-2.16	2.01	2.06
15	V	101	BCL	C1B-CHB	2.16	1.47	1.41
15	V	101	BCL	MG-NA	-2.16	2.01	2.06
15	Z	102	BCL	C1B-CHB	2.16	1.47	1.41
15	9	102	BCL	MG-NA	-2.15	2.01	2.06
15	2	102	BCL	C1B-CHB	2.15	1.47	1.41
15	9	102	BCL	C1B-CHB	2.14	1.46	1.41
15	4	102	BCL	C1D-C2D	2.14	1.49	1.45
15	M	403	BCL	C4B-CHC	2.14	1.46	1.41
15	8	102	BCL	C1B-CHB	2.14	1.46	1.41
15	P	102	BCL	MG-NA	-2.14	2.01	2.06
15	F	502	BCL	MG-NC	-2.14	2.01	2.06
15	U	101	BCL	C1B-CHB	2.13	1.46	1.41
15	R	101	BCL	C1D-C2D	2.13	1.49	1.45
15	Q	102	BCL	MG-NA	-2.13	2.01	2.06
15	Z	102	BCL	MG-NA	-2.13	2.01	2.06
15	B	102	BCL	MG-NA	-2.12	2.01	2.06
15	L	301	BCL	C4B-CHC	2.12	1.46	1.41
15	J	102	BCL	C1D-C2D	2.12	1.49	1.45
15	E	102	BCL	MG-NA	-2.12	2.01	2.06
15	U	101	BCL	MG-NA	-2.12	2.01	2.06
15	0	101	BCL	MG-NA	-2.12	2.01	2.06
15	1	402	BCL	MG-NC	-2.12	2.01	2.06
15	W	101	BCL	C1B-CHB	2.10	1.46	1.41
15	W	101	BCL	MG-NC	-2.10	2.01	2.06
15	N	101	BCL	C1B-CHB	2.10	1.46	1.41
10	C	402	HEM	C1D-ND	-2.08	1.34	1.38
15	R	101	BCL	MG-NA	-2.08	2.01	2.06
15	5	102	BCL	MG-NC	-2.07	2.01	2.06
15	M	403	BCL	C1B-CHB	2.07	1.46	1.41
15	I	101	BCL	C1B-CHB	2.07	1.46	1.41
15	V	101	BCL	C4B-CHC	2.07	1.46	1.41
15	4	102	BCL	C1B-CHB	2.06	1.46	1.41
15	A	502	BCL	C4B-CHC	2.06	1.46	1.41
15	M	403	BCL	MG-NC	-2.06	2.01	2.06
15	I	101	BCL	C4B-CHC	2.06	1.46	1.41
15	K	102	BCL	MG-NC	-2.06	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	102	BCL	C1B-CHB	2.06	1.46	1.41
15	J	102	BCL	MG-NC	-2.06	2.01	2.06
15	7	101	BCL	C1B-CHB	2.06	1.46	1.41
15	8	102	BCL	MG-NA	-2.05	2.01	2.06
15	T	101	BCL	MG-NA	-2.05	2.01	2.06
15	B	102	BCL	MG-NC	-2.04	2.01	2.06
15	G	102	BCL	C4B-CHC	2.03	1.46	1.41
15	Z	102	BCL	C4B-CHC	2.03	1.46	1.41
10	C	403	HEM	C1D-ND	-2.03	1.34	1.38
15	Q	102	BCL	C1B-CHB	2.03	1.46	1.41
15	6	101	BCL	MG-NC	-2.02	2.01	2.06
15	V	101	BCL	C1D-C2D	2.02	1.49	1.45
15	S	102	BCL	C4B-CHC	2.02	1.46	1.41
15	M	402	BCL	MG-NC	-2.02	2.01	2.06
10	C	402	HEM	CHB-C1B	2.01	1.40	1.35
15	B	102	BCL	C4B-CHC	2.01	1.46	1.41
15	P	102	BCL	C4B-CHC	2.01	1.46	1.41
15	J	102	BCL	C4B-CHC	2.01	1.46	1.41
15	1	402	BCL	C4B-CHC	2.01	1.46	1.41
15	X	102	BCL	C4B-CHC	2.01	1.46	1.41
15	U	101	BCL	MG-NC	-2.00	2.01	2.06
15	F	502	BCL	C4B-CHC	2.00	1.46	1.41
15	X	102	BCL	C1D-C2D	2.00	1.49	1.45
10	C	403	HEM	C4B-NB	-2.00	1.34	1.38
15	J	102	BCL	C1B-CHB	2.00	1.46	1.41

All (1145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	J	103	CRT	C3-C1-C4	-17.03	84.72	110.86
22	J	103	CRT	C2-C1-C4	-15.82	86.57	110.86
22	P	103	CRT	C3-C1-C4	-15.60	86.91	110.86
22	P	103	CRT	C2-C1-C4	-15.40	87.21	110.86
15	Q	102	BCL	CHD-C1D-ND	-8.78	116.38	124.45
15	F	502	BCL	CHD-C1D-ND	-8.75	116.41	124.45
15	5	102	BCL	CHD-C1D-ND	-8.72	116.44	124.45
15	K	102	BCL	CHD-C1D-ND	-8.68	116.47	124.45
15	L	308	BCL	CHD-C1D-ND	-8.68	116.48	124.45
15	O	502	BCL	CHD-C1D-ND	-8.64	116.51	124.45
15	I	101	BCL	CHD-C1D-ND	-8.59	116.56	124.45
15	Y	102	BCL	CHD-C1D-ND	-8.59	116.56	124.45
15	U	101	BCL	CHD-C1D-ND	-8.55	116.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	402	BCL	CHD-C1D-ND	-8.54	116.61	124.45
15	M	403	BCL	CHD-C1D-ND	-8.47	116.67	124.45
15	W	101	BCL	CHD-C1D-ND	-8.46	116.68	124.45
15	3	101	BCL	CHD-C1D-ND	-8.44	116.69	124.45
15	D	102	BCL	CHD-C1D-ND	-8.41	116.73	124.45
15	9	102	BCL	CHD-C1D-ND	-8.33	116.80	124.45
15	S	102	BCL	CHD-C1D-ND	-8.24	116.89	124.45
15	M	402	BCL	CHD-C1D-ND	-8.22	116.90	124.45
15	U	101	BCL	CMD-C2D-C1D	8.21	139.18	124.71
15	7	101	BCL	CHD-C1D-ND	-8.15	116.96	124.45
15	A	502	BCL	CHD-C1D-ND	-8.11	117.00	124.45
15	M	403	BCL	CMD-C2D-C1D	8.01	138.83	124.71
15	K	102	BCL	CMD-C2D-C1D	8.00	138.82	124.71
15	9	102	BCL	CMD-C2D-C1D	7.99	138.80	124.71
15	3	101	BCL	CMD-C2D-C1D	7.98	138.78	124.71
15	F	502	BCL	CMD-C2D-C1D	7.98	138.77	124.71
15	Y	102	BCL	CMD-C2D-C1D	7.95	138.73	124.71
15	Q	102	BCL	CMD-C2D-C1D	7.95	138.72	124.71
15	1	402	BCL	CMD-C2D-C1D	7.82	138.49	124.71
15	5	102	BCL	CMD-C2D-C1D	7.81	138.47	124.71
15	G	102	BCL	CHD-C1D-ND	-7.71	117.37	124.45
15	N	101	BCL	CHD-C1D-ND	-7.69	117.38	124.45
15	D	102	BCL	CMD-C2D-C1D	7.69	138.27	124.71
15	W	101	BCL	CMD-C2D-C1D	7.69	138.26	124.71
15	Z	102	BCL	CHD-C1D-ND	-7.68	117.40	124.45
15	I	101	BCL	CMD-C2D-C1D	7.67	138.22	124.71
15	O	502	BCL	CMD-C2D-C1D	7.65	138.20	124.71
15	6	101	BCL	CHD-C1D-ND	-7.64	117.44	124.45
15	S	102	BCL	CMD-C2D-C1D	7.63	138.17	124.71
15	L	301	BCL	CMD-C2D-C1D	7.57	138.05	124.71
15	L	301	BCL	CHD-C1D-ND	-7.56	117.50	124.45
15	7	101	BCL	CMD-C2D-C1D	7.45	137.84	124.71
15	A	502	BCL	CMD-C2D-C1D	7.37	137.70	124.71
15	X	102	BCL	CHD-C1D-ND	-7.36	117.69	124.45
15	4	102	BCL	CHD-C1D-ND	-7.36	117.69	124.45
15	J	102	BCL	CHD-C1D-ND	-7.34	117.71	124.45
15	L	308	BCL	CMD-C2D-C1D	7.33	137.63	124.71
15	V	101	BCL	CHD-C1D-ND	-7.28	117.77	124.45
15	8	102	BCL	CHD-C1D-ND	-7.26	117.78	124.45
15	2	102	BCL	CHD-C1D-ND	-7.22	117.82	124.45
15	P	102	BCL	CHD-C1D-ND	-7.21	117.83	124.45
15	E	102	BCL	CHD-C1D-ND	-7.17	117.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	0	101	BCL	CHD-C1D-ND	-7.13	117.91	124.45
22	4	103	CRT	C31-C32-C33	-7.06	117.24	127.31
15	R	101	BCL	CHD-C1D-ND	-7.04	117.98	124.45
15	6	101	BCL	CMD-C2D-C1D	7.03	137.10	124.71
15	Z	102	BCL	CMD-C2D-C1D	7.02	137.08	124.71
15	T	101	BCL	CHD-C1D-ND	-6.97	118.05	124.45
15	B	102	BCL	CHD-C1D-ND	-6.95	118.07	124.45
15	4	102	BCL	CMD-C2D-C1D	6.93	136.93	124.71
15	G	102	BCL	CMD-C2D-C1D	6.93	136.92	124.71
15	N	101	BCL	CMD-C2D-C1D	6.90	136.87	124.71
15	M	402	BCL	CMD-C2D-C1D	6.65	136.43	124.71
15	J	102	BCL	CMD-C2D-C1D	6.65	136.43	124.71
15	T	101	BCL	CMD-C2D-C1D	6.64	136.41	124.71
15	0	101	BCL	CMD-C2D-C1D	6.57	136.30	124.71
15	2	102	BCL	CMD-C2D-C1D	6.57	136.28	124.71
15	V	101	BCL	CMD-C2D-C1D	6.56	136.27	124.71
15	8	102	BCL	CMD-C2D-C1D	6.55	136.26	124.71
15	R	101	BCL	CMD-C2D-C1D	6.53	136.22	124.71
15	X	102	BCL	CMD-C2D-C1D	6.53	136.22	124.71
22	M	406	CRT	C40-C38-C37	6.50	120.83	110.86
15	P	102	BCL	CMD-C2D-C1D	6.48	136.13	124.71
15	E	102	BCL	CMD-C2D-C1D	6.41	136.01	124.71
15	B	102	BCL	CMD-C2D-C1D	6.31	135.82	124.71
15	P	102	BCL	C2D-C1D-ND	5.83	114.40	110.10
22	2	103	CRT	C40-C38-C37	5.76	119.70	110.86
15	N	101	BCL	C2D-C1D-ND	5.75	114.34	110.10
22	V	102	CRT	C39-C38-C37	5.72	119.64	110.86
22	J	103	CRT	C3-C1-C2	5.67	121.03	110.37
22	V	102	CRT	C40-C38-C39	5.64	120.97	110.37
15	X	102	BCL	C2D-C1D-ND	5.64	114.26	110.10
15	M	403	BCL	O2D-CGD-CBD	5.63	121.27	111.27
15	6	101	BCL	C2D-C1D-ND	5.62	114.25	110.10
15	V	101	BCL	C2D-C1D-ND	5.61	114.24	110.10
15	M	402	BCL	O2D-CGD-CBD	5.61	121.23	111.27
15	E	102	BCL	C2D-C1D-ND	5.54	114.19	110.10
15	G	102	BCL	C2D-C1D-ND	5.51	114.17	110.10
15	Z	102	BCL	C2D-C1D-ND	5.46	114.12	110.10
22	P	103	CRT	C3-C1-C2	5.44	120.61	110.37
15	T	101	BCL	C2D-C1D-ND	5.44	114.11	110.10
15	8	102	BCL	C2D-C1D-ND	5.44	114.11	110.10
22	M	406	CRT	C40-C38-C39	5.43	120.58	110.37
15	O	502	BCL	C2D-C1D-ND	5.42	114.10	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	102	BCL	C2D-C1D-ND	5.39	114.08	110.10
15	0	101	BCL	C2D-C1D-ND	5.37	114.06	110.10
22	2	103	CRT	C39-C38-C37	5.34	119.05	110.86
15	Y	102	BCL	C2D-C1D-ND	5.32	114.02	110.10
10	C	401	HEM	CHC-C4B-NB	5.32	130.21	124.43
14	H	301	PGV	O01-C1-C2	5.28	122.89	111.50
15	S	102	BCL	C2D-C1D-ND	5.28	113.99	110.10
15	1	402	BCL	C2D-C1D-ND	5.26	113.98	110.10
15	K	102	BCL	C2D-C1D-ND	5.25	113.97	110.10
15	A	502	BCL	C2D-C1D-ND	5.25	113.97	110.10
15	W	101	BCL	O2D-CGD-CBD	5.25	120.59	111.27
15	W	101	BCL	C2D-C1D-ND	5.24	113.97	110.10
22	2	103	CRT	C40-C38-C39	5.24	120.22	110.37
15	Q	102	BCL	C2D-C1D-ND	5.22	113.95	110.10
15	5	102	BCL	C2D-C1D-ND	5.21	113.95	110.10
15	L	301	BCL	C2D-C1D-ND	5.18	113.92	110.10
15	F	502	BCL	C2D-C1D-ND	5.18	113.92	110.10
22	M	406	CRT	C36-C35-C33	-5.18	118.06	125.89
15	9	102	BCL	C2D-C1D-ND	5.17	113.91	110.10
15	4	102	BCL	C2D-C1D-ND	5.16	113.91	110.10
15	U	101	BCL	C2D-C1D-ND	5.16	113.90	110.10
15	M	402	BCL	C2D-C1D-ND	5.13	113.88	110.10
15	J	102	BCL	C2D-C1D-ND	5.12	113.88	110.10
15	2	102	BCL	C2D-C1D-ND	5.12	113.88	110.10
15	9	102	BCL	C3D-C2D-C1D	-5.11	98.86	105.83
15	7	101	BCL	C2D-C1D-ND	5.11	113.87	110.10
15	O	502	BCL	C3D-C2D-C1D	-5.09	98.88	105.83
15	K	102	BCL	C3D-C2D-C1D	-5.09	98.88	105.83
15	I	101	BCL	C2D-C1D-ND	5.09	113.85	110.10
15	M	403	BCL	C3D-C2D-C1D	-5.08	98.90	105.83
15	S	102	BCL	C3D-C2D-C1D	-5.08	98.90	105.83
15	Y	102	BCL	C3D-C2D-C1D	-5.07	98.91	105.83
15	U	101	BCL	C3D-C2D-C1D	-5.06	98.92	105.83
15	D	102	BCL	C2D-C1D-ND	5.06	113.83	110.10
15	R	101	BCL	C2D-C1D-ND	5.06	113.83	110.10
15	S	102	BCL	O2D-CGD-CBD	5.04	120.22	111.27
15	F	502	BCL	C3D-C2D-C1D	-5.02	98.97	105.83
15	1	402	BCL	C3D-C2D-C1D	-5.02	98.97	105.83
15	W	101	BCL	C3D-C2D-C1D	-5.02	98.98	105.83
15	Q	102	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
15	A	502	BCL	C3D-C2D-C1D	-4.99	99.02	105.83
15	I	101	BCL	O2D-CGD-CBD	4.99	120.14	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	102	CRT	C5-C6-C7	-4.99	118.36	125.89
22	M	406	CRT	C21-C22-C23	-4.97	120.21	127.31
15	3	101	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
15	K	102	BCL	O2D-CGD-CBD	4.95	120.06	111.27
15	L	301	BCL	C3D-C2D-C1D	-4.94	99.09	105.83
15	N	101	BCL	C3D-C2D-C1D	-4.93	99.10	105.83
15	Q	102	BCL	O2D-CGD-CBD	4.93	120.03	111.27
15	5	102	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
15	D	102	BCL	C3D-C2D-C1D	-4.92	99.11	105.83
15	O	502	BCL	O2D-CGD-CBD	4.92	120.01	111.27
22	V	102	CRT	C40-C38-C37	4.91	118.40	110.86
15	3	101	BCL	C2D-C1D-ND	4.90	113.72	110.10
15	7	101	BCL	C3D-C2D-C1D	-4.88	99.17	105.83
15	U	101	BCL	O2D-CGD-CBD	4.88	119.94	111.27
15	V	101	BCL	C3C-C4C-CHD	-4.87	113.00	123.39
15	Q	102	BCL	CMB-C2B-C3B	4.86	133.78	124.68
15	I	101	BCL	C3D-C2D-C1D	-4.86	99.19	105.83
10	C	404	HEM	CHC-C4B-NB	4.84	129.68	124.43
15	T	101	BCL	C3C-C4C-CHD	-4.83	113.07	123.39
15	I	101	BCL	CMB-C2B-C3B	4.83	133.71	124.68
15	6	101	BCL	C3D-C2D-C1D	-4.83	99.24	105.83
10	C	403	HEM	CHC-C4B-NB	4.83	129.68	124.43
15	5	102	BCL	O2D-CGD-CBD	4.81	119.82	111.27
15	9	102	BCL	O2D-CGD-CBD	4.81	119.81	111.27
15	P	102	BCL	C3C-C4C-CHD	-4.81	113.12	123.39
15	L	308	BCL	C2D-C1D-ND	4.80	113.64	110.10
22	E	103	CRT	C21-C22-C23	-4.79	120.47	127.31
15	X	102	BCL	C3C-C4C-CHD	-4.79	113.17	123.39
15	P	102	BCL	C3D-C2D-C1D	-4.78	99.30	105.83
22	0	102	CRT	C21-C22-C23	-4.78	120.50	127.31
15	B	102	BCL	C3C-C4C-CHD	-4.77	113.21	123.39
15	8	102	BCL	C3D-C2D-C1D	-4.77	99.33	105.83
15	L	308	BCL	C3D-C2D-C1D	-4.76	99.34	105.83
15	N	101	BCL	CHD-C4C-NC	4.75	130.35	125.08
15	M	403	BCL	C2D-C1D-ND	4.75	113.61	110.10
15	Z	102	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
15	P	102	BCL	CHD-C4C-NC	4.74	130.34	125.08
15	A	502	BCL	O2D-CGD-CBD	4.74	119.69	111.27
15	9	102	BCL	CMB-C2B-C3B	4.74	133.54	124.68
15	G	102	BCL	C3D-C2D-C1D	-4.74	99.37	105.83
15	E	102	BCL	C3C-C4C-CHD	-4.73	113.28	123.39
15	M	402	BCL	C3D-C2D-C1D	-4.73	99.38	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	V	101	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
15	E	102	BCL	C3D-C2D-C1D	-4.71	99.40	105.83
10	C	402	HEM	CHC-C4B-NB	4.71	129.55	124.43
15	1	402	BCL	CMB-C2B-C3B	4.71	133.48	124.68
22	N	102	CRT	C5-C6-C7	-4.70	118.78	125.89
15	V	101	BCL	CHD-C4C-NC	4.70	130.30	125.08
15	0	101	BCL	C3C-C4C-CHD	-4.69	113.37	123.39
22	N	102	CRT	C21-C22-C23	-4.68	120.63	127.31
15	S	102	BCL	CMB-C2B-C3B	4.67	133.42	124.68
15	4	102	BCL	C3C-C4C-CHD	-4.66	113.44	123.39
15	A	502	BCL	CMB-C2B-C3B	4.66	133.39	124.68
15	4	102	BCL	C3D-C2D-C1D	-4.65	99.48	105.83
15	B	102	BCL	C3D-C2D-C1D	-4.65	99.48	105.83
15	Y	102	BCL	O2D-CGD-CBD	4.65	119.53	111.27
15	Z	102	BCL	CHD-C4C-NC	4.65	130.24	125.08
15	M	403	BCL	CMB-C2B-C3B	4.65	133.38	124.68
17	L	304	UQ8	C7-C6-C5	4.64	124.07	118.48
15	F	502	BCL	O2D-CGD-CBD	4.64	119.52	111.27
15	D	102	BCL	O2D-CGD-CBD	4.64	119.52	111.27
15	N	101	BCL	C3C-C4C-CHD	-4.64	113.49	123.39
15	0	101	BCL	C3D-C2D-C1D	-4.64	99.50	105.83
15	4	102	BCL	CHD-C4C-NC	4.63	130.22	125.08
15	3	101	BCL	O2D-CGD-CBD	4.62	119.48	111.27
15	T	101	BCL	C3D-C2D-C1D	-4.62	99.52	105.83
15	D	102	BCL	CMB-C2B-C3B	4.62	133.33	124.68
15	B	102	BCL	CHD-C4C-NC	4.62	130.21	125.08
15	X	102	BCL	C3D-C2D-C1D	-4.61	99.53	105.83
15	0	101	BCL	CHD-C4C-NC	4.61	130.20	125.08
15	U	101	BCL	CMB-C2B-C3B	4.61	133.30	124.68
15	G	102	BCL	C3C-C4C-CHD	-4.61	113.55	123.39
15	T	101	BCL	CHD-C4C-NC	4.61	130.19	125.08
15	Z	102	BCL	CMB-C2B-C3B	4.61	133.29	124.68
15	7	101	BCL	CMB-C2B-C3B	4.60	133.29	124.68
15	J	102	BCL	CMB-C2B-C3B	4.59	133.27	124.68
15	N	101	BCL	CMB-C2B-C3B	4.59	133.26	124.68
15	E	102	BCL	CHD-C4C-NC	4.59	130.17	125.08
15	V	101	BCL	CMB-C2B-C3B	4.58	133.25	124.68
22	V	102	CRT	C21-C22-C23	-4.58	120.77	127.31
15	R	101	BCL	C3D-C2D-C1D	-4.58	99.58	105.83
15	0	101	BCL	CMB-C2B-C3B	4.56	133.22	124.68
15	Z	102	BCL	C3C-C4C-CHD	-4.56	113.66	123.39
15	K	102	BCL	CMB-C2B-C3B	4.56	133.20	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	X	102	BCL	CHD-C4C-NC	4.56	130.14	125.08
15	X	102	BCL	CMB-C2B-C3B	4.55	133.20	124.68
15	6	101	BCL	C1D-ND-C4D	-4.53	103.12	106.33
15	J	102	BCL	C3D-C2D-C1D	-4.53	99.65	105.83
15	M	403	BCL	CHD-C4C-NC	4.51	130.09	125.08
15	F	502	BCL	CMB-C2B-C3B	4.51	133.11	124.68
15	M	402	BCL	CMB-C2B-C3B	4.50	133.09	124.68
15	O	502	BCL	CHD-C4C-NC	4.50	130.07	125.08
15	B	102	BCL	CMB-C2B-C3B	4.49	133.08	124.68
15	6	101	BCL	C3C-C4C-CHD	-4.49	113.80	123.39
22	B	103	CRT	C21-C22-C23	-4.48	120.92	127.31
15	2	102	BCL	C3C-C4C-CHD	-4.48	113.83	123.39
15	S	102	BCL	CHD-C4C-NC	4.48	130.05	125.08
15	Z	102	BCL	C1D-ND-C4D	-4.48	103.16	106.33
22	E	103	CRT	C20-C19-C17	-4.47	120.93	127.31
15	L	301	BCL	C3C-C4C-CHD	-4.47	113.85	123.39
15	2	102	BCL	C3D-C2D-C1D	-4.46	99.74	105.83
15	G	102	BCL	CHD-C4C-NC	4.46	130.03	125.08
15	J	102	BCL	C3C-C4C-CHD	-4.45	113.88	123.39
22	Z	103	CRT	C5-C6-C7	-4.44	119.19	125.89
10	C	401	HEM	CHD-C1D-ND	4.43	129.25	124.43
15	X	102	BCL	C1D-ND-C4D	-4.42	103.20	106.33
15	6	101	BCL	CHD-C4C-NC	4.42	129.98	125.08
15	1	402	BCL	CHD-C4C-NC	4.41	129.98	125.08
15	5	102	BCL	CMB-C2B-C3B	4.41	132.93	124.68
15	J	102	BCL	CHD-C4C-NC	4.41	129.98	125.08
15	9	102	BCL	CHD-C4C-NC	4.41	129.97	125.08
15	4	102	BCL	CMB-C2B-C3B	4.41	132.93	124.68
19	M	409	CDL	OA6-CA5-C11	4.41	121.00	111.50
15	L	301	BCL	CMB-C2B-C3B	4.41	132.92	124.68
15	W	101	BCL	CMB-C2B-C3B	4.41	132.92	124.68
15	2	102	BCL	CMB-C2B-C3B	4.40	132.92	124.68
15	R	101	BCL	C3C-C4C-CHD	-4.40	113.99	123.39
15	L	308	BCL	CMB-C2B-C3B	4.39	132.89	124.68
15	L	308	BCL	O2D-CGD-CBD	4.38	119.06	111.27
15	3	101	BCL	CHD-C4C-NC	4.38	129.94	125.08
15	Y	102	BCL	CHD-C4C-NC	4.38	129.94	125.08
15	8	102	BCL	C3C-C4C-CHD	-4.38	114.04	123.39
15	7	101	BCL	O2D-CGD-CBD	4.38	119.05	111.27
15	K	102	BCL	CHD-C4C-NC	4.38	129.94	125.08
22	P	103	CRT	C21-C22-C23	-4.37	121.07	127.31
15	V	101	BCL	C1D-ND-C4D	-4.37	103.23	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	102	CRT	C21-C22-C23	-4.36	121.08	127.31
15	8	102	BCL	CHD-C4C-NC	4.36	129.91	125.08
15	I	101	BCL	C1D-ND-C4D	-4.36	103.24	106.33
15	L	308	BCL	CHD-C4C-NC	4.35	129.91	125.08
15	T	101	BCL	CMB-C2B-C3B	4.33	132.77	124.68
15	P	102	BCL	C1D-ND-C4D	-4.32	103.26	106.33
15	8	102	BCL	CMB-C2B-C3B	4.32	132.76	124.68
19	L	311	CDL	OB6-CB5-C51	4.32	120.81	111.50
15	N	101	BCL	C1D-ND-C4D	-4.32	103.27	106.33
15	Y	102	BCL	C1D-ND-C4D	-4.31	103.27	106.33
15	G	102	BCL	CMB-C2B-C3B	4.31	132.75	124.68
15	F	502	BCL	CHD-C4C-NC	4.31	129.86	125.08
22	Y	101	CRT	C10-C9-C7	-4.30	121.17	127.31
19	L	311	CDL	OA6-CA5-C11	4.29	118.99	111.09
22	T	102	CRT	C21-C22-C23	-4.29	121.18	127.31
15	M	403	BCL	C3C-C4C-CHD	-4.29	114.23	123.39
15	1	402	BCL	O2D-CGD-CBD	4.28	118.88	111.27
15	B	102	BCL	C1-C2-C3	-4.28	118.64	126.04
15	L	308	BCL	C3C-C4C-CHD	-4.28	114.24	123.39
22	M	406	CRT	C39-C38-C37	4.28	117.43	110.86
15	5	102	BCL	CHD-C4C-NC	4.27	129.82	125.08
15	Q	102	BCL	CHD-C4C-NC	4.27	129.82	125.08
18	S	101	LMT	C1B-O5B-C5B	4.26	122.06	113.69
15	O	502	BCL	C3C-C4C-CHD	-4.26	114.30	123.39
15	2	102	BCL	CHD-C4C-NC	4.26	129.81	125.08
15	J	102	BCL	O2D-CGD-CBD	4.26	118.83	111.27
14	L	305	PGV	O01-C1-C2	4.25	120.67	111.50
15	E	102	BCL	O2D-CGD-CBD	4.25	118.82	111.27
22	2	103	CRT	C21-C22-C23	-4.23	121.27	127.31
15	P	102	BCL	CMB-C2B-C3B	4.23	132.59	124.68
15	6	101	BCL	CMB-C2B-C3B	4.23	132.59	124.68
15	R	101	BCL	CMB-C2B-C3B	4.23	132.59	124.68
15	E	102	BCL	C1D-ND-C4D	-4.21	103.34	106.33
22	J	103	CRT	C10-C9-C7	-4.21	121.30	127.31
18	5	101	LMT	C1-O1'-C1'	-4.21	106.86	113.84
15	W	101	BCL	CHD-C4C-NC	4.21	129.75	125.08
15	Q	102	BCL	C1D-ND-C4D	-4.21	103.35	106.33
15	O	502	BCL	CMB-C2B-C3B	4.20	132.54	124.68
15	G	102	BCL	C1D-ND-C4D	-4.20	103.35	106.33
15	A	502	BCL	CHD-C4C-NC	4.20	129.74	125.08
15	M	403	BCL	O2D-CGD-O1D	-4.20	115.63	123.84
15	F	502	BCL	C1D-ND-C4D	-4.19	103.36	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	U	101	BCL	C1D-ND-C4D	-4.19	103.36	106.33
22	J	103	CRT	C21-C22-C23	-4.19	121.33	127.31
22	N	102	CRT	C10-C9-C7	-4.18	121.34	127.31
15	1	402	BCL	C1D-ND-C4D	-4.17	103.37	106.33
15	E	102	BCL	CMB-C2B-C3B	4.16	132.47	124.68
15	I	101	BCL	CHD-C4C-NC	4.16	129.70	125.08
15	B	102	BCL	C1D-ND-C4D	-4.16	103.38	106.33
19	M	407	CDL	OB6-CB5-C51	4.15	120.44	111.50
15	5	102	BCL	C1D-ND-C4D	-4.14	103.39	106.33
15	M	402	BCL	CHD-C4C-NC	4.14	129.68	125.08
19	M	409	CDL	OB6-CB5-C51	4.14	120.42	111.50
15	R	101	BCL	CHD-C4C-NC	4.14	129.67	125.08
15	K	102	BCL	C1D-ND-C4D	-4.13	103.40	106.33
19	D	101	CDL	OA6-CA5-C11	4.13	120.39	111.50
22	T	102	CRT	C5-C6-C7	-4.12	119.67	125.89
15	T	101	BCL	C1D-ND-C4D	-4.12	103.41	106.33
15	3	101	BCL	CMB-C2B-C3B	4.12	132.38	124.68
10	C	402	HEM	CHD-C1D-ND	4.12	128.90	124.43
22	G	103	CRT	C21-C22-C23	-4.11	121.44	127.31
15	O	502	BCL	C1D-ND-C4D	-4.11	103.42	106.33
15	0	101	BCL	C1D-ND-C4D	-4.10	103.42	106.33
22	M	406	CRT	C20-C19-C17	-4.08	121.48	127.31
14	1	401	PGV	O01-C1-C2	4.07	120.28	111.50
15	U	101	BCL	CHD-C4C-NC	4.06	129.59	125.08
15	Y	102	BCL	CMB-C2B-C3B	4.06	132.27	124.68
15	Q	102	BCL	C3C-C4C-CHD	-4.05	114.74	123.39
15	D	102	BCL	C3C-C4C-CHD	-4.04	114.76	123.39
15	W	101	BCL	C1D-ND-C4D	-4.04	103.47	106.33
10	C	404	HEM	CHD-C1D-ND	4.04	128.82	124.43
15	7	101	BCL	CHD-C4C-NC	4.04	129.56	125.08
15	8	102	BCL	C1D-ND-C4D	-4.03	103.47	106.33
15	L	301	BCL	CHD-C4C-NC	4.03	129.55	125.08
15	W	101	BCL	C3C-C4C-CHD	-4.03	114.79	123.39
14	A	501	PGV	O01-C1-C2	4.02	120.17	111.50
15	6	101	BCL	O2D-CGD-CBD	4.02	118.41	111.27
14	F	501	PGV	O01-C1-C2	4.02	120.16	111.50
22	9	101	CRT	C21-C22-C23	-4.02	121.57	127.31
15	4	102	BCL	C1D-ND-C4D	-4.02	103.48	106.33
22	P	103	CRT	C5-C6-C7	-4.02	119.82	125.89
22	N	102	CRT	C20-C19-C17	-4.01	121.58	127.31
15	7	101	BCL	C1D-ND-C4D	-3.99	103.50	106.33
15	A	502	BCL	C1D-ND-C4D	-3.99	103.50	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	402	BCL	C3C-C4C-CHD	-3.99	114.87	123.39
15	S	102	BCL	C3C-C4C-CHD	-3.98	114.88	123.39
15	S	102	BCL	C1D-ND-C4D	-3.98	103.51	106.33
22	6	102	CRT	C10-C9-C7	-3.97	121.65	127.31
15	2	102	BCL	C1D-ND-C4D	-3.96	103.52	106.33
19	H	302	CDL	OB6-CB5-C51	3.96	120.03	111.50
10	C	403	HEM	CHD-C1D-ND	3.95	128.73	124.43
15	9	102	BCL	C1D-ND-C4D	-3.95	103.53	106.33
15	U	101	BCL	C3C-C4C-CHD	-3.94	114.97	123.39
14	M	408	PGV	O01-C1-C2	3.93	119.98	111.50
15	J	102	BCL	C1D-ND-C4D	-3.93	103.54	106.33
22	Z	103	CRT	C10-C9-C7	-3.93	121.70	127.31
21	M	405	MQ8	C45-C43-C44	3.93	121.88	115.27
15	4	102	BCL	O2D-CGD-CBD	3.93	118.25	111.27
15	M	402	BCL	C1D-ND-C4D	-3.92	103.55	106.33
15	L	308	BCL	C1-C2-C3	-3.92	119.26	126.04
15	D	102	BCL	CHD-C4C-NC	3.90	129.41	125.08
15	0	101	BCL	O2D-CGD-CBD	3.90	118.20	111.27
10	C	402	HEM	CBA-CAA-C2A	-3.90	105.97	112.62
15	9	102	BCL	C3C-C4C-CHD	-3.89	115.09	123.39
14	C	408	PGV	O01-C1-C2	3.88	119.86	111.50
10	C	401	HEM	C1B-NB-C4B	3.88	109.08	105.07
22	Z	103	CRT	C21-C22-C23	-3.87	121.79	127.31
10	C	403	HEM	C1B-NB-C4B	3.86	109.06	105.07
22	4	103	CRT	C29-C28-C30	3.86	124.16	118.08
22	T	102	CRT	C10-C9-C7	-3.86	121.81	127.31
15	Y	102	BCL	C3C-C4C-CHD	-3.83	115.20	123.39
15	L	301	BCL	C1D-ND-C4D	-3.83	103.62	106.33
22	6	102	CRT	C20-C19-C17	-3.83	121.85	127.31
15	N	101	BCL	O2D-CGD-CBD	3.82	118.06	111.27
14	L	310	PGV	O01-C1-C2	3.82	119.73	111.50
15	D	102	BCL	C1D-ND-C4D	-3.80	103.64	106.33
15	3	101	BCL	C1D-ND-C4D	-3.80	103.64	106.33
14	A	503	PGV	O01-C1-C2	3.79	119.67	111.50
15	R	101	BCL	C1D-ND-C4D	-3.79	103.64	106.33
22	4	103	CRT	C21-C22-C23	-3.79	121.90	127.31
15	Z	102	BCL	O2D-CGD-CBD	3.78	117.99	111.27
10	C	401	HEM	CHA-C4D-ND	3.77	129.04	124.38
15	A	502	BCL	C3C-C4C-CHD	-3.77	115.34	123.39
15	5	102	BCL	C1-C2-C3	-3.76	119.53	126.04
10	C	402	HEM	C1B-NB-C4B	3.76	108.96	105.07
22	9	101	CRT	C8-C7-C6	3.75	123.98	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	V	101	BCL	C1-C2-C3	-3.74	119.58	126.04
15	B	102	BCL	O2D-CGD-CBD	3.73	117.90	111.27
15	2	102	BCL	O2D-CGD-CBD	3.71	117.87	111.27
15	6	101	BCL	C4-C3-C5	3.70	121.49	115.27
19	D	101	CDL	OB6-CB5-C51	3.69	119.45	111.50
22	Y	101	CRT	C20-C19-C17	-3.68	122.05	127.31
14	Q	101	PGV	O01-C1-C2	3.68	119.44	111.50
15	1	402	BCL	C3C-C4C-CHD	-3.68	115.53	123.39
15	K	102	BCL	C3C-C4C-CHD	-3.66	115.57	123.39
15	F	502	BCL	C3C-C4C-CHD	-3.65	115.59	123.39
15	G	102	BCL	O2D-CGD-CBD	3.64	117.73	111.27
15	0	101	BCL	C1-C2-C3	-3.63	119.76	126.04
15	P	102	BCL	O2D-CGD-CBD	3.62	117.70	111.27
15	P	102	BCL	C1-C2-C3	-3.61	119.80	126.04
15	8	102	BCL	O2D-CGD-CBD	3.61	117.67	111.27
22	Z	103	CRT	C20-C19-C17	-3.60	122.18	127.31
15	Q	102	BCL	C4-C3-C5	3.59	121.30	115.27
18	5	101	LMT	O1'-C1'-C2'	3.58	113.90	108.30
22	2	103	CRT	C20-C19-C17	-3.58	122.20	127.31
14	L	306	PGV	O01-C1-C2	3.56	119.17	111.50
15	I	101	BCL	C3D-C4D-ND	3.56	115.99	110.24
22	Y	101	CRT	C5-C6-C7	-3.55	120.52	125.89
15	M	403	BCL	C1D-ND-C4D	-3.55	103.82	106.33
10	C	403	HEM	CHA-C4D-ND	3.54	128.76	124.38
10	C	402	HEM	CHB-C1B-NB	3.53	128.75	124.38
18	G	101	LMT	C1B-O1B-C4'	-3.53	109.24	117.96
15	T	101	BCL	O2D-CGD-CBD	3.52	117.53	111.27
15	K	102	BCL	C1-C2-C3	-3.52	119.96	126.04
19	H	302	CDL	OA6-CA5-C11	3.51	119.07	111.50
10	C	404	HEM	C1B-NB-C4B	3.51	108.70	105.07
15	X	102	BCL	O2D-CGD-CBD	3.50	117.50	111.27
15	Y	102	BCL	C1-C2-C3	-3.50	119.99	126.04
17	L	303	UQ8	C7-C8-C9	-3.49	120.97	126.79
10	C	404	HEM	CHA-C4D-ND	3.49	128.70	124.38
15	M	402	BCL	C3D-C4D-ND	3.49	115.89	110.24
15	I	101	BCL	C3C-C4C-CHD	-3.48	115.97	123.39
15	7	101	BCL	C3C-C4C-CHD	-3.47	115.99	123.39
17	L	303	UQ8	C12-C13-C14	-3.46	119.33	127.66
15	7	101	BCL	C1-C2-C3	-3.45	120.08	126.04
15	5	102	BCL	C3C-C4C-CHD	-3.43	116.06	123.39
15	6	101	BCL	C3D-C4D-ND	3.42	115.77	110.24
22	J	103	CRT	C5-C6-C7	-3.42	120.72	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	308	BCL	C1D-ND-C4D	-3.42	103.91	106.33
15	Q	102	BCL	C3D-C4D-ND	3.41	115.76	110.24
17	L	304	UQ8	C7-C8-C9	-3.41	121.11	126.79
15	X	102	BCL	C3D-C4D-ND	3.41	115.75	110.24
15	R	101	BCL	O2D-CGD-CBD	3.41	117.32	111.27
15	Y	102	BCL	C3D-C4D-ND	3.41	115.75	110.24
10	C	401	HEM	CBA-CAA-C2A	-3.40	106.82	112.62
22	E	103	CRT	C26-C27-C28	-3.40	122.46	127.31
22	P	103	CRT	C20-C19-C17	-3.40	122.46	127.31
15	3	101	BCL	C3C-C4C-CHD	-3.39	116.15	123.39
15	Z	102	BCL	C3D-C4D-ND	3.38	115.71	110.24
15	F	502	BCL	C3D-C4D-ND	3.38	115.70	110.24
10	C	401	HEM	CHB-C1B-NB	3.38	128.56	124.38
22	T	102	CRT	C20-C19-C17	-3.37	122.50	127.31
15	I	101	BCL	C1-C2-C3	-3.37	120.22	126.04
15	T	101	BCL	C1C-NC-C4C	-3.37	105.19	106.71
10	C	402	HEM	CHA-C4D-ND	3.36	128.53	124.38
15	R	101	BCL	C1C-NC-C4C	-3.36	105.19	106.71
15	1	402	BCL	C3D-C4D-ND	3.36	115.67	110.24
22	Z	103	CRT	C15-C14-C12	-3.36	122.52	127.31
15	V	101	BCL	C3D-C4D-ND	3.35	115.66	110.24
15	U	101	BCL	C3D-C4D-ND	3.34	115.64	110.24
22	P	103	CRT	C15-C14-C12	-3.33	122.56	127.31
15	N	101	BCL	C4-C3-C5	3.33	120.87	115.27
15	7	101	BCL	C3D-C4D-ND	3.33	115.62	110.24
15	W	101	BCL	C3D-C4D-ND	3.32	115.61	110.24
15	K	102	BCL	C3D-C4D-ND	3.32	115.61	110.24
15	1	402	BCL	C4-C3-C5	3.32	120.85	115.27
15	5	102	BCL	C3D-C4D-ND	3.31	115.59	110.24
22	9	101	CRT	C10-C9-C7	-3.31	122.59	127.31
15	X	102	BCL	C1-C2-C3	-3.31	120.32	126.04
17	L	303	UQ8	C15-C14-C16	3.31	120.83	115.27
15	L	308	BCL	C3D-C4D-ND	3.31	115.59	110.24
22	G	103	CRT	C32-C31-C30	-3.30	112.91	123.22
15	J	102	BCL	C3D-C4D-ND	3.30	115.58	110.24
15	4	102	BCL	C3D-C4D-ND	3.30	115.57	110.24
15	G	102	BCL	C3D-C4D-ND	3.30	115.57	110.24
15	V	101	BCL	O2D-CGD-CBD	3.29	117.11	111.27
15	N	101	BCL	C3D-C4D-ND	3.28	115.54	110.24
15	D	102	BCL	C3D-C4D-ND	3.28	115.54	110.24
15	O	502	BCL	C3D-C4D-ND	3.27	115.53	110.24
14	F	501	PGV	C02-O01-C1	-3.27	109.73	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	102	BCL	C3D-C4D-ND	3.27	115.53	110.24
15	A	502	BCL	C3D-C4D-ND	3.27	115.53	110.24
17	L	304	UQ8	C37-C38-C39	-3.27	119.79	127.66
15	2	102	BCL	C3D-C4D-ND	3.26	115.51	110.24
22	P	103	CRT	C32-C31-C30	-3.25	113.06	123.22
15	3	101	BCL	C1C-NC-C4C	-3.25	105.24	106.71
15	E	102	BCL	C3D-C4D-ND	3.25	115.49	110.24
17	L	309	UQ8	C7-C8-C9	-3.25	121.39	126.79
22	V	102	CRT	O2-C38-C39	-3.25	86.65	108.97
21	M	405	MQ8	C34-C33-C35	3.24	120.73	115.27
15	T	101	BCL	C3D-C4D-ND	3.24	115.48	110.24
15	P	102	BCL	C3D-C4D-ND	3.24	115.48	110.24
15	2	102	BCL	C4-C3-C5	3.24	120.72	115.27
22	M	406	CRT	C10-C9-C7	-3.23	122.70	127.31
22	9	101	CRT	C20-C19-C17	-3.22	122.71	127.31
15	R	101	BCL	C3D-C4D-ND	3.22	115.45	110.24
15	M	403	BCL	C3D-C4D-ND	3.22	115.44	110.24
19	M	407	CDL	OA8-CA7-C31	3.22	119.81	111.38
15	0	101	BCL	C3D-C4D-ND	3.21	115.43	110.24
22	M	406	CRT	O2-C38-C40	-3.20	86.96	108.97
15	Z	102	BCL	C1-C2-C3	-3.20	120.51	126.04
15	3	101	BCL	C4-C3-C5	3.19	120.64	115.27
15	S	102	BCL	C3D-C4D-ND	3.19	115.40	110.24
15	8	102	BCL	C3D-C4D-ND	3.19	115.40	110.24
21	M	405	MQ8	C41-C42-C43	-3.18	120.00	127.66
17	L	304	UQ8	C27-C28-C29	-3.18	120.00	127.66
15	J	102	BCL	C4-C3-C5	3.17	120.60	115.27
15	L	301	BCL	O2D-CGD-CBD	3.15	116.87	111.27
15	M	402	BCL	C1C-NC-C4C	-3.15	105.29	106.71
17	L	304	UQ8	C17-C18-C19	-3.15	120.09	127.66
15	3	101	BCL	C3D-C4D-ND	3.13	115.31	110.24
22	Y	101	CRT	C21-C22-C23	-3.13	122.84	127.31
15	8	102	BCL	O2A-CGA-CBA	3.13	121.72	111.91
15	L	301	BCL	CED-O2D-CGD	3.13	123.01	115.94
15	L	301	BCL	O2A-CGA-CBA	3.12	121.71	111.91
22	J	103	CRT	C20-C19-C17	-3.12	122.85	127.31
22	T	102	CRT	C15-C14-C12	-3.12	122.86	127.31
22	B	103	CRT	C5-C6-C7	-3.12	121.18	125.89
10	C	404	HEM	CHB-C1B-NB	3.11	128.22	124.38
15	8	102	BCL	C1-C2-C3	-3.11	120.67	126.04
14	A	503	PGV	C02-O01-C1	-3.11	110.14	117.79
15	O	502	BCL	CHC-C1C-NC	3.09	128.79	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	102	CRT	C20-C19-C17	-3.09	122.90	127.31
21	M	405	MQ8	C29-C28-C30	3.09	120.46	115.27
17	L	304	UQ8	C1M-C1-C6	-3.08	119.38	124.40
15	D	102	BCL	CHC-C1C-NC	3.07	128.76	124.51
15	E	102	BCL	C1C-NC-C4C	-3.07	105.32	106.71
22	B	103	CRT	C32-C31-C30	-3.07	113.64	123.22
15	9	102	BCL	C3D-C4D-ND	3.07	115.20	110.24
21	M	405	MQ8	C36-C37-C38	-3.07	120.28	127.66
15	U	101	BCL	C4-C3-C5	3.06	120.42	115.27
22	6	102	CRT	C32-C31-C30	-3.06	113.68	123.22
15	4	102	BCL	CHB-C4A-NA	3.05	128.73	124.51
15	L	301	BCL	C3D-C4D-ND	3.05	115.17	110.24
22	6	102	CRT	C21-C22-C23	-3.04	122.97	127.31
15	A	502	BCL	C4-C3-C5	3.03	120.36	115.27
15	Q	102	BCL	C1-C2-C3	-3.03	120.81	126.04
15	M	403	BCL	CAA-C2A-C3A	-3.03	104.49	112.78
15	X	102	BCL	CHB-C4A-NA	3.02	128.69	124.51
17	L	303	UQ8	C10-C9-C11	3.02	120.34	115.27
15	Y	102	BCL	CHC-C1C-NC	3.02	128.68	124.51
15	B	102	BCL	C1C-NC-C4C	-3.01	105.35	106.71
22	Z	103	CRT	C31-C32-C33	-3.01	123.01	127.31
15	S	102	BCL	C4-C3-C5	3.01	120.34	115.27
15	0	101	BCL	CHB-C4A-NA	3.01	128.68	124.51
15	N	101	BCL	C1C-NC-C4C	-3.01	105.35	106.71
15	K	102	BCL	C4-C3-C5	3.01	120.33	115.27
15	2	102	BCL	O2A-CGA-CBA	3.00	121.34	111.91
22	2	103	CRT	O2-C38-C40	-3.00	88.31	108.97
15	X	102	BCL	O2A-CGA-CBA	3.00	121.33	111.91
17	L	304	UQ8	C15-C14-C16	3.00	120.32	115.27
15	R	101	BCL	C4-C3-C5	3.00	120.31	115.27
15	L	308	BCL	C1C-NC-C4C	-2.99	105.36	106.71
15	B	102	BCL	C4-C3-C5	2.99	120.30	115.27
15	G	102	BCL	O2A-CGA-CBA	2.99	121.29	111.91
22	V	102	CRT	O2-C38-C40	-2.99	88.43	108.97
22	2	103	CRT	O2-C38-C39	-2.98	88.45	108.97
22	4	103	CRT	C36-C35-C33	-2.98	121.39	125.89
17	L	309	UQ8	C25-C24-C26	2.98	120.28	115.27
15	A	502	BCL	C1C-NC-C4C	-2.97	105.37	106.71
15	L	301	BCL	C4-C3-C5	2.97	120.27	115.27
15	6	101	BCL	O2A-CGA-CBA	2.97	121.22	111.91
17	L	304	UQ8	C12-C13-C14	-2.96	120.53	127.66
17	L	304	UQ8	C10-C9-C11	2.96	120.25	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	V	101	BCL	C4-C3-C5	2.96	120.25	115.27
15	M	402	BCL	C1-C2-C3	-2.96	120.93	126.04
22	9	101	CRT	C8-C7-C9	-2.95	118.79	122.92
22	P	103	CRT	C10-C9-C7	-2.95	123.10	127.31
22	0	102	CRT	C32-C31-C30	-2.95	114.01	123.22
22	9	101	CRT	C32-C31-C30	-2.95	114.02	123.22
14	L	305	PGV	C02-O01-C1	-2.94	110.54	117.79
15	T	101	BCL	CHB-C4A-NA	2.94	128.58	124.51
15	V	101	BCL	CHB-C4A-NA	2.94	128.58	124.51
22	R	102	CRT	C13-C12-C11	2.94	122.70	118.08
22	R	102	CRT	C20-C19-C17	-2.93	123.13	127.31
15	P	102	BCL	C1C-NC-C4C	-2.93	105.39	106.71
22	E	103	CRT	C32-C31-C30	-2.92	114.09	123.22
15	O	502	BCL	C1C-NC-C4C	-2.92	105.39	106.71
18	E	101	LMT	C1B-O1B-C4'	-2.91	110.75	117.96
15	Q	102	BCL	CHC-C1C-NC	2.91	128.54	124.51
14	L	310	PGV	O03-C19-C20	2.91	121.04	111.91
15	I	101	BCL	C4-C3-C5	2.91	120.17	115.27
15	Y	102	BCL	C4-C3-C5	2.91	120.16	115.27
14	H	301	PGV	C02-O01-C1	-2.90	110.65	117.79
14	M	408	PGV	C02-O01-C1	-2.90	110.65	117.79
14	A	501	PGV	C02-O01-C1	-2.90	110.66	117.79
14	H	301	PGV	O03-C19-C20	2.89	120.99	111.91
15	4	102	BCL	C1-C2-C3	-2.89	121.04	126.04
19	L	311	CDL	CB4-OB6-CB5	-2.89	110.67	117.79
15	2	102	BCL	C1-C2-C3	-2.89	121.05	126.04
19	M	407	CDL	OA6-CA5-C11	2.89	118.85	110.80
15	U	101	BCL	C1-C2-C3	-2.88	121.05	126.04
15	E	102	BCL	O2A-CGA-CBA	2.88	120.94	111.91
17	L	304	UQ8	C35-C34-C36	2.88	120.11	115.27
15	M	403	BCL	O2A-CGA-CBA	2.87	120.92	111.91
22	V	102	CRT	C9-C10-C11	-2.87	114.26	123.22
19	M	409	CDL	OB8-CB7-C71	2.87	120.90	111.91
15	J	102	BCL	C1-C2-C3	-2.86	121.09	126.04
15	F	502	BCL	C4-C3-C5	2.86	120.08	115.27
15	W	101	BCL	CHC-C1C-NC	2.86	128.46	124.51
15	N	101	BCL	CHC-C1C-NC	2.86	128.46	124.51
14	Q	101	PGV	O03-C19-C20	2.85	120.87	111.91
15	0	101	BCL	C4-C3-C5	2.85	120.07	115.27
15	L	301	BCL	C1-C2-C3	-2.85	121.12	126.04
22	R	102	CRT	C32-C31-C30	-2.85	114.33	123.22
10	C	403	HEM	CHB-C1B-NB	2.85	127.90	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	8	102	BCL	C4-C3-C5	2.85	120.06	115.27
17	L	309	UQ8	C20-C19-C21	2.85	120.06	115.27
17	L	304	UQ8	C6-C1-C2	2.84	121.43	119.18
17	L	303	UQ8	C1M-C1-C6	-2.84	119.77	124.40
22	R	102	CRT	C9-C10-C11	-2.84	114.36	123.22
14	H	301	PGV	O01-C1-O02	-2.84	116.84	123.70
17	L	309	UQ8	C12-C13-C14	-2.84	120.82	127.66
15	9	102	BCL	C1C-NC-C4C	-2.84	105.43	106.71
15	N	101	BCL	O2A-CGA-CBA	2.83	120.80	111.91
17	L	304	UQ8	C32-C33-C34	-2.83	120.84	127.66
22	J	103	CRT	C32-C31-C30	-2.83	114.38	123.22
15	W	101	BCL	C4-C3-C5	2.83	120.03	115.27
22	4	103	CRT	C10-C9-C7	-2.83	123.27	127.31
15	Y	102	BCL	O2A-CGA-CBA	2.83	120.78	111.91
15	M	403	BCL	C4A-NA-C1A	2.82	107.97	106.71
15	7	101	BCL	CHC-C1C-NC	2.82	128.41	124.51
19	H	302	CDL	OB8-CB7-C71	2.82	120.75	111.91
21	M	405	MQ8	C16-C17-C18	-2.82	120.88	127.66
14	L	306	PGV	O03-C19-C20	2.81	120.74	111.91
22	M	406	CRT	C32-C31-C30	-2.81	114.44	123.22
15	5	102	BCL	C4-C3-C5	2.81	120.00	115.27
15	G	102	BCL	C4-C3-C5	2.81	120.00	115.27
15	G	102	BCL	CHB-C4A-NA	2.81	128.40	124.51
15	V	101	BCL	O2A-CGA-CBA	2.81	120.73	111.91
22	E	103	CRT	C9-C10-C11	-2.81	114.46	123.22
22	V	102	CRT	C14-C15-C16	-2.80	114.47	123.22
15	U	101	BCL	CHC-C1C-NC	2.80	128.39	124.51
15	8	102	BCL	CHB-C4A-NA	2.80	128.38	124.51
22	0	102	CRT	C10-C9-C7	-2.80	123.32	127.31
18	4	104	LMT	C1B-O1B-C4'	-2.80	111.05	117.96
15	1	402	BCL	CHC-C1C-NC	2.79	128.38	124.51
15	0	101	BCL	C1C-NC-C4C	-2.79	105.45	106.71
15	Z	102	BCL	C4-C3-C5	2.79	119.97	115.27
15	2	102	BCL	CHB-C4A-NA	2.79	128.37	124.51
22	E	103	CRT	C14-C15-C16	-2.79	114.51	123.22
15	V	101	BCL	C1C-NC-C4C	-2.79	105.45	106.71
17	L	304	UQ8	C20-C19-C21	2.79	119.96	115.27
22	0	102	CRT	C13-C12-C11	2.79	122.47	118.08
15	3	101	BCL	C4A-NA-C1A	2.79	107.96	106.71
15	Z	102	BCL	O2A-CGA-CBA	2.79	120.65	111.91
19	D	101	CDL	OB8-CB7-C71	2.78	120.63	111.91
22	M	406	CRT	O2-C38-C39	-2.78	89.87	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	S	102	BCL	CHC-C1C-NC	2.78	128.35	124.51
17	L	304	UQ8	C30-C29-C31	2.77	119.94	115.27
17	L	309	UQ8	C10-C9-C11	2.77	119.94	115.27
15	2	102	BCL	C1C-NC-C4C	-2.77	105.46	106.71
15	K	102	BCL	CHC-C1C-NC	2.77	128.34	124.51
15	E	102	BCL	CHB-C4A-NA	2.77	128.34	124.51
21	M	405	MQ8	C19-C18-C20	2.77	119.93	115.27
15	P	102	BCL	CHB-C4A-NA	2.75	128.32	124.51
15	1	402	BCL	C1-C2-C3	-2.75	121.29	126.04
22	T	102	CRT	C32-C31-C30	-2.75	114.65	123.22
15	B	102	BCL	CHB-C4A-NA	2.74	128.30	124.51
15	E	102	BCL	CHC-C1C-NC	2.74	128.30	124.51
17	L	303	UQ8	C25-C24-C26	2.74	120.65	114.60
14	L	305	PGV	O03-C19-C20	2.74	120.49	111.91
15	K	102	BCL	O2D-CGD-O1D	-2.74	118.49	123.84
15	X	102	BCL	C1C-NC-C4C	-2.73	105.48	106.71
15	F	502	BCL	CHC-C1C-NC	2.73	128.29	124.51
15	6	101	BCL	CHB-C4A-NA	2.73	128.29	124.51
15	7	101	BCL	C4-C3-C5	2.73	119.86	115.27
15	5	102	BCL	CHC-C1C-NC	2.73	128.28	124.51
15	E	102	BCL	C4-C3-C5	2.73	119.86	115.27
15	6	101	BCL	C2A-C1A-CHA	-2.73	119.09	123.86
22	M	406	CRT	C14-C15-C16	-2.72	114.73	123.22
15	M	403	BCL	C4-C3-C5	2.72	119.84	115.27
15	P	102	BCL	C4-C3-C5	2.71	119.83	115.27
15	7	101	BCL	CHB-C4A-NA	2.71	128.26	124.51
15	9	102	BCL	CHC-C1C-NC	2.71	128.26	124.51
18	8	101	LMT	C1B-O1B-C4'	-2.71	111.27	117.96
22	B	103	CRT	C20-C19-C17	-2.70	123.45	127.31
15	3	101	BCL	C1-C2-C3	-2.70	121.37	126.04
15	T	101	BCL	C1-C2-C3	-2.70	121.37	126.04
15	O	502	BCL	C4-C3-C5	2.70	119.81	115.27
22	E	103	CRT	C34-C33-C35	2.70	122.33	118.08
15	M	403	BCL	C1-C2-C3	-2.70	121.38	126.04
15	X	102	BCL	CHC-C1C-NC	2.70	128.24	124.51
15	4	102	BCL	O2A-CGA-CBA	2.70	120.37	111.91
15	0	101	BCL	C2A-C1A-CHA	-2.69	119.15	123.86
15	R	101	BCL	C1-C2-C3	-2.69	121.38	126.04
15	I	101	BCL	CHC-C1C-NC	2.69	128.24	124.51
15	Q	102	BCL	O2D-CGD-O1D	-2.69	118.58	123.84
22	0	102	CRT	C18-C17-C16	2.69	122.31	118.08
15	M	402	BCL	CHC-C1C-NC	2.69	128.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	101	BCL	O2A-CGA-CBA	2.68	120.33	111.91
17	L	309	UQ8	C17-C18-C19	-2.68	121.20	127.66
15	G	102	BCL	C1C-NC-C4C	-2.68	105.50	106.71
22	Y	101	CRT	C32-C31-C30	-2.68	114.85	123.22
15	I	101	BCL	O2D-CGD-O1D	-2.68	118.60	123.84
19	M	407	CDL	CB4-OB6-CB5	-2.68	111.20	117.79
14	M	408	PGV	O03-C19-C20	2.67	120.30	111.91
15	F	502	BCL	O2D-CGD-O1D	-2.67	118.61	123.84
22	V	102	CRT	C13-C12-C11	2.67	122.29	118.08
17	L	304	UQ8	C40-C39-C41	2.67	119.77	115.27
18	4	101	LMT	C1B-O1B-C4'	-2.67	111.35	117.96
15	J	102	BCL	O2A-CGA-CBA	2.67	120.29	111.91
15	A	502	BCL	C1-C2-C3	-2.67	121.43	126.04
22	2	103	CRT	C32-C31-C30	-2.67	114.89	123.22
15	V	101	BCL	C2A-C1A-CHA	-2.67	119.20	123.86
15	B	102	BCL	C2A-C1A-CHA	-2.67	119.20	123.86
15	O	502	BCL	O2A-CGA-CBA	2.67	120.27	111.91
15	K	102	BCL	C1C-NC-C4C	-2.66	105.51	106.71
21	M	405	MQ8	C31-C32-C33	-2.66	121.26	127.66
15	D	102	BCL	C1C-NC-C4C	-2.66	105.51	106.71
15	E	102	BCL	C1-C2-C3	-2.66	121.45	126.04
15	O	502	BCL	O2D-CGD-O1D	-2.66	118.65	123.84
22	J	103	CRT	C14-C15-C16	-2.65	114.95	123.22
18	S	101	LMT	C3'-C4'-C5'	-2.65	104.85	110.93
15	G	102	BCL	C1-C2-C3	-2.64	121.47	126.04
18	2	101	LMT	C1-O1'-C1'	-2.64	109.46	113.84
15	J	102	BCL	O2D-CGD-O1D	-2.64	118.68	123.84
15	3	101	BCL	CHC-C1C-NC	2.64	128.16	124.51
18	S	101	LMT	O1B-C1B-C2B	2.64	114.93	108.10
15	I	101	BCL	CHB-C4A-NA	2.64	128.16	124.51
15	R	101	BCL	CHB-C4A-NA	2.64	128.16	124.51
15	G	102	BCL	CHC-C1C-NC	2.64	128.16	124.51
15	B	102	BCL	CHC-C1C-NC	2.63	128.15	124.51
15	M	402	BCL	C1D-CHD-C4C	-2.63	120.27	126.62
15	9	102	BCL	C1-C2-C3	-2.63	121.49	126.04
15	7	101	BCL	O2A-CGA-CBA	2.63	120.16	111.91
14	A	503	PGV	O03-C19-C20	2.63	120.16	111.91
15	5	102	BCL	C4A-NA-C1A	2.63	107.89	106.71
22	0	102	CRT	C14-C15-C16	-2.63	115.02	123.22
22	V	102	CRT	C26-C27-C28	-2.63	123.56	127.31
22	E	103	CRT	C21-C20-C19	-2.62	118.10	123.47
22	V	102	CRT	C32-C31-C30	-2.62	115.04	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	309	UQ8	C30-C29-C28	-2.62	116.96	123.68
15	4	102	BCL	C1C-NC-C4C	-2.62	105.53	106.71
15	V	101	BCL	C1-O2A-CGA	2.61	123.30	116.44
22	Y	101	CRT	C14-C15-C16	-2.61	115.06	123.22
15	R	101	BCL	C2A-C1A-CHA	-2.61	119.30	123.86
15	J	102	BCL	CHB-C4A-NA	2.61	128.12	124.51
15	F	502	BCL	CHB-C4A-NA	2.60	128.11	124.51
10	C	403	HEM	CBA-CAA-C2A	-2.60	108.18	112.62
15	1	402	BCL	O2A-CGA-CBA	2.60	120.07	111.91
15	S	102	BCL	C1C-NC-C4C	-2.59	105.54	106.71
22	J	103	CRT	C8-C7-C9	-2.59	119.29	122.92
22	9	101	CRT	C34-C33-C35	2.59	122.16	118.08
15	3	101	BCL	C1D-CHD-C4C	-2.59	120.37	126.62
15	N	101	BCL	CHB-C4A-NA	2.59	128.09	124.51
17	L	304	UQ8	C42-C43-C44	-2.59	118.90	127.75
15	8	102	BCL	C1C-NC-C4C	-2.59	105.54	106.71
17	L	309	UQ8	C22-C23-C24	-2.59	121.43	127.66
15	K	102	BCL	O2A-CGA-CBA	2.59	120.02	111.91
14	A	501	PGV	O03-C19-C20	2.58	120.01	111.91
15	U	101	BCL	O2A-CGA-CBA	2.58	120.01	111.91
15	T	101	BCL	CHC-C1C-NC	2.58	128.08	124.51
22	9	101	CRT	C5-C6-C7	2.58	129.78	125.89
15	Z	102	BCL	CHB-C4A-NA	2.58	128.07	124.51
15	J	102	BCL	CHC-C1C-NC	2.58	128.07	124.51
18	Z	101	LMT	C1-O1'-C1'	-2.57	109.58	113.84
15	S	102	BCL	O2D-CGD-O1D	-2.57	118.81	123.84
15	6	101	BCL	O2D-CGD-O1D	-2.57	118.81	123.84
15	P	102	BCL	C2A-C1A-CHA	-2.57	119.37	123.86
15	R	101	BCL	CHC-C1C-NC	2.57	128.06	124.51
15	8	102	BCL	CHC-C1C-NC	2.57	128.06	124.51
15	L	308	BCL	O2A-CGA-CBA	2.57	119.97	111.91
15	M	402	BCL	C4-C3-C5	2.57	119.59	115.27
15	J	102	BCL	C2A-C1A-CHA	-2.57	119.37	123.86
15	X	102	BCL	C4-C3-C5	2.56	119.58	115.27
15	0	101	BCL	CHC-C1C-NC	2.56	128.05	124.51
22	B	103	CRT	C14-C15-C16	-2.56	115.24	123.22
21	M	405	MQ8	C50-C48-C49	2.56	120.25	114.60
21	M	405	MQ8	C26-C27-C28	-2.55	121.51	127.66
22	V	102	CRT	C5-C6-C7	-2.55	122.03	125.89
22	N	102	CRT	C32-C31-C30	-2.55	115.25	123.22
22	B	103	CRT	C29-C28-C30	2.55	122.10	118.08
15	2	102	BCL	CHC-C1C-NC	2.55	128.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	6	101	BCL	CHC-C1C-NC	2.55	128.04	124.51
21	M	405	MQ8	C21-C22-C23	-2.55	121.52	127.66
15	5	102	BCL	CHB-C4A-NA	2.55	128.03	124.51
15	X	102	BCL	C2A-C1A-CHA	-2.54	119.41	123.86
15	Z	102	BCL	CHC-C1C-NC	2.54	128.03	124.51
22	B	103	CRT	C34-C33-C35	2.54	122.08	118.08
15	J	102	BCL	C1C-NC-C4C	-2.54	105.56	106.71
22	4	103	CRT	C21-C20-C19	-2.54	118.27	123.47
19	M	409	CDL	CA4-OA6-CA5	-2.54	111.54	117.79
18	T	103	LMT	C1B-O1B-C4'	-2.54	111.68	117.96
22	4	103	CRT	C31-C30-C28	2.54	133.54	126.42
22	Y	101	CRT	C26-C27-C28	-2.54	123.69	127.31
18	P	104	LMT	C1B-O1B-C4'	-2.53	111.69	117.96
17	L	309	UQ8	C37-C38-C39	-2.53	121.56	127.66
15	4	102	BCL	C2A-C1A-CHA	-2.53	119.43	123.86
22	0	102	CRT	C21-C20-C19	-2.53	118.29	123.47
15	N	101	BCL	C1-C2-C3	-2.53	121.67	126.04
15	D	102	BCL	O2D-CGD-O1D	-2.53	118.90	123.84
15	7	101	BCL	C1C-NC-C4C	-2.53	105.57	106.71
15	S	102	BCL	C1-C2-C3	-2.52	121.68	126.04
18	5	101	LMT	O1B-C4'-C3'	2.52	114.00	107.28
18	B	101	LMT	C1B-O1B-C4'	-2.52	111.72	117.96
15	P	102	BCL	CHC-C1C-NC	2.52	128.00	124.51
15	9	102	BCL	O2A-CGA-CBA	2.52	119.82	111.91
17	L	303	UQ8	C20-C19-C21	2.52	119.51	115.27
15	3	101	BCL	O2A-CGA-CBA	2.52	119.81	111.91
15	6	101	BCL	C1-C2-C3	-2.52	121.69	126.04
15	G	102	BCL	C2A-C1A-CHA	-2.52	119.46	123.86
15	Y	102	BCL	CHB-C4A-NA	2.51	127.99	124.51
15	M	403	BCL	CHB-C4A-NA	2.51	127.98	124.51
15	9	102	BCL	CHB-C4A-NA	2.51	127.98	124.51
14	1	401	PGV	O03-C19-C20	2.50	119.75	111.91
15	U	101	BCL	O2D-CGD-O1D	-2.50	118.95	123.84
22	0	102	CRT	C27-C26-C25	-2.50	115.43	123.22
22	0	102	CRT	C34-C33-C35	2.49	122.00	118.08
15	U	101	BCL	CMD-C2D-C3D	-2.48	121.90	127.61
22	6	102	CRT	C34-C33-C35	2.48	121.99	118.08
15	9	102	BCL	O2D-CGD-O1D	-2.48	118.98	123.84
21	M	405	MQ8	C14-C13-C15	2.48	119.44	115.27
15	I	101	BCL	C2A-C1A-CHA	-2.48	119.53	123.86
15	2	102	BCL	C4A-NA-C1A	2.48	107.82	106.71
15	Z	102	BCL	C2A-C1A-CHA	-2.48	119.53	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	103	CRT	C18-C17-C16	2.48	121.98	118.08
15	4	102	BCL	C4-C3-C5	2.47	119.42	115.27
15	L	301	BCL	C1C-NC-C4C	-2.46	105.60	106.71
15	F	502	BCL	O2A-CGA-CBA	2.46	119.64	111.91
15	2	102	BCL	C2A-C1A-CHA	-2.46	119.55	123.86
15	E	102	BCL	C2A-C1A-CHA	-2.46	119.55	123.86
15	3	101	BCL	O2D-CGD-O1D	-2.46	119.03	123.84
22	0	102	CRT	C5-C6-C7	-2.46	122.18	125.89
15	T	101	BCL	C4-C3-C5	2.45	119.40	115.27
22	P	103	CRT	C34-C33-C35	2.45	121.94	118.08
15	D	102	BCL	C1-C2-C3	-2.45	121.80	126.04
22	0	102	CRT	C20-C19-C17	-2.45	123.81	127.31
17	L	309	UQ8	C40-C39-C41	2.45	119.40	115.27
15	9	102	BCL	C1D-CHD-C4C	-2.45	120.71	126.62
17	L	303	UQ8	C17-C18-C19	-2.45	121.77	127.66
15	D	102	BCL	C4-C3-C5	2.45	119.39	115.27
15	W	101	BCL	O2D-CGD-O1D	-2.45	119.05	123.84
17	L	309	UQ8	C15-C14-C16	2.44	119.38	115.27
15	M	403	BCL	C1D-CHD-C4C	-2.44	120.73	126.62
15	L	301	BCL	O2A-CGA-O1A	-2.44	117.43	123.59
15	5	102	BCL	C1C-NC-C4C	-2.44	105.61	106.71
22	R	102	CRT	C21-C20-C19	-2.44	118.48	123.47
15	L	301	BCL	CHC-C1C-NC	2.44	127.88	124.51
15	X	102	BCL	C4A-NA-C1A	2.44	107.80	106.71
17	L	309	UQ8	C1M-C1-C6	-2.44	120.42	124.40
15	M	402	BCL	O2D-CGD-O1D	-2.44	119.08	123.84
10	C	401	HEM	CHD-C1D-C2D	-2.43	121.18	124.98
15	Z	102	BCL	C1C-NC-C4C	-2.43	105.61	106.71
22	B	103	CRT	C13-C12-C11	2.42	121.90	118.08
19	L	311	CDL	OB8-CB7-C71	2.42	119.51	111.91
15	P	102	BCL	O2A-CGA-CBA	2.41	119.48	111.91
15	7	101	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
18	5	101	LMT	O1B-C4'-C5'	-2.41	102.84	109.45
15	8	102	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
22	B	103	CRT	C9-C10-C11	-2.41	115.69	123.22
22	V	102	CRT	C11-C12-C14	-2.41	115.24	118.94
15	D	102	BCL	CHB-C4A-NA	2.41	127.84	124.51
15	A	502	BCL	CHC-C1C-NC	2.41	127.84	124.51
15	5	102	BCL	C1D-CHD-C4C	-2.41	120.81	126.62
18	L	307	LMT	C1B-O1B-C4'	-2.41	112.00	117.96
15	Z	102	BCL	O2D-CGD-O1D	-2.40	119.14	123.84
15	T	101	BCL	C2A-C1A-CHA	-2.40	119.66	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	101	CRT	C27-C26-C25	-2.40	115.72	123.22
15	O	502	BCL	C1-C2-C3	-2.40	121.89	126.04
15	E	102	BCL	C1D-CHD-C4C	-2.40	120.83	126.62
22	T	102	CRT	C27-C26-C25	-2.40	115.73	123.22
22	0	102	CRT	C29-C28-C30	2.40	121.86	118.08
15	K	102	BCL	C1D-CHD-C4C	-2.40	120.84	126.62
15	8	102	BCL	C2A-C1A-CHA	-2.40	119.67	123.86
15	5	102	BCL	O2D-CGD-O1D	-2.40	119.15	123.84
15	B	102	BCL	C1D-CHD-C4C	-2.40	120.84	126.62
22	R	102	CRT	C14-C15-C16	-2.39	115.75	123.22
10	C	401	HEM	C4D-ND-C1D	2.39	107.54	105.07
15	K	102	BCL	C4A-NA-C1A	2.39	107.78	106.71
22	2	103	CRT	C26-C27-C28	-2.39	123.90	127.31
15	E	102	BCL	O2D-CGD-O1D	-2.39	119.17	123.84
15	P	102	BCL	C1-O2A-CGA	2.39	122.70	116.44
19	M	409	CDL	OA8-CA7-C31	2.38	119.39	111.91
22	V	102	CRT	C34-C33-C35	2.38	121.83	118.08
22	B	103	CRT	C10-C9-C7	-2.38	123.91	127.31
18	J	104	LMT	C1B-O1B-C4'	-2.38	112.07	117.96
15	T	101	BCL	C1D-CHD-C4C	-2.38	120.88	126.62
15	A	502	BCL	O2D-CGD-O1D	-2.38	119.19	123.84
15	A	502	BCL	CHB-C4A-NA	2.38	127.80	124.51
10	C	402	HEM	CHD-C1D-C2D	-2.38	121.27	124.98
15	3	101	BCL	CMD-C2D-C3D	-2.37	122.15	127.61
15	N	101	BCL	C1D-CHD-C4C	-2.37	120.90	126.62
18	P	101	LMT	C1B-O1B-C4'	-2.37	112.10	117.96
15	1	402	BCL	C1C-NC-C4C	-2.37	105.64	106.71
15	6	101	BCL	C1C-NC-C4C	-2.37	105.64	106.71
22	T	102	CRT	C36-C35-C33	-2.37	122.32	125.89
15	V	101	BCL	CHC-C1C-NC	2.36	127.78	124.51
15	K	102	BCL	C2A-C1A-CHA	-2.36	119.73	123.86
15	B	102	BCL	CED-O2D-CGD	2.36	121.28	115.94
15	7	101	BCL	C1D-CHD-C4C	-2.36	120.93	126.62
15	Q	102	BCL	CHB-C4A-NA	2.36	127.77	124.51
15	Y	102	BCL	C1C-NC-C4C	-2.36	105.65	106.71
15	T	101	BCL	CED-O2D-CGD	2.35	121.26	115.94
19	H	302	CDL	OA8-CA7-C31	2.35	119.29	111.91
17	L	309	UQ8	C27-C26-C24	-2.35	105.25	112.98
10	C	401	HEM	CHA-C4D-C3D	-2.35	120.92	125.33
15	1	402	BCL	C1D-CHD-C4C	-2.35	120.96	126.62
15	S	102	BCL	C1D-CHD-C4C	-2.35	120.96	126.62
15	P	102	BCL	C1D-CHD-C4C	-2.34	120.97	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3	101	BCL	CHB-C4A-NA	2.34	127.75	124.51
15	4	102	BCL	C1D-CHD-C4C	-2.34	120.97	126.62
10	C	403	HEM	CHD-C1D-C2D	-2.34	121.32	124.98
15	X	102	BCL	O2D-CGD-O1D	-2.34	119.26	123.84
18	M	411	LMT	C1B-O1B-C4'	-2.34	112.17	117.96
15	Z	102	BCL	C1D-CHD-C4C	-2.34	120.97	126.62
15	4	102	BCL	O2D-CGD-O1D	-2.34	119.26	123.84
14	F	501	PGV	O03-C19-C20	2.34	119.26	111.91
15	M	402	BCL	O1D-CGD-CBD	-2.34	119.69	124.48
22	R	102	CRT	C29-C28-C30	2.34	121.77	118.08
22	R	102	CRT	C18-C17-C16	2.34	121.76	118.08
22	N	102	CRT	C21-C20-C19	-2.34	118.69	123.47
10	C	404	HEM	CHD-C1D-C2D	-2.33	121.34	124.98
17	L	304	UQ8	C22-C23-C24	-2.33	122.05	127.66
22	4	103	CRT	C32-C31-C30	2.33	130.49	123.22
22	Z	103	CRT	C36-C35-C33	-2.33	122.37	125.89
15	F	502	BCL	CMD-C2D-C3D	-2.33	122.26	127.61
15	U	101	BCL	CHB-C4A-NA	2.33	127.73	124.51
15	0	101	BCL	O2D-CGD-O1D	-2.33	119.29	123.84
15	M	403	BCL	CMD-C2D-C3D	-2.33	122.26	127.61
15	0	101	BCL	C1D-CHD-C4C	-2.33	121.01	126.62
15	W	101	BCL	C1-C2-C3	-2.32	122.02	126.04
15	P	102	BCL	O2D-CGD-O1D	-2.32	119.30	123.84
18	2	101	LMT	C1B-O1B-C4'	-2.32	112.22	117.96
15	L	308	BCL	CHC-C1C-NC	2.32	127.72	124.51
15	Q	102	BCL	CMD-C2D-C3D	-2.32	122.28	127.61
15	T	101	BCL	C1-O2A-CGA	2.32	122.53	116.44
14	L	305	PGV	O01-C1-O02	-2.32	118.10	123.70
15	4	102	BCL	CHC-C1C-NC	2.31	127.71	124.51
15	F	502	BCL	C1-C2-C3	-2.31	122.04	126.04
22	6	102	CRT	C21-C20-C19	-2.31	118.73	123.47
15	K	102	BCL	CMD-C2D-C3D	-2.31	122.29	127.61
15	S	102	BCL	O2A-CGA-CBA	2.31	119.16	111.91
22	E	103	CRT	C18-C17-C16	2.31	121.72	118.08
22	9	101	CRT	C35-C33-C32	-2.31	115.40	118.94
15	R	101	BCL	C1-O2A-CGA	2.31	122.50	116.44
14	F	501	PGV	O14-P-O13	2.31	119.71	110.68
15	A	502	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
22	2	103	CRT	C34-C33-C35	2.30	121.70	118.08
22	N	102	CRT	C13-C12-C11	2.30	121.70	118.08
15	R	101	BCL	CED-O2D-CGD	2.30	121.14	115.94
19	M	409	CDL	CB4-OB6-CB5	-2.30	112.13	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Q	102	BCL	C2A-C1A-CHA	-2.30	119.84	123.86
14	M	408	PGV	O14-P-O13	2.30	119.68	110.68
14	C	408	PGV	O03-C19-C20	2.29	119.11	111.91
22	6	102	CRT	C35-C33-C32	-2.29	115.42	118.94
15	L	308	BCL	C4A-NA-C1A	2.29	107.74	106.71
15	9	102	BCL	CMD-C2D-C3D	-2.29	122.34	127.61
15	O	502	BCL	C4B-CHC-C1C	-2.29	125.58	130.12
15	Y	102	BCL	CMD-C2D-C3D	-2.29	122.35	127.61
17	L	309	UQ8	C46-C44-C45	2.29	119.65	114.60
22	4	103	CRT	C30-C28-C27	-2.28	115.44	118.94
15	A	502	BCL	O2A-CGA-CBA	2.28	119.08	111.91
15	K	102	BCL	CHB-C4A-NA	2.28	127.67	124.51
15	B	102	BCL	O2D-CGD-O1D	-2.28	119.37	123.84
15	M	402	BCL	O2A-CGA-CBA	2.28	119.07	111.91
15	L	308	BCL	O2D-CGD-O1D	-2.28	119.38	123.84
15	T	101	BCL	C4A-NA-C1A	2.28	107.73	106.71
22	R	102	CRT	C11-C12-C14	-2.28	115.45	118.94
18	M	410	LMT	C1B-O1B-C4'	-2.28	112.33	117.96
21	M	405	MQ8	C24-C23-C25	2.27	119.10	115.27
22	Z	103	CRT	C26-C27-C28	-2.27	124.07	127.31
22	E	103	CRT	C13-C12-C11	2.27	121.66	118.08
15	L	308	BCL	C4-C3-C5	2.27	119.09	115.27
15	L	308	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
15	V	101	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
15	I	101	BCL	O2A-CGA-CBA	2.26	119.02	111.91
22	J	103	CRT	C18-C17-C16	2.26	121.64	118.08
15	E	102	BCL	C4A-NA-C1A	2.26	107.72	106.71
15	T	101	BCL	O2D-CGD-O1D	-2.26	119.42	123.84
15	D	102	BCL	O2A-CGA-CBA	2.26	119.00	111.91
15	5	102	BCL	CMD-C2D-C3D	-2.26	122.42	127.61
22	B	103	CRT	C30-C28-C27	-2.25	115.48	118.94
22	Z	103	CRT	C32-C31-C30	-2.25	116.20	123.22
14	Q	101	PGV	O14-P-O13	2.25	119.48	110.68
10	C	404	HEM	C4D-ND-C1D	2.25	107.39	105.07
15	Y	102	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
15	2	102	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
15	R	101	BCL	O2D-CGD-O1D	-2.24	119.45	123.84
15	R	101	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
15	L	308	BCL	C4B-CHC-C1C	-2.24	125.68	130.12
22	6	102	CRT	C9-C10-C11	-2.24	116.23	123.22
15	8	102	BCL	C1D-CHD-C4C	-2.24	121.22	126.62
22	V	102	CRT	C27-C26-C25	-2.24	116.24	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	103	CRT	C34-C33-C35	2.24	121.60	118.08
15	Y	102	BCL	O2D-CGD-O1D	-2.23	119.47	123.84
18	Z	101	LMT	O1'-C1'-C2'	2.23	111.79	108.30
15	N	101	BCL	C4A-NA-C1A	2.23	107.71	106.71
15	G	102	BCL	O2D-CGD-O1D	-2.23	119.48	123.84
15	F	502	BCL	C1D-CHD-C4C	-2.23	121.25	126.62
15	8	102	BCL	O2A-CGA-O1A	-2.23	117.97	123.59
15	L	301	BCL	C1D-CHD-C4C	-2.23	121.25	126.62
22	G	103	CRT	C20-C19-C17	-2.22	124.14	127.31
14	L	310	PGV	C02-O01-C1	-2.22	112.32	117.79
22	N	102	CRT	C34-C33-C35	2.22	121.57	118.08
15	J	102	BCL	C1D-CHD-C4C	-2.22	121.27	126.62
19	L	311	CDL	OA8-CA7-C31	2.22	118.87	111.91
15	Y	102	BCL	C2A-C1A-CHA	-2.22	119.98	123.86
22	P	103	CRT	C35-C33-C32	-2.22	115.54	118.94
10	C	403	HEM	C4D-ND-C1D	2.21	107.36	105.07
22	B	103	CRT	C21-C20-C19	-2.21	118.94	123.47
15	1	402	BCL	CMD-C2D-C3D	-2.21	122.53	127.61
22	Y	101	CRT	C34-C33-C35	2.21	121.56	118.08
15	Q	102	BCL	O2A-CGA-CBA	2.21	118.83	111.91
18	S	101	LMT	O5B-C5B-C4B	2.21	113.70	109.69
19	H	302	CDL	CB4-OB6-CB5	-2.21	112.36	117.79
22	N	102	CRT	C8-C7-C9	-2.20	119.84	122.92
15	M	403	BCL	O2A-CGA-O1A	-2.20	118.05	123.59
10	C	402	HEM	C4D-ND-C1D	2.20	107.34	105.07
22	V	102	CRT	C29-C28-C30	2.20	121.54	118.08
22	E	103	CRT	C20-C21-C22	-2.20	118.97	123.47
15	6	101	BCL	C1D-CHD-C4C	-2.20	121.32	126.62
19	M	407	CDL	OB6-CB5-OB7	-2.20	118.39	123.70
22	T	102	CRT	C21-C20-C19	-2.20	118.98	123.47
15	U	101	BCL	C2A-C1A-CHA	-2.19	120.02	123.86
17	L	304	UQ8	C42-C41-C39	-2.19	105.77	112.98
15	X	102	BCL	C1D-CHD-C4C	-2.19	121.34	126.62
22	N	102	CRT	C15-C14-C12	-2.19	124.19	127.31
15	9	102	BCL	C4-C3-C5	2.19	118.95	115.27
15	2	102	BCL	O2D-CGD-O1D	-2.19	119.56	123.84
15	L	301	BCL	C2A-C1A-CHA	-2.19	120.03	123.86
22	N	102	CRT	C26-C27-C28	-2.19	124.19	127.31
22	9	101	CRT	C15-C14-C12	-2.19	124.19	127.31
15	I	101	BCL	CMD-C2D-C3D	-2.19	122.58	127.61
22	P	103	CRT	C29-C28-C30	2.18	121.52	118.08
22	T	102	CRT	C14-C15-C16	-2.18	116.41	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	N	101	BCL	O2D-CGD-O1D	-2.18	119.58	123.84
10	C	404	HEM	CHA-C4D-C3D	-2.18	121.24	125.33
15	M	403	BCL	CHC-C1C-NC	2.18	127.52	124.51
10	C	402	HEM	CHA-C4D-C3D	-2.17	121.25	125.33
15	D	102	BCL	CMD-C2D-C3D	-2.17	122.62	127.61
18	H	303	LMT	O5'-C5'-C6'	2.17	111.83	106.44
22	J	103	CRT	C21-C20-C19	-2.17	119.04	123.47
22	N	102	CRT	C14-C15-C16	-2.17	116.46	123.22
15	S	102	BCL	CHB-C4A-NA	2.16	127.50	124.51
14	1	401	PGV	C02-O01-C1	-2.16	112.47	117.79
22	4	103	CRT	C5-C6-C7	-2.16	122.62	125.89
15	N	101	BCL	C2A-C1A-CHA	-2.16	120.08	123.86
22	4	103	CRT	C27-C26-C25	-2.16	116.48	123.22
22	E	103	CRT	C29-C28-C30	2.16	121.48	118.08
15	1	402	BCL	CED-O2D-CGD	2.16	120.82	115.94
22	V	102	CRT	C21-C20-C19	-2.16	119.05	123.47
22	6	102	CRT	C15-C14-C12	-2.16	124.23	127.31
15	M	402	BCL	CHB-C4A-NA	2.16	127.49	124.51
15	B	102	BCL	O2A-CGA-CBA	2.15	118.67	111.91
22	G	103	CRT	C14-C15-C16	-2.15	116.50	123.22
15	5	102	BCL	O2A-CGA-CBA	2.15	118.66	111.91
10	C	403	HEM	CHA-C4D-C3D	-2.15	121.29	125.33
15	O	502	BCL	CHB-C4A-NA	2.15	127.48	124.51
15	W	101	BCL	C1D-CHD-C4C	-2.15	121.44	126.62
22	G	103	CRT	C29-C28-C30	2.15	121.46	118.08
17	L	304	UQ8	C46-C44-C45	2.15	119.34	114.60
15	7	101	BCL	C4A-NA-C1A	2.14	107.67	106.71
15	V	101	BCL	CED-O2D-CGD	2.14	120.78	115.94
21	M	405	MQ8	C39-C38-C40	2.14	118.87	115.27
16	L	302	BPH	CMA-C3A-C4A	-2.14	109.69	114.38
14	1	401	PGV	O01-C1-O02	-2.14	118.54	123.70
15	G	102	BCL	C1D-CHD-C4C	-2.13	121.47	126.62
15	P	102	BCL	C11-C12-C13	-2.13	109.03	115.92
22	B	103	CRT	C27-C26-C25	-2.13	116.57	123.22
21	M	405	MQ8	C41-C40-C38	-2.13	105.99	112.98
15	4	102	BCL	CED-O2D-CGD	2.13	120.74	115.94
15	I	101	BCL	C1D-CHD-C4C	-2.12	121.50	126.62
15	0	101	BCL	CED-O2D-CGD	2.12	120.74	115.94
15	K	102	BCL	C4B-CHC-C1C	-2.12	125.92	130.12
15	8	102	BCL	CED-O2D-CGD	2.12	120.73	115.94
15	L	301	BCL	CHB-C4A-NA	2.12	127.44	124.51
15	2	102	BCL	C4D-CHA-C1A	-2.12	118.67	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	408	PGV	O01-C1-O02	-2.12	118.58	123.70
15	M	402	BCL	C2A-C1A-CHA	-2.12	120.16	123.86
15	9	102	BCL	C4A-NA-C1A	2.12	107.66	106.71
22	E	103	CRT	C27-C26-C25	-2.11	116.62	123.22
15	W	101	BCL	CMD-C2D-C3D	-2.11	122.76	127.61
15	3	101	BCL	CED-O2D-CGD	2.11	120.71	115.94
15	M	403	BCL	C1C-NC-C4C	-2.11	105.76	106.71
10	C	402	HEM	CAD-CBD-CGD	-2.11	109.06	113.60
15	F	502	BCL	C2A-C1A-CHA	-2.11	120.17	123.86
10	C	401	HEM	CBD-CAD-C3D	-2.11	106.77	112.63
15	D	102	BCL	C1-O2A-CGA	2.11	121.98	116.44
10	C	403	HEM	O2D-CGD-CBD	2.11	120.80	114.03
22	P	103	CRT	C13-C12-C14	-2.11	119.97	122.92
15	2	102	BCL	O2A-CGA-O1A	-2.11	118.28	123.59
22	R	102	CRT	C27-C26-C25	-2.10	116.65	123.22
18	8	103	LMT	C3'-C4'-C5'	-2.10	106.11	110.93
15	A	502	BCL	C2A-C1A-CHA	-2.10	120.19	123.86
22	N	102	CRT	C24-C23-C22	-2.10	119.98	122.92
22	6	102	CRT	C27-C26-C25	-2.10	116.67	123.22
15	L	308	BCL	CHD-C1D-C2D	2.10	129.88	125.48
22	J	103	CRT	C29-C28-C30	2.10	121.38	118.08
17	L	303	UQ8	C22-C23-C24	-2.09	120.60	127.75
22	4	103	CRT	C15-C14-C12	-2.09	124.32	127.31
22	6	102	CRT	C26-C27-C28	-2.09	124.33	127.31
22	6	102	CRT	C29-C28-C30	2.09	121.36	118.08
18	R	103	LMT	C1B-O1B-C4'	-2.09	112.80	117.96
22	T	102	CRT	C8-C7-C9	-2.08	120.00	122.92
22	G	103	CRT	C35-C33-C32	-2.08	115.74	118.94
22	T	102	CRT	C34-C33-C35	2.08	121.36	118.08
15	B	102	BCL	C1-O2A-CGA	2.08	121.91	116.44
22	G	103	CRT	C21-C20-C19	-2.08	119.21	123.47
14	A	503	PGV	O03-C19-O04	-2.08	118.35	123.59
15	W	101	BCL	CHB-C4A-NA	2.08	127.39	124.51
15	1	402	BCL	O2D-CGD-O1D	-2.07	119.79	123.84
22	P	103	CRT	C27-C26-C25	-2.07	116.75	123.22
15	R	101	BCL	O2A-CGA-CBA	2.07	118.40	111.91
15	L	301	BCL	CMD-C2D-C3D	-2.07	122.86	127.61
22	4	103	CRT	C14-C15-C16	-2.07	116.77	123.22
22	R	102	CRT	C34-C33-C35	2.07	121.33	118.08
22	E	103	CRT	C11-C12-C14	-2.07	115.77	118.94
15	V	101	BCL	O2D-CGD-O1D	-2.06	119.80	123.84
22	T	102	CRT	C29-C28-C30	2.06	121.33	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	402	BCL	C4B-CHC-C1C	-2.06	126.04	130.12
15	G	102	BCL	O2A-CGA-O1A	-2.06	118.40	123.59
16	M	404	BPH	CMA-C3A-C4A	-2.05	109.88	114.38
15	3	101	BCL	C4B-CHC-C1C	-2.05	126.05	130.12
18	X	101	LMT	C1-O1'-C1'	-2.05	110.44	113.84
15	D	102	BCL	C1D-CHD-C4C	-2.05	121.68	126.62
18	X	101	LMT	C1B-O1B-C4'	-2.05	112.89	117.96
15	Y	102	BCL	C4B-CHC-C1C	-2.05	126.06	130.12
22	N	102	CRT	C35-C33-C32	-2.05	115.80	118.94
22	0	102	CRT	C24-C23-C25	2.04	121.29	118.08
15	O	502	BCL	CMD-C2D-C3D	-2.04	122.92	127.61
18	5	101	LMT	O5'-C5'-C4'	2.04	114.05	109.75
22	T	102	CRT	C31-C32-C33	-2.04	124.40	127.31
10	C	402	HEM	CHB-C1B-C2B	-2.04	121.08	126.72
22	0	102	CRT	C9-C10-C11	-2.04	116.86	123.22
15	S	102	BCL	CMD-C2D-C3D	-2.04	122.93	127.61
15	G	102	BCL	CED-O2D-CGD	2.03	120.54	115.94
22	0	102	CRT	C16-C17-C19	-2.03	115.82	118.94
22	B	103	CRT	C20-C21-C22	-2.03	119.32	123.47
22	9	101	CRT	C21-C20-C19	-2.02	119.33	123.47
15	W	101	BCL	O1D-CGD-CBD	-2.02	120.35	124.48
15	J	102	BCL	C4D-CHA-C1A	-2.02	118.79	121.25
15	0	101	BCL	C4D-CHA-C1A	-2.02	118.79	121.25
19	M	409	CDL	OB8-CB7-OB9	-2.02	118.49	123.59
15	D	102	BCL	CAC-C3C-C2C	-2.02	109.22	114.26
15	P	102	BCL	C4A-NA-C1A	2.02	107.61	106.71
22	M	406	CRT	C5-C6-C7	-2.02	122.84	125.89
22	Y	101	CRT	C29-C28-C30	2.02	121.25	118.08
15	O	502	BCL	C1D-CHD-C4C	-2.01	121.76	126.62
15	X	102	BCL	CED-O2D-CGD	2.01	120.49	115.94
15	M	403	BCL	CHD-C1D-C2D	2.01	129.70	125.48
22	V	102	CRT	C18-C17-C16	2.01	121.25	118.08
15	W	101	BCL	C11-C12-C13	-2.01	109.42	115.92
22	P	103	CRT	C30-C28-C27	-2.01	115.86	118.94
22	J	103	CRT	C26-C27-C28	-2.01	124.44	127.31
15	7	101	BCL	CMD-C2D-C3D	-2.01	123.00	127.61
22	0	102	CRT	C30-C28-C27	-2.00	115.86	118.94
15	Z	102	BCL	C11-C10-C8	-2.00	109.44	115.92
15	O	502	BCL	O2A-CGA-O1A	-2.00	118.54	123.59
15	D	102	BCL	C2A-C1A-CHA	-2.00	120.36	123.86

There are no chirality outliers.

All (1053) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	401	HEM	C2B-C3B-CAB-CBB
10	C	402	HEM	C2B-C3B-CAB-CBB
10	C	403	HEM	C2B-C3B-CAB-CBB
10	C	403	HEM	C4B-C3B-CAB-CBB
10	C	404	HEM	C2B-C3B-CAB-CBB
14	L	305	PGV	C03-O11-P-O13
14	L	305	PGV	C04-O12-P-O13
14	L	305	PGV	O12-C04-C05-C06
14	L	306	PGV	C04-O12-P-O14
14	L	310	PGV	C03-O11-P-O12
14	L	310	PGV	C03-O11-P-O14
14	L	310	PGV	C04-O12-P-O14
14	H	301	PGV	C04-C05-C06-O06
14	A	501	PGV	C03-O11-P-O13
14	A	501	PGV	C03-O11-P-O14
14	A	501	PGV	C04-O12-P-O11
14	A	501	PGV	C04-O12-P-O13
14	A	501	PGV	O02-C1-O01-C02
14	A	501	PGV	C2-C1-O01-C02
14	A	503	PGV	C04-O12-P-O13
14	Q	101	PGV	C03-O11-P-O12
14	Q	101	PGV	C03-O11-P-O14
15	M	403	BCL	CAD-CBD-CGD-O1D
15	M	403	BCL	CAD-CBD-CGD-O2D
15	A	502	BCL	C2C-C3C-CAC-CBC
15	D	102	BCL	C2C-C3C-CAC-CBC
15	D	102	BCL	C4C-C3C-CAC-CBC
15	E	102	BCL	C6-C7-C8-C9
15	F	502	BCL	C4-C3-C5-C6
15	G	102	BCL	C4C-C3C-CAC-CBC
15	G	102	BCL	C11-C12-C13-C14
15	J	102	BCL	C1A-C2A-CAA-CBA
15	N	101	BCL	C2C-C3C-CAC-CBC
15	N	101	BCL	C4C-C3C-CAC-CBC
15	N	101	BCL	C2-C3-C5-C6
15	N	101	BCL	C4-C3-C5-C6
15	O	502	BCL	C1A-C2A-CAA-CBA
15	O	502	BCL	C3A-C2A-CAA-CBA
15	O	502	BCL	C4C-C3C-CAC-CBC
15	Q	102	BCL	C2C-C3C-CAC-CBC
15	Q	102	BCL	C4C-C3C-CAC-CBC
15	R	101	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
15	R	101	BCL	C4C-C3C-CAC-CBC
15	R	101	BCL	C2-C3-C5-C6
15	R	101	BCL	C4-C3-C5-C6
15	S	102	BCL	C4-C3-C5-C6
15	T	101	BCL	C1A-C2A-CAA-CBA
15	T	101	BCL	C3A-C2A-CAA-CBA
15	T	101	BCL	O1A-CGA-O2A-C1
15	T	101	BCL	C6-C7-C8-C9
15	U	101	BCL	C2C-C3C-CAC-CBC
15	U	101	BCL	C4C-C3C-CAC-CBC
15	V	101	BCL	C1A-C2A-CAA-CBA
15	W	101	BCL	C1A-C2A-CAA-CBA
15	W	101	BCL	C2C-C3C-CAC-CBC
15	W	101	BCL	C4C-C3C-CAC-CBC
15	X	102	BCL	C1A-C2A-CAA-CBA
15	Z	102	BCL	C2C-C3C-CAC-CBC
15	Z	102	BCL	C4C-C3C-CAC-CBC
15	Z	102	BCL	C6-C7-C8-C9
15	2	102	BCL	C1A-C2A-CAA-CBA
15	2	102	BCL	C2-C3-C5-C6
15	2	102	BCL	C4-C3-C5-C6
15	2	102	BCL	C11-C10-C8-C9
15	3	101	BCL	C1A-C2A-CAA-CBA
15	3	101	BCL	C2C-C3C-CAC-CBC
15	4	102	BCL	C6-C7-C8-C9
15	6	101	BCL	C2C-C3C-CAC-CBC
15	6	101	BCL	C4C-C3C-CAC-CBC
15	8	102	BCL	C1A-C2A-CAA-CBA
15	0	101	BCL	C3A-C2A-CAA-CBA
17	L	304	UQ8	C9-C11-C12-C13
17	L	304	UQ8	C1-C6-C7-C8
17	L	304	UQ8	C5-C6-C7-C8
17	L	309	UQ8	C40-C39-C41-C42
17	L	309	UQ8	C38-C39-C41-C42
17	L	309	UQ8	C35-C34-C36-C37
17	L	309	UQ8	C19-C21-C22-C23
18	M	411	LMT	O5'-C1'-O1'-C1
18	H	303	LMT	O5'-C1'-O1'-C1
18	J	104	LMT	O5'-C1'-O1'-C1
19	L	311	CDL	CA2-OA2-PA1-OA5
19	L	311	CDL	CA3-OA5-PA1-OA3
19	M	407	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
19	M	407	CDL	CB2-OB2-PB2-OB3
19	M	407	CDL	CB2-OB2-PB2-OB4
19	M	407	CDL	CB3-OB5-PB2-OB2
19	M	409	CDL	CA2-OA2-PA1-OA4
19	M	409	CDL	CB3-OB5-PB2-OB3
19	M	409	CDL	CB3-OB5-PB2-OB4
19	M	409	CDL	OB5-CB3-CB4-OB6
19	H	302	CDL	O1-C1-CB2-OB2
19	H	302	CDL	CA3-OA5-PA1-OA2
19	H	302	CDL	CA3-OA5-PA1-OA3
19	H	302	CDL	CB3-OB5-PB2-OB4
19	D	101	CDL	O1-C1-CB2-OB2
19	D	101	CDL	CA2-OA2-PA1-OA3
19	D	101	CDL	CA2-OA2-PA1-OA4
19	D	101	CDL	CA3-OA5-PA1-OA4
19	D	101	CDL	C11-CA5-OA6-CA4
19	D	101	CDL	CB3-OB5-PB2-OB2
19	D	101	CDL	CB3-OB5-PB2-OB3
21	M	405	MQ8	C42-C43-C44-C46
21	M	405	MQ8	C45-C43-C44-C46
22	M	406	CRT	C32-C33-C35-C36
22	M	406	CRT	C34-C33-C35-C36
22	M	406	CRT	C36-C37-C38-C39
22	B	103	CRT	C5-C6-C7-C8
22	B	103	CRT	C5-C6-C7-C9
22	E	103	CRT	C2-C1-O1-C1M
22	E	103	CRT	C36-C37-C38-C39
22	E	103	CRT	C36-C37-C38-C40
22	G	103	CRT	C5-C6-C7-C8
22	G	103	CRT	C5-C6-C7-C9
22	G	103	CRT	C40-C38-O2-C2M
22	J	103	CRT	C2-C1-O1-C1M
22	J	103	CRT	O1-C1-C4-C5
22	J	103	CRT	C2-C1-C4-C5
22	J	103	CRT	C3-C1-C4-C5
22	J	103	CRT	C40-C38-O2-C2M
22	N	102	CRT	C2-C1-C4-C5
22	N	102	CRT	C3-C1-C4-C5
22	N	102	CRT	C36-C37-C38-C39
22	N	102	CRT	C36-C37-C38-C40
22	N	102	CRT	C36-C37-C38-O2
22	P	103	CRT	C2-C1-O1-C1M

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Mol	Chain	Res	Type	Atoms
22	P	103	CRT	C10-C11-C12-C13
22	P	103	CRT	C10-C11-C12-C14
22	P	103	CRT	C15-C16-C17-C18
22	P	103	CRT	C15-C16-C17-C19
22	T	102	CRT	O1-C1-C4-C5
22	T	102	CRT	C2-C1-C4-C5
22	T	102	CRT	C3-C1-C4-C5
22	T	102	CRT	C10-C11-C12-C13
22	T	102	CRT	C10-C11-C12-C14
22	T	102	CRT	C15-C16-C17-C18
22	T	102	CRT	C15-C16-C17-C19
22	V	102	CRT	O1-C1-C4-C5
22	V	102	CRT	C2-C1-C4-C5
22	V	102	CRT	C3-C1-C4-C5
22	V	102	CRT	C36-C37-C38-C39
22	V	102	CRT	C36-C37-C38-C40
22	Y	101	CRT	C10-C11-C12-C13
22	Y	101	CRT	C10-C11-C12-C14
22	Z	103	CRT	C2-C1-C4-C5
22	Z	103	CRT	C3-C1-C4-C5
22	Z	103	CRT	C10-C11-C12-C13
22	Z	103	CRT	C10-C11-C12-C14
22	Z	103	CRT	C32-C33-C35-C36
22	Z	103	CRT	C34-C33-C35-C36
22	Z	103	CRT	C36-C37-C38-C39
22	2	103	CRT	C5-C6-C7-C8
22	2	103	CRT	C5-C6-C7-C9
22	2	103	CRT	C36-C37-C38-C40
22	4	103	CRT	C5-C6-C7-C8
22	4	103	CRT	C5-C6-C7-C9
22	6	102	CRT	C2-C1-C4-C5
22	6	102	CRT	C5-C6-C7-C8
22	6	102	CRT	C5-C6-C7-C9
22	9	101	CRT	C5-C6-C7-C8
22	9	101	CRT	C5-C6-C7-C9
19	L	311	CDL	C11-CA5-OA6-CA4
18	5	101	LMT	C3'-C4'-O1B-C1B
18	S	101	LMT	C2B-C1B-O1B-C4'
19	L	311	CDL	OA7-CA5-OA6-CA4
15	T	101	BCL	CBA-CGA-O2A-C1
15	4	102	BCL	CBD-CGD-O2D-CED
15	7	101	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	L	310	PGV	O04-C19-O03-C01
15	B	102	BCL	CBD-CGD-O2D-CED
15	S	102	BCL	CBD-CGD-O2D-CED
19	D	101	CDL	OA7-CA5-OA6-CA4
15	A	502	BCL	C3-C5-C6-C7
15	E	102	BCL	C3-C5-C6-C7
15	U	101	BCL	C3-C5-C6-C7
14	L	310	PGV	C20-C19-O03-C01
18	E	101	LMT	O5B-C5B-C6B-O6B
18	L	307	LMT	O5B-C5B-C6B-O6B
15	I	101	BCL	C4-C3-C5-C6
15	1	402	BCL	C4-C3-C5-C6
15	0	101	BCL	C4-C3-C5-C6
15	I	101	BCL	C2-C3-C5-C6
15	S	102	BCL	C2-C3-C5-C6
17	L	309	UQ8	C33-C34-C36-C37
15	E	102	BCL	C2A-CAA-CBA-CGA
15	N	101	BCL	C2A-CAA-CBA-CGA
15	Z	102	BCL	C2A-CAA-CBA-CGA
15	6	101	BCL	C2A-CAA-CBA-CGA
15	D	102	BCL	C3-C5-C6-C7
14	A	503	PGV	C20-C19-O03-C01
14	A	503	PGV	O04-C19-O03-C01
15	0	101	BCL	O1A-CGA-O2A-C1
19	D	101	CDL	OA9-CA7-OA8-CA6
18	L	307	LMT	C4B-C5B-C6B-O6B
15	L	308	BCL	CBD-CGD-O2D-CED
15	J	102	BCL	CBD-CGD-O2D-CED
14	L	306	PGV	O12-C04-C05-O05
19	L	311	CDL	O1-C1-CA2-OA2
15	Z	102	BCL	C3-C5-C6-C7
15	0	101	BCL	CBA-CGA-O2A-C1
19	D	101	CDL	C31-CA7-OA8-CA6
15	I	101	BCL	CBD-CGD-O2D-CED
18	P	101	LMT	O5B-C5B-C6B-O6B
18	E	101	LMT	C4B-C5B-C6B-O6B
18	M	410	LMT	O5'-C5'-C6'-O6'
15	Q	102	BCL	C4-C3-C5-C6
15	3	101	BCL	C4-C3-C5-C6
15	F	502	BCL	C2-C3-C5-C6
15	Q	102	BCL	C2-C3-C5-C6
15	3	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	R	103	LMT	O5'-C1'-O1'-C1
18	T	103	LMT	O5'-C1'-O1'-C1
17	L	303	UQ8	C19-C21-C22-C23
17	L	309	UQ8	C39-C41-C42-C43
17	L	309	UQ8	C24-C26-C27-C28
15	W	101	BCL	CBA-CGA-O2A-C1
15	T	101	BCL	CBD-CGD-O2D-CED
15	7	101	BCL	O1D-CGD-O2D-CED
19	D	101	CDL	CA2-C1-CB2-OB2
15	W	101	BCL	O1A-CGA-O2A-C1
15	K	102	BCL	CBA-CGA-O2A-C1
15	U	101	BCL	CBA-CGA-O2A-C1
14	1	401	PGV	C19-C20-C21-C22
15	0	101	BCL	C10-C11-C12-C13
14	M	408	PGV	O01-C02-C03-O11
15	J	102	BCL	C5-C6-C7-C8
15	U	101	BCL	C10-C11-C12-C13
19	M	407	CDL	O1-C1-CB2-OB2
15	1	402	BCL	C2-C3-C5-C6
15	0	101	BCL	C2-C3-C5-C6
15	L	308	BCL	C11-C10-C8-C9
15	B	102	BCL	C11-C10-C8-C9
15	G	102	BCL	C6-C7-C8-C9
15	G	102	BCL	C11-C10-C8-C9
15	I	101	BCL	C11-C10-C8-C9
15	J	102	BCL	C6-C7-C8-C9
15	N	101	BCL	C11-C10-C8-C9
15	P	102	BCL	C11-C10-C8-C9
15	R	101	BCL	C6-C7-C8-C9
15	R	101	BCL	C11-C10-C8-C9
15	V	101	BCL	C6-C7-C8-C9
15	X	102	BCL	C6-C7-C8-C9
15	Z	102	BCL	C11-C12-C13-C14
15	6	101	BCL	C6-C7-C8-C9
15	6	101	BCL	C11-C10-C8-C9
15	8	102	BCL	C11-C12-C13-C14
15	9	102	BCL	C11-C10-C8-C9
15	P	102	BCL	C8-C10-C11-C12
15	G	102	BCL	C2A-CAA-CBA-CGA
22	B	103	CRT	C15-C16-C17-C18
19	D	101	CDL	CA5-C11-C12-C13
15	K	102	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	U	101	BCL	O1A-CGA-O2A-C1
15	A	502	BCL	C10-C11-C12-C13
15	O	502	BCL	C10-C11-C12-C13
15	S	102	BCL	C5-C6-C7-C8
15	F	502	BCL	C10-C11-C12-C13
15	O	502	BCL	C5-C6-C7-C8
15	O	502	BCL	C8-C10-C11-C12
15	6	101	BCL	C5-C6-C7-C8
15	6	101	BCL	C15-C16-C17-C18
15	7	101	BCL	C5-C6-C7-C8
15	E	102	BCL	C13-C15-C16-C17
15	G	102	BCL	C5-C6-C7-C8
15	W	101	BCL	C5-C6-C7-C8
15	Z	102	BCL	C5-C6-C7-C8
15	3	101	BCL	C5-C6-C7-C8
15	5	102	BCL	C5-C6-C7-C8
15	5	102	BCL	C15-C16-C17-C18
15	4	102	BCL	O1D-CGD-O2D-CED
14	M	408	PGV	C19-C20-C21-C22
19	M	409	CDL	CA5-C11-C12-C13
19	M	409	CDL	C52-C53-C54-C55
15	B	102	BCL	C5-C6-C7-C8
15	B	102	BCL	C15-C16-C17-C18
15	D	102	BCL	C10-C11-C12-C13
15	F	502	BCL	C15-C16-C17-C18
15	A	502	BCL	C13-C15-C16-C17
15	W	101	BCL	C10-C11-C12-C13
15	L	301	BCL	C11-C10-C8-C7
15	I	101	BCL	C6-C7-C8-C10
15	N	101	BCL	C6-C7-C8-C10
15	X	102	BCL	C6-C7-C8-C10
15	X	102	BCL	C11-C10-C8-C7
15	Y	102	BCL	C11-C10-C8-C7
15	4	102	BCL	C11-C10-C8-C7
15	0	101	BCL	C6-C7-C8-C10
15	S	102	BCL	C3-C5-C6-C7
15	J	102	BCL	C2A-CAA-CBA-CGA
15	S	102	BCL	O1D-CGD-O2D-CED
15	T	101	BCL	C5-C6-C7-C8
18	2	101	LMT	O5'-C1'-O1'-C1
15	B	102	BCL	O1D-CGD-O2D-CED
17	L	303	UQ8	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	L	309	UQ8	C34-C36-C37-C38
17	L	309	UQ8	C14-C16-C17-C18
14	L	305	PGV	O12-C04-C05-O05
15	P	102	BCL	C3-C5-C6-C7
15	T	101	BCL	C10-C11-C12-C13
15	0	101	BCL	C15-C16-C17-C18
15	E	102	BCL	C5-C6-C7-C8
15	E	102	BCL	C10-C11-C12-C13
15	P	102	BCL	C5-C6-C7-C8
15	U	101	BCL	C5-C6-C7-C8
15	Y	102	BCL	C5-C6-C7-C8
15	2	102	BCL	C15-C16-C17-C18
18	L	307	LMT	C4-C5-C6-C7
18	P	101	LMT	C4-C5-C6-C7
15	F	502	BCL	C13-C15-C16-C17
15	N	101	BCL	C8-C10-C11-C12
15	V	101	BCL	C10-C11-C12-C13
15	2	102	BCL	C13-C15-C16-C17
15	4	102	BCL	C15-C16-C17-C18
14	H	301	PGV	C04-O12-P-O11
14	A	501	PGV	C03-O11-P-O12
19	L	311	CDL	CB3-OB5-PB2-OB2
19	M	407	CDL	CA2-OA2-PA1-OA5
19	M	407	CDL	CB2-OB2-PB2-OB5
19	M	409	CDL	CA2-OA2-PA1-OA5
19	M	409	CDL	CA3-OA5-PA1-OA2
19	M	409	CDL	CB3-OB5-PB2-OB2
19	H	302	CDL	CB3-OB5-PB2-OB2
19	D	101	CDL	CA2-OA2-PA1-OA5
19	D	101	CDL	CA3-OA5-PA1-OA2
19	D	101	CDL	CB2-OB2-PB2-OB5
15	N	101	BCL	C3-C5-C6-C7
15	X	102	BCL	C3-C5-C6-C7
14	A	501	PGV	C20-C19-O03-C01
15	R	101	BCL	C13-C15-C16-C17
18	4	104	LMT	C5'-C4'-O1B-C1B
14	L	306	PGV	O12-C04-C05-C06
18	S	101	LMT	O5B-C5B-C6B-O6B
15	6	101	BCL	C4-C3-C5-C6
15	5	102	BCL	CBD-CGD-O2D-CED
18	2	101	LMT	O5B-C5B-C6B-O6B
18	S	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
15	U	101	BCL	C13-C15-C16-C17
18	M	410	LMT	C4'-C5'-C6'-O6'
14	M	408	PGV	C21-C22-C23-C24
14	Q	101	PGV	C2-C1-O01-C02
15	V	101	BCL	C15-C16-C17-C18
14	C	408	PGV	C3-C4-C5-C6
18	T	103	LMT	C6-C7-C8-C9
18	5	101	LMT	C3-C4-C5-C6
19	L	311	CDL	C34-C35-C36-C37
19	D	101	CDL	C54-C55-C56-C57
12	C	406	Z41	C25-C26-C27-C28
19	L	311	CDL	C54-C55-C56-C57
19	L	311	CDL	CA6-CA4-OA6-CA5
14	Q	101	PGV	O02-C1-O01-C02
18	R	103	LMT	C2-C3-C4-C5
19	H	302	CDL	C59-C60-C61-C62
15	J	102	BCL	O1D-CGD-O2D-CED
14	L	310	PGV	O12-C04-C05-O05
19	L	311	CDL	C62-C63-C64-C65
14	1	401	PGV	C1-C2-C3-C4
15	V	101	BCL	CBA-CGA-O2A-C1
19	H	302	CDL	C16-C17-C18-C19
15	5	102	BCL	C4-C3-C5-C6
18	T	103	LMT	C5-C6-C7-C8
15	X	102	BCL	C2-C3-C5-C6
15	L	301	BCL	C11-C10-C8-C9
15	A	502	BCL	C11-C10-C8-C9
15	D	102	BCL	C11-C10-C8-C9
18	L	307	LMT	C3-C4-C5-C6
19	L	311	CDL	C63-C64-C65-C66
19	L	311	CDL	C79-C80-C81-C82
19	M	409	CDL	C55-C56-C57-C58
22	M	406	CRT	C5-C6-C7-C8
22	J	103	CRT	C5-C6-C7-C8
14	A	503	PGV	C04-C05-C06-O06
22	M	406	CRT	C5-C6-C7-C9
22	J	103	CRT	C5-C6-C7-C9
18	R	103	LMT	O5B-C5B-C6B-O6B
14	H	301	PGV	C2-C1-O01-C02
18	2	101	LMT	O1'-C1-C2-C3
14	A	503	PGV	C19-C20-C21-C22
15	L	308	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	4	101	LMT	C5-C6-C7-C8
18	4	104	LMT	C3'-C4'-O1B-C1B
19	L	311	CDL	C80-C81-C82-C83
18	M	411	LMT	C2'-C1'-O1'-C1
14	C	408	PGV	C1-C2-C3-C4
19	L	311	CDL	CB5-C51-C52-C53
15	L	301	BCL	C15-C16-C17-C18
15	R	101	BCL	C8-C10-C11-C12
14	A	501	PGV	O04-C19-O03-C01
19	M	409	CDL	C36-C37-C38-C39
19	H	302	CDL	C17-C18-C19-C20
15	6	101	BCL	C3-C5-C6-C7
15	O	502	BCL	CBA-CGA-O2A-C1
14	L	305	PGV	C2-C3-C4-C5
15	J	102	BCL	C3A-C2A-CAA-CBA
15	V	101	BCL	C3A-C2A-CAA-CBA
15	W	101	BCL	C3A-C2A-CAA-CBA
15	X	102	BCL	C3A-C2A-CAA-CBA
15	Y	102	BCL	C3A-C2A-CAA-CBA
15	1	402	BCL	C3A-C2A-CAA-CBA
15	2	102	BCL	C3A-C2A-CAA-CBA
15	3	101	BCL	C3A-C2A-CAA-CBA
15	8	102	BCL	C3A-C2A-CAA-CBA
15	Y	102	BCL	C8-C10-C11-C12
15	6	101	BCL	C8-C10-C11-C12
15	0	101	BCL	C13-C15-C16-C17
18	8	101	LMT	C2-C1-O1'-C1'
14	C	408	PGV	C2-C3-C4-C5
18	4	101	LMT	O5'-C5'-C6'-O6'
14	H	301	PGV	O02-C1-O01-C02
15	7	101	BCL	C3-C5-C6-C7
18	Z	101	LMT	C6-C7-C8-C9
15	G	102	BCL	C4-C3-C5-C6
15	V	101	BCL	C4-C3-C5-C6
15	X	102	BCL	C4-C3-C5-C6
15	Y	102	BCL	C4-C3-C5-C6
15	9	102	BCL	C4-C3-C5-C6
16	L	302	BPH	C4-C3-C5-C6
15	G	102	BCL	C2-C3-C5-C6
15	U	101	BCL	C2-C3-C5-C6
19	M	407	CDL	C11-CA5-OA6-CA4
18	L	307	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
18	H	303	LMT	C4-C5-C6-C7
15	2	102	BCL	C2A-CAA-CBA-CGA
14	H	301	PGV	O05-C05-C06-O06
19	M	409	CDL	C16-C17-C18-C19
15	X	102	BCL	C15-C16-C17-C18
15	V	101	BCL	O1A-CGA-O2A-C1
19	H	302	CDL	CA2-C1-CB2-OB2
19	M	407	CDL	OA7-CA5-OA6-CA4
15	8	102	BCL	C15-C16-C17-C18
15	O	502	BCL	O1A-CGA-O2A-C1
19	H	302	CDL	CA7-C31-C32-C33
15	Q	102	BCL	C3-C5-C6-C7
14	L	310	PGV	C25-C26-C27-C28
15	5	102	BCL	C8-C10-C11-C12
15	F	502	BCL	CBD-CGD-O2D-CED
15	U	101	BCL	C4-C3-C5-C6
15	7	101	BCL	C4-C3-C5-C6
15	I	101	BCL	O1D-CGD-O2D-CED
15	A	502	BCL	C6-C7-C8-C10
15	A	502	BCL	C11-C10-C8-C7
15	J	102	BCL	C6-C7-C8-C10
15	K	102	BCL	C6-C7-C8-C10
15	P	102	BCL	C11-C10-C8-C7
15	Q	102	BCL	C12-C13-C15-C16
15	U	101	BCL	C12-C13-C15-C16
15	Y	102	BCL	C2-C3-C5-C6
15	5	102	BCL	C2-C3-C5-C6
15	6	101	BCL	C2-C3-C5-C6
15	6	101	BCL	C6-C7-C8-C10
15	7	101	BCL	C2-C3-C5-C6
15	9	102	BCL	C2-C3-C5-C6
15	9	102	BCL	C6-C7-C8-C10
15	N	101	BCL	C16-C17-C18-C19
15	U	101	BCL	C16-C17-C18-C20
15	8	102	BCL	CBA-CGA-O2A-C1
19	M	409	CDL	C42-C43-C44-C45
14	1	401	PGV	C2-C3-C4-C5
15	T	101	BCL	O1D-CGD-O2D-CED
15	5	102	BCL	C10-C11-C12-C13
19	H	302	CDL	C54-C55-C56-C57
19	H	302	CDL	C58-C59-C60-C61
19	L	311	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
14	L	305	PGV	C2-C1-O01-C02
14	L	310	PGV	C2-C1-O01-C02
14	A	503	PGV	C2-C1-O01-C02
14	F	501	PGV	C2-C1-O01-C02
10	C	401	HEM	C4B-C3B-CAB-CBB
10	C	402	HEM	C4B-C3B-CAB-CBB
10	C	404	HEM	C4B-C3B-CAB-CBB
15	M	402	BCL	C10-C11-C12-C13
18	J	104	LMT	C4-C5-C6-C7
14	L	310	PGV	O02-C1-O01-C02
14	F	501	PGV	O02-C1-O01-C02
15	3	101	BCL	C3-C5-C6-C7
18	L	307	LMT	C11-C10-C9-C8
19	D	101	CDL	OB6-CB4-CB6-OB8
18	8	103	LMT	O5B-C5B-C6B-O6B
15	J	102	BCL	C8-C10-C11-C12
15	V	101	BCL	C2-C3-C5-C6
17	L	304	UQ8	C38-C39-C41-C42
19	L	311	CDL	C71-C72-C73-C74
15	A	502	BCL	C6-C7-C8-C9
15	Q	102	BCL	C14-C13-C15-C16
15	U	101	BCL	C14-C13-C15-C16
15	X	102	BCL	C11-C10-C8-C9
15	X	102	BCL	C2A-CAA-CBA-CGA
18	M	411	LMT	O5'-C5'-C6'-O6'
18	R	103	LMT	O5'-C5'-C6'-O6'
22	E	103	CRT	C34-C33-C35-C36
18	G	101	LMT	C3'-C4'-O1B-C1B
19	M	409	CDL	C51-C52-C53-C54
15	8	102	BCL	O1A-CGA-O2A-C1
15	Y	102	BCL	C1A-C2A-CAA-CBA
15	1	402	BCL	C1A-C2A-CAA-CBA
15	0	101	BCL	C1A-C2A-CAA-CBA
18	E	101	LMT	O5'-C5'-C6'-O6'
15	V	101	BCL	C16-C17-C18-C20
14	L	305	PGV	O02-C1-O01-C02
22	Z	103	CRT	C11-C10-C9-C7
14	L	305	PGV	C03-O11-P-O12
14	L	310	PGV	C04-O12-P-O11
18	X	101	LMT	O5B-C5B-C6B-O6B
19	M	409	CDL	C59-C60-C61-C62
18	X	101	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
14	L	310	PGV	C01-C02-C03-O11
14	M	408	PGV	C01-C02-C03-O11
15	L	308	BCL	C8-C10-C11-C12
15	V	101	BCL	C5-C6-C7-C8
22	M	406	CRT	C1-C4-C5-C6
22	Z	103	CRT	C1-C4-C5-C6
14	A	503	PGV	O12-C04-C05-C06
18	T	103	LMT	O5B-C5B-C6B-O6B
19	L	311	CDL	CB2-C1-CA2-OA2
15	B	102	BCL	C2C-C3C-CAC-CBC
15	G	102	BCL	C2C-C3C-CAC-CBC
15	J	102	BCL	C2C-C3C-CAC-CBC
15	O	502	BCL	C2C-C3C-CAC-CBC
15	7	101	BCL	C2C-C3C-CAC-CBC
15	8	102	BCL	C2C-C3C-CAC-CBC
13	C	407	PLM	C6-C7-C8-C9
15	L	308	BCL	C5-C6-C7-C8
15	G	102	BCL	C13-C15-C16-C17
15	2	102	BCL	C5-C6-C7-C8
15	G	102	BCL	C3-C5-C6-C7
14	F	501	PGV	O03-C01-C02-C03
18	E	101	LMT	C3'-C4'-O1B-C1B
19	M	409	CDL	CB3-CB4-CB6-OB8
15	N	101	BCL	C13-C15-C16-C17
18	8	101	LMT	C3-C4-C5-C6
18	5	101	LMT	O5'-C5'-C6'-O6'
15	V	101	BCL	CAA-CBA-CGA-O2A
18	Z	101	LMT	C7-C8-C9-C10
12	C	406	Z41	C11-C10-C9-C8
18	T	103	LMT	O5'-C5'-C6'-O6'
15	8	102	BCL	C4-C3-C5-C6
17	L	304	UQ8	C40-C39-C41-C42
19	M	409	CDL	C31-CA7-OA8-CA6
18	G	101	LMT	O5'-C5'-C6'-O6'
18	8	103	LMT	O5'-C5'-C6'-O6'
18	L	307	LMT	C7-C8-C9-C10
15	O	502	BCL	C2A-CAA-CBA-CGA
15	S	102	BCL	C2-C1-O2A-CGA
14	L	310	PGV	C21-C22-C23-C24
18	M	410	LMT	C2-C3-C4-C5
14	F	501	PGV	O01-C02-C03-O11
19	M	407	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
15	A	502	BCL	C16-C17-C18-C19
15	N	101	BCL	C16-C17-C18-C20
15	U	101	BCL	C16-C17-C18-C19
14	L	305	PGV	C4-C5-C6-C7
18	G	101	LMT	C5'-C4'-O1B-C1B
15	K	102	BCL	C15-C16-C17-C18
15	Q	102	BCL	C15-C16-C17-C18
22	E	103	CRT	C3-C1-O1-C1M
22	G	103	CRT	C39-C38-O2-C2M
22	J	103	CRT	C3-C1-O1-C1M
22	J	103	CRT	C39-C38-O2-C2M
22	N	102	CRT	C39-C38-O2-C2M
22	P	103	CRT	C3-C1-O1-C1M
22	Z	103	CRT	C39-C38-O2-C2M
14	L	310	PGV	O03-C01-C02-O01
14	A	503	PGV	O02-C1-O01-C02
19	M	409	CDL	OA9-CA7-OA8-CA6
22	G	103	CRT	C36-C37-C38-C39
22	Z	103	CRT	C36-C37-C38-C40
22	6	102	CRT	C3-C1-C4-C5
18	E	101	LMT	C5'-C4'-O1B-C1B
15	B	102	BCL	C11-C10-C8-C7
15	D	102	BCL	C11-C12-C13-C15
15	G	102	BCL	C6-C7-C8-C10
15	J	102	BCL	C12-C13-C15-C16
15	K	102	BCL	C11-C10-C8-C7
15	Q	102	BCL	C11-C10-C8-C7
15	Q	102	BCL	C11-C12-C13-C15
15	S	102	BCL	C11-C10-C8-C7
15	U	101	BCL	C6-C7-C8-C10
15	W	101	BCL	C11-C10-C8-C7
15	2	102	BCL	C11-C10-C8-C7
15	5	102	BCL	C11-C10-C8-C7
15	M	402	BCL	C11-C10-C8-C9
15	G	102	BCL	C14-C13-C15-C16
15	J	102	BCL	C14-C13-C15-C16
15	O	502	BCL	C11-C10-C8-C9
15	Q	102	BCL	C11-C10-C8-C9
15	S	102	BCL	C11-C10-C8-C9
15	T	101	BCL	C14-C13-C15-C16
15	U	101	BCL	C6-C7-C8-C9
15	Y	102	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	5	102	BCL	C11-C10-C8-C9
15	9	102	BCL	C6-C7-C8-C9
22	M	406	CRT	C36-C37-C38-O2
22	Z	103	CRT	C36-C37-C38-O2
18	B	101	LMT	C4B-C5B-C6B-O6B
18	B	101	LMT	C2-C3-C4-C5
14	M	408	PGV	C20-C19-O03-C01
15	Y	102	BCL	C10-C11-C12-C13
19	H	302	CDL	C71-C72-C73-C74
14	C	408	PGV	C01-C02-C03-O11
19	M	409	CDL	OB5-CB3-CB4-CB6
21	M	405	MQ8	C28-C30-C31-C32
15	W	101	BCL	C4-C3-C5-C6
15	8	102	BCL	C2-C3-C5-C6
14	A	503	PGV	O12-C04-C05-O05
14	C	408	PGV	C21-C22-C23-C24
15	2	102	BCL	C16-C17-C18-C19
18	P	101	LMT	C4B-C5B-C6B-O6B
19	L	311	CDL	CB7-C71-C72-C73
15	5	102	BCL	O1D-CGD-O2D-CED
14	A	501	PGV	C24-C25-C26-C27
14	1	401	PGV	C21-C22-C23-C24
15	1	402	BCL	CBA-CGA-O2A-C1
19	H	302	CDL	C78-C79-C80-C81
15	2	102	BCL	C8-C10-C11-C12
19	L	311	CDL	C33-C34-C35-C36
16	M	404	BPH	C4-C3-C5-C6
15	P	102	BCL	CBA-CGA-O2A-C1
18	H	303	LMT	O1'-C1-C2-C3
12	C	406	Z41	C13-C14-C15-C16
14	L	310	PGV	O01-C02-C03-O11
15	J	102	BCL	CBA-CGA-O2A-C1
19	L	311	CDL	C81-C82-C83-C84
18	P	101	LMT	O1'-C1-C2-C3
19	M	409	CDL	OB6-CB4-CB6-OB8
14	F	501	PGV	C20-C19-O03-C01
15	F	502	BCL	O1D-CGD-O2D-CED
15	L	301	BCL	C16-C17-C18-C19
15	A	502	BCL	C16-C17-C18-C20
12	C	406	Z41	C21-C22-C23-C24
15	D	102	BCL	C2-C1-O2A-CGA
15	U	101	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	W	101	BCL	C2-C3-C5-C6
15	W	101	BCL	C8-C10-C11-C12
15	X	102	BCL	C8-C10-C11-C12
15	D	102	BCL	C11-C12-C13-C14
15	J	102	BCL	C11-C10-C8-C9
15	K	102	BCL	C11-C10-C8-C9
15	Q	102	BCL	C11-C12-C13-C14
15	V	101	BCL	C11-C10-C8-C9
15	W	101	BCL	C11-C10-C8-C9
15	4	102	BCL	C11-C10-C8-C9
15	0	101	BCL	C6-C7-C8-C9
15	0	101	BCL	C11-C10-C8-C9
19	M	409	CDL	C43-C44-C45-C46
19	L	311	CDL	CA4-CA3-OA5-PA1
15	V	101	BCL	C16-C17-C18-C19
15	Z	102	BCL	CBD-CGD-O2D-CED
15	V	101	BCL	C8-C10-C11-C12
15	M	402	BCL	C4C-C3C-CAC-CBC
22	B	103	CRT	C15-C16-C17-C19
15	I	101	BCL	C8-C10-C11-C12
15	4	102	BCL	C5-C6-C7-C8
10	C	402	HEM	C3D-CAD-CBD-CGD
15	Y	102	BCL	C16-C17-C18-C19
15	0	101	BCL	C16-C17-C18-C19
14	L	306	PGV	C01-C02-C03-O11
14	1	401	PGV	C20-C21-C22-C23
15	L	308	BCL	C6-C7-C8-C10
15	L	308	BCL	C11-C10-C8-C7
15	A	502	BCL	C11-C12-C13-C15
15	E	102	BCL	C6-C7-C8-C10
15	F	502	BCL	C6-C7-C8-C10
15	F	502	BCL	C11-C10-C8-C7
15	G	102	BCL	C11-C12-C13-C15
15	R	101	BCL	C6-C7-C8-C10
15	T	101	BCL	C6-C7-C8-C10
15	V	101	BCL	C6-C7-C8-C10
15	Y	102	BCL	C6-C7-C8-C10
15	Z	102	BCL	C6-C7-C8-C10
15	9	102	BCL	C12-C13-C15-C16
16	L	302	BPH	C2-C3-C5-C6
16	M	404	BPH	C11-C12-C13-C15
16	M	404	BPH	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	H	301	PGV	C3-C4-C5-C6
18	Z	101	LMT	C1-C2-C3-C4
14	F	501	PGV	C20-C21-C22-C23
18	T	103	LMT	C4-C5-C6-C7
15	2	102	BCL	C16-C17-C18-C20
14	L	305	PGV	C3-C4-C5-C6
15	Q	102	BCL	CBD-CGD-O2D-CED
14	A	503	PGV	C2-C3-C4-C5
15	L	301	BCL	CAD-CBD-CGD-O2D
16	M	404	BPH	CAD-CBD-CGD-O2D
19	M	407	CDL	CA6-CA4-OA6-CA5
15	0	101	BCL	CBD-CGD-O2D-CED
15	I	101	BCL	CBA-CGA-O2A-C1
15	7	101	BCL	CBA-CGA-O2A-C1
15	R	101	BCL	C16-C17-C18-C19
15	4	102	BCL	C16-C17-C18-C19
18	E	101	LMT	O5'-C1'-O1'-C1
18	G	101	LMT	O5'-C1'-O1'-C1
16	M	404	BPH	C2-C3-C5-C6
18	P	101	LMT	C9-C10-C11-C12
14	L	306	PGV	O01-C02-C03-O11
15	8	102	BCL	C2A-CAA-CBA-CGA
18	X	101	LMT	C3'-C4'-O1B-C1B
15	I	101	BCL	C3-C5-C6-C7
14	M	408	PGV	O04-C19-O03-C01
15	P	102	BCL	O1A-CGA-O2A-C1
18	H	303	LMT	C2'-C1'-O1'-C1
18	4	101	LMT	C6-C7-C8-C9
14	C	408	PGV	O03-C01-C02-O01
15	J	102	BCL	O1A-CGA-O2A-C1
15	Z	102	BCL	O1D-CGD-O2D-CED
15	O	502	BCL	C4-C3-C5-C6
15	Z	102	BCL	C4-C3-C5-C6
15	4	102	BCL	C4-C3-C5-C6
18	R	103	LMT	C5-C6-C7-C8
15	1	402	BCL	O1A-CGA-O2A-C1
15	E	102	BCL	C11-C10-C8-C9
15	I	101	BCL	C6-C7-C8-C9
14	F	501	PGV	O04-C19-O03-C01
18	B	101	LMT	C6-C7-C8-C9
22	0	102	CRT	C15-C16-C17-C18
19	H	302	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
15	3	101	BCL	C16-C17-C18-C19
14	C	408	PGV	C04-O12-P-O11
14	L	305	PGV	C04-O12-P-O11
14	1	401	PGV	C03-O11-P-O12
19	M	407	CDL	CA3-OA5-PA1-OA2
15	0	101	BCL	O1D-CGD-O2D-CED
15	Q	102	BCL	O1D-CGD-O2D-CED
15	7	101	BCL	O1A-CGA-O2A-C1
14	L	306	PGV	C04-O12-P-O13
14	L	310	PGV	C03-O11-P-O13
14	L	310	PGV	C04-O12-P-O13
14	H	301	PGV	C04-O12-P-O13
19	L	311	CDL	CA2-OA2-PA1-OA4
19	L	311	CDL	CB3-OB5-PB2-OB3
19	M	407	CDL	CA3-OA5-PA1-OA4
19	M	407	CDL	CB3-OB5-PB2-OB4
19	M	409	CDL	CA3-OA5-PA1-OA3
19	H	302	CDL	CB3-OB5-PB2-OB3
19	D	101	CDL	CA3-OA5-PA1-OA3
19	D	101	CDL	CB2-OB2-PB2-OB3
14	F	501	PGV	C23-C24-C25-C26
14	A	503	PGV	C01-C02-C03-O11
19	M	407	CDL	OB5-CB3-CB4-CB6
19	M	409	CDL	OA5-CA3-CA4-CA6
17	L	304	UQ8	C14-C16-C17-C18
15	I	101	BCL	O1A-CGA-O2A-C1
15	D	102	BCL	C5-C6-C7-C8
22	6	102	CRT	C1-C4-C5-C6
22	9	101	CRT	C1-C4-C5-C6
14	1	401	PGV	C4-C5-C6-C7
19	M	407	CDL	CA2-C1-CB2-OB2
18	T	103	LMT	O1'-C1-C2-C3
14	C	408	PGV	O01-C02-C03-O11
14	A	503	PGV	O01-C02-C03-O11
15	F	502	BCL	C11-C12-C13-C15
15	N	101	BCL	C11-C10-C8-C7
15	P	102	BCL	C11-C12-C13-C15
15	R	101	BCL	C11-C10-C8-C7
15	4	102	BCL	C2C-C3C-CAC-CBC
15	5	102	BCL	C2C-C3C-CAC-CBC
19	M	409	CDL	OA5-CA3-CA4-OA6
19	D	101	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
18	R	103	LMT	C3-C4-C5-C6
15	P	102	BCL	CAA-CBA-CGA-O2A
14	H	301	PGV	C23-C24-C25-C26
15	6	101	BCL	C13-C15-C16-C17
14	L	310	PGV	O03-C01-C02-C03
19	D	101	CDL	CB3-CB4-CB6-OB8
24	K	101	LDA	C4-C5-C6-C7
14	F	501	PGV	O03-C01-C02-O01
18	B	101	LMT	C4-C5-C6-C7
15	L	301	BCL	C16-C17-C18-C20
15	0	101	BCL	C16-C17-C18-C20
15	E	102	BCL	O1D-CGD-O2D-CED
14	A	501	PGV	C05-C04-O12-P
15	6	101	BCL	CBA-CGA-O2A-C1
18	T	103	LMT	C2-C3-C4-C5
15	4	102	BCL	C2-C3-C5-C6
15	9	102	BCL	C5-C6-C7-C8
15	A	502	BCL	C11-C12-C13-C14
15	F	502	BCL	C6-C7-C8-C9
15	F	502	BCL	C11-C10-C8-C9
15	T	101	BCL	C11-C10-C8-C9
15	8	102	BCL	C14-C13-C15-C16
15	9	102	BCL	C14-C13-C15-C16
16	M	404	BPH	C11-C12-C13-C14
22	4	103	CRT	C28-C30-C31-C32
18	B	101	LMT	O1'-C1-C2-C3
15	J	102	BCL	C16-C17-C18-C19
17	L	309	UQ8	C5-C4-O4-C4M
18	X	101	LMT	C5'-C4'-O1B-C1B
18	8	103	LMT	C6-C7-C8-C9
14	M	408	PGV	C1-C2-C3-C4
14	Q	101	PGV	C01-C02-O01-C1
19	D	101	CDL	CA6-CA4-OA6-CA5
14	F	501	PGV	C01-C02-C03-O11
15	2	102	BCL	O1D-CGD-O2D-CED
15	L	301	BCL	C2-C1-O2A-CGA
15	W	101	BCL	C2-C1-O2A-CGA
15	5	102	BCL	C2-C1-O2A-CGA
15	6	101	BCL	C2-C1-O2A-CGA
19	H	302	CDL	CA4-CA3-OA5-PA1
19	L	311	CDL	C73-C74-C75-C76
14	Q	101	PGV	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
15	6	101	BCL	O1D-CGD-O2D-CED
18	T	103	LMT	C2B-C1B-O1B-C4'
15	O	502	BCL	C2-C3-C5-C6
15	Z	102	BCL	C2-C3-C5-C6
17	L	309	UQ8	C29-C31-C32-C33
22	N	102	CRT	C40-C38-O2-C2M
22	Z	103	CRT	C40-C38-O2-C2M
14	L	306	PGV	C6-C7-C8-C9
14	L	306	PGV	C04-O12-P-O11
14	A	503	PGV	C04-O12-P-O11
19	M	409	CDL	CB2-OB2-PB2-OB5
19	H	302	CDL	CB2-OB2-PB2-OB5
14	1	401	PGV	C04-O12-P-O13
22	G	103	CRT	C36-C37-C38-C40
22	P	103	CRT	C36-C37-C38-C39
22	2	103	CRT	C36-C37-C38-C39
22	6	102	CRT	C36-C37-C38-C39
18	4	104	LMT	C5-C6-C7-C8
15	E	102	BCL	C11-C10-C8-C7
15	T	101	BCL	C12-C13-C15-C16
15	8	102	BCL	C11-C12-C13-C15
14	Q	101	PGV	O01-C1-C2-C3
15	L	308	BCL	C6-C7-C8-C9
15	Y	102	BCL	C6-C7-C8-C9
19	M	409	CDL	OA7-CA5-OA6-CA4
18	J	101	LMT	C4-C5-C6-C7
15	F	502	BCL	C8-C10-C11-C12
22	G	103	CRT	C36-C37-C38-O2
19	M	409	CDL	CB5-C51-C52-C53
18	Z	101	LMT	O1'-C1-C2-C3
18	2	101	LMT	C2-C3-C4-C5
18	J	104	LMT	O1'-C1-C2-C3
15	6	101	BCL	CBD-CGD-O2D-CED
14	F	501	PGV	C19-C20-C21-C22
14	L	310	PGV	C29-C30-C31-C32
18	4	101	LMT	C4-C5-C6-C7
15	B	102	BCL	C13-C15-C16-C17
19	H	302	CDL	C60-C61-C62-C63
19	M	409	CDL	C11-CA5-OA6-CA4
15	F	502	BCL	C16-C17-C18-C19
15	6	101	BCL	O1A-CGA-O2A-C1
15	8	102	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	9	102	BCL	C2-C1-O2A-CGA
18	4	101	LMT	C7-C8-C9-C10
15	Y	102	BCL	C2A-CAA-CBA-CGA
14	H	301	PGV	C02-C03-O11-P
15	U	101	BCL	C3A-C2A-CAA-CBA
15	Y	102	BCL	C16-C17-C18-C20
15	T	101	BCL	C4-C3-C5-C6
15	E	102	BCL	C14-C13-C15-C16
15	F	502	BCL	C11-C12-C13-C14
15	P	102	BCL	C11-C12-C13-C14
15	Q	102	BCL	C6-C7-C8-C9
15	S	102	BCL	C6-C7-C8-C9
15	Z	102	BCL	C14-C13-C15-C16
15	4	102	BCL	C14-C13-C15-C16
15	L	308	BCL	C16-C17-C18-C20
15	E	102	BCL	C8-C10-C11-C12
14	C	408	PGV	O03-C01-C02-C03
22	4	103	CRT	C31-C32-C33-C34
10	C	402	HEM	CAD-CBD-CGD-O1D
16	L	302	BPH	O2A-C1-C2-C3
18	5	101	LMT	O5'-C1'-O1'-C1
22	M	406	CRT	C29-C28-C30-C31
22	G	103	CRT	C15-C16-C17-C18
22	T	102	CRT	C5-C6-C7-C8
22	2	103	CRT	C15-C16-C17-C18
15	B	102	BCL	C1A-C2A-CAA-CBA
15	G	102	BCL	C1A-C2A-CAA-CBA
15	U	101	BCL	C1A-C2A-CAA-CBA
15	Z	102	BCL	C1A-C2A-CAA-CBA
15	D	102	BCL	C6-C7-C8-C10
15	6	101	BCL	C11-C10-C8-C7
15	S	102	BCL	C8-C10-C11-C12
22	J	103	CRT	C11-C10-C9-C7
10	C	401	HEM	CAA-CBA-CGA-O2A
15	N	101	BCL	C10-C11-C12-C13
15	P	102	BCL	C2A-CAA-CBA-CGA
15	D	102	BCL	C15-C16-C17-C18
15	1	402	BCL	C13-C15-C16-C17
15	3	101	BCL	C15-C16-C17-C18
16	M	404	BPH	C5-C6-C7-C8
10	C	401	HEM	CAA-CBA-CGA-O1A
18	5	101	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
14	Q	101	PGV	C19-C20-C21-C22
19	D	101	CDL	OB5-CB3-CB4-CB6
15	T	101	BCL	C13-C15-C16-C17
15	E	102	BCL	C4-C3-C5-C6
17	L	309	UQ8	C30-C29-C31-C32
18	8	101	LMT	C3'-C4'-O1B-C1B
19	H	302	CDL	C31-CA7-OA8-CA6
15	L	301	BCL	C3-C5-C6-C7
15	J	102	BCL	C16-C17-C18-C20
22	4	103	CRT	C31-C32-C33-C35
10	C	402	HEM	CAD-CBD-CGD-O2D
18	B	101	LMT	O5B-C5B-C6B-O6B
22	6	102	CRT	C11-C10-C9-C7
22	2	103	CRT	C1-C4-C5-C6
24	K	101	LDA	C2-C3-C4-C5
15	M	403	BCL	C5-C6-C7-C8
17	L	304	UQ8	C19-C21-C22-C23
15	A	502	BCL	C2-C1-O2A-CGA
15	I	101	BCL	C2-C1-O2A-CGA
15	O	502	BCL	C2-C1-O2A-CGA
15	0	101	BCL	C2C-C3C-CAC-CBC
24	O	501	LDA	C2-C3-C4-C5
15	5	102	BCL	C6-C7-C8-C9
15	5	102	BCL	C14-C13-C15-C16
14	A	503	PGV	C22-C23-C24-C25
15	G	102	BCL	O1D-CGD-O2D-CED
15	D	102	BCL	C16-C17-C18-C19
15	P	102	BCL	C16-C17-C18-C19
15	V	101	BCL	CAA-CBA-CGA-O1A
15	Q	102	BCL	C13-C15-C16-C17
19	H	302	CDL	OA9-CA7-OA8-CA6
15	B	102	BCL	C4C-C3C-CAC-CBC
15	J	102	BCL	C4C-C3C-CAC-CBC
15	8	102	BCL	C4C-C3C-CAC-CBC
22	0	102	CRT	C15-C16-C17-C19
18	M	410	LMT	O5B-C1B-O1B-C4'
15	T	101	BCL	C2-C3-C5-C6
15	S	102	BCL	C10-C11-C12-C13
15	U	101	BCL	C15-C16-C17-C18
19	M	409	CDL	C58-C59-C60-C61
18	P	104	LMT	C2-C3-C4-C5
16	L	302	BPH	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	L	305	PGV	O01-C02-C03-O11
19	L	311	CDL	C84-C85-C86-C87
15	E	102	BCL	CBD-CGD-O2D-CED
16	L	302	BPH	C11-C12-C13-C15
17	L	309	UQ8	C28-C29-C31-C32
18	8	103	LMT	C11-C10-C9-C8
19	M	407	CDL	OB6-CB4-CB6-OB8
18	5	101	LMT	C2'-C1'-O1'-C1
12	C	406	Z41	C30-C31-C32-C33
18	J	101	LMT	C11-C10-C9-C8
15	E	102	BCL	C2-C3-C5-C6
18	J	104	LMT	C4'-C5'-C6'-O6'
15	M	402	BCL	C6-C7-C8-C9
15	D	102	BCL	C6-C7-C8-C9
18	X	101	LMT	C7-C8-C9-C10
15	G	102	BCL	C3A-C2A-CAA-CBA
15	R	101	BCL	CAA-CBA-CGA-O2A
15	7	101	BCL	CAA-CBA-CGA-O2A
15	L	308	BCL	CAD-CBD-CGD-O2D
15	M	402	BCL	CAD-CBD-CGD-O2D
15	L	308	BCL	C16-C17-C18-C19
15	L	301	BCL	C2A-CAA-CBA-CGA
15	2	102	BCL	CBD-CGD-O2D-CED
15	X	102	BCL	C2-C1-O2A-CGA
15	K	102	BCL	C4-C3-C5-C6
14	1	401	PGV	O01-C1-C2-C3
22	E	103	CRT	C32-C33-C35-C36
22	R	102	CRT	C22-C23-C25-C26
22	2	103	CRT	C15-C16-C17-C19
21	M	405	MQ8	C43-C44-C46-C47
15	X	102	BCL	CAA-CBA-CGA-O2A
19	D	101	CDL	C52-C51-CB5-OB6
15	D	102	BCL	O2A-C1-C2-C3
15	R	101	BCL	O2A-C1-C2-C3
15	L	308	BCL	CHA-CBD-CGD-O2D
15	M	403	BCL	CHA-CBD-CGD-O1D
15	M	403	BCL	CHA-CBD-CGD-O2D
15	F	502	BCL	CHA-CBD-CGD-O1D
15	F	502	BCL	CHA-CBD-CGD-O2D
15	I	101	BCL	CHA-CBD-CGD-O1D
15	I	101	BCL	CHA-CBD-CGD-O2D
15	K	102	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	K	102	BCL	CHA-CBD-CGD-O2D
15	O	502	BCL	CHA-CBD-CGD-O2D
15	W	101	BCL	CHA-CBD-CGD-O1D
15	W	101	BCL	CHA-CBD-CGD-O2D
15	1	402	BCL	CHA-CBD-CGD-O1D
15	1	402	BCL	CHA-CBD-CGD-O2D
15	3	101	BCL	CHA-CBD-CGD-O1D
15	3	101	BCL	CHA-CBD-CGD-O2D
15	5	102	BCL	CHA-CBD-CGD-O1D
15	5	102	BCL	CHA-CBD-CGD-O2D
15	7	101	BCL	CHA-CBD-CGD-O1D
15	7	101	BCL	CHA-CBD-CGD-O2D
14	Q	101	PGV	C01-C02-C03-O11
19	M	409	CDL	C17-C18-C19-C20
14	L	310	PGV	C23-C24-C25-C26
15	N	101	BCL	C15-C16-C17-C18
15	8	102	BCL	CAA-CBA-CGA-O2A
18	T	103	LMT	O5B-C1B-O1B-C4'
15	M	402	BCL	C6-C7-C8-C10
15	M	403	BCL	C12-C13-C15-C16
15	K	102	BCL	C2-C3-C5-C6
15	4	102	BCL	C6-C7-C8-C10
15	9	102	BCL	C11-C10-C8-C7
19	D	101	CDL	C72-C71-CB7-OB8
15	M	403	BCL	C14-C13-C15-C16
15	N	101	BCL	C6-C7-C8-C9
17	L	309	UQ8	C9-C11-C12-C13
14	A	501	PGV	C25-C26-C27-C28
18	8	101	LMT	C5'-C4'-O1B-C1B
15	4	102	BCL	CAA-CBA-CGA-O2A
16	M	404	BPH	C2C-C3C-CAC-CBC
15	F	502	BCL	C16-C17-C18-C20
14	1	401	PGV	O02-C1-C2-C3
22	G	103	CRT	C15-C16-C17-C19
22	T	102	CRT	C5-C6-C7-C9
15	P	102	BCL	C1A-C2A-CAA-CBA
15	R	101	BCL	C1A-C2A-CAA-CBA
15	6	101	BCL	C1A-C2A-CAA-CBA
15	7	101	BCL	CAA-CBA-CGA-O1A
15	9	102	BCL	C16-C17-C18-C19
14	H	301	PGV	C6-C7-C8-C9
15	P	102	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	A	503	PGV	C04-O12-P-O14
19	H	302	CDL	CA2-OA2-PA1-OA4
15	1	402	BCL	C5-C6-C7-C8
19	D	101	CDL	C72-C71-CB7-OB9
15	4	102	BCL	C16-C17-C18-C20
15	K	102	BCL	C2A-CAA-CBA-CGA
15	E	102	BCL	C15-C16-C17-C18
10	C	404	HEM	CAA-CBA-CGA-O2A
15	O	502	BCL	CAD-CBD-CGD-O1D
15	Y	102	BCL	CAD-CBD-CGD-O1D
15	1	402	BCL	CAD-CBD-CGD-O1D
15	5	102	BCL	CAD-CBD-CGD-O1D
15	9	102	BCL	CAD-CBD-CGD-O1D
19	D	101	CDL	C52-C51-CB5-OB7
12	C	406	Z41	C28-C29-C30-C31
14	M	408	PGV	O03-C19-C20-C21
15	U	101	BCL	C11-C10-C8-C9
15	V	101	BCL	C11-C12-C13-C14
19	L	311	CDL	C75-C76-C77-C78
19	H	302	CDL	C55-C56-C57-C58
16	M	404	BPH	C10-C11-C12-C13
19	H	302	CDL	C72-C73-C74-C75
15	F	502	BCL	CAA-CBA-CGA-O2A
14	H	301	PGV	O12-C04-C05-C06
19	M	409	CDL	C77-C78-C79-C80
15	P	102	BCL	C16-C17-C18-C20
17	L	309	UQ8	C20-C19-C21-C22
15	B	102	BCL	C3A-C2A-CAA-CBA
15	I	101	BCL	C11-C10-C8-C7
15	V	101	BCL	C11-C12-C13-C15
15	Z	102	BCL	C3A-C2A-CAA-CBA
15	8	102	BCL	C12-C13-C15-C16
14	H	301	PGV	O03-C19-C20-C21
19	L	311	CDL	C52-C51-CB5-OB6
19	H	302	CDL	C82-C83-C84-C85
24	O	501	LDA	C4-C5-C6-C7
22	N	102	CRT	C15-C16-C17-C19
22	N	102	CRT	C22-C23-C25-C26
22	Y	101	CRT	C15-C16-C17-C19
22	6	102	CRT	C10-C11-C12-C14
10	C	404	HEM	CAA-CBA-CGA-O1A
15	X	102	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	H	302	CDL	C18-C19-C20-C21
15	Q	102	BCL	C10-C11-C12-C13
14	M	408	PGV	O01-C1-C2-C3

There are no ring outliers.

100 monomers are involved in 463 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	E	103	CRT	7	0
15	Q	102	BCL	5	0
15	N	101	BCL	10	0
17	L	303	UQ8	4	0
22	B	103	CRT	6	0
15	O	502	BCL	2	0
15	U	101	BCL	6	0
22	Y	101	CRT	6	0
18	B	101	LMT	3	0
24	O	501	LDA	1	0
14	L	305	PGV	5	0
18	P	104	LMT	3	0
18	2	101	LMT	4	0
16	L	302	BPH	6	0
22	4	103	CRT	10	0
15	B	102	BCL	9	0
18	P	101	LMT	1	0
14	C	408	PGV	2	0
15	3	101	BCL	9	0
18	H	303	LMT	3	0
13	C	407	PLM	2	0
18	T	103	LMT	3	0
14	A	503	PGV	4	0
15	E	102	BCL	10	0
15	G	102	BCL	9	0
15	4	102	BCL	8	0
18	J	104	LMT	1	0
21	M	405	MQ8	8	0
14	Q	101	PGV	1	0
22	Z	103	CRT	7	0
15	P	102	BCL	4	0
15	R	101	BCL	6	0
15	L	301	BCL	4	0
22	V	102	CRT	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	402	HEM	5	0
15	9	102	BCL	5	0
18	4	104	LMT	2	0
22	0	102	CRT	8	0
15	7	101	BCL	8	0
14	L	310	PGV	4	0
10	C	401	HEM	7	0
10	C	404	HEM	3	0
22	P	103	CRT	3	0
15	M	402	BCL	3	0
18	Z	101	LMT	2	0
19	L	311	CDL	7	0
15	S	102	BCL	5	0
19	M	407	CDL	1	0
15	0	101	BCL	8	0
19	M	409	CDL	8	0
22	M	406	CRT	5	0
22	G	103	CRT	5	0
15	Z	102	BCL	6	0
18	G	101	LMT	1	0
15	8	102	BCL	11	0
22	9	101	CRT	6	0
22	J	103	CRT	9	0
14	M	408	PGV	3	0
18	X	101	LMT	3	0
14	L	306	PGV	4	0
15	F	502	BCL	1	0
15	W	101	BCL	2	0
14	A	501	PGV	3	0
15	X	102	BCL	5	0
15	V	101	BCL	6	0
14	H	301	PGV	3	0
15	Y	102	BCL	4	0
18	5	101	LMT	1	0
18	M	411	LMT	1	0
18	E	101	LMT	2	0
22	2	103	CRT	11	0
22	R	102	CRT	4	0
15	1	402	BCL	11	0
17	L	309	UQ8	5	0
15	5	102	BCL	7	0
18	M	410	LMT	2	0

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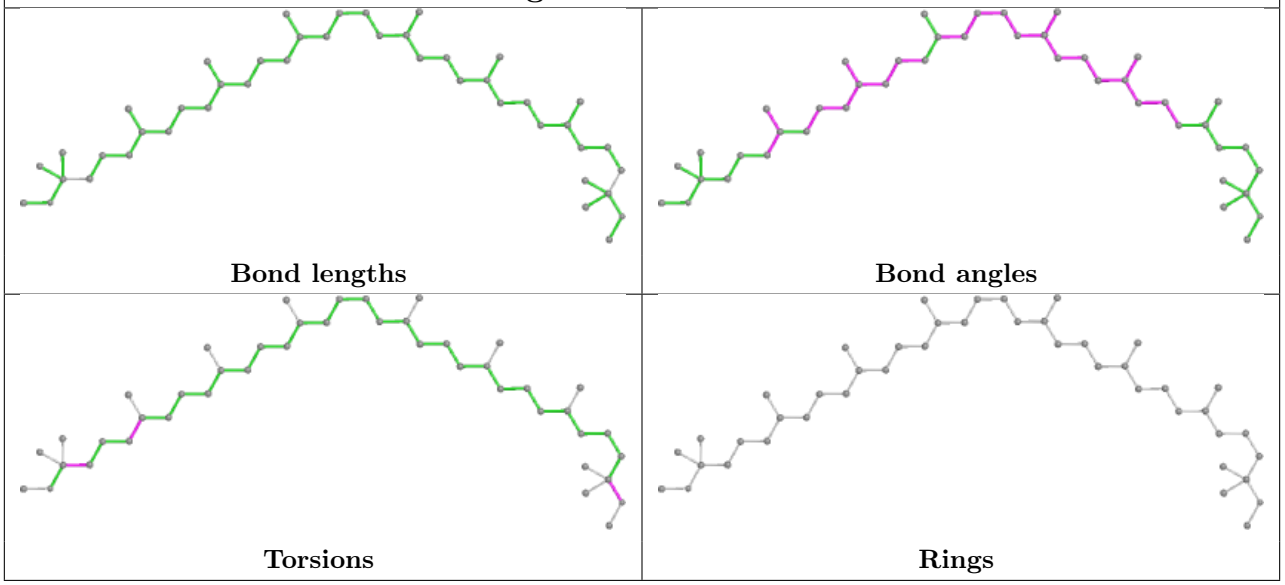
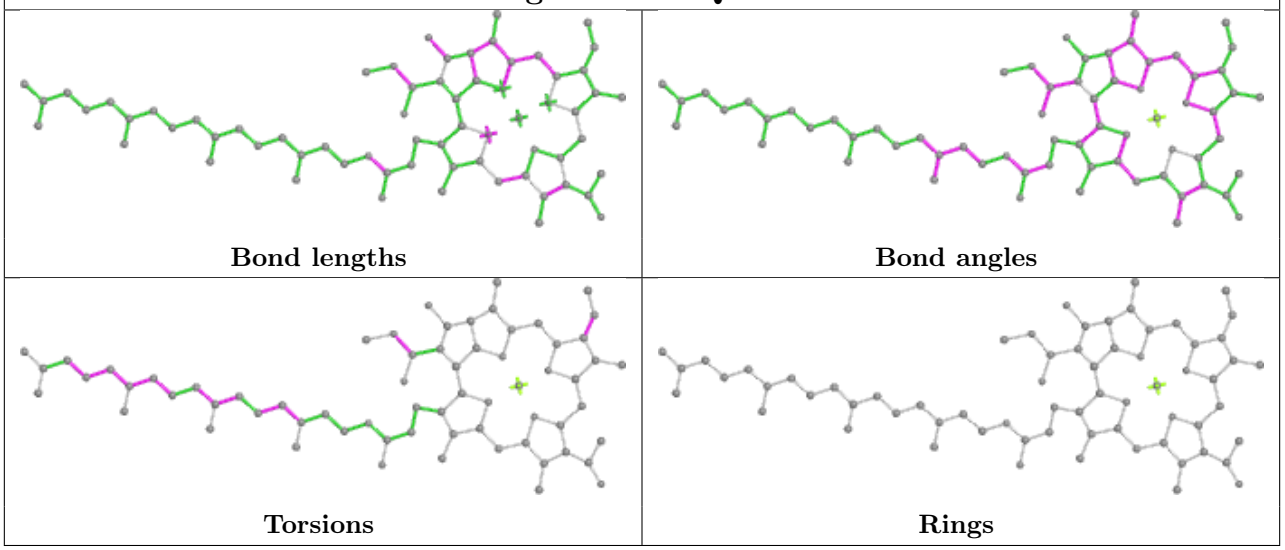
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	502	BCL	5	0
18	J	101	LMT	3	0
15	K	102	BCL	8	0
15	6	101	BCL	7	0
18	S	101	LMT	3	0
10	C	403	HEM	6	0
15	I	101	BCL	6	0
18	4	101	LMT	6	0
16	M	404	BPH	6	0
19	H	302	CDL	2	0
22	6	102	CRT	5	0
14	1	401	PGV	5	0
15	T	101	BCL	4	0
17	L	304	UQ8	15	0
15	2	102	BCL	9	0
18	L	307	LMT	3	0
15	J	102	BCL	6	0
22	N	102	CRT	9	0
15	D	102	BCL	4	0
15	L	308	BCL	4	0
18	R	103	LMT	4	0
18	8	103	LMT	3	0
22	T	102	CRT	8	0
15	M	403	BCL	2	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.

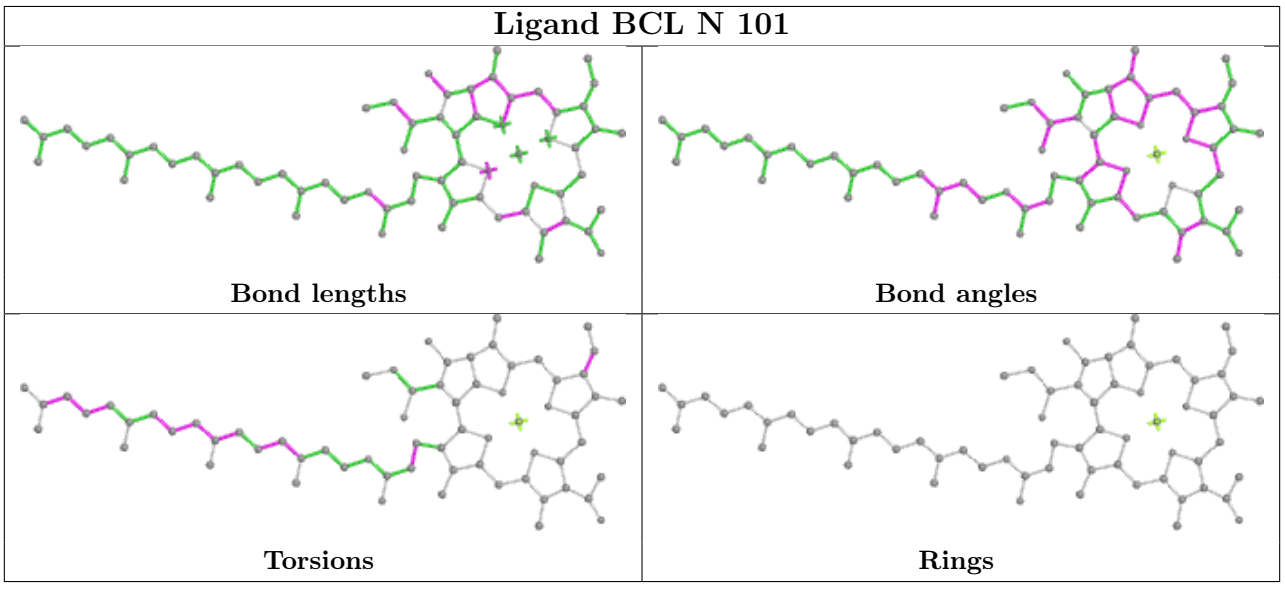
Ligand CRT E 103



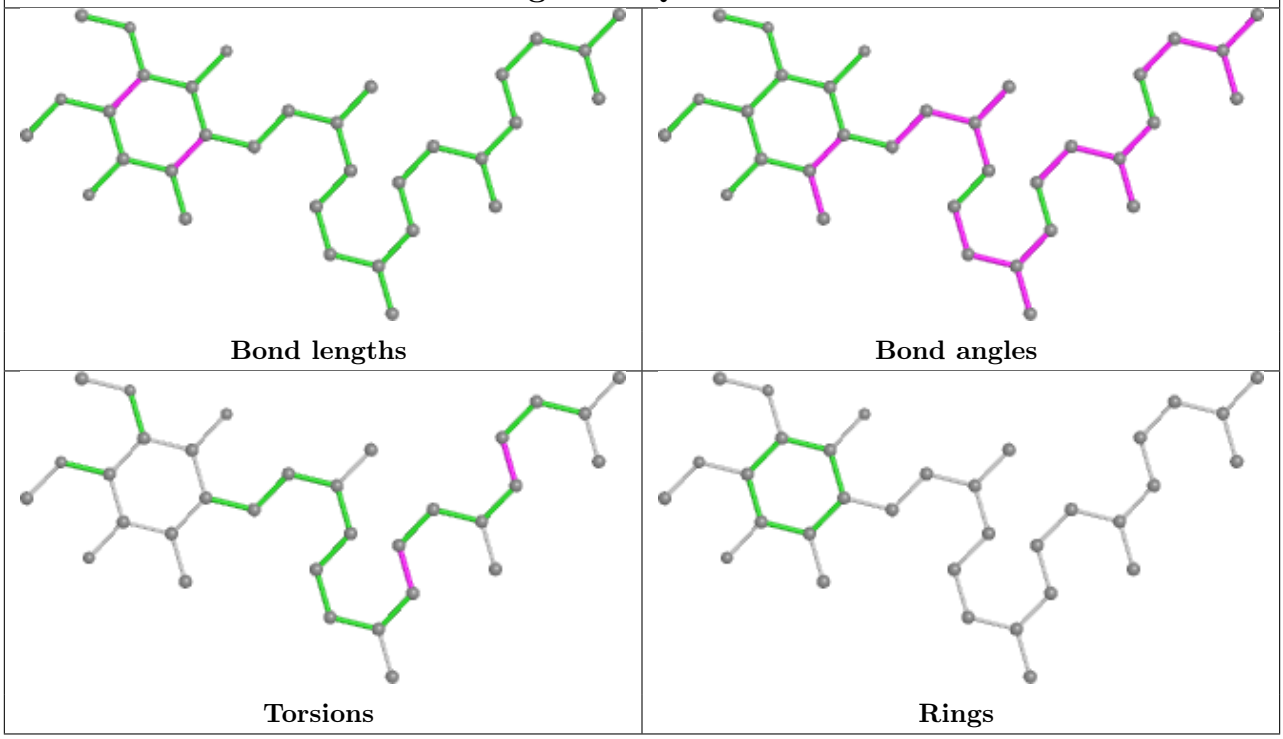
Ligand BCL Q 102



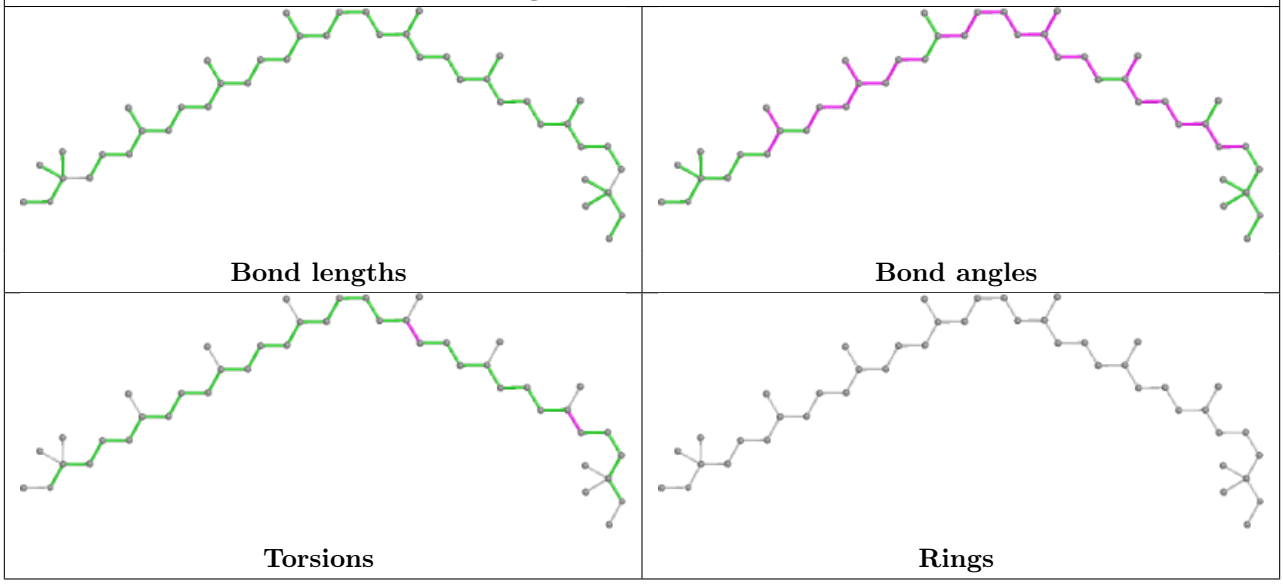
Ligand BCL N 101



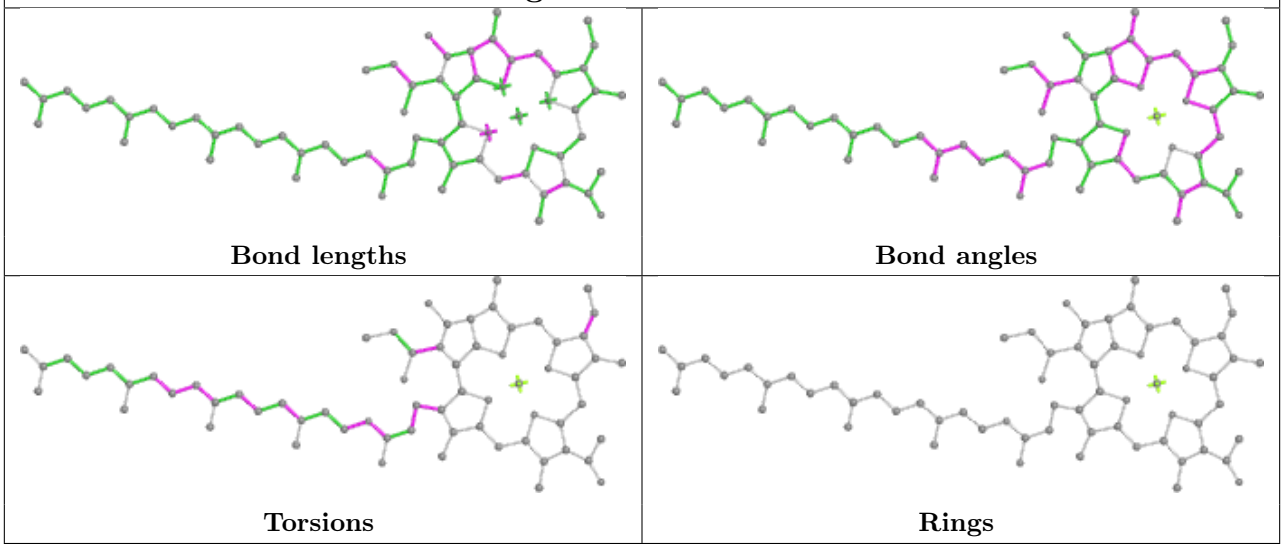
Ligand UQ8 L 303



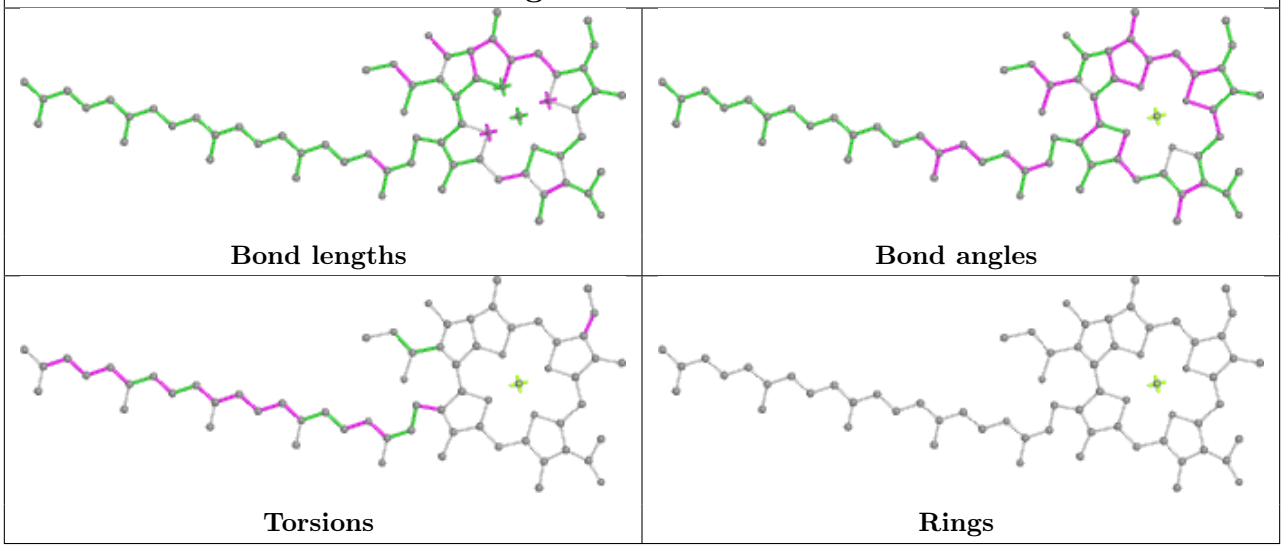
Ligand CRT B 103



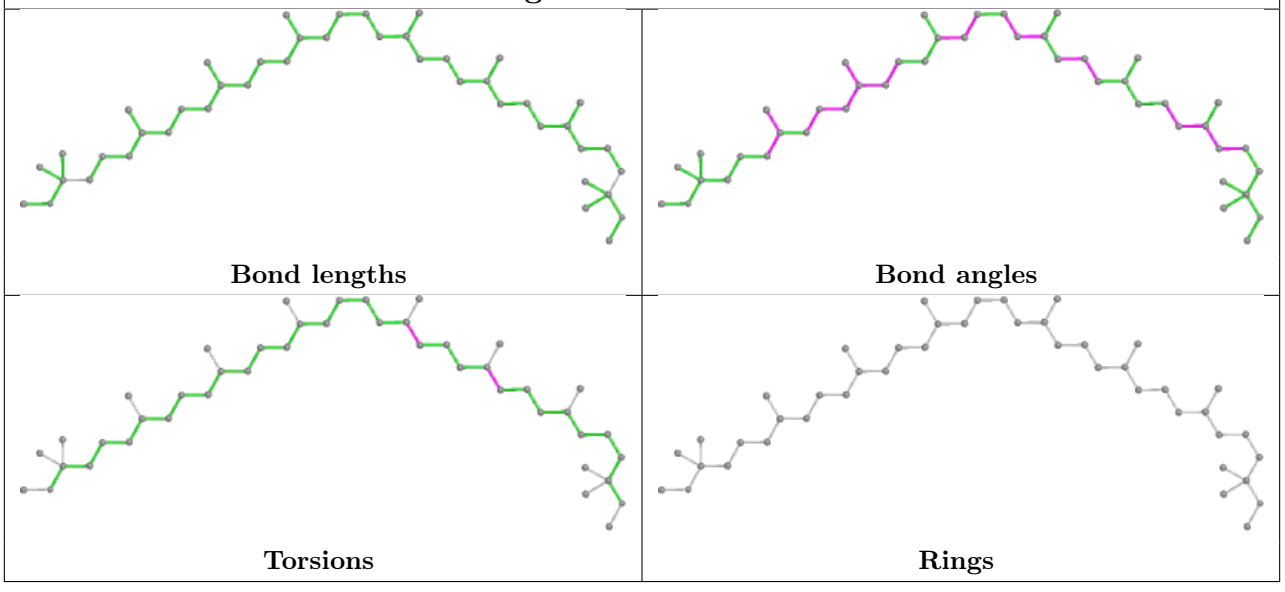
Ligand BCL O 502



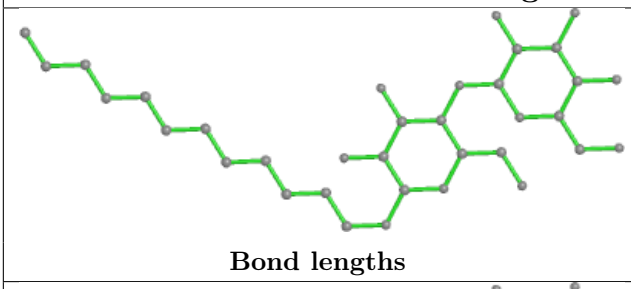
Ligand BCL U 101



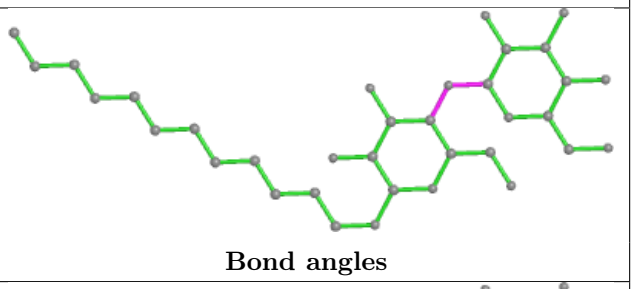
Ligand CRT Y 101



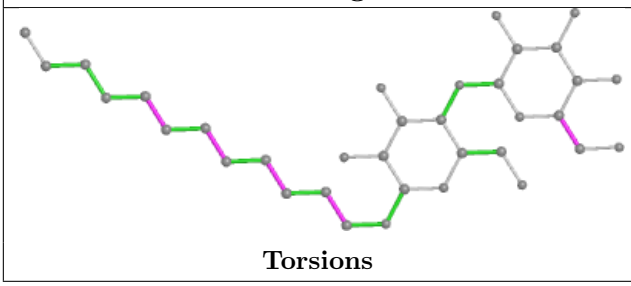
Ligand LMT B 101



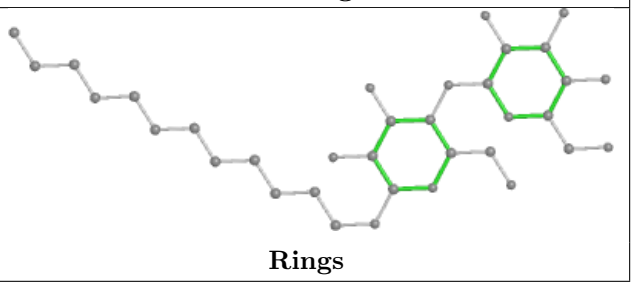
Bond lengths



Bond angles

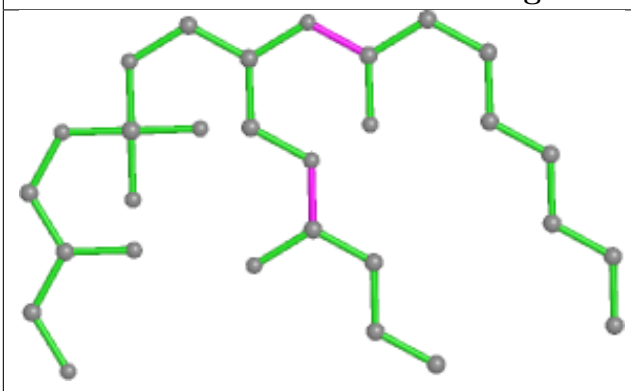


Torsions

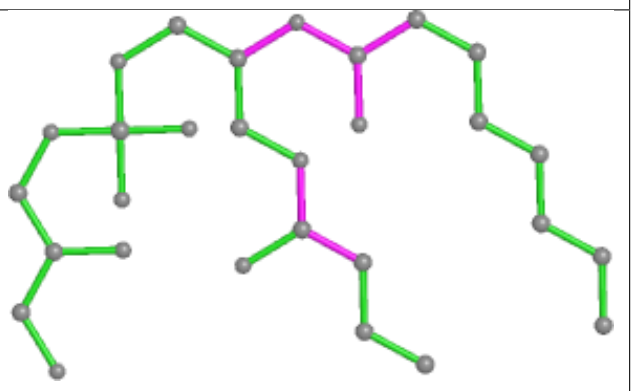


Rings

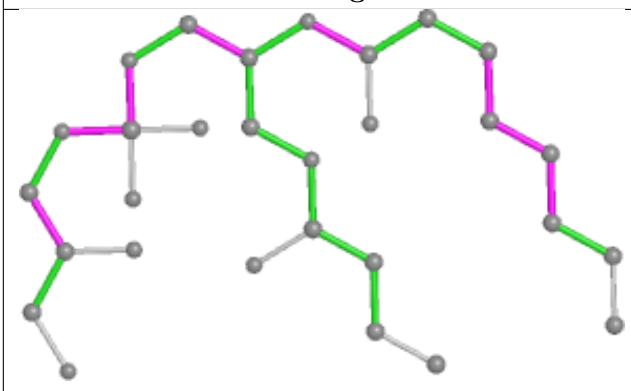
Ligand PGV L 305



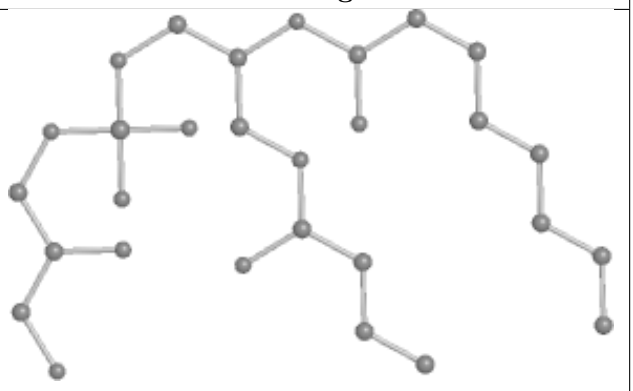
Bond lengths



Bond angles

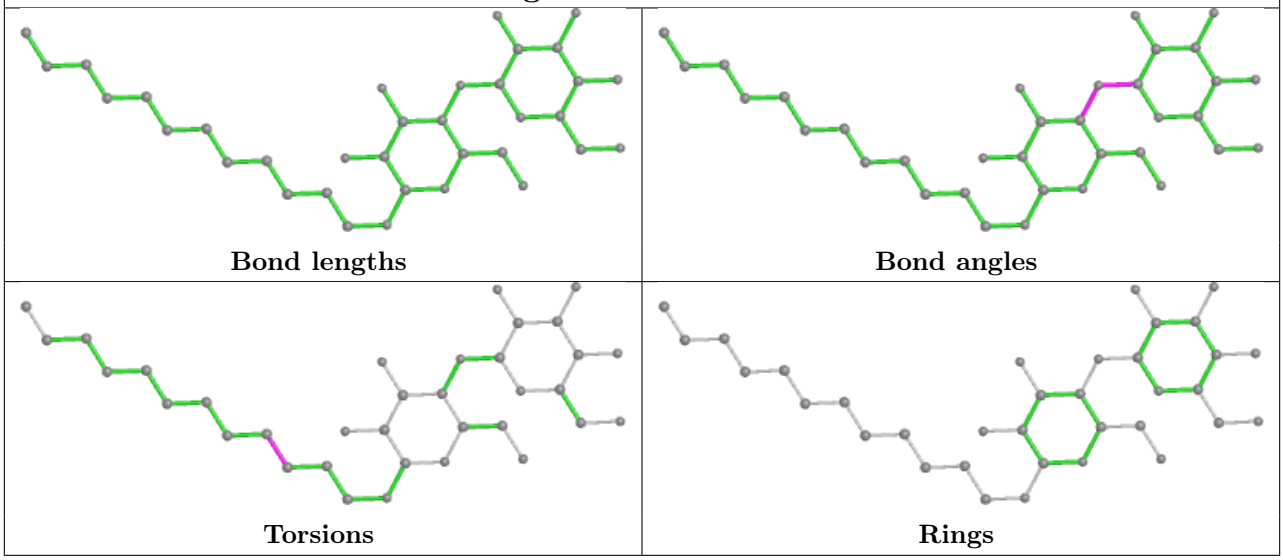


Torsions

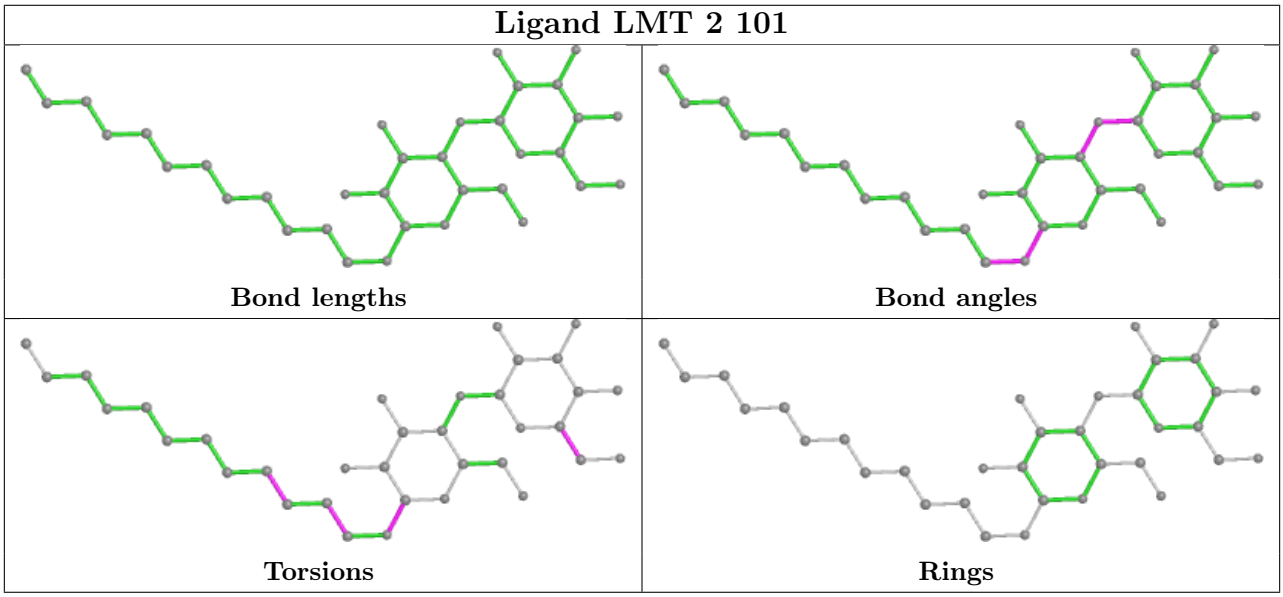


Rings

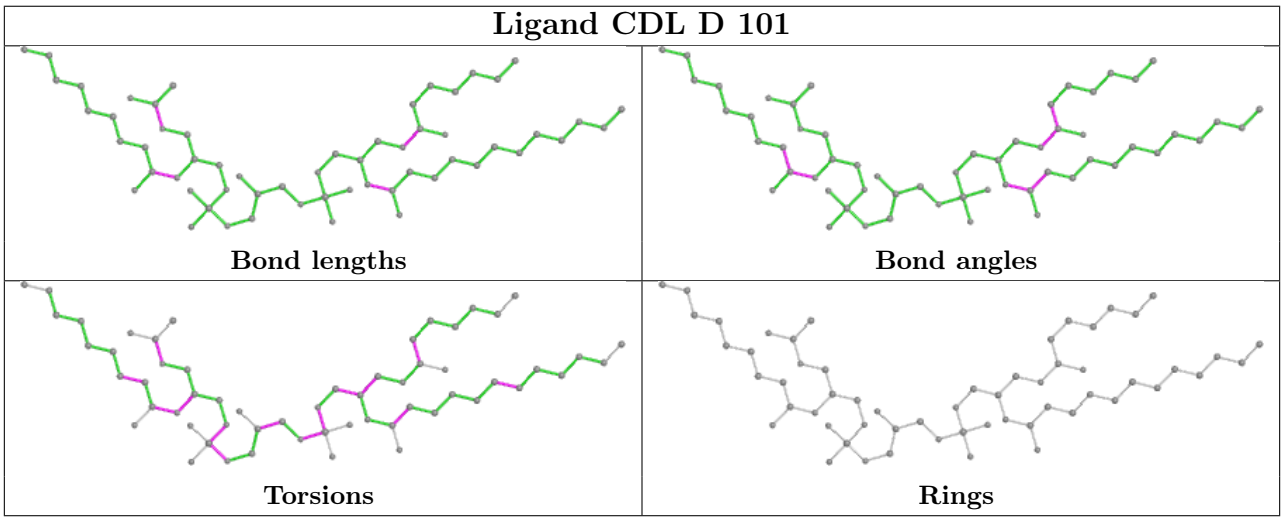
Ligand LMT P 104



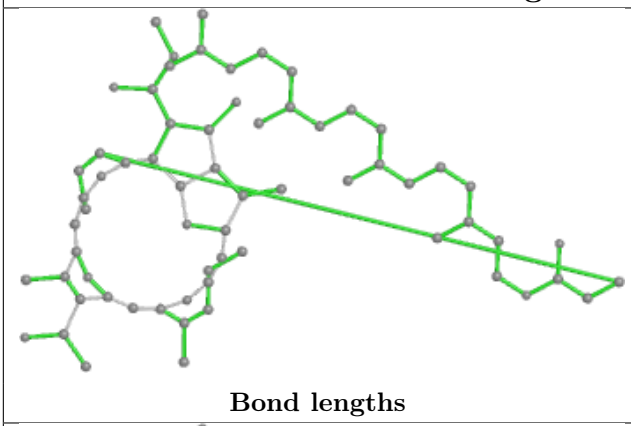
Ligand LMT 2 101



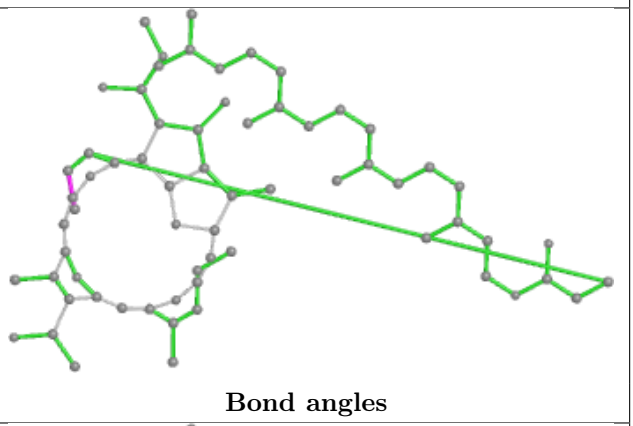
Ligand CDL D 101



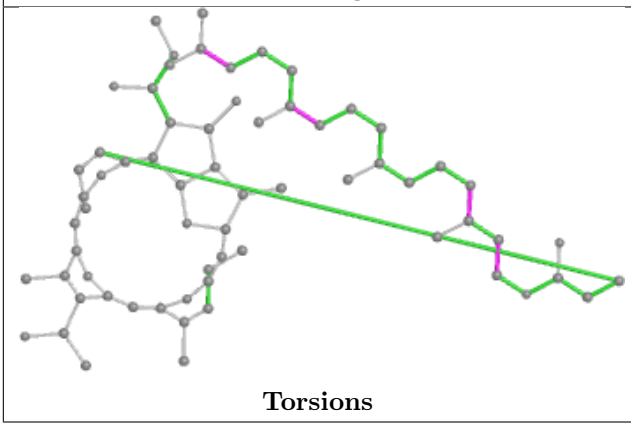
Ligand BPH L 302



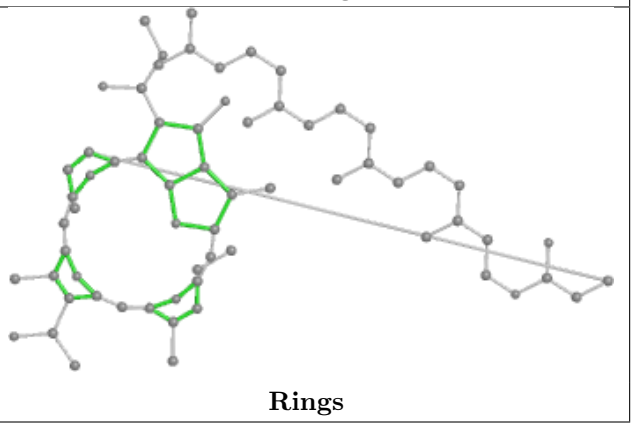
Bond lengths



Bond angles

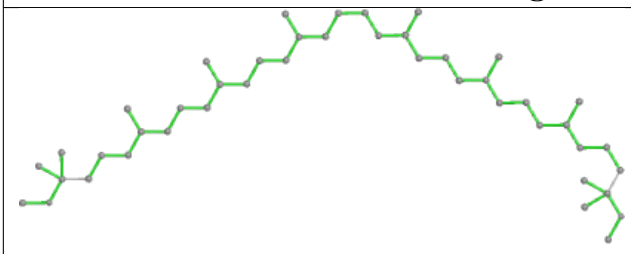


Torsions

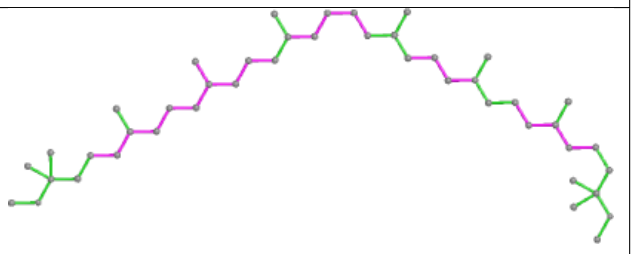


Rings

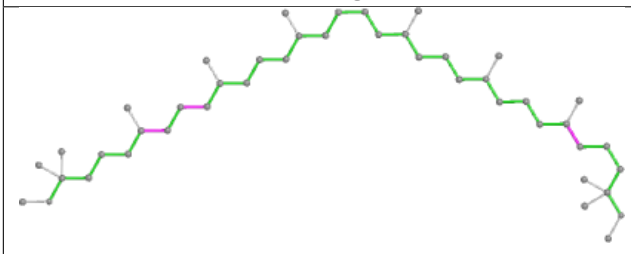
Ligand CRT 4 103



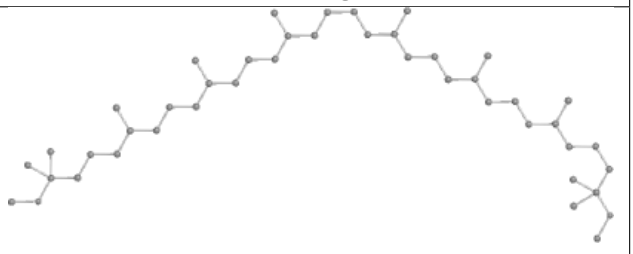
Bond lengths



Bond angles

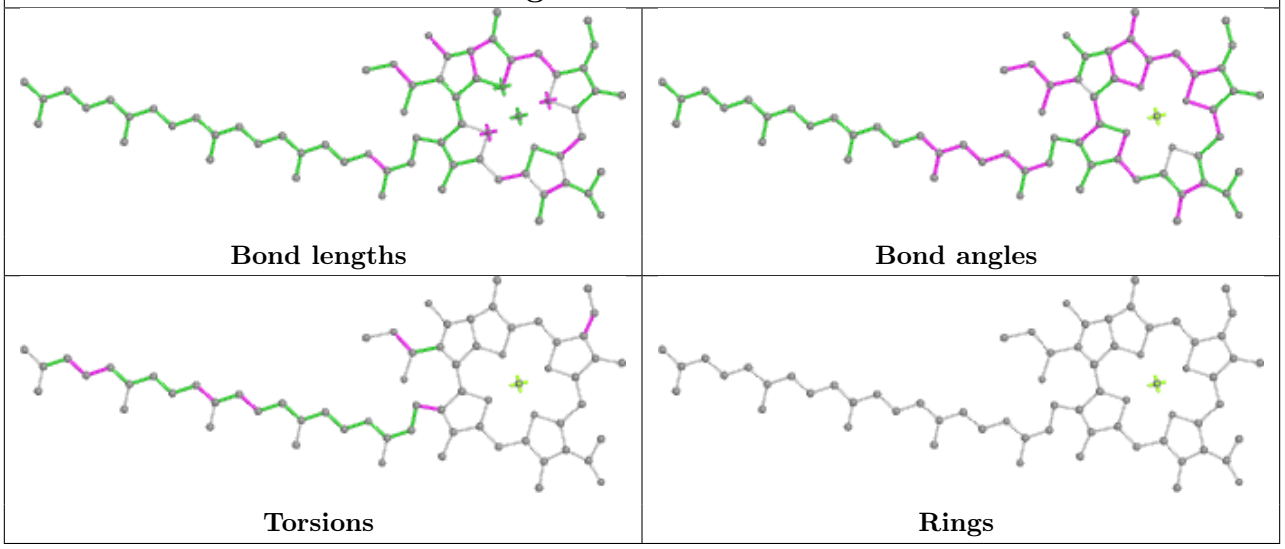


Torsions

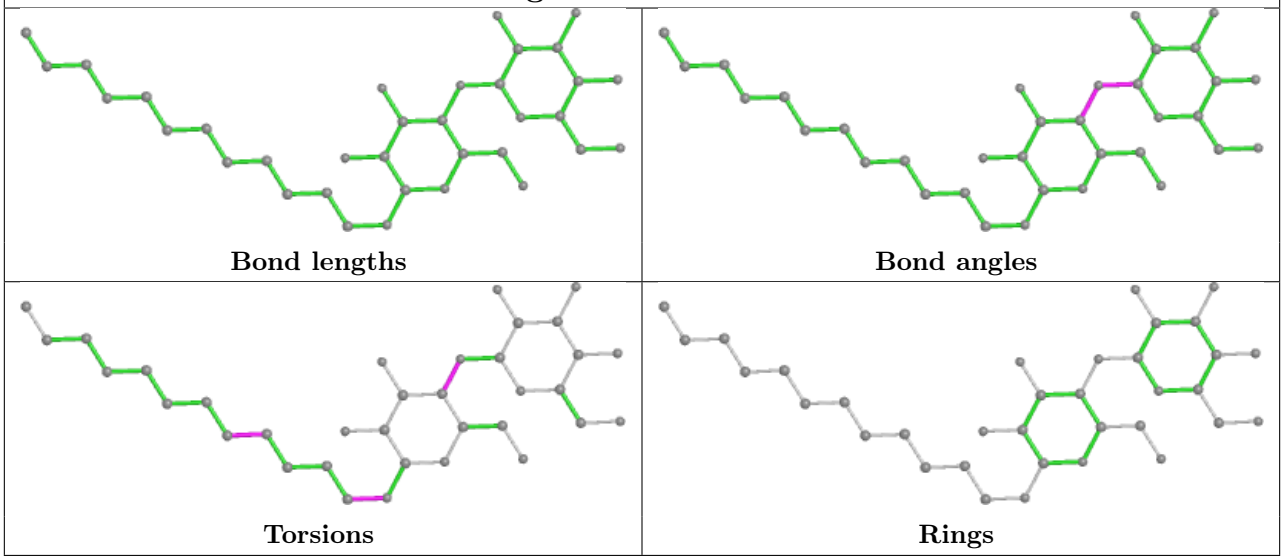


Rings

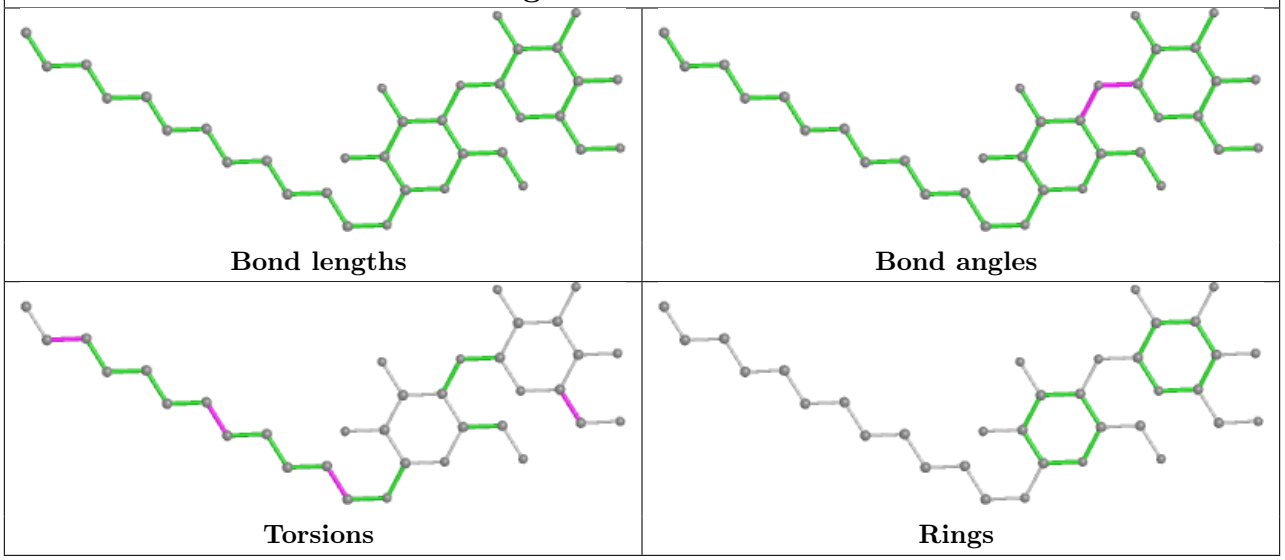
Ligand BCL B 102



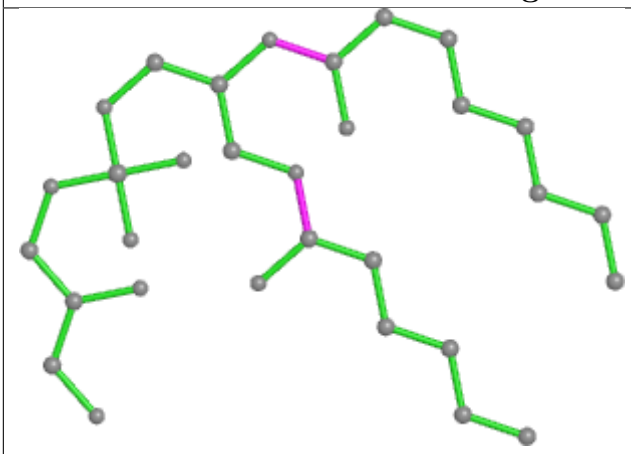
Ligand LMT 8 101



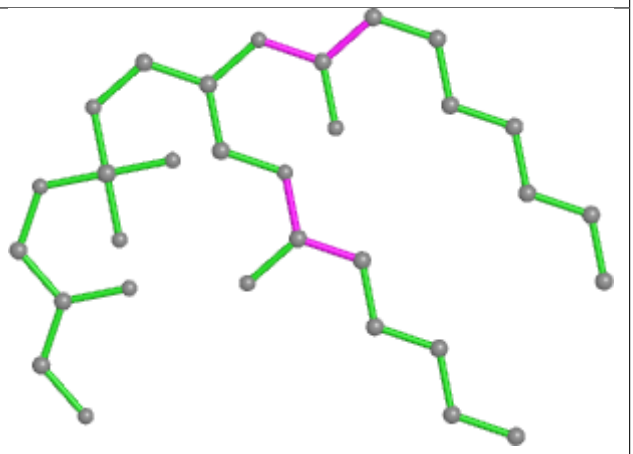
Ligand LMT P 101



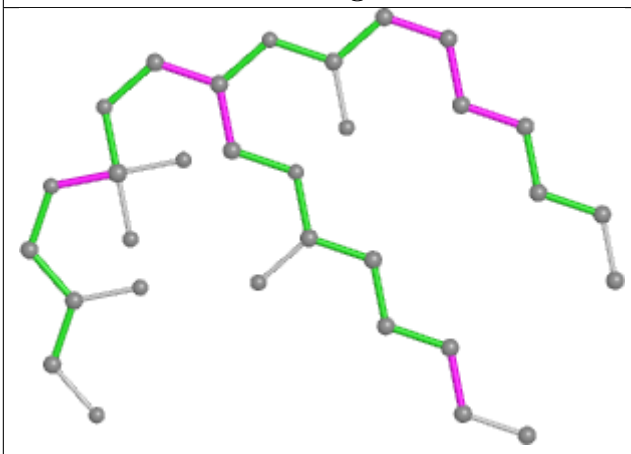
Ligand PGV C 408



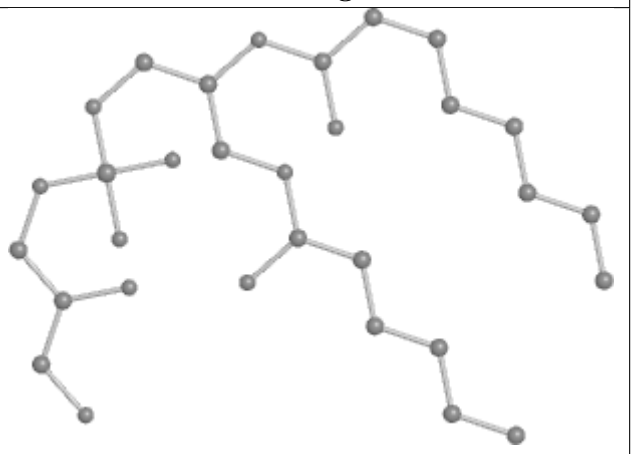
Bond lengths



Bond angles

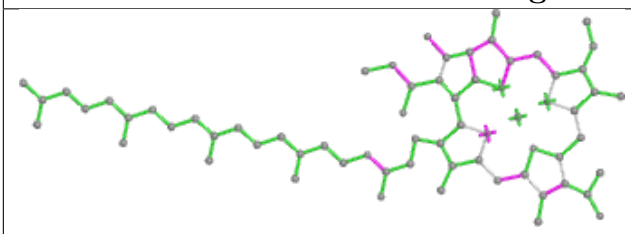


Torsions

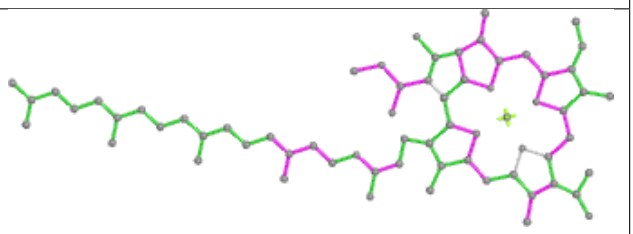


Rings

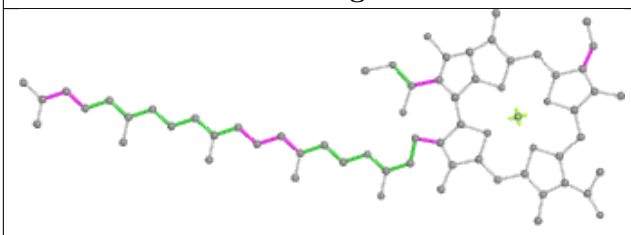
Ligand BCL 3 101



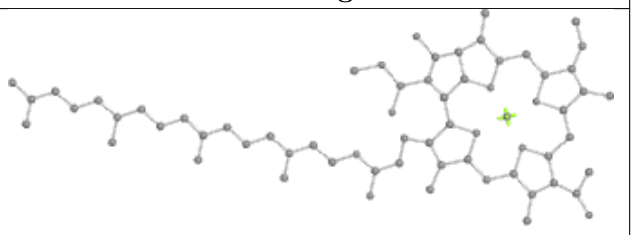
Bond lengths



Bond angles

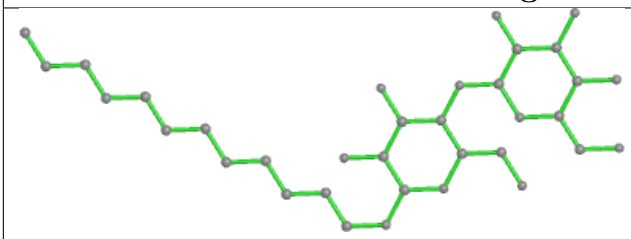


Torsions

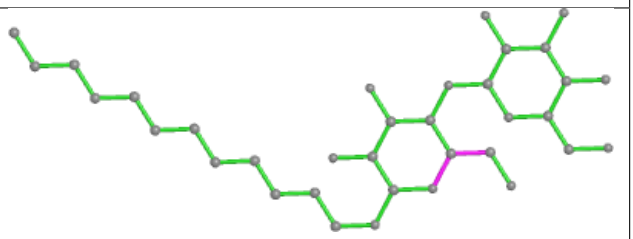


Rings

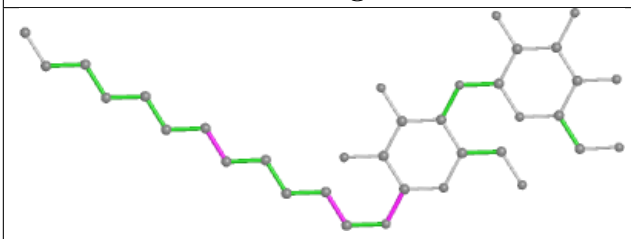
Ligand LMT H 303



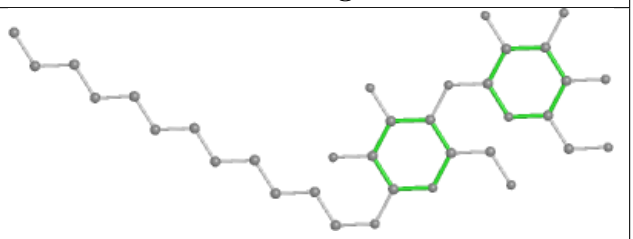
Bond lengths



Bond angles

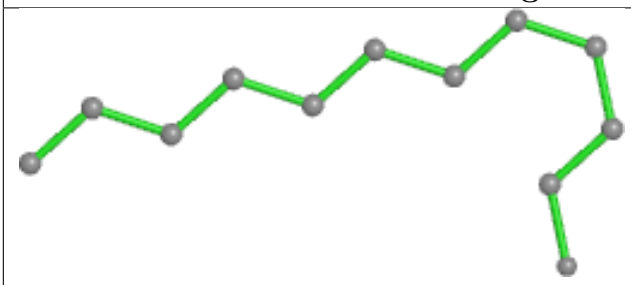


Torsions

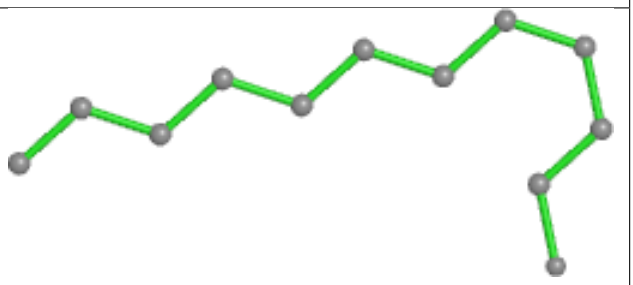


Rings

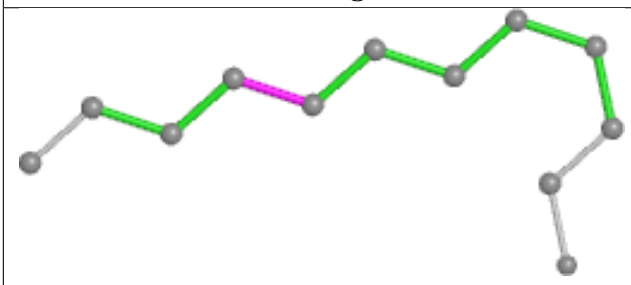
Ligand PLM C 407



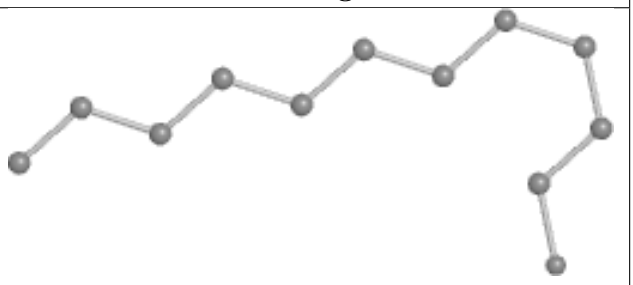
Bond lengths



Bond angles

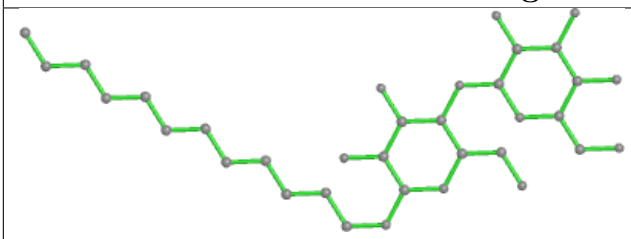


Torsions

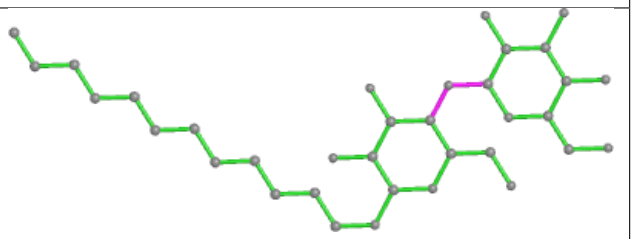


Rings

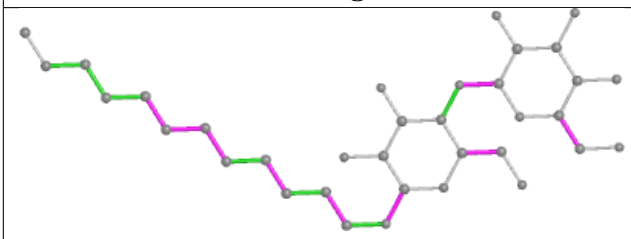
Ligand LMT T 103



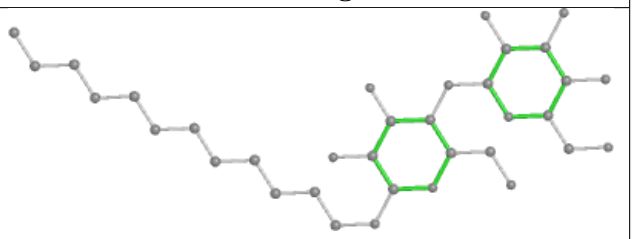
Bond lengths



Bond angles

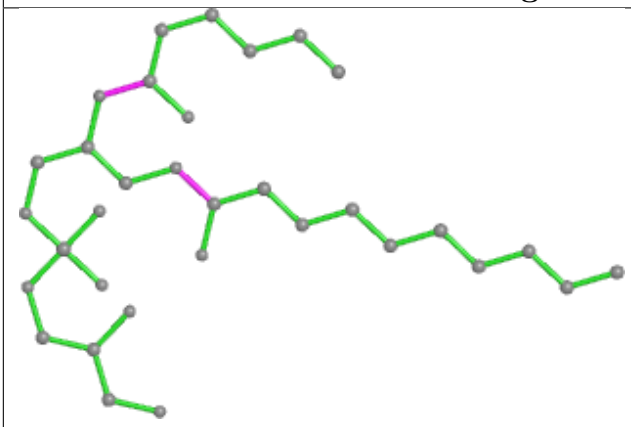


Torsions

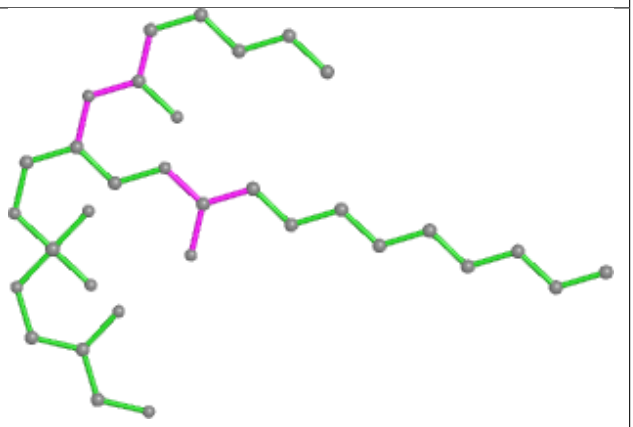


Rings

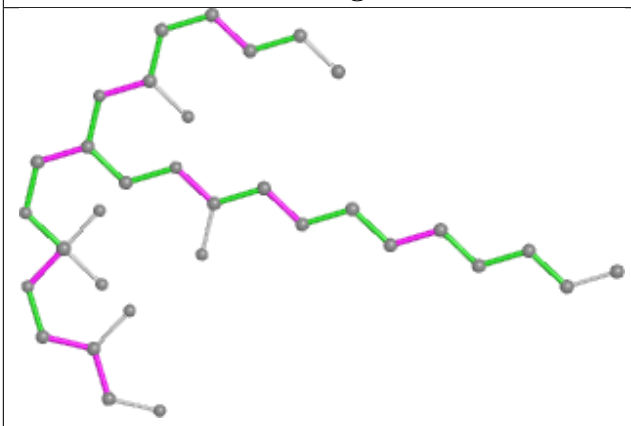
Ligand PGV A 503



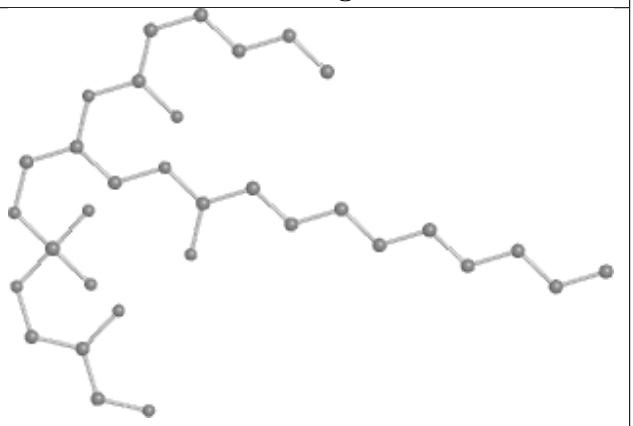
Bond lengths



Bond angles

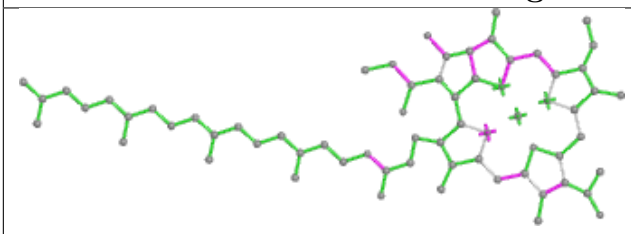


Torsions

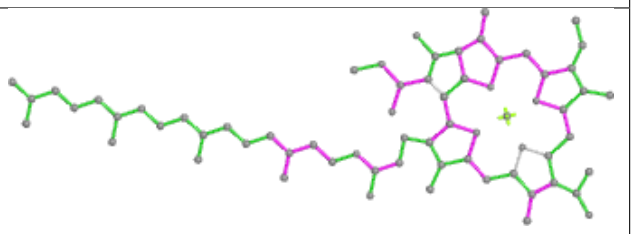


Rings

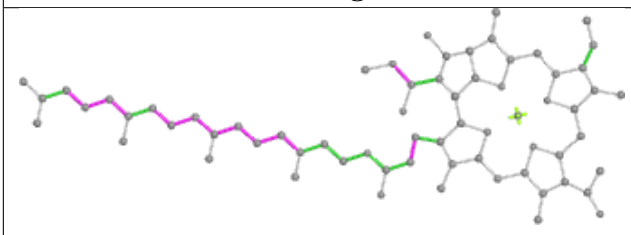
Ligand BCL E 102



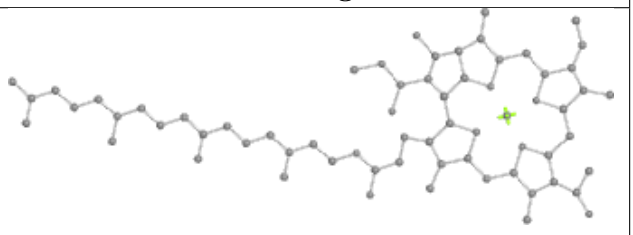
Bond lengths



Bond angles

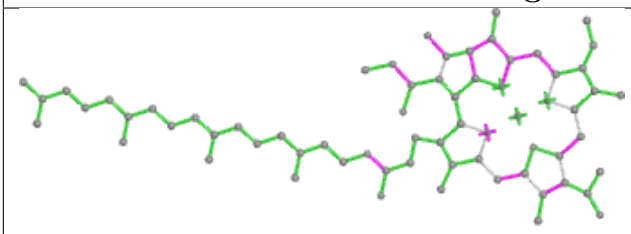


Torsions

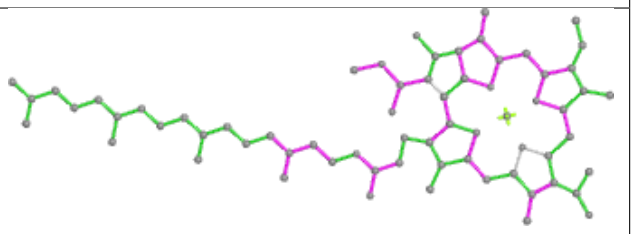


Rings

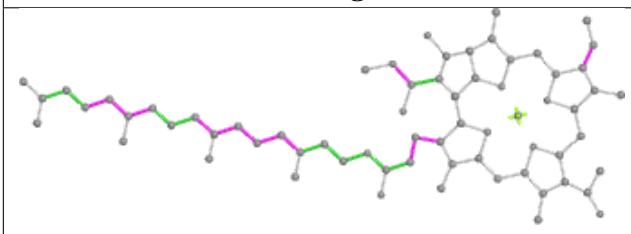
Ligand BCL G 102



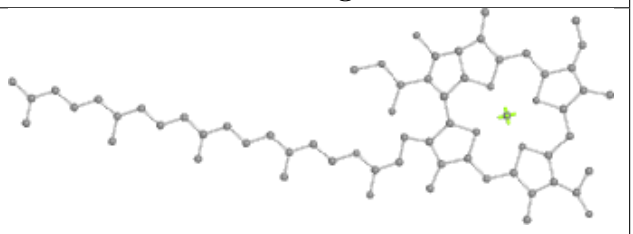
Bond lengths



Bond angles

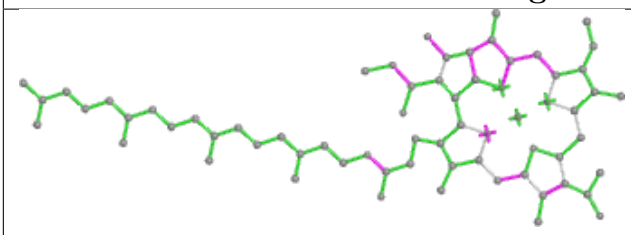


Torsions

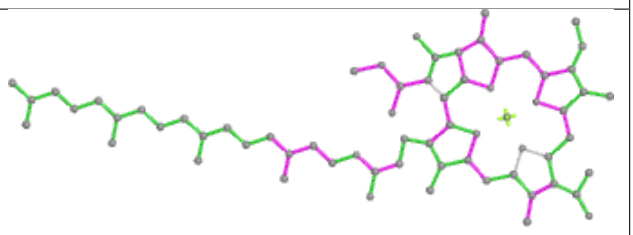


Rings

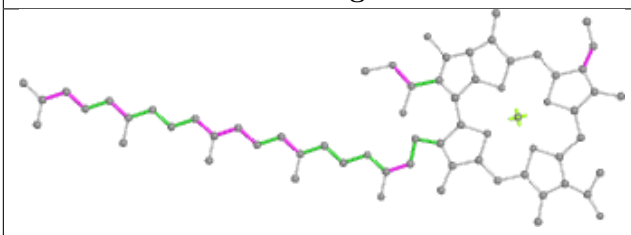
Ligand BCL 4 102



Bond lengths



Bond angles



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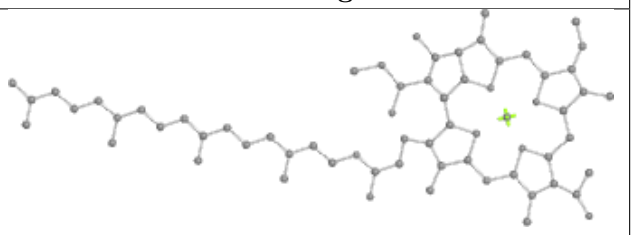
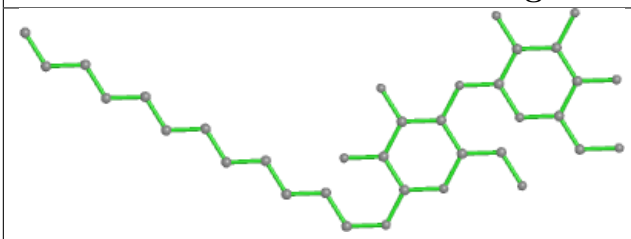
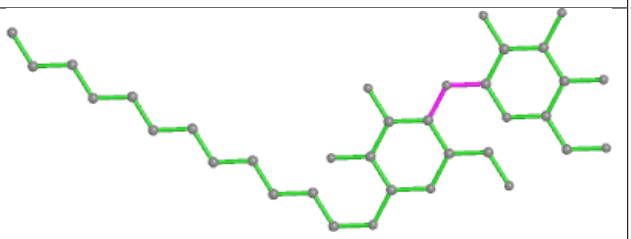
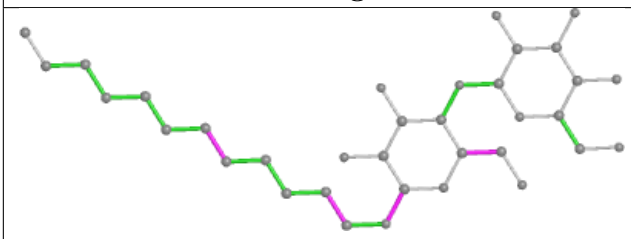


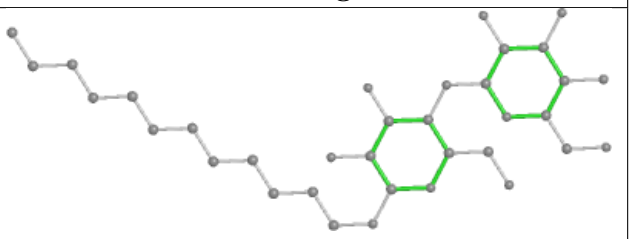
Rings

Ligand LMT J 104

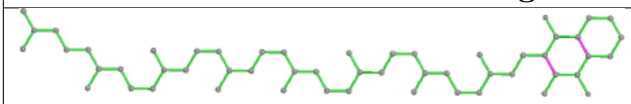

Bond lengths


Bond angles


Torsions


Rings

Ligand MQ8 M 405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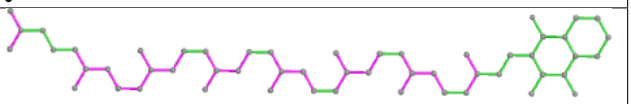
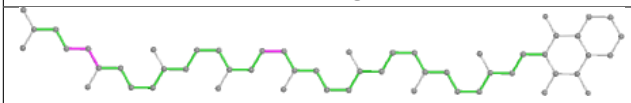
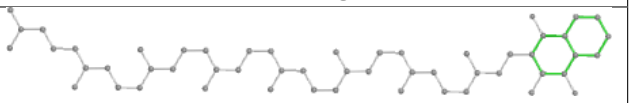
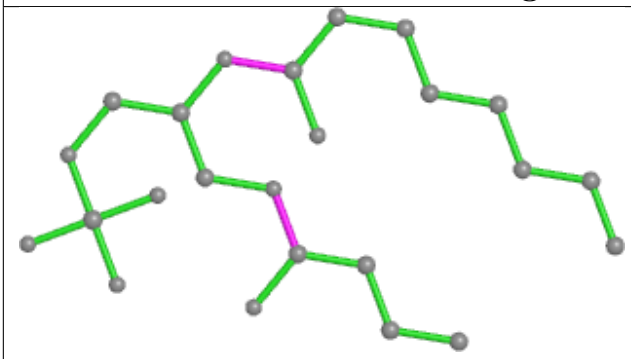
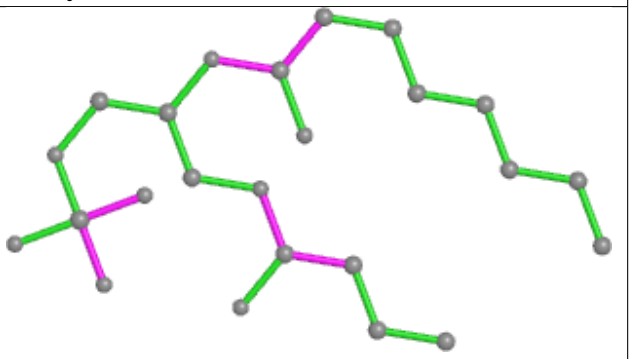

Bond angles

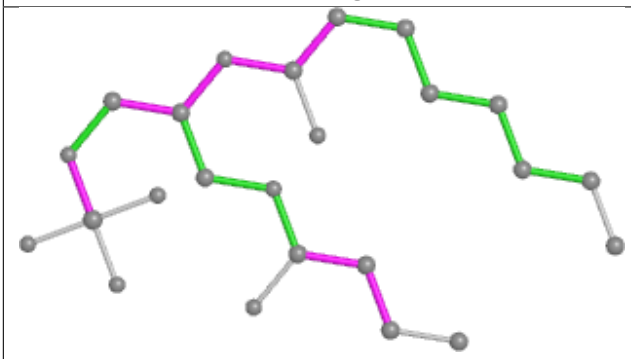

Torsions

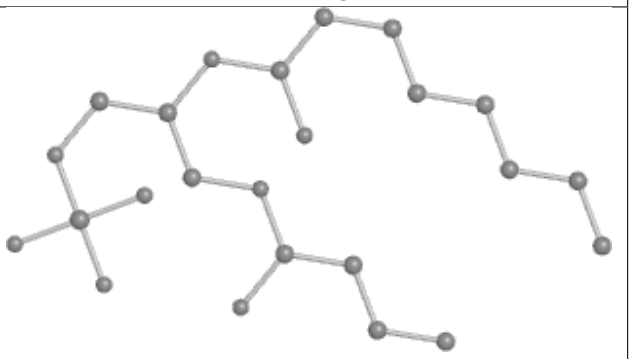

Rings

Ligand PGV Q 101

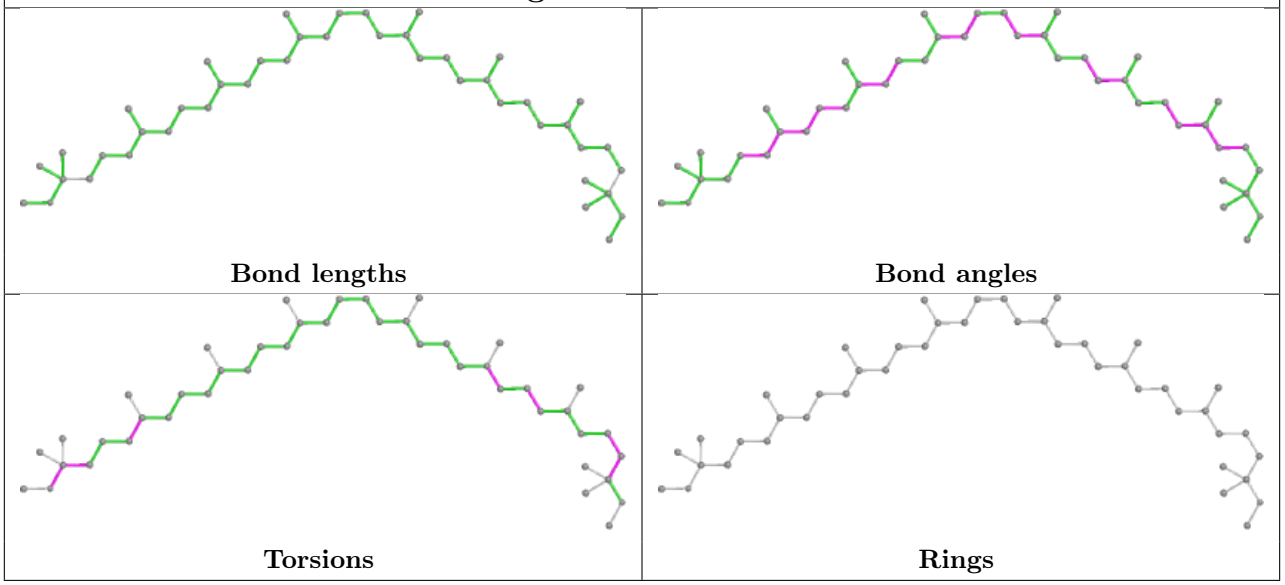

Bond lengths


Bond angles

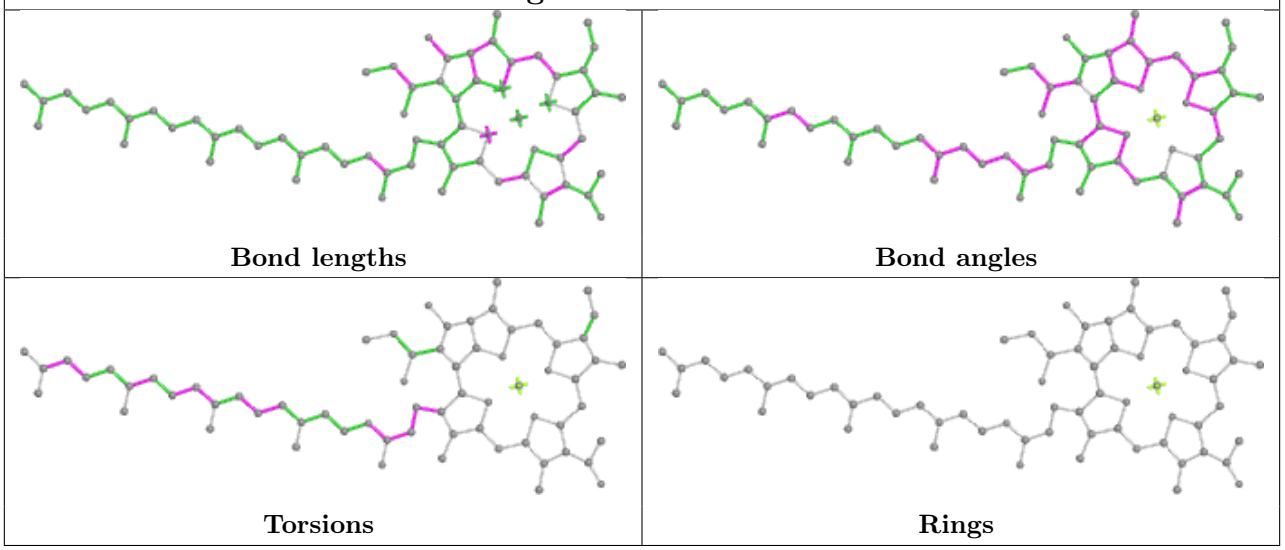

Torsions


Rings

Ligand CRT Z 103



Ligand BCL P 102



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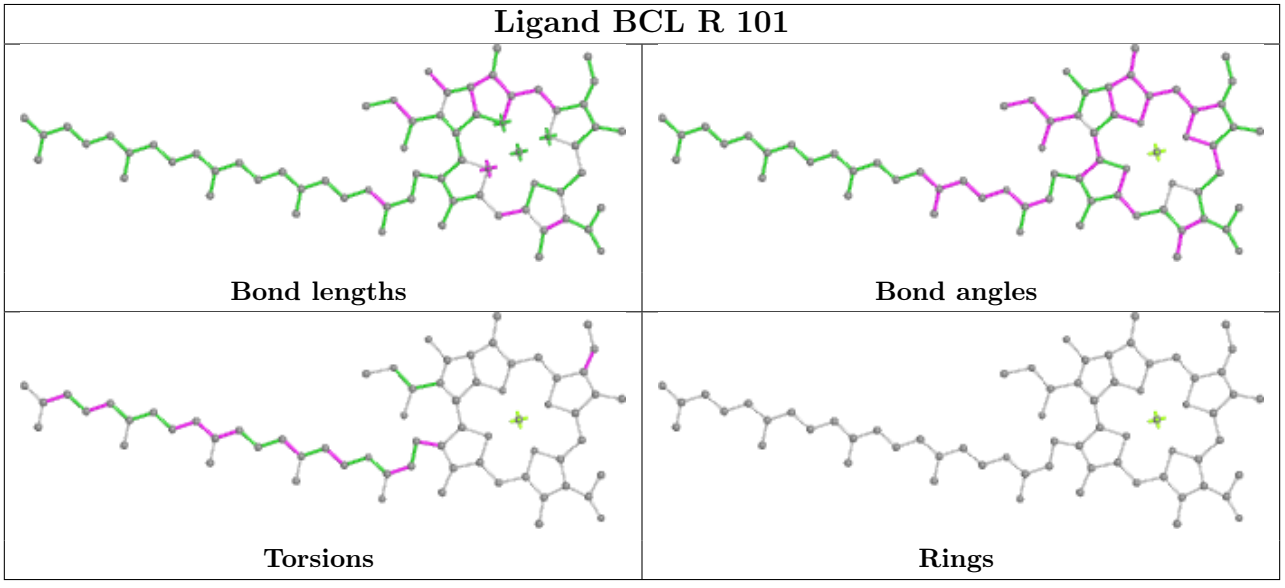

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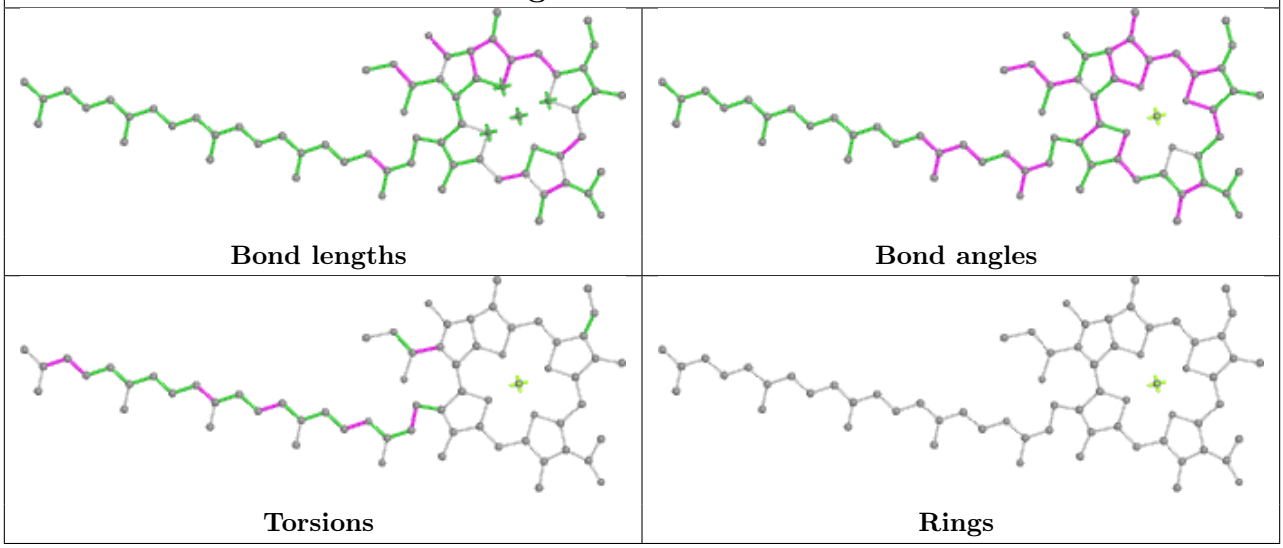
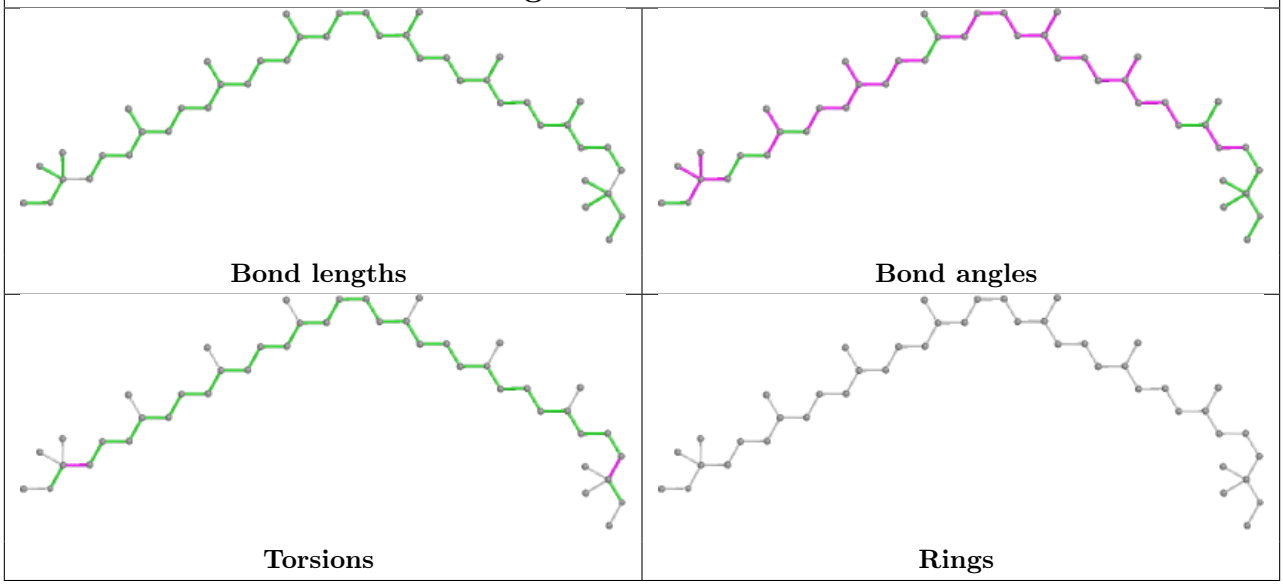
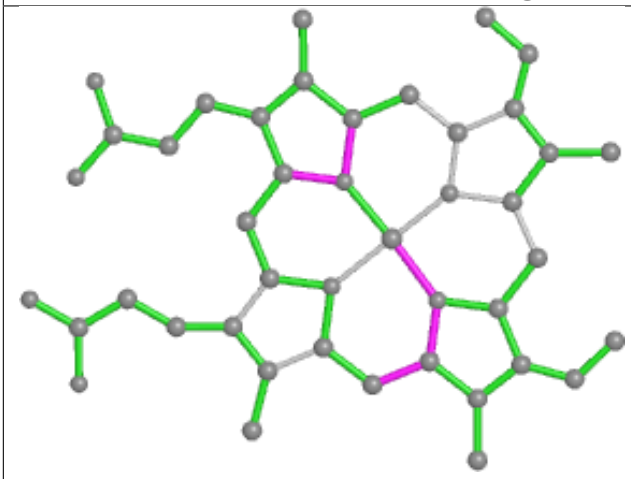


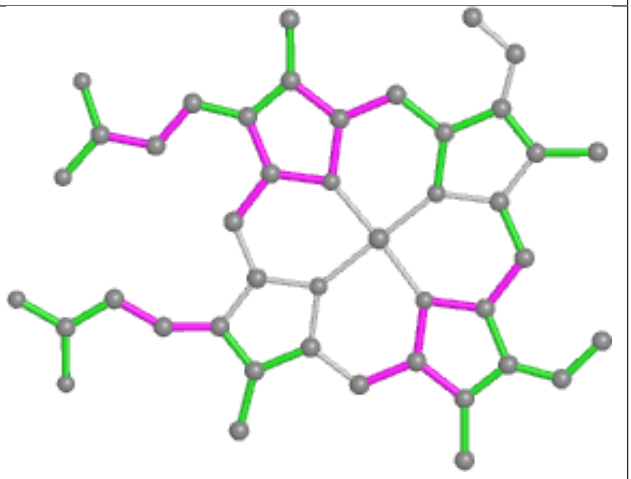
Ligand CRT V 102



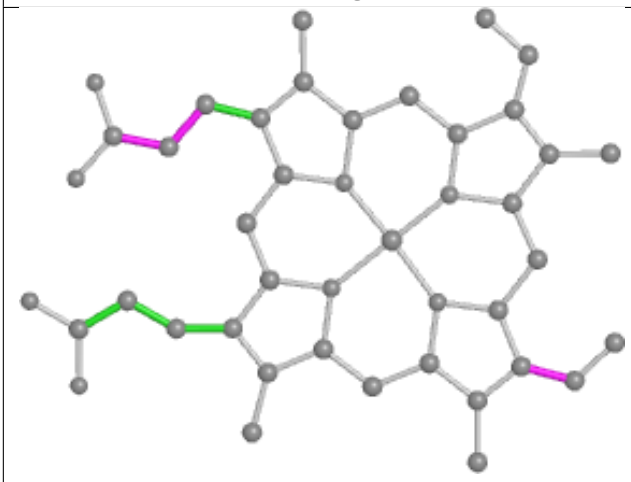
Ligand HEM C 402



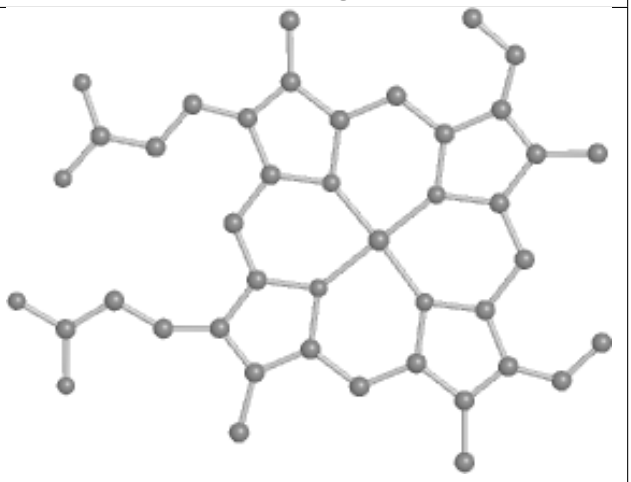
Bond lengths



Bond angles

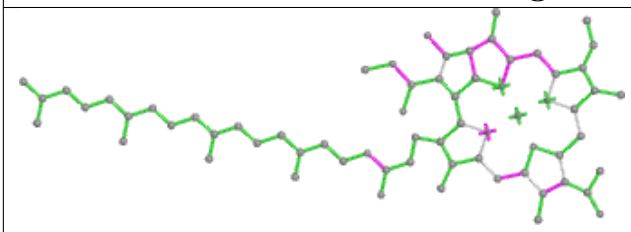


Torsions



Rings

Ligand BCL 9 102



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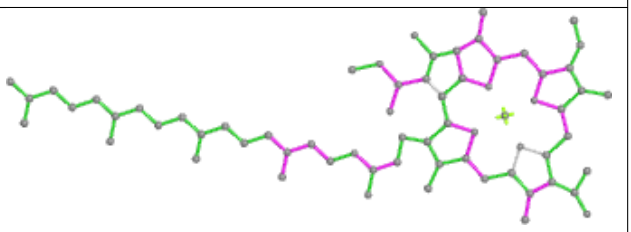
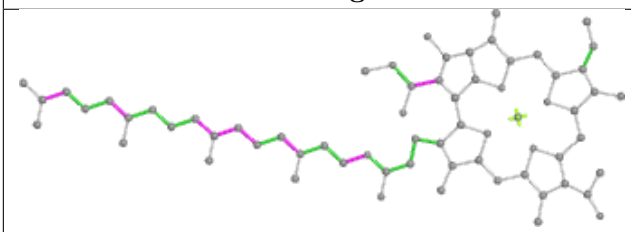


Bond angles



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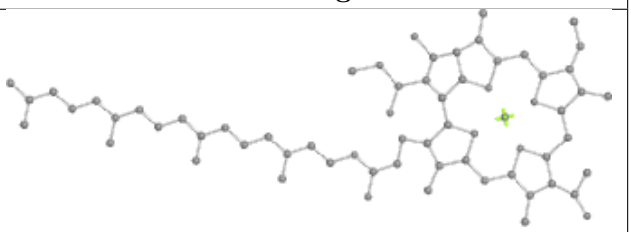
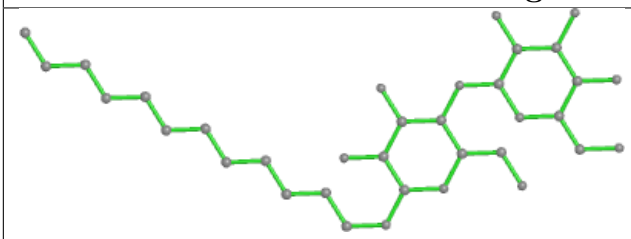
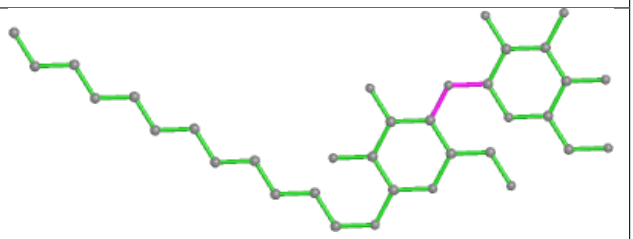


Rings

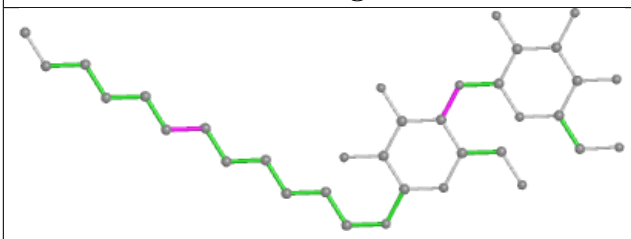
Ligand LMT 4 104



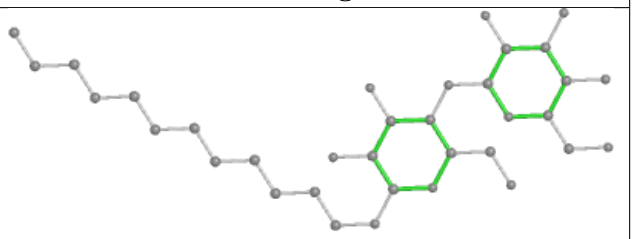
Bond lengths



Bond angles

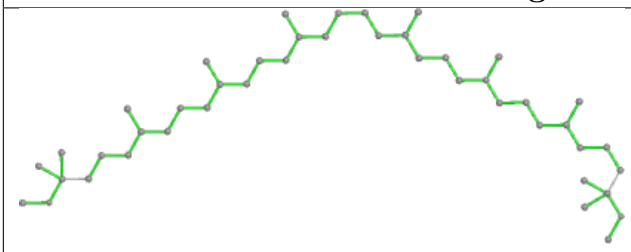


Torsions

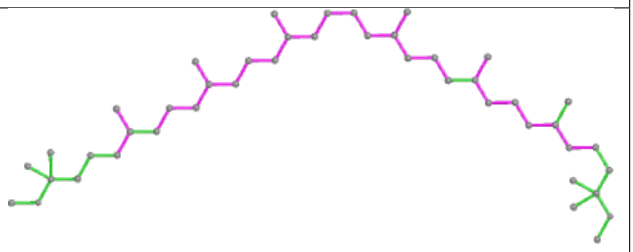


Rings

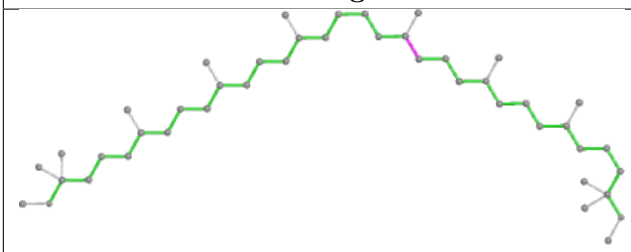
Ligand CRT 0 102



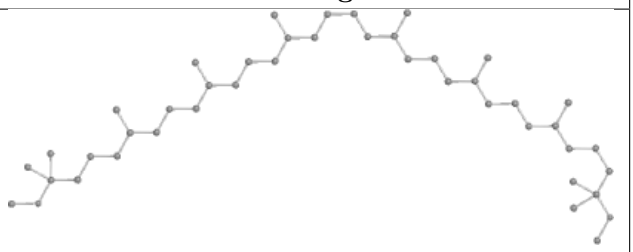
Bond lengths



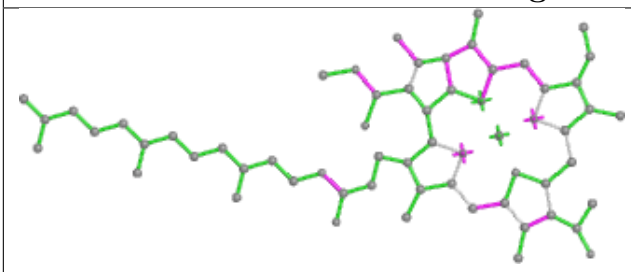
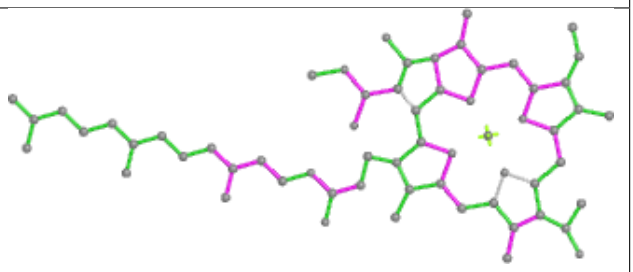
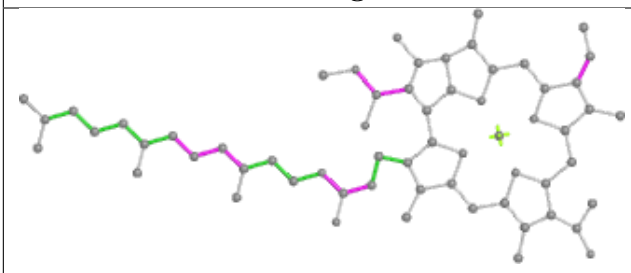
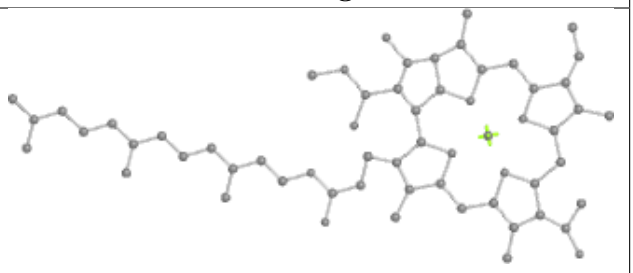
Bond angles

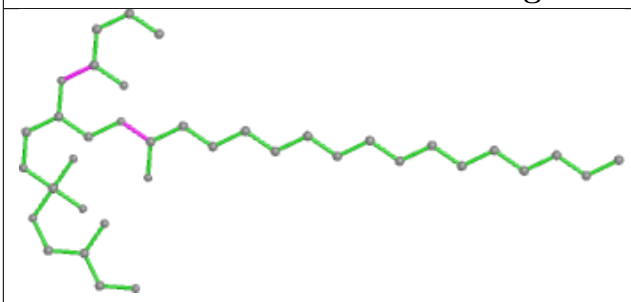
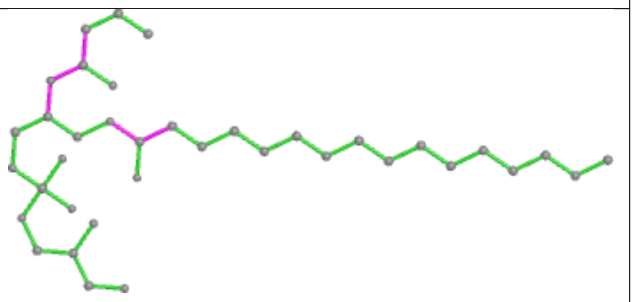
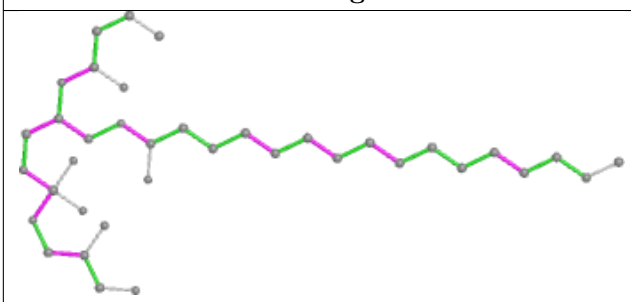
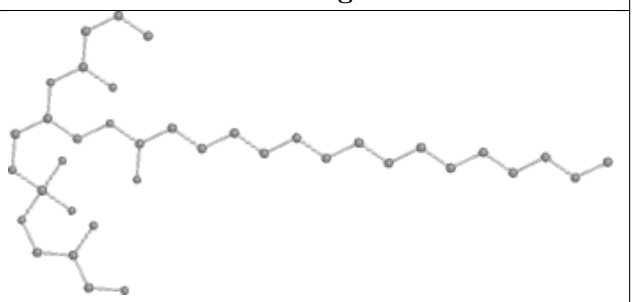


Torsions

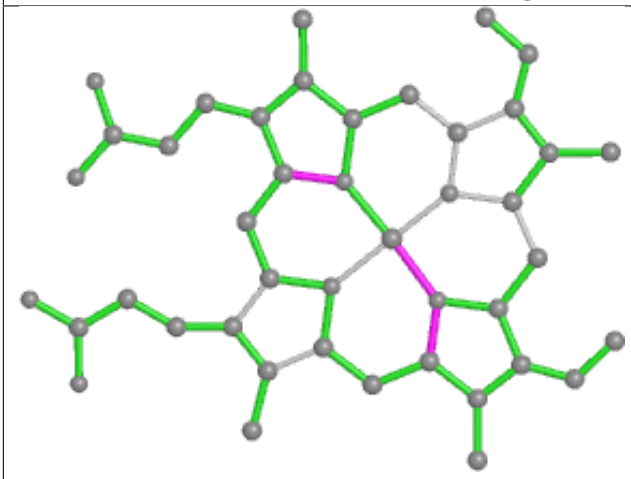


Rings

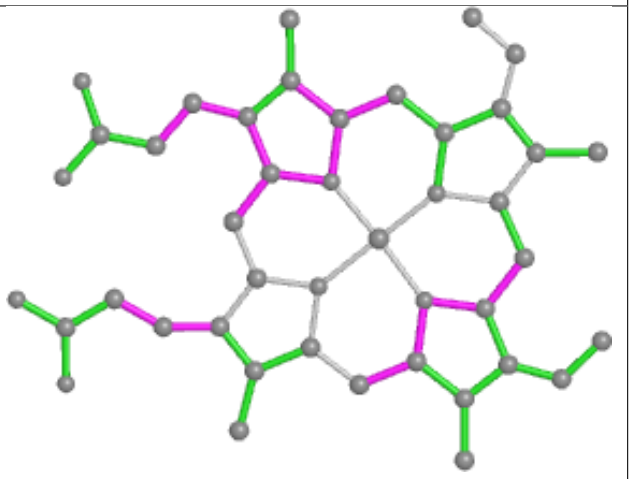
Ligand BCL 7 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV L 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

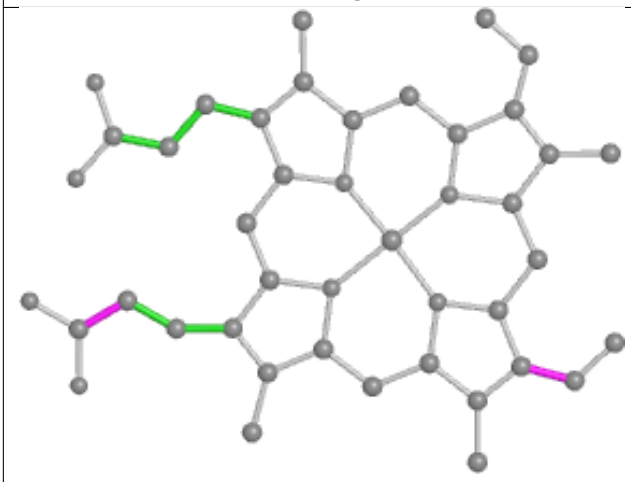
Ligand HEM C 401



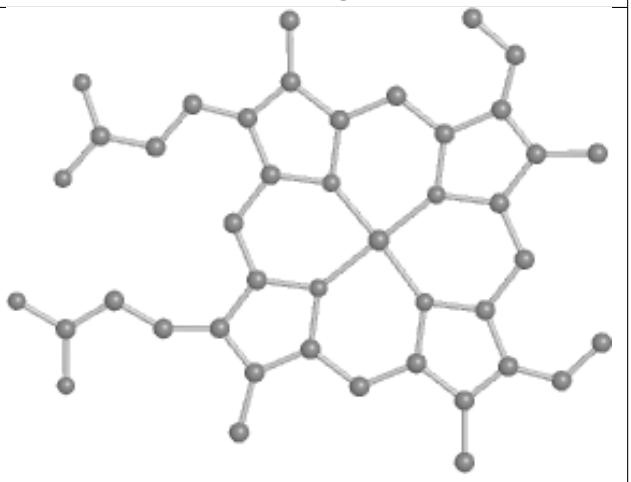
Bond lengths



Bond angles

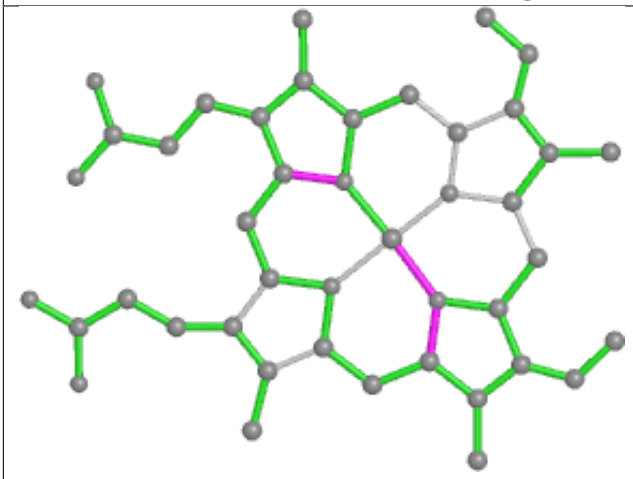


Torsions

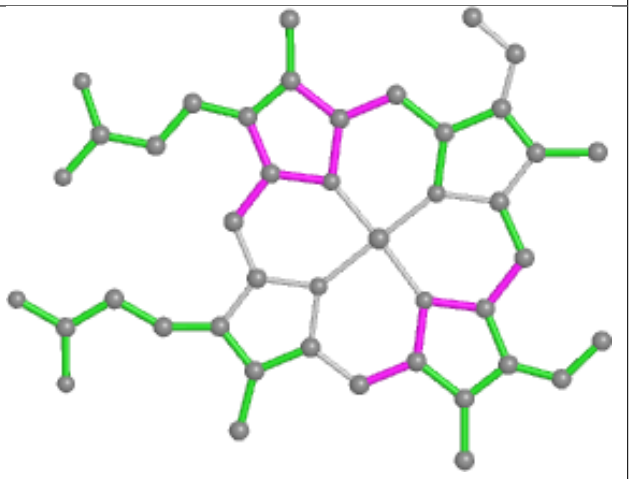


Rings

Ligand HEM C 404



Bond lengths



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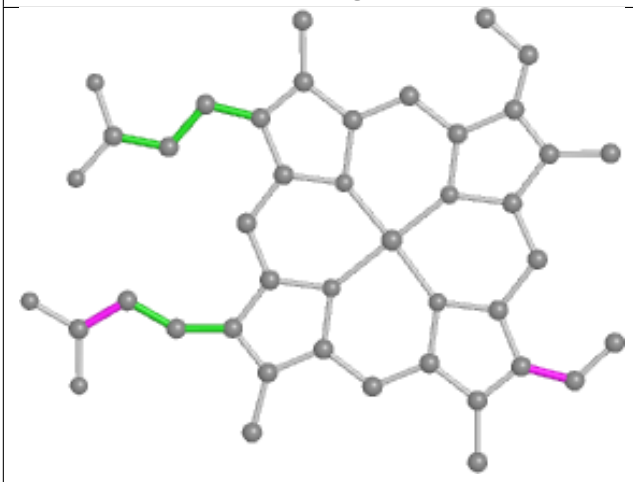
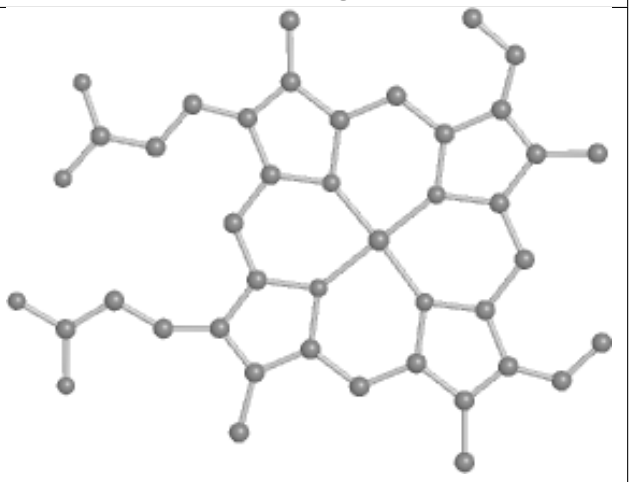
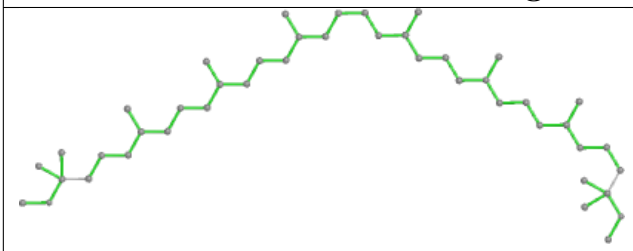


Torsions

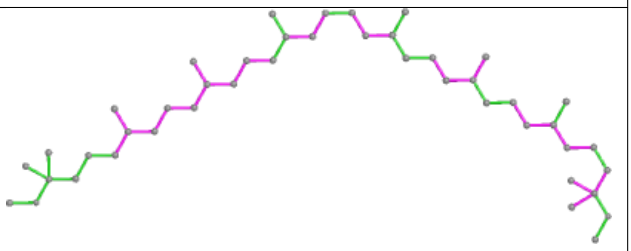


Rings

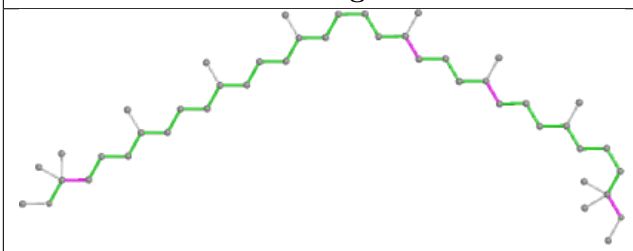
Ligand CRT P 103



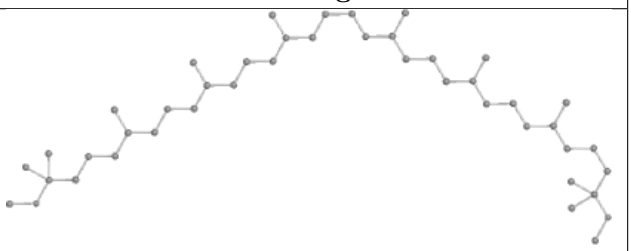
Bond lengths



Bond angles

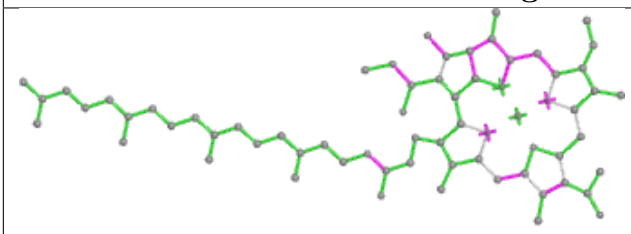


Torsions

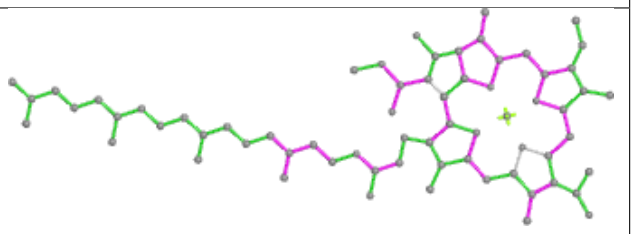


Rings

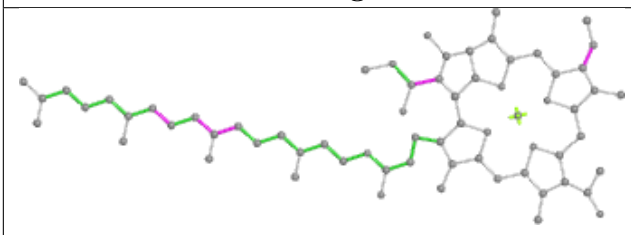
Ligand BCL M 402



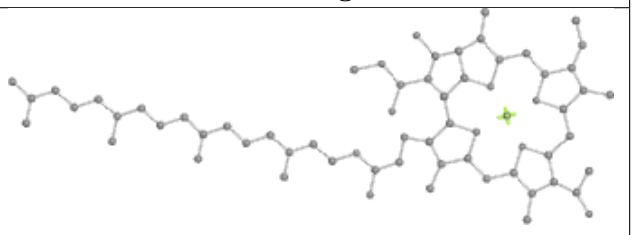
Bond lengths



Bond angles

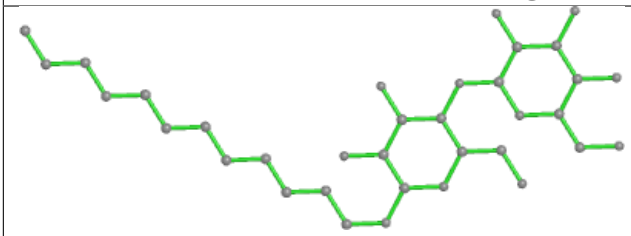


Torsions

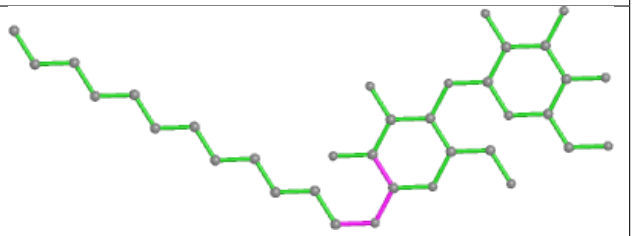


Rings

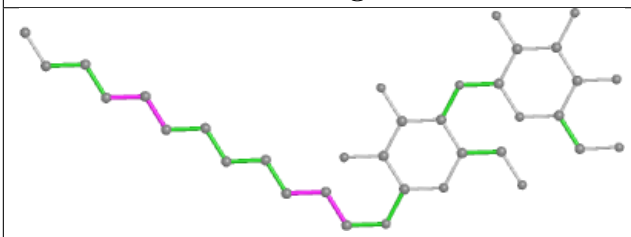
Ligand LMT Z 101



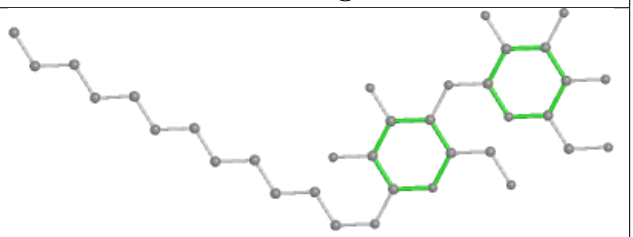
Bond lengths



Bond angles

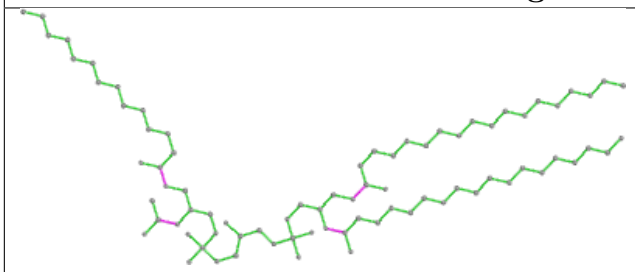


Torsions

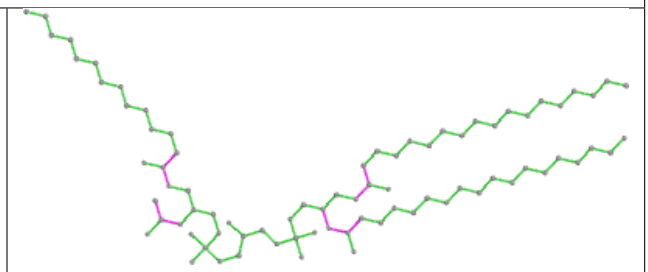


Rings

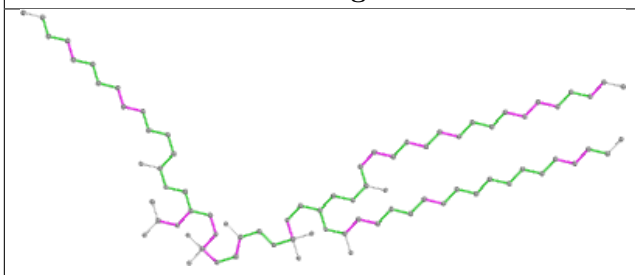
Ligand CDL L 311



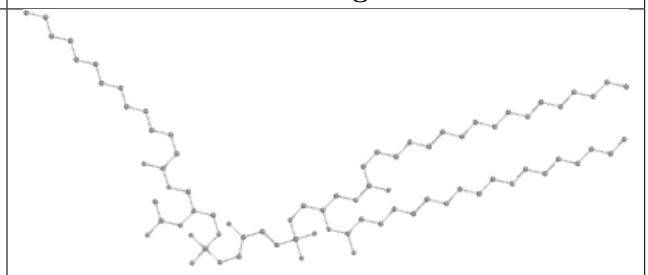
Bond lengths



Bond angles

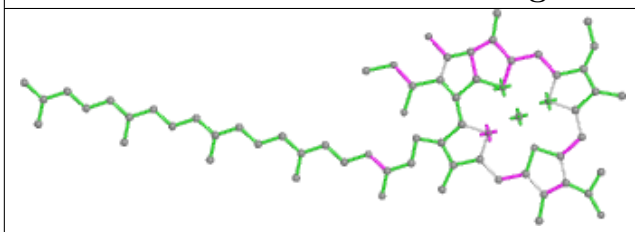


Torsions

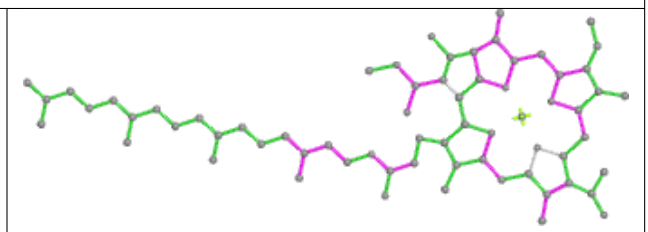


Rings

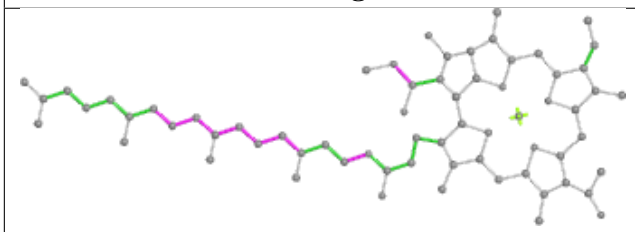
Ligand BCL S 102



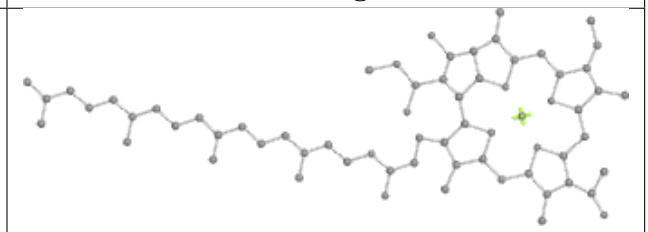
Bond lengths



Bond angles

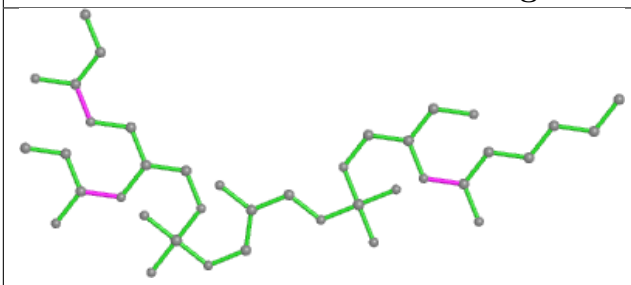


Torsions

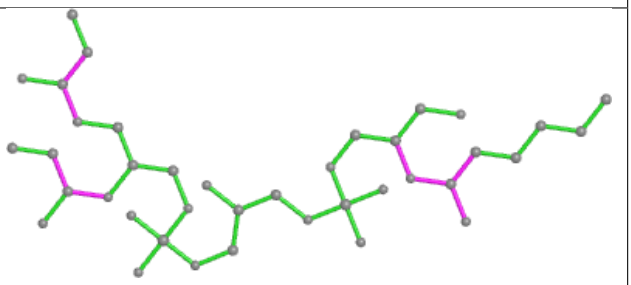


Rings

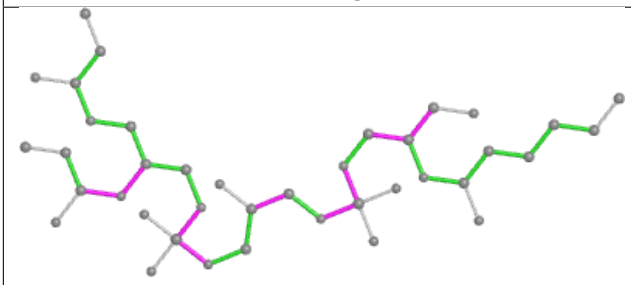
Ligand CDL M 407



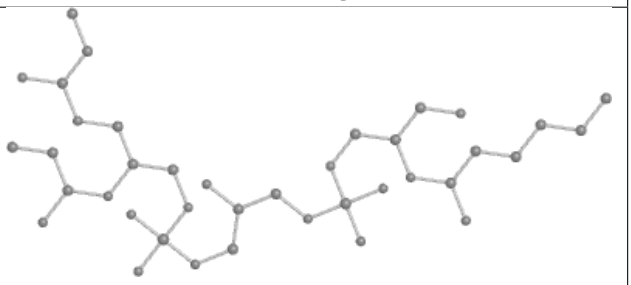
Bond lengths



Bond angles

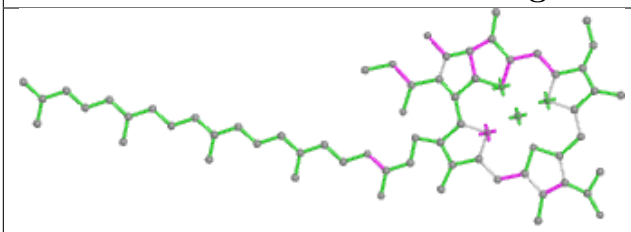


Torsions

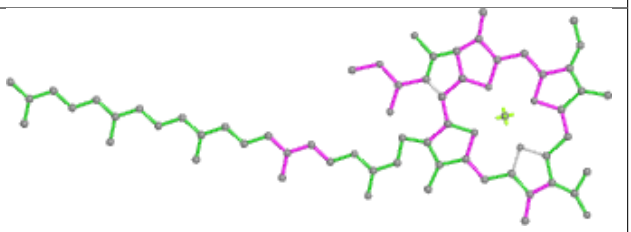


Rings

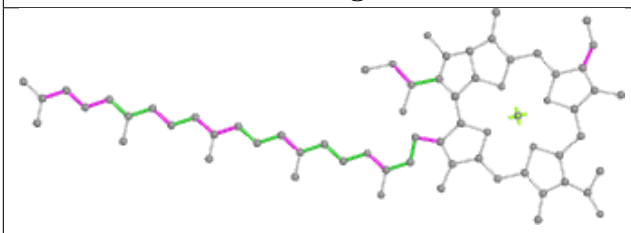
Ligand BCL 0 101



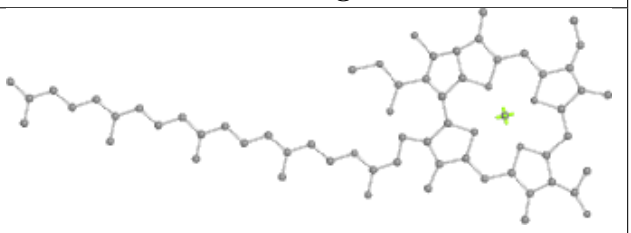
Bond lengths



Bond angles

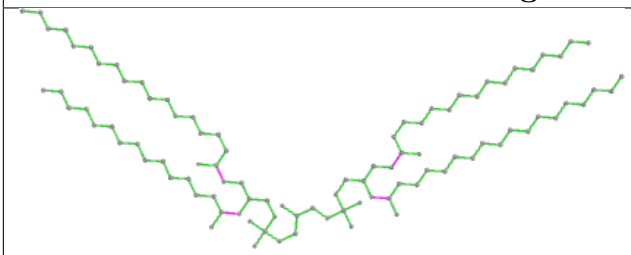


Torsions

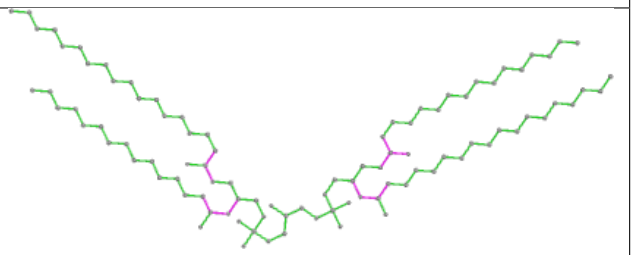


Rings

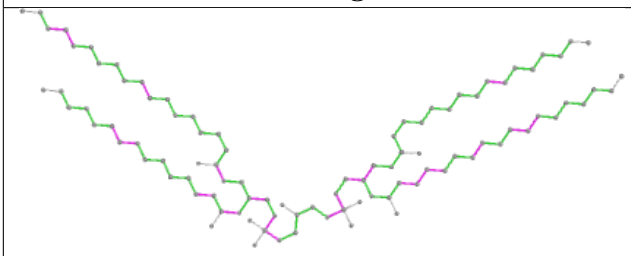
Ligand CDL M 409



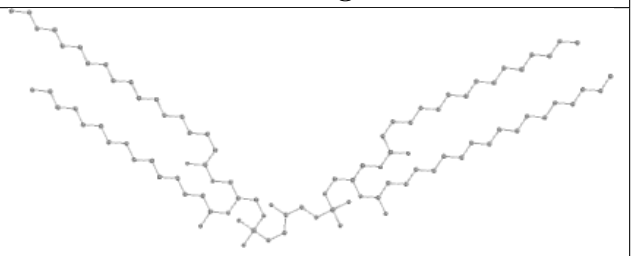
Bond lengths



Bond angles

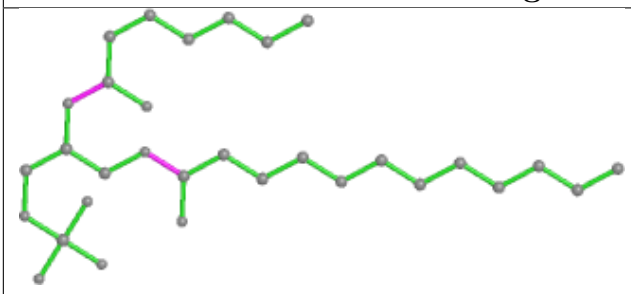


Torsions

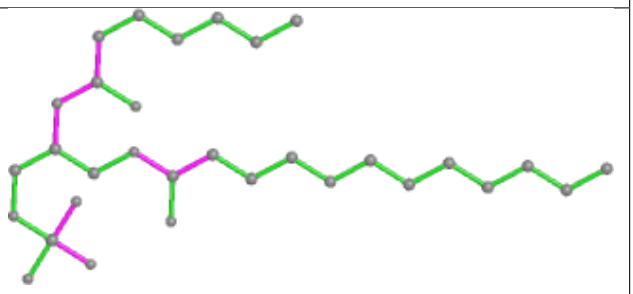


Rings

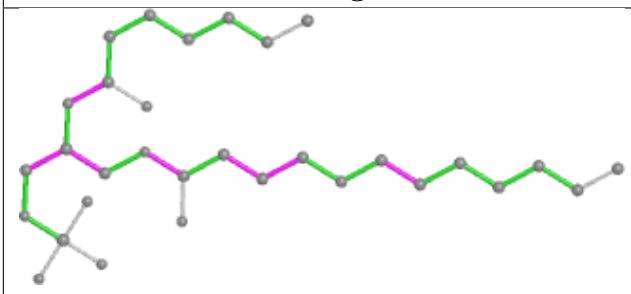
Ligand PGV F 501



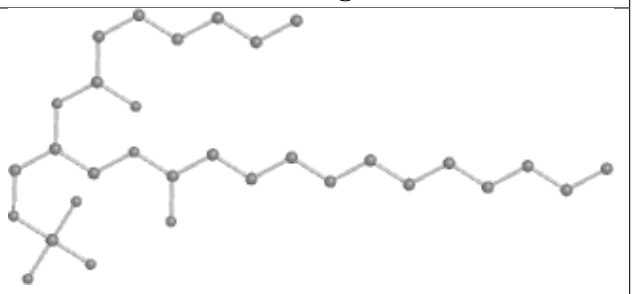
Bond lengths



Bond angles

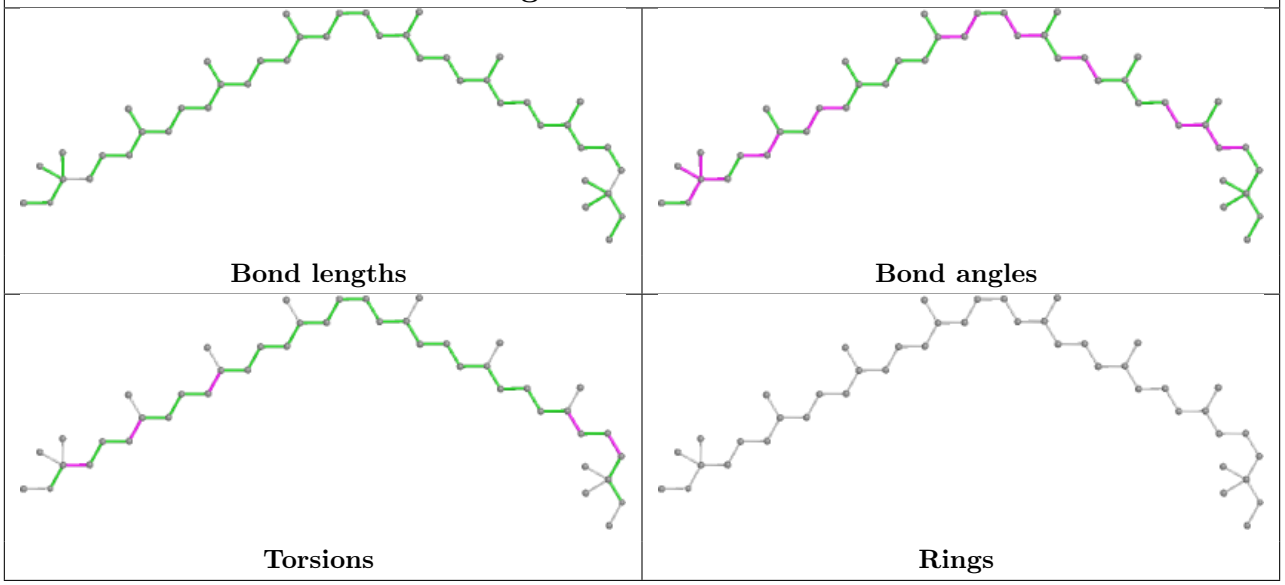


Torsions

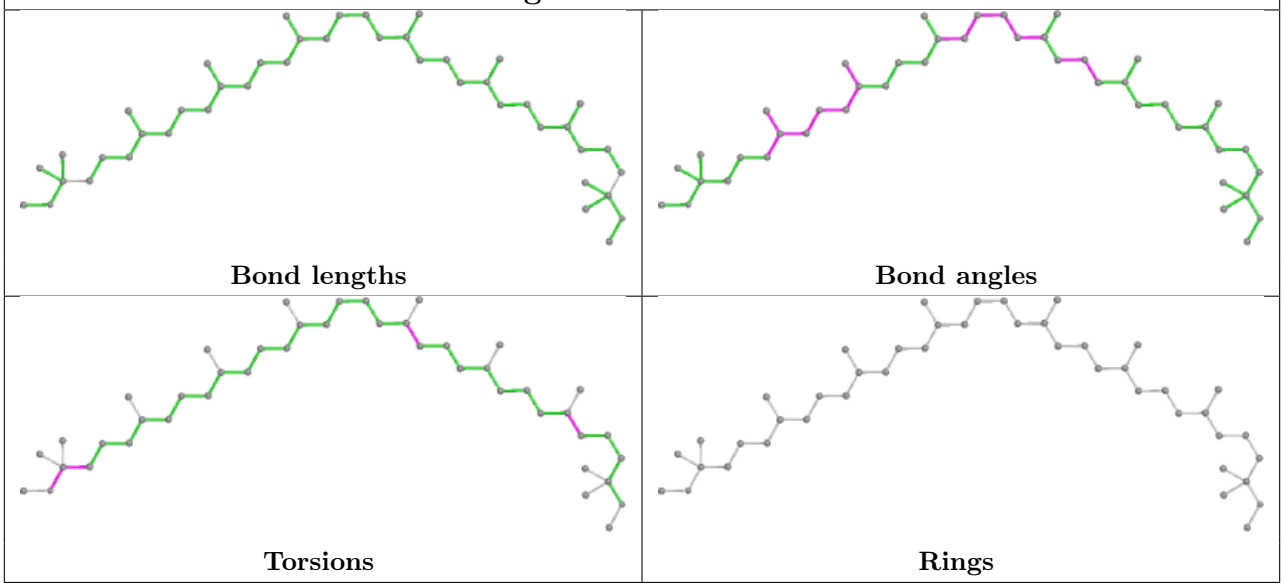


Rings

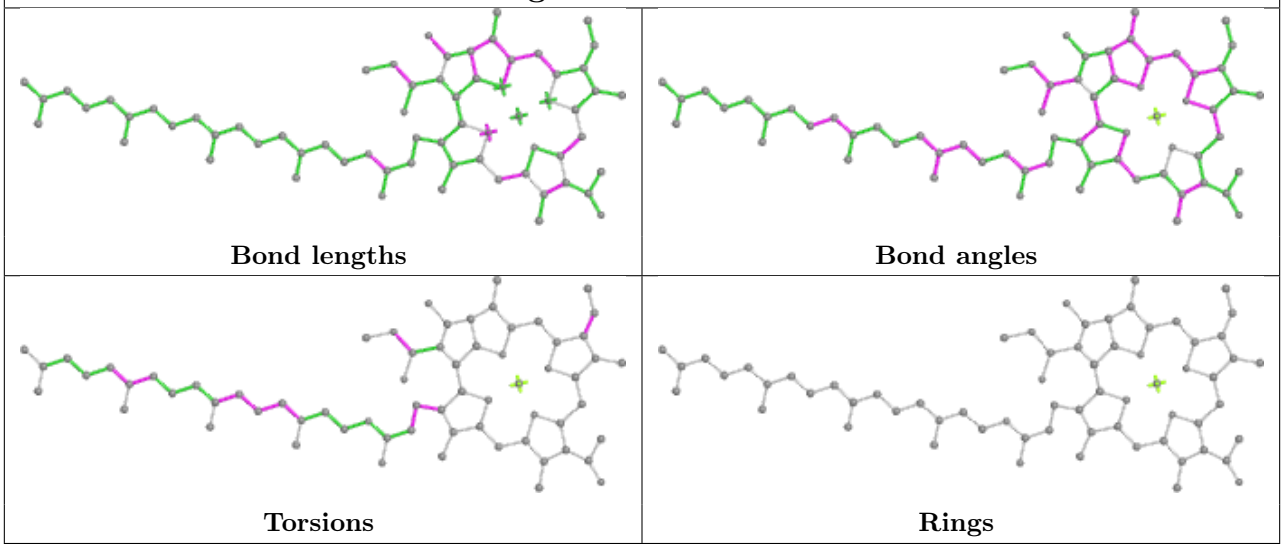
Ligand CRT M 406



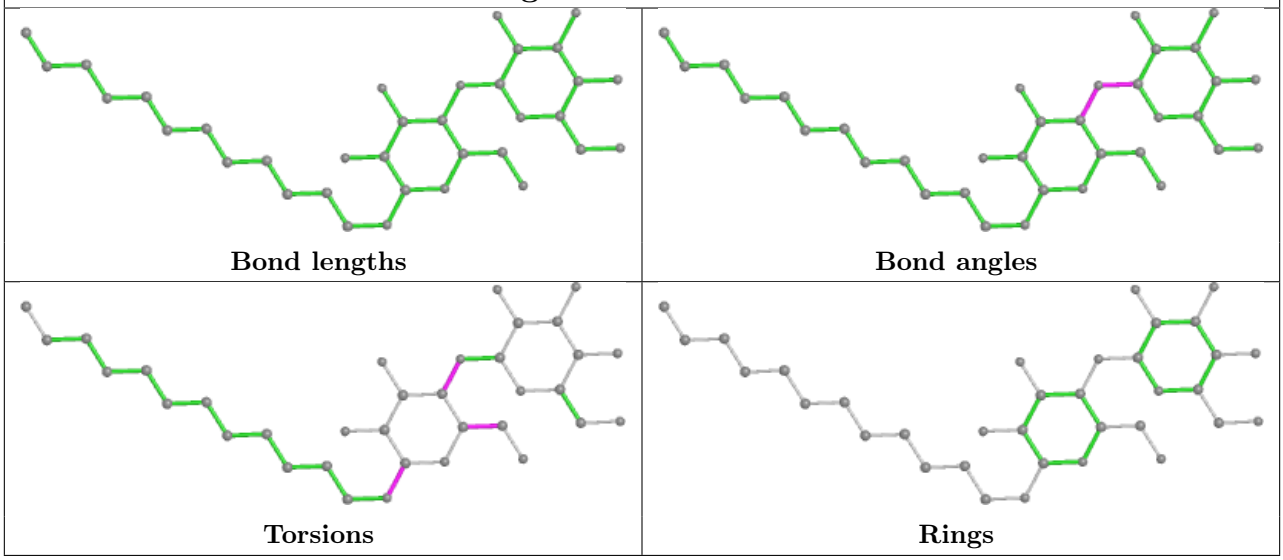
Ligand CRT G 103



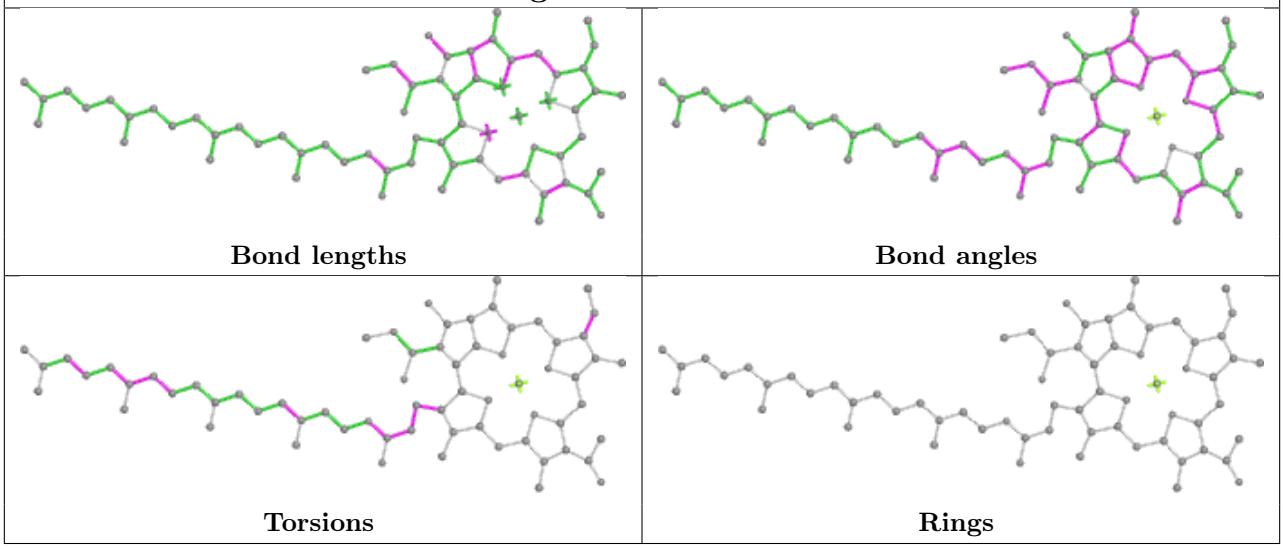
Ligand BCL Z 102



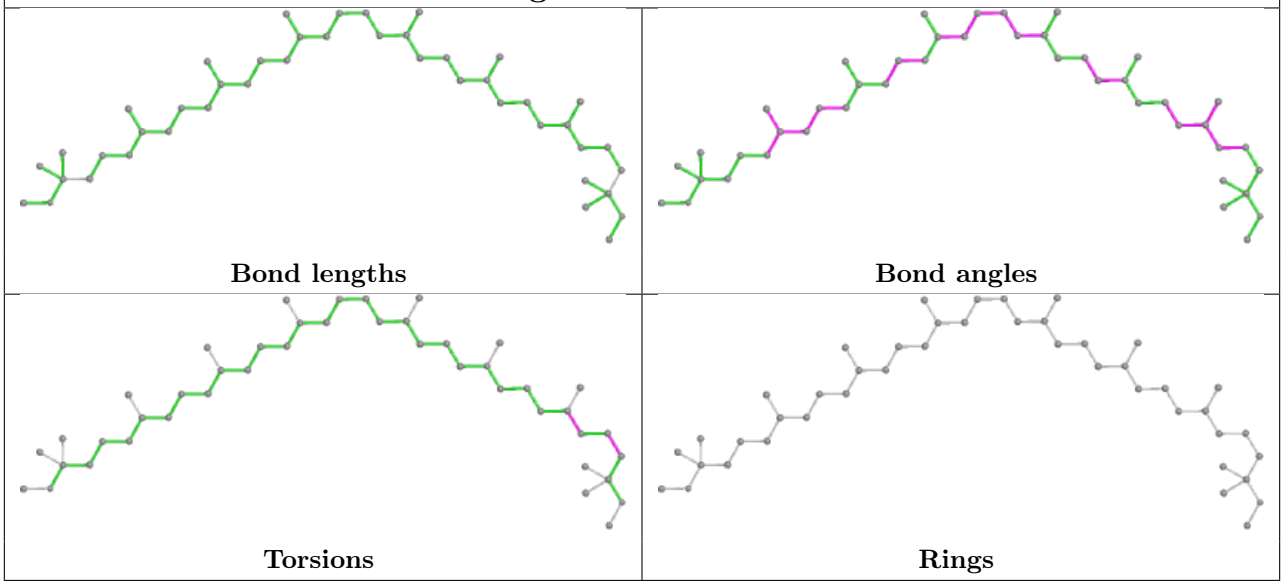
Ligand LMT G 101



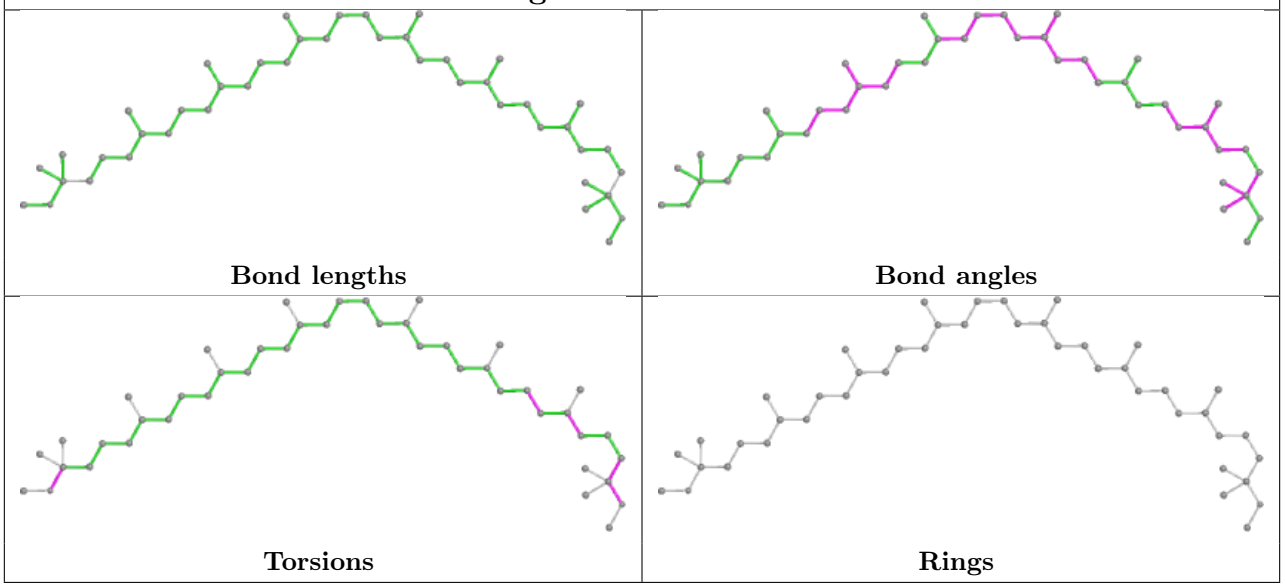
Ligand BCL 8 102



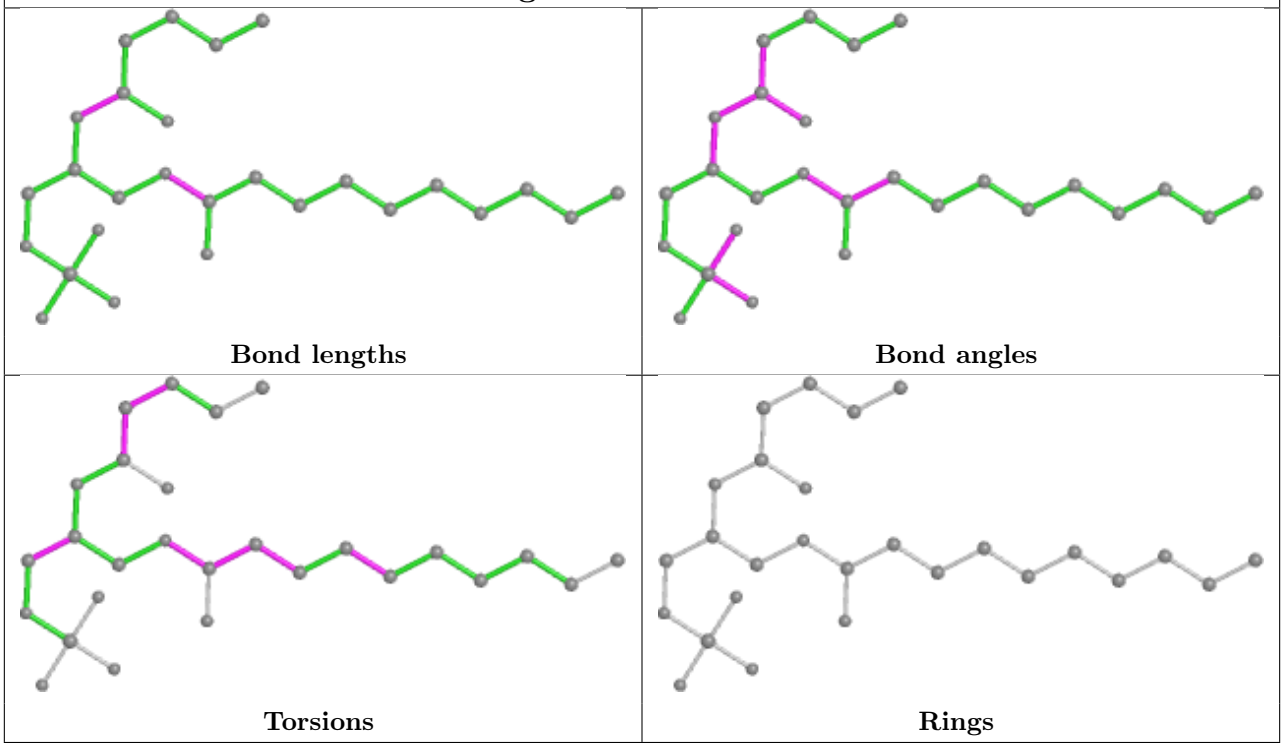
Ligand CRT 9 101



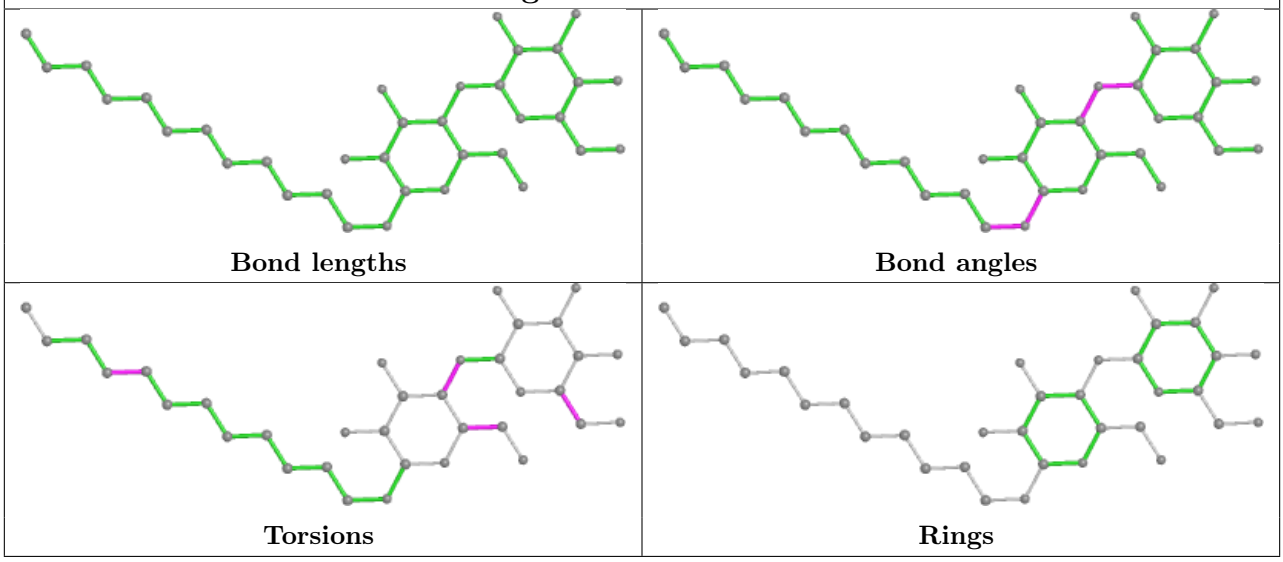
Ligand CRT J 103



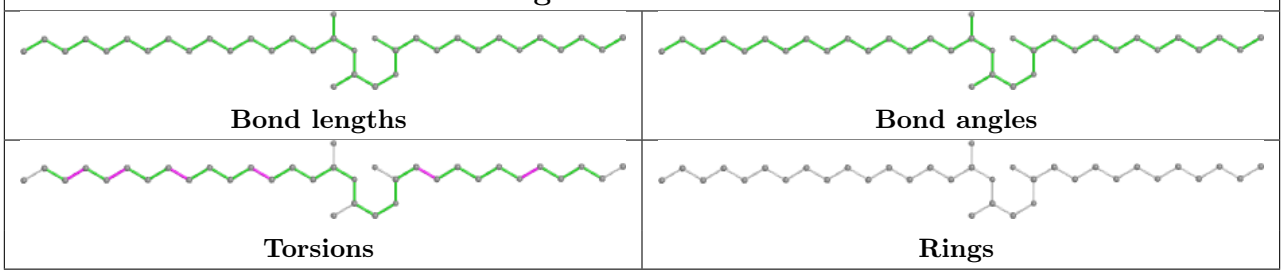
Ligand PGV M 408



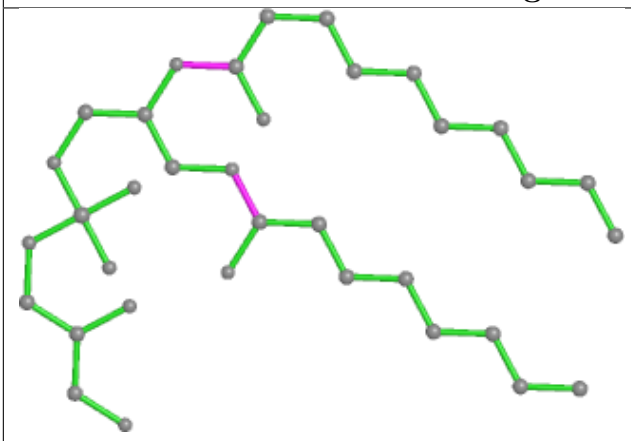
Ligand LMT X 101



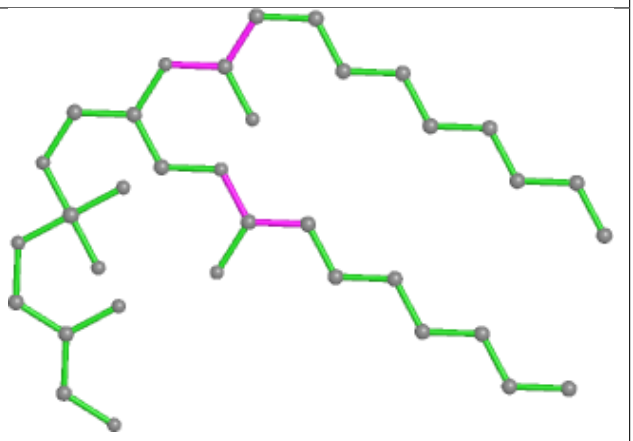
Ligand Z41 C 406



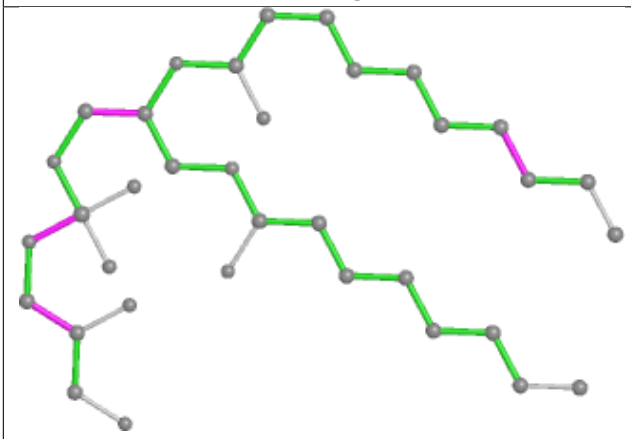
Ligand PGV L 306



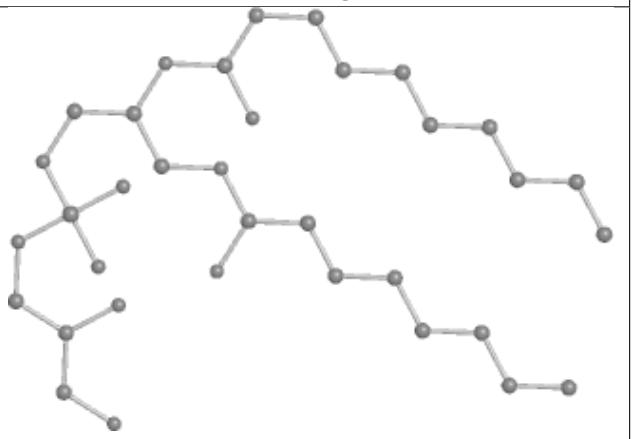
Bond lengths



Bond angles

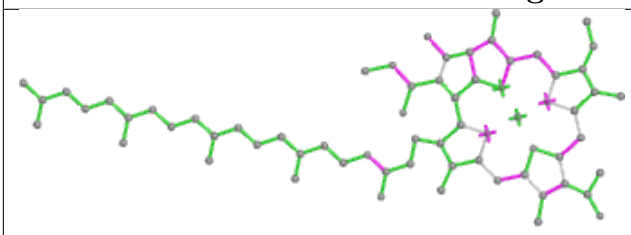


Torsions

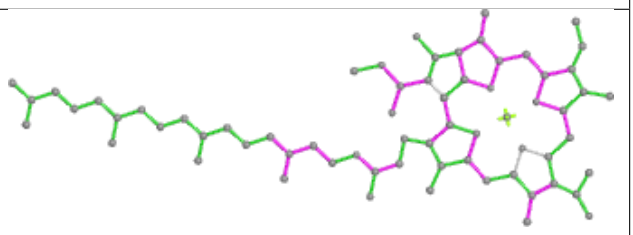


Rings

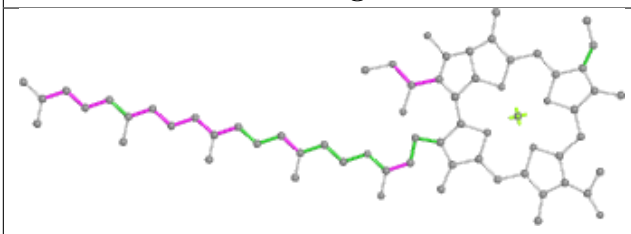
Ligand BCL F 502



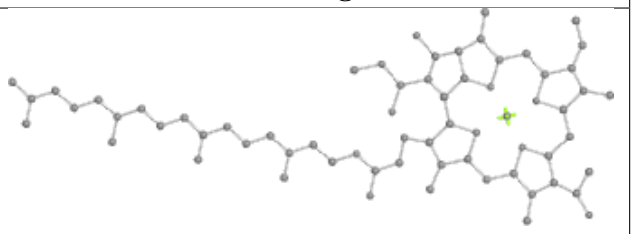
Bond lengths



Bond angles

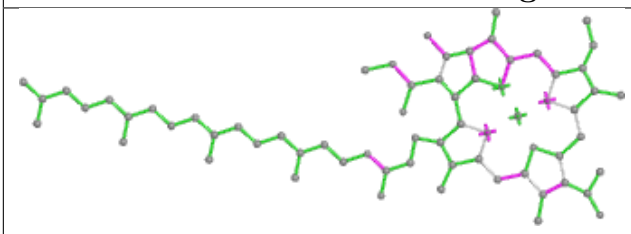


Torsions

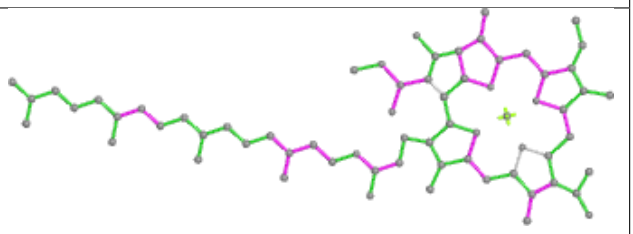


Rings

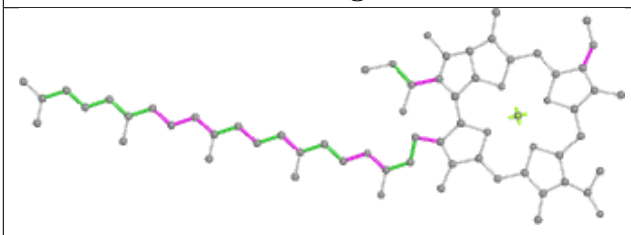
Ligand BCL W 101



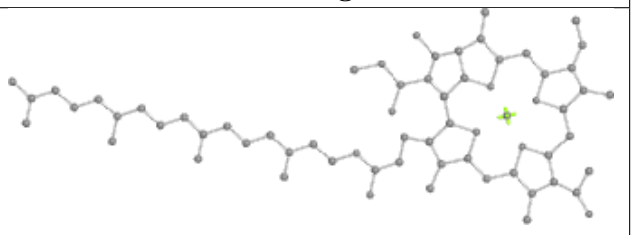
Bond lengths



Bond angles

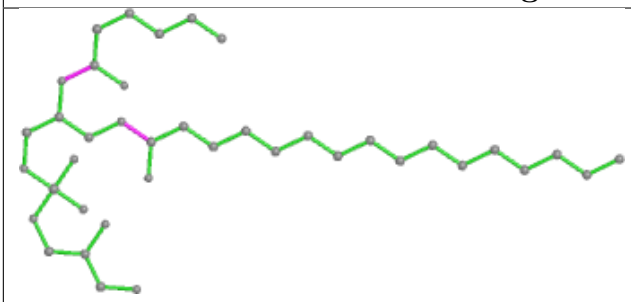


Torsions

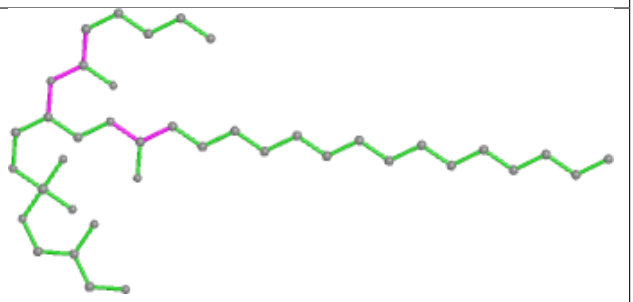


Rings

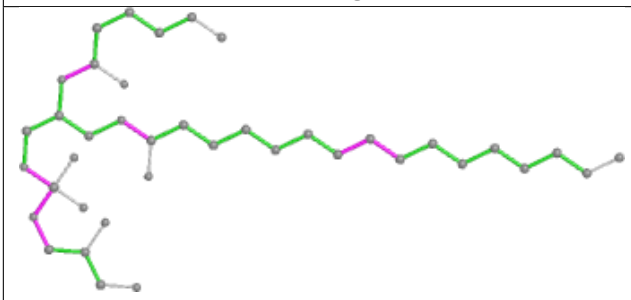
Ligand PGV A 501



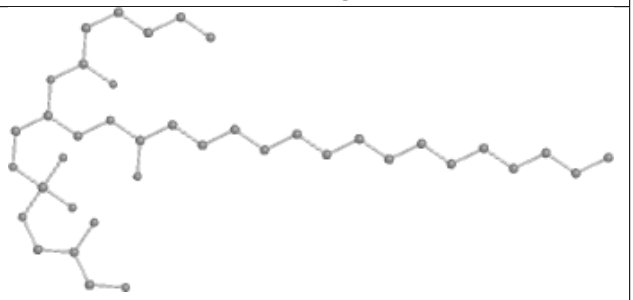
Bond lengths



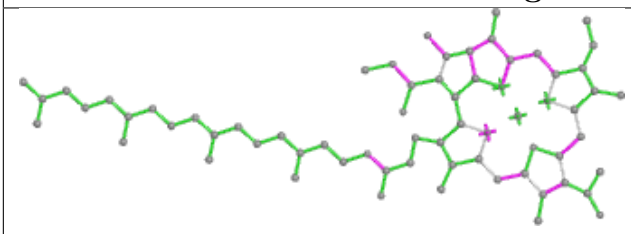
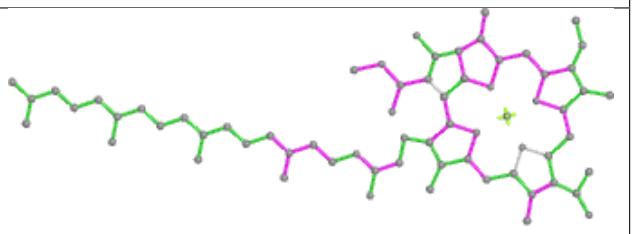
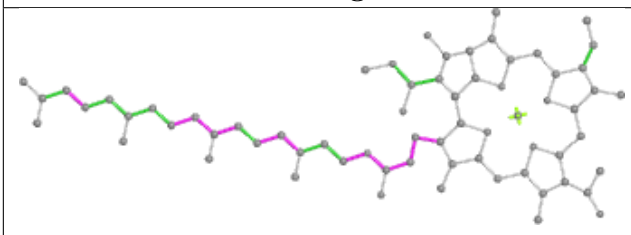
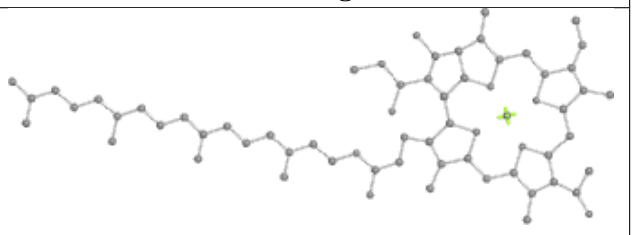
Bond angles



Torsions



Rings

Ligand BCL X 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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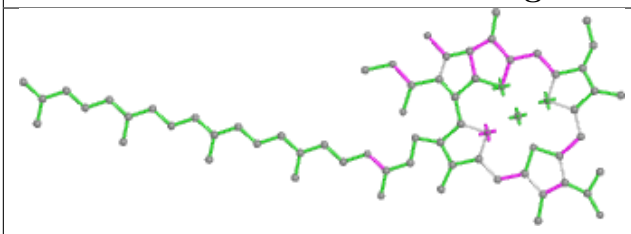
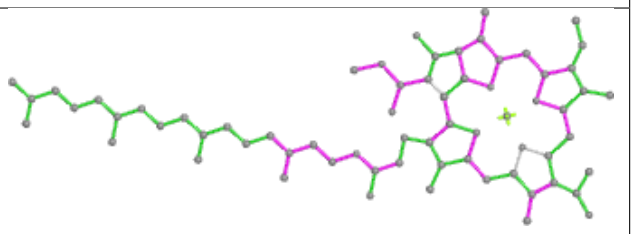
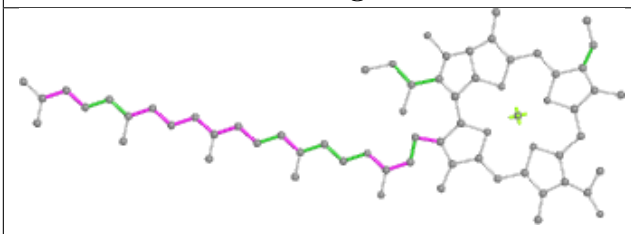
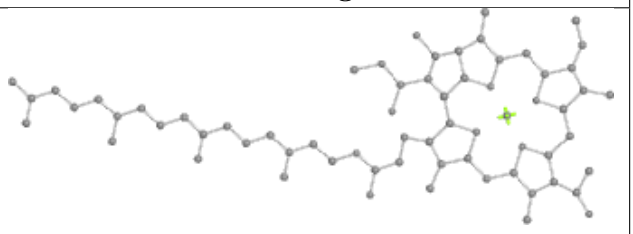
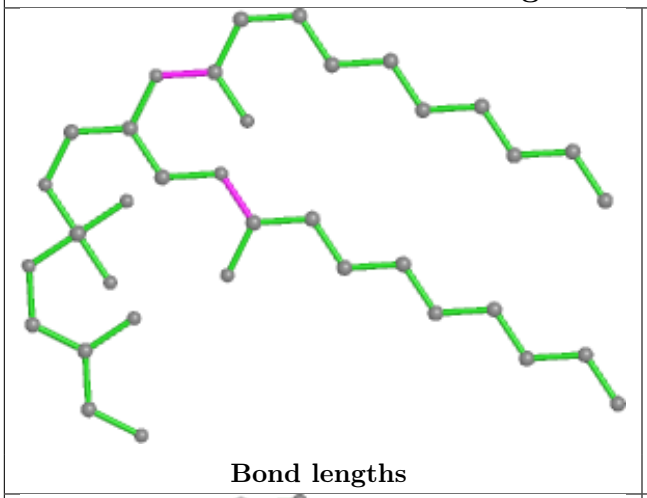
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV H 301



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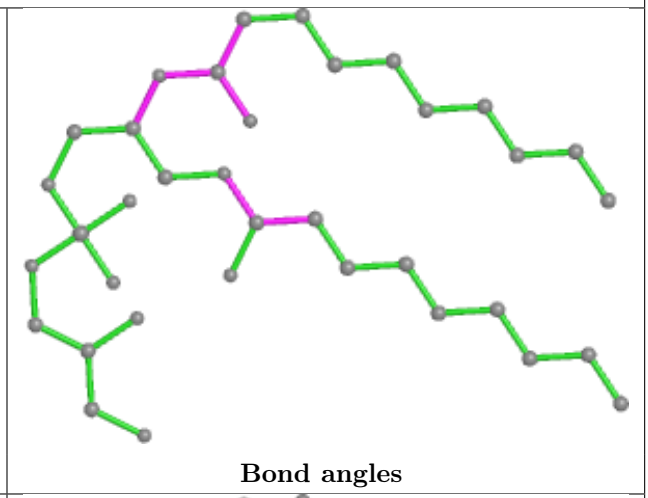
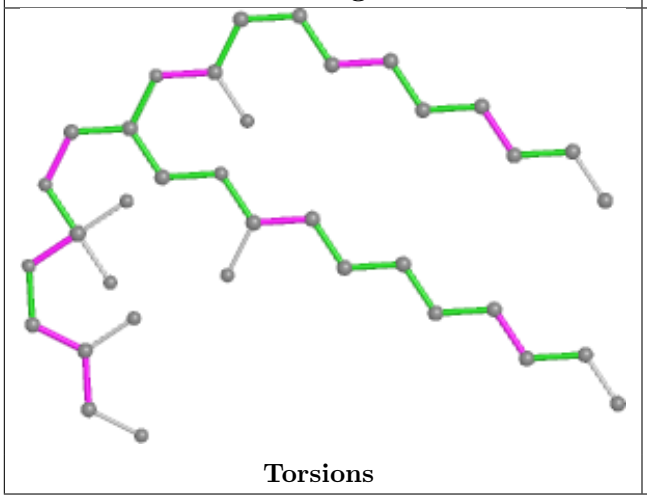
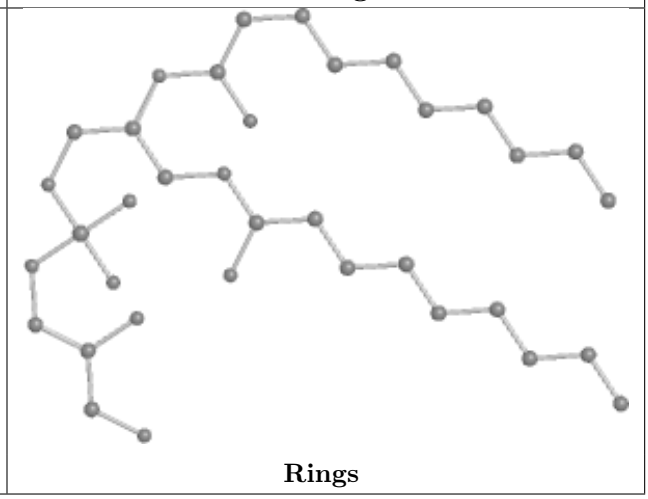


Bond angles

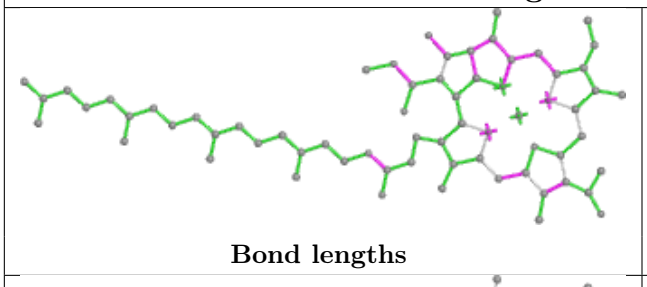


Torsions

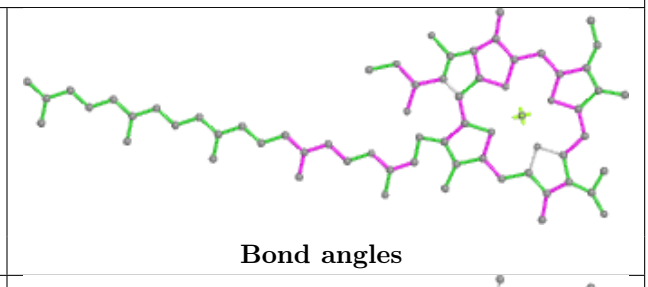


Rings

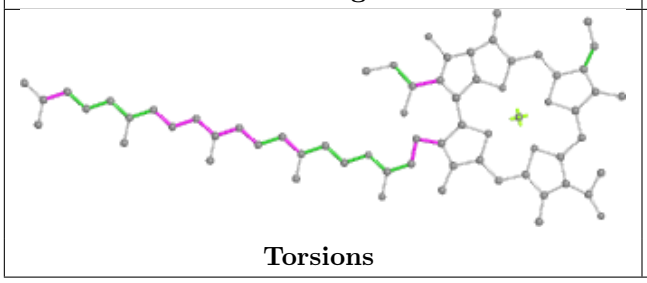
Ligand BCL Y 102



Bond lengths



Bond angles



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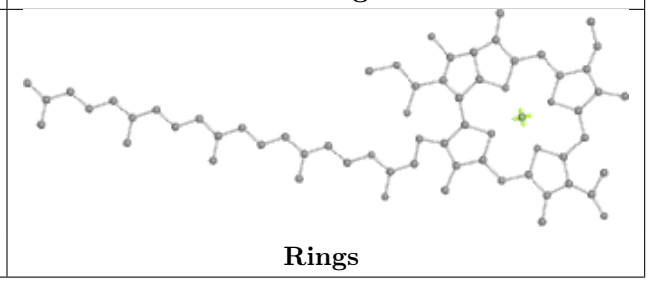
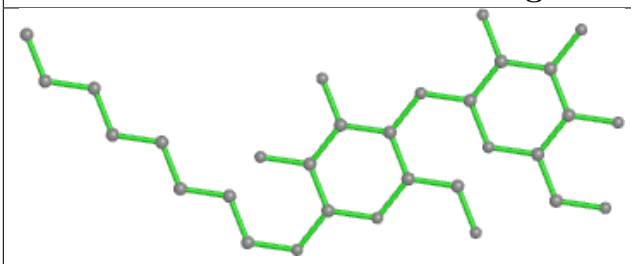


Rings

Ligand LMT 5 101



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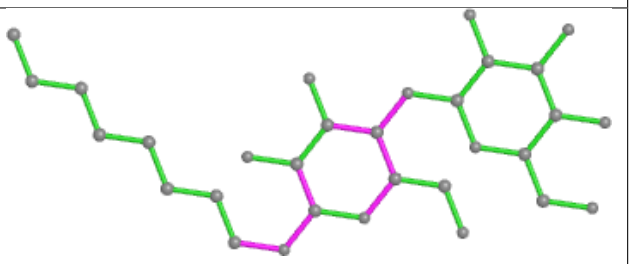

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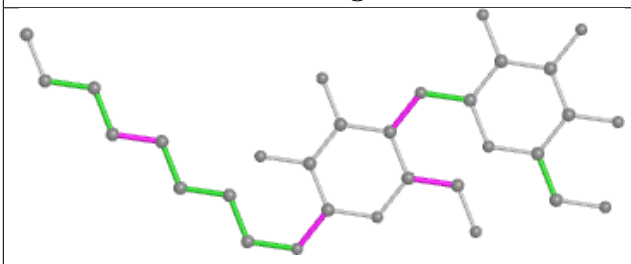

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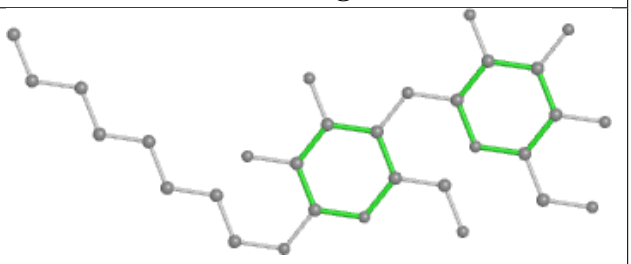
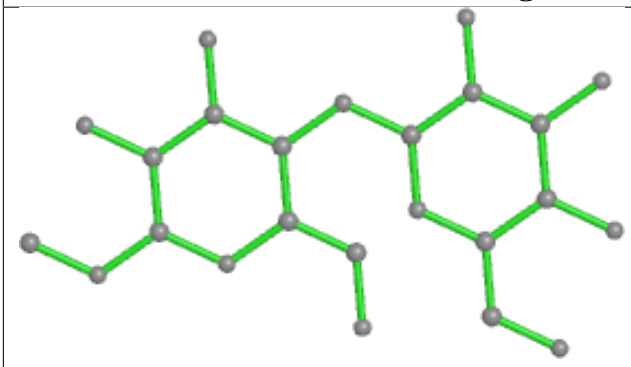


Rings

Ligand LMT M 411



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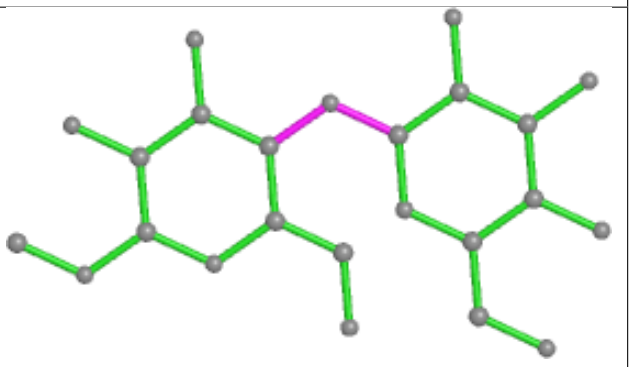
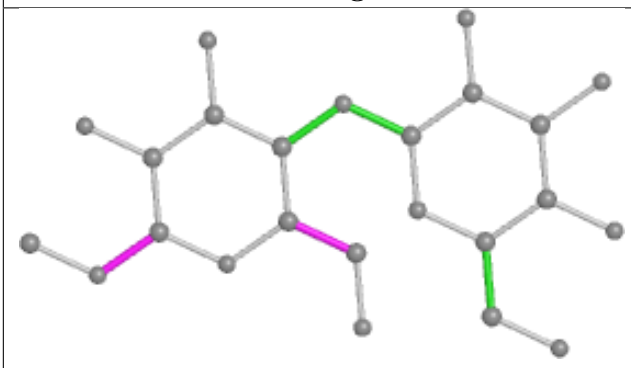


Bond angles



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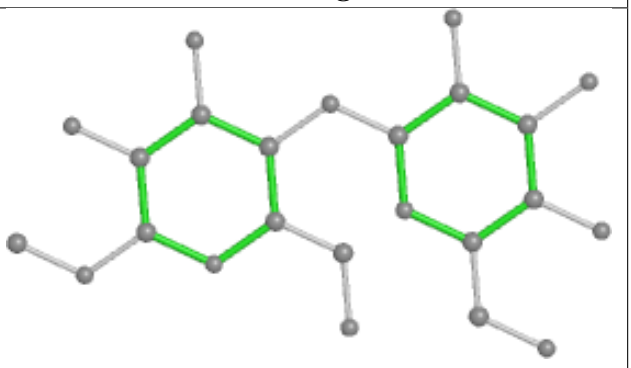
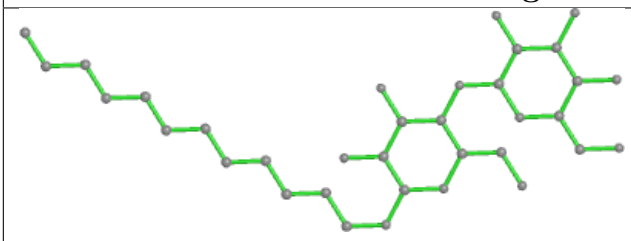
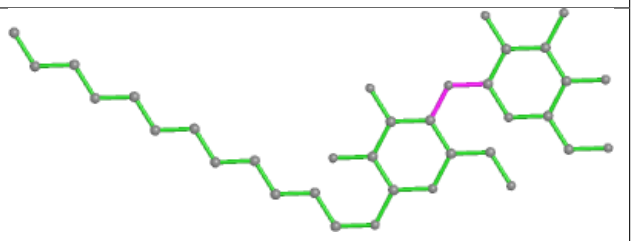


Rings

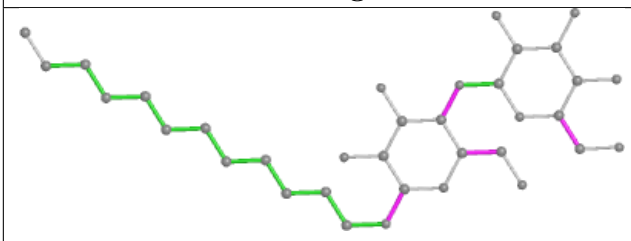
Ligand LMT E 101



Bond lengths



Bond angles



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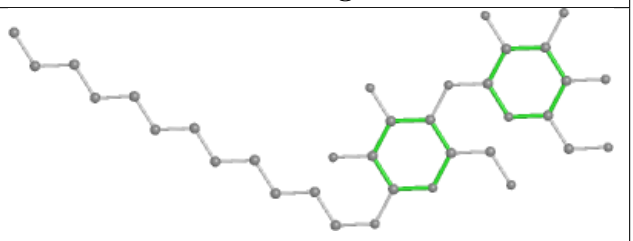
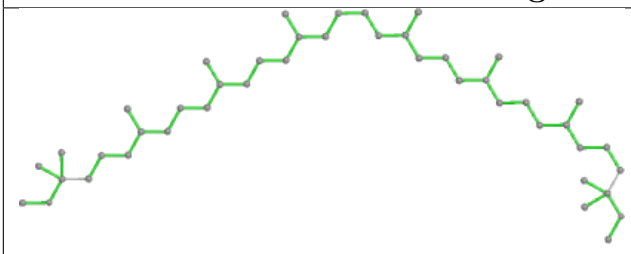
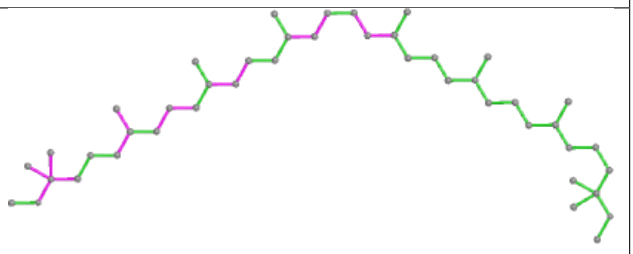


Rings

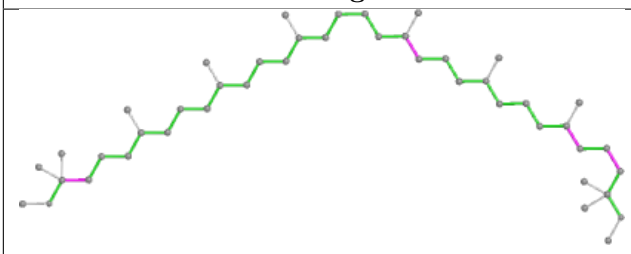
Ligand CRT 2 103



Bond lengths



Bond angles



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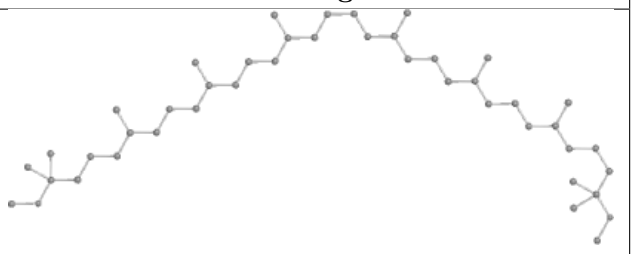
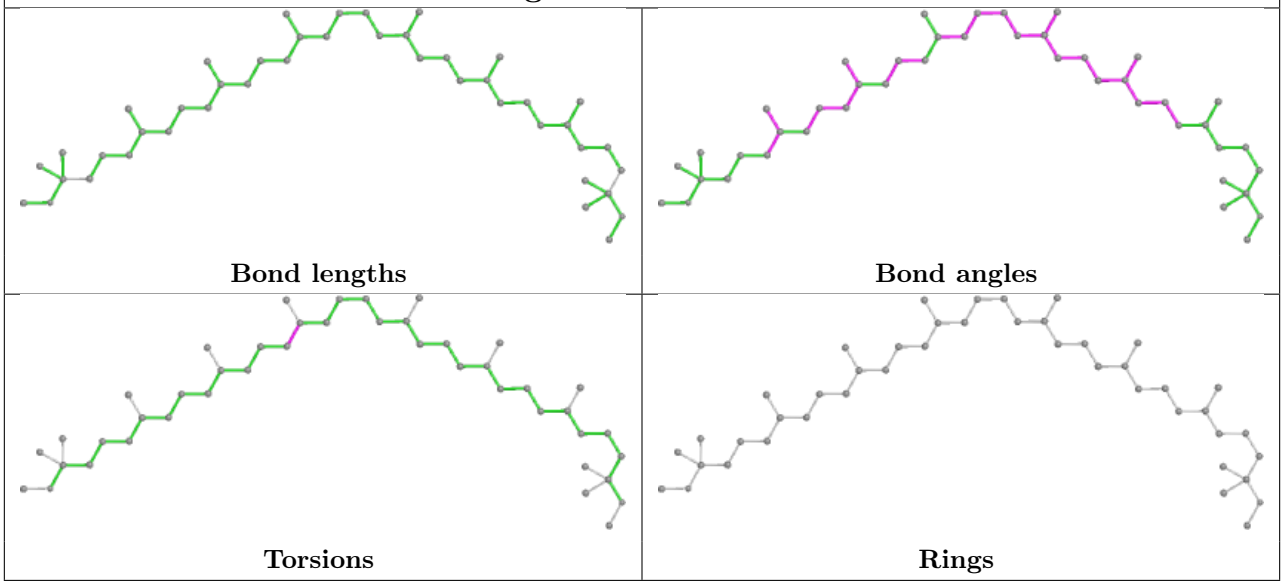
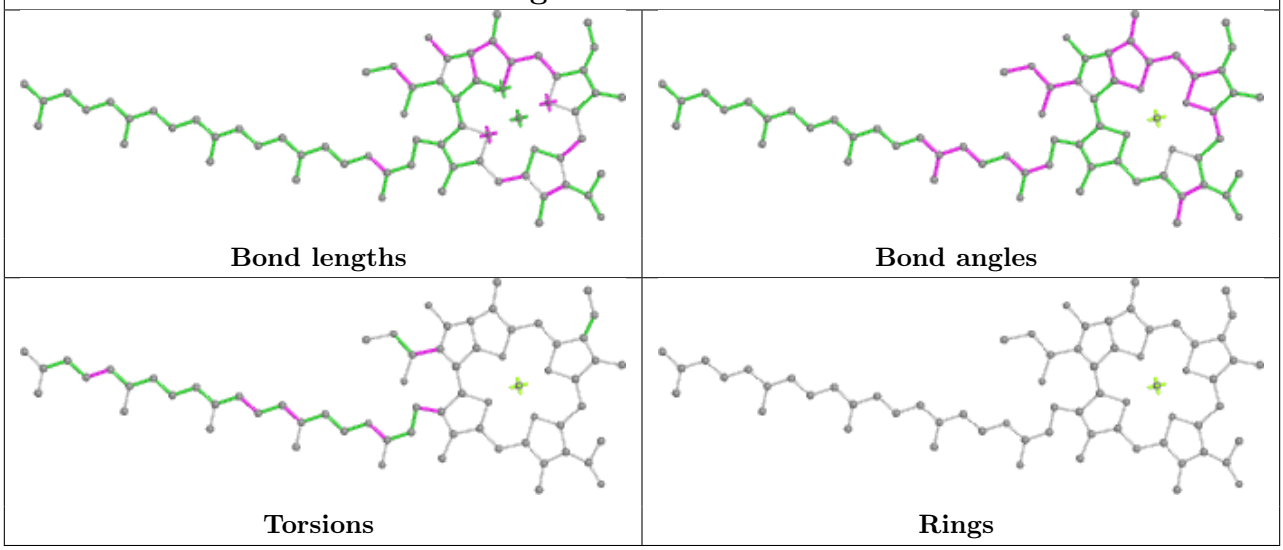


Rings

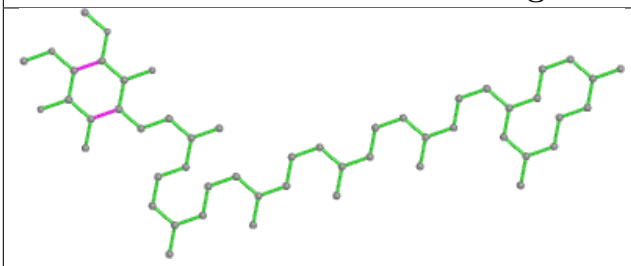
Ligand CRT R 102



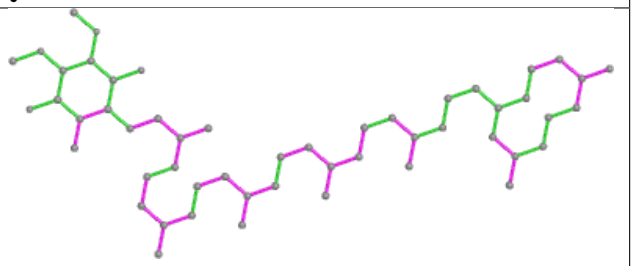
Ligand BCL 1 402



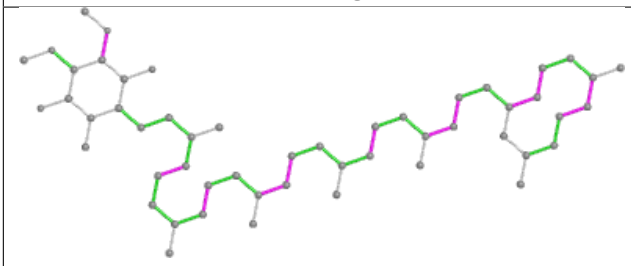
Ligand UQ8 L 309



Bond lengths



Bond angles



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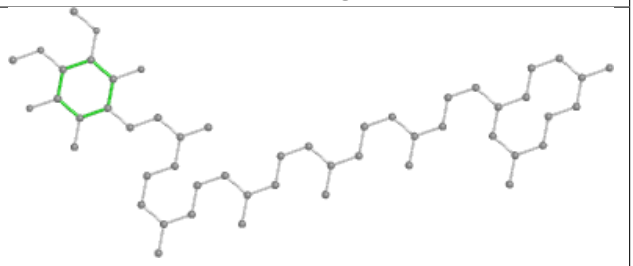
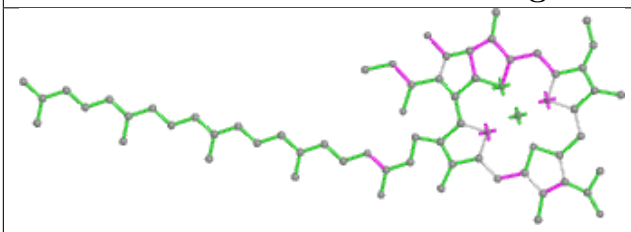
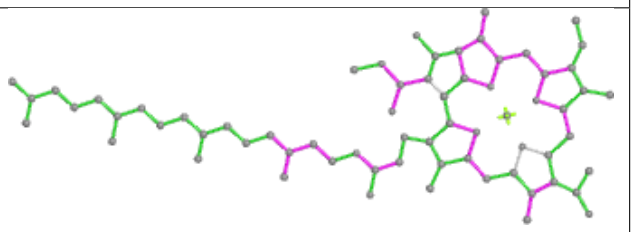


Rings

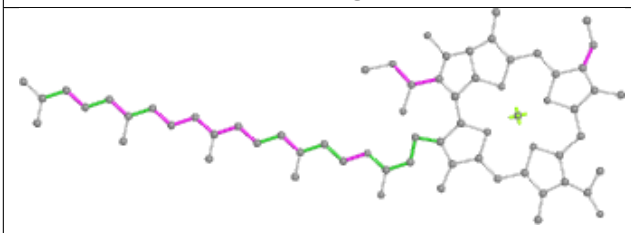
Ligand BCL 5 102



Bond lengths



Bond angles



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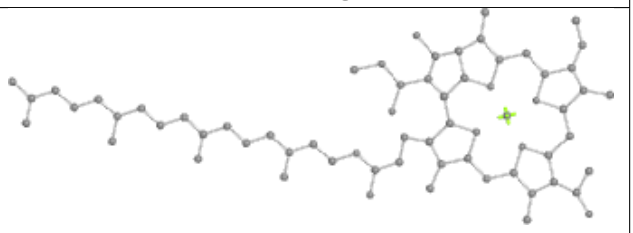
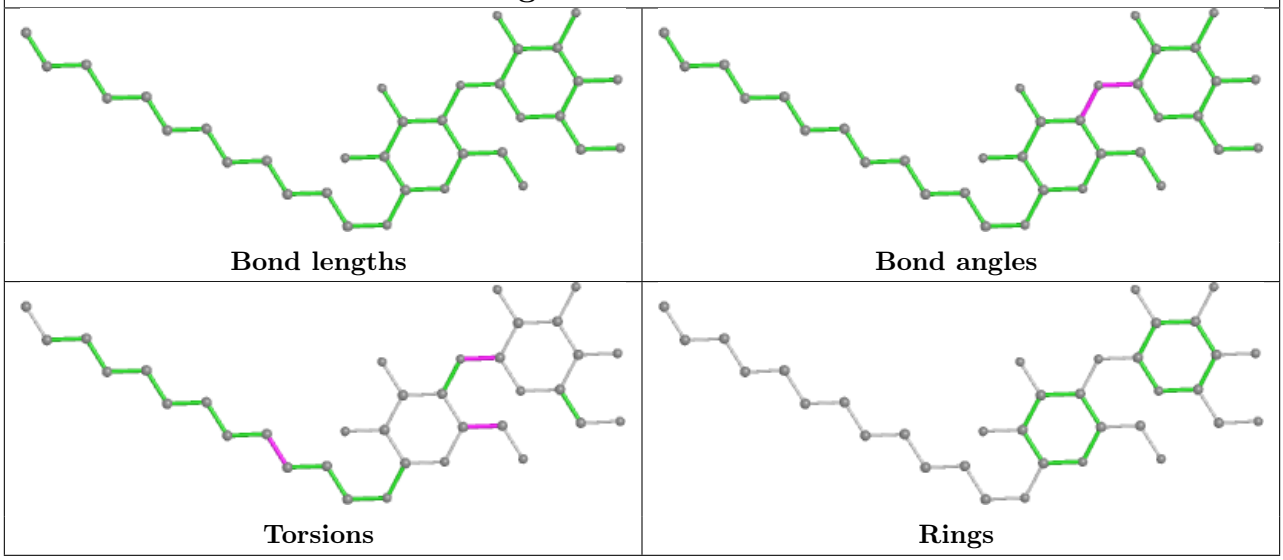
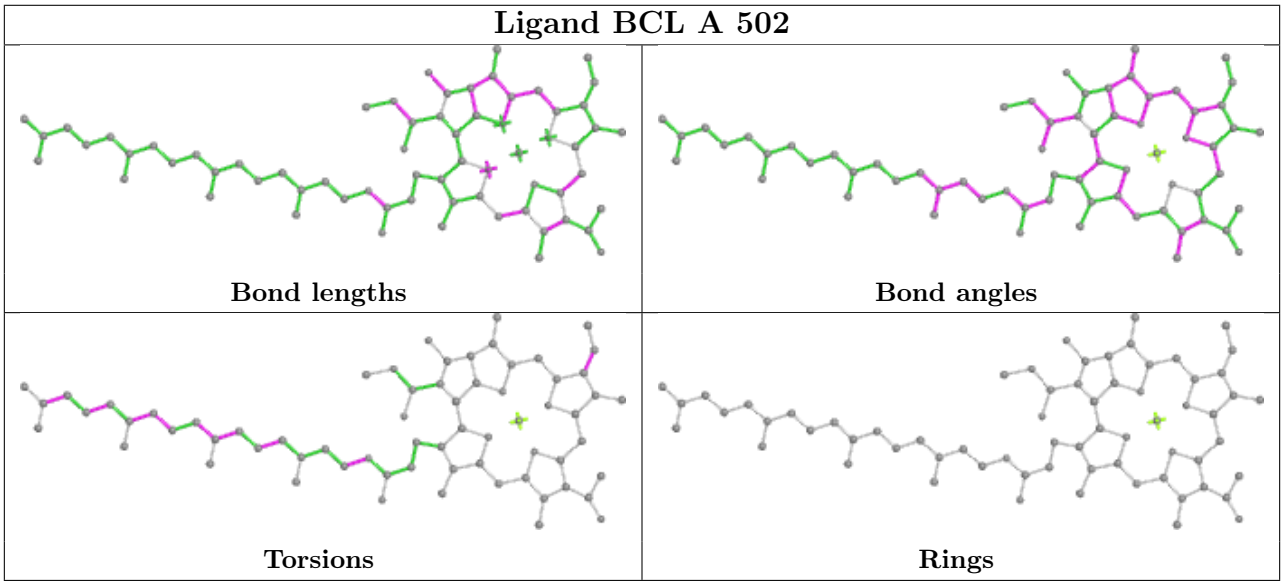


Rings

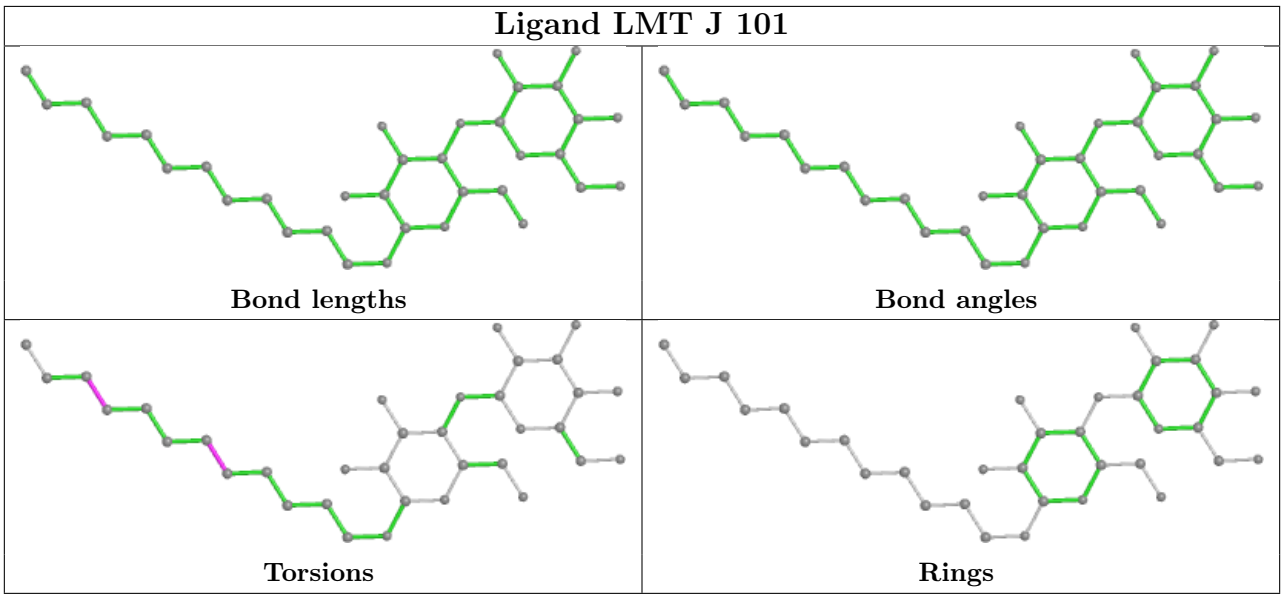
Ligand LMT M 410

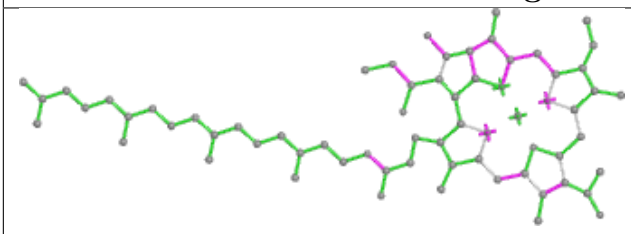
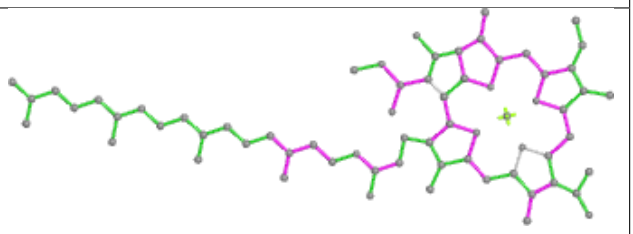
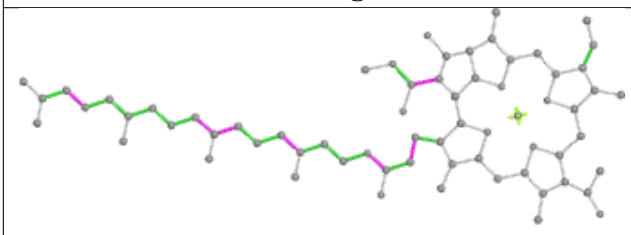
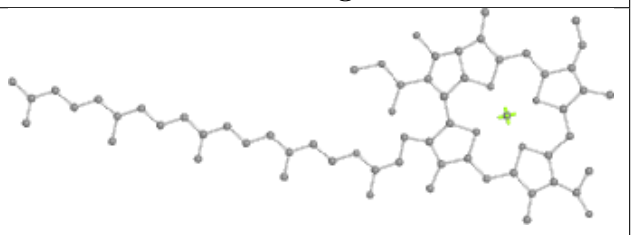


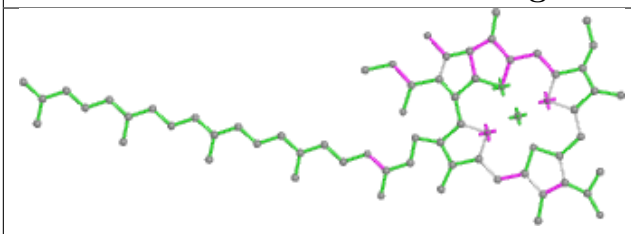
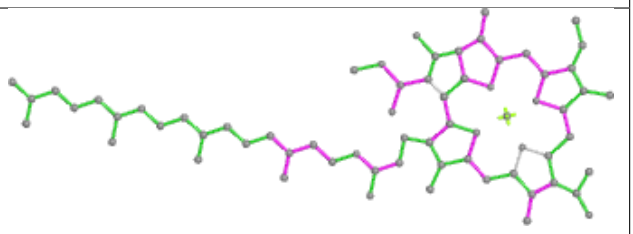
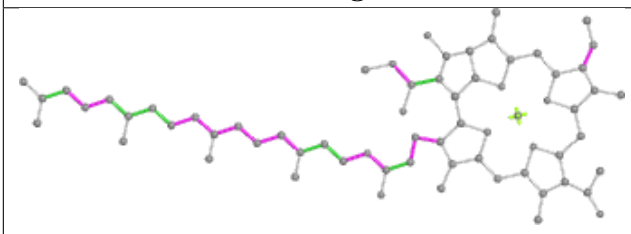
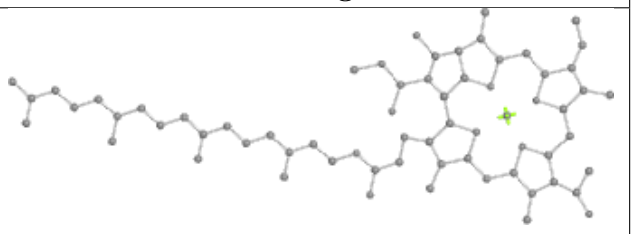
Ligand BCL A 502



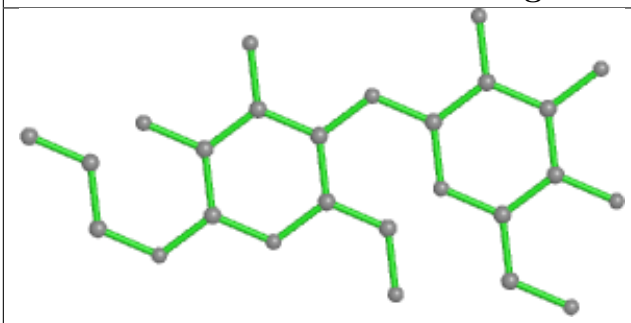
Ligand LMT J 101



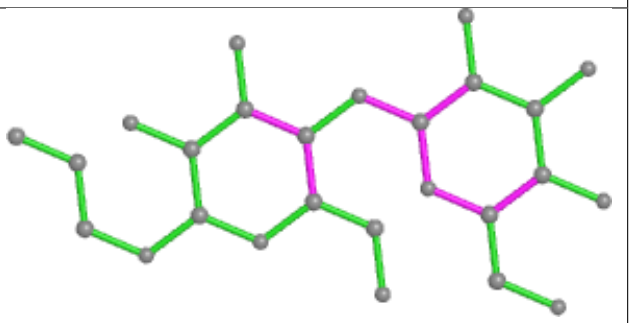
Ligand BCL K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 6 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

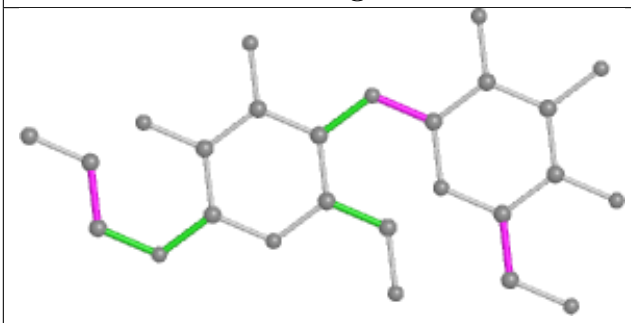
Ligand LMT S 101



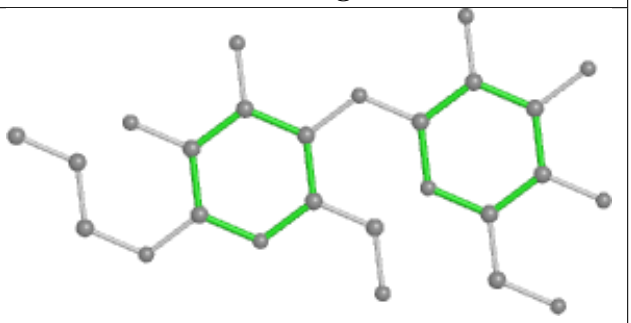
Bond lengths



Bond angles

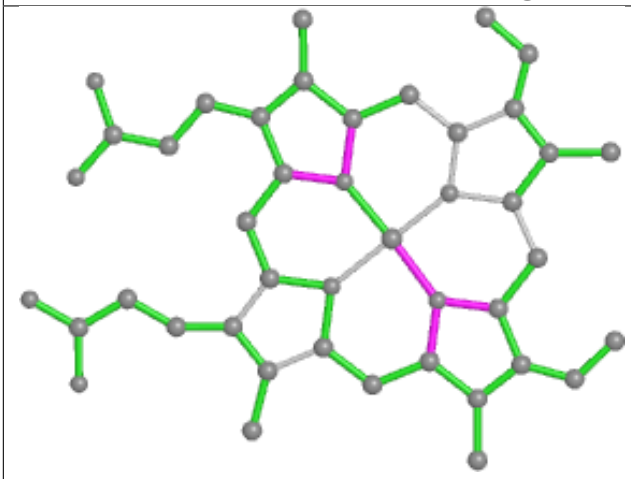


Torsions

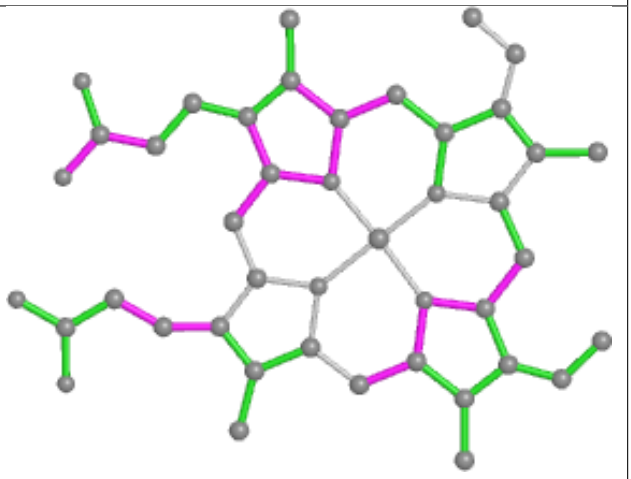


Rings

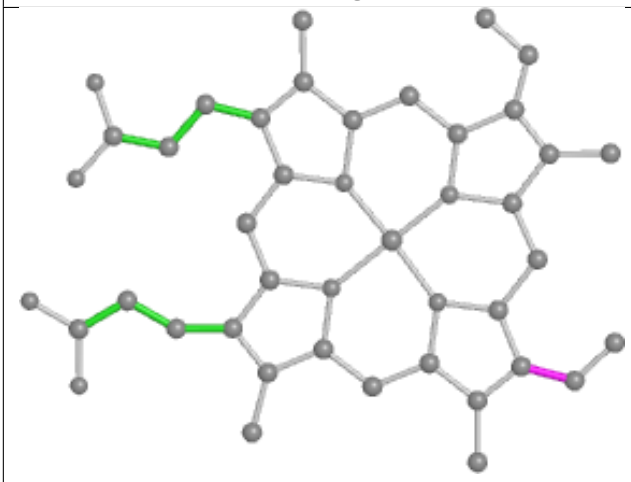
Ligand HEM C 403



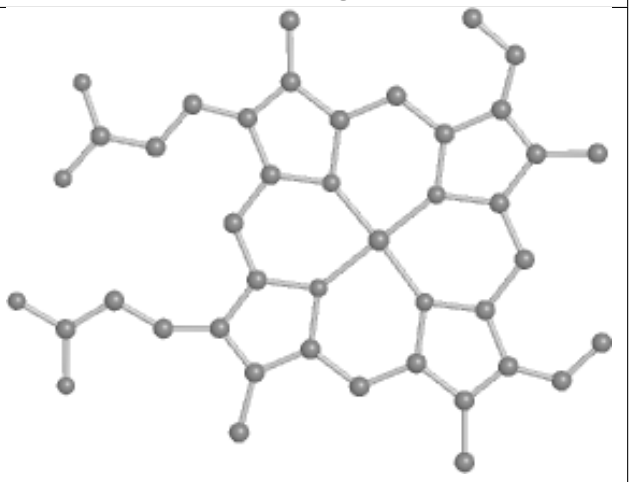
Bond lengths



Bond angles

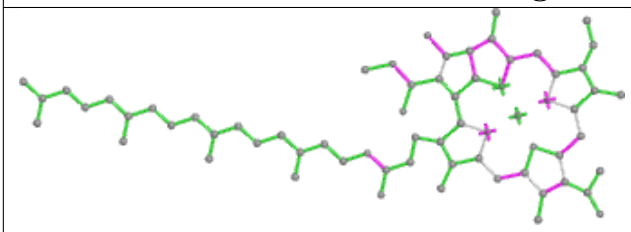


Torsions

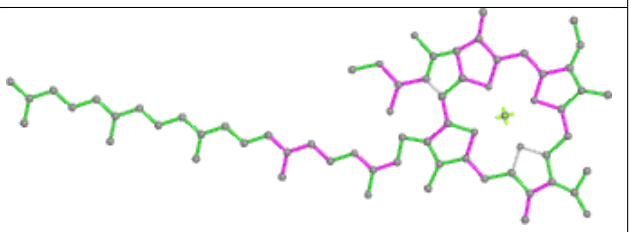


Rings

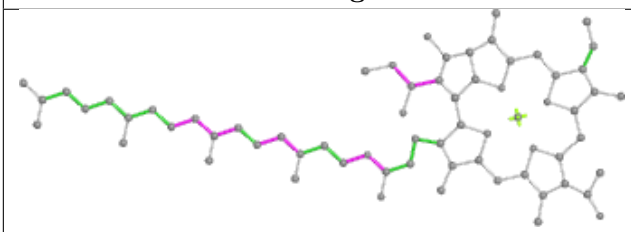
Ligand BCL I 101



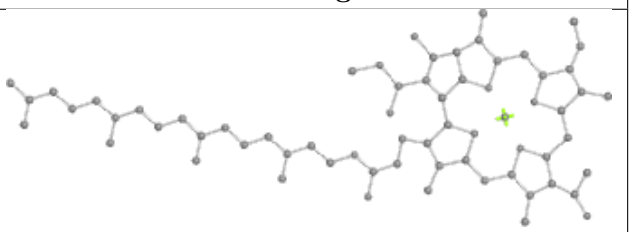
Bond lengths



Bond angles

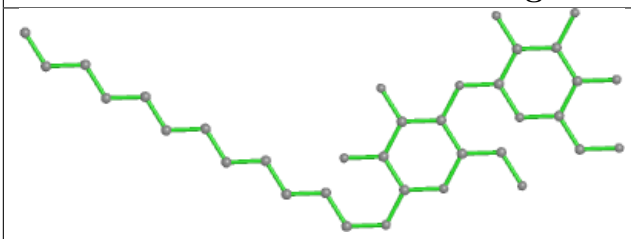


Torsions

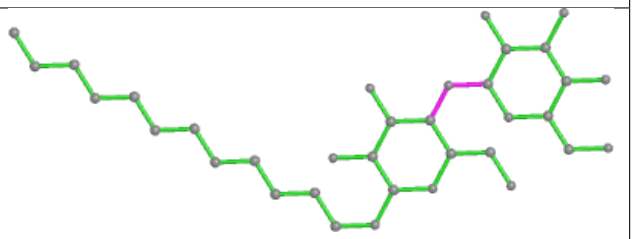


Rings

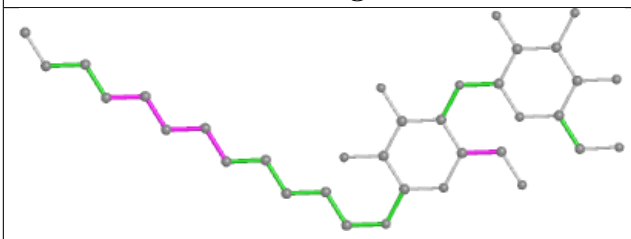
Ligand LMT 4 101



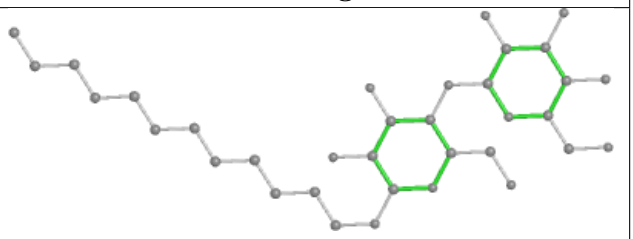
Bond lengths



Bond angles

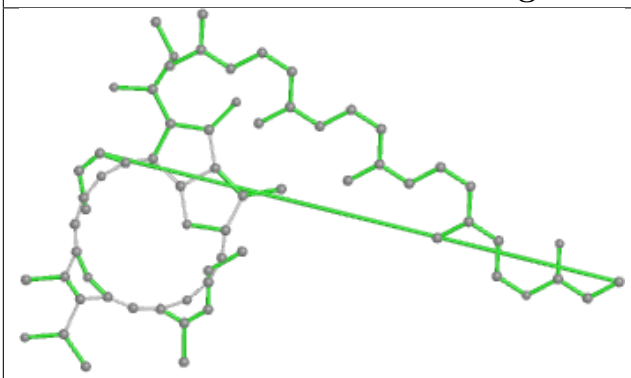


Torsions

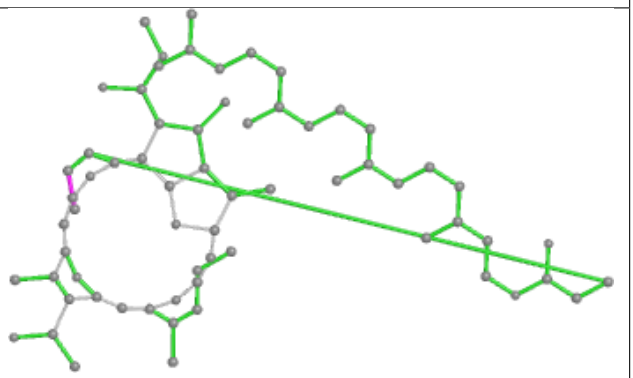


Rings

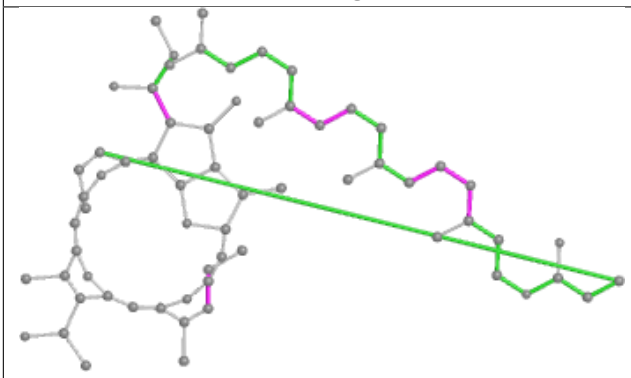
Ligand BPH M 404



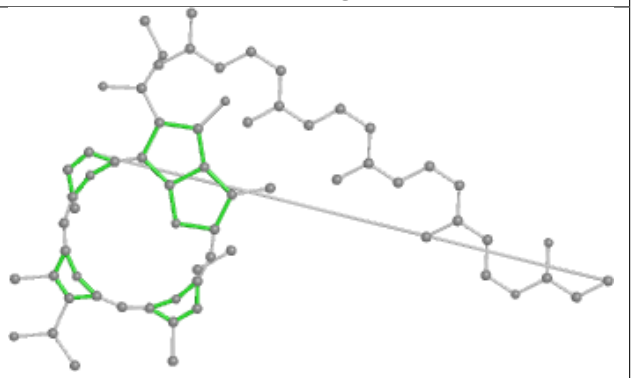
Bond lengths



Bond angles

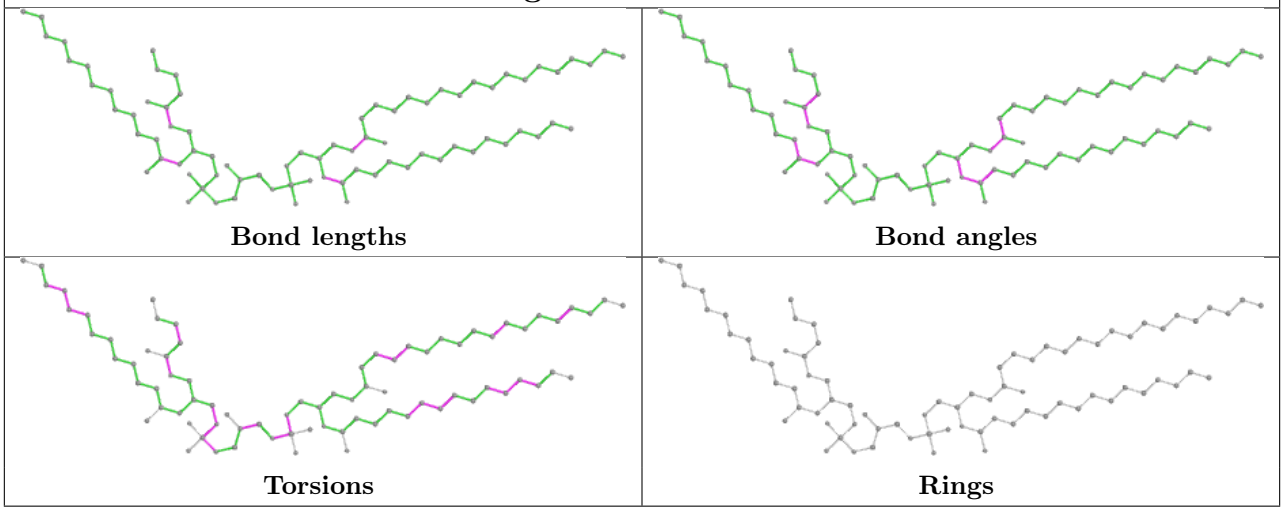


Torsions

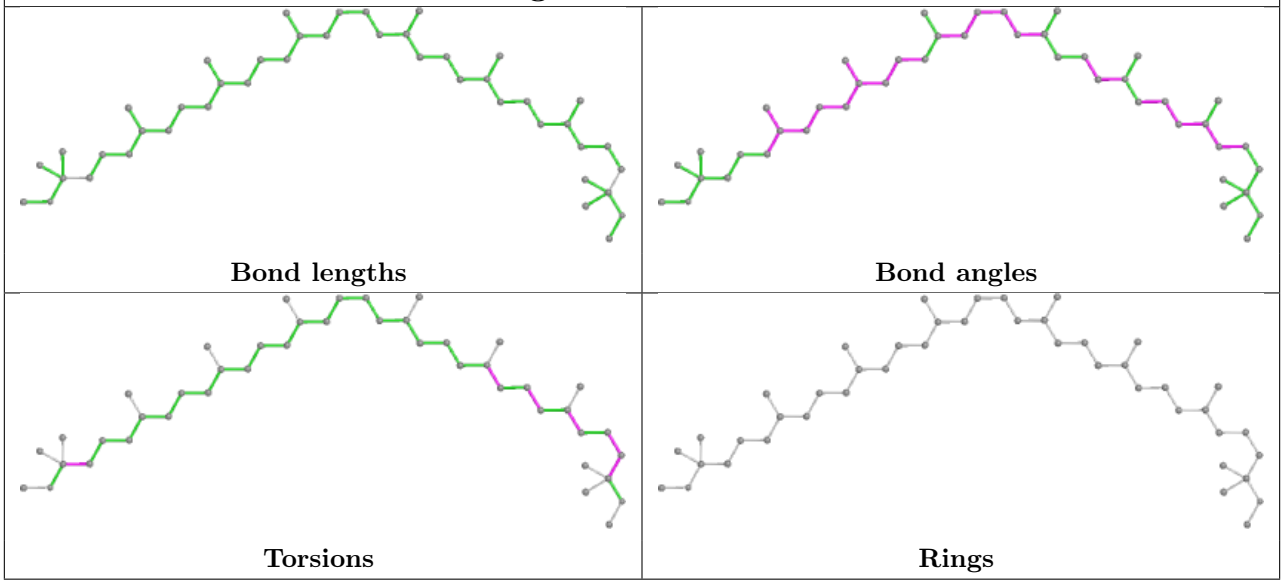


Rings

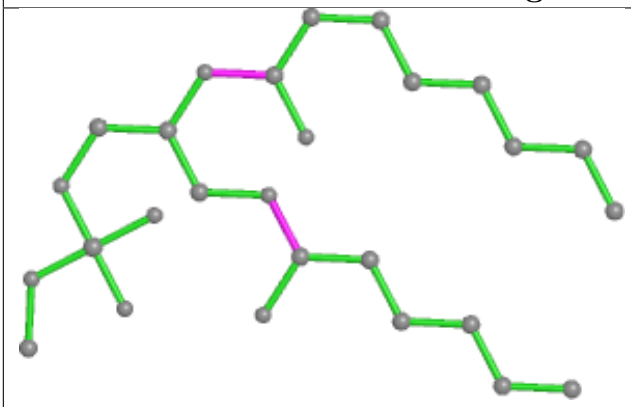
Ligand CDL H 302



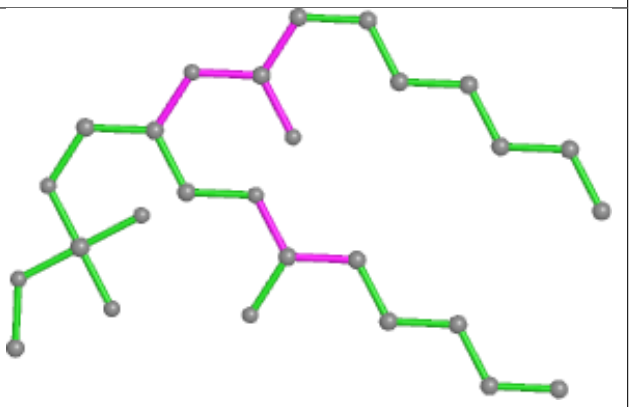
Ligand CRT 6 102



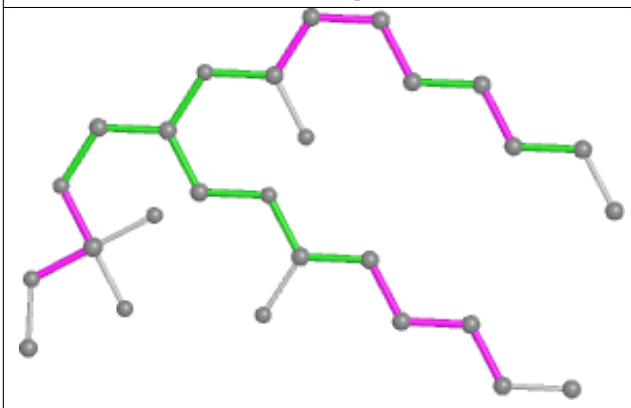
Ligand PGV 1 401



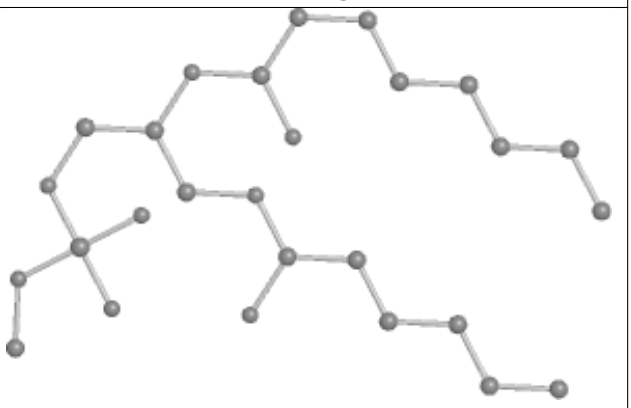
Bond lengths



Bond angles

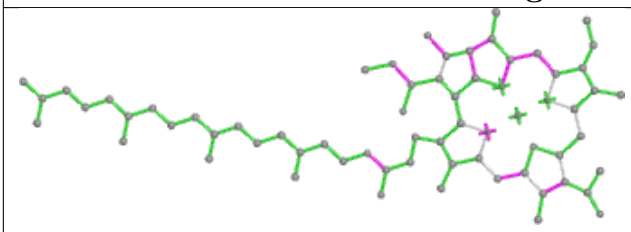


Torsions

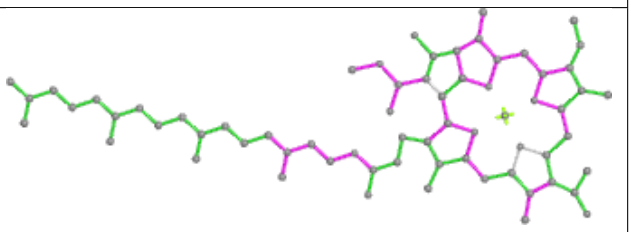


Rings

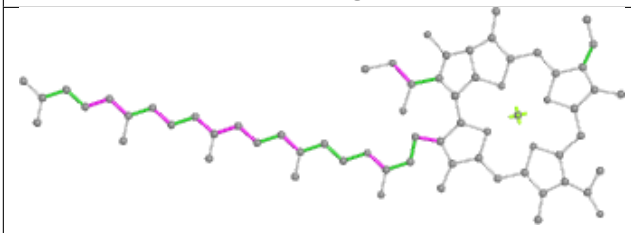
Ligand BCL T 101



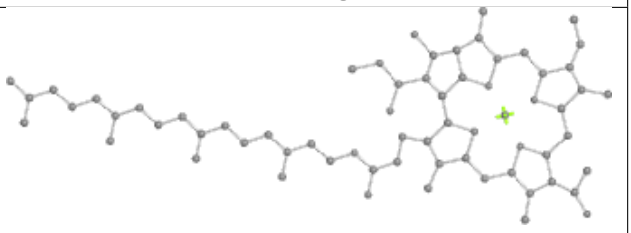
Bond lengths



Bond angles

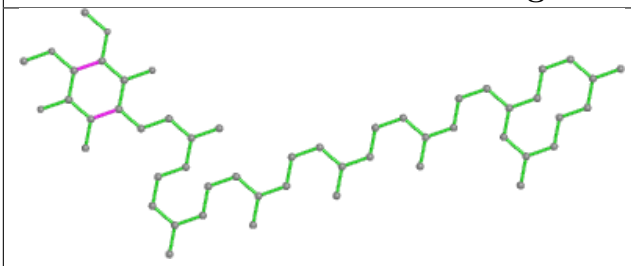


Torsions

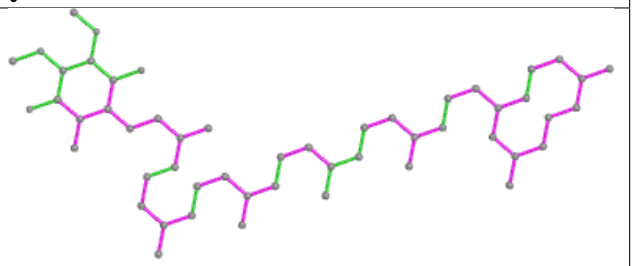


Rings

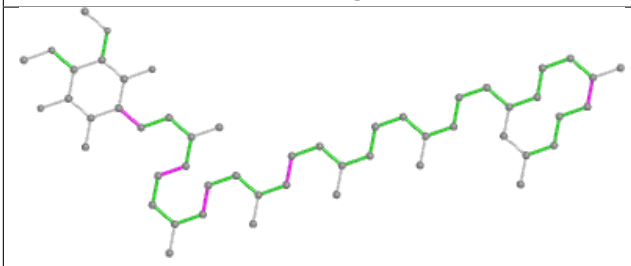
Ligand UQ8 L 304



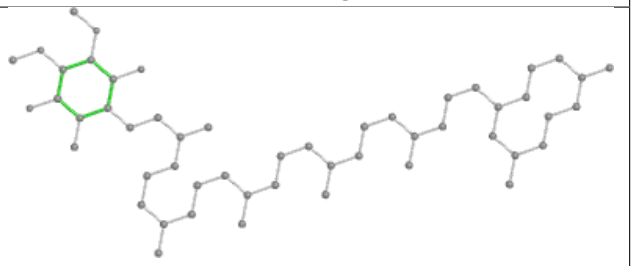
Bond lengths



Bond angles

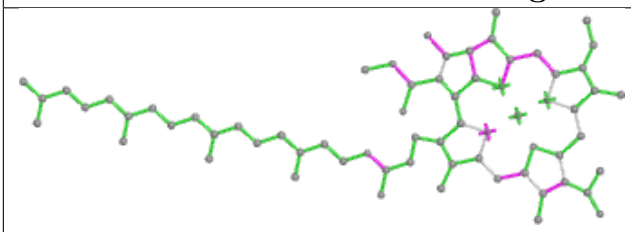


Torsions

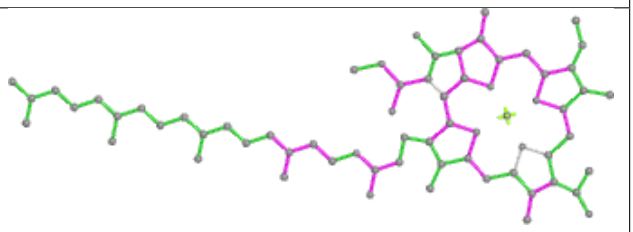


Rings

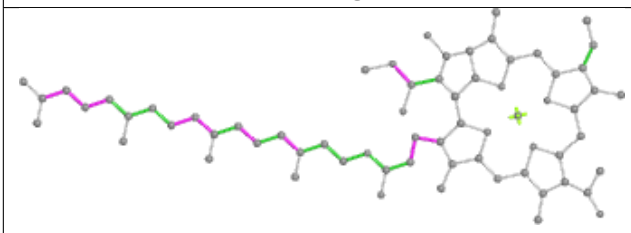
Ligand BCL 2 102



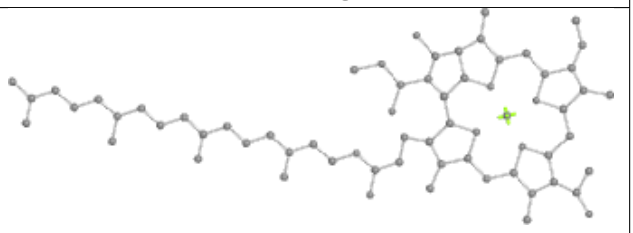
Bond lengths



Bond angles

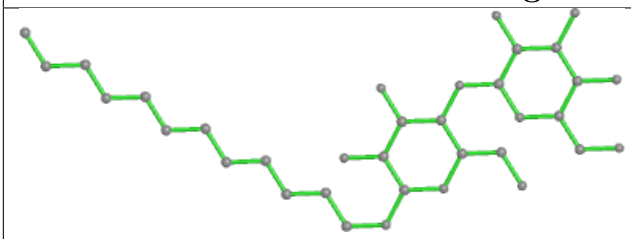


Torsions

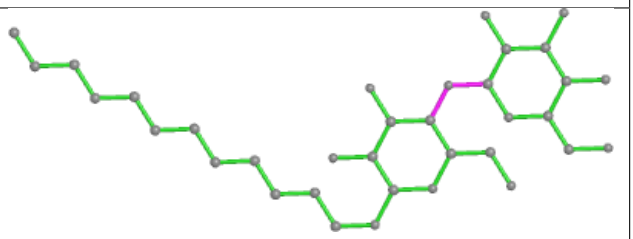


Rings

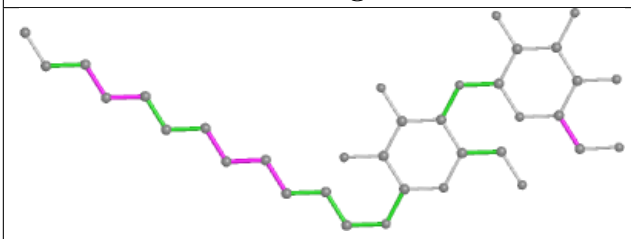
Ligand LMT L 307



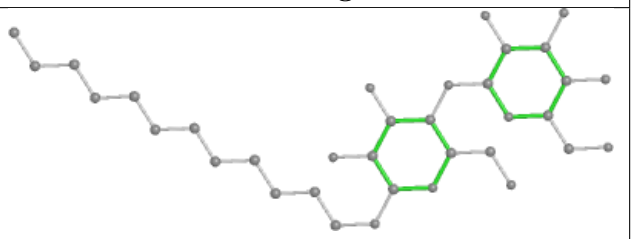
Bond lengths



Bond angles

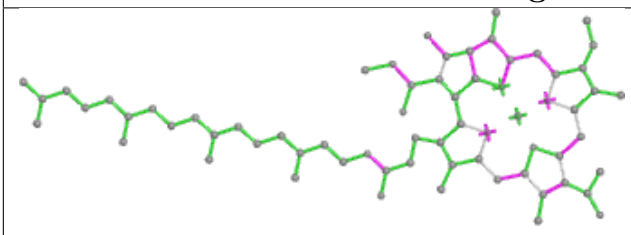


Torsions

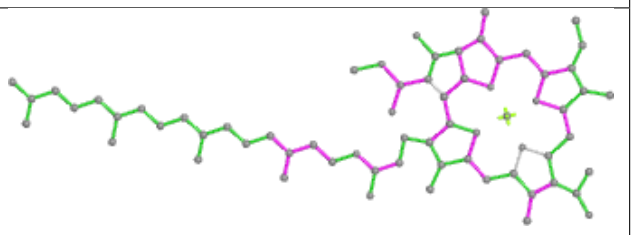


Rings

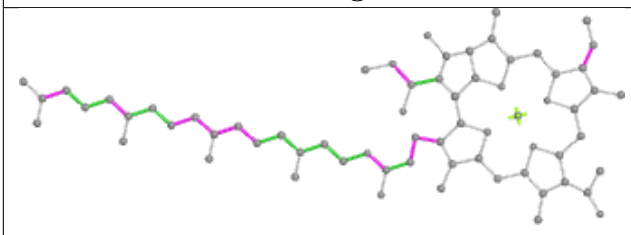
Ligand BCL J 102



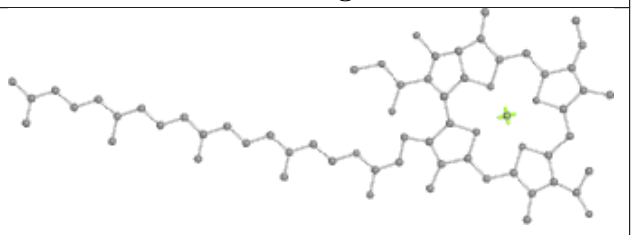
Bond lengths



Bond angles

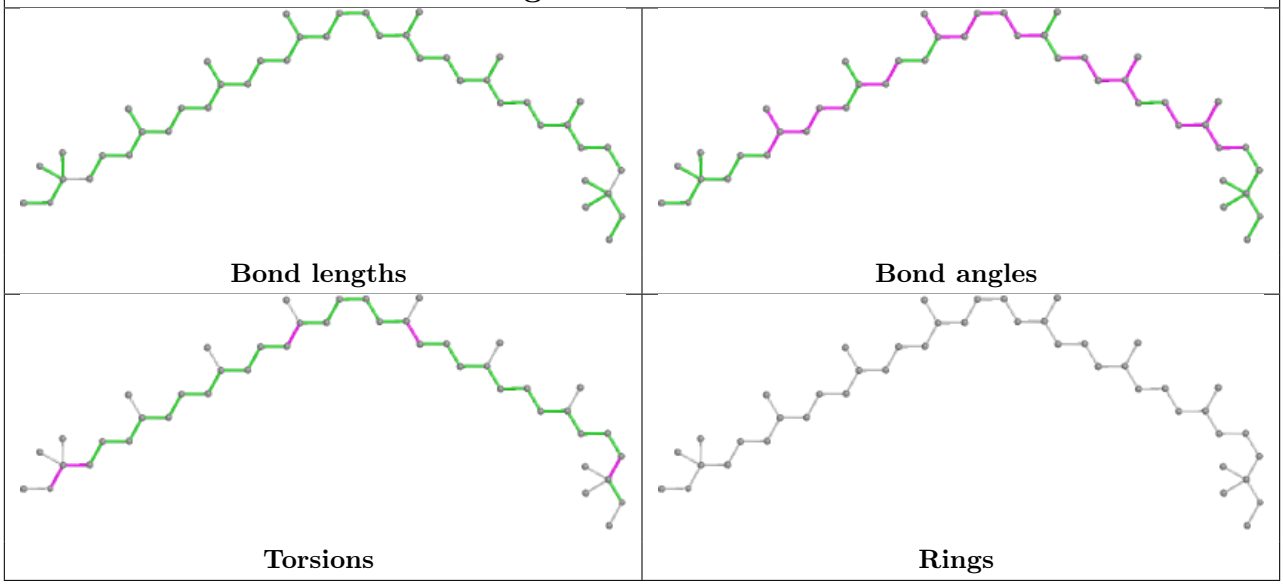


Torsions

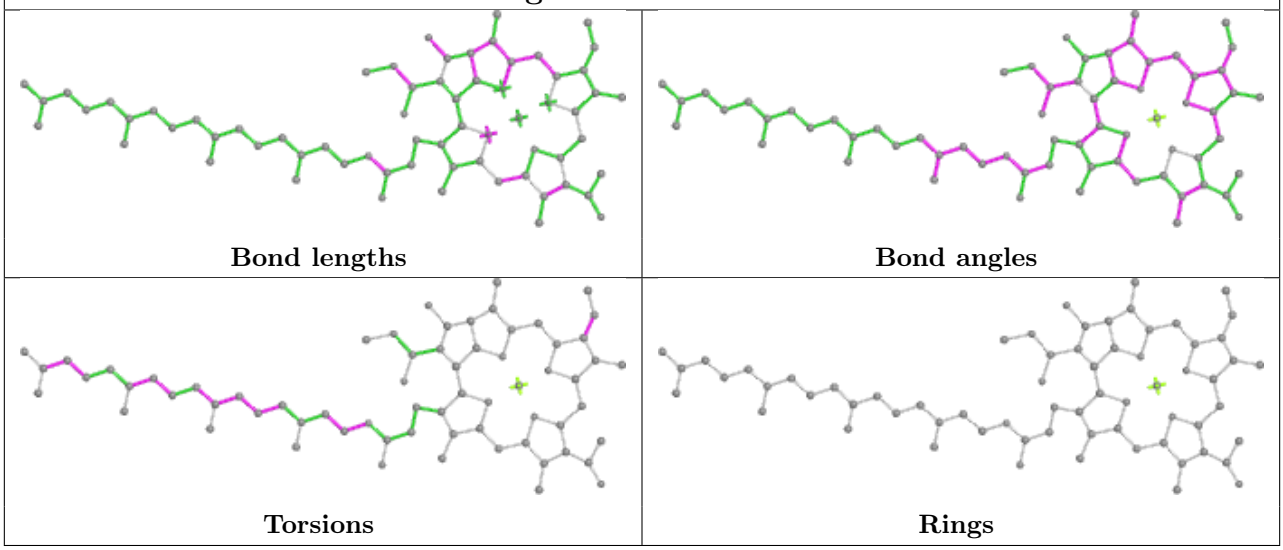


Rings

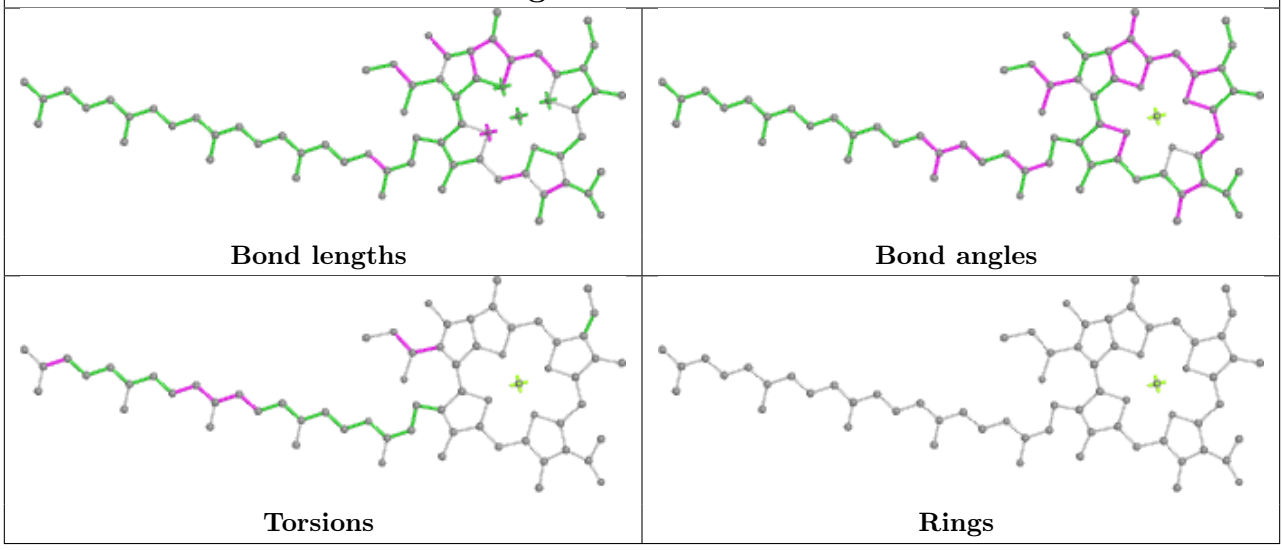
Ligand CRT N 102



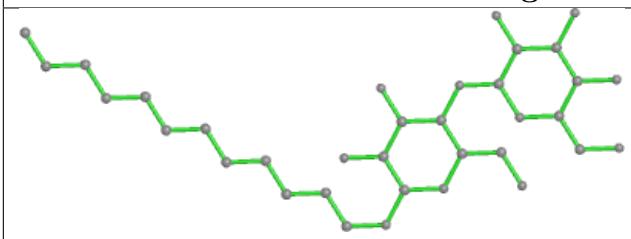
Ligand BCL D 102



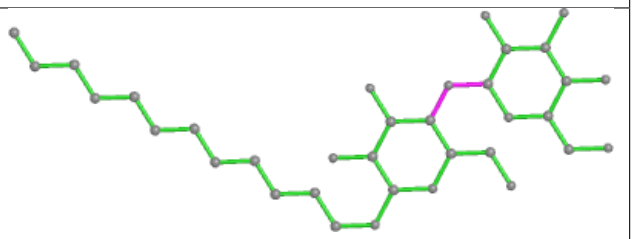
Ligand BCL L 308



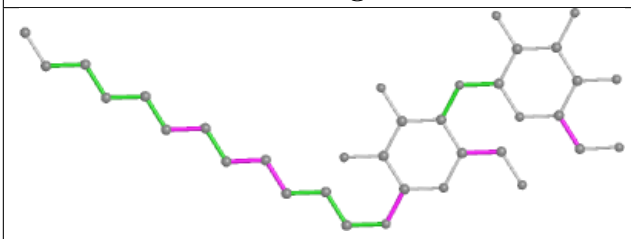
Ligand LMT R 103



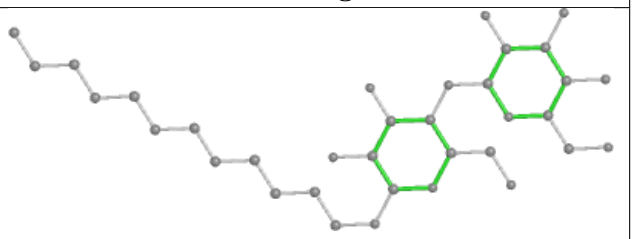
Bond lengths



Bond angles

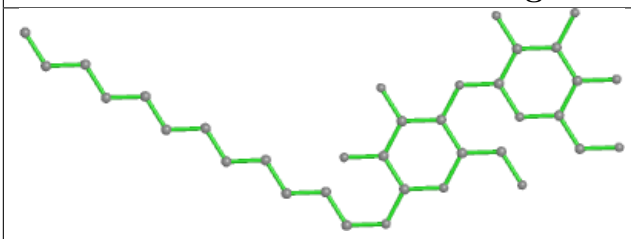


Torsions

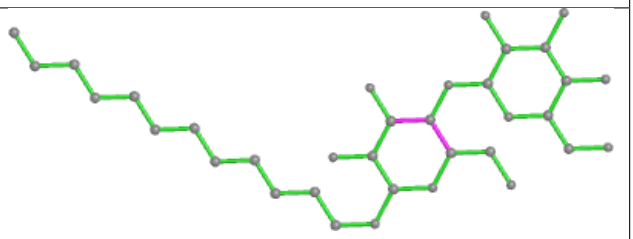


Rings

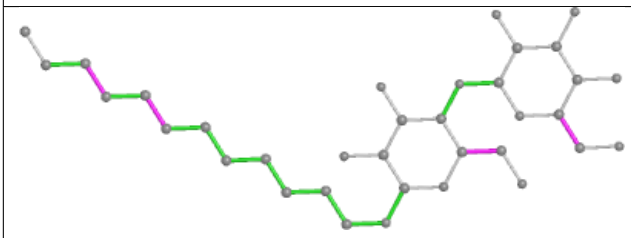
Ligand LMT 8 103



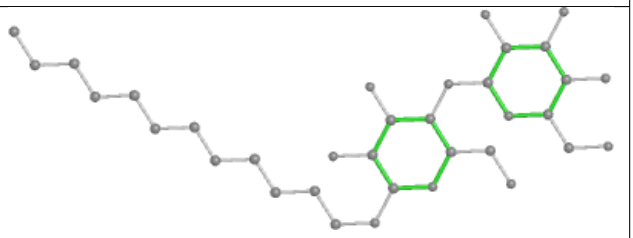
Bond lengths



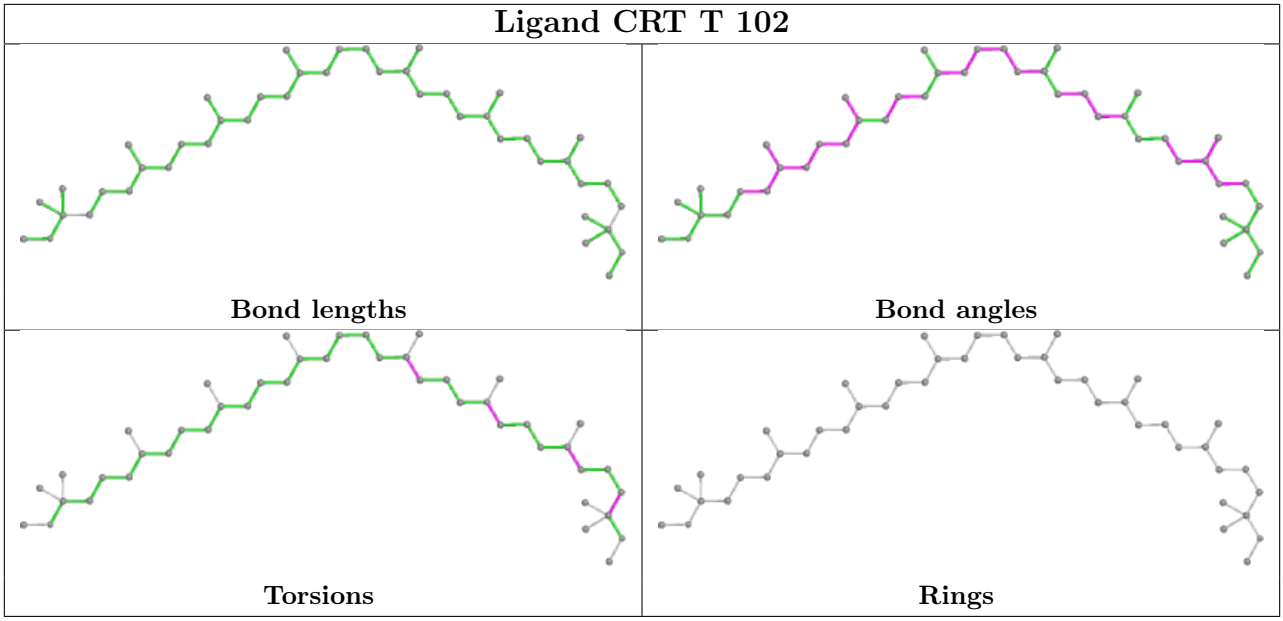
Bond angles

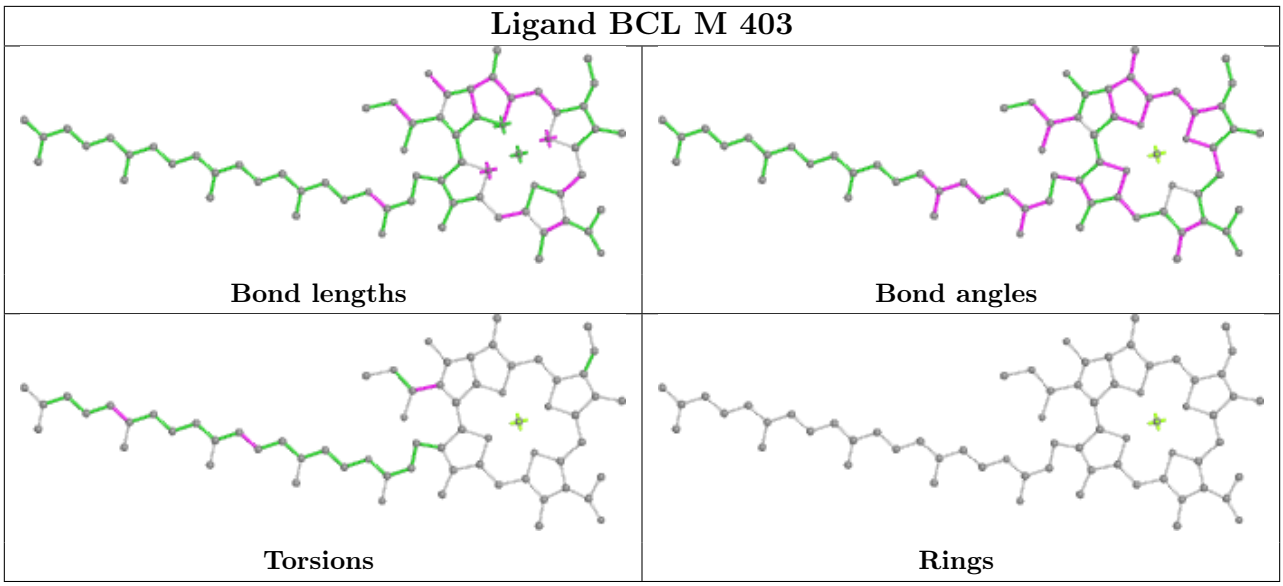


Torsions



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.

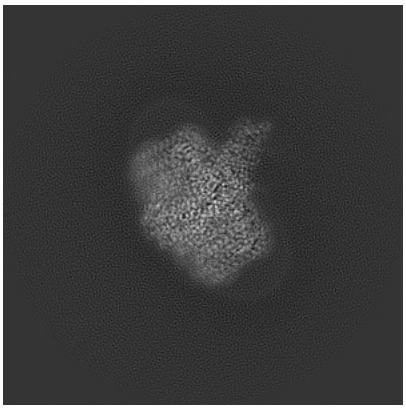
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37465. These allow visual inspection of the internal detail of the map and identification of artifacts.

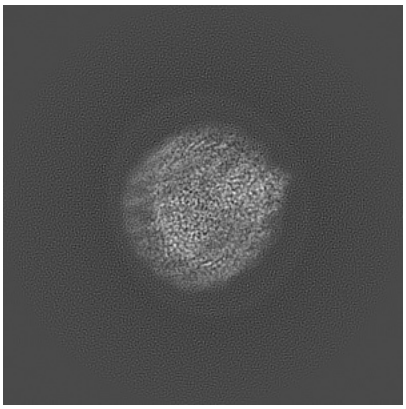
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

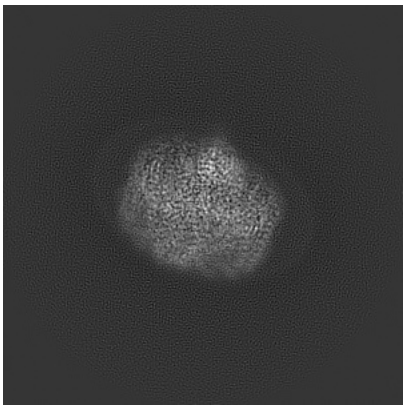
6.1.1 Primary map



X

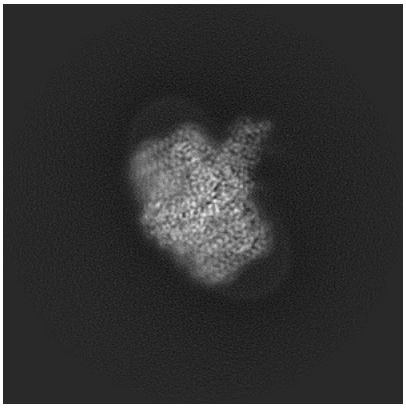


Y

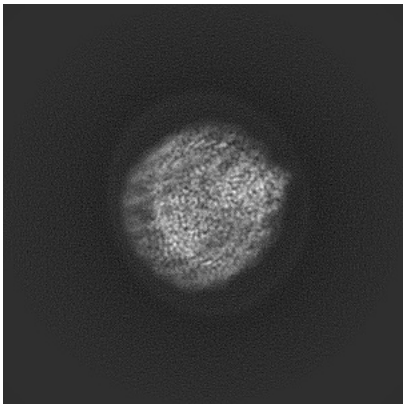


Z

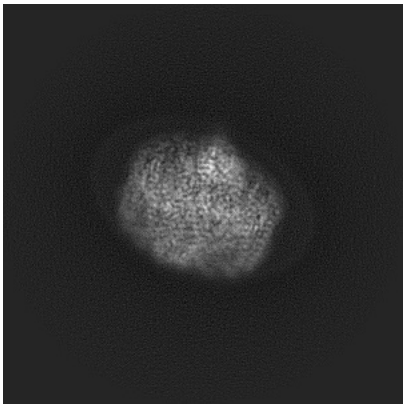
6.1.2 Raw map



X



Y

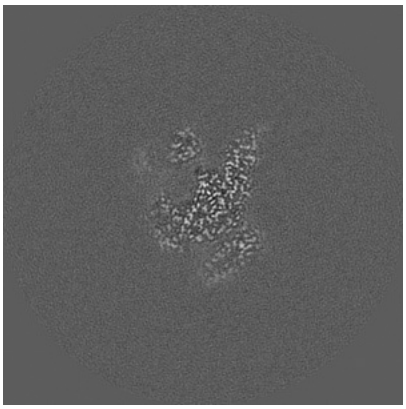


Z

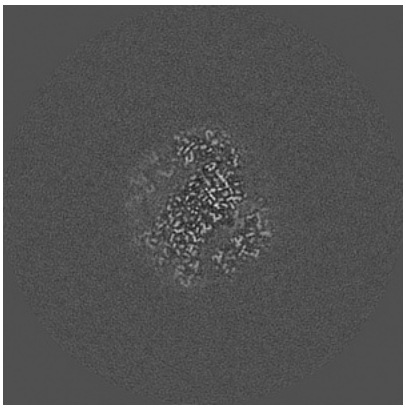
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

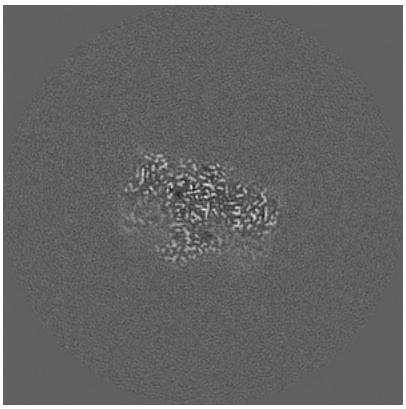
6.2.1 Primary map



X Index: 240

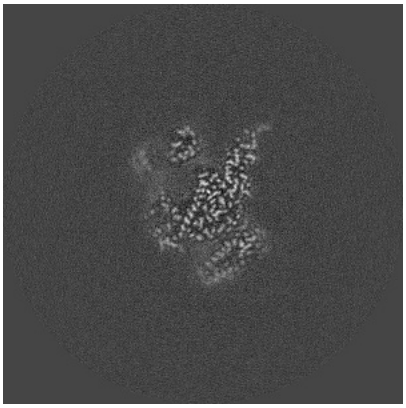


Y Index: 240

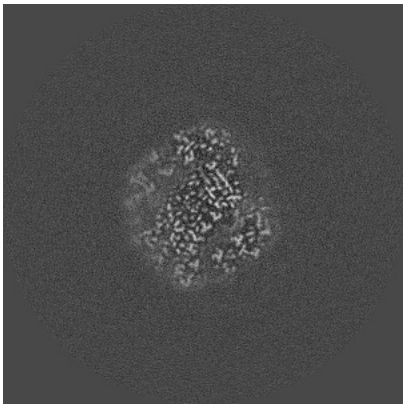


Z Index: 240

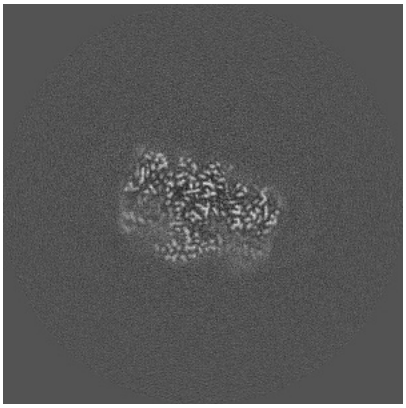
6.2.2 Raw map



X Index: 240



Y Index: 240

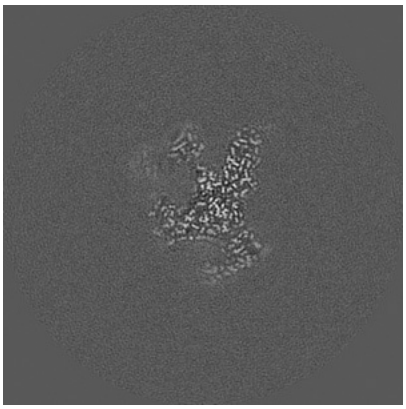


Z Index: 240

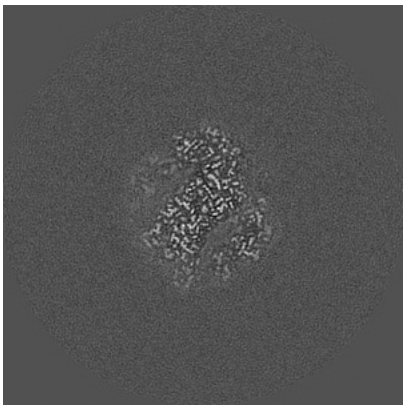
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

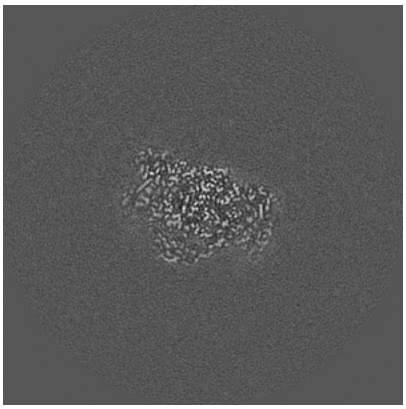
6.3.1 Primary map



X Index: 246

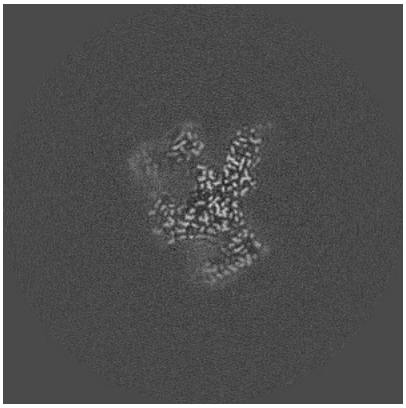


Y Index: 238

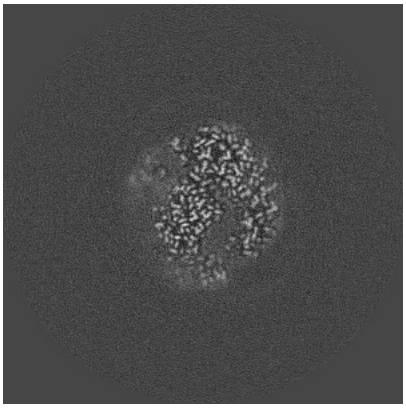


Z Index: 231

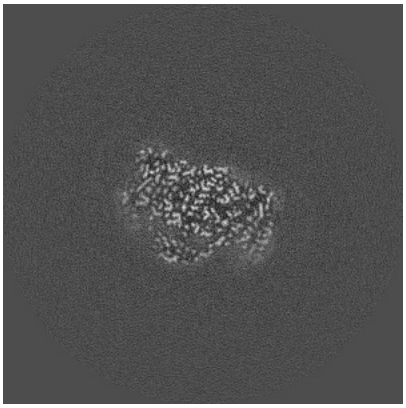
6.3.2 Raw map



X Index: 246



Y Index: 228

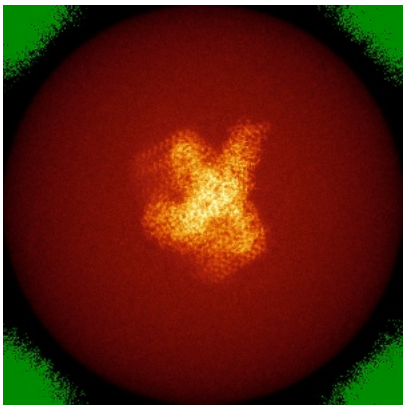


Z Index: 231

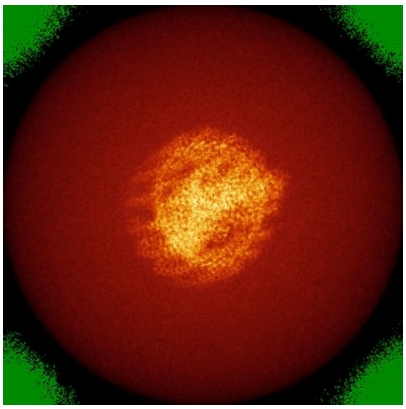
The images above show the largest variance slices of the map in three orthogonal directions.

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

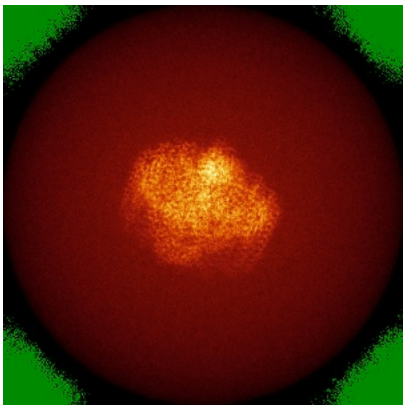
6.4.1 Primary map



X

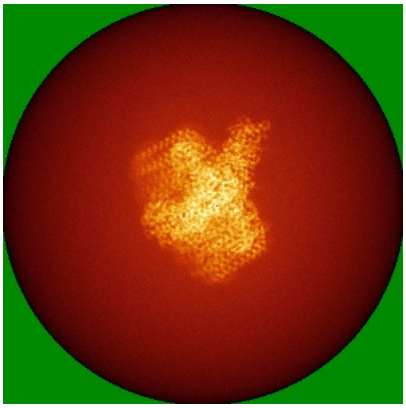


Y

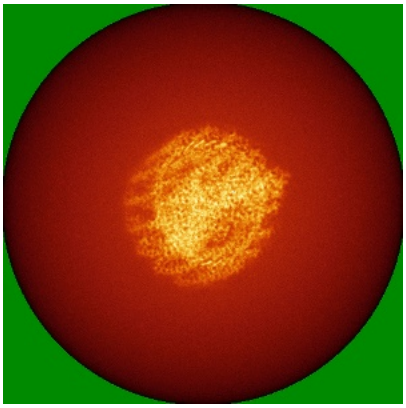


Z

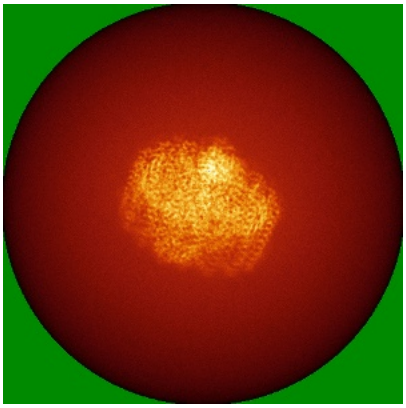
6.4.2 Raw map



X



Y

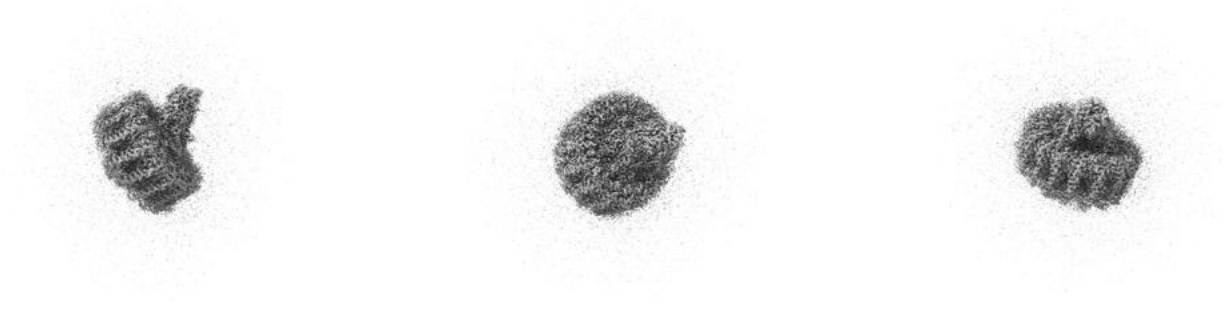


Z

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 0.013. 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.

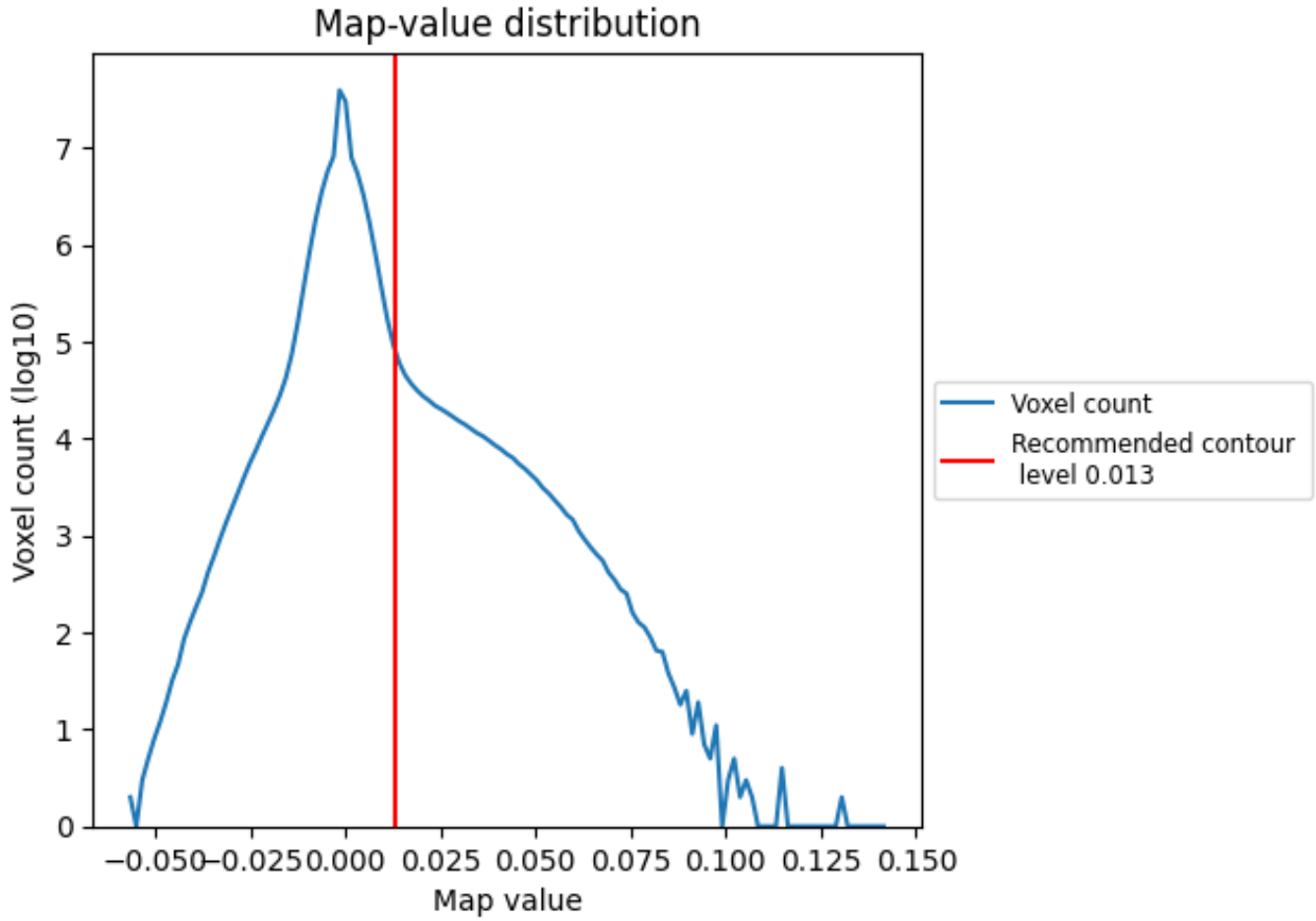
6.6 Mask visualisation (i)

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

7 Map analysis

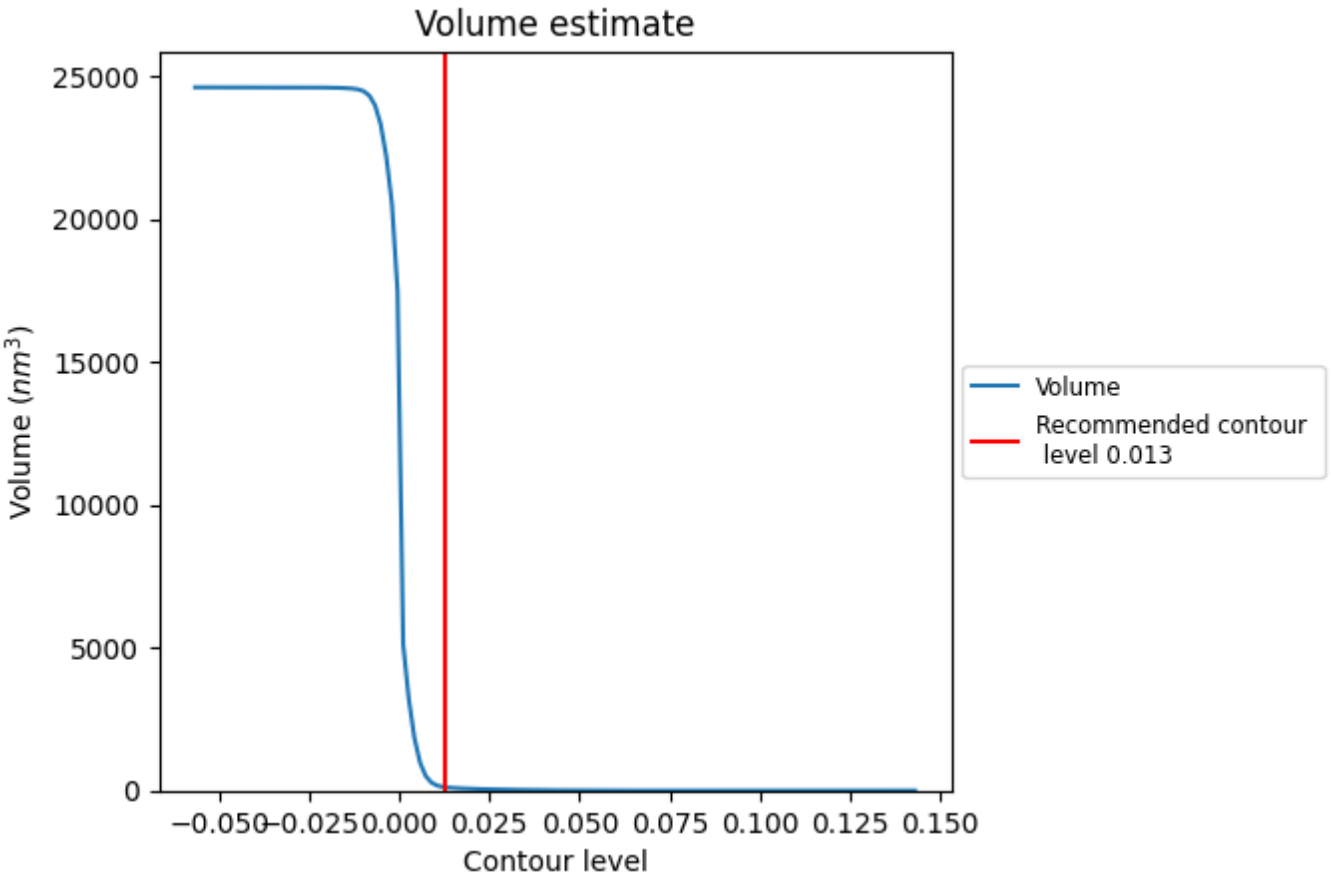
This section contains the results of statistical analysis of the map.

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.

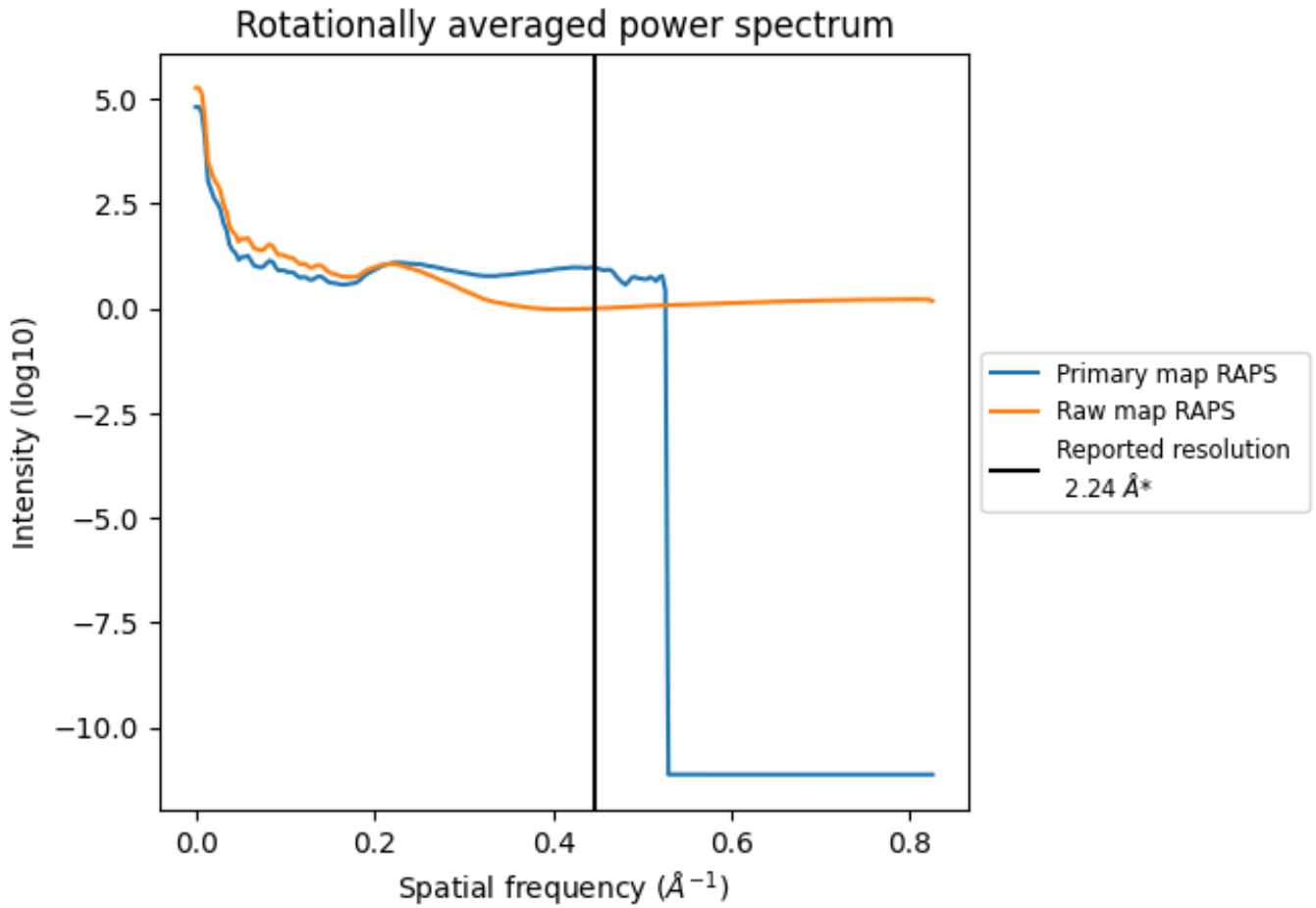
7.2 Volume estimate



The volume at the recommended contour level is 115 nm^3; this corresponds to an approximate mass of 103 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)

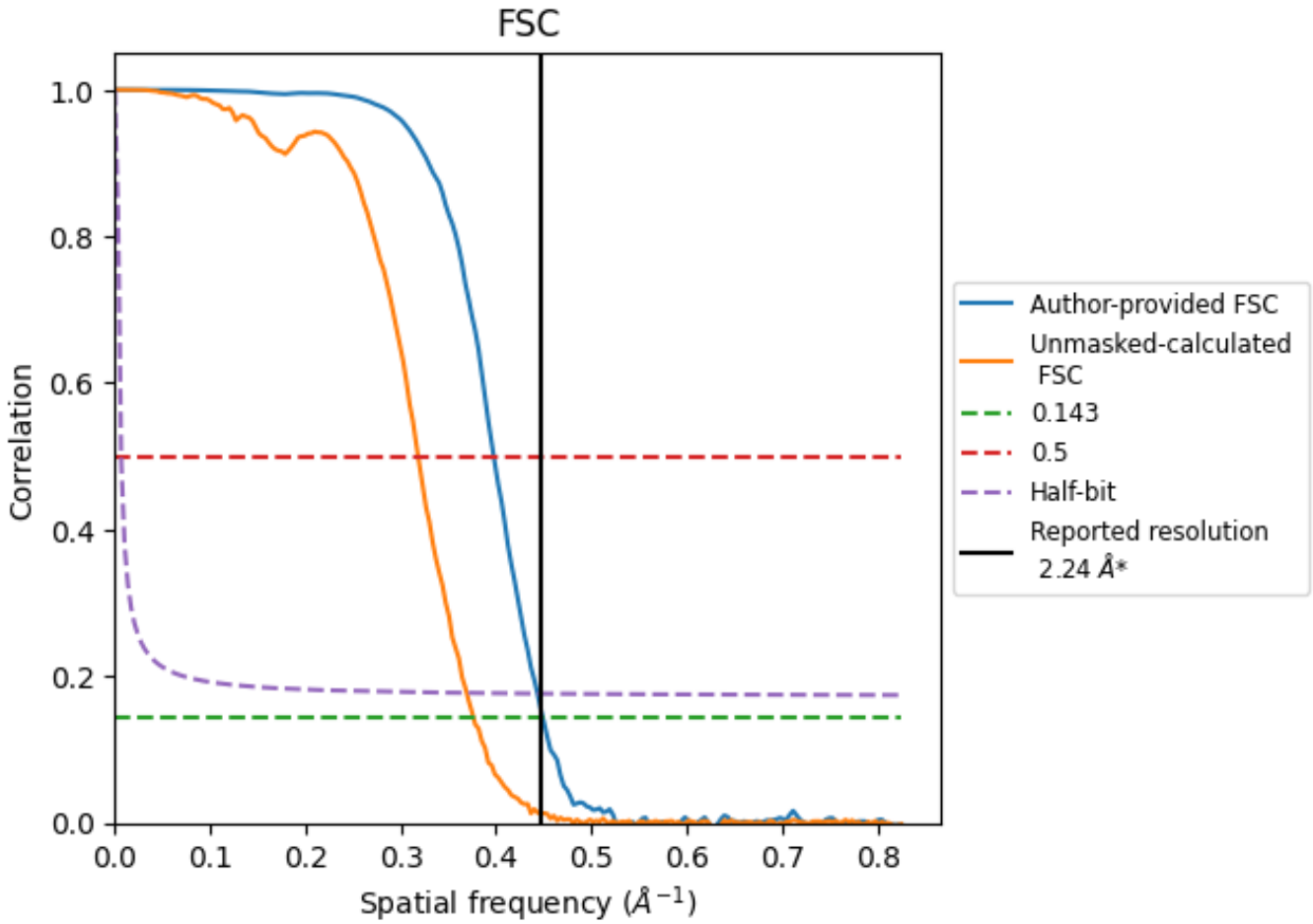


*Reported resolution corresponds to spatial frequency of 0.446 $Å^{-1}$

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 0.446 Å^{-1}

8.2 Resolution estimates (i)

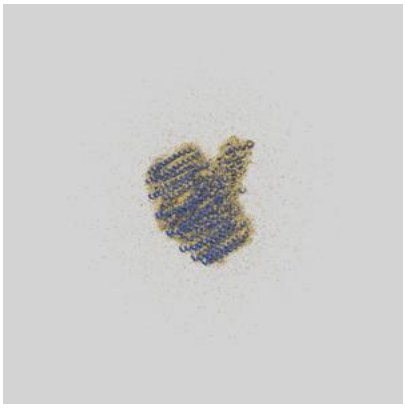
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.23	2.52	2.25
Unmasked-calculated*	2.66	3.14	2.71

*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 2.66 differs from the reported value 2.24 by more than 10 %

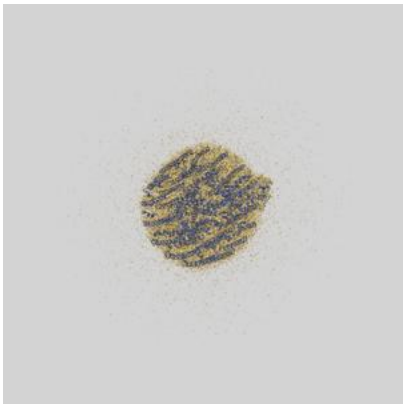
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37465 and PDB model 8WDU. Per-residue inclusion information can be found in section 3 on page 21.

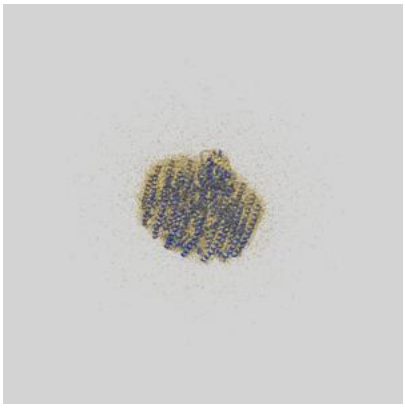
9.1 Map-model overlay



X



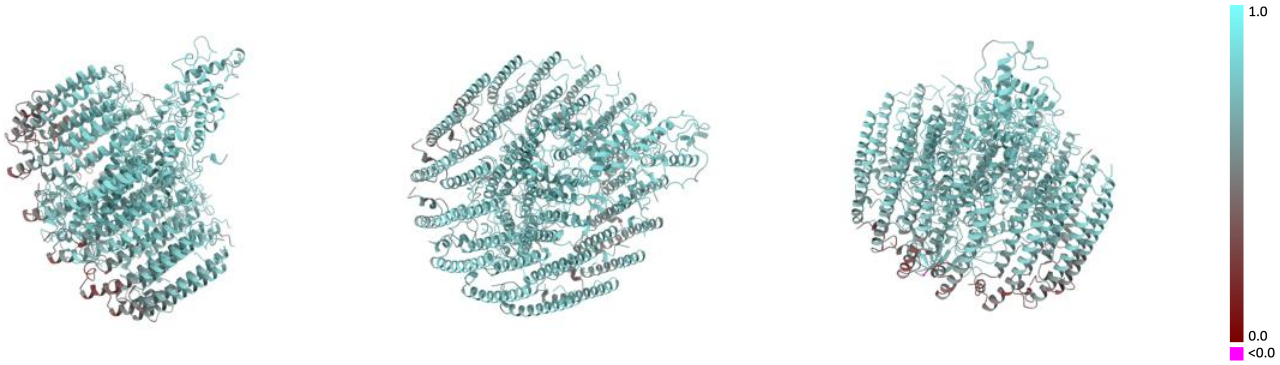
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

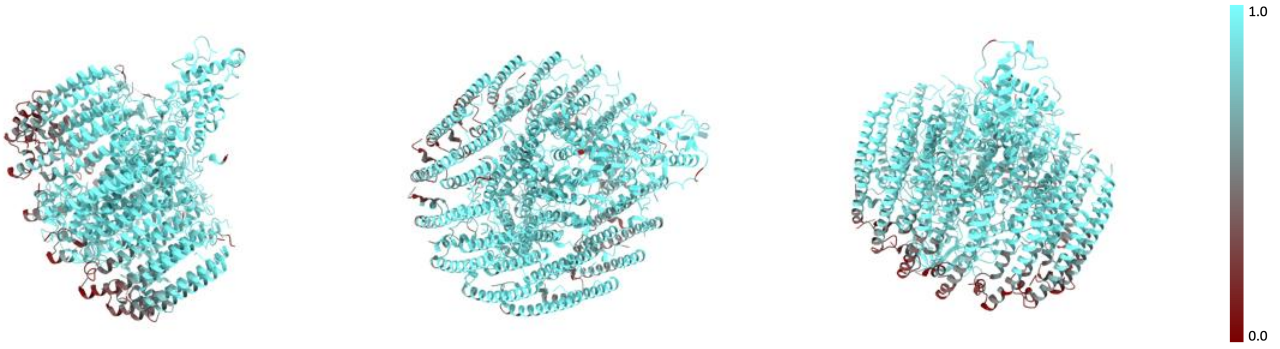
9.2 Q-score mapped to coordinate model



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.

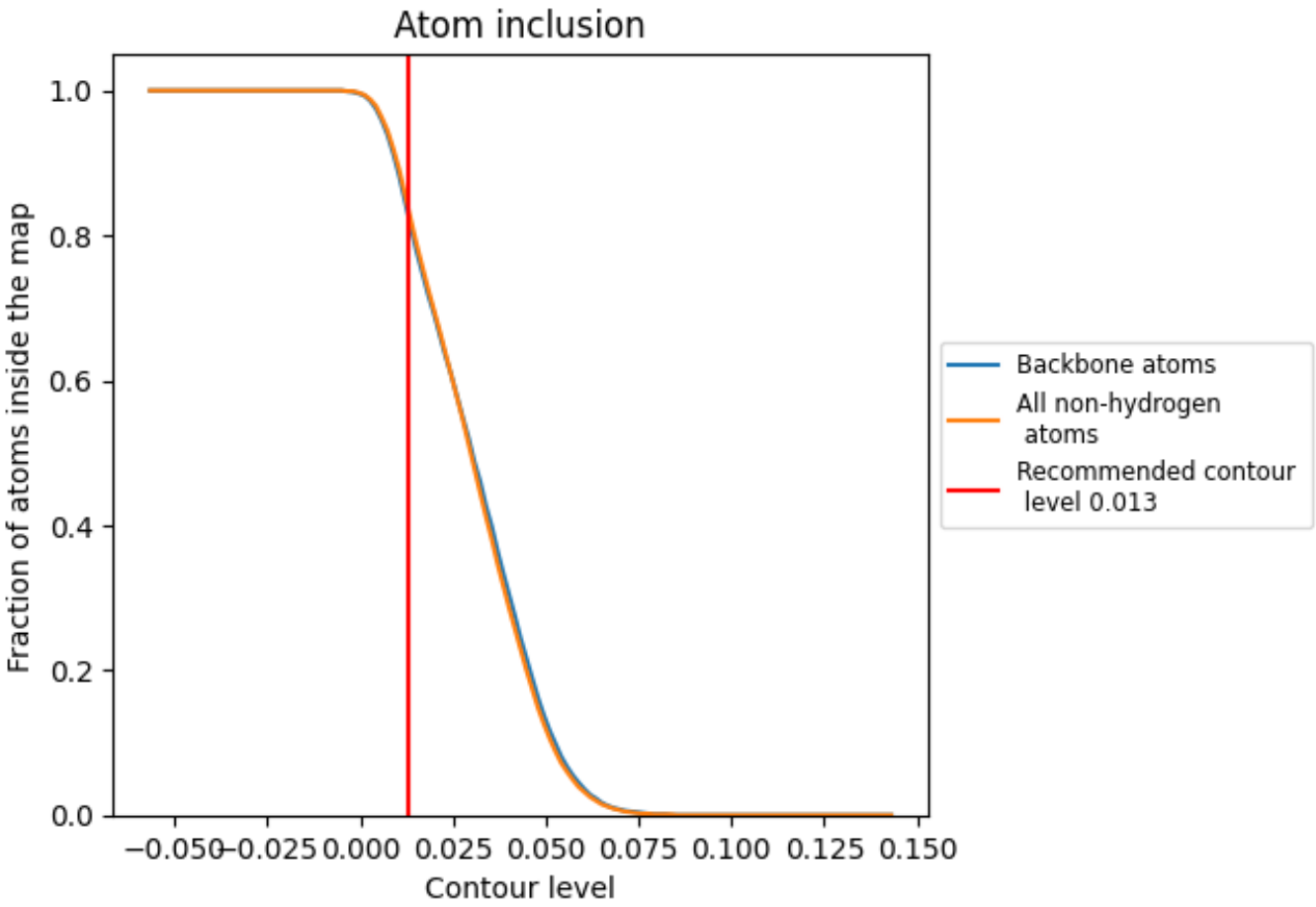
9.3 Atom inclusion mapped to coordinate model



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.6760
0	0.9090	0.7090
1	0.7440	0.6370
2	0.5920	0.5390
3	0.7870	0.6490
4	0.6360	0.5700
5	0.8460	0.6710
6	0.8050	0.6540
7	0.9350	0.7170
8	0.8050	0.6450
9	0.9480	0.7270
A	0.9240	0.7070
B	0.8770	0.6870
C	0.9620	0.7430
D	0.8530	0.6830
E	0.7970	0.6520
F	0.7340	0.6280
G	0.7390	0.6240
H	0.9220	0.7140
I	0.7470	0.6370
J	0.6730	0.5870
K	0.6900	0.5930
L	0.9300	0.7400
M	0.9460	0.7430
N	0.6370	0.5700
O	0.8080	0.6510
P	0.7110	0.5980
Q	0.8220	0.6620
R	0.7710	0.6370
S	0.7500	0.6510
T	0.7120	0.6050
U	0.7360	0.6320
V	0.7320	0.6130
W	0.7180	0.6230
X	0.6760	0.5960

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.6850	0.5950
Z	0.6680	0.5650