Full wwPDB EM Validation Report

Feb 13, 2024 – 06:46 PM JST

PDB ID	:	8WDV
EMDB ID	:	EMD-37466
Title	:	Photosynthetic LH1-RC complex from the purple sulfur bacterium Allochromatium vinosum purified by Ca2+-DEAE
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:

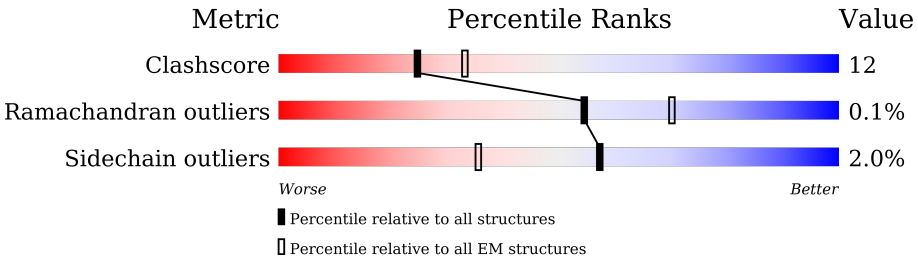
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.24 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	68% 13% 19%
2	L	278	78% 21%
3	M	325	83% 14%
4	H	259	10% 78% 21%
5	1	44	70% 27%
5	5	44	11% 80% 16%
5	7	44	11% 68% 25% 7%

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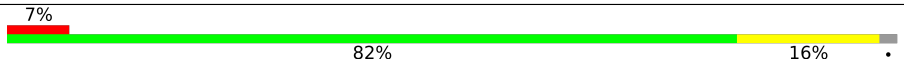
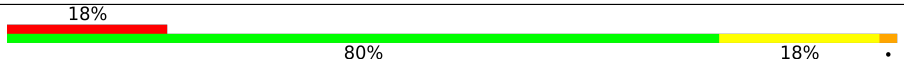
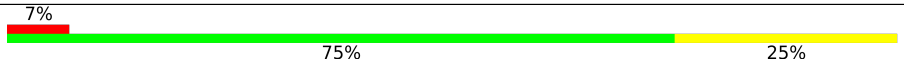
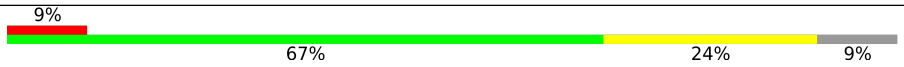
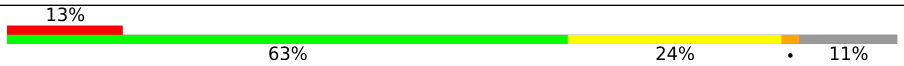
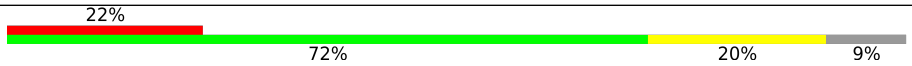
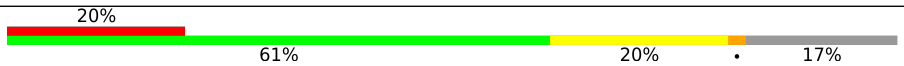
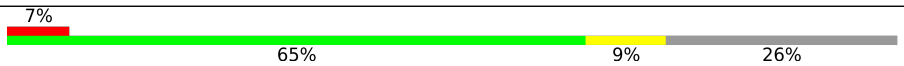
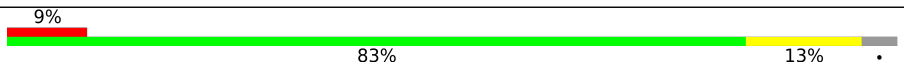
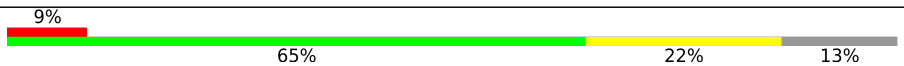
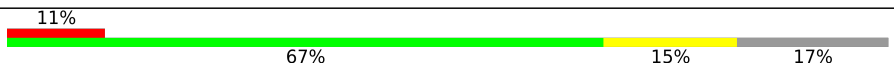
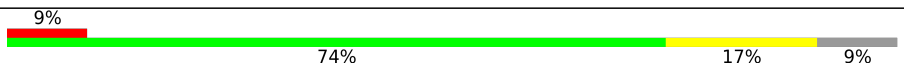
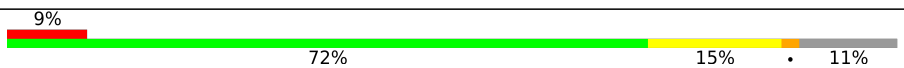
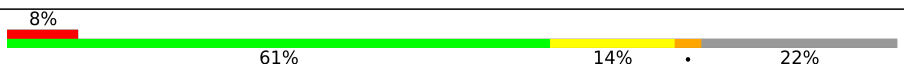
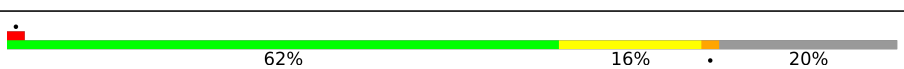
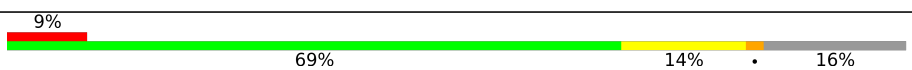
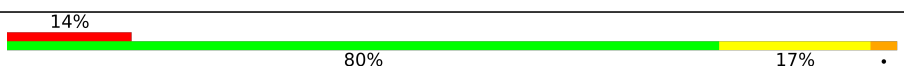
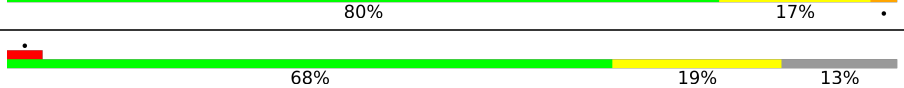
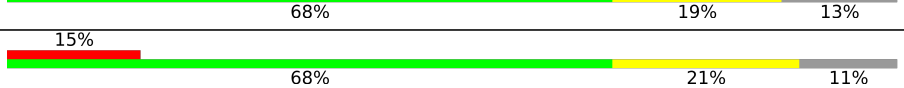
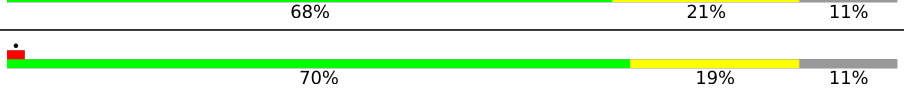
Mol	Chain	Length	Quality of chain
5	9	44	
5	A	44	
5	I	44	
5	K	44	
5	O	44	
5	Q	44	
6	0	46	
6	2	46	
6	4	46	
6	6	46	
6	8	46	
6	B	46	
6	J	46	
6	N	46	
6	P	46	
6	R	46	
7	D	64	
7	F	64	
7	S	64	
7	U	64	
7	W	64	
7	Y	64	
8	E	47	
8	G	47	
8	T	47	

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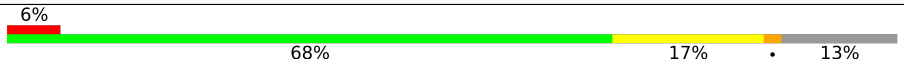
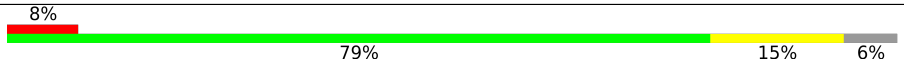
Mol	Chain	Length	Quality of chain
8	V	47	
8	X	47	
8	Z	47	
9	3	66	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 26261 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	41	Total	C	N	O		0	0
			341	237	55	49			
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	40	Total	C	N	O	S	0	0
			331	223	53	54	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	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
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	34	Total	C	N	O	S	0	0
			287	197	46	43	1		
6	0	42	Total	C	N	O	S	0	0
			345	231	55	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	50	Total	C	N	O	S	0	0
			407	276	63	66	2		
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	51	Total	C	N	O	S	0	0
			412	279	64	67	2		
7	U	51	Total	C	N	O	S	0	0
			412	279	64	67	2		
7	W	54	Total	C	N	O	S	0	0
			431	291	67	71	2		
7	Y	64	Total	C	N	O	S	0	0
			511	341	83	85	2		

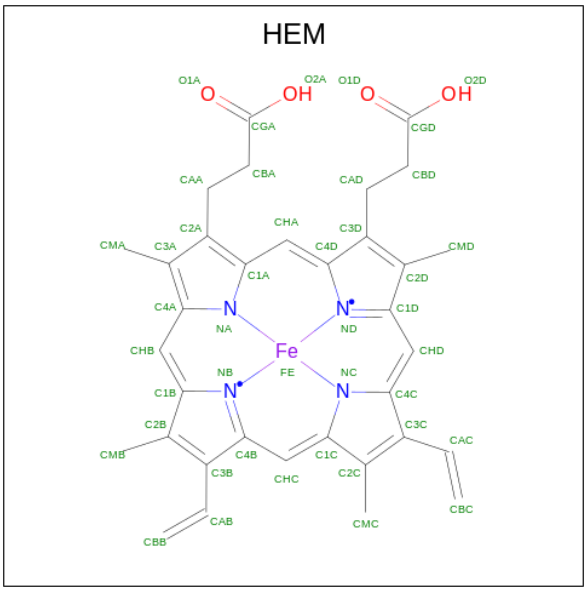
- Molecule 8 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	41	Total	C	N	O	S	0	0
			343	231	53	56	3		
8	G	42	Total	C	N	O	S	0	0
			349	234	54	58	3		
8	T	42	Total	C	N	O	S	0	0
			349	234	54	58	3		
8	V	42	Total	C	N	O	S	0	0
			349	234	54	58	3		
8	X	42	Total	C	N	O	S	0	0
			349	234	54	58	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	62	Total	C	N	O	S	0	0
			489	332	76	78	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
12	C	1	Total	Ca	0
			1	1	
12	M	1	Total	Ca	0
			1	1	
12	D	1	Total	Ca	0
			1	1	
12	F	1	Total	Ca	0
			1	1	

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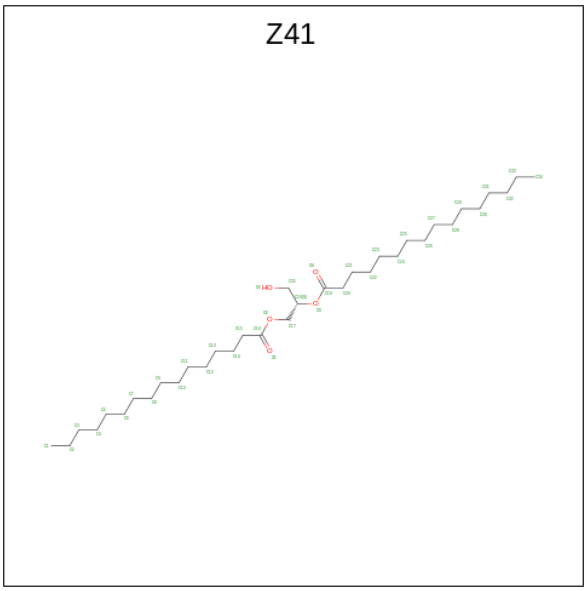
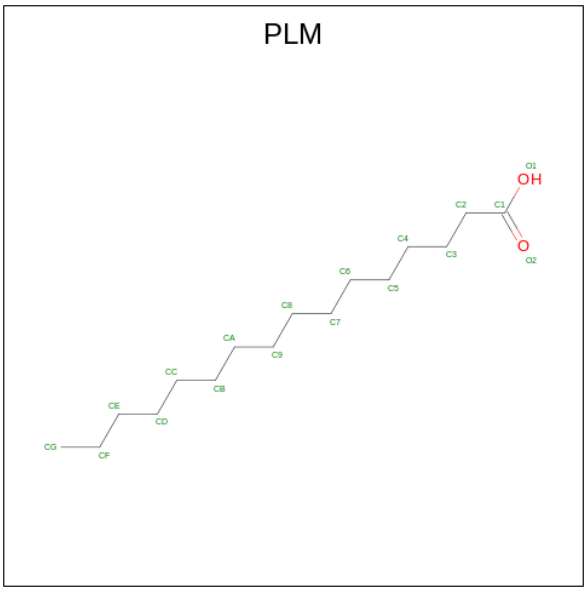
Mol	Chain	Residues	Atoms	AltConf
12	S	1	Total Ca 1 1	0
12	U	1	Total Ca 1 1	0
12	W	1	Total Ca 1 1	0
12	Y	1	Total Ca 1 1	0

- Molecule 13 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (three-letter code: Z41) (formula: $C_{35}H_{68}O_5$).



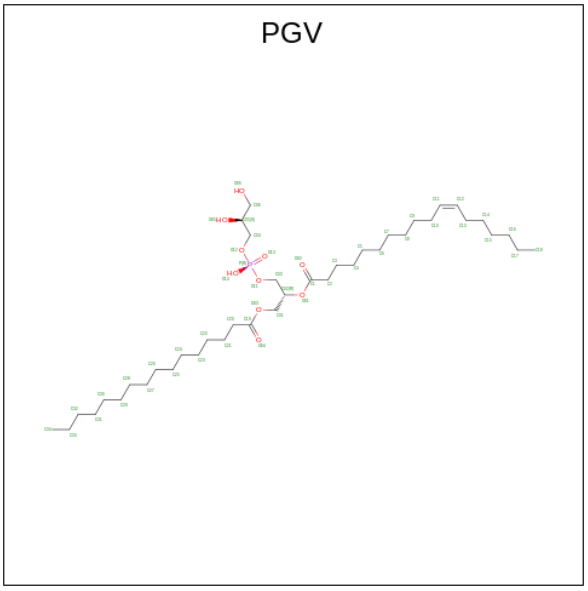
Mol	Chain	Residues	Atoms	AltConf
13	C	1	Total C O 35 31 4	0

- Molecule 14 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



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

- Molecule 15 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
15	C	1	Total	C	O	P	0
			31	20	10	1	
15	L	1	Total	C	O	P	0
			29	18	10	1	

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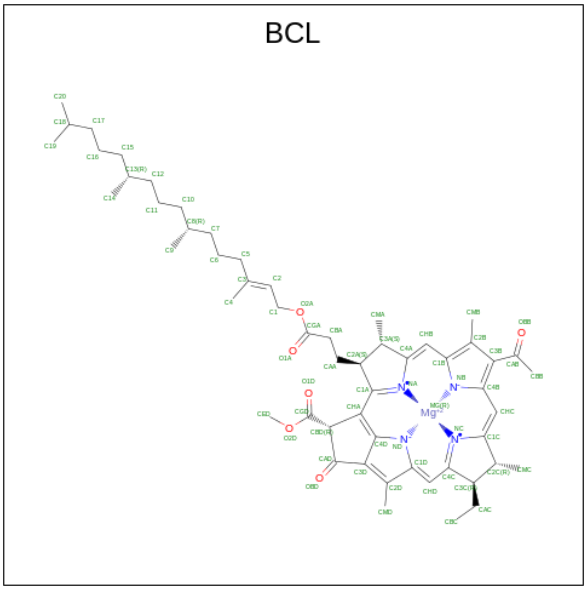
Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total	C	O	P	0
			35	24	10	1	
15	L	1	Total	C	O	P	0
			33	22	10	1	
15	M	1	Total	C	O	P	0
			37	26	10	1	
15	M	1	Total	C	O	P	0
			27	18	8	1	
15	H	1	Total	C	O	P	0
			36	25	10	1	
15	D	1	Total	C	O	P	0
			39	28	10	1	
15	F	1	Total	C	O	P	0
			36	25	10	1	
15	1	1	Total	C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

- Molecule 16 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
16	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
16	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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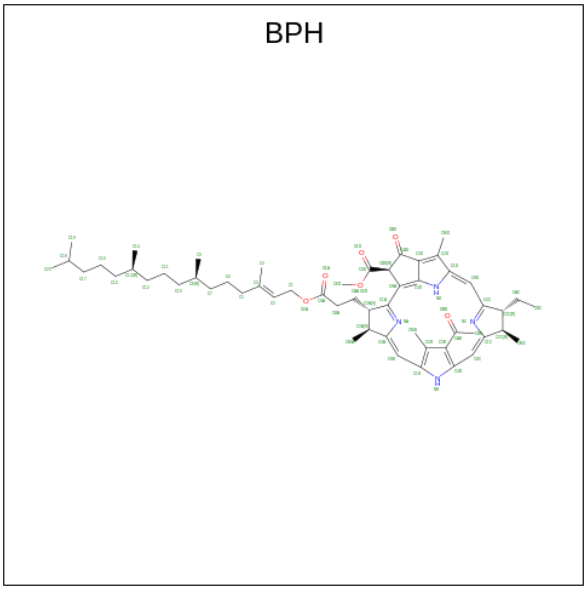
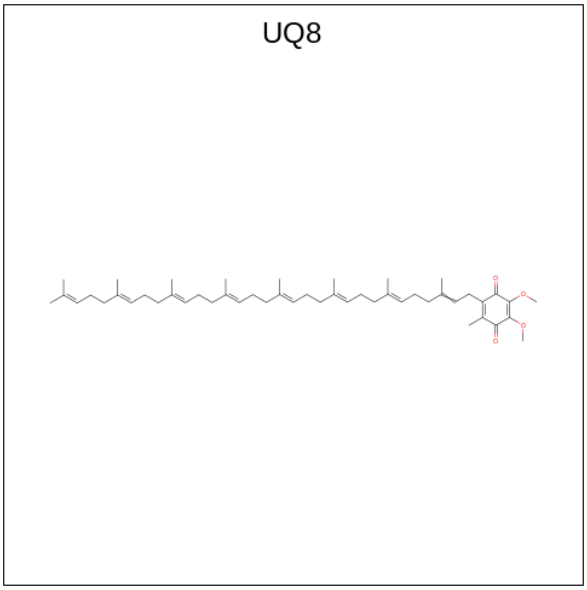
Mol	Chain	Residues	Atoms					AltConf
16	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 17 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 18 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).

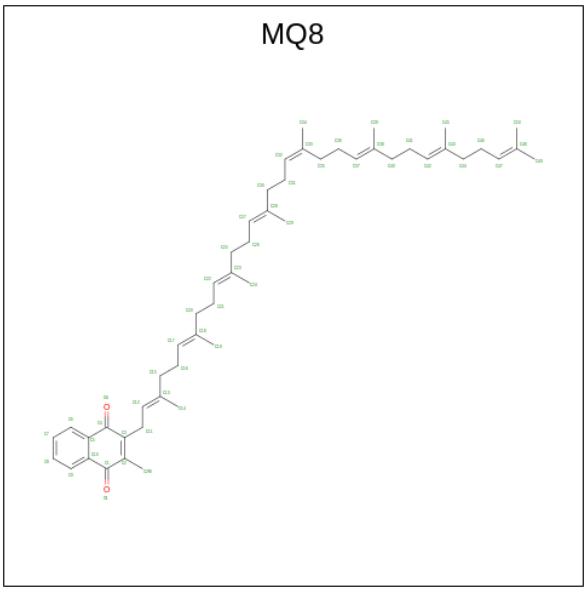


Mol	Chain	Residues	Atoms	AltConf
18	L	1	Total C O 33 29 4	0
18	L	1	Total C O 53 49 4	0
18	L	1	Total C O 53 49 4	0

- Molecule 19 is FE (III) ION (three-letter code: FE) (formula: Fe).

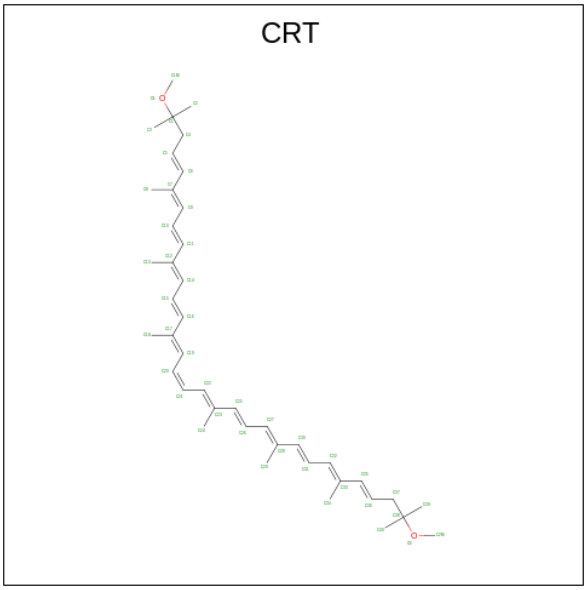
Mol	Chain	Residues	Atoms	AltConf
19	M	1	Total Fe 1 1	0

- Molecule 20 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



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

- Molecule 21 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



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

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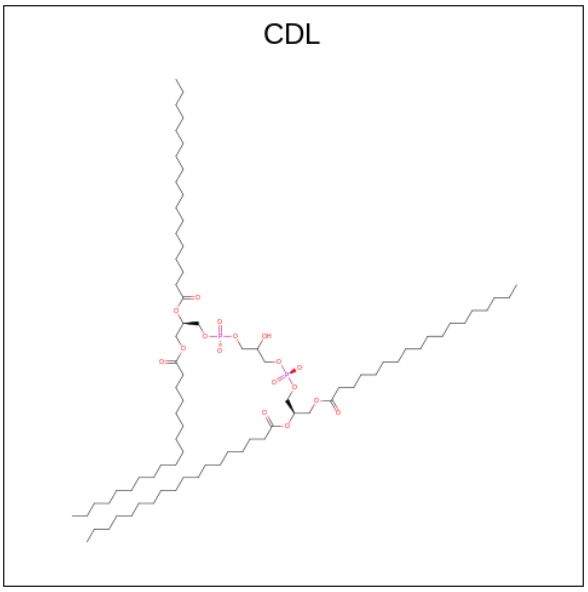
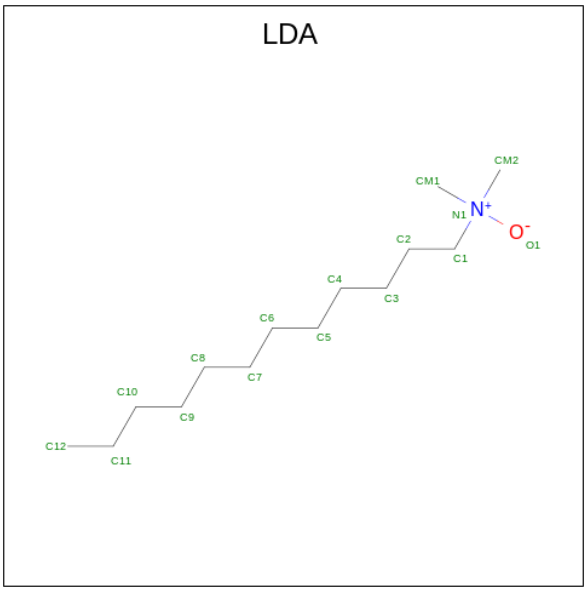
Mol	Chain	Residues	Atoms	AltConf
21	G	1	Total C O 44 42 2	0
21	K	1	Total C O 44 42 2	0
21	N	1	Total C O 44 42 2	0
21	Q	1	Total C O 44 42 2	0
21	R	1	Total C O 44 42 2	0
21	T	1	Total C O 44 42 2	0
21	V	1	Total C O 44 42 2	0
21	X	1	Total C O 44 42 2	0
21	Z	1	Total C O 44 42 2	0
21	2	1	Total C O 44 42 2	0
21	4	1	Total C O 44 42 2	0
21	7	1	Total C O 44 42 2	0
21	8	1	Total C O 44 42 2	0
21	0	1	Total C O 44 42 2	0

- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



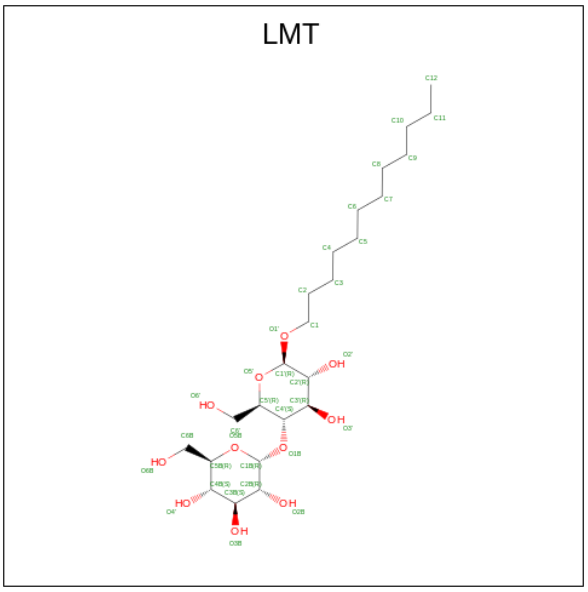
Mol	Chain	Residues	Atoms				AltConf
22	M	1	Total	C	O	P	0
			39	21	16	2	
22	M	1	Total	C	O	P	0
			95	76	17	2	
22	M	1	Total	C	O	P	0
			84	65	17	2	
22	H	1	Total	C	O	P	0
			79	60	17	2	
22	D	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 23 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				AltConf
23	M	1	Total	C	N	O	0
			16	14	1	1	
23	O	1	Total	C	N	O	0
			16	14	1	1	

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



Mol	Chain	Residues	Atoms			AltConf
24	M	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms	AltConf
24	H	1	Total C O 35 24 11	0
24	B	1	Total C O 35 24 11	0
24	E	1	Total C O 35 24 11	0
24	G	1	Total C O 35 24 11	0
24	G	1	Total C O 35 24 11	0
24	J	1	Total C O 35 24 11	0
24	P	1	Total C O 35 24 11	0
24	P	1	Total C O 35 24 11	0
24	R	1	Total C O 35 24 11	0
24	V	1	Total C O 35 24 11	0
24	X	1	Total C O 35 24 11	0
24	Z	1	Total C O 35 24 11	0
24	2	1	Total C O 35 24 11	0
24	2	1	Total C O 35 24 11	0
24	4	1	Total C O 35 24 11	0
24	5	1	Total C O 31 20 11	0
24	8	1	Total C O 35 24 11	0
24	0	1	Total C O 35 24 11	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	AltConf
25	C	134	Total O 134 134	0

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Mol	Chain	Residues	Atoms	AltConf
25	L	50	Total O 50 50	0
25	M	73	Total O 73 73	0
25	H	16	Total O 16 16	0
25	A	2	Total O 2 2	0
25	D	7	Total O 7 7	0
25	E	2	Total O 2 2	0
25	F	3	Total O 3 3	0
25	I	2	Total O 2 2	0
25	K	1	Total O 1 1	0
25	Q	3	Total O 3 3	0
25	R	1	Total O 1 1	0
25	S	6	Total O 6 6	0
25	T	4	Total O 4 4	0
25	U	12	Total O 12 12	0
25	V	3	Total O 3 3	0
25	W	6	Total O 6 6	0
25	X	2	Total O 2 2	0
25	Y	8	Total O 8 8	0
25	Z	2	Total O 2 2	0
25	1	1	Total O 1 1	0
25	2	1	Total O 1 1	0

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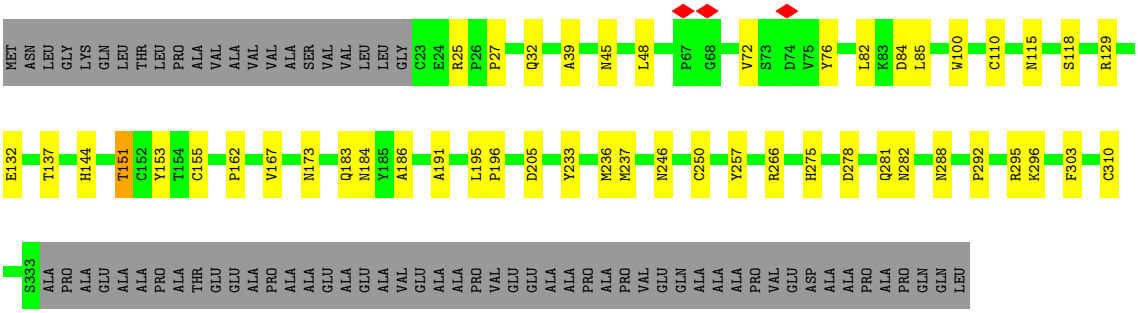
Mol	Chain	Residues	Atoms	AltConf
25	3	10	Total O 10 10	0
25	5	1	Total O 1 1	0
25	7	1	Total O 1 1	0
25	9	3	Total O 3 3	0

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.

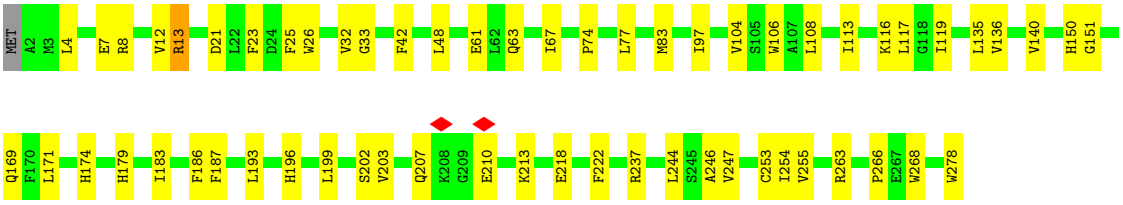
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



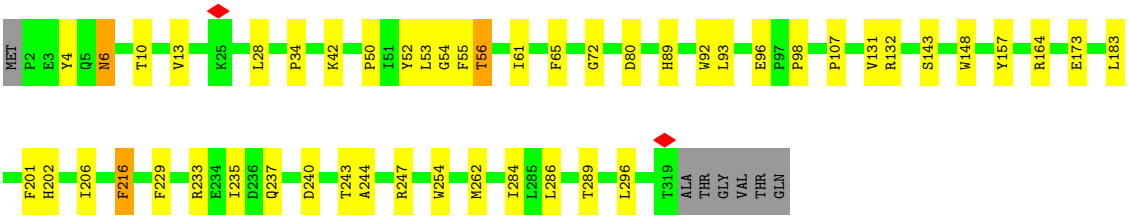
• Molecule 2: Reaction center protein L chain

Chain L:



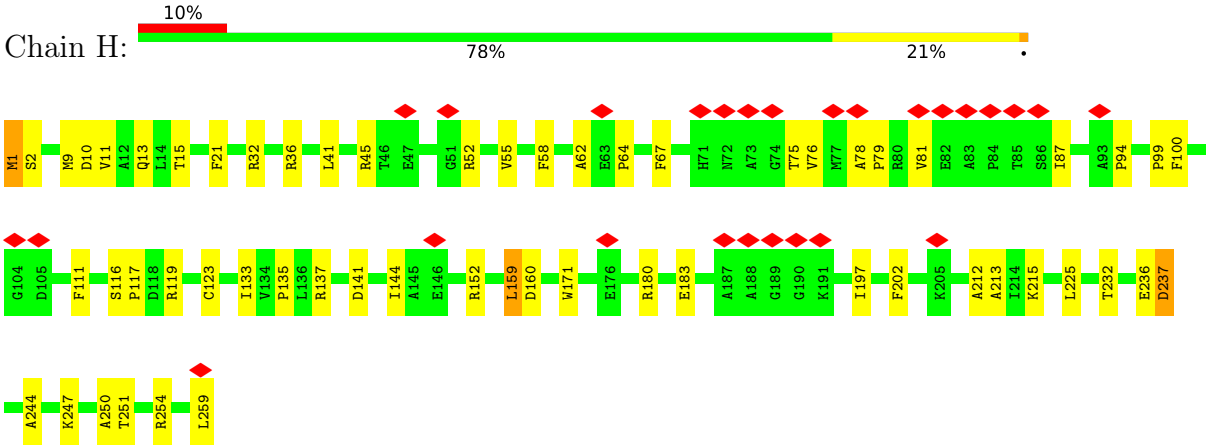
• Molecule 3: Reaction center protein M chain

Chain M:



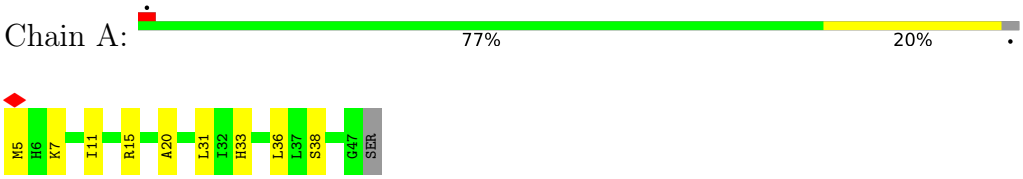
• Molecule 4: Photosynthetic reaction center H subunit

Chain H:



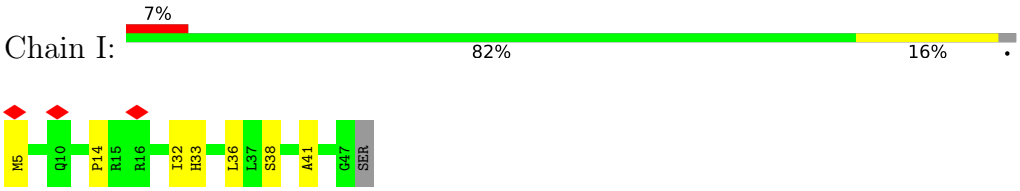
• Molecule 5: Antenna complex alpha/beta subunit

Chain A:



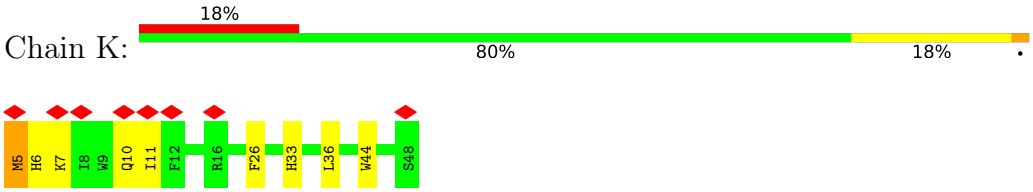
• Molecule 5: Antenna complex alpha/beta subunit

Chain I:



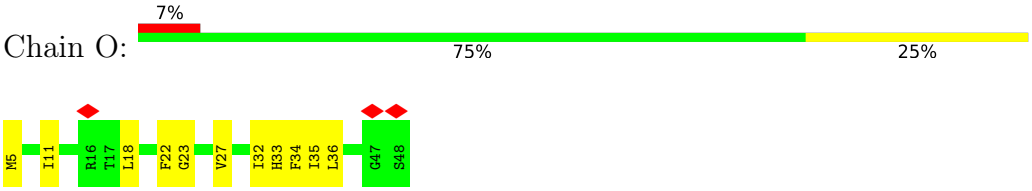
• Molecule 5: Antenna complex alpha/beta subunit

Chain K:



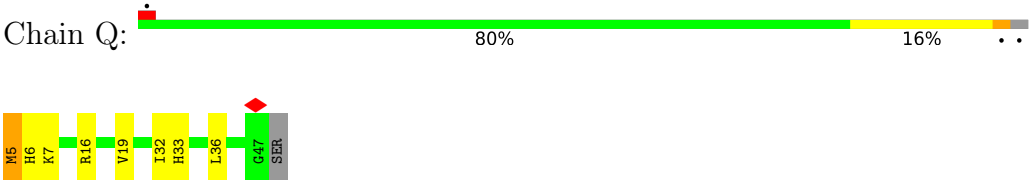
• Molecule 5: Antenna complex alpha/beta subunit

Chain O:



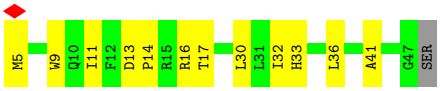
• Molecule 5: Antenna complex alpha/beta subunit

Chain Q:



• Molecule 5: Antenna complex alpha/beta subunit

Chain 1:

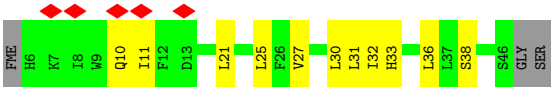


• Molecule 5: Antenna complex alpha/beta subunit

Chain 5:

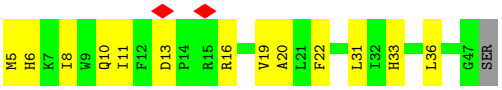
• Molecule 5: Antenna complex alpha/beta subunit

Chain 7:



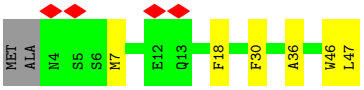
• Molecule 5: Antenna complex alpha/beta subunit

Chain 9:



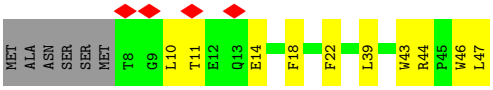
• Molecule 6: Antenna complex alpha/beta subunit

Chain B:



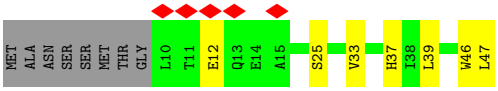
• Molecule 6: Antenna complex alpha/beta subunit

Chain J:



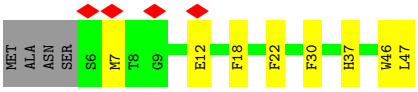
• Molecule 6: Antenna complex alpha/beta subunit

Chain N:



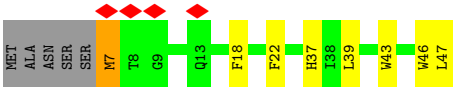
• Molecule 6: Antenna complex alpha/beta subunit

Chain P:



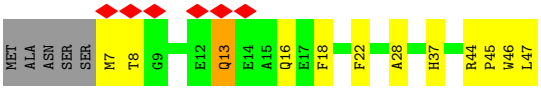
• Molecule 6: Antenna complex alpha/beta subunit

Chain R:



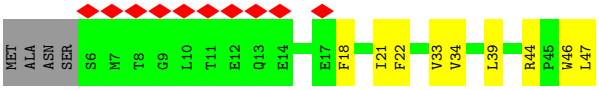
• Molecule 6: Antenna complex alpha/beta subunit

Chain 2:



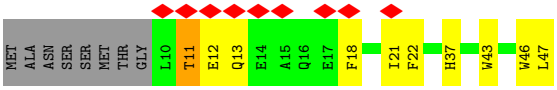
• Molecule 6: Antenna complex alpha/beta subunit

Chain 4:



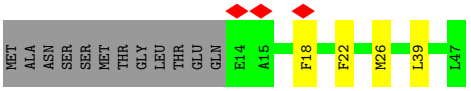
• Molecule 6: Antenna complex alpha/beta subunit

Chain 6:



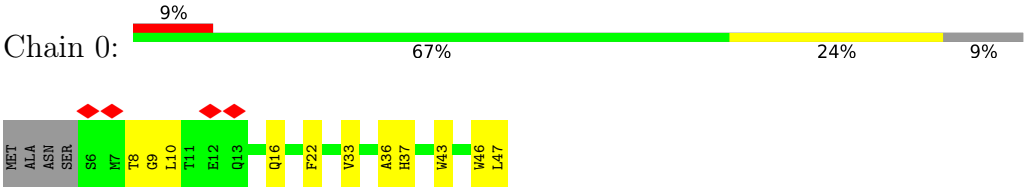
• Molecule 6: Antenna complex alpha/beta subunit

Chain 8:



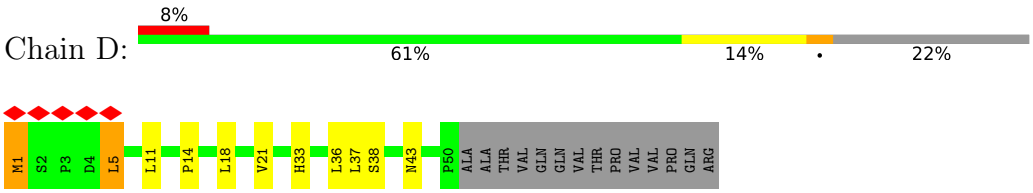
• Molecule 6: Antenna complex alpha/beta subunit

Chain 0:



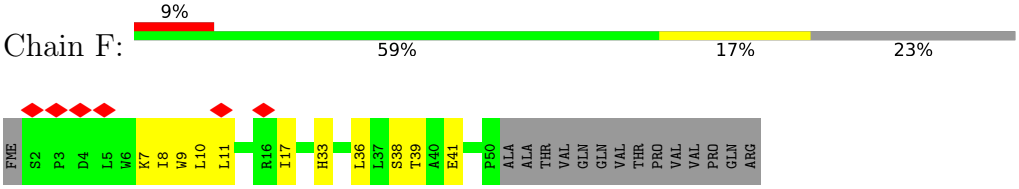
• Molecule 7: Antenna complex alpha/beta subunit

Chain D:



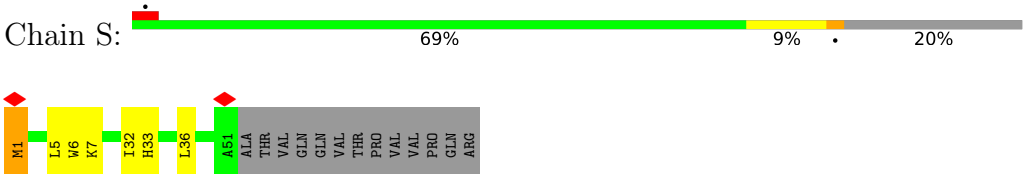
• Molecule 7: Antenna complex alpha/beta subunit

Chain F:



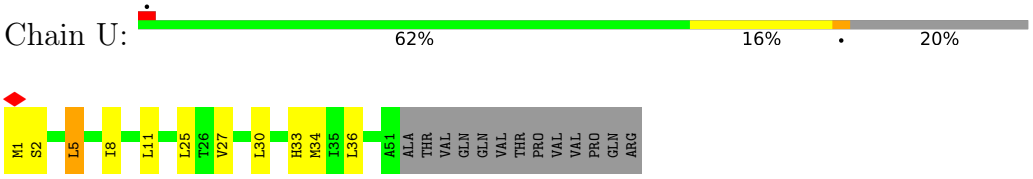
• Molecule 7: Antenna complex alpha/beta subunit

Chain S:



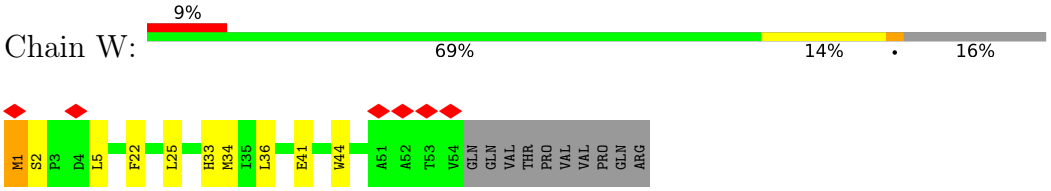
• Molecule 7: Antenna complex alpha/beta subunit

Chain U:



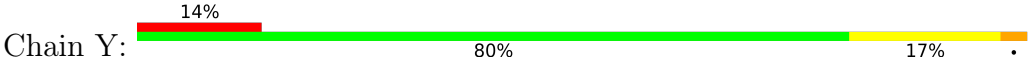
• Molecule 7: Antenna complex alpha/beta subunit

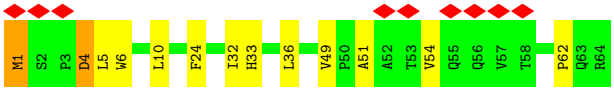
Chain W:



• Molecule 7: Antenna complex alpha/beta subunit

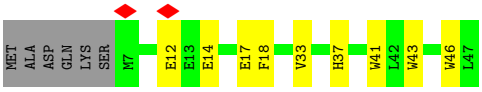
Chain Y:





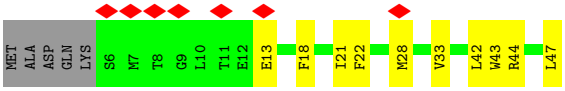
• Molecule 8: Antenna complex alpha/beta subunit

Chain E:



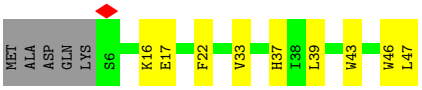
• Molecule 8: Antenna complex alpha/beta subunit

Chain G:



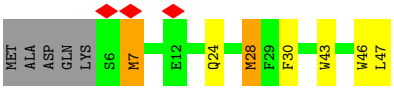
• Molecule 8: Antenna complex alpha/beta subunit

Chain T:



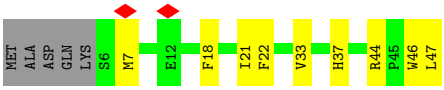
• Molecule 8: Antenna complex alpha/beta subunit

Chain V:



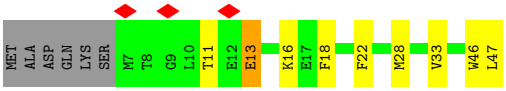
• Molecule 8: Antenna complex alpha/beta subunit

Chain X:



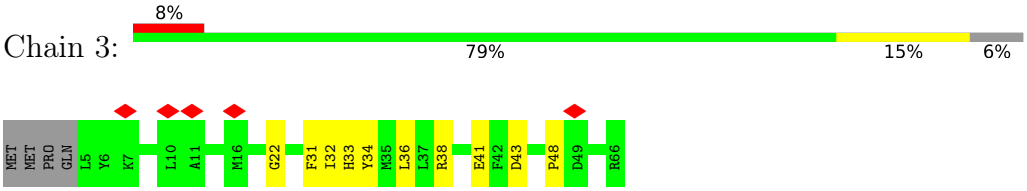
• Molecule 8: Antenna complex alpha/beta subunit

Chain Z:



• Molecule 9: Antenna complex alpha/beta subunit

Chain 3:


8%
79%
15%
6%
MET
MET
PRO
GLN
L5
Y6
K7
L10
A11
M16
G22
F31
I32
H33
Y34
M35
L36
L37
R38
E41
F42
D43
P48
D49
R66

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219233	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.244	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	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: UQ8, LMT, FME, PLM, CA, CDL, HEM, LDA, BPH, PGV, FE, BCL, MG, CRT, Z41, MQ8

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	0.32	0/2502	0.47	0/3426
2	L	0.30	0/2295	0.44	0/3135
3	M	0.31	0/2632	0.43	0/3601
4	H	0.27	0/2039	0.48	0/2776
5	1	0.27	0/362	0.41	0/492
5	5	0.26	0/358	0.41	0/488
5	7	0.26	0/354	0.43	0/483
5	9	0.26	0/362	0.40	0/492
5	A	0.27	0/362	0.42	0/492
5	I	0.26	0/362	0.40	0/492
5	K	0.26	0/369	0.41	0/500
5	O	0.26	0/369	0.42	0/500
5	Q	0.28	0/362	0.40	0/492
6	0	0.24	0/357	0.37	0/485
6	2	0.24	0/351	0.36	0/477
6	4	0.24	0/357	0.37	0/485
6	6	0.24	0/332	0.35	0/452
6	8	0.25	0/299	0.36	0/407
6	B	0.25	0/371	0.38	0/504
6	J	0.24	0/343	0.38	0/467
6	N	0.24	0/332	0.36	0/452
6	P	0.24	0/357	0.38	0/485
6	R	0.24	0/351	0.37	0/477
7	D	0.24	0/409	0.42	0/561
7	F	0.24	0/409	0.43	0/561
7	S	0.25	0/414	0.41	0/568
7	U	0.25	0/414	0.42	0/568
7	W	0.25	0/433	0.42	0/595
7	Y	0.25	0/515	0.48	0/709
8	E	0.25	0/355	0.38	0/480
8	G	0.24	0/361	0.38	0/488
8	T	0.25	0/361	0.39	0/488

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
8	V	0.25	0/361	0.38	0/488
8	X	0.24	0/361	0.37	0/488
8	Z	0.24	0/355	0.38	0/480
9	3	0.28	0/506	0.43	0/688
All	All	0.28	0/21432	0.42	0/29222

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2328	54	0
2	L	2210	0	2166	49	0
3	M	2533	0	2490	47	0
4	H	1993	0	1994	43	0
5	1	359	0	371	10	0
5	5	355	0	360	7	0
5	7	341	0	346	14	0
5	9	359	0	371	10	0
5	A	359	0	371	8	0
5	I	359	0	371	7	0
5	K	366	0	376	12	0
5	O	366	0	376	10	0
5	Q	359	0	371	10	0
6	0	345	0	334	11	0
6	2	339	0	329	13	0
6	4	345	0	334	10	0
6	6	320	0	310	9	0
6	8	287	0	278	6	0
6	B	359	0	345	7	0
6	J	331	0	320	11	0
6	N	320	0	310	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	345	0	334	6	0
6	R	339	0	329	9	0
7	D	407	0	424	10	0
7	F	397	0	413	9	0
7	S	412	0	429	7	0
7	U	412	0	429	11	0
7	W	431	0	450	11	0
7	Y	511	0	535	11	0
8	E	343	0	336	12	0
8	G	349	0	341	10	0
8	T	349	0	341	12	0
8	V	349	0	341	10	0
8	X	349	0	341	11	0
8	Z	343	0	336	10	0
9	3	489	0	497	10	0
10	C	172	0	120	23	0
11	C	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
12	F	1	0	0	0	0
12	M	1	0	0	0	0
12	S	1	0	0	0	0
12	U	1	0	0	0	0
12	W	1	0	0	0	0
12	Y	1	0	0	0	0
13	C	35	0	0	0	0
14	C	12	0	18	3	0
15	1	27	0	25	3	0
15	C	31	0	32	2	0
15	D	39	0	51	4	0
15	F	36	0	42	3	0
15	H	36	0	42	3	0
15	L	97	0	104	11	0
15	M	64	0	74	3	0
16	0	66	0	74	8	0
16	1	66	0	74	3	0
16	2	66	0	74	10	0
16	3	66	0	74	7	0
16	4	66	0	74	6	0
16	5	66	0	74	8	0
16	6	66	0	74	6	0
16	7	61	0	61	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	8	66	0	74	4	0
16	9	66	0	74	5	0
16	A	66	0	74	2	0
16	B	66	0	74	8	0
16	D	66	0	74	5	0
16	E	66	0	74	7	0
16	F	66	0	74	1	0
16	G	66	0	74	5	0
16	I	66	0	74	6	0
16	J	66	0	74	5	0
16	K	66	0	74	8	0
16	L	132	0	148	10	0
16	M	132	0	148	8	0
16	N	66	0	74	8	0
16	O	66	0	74	4	0
16	P	66	0	74	7	0
16	Q	66	0	74	5	0
16	R	66	0	74	7	0
16	S	66	0	74	7	0
16	T	66	0	74	10	0
16	U	66	0	74	6	0
16	V	66	0	74	8	0
16	W	66	0	74	3	0
16	X	66	0	74	7	0
16	Y	66	0	74	3	0
16	Z	66	0	74	8	0
17	L	65	0	76	5	0
17	M	65	0	76	7	0
18	L	139	0	187	25	0
19	M	1	0	0	0	0
20	M	53	0	72	3	0
21	0	44	0	60	5	0
21	2	44	0	60	8	0
21	4	44	0	60	12	0
21	7	44	0	60	11	0
21	8	44	0	60	7	0
21	B	44	0	60	5	0
21	E	44	0	60	4	0
21	G	44	0	60	7	0
21	K	44	0	60	10	0
21	M	44	0	60	5	0
21	N	44	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Q	44	0	60	8	0
21	R	44	0	60	5	0
21	T	44	0	60	8	0
21	V	44	0	60	4	0
21	X	44	0	60	9	0
21	Z	44	0	60	6	0
22	D	58	0	60	3	0
22	H	79	0	105	2	0
22	M	218	0	289	13	0
23	M	16	0	31	0	0
23	O	16	0	31	1	0
24	0	35	0	46	3	0
24	2	70	0	92	4	0
24	4	35	0	46	2	0
24	5	31	0	35	1	0
24	8	35	0	46	4	0
24	B	35	0	46	3	0
24	E	35	0	46	2	0
24	G	70	0	92	6	0
24	H	35	0	46	3	0
24	J	35	0	46	3	0
24	M	35	0	46	2	0
24	P	70	0	92	6	0
24	R	35	0	46	2	0
24	V	35	0	46	2	0
24	X	35	0	46	0	0
24	Z	35	0	46	2	0
25	1	1	0	0	0	0
25	2	1	0	0	0	0
25	3	10	0	0	0	0
25	5	1	0	0	0	0
25	7	1	0	0	0	0
25	9	3	0	0	0	0
25	A	2	0	0	0	0
25	C	134	0	0	1	0
25	D	7	0	0	0	0
25	E	2	0	0	0	0
25	F	3	0	0	0	0
25	H	16	0	0	0	0
25	I	2	0	0	0	0
25	K	1	0	0	0	0
25	L	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	M	73	0	0	2	0
25	Q	3	0	0	0	0
25	R	1	0	0	0	0
25	S	6	0	0	0	0
25	T	4	0	0	0	0
25	U	12	0	0	0	0
25	V	3	0	0	0	0
25	W	6	0	0	0	0
25	X	2	0	0	0	0
25	Y	8	0	0	0	0
25	Z	2	0	0	0	0
All	All	26261	0	26696	617	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 12.

All (617) 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	1.62	1.39
1:C:250:CYS:SG	10:C:403:HEM:HAC	1.60	1.39
1:C:310:CYS:SG	10:C:404:HEM:CAC	2.15	1.34
1:C:155:CYS:SG	10:C:402:HEM:CAC	2.15	1.33
1:C:250:CYS:SG	10:C:403:HEM:CAC	2.19	1.30
1:C:110:CYS:SG	10:C:401:HEM:HAC	1.72	1.28
1:C:310:CYS:SG	10:C:404:HEM:HAC	1.73	1.25
1:C:110:CYS:SG	10:C:401:HEM:CAC	2.24	1.24
1:C:250:CYS:HG	10:C:403:HEM:HAC	0.88	0.96
1:C:155:CYS:HG	10:C:402:HEM:HAC	0.81	0.93
1:C:155:CYS:HG	10:C:402:HEM:CAC	1.70	0.87
6:0:8:THR:HG23	6:0:10:LEU:H	1.45	0.81
1:C:151:THR:HG22	1:C:153:TYR:H	1.48	0.77
14:C:408:PLM:H51	15:L:305:PGV:H42	1.66	0.75
21:N:102:CRT:H35	16:O:502:BCL:HMB2	1.67	0.75
1:C:155:CYS:SG	10:C:402:HEM:C3C	2.80	0.73
1:C:310:CYS:SG	10:C:404:HEM:C3C	2.82	0.73
16:L:307:BCL:HHC	16:M:404:BCL:H42	1.71	0.72
8:V:43:TRP:HB2	24:V:101:LMT:H31	1.72	0.72
4:H:45:ARG:NH1	6:B:7:MET:O	2.22	0.72
1:C:250:CYS:HG	10:C:403:HEM:CAC	1.79	0.72
21:E:103:CRT:H35	16:F:502:BCL:HMB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:203:VAL:HG13	2:L:213:LYS:HB2	1.73	0.71
21:G:103:CRT:H35	16:I:101:BCL:HMB2	1.71	0.70
5:A:31:LEU:HD11	15:D:501:PGV:H201	1.73	0.70
4:H:58:PHE:HB3	22:D:502:CDL:H141	1.72	0.70
24:2:104:LMT:H42	6:4:39:LEU:HB3	1.75	0.69
7:U:2:SER:H	7:U:5:LEU:HD23	1.56	0.69
8:G:47:LEU:HD13	24:G:104:LMT:H32	1.76	0.68
6:2:18:PHE:HA	21:2:103:CRT:H6	1.76	0.68
7:S:33:HIS:CE1	16:T:101:BCL:HMD1	2.30	0.67
7:F:39:THR:HG22	7:F:41:GLU:H	1.59	0.67
4:H:133:ILE:HD12	4:H:180:ARG:HG3	1.76	0.66
7:D:11:LEU:HD11	21:G:103:CRT:H23	1.77	0.66
24:P:103:LMT:H42	6:R:39:LEU:HB3	1.77	0.66
5:9:33:HIS:CE1	16:0:102:BCL:HMD1	2.31	0.66
5:K:33:HIS:CE1	16:N:101:BCL:HMD1	2.31	0.65
5:O:33:HIS:CE1	16:P:102:BCL:HMD1	2.31	0.65
17:M:405:BPH:HBB3	17:M:405:BPH:HHC	1.76	0.65
22:M:411:CDL:H141	22:M:411:CDL:H532	1.77	0.65
5:Q:33:HIS:CE1	16:R:101:BCL:HMD1	2.31	0.65
4:H:137:ARG:NH2	4:H:183:GLU:OE1	2.30	0.65
7:U:33:HIS:CE1	16:V:102:BCL:HMD1	2.31	0.65
7:W:33:HIS:CE1	16:X:102:BCL:HMD1	2.32	0.65
2:L:237:ARG:HH21	3:M:6:ASN:HD22	1.46	0.64
8:G:42:LEU:O	24:G:101:LMT:O3'	2.14	0.64
2:L:23:PHE:HE1	5:9:19:VAL:HG21	1.61	0.64
15:L:306:PGV:H232	15:H:301:PGV:H201	1.78	0.64
5:A:33:HIS:CE1	16:B:102:BCL:HMD1	2.33	0.64
7:D:33:HIS:CE1	16:E:102:BCL:HMD1	2.32	0.64
5:A:11:ILE:HD11	21:E:103:CRT:H23	1.79	0.63
8:X:22:PHE:HA	21:X:103:CRT:H14	1.79	0.63
15:1:401:PGV:H011	15:1:401:PGV:H32	1.80	0.63
16:A:101:BCL:HMB2	21:0:103:CRT:H35	1.81	0.63
7:U:11:LEU:HD12	21:X:103:CRT:H82	1.81	0.63
3:M:98:PRO:HB3	3:M:107:PRO:HG3	1.80	0.63
5:1:13:ASP:HB3	5:1:16:ARG:HG2	1.80	0.63
9:3:33:HIS:CE1	16:4:101:BCL:HMD1	2.34	0.63
5:I:33:HIS:CE1	16:J:101:BCL:HMD1	2.34	0.63
7:Y:33:HIS:CE1	16:Z:102:BCL:HMD1	2.33	0.62
1:C:278:ASP:OD1	1:C:282:ASN:ND2	2.30	0.62
6:N:47:LEU:HD13	24:P:101:LMT:H32	1.81	0.62
8:T:33:VAL:HG11	16:T:101:BCL:HBA2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:33:HIS:CE1	16:2:102:BCL:HMD1	2.34	0.62
9:3:36:LEU:HD11	16:4:101:BCL:HHD	1.80	0.62
1:C:72:VAL:HG13	1:C:76:TYR:HD2	1.65	0.62
15:M:410:PGV:H251	5:O:27:VAL:HG21	1.82	0.61
8:G:43:TRP:HB2	24:G:101:LMT:H52	1.80	0.61
15:L:309:PGV:O14	5:A:15:ARG:NH1	2.32	0.61
21:G:103:CRT:H393	5:I:33:HIS:HB3	1.83	0.61
2:L:97:ILE:HG21	18:L:304:UQ8:H22A	1.83	0.61
4:H:212:ALA:O	4:H:254:ARG:NH2	2.25	0.61
5:Q:7:LYS:NZ	8:T:17:GLU:OE2	2.26	0.61
5:7:33:HIS:CE1	16:8:102:BCL:HMD1	2.36	0.61
5:K:7:LYS:HB3	21:Q:101:CRT:H41	1.81	0.61
5:5:33:HIS:CE1	16:6:101:BCL:HMD1	2.35	0.61
7:F:41:GLU:O	8:G:44:ARG:NH1	2.33	0.61
24:G:104:LMT:H31	6:J:43:TRP:HB2	1.83	0.61
21:T:102:CRT:H35	16:U:101:BCL:HMB2	1.83	0.60
5:I:36:LEU:HD11	16:J:101:BCL:HHD	1.83	0.60
7:Y:1:FME:SD	7:Y:1:FME:N	2.74	0.60
4:H:32:ARG:HG2	4:H:62:ALA:HB2	1.83	0.60
17:M:405:BPH:HBC3	17:M:405:BPH:HHD	1.84	0.60
4:H:78:ALA:HB3	4:H:79:PRO:HD3	1.83	0.60
24:4:103:LMT:H22	6:6:43:TRP:HB2	1.82	0.60
2:L:174:HIS:HB3	3:M:183:LEU:HD13	1.84	0.60
14:C:408:PLM:H32	15:L:305:PGV:H21	1.84	0.59
3:M:28:LEU:HD12	3:M:54:GLY:HA2	1.82	0.59
7:F:33:HIS:CE1	16:G:102:BCL:HMD1	2.37	0.59
1:C:250:CYS:SG	10:C:403:HEM:C3C	2.94	0.59
16:U:101:BCL:H152	8:V:28:MET:HB3	1.84	0.59
7:Y:4:ASP:OD1	7:Y:4:ASP:N	2.35	0.59
7:U:8:ILE:HA	21:X:103:CRT:H83	1.84	0.59
8:V:7:MET:SD	8:V:7:MET:N	2.70	0.59
4:H:67:PHE:HB2	4:H:76:VAL:HG13	1.84	0.59
5:O:36:LEU:HD11	16:P:102:BCL:HHD	1.84	0.59
24:R:103:LMT:H31	8:T:43:TRP:HB2	1.83	0.59
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.84	0.59
16:M:404:BCL:H12	17:M:405:BPH:HBB3	1.84	0.58
6:R:7:MET:SD	6:R:7:MET:N	2.75	0.58
22:H:302:CDL:OA3	22:D:502:CDL:O1	2.20	0.58
5:O:11:ILE:HD11	21:R:102:CRT:H23	1.86	0.58
5:Q:5:FME:O	5:Q:7:LYS:N	2.31	0.58
5:5:22:PHE:HE1	21:7:101:CRT:H182	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:101:CRT:H35	16:7:102:BCL:HMB2	1.84	0.58
5:A:7:LYS:NZ	8:E:17:GLU:OE2	2.26	0.58
1:C:27:PRO:HD3	9:3:38:ARG:HG2	1.85	0.58
17:L:302:BPH:HHC	17:L:302:BPH:HBB3	1.85	0.58
7:D:5:LEU:HD23	8:G:21:ILE:HD11	1.86	0.58
2:L:8:ARG:HG2	4:H:87:ILE:HG21	1.85	0.57
18:L:304:UQ8:H20A	5:7:31:LEU:HA	1.86	0.57
3:M:233:ARG:NH1	4:H:236:GLU:OE1	2.37	0.57
21:Z:103:CRT:H36	5:1:30:LEU:HD23	1.86	0.57
5:5:36:LEU:HD11	16:6:101:BCL:HHD	1.86	0.57
21:B:103:CRT:H23	5:9:11:ILE:HD11	1.87	0.57
4:H:13:GLN:NE2	15:H:301:PGV:O13	2.38	0.57
2:L:13:ARG:HH11	2:L:13:ARG:HB2	1.70	0.56
6:6:37:HIS:HB3	16:6:101:BCL:H92	1.86	0.56
5:7:36:LEU:HD11	16:8:102:BCL:HHD	1.88	0.56
1:C:129:ARG:NH1	1:C:132:GLU:OE1	2.38	0.56
7:F:36:LEU:HD11	16:G:102:BCL:HHD	1.88	0.56
24:P:101:LMT:H5B	24:P:101:LMT:H6E	1.87	0.56
4:H:159:LEU:HD22	4:H:215:LYS:HG2	1.87	0.56
5:Q:36:LEU:HD11	16:R:101:BCL:HHD	1.88	0.56
7:F:38:SER:OG	15:F:501:PGV:O04	2.21	0.56
15:M:410:PGV:H201	5:O:23:GLY:HA3	1.86	0.56
24:G:104:LMT:H42	6:J:39:LEU:HB3	1.88	0.55
5:1:11:ILE:HD11	21:4:102:CRT:H23	1.88	0.55
15:L:305:PGV:H22	15:1:401:PGV:H202	1.87	0.55
4:H:1:FME:HB2	24:H:303:LMT:H21	1.89	0.55
1:C:25:ARG:NH2	9:3:43:ASP:OD2	2.40	0.55
6:P:47:LEU:HD13	24:P:103:LMT:H32	1.88	0.55
2:L:179:HIS:CE1	2:L:183:ILE:HD11	2.42	0.55
24:P:103:LMT:H31	6:R:43:TRP:HB2	1.88	0.55
6:B:18:PHE:HB2	21:B:103:CRT:H21A	1.87	0.55
1:C:246:ASN:HA	2:L:171:LEU:HD21	1.90	0.54
22:M:412:CDL:H801	22:M:412:CDL:H561	1.89	0.54
8:G:18:PHE:HA	21:G:103:CRT:H6	1.88	0.54
24:R:103:LMT:H52	8:T:39:LEU:HB3	1.90	0.54
5:1:36:LEU:HD11	16:2:102:BCL:HHD	1.90	0.54
7:Y:10:LEU:HB2	21:2:103:CRT:H1M1	1.89	0.54
8:E:18:PHE:HB2	21:E:103:CRT:H21A	1.89	0.54
3:M:61:ILE:HG23	17:M:405:BPH:H121	1.89	0.54
3:M:206:ILE:HD13	16:M:403:BCL:HMD1	1.89	0.54
16:Y:101:BCL:H3C	24:Z:101:LMT:H62	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:38:SER:O	15:D:501:PGV:O06	2.25	0.54
21:4:102:CRT:H371	16:5:102:BCL:HMB2	1.88	0.54
1:C:32:GLN:HB2	2:L:77:LEU:HD12	1.90	0.53
8:G:18:PHE:HB2	21:G:103:CRT:H21A	1.90	0.53
24:2:101:LMT:H5B	24:2:101:LMT:H6E	1.90	0.53
6:6:18:PHE:HB2	21:7:101:CRT:H21A	1.89	0.53
5:7:25:LEU:HB2	16:7:102:BCL:H43	1.90	0.53
3:M:13:VAL:HG12	4:H:144:ILE:HD13	1.90	0.53
7:F:7:LYS:HA	7:F:10:LEU:HD13	1.90	0.53
7:W:41:GLU:O	8:X:44:ARG:NH1	2.40	0.53
16:6:101:BCL:H172	24:8:101:LMT:H41	1.91	0.53
1:C:205:ASP:OD1	1:C:281:GLN:NE2	2.42	0.53
21:K:101:CRT:H35	16:K:102:BCL:HMB2	1.89	0.53
7:Y:1:FME:HG2	6:2:28:ALA:HB2	1.91	0.53
3:M:157:TYR:CZ	21:M:407:CRT:H293	2.43	0.53
7:W:36:LEU:HD11	16:X:102:BCL:HHD	1.90	0.53
7:W:2:SER:HB3	7:W:5:LEU:HG	1.91	0.53
21:K:101:CRT:H342	16:K:102:BCL:HBA2	1.91	0.53
21:Z:103:CRT:H372	5:1:33:HIS:CG	2.44	0.53
5:5:18:LEU:HD21	21:7:101:CRT:H132	1.90	0.53
5:I:41:ALA:O	6:J:44:ARG:NH1	2.39	0.52
3:M:10:THR:HG21	4:H:202:PHE:HB2	1.91	0.52
8:Z:18:PHE:HA	21:Z:103:CRT:H6	1.92	0.52
21:Q:101:CRT:H35	16:Q:102:BCL:HMB2	1.91	0.52
6:8:22:PHE:CD1	21:8:103:CRT:H14	2.45	0.52
22:H:302:CDL:H862	22:H:302:CDL:H592	1.91	0.52
5:7:10:GLN:HB2	21:0:103:CRT:H1M1	1.91	0.52
1:C:167:VAL:HG22	7:Y:62:PRO:HD2	1.91	0.52
2:L:32:VAL:HG23	2:L:33:GLY:H	1.75	0.52
6:0:36:ALA:HB1	24:0:101:LMT:H101	1.92	0.52
4:H:41:LEU:HD12	4:H:55:VAL:HG12	1.91	0.52
7:W:22:PHE:HE1	21:X:103:CRT:H182	1.75	0.52
1:C:236:MET:HB3	10:C:403:HEM:C4B	2.45	0.52
1:C:25:ARG:HD3	15:C:409:PGV:H31	1.92	0.51
24:2:104:LMT:H61	16:3:101:BCL:H3C	1.91	0.51
21:4:102:CRT:H291	21:4:102:CRT:H32	1.93	0.51
2:L:13:ARG:NH1	2:L:21:ASP:OD1	2.43	0.51
15:L:309:PGV:H41	5:A:20:ALA:HB2	1.93	0.51
8:Z:11:THR:OG1	8:Z:13:GLU:OE1	2.24	0.51
4:H:141:ASP:OD1	4:H:141:ASP:N	2.38	0.51
6:0:43:TRP:HB2	24:0:101:LMT:H22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:37:LEU:O	7:D:43:ASN:ND2	2.40	0.51
7:S:1:FME:O	8:V:24:GLN:NE2	2.44	0.51
1:C:110:CYS:HB2	10:C:401:HEM:C3C	2.45	0.51
21:B:103:CRT:H35	16:D:503:BCL:HMB2	1.93	0.51
4:H:64:PRO:HA	4:H:79:PRO:HD2	1.92	0.51
7:W:1:FME:HB3	8:Z:28:MET:HE1	1.92	0.51
6:4:21:ILE:HD11	21:4:102:CRT:H6	1.93	0.51
6:4:21:ILE:HG13	21:4:102:CRT:H9	1.92	0.51
1:C:184:ASN:ND2	3:M:96:GLU:HG2	2.26	0.50
1:C:288:ASN:O	1:C:296:LYS:NZ	2.41	0.50
17:L:302:BPH:HHC	17:L:302:BPH:CBB	2.40	0.50
5:Q:5:FME:C	5:Q:7:LYS:H	2.23	0.50
8:X:21:ILE:HD12	21:X:103:CRT:H6	1.92	0.50
2:L:83:MET:HB3	5:7:38:SER:HB3	1.93	0.50
3:M:148:TRP:HE1	22:M:411:CDL:H361	1.76	0.50
22:M:411:CDL:H801	4:H:21:PHE:HB3	1.94	0.50
16:2:102:BCL:H203	16:2:102:BCL:H13	1.93	0.50
5:O:22:PHE:HE1	21:Q:101:CRT:H182	1.77	0.50
1:C:48:LEU:HD21	15:C:409:PGV:H05	1.94	0.50
2:L:207:GLN:HB2	2:L:210:GLU:HG3	1.93	0.50
21:R:102:CRT:H372	7:S:33:HIS:CG	2.46	0.50
4:H:11:VAL:HG21	24:H:303:LMT:H32	1.94	0.50
1:C:45:ASN:HB3	1:C:48:LEU:HB2	1.94	0.50
3:M:65:PHE:HD1	17:M:405:BPH:H112	1.77	0.49
5:K:36:LEU:HD11	16:N:101:BCL:HHD	1.94	0.49
1:C:184:ASN:HD21	3:M:96:GLU:HG2	1.76	0.49
3:M:131:VAL:HG21	15:M:410:PGV:H212	1.94	0.49
22:M:411:CDL:H672	24:H:303:LMT:H123	1.94	0.49
7:D:36:LEU:HD11	16:E:102:BCL:HHD	1.94	0.49
4:H:215:LYS:NZ	4:H:250:ALA:O	2.45	0.49
8:T:22:PHE:HA	21:T:102:CRT:H14	1.94	0.49
3:M:65:PHE:CD1	17:M:405:BPH:H112	2.47	0.49
1:C:151:THR:HG22	1:C:153:TYR:N	2.23	0.49
18:L:304:UQ8:H23	5:7:27:VAL:HG13	1.94	0.49
8:E:33:VAL:HG11	16:E:102:BCL:HAA1	1.95	0.49
6:R:46:TRP:CD1	6:R:47:LEU:HG	2.46	0.49
4:H:36:ARG:HG2	4:H:79:PRO:HG3	1.94	0.49
7:S:7:LYS:HB3	21:V:103:CRT:H23	1.95	0.49
2:L:108:LEU:HD11	22:M:412:CDL:H602	1.95	0.49
3:M:289:THR:HB	24:M:414:LMT:H11	1.95	0.49
4:H:197:ILE:HD11	4:H:202:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:22:PHE:HA	21:2:103:CRT:H11	1.93	0.49
2:L:136:VAL:HA	2:L:140:VAL:HB	1.95	0.49
2:L:187:PHE:HB3	17:M:405:BPH:HBB2	1.93	0.49
5:K:10:GLN:HE21	6:N:12:GLU:HG2	1.78	0.49
7:U:36:LEU:HD11	16:V:102:BCL:HHD	1.94	0.49
2:L:104:VAL:HG22	22:M:412:CDL:H821	1.93	0.49
6:B:46:TRP:CD1	6:B:47:LEU:HG	2.48	0.49
1:C:292:PRO:HD2	1:C:295:ARG:HG2	1.95	0.48
6:B:46:TRP:CE2	16:B:102:BCL:H2C	2.48	0.48
6:P:30:PHE:CE1	16:P:102:BCL:H11	2.48	0.48
9:3:31:PHE:HE2	21:4:102:CRT:H2M2	1.77	0.48
1:C:162:PRO:HD2	10:C:402:HEM:HBD2	1.94	0.48
3:M:52:TYR:O	3:M:132:ARG:NH1	2.41	0.48
2:L:25:PHE:CE1	2:L:32:VAL:HG21	2.48	0.48
22:M:411:CDL:H371	22:M:411:CDL:H121	1.95	0.48
1:C:110:CYS:CB	10:C:401:HEM:HAC	2.40	0.48
15:L:306:PGV:H202	15:H:301:PGV:H062	1.95	0.48
7:F:9:TRP:HZ3	7:F:17:ILE:HG21	1.78	0.48
6:2:18:PHE:HB2	21:2:103:CRT:H21A	1.94	0.48
16:L:301:BCL:H2	17:L:302:BPH:HBB3	1.96	0.48
4:H:52:ARG:NH2	8:E:14:GLU:OE1	2.47	0.48
6:J:11:THR:N	6:J:14:GLU:OE2	2.44	0.48
8:T:33:VAL:HG11	16:T:101:BCL:CBA	2.44	0.48
6:4:18:PHE:HB2	21:4:102:CRT:H21A	1.95	0.48
1:C:144:HIS:HE1	10:C:404:HEM:C1C	2.32	0.48
16:L:307:BCL:CHC	16:M:404:BCL:H42	2.43	0.48
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.49	0.48
16:1:402:BCL:HMD1	6:2:37:HIS:CE1	2.48	0.48
21:2:103:CRT:H35	16:3:101:BCL:HMB2	1.95	0.48
6:P:18:PHE:HB2	21:Q:101:CRT:H32A	1.96	0.48
16:9:101:BCL:HMD1	6:0:37:HIS:CE1	2.48	0.48
8:G:22:PHE:CD2	21:G:103:CRT:H14	2.49	0.48
16:R:101:BCL:H41	16:R:101:BCL:H61	1.54	0.48
3:M:229:PHE:HE1	4:H:244:ALA:HB2	1.79	0.47
18:L:303:UQ8:H22	18:L:303:UQ8:H25	1.62	0.47
18:L:308:UQ8:H41A	7:U:27:VAL:HG12	1.96	0.47
8:E:43:TRP:O	24:E:101:LMT:O3'	2.31	0.47
2:L:247:VAL:HG21	17:L:302:BPH:HBC3	1.96	0.47
16:2:102:BCL:H162	24:2:104:LMT:H41	1.96	0.47
5:9:13:ASP:OD2	5:9:16:ARG:HG3	2.15	0.47
1:C:100:TRP:CD1	1:C:153:TYR:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:46:TRP:CE2	16:T:101:BCL:H2C	2.50	0.47
16:Y:101:BCL:H112	16:Y:101:BCL:H72	1.49	0.47
6:8:22:PHE:CE1	21:8:103:CRT:H16	2.49	0.47
16:8:102:BCL:HBB2	24:0:101:LMT:H111	1.95	0.47
4:H:9:MET:HA	4:H:13:GLN:OE1	2.14	0.47
21:T:102:CRT:H392	7:U:33:HIS:HB2	1.96	0.47
8:X:18:PHE:HB2	21:X:103:CRT:H21A	1.96	0.47
4:H:2:SER:H	5:I:38:SER:HB2	1.80	0.47
7:W:25:LEU:HB2	16:W:101:BCL:H43	1.97	0.47
6:6:46:TRP:HZ2	16:6:101:BCL:H91	1.78	0.47
16:I:101:BCL:H141	16:I:101:BCL:H161	1.75	0.47
16:T:101:BCL:HBA1	16:T:101:BCL:H3A	1.50	0.47
7:U:25:LEU:HB2	16:U:101:BCL:H43	1.96	0.47
9:3:41:GLU:O	6:4:44:ARG:NH1	2.46	0.47
3:M:243:THR:HB	4:H:117:PRO:HD2	1.96	0.47
4:H:100:PHE:HB2	4:H:111:PHE:CZ	2.50	0.47
5:9:36:LEU:HD11	16:0:102:BCL:HHD	1.96	0.47
1:C:115:ASN:ND2	1:C:118:SER:HB2	2.30	0.46
2:L:119:ILE:HG22	3:M:229:PHE:HE2	1.80	0.46
18:L:304:UQ8:H40A	5:9:22:PHE:HB3	1.97	0.46
21:M:407:CRT:H2M3	5:O:35:ILE:HG12	1.97	0.46
8:V:30:PHE:CE1	16:V:102:BCL:H11	2.51	0.46
6:2:46:TRP:CD2	16:2:102:BCL:H2C	2.50	0.46
6:4:34:VAL:HG22	16:4:101:BCL:H62	1.97	0.46
6:6:47:LEU:HD13	24:8:101:LMT:H51	1.96	0.46
2:L:12:VAL:O	2:L:116:LYS:NZ	2.40	0.46
4:H:94:PRO:HB2	6:0:9:GLY:HA3	1.97	0.46
5:I:32:ILE:HD12	16:J:101:BCL:O1D	2.15	0.46
7:Y:36:LEU:HD11	16:Z:102:BCL:HHD	1.97	0.46
6:4:21:ILE:HD11	21:4:102:CRT:C6	2.45	0.46
6:4:46:TRP:CD1	6:4:47:LEU:HG	2.51	0.46
5:9:10:GLN:HA	6:0:8:THR:HG21	1.97	0.46
5:A:36:LEU:HD11	16:B:102:BCL:HHD	1.97	0.46
7:Y:49:VAL:HA	7:Y:51:ALA:H	1.80	0.46
16:0:102:BCL:H3A	16:0:102:BCL:H43	1.97	0.46
1:C:110:CYS:SG	10:C:401:HEM:CBC	2.96	0.46
18:L:308:UQ8:H33	7:W:34:MET:SD	2.55	0.46
5:I:14:PRO:HB3	6:J:18:PHE:CZ	2.51	0.46
8:V:46:TRP:CE2	16:V:102:BCL:H2C	2.51	0.46
5:K:11:ILE:HD13	21:Q:101:CRT:H1M1	1.96	0.46
8:X:37:HIS:CG	16:X:102:BCL:H91	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:101:BCL:H192	16:4:101:BCL:H161	1.74	0.46
18:L:303:UQ8:H16	18:L:303:UQ8:H12	1.66	0.46
15:L:309:PGV:H241	5:9:20:ALA:HB2	1.98	0.46
3:M:89:HIS:O	3:M:93:LEU:HG	2.16	0.46
6:6:22:PHE:HA	21:7:101:CRT:H14	1.98	0.46
7:D:18:LEU:HA	7:D:21:VAL:HG12	1.98	0.46
5:7:32:ILE:HD12	16:8:102:BCL:O1D	2.15	0.46
21:7:101:CRT:H392	16:7:102:BCL:HBB2	1.98	0.46
6:8:18:PHE:CE1	21:8:103:CRT:H9	2.51	0.46
18:L:304:UQ8:H17A	5:7:30:LEU:HD13	1.98	0.46
16:G:102:BCL:H192	16:G:102:BCL:H161	1.72	0.46
6:N:33:VAL:HG11	16:N:101:BCL:HAA1	1.98	0.46
5:O:34:PHE:HD1	23:O:501:LDA:H111	1.80	0.46
8:T:46:TRP:CD2	16:T:101:BCL:H2C	2.51	0.46
6:0:22:PHE:CD1	21:0:103:CRT:H14	2.51	0.46
1:C:173:ASN:O	3:M:80:ASP:HB2	2.15	0.45
4:H:55:VAL:HG13	22:D:502:CDL:HA21	1.98	0.45
21:B:103:CRT:H372	7:D:33:HIS:CG	2.51	0.45
16:D:503:BCL:HBC2	8:E:43:TRP:CZ3	2.51	0.45
16:N:101:BCL:H91	16:N:101:BCL:H111	1.73	0.45
4:H:247:LYS:HE2	4:H:247:LYS:HA	1.97	0.45
7:S:6:TRP:CD2	8:T:16:LYS:HG2	2.51	0.45
16:3:101:BCL:H62	16:3:101:BCL:H41	1.50	0.45
1:C:183:GLN:HB3	1:C:196:PRO:HA	1.98	0.45
16:L:307:BCL:H201	18:L:308:UQ8:H13	1.98	0.45
18:L:308:UQ8:H17	18:L:308:UQ8:H20	1.75	0.45
16:A:101:BCL:H61	16:A:101:BCL:H102	1.40	0.45
5:K:5:FME:HE3	16:O:502:BCL:H161	1.98	0.45
16:K:102:BCL:H102	16:K:102:BCL:H61	1.48	0.45
16:Z:102:BCL:O2A	16:Z:102:BCL:H3A	2.15	0.45
6:8:39:LEU:HB3	24:8:101:LMT:H42	1.98	0.45
15:L:305:PGV:H211	15:1:401:PGV:H71	1.99	0.45
16:G:102:BCL:H161	16:G:102:BCL:H143	1.74	0.45
7:U:30:LEU:O	7:U:34:MET:HG2	2.17	0.45
16:V:102:BCL:H93	16:V:102:BCL:H62	1.78	0.45
21:2:103:CRT:H10	21:2:103:CRT:H81	1.85	0.45
6:J:22:PHE:CD2	21:K:101:CRT:H14	2.52	0.45
16:S:101:BCL:H8	16:S:101:BCL:H122	1.73	0.45
8:V:46:TRP:CD1	8:V:47:LEU:HG	2.52	0.45
21:Z:103:CRT:H20	21:Z:103:CRT:H181	1.86	0.45
6:2:7:MET:SD	6:2:8:THR:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:26:TRP:HZ3	4:H:99:PRO:HB3	1.81	0.45
5:5:18:LEU:HD23	16:5:102:BCL:H203	1.99	0.45
6:0:33:VAL:HG11	16:0:102:BCL:HBA2	1.98	0.45
16:B:102:BCL:H141	16:B:102:BCL:H161	1.79	0.45
6:R:47:LEU:HD12	16:R:101:BCL:H162	1.99	0.45
21:T:102:CRT:H372	7:U:33:HIS:CG	2.51	0.45
8:X:21:ILE:HB	21:X:103:CRT:H9	1.97	0.45
2:L:202:SER:HA	3:M:143:SER:HB2	1.99	0.45
16:L:307:BCL:H91	16:L:307:BCL:H111	1.83	0.45
16:M:403:BCL:H61	20:M:406:MQ8:H243	1.99	0.45
6:J:46:TRP:CD2	16:J:101:BCL:H2C	2.52	0.45
21:Q:101:CRT:H10	21:Q:101:CRT:H81	1.82	0.45
6:J:47:LEU:O	24:J:102:LMT:O3'	2.33	0.45
16:L:307:BCL:H201	18:L:308:UQ8:H15	1.98	0.45
3:M:284:ILE:HD13	3:M:284:ILE:HA	1.82	0.45
7:F:8:ILE:HD12	7:F:11:LEU:HD11	2.00	0.45
16:I:101:BCL:H62	16:I:101:BCL:H41	1.57	0.45
16:S:101:BCL:H61	16:S:101:BCL:H41	1.54	0.45
6:2:45:PRO:O	9:3:48:PRO:HG3	2.17	0.45
2:L:106:TRP:HH2	20:M:406:MQ8:H301	1.82	0.44
18:L:308:UQ8:H27	18:L:308:UQ8:H30	1.75	0.44
21:B:103:CRT:H20	21:B:103:CRT:H181	1.88	0.44
21:V:103:CRT:H35	16:W:101:BCL:HMB2	1.99	0.44
21:X:103:CRT:H20	21:X:103:CRT:H181	1.85	0.44
9:3:32:ILE:HD12	16:4:101:BCL:O1D	2.17	0.44
16:5:102:BCL:HBC3	16:5:102:BCL:H2C	1.81	0.44
1:C:110:CYS:CB	10:C:401:HEM:CAC	2.95	0.44
3:M:80:ASP:OD1	25:M:502:HOH:O	2.20	0.44
7:D:14:PRO:HB3	8:E:18:PHE:CZ	2.53	0.44
6:J:10:LEU:HG	6:J:14:GLU:HG2	1.98	0.44
8:X:33:VAL:HG11	16:X:102:BCL:HAA1	1.99	0.44
8:Z:22:PHE:HA	21:Z:103:CRT:H14	1.98	0.44
8:X:46:TRP:CE2	16:X:102:BCL:H2C	2.52	0.44
16:U:101:BCL:H2	16:U:101:BCL:H61	1.73	0.44
8:Z:46:TRP:CD2	16:Z:102:BCL:H2C	2.51	0.44
16:5:102:BCL:H93	16:5:102:BCL:H61	1.72	0.44
16:Q:102:BCL:H172	16:Q:102:BCL:H111	1.98	0.44
16:1:402:BCL:H152	16:1:402:BCL:H18	1.53	0.44
16:2:102:BCL:H62	16:2:102:BCL:H41	1.72	0.44
18:L:304:UQ8:H45B	5:7:21:LEU:HD23	1.98	0.44
16:M:403:BCL:HBB2	16:M:403:BCL:HMB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:102:BCL:H93	16:B:102:BCL:H61	1.69	0.44
6:2:46:TRP:CE2	16:2:102:BCL:H2C	2.53	0.44
21:2:103:CRT:H26	21:2:103:CRT:H241	1.86	0.44
16:0:102:BCL:H93	16:0:102:BCL:H61	1.69	0.44
2:L:186:PHE:CD2	2:L:246:ALA:HB1	2.53	0.44
7:Y:6:TRP:CD2	8:Z:16:LYS:HG2	2.53	0.44
7:Y:32:ILE:HD12	16:Z:102:BCL:O1D	2.17	0.44
8:Z:46:TRP:CE2	16:Z:102:BCL:H2C	2.53	0.44
5:7:11:ILE:HG23	21:0:103:CRT:H1M2	2.00	0.44
24:G:104:LMT:H122	16:I:101:BCL:HMA3	2.00	0.44
16:S:101:BCL:HBC3	16:S:101:BCL:H2C	1.87	0.44
21:T:102:CRT:H10	21:T:102:CRT:H81	1.75	0.44
18:L:308:UQ8:H46	18:L:308:UQ8:H42	1.64	0.44
5:K:33:HIS:CD2	21:K:101:CRT:H372	2.53	0.44
6:6:21:ILE:HD12	21:7:101:CRT:H6	2.00	0.44
5:7:33:HIS:CD2	21:7:101:CRT:H372	2.53	0.44
2:L:193:LEU:HD13	3:M:216:PHE:CG	2.53	0.43
2:L:199:LEU:HD22	2:L:222:PHE:CE2	2.53	0.43
18:L:304:UQ8:H32	18:L:304:UQ8:H35	1.67	0.43
16:3:101:BCL:H192	16:3:101:BCL:H161	1.82	0.43
16:9:101:BCL:HBC3	16:9:101:BCL:H2C	1.82	0.43
18:L:304:UQ8:H7A	18:L:304:UQ8:H10	1.52	0.43
16:N:101:BCL:HMB1	24:P:101:LMT:H102	1.99	0.43
8:Z:33:VAL:HG11	16:Z:102:BCL:HAA1	2.00	0.43
16:0:102:BCL:H41	16:0:102:BCL:H62	1.84	0.43
18:L:308:UQ8:H40	18:L:308:UQ8:H37	1.77	0.43
16:D:503:BCL:HMD1	8:E:37:HIS:CE1	2.53	0.43
16:Q:102:BCL:HMD1	6:R:37:HIS:CE1	2.53	0.43
6:2:22:PHE:CD2	21:2:103:CRT:H14	2.53	0.43
3:M:4:TYR:HE1	22:M:409:CDL:HA22	1.82	0.43
16:O:502:BCL:H192	16:O:502:BCL:H162	1.76	0.43
16:Q:102:BCL:H41	16:Q:102:BCL:H61	1.54	0.43
16:2:102:BCL:H91	16:2:102:BCL:H111	1.77	0.43
1:C:191:ALA:O	2:L:266:PRO:HB2	2.18	0.43
8:E:46:TRP:CD2	16:E:102:BCL:H2C	2.54	0.43
21:K:101:CRT:H10	21:K:101:CRT:H81	1.88	0.43
21:T:102:CRT:H20	21:T:102:CRT:H181	1.86	0.43
16:V:102:BCL:HBA2	16:V:102:BCL:HED3	2.00	0.43
5:1:9:TRP:HZ3	5:1:17:THR:HG21	1.83	0.43
21:7:101:CRT:H371	16:7:102:BCL:C2B	2.48	0.43
18:L:308:UQ8:H32	18:L:308:UQ8:H35	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:201:PHE:CZ	4:H:15:THR:HG22	2.54	0.43
5:K:26:PHE:CE1	21:K:101:CRT:H343	2.53	0.43
2:L:42:PHE:HA	18:L:304:UQ8:H30B	2.00	0.43
2:L:48:LEU:HD13	5:9:31:LEU:HD22	2.00	0.43
2:L:113:ILE:HG23	3:M:254:TRP:HE3	1.83	0.43
8:T:47:LEU:HD12	16:T:101:BCL:H161	2.00	0.43
5:Q:32:ILE:HD12	16:R:101:BCL:O1D	2.19	0.43
6:R:18:PHE:HA	21:R:102:CRT:H6	2.01	0.43
16:3:101:BCL:HHD	16:3:101:BCL:HAC2	1.80	0.43
6:J:14:GLU:OE1	6:J:14:GLU:N	2.50	0.43
6:P:22:PHE:HA	21:Q:101:CRT:H14	2.00	0.43
16:S:101:BCL:HAC2	16:S:101:BCL:HHD	1.82	0.43
7:W:41:GLU:HA	7:Y:54:VAL:HG11	2.01	0.43
5:1:14:PRO:HA	5:1:17:THR:HG22	2.01	0.43
5:1:41:ALA:O	6:2:44:ARG:NH1	2.52	0.43
6:6:11:THR:HG22	6:6:12:GLU:H	1.83	0.43
16:7:102:BCL:HMB1	16:7:102:BCL:HBB3	2.01	0.43
3:M:55:PHE:CD1	5:Q:19:VAL:HG21	2.55	0.42
16:K:102:BCL:HMD1	6:N:37:HIS:CE1	2.54	0.42
16:S:101:BCL:H202	16:S:101:BCL:H162	1.79	0.42
8:X:46:TRP:CD1	8:X:47:LEU:HG	2.54	0.42
3:M:240:ASP:OD2	4:H:119:ARG:HB3	2.19	0.42
4:H:213:ALA:HA	4:H:247:LYS:HE3	2.00	0.42
16:S:101:BCL:HMD1	8:T:37:HIS:CE1	2.54	0.42
24:V:101:LMT:O3'	24:V:101:LMT:O2B	2.24	0.42
8:X:47:LEU:HD13	24:Z:101:LMT:H32	2.00	0.42
14:C:408:PLM:H62	2:L:268:TRP:CZ2	2.54	0.42
3:M:53:LEU:O	5:Q:16:ARG:NH1	2.34	0.42
4:H:123:CYS:HA	4:H:232:THR:HA	2.01	0.42
7:W:44:TRP:CD2	16:W:101:BCL:H2C	2.55	0.42
9:3:34:TYR:CE2	9:3:38:ARG:HD2	2.55	0.42
21:4:102:CRT:H36	21:4:102:CRT:H341	1.85	0.42
2:L:117:LEU:O	3:M:247:ARG:NH1	2.51	0.42
4:H:67:PHE:HE2	4:H:78:ALA:HB2	1.84	0.42
8:E:12:GLU:H	8:E:12:GLU:HG3	1.67	0.42
16:I:101:BCL:H192	16:I:101:BCL:H162	1.76	0.42
16:J:101:BCL:H111	16:J:101:BCL:H91	1.65	0.42
5:Q:5:FME:C	5:Q:7:LYS:N	2.82	0.42
16:7:102:BCL:HBC3	16:7:102:BCL:H2C	1.83	0.42
6:0:46:TRP:CE2	16:0:102:BCL:H2C	2.55	0.42
21:M:407:CRT:H10	21:M:407:CRT:H81	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:46:TRP:HZ2	16:X:102:BCL:H13	1.84	0.42
16:1:402:BCL:HAC2	16:1:402:BCL:HHD	1.85	0.42
16:3:101:BCL:HBC3	16:3:101:BCL:H2C	1.79	0.42
21:7:101:CRT:H20	21:7:101:CRT:H181	1.81	0.42
16:9:101:BCL:H8	16:9:101:BCL:H52	1.75	0.42
2:L:135:LEU:HD12	22:M:412:CDL:H861	2.01	0.42
2:L:174:HIS:NE2	16:L:301:BCL:HMC2	2.35	0.42
3:M:72:GLY:HA3	21:M:407:CRT:C6	2.50	0.42
4:H:21:PHE:HE2	15:F:501:PGV:H292	1.83	0.42
6:J:22:PHE:CE2	21:K:101:CRT:H16	2.54	0.42
16:L:307:BCL:H202	16:L:307:BCL:H162	1.76	0.42
7:D:1:FME:HG3	8:G:28:MET:SD	2.59	0.42
8:E:43:TRP:HB2	24:E:101:LMT:H22	2.01	0.42
16:K:102:BCL:H202	16:K:102:BCL:H162	1.88	0.42
21:R:102:CRT:H20	21:R:102:CRT:H181	1.89	0.42
16:7:102:BCL:H71	16:7:102:BCL:H112	1.69	0.42
6:8:18:PHE:HE1	21:8:103:CRT:H9	1.85	0.42
21:8:103:CRT:H292	16:9:101:BCL:H61	2.02	0.42
4:H:13:GLN:NE2	15:F:501:PGV:H211	2.35	0.42
8:E:41:TRP:CZ2	16:E:102:BCL:H18	2.54	0.42
1:C:39:ALA:O	2:L:169:GLN:NE2	2.45	0.42
15:L:306:PGV:H061	7:D:38:SER:HA	2.02	0.42
3:M:42:LYS:NZ	25:M:506:HOH:O	2.44	0.42
21:M:407:CRT:H20	21:M:407:CRT:H181	1.77	0.42
24:J:102:LMT:H122	16:K:102:BCL:HMA3	2.02	0.42
16:P:102:BCL:O2A	16:P:102:BCL:H3A	2.20	0.42
6:R:46:TRP:CE2	16:R:101:BCL:H2C	2.55	0.42
7:S:32:ILE:HD12	16:T:101:BCL:O1D	2.20	0.42
16:X:102:BCL:H161	16:X:102:BCL:H192	1.82	0.42
16:Y:101:BCL:H101	16:Y:101:BCL:H13	1.62	0.42
8:Z:22:PHE:HA	21:Z:103:CRT:H11	2.02	0.42
16:2:102:BCL:H93	16:2:102:BCL:H61	1.67	0.42
2:L:63:GLN:OE1	15:D:501:PGV:H05	2.19	0.42
3:M:34:PRO:HG3	3:M:50:PRO:HD3	2.02	0.42
3:M:286:LEU:HD23	24:M:414:LMT:H52	2.01	0.42
16:D:503:BCL:H162	16:D:503:BCL:H122	1.74	0.42
7:F:7:LYS:HD3	21:K:101:CRT:H31A	2.02	0.42
5:K:33:HIS:CG	21:K:101:CRT:H372	2.55	0.42
16:Z:102:BCL:H141	16:Z:102:BCL:H162	1.68	0.42
21:4:102:CRT:H35	21:4:102:CRT:H31	1.67	0.42
6:8:22:PHE:O	6:8:26:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ALA:HB2	3:M:92:TRP:CD2	2.55	0.41
16:L:307:BCL:HMB1	16:L:307:BCL:HBB2	2.01	0.41
20:M:406:MQ8:H241	20:M:406:MQ8:H261	1.80	0.41
24:B:101:LMT:H62	24:B:101:LMT:H91	1.89	0.41
16:E:102:BCL:H141	16:E:102:BCL:H161	1.79	0.41
6:N:37:HIS:CG	16:N:101:BCL:H92	2.55	0.41
6:N:46:TRP:CE2	16:N:101:BCL:H2C	2.55	0.41
7:S:36:LEU:HD11	16:T:101:BCL:HHD	2.01	0.41
21:T:102:CRT:H15	21:T:102:CRT:H131	1.97	0.41
6:4:22:PHE:HA	21:4:102:CRT:H14	2.01	0.41
24:8:101:LMT:H81	24:8:101:LMT:H52	1.88	0.41
1:C:137:THR:HG23	1:C:275:HIS:CE1	2.55	0.41
18:L:304:UQ8:H42	18:L:304:UQ8:H46	1.72	0.41
3:M:237:GLN:HB2	3:M:262:MET:HG2	2.02	0.41
4:H:116:SER:OG	4:H:237:ASP:HB3	2.20	0.41
4:H:160:ASP:OD1	4:H:160:ASP:N	2.44	0.41
6:B:36:ALA:HB1	24:B:101:LMT:H111	2.02	0.41
16:K:102:BCL:H193	6:N:25:SER:HA	2.01	0.41
16:P:102:BCL:H162	16:P:102:BCL:H192	1.74	0.41
24:4:103:LMT:H1B	24:4:103:LMT:H3'	1.73	0.41
16:5:102:BCL:HAC2	16:5:102:BCL:HHD	1.84	0.41
5:7:33:HIS:CG	21:7:101:CRT:H372	2.54	0.41
21:0:103:CRT:H20	21:0:103:CRT:H181	1.92	0.41
17:L:302:BPH:H6C1	17:L:302:BPH:H102	1.85	0.41
18:L:303:UQ8:H15B	18:L:303:UQ8:H17A	1.95	0.41
6:B:46:TRP:CD2	16:B:102:BCL:H2C	2.55	0.41
5:O:18:LEU:HD12	5:O:18:LEU:HA	1.92	0.41
5:O:32:ILE:HD12	16:P:102:BCL:O1D	2.20	0.41
21:V:103:CRT:H372	7:W:33:HIS:CG	2.55	0.41
21:X:103:CRT:H15	21:X:103:CRT:H131	1.93	0.41
6:4:33:VAL:HG11	16:4:101:BCL:HAA1	2.03	0.41
24:5:101:LMT:H3'	24:5:101:LMT:H1B	1.77	0.41
16:9:101:BCL:H13	16:9:101:BCL:H102	1.72	0.41
16:0:102:BCL:H3A	16:0:102:BCL:HBA1	1.63	0.41
18:L:304:UQ8:H27	18:L:304:UQ8:H30	1.66	0.41
3:M:164:ARG:HH12	3:M:173:GLU:HB3	1.85	0.41
22:M:412:CDL:H802	22:M:412:CDL:H831	1.77	0.41
8:G:33:VAL:HG11	16:G:102:BCL:HAA1	2.02	0.41
16:O:502:BCL:HMD1	6:P:37:HIS:CE1	2.55	0.41
16:R:101:BCL:H141	16:R:101:BCL:H161	1.79	0.41
21:4:102:CRT:H15	21:4:102:CRT:H131	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:108:LEU:HD21	22:M:412:CDL:H562	2.02	0.41
2:L:244:LEU:HD12	22:M:412:CDL:H392	2.02	0.41
5:K:33:HIS:HB3	21:K:101:CRT:H393	2.01	0.41
5:Q:36:LEU:HD13	16:Q:102:BCL:HBC1	2.02	0.41
16:S:101:BCL:H162	16:S:101:BCL:H141	1.85	0.41
6:2:13:GLN:HE21	6:2:13:GLN:HB3	1.62	0.41
5:9:6:HIS:HB2	6:0:16:GLN:HA	2.03	0.41
2:L:199:LEU:HD22	2:L:222:PHE:CD2	2.56	0.41
16:T:101:BCL:H62	16:T:101:BCL:H92	1.82	0.41
1:C:25:ARG:NH1	25:C:521:HOH:O	2.54	0.41
2:L:218:GLU:CD	3:M:235:ILE:HD11	2.40	0.41
16:M:404:BCL:H41	16:M:404:BCL:H62	1.64	0.41
8:T:46:TRP:CD1	8:T:47:LEU:HG	2.56	0.41
16:5:102:BCL:H192	16:5:102:BCL:H162	1.76	0.41
6:P:46:TRP:CE2	16:P:102:BCL:H2C	2.55	0.41
21:Q:101:CRT:H26	21:Q:101:CRT:H241	1.93	0.41
6:2:46:TRP:CD1	6:2:47:LEU:HG	2.56	0.41
5:7:32:ILE:HG12	21:8:103:CRT:H403	2.03	0.41
1:C:195:LEU:HD12	1:C:237:MET:HG3	2.03	0.41
2:L:7:GLU:OE2	3:M:254:TRP:NE1	2.36	0.41
2:L:67:ILE:HG23	15:D:501:PGV:H41	2.03	0.41
2:L:150:HIS:HE1	25:L:441:HOH:O	2.03	0.41
18:L:304:UQ8:H37	18:L:304:UQ8:H40	1.57	0.41
16:E:102:BCL:H142	16:E:102:BCL:H111	1.83	0.41
24:J:102:LMT:H42	6:N:39:LEU:HB3	2.02	0.41
5:K:6:HIS:CE1	5:K:7:LYS:HD3	2.56	0.41
21:T:102:CRT:H393	7:U:30:LEU:HD23	2.02	0.41
5:1:32:ILE:HD12	16:2:102:BCL:O1D	2.20	0.41
16:5:102:BCL:HMD1	6:6:37:HIS:CE1	2.55	0.41
16:7:102:BCL:H92	16:7:102:BCL:H61	1.88	0.41
2:L:4:LEU:HB2	2:L:7:GLU:HB2	2.03	0.41
21:G:103:CRT:H10	21:G:103:CRT:H81	1.90	0.41
8:Z:46:TRP:CD1	8:Z:47:LEU:HG	2.56	0.41
5:5:22:PHE:HB3	16:5:102:BCL:H71	2.03	0.41
16:I:101:BCL:HBB3	16:I:101:BCL:HMB1	2.03	0.40
6:N:37:HIS:CD2	16:N:101:BCL:H92	2.56	0.40
1:C:250:CYS:HB3	1:C:266:ARG:HB2	2.04	0.40
2:L:254:ILE:HD12	2:L:254:ILE:HA	1.92	0.40
16:L:307:BCL:H152	16:M:404:BCL:H193	2.03	0.40
21:V:103:CRT:H20	21:V:103:CRT:H181	1.87	0.40
1:C:82:LEU:HB3	1:C:85:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:135:PRO:HA	4:H:171:TRP:HA	2.03	0.40
21:E:103:CRT:H26	21:E:103:CRT:H241	1.91	0.40
5:K:44:TRP:NE1	16:K:102:BCL:OBB	2.53	0.40
15:L:309:PGV:H231	15:L:309:PGV:H202	1.88	0.40
3:M:56:THR:HG21	3:M:131:VAL:HB	2.03	0.40
16:D:503:BCL:H162	16:D:503:BCL:H192	1.69	0.40
16:U:101:BCL:HBC2	8:V:43:TRP:CZ3	2.56	0.40
8:V:46:TRP:CD2	16:V:102:BCL:H2C	2.56	0.40
8:V:46:TRP:HZ2	16:V:102:BCL:H122	1.87	0.40
9:3:22:GLY:HA3	16:3:101:BCL:H172	2.03	0.40
5:5:32:ILE:HD12	16:6:101:BCL:O1D	2.20	0.40
21:8:103:CRT:H15	21:8:103:CRT:H131	1.91	0.40
1:C:257:TYR:OH	3:M:296:LEU:HD21	2.21	0.40
1:C:303:PHE:HB2	10:C:402:HEM:HBD1	2.04	0.40
2:L:74:PRO:HG3	2:L:151:GLY:O	2.21	0.40
2:L:196:HIS:ND1	18:L:303:UQ8:O2	2.38	0.40
6:B:30:PHE:CE1	16:B:102:BCL:H11	2.57	0.40
24:B:101:LMT:H41	6:0:47:LEU:HD13	2.03	0.40
16:B:102:BCL:H91	16:B:102:BCL:H111	1.85	0.40
6:R:22:PHE:HA	21:R:102:CRT:H14	2.03	0.40
16:U:101:BCL:H112	16:U:101:BCL:H72	1.95	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%)	301 (97%)	8 (3%)	0	100	100
2	L	275/278 (99%)	269 (98%)	6 (2%)	0	100	100
3	M	316/325 (97%)	311 (98%)	5 (2%)	0	100	100
4	H	258/259 (100%)	249 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1	41/44 (93%)	41 (100%)	0	0	100	100
5	5	41/44 (93%)	38 (93%)	2 (5%)	1 (2%)	6	2
5	7	39/44 (89%)	39 (100%)	0	0	100	100
5	9	41/44 (93%)	40 (98%)	1 (2%)	0	100	100
5	A	41/44 (93%)	41 (100%)	0	0	100	100
5	I	41/44 (93%)	41 (100%)	0	0	100	100
5	K	42/44 (96%)	42 (100%)	0	0	100	100
5	O	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
5	Q	41/44 (93%)	40 (98%)	0	1 (2%)	6	2
6	0	40/46 (87%)	38 (95%)	2 (5%)	0	100	100
6	2	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
6	4	40/46 (87%)	40 (100%)	0	0	100	100
6	6	36/46 (78%)	36 (100%)	0	0	100	100
6	8	32/46 (70%)	32 (100%)	0	0	100	100
6	B	42/46 (91%)	42 (100%)	0	0	100	100
6	J	38/46 (83%)	38 (100%)	0	0	100	100
6	N	36/46 (78%)	36 (100%)	0	0	100	100
6	P	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
6	R	39/46 (85%)	39 (100%)	0	0	100	100
7	D	48/64 (75%)	46 (96%)	2 (4%)	0	100	100
7	F	47/64 (73%)	45 (96%)	2 (4%)	0	100	100
7	S	49/64 (77%)	49 (100%)	0	0	100	100
7	U	49/64 (77%)	49 (100%)	0	0	100	100
7	W	52/64 (81%)	49 (94%)	3 (6%)	0	100	100
7	Y	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
8	E	39/47 (83%)	39 (100%)	0	0	100	100
8	G	40/47 (85%)	40 (100%)	0	0	100	100
8	T	40/47 (85%)	40 (100%)	0	0	100	100
8	V	40/47 (85%)	40 (100%)	0	0	100	100
8	X	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
8	Z	39/47 (83%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	3	60/66 (91%)	60 (100%)	0	0	100 100
All	All	2514/2833 (89%)	2465 (98%)	47 (2%)	2 (0%)	54 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Q	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%)	217 (97%)	6 (3%)	44 51
3	M	252/257 (98%)	249 (99%)	3 (1%)	71 78
4	H	206/206 (100%)	197 (96%)	9 (4%)	28 30
5	1	37/38 (97%)	37 (100%)	0	100 100
5	5	36/38 (95%)	34 (94%)	2 (6%)	21 19
5	7	36/38 (95%)	36 (100%)	0	100 100
5	9	37/38 (97%)	36 (97%)	1 (3%)	44 51
5	A	37/38 (97%)	37 (100%)	0	100 100
5	I	37/38 (97%)	37 (100%)	0	100 100
5	K	38/38 (100%)	38 (100%)	0	100 100
5	O	38/38 (100%)	38 (100%)	0	100 100
5	Q	37/38 (97%)	37 (100%)	0	100 100
6	0	35/38 (92%)	35 (100%)	0	100 100
6	2	34/38 (90%)	32 (94%)	2 (6%)	19 17
6	4	35/38 (92%)	35 (100%)	0	100 100
6	6	32/38 (84%)	30 (94%)	2 (6%)	18 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	8	28/38 (74%)	28 (100%)	0	100	100
6	B	37/38 (97%)	37 (100%)	0	100	100
6	J	33/38 (87%)	33 (100%)	0	100	100
6	N	32/38 (84%)	32 (100%)	0	100	100
6	P	35/38 (92%)	33 (94%)	2 (6%)	20	19
6	R	34/38 (90%)	33 (97%)	1 (3%)	42	48
7	D	43/55 (78%)	42 (98%)	1 (2%)	50	57
7	F	43/55 (78%)	43 (100%)	0	100	100
7	S	43/55 (78%)	42 (98%)	1 (2%)	50	57
7	U	43/55 (78%)	42 (98%)	1 (2%)	50	57
7	W	45/55 (82%)	45 (100%)	0	100	100
7	Y	55/55 (100%)	52 (94%)	3 (6%)	21	20
8	E	35/40 (88%)	35 (100%)	0	100	100
8	G	36/40 (90%)	35 (97%)	1 (3%)	43	49
8	T	36/40 (90%)	36 (100%)	0	100	100
8	V	36/40 (90%)	34 (94%)	2 (6%)	21	19
8	X	36/40 (90%)	35 (97%)	1 (3%)	43	49
8	Z	35/40 (88%)	34 (97%)	1 (3%)	42	48
9	3	48/52 (92%)	48 (100%)	0	100	100
All	All	2148/2342 (92%)	2106 (98%)	42 (2%)	57	62

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	84	ASP
1	C	151	THR
1	C	233	TYR
2	L	13	ARG
2	L	61	GLU
2	L	253	CYS
2	L	255	VAL
2	L	263	ARG
2	L	278	TRP
3	M	6	ASN
3	M	56	THR

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Mol	Chain	Res	Type
3	M	216	PHE
4	H	10	ASP
4	H	75	THR
4	H	81	VAL
4	H	152	ARG
4	H	159	LEU
4	H	225	LEU
4	H	237	ASP
4	H	251	THR
4	H	259	LEU
7	D	5	LEU
8	G	13	GLU
6	P	7	MET
6	P	12	GLU
6	R	7	MET
7	S	5	LEU
7	U	5	LEU
8	V	7	MET
8	V	28	MET
8	X	7	MET
7	Y	4	ASP
7	Y	5	LEU
7	Y	24	PHE
8	Z	13	GLU
6	2	13	GLN
6	2	16	GLN
5	5	6	HIS
5	5	10	GLN
6	6	11	THR
6	6	13	GLN
5	9	8	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	322	GLN
2	L	150	HIS
3	M	6	ASN
8	E	24	GLN
5	K	6	HIS
5	Q	10	GLN
6	R	24	GLN

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Mol	Chain	Res	Type
8	Z	24	GLN
6	2	13	GLN
6	8	24	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

14 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	1	5	5	8,9,10	0.50	0	7,9,11	0.96	1 (14%)
7	FME	U	1	7	8,9,10	0.53	0	7,9,11	0.88	1 (14%)
7	FME	D	1	7	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
5	FME	K	5	5	8,9,10	0.50	0	7,9,11	1.23	1 (14%)
4	FME	H	1	4	8,9,10	0.51	0	7,9,11	0.97	1 (14%)
5	FME	O	5	5	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
5	FME	Q	5	5	8,9,10	0.51	0	7,9,11	1.00	1 (14%)
7	FME	S	1	7	8,9,10	0.53	0	7,9,11	0.93	1 (14%)
5	FME	5	5	5	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
7	FME	Y	1	7	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
5	FME	9	5	5	8,9,10	0.50	0	7,9,11	1.11	1 (14%)
5	FME	A	5	5	8,9,10	0.49	0	7,9,11	1.12	1 (14%)
5	FME	I	5	5	8,9,10	0.49	0	7,9,11	1.14	1 (14%)
7	FME	W	1	7	8,9,10	0.53	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	1	5	5	-	1/7/9/11	-
7	FME	U	1	7	-	1/7/9/11	-
7	FME	D	1	7	-	0/7/9/11	-
5	FME	K	5	5	-	1/7/9/11	-
4	FME	H	1	4	-	3/7/9/11	-
5	FME	O	5	5	-	0/7/9/11	-
5	FME	Q	5	5	-	3/7/9/11	-
7	FME	S	1	7	-	1/7/9/11	-
5	FME	5	5	5	-	2/7/9/11	-
7	FME	Y	1	7	-	1/7/9/11	-
5	FME	9	5	5	-	0/7/9/11	-
5	FME	A	5	5	-	0/7/9/11	-
5	FME	I	5	5	-	0/7/9/11	-
7	FME	W	1	7	-	0/7/9/11	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1	FME	O-C-CA	-2.71	117.68	124.78
5	K	5	FME	O-C-CA	-2.70	117.69	124.78
5	I	5	FME	O-C-CA	-2.70	117.70	124.78
5	9	5	FME	O-C-CA	-2.67	117.79	124.78
5	A	5	FME	O-C-CA	-2.64	117.85	124.78
7	W	1	FME	O-C-CA	-2.58	118.02	124.78
5	5	5	FME	O-C-CA	-2.52	118.16	124.78
5	Q	5	FME	O-C-CA	-2.50	118.22	124.78
5	O	5	FME	O-C-CA	-2.48	118.27	124.78
7	Y	1	FME	O-C-CA	-2.46	118.33	124.78
5	1	5	FME	O-C-CA	-2.45	118.36	124.78
7	S	1	FME	O-C-CA	-2.39	118.52	124.78
7	U	1	FME	O-C-CA	-2.24	118.91	124.78
4	H	1	FME	O-C-CA	-2.20	119.01	124.78

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
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	Q	5	FME	O-C-CA-CB
7	S	1	FME	O1-CN-N-CA
7	U	1	FME	O1-CN-N-CA
7	Y	1	FME	O1-CN-N-CA
5	1	5	FME	O1-CN-N-CA
5	5	5	FME	CA-CB-CG-SD
4	H	1	FME	CB-CA-N-CN
5	5	5	FME	N-CA-CB-CG
4	H	1	FME	CA-CB-CG-SD

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1	FME	1	0
5	K	5	FME	1	0
4	H	1	FME	1	0
5	Q	5	FME	3	0
7	S	1	FME	1	0
7	Y	1	FME	2	0
7	W	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 111 ligands modelled in this entry, 10 are monoatomic - leaving 101 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LMT	P	101	-	36,36,36	0.41	0	47,47,47	0.60	0
18	UQ8	L	303	-	33,33,53	1.46	2 (6%)	40,43,67	1.61	9 (22%)
16	BCL	5	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.27	21 (26%)
10	HEM	C	401	1	41,50,50	1.35	5 (12%)	45,82,82	1.90	11 (24%)
16	BCL	M	404	-	64,74,74	1.70	14 (21%)	78,115,115	2.44	24 (30%)
15	PGV	D	501	-	38,38,50	1.01	2 (5%)	41,44,56	1.17	3 (7%)
24	LMT	2	101	-	36,36,36	0.40	0	47,47,47	0.66	1 (2%)
15	PGV	M	408	-	36,36,50	1.07	2 (5%)	39,42,56	1.15	3 (7%)
24	LMT	G	101	-	36,36,36	0.41	0	47,47,47	0.67	1 (2%)
24	LMT	0	101	-	36,36,36	0.40	0	47,47,47	0.77	1 (2%)
24	LMT	H	303	-	36,36,36	0.38	0	47,47,47	0.78	1 (2%)
21	CRT	2	103	-	41,43,43	0.74	0	50,54,54	2.22	17 (34%)
24	LMT	M	414	-	36,36,36	0.39	0	47,47,47	0.76	1 (2%)
16	BCL	9	101	-	64,74,74	1.70	13 (20%)	78,115,115	2.23	21 (26%)
16	BCL	L	307	-	64,74,74	1.69	14 (21%)	78,115,115	2.21	17 (21%)
16	BCL	Z	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.21	19 (24%)
24	LMT	8	101	-	36,36,36	0.39	0	47,47,47	0.77	2 (4%)
24	LMT	5	101	-	32,32,36	0.43	0	43,43,47	1.13	3 (6%)
16	BCL	I	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.25	20 (25%)
16	BCL	1	402	-	64,74,74	1.69	14 (21%)	78,115,115	2.25	21 (26%)
20	MQ8	M	406	-	54,54,54	1.31	2 (3%)	66,69,69	1.50	14 (21%)
24	LMT	2	104	-	36,36,36	0.42	0	47,47,47	0.66	1 (2%)
21	CRT	Q	101	-	41,43,43	0.72	0	50,54,54	3.76	15 (30%)
21	CRT	T	102	-	41,43,43	0.75	0	50,54,54	1.97	15 (30%)
15	PGV	F	501	-	35,35,50	1.09	2 (5%)	38,41,56	1.14	3 (7%)
16	BCL	L	301	-	64,74,74	1.68	13 (20%)	78,115,115	2.24	21 (26%)
16	BCL	6	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.20	21 (26%)
16	BCL	D	503	-	64,74,74	1.69	13 (20%)	78,115,115	2.30	18 (23%)
16	BCL	W	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.27	19 (24%)
21	CRT	E	103	-	41,43,43	0.73	0	50,54,54	1.80	15 (30%)
24	LMT	X	101	-	36,36,36	0.42	0	47,47,47	0.82	1 (2%)
22	CDL	H	302	-	78,78,99	1.02	4 (5%)	84,90,111	1.08	6 (7%)
10	HEM	C	403	1	41,50,50	1.35	5 (12%)	45,82,82	1.82	9 (20%)
16	BCL	K	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.31	21 (26%)
22	CDL	M	409	-	38,38,99	1.31	3 (7%)	43,49,111	1.22	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCL	S	101	-	64,74,74	1.69	14 (21%)	78,115,115	2.25	19 (24%)
21	CRT	M	407	-	41,43,43	0.71	0	50,54,54	2.28	16 (32%)
21	CRT	R	102	-	41,43,43	0.72	0	50,54,54	1.66	14 (28%)
16	BCL	B	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.18	22 (28%)
21	CRT	4	102	-	41,43,43	0.69	0	50,54,54	1.96	12 (24%)
23	LDA	O	501	-	12,15,15	2.07	1 (8%)	14,17,17	0.50	0
16	BCL	V	102	-	64,74,74	1.68	11 (17%)	78,115,115	2.15	20 (25%)
24	LMT	P	103	-	36,36,36	0.38	0	47,47,47	0.71	1 (2%)
21	CRT	7	101	-	41,43,43	0.69	0	50,54,54	1.54	8 (16%)
16	BCL	X	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.16	19 (24%)
16	BCL	M	403	-	64,74,74	1.69	13 (20%)	78,115,115	2.21	22 (28%)
21	CRT	V	103	-	41,43,43	0.74	0	50,54,54	2.23	19 (38%)
16	BCL	3	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.32	23 (29%)
22	CDL	M	412	-	83,83,99	1.03	4 (4%)	89,95,111	1.14	6 (6%)
15	PGV	L	306	-	34,34,50	1.09	2 (5%)	37,40,56	1.16	3 (8%)
16	BCL	Y	101	-	64,74,74	1.68	13 (20%)	78,115,115	2.27	19 (24%)
16	BCL	2	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.22	21 (26%)
15	PGV	M	410	-	26,26,50	1.28	2 (7%)	30,31,56	1.37	6 (20%)
21	CRT	B	103	-	41,43,43	0.71	0	50,54,54	1.71	14 (28%)
21	CRT	X	103	-	41,43,43	0.74	0	50,54,54	1.86	15 (30%)
16	BCL	G	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.21	22 (28%)
16	BCL	A	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.32	19 (24%)
16	BCL	4	101	-	64,74,74	1.70	14 (21%)	78,115,115	2.23	22 (28%)
21	CRT	K	101	-	41,43,43	0.74	0	50,54,54	3.39	14 (28%)
23	LDA	M	413	-	12,15,15	2.07	1 (8%)	14,17,17	0.50	0
16	BCL	E	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.22	20 (25%)
15	PGV	L	309	-	32,32,50	1.14	2 (6%)	35,38,56	1.28	3 (8%)
16	BCL	J	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.21	19 (24%)
18	UQ8	L	304	-	53,53,53	1.19	2 (3%)	64,67,67	1.69	15 (23%)
13	Z41	C	407	-	34,34,39	0.28	0	36,36,41	0.31	0
16	BCL	8	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.21	20 (25%)
16	BCL	Q	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.29	20 (25%)
24	LMT	Z	101	-	36,36,36	0.39	0	47,47,47	0.99	3 (6%)
16	BCL	N	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.21	20 (25%)
24	LMT	G	104	-	36,36,36	0.39	0	47,47,47	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LMT	R	103	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
16	BCL	U	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.25	18 (23%)
24	LMT	J	102	-	36,36,36	0.39	0	47,47,47	0.73	1 (2%)
17	BPH	L	302	-	51,70,70	0.56	2 (3%)	52,101,101	0.68	1 (1%)
16	BCL	F	502	-	64,74,74	1.70	14 (21%)	78,115,115	2.28	19 (24%)
22	CDL	M	411	-	94,94,99	0.95	4 (4%)	100,106,111	1.09	7 (7%)
21	CRT	0	103	-	41,43,43	0.72	0	50,54,54	1.67	14 (28%)
16	BCL	R	101	-	64,74,74	1.67	12 (18%)	78,115,115	2.18	19 (24%)
15	PGV	1	401	-	26,26,50	1.28	2 (7%)	29,31,56	1.19	2 (6%)
24	LMT	E	101	-	36,36,36	0.43	0	47,47,47	0.80	1 (2%)
24	LMT	4	103	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
15	PGV	H	301	-	35,35,50	1.07	2 (5%)	38,41,56	1.21	4 (10%)
16	BCL	T	101	-	64,74,74	1.67	11 (17%)	78,115,115	2.18	18 (23%)
15	PGV	C	409	-	30,30,50	1.16	2 (6%)	33,36,56	1.11	4 (12%)
24	LMT	B	101	-	36,36,36	0.42	0	47,47,47	0.66	1 (2%)
21	CRT	G	103	-	41,43,43	0.70	0	50,54,54	1.64	14 (28%)
16	BCL	P	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.18	21 (26%)
21	CRT	Z	103	-	41,43,43	0.73	0	50,54,54	1.89	15 (30%)
22	CDL	D	502	-	57,57,99	1.11	4 (7%)	63,69,111	1.18	5 (7%)
10	HEM	C	404	1	41,50,50	1.36	5 (12%)	45,82,82	1.82	11 (24%)
21	CRT	8	103	-	41,43,43	0.70	0	50,54,54	1.68	12 (24%)
16	BCL	0	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.15	18 (23%)
17	BPH	M	405	-	51,70,70	0.54	1 (1%)	52,101,101	0.61	0
15	PGV	L	305	-	28,28,50	1.21	2 (7%)	31,34,56	1.23	3 (9%)
16	BCL	O	502	-	64,74,74	1.69	13 (20%)	78,115,115	2.30	19 (24%)
24	LMT	V	101	-	36,36,36	0.38	0	47,47,47	0.74	0
21	CRT	N	102	-	41,43,43	0.71	0	50,54,54	1.77	14 (28%)
14	PLM	C	408	1	11,11,17	0.37	0	10,10,17	0.42	0
10	HEM	C	402	1	41,50,50	1.33	5 (12%)	45,82,82	1.87	9 (20%)
16	BCL	7	102	-	59,69,74	1.77	14 (23%)	72,109,115	2.33	21 (29%)
18	UQ8	L	308	-	53,53,53	1.22	2 (3%)	64,67,67	1.60	14 (21%)

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
24	LMT	P	101	-	-	4/21/61/61	0/2/2/2
18	UQ8	L	303	-	-	4/27/51/75	0/1/1/1
16	BCL	5	102	-	-	12/37/137/137	-
10	HEM	C	401	1	-	4/12/54/54	-
16	BCL	M	404	-	-	12/37/137/137	-
15	PGV	D	501	-	-	15/43/43/55	-
24	LMT	2	101	-	-	2/21/61/61	0/2/2/2
15	PGV	M	408	-	-	6/41/41/55	-
24	LMT	G	101	-	-	5/21/61/61	0/2/2/2
24	LMT	0	101	-	-	6/21/61/61	0/2/2/2
24	LMT	H	303	-	-	1/21/61/61	0/2/2/2
21	CRT	2	103	-	-	2/51/51/51	-
24	LMT	M	414	-	-	6/21/61/61	0/2/2/2
16	BCL	9	101	-	-	17/37/137/137	-
16	BCL	L	307	-	-	14/37/137/137	-
16	BCL	Z	102	-	-	17/37/137/137	-
24	LMT	8	101	-	-	3/21/61/61	0/2/2/2
24	LMT	5	101	-	-	6/17/57/61	0/2/2/2
16	BCL	I	101	-	-	14/37/137/137	-
16	BCL	1	402	-	-	17/37/137/137	-
20	MQ8	M	406	-	-	4/47/67/67	0/2/2/2
24	LMT	2	104	-	-	3/21/61/61	0/2/2/2
21	CRT	Q	101	-	-	9/51/51/51	-
21	CRT	T	102	-	-	4/51/51/51	-
15	PGV	F	501	-	-	6/40/40/55	-
16	BCL	L	301	-	-	9/37/137/137	-
16	BCL	6	101	-	-	14/37/137/137	-
16	BCL	D	503	-	-	10/37/137/137	-
16	BCL	W	101	-	-	20/37/137/137	-
21	CRT	E	103	-	-	0/51/51/51	-
24	LMT	X	101	-	-	3/21/61/61	0/2/2/2
22	CDL	H	302	-	-	25/89/89/110	-
10	HEM	C	403	1	-	2/12/54/54	-
16	BCL	K	102	-	-	12/37/137/137	-
22	CDL	M	409	-	-	19/48/48/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCL	S	101	-	-	11/37/137/137	-
21	CRT	M	407	-	-	8/51/51/51	-
21	CRT	R	102	-	-	2/51/51/51	-
16	BCL	B	102	-	-	17/37/137/137	-
21	CRT	4	102	-	-	7/51/51/51	-
23	LDA	O	501	-	-	0/13/13/13	-
16	BCL	V	102	-	-	22/37/137/137	-
24	LMT	P	103	-	-	1/21/61/61	0/2/2/2
21	CRT	7	101	-	-	5/51/51/51	-
16	BCL	X	102	-	-	16/37/137/137	-
16	BCL	M	403	-	-	6/37/137/137	-
21	CRT	V	103	-	-	5/51/51/51	-
16	BCL	3	101	-	-	12/37/137/137	-
22	CDL	M	412	-	-	32/93/93/110	-
15	PGV	L	306	-	-	7/39/39/55	-
16	BCL	Y	101	-	-	20/37/137/137	-
16	BCL	2	102	-	-	14/37/137/137	-
15	PGV	M	410	-	-	7/28/28/55	-
21	CRT	B	103	-	-	2/51/51/51	-
21	CRT	X	103	-	-	4/51/51/51	-
16	BCL	G	102	-	-	18/37/137/137	-
16	BCL	A	101	-	-	13/37/137/137	-
16	BCL	4	101	-	-	10/37/137/137	-
21	CRT	K	101	-	-	10/51/51/51	-
23	LDA	M	413	-	-	3/13/13/13	-
16	BCL	E	102	-	-	13/37/137/137	-
15	PGV	L	309	-	-	6/37/37/55	-
16	BCL	J	101	-	-	14/37/137/137	-
18	UQ8	L	304	-	-	14/51/75/75	0/1/1/1
13	Z41	C	407	-	-	6/35/35/41	-
16	BCL	8	102	-	-	15/37/137/137	-
16	BCL	Q	102	-	-	13/37/137/137	-
24	LMT	Z	101	-	-	5/21/61/61	0/2/2/2
16	BCL	N	101	-	-	15/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	G	104	-	-	2/21/61/61	0/2/2/2
24	LMT	R	103	-	-	7/21/61/61	0/2/2/2
16	BCL	U	101	-	-	18/37/137/137	-
24	LMT	J	102	-	-	3/21/61/61	0/2/2/2
17	BPH	L	302	-	-	4/37/105/105	0/5/6/6
16	BCL	F	502	-	-	14/37/137/137	-
22	CDL	M	411	-	-	30/105/105/110	-
21	CRT	0	103	-	-	2/51/51/51	-
16	BCL	R	101	-	-	13/37/137/137	-
15	PGV	1	401	-	-	12/30/30/55	-
24	LMT	E	101	-	-	1/21/61/61	0/2/2/2
24	LMT	4	103	-	-	2/21/61/61	0/2/2/2
15	PGV	H	301	-	-	15/40/40/55	-
16	BCL	T	101	-	-	17/37/137/137	-
15	PGV	C	409	-	-	6/35/35/55	-
24	LMT	B	101	-	-	1/21/61/61	0/2/2/2
21	CRT	G	103	-	-	5/51/51/51	-
16	BCL	P	102	-	-	21/37/137/137	-
21	CRT	Z	103	-	-	8/51/51/51	-
22	CDL	D	502	-	-	23/67/67/110	-
10	HEM	C	404	1	-	4/12/54/54	-
21	CRT	8	103	-	-	3/51/51/51	-
16	BCL	0	102	-	-	17/37/137/137	-
17	BPH	M	405	-	-	5/37/105/105	0/5/6/6
15	PGV	L	305	-	-	14/33/33/55	-
16	BCL	O	502	-	-	19/37/137/137	-
24	LMT	V	101	-	-	9/21/61/61	0/2/2/2
21	CRT	N	102	-	-	5/51/51/51	-
14	PLM	C	408	1	-	1/8/9/15	-
10	HEM	C	402	1	-	5/12/54/54	-
16	BCL	7	102	-	-	12/31/131/137	-
18	UQ8	L	308	-	-	8/51/75/75	0/1/1/1

All (535) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	406	MQ8	C3-C2	7.86	1.49	1.35
18	L	308	UQ8	C6-C1	7.60	1.49	1.35
18	L	304	UQ8	C6-C1	7.56	1.49	1.35
18	L	303	UQ8	C6-C1	7.40	1.48	1.35
23	M	413	LDA	O1-N1	-7.14	1.25	1.42
23	O	501	LDA	O1-N1	-7.14	1.25	1.42
16	L	301	BCL	O2D-CGD	5.18	1.45	1.33
16	N	101	BCL	O2D-CGD	5.12	1.45	1.33
16	5	102	BCL	O2D-CGD	5.08	1.45	1.33
16	B	102	BCL	O2D-CGD	5.07	1.45	1.33
16	J	101	BCL	O2D-CGD	5.06	1.45	1.33
16	0	102	BCL	O2D-CGD	5.05	1.45	1.33
16	7	102	BCL	O2D-CGD	5.04	1.45	1.33
16	V	102	BCL	O2D-CGD	5.04	1.45	1.33
16	G	102	BCL	O2D-CGD	5.03	1.45	1.33
16	8	102	BCL	O2D-CGD	5.03	1.45	1.33
16	2	102	BCL	O2D-CGD	5.03	1.45	1.33
16	4	101	BCL	O2D-CGD	5.02	1.45	1.33
16	E	102	BCL	O2D-CGD	5.01	1.45	1.33
16	S	101	BCL	O2D-CGD	5.00	1.45	1.33
16	1	402	BCL	O2D-CGD	5.00	1.45	1.33
16	I	101	BCL	O2D-CGD	5.00	1.45	1.33
16	F	502	BCL	O2D-CGD	4.99	1.45	1.33
16	6	101	BCL	O2D-CGD	4.99	1.45	1.33
16	K	102	BCL	O2D-CGD	4.99	1.45	1.33
16	X	102	BCL	O2D-CGD	4.99	1.45	1.33
16	A	101	BCL	O2D-CGD	4.98	1.45	1.33
16	U	101	BCL	O2D-CGD	4.98	1.45	1.33
16	P	102	BCL	O2D-CGD	4.98	1.45	1.33
16	W	101	BCL	O2D-CGD	4.97	1.45	1.33
16	Q	102	BCL	O2D-CGD	4.97	1.45	1.33
16	D	503	BCL	O2D-CGD	4.97	1.45	1.33
16	Y	101	BCL	O2D-CGD	4.97	1.45	1.33
16	R	101	BCL	O2D-CGD	4.97	1.45	1.33
16	T	101	BCL	O2D-CGD	4.96	1.45	1.33
16	O	502	BCL	O2D-CGD	4.96	1.45	1.33
16	M	404	BCL	O2D-CGD	4.96	1.45	1.33
16	3	101	BCL	O2D-CGD	4.95	1.45	1.33
16	Z	102	BCL	O2D-CGD	4.92	1.45	1.33
16	9	101	BCL	O2D-CGD	4.92	1.45	1.33
16	M	403	BCL	O2D-CGD	4.90	1.45	1.33
16	G	102	BCL	C3B-C2B	4.89	1.48	1.39
16	B	102	BCL	C3B-C2B	4.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	404	BCL	C3D-C4D	-4.84	1.33	1.44
16	6	101	BCL	C3B-C2B	4.83	1.48	1.39
16	Z	102	BCL	C3B-C2B	4.82	1.48	1.39
16	L	307	BCL	C3B-C2B	4.82	1.48	1.39
16	4	101	BCL	C3B-C2B	4.82	1.48	1.39
16	F	502	BCL	C3B-C2B	4.80	1.48	1.39
16	T	101	BCL	C3B-C2B	4.80	1.48	1.39
16	E	102	BCL	C3B-C2B	4.80	1.48	1.39
16	J	101	BCL	C3B-C2B	4.80	1.48	1.39
16	L	307	BCL	C3D-C4D	-4.79	1.33	1.44
16	K	102	BCL	C3B-C2B	4.79	1.48	1.39
16	I	101	BCL	C3B-C2B	4.78	1.48	1.39
16	R	101	BCL	C3B-C2B	4.77	1.48	1.39
16	N	101	BCL	C3B-C2B	4.77	1.48	1.39
16	M	403	BCL	C3D-C4D	-4.77	1.33	1.44
16	D	503	BCL	C3D-C4D	-4.77	1.33	1.44
16	2	102	BCL	C3B-C2B	4.76	1.48	1.39
16	P	102	BCL	C3B-C2B	4.76	1.48	1.39
16	5	102	BCL	C3B-C2B	4.76	1.48	1.39
22	M	412	CDL	OA6-CA5	4.75	1.45	1.35
16	X	102	BCL	C3B-C2B	4.74	1.47	1.39
16	1	402	BCL	C3B-C2B	4.74	1.47	1.39
16	U	101	BCL	C3B-C2B	4.74	1.47	1.39
16	9	101	BCL	C3D-C4D	-4.73	1.33	1.44
16	D	503	BCL	C3B-C2B	4.73	1.47	1.39
16	L	307	BCL	O2D-CGD	4.73	1.44	1.33
16	L	301	BCL	C3B-C2B	4.72	1.47	1.39
16	M	404	BCL	C3B-C2B	4.72	1.47	1.39
16	7	102	BCL	C3D-C4D	-4.72	1.33	1.44
16	W	101	BCL	C3B-C2B	4.71	1.47	1.39
16	S	101	BCL	C3D-C4D	-4.71	1.33	1.44
16	O	502	BCL	C3D-C4D	-4.70	1.33	1.44
16	U	101	BCL	C3D-C4D	-4.70	1.33	1.44
16	W	101	BCL	C3D-C4D	-4.70	1.33	1.44
16	V	102	BCL	C3B-C2B	4.70	1.47	1.39
16	8	102	BCL	C3B-C2B	4.70	1.47	1.39
16	K	102	BCL	C3D-C4D	-4.70	1.33	1.44
16	A	101	BCL	C3D-C4D	-4.70	1.33	1.44
16	F	502	BCL	C3D-C4D	-4.70	1.33	1.44
16	3	101	BCL	C3B-C2B	4.70	1.47	1.39
16	L	301	BCL	C3D-C4D	-4.69	1.33	1.44
16	I	101	BCL	C3D-C4D	-4.69	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	102	BCL	C3D-C4D	-4.69	1.33	1.44
16	0	102	BCL	C3B-C2B	4.69	1.47	1.39
16	5	102	BCL	C3D-C4D	-4.68	1.33	1.44
16	7	102	BCL	C3B-C2B	4.67	1.47	1.39
16	Q	102	BCL	C3B-C2B	4.67	1.47	1.39
20	M	406	MQ8	C10-C5	4.67	1.48	1.40
16	O	502	BCL	C3B-C2B	4.66	1.47	1.39
16	A	101	BCL	C3B-C2B	4.66	1.47	1.39
16	G	102	BCL	C3D-C4D	-4.66	1.33	1.44
16	2	102	BCL	C3D-C4D	-4.66	1.33	1.44
16	0	102	BCL	C3D-C4D	-4.66	1.33	1.44
16	Y	101	BCL	C3D-C4D	-4.66	1.33	1.44
16	M	403	BCL	C3B-C2B	4.66	1.47	1.39
16	3	101	BCL	C3D-C4D	-4.65	1.33	1.44
16	S	101	BCL	C3B-C2B	4.65	1.47	1.39
16	B	102	BCL	C3D-C4D	-4.64	1.33	1.44
16	9	101	BCL	C3B-C2B	4.64	1.47	1.39
16	1	402	BCL	C3D-C4D	-4.62	1.33	1.44
16	N	101	BCL	C3D-C4D	-4.61	1.33	1.44
16	R	101	BCL	C3D-C4D	-4.60	1.33	1.44
16	Z	102	BCL	C3D-C4D	-4.60	1.33	1.44
16	Y	101	BCL	C3B-C2B	4.60	1.47	1.39
16	8	102	BCL	C3D-C4D	-4.59	1.33	1.44
16	6	101	BCL	C3D-C4D	-4.58	1.33	1.44
16	J	101	BCL	C3D-C4D	-4.58	1.33	1.44
16	X	102	BCL	C3D-C4D	-4.58	1.33	1.44
16	4	101	BCL	C3D-C4D	-4.57	1.33	1.44
16	E	102	BCL	C3D-C4D	-4.56	1.33	1.44
16	P	102	BCL	C3D-C4D	-4.56	1.33	1.44
16	T	101	BCL	C3D-C4D	-4.55	1.33	1.44
16	V	102	BCL	C3D-C4D	-4.52	1.34	1.44
15	1	401	PGV	O01-C1	4.44	1.46	1.34
22	M	409	CDL	OA6-CA5	4.37	1.46	1.34
22	M	409	CDL	OA8-CA7	4.36	1.46	1.33
16	M	403	BCL	O2A-CGA	4.35	1.46	1.33
16	1	402	BCL	O2A-CGA	4.34	1.46	1.33
22	M	411	CDL	OA6-CA5	4.33	1.46	1.34
16	Z	102	BCL	O2A-CGA	4.29	1.45	1.33
16	4	101	BCL	O2A-CGA	4.28	1.45	1.33
16	E	102	BCL	O2A-CGA	4.27	1.45	1.33
16	F	502	BCL	O2A-CGA	4.27	1.45	1.33
16	3	101	BCL	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	102	BCL	O2A-CGA	4.24	1.45	1.33
16	X	102	BCL	O2A-CGA	4.24	1.45	1.33
16	L	301	BCL	O2A-CGA	4.23	1.45	1.33
16	I	101	BCL	O2A-CGA	4.23	1.45	1.33
16	O	502	BCL	O2A-CGA	4.23	1.45	1.33
16	9	101	BCL	O2A-CGA	4.22	1.45	1.33
15	M	410	PGV	O03-C19	4.22	1.45	1.33
22	M	411	CDL	OA8-CA7	4.22	1.45	1.33
15	1	401	PGV	O03-C19	4.21	1.45	1.33
16	G	102	BCL	O2A-CGA	4.21	1.45	1.33
16	S	101	BCL	O2A-CGA	4.21	1.45	1.33
16	M	404	BCL	O2A-CGA	4.21	1.45	1.33
16	J	101	BCL	O2A-CGA	4.21	1.45	1.33
16	U	101	BCL	O2A-CGA	4.21	1.45	1.33
22	M	412	CDL	OA8-CA7	4.20	1.45	1.33
16	5	102	BCL	O2A-CGA	4.20	1.45	1.33
15	L	305	PGV	O01-C1	4.20	1.46	1.34
16	6	101	BCL	O2A-CGA	4.20	1.45	1.33
16	K	102	BCL	O2A-CGA	4.19	1.45	1.33
15	L	309	PGV	O03-C19	4.19	1.45	1.33
16	R	101	BCL	O2A-CGA	4.19	1.45	1.33
15	C	409	PGV	O03-C19	4.19	1.45	1.33
15	M	408	PGV	O03-C19	4.19	1.45	1.33
22	M	412	CDL	OB8-CB7	4.19	1.45	1.33
15	F	501	PGV	O03-C19	4.19	1.45	1.33
15	L	306	PGV	O03-C19	4.18	1.45	1.33
22	D	502	CDL	OB8-CB7	4.18	1.45	1.33
16	Q	102	BCL	O2A-CGA	4.17	1.45	1.33
16	7	102	BCL	O2A-CGA	4.16	1.45	1.33
16	D	503	BCL	O2A-CGA	4.16	1.45	1.33
16	N	101	BCL	O2A-CGA	4.16	1.45	1.33
22	H	302	CDL	OA8-CA7	4.16	1.45	1.33
16	P	102	BCL	O2A-CGA	4.15	1.45	1.33
15	F	501	PGV	O01-C1	4.15	1.46	1.34
16	B	102	BCL	O2A-CGA	4.15	1.45	1.33
15	L	309	PGV	O01-C1	4.15	1.46	1.34
15	H	301	PGV	O03-C19	4.14	1.45	1.33
16	T	101	BCL	O2A-CGA	4.14	1.45	1.33
16	0	102	BCL	O2A-CGA	4.14	1.45	1.33
22	M	411	CDL	OB8-CB7	4.14	1.45	1.33
16	W	101	BCL	O2A-CGA	4.14	1.45	1.33
16	A	101	BCL	O2A-CGA	4.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	305	PGV	O03-C19	4.11	1.45	1.33
22	D	502	CDL	OB6-CB5	4.10	1.45	1.34
22	H	302	CDL	OB8-CB7	4.10	1.45	1.33
22	D	502	CDL	OA6-CA5	4.10	1.45	1.34
16	Y	101	BCL	O2A-CGA	4.10	1.45	1.33
16	2	102	BCL	O2A-CGA	4.09	1.45	1.33
16	8	102	BCL	O2A-CGA	4.09	1.45	1.33
15	M	408	PGV	O01-C1	4.08	1.45	1.34
16	L	307	BCL	O2A-CGA	4.08	1.45	1.33
22	M	412	CDL	OB6-CB5	4.07	1.45	1.34
22	H	302	CDL	OA6-CA5	4.06	1.45	1.34
22	M	411	CDL	OB6-CB5	4.04	1.45	1.34
22	M	409	CDL	OB6-CB5	4.04	1.45	1.34
22	H	302	CDL	OB6-CB5	4.00	1.45	1.34
15	H	301	PGV	O01-C1	3.99	1.45	1.34
15	M	410	PGV	O01-C1	3.99	1.45	1.34
15	D	501	PGV	O03-C19	3.99	1.45	1.33
15	L	306	PGV	O01-C1	3.98	1.45	1.34
15	C	409	PGV	O01-C1	3.97	1.45	1.34
15	D	501	PGV	O01-C1	3.97	1.45	1.34
16	7	102	BCL	CHD-C1D	3.78	1.45	1.38
16	F	502	BCL	CHD-C1D	3.70	1.45	1.38
16	I	101	BCL	CHD-C1D	3.67	1.45	1.38
16	5	102	BCL	CHD-C1D	3.66	1.45	1.38
16	9	101	BCL	CHD-C1D	3.64	1.45	1.38
10	C	404	HEM	C1B-NB	-3.59	1.34	1.40
16	W	101	BCL	CHD-C1D	3.58	1.45	1.38
16	A	101	BCL	CHD-C1D	3.57	1.45	1.38
10	C	401	HEM	C1B-NB	-3.56	1.34	1.40
16	Y	101	BCL	CHD-C1D	3.56	1.45	1.38
16	J	101	BCL	OBD-CAD	3.56	1.28	1.22
16	B	102	BCL	OBD-CAD	3.55	1.28	1.22
16	U	101	BCL	CHD-C1D	3.53	1.45	1.38
16	G	102	BCL	OBD-CAD	3.53	1.28	1.22
10	C	403	HEM	C1B-NB	-3.53	1.34	1.40
16	6	101	BCL	OBD-CAD	3.51	1.28	1.22
16	S	101	BCL	CHD-C1D	3.51	1.45	1.38
16	M	403	BCL	CHD-C1D	3.49	1.45	1.38
16	D	503	BCL	CHD-C1D	3.49	1.45	1.38
16	Y	101	BCL	OBD-CAD	3.49	1.28	1.22
16	Q	102	BCL	CHD-C1D	3.49	1.45	1.38
16	U	101	BCL	OBD-CAD	3.48	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	102	BCL	OBD-CAD	3.48	1.28	1.22
16	O	502	BCL	CHD-C1D	3.48	1.45	1.38
16	5	102	BCL	OBD-CAD	3.47	1.28	1.22
16	P	102	BCL	OBD-CAD	3.47	1.28	1.22
16	1	402	BCL	OBD-CAD	3.47	1.28	1.22
16	4	101	BCL	OBD-CAD	3.47	1.28	1.22
16	I	101	BCL	OBD-CAD	3.47	1.28	1.22
16	W	101	BCL	OBD-CAD	3.47	1.28	1.22
16	0	102	BCL	OBD-CAD	3.47	1.28	1.22
16	R	101	BCL	OBD-CAD	3.46	1.28	1.22
16	1	402	BCL	CHD-C1D	3.46	1.45	1.38
16	O	502	BCL	OBD-CAD	3.46	1.28	1.22
16	3	101	BCL	OBD-CAD	3.46	1.28	1.22
16	D	503	BCL	OBD-CAD	3.45	1.28	1.22
16	9	101	BCL	OBD-CAD	3.45	1.28	1.22
16	F	502	BCL	OBD-CAD	3.45	1.28	1.22
16	K	102	BCL	CHD-C1D	3.45	1.45	1.38
16	2	102	BCL	OBD-CAD	3.45	1.28	1.22
16	3	101	BCL	CHD-C1D	3.44	1.45	1.38
16	L	307	BCL	CHD-C1D	3.44	1.45	1.38
16	T	101	BCL	OBD-CAD	3.44	1.28	1.22
16	8	102	BCL	OBD-CAD	3.44	1.28	1.22
16	L	307	BCL	OBD-CAD	3.43	1.28	1.22
16	Z	102	BCL	OBD-CAD	3.43	1.28	1.22
10	C	402	HEM	C1B-NB	-3.43	1.34	1.40
16	K	102	BCL	OBD-CAD	3.43	1.28	1.22
16	Q	102	BCL	OBD-CAD	3.43	1.28	1.22
16	V	102	BCL	OBD-CAD	3.42	1.28	1.22
10	C	403	HEM	C4D-ND	-3.42	1.34	1.40
16	7	102	BCL	OBD-CAD	3.42	1.28	1.22
16	X	102	BCL	OBD-CAD	3.41	1.28	1.22
16	N	101	BCL	OBD-CAD	3.40	1.28	1.22
16	A	101	BCL	OBD-CAD	3.39	1.28	1.22
16	R	101	BCL	C1D-ND	-3.39	1.33	1.37
16	L	301	BCL	CHD-C1D	3.39	1.45	1.38
16	S	101	BCL	OBD-CAD	3.39	1.28	1.22
16	L	301	BCL	OBD-CAD	3.39	1.28	1.22
16	T	101	BCL	C1D-ND	-3.37	1.33	1.37
10	C	404	HEM	C4D-ND	-3.36	1.34	1.40
16	V	102	BCL	C1D-ND	-3.35	1.33	1.37
16	L	307	BCL	C1D-ND	-3.34	1.33	1.37
16	M	403	BCL	OBD-CAD	3.34	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	102	BCL	C1D-ND	-3.34	1.33	1.37
10	C	401	HEM	C4D-ND	-3.33	1.34	1.40
16	4	101	BCL	C1D-ND	-3.33	1.33	1.37
16	M	404	BCL	CHD-C1D	3.32	1.44	1.38
16	8	102	BCL	C1D-ND	-3.30	1.33	1.37
16	Z	102	BCL	CHD-C1D	3.30	1.44	1.38
16	X	102	BCL	C1D-ND	-3.30	1.33	1.37
16	Z	102	BCL	C1D-ND	-3.29	1.33	1.37
16	2	102	BCL	C1D-ND	-3.28	1.33	1.37
10	C	402	HEM	C4D-ND	-3.28	1.34	1.40
16	E	102	BCL	C1D-ND	-3.27	1.33	1.37
16	P	102	BCL	CHD-C1D	3.27	1.44	1.38
16	0	102	BCL	C1D-ND	-3.27	1.33	1.37
16	N	101	BCL	CHD-C1D	3.27	1.44	1.38
16	B	102	BCL	CHD-C1D	3.26	1.44	1.38
16	2	102	BCL	CHD-C1D	3.26	1.44	1.38
16	8	102	BCL	CHD-C1D	3.25	1.44	1.38
16	J	101	BCL	C1D-ND	-3.24	1.33	1.37
18	L	308	UQ8	C4-C3	3.24	1.49	1.36
16	B	102	BCL	C1D-ND	-3.24	1.33	1.37
16	N	101	BCL	C1D-ND	-3.24	1.33	1.37
16	6	101	BCL	C1D-ND	-3.21	1.33	1.37
16	4	101	BCL	CHD-C1D	3.20	1.44	1.38
16	T	101	BCL	CHD-C1D	3.20	1.44	1.38
16	J	101	BCL	CHD-C1D	3.19	1.44	1.38
16	G	102	BCL	CHD-C1D	3.19	1.44	1.38
16	G	102	BCL	C1D-ND	-3.18	1.33	1.37
16	0	102	BCL	CHD-C1D	3.18	1.44	1.38
16	V	102	BCL	CHD-C1D	3.18	1.44	1.38
16	X	102	BCL	CHD-C1D	3.15	1.44	1.38
16	M	404	BCL	OBD-CAD	3.14	1.27	1.22
16	R	101	BCL	CHD-C1D	3.11	1.44	1.38
16	6	101	BCL	CHD-C1D	3.10	1.44	1.38
16	E	102	BCL	CHD-C1D	3.08	1.44	1.38
16	M	403	BCL	C1D-ND	-3.08	1.34	1.37
16	M	403	BCL	C3D-C2D	3.07	1.47	1.39
18	L	304	UQ8	C4-C3	3.06	1.48	1.36
18	L	303	UQ8	C4-C3	3.05	1.48	1.36
16	K	102	BCL	C1D-ND	-3.04	1.34	1.37
16	P	102	BCL	C3D-C2D	2.99	1.47	1.39
16	L	307	BCL	C3D-C2D	2.99	1.47	1.39
16	9	101	BCL	C1D-ND	-2.98	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	404	BCL	C1D-ND	-2.97	1.34	1.37
16	U	101	BCL	C3D-C2D	2.96	1.47	1.39
16	2	102	BCL	C3D-C2D	2.96	1.47	1.39
16	1	402	BCL	C3D-C2D	2.95	1.47	1.39
16	D	503	BCL	C1D-ND	-2.95	1.34	1.37
16	1	402	BCL	C1D-ND	-2.94	1.34	1.37
16	V	102	BCL	C3D-C2D	2.94	1.47	1.39
10	C	404	HEM	FE-NB	2.94	2.11	1.96
16	W	101	BCL	C3D-C2D	2.94	1.47	1.39
16	N	101	BCL	C3D-C2D	2.93	1.47	1.39
16	Z	102	BCL	C3D-C2D	2.93	1.47	1.39
10	C	403	HEM	FE-NB	2.92	2.11	1.96
16	6	101	BCL	C3D-C2D	2.92	1.47	1.39
16	S	101	BCL	C3D-C2D	2.92	1.47	1.39
16	4	101	BCL	C3D-C2D	2.92	1.47	1.39
16	5	102	BCL	C3D-C2D	2.92	1.47	1.39
16	O	502	BCL	C3D-C2D	2.91	1.47	1.39
16	I	101	BCL	C3D-C2D	2.91	1.47	1.39
16	Q	102	BCL	C3D-C2D	2.91	1.47	1.39
16	R	101	BCL	C3D-C2D	2.91	1.47	1.39
16	3	101	BCL	C3D-C2D	2.91	1.47	1.39
16	D	503	BCL	C3D-C2D	2.90	1.47	1.39
16	J	101	BCL	C3D-C2D	2.90	1.47	1.39
16	K	102	BCL	C3D-C2D	2.90	1.47	1.39
16	L	301	BCL	C1D-ND	-2.89	1.34	1.37
16	0	102	BCL	C3D-C2D	2.89	1.47	1.39
16	3	101	BCL	C1D-ND	-2.89	1.34	1.37
16	F	502	BCL	C3D-C2D	2.88	1.47	1.39
16	X	102	BCL	C3D-C2D	2.88	1.47	1.39
16	9	101	BCL	C3D-C2D	2.88	1.47	1.39
16	W	101	BCL	C1D-ND	-2.88	1.34	1.37
16	Q	102	BCL	C1D-ND	-2.88	1.34	1.37
16	7	102	BCL	C3D-C2D	2.88	1.47	1.39
16	8	102	BCL	C3D-C2D	2.88	1.47	1.39
16	U	101	BCL	C1D-ND	-2.87	1.34	1.37
16	Y	101	BCL	C3D-C2D	2.86	1.46	1.39
16	G	102	BCL	C3D-C2D	2.86	1.46	1.39
16	B	102	BCL	C3D-C2D	2.86	1.46	1.39
16	S	101	BCL	C1D-ND	-2.85	1.34	1.37
10	C	402	HEM	FE-NB	2.85	2.11	1.96
16	O	502	BCL	C1D-ND	-2.84	1.34	1.37
16	A	101	BCL	C1D-ND	-2.84	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	102	BCL	C3D-C2D	2.84	1.46	1.39
16	I	101	BCL	CHD-C4C	2.84	1.47	1.39
16	A	101	BCL	C3D-C2D	2.83	1.46	1.39
10	C	401	HEM	FE-NB	2.82	2.10	1.96
16	T	101	BCL	C3D-C2D	2.81	1.46	1.39
16	7	102	BCL	CHD-C4C	2.80	1.47	1.39
16	F	502	BCL	CHD-C4C	2.80	1.47	1.39
16	Y	101	BCL	C1D-ND	-2.79	1.34	1.37
16	I	101	BCL	C1D-C2D	2.75	1.50	1.45
16	Y	101	BCL	CHD-C4C	2.74	1.47	1.39
16	O	502	BCL	CHD-C4C	2.74	1.47	1.39
16	5	102	BCL	CHD-C4C	2.74	1.46	1.39
16	9	101	BCL	CHD-C4C	2.74	1.46	1.39
16	L	301	BCL	C3D-C2D	2.73	1.46	1.39
16	I	101	BCL	C1D-ND	-2.72	1.34	1.37
16	A	101	BCL	CHD-C4C	2.71	1.46	1.39
16	K	102	BCL	CHD-C4C	2.70	1.46	1.39
16	F	502	BCL	C1D-ND	-2.69	1.34	1.37
16	S	101	BCL	CHD-C4C	2.69	1.46	1.39
16	7	102	BCL	C1D-C2D	2.69	1.50	1.45
16	M	404	BCL	C3D-C2D	2.68	1.46	1.39
16	5	102	BCL	C1D-ND	-2.67	1.34	1.37
16	3	101	BCL	CHD-C4C	2.67	1.46	1.39
16	W	101	BCL	CHD-C4C	2.67	1.46	1.39
16	D	503	BCL	CHD-C4C	2.67	1.46	1.39
16	U	101	BCL	CHD-C4C	2.66	1.46	1.39
16	Q	102	BCL	CHD-C4C	2.66	1.46	1.39
16	A	101	BCL	C1D-C2D	2.66	1.50	1.45
16	F	502	BCL	C1D-C2D	2.66	1.50	1.45
16	7	102	BCL	C1D-ND	-2.65	1.34	1.37
16	1	402	BCL	CHD-C4C	2.64	1.46	1.39
16	5	102	BCL	C1D-C2D	2.63	1.50	1.45
16	L	307	BCL	CHD-C4C	2.61	1.46	1.39
16	3	101	BCL	C1D-C2D	2.61	1.50	1.45
16	W	101	BCL	C1D-C2D	2.60	1.50	1.45
16	M	403	BCL	CHD-C4C	2.59	1.46	1.39
16	O	502	BCL	C1D-C2D	2.56	1.50	1.45
16	K	102	BCL	C1D-C2D	2.56	1.50	1.45
16	U	101	BCL	C1D-C2D	2.55	1.50	1.45
16	S	101	BCL	C1D-C2D	2.55	1.50	1.45
16	9	101	BCL	C1D-C2D	2.54	1.50	1.45
16	Y	101	BCL	C1D-C2D	2.52	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	402	BCL	C1D-C2D	2.51	1.50	1.45
16	L	301	BCL	CHD-C4C	2.51	1.46	1.39
16	M	404	BCL	C1D-C2D	2.50	1.50	1.45
16	Q	102	BCL	C1D-C2D	2.50	1.50	1.45
16	M	404	BCL	CHD-C4C	2.48	1.46	1.39
16	D	503	BCL	C1D-C2D	2.46	1.50	1.45
16	M	404	BCL	MG-NA	-2.45	2.00	2.06
22	D	502	CDL	OA8-CA7	2.45	1.45	1.33
16	4	101	BCL	MG-NA	-2.44	2.00	2.06
16	L	307	BCL	C1D-C2D	2.44	1.50	1.45
16	K	102	BCL	MG-NA	-2.43	2.00	2.06
16	Z	102	BCL	CHD-C4C	2.43	1.46	1.39
16	3	101	BCL	MG-NA	-2.43	2.00	2.06
16	L	307	BCL	MG-NA	-2.43	2.00	2.06
16	G	102	BCL	CHD-C4C	2.42	1.46	1.39
16	5	102	BCL	MG-NA	-2.41	2.00	2.06
16	4	101	BCL	CHD-C4C	2.40	1.46	1.39
16	9	101	BCL	MG-NA	-2.40	2.00	2.06
16	8	102	BCL	CHD-C4C	2.39	1.46	1.39
16	M	403	BCL	MG-NA	-2.39	2.00	2.06
16	P	102	BCL	CHD-C4C	2.38	1.45	1.39
16	0	102	BCL	CHD-C4C	2.37	1.45	1.39
16	B	102	BCL	CHD-C4C	2.36	1.45	1.39
16	E	102	BCL	CHD-C4C	2.36	1.45	1.39
16	2	102	BCL	CHD-C4C	2.36	1.45	1.39
16	Y	101	BCL	MG-NA	-2.36	2.00	2.06
16	N	101	BCL	CHD-C4C	2.35	1.45	1.39
16	I	101	BCL	MG-NC	-2.35	2.00	2.06
16	T	101	BCL	CHD-C4C	2.34	1.45	1.39
16	X	102	BCL	CHD-C4C	2.34	1.45	1.39
16	7	102	BCL	MG-NC	-2.34	2.00	2.06
16	6	101	BCL	CHD-C4C	2.34	1.45	1.39
16	M	403	BCL	C1D-C2D	2.34	1.49	1.45
16	G	102	BCL	MG-NA	-2.33	2.00	2.06
16	J	101	BCL	CHD-C4C	2.33	1.45	1.39
16	V	102	BCL	CHD-C4C	2.33	1.45	1.39
16	L	301	BCL	C1D-C2D	2.32	1.49	1.45
16	F	502	BCL	MG-NC	-2.32	2.00	2.06
16	I	101	BCL	MG-NA	-2.31	2.00	2.06
16	6	101	BCL	MG-NA	-2.31	2.00	2.06
16	R	101	BCL	CHD-C4C	2.30	1.45	1.39
16	7	102	BCL	MG-NA	-2.28	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	102	BCL	MG-NA	-2.28	2.00	2.06
16	2	102	BCL	MG-NA	-2.28	2.00	2.06
16	F	502	BCL	MG-NA	-2.26	2.00	2.06
16	M	404	BCL	MG-NC	-2.26	2.00	2.06
16	O	502	BCL	MG-NA	-2.25	2.00	2.06
16	N	101	BCL	MG-NA	-2.24	2.00	2.06
16	3	101	BCL	C1B-CHB	2.24	1.47	1.41
16	6	101	BCL	C1B-CHB	2.24	1.47	1.41
16	S	101	BCL	MG-NA	-2.23	2.01	2.06
16	5	102	BCL	MG-NC	-2.23	2.01	2.06
16	V	102	BCL	MG-NA	-2.23	2.01	2.06
16	1	402	BCL	MG-NA	-2.23	2.01	2.06
16	R	101	BCL	MG-NA	-2.22	2.01	2.06
16	9	101	BCL	MG-NC	-2.22	2.01	2.06
16	Z	102	BCL	MG-NA	-2.22	2.01	2.06
16	P	102	BCL	MG-NA	-2.21	2.01	2.06
16	X	102	BCL	MG-NA	-2.21	2.01	2.06
16	0	102	BCL	MG-NA	-2.21	2.01	2.06
16	G	102	BCL	MG-NC	-2.20	2.01	2.06
16	8	102	BCL	MG-NA	-2.20	2.01	2.06
16	4	101	BCL	MG-NC	-2.20	2.01	2.06
16	Q	102	BCL	MG-NA	-2.19	2.01	2.06
16	B	102	BCL	MG-NA	-2.19	2.01	2.06
16	D	503	BCL	MG-NC	-2.19	2.01	2.06
16	M	403	BCL	C1B-CHB	2.18	1.47	1.41
16	D	503	BCL	MG-NA	-2.18	2.01	2.06
16	J	101	BCL	MG-NA	-2.18	2.01	2.06
16	A	101	BCL	MG-NA	-2.18	2.01	2.06
16	U	101	BCL	MG-NA	-2.17	2.01	2.06
16	Y	101	BCL	MG-NC	-2.17	2.01	2.06
16	K	102	BCL	C1B-CHB	2.16	1.47	1.41
16	8	102	BCL	MG-NC	-2.16	2.01	2.06
16	S	101	BCL	C1B-CHB	2.16	1.47	1.41
16	Z	102	BCL	C1D-C2D	2.15	1.49	1.45
16	6	101	BCL	MG-NC	-2.15	2.01	2.06
16	X	102	BCL	C1B-CHB	2.15	1.47	1.41
16	T	101	BCL	C1B-CHB	2.15	1.47	1.41
16	1	402	BCL	MG-NC	-2.14	2.01	2.06
16	I	101	BCL	C1B-CHB	2.14	1.47	1.41
16	G	102	BCL	C1D-C2D	2.14	1.49	1.45
17	M	405	BPH	C3A-C2A	-2.14	1.52	1.54
16	J	101	BCL	C1B-CHB	2.14	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	402	BCL	C1B-CHB	2.13	1.46	1.41
16	W	101	BCL	MG-NA	-2.13	2.01	2.06
16	M	404	BCL	C4B-CHC	2.13	1.46	1.41
16	Y	101	BCL	C1B-CHB	2.13	1.46	1.41
16	R	101	BCL	C1B-CHB	2.12	1.46	1.41
16	S	101	BCL	MG-NC	-2.11	2.01	2.06
16	L	307	BCL	C4B-CHC	2.11	1.46	1.41
16	K	102	BCL	MG-NC	-2.11	2.01	2.06
16	N	101	BCL	MG-NC	-2.11	2.01	2.06
16	4	101	BCL	C1B-CHB	2.11	1.46	1.41
16	5	102	BCL	C1B-CHB	2.11	1.46	1.41
10	C	402	HEM	C1D-ND	-2.11	1.34	1.38
16	4	101	BCL	C1D-C2D	2.11	1.49	1.45
16	O	502	BCL	MG-NC	-2.10	2.01	2.06
16	0	102	BCL	C1B-CHB	2.10	1.46	1.41
16	U	101	BCL	C1B-CHB	2.10	1.46	1.41
16	L	307	BCL	C1B-CHB	2.10	1.46	1.41
16	P	102	BCL	MG-NC	-2.10	2.01	2.06
16	9	101	BCL	C1B-CHB	2.10	1.46	1.41
10	C	403	HEM	C4B-NB	-2.09	1.34	1.38
16	L	301	BCL	C4B-CHC	2.09	1.46	1.41
16	3	101	BCL	MG-NC	-2.09	2.01	2.06
16	D	503	BCL	C1B-CHB	2.09	1.46	1.41
16	B	102	BCL	MG-NC	-2.09	2.01	2.06
16	7	102	BCL	C1B-CHB	2.09	1.46	1.41
10	C	404	HEM	C1D-ND	-2.08	1.34	1.38
16	Z	102	BCL	MG-NC	-2.08	2.01	2.06
10	C	403	HEM	C1D-ND	-2.08	1.34	1.38
16	B	102	BCL	C1B-CHB	2.08	1.46	1.41
16	L	301	BCL	MG-NC	-2.08	2.01	2.06
16	P	102	BCL	C1B-CHB	2.08	1.46	1.41
16	2	102	BCL	C1B-CHB	2.08	1.46	1.41
16	L	301	BCL	C1B-CHB	2.08	1.46	1.41
16	U	101	BCL	MG-NC	-2.07	2.01	2.06
16	E	102	BCL	C1D-C2D	2.07	1.49	1.45
16	O	502	BCL	C1B-CHB	2.07	1.46	1.41
16	F	502	BCL	C1B-CHB	2.07	1.46	1.41
16	F	502	BCL	C4B-CHC	2.07	1.46	1.41
16	E	102	BCL	MG-NC	-2.07	2.01	2.06
16	T	101	BCL	MG-NA	-2.07	2.01	2.06
10	C	401	HEM	C4B-NB	-2.07	1.34	1.38
16	Q	102	BCL	C1B-CHB	2.06	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	102	BCL	C1B-CHB	2.06	1.46	1.41
10	C	404	HEM	C4B-NB	-2.06	1.34	1.38
16	2	102	BCL	C1D-C2D	2.06	1.49	1.45
16	Z	102	BCL	C1B-CHB	2.06	1.46	1.41
16	R	101	BCL	MG-NC	-2.06	2.01	2.06
16	0	102	BCL	MG-NC	-2.05	2.01	2.06
16	G	102	BCL	C1B-CHB	2.05	1.46	1.41
16	V	102	BCL	C1B-CHB	2.05	1.46	1.41
16	A	101	BCL	MG-NC	-2.05	2.01	2.06
16	L	307	BCL	MG-NC	-2.04	2.01	2.06
16	N	101	BCL	C1B-CHB	2.04	1.46	1.41
16	X	102	BCL	MG-NC	-2.04	2.01	2.06
16	M	404	BCL	C1B-CHB	2.04	1.46	1.41
16	Q	102	BCL	MG-NC	-2.04	2.01	2.06
10	C	402	HEM	C4B-NB	-2.03	1.34	1.38
16	M	403	BCL	MG-NC	-2.03	2.01	2.06
16	1	402	BCL	C4B-CHC	2.03	1.46	1.41
16	2	102	BCL	MG-NC	-2.03	2.01	2.06
16	W	101	BCL	MG-NC	-2.03	2.01	2.06
16	4	101	BCL	C3C-C4C	-2.03	1.49	1.51
16	P	102	BCL	C1D-C2D	2.03	1.49	1.45
10	C	401	HEM	C1D-ND	-2.03	1.34	1.38
17	L	302	BPH	C3A-C2A	-2.03	1.52	1.54
17	L	302	BPH	CBD-CGD	-2.02	1.49	1.52
16	8	102	BCL	C1B-CHB	2.02	1.46	1.41
16	S	101	BCL	C4B-CHC	2.02	1.46	1.41
16	N	101	BCL	C1D-C2D	2.01	1.49	1.45
16	7	102	BCL	C4B-CHC	2.01	1.46	1.41
16	W	101	BCL	C4B-CHC	2.01	1.46	1.41
16	J	101	BCL	MG-NC	-2.00	2.01	2.06

All (1142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	K	101	CRT	C2-C1-C4	-16.37	85.73	110.86
21	Q	101	CRT	C3-C1-C4	-16.32	85.80	110.86
21	Q	101	CRT	C2-C1-C4	-15.78	86.63	110.86
21	K	101	CRT	C3-C1-C4	-11.94	92.53	110.86
16	3	101	BCL	CHD-C1D-ND	-8.70	116.46	124.45
16	M	404	BCL	CHD-C1D-ND	-8.67	116.49	124.45
16	A	101	BCL	CHD-C1D-ND	-8.67	116.49	124.45
16	5	102	BCL	CHD-C1D-ND	-8.65	116.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	7	102	BCL	CHD-C1D-ND	-8.61	116.55	124.45
16	F	502	BCL	CHD-C1D-ND	-8.58	116.57	124.45
16	Y	101	BCL	CHD-C1D-ND	-8.55	116.60	124.45
16	K	102	BCL	CHD-C1D-ND	-8.54	116.61	124.45
16	I	101	BCL	CHD-C1D-ND	-8.52	116.62	124.45
16	D	503	BCL	CHD-C1D-ND	-8.51	116.63	124.45
16	M	404	BCL	CMD-C2D-C1D	8.44	139.59	124.71
16	O	502	BCL	CHD-C1D-ND	-8.40	116.73	124.45
16	Q	102	BCL	CHD-C1D-ND	-8.38	116.75	124.45
16	S	101	BCL	CHD-C1D-ND	-8.35	116.78	124.45
16	U	101	BCL	CHD-C1D-ND	-8.35	116.78	124.45
16	1	402	BCL	CHD-C1D-ND	-8.34	116.79	124.45
16	9	101	BCL	CHD-C1D-ND	-8.34	116.79	124.45
16	W	101	BCL	CHD-C1D-ND	-8.26	116.86	124.45
16	L	307	BCL	CHD-C1D-ND	-8.20	116.92	124.45
16	7	102	BCL	CMD-C2D-C1D	8.13	139.05	124.71
16	A	101	BCL	CMD-C2D-C1D	8.09	138.96	124.71
16	F	502	BCL	CMD-C2D-C1D	8.06	138.92	124.71
16	I	101	BCL	CMD-C2D-C1D	8.02	138.85	124.71
16	5	102	BCL	CMD-C2D-C1D	7.94	138.71	124.71
16	M	403	BCL	CHD-C1D-ND	-7.89	117.20	124.45
16	O	502	BCL	CMD-C2D-C1D	7.88	138.60	124.71
16	L	301	BCL	CMD-C2D-C1D	7.85	138.54	124.71
16	3	101	BCL	CMD-C2D-C1D	7.83	138.51	124.71
16	Q	102	BCL	CMD-C2D-C1D	7.81	138.47	124.71
16	L	301	BCL	CHD-C1D-ND	-7.80	117.28	124.45
16	K	102	BCL	CMD-C2D-C1D	7.80	138.46	124.71
16	W	101	BCL	CMD-C2D-C1D	7.79	138.45	124.71
16	Y	101	BCL	CMD-C2D-C1D	7.78	138.43	124.71
16	9	101	BCL	CMD-C2D-C1D	7.74	138.36	124.71
16	S	101	BCL	CMD-C2D-C1D	7.70	138.28	124.71
16	U	101	BCL	CMD-C2D-C1D	7.68	138.24	124.71
16	D	503	BCL	CMD-C2D-C1D	7.67	138.23	124.71
16	4	101	BCL	CHD-C1D-ND	-7.57	117.50	124.45
16	1	402	BCL	CMD-C2D-C1D	7.57	138.05	124.71
16	G	102	BCL	CHD-C1D-ND	-7.45	117.61	124.45
16	Z	102	BCL	CHD-C1D-ND	-7.43	117.63	124.45
16	2	102	BCL	CHD-C1D-ND	-7.38	117.67	124.45
16	E	102	BCL	CHD-C1D-ND	-7.31	117.74	124.45
16	N	101	BCL	CHD-C1D-ND	-7.28	117.76	124.45
16	L	307	BCL	CMD-C2D-C1D	7.26	137.50	124.71
16	J	101	BCL	CHD-C1D-ND	-7.18	117.85	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	8	102	BCL	CHD-C1D-ND	-7.17	117.87	124.45
16	R	101	BCL	CHD-C1D-ND	-7.15	117.89	124.45
16	P	102	BCL	CHD-C1D-ND	-7.13	117.90	124.45
16	6	101	BCL	CHD-C1D-ND	-7.11	117.92	124.45
16	T	101	BCL	CHD-C1D-ND	-7.10	117.93	124.45
21	4	102	CRT	C31-C32-C33	-7.04	117.26	127.31
16	V	102	BCL	CHD-C1D-ND	-7.00	118.02	124.45
16	0	102	BCL	CHD-C1D-ND	-6.97	118.05	124.45
16	B	102	BCL	CHD-C1D-ND	-6.96	118.06	124.45
16	X	102	BCL	CHD-C1D-ND	-6.96	118.06	124.45
16	M	403	BCL	CMD-C2D-C1D	6.93	136.92	124.71
16	G	102	BCL	CMD-C2D-C1D	6.93	136.92	124.71
16	E	102	BCL	CMD-C2D-C1D	6.83	136.75	124.71
16	2	102	BCL	CMD-C2D-C1D	6.78	136.66	124.71
16	8	102	BCL	CMD-C2D-C1D	6.77	136.65	124.71
16	Z	102	BCL	CMD-C2D-C1D	6.76	136.63	124.71
16	4	101	BCL	CMD-C2D-C1D	6.74	136.59	124.71
16	B	102	BCL	CMD-C2D-C1D	6.69	136.51	124.71
16	J	101	BCL	CMD-C2D-C1D	6.66	136.46	124.71
16	6	101	BCL	CMD-C2D-C1D	6.66	136.44	124.71
16	N	101	BCL	CMD-C2D-C1D	6.58	136.31	124.71
16	P	102	BCL	CMD-C2D-C1D	6.53	136.22	124.71
16	0	102	BCL	CMD-C2D-C1D	6.53	136.22	124.71
16	T	101	BCL	CMD-C2D-C1D	6.53	136.21	124.71
16	X	102	BCL	CMD-C2D-C1D	6.51	136.18	124.71
16	R	101	BCL	CMD-C2D-C1D	6.43	136.05	124.71
16	V	102	BCL	CMD-C2D-C1D	6.25	135.73	124.71
21	2	103	CRT	C40-C38-C37	6.01	120.09	110.86
21	M	407	CRT	C40-C38-C37	5.95	119.99	110.86
21	V	103	CRT	C39-C38-C37	5.72	119.63	110.86
16	R	101	BCL	C2D-C1D-ND	5.60	114.23	110.10
16	M	403	BCL	O2D-CGD-CBD	5.59	121.20	111.27
16	M	404	BCL	O2D-CGD-CBD	5.53	121.10	111.27
16	E	102	BCL	C2D-C1D-ND	5.49	114.15	110.10
16	T	101	BCL	C2D-C1D-ND	5.45	114.12	110.10
16	4	101	BCL	C2D-C1D-ND	5.43	114.11	110.10
16	6	101	BCL	C2D-C1D-ND	5.41	114.09	110.10
16	2	102	BCL	C2D-C1D-ND	5.40	114.08	110.10
21	Q	101	CRT	C3-C1-C2	5.40	120.52	110.37
16	X	102	BCL	C2D-C1D-ND	5.39	114.08	110.10
16	Z	102	BCL	C2D-C1D-ND	5.39	114.08	110.10
16	N	101	BCL	C2D-C1D-ND	5.37	114.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	8	102	BCL	C2D-C1D-ND	5.36	114.05	110.10
21	V	103	CRT	C40-C38-C37	5.35	119.07	110.86
16	V	102	BCL	C2D-C1D-ND	5.33	114.03	110.10
21	V	103	CRT	C40-C38-C39	5.27	120.28	110.37
21	2	103	CRT	C40-C38-C39	5.26	120.26	110.37
16	L	307	BCL	O2D-CGD-CBD	5.24	120.57	111.27
16	L	301	BCL	C2D-C1D-ND	5.23	113.96	110.10
16	D	503	BCL	C2D-C1D-ND	5.22	113.95	110.10
16	J	101	BCL	C2D-C1D-ND	5.22	113.95	110.10
16	0	102	BCL	C2D-C1D-ND	5.22	113.95	110.10
16	M	404	BCL	C3D-C2D-C1D	-5.21	98.72	105.83
21	M	407	CRT	C40-C38-C39	5.21	120.17	110.37
16	P	102	BCL	C2D-C1D-ND	5.21	113.94	110.10
16	K	102	BCL	C2D-C1D-ND	5.20	113.94	110.10
16	1	402	BCL	C2D-C1D-ND	5.19	113.93	110.10
16	Y	101	BCL	C2D-C1D-ND	5.17	113.91	110.10
16	B	102	BCL	C2D-C1D-ND	5.16	113.91	110.10
10	C	402	HEM	CHC-C4B-NB	5.15	130.03	124.43
16	U	101	BCL	C2D-C1D-ND	5.13	113.88	110.10
16	D	503	BCL	O2D-CGD-CBD	5.08	120.30	111.27
16	3	101	BCL	C2D-C1D-ND	5.07	113.84	110.10
16	G	102	BCL	C2D-C1D-ND	5.04	113.82	110.10
21	2	103	CRT	C39-C38-C37	5.03	118.58	110.86
22	M	412	CDL	OA6-CA5-C11	5.03	120.34	111.09
10	C	403	HEM	CHC-C4B-NB	5.03	129.89	124.43
16	A	101	BCL	C2D-C1D-ND	5.02	113.80	110.10
21	T	102	CRT	C21-C22-C23	-5.01	120.15	127.31
16	O	502	BCL	C2D-C1D-ND	5.01	113.80	110.10
21	E	103	CRT	C21-C22-C23	-5.01	120.16	127.31
21	M	407	CRT	C39-C38-C37	5.01	118.55	110.86
16	F	502	BCL	C2D-C1D-ND	5.01	113.80	110.10
16	9	101	BCL	O2D-CGD-CBD	5.01	120.16	111.27
16	Q	102	BCL	C2D-C1D-ND	5.00	113.79	110.10
16	K	102	BCL	C3D-C2D-C1D	-4.99	99.02	105.83
16	L	301	BCL	C3D-C2D-C1D	-4.99	99.03	105.83
16	O	502	BCL	O2D-CGD-CBD	4.97	120.11	111.27
16	F	502	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
16	O	502	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
16	W	101	BCL	O2D-CGD-CBD	4.96	120.09	111.27
16	D	503	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
16	W	101	BCL	C2D-C1D-ND	4.96	113.76	110.10
16	A	101	BCL	O2D-CGD-CBD	4.95	120.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	101	BCL	C3D-C2D-C1D	-4.95	99.08	105.83
16	S	101	BCL	C2D-C1D-ND	4.95	113.75	110.10
16	U	101	BCL	C3D-C2D-C1D	-4.94	99.09	105.83
16	3	101	BCL	C3D-C2D-C1D	-4.94	99.09	105.83
10	C	401	HEM	CHC-C4B-NB	4.94	129.79	124.43
16	W	101	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
16	1	402	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
21	T	102	CRT	C10-C9-C7	-4.93	120.28	127.31
16	7	102	BCL	O2D-CGD-CBD	4.93	120.02	111.27
16	S	101	BCL	C3D-C2D-C1D	-4.92	99.11	105.83
16	M	404	BCL	CHD-C4C-NC	4.92	130.54	125.08
16	Q	102	BCL	C3D-C2D-C1D	-4.92	99.12	105.83
16	M	404	BCL	C2D-C1D-ND	4.91	113.73	110.10
16	W	101	BCL	CMB-C2B-C3B	4.89	133.82	124.68
16	A	101	BCL	C3D-C2D-C1D	-4.88	99.17	105.83
16	I	101	BCL	C3D-C2D-C1D	-4.88	99.18	105.83
10	C	404	HEM	CHC-C4B-NB	4.87	129.72	124.43
21	Z	103	CRT	C21-C22-C23	-4.87	120.36	127.31
16	1	402	BCL	O2D-CGD-CBD	4.87	119.92	111.27
16	7	102	BCL	C3D-C2D-C1D	-4.86	99.20	105.83
16	F	502	BCL	O2D-CGD-CBD	4.86	119.91	111.27
21	M	407	CRT	C21-C22-C23	-4.85	120.39	127.31
16	5	102	BCL	C3D-C2D-C1D	-4.84	99.22	105.83
16	Q	102	BCL	O2D-CGD-CBD	4.84	119.87	111.27
16	E	102	BCL	C3C-C4C-CHD	-4.84	113.06	123.39
16	I	101	BCL	O2D-CGD-CBD	4.83	119.85	111.27
18	L	304	UQ8	C7-C8-C9	-4.82	118.77	126.79
21	2	103	CRT	C21-C22-C23	-4.82	120.44	127.31
16	6	101	BCL	C3C-C4C-CHD	-4.81	113.11	123.39
16	T	101	BCL	C3C-C4C-CHD	-4.81	113.11	123.39
16	J	101	BCL	C3C-C4C-CHD	-4.81	113.12	123.39
16	S	101	BCL	O2D-CGD-CBD	4.80	119.80	111.27
16	4	101	BCL	CHD-C4C-NC	4.79	130.40	125.08
16	Q	102	BCL	CMB-C2B-C3B	4.79	133.64	124.68
21	K	101	CRT	C3-C1-C2	4.79	119.38	110.37
16	5	102	BCL	C2D-C1D-ND	4.79	113.63	110.10
16	3	101	BCL	O2D-CGD-CBD	4.79	119.77	111.27
16	U	101	BCL	O2D-CGD-CBD	4.78	119.76	111.27
16	9	101	BCL	C3D-C2D-C1D	-4.77	99.32	105.83
16	I	101	BCL	C2D-C1D-ND	4.77	113.62	110.10
16	K	102	BCL	O2D-CGD-CBD	4.76	119.72	111.27
16	Z	102	BCL	C3D-C2D-C1D	-4.75	99.35	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	402	BCL	CMB-C2B-C3B	4.74	133.55	124.68
21	B	103	CRT	C21-C22-C23	-4.74	120.54	127.31
16	8	102	BCL	C3C-C4C-CHD	-4.74	113.26	123.39
16	X	102	BCL	C3C-C4C-CHD	-4.74	113.27	123.39
16	4	101	BCL	C3D-C2D-C1D	-4.74	99.37	105.83
21	X	103	CRT	C21-C22-C23	-4.73	120.56	127.31
16	A	101	BCL	CMB-C2B-C3B	4.72	133.52	124.68
16	9	101	BCL	C2D-C1D-ND	4.72	113.58	110.10
16	2	102	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
16	2	102	BCL	C3C-C4C-CHD	-4.71	113.32	123.39
16	M	404	BCL	CMB-C2B-C3B	4.71	133.49	124.68
16	5	102	BCL	CMB-C2B-C3B	4.71	133.49	124.68
16	N	101	BCL	C3C-C4C-CHD	-4.71	113.34	123.39
16	V	102	BCL	C3C-C4C-CHD	-4.70	113.34	123.39
16	6	101	BCL	CHD-C4C-NC	4.70	130.30	125.08
21	8	103	CRT	C21-C22-C23	-4.70	120.60	127.31
16	B	102	BCL	C3C-C4C-CHD	-4.70	113.35	123.39
16	4	101	BCL	C3C-C4C-CHD	-4.69	113.37	123.39
16	R	101	BCL	C3C-C4C-CHD	-4.69	113.38	123.39
16	L	307	BCL	C2D-C1D-ND	4.69	113.56	110.10
16	Z	102	BCL	C3C-C4C-CHD	-4.69	113.38	123.39
16	E	102	BCL	C3D-C2D-C1D	-4.68	99.44	105.83
16	R	101	BCL	C3D-C2D-C1D	-4.68	99.44	105.83
16	E	102	BCL	CHD-C4C-NC	4.68	130.27	125.08
16	N	101	BCL	C3D-C2D-C1D	-4.68	99.45	105.83
16	X	102	BCL	C3D-C2D-C1D	-4.67	99.46	105.83
16	D	503	BCL	CMB-C2B-C3B	4.67	133.41	124.68
16	S	101	BCL	CMB-C2B-C3B	4.66	133.40	124.68
16	L	307	BCL	C3D-C2D-C1D	-4.66	99.48	105.83
16	8	102	BCL	C3D-C2D-C1D	-4.65	99.48	105.83
16	F	502	BCL	CMB-C2B-C3B	4.65	133.38	124.68
16	N	101	BCL	CHD-C4C-NC	4.65	130.24	125.08
16	6	101	BCL	C3D-C2D-C1D	-4.65	99.49	105.83
16	5	102	BCL	O2D-CGD-CBD	4.65	119.53	111.27
16	M	403	BCL	C3D-C2D-C1D	-4.64	99.49	105.83
16	8	102	BCL	CHD-C4C-NC	4.64	130.23	125.08
16	0	102	BCL	C3C-C4C-CHD	-4.64	113.48	123.39
16	P	102	BCL	C3C-C4C-CHD	-4.63	113.50	123.39
16	T	101	BCL	C3D-C2D-C1D	-4.61	99.53	105.83
21	N	102	CRT	C21-C22-C23	-4.61	120.73	127.31
16	B	102	BCL	CHD-C4C-NC	4.61	130.19	125.08
16	T	101	BCL	CMB-C2B-C3B	4.60	133.29	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	7	102	BCL	C2D-C1D-ND	4.60	113.50	110.10
16	K	102	BCL	CMB-C2B-C3B	4.60	133.29	124.68
10	C	401	HEM	CHD-C1D-ND	4.60	129.43	124.43
16	J	101	BCL	CHD-C4C-NC	4.59	130.18	125.08
16	T	101	BCL	CHD-C4C-NC	4.59	130.18	125.08
16	Z	102	BCL	CMB-C2B-C3B	4.58	133.25	124.68
16	M	403	BCL	C2D-C1D-ND	4.58	113.48	110.10
16	X	102	BCL	CHD-C4C-NC	4.58	130.16	125.08
16	G	102	BCL	C3C-C4C-CHD	-4.57	113.63	123.39
16	J	101	BCL	C3D-C2D-C1D	-4.57	99.59	105.83
16	G	102	BCL	CHD-C4C-NC	4.57	130.15	125.08
16	Y	101	BCL	O2D-CGD-CBD	4.56	119.37	111.27
16	G	102	BCL	C3D-C2D-C1D	-4.56	99.61	105.83
16	Z	102	BCL	CHD-C4C-NC	4.56	130.14	125.08
16	9	101	BCL	CMB-C2B-C3B	4.56	133.20	124.68
16	V	102	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
16	0	102	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
16	B	102	BCL	C3D-C2D-C1D	-4.54	99.63	105.83
16	2	102	BCL	CHD-C4C-NC	4.54	130.12	125.08
21	M	407	CRT	C20-C19-C17	-4.53	120.84	127.31
21	R	102	CRT	C21-C22-C23	-4.53	120.85	127.31
16	O	502	BCL	CMB-C2B-C3B	4.53	133.15	124.68
16	L	301	BCL	CHD-C4C-NC	4.52	130.10	125.08
16	B	102	BCL	CMB-C2B-C3B	4.52	133.14	124.68
16	V	102	BCL	CHD-C4C-NC	4.51	130.09	125.08
16	3	101	BCL	CHD-C4C-NC	4.51	130.08	125.08
16	N	101	BCL	CMB-C2B-C3B	4.51	133.11	124.68
16	0	102	BCL	CHD-C4C-NC	4.50	130.08	125.08
16	P	102	BCL	C3D-C2D-C1D	-4.50	99.69	105.83
16	M	404	BCL	C3C-C4C-CHD	-4.50	113.79	123.39
16	L	301	BCL	C3C-C4C-CHD	-4.49	113.81	123.39
16	R	101	BCL	CHD-C4C-NC	4.48	130.05	125.08
16	R	101	BCL	CMB-C2B-C3B	4.47	133.04	124.68
16	L	307	BCL	CMB-C2B-C3B	4.47	133.03	124.68
16	7	102	BCL	CMB-C2B-C3B	4.47	133.03	124.68
16	P	102	BCL	CHD-C4C-NC	4.46	130.03	125.08
21	K	101	CRT	C21-C22-C23	-4.46	120.95	127.31
16	L	301	BCL	CMB-C2B-C3B	4.42	132.96	124.68
16	M	403	BCL	CHD-C4C-NC	4.42	129.99	125.08
16	Y	101	BCL	CMB-C2B-C3B	4.42	132.96	124.68
21	T	102	CRT	C5-C6-C7	-4.42	119.21	125.89
22	D	502	CDL	OB6-CB5-C51	4.42	121.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	E	102	BCL	CMB-C2B-C3B	4.42	132.94	124.68
16	8	102	BCL	CMB-C2B-C3B	4.42	132.94	124.68
16	2	102	BCL	CMB-C2B-C3B	4.41	132.92	124.68
15	H	301	PGV	O01-C1-C2	4.39	120.97	111.50
21	V	103	CRT	C21-C22-C23	-4.39	121.04	127.31
21	0	103	CRT	C21-C22-C23	-4.38	121.05	127.31
16	G	102	BCL	CMB-C2B-C3B	4.38	132.88	124.68
16	L	307	BCL	CHD-C4C-NC	4.38	129.94	125.08
16	V	102	BCL	CMB-C2B-C3B	4.38	132.87	124.68
16	M	403	BCL	CMB-C2B-C3B	4.37	132.84	124.68
16	U	101	BCL	CMB-C2B-C3B	4.36	132.84	124.68
21	Q	101	CRT	C10-C9-C7	-4.36	121.08	127.31
16	I	101	BCL	CMB-C2B-C3B	4.36	132.83	124.68
10	C	404	HEM	CHD-C1D-ND	4.35	129.16	124.43
15	L	309	PGV	O01-C1-C2	4.35	120.87	111.50
16	J	101	BCL	CMB-C2B-C3B	4.34	132.80	124.68
16	P	102	BCL	CMB-C2B-C3B	4.33	132.78	124.68
16	S	101	BCL	CHD-C4C-NC	4.33	129.88	125.08
16	E	102	BCL	C1D-ND-C4D	-4.32	103.26	106.33
16	J	101	BCL	O2D-CGD-CBD	4.31	118.93	111.27
16	4	101	BCL	CMB-C2B-C3B	4.31	132.74	124.68
16	Y	101	BCL	CHD-C4C-NC	4.27	129.82	125.08
16	O	502	BCL	CHD-C4C-NC	4.26	129.81	125.08
16	K	102	BCL	CHD-C4C-NC	4.26	129.80	125.08
21	G	103	CRT	C21-C22-C23	-4.25	121.24	127.31
16	X	102	BCL	CMB-C2B-C3B	4.25	132.63	124.68
16	Y	101	BCL	C1D-ND-C4D	-4.25	103.32	106.33
22	M	411	CDL	OA6-CA5-C11	4.25	120.65	111.50
16	A	101	BCL	C1D-ND-C4D	-4.24	103.33	106.33
10	C	402	HEM	CHD-C1D-ND	4.24	129.03	124.43
16	3	101	BCL	CMB-C2B-C3B	4.23	132.59	124.68
16	1	402	BCL	CHD-C4C-NC	4.22	129.76	125.08
16	R	101	BCL	C1D-ND-C4D	-4.22	103.34	106.33
16	0	102	BCL	CMB-C2B-C3B	4.20	132.54	124.68
16	T	101	BCL	C1D-ND-C4D	-4.19	103.36	106.33
16	D	503	BCL	C1D-ND-C4D	-4.19	103.36	106.33
15	L	306	PGV	O01-C1-C2	4.17	120.50	111.50
16	L	307	BCL	C3C-C4C-CHD	-4.17	114.49	123.39
16	2	102	BCL	C1D-ND-C4D	-4.17	103.38	106.33
16	F	502	BCL	CHD-C4C-NC	4.16	129.70	125.08
16	M	403	BCL	C3C-C4C-CHD	-4.15	114.52	123.39
21	Q	101	CRT	C5-C6-C7	-4.15	119.62	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	305	PGV	O01-C1-C2	4.15	120.45	111.50
16	U	101	BCL	C1D-ND-C4D	-4.15	103.39	106.33
16	Z	102	BCL	C1D-ND-C4D	-4.14	103.39	106.33
16	Q	102	BCL	CHD-C4C-NC	4.14	129.67	125.08
16	N	101	BCL	C1D-ND-C4D	-4.13	103.40	106.33
16	F	502	BCL	C1D-ND-C4D	-4.12	103.41	106.33
16	4	101	BCL	O2D-CGD-CBD	4.12	118.58	111.27
16	D	503	BCL	CHD-C4C-NC	4.11	129.65	125.08
16	8	102	BCL	C1D-ND-C4D	-4.11	103.41	106.33
16	K	102	BCL	C1D-ND-C4D	-4.11	103.41	106.33
16	6	101	BCL	C1D-ND-C4D	-4.11	103.42	106.33
16	6	101	BCL	CMB-C2B-C3B	4.10	132.35	124.68
16	0	102	BCL	C1D-ND-C4D	-4.10	103.42	106.33
16	5	102	BCL	CHD-C4C-NC	4.09	129.62	125.08
10	C	403	HEM	CHD-C1D-ND	4.08	128.87	124.43
21	4	102	CRT	C29-C28-C30	4.08	124.51	118.08
16	A	101	BCL	CHD-C4C-NC	4.07	129.60	125.08
16	O	502	BCL	C3C-C4C-CHD	-4.07	114.70	123.39
16	G	102	BCL	C1D-ND-C4D	-4.07	103.44	106.33
21	Z	103	CRT	C5-C6-C7	-4.07	119.75	125.89
16	4	101	BCL	C1D-ND-C4D	-4.06	103.45	106.33
16	B	102	BCL	C1D-ND-C4D	-4.05	103.46	106.33
15	M	408	PGV	O01-C1-C2	4.05	120.22	111.50
16	1	402	BCL	C1D-ND-C4D	-4.05	103.46	106.33
16	8	102	BCL	O2D-CGD-CBD	4.04	118.45	111.27
21	Q	101	CRT	C21-C22-C23	-4.04	121.54	127.31
16	P	102	BCL	C1D-ND-C4D	-4.03	103.47	106.33
16	Q	102	BCL	C3C-C4C-CHD	-4.03	114.78	123.39
16	X	102	BCL	C1D-ND-C4D	-4.01	103.48	106.33
16	D	503	BCL	C3C-C4C-CHD	-4.01	114.82	123.39
16	A	101	BCL	C3C-C4C-CHD	-4.00	114.84	123.39
16	L	301	BCL	C1D-ND-C4D	-4.00	103.49	106.33
15	M	410	PGV	O01-C1-C2	4.00	120.11	111.50
16	O	502	BCL	C1D-ND-C4D	-3.99	103.50	106.33
22	M	409	CDL	OB6-CB5-C51	3.98	120.09	111.50
16	J	101	BCL	C1D-ND-C4D	-3.98	103.51	106.33
16	3	101	BCL	C1D-ND-C4D	-3.97	103.51	106.33
22	M	411	CDL	OB6-CB5-C51	3.97	120.06	111.50
16	W	101	BCL	CHD-C4C-NC	3.97	129.49	125.08
10	C	402	HEM	CBA-CAA-C2A	-3.96	105.86	112.62
16	9	101	BCL	CHD-C4C-NC	3.96	129.48	125.08
16	I	101	BCL	C1D-ND-C4D	-3.96	103.53	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	102	BCL	C1D-ND-C4D	-3.95	103.53	106.33
21	Z	103	CRT	C10-C9-C7	-3.95	121.67	127.31
16	V	102	BCL	C1D-ND-C4D	-3.95	103.53	106.33
16	5	102	BCL	C1D-ND-C4D	-3.95	103.53	106.33
16	6	101	BCL	O2D-CGD-CBD	3.93	118.25	111.27
21	E	103	CRT	C20-C19-C17	-3.91	121.73	127.31
10	C	402	HEM	C1B-NB-C4B	3.91	109.11	105.07
16	W	101	BCL	C1D-ND-C4D	-3.90	103.56	106.33
16	0	102	BCL	O2D-CGD-CBD	3.90	118.20	111.27
16	U	101	BCL	CHD-C4C-NC	3.90	129.41	125.08
15	D	501	PGV	O01-C1-C2	3.90	119.90	111.50
16	S	101	BCL	C1D-ND-C4D	-3.90	103.57	106.33
16	W	101	BCL	C3C-C4C-CHD	-3.89	115.09	123.39
16	7	102	BCL	CHD-C4C-NC	3.89	129.39	125.08
16	3	101	BCL	C3C-C4C-CHD	-3.88	115.09	123.39
16	U	101	BCL	C3C-C4C-CHD	-3.87	115.12	123.39
16	2	102	BCL	O2D-CGD-CBD	3.85	118.11	111.27
16	N	101	BCL	O2D-CGD-CBD	3.85	118.11	111.27
16	Z	102	BCL	O2D-CGD-CBD	3.85	118.10	111.27
21	4	102	CRT	C21-C22-C23	-3.85	121.82	127.31
16	G	102	BCL	O2D-CGD-CBD	3.84	118.09	111.27
10	C	403	HEM	C1B-NB-C4B	3.82	109.02	105.07
16	B	102	BCL	O2D-CGD-CBD	3.81	118.04	111.27
21	X	103	CRT	C10-C9-C7	-3.81	121.87	127.31
16	R	101	BCL	O2D-CGD-CBD	3.81	118.04	111.27
16	9	101	BCL	C1D-ND-C4D	-3.81	103.63	106.33
16	I	101	BCL	CHD-C4C-NC	3.81	129.30	125.08
10	C	401	HEM	C1B-NB-C4B	3.80	109.00	105.07
10	C	404	HEM	C1B-NB-C4B	3.78	108.98	105.07
16	S	101	BCL	C3C-C4C-CHD	-3.78	115.32	123.39
16	1	402	BCL	C3C-C4C-CHD	-3.77	115.34	123.39
22	H	302	CDL	OA6-CA5-C11	3.76	119.61	111.50
16	P	102	BCL	O2D-CGD-CBD	3.75	117.94	111.27
16	K	102	BCL	C3C-C4C-CHD	-3.75	115.38	123.39
21	4	102	CRT	C20-C19-C17	-3.75	121.96	127.31
21	X	103	CRT	C5-C6-C7	-3.75	120.23	125.89
10	C	401	HEM	CHA-C4D-ND	3.75	129.01	124.38
16	7	102	BCL	C1D-ND-C4D	-3.74	103.68	106.33
15	1	401	PGV	O01-C1-C2	3.73	119.53	111.50
22	H	302	CDL	OB6-CB5-C51	3.71	119.51	111.50
16	Y	101	BCL	C3C-C4C-CHD	-3.71	115.47	123.39
24	5	101	LMT	C1-O1'-C1'	-3.69	107.72	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	102	BCL	O2D-CGD-CBD	3.69	117.83	111.27
16	L	307	BCL	C1D-ND-C4D	-3.69	103.72	106.33
16	M	404	BCL	C1D-ND-C4D	-3.68	103.72	106.33
22	D	502	CDL	OA6-CA5-C11	3.68	119.42	111.50
16	X	102	BCL	O2D-CGD-CBD	3.67	117.80	111.27
10	C	401	HEM	CHB-C1B-NB	3.66	128.91	124.38
22	M	412	CDL	OB6-CB5-C51	3.66	119.39	111.50
21	N	102	CRT	C10-C9-C7	-3.66	122.09	127.31
16	T	101	BCL	C1-C2-C3	-3.65	119.72	126.04
15	F	501	PGV	O01-C1-C2	3.65	119.36	111.50
21	N	102	CRT	C20-C19-C17	-3.64	122.11	127.31
15	C	409	PGV	O01-C1-C2	3.64	119.35	111.50
16	T	101	BCL	O2D-CGD-CBD	3.64	117.73	111.27
10	C	403	HEM	CHA-C4D-ND	3.63	128.87	124.38
16	M	404	BCL	O2D-CGD-O1D	-3.62	116.76	123.84
21	Q	101	CRT	C20-C19-C17	-3.61	122.15	127.31
16	L	307	BCL	C1-C2-C3	-3.60	119.82	126.04
21	X	103	CRT	C20-C19-C17	-3.60	122.17	127.31
21	7	101	CRT	C20-C19-C17	-3.58	122.19	127.31
16	4	101	BCL	C1-C2-C3	-3.58	119.86	126.04
16	E	102	BCL	O2D-CGD-CBD	3.57	117.60	111.27
10	C	401	HEM	CBA-CAA-C2A	-3.54	106.57	112.62
16	F	502	BCL	C3C-C4C-CHD	-3.53	115.84	123.39
16	O	502	BCL	C1-C2-C3	-3.52	119.96	126.04
16	P	102	BCL	C1-C2-C3	-3.51	119.98	126.04
21	8	103	CRT	C20-C19-C17	-3.50	122.31	127.31
16	M	403	BCL	C1D-ND-C4D	-3.50	103.85	106.33
16	L	301	BCL	O2D-CGD-CBD	3.49	117.48	111.27
16	9	101	BCL	C3C-C4C-CHD	-3.49	115.93	123.39
18	L	308	UQ8	C7-C8-C9	-3.48	121.00	126.79
16	K	102	BCL	C1-C2-C3	-3.46	120.06	126.04
16	Y	101	BCL	C1-C2-C3	-3.45	120.08	126.04
16	L	307	BCL	C3D-C4D-ND	3.44	115.81	110.24
16	Y	101	BCL	C3D-C4D-ND	3.43	115.79	110.24
16	A	101	BCL	C3D-C4D-ND	3.43	115.79	110.24
10	C	404	HEM	CHB-C1B-NB	3.43	128.62	124.38
21	G	103	CRT	C20-C19-C17	-3.43	122.42	127.31
22	M	412	CDL	CA4-OA6-CA5	-3.43	111.51	117.90
16	I	101	BCL	C3D-C4D-ND	3.41	115.76	110.24
16	U	101	BCL	C3D-C4D-ND	3.41	115.76	110.24
16	5	102	BCL	C3C-C4C-CHD	-3.40	116.12	123.39
21	Z	103	CRT	C20-C19-C17	-3.40	122.45	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	T	102	CRT	C20-C19-C17	-3.39	122.48	127.31
20	M	406	MQ8	C34-C33-C35	3.38	120.96	115.27
21	K	101	CRT	C20-C19-C17	-3.38	122.48	127.31
16	P	102	BCL	C3D-C4D-ND	3.38	115.71	110.24
16	K	102	BCL	C3D-C4D-ND	3.38	115.71	110.24
18	L	304	UQ8	C12-C13-C14	-3.38	119.52	127.66
16	N	101	BCL	C1-C2-C3	-3.37	120.21	126.04
16	V	102	BCL	C1-C2-C3	-3.37	120.21	126.04
16	7	102	BCL	C1-C2-C3	-3.37	120.22	126.04
16	F	502	BCL	C3D-C4D-ND	3.37	115.68	110.24
16	D	503	BCL	C3D-C4D-ND	3.36	115.68	110.24
16	9	101	BCL	C3D-C4D-ND	3.36	115.67	110.24
16	5	102	BCL	C3D-C4D-ND	3.35	115.67	110.24
16	O	502	BCL	C3D-C4D-ND	3.35	115.66	110.24
16	Z	102	BCL	C3D-C4D-ND	3.35	115.66	110.24
16	G	102	BCL	C3D-C4D-ND	3.35	115.66	110.24
10	C	402	HEM	CHB-C1B-NB	3.35	128.52	124.38
16	M	403	BCL	C3D-C4D-ND	3.35	115.65	110.24
16	E	102	BCL	C3D-C4D-ND	3.34	115.63	110.24
16	2	102	BCL	C3D-C4D-ND	3.33	115.63	110.24
21	M	407	CRT	C10-C9-C7	-3.33	122.56	127.31
18	L	304	UQ8	C40-C39-C41	3.33	120.87	115.27
21	N	102	CRT	C5-C6-C7	-3.33	120.86	125.89
16	0	102	BCL	C3D-C4D-ND	3.32	115.62	110.24
16	Q	102	BCL	C3D-C4D-ND	3.32	115.61	110.24
16	W	101	BCL	C3D-C4D-ND	3.32	115.61	110.24
16	1	402	BCL	C3D-C4D-ND	3.32	115.60	110.24
16	S	101	BCL	C3D-C4D-ND	3.31	115.59	110.24
16	M	404	BCL	O2A-CGA-CBA	3.31	122.29	111.91
16	N	101	BCL	C3D-C4D-ND	3.30	115.58	110.24
16	3	101	BCL	C3D-C4D-ND	3.30	115.58	110.24
16	8	102	BCL	C1-C2-C3	-3.30	120.33	126.04
16	M	403	BCL	C1-C2-C3	-3.30	120.34	126.04
16	8	102	BCL	C3D-C4D-ND	3.29	115.56	110.24
16	I	101	BCL	C3C-C4C-CHD	-3.29	116.36	123.39
16	R	101	BCL	C1-C2-C3	-3.29	120.36	126.04
22	M	411	CDL	OB8-CB7-C71	3.28	122.21	111.91
21	M	407	CRT	O2-C38-C40	-3.28	86.40	108.97
16	B	102	BCL	C3D-C4D-ND	3.28	115.55	110.24
16	7	102	BCL	C3D-C4D-ND	3.28	115.54	110.24
15	D	501	PGV	C02-O01-C1	-3.28	109.72	117.79
10	C	404	HEM	CHA-C4D-ND	3.27	128.42	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	303	UQ8	C7-C8-C9	-3.26	121.37	126.79
21	2	103	CRT	C20-C19-C17	-3.26	122.66	127.31
21	7	101	CRT	C10-C9-C7	-3.26	122.66	127.31
22	M	409	CDL	OA8-CA7-C31	3.26	119.92	111.38
16	R	101	BCL	C3D-C4D-ND	3.26	115.50	110.24
21	7	101	CRT	C21-C22-C23	-3.25	122.67	127.31
16	J	101	BCL	C3D-C4D-ND	3.25	115.50	110.24
16	4	101	BCL	C3D-C4D-ND	3.25	115.49	110.24
16	T	101	BCL	C3D-C4D-ND	3.25	115.49	110.24
16	L	301	BCL	O2A-CGA-CBA	3.24	122.09	111.91
16	X	102	BCL	C1-C2-C3	-3.24	120.44	126.04
16	0	102	BCL	C1-C2-C3	-3.24	120.45	126.04
16	2	102	BCL	C1-C2-C3	-3.24	120.45	126.04
16	6	101	BCL	C3D-C4D-ND	3.23	115.47	110.24
21	T	102	CRT	C32-C31-C30	-3.23	113.14	123.22
21	M	407	CRT	C32-C31-C30	-3.23	113.14	123.22
21	Q	101	CRT	C32-C31-C30	-3.23	113.14	123.22
18	L	308	UQ8	C30-C29-C31	3.22	120.69	115.27
16	0	102	BCL	C4-C3-C5	3.22	120.69	115.27
18	L	304	UQ8	C37-C38-C39	-3.22	119.91	127.66
21	2	103	CRT	C10-C9-C7	-3.22	122.72	127.31
10	C	402	HEM	CHA-C4D-ND	3.21	128.35	124.38
15	F	501	PGV	O03-C19-C20	3.21	122.00	111.91
16	V	102	BCL	C3D-C4D-ND	3.20	115.42	110.24
16	Q	102	BCL	C4-C3-C5	3.20	120.65	115.27
16	X	102	BCL	C3D-C4D-ND	3.18	115.38	110.24
18	L	303	UQ8	C15-C14-C16	3.18	120.62	115.27
18	L	303	UQ8	C1M-C1-C6	-3.17	119.23	124.40
18	L	304	UQ8	C27-C28-C29	-3.17	120.04	127.66
18	L	303	UQ8	C12-C13-C14	-3.16	120.05	127.66
21	V	103	CRT	O2-C38-C39	-3.15	87.28	108.97
16	T	101	BCL	C1C-NC-C4C	-3.15	105.29	106.71
21	X	103	CRT	C32-C31-C30	-3.15	113.38	123.22
16	7	102	BCL	C3C-C4C-CHD	-3.15	116.66	123.39
16	M	404	BCL	C3D-C4D-ND	3.14	115.32	110.24
16	E	102	BCL	C1C-NC-C4C	-3.14	105.30	106.71
16	D	503	BCL	C4-C3-C5	3.14	120.55	115.27
20	M	406	MQ8	C36-C37-C38	-3.13	120.12	127.66
16	3	101	BCL	C1C-NC-C4C	-3.12	105.30	106.71
21	4	102	CRT	C36-C35-C33	-3.12	121.17	125.89
21	Z	103	CRT	C31-C32-C33	-3.12	122.86	127.31
16	K	102	BCL	C4-C3-C5	3.11	120.51	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	101	CRT	C5-C6-C7	-3.11	121.19	125.89
16	J	101	BCL	C1C-NC-C4C	-3.11	105.31	106.71
16	W	101	BCL	C1-C2-C3	-3.11	120.67	126.04
16	6	101	BCL	C1-C2-C3	-3.10	120.67	126.04
21	Z	103	CRT	C26-C27-C28	-3.10	122.88	127.31
16	A	101	BCL	C1-C2-C3	-3.10	120.68	126.04
16	L	301	BCL	C3D-C4D-ND	3.10	115.25	110.24
16	R	101	BCL	C4-C3-C5	3.10	120.49	115.27
16	X	102	BCL	C1C-NC-C4C	-3.10	105.31	106.71
20	M	406	MQ8	C29-C28-C30	3.09	120.47	115.27
21	2	103	CRT	O2-C38-C40	-3.08	87.77	108.97
16	I	101	BCL	C1-C2-C3	-3.08	120.72	126.04
21	8	103	CRT	C10-C9-C7	-3.07	122.92	127.31
16	P	102	BCL	CHB-C4A-NA	3.06	128.74	124.51
16	D	503	BCL	C1-C2-C3	-3.06	120.75	126.04
16	G	102	BCL	C1-C2-C3	-3.06	120.75	126.04
16	V	102	BCL	C1C-NC-C4C	-3.06	105.33	106.71
21	B	103	CRT	C32-C31-C30	-3.06	113.68	123.22
21	4	102	CRT	C10-C9-C7	-3.05	122.95	127.31
21	M	407	CRT	C14-C15-C16	-3.05	113.70	123.22
21	B	103	CRT	C20-C19-C17	-3.04	122.98	127.31
21	N	102	CRT	C32-C31-C30	-3.03	113.76	123.22
16	Z	102	BCL	C1C-NC-C4C	-3.03	105.34	106.71
16	B	102	BCL	C1-C2-C3	-3.02	120.81	126.04
21	2	103	CRT	O2-C38-C39	-3.02	88.22	108.97
16	S	101	BCL	C4-C3-C5	3.02	120.34	115.27
21	Q	101	CRT	C15-C14-C12	-3.02	123.01	127.31
16	2	102	BCL	C4-C3-C5	3.01	120.34	115.27
16	Z	102	BCL	O2A-CGA-CBA	3.01	121.36	111.91
16	3	101	BCL	C4-C3-C5	3.01	120.33	115.27
21	K	101	CRT	C10-C9-C7	-3.01	123.02	127.31
16	4	101	BCL	CHB-C4A-NA	3.00	128.66	124.51
16	L	301	BCL	CED-O2D-CGD	3.00	122.72	115.94
16	A	101	BCL	CHC-C1C-NC	3.00	128.65	124.51
18	L	304	UQ8	C22-C23-C24	-2.99	120.45	127.66
21	0	103	CRT	C32-C31-C30	-2.99	113.89	123.22
16	R	101	BCL	C1C-NC-C4C	-2.99	105.36	106.71
16	J	101	BCL	C1-C2-C3	-2.99	120.88	126.04
21	Z	103	CRT	C14-C15-C16	-2.98	113.92	123.22
16	B	102	BCL	CHB-C4A-NA	2.98	128.63	124.51
16	B	102	BCL	C4-C3-C5	2.98	120.28	115.27
16	F	502	BCL	C4-C3-C5	2.98	120.28	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	101	LMT	C1B-O1B-C4'	-2.97	110.61	117.96
18	L	308	UQ8	C40-C39-C41	2.96	120.26	115.27
15	M	410	PGV	O03-C19-C20	2.96	121.20	111.91
18	L	304	UQ8	C35-C34-C36	2.96	120.25	115.27
21	E	103	CRT	C32-C31-C30	-2.96	113.98	123.22
16	2	102	BCL	O2A-CGA-CBA	2.96	121.20	111.91
16	5	102	BCL	C1-C2-C3	-2.96	120.92	126.04
21	V	103	CRT	C20-C19-C17	-2.96	123.09	127.31
21	G	103	CRT	C32-C31-C30	-2.96	113.98	123.22
16	P	102	BCL	C4-C3-C5	2.95	120.24	115.27
16	0	102	BCL	C1C-NC-C4C	-2.95	105.38	106.71
21	8	103	CRT	C32-C31-C30	-2.94	114.03	123.22
16	E	102	BCL	CHB-C4A-NA	2.94	128.58	124.51
16	E	102	BCL	O2A-CGA-CBA	2.94	121.14	111.91
21	K	101	CRT	C21-C20-C19	-2.94	117.45	123.47
16	M	404	BCL	C4A-NA-C1A	2.94	108.03	106.71
16	J	101	BCL	C4-C3-C5	2.94	120.21	115.27
16	A	101	BCL	C4-C3-C5	2.94	120.21	115.27
16	Q	102	BCL	CHC-C1C-NC	2.93	128.57	124.51
18	L	308	UQ8	C32-C33-C34	-2.93	120.60	127.66
21	V	103	CRT	O2-C38-C40	-2.93	88.81	108.97
10	C	403	HEM	CBA-CAA-C2A	-2.93	107.62	112.62
21	X	103	CRT	C21-C20-C19	-2.93	117.48	123.47
16	O	502	BCL	CHC-C1C-NC	2.92	128.54	124.51
16	8	102	BCL	CHB-C4A-NA	2.91	128.54	124.51
16	8	102	BCL	O2A-CGA-CBA	2.91	121.04	111.91
16	N	101	BCL	CHB-C4A-NA	2.90	128.53	124.51
16	N	101	BCL	O2A-CGA-CBA	2.89	120.99	111.91
16	6	101	BCL	C1C-NC-C4C	-2.89	105.41	106.71
16	K	102	BCL	CHC-C1C-NC	2.89	128.51	124.51
16	8	102	BCL	C4-C3-C5	2.89	120.13	115.27
16	G	102	BCL	C4-C3-C5	2.88	120.12	115.27
16	5	102	BCL	C4-C3-C5	2.88	120.12	115.27
21	G	103	CRT	C14-C15-C16	-2.88	114.23	123.22
16	0	102	BCL	CHB-C4A-NA	2.88	128.50	124.51
16	6	101	BCL	O2A-CGA-CBA	2.88	120.94	111.91
20	M	406	MQ8	C16-C17-C18	-2.88	120.73	127.66
15	M	408	PGV	C02-O01-C1	-2.88	110.71	117.79
16	6	101	BCL	CHB-C4A-NA	2.88	128.49	124.51
16	W	101	BCL	C4-C3-C5	2.87	120.11	115.27
16	V	102	BCL	CHB-C4A-NA	2.87	128.48	124.51
18	L	308	UQ8	C20-C19-C21	2.87	120.10	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	102	BCL	C1-C2-C3	-2.87	121.08	126.04
15	L	309	PGV	C02-O01-C1	-2.87	110.74	117.79
22	H	302	CDL	OA8-CA7-C31	2.86	120.90	111.91
21	T	102	CRT	C14-C15-C16	-2.86	114.28	123.22
21	T	102	CRT	C21-C20-C19	-2.86	117.62	123.47
24	E	101	LMT	C1B-O1B-C4'	-2.86	110.89	117.96
16	3	101	BCL	CHC-C1C-NC	2.85	128.46	124.51
15	L	309	PGV	O03-C19-C20	2.85	120.86	111.91
16	G	102	BCL	O2A-CGA-CBA	2.85	120.86	111.91
16	Q	102	BCL	C1-C2-C3	-2.85	121.11	126.04
18	L	304	UQ8	C15-C14-C16	2.85	120.06	115.27
16	J	101	BCL	CHB-C4A-NA	2.84	128.45	124.51
16	J	101	BCL	O2A-CGA-CBA	2.84	120.83	111.91
21	Z	103	CRT	C36-C35-C33	-2.84	121.60	125.89
16	2	102	BCL	CHB-C4A-NA	2.84	128.44	124.51
16	B	102	BCL	O2A-CGA-CBA	2.84	120.82	111.91
16	V	102	BCL	O2A-CGA-CBA	2.82	120.77	111.91
16	5	102	BCL	CHC-C1C-NC	2.82	128.42	124.51
16	6	101	BCL	C4-C3-C5	2.82	120.02	115.27
16	G	102	BCL	CHB-C4A-NA	2.82	128.41	124.51
21	E	103	CRT	C9-C10-C11	-2.81	114.44	123.22
16	L	301	BCL	C4-C3-C5	2.81	120.00	115.27
16	2	102	BCL	C1C-NC-C4C	-2.81	105.44	106.71
16	U	101	BCL	CHC-C1C-NC	2.81	128.40	124.51
16	U	101	BCL	C4-C3-C5	2.81	119.99	115.27
16	T	101	BCL	CHB-C4A-NA	2.80	128.39	124.51
21	R	102	CRT	C21-C20-C19	-2.80	117.73	123.47
18	L	308	UQ8	C35-C34-C36	2.80	119.99	115.27
21	0	103	CRT	C21-C20-C19	-2.80	117.74	123.47
21	V	103	CRT	C14-C15-C16	-2.80	114.48	123.22
21	R	102	CRT	C32-C31-C30	-2.80	114.49	123.22
16	S	101	BCL	C1-C2-C3	-2.80	121.21	126.04
16	M	403	BCL	C1C-NC-C4C	-2.79	105.45	106.71
16	I	101	BCL	C4-C3-C5	2.79	119.96	115.27
21	2	103	CRT	C32-C31-C30	-2.79	114.52	123.22
22	H	302	CDL	OB8-CB7-C71	2.79	120.65	111.91
21	M	407	CRT	C35-C33-C32	-2.79	114.67	118.94
16	F	502	BCL	C1-C2-C3	-2.78	121.23	126.04
16	8	102	BCL	C2A-C1A-CHA	-2.78	118.99	123.86
16	W	101	BCL	CHC-C1C-NC	2.78	128.36	124.51
16	M	403	BCL	CHC-C1C-NC	2.78	128.35	124.51
15	H	301	PGV	O03-C19-C20	2.77	120.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	402	BCL	C1-C2-C3	-2.77	121.25	126.04
21	B	103	CRT	C21-C20-C19	-2.77	117.80	123.47
16	F	502	BCL	CHC-C1C-NC	2.77	128.34	124.51
16	E	102	BCL	C4-C3-C5	2.76	119.92	115.27
21	V	103	CRT	C32-C31-C30	-2.76	114.60	123.22
16	M	403	BCL	O2D-CGD-O1D	-2.76	118.44	123.84
16	L	307	BCL	O2D-CGD-O1D	-2.75	118.45	123.84
21	R	102	CRT	C20-C19-C17	-2.75	123.38	127.31
16	P	102	BCL	O2A-CGA-CBA	2.75	120.54	111.91
21	M	407	CRT	O2-C38-C39	-2.75	90.06	108.97
10	C	404	HEM	CHD-C1D-C2D	-2.75	120.69	124.98
16	Y	101	BCL	O2A-CGA-CBA	2.74	120.52	111.91
10	C	403	HEM	CHB-C1B-NB	2.74	127.77	124.38
16	P	102	BCL	C2A-C1A-CHA	-2.74	119.07	123.86
16	4	101	BCL	C4A-NA-C1A	2.74	107.94	106.71
20	M	406	MQ8	C26-C27-C28	-2.73	121.08	127.66
16	B	102	BCL	C2A-C1A-CHA	-2.73	119.08	123.86
16	D	503	BCL	CHC-C1C-NC	2.73	128.28	124.51
16	4	101	BCL	O2A-CGA-CBA	2.73	120.47	111.91
18	L	308	UQ8	C1M-C1-C6	-2.72	119.96	124.40
21	M	407	CRT	C34-C33-C35	2.72	122.37	118.08
16	T	101	BCL	C2A-C1A-CHA	-2.72	119.10	123.86
16	X	102	BCL	CHB-C4A-NA	2.72	128.27	124.51
18	L	303	UQ8	C10-C9-C11	2.71	119.84	115.27
18	L	304	UQ8	C32-C33-C34	-2.71	121.13	127.66
21	4	102	CRT	C30-C28-C27	-2.71	114.78	118.94
15	1	401	PGV	O03-C19-C20	2.71	120.42	111.91
16	6	101	BCL	C2A-C1A-CHA	-2.71	119.12	123.86
16	N	101	BCL	C1C-NC-C4C	-2.71	105.49	106.71
21	E	103	CRT	C13-C12-C11	2.71	122.34	118.08
15	L	306	PGV	O03-C19-C20	2.71	120.40	111.91
16	L	307	BCL	O2A-CGA-CBA	2.70	120.39	111.91
16	2	102	BCL	C2A-C1A-CHA	-2.70	119.13	123.86
16	0	102	BCL	C2A-C1A-CHA	-2.70	119.13	123.86
21	K	101	CRT	C15-C14-C12	-2.70	123.45	127.31
16	Z	102	BCL	CHB-C4A-NA	2.70	128.24	124.51
21	0	103	CRT	C14-C15-C16	-2.70	114.80	123.22
16	P	102	BCL	C1C-NC-C4C	-2.70	105.49	106.71
16	X	102	BCL	C4-C3-C5	2.69	119.80	115.27
16	D	503	BCL	O2D-CGD-O1D	-2.69	118.57	123.84
16	U	101	BCL	O2A-CGA-CBA	2.69	120.35	111.91
16	Y	101	BCL	C4-C3-C5	2.69	119.80	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	7	102	BCL	C4-C3-C5	2.69	119.80	115.27
21	B	103	CRT	C5-C6-C7	-2.69	121.83	125.89
21	E	103	CRT	C14-C15-C16	-2.69	114.83	123.22
16	R	101	BCL	CHB-C4A-NA	2.68	128.22	124.51
16	9	101	BCL	C4-C3-C5	2.68	119.79	115.27
20	M	406	MQ8	C14-C13-C15	2.68	119.78	115.27
18	L	308	UQ8	C17-C18-C19	-2.68	121.20	127.66
16	Z	102	BCL	C2A-C1A-CHA	-2.68	119.17	123.86
16	M	404	BCL	C1D-CHD-C4C	-2.68	120.16	126.62
22	M	409	CDL	OA6-CA5-C11	2.68	118.27	110.80
21	7	101	CRT	C32-C31-C30	-2.68	114.86	123.22
16	N	101	BCL	C4-C3-C5	2.68	119.77	115.27
16	Y	101	BCL	CHC-C1C-NC	2.67	128.20	124.51
16	W	101	BCL	O2D-CGD-O1D	-2.67	118.62	123.84
24	B	101	LMT	C1B-O1B-C4'	-2.67	111.36	117.96
16	X	102	BCL	CHC-C1C-NC	2.67	128.20	124.51
21	K	101	CRT	C32-C31-C30	-2.66	114.91	123.22
16	M	404	BCL	CAA-C2A-C3A	-2.66	105.49	112.78
16	S	101	BCL	CHC-C1C-NC	2.66	128.19	124.51
16	B	102	BCL	CHC-C1C-NC	2.65	128.18	124.51
16	M	403	BCL	C4-C3-C5	2.65	119.73	115.27
16	I	101	BCL	CHC-C1C-NC	2.65	128.18	124.51
10	C	401	HEM	CHD-C1D-C2D	-2.65	120.84	124.98
16	P	102	BCL	CHC-C1C-NC	2.65	128.17	124.51
16	E	102	BCL	C1-C2-C3	-2.65	121.47	126.04
16	S	101	BCL	O2D-CGD-O1D	-2.64	118.67	123.84
16	T	101	BCL	C4-C3-C5	2.64	119.72	115.27
21	T	102	CRT	C8-C7-C9	-2.64	119.22	122.92
16	Z	102	BCL	CHC-C1C-NC	2.64	128.16	124.51
16	7	102	BCL	CHC-C1C-NC	2.64	128.16	124.51
20	M	406	MQ8	C45-C43-C44	2.64	119.70	115.27
21	0	103	CRT	C27-C26-C25	-2.63	115.00	123.22
20	M	406	MQ8	C24-C23-C25	2.63	119.70	115.27
16	K	102	BCL	O2A-CGA-CBA	2.63	120.17	111.91
21	R	102	CRT	C14-C15-C16	-2.63	115.02	123.22
21	G	103	CRT	C13-C12-C11	2.63	122.22	118.08
18	L	304	UQ8	C25-C24-C26	2.63	119.69	115.27
16	8	102	BCL	C1C-NC-C4C	-2.62	105.53	106.71
16	R	101	BCL	CHC-C1C-NC	2.62	128.14	124.51
16	E	102	BCL	C2A-C1A-CHA	-2.62	119.28	123.86
24	5	101	LMT	O1'-C1'-C2'	2.62	112.39	108.30
21	2	103	CRT	C5-C6-C7	-2.62	121.93	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	9	101	BCL	CHC-C1C-NC	2.62	128.13	124.51
16	A	101	BCL	O2D-CGD-O1D	-2.62	118.72	123.84
16	O	502	BCL	O2A-CGA-CBA	2.62	120.11	111.91
21	B	103	CRT	C14-C15-C16	-2.61	115.06	123.22
16	V	102	BCL	CHC-C1C-NC	2.61	128.13	124.51
16	3	101	BCL	C1D-CHD-C4C	-2.61	120.33	126.62
16	1	402	BCL	CHC-C1C-NC	2.61	128.12	124.51
16	9	101	BCL	O2A-CGA-CBA	2.61	120.09	111.91
16	O	502	BCL	C4-C3-C5	2.61	119.66	115.27
16	X	102	BCL	C2A-C1A-CHA	-2.61	119.30	123.86
16	3	101	BCL	C1-C2-C3	-2.61	121.54	126.04
21	G	103	CRT	C10-C9-C7	-2.61	123.59	127.31
21	Q	101	CRT	C34-C33-C35	2.60	122.18	118.08
16	X	102	BCL	O2A-CGA-CBA	2.60	120.07	111.91
16	Z	102	BCL	C4-C3-C5	2.60	119.64	115.27
22	M	411	CDL	OA8-CA7-C31	2.59	120.05	111.91
16	G	102	BCL	C2A-C1A-CHA	-2.59	119.32	123.86
21	4	102	CRT	C5-C6-C7	-2.59	121.98	125.89
10	C	402	HEM	CHD-C1D-C2D	-2.59	120.93	124.98
16	J	101	BCL	C2A-C1A-CHA	-2.59	119.33	123.86
16	4	101	BCL	C4-C3-C5	2.59	119.62	115.27
16	U	101	BCL	C1-C2-C3	-2.59	121.57	126.04
21	E	103	CRT	C21-C20-C19	-2.59	118.18	123.47
24	R	103	LMT	C1B-O1B-C4'	-2.58	111.57	117.96
16	M	403	BCL	C1D-CHD-C4C	-2.58	120.39	126.62
21	T	102	CRT	C36-C35-C33	-2.58	121.99	125.89
16	B	102	BCL	C1C-NC-C4C	-2.58	105.55	106.71
16	L	301	BCL	CHB-C4A-NA	2.58	128.08	124.51
16	M	404	BCL	CMD-C2D-C3D	-2.58	121.68	127.61
21	Z	103	CRT	C32-C31-C30	-2.57	115.18	123.22
21	E	103	CRT	C26-C27-C28	-2.57	123.64	127.31
21	B	103	CRT	C9-C10-C11	-2.57	115.19	123.22
21	Z	103	CRT	C13-C12-C11	2.57	122.13	118.08
16	J	101	BCL	CHC-C1C-NC	2.57	128.07	124.51
16	R	101	BCL	C2A-C1A-CHA	-2.57	119.37	123.86
20	M	406	MQ8	C41-C42-C43	-2.57	121.48	127.66
21	Z	103	CRT	C21-C20-C19	-2.56	118.22	123.47
16	7	102	BCL	O2A-CGA-CBA	2.56	119.95	111.91
16	M	404	BCL	CHB-C4A-NA	2.56	128.05	124.51
20	M	406	MQ8	C21-C22-C23	-2.56	121.50	127.66
16	V	102	BCL	C4-C3-C5	2.56	119.57	115.27
18	L	308	UQ8	C25-C24-C26	2.55	119.57	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	103	CRT	C26-C27-C28	-2.55	123.66	127.31
24	P	103	LMT	C1B-O1B-C4'	-2.55	111.64	117.96
21	K	101	CRT	C26-C27-C28	-2.55	123.67	127.31
24	J	102	LMT	C1B-O1B-C4'	-2.55	111.66	117.96
16	L	301	BCL	CHC-C1C-NC	2.55	128.03	124.51
21	X	103	CRT	C27-C26-C25	-2.55	115.27	123.22
10	C	404	HEM	CBA-CAA-C2A	-2.55	108.28	112.62
16	7	102	BCL	CMD-C2D-C3D	-2.55	121.76	127.61
16	0	102	BCL	CHC-C1C-NC	2.55	128.03	124.51
10	C	402	HEM	CAD-CBD-CGD	-2.54	108.13	113.60
24	G	101	LMT	C1B-O1B-C4'	-2.54	111.67	117.96
21	V	103	CRT	C21-C20-C19	-2.54	118.27	123.47
16	3	101	BCL	O2A-CGA-CBA	2.54	119.87	111.91
15	L	305	PGV	O03-C19-C20	2.53	119.86	111.91
21	B	103	CRT	C13-C12-C11	2.53	122.06	118.08
16	T	101	BCL	CHC-C1C-NC	2.53	128.01	124.51
16	I	101	BCL	CHB-C4A-NA	2.53	128.01	124.51
16	N	101	BCL	CHC-C1C-NC	2.53	128.00	124.51
15	D	501	PGV	O03-C19-C20	2.52	119.82	111.91
16	9	101	BCL	O2D-CGD-O1D	-2.52	118.91	123.84
21	R	102	CRT	C9-C10-C11	-2.52	115.36	123.22
22	M	412	CDL	OB8-CB7-C71	2.52	119.81	111.91
20	M	406	MQ8	C19-C18-C20	2.51	119.50	115.27
16	U	101	BCL	O2D-CGD-O1D	-2.51	118.92	123.84
21	Q	101	CRT	C35-C33-C32	-2.51	115.09	118.94
16	6	101	BCL	CHC-C1C-NC	2.51	127.98	124.51
18	L	303	UQ8	C20-C19-C21	2.51	119.50	115.27
16	2	102	BCL	CHC-C1C-NC	2.51	127.98	124.51
24	Z	101	LMT	O1'-C1'-C2'	2.51	112.22	108.30
16	M	404	BCL	C1C-NC-C4C	-2.50	105.58	106.71
21	X	103	CRT	C14-C15-C16	-2.50	115.40	123.22
16	8	102	BCL	CHC-C1C-NC	2.50	127.97	124.51
16	N	101	BCL	C2A-C1A-CHA	-2.50	119.48	123.86
16	D	503	BCL	O2A-CGA-CBA	2.50	119.75	111.91
21	X	103	CRT	C29-C28-C30	2.50	122.01	118.08
21	X	103	CRT	C34-C33-C35	2.50	122.01	118.08
18	L	304	UQ8	C20-C19-C21	2.50	119.47	115.27
16	A	101	BCL	CMD-C2D-C3D	-2.50	121.87	127.61
21	0	103	CRT	C20-C19-C17	-2.50	123.75	127.31
16	E	102	BCL	CHC-C1C-NC	2.50	127.96	124.51
16	O	502	BCL	O2D-CGD-O1D	-2.50	118.96	123.84
22	D	502	CDL	OB8-CB7-C71	2.50	119.74	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	308	UQ8	C46-C44-C45	2.49	120.11	114.60
24	Z	101	LMT	C1-O1'-C1'	-2.49	109.71	113.84
21	R	102	CRT	C18-C17-C16	2.49	122.00	118.08
18	L	304	UQ8	C46-C44-C45	2.49	120.10	114.60
16	V	102	BCL	C2A-C1A-CHA	-2.48	119.52	123.86
21	0	103	CRT	C9-C10-C11	-2.48	115.47	123.22
16	8	102	BCL	O2D-CGD-O1D	-2.48	118.99	123.84
22	M	409	CDL	CB4-OB6-CB5	-2.48	111.68	117.79
16	J	101	BCL	O2D-CGD-O1D	-2.48	118.99	123.84
15	C	409	PGV	O03-C19-C20	2.48	119.69	111.91
16	3	101	BCL	C4A-NA-C1A	2.48	107.82	106.71
18	L	303	UQ8	C25-C24-C26	2.48	120.08	114.60
21	G	103	CRT	C26-C27-C28	-2.47	123.78	127.31
16	L	301	BCL	C1-C2-C3	-2.47	121.77	126.04
15	C	409	PGV	C02-O01-C1	-2.47	111.71	117.79
21	E	103	CRT	C34-C33-C35	2.46	121.96	118.08
16	W	101	BCL	O2A-CGA-CBA	2.46	119.62	111.91
20	M	406	MQ8	C39-C38-C40	2.46	119.41	115.27
21	8	103	CRT	C15-C14-C12	-2.46	123.80	127.31
16	1	402	BCL	O2A-CGA-CBA	2.46	119.62	111.91
21	T	102	CRT	C13-C12-C11	2.46	121.95	118.08
18	L	303	UQ8	C17-C18-C19	-2.45	121.75	127.66
21	R	102	CRT	C34-C33-C35	2.45	121.94	118.08
16	K	102	BCL	O2D-CGD-O1D	-2.45	119.04	123.84
16	K	102	BCL	C1C-NC-C4C	-2.45	105.60	106.71
15	L	306	PGV	C02-O01-C1	-2.45	111.75	117.79
16	L	307	BCL	C4-C3-C5	2.45	119.39	115.27
21	N	102	CRT	C34-C33-C35	2.45	121.94	118.08
16	I	101	BCL	CMD-C2D-C3D	-2.45	121.98	127.61
21	X	103	CRT	C26-C27-C28	-2.45	123.81	127.31
15	M	408	PGV	O03-C19-C20	2.45	119.60	111.91
21	V	103	CRT	C9-C10-C11	-2.45	115.58	123.22
21	T	102	CRT	C27-C26-C25	-2.45	115.58	123.22
21	K	101	CRT	C14-C15-C16	-2.45	115.58	123.22
16	4	101	BCL	CHC-C1C-NC	2.45	127.89	124.51
16	3	101	BCL	CHB-C4A-NA	2.44	127.89	124.51
21	T	102	CRT	C29-C28-C30	2.44	121.92	118.08
10	C	401	HEM	C4D-ND-C1D	2.44	107.59	105.07
21	V	103	CRT	C10-C9-C7	-2.44	123.83	127.31
21	0	103	CRT	C13-C12-C11	2.44	121.92	118.08
21	Q	101	CRT	C27-C26-C25	-2.44	115.60	123.22
21	N	102	CRT	C21-C20-C19	-2.44	118.48	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	R	101	BCL	O2A-CGA-CBA	2.44	119.56	111.91
21	M	407	CRT	C13-C12-C11	2.44	121.91	118.08
16	Q	102	BCL	O2D-CGD-O1D	-2.43	119.08	123.84
18	L	308	UQ8	C22-C23-C24	-2.43	121.80	127.66
16	R	101	BCL	O2D-CGD-O1D	-2.43	119.08	123.84
16	1	402	BCL	C4-C3-C5	2.43	119.36	115.27
16	G	102	BCL	CHC-C1C-NC	2.43	127.87	124.51
21	B	103	CRT	C34-C33-C35	2.43	121.90	118.08
16	F	502	BCL	CMD-C2D-C3D	-2.43	122.03	127.61
21	V	103	CRT	C18-C17-C16	2.43	121.90	118.08
15	L	305	PGV	C02-O01-C1	-2.43	111.81	117.79
21	N	102	CRT	C29-C28-C30	2.43	121.90	118.08
16	A	101	BCL	O2A-CGA-CBA	2.42	119.52	111.91
21	E	103	CRT	C29-C28-C30	2.42	121.89	118.08
16	I	101	BCL	O2D-CGD-O1D	-2.42	119.11	123.84
16	X	102	BCL	C1D-CHD-C4C	-2.42	120.79	126.62
16	9	101	BCL	C1-C2-C3	-2.42	121.86	126.04
16	L	307	BCL	CHB-C4A-NA	2.42	127.85	124.51
21	V	103	CRT	C26-C27-C28	-2.42	123.86	127.31
16	6	101	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
21	V	103	CRT	C13-C12-C11	2.41	121.88	118.08
16	X	102	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
16	A	101	BCL	CHB-C4A-NA	2.41	127.84	124.51
16	5	102	BCL	CMD-C2D-C3D	-2.41	122.07	127.61
24	2	104	LMT	C1B-O1B-C4'	-2.41	112.00	117.96
16	1	402	BCL	O2D-CGD-O1D	-2.41	119.13	123.84
21	M	407	CRT	C9-C10-C11	-2.41	115.71	123.22
16	L	301	BCL	C1D-CHD-C4C	-2.40	120.83	126.62
16	4	101	BCL	C2A-C1A-CHA	-2.40	119.66	123.86
16	L	301	BCL	O2A-CGA-O1A	-2.40	117.54	123.59
21	2	103	CRT	C13-C12-C11	2.40	121.86	118.08
21	2	103	CRT	C14-C15-C16	-2.39	115.75	123.22
22	D	502	CDL	CB4-OB6-CB5	-2.39	111.91	117.79
16	2	102	BCL	O2D-CGD-O1D	-2.39	119.17	123.84
16	M	403	BCL	O2A-CGA-CBA	2.39	119.40	111.91
16	7	102	BCL	O2D-CGD-O1D	-2.39	119.17	123.84
21	N	102	CRT	C15-C14-C12	-2.39	123.91	127.31
10	C	403	HEM	CHD-C1D-C2D	-2.38	121.25	124.98
16	4	101	BCL	O2D-CGD-O1D	-2.38	119.19	123.84
16	9	101	BCL	C1D-CHD-C4C	-2.38	120.89	126.62
21	G	103	CRT	C34-C33-C35	2.38	121.82	118.08
21	R	102	CRT	C27-C26-C25	-2.38	115.80	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	102	BCL	O2D-CGD-O1D	-2.37	119.19	123.84
20	M	406	MQ8	C50-C48-C49	2.37	119.84	114.60
16	E	102	BCL	C1D-CHD-C4C	-2.37	120.90	126.62
16	N	101	BCL	C1D-CHD-C4C	-2.37	120.90	126.62
21	0	103	CRT	C18-C17-C16	2.37	121.81	118.08
16	V	102	BCL	O2D-CGD-O1D	-2.37	119.20	123.84
16	Y	101	BCL	O2D-CGD-O1D	-2.37	119.21	123.84
21	2	103	CRT	C21-C20-C19	-2.37	118.62	123.47
16	M	404	BCL	CHC-C1C-NC	2.37	127.79	124.51
16	9	101	BCL	CHB-C4A-NA	2.37	127.78	124.51
16	I	101	BCL	O2A-CGA-CBA	2.37	119.33	111.91
16	F	502	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
16	P	102	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
21	0	103	CRT	C29-C28-C30	2.36	121.80	118.08
16	Z	102	BCL	C1D-CHD-C4C	-2.36	120.92	126.62
16	0	102	BCL	C1D-CHD-C4C	-2.36	120.92	126.62
16	B	102	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
24	0	101	LMT	C1B-O1B-C4'	-2.36	112.12	117.96
21	X	103	CRT	C15-C14-C12	-2.36	123.94	127.31
16	M	404	BCL	O2A-CGA-O1A	-2.36	117.64	123.59
16	6	101	BCL	C1D-CHD-C4C	-2.36	120.93	126.62
21	B	103	CRT	C10-C9-C7	-2.36	123.95	127.31
21	E	103	CRT	C5-C6-C7	-2.35	122.33	125.89
16	5	102	BCL	O2D-CGD-O1D	-2.35	119.24	123.84
16	B	102	BCL	C1D-CHD-C4C	-2.35	120.95	126.62
21	4	102	CRT	C27-C26-C25	-2.35	115.89	123.22
18	L	304	UQ8	C17-C18-C19	-2.35	122.01	127.66
18	L	308	UQ8	C37-C38-C39	-2.35	122.01	127.66
18	L	308	UQ8	C10-C9-C11	2.34	119.21	115.27
21	G	103	CRT	C9-C10-C11	-2.34	115.91	123.22
16	Q	102	BCL	O2A-CGA-CBA	2.34	119.25	111.91
16	J	101	BCL	C1D-CHD-C4C	-2.34	120.98	126.62
16	T	101	BCL	C1D-CHD-C4C	-2.34	120.98	126.62
10	C	403	HEM	C4D-ND-C1D	2.33	107.48	105.07
15	M	410	PGV	O14-P-O13	2.33	119.81	110.68
16	M	404	BCL	C6-C5-C3	-2.33	107.34	113.45
21	8	103	CRT	C5-C6-C7	-2.33	122.37	125.89
24	4	103	LMT	C1B-O1B-C4'	-2.33	112.20	117.96
21	T	102	CRT	C26-C27-C28	-2.33	123.99	127.31
21	N	102	CRT	C27-C26-C25	-2.33	115.95	123.22
21	B	103	CRT	C18-C17-C16	2.33	121.74	118.08
16	V	102	BCL	C1D-CHD-C4C	-2.33	121.01	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	M	404	BCL	C4-C3-C2	-2.32	117.72	123.68
16	5	102	BCL	CHB-C4A-NA	2.32	127.72	124.51
16	4	101	BCL	C1D-CHD-C4C	-2.32	121.02	126.62
16	9	101	BCL	C1C-NC-C4C	-2.32	105.66	106.71
16	O	502	BCL	CHB-C4A-NA	2.32	127.72	124.51
16	F	502	BCL	CHB-C4A-NA	2.31	127.71	124.51
16	7	102	BCL	CHB-C4A-NA	2.31	127.71	124.51
16	3	101	BCL	O2D-CGD-O1D	-2.31	119.32	123.84
16	K	102	BCL	CHB-C4A-NA	2.31	127.71	124.51
21	V	103	CRT	C34-C33-C35	2.31	121.72	118.08
16	G	102	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
16	S	101	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
16	8	102	BCL	C1D-CHD-C4C	-2.30	121.06	126.62
21	B	103	CRT	C26-C27-C28	-2.30	124.02	127.31
21	R	102	CRT	C10-C9-C7	-2.30	124.02	127.31
16	9	101	BCL	CMD-C2D-C3D	-2.30	122.32	127.61
16	T	101	BCL	O2D-CGD-O1D	-2.30	119.34	123.84
16	A	101	BCL	C2A-C1A-CHA	-2.30	119.84	123.86
21	R	102	CRT	C29-C28-C30	2.30	121.70	118.08
16	5	102	BCL	C1D-CHD-C4C	-2.30	121.08	126.62
21	E	103	CRT	C27-C26-C25	-2.30	116.05	123.22
16	K	102	BCL	C2A-C1A-CHA	-2.30	119.84	123.86
16	F	502	BCL	O2A-CGA-CBA	2.30	119.11	111.91
21	E	103	CRT	C10-C9-C7	-2.29	124.04	127.31
16	Q	102	BCL	CHB-C4A-NA	2.29	127.68	124.51
16	O	502	BCL	CMD-C2D-C3D	-2.29	122.35	127.61
16	L	307	BCL	C4B-CHC-C1C	-2.29	125.59	130.12
18	L	304	UQ8	C1M-C1-C6	-2.28	120.67	124.40
10	C	401	HEM	CHB-C1B-C2B	-2.28	120.41	126.72
16	5	102	BCL	O2A-CGA-CBA	2.28	119.06	111.91
21	Z	103	CRT	C8-C7-C9	-2.28	119.73	122.92
21	V	103	CRT	C29-C28-C30	2.28	121.67	118.08
10	C	404	HEM	CAD-CBD-CGD	-2.28	108.71	113.60
16	S	101	BCL	O2A-CGA-CBA	2.27	119.05	111.91
16	B	102	BCL	C4D-CHA-C1A	-2.27	118.48	121.25
16	0	102	BCL	O2D-CGD-O1D	-2.27	119.40	123.84
16	3	101	BCL	CMD-C2D-C3D	-2.27	122.39	127.61
21	R	102	CRT	C13-C12-C11	2.27	121.65	118.08
16	7	102	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
16	K	102	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
24	8	101	LMT	C1B-O1B-C4'	-2.27	112.35	117.96
21	7	101	CRT	C15-C14-C12	-2.27	124.07	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	G	103	CRT	C29-C28-C30	2.27	121.65	118.08
16	Q	102	BCL	CMD-C2D-C3D	-2.26	122.41	127.61
16	G	102	BCL	O2D-CGD-O1D	-2.26	119.41	123.84
21	T	102	CRT	C18-C17-C16	2.26	121.64	118.08
16	G	102	BCL	C1C-NC-C4C	-2.26	105.69	106.71
16	R	101	BCL	C1D-CHD-C4C	-2.26	121.17	126.62
21	0	103	CRT	C34-C33-C35	2.26	121.63	118.08
16	L	301	BCL	CMD-C2D-C3D	-2.26	122.42	127.61
24	5	101	LMT	O1B-C4'-C3'	2.26	113.28	107.28
21	0	103	CRT	C10-C9-C7	-2.25	124.09	127.31
21	B	103	CRT	C29-C28-C30	2.25	121.63	118.08
16	2	102	BCL	C1D-CHD-C4C	-2.25	121.18	126.62
15	M	410	PGV	C02-O01-C1	-2.25	112.24	117.79
21	N	102	CRT	C26-C27-C28	-2.25	124.09	127.31
21	0	103	CRT	C26-C27-C28	-2.25	124.09	127.31
16	Q	102	BCL	C1C-NC-C4C	-2.25	105.69	106.71
21	R	102	CRT	C26-C27-C28	-2.25	124.10	127.31
16	W	101	BCL	CMD-C2D-C3D	-2.25	122.44	127.61
16	S	101	BCL	CHB-C4A-NA	2.25	127.62	124.51
21	8	103	CRT	C29-C28-C30	2.24	121.60	118.08
16	U	101	BCL	C2A-C1A-CHA	-2.23	119.95	123.86
18	L	304	UQ8	C30-C29-C31	2.23	119.03	115.27
22	H	302	CDL	CA4-OA6-CA5	-2.23	112.30	117.79
21	Z	103	CRT	C9-C10-C11	-2.23	116.25	123.22
16	Y	101	BCL	CHB-C4A-NA	2.23	127.60	124.51
16	Y	101	BCL	CMD-C2D-C3D	-2.23	122.49	127.61
21	8	103	CRT	C34-C33-C35	2.23	121.59	118.08
16	6	101	BCL	C4D-CHA-C1A	-2.23	118.54	121.25
21	V	103	CRT	C27-C26-C25	-2.23	116.27	123.22
16	P	102	BCL	C1D-CHD-C4C	-2.22	121.26	126.62
16	1	402	BCL	C1D-CHD-C4C	-2.22	121.26	126.62
16	Q	102	BCL	C1D-CHD-C4C	-2.22	121.27	126.62
21	G	103	CRT	C21-C20-C19	-2.22	118.93	123.47
10	C	402	HEM	C4D-ND-C1D	2.22	107.36	105.07
16	8	102	BCL	C4D-CHA-C1A	-2.22	118.55	121.25
21	0	103	CRT	C5-C6-C7	-2.21	122.55	125.89
10	C	401	HEM	CHA-C4D-C3D	-2.21	121.17	125.33
16	U	101	BCL	CHB-C4A-NA	2.21	127.57	124.51
21	8	103	CRT	C27-C26-C25	-2.21	116.31	123.22
16	K	102	BCL	CMD-C2D-C3D	-2.21	122.53	127.61
21	2	103	CRT	C34-C33-C35	2.21	121.56	118.08
16	F	502	BCL	C1D-CHD-C4C	-2.21	121.29	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	I	101	BCL	C2A-C1A-CHA	-2.21	120.00	123.86
21	K	101	CRT	C34-C33-C35	2.21	121.55	118.08
16	4	101	BCL	C1C-NC-C4C	-2.21	105.71	106.71
16	1	402	BCL	CHB-C4A-NA	2.21	127.56	124.51
16	Q	102	BCL	C2A-C1A-CHA	-2.20	120.00	123.86
21	V	103	CRT	C31-C32-C33	-2.20	124.17	127.31
24	H	303	LMT	C1B-O1B-C4'	-2.20	112.53	117.96
16	L	301	BCL	C2A-C1A-CHA	-2.19	120.02	123.86
24	8	101	LMT	C1-O1'-C1'	-2.19	110.21	113.84
16	N	101	BCL	O2D-CGD-O1D	-2.19	119.55	123.84
21	B	103	CRT	C27-C26-C25	-2.18	116.40	123.22
16	L	307	BCL	C1D-CHD-C4C	-2.18	121.36	126.62
15	H	301	PGV	C02-O01-C1	-2.18	112.42	117.79
21	8	103	CRT	C26-C27-C28	-2.18	124.20	127.31
16	S	101	BCL	CMD-C2D-C3D	-2.18	122.61	127.61
21	T	102	CRT	C34-C33-C35	2.18	121.51	118.08
21	7	101	CRT	C27-C26-C25	-2.18	116.43	123.22
21	N	102	CRT	C14-C15-C16	-2.17	116.44	123.22
21	8	103	CRT	C21-C20-C19	-2.17	119.04	123.47
16	9	101	BCL	C2A-C1A-CHA	-2.17	120.07	123.86
21	K	101	CRT	C18-C17-C16	2.17	121.49	118.08
21	7	101	CRT	C29-C28-C30	2.16	121.48	118.08
21	2	103	CRT	C29-C28-C30	2.16	121.48	118.08
22	M	411	CDL	OB8-CB7-OB9	-2.16	118.15	123.59
21	4	102	CRT	C31-C30-C28	2.16	132.47	126.42
10	C	403	HEM	CHA-C4D-C3D	-2.15	121.29	125.33
16	U	101	BCL	CMD-C2D-C3D	-2.15	122.67	127.61
16	P	102	BCL	C1-O2A-CGA	2.15	122.08	116.44
16	B	102	BCL	CED-O2D-CGD	2.15	120.80	115.94
16	W	101	BCL	CHB-C4A-NA	2.15	127.48	124.51
16	D	503	BCL	C2A-C1A-CHA	-2.15	120.11	123.86
16	7	102	BCL	C2A-C1A-CHA	-2.15	120.11	123.86
16	1	402	BCL	C2A-C1A-CHA	-2.14	120.11	123.86
21	G	103	CRT	C18-C17-C16	2.14	121.45	118.08
21	4	102	CRT	C14-C15-C16	-2.14	116.53	123.22
20	M	406	MQ8	C31-C32-C33	-2.14	122.50	127.66
16	3	101	BCL	C4B-CHC-C1C	-2.14	125.89	130.12
16	Y	101	BCL	C1D-CHD-C4C	-2.14	121.47	126.62
16	I	101	BCL	C1D-CHD-C4C	-2.14	121.47	126.62
16	O	502	BCL	C1D-CHD-C4C	-2.13	121.47	126.62
16	D	503	BCL	CMD-C2D-C3D	-2.13	122.71	127.61
16	W	101	BCL	C1D-CHD-C4C	-2.13	121.49	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	7	102	BCL	CHD-C1D-C2D	2.13	129.94	125.48
22	M	412	CDL	OA8-CA7-C31	2.13	118.58	111.91
16	1	402	BCL	C6-C5-C3	-2.13	107.88	113.45
16	F	502	BCL	C2A-C1A-CHA	-2.13	120.14	123.86
10	C	401	HEM	CBD-CAD-C3D	-2.12	106.72	112.63
16	2	102	BCL	O2A-CGA-O1A	-2.12	118.24	123.59
21	K	101	CRT	C1-C4-C5	2.12	118.67	113.06
21	Q	101	CRT	C8-C7-C9	-2.12	119.95	122.92
21	M	407	CRT	C30-C28-C27	-2.11	115.70	118.94
21	Z	103	CRT	C18-C17-C16	2.11	121.41	118.08
21	R	102	CRT	C5-C6-C7	-2.11	122.70	125.89
16	O	502	BCL	C2A-C1A-CHA	-2.11	120.17	123.86
16	M	403	BCL	C1-O2A-CGA	2.11	121.98	116.44
21	X	103	CRT	C13-C12-C11	2.11	121.40	118.08
16	D	503	BCL	CHB-C4A-NA	2.11	127.43	124.51
21	M	407	CRT	C27-C26-C25	-2.11	116.64	123.22
16	5	102	BCL	C2A-C1A-CHA	-2.11	120.18	123.86
16	M	403	BCL	CHB-C4A-NA	2.11	127.42	124.51
22	M	411	CDL	CB6-CB4-CB3	-2.10	106.81	111.79
10	C	404	HEM	C4D-ND-C1D	2.10	107.24	105.07
22	M	412	CDL	CB4-OB6-CB5	-2.10	112.63	117.79
16	V	102	BCL	C1-O2A-CGA	2.10	121.94	116.44
16	Y	101	BCL	C2A-C1A-CHA	-2.09	120.20	123.86
16	4	101	BCL	C4B-CHC-C1C	-2.09	125.97	130.12
16	W	101	BCL	C2A-C1A-CHA	-2.09	120.20	123.86
15	F	501	PGV	O03-C19-O04	-2.09	118.31	123.59
16	E	102	BCL	O2D-CGD-O1D	-2.09	119.75	123.84
21	2	103	CRT	C9-C10-C11	-2.09	116.70	123.22
15	M	410	PGV	O03-C19-O04	-2.09	118.33	123.59
16	G	102	BCL	C4B-CHC-C1C	-2.08	125.99	130.12
16	P	102	BCL	C4D-CHA-C1A	-2.08	118.71	121.25
21	G	103	CRT	C27-C26-C25	-2.08	116.72	123.22
16	6	101	BCL	O2A-CGA-O1A	-2.08	118.33	123.59
16	L	301	BCL	C4D-CHA-C1A	-2.08	118.72	121.25
15	H	301	PGV	O01-C1-O02	-2.08	118.68	123.70
24	Z	101	LMT	O5'-C5'-C4'	2.08	114.14	109.75
16	5	102	BCL	CHD-C1D-C2D	2.08	129.84	125.48
22	M	411	CDL	CB4-OB6-CB5	-2.08	112.68	117.79
21	E	103	CRT	C11-C12-C14	-2.08	115.75	118.94
21	G	103	CRT	C35-C33-C32	-2.08	115.75	118.94
16	B	102	BCL	C1-O2A-CGA	2.07	121.89	116.44
16	M	403	BCL	C4B-CHC-C1C	-2.07	126.01	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	402	BCL	CMD-C2D-C3D	-2.07	122.84	127.61
16	S	101	BCL	C2A-C1A-CHA	-2.07	120.24	123.86
21	Q	101	CRT	C21-C20-C19	-2.07	119.23	123.47
16	E	102	BCL	C4A-NA-C1A	2.07	107.64	106.71
21	X	103	CRT	C18-C17-C16	2.06	121.32	118.08
16	M	404	BCL	CGD-CBD-CAD	-2.06	104.06	110.73
21	8	103	CRT	C14-C15-C16	-2.06	116.79	123.22
16	M	403	BCL	C2A-C1A-CHA	-2.06	120.26	123.86
16	7	102	BCL	C4B-CHC-C1C	-2.06	126.04	130.12
21	E	103	CRT	C18-C17-C16	2.06	121.32	118.08
18	L	308	UQ8	C32-C31-C29	-2.05	106.22	112.98
16	3	101	BCL	C2A-C1A-CHA	-2.04	120.29	123.86
16	G	102	BCL	C11-C10-C8	-2.04	109.32	115.92
22	H	302	CDL	OA8-CA7-OA9	-2.04	118.44	123.59
16	M	404	BCL	CHD-C1D-C2D	2.04	129.76	125.48
16	K	102	BCL	C4A-NA-C1A	2.04	107.62	106.71
16	N	101	BCL	C4A-NA-C1A	2.04	107.62	106.71
16	5	102	BCL	C1C-NC-C4C	-2.04	105.79	106.71
10	C	404	HEM	CHA-C4D-C3D	-2.04	121.50	125.33
15	M	410	PGV	O01-C1-O02	-2.04	118.78	123.70
16	9	101	BCL	C4B-CHC-C1C	-2.04	126.08	130.12
18	L	303	UQ8	C22-C23-C24	-2.04	120.79	127.75
16	I	101	BCL	CHD-C1D-C2D	2.03	129.75	125.48
24	M	414	LMT	C1-O1'-C1'	-2.03	110.47	113.84
16	G	102	BCL	C11-C12-C13	-2.03	109.36	115.92
24	2	101	LMT	C1B-O1B-C4'	-2.03	112.95	117.96
21	N	102	CRT	C18-C17-C16	2.02	121.27	118.08
16	M	403	BCL	O1D-CGD-CBD	-2.02	120.34	124.48
16	2	102	BCL	C4D-CHA-C1A	-2.02	118.79	121.25
21	Z	103	CRT	C27-C26-C25	-2.02	116.91	123.22
22	D	502	CDL	OB6-CB5-OB7	-2.02	118.82	123.70
21	Q	101	CRT	C29-C28-C30	2.02	121.26	118.08
21	N	102	CRT	C35-C33-C32	-2.02	115.84	118.94
21	X	103	CRT	C9-C10-C11	-2.01	116.93	123.22
17	L	302	BPH	CMA-C3A-C4A	-2.01	109.97	114.38
16	A	101	BCL	CHD-C1D-C2D	2.01	129.70	125.48
16	3	101	BCL	CHD-C1D-C2D	2.01	129.70	125.48
10	C	404	HEM	CHB-C1B-C2B	-2.01	121.16	126.72
16	1	402	BCL	C1C-NC-C4C	-2.01	105.80	106.71
16	4	101	BCL	C4D-CHA-C1A	-2.01	118.81	121.25
15	C	409	PGV	O01-C1-O02	-2.00	118.86	123.70
21	4	102	CRT	C9-C10-C11	-2.00	116.97	123.22

There are no chirality outliers.

All (966) 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
10	C	404	HEM	C4B-C3B-CAB-CBB
15	C	409	PGV	C03-O11-P-O12
15	C	409	PGV	C03-O11-P-O13
15	C	409	PGV	C03-O11-P-O14
15	L	305	PGV	C04-O12-P-O11
15	L	305	PGV	C04-O12-P-O13
15	L	305	PGV	O12-C04-C05-C06
15	M	408	PGV	C03-O11-P-O14
15	D	501	PGV	C03-O11-P-O12
15	D	501	PGV	C03-O11-P-O13
15	D	501	PGV	C03-O11-P-O14
15	F	501	PGV	C04-O12-P-O13
15	1	401	PGV	C2-C1-O01-C02
16	M	404	BCL	CAD-CBD-CGD-O1D
16	M	404	BCL	CAD-CBD-CGD-O2D
16	A	101	BCL	C2C-C3C-CAC-CBC
16	A	101	BCL	C4C-C3C-CAC-CBC
16	B	102	BCL	C1A-C2A-CAA-CBA
16	B	102	BCL	C2C-C3C-CAC-CBC
16	B	102	BCL	C4C-C3C-CAC-CBC
16	D	503	BCL	C2C-C3C-CAC-CBC
16	D	503	BCL	C4C-C3C-CAC-CBC
16	F	502	BCL	CHA-CBD-CGD-O1D
16	G	102	BCL	C6-C7-C8-C9
16	I	101	BCL	C2-C3-C5-C6
16	I	101	BCL	C4-C3-C5-C6
16	O	502	BCL	C2C-C3C-CAC-CBC
16	O	502	BCL	C4C-C3C-CAC-CBC
16	Q	102	BCL	C2C-C3C-CAC-CBC
16	Q	102	BCL	C4C-C3C-CAC-CBC
16	Q	102	BCL	C2-C3-C5-C6
16	Q	102	BCL	C4-C3-C5-C6
16	R	101	BCL	C4-C3-C5-C6
16	S	101	BCL	C2-C3-C5-C6
16	S	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	T	101	BCL	C3A-C2A-CAA-CBA
16	T	101	BCL	C4C-C3C-CAC-CBC
16	U	101	BCL	C1A-C2A-CAA-CBA
16	U	101	BCL	C3A-C2A-CAA-CBA
16	U	101	BCL	C2C-C3C-CAC-CBC
16	U	101	BCL	C4C-C3C-CAC-CBC
16	V	102	BCL	C4C-C3C-CAC-CBC
16	W	101	BCL	C1A-C2A-CAA-CBA
16	W	101	BCL	C3A-C2A-CAA-CBA
16	W	101	BCL	C2C-C3C-CAC-CBC
16	W	101	BCL	C4C-C3C-CAC-CBC
16	Y	101	BCL	C3A-C2A-CAA-CBA
16	Y	101	BCL	C11-C10-C8-C7
16	Z	102	BCL	C2C-C3C-CAC-CBC
16	Z	102	BCL	C4C-C3C-CAC-CBC
16	1	402	BCL	C1A-C2A-CAA-CBA
16	1	402	BCL	C3A-C2A-CAA-CBA
16	2	102	BCL	C1A-C2A-CAA-CBA
16	3	101	BCL	C1A-C2A-CAA-CBA
16	3	101	BCL	C4-C3-C5-C6
16	7	102	BCL	C1A-C2A-CAA-CBA
16	7	102	BCL	C3A-C2A-CAA-CBA
16	7	102	BCL	C6-C7-C8-C9
16	8	102	BCL	C1A-C2A-CAA-CBA
16	9	101	BCL	C1A-C2A-CAA-CBA
16	9	101	BCL	C3A-C2A-CAA-CBA
16	0	102	BCL	C1A-C2A-CAA-CBA
16	0	102	BCL	C3A-C2A-CAA-CBA
18	L	303	UQ8	C14-C16-C17-C18
18	L	304	UQ8	C14-C16-C17-C18
18	L	308	UQ8	C14-C16-C17-C18
21	M	407	CRT	C32-C33-C35-C36
21	M	407	CRT	C34-C33-C35-C36
21	M	407	CRT	C35-C36-C37-C38
21	M	407	CRT	C36-C37-C38-C39
21	G	103	CRT	C36-C37-C38-C39
21	G	103	CRT	C36-C37-C38-C40
21	G	103	CRT	C36-C37-C38-O2
21	K	101	CRT	C1-C4-C5-C6
21	N	102	CRT	C10-C11-C12-C13
21	N	102	CRT	C15-C16-C17-C18
21	N	102	CRT	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
21	Q	101	CRT	C2-C1-O1-C1M
21	Q	101	CRT	C10-C11-C12-C13
21	Q	101	CRT	C10-C11-C12-C14
21	T	102	CRT	C2-C1-C4-C5
21	T	102	CRT	C3-C1-C4-C5
21	T	102	CRT	C5-C6-C7-C8
21	T	102	CRT	C5-C6-C7-C9
21	V	103	CRT	O1-C1-C4-C5
21	V	103	CRT	C2-C1-C4-C5
21	V	103	CRT	C3-C1-C4-C5
21	V	103	CRT	C36-C37-C38-C39
21	X	103	CRT	C10-C11-C12-C13
21	X	103	CRT	C10-C11-C12-C14
21	Z	103	CRT	C32-C33-C35-C36
21	Z	103	CRT	C34-C33-C35-C36
21	Z	103	CRT	C36-C37-C38-C39
21	Z	103	CRT	C36-C37-C38-C40
21	2	103	CRT	C36-C37-C38-C40
21	4	102	CRT	C10-C11-C12-C13
21	4	102	CRT	C10-C11-C12-C14
21	4	102	CRT	C15-C16-C17-C18
21	4	102	CRT	C15-C16-C17-C19
21	7	101	CRT	C10-C11-C12-C13
22	M	409	CDL	CA2-OA2-PA1-OA3
22	M	409	CDL	CA2-OA2-PA1-OA4
22	M	409	CDL	CA2-OA2-PA1-OA5
22	M	409	CDL	CA3-OA5-PA1-OA4
22	M	409	CDL	CB2-OB2-PB2-OB5
22	M	409	CDL	OB6-CB4-CB6-OB8
22	M	411	CDL	CB3-OB5-PB2-OB3
22	M	412	CDL	CA3-OA5-PA1-OA4
22	M	412	CDL	CB3-OB5-PB2-OB2
22	M	412	CDL	CB3-OB5-PB2-OB3
22	H	302	CDL	O1-C1-CB2-OB2
22	H	302	CDL	CA2-C1-CB2-OB2
22	H	302	CDL	CA3-OA5-PA1-OA3
22	H	302	CDL	CB2-OB2-PB2-OB4
22	D	502	CDL	CA2-C1-CB2-OB2
22	D	502	CDL	CA2-OA2-PA1-OA5
22	D	502	CDL	OA5-CA3-CA4-OA6
22	D	502	CDL	C11-CA5-OA6-CA4
24	5	101	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
16	G	102	BCL	CBD-CGD-O2D-CED
16	T	101	BCL	O1A-CGA-O2A-C1
16	0	102	BCL	O1A-CGA-O2A-C1
16	X	102	BCL	CBD-CGD-O2D-CED
16	2	102	BCL	CBD-CGD-O2D-CED
16	0	102	BCL	CBD-CGD-O2D-CED
15	1	401	PGV	O02-C1-O01-C02
22	D	502	CDL	OA7-CA5-OA6-CA4
16	E	102	BCL	C3-C5-C6-C7
16	4	101	BCL	C3-C5-C6-C7
17	M	405	BPH	C3-C5-C6-C7
16	K	102	BCL	CBA-CGA-O2A-C1
16	T	101	BCL	CBA-CGA-O2A-C1
16	0	102	BCL	CBA-CGA-O2A-C1
16	N	101	BCL	CBD-CGD-O2D-CED
16	A	101	BCL	C4-C3-C5-C6
16	1	402	BCL	C4-C3-C5-C6
16	R	101	BCL	C2-C3-C5-C6
16	3	101	BCL	C2-C3-C5-C6
16	E	102	BCL	C2A-CAA-CBA-CGA
16	N	101	BCL	C2A-CAA-CBA-CGA
16	6	101	BCL	C2A-CAA-CBA-CGA
16	M	404	BCL	C3-C5-C6-C7
16	G	102	BCL	C3-C5-C6-C7
16	I	101	BCL	C3-C5-C6-C7
16	Y	101	BCL	C3-C5-C6-C7
16	6	101	BCL	C3-C5-C6-C7
16	9	101	BCL	C3-C5-C6-C7
15	1	401	PGV	C20-C19-O03-C01
16	K	102	BCL	O1A-CGA-O2A-C1
16	L	307	BCL	CBD-CGD-O2D-CED
16	V	102	BCL	CBD-CGD-O2D-CED
16	G	102	BCL	O1D-CGD-O2D-CED
22	H	302	CDL	O1-C1-CA2-OA2
22	D	502	CDL	O1-C1-CB2-OB2
16	Z	102	BCL	C3-C5-C6-C7
15	D	501	PGV	C2-C1-O01-C02
16	F	502	BCL	C4-C3-C5-C6
17	M	405	BPH	C4-C3-C5-C6
18	L	304	UQ8	C15-C14-C16-C17
16	F	502	BCL	C2-C3-C5-C6
17	M	405	BPH	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	L	304	UQ8	C13-C14-C16-C17
16	G	102	BCL	C2A-CAA-CBA-CGA
16	Z	102	BCL	C2A-CAA-CBA-CGA
24	R	103	LMT	O5'-C1'-O1'-C1
18	L	303	UQ8	C19-C21-C22-C23
15	1	401	PGV	O04-C19-O03-C01
16	B	102	BCL	CBD-CGD-O2D-CED
15	D	501	PGV	O02-C1-O01-C02
24	Z	101	LMT	C4'-C5'-C6'-O6'
16	U	101	BCL	CBA-CGA-O2A-C1
16	W	101	BCL	CBA-CGA-O2A-C1
16	Y	101	BCL	CBD-CGD-O2D-CED
16	E	102	BCL	C13-C15-C16-C17
16	F	502	BCL	C13-C15-C16-C17
15	L	305	PGV	O12-C04-C05-O05
22	M	409	CDL	O1-C1-CB2-OB2
22	M	412	CDL	O1-C1-CB2-OB2
16	0	102	BCL	C4-C3-C5-C6
16	0	102	BCL	C2-C3-C5-C6
16	L	307	BCL	C11-C10-C8-C9
16	B	102	BCL	C11-C10-C8-C9
16	E	102	BCL	C6-C7-C8-C9
16	I	101	BCL	C11-C10-C8-C9
16	J	101	BCL	C6-C7-C8-C9
16	J	101	BCL	C11-C10-C8-C9
16	N	101	BCL	C11-C10-C8-C9
16	P	102	BCL	C11-C10-C8-C9
16	R	101	BCL	C11-C10-C8-C9
16	T	101	BCL	C11-C10-C8-C9
16	V	102	BCL	C6-C7-C8-C9
16	X	102	BCL	C6-C7-C8-C9
16	Z	102	BCL	C6-C7-C8-C9
16	2	102	BCL	C11-C10-C8-C9
16	6	101	BCL	C11-C10-C8-C9
16	9	101	BCL	C11-C10-C8-C9
16	0	102	BCL	C11-C10-C8-C9
16	L	301	BCL	C15-C16-C17-C18
16	9	101	BCL	C5-C6-C7-C8
21	M	407	CRT	C5-C6-C7-C8
21	K	101	CRT	C5-C6-C7-C8
21	K	101	CRT	C10-C11-C12-C13
21	Q	101	CRT	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	X	103	CRT	C15-C16-C17-C18
21	7	101	CRT	C15-C16-C17-C18
21	0	103	CRT	C5-C6-C7-C8
21	K	101	CRT	C5-C6-C7-C9
24	X	101	LMT	O5'-C5'-C6'-O6'
16	W	101	BCL	O1A-CGA-O2A-C1
16	Z	102	BCL	C15-C16-C17-C18
16	1	402	BCL	C13-C15-C16-C17
16	J	101	BCL	C5-C6-C7-C8
16	O	502	BCL	C8-C10-C11-C12
16	P	102	BCL	C13-C15-C16-C17
16	T	101	BCL	C5-C6-C7-C8
16	U	101	BCL	C10-C11-C12-C13
16	Z	102	BCL	C10-C11-C12-C13
16	E	102	BCL	C10-C11-C12-C13
16	N	101	BCL	C5-C6-C7-C8
16	P	102	BCL	C8-C10-C11-C12
16	Y	101	BCL	C5-C6-C7-C8
16	Z	102	BCL	C8-C10-C11-C12
16	6	101	BCL	C10-C11-C12-C13
15	L	306	PGV	C1-C2-C3-C4
22	H	302	CDL	CA5-C11-C12-C13
22	M	412	CDL	C71-CB7-OB8-CB6
16	P	102	BCL	CBD-CGD-O2D-CED
16	V	102	BCL	C10-C11-C12-C13
16	X	102	BCL	O1D-CGD-O2D-CED
16	2	102	BCL	O1D-CGD-O2D-CED
16	L	301	BCL	C11-C10-C8-C7
16	A	101	BCL	C6-C7-C8-C10
16	K	102	BCL	C6-C7-C8-C10
16	Q	102	BCL	C11-C10-C8-C7
16	1	402	BCL	C11-C10-C8-C7
16	8	102	BCL	C12-C13-C15-C16
16	D	503	BCL	C3-C5-C6-C7
22	D	502	CDL	CA5-C11-C12-C13
16	1	402	BCL	C15-C16-C17-C18
16	0	102	BCL	O1D-CGD-O2D-CED
18	L	308	UQ8	C19-C21-C22-C23
16	1	402	BCL	C3-C5-C6-C7
16	P	102	BCL	C15-C16-C17-C18
16	8	102	BCL	C5-C6-C7-C8
16	U	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	I	101	BCL	C13-C15-C16-C17
16	2	102	BCL	C15-C16-C17-C18
24	4	103	LMT	C5'-C4'-O1B-C1B
16	N	101	BCL	O1D-CGD-O2D-CED
16	G	102	BCL	C5-C6-C7-C8
16	I	101	BCL	C5-C6-C7-C8
17	L	302	BPH	C15-C16-C17-C18
15	L	305	PGV	C03-O11-P-O12
15	H	301	PGV	C04-O12-P-O11
15	1	401	PGV	C03-O11-P-O12
22	M	409	CDL	CA3-OA5-PA1-OA2
22	M	411	CDL	CA2-OA2-PA1-OA5
22	M	412	CDL	CA3-OA5-PA1-OA2
22	M	412	CDL	CB2-OB2-PB2-OB5
22	H	302	CDL	CB2-OB2-PB2-OB5
22	D	502	CDL	CA3-OA5-PA1-OA2
16	J	101	BCL	CBA-CGA-O2A-C1
16	7	102	BCL	CBA-CGA-O2A-C1
16	2	102	BCL	C4-C3-C5-C6
16	E	102	BCL	C15-C16-C17-C18
16	Q	102	BCL	C3-C5-C6-C7
16	O	502	BCL	CBA-CGA-O2A-C1
16	2	102	BCL	C5-C6-C7-C8
23	M	413	LDA	C4-C5-C6-C7
24	2	104	LMT	C6-C7-C8-C9
15	H	301	PGV	C2-C1-O01-C02
13	C	407	Z41	C11-C10-C9-C8
22	M	411	CDL	C42-C43-C44-C45
22	H	302	CDL	C59-C60-C61-C62
15	H	301	PGV	O02-C1-O01-C02
16	V	102	BCL	O1D-CGD-O2D-CED
16	M	404	BCL	CBA-CGA-O2A-C1
16	G	102	BCL	C15-C16-C17-C18
16	3	101	BCL	C5-C6-C7-C8
16	J	101	BCL	O1A-CGA-O2A-C1
16	N	101	BCL	C16-C17-C18-C19
16	U	101	BCL	C4-C3-C5-C6
16	W	101	BCL	C4-C3-C5-C6
18	L	304	UQ8	C30-C29-C31-C32
22	H	302	CDL	C12-C13-C14-C15
24	Z	101	LMT	C6-C7-C8-C9
16	A	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	W	101	BCL	C2-C3-C5-C6
16	1	402	BCL	C2-C3-C5-C6
16	L	301	BCL	C11-C10-C8-C9
16	J	101	BCL	C14-C13-C15-C16
16	Y	101	BCL	C11-C10-C8-C9
13	C	407	Z41	C10-C11-C12-C13
24	2	104	LMT	C5-C6-C7-C8
16	2	102	BCL	C2A-CAA-CBA-CGA
22	M	412	CDL	OB9-CB7-OB8-CB6
15	H	301	PGV	C04-C05-C06-O06
15	D	501	PGV	C04-C05-C06-O06
21	7	101	CRT	C10-C11-C12-C14
16	R	101	BCL	C3-C5-C6-C7
16	E	102	BCL	C5-C6-C7-C8
24	4	103	LMT	C3'-C4'-O1B-C1B
16	2	102	BCL	C13-C15-C16-C17
20	M	406	MQ8	C28-C30-C31-C32
24	H	303	LMT	C6-C7-C8-C9
16	7	102	BCL	O1A-CGA-O2A-C1
22	M	412	CDL	C41-C42-C43-C44
16	9	101	BCL	CBA-CGA-O2A-C1
16	B	102	BCL	C3A-C2A-CAA-CBA
16	J	101	BCL	C3A-C2A-CAA-CBA
16	O	502	BCL	C3A-C2A-CAA-CBA
16	V	102	BCL	C3A-C2A-CAA-CBA
16	2	102	BCL	C3A-C2A-CAA-CBA
16	3	101	BCL	C3A-C2A-CAA-CBA
16	8	102	BCL	C3A-C2A-CAA-CBA
24	M	414	LMT	O5'-C5'-C6'-O6'
16	L	307	BCL	O1D-CGD-O2D-CED
24	X	101	LMT	O5B-C5B-C6B-O6B
24	P	101	LMT	C2-C3-C4-C5
18	L	304	UQ8	C12-C11-C9-C10
16	U	101	BCL	C2-C3-C5-C6
18	L	304	UQ8	C28-C29-C31-C32
18	L	304	UQ8	C12-C11-C9-C8
15	D	501	PGV	O05-C05-C06-O06
16	O	502	BCL	O1A-CGA-O2A-C1
24	Z	101	LMT	O5'-C5'-C6'-O6'
16	U	101	BCL	C5-C6-C7-C8
16	X	102	BCL	C10-C11-C12-C13
24	V	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
16	Z	102	BCL	C13-C15-C16-C17
15	H	301	PGV	C3-C4-C5-C6
22	M	412	CDL	C58-C59-C60-C61
16	O	502	BCL	C4-C3-C5-C6
16	E	102	BCL	C6-C7-C8-C10
16	J	101	BCL	C12-C13-C15-C16
16	O	502	BCL	C2-C3-C5-C6
16	S	101	BCL	C6-C7-C8-C10
16	U	101	BCL	C11-C10-C8-C7
16	X	102	BCL	C6-C7-C8-C10
16	5	102	BCL	C11-C10-C8-C7
16	3	101	BCL	C3-C5-C6-C7
16	M	404	BCL	O1A-CGA-O2A-C1
16	9	101	BCL	O1A-CGA-O2A-C1
16	B	102	BCL	C5-C6-C7-C8
16	N	101	BCL	C16-C17-C18-C20
22	M	411	CDL	C55-C56-C57-C58
16	J	101	BCL	C2A-CAA-CBA-CGA
16	K	102	BCL	C2A-CAA-CBA-CGA
16	Y	101	BCL	C2A-CAA-CBA-CGA
16	8	102	BCL	C2A-CAA-CBA-CGA
16	0	102	BCL	C8-C10-C11-C12
15	M	410	PGV	C21-C22-C23-C24
15	H	301	PGV	C1-C2-C3-C4
15	H	301	PGV	C4-C5-C6-C7
22	H	302	CDL	C54-C55-C56-C57
24	V	101	LMT	C5-C6-C7-C8
24	V	101	LMT	C6-C7-C8-C9
24	V	101	LMT	O5'-C1'-O1'-C1
16	B	102	BCL	O1D-CGD-O2D-CED
20	M	406	MQ8	C38-C40-C41-C42
22	M	412	CDL	C51-CB5-OB6-CB4
15	M	408	PGV	O01-C02-C03-O11
15	D	501	PGV	C22-C23-C24-C25
10	C	401	HEM	C4B-C3B-CAB-CBB
10	C	402	HEM	C4B-C3B-CAB-CBB
16	Z	102	BCL	C5-C6-C7-C8
16	0	102	BCL	C5-C6-C7-C8
24	0	101	LMT	C3'-C4'-O1B-C1B
22	M	412	CDL	O1-C1-CA2-OA2
15	M	410	PGV	C22-C23-C24-C25
22	M	412	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
24	G	101	LMT	O5'-C5'-C6'-O6'
24	V	101	LMT	O5'-C5'-C6'-O6'
16	M	404	BCL	C4-C3-C5-C6
16	B	102	BCL	C4-C3-C5-C6
16	2	102	BCL	C2-C3-C5-C6
16	9	101	BCL	C2-C3-C5-C6
16	A	101	BCL	C6-C7-C8-C9
16	K	102	BCL	C6-C7-C8-C9
16	Q	102	BCL	C11-C10-C8-C9
16	5	102	BCL	C11-C10-C8-C9
24	E	101	LMT	O5'-C5'-C6'-O6'
24	R	103	LMT	C2-C3-C4-C5
24	B	101	LMT	O5B-C5B-C6B-O6B
21	R	102	CRT	C15-C16-C17-C18
16	J	101	BCL	C1A-C2A-CAA-CBA
16	O	502	BCL	C1A-C2A-CAA-CBA
16	T	101	BCL	C1A-C2A-CAA-CBA
16	V	102	BCL	C1A-C2A-CAA-CBA
16	Y	101	BCL	C1A-C2A-CAA-CBA
16	D	503	BCL	C15-C16-C17-C18
22	M	409	CDL	CB3-OB5-PB2-OB2
22	M	411	CDL	CB3-OB5-PB2-OB2
16	M	404	BCL	CBD-CGD-O2D-CED
16	U	101	BCL	C3-C5-C6-C7
16	8	102	BCL	C3-C5-C6-C7
16	Y	101	BCL	O1D-CGD-O2D-CED
15	M	410	PGV	C20-C19-O03-C01
16	1	402	BCL	CBA-CGA-O2A-C1
22	H	302	CDL	OA5-CA3-CA4-CA6
22	D	502	CDL	OA5-CA3-CA4-CA6
24	R	103	LMT	O5'-C5'-C6'-O6'
16	1	402	BCL	C8-C10-C11-C12
22	D	502	CDL	C56-C57-C58-C59
24	V	101	LMT	O5B-C5B-C6B-O6B
22	M	412	CDL	C57-C58-C59-C60
21	M	407	CRT	C1-C4-C5-C6
24	V	101	LMT	O5B-C1B-O1B-C4'
16	9	101	BCL	C4-C3-C5-C6
16	T	101	BCL	C2C-C3C-CAC-CBC
16	V	102	BCL	C2C-C3C-CAC-CBC
16	X	102	BCL	C2C-C3C-CAC-CBC
16	3	101	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
16	7	102	BCL	C2C-C3C-CAC-CBC
22	M	411	CDL	C16-C17-C18-C19
24	0	101	LMT	C5'-C4'-O1B-C1B
16	J	101	BCL	C8-C10-C11-C12
16	K	102	BCL	C15-C16-C17-C18
22	M	412	CDL	C71-C72-C73-C74
13	C	407	Z41	C25-C26-C27-C28
24	P	101	LMT	O5B-C5B-C6B-O6B
16	S	101	BCL	C3-C5-C6-C7
24	P	101	LMT	C4'-C5'-C6'-O6'
15	D	501	PGV	O03-C01-C02-C03
16	P	102	BCL	O1D-CGD-O2D-CED
15	D	501	PGV	C24-C25-C26-C27
24	2	101	LMT	O5B-C5B-C6B-O6B
22	M	411	CDL	CA5-C11-C12-C13
18	L	308	UQ8	C39-C41-C42-C43
24	X	101	LMT	C4'-C5'-C6'-O6'
24	0	101	LMT	C4-C5-C6-C7
16	G	102	BCL	C4-C3-C5-C6
16	N	101	BCL	C4-C3-C5-C6
16	4	101	BCL	C4-C3-C5-C6
16	N	101	BCL	C2-C3-C5-C6
16	F	502	BCL	C16-C17-C18-C19
16	T	101	BCL	C16-C17-C18-C19
22	M	412	CDL	C31-CA7-OA8-CA6
16	T	101	BCL	CBD-CGD-O2D-CED
16	4	101	BCL	C15-C16-C17-C18
24	R	103	LMT	O5B-C5B-C6B-O6B
24	0	101	LMT	O5B-C5B-C6B-O6B
16	7	102	BCL	C2-C1-O2A-CGA
24	2	104	LMT	O5'-C5'-C6'-O6'
16	7	102	BCL	C5-C6-C7-C8
16	L	307	BCL	CBA-CGA-O2A-C1
24	G	101	LMT	C3'-C4'-O1B-C1B
16	0	102	BCL	C15-C16-C17-C18
16	1	402	BCL	O1A-CGA-O2A-C1
10	C	402	HEM	C3D-CAD-CBD-CGD
16	W	101	BCL	C15-C16-C17-C18
21	G	103	CRT	C39-C38-O2-C2M
21	G	103	CRT	C40-C38-O2-C2M
21	K	101	CRT	C3-C1-O1-C1M
21	Q	101	CRT	C3-C1-O1-C1M

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Mol	Chain	Res	Type	Atoms
24	5	101	LMT	C2'-C1'-O1'-C1
15	L	305	PGV	O03-C01-C02-O01
22	M	412	CDL	OB7-CB5-OB6-CB4
21	K	101	CRT	C2-C1-C4-C5
21	K	101	CRT	C3-C1-C4-C5
21	K	101	CRT	C36-C37-C38-C39
21	N	102	CRT	C36-C37-C38-C39
21	Q	101	CRT	C2-C1-C4-C5
21	V	103	CRT	C36-C37-C38-C40
21	Z	103	CRT	C2-C1-C4-C5
21	2	103	CRT	C36-C37-C38-C39
22	M	412	CDL	C53-C54-C55-C56
16	A	101	BCL	C11-C10-C8-C7
16	B	102	BCL	C11-C10-C8-C7
16	D	503	BCL	C6-C7-C8-C10
16	E	102	BCL	C11-C10-C8-C7
16	G	102	BCL	C2-C3-C5-C6
16	U	101	BCL	C6-C7-C8-C10
16	V	102	BCL	C6-C7-C8-C10
16	W	101	BCL	C11-C10-C8-C7
16	Z	102	BCL	C6-C7-C8-C10
16	0	102	BCL	C11-C10-C8-C7
22	M	412	CDL	OA9-CA7-OA8-CA6
16	A	101	BCL	C11-C10-C8-C9
16	E	102	BCL	C11-C10-C8-C9
16	K	102	BCL	C11-C10-C8-C9
16	N	101	BCL	C6-C7-C8-C9
16	O	502	BCL	C14-C13-C15-C16
16	W	101	BCL	C11-C10-C8-C9
16	X	102	BCL	C11-C10-C8-C9
16	Z	102	BCL	C11-C10-C8-C9
16	9	101	BCL	C6-C7-C8-C9
15	M	410	PGV	C19-C20-C21-C22
22	M	412	CDL	C72-C73-C74-C75
21	M	407	CRT	C36-C37-C38-O2
21	Z	103	CRT	C36-C37-C38-O2
16	F	502	BCL	C15-C16-C17-C18
24	G	101	LMT	C5'-C4'-O1B-C1B
16	W	101	BCL	C13-C15-C16-C17
15	M	408	PGV	C01-C02-C03-O11
22	M	411	CDL	OA5-CA3-CA4-CA6
15	L	309	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	M	411	CDL	CB7-C71-C72-C73
16	V	102	BCL	C4-C3-C5-C6
18	L	304	UQ8	C40-C39-C41-C42
16	4	101	BCL	C2-C3-C5-C6
16	8	102	BCL	C13-C15-C16-C17
16	1	402	BCL	C16-C17-C18-C19
16	2	102	BCL	C16-C17-C18-C19
16	P	102	BCL	CBA-CGA-O2A-C1
15	M	410	PGV	O04-C19-O03-C01
16	Y	101	BCL	C8-C10-C11-C12
16	6	101	BCL	CBA-CGA-O2A-C1
22	H	302	CDL	C17-C18-C19-C20
16	7	102	BCL	C4-C3-C5-C6
16	M	404	BCL	C2-C3-C5-C6
16	B	102	BCL	C2-C3-C5-C6
16	V	102	BCL	C2-C3-C5-C6
22	M	412	CDL	C56-C57-C58-C59
16	L	307	BCL	O1A-CGA-O2A-C1
15	H	301	PGV	O05-C05-C06-O06
22	M	411	CDL	OA5-CA3-CA4-OA6
24	0	101	LMT	C11-C10-C9-C8
13	C	407	Z41	O2-C17-C18-O3
15	D	501	PGV	O03-C01-C02-O01
22	D	502	CDL	OB6-CB4-CB6-OB8
16	B	102	BCL	CBA-CGA-O2A-C1
24	5	101	LMT	O5'-C1'-O1'-C1
16	W	101	BCL	C5-C6-C7-C8
22	M	409	CDL	CB3-CB4-CB6-OB8
22	H	302	CDL	CB2-C1-CA2-OA2
16	E	102	BCL	C4-C3-C5-C6
16	F	502	BCL	C2-C1-O2A-CGA
16	O	502	BCL	C2-C1-O2A-CGA
16	P	102	BCL	C2-C1-O2A-CGA
24	V	101	LMT	C2B-C1B-O1B-C4'
16	M	403	BCL	C11-C10-C8-C9
16	D	503	BCL	C11-C10-C8-C9
16	F	502	BCL	C11-C10-C8-C9
16	T	101	BCL	C14-C13-C15-C16
24	R	103	LMT	O1'-C1-C2-C3
16	F	502	BCL	C16-C17-C18-C20
16	T	101	BCL	C16-C17-C18-C20
16	M	403	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
16	X	102	BCL	C4C-C3C-CAC-CBC
21	M	407	CRT	C5-C6-C7-C9
21	N	102	CRT	C10-C11-C12-C14
21	7	101	CRT	C15-C16-C17-C19
16	3	101	BCL	C10-C11-C12-C13
24	Z	101	LMT	C1-C2-C3-C4
24	M	414	LMT	C4B-C5B-C6B-O6B
13	C	407	Z41	C12-C13-C14-C15
16	T	101	BCL	O1D-CGD-O2D-CED
22	M	409	CDL	OB5-CB3-CB4-CB6
22	D	502	CDL	OB5-CB3-CB4-CB6
16	L	307	BCL	C11-C10-C8-C7
16	E	102	BCL	C2-C3-C5-C6
16	F	502	BCL	C11-C10-C8-C7
16	G	102	BCL	C6-C7-C8-C10
16	I	101	BCL	C11-C10-C8-C7
16	J	101	BCL	C6-C7-C8-C10
16	K	102	BCL	C11-C10-C8-C7
16	N	101	BCL	C6-C7-C8-C10
16	N	101	BCL	C11-C10-C8-C7
16	O	502	BCL	C12-C13-C15-C16
16	P	102	BCL	C6-C7-C8-C10
16	P	102	BCL	C11-C10-C8-C7
16	Q	102	BCL	C12-C13-C15-C16
16	R	101	BCL	C11-C10-C8-C7
16	S	101	BCL	C11-C10-C8-C7
16	T	101	BCL	C12-C13-C15-C16
16	W	101	BCL	C6-C7-C8-C10
16	X	102	BCL	C11-C12-C13-C15
16	Z	102	BCL	C11-C10-C8-C7
16	1	402	BCL	C6-C7-C8-C10
16	2	102	BCL	C11-C10-C8-C7
16	6	101	BCL	C11-C10-C8-C7
16	7	102	BCL	C2-C3-C5-C6
16	7	102	BCL	C6-C7-C8-C10
16	9	101	BCL	C6-C7-C8-C10
16	9	101	BCL	C11-C10-C8-C7
24	M	414	LMT	C5'-C4'-O1B-C1B
22	M	411	CDL	C54-C55-C56-C57
15	D	501	PGV	C31-C32-C33-C34
24	M	414	LMT	C3'-C4'-O1B-C1B
16	A	101	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	L	307	BCL	C5-C6-C7-C8
16	A	101	BCL	C13-C15-C16-C17
16	G	102	BCL	C13-C15-C16-C17
16	L	301	BCL	CAD-CBD-CGD-O2D
16	L	307	BCL	CAD-CBD-CGD-O2D
24	5	101	LMT	C4-C5-C6-C7
16	P	102	BCL	CAA-CBA-CGA-O2A
16	Y	101	BCL	C4-C3-C5-C6
18	L	308	UQ8	C5-C4-O4-C4M
15	L	306	PGV	C21-C22-C23-C24
22	M	409	CDL	OB5-CB3-CB4-OB6
16	N	101	BCL	C15-C16-C17-C18
22	M	412	CDL	C38-C39-C40-C41
16	1	402	BCL	C16-C17-C18-C20
16	2	102	BCL	C16-C17-C18-C20
16	0	102	BCL	C16-C17-C18-C19
16	F	502	BCL	CHA-CBD-CGD-O2D
16	P	102	BCL	O1A-CGA-O2A-C1
22	H	302	CDL	OB6-CB4-CB6-OB8
16	6	101	BCL	O1A-CGA-O2A-C1
16	W	101	BCL	C16-C17-C18-C19
16	T	101	BCL	C3-C5-C6-C7
16	5	102	BCL	C4-C3-C5-C6
16	B	102	BCL	O1A-CGA-O2A-C1
16	Y	101	BCL	C10-C11-C12-C13
16	V	102	BCL	CAA-CBA-CGA-O2A
16	Q	102	BCL	C14-C13-C15-C16
16	W	101	BCL	C6-C7-C8-C9
23	M	413	LDA	C5-C6-C7-C8
24	8	101	LMT	C1-C2-C3-C4
21	Q	101	CRT	C15-C16-C17-C19
21	R	102	CRT	C15-C16-C17-C19
21	X	103	CRT	C15-C16-C17-C19
16	5	102	BCL	C10-C11-C12-C13
15	L	305	PGV	C03-O11-P-O13
15	H	301	PGV	C04-O12-P-O13
15	1	401	PGV	C03-O11-P-O13
22	M	409	CDL	CB2-OB2-PB2-OB4
22	M	409	CDL	CB3-OB5-PB2-OB4
22	M	411	CDL	CA2-OA2-PA1-OA4
22	M	411	CDL	CA3-OA5-PA1-OA3
22	M	412	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
22	D	502	CDL	CA2-OA2-PA1-OA4
22	D	502	CDL	CA3-OA5-PA1-OA3
24	G	104	LMT	C4-C5-C6-C7
22	H	302	CDL	C71-CB7-OB8-CB6
15	L	306	PGV	C01-C02-C03-O11
21	7	101	CRT	C1-C4-C5-C6
16	4	101	BCL	C16-C17-C18-C19
16	8	102	BCL	C4-C3-C5-C6
15	L	306	PGV	O01-C02-C03-O11
15	L	309	PGV	O01-C02-C03-O11
16	M	403	BCL	C6-C7-C8-C10
16	F	502	BCL	C6-C7-C8-C10
16	G	102	BCL	C11-C10-C8-C7
16	R	101	BCL	C2C-C3C-CAC-CBC
16	T	101	BCL	C11-C10-C8-C7
16	W	101	BCL	C12-C13-C15-C16
16	Y	101	BCL	C6-C7-C8-C10
16	6	101	BCL	C6-C7-C8-C10
16	8	102	BCL	C11-C12-C13-C15
16	9	101	BCL	C11-C12-C13-C15
22	M	412	CDL	OB5-CB3-CB4-OB6
22	D	502	CDL	OB5-CB3-CB4-OB6
16	P	102	BCL	C10-C11-C12-C13
24	M	414	LMT	O5B-C5B-C6B-O6B
15	L	305	PGV	O03-C01-C02-C03
22	M	412	CDL	CB3-CB4-CB6-OB8
22	M	409	CDL	OA6-CA4-CA6-OA8
22	M	412	CDL	C78-C79-C80-C81
16	V	102	BCL	O1A-CGA-O2A-C1
16	Z	102	BCL	C4-C3-C5-C6
15	L	309	PGV	C20-C19-O03-C01
16	Q	102	BCL	C11-C12-C13-C14
16	S	101	BCL	C11-C10-C8-C9
16	U	101	BCL	C6-C7-C8-C9
16	1	402	BCL	C11-C10-C8-C9
16	5	102	BCL	C6-C7-C8-C9
22	H	302	CDL	OB9-CB7-OB8-CB6
22	H	302	CDL	C78-C79-C80-C81
21	4	102	CRT	C28-C30-C31-C32
15	D	501	PGV	C25-C26-C27-C28
16	4	101	BCL	CAA-CBA-CGA-O2A
24	M	414	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
16	5	102	BCL	C2-C3-C5-C6
16	A	101	BCL	C16-C17-C18-C20
16	Y	101	BCL	C16-C17-C18-C20
24	R	103	LMT	C5-C6-C7-C8
16	O	502	BCL	O1D-CGD-O2D-CED
15	1	401	PGV	C03-C02-O01-C1
15	L	309	PGV	C01-C02-C03-O11
16	P	102	BCL	C2A-CAA-CBA-CGA
16	V	102	BCL	C2A-CAA-CBA-CGA
16	V	102	BCL	CBA-CGA-O2A-C1
16	L	301	BCL	C2-C1-O2A-CGA
16	D	503	BCL	C2-C1-O2A-CGA
16	U	101	BCL	C2-C1-O2A-CGA
16	W	101	BCL	C2-C1-O2A-CGA
15	L	306	PGV	C22-C23-C24-C25
23	M	413	LDA	C1-C2-C3-C4
24	G	104	LMT	C11-C10-C9-C8
16	B	102	BCL	CAA-CBA-CGA-O2A
22	M	412	CDL	C31-C32-C33-C34
15	H	301	PGV	O01-C02-C03-O11
22	H	302	CDL	OA5-CA3-CA4-OA6
16	P	102	BCL	C3-C5-C6-C7
16	Y	101	BCL	C2-C3-C5-C6
18	L	304	UQ8	C38-C39-C41-C42
16	9	101	BCL	C10-C11-C12-C13
16	M	403	BCL	C10-C11-C12-C13
15	C	409	PGV	C04-O12-P-O11
15	D	501	PGV	C04-O12-P-O11
15	F	501	PGV	C03-O11-P-O12
15	F	501	PGV	C04-O12-P-O11
22	M	411	CDL	CA3-OA5-PA1-OA2
22	M	411	CDL	CB2-OB2-PB2-OB5
22	M	412	CDL	CA2-OA2-PA1-OA5
22	H	302	CDL	CA3-OA5-PA1-OA2
22	H	302	CDL	CB3-OB5-PB2-OB2
22	D	502	CDL	CB2-OB2-PB2-OB5
22	D	502	CDL	CB3-OB5-PB2-OB2
15	1	401	PGV	C04-O12-P-O13
21	Z	103	CRT	C3-C1-C4-C5
21	8	103	CRT	C2-C1-C4-C5
15	L	309	PGV	O03-C01-C02-C03
18	L	304	UQ8	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
16	S	101	BCL	C5-C6-C7-C8
16	X	102	BCL	C15-C16-C17-C18
16	X	102	BCL	C11-C10-C8-C7
16	4	101	BCL	C11-C10-C8-C7
15	F	501	PGV	C1-C2-C3-C4
16	L	301	BCL	C3-C5-C6-C7
16	D	503	BCL	C6-C7-C8-C9
16	F	502	BCL	C6-C7-C8-C9
16	P	102	BCL	C6-C7-C8-C9
16	6	101	BCL	C6-C7-C8-C9
16	8	102	BCL	C11-C12-C13-C14
16	8	102	BCL	C14-C13-C15-C16
16	R	101	BCL	O1D-CGD-O2D-CED
16	W	101	BCL	C16-C17-C18-C20
24	8	101	LMT	C3-C4-C5-C6
18	L	304	UQ8	C2-C3-O3-C3M
15	H	301	PGV	C6-C7-C8-C9
21	Z	103	CRT	O1-C1-C4-C5
22	H	302	CDL	C13-C14-C15-C16
22	M	411	CDL	C1-CA2-OA2-PA1
16	J	101	BCL	CAA-CBA-CGA-O2A
15	L	309	PGV	O04-C19-O03-C01
22	M	409	CDL	CA2-C1-CB2-OB2
15	H	301	PGV	C23-C24-C25-C26
22	H	302	CDL	C18-C19-C20-C21
16	O	502	BCL	CBD-CGD-O2D-CED
22	M	411	CDL	C35-C36-C37-C38
16	4	101	BCL	C2A-CAA-CBA-CGA
21	8	103	CRT	C11-C10-C9-C7
24	R	103	LMT	C3-C4-C5-C6
22	D	502	CDL	CB5-C51-C52-C53
24	J	102	LMT	C6-C7-C8-C9
20	M	406	MQ8	C24-C23-C25-C26
16	S	101	BCL	C2-C1-O2A-CGA
16	B	102	BCL	C2A-CAA-CBA-CGA
16	V	102	BCL	C8-C10-C11-C12
16	M	403	BCL	C6-C7-C8-C9
16	N	101	BCL	C11-C12-C13-C14
16	O	502	BCL	C11-C10-C8-C9
16	V	102	BCL	C11-C10-C8-C9
16	W	101	BCL	C14-C13-C15-C16
16	9	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	0	102	BCL	C6-C7-C8-C9
24	Z	101	LMT	C7-C8-C9-C10
21	4	102	CRT	C31-C32-C33-C34
22	M	412	CDL	CA2-C1-CB2-OB2
22	M	412	CDL	CA3-CA4-CA6-OA8
22	D	502	CDL	CA3-CA4-CA6-OA8
16	8	102	BCL	O1A-CGA-O2A-C1
16	G	102	BCL	C16-C17-C18-C19
16	Y	101	BCL	C16-C17-C18-C19
17	L	302	BPH	O2A-C1-C2-C3
24	G	101	LMT	O5'-C1'-O1'-C1
21	B	103	CRT	C5-C6-C7-C8
16	Q	102	BCL	C13-C15-C16-C17
16	G	102	BCL	C1A-C2A-CAA-CBA
16	P	102	BCL	C1A-C2A-CAA-CBA
16	X	102	BCL	CAA-CBA-CGA-O2A
16	Z	102	BCL	C2-C3-C5-C6
16	7	102	BCL	C11-C10-C8-C7
16	5	102	BCL	C8-C10-C11-C12
10	C	401	HEM	CAA-CBA-CGA-O1A
15	M	408	PGV	C03-O11-P-O12
10	C	401	HEM	CAA-CBA-CGA-O2A
16	P	102	BCL	C5-C6-C7-C8
16	R	101	BCL	C13-C15-C16-C17
15	H	301	PGV	C01-C02-C03-O11
22	M	411	CDL	C43-C44-C45-C46
18	L	303	UQ8	C15-C14-C16-C17
16	B	102	BCL	C13-C15-C16-C17
21	4	102	CRT	C31-C32-C33-C35
16	3	101	BCL	C15-C16-C17-C18
22	D	502	CDL	C12-C13-C14-C15
24	G	101	LMT	C3-C4-C5-C6
16	8	102	BCL	CBA-CGA-O2A-C1
16	A	101	BCL	O1D-CGD-O2D-CED
21	8	103	CRT	C1-C4-C5-C6
15	L	305	PGV	C4-C5-C6-C7
16	Y	101	BCL	C13-C15-C16-C17
16	M	404	BCL	C2-C1-O2A-CGA
16	I	101	BCL	C2-C1-O2A-CGA
16	1	402	BCL	C2-C1-O2A-CGA
22	M	411	CDL	C15-C16-C17-C18
16	4	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	S	101	BCL	C8-C10-C11-C12
16	E	102	BCL	C8-C10-C11-C12
22	M	409	CDL	C1-CB2-OB2-PB2
16	I	101	BCL	O1D-CGD-O2D-CED
24	P	101	LMT	O5'-C5'-C6'-O6'
16	6	101	BCL	C13-C15-C16-C17
16	K	102	BCL	C4-C3-C5-C6
16	P	102	BCL	C4-C3-C5-C6
21	0	103	CRT	C5-C6-C7-C9
18	L	304	UQ8	C23-C24-C26-C27
16	V	102	BCL	C5-C6-C7-C8
22	M	411	CDL	CA7-C31-C32-C33
15	C	409	PGV	C4-C5-C6-C7
16	I	101	BCL	C16-C17-C18-C19
16	R	101	BCL	C16-C17-C18-C19
16	3	101	BCL	C16-C17-C18-C19
16	6	101	BCL	C16-C17-C18-C20
15	1	401	PGV	O01-C02-C03-O11
16	Z	102	BCL	O1D-CGD-O2D-CED
15	L	305	PGV	C5-C6-C7-C8
16	U	101	BCL	C15-C16-C17-C18
16	K	102	BCL	C2-C3-C5-C6
16	Q	102	BCL	C11-C12-C13-C15
22	M	411	CDL	C31-CA7-OA8-CA6
16	A	101	BCL	CBD-CGD-O2D-CED
22	M	411	CDL	OA9-CA7-OA8-CA6
22	M	411	CDL	OA6-CA4-CA6-OA8
16	S	101	BCL	C16-C17-C18-C20
16	G	102	BCL	CBA-CGA-O2A-C1
16	6	101	BCL	C4-C3-C5-C6
18	L	304	UQ8	C20-C19-C21-C22
10	C	402	HEM	CAD-CBD-CGD-O1D
16	8	102	BCL	C2-C3-C5-C6
16	8	102	BCL	CAA-CBA-CGA-O2A
16	G	102	BCL	C11-C10-C8-C9
16	Q	102	BCL	C6-C7-C8-C9
16	R	101	BCL	C6-C7-C8-C9
16	S	101	BCL	C6-C7-C8-C9
16	U	101	BCL	C11-C10-C8-C9
16	X	102	BCL	C11-C12-C13-C14
16	Y	101	BCL	C6-C7-C8-C9
16	1	402	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	P	102	BCL	C3A-C2A-CAA-CBA
16	M	403	BCL	CAD-CBD-CGD-O2D
17	L	302	BPH	CAD-CBD-CGD-O2D
22	M	409	CDL	CA3-CA4-OA6-CA5
24	5	101	LMT	C4'-C5'-C6'-O6'
16	F	502	BCL	C10-C11-C12-C13
16	V	102	BCL	C2-C1-O2A-CGA
16	G	102	BCL	O1A-CGA-O2A-C1
16	X	102	BCL	C4-C3-C5-C6
18	L	308	UQ8	C35-C34-C36-C37
16	5	102	BCL	C16-C17-C18-C19
16	6	101	BCL	C2-C3-C5-C6
15	H	301	PGV	O01-C1-C2-C3
21	K	101	CRT	C10-C11-C12-C14
22	D	502	CDL	CB3-CB4-CB6-OB8
16	R	101	BCL	CBD-CGD-O2D-CED
22	D	502	CDL	C53-C54-C55-C56
22	M	411	CDL	C77-C78-C79-C80
17	M	405	BPH	O2A-C1-C2-C3
16	O	502	BCL	C2A-CAA-CBA-CGA
16	U	101	BCL	C16-C17-C18-C19
16	M	404	BCL	CHA-CBD-CGD-O1D
16	M	404	BCL	CHA-CBD-CGD-O2D
16	D	503	BCL	CHA-CBD-CGD-O1D
16	D	503	BCL	CHA-CBD-CGD-O2D
16	I	101	BCL	CHA-CBD-CGD-O2D
16	K	102	BCL	CHA-CBD-CGD-O1D
16	K	102	BCL	CHA-CBD-CGD-O2D
16	O	502	BCL	CHA-CBD-CGD-O2D
16	Y	101	BCL	CHA-CBD-CGD-O2D
16	3	101	BCL	CHA-CBD-CGD-O1D
16	3	101	BCL	CHA-CBD-CGD-O2D
16	5	102	BCL	CHA-CBD-CGD-O1D
16	5	102	BCL	CHA-CBD-CGD-O2D
20	M	406	MQ8	C19-C18-C20-C21
24	P	103	LMT	C4-C5-C6-C7
21	K	101	CRT	C39-C38-O2-C2M
16	L	307	BCL	C16-C17-C18-C20
15	F	501	PGV	O03-C01-C02-O01
15	M	410	PGV	O01-C1-C2-C3
16	L	307	BCL	CAA-CBA-CGA-O2A
16	9	101	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	Q	101	CRT	C3-C1-C4-C5
21	Q	101	CRT	C36-C37-C38-C39
15	1	401	PGV	O01-C1-C2-C3
16	I	101	BCL	CBD-CGD-O2D-CED
16	L	307	BCL	C6-C7-C8-C10
16	J	101	BCL	C11-C10-C8-C7
16	X	102	BCL	C2-C3-C5-C6
18	L	308	UQ8	C33-C34-C36-C37
24	0	101	LMT	O5'-C1'-O1'-C1
22	H	302	CDL	C12-C11-CA5-OA6
15	D	501	PGV	C20-C21-C22-C23
18	L	304	UQ8	C4-C3-O3-C3M
18	L	308	UQ8	C3-C4-O4-C4M
10	C	402	HEM	CAD-CBD-CGD-O2D
10	C	404	HEM	CAA-CBA-CGA-O2A
15	M	408	PGV	C27-C28-C29-C30
22	M	412	CDL	C72-C71-CB7-OB8
15	L	305	PGV	C20-C19-O03-C01
16	V	102	BCL	C16-C17-C18-C20
16	6	101	BCL	C16-C17-C18-C19
24	2	101	LMT	O1'-C1-C2-C3
16	I	101	BCL	C1A-C2A-CAA-CBA
16	R	101	BCL	C1A-C2A-CAA-CBA
16	X	102	BCL	C1A-C2A-CAA-CBA
24	J	102	LMT	C4'-C5'-C6'-O6'
22	M	411	CDL	C71-CB7-OB8-CB6
22	M	409	CDL	CA3-CA4-CA6-OA8
22	M	411	CDL	CA3-CA4-CA6-OA8
16	B	102	BCL	C16-C17-C18-C20
15	L	305	PGV	C02-C03-O11-P
15	H	301	PGV	C02-C03-O11-P
15	M	410	PGV	O02-C1-C2-C3
15	1	401	PGV	O02-C1-C2-C3
24	J	102	LMT	C4-C5-C6-C7
15	C	409	PGV	C04-O12-P-O13
15	L	306	PGV	C04-O12-P-O13
15	M	408	PGV	C03-O11-P-O13
22	M	411	CDL	CB2-OB2-PB2-OB3
22	D	502	CDL	CB2-OB2-PB2-OB3
16	L	307	BCL	CAA-CBA-CGA-O1A
16	P	102	BCL	CAA-CBA-CGA-O1A
22	H	302	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
15	F	501	PGV	C22-C23-C24-C25
22	M	411	CDL	C80-C81-C82-C83
16	L	301	BCL	CBA-CGA-O2A-C1
18	L	303	UQ8	C13-C14-C16-C17
16	I	101	BCL	CAD-CBD-CGD-O1D
16	O	502	BCL	CAD-CBD-CGD-O1D
16	Y	101	BCL	CAD-CBD-CGD-O1D
16	9	101	BCL	CAD-CBD-CGD-O1D
16	L	301	BCL	O1A-CGA-O2A-C1
17	M	405	BPH	C5-C6-C7-C8
16	L	307	BCL	C6-C7-C8-C9
15	L	305	PGV	C2-C3-C4-C5
15	L	306	PGV	C4-C5-C6-C7
24	V	101	LMT	C4-C5-C6-C7
16	Z	102	BCL	CBD-CGD-O2D-CED
10	C	404	HEM	CAA-CBA-CGA-O1A
15	1	401	PGV	O03-C19-C20-C21
16	4	101	BCL	C5-C6-C7-C8
22	M	411	CDL	C36-C37-C38-C39
22	H	302	CDL	C31-C32-C33-C34
16	L	307	BCL	C12-C13-C15-C16
16	M	404	BCL	C6-C7-C8-C10
16	G	102	BCL	C3A-C2A-CAA-CBA
16	N	101	BCL	C2C-C3C-CAC-CBC
16	V	102	BCL	C11-C12-C13-C15
16	5	102	BCL	C2C-C3C-CAC-CBC
16	5	102	BCL	C6-C7-C8-C10
16	0	102	BCL	C2C-C3C-CAC-CBC
16	0	102	BCL	C6-C7-C8-C10
22	M	411	CDL	C71-C72-C73-C74
21	B	103	CRT	C5-C6-C7-C9
24	5	101	LMT	C2-C1-O1'-C1'
24	8	101	LMT	C2-C1-O1'-C1'
16	O	502	BCL	C15-C16-C17-C18
16	V	102	BCL	CAA-CBA-CGA-O1A
18	L	308	UQ8	C9-C11-C12-C13
16	T	101	BCL	C13-C15-C16-C17
16	R	101	BCL	CAA-CBA-CGA-O2A
17	L	302	BPH	C8-C10-C11-C12
22	M	412	CDL	C72-C71-CB7-OB9
16	L	301	BCL	C2A-CAA-CBA-CGA
14	C	408	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
15	L	305	PGV	O04-C19-O03-C01
13	C	407	Z41	O3-C19-C20-C21

There are no ring outliers.

97 monomers are involved in 447 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	P	101	LMT	3	0
18	L	303	UQ8	4	0
16	5	102	BCL	8	0
10	C	401	HEM	6	0
16	M	404	BCL	5	0
15	D	501	PGV	4	0
24	2	101	LMT	1	0
24	G	101	LMT	2	0
24	0	101	LMT	3	0
24	H	303	LMT	3	0
21	2	103	CRT	8	0
24	M	414	LMT	2	0
16	9	101	BCL	5	0
16	L	307	BCL	8	0
16	Z	102	BCL	8	0
24	8	101	LMT	4	0
24	5	101	LMT	1	0
16	I	101	BCL	6	0
16	1	402	BCL	3	0
20	M	406	MQ8	3	0
24	2	104	LMT	3	0
21	Q	101	CRT	8	0
21	T	102	CRT	8	0
15	F	501	PGV	3	0
16	L	301	BCL	2	0
16	6	101	BCL	6	0
16	D	503	BCL	5	0
16	W	101	BCL	3	0
21	E	103	CRT	4	0
22	H	302	CDL	2	0
10	C	403	HEM	6	0
16	K	102	BCL	8	0
22	M	409	CDL	1	0
16	S	101	BCL	7	0
21	M	407	CRT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	R	102	CRT	5	0
16	B	102	BCL	8	0
21	4	102	CRT	12	0
23	O	501	LDA	1	0
16	V	102	BCL	8	0
24	P	103	LMT	3	0
21	7	101	CRT	11	0
16	X	102	BCL	7	0
16	M	403	BCL	3	0
21	V	103	CRT	4	0
16	3	101	BCL	7	0
22	M	412	CDL	7	0
15	L	306	PGV	3	0
16	Y	101	BCL	3	0
16	2	102	BCL	10	0
15	M	410	PGV	3	0
21	B	103	CRT	5	0
21	X	103	CRT	9	0
16	G	102	BCL	5	0
16	A	101	BCL	2	0
16	4	101	BCL	6	0
21	K	101	CRT	10	0
16	E	102	BCL	7	0
15	L	309	PGV	4	0
16	J	101	BCL	5	0
18	L	304	UQ8	12	0
16	8	102	BCL	4	0
16	Q	102	BCL	5	0
24	Z	101	LMT	2	0
16	N	101	BCL	8	0
24	G	104	LMT	4	0
24	R	103	LMT	2	0
16	U	101	BCL	6	0
24	J	102	LMT	3	0
17	L	302	BPH	5	0
16	F	502	BCL	1	0
22	M	411	CDL	5	0
21	0	103	CRT	5	0
16	R	101	BCL	7	0
15	1	401	PGV	3	0
24	E	101	LMT	2	0
24	4	103	LMT	2	0

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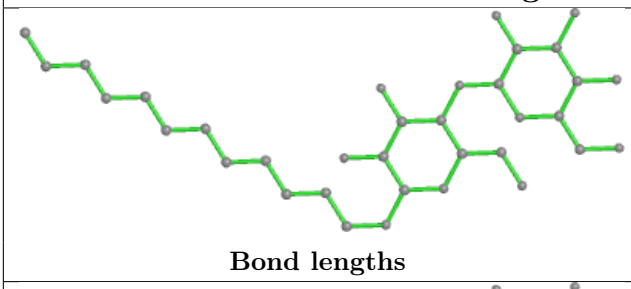
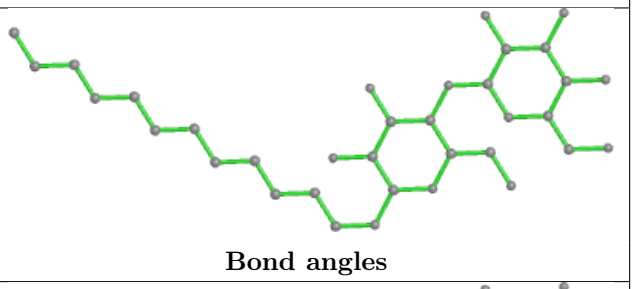
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	301	PGV	3	0
16	T	101	BCL	10	0
15	C	409	PGV	2	0
24	B	101	LMT	3	0
21	G	103	CRT	7	0
16	P	102	BCL	7	0
21	Z	103	CRT	6	0
22	D	502	CDL	3	0
10	C	404	HEM	4	0
21	8	103	CRT	7	0
16	0	102	BCL	8	0
17	M	405	BPH	7	0
15	L	305	PGV	4	0
16	O	502	BCL	4	0
24	V	101	LMT	2	0
21	N	102	CRT	1	0
14	C	408	PLM	3	0
10	C	402	HEM	7	0
16	7	102	BCL	8	0
18	L	308	UQ8	9	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.

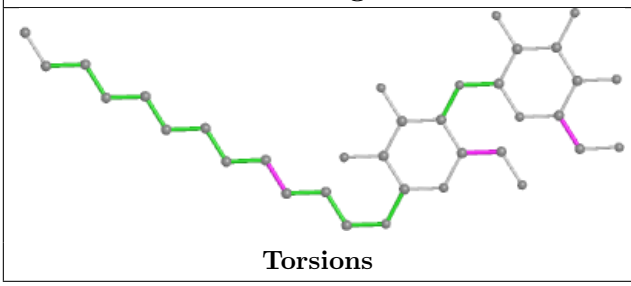
Ligand LMT P 101



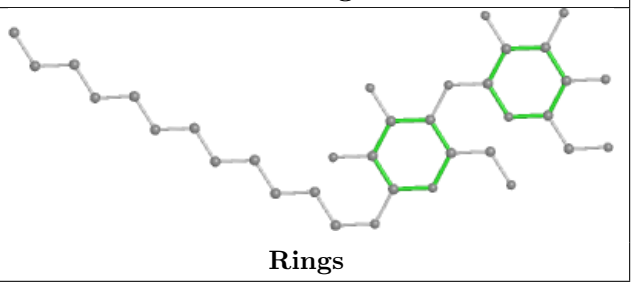
Bond lengths



Bond angles

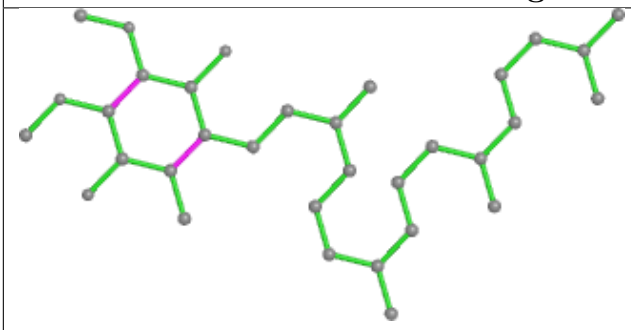


Torsions

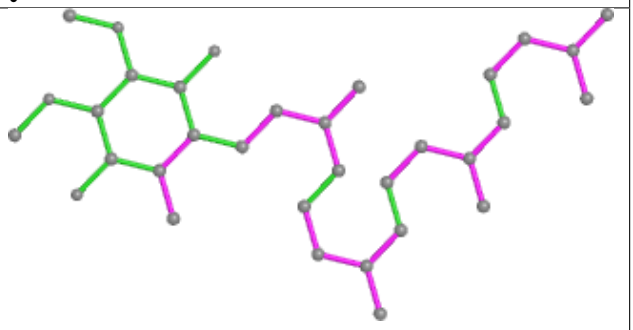


Rings

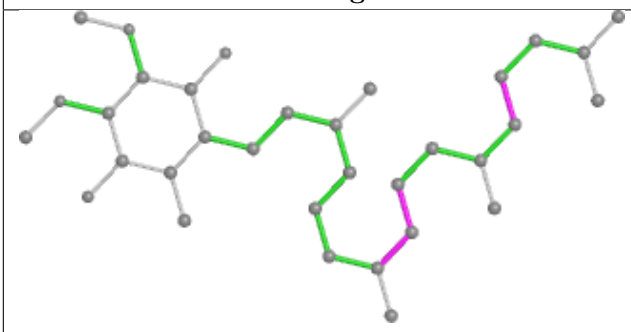
Ligand UQ8 L 303



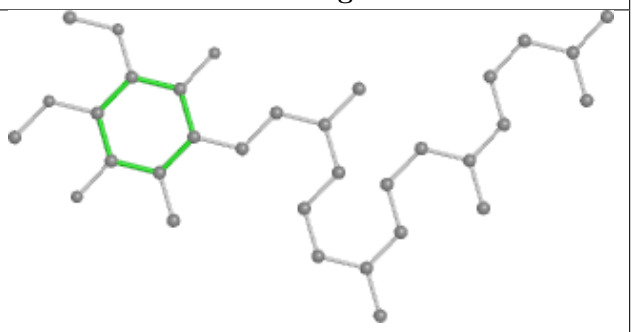
Bond lengths



Bond angles

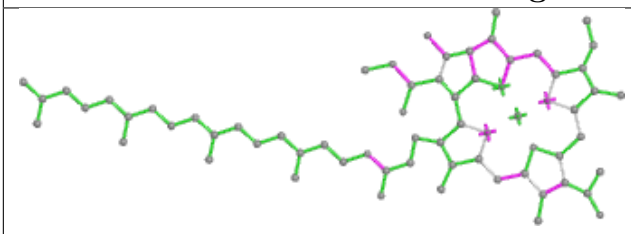


Torsions

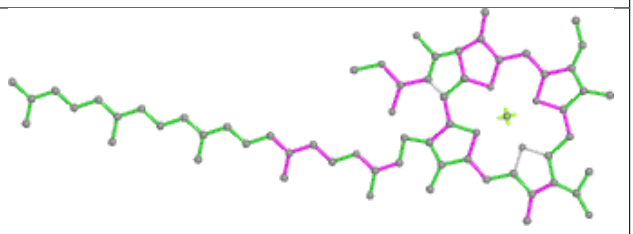


Rings

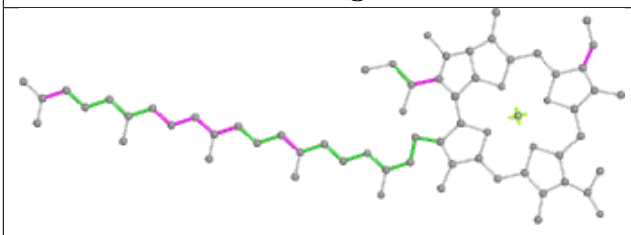
Ligand BCL 5 102



Bond lengths



Bond angles



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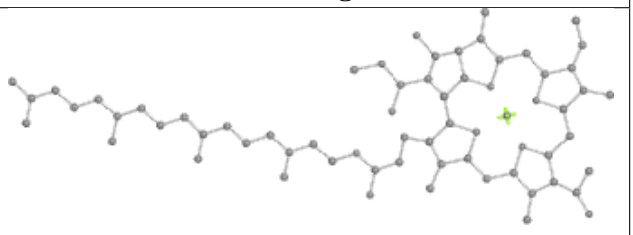
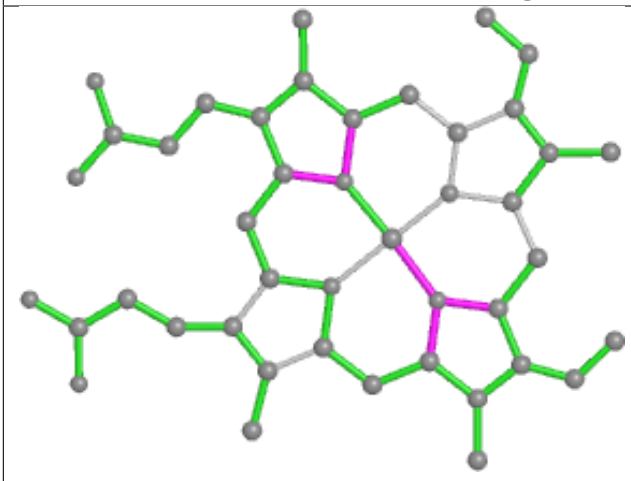
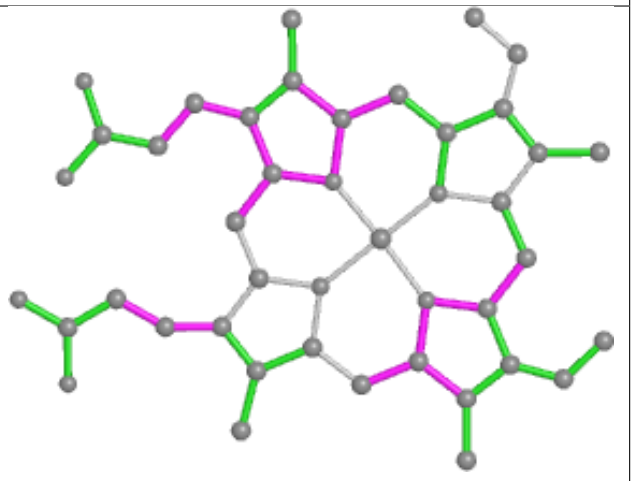


Rings

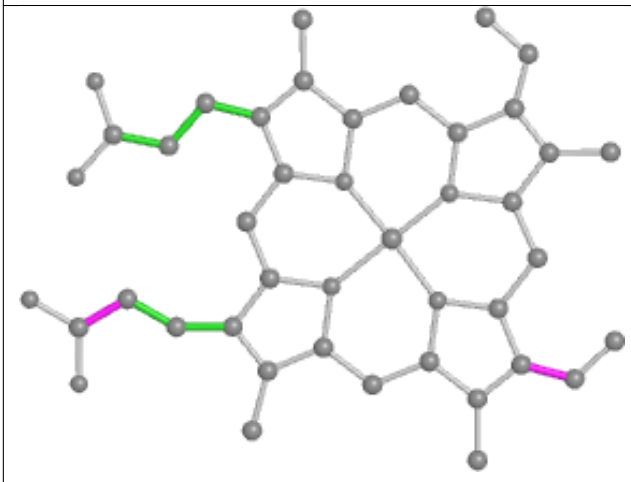
Ligand HEM C 401



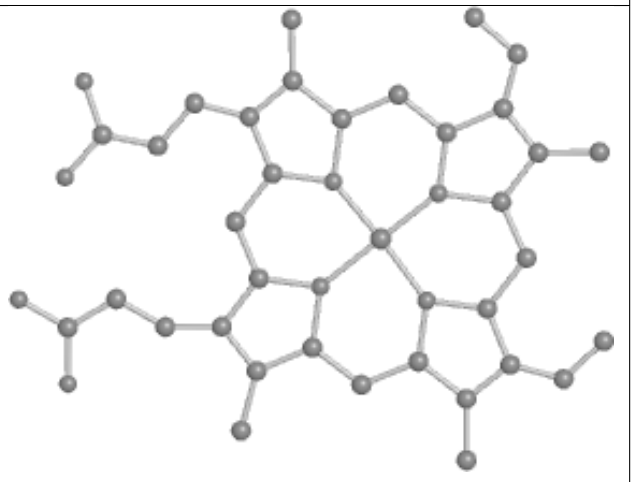
Bond lengths



Bond angles

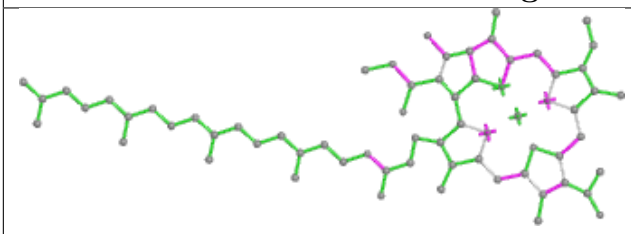


Torsions

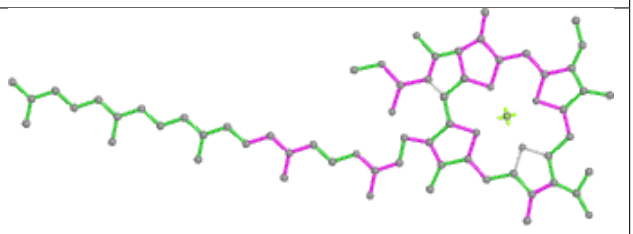


Rings

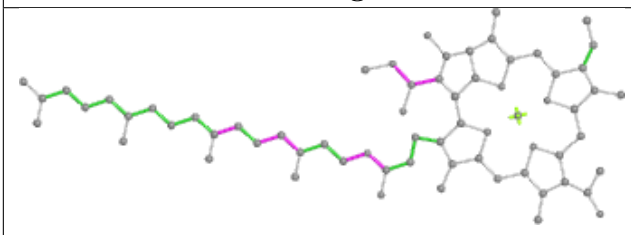
Ligand BCL M 404



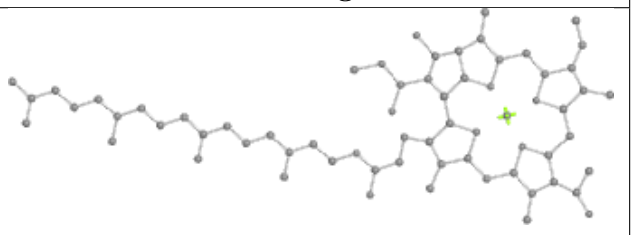
Bond lengths



Bond angles

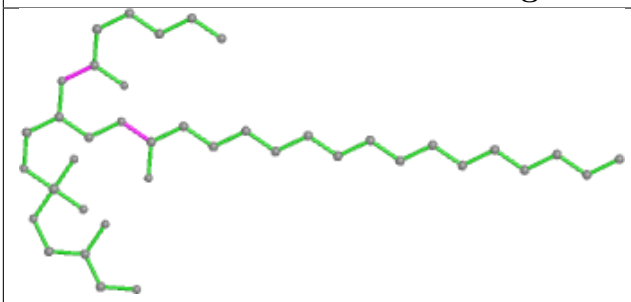


Torsions

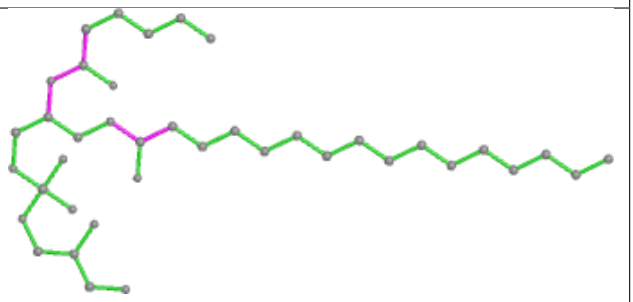


Rings

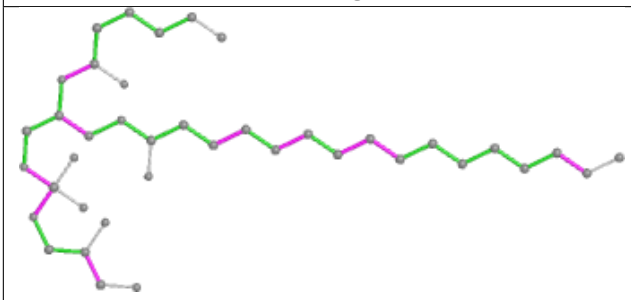
Ligand PGV D 501



Bond lengths



Bond angles



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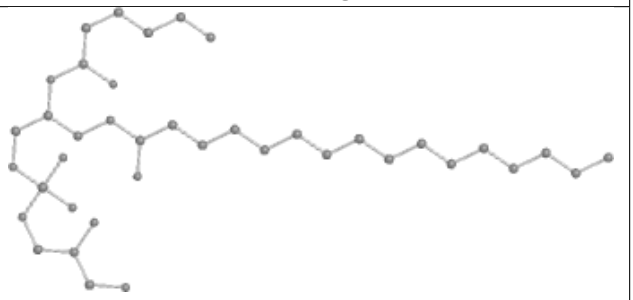
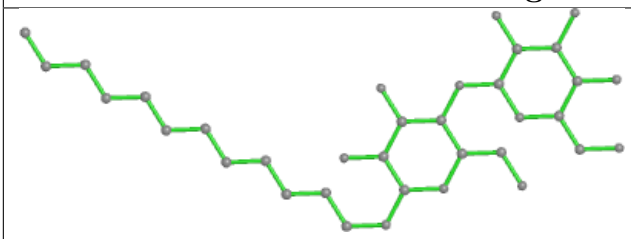
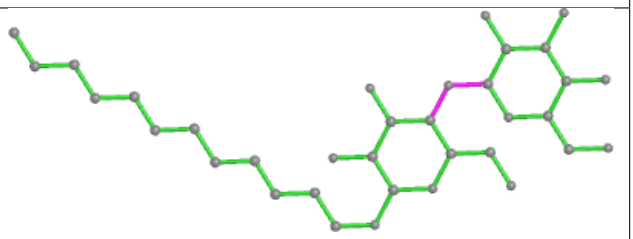


Rings

Ligand LMT 2 101



Bond lengths



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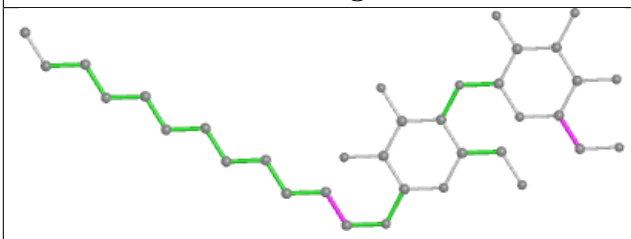

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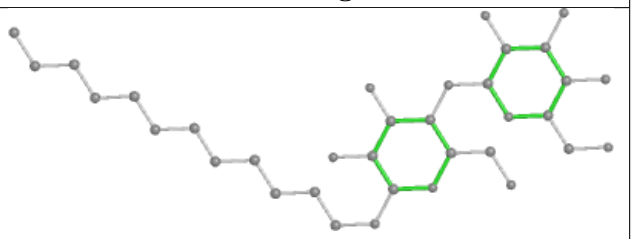
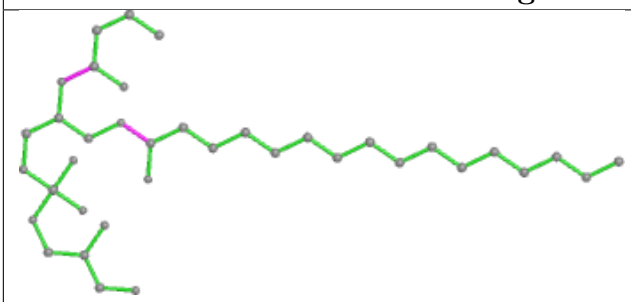
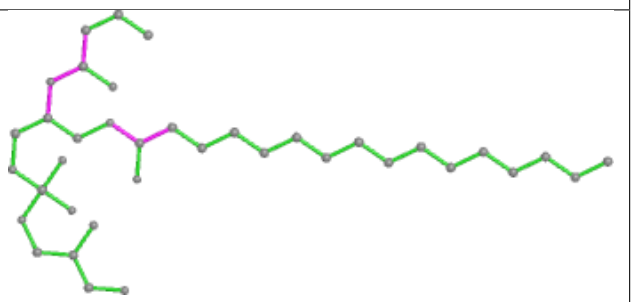


Rings

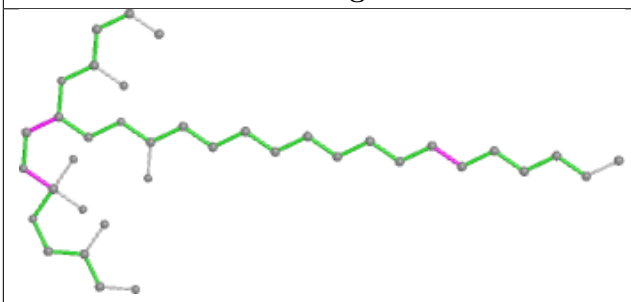
Ligand PGV M 408



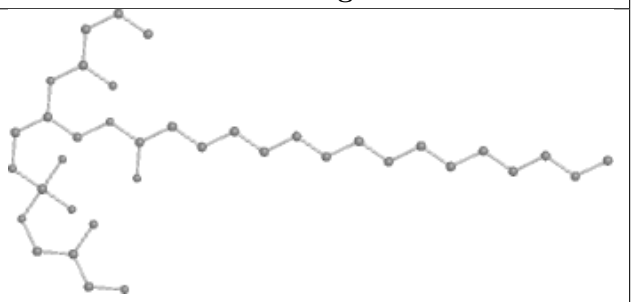
Bond lengths



Bond angles

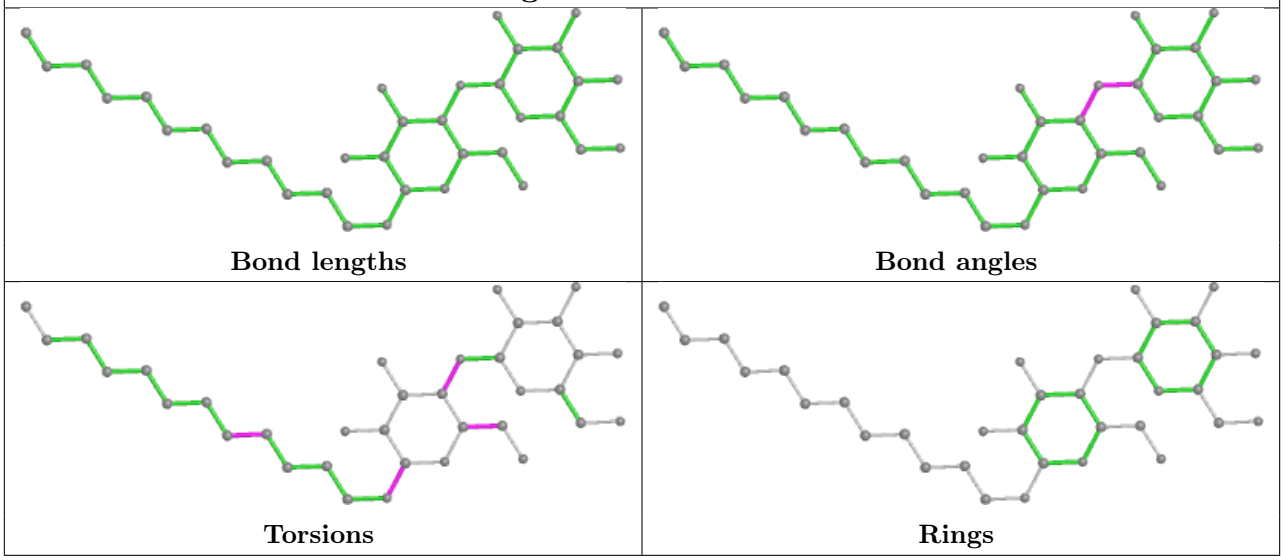


Torsions

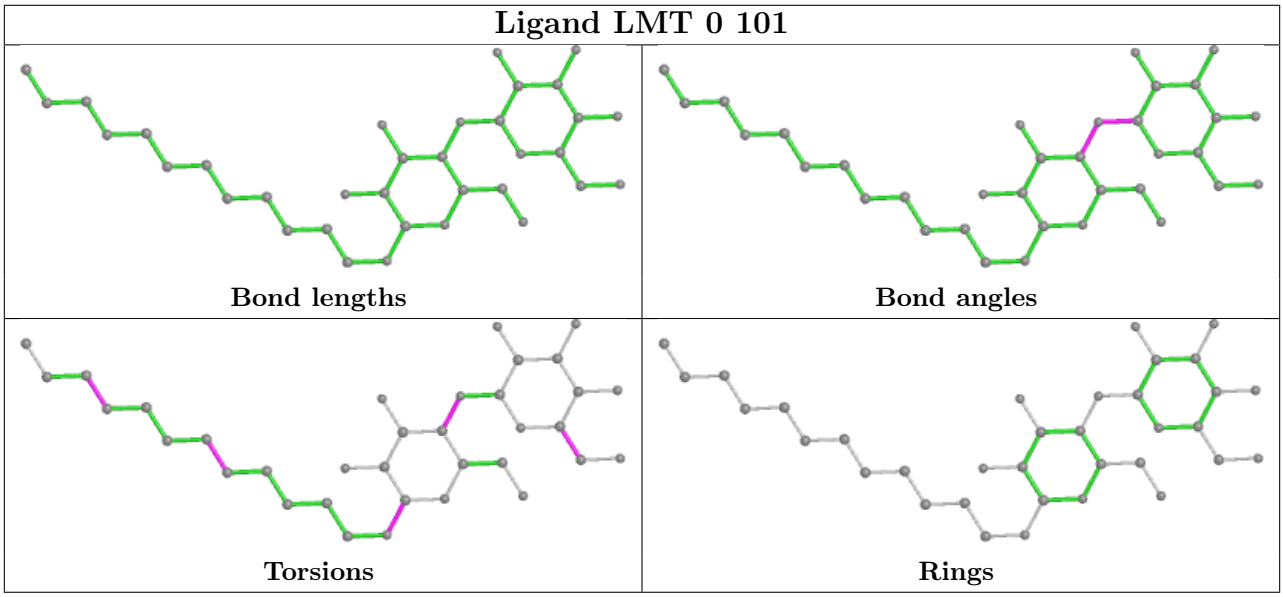


Rings

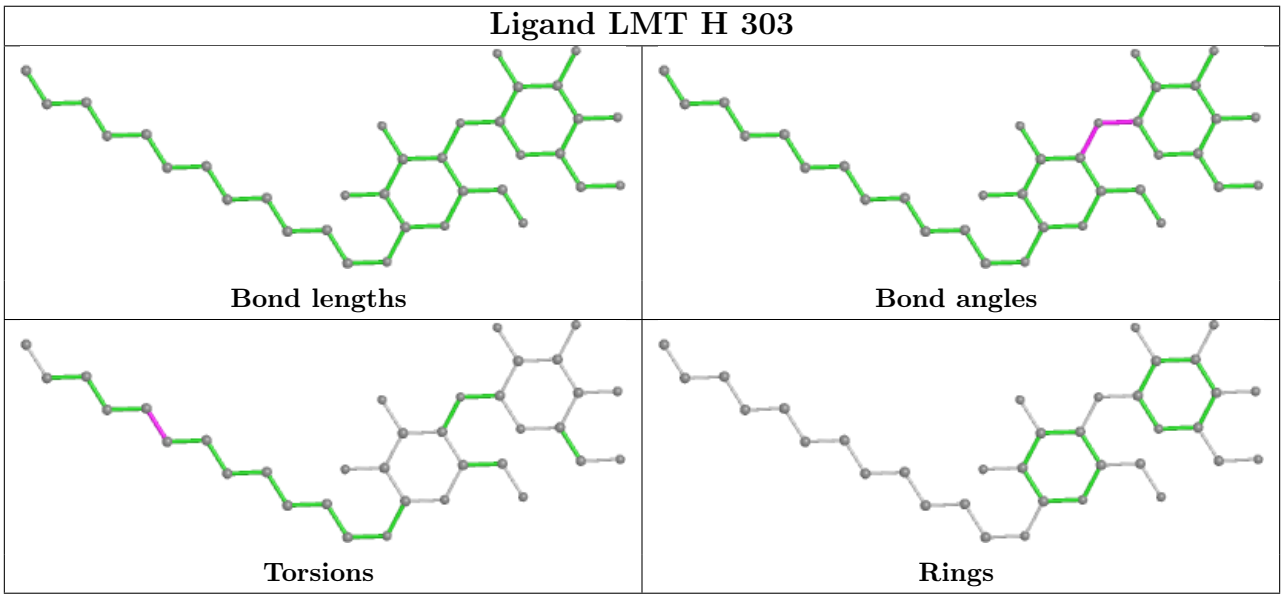
Ligand LMT G 101



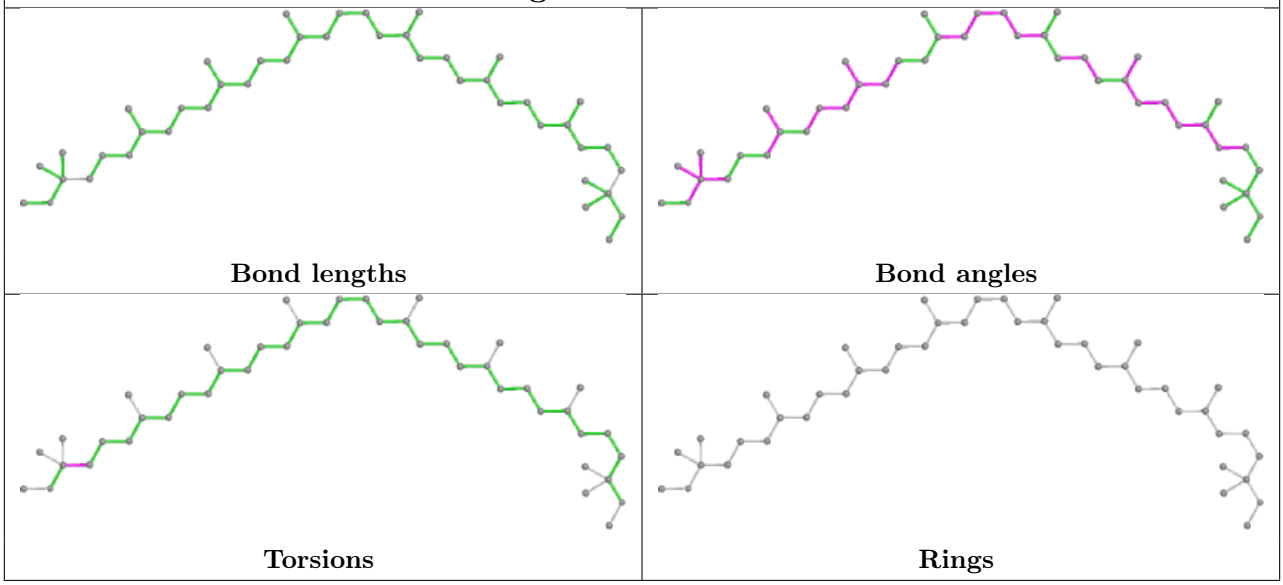
Ligand LMT 0 101



Ligand LMT H 303



Ligand CRT 2 103



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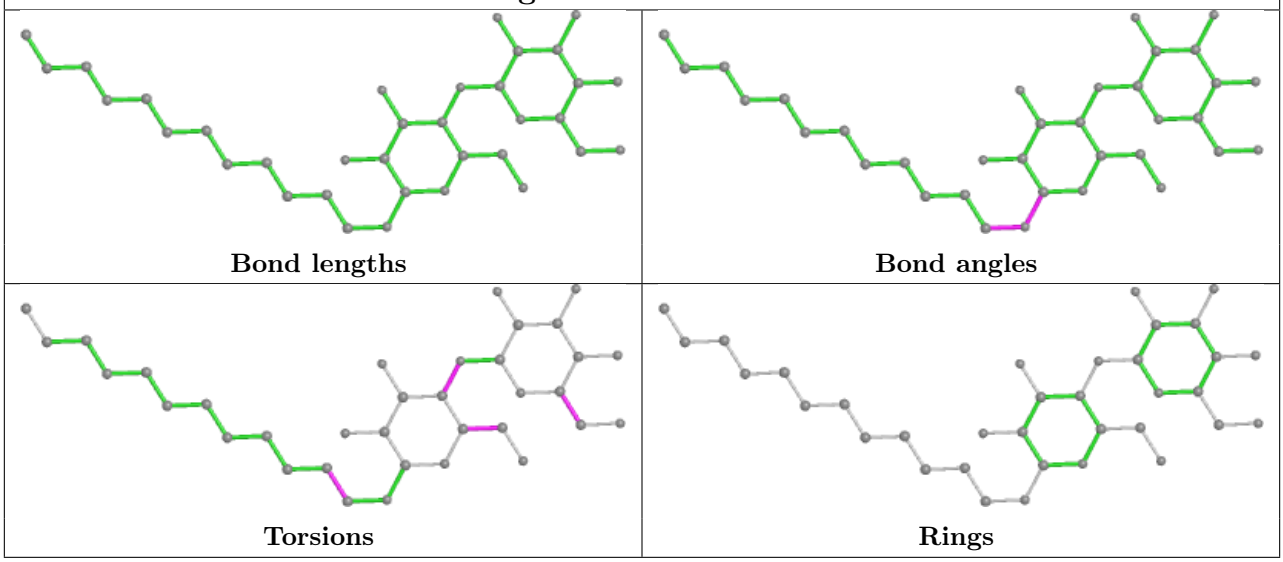
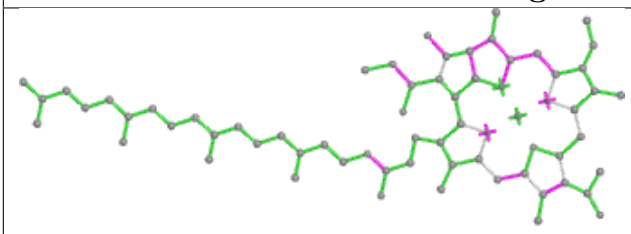
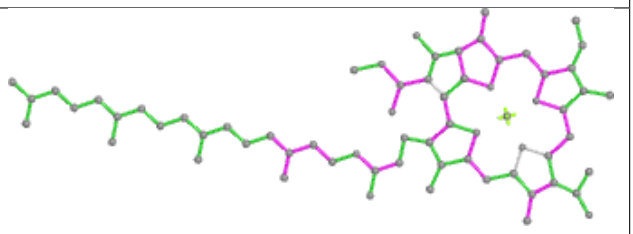


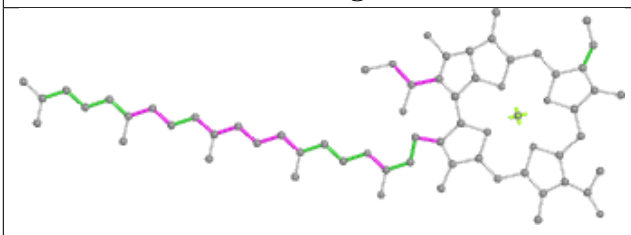
Ligand BCL 9 101



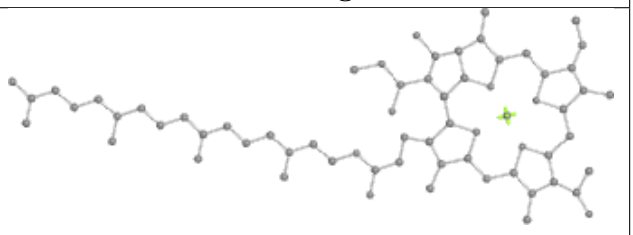
Bond lengths



Bond angles

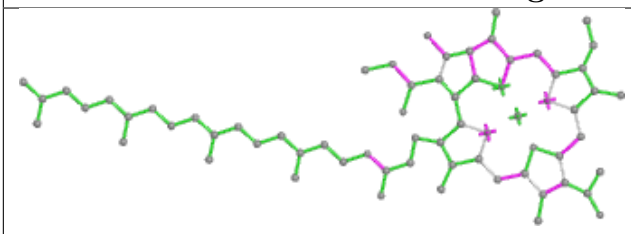


Torsions

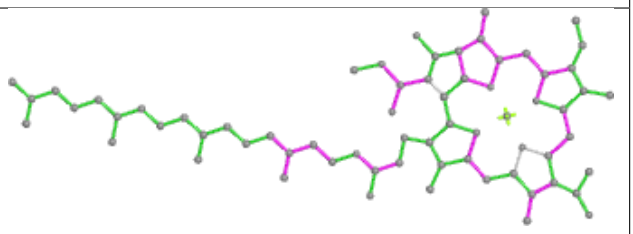


Rings

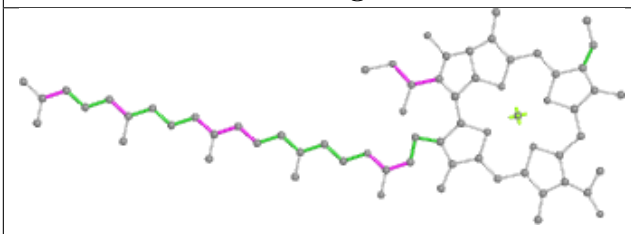
Ligand BCL L 307



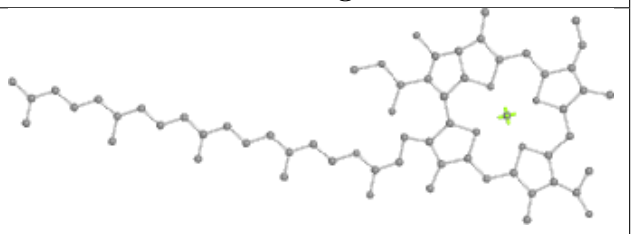
Bond lengths



Bond angles

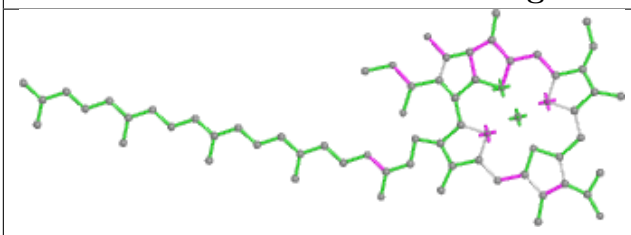


Torsions

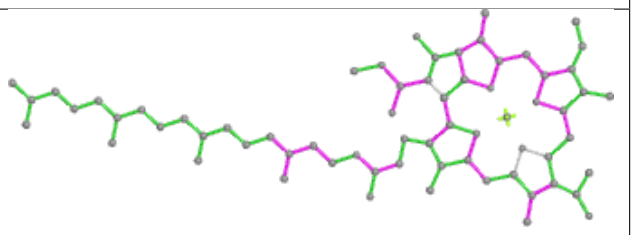


Rings

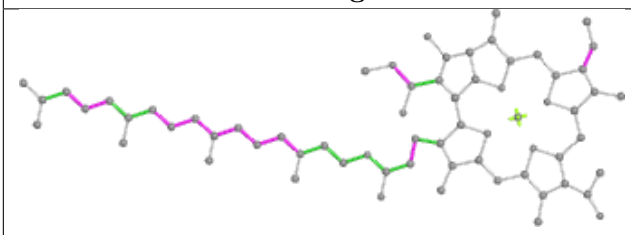
Ligand BCL Z 102



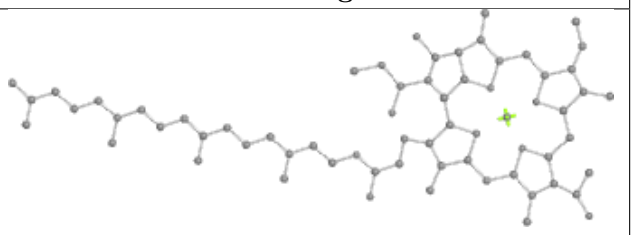
Bond lengths



Bond angles

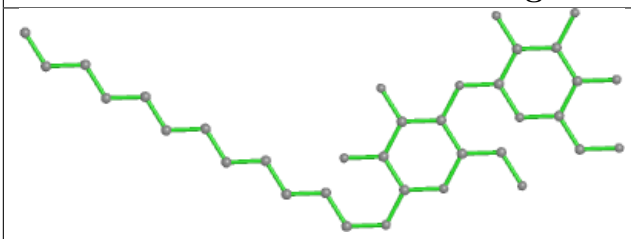


Torsions



Rings

Ligand LMT 8 101



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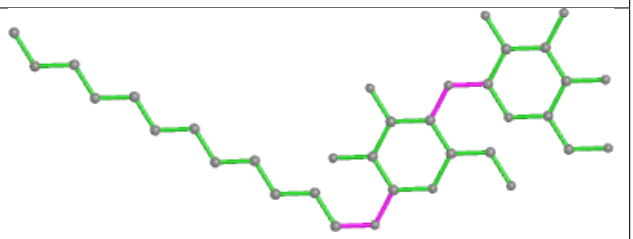
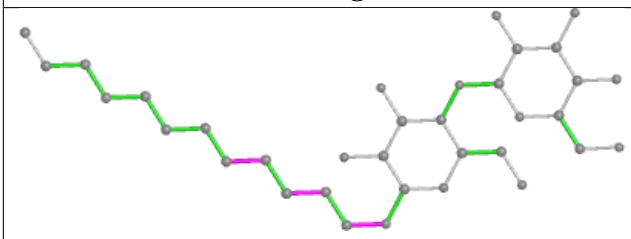
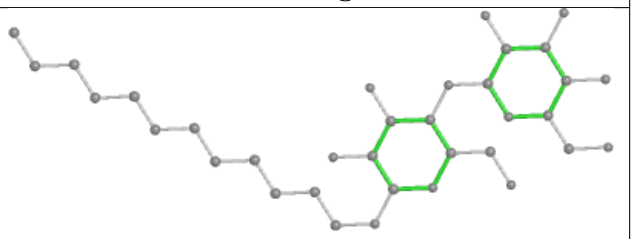


Bond angles

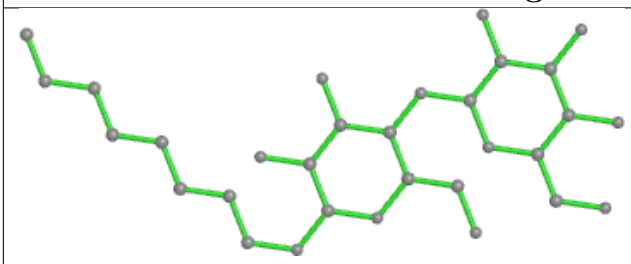


Torsions

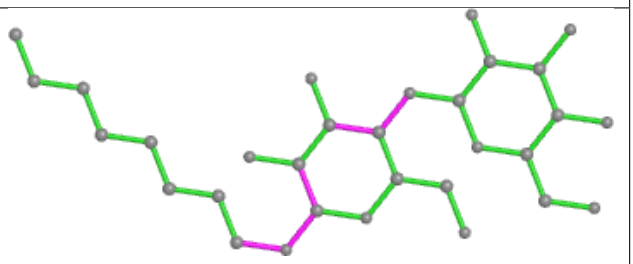


Rings

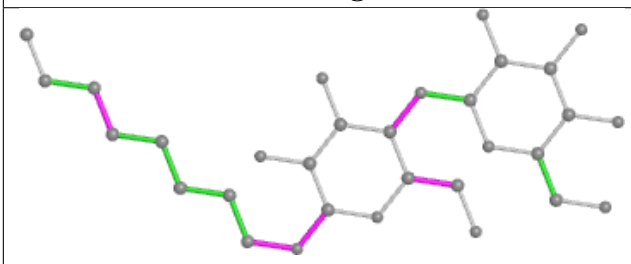
Ligand LMT 5 101



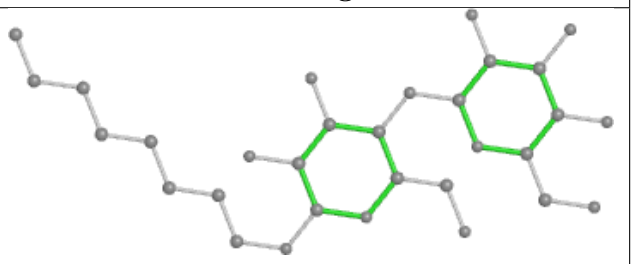
Bond lengths



Bond angles

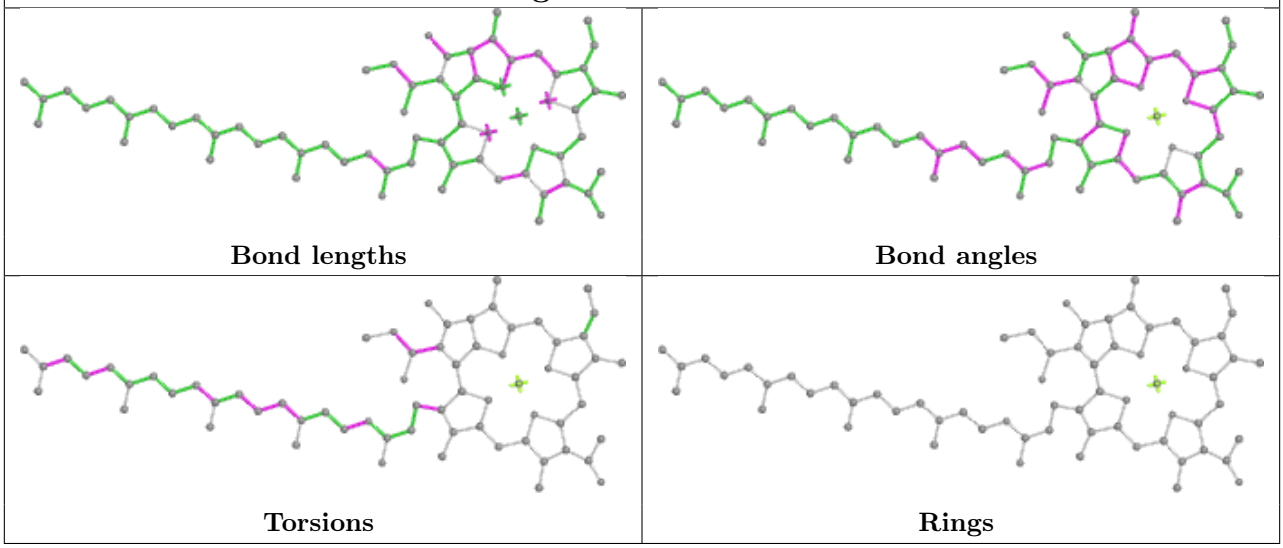


Torsions

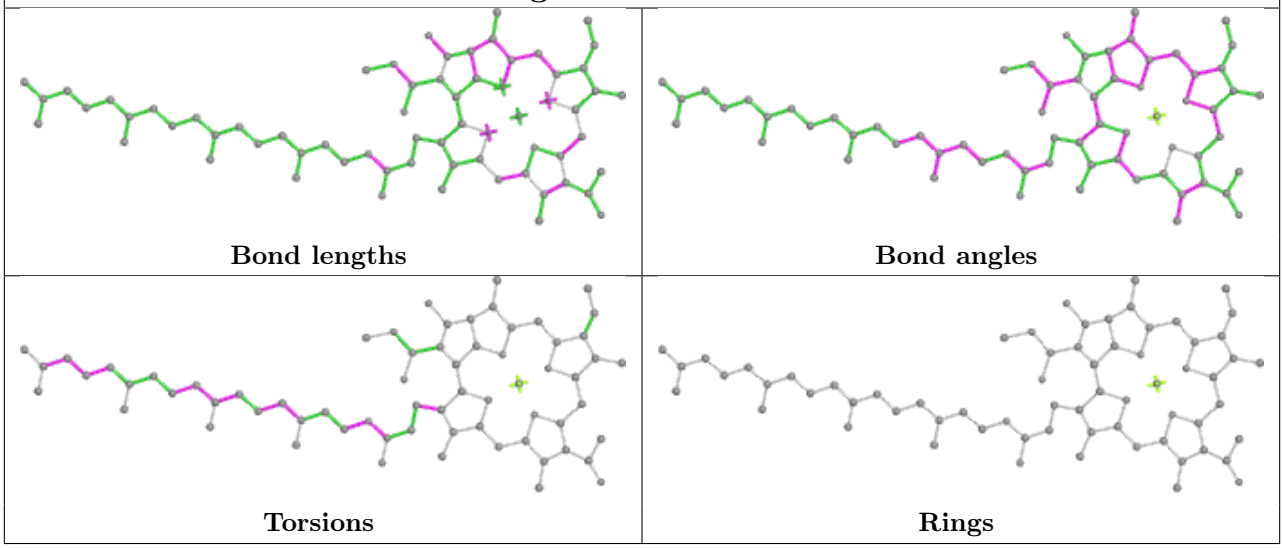


Rings

Ligand BCL I 101



Ligand BCL 1 402



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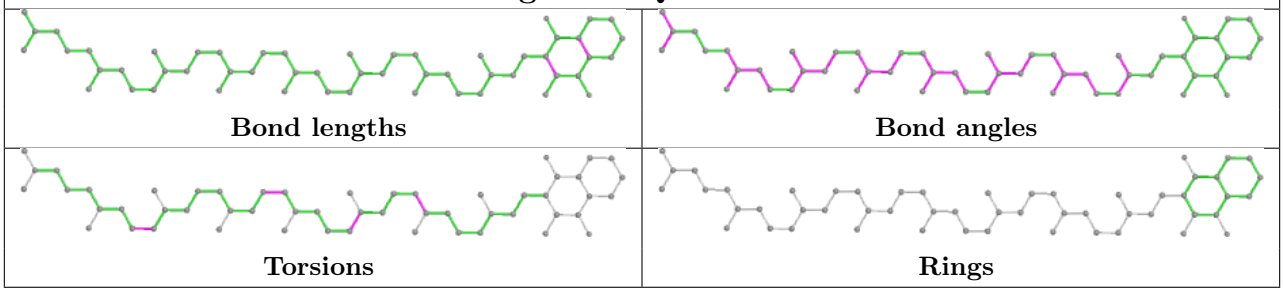
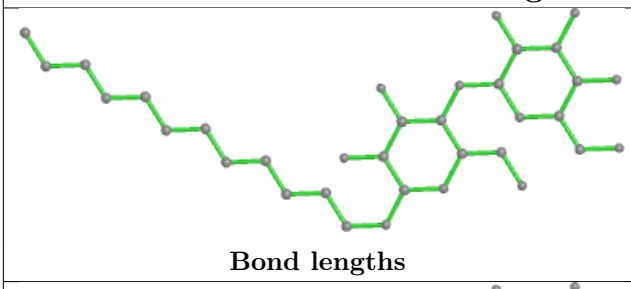
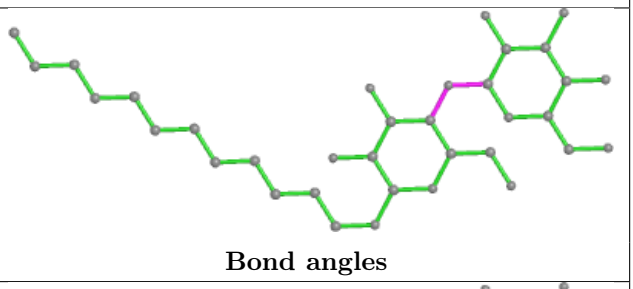


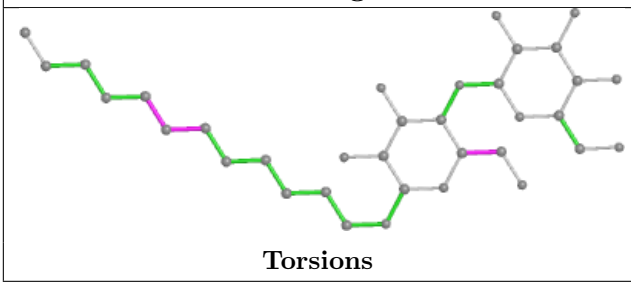
Ligand LMT 2 104



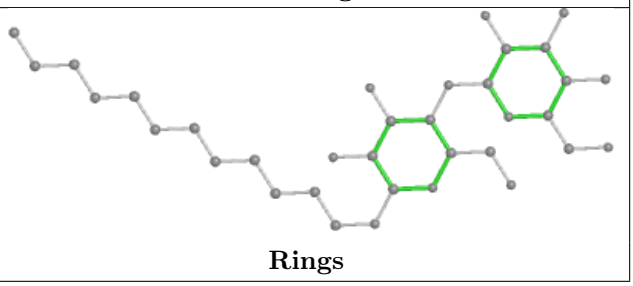
Bond lengths



Bond angles

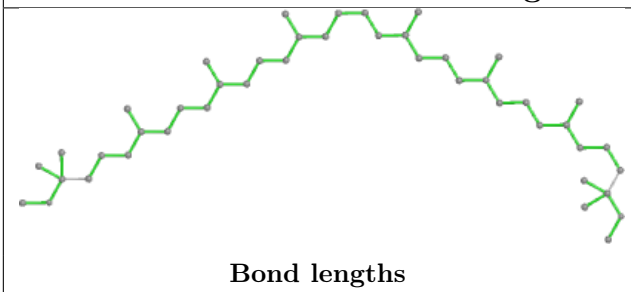


Torsions

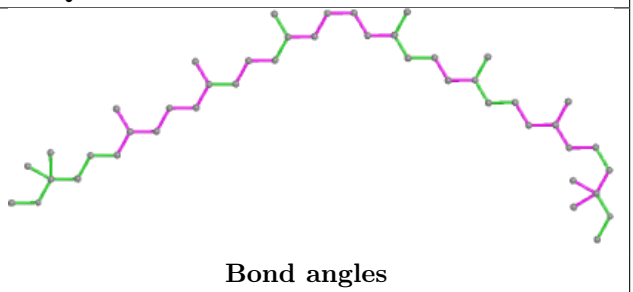


Rings

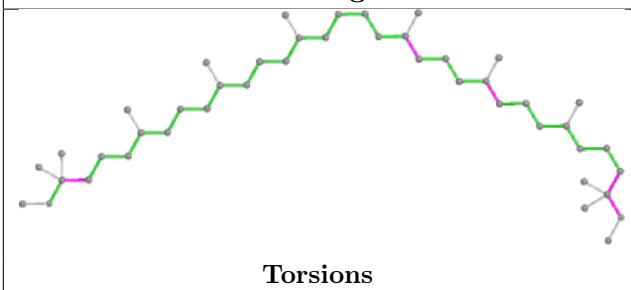
Ligand CRT Q 101



Bond lengths



Bond angles



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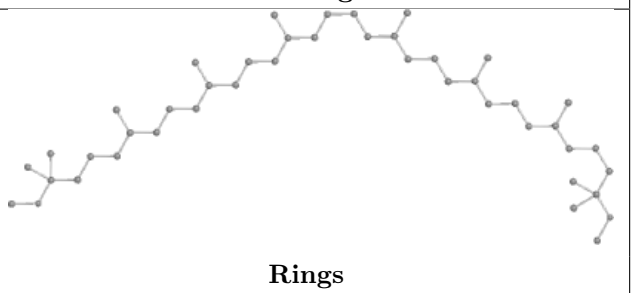
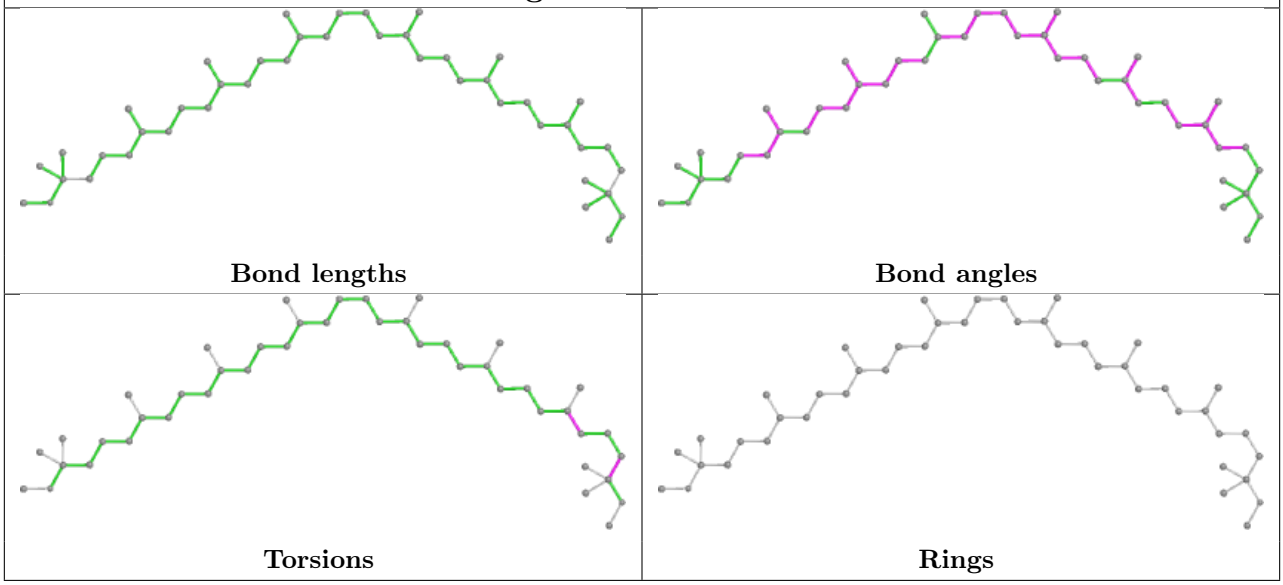
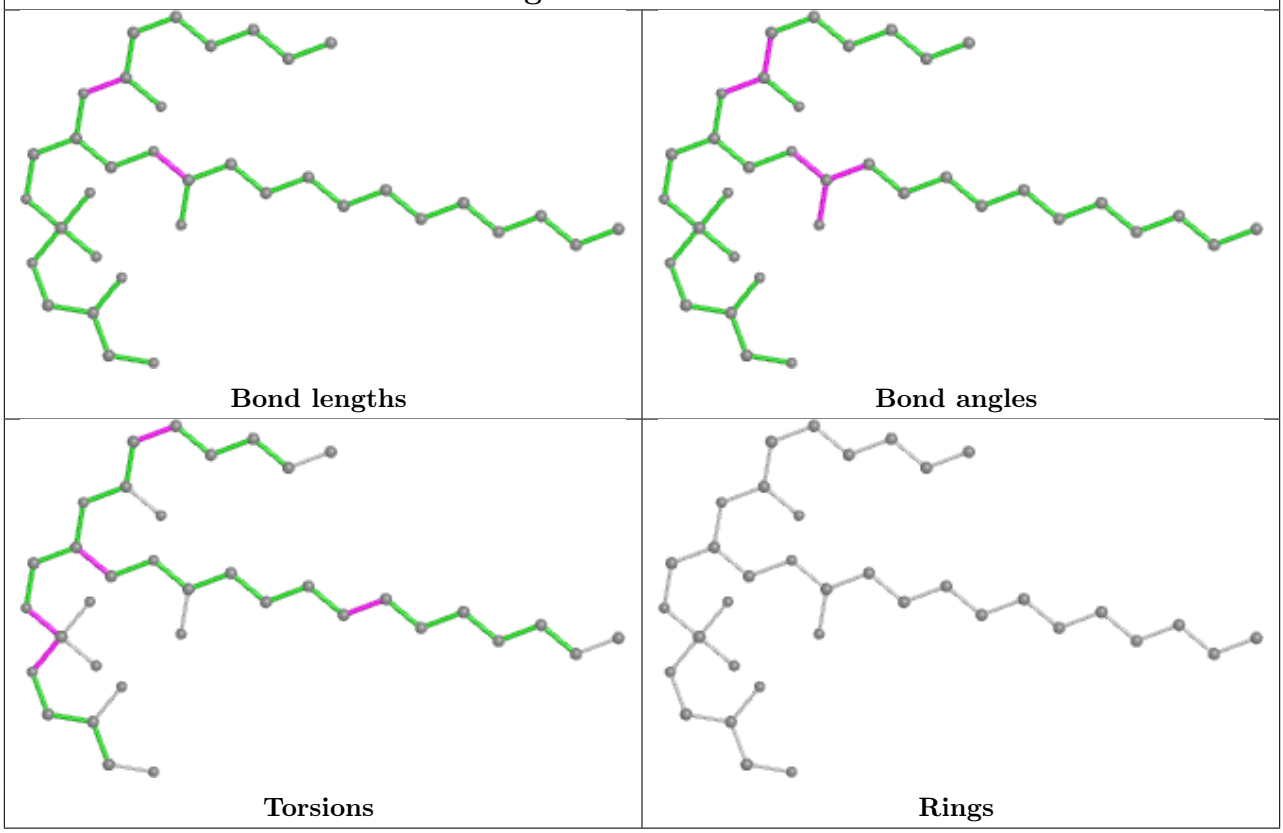


Rings

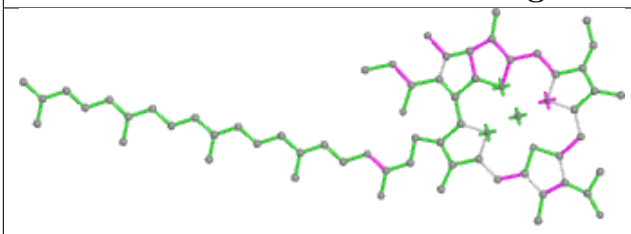
Ligand CRT T 102



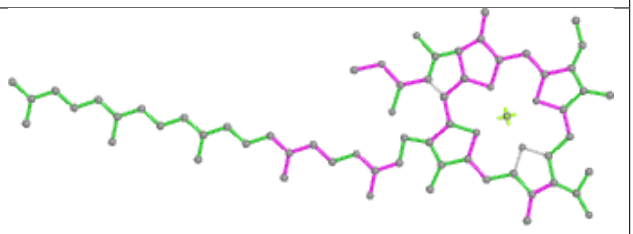
Ligand PGV F 501



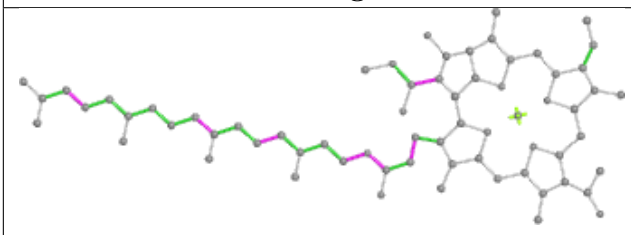
Ligand BCL L 301



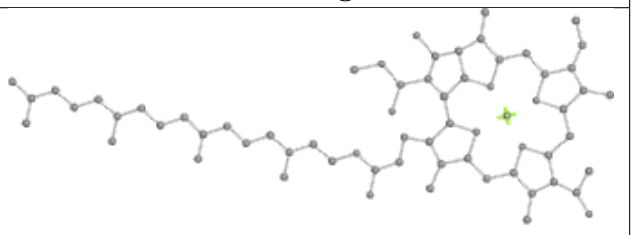
Bond lengths



Bond angles

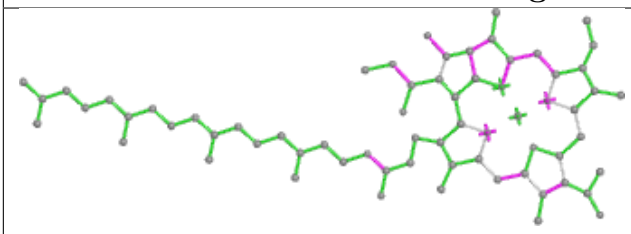


Torsions

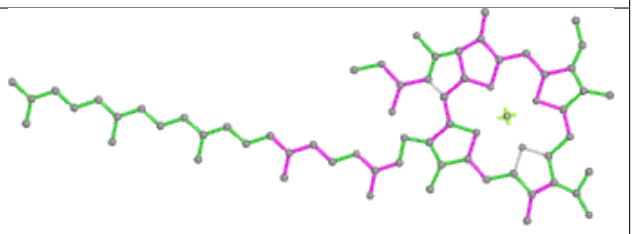


Rings

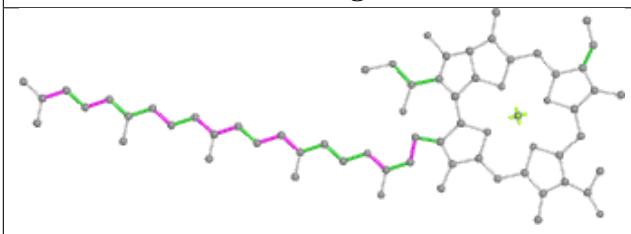
Ligand BCL 6 101



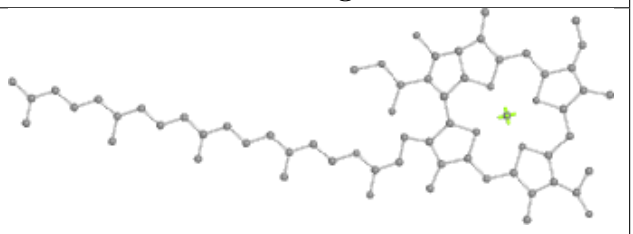
Bond lengths



Bond angles

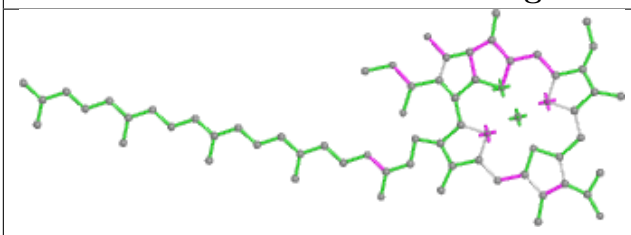


Torsions

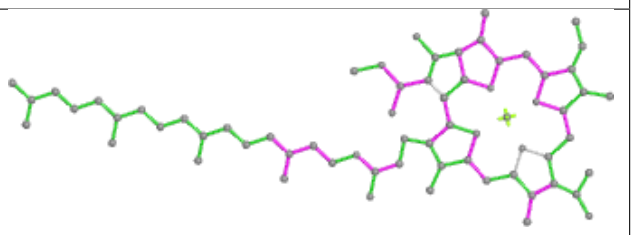


Rings

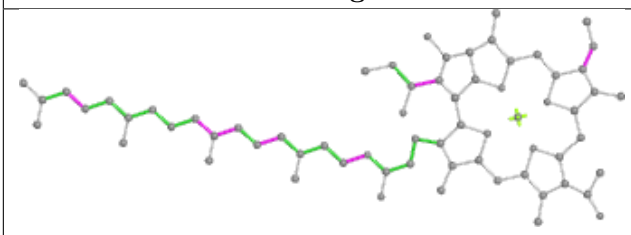
Ligand BCL D 503



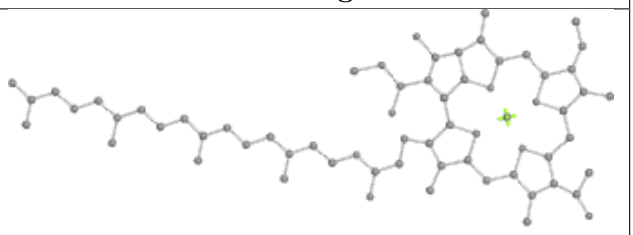
Bond lengths



Bond angles

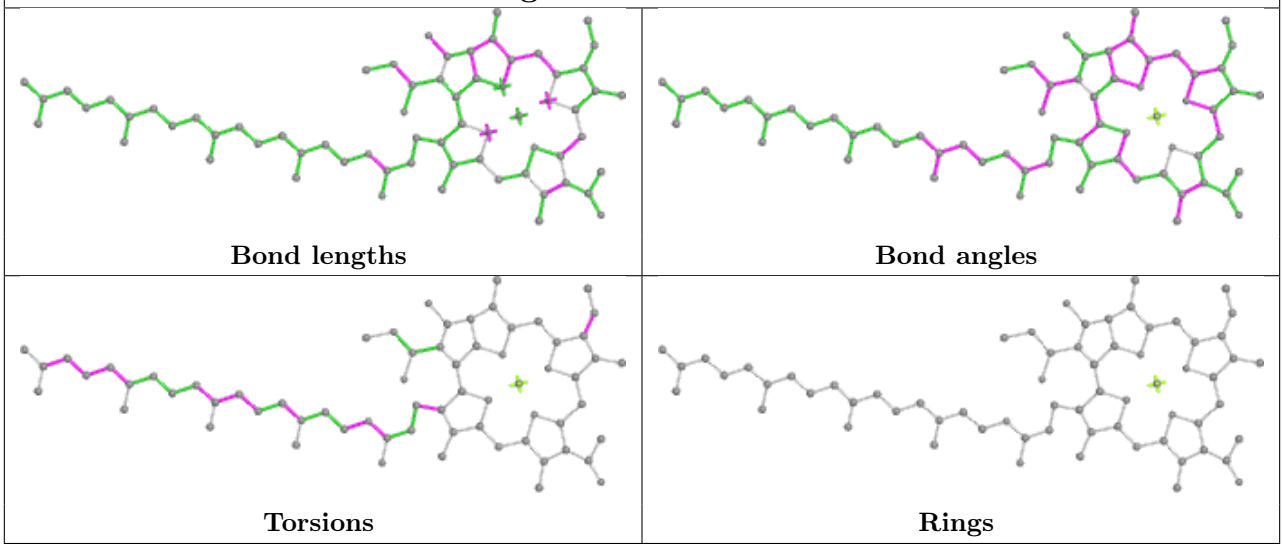


Torsions

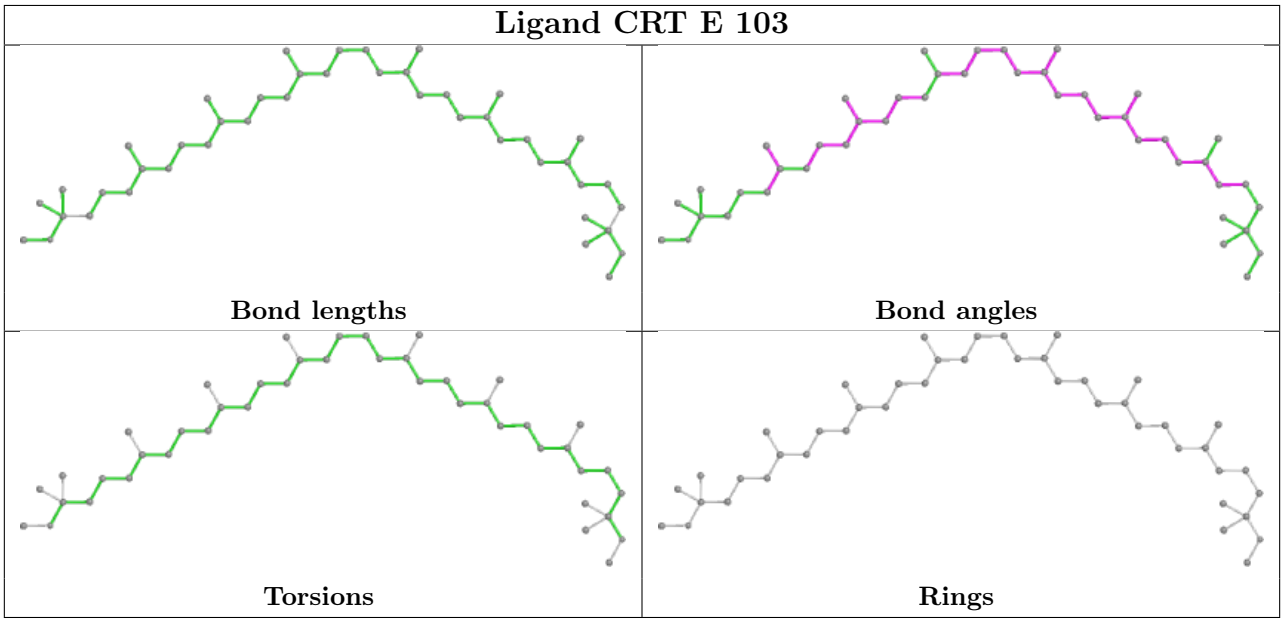


Rings

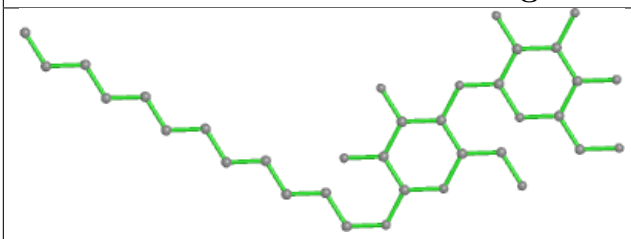
Ligand BCL W 101



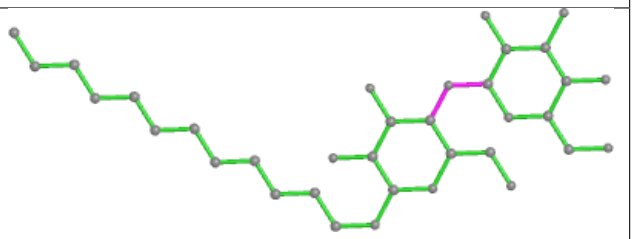
Ligand CRT E 103



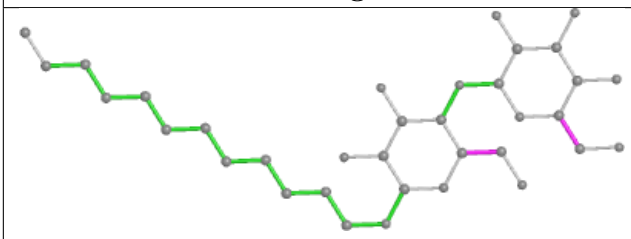
Ligand LMT X 101



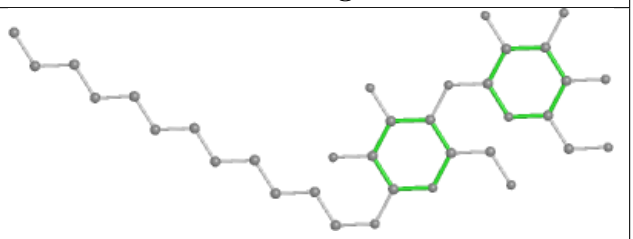
Bond lengths



Bond angles

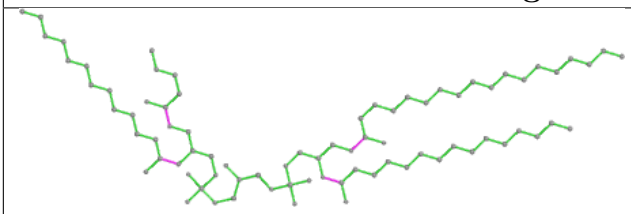


Torsions

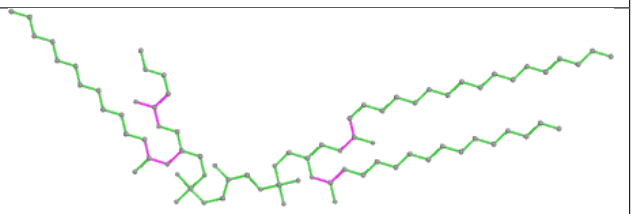


Rings

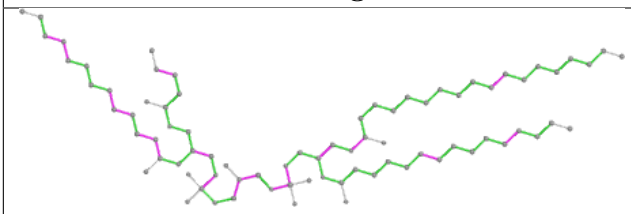
Ligand CDL H 302



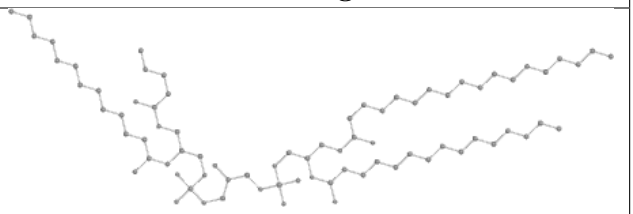
Bond lengths



Bond angles

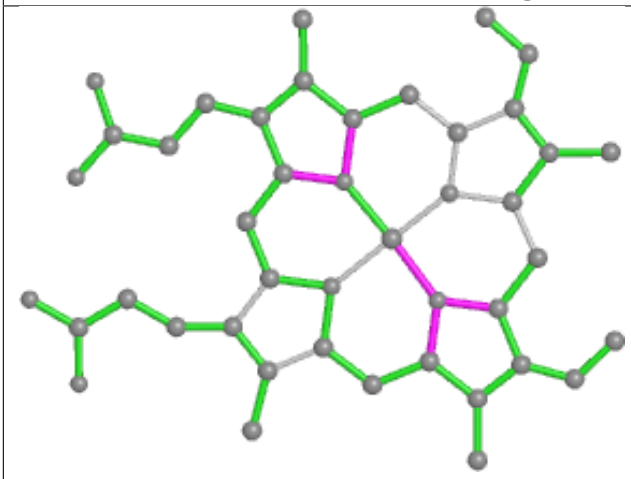


Torsions

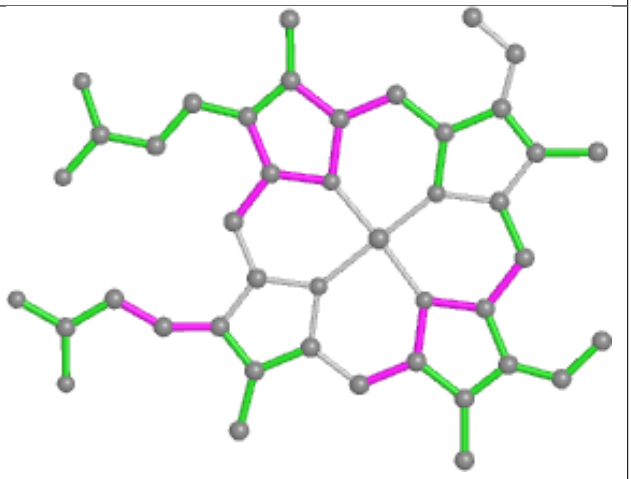


Rings

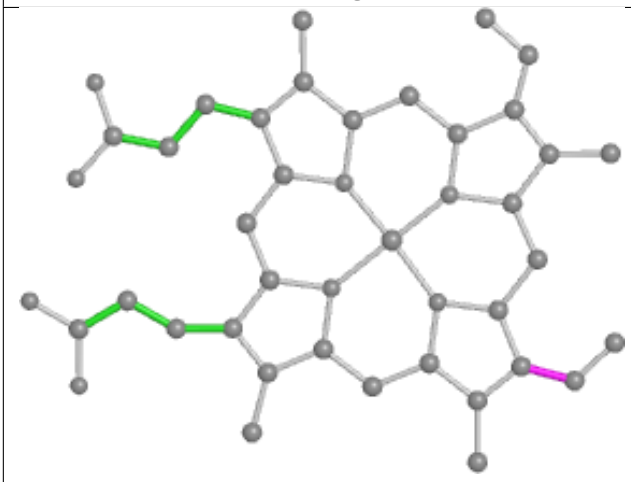
Ligand HEM C 403



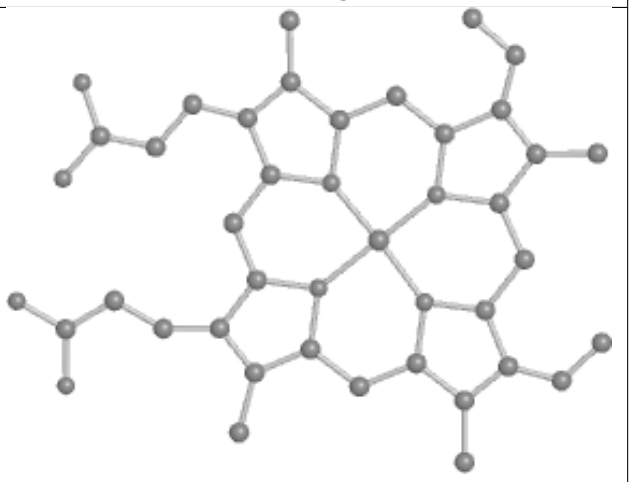
Bond lengths



Bond angles

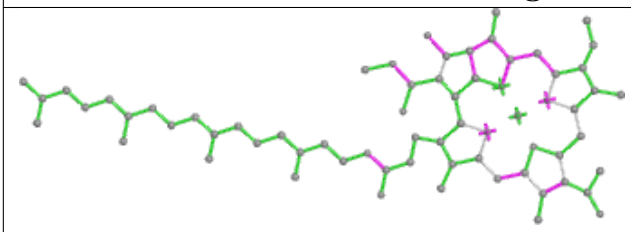


Torsions

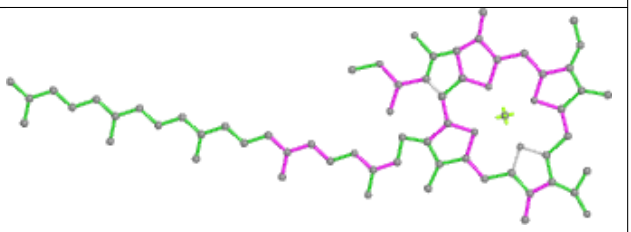


Rings

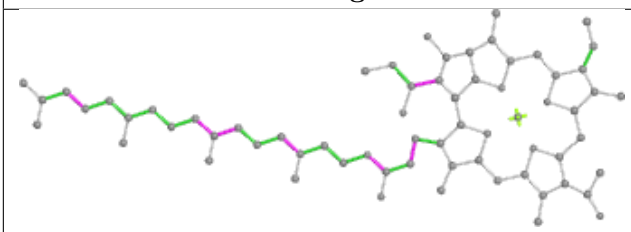
Ligand BCL K 102



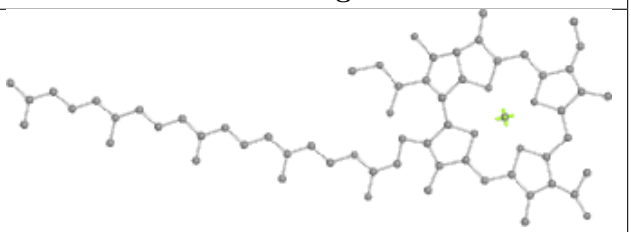
Bond lengths



Bond angles

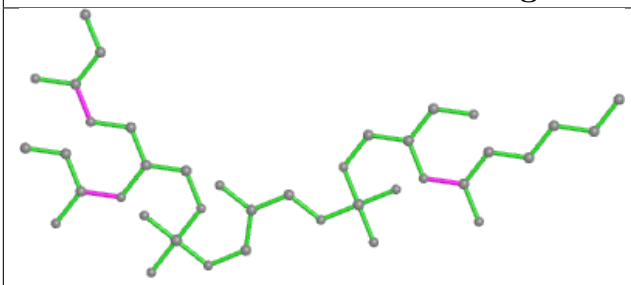


Torsions

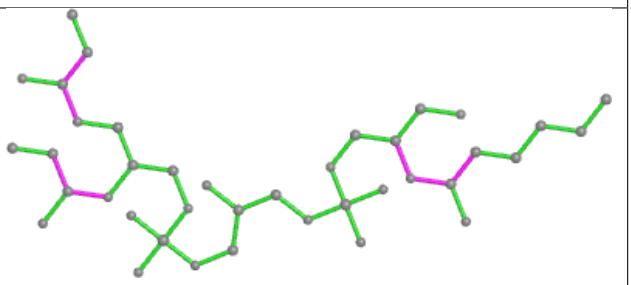


Rings

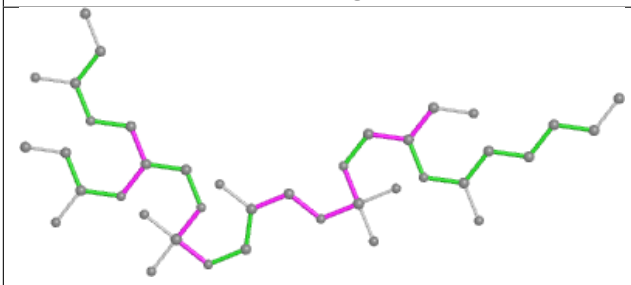
Ligand CDL M 409



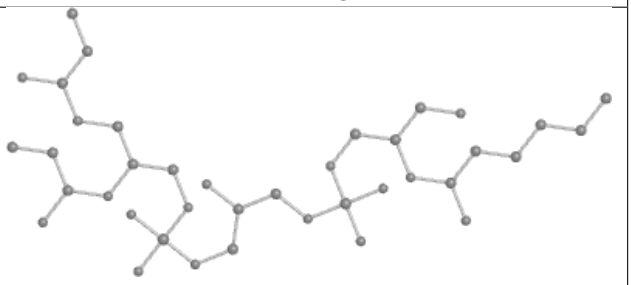
Bond lengths



Bond angles

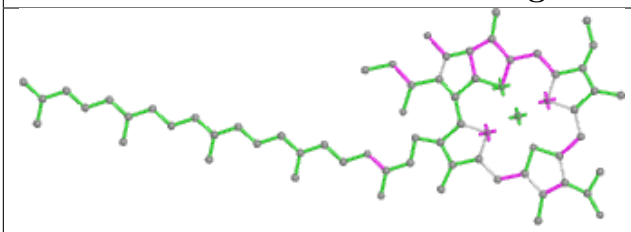


Torsions

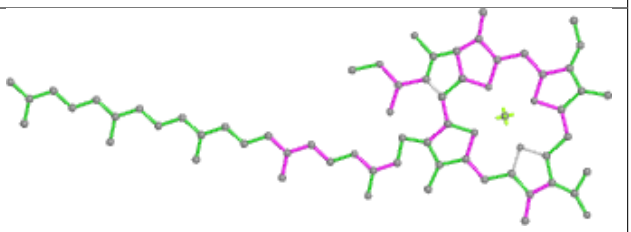


Rings

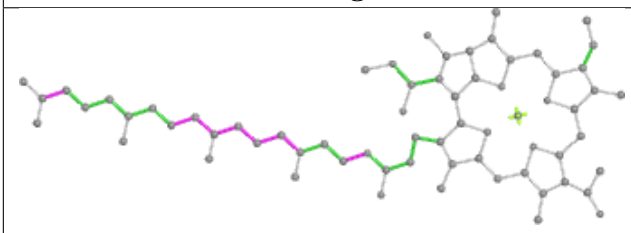
Ligand BCL S 101



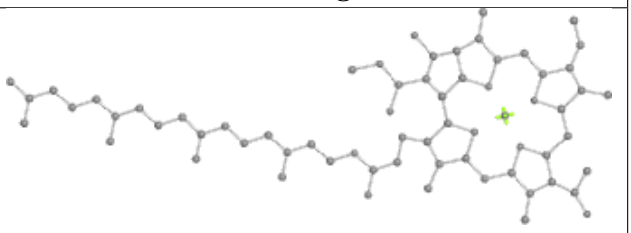
Bond lengths



Bond angles

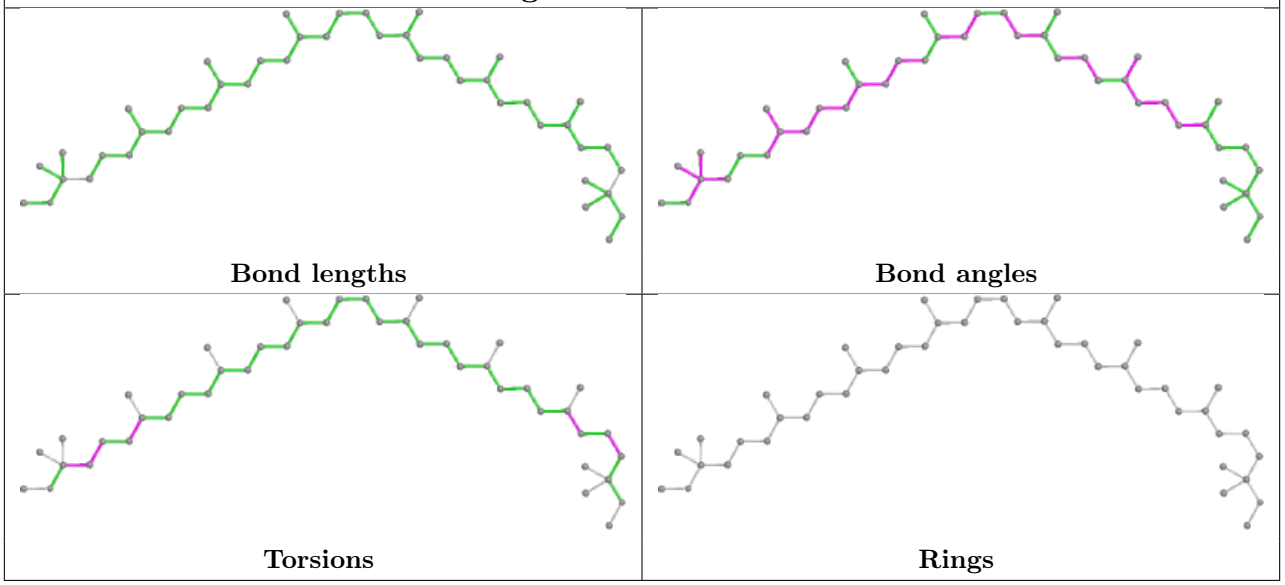


Torsions

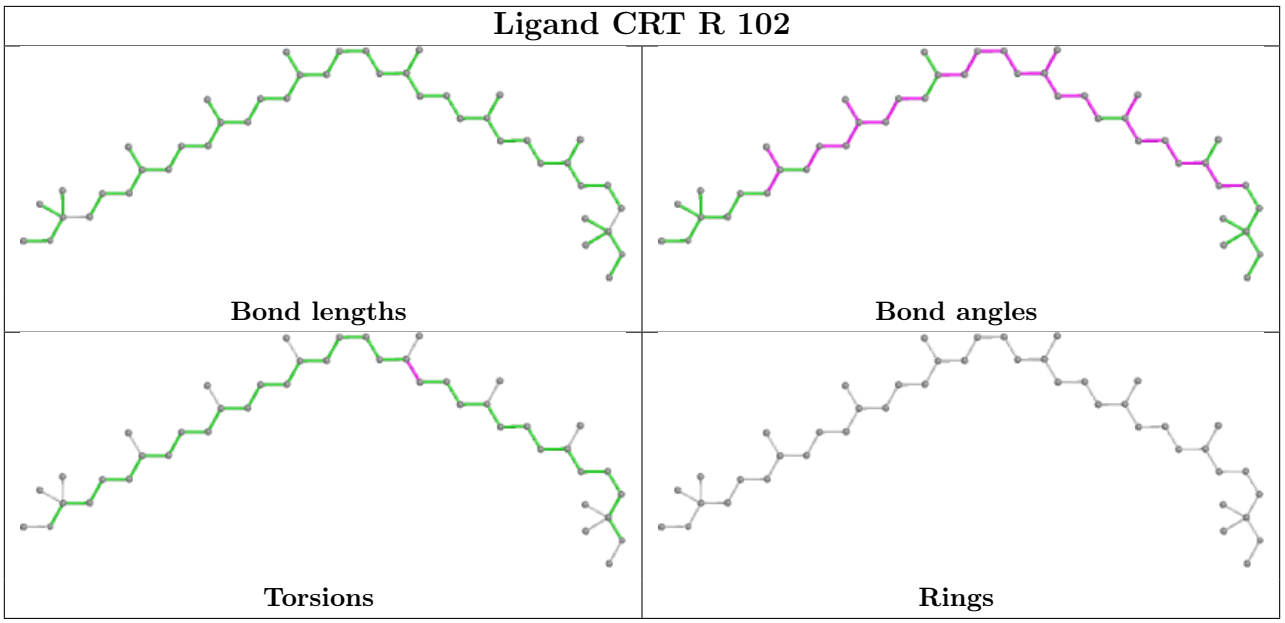


Rings

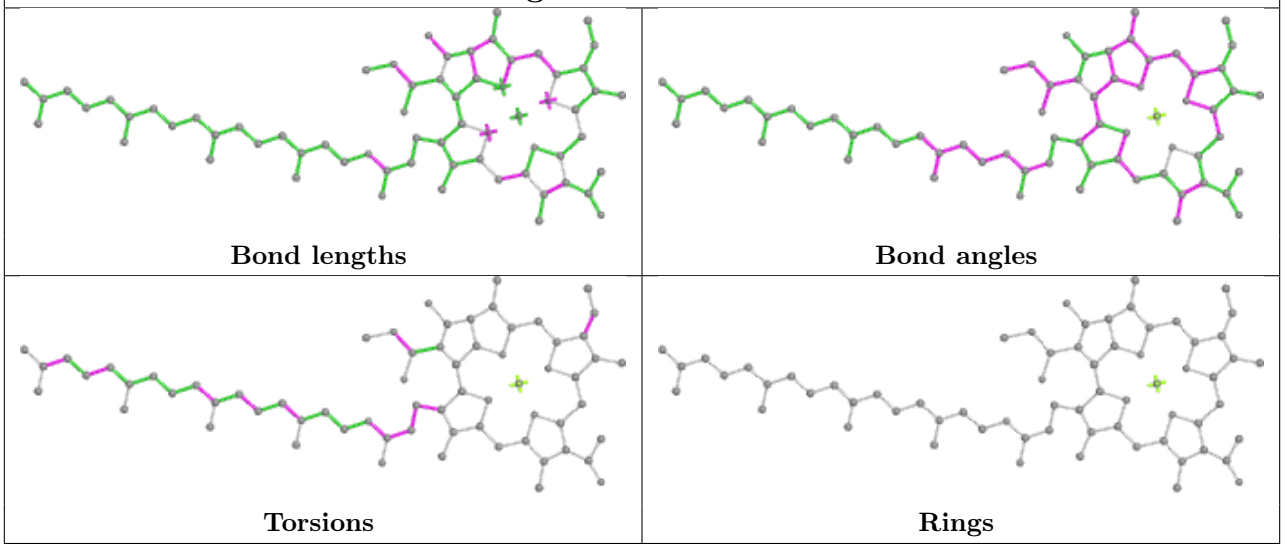
Ligand CRT M 407



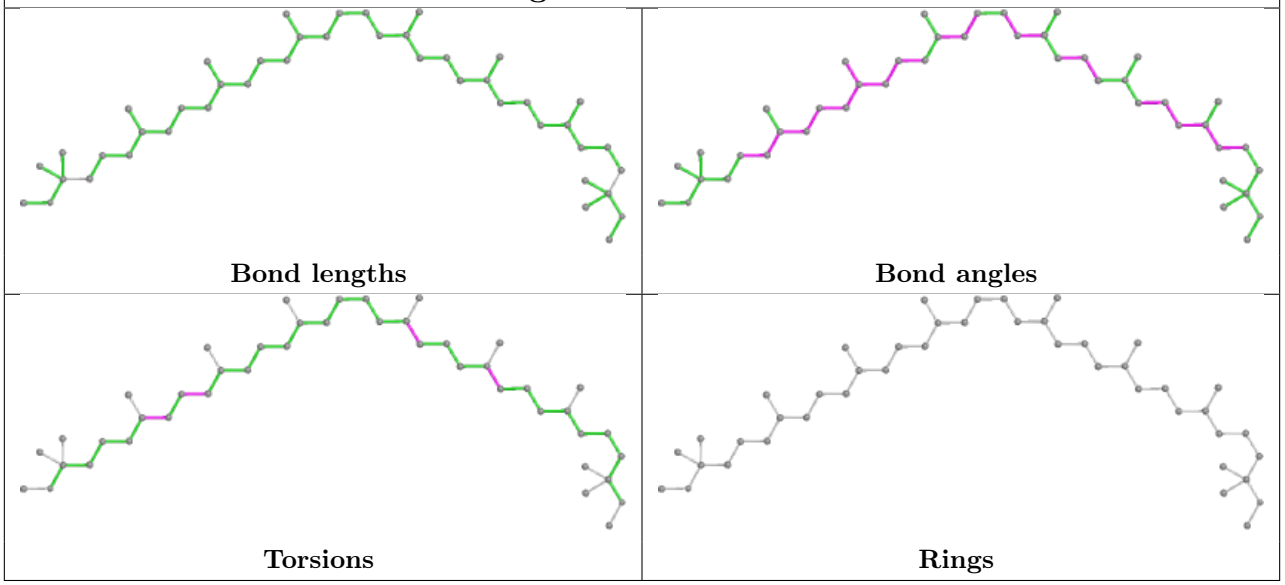
Ligand CRT R 102



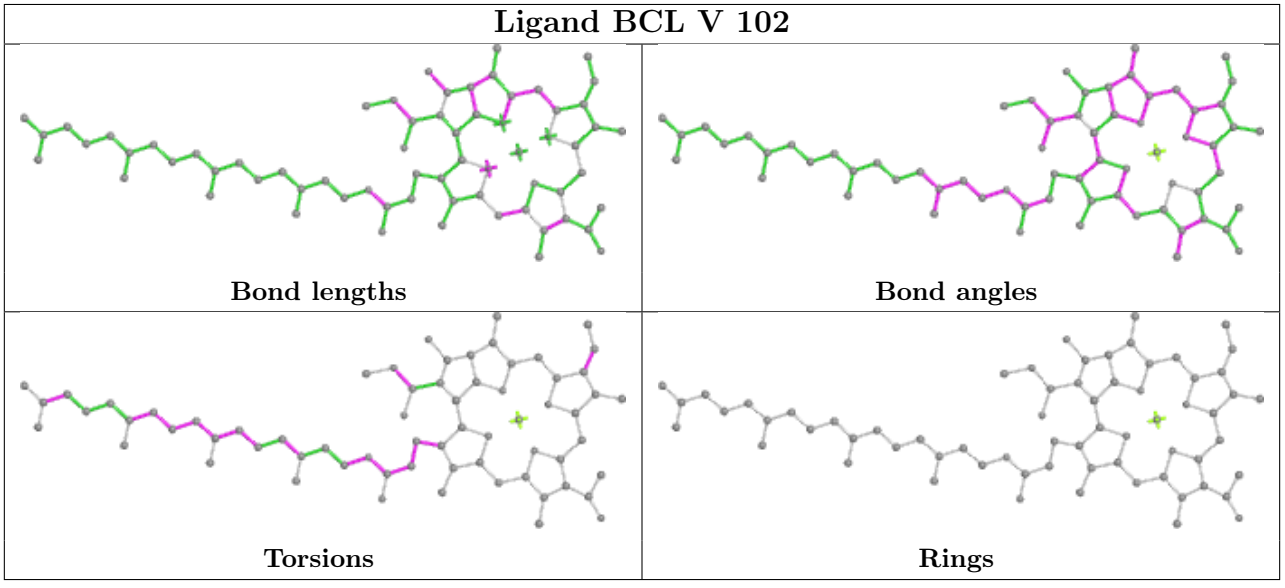
Ligand BCL B 102



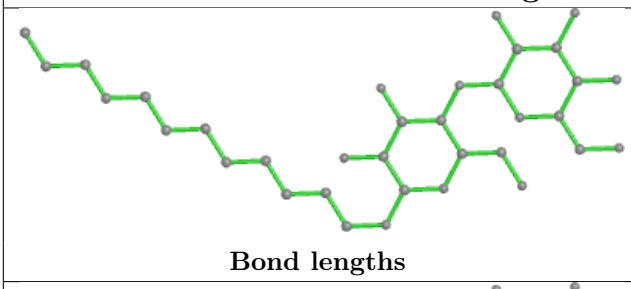
Ligand CRT 4 102



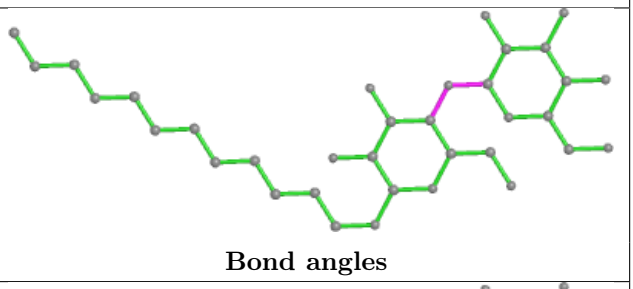
Ligand BCL V 102



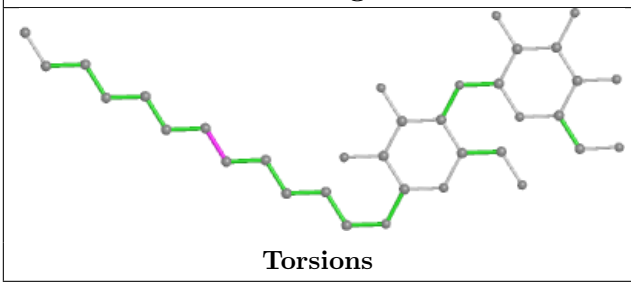
Ligand LMT P 103



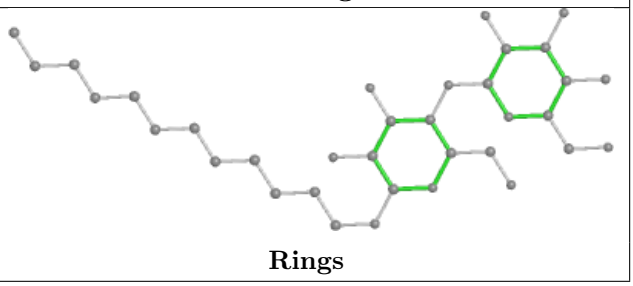
Bond lengths



Bond angles

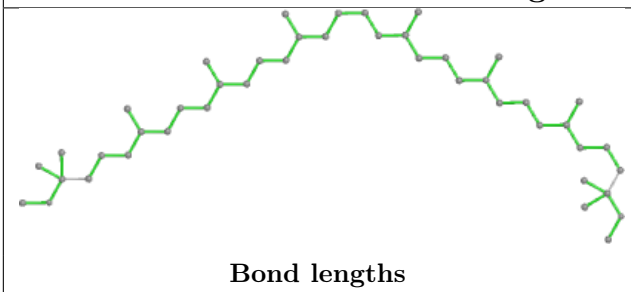


Torsions

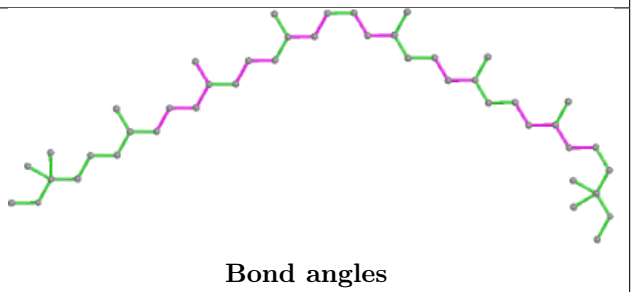


Rings

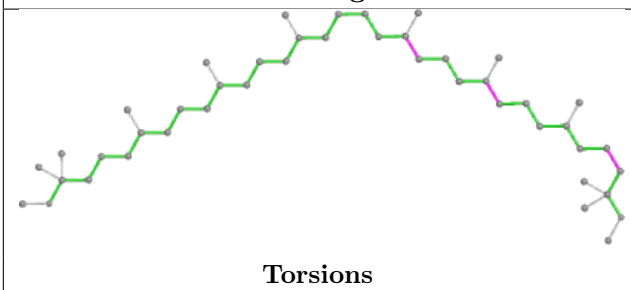
Ligand CRT 7 101



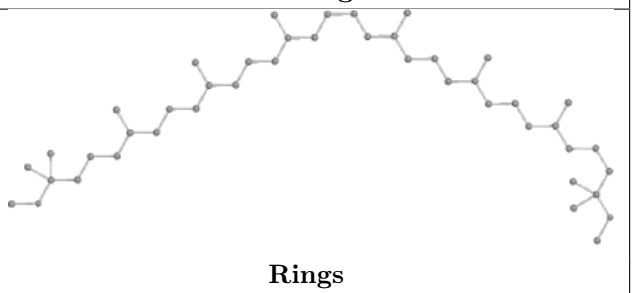
Bond lengths



Bond angles

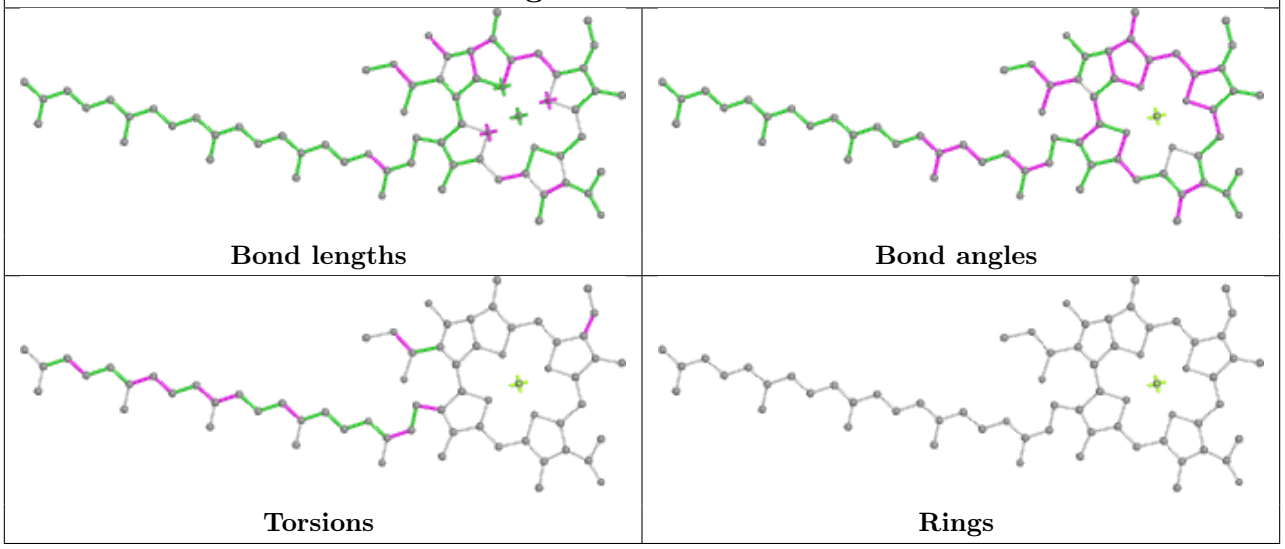


Torsions

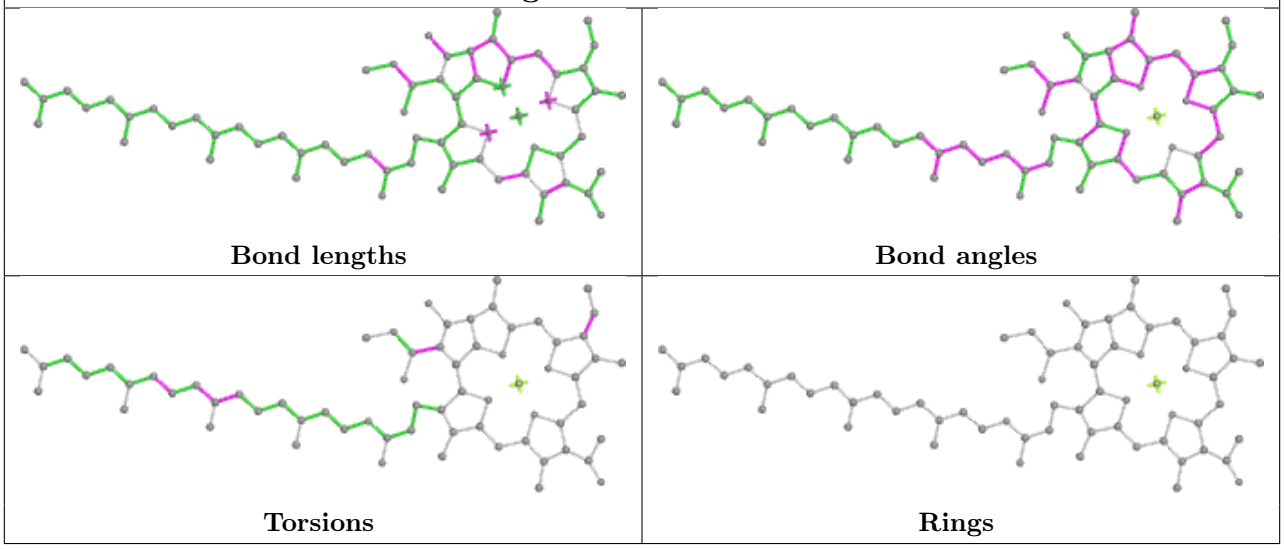


Rings

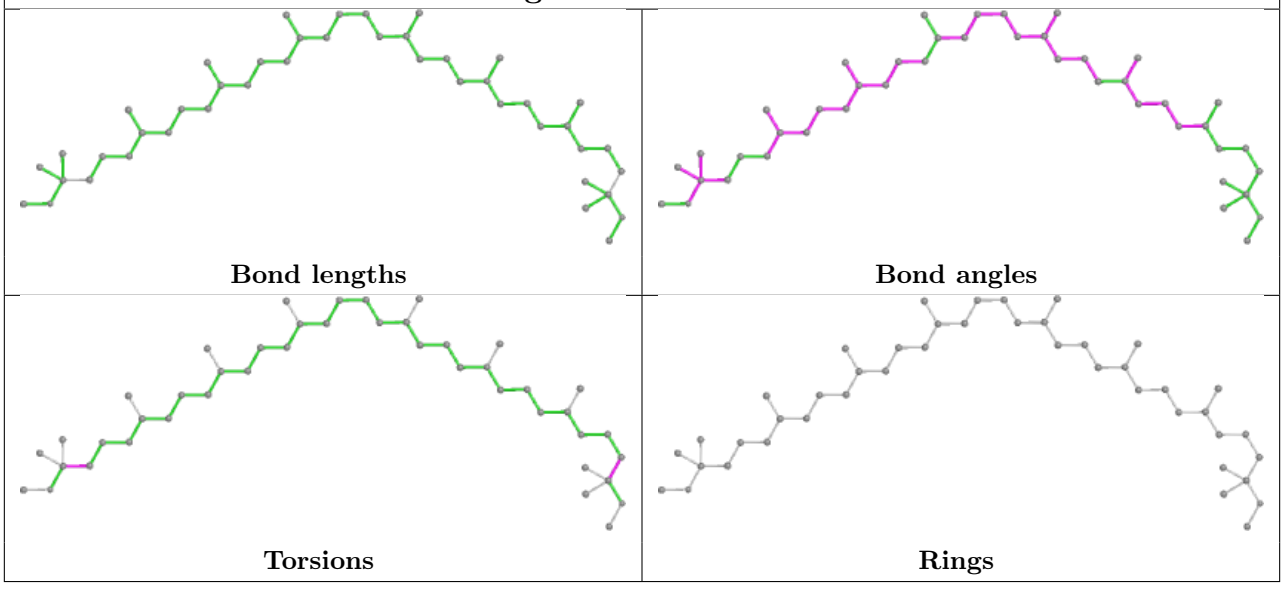
Ligand BCL X 102



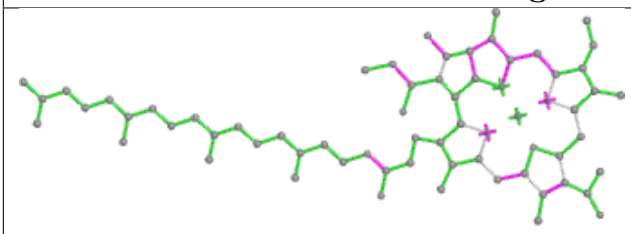
Ligand BCL M 403



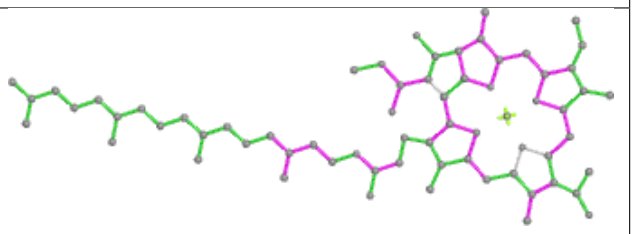
Ligand CRT V 103



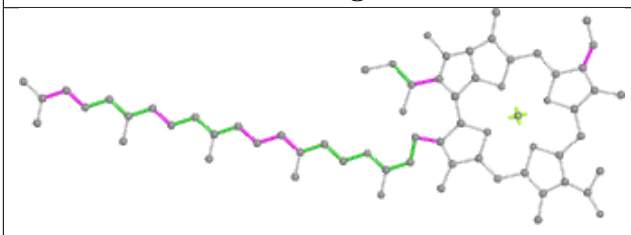
Ligand BCL 3 101



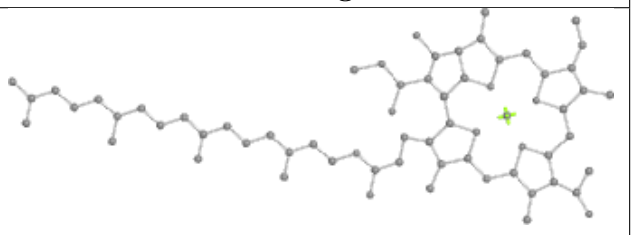
Bond lengths



Bond angles

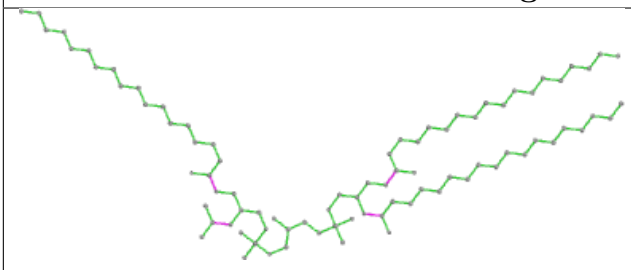


Torsions

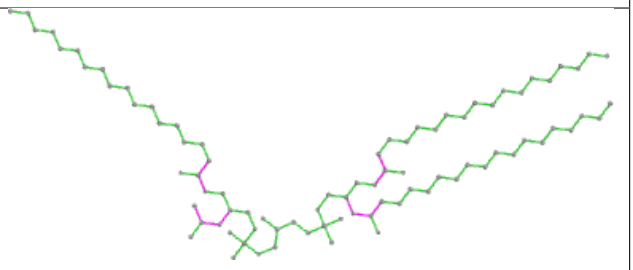


Rings

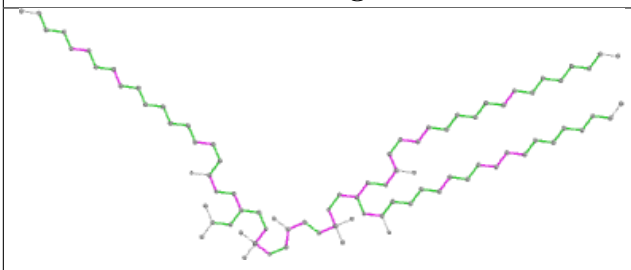
Ligand CDL M 412



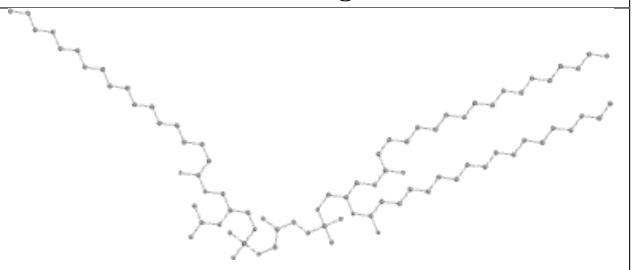
Bond lengths



Bond angles

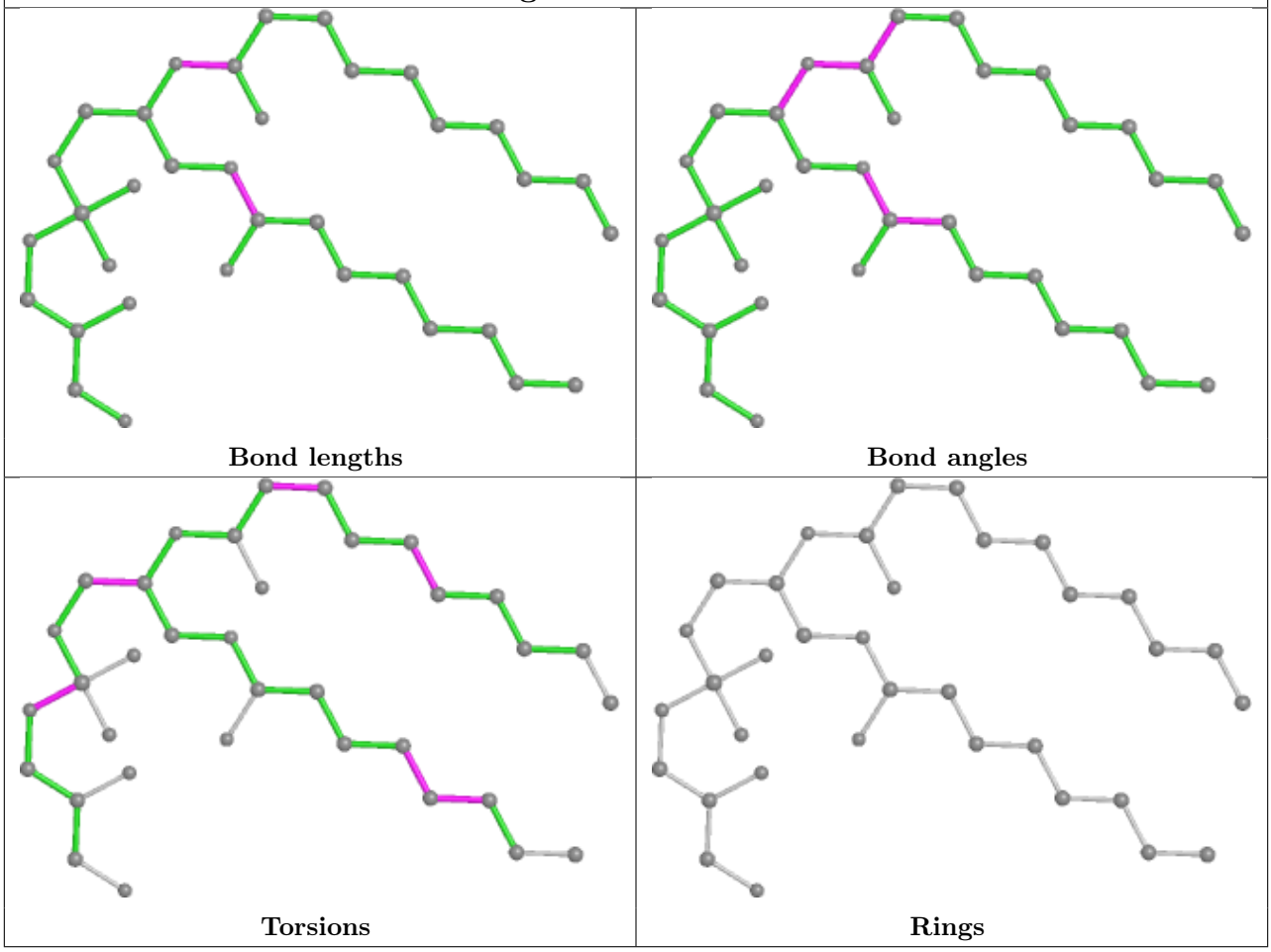


Torsions

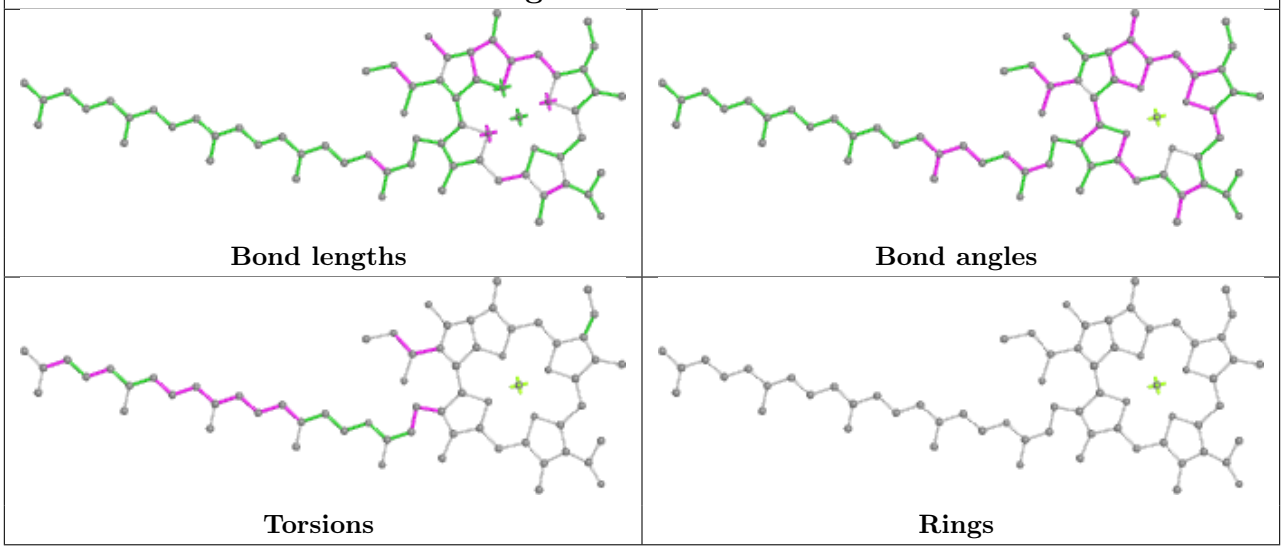


Rings

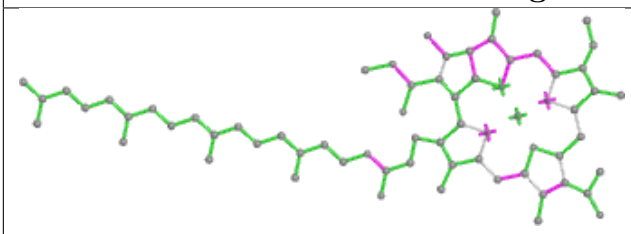
Ligand PGV L 306



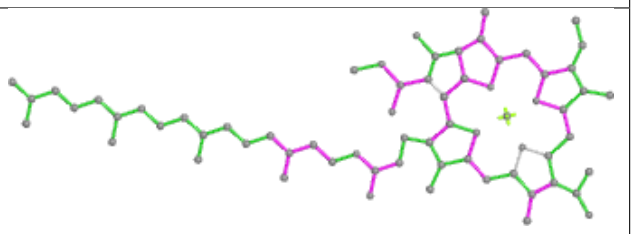
Ligand BCL Y 101



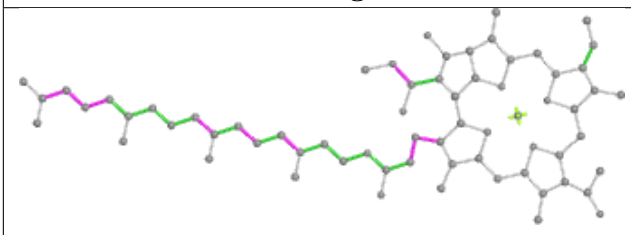
Ligand BCL 2 102



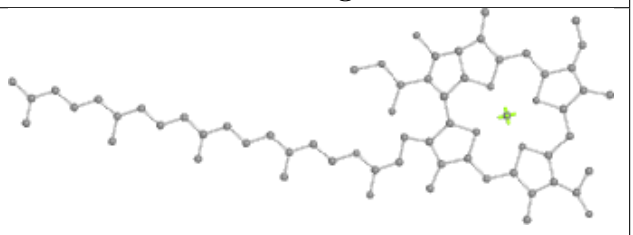
Bond lengths



Bond angles

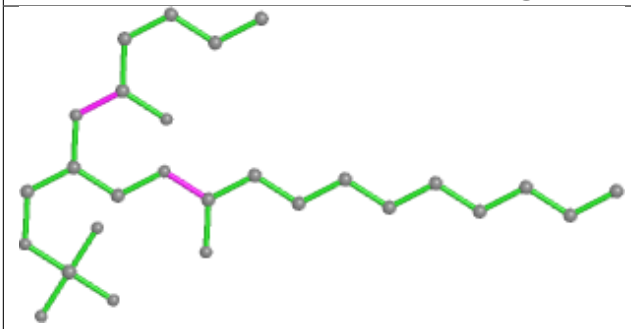


Torsions

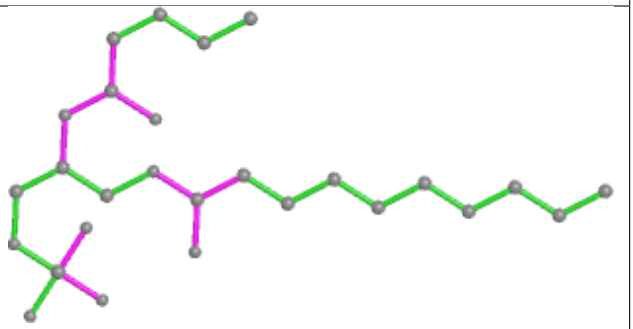


Rings

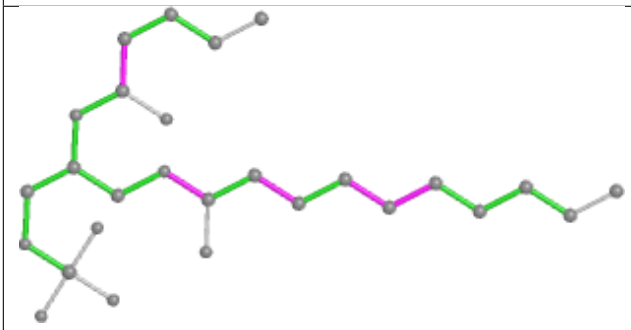
Ligand PGV M 410



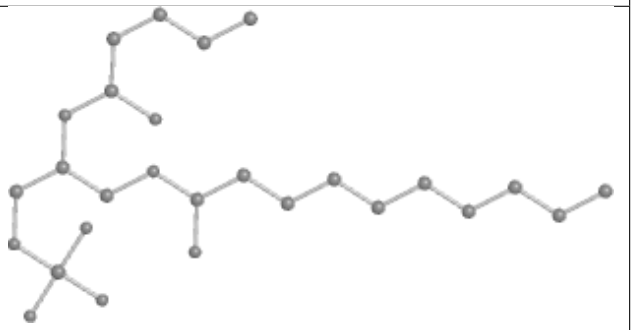
Bond lengths



Bond angles

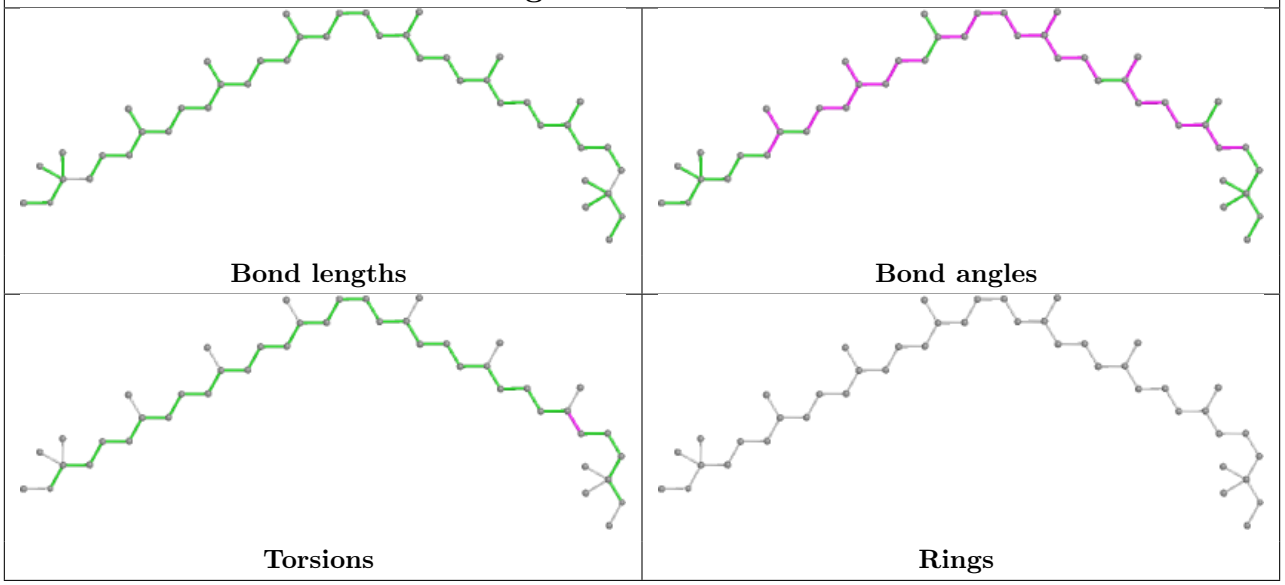


Torsions

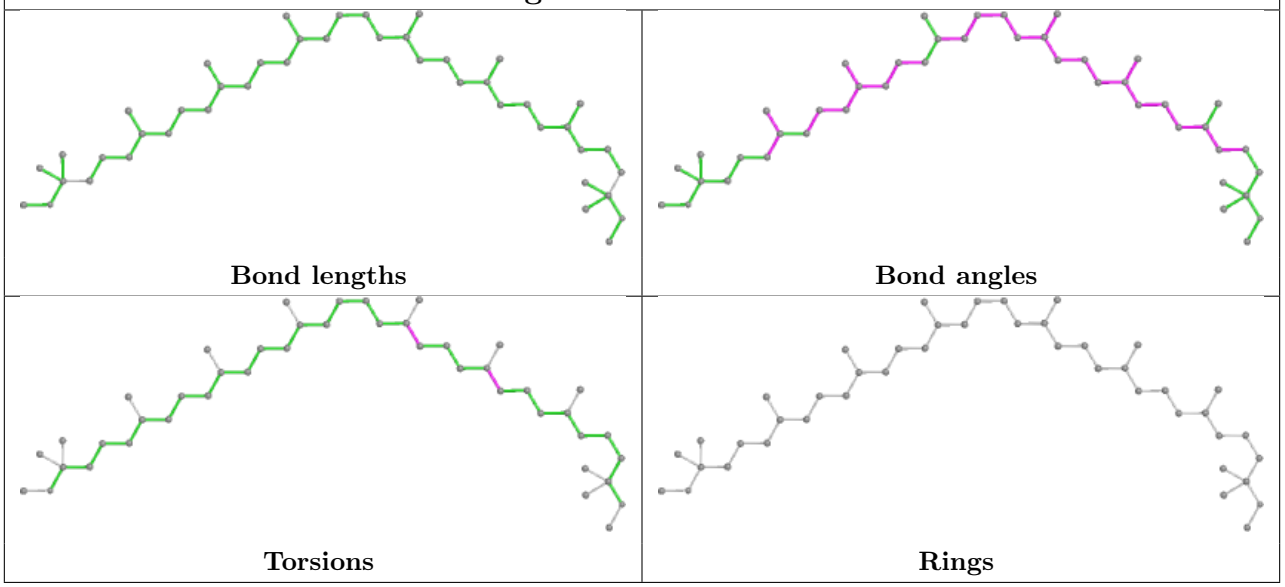


Rings

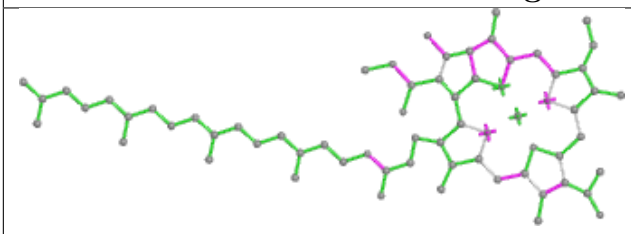
Ligand CRT B 103



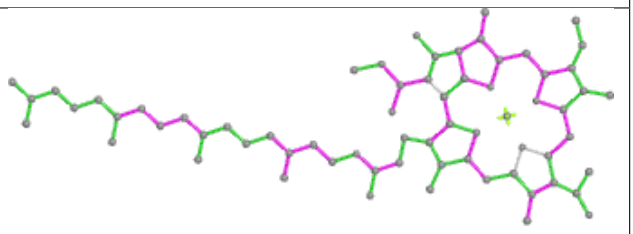
Ligand CRT X 103



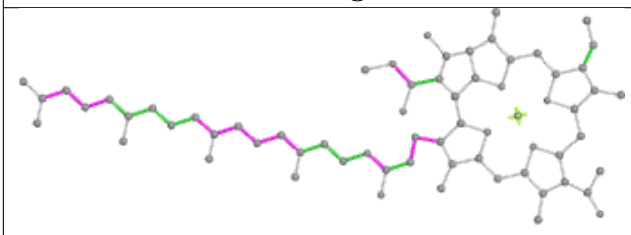
Ligand BCL G 102



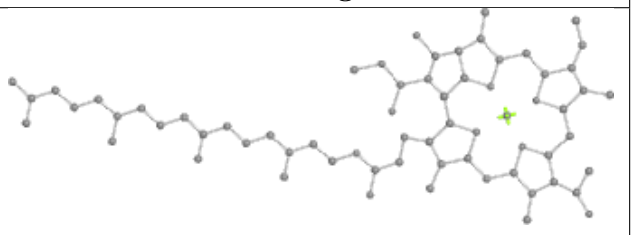
Bond lengths



Bond angles

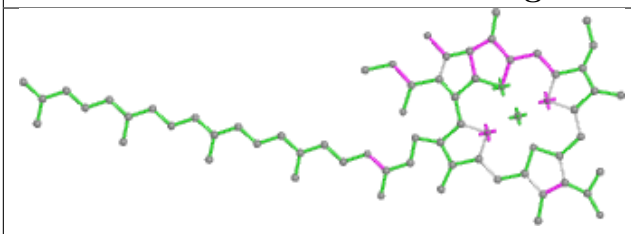


Torsions

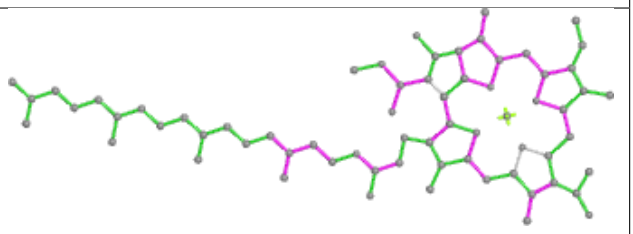


Rings

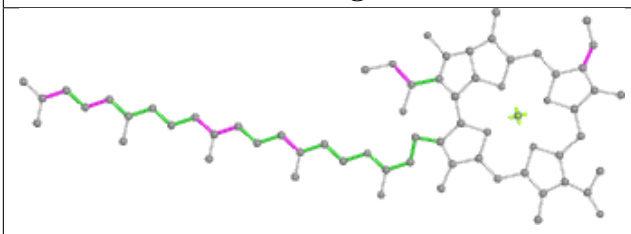
Ligand BCL A 101



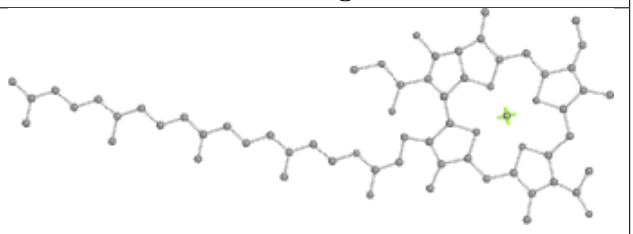
Bond lengths



Bond angles

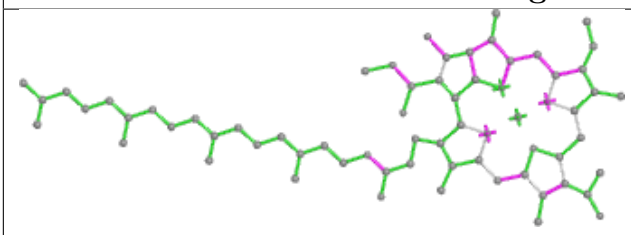


Torsions

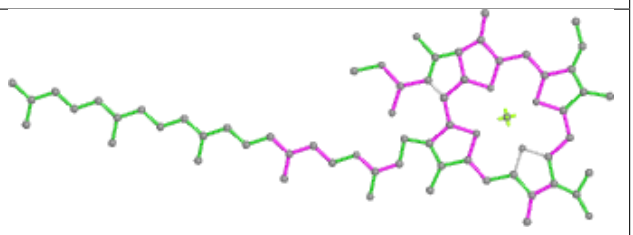


Rings

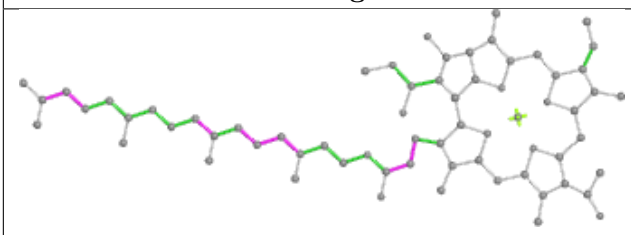
Ligand BCL 4 101



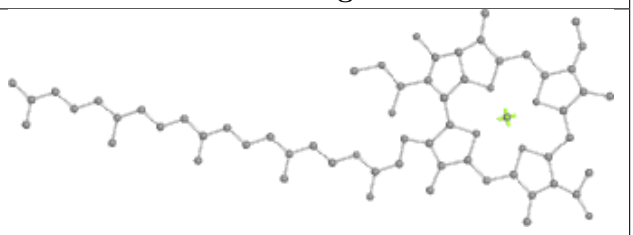
Bond lengths



Bond angles

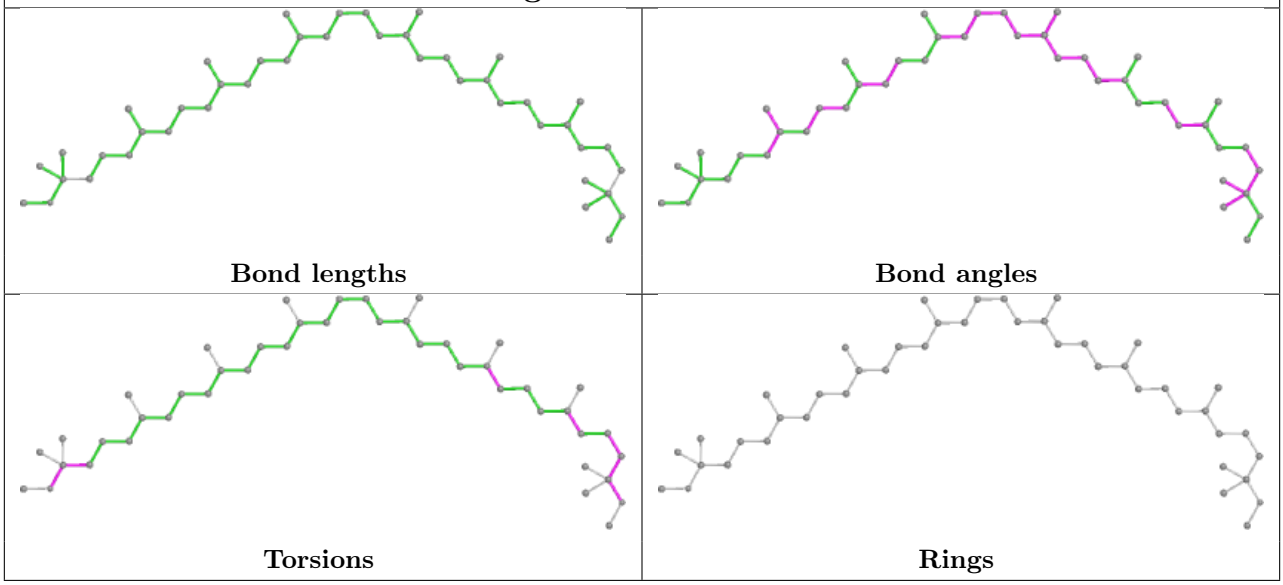


Torsions

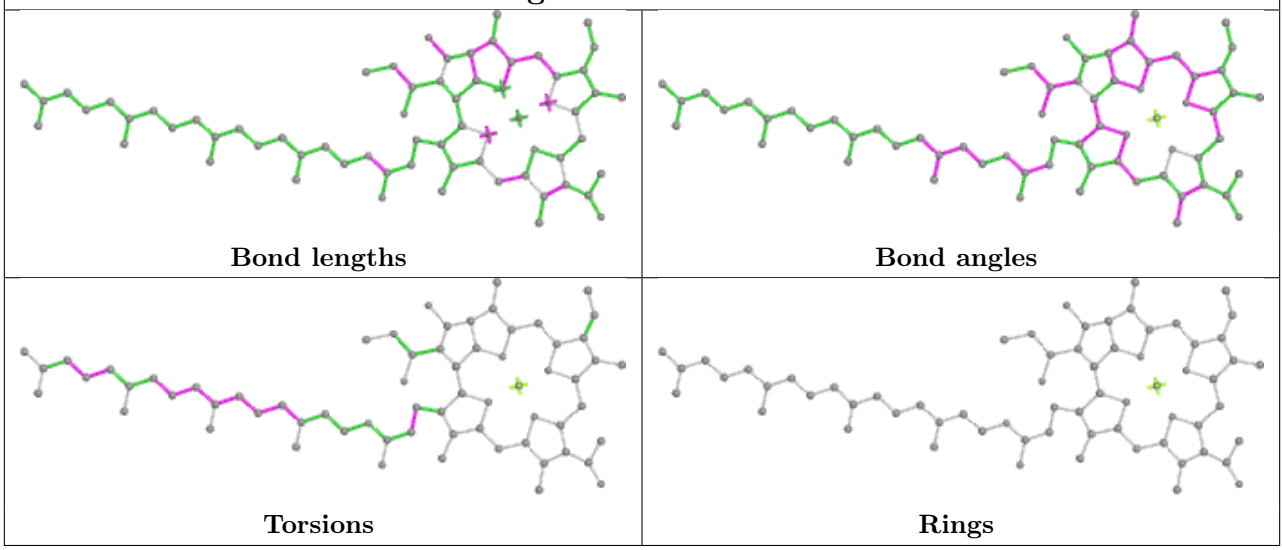


Rings

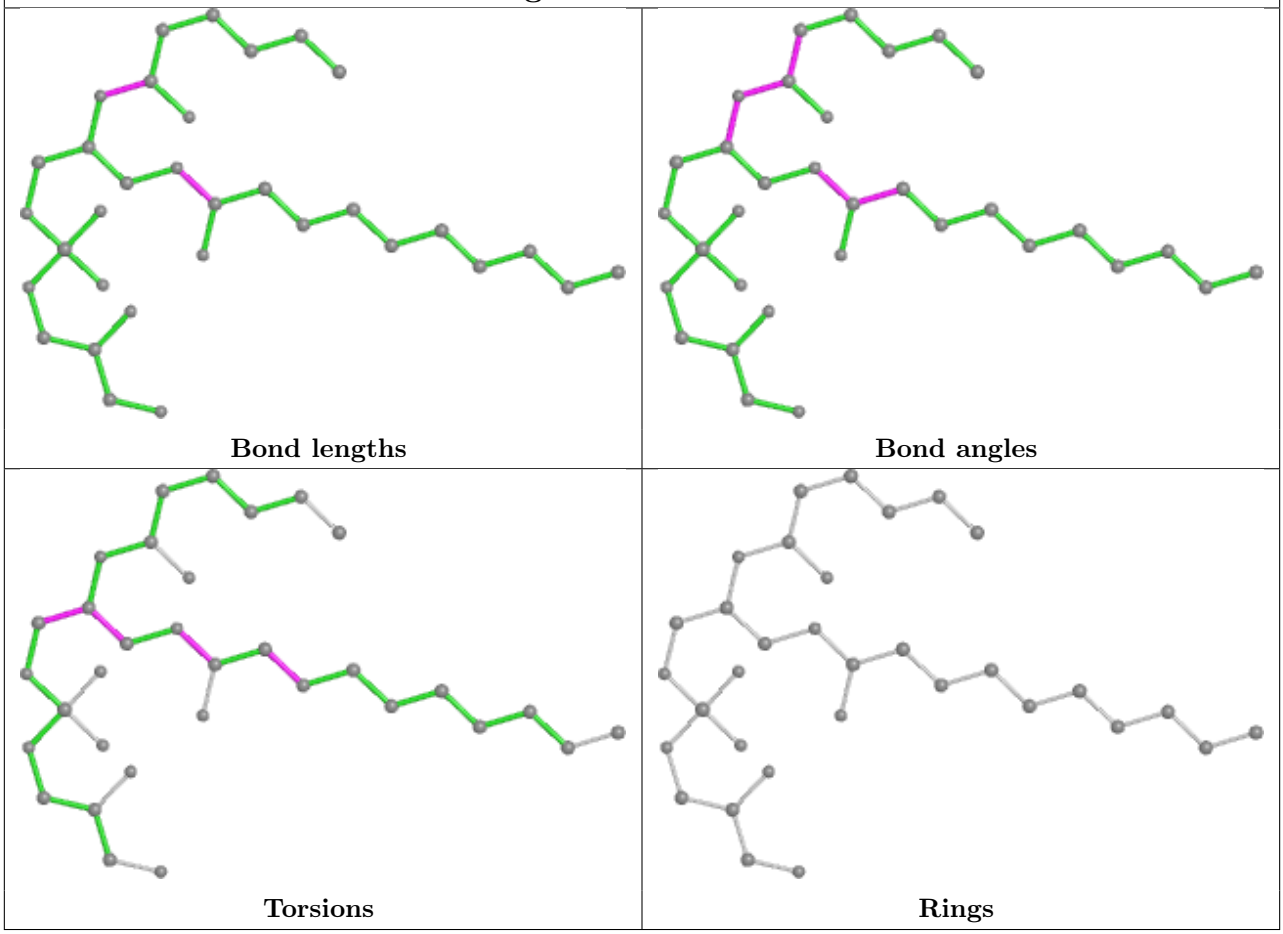
Ligand CRT K 101



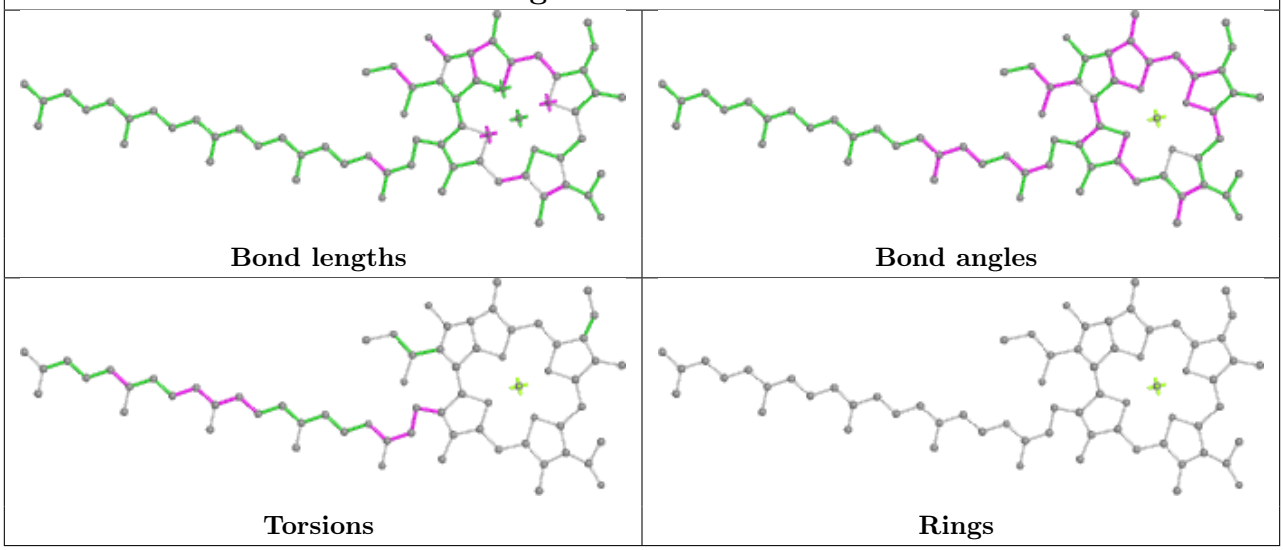
Ligand BCL E 102



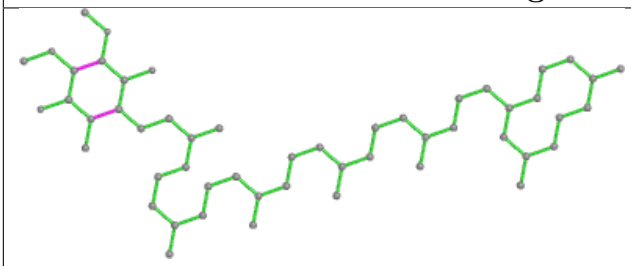
Ligand PGV L 309

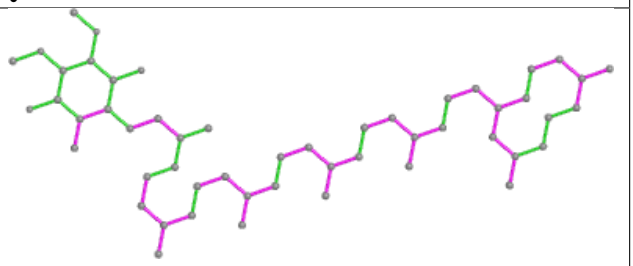


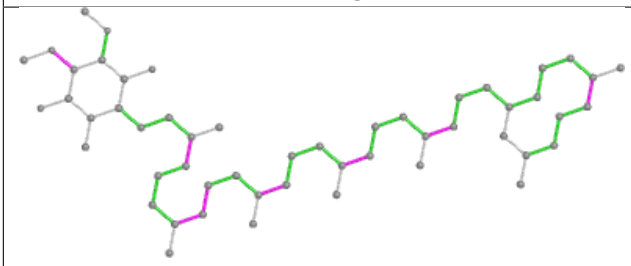
Ligand BCL J 101

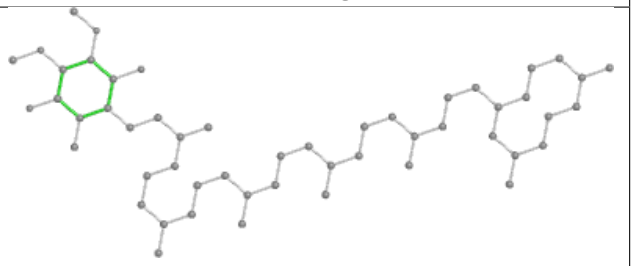


Ligand UQ8 L 304

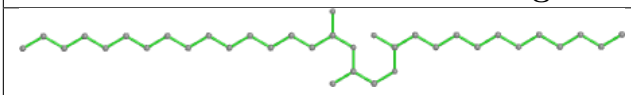

Bond lengths

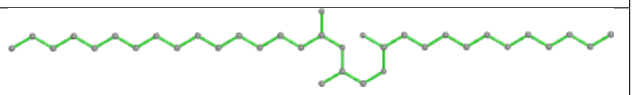

Bond angles

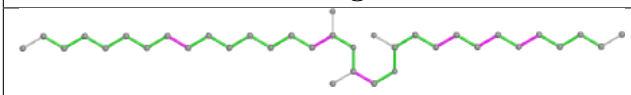

Torsions

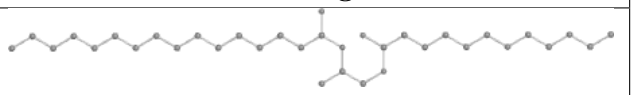

Rings

Ligand Z41 C 407

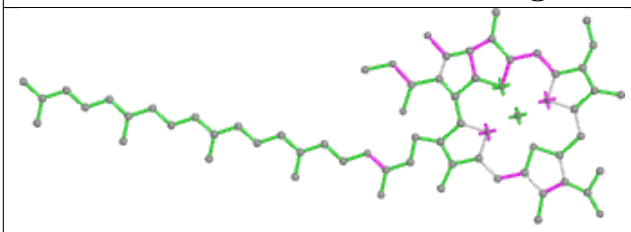

Bond lengths

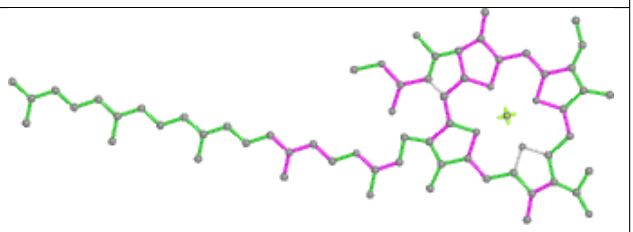

Bond angles

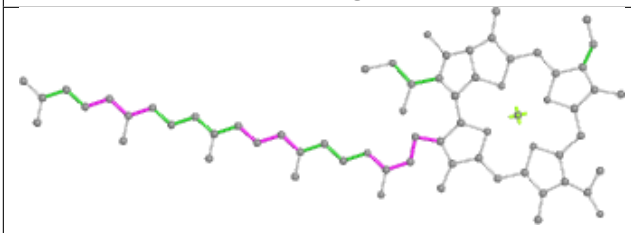

Torsions

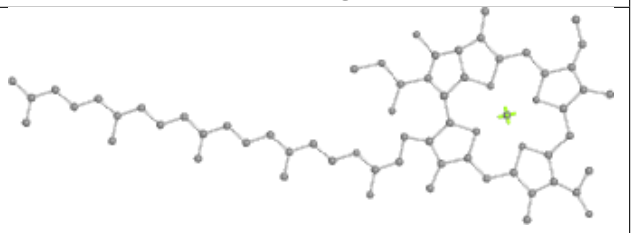

Rings

Ligand BCL 8 102

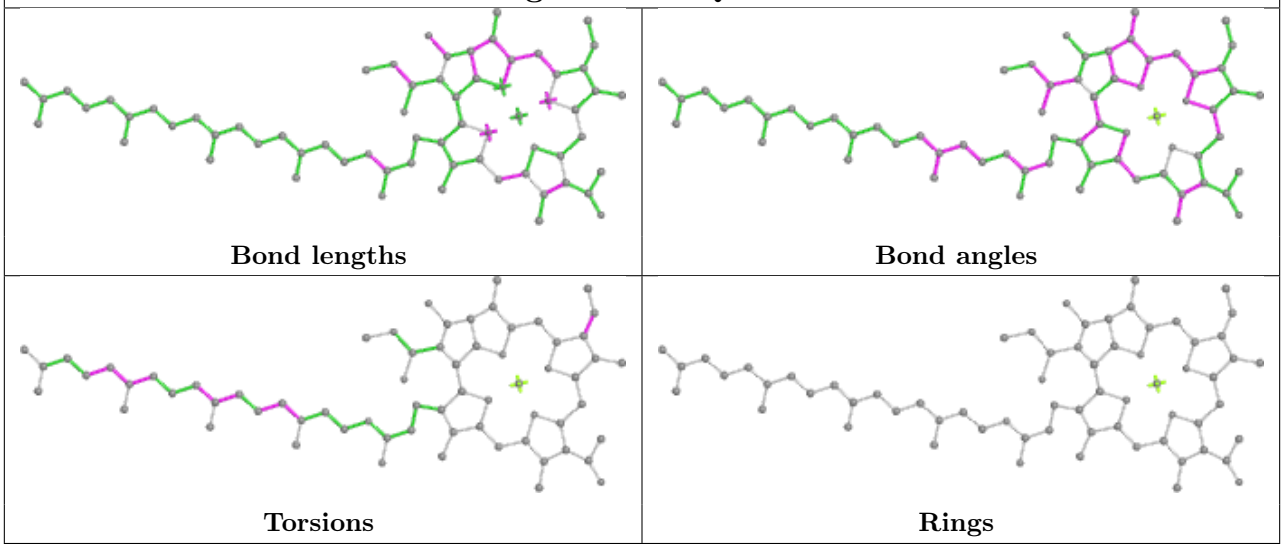

Bond lengths


Bond angles


Torsions


Rings

Ligand BCL Q 102



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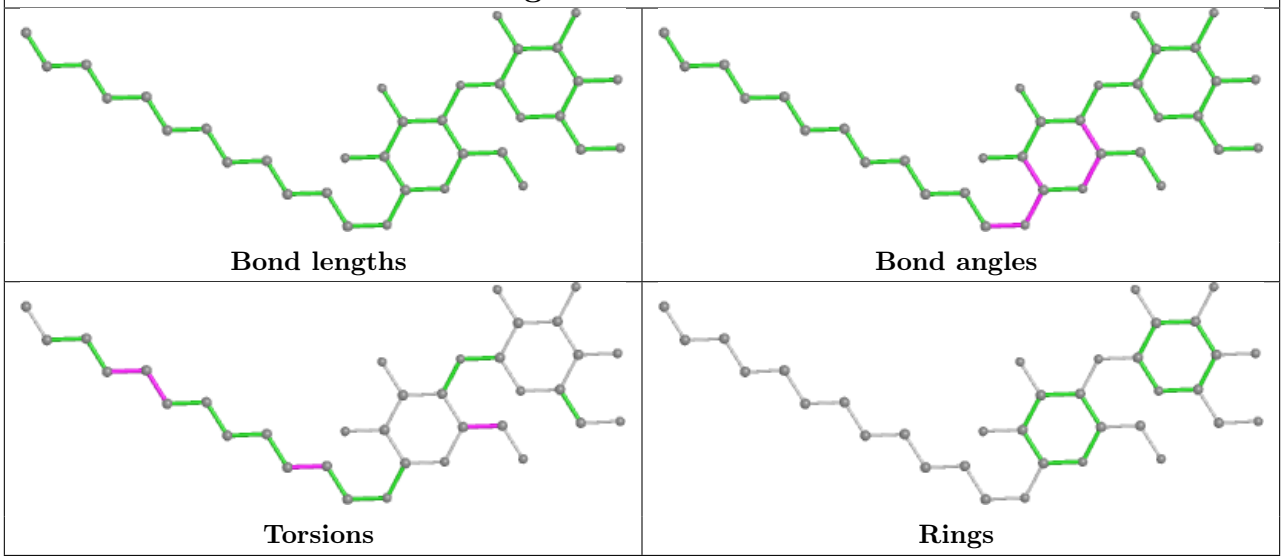

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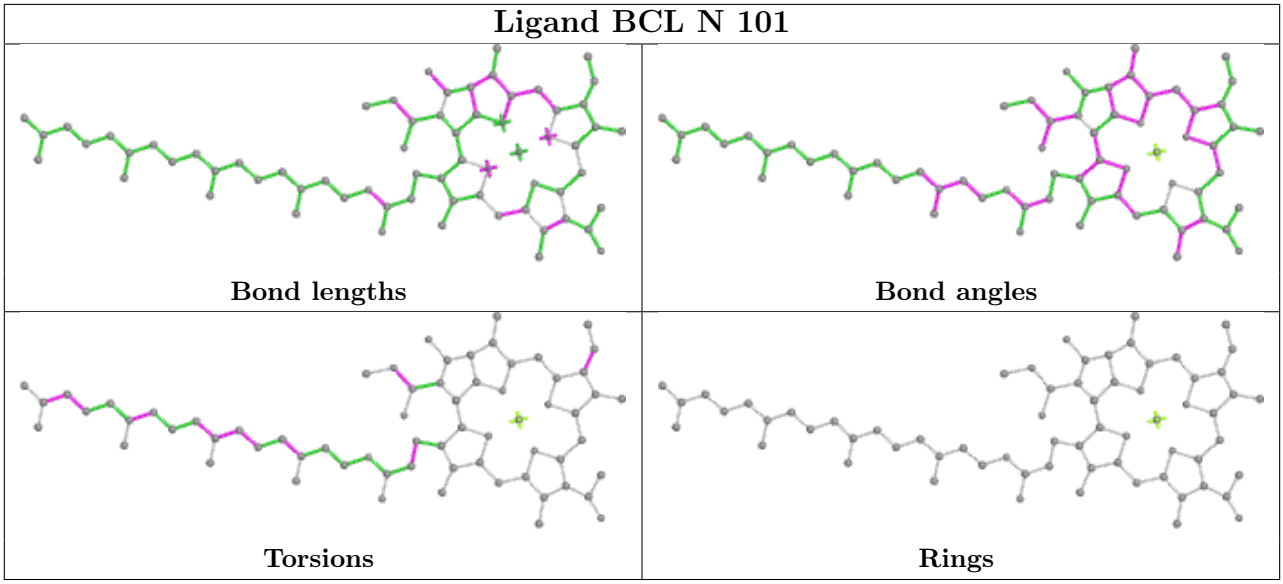
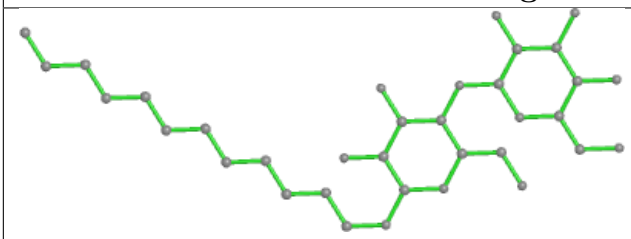
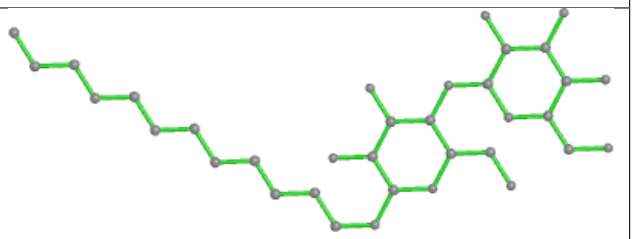


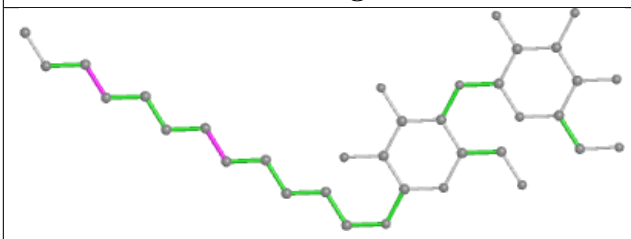
Ligand LMT G 104



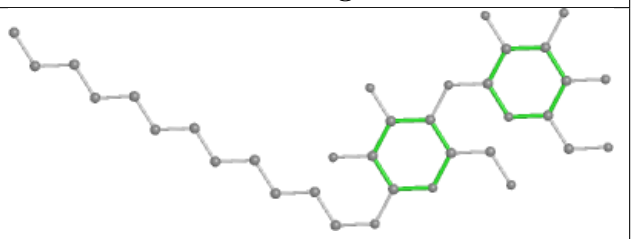
Bond lengths



Bond angles

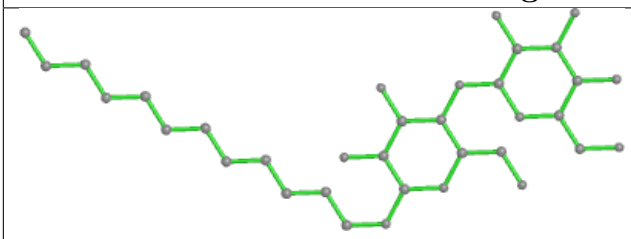


Torsions



Rings

Ligand LMT R 103



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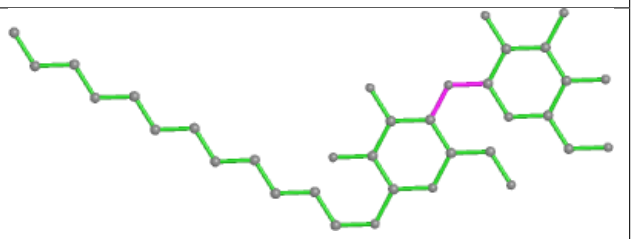
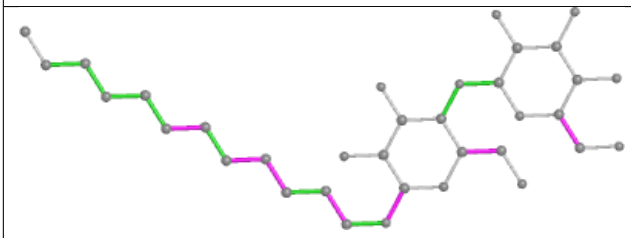
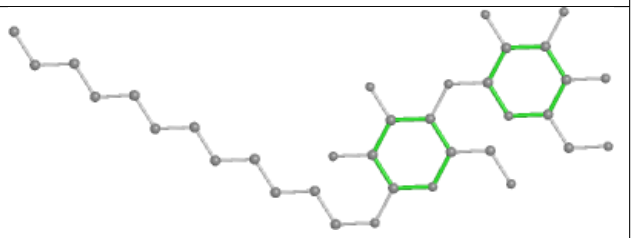


Bond angles

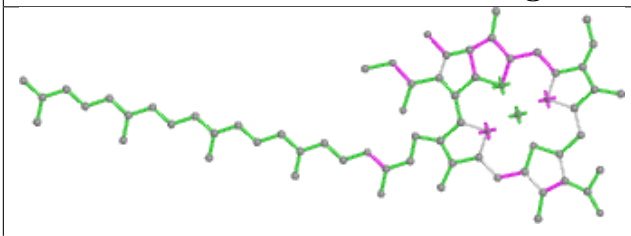


Torsions

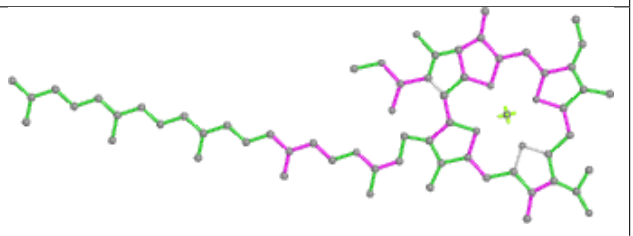


Rings

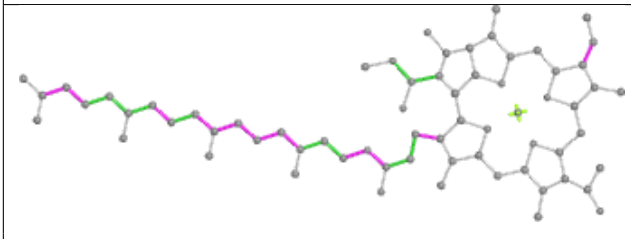
Ligand BCL U 101



Bond lengths



Bond angles



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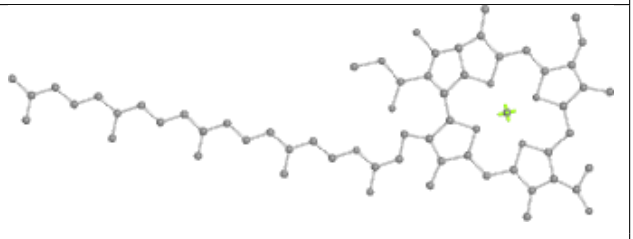
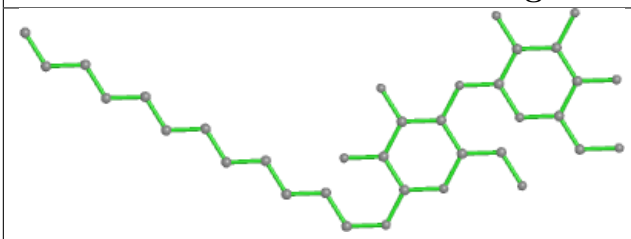
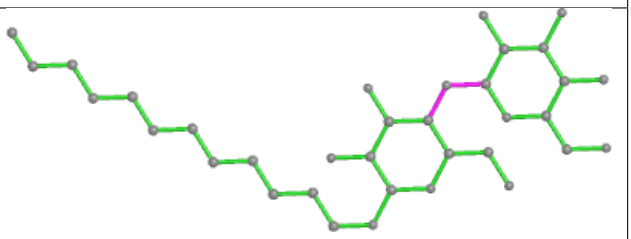


Rings

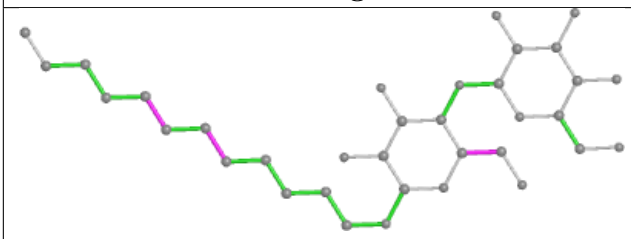
Ligand LMT J 102



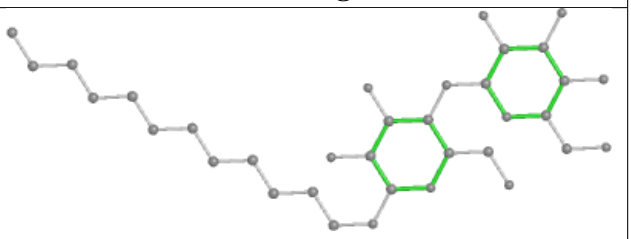
Bond lengths



Bond angles

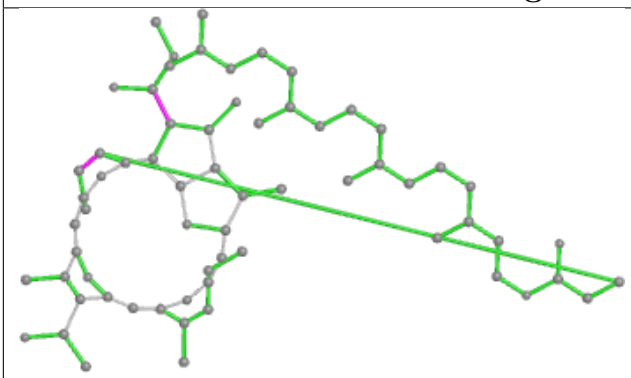


Torsions

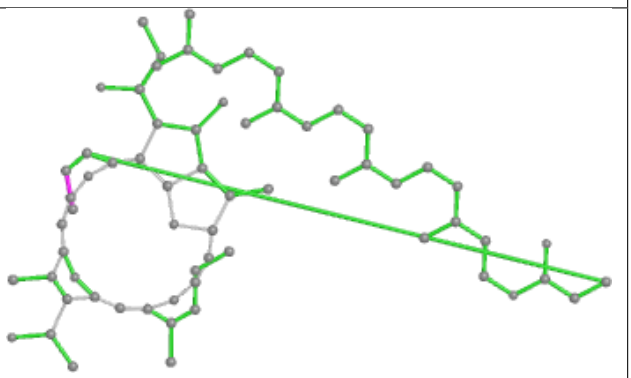


Rings

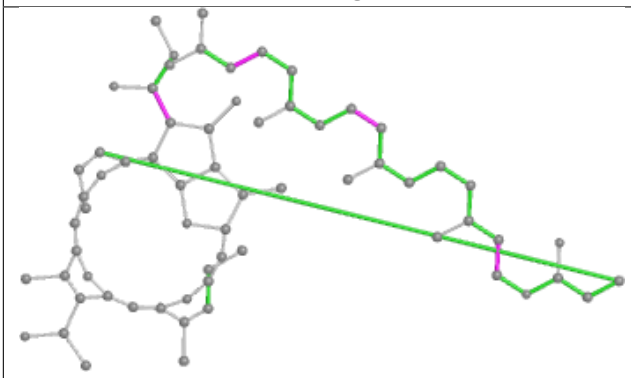
Ligand BPH L 302



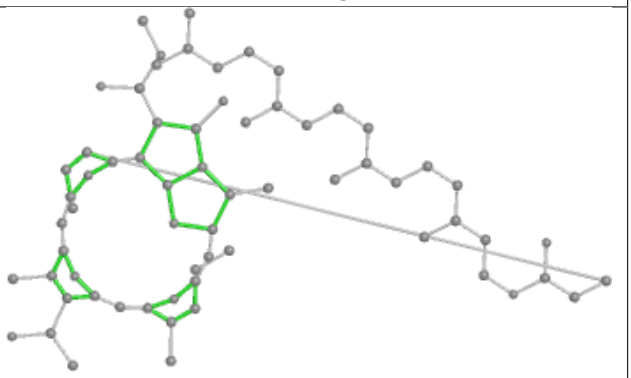
Bond lengths



Bond angles

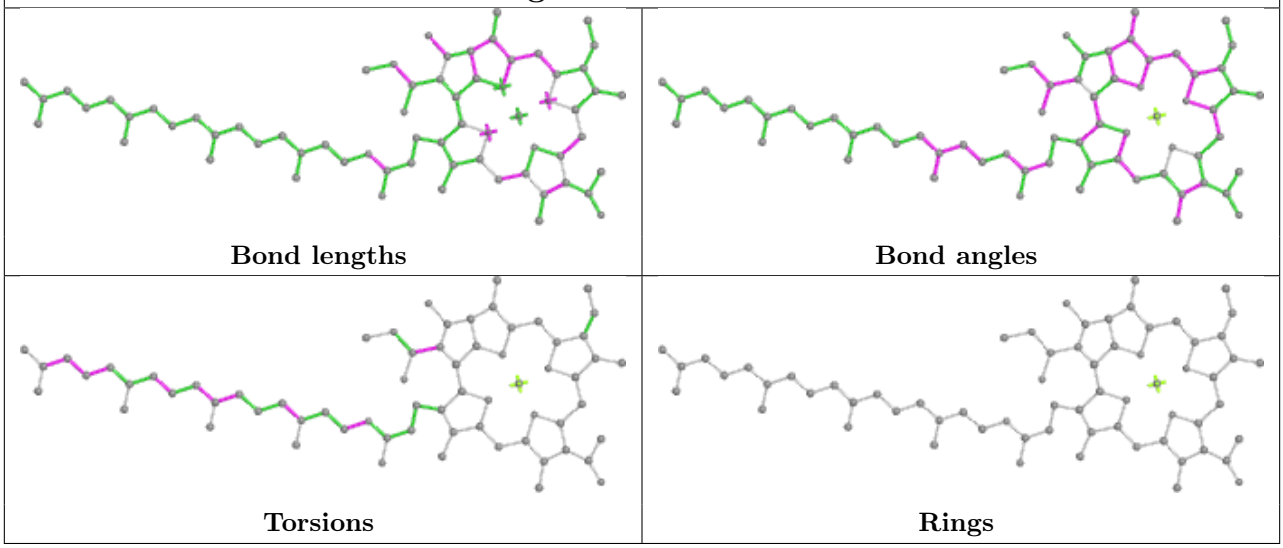


Torsions

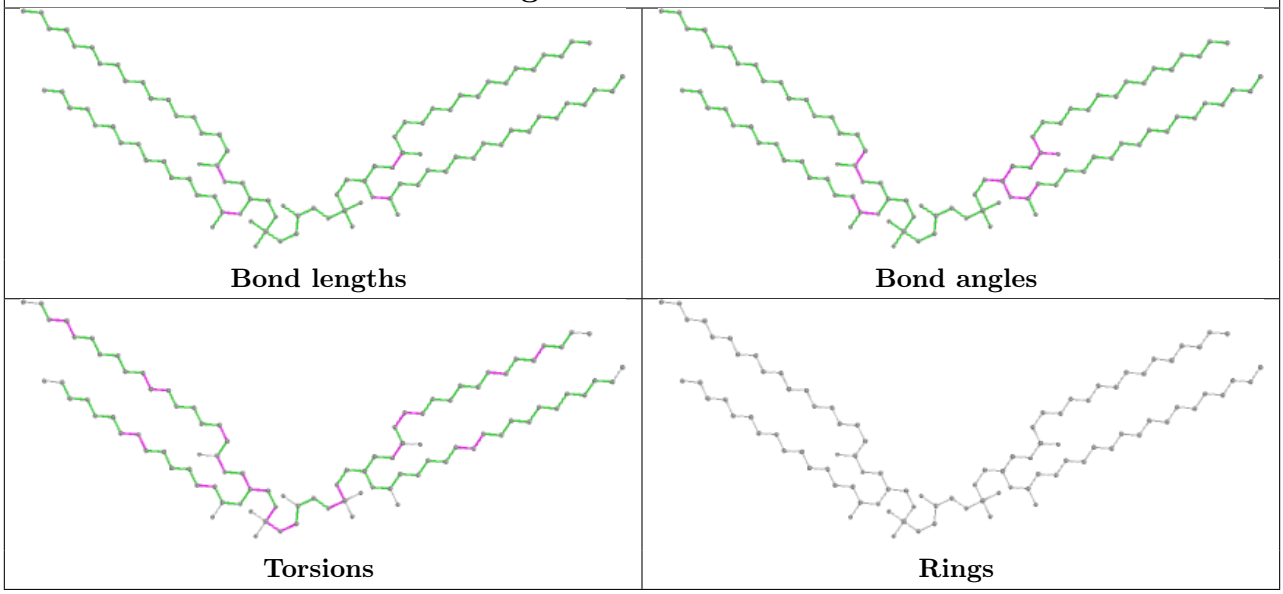


Rings

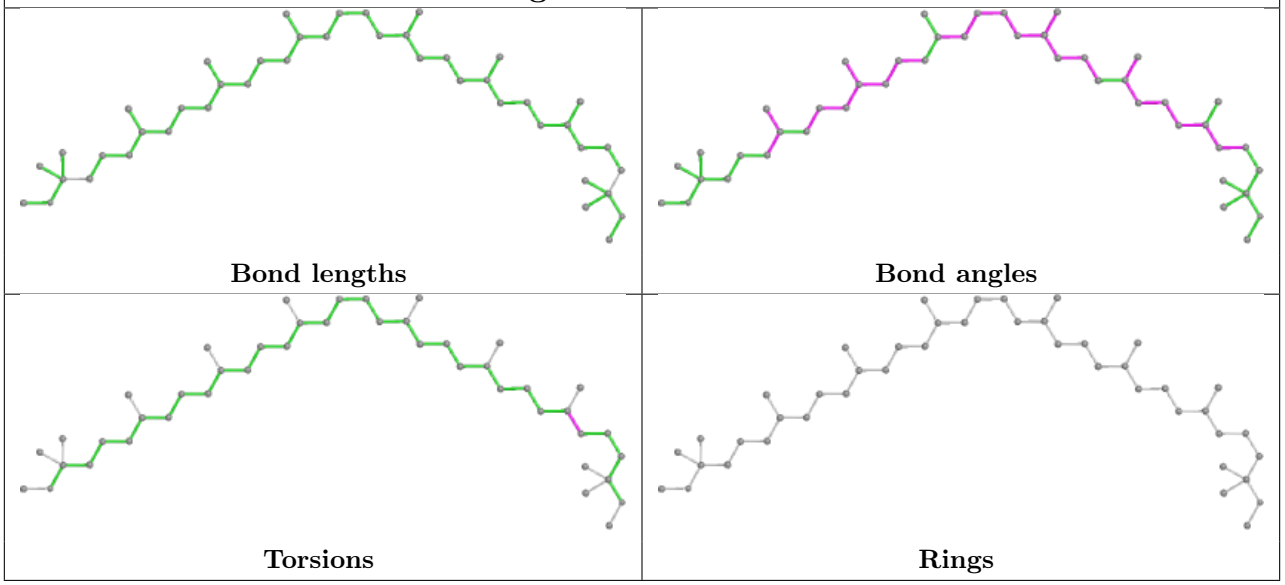
Ligand BCL F 502



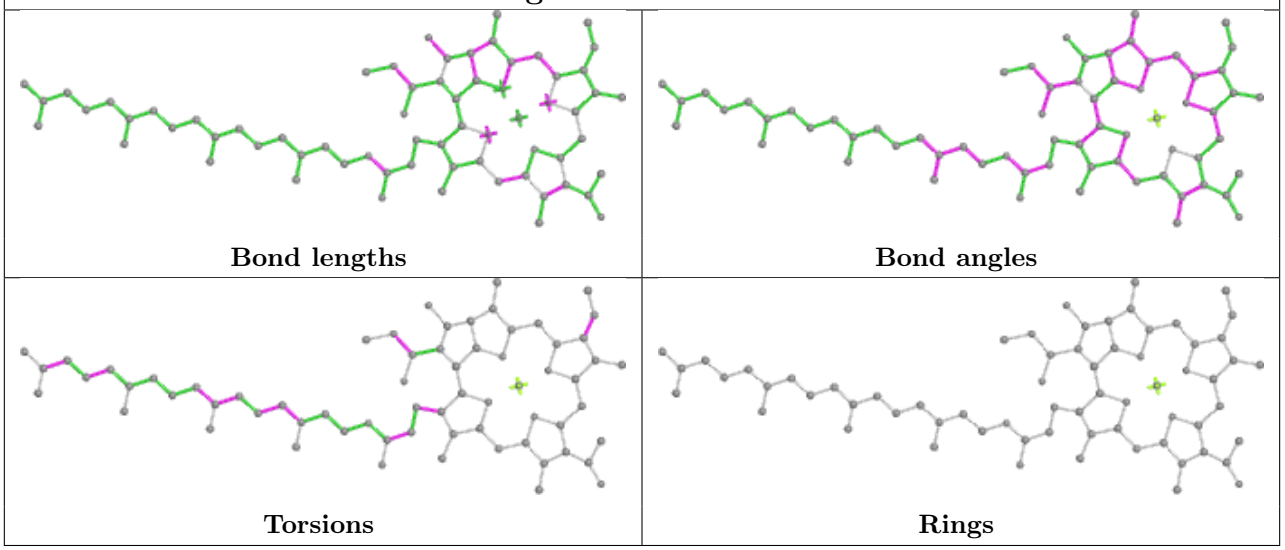
Ligand CDL M 411



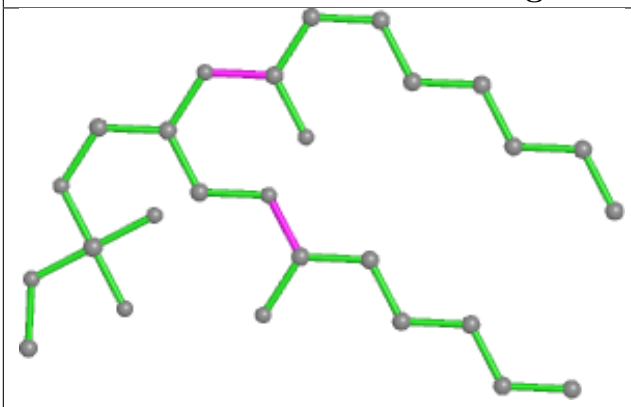
Ligand CRT 0 103



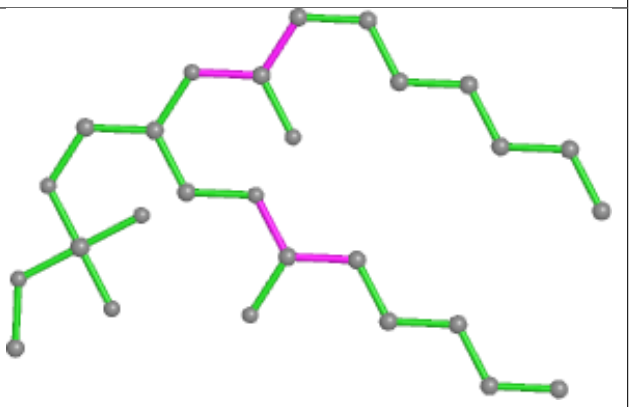
Ligand BCL R 101



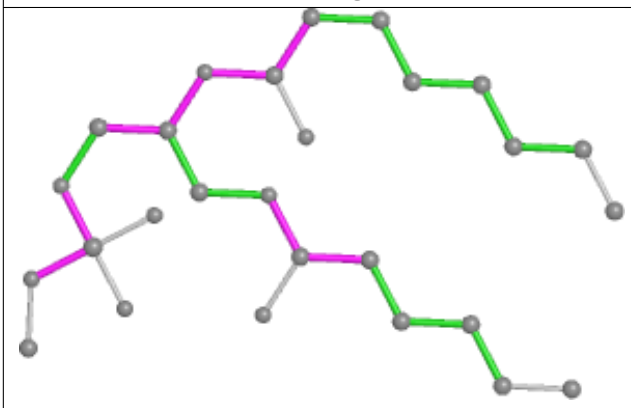
Ligand PGV 1 401



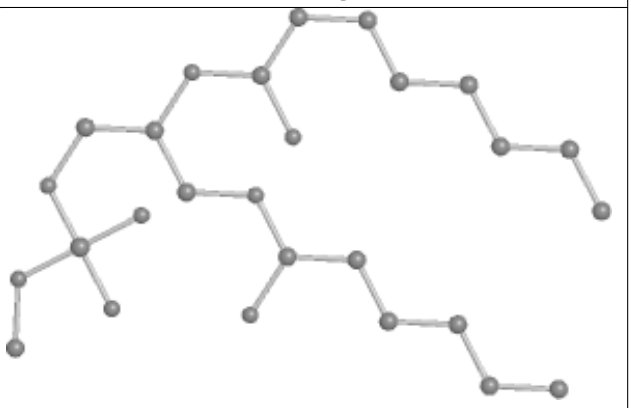
Bond lengths



Bond angles

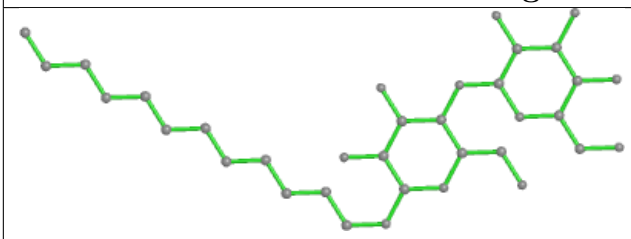


Torsions



Rings

Ligand LMT E 101



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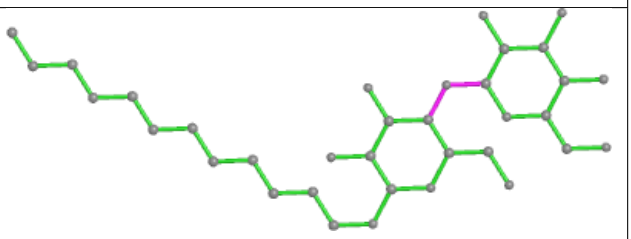
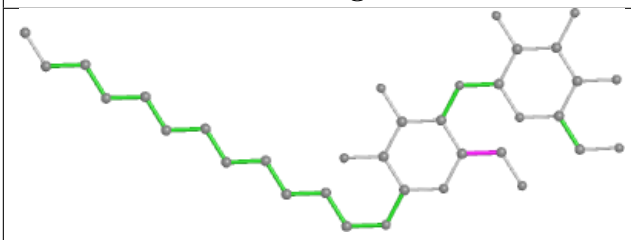


Bond angles



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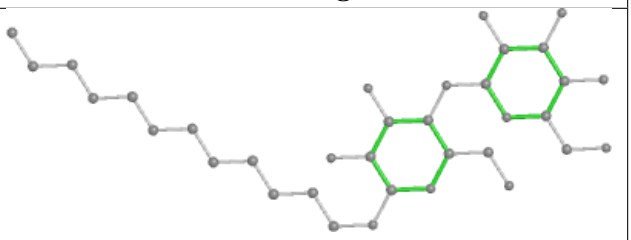
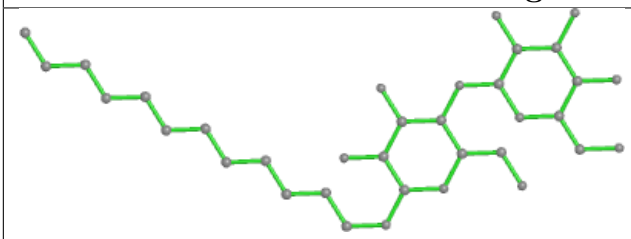
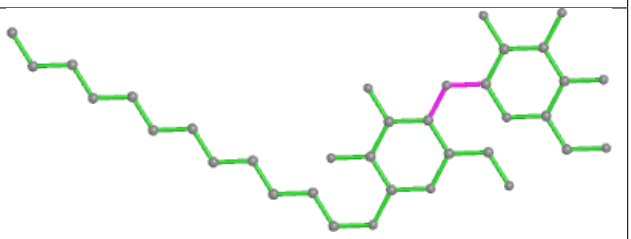


Rings

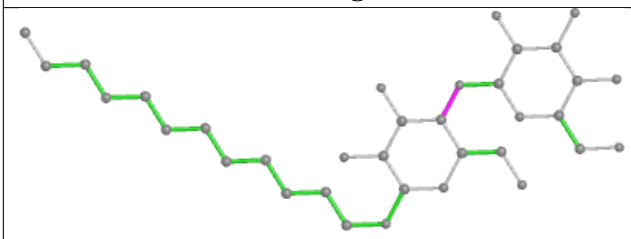
Ligand LMT 4 103



Bond lengths



Bond angles



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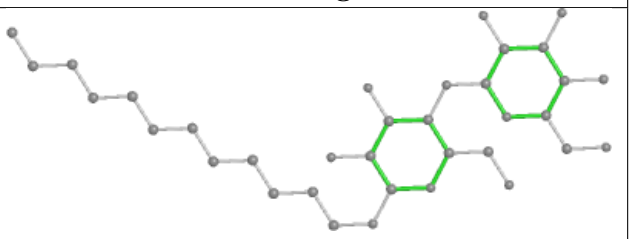
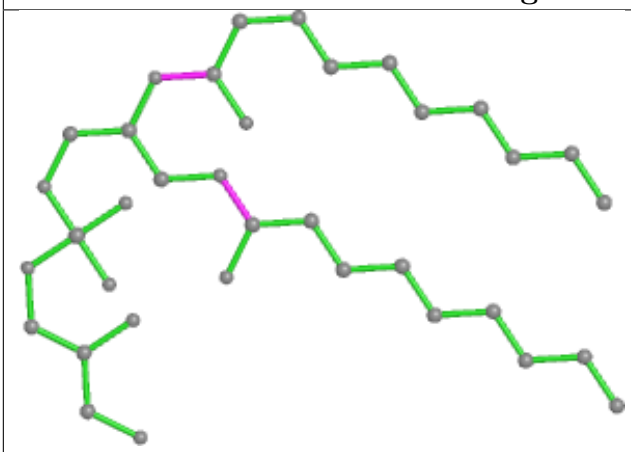
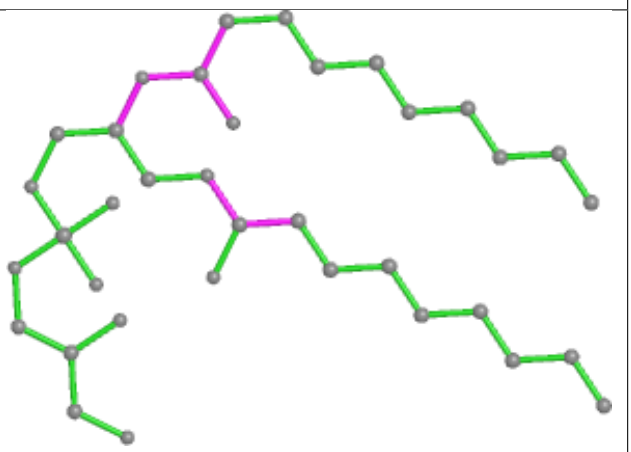


Rings

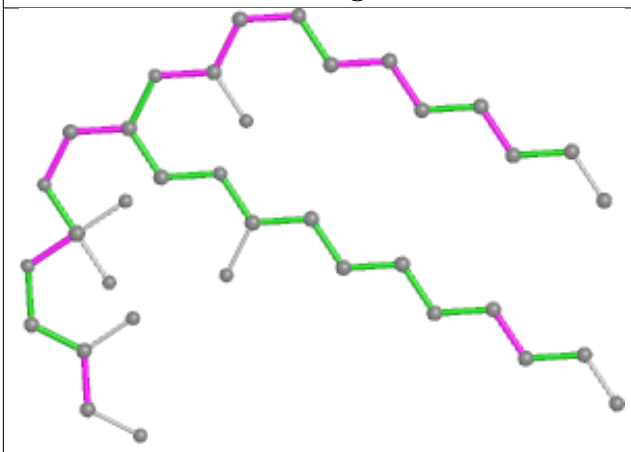
Ligand PGV H 301



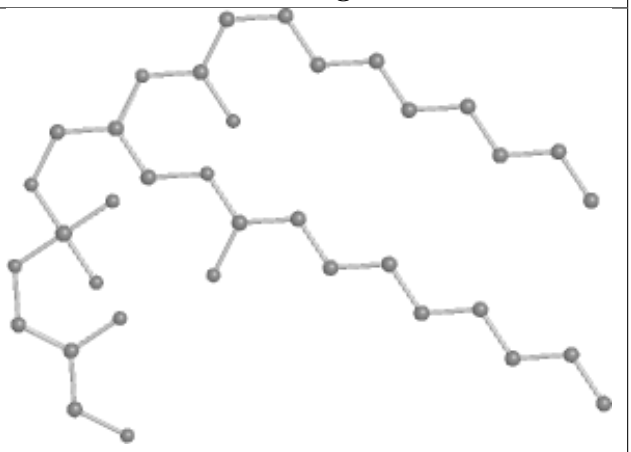
Bond lengths



Bond angles

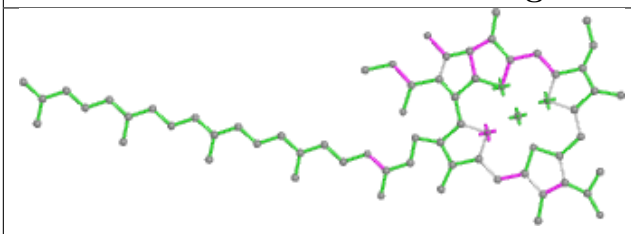


Torsions

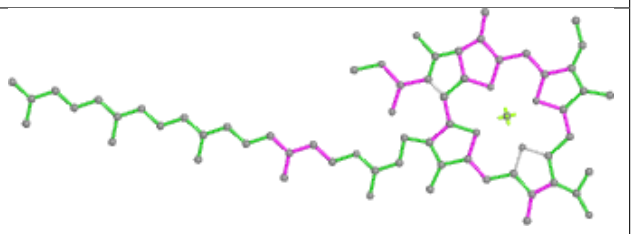


Rings

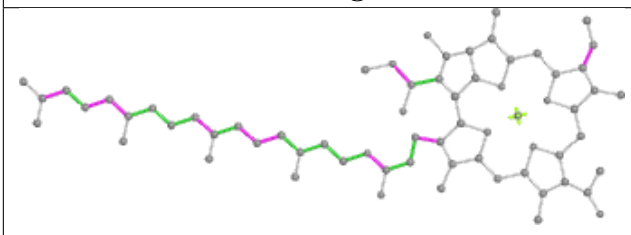
Ligand BCL T 101



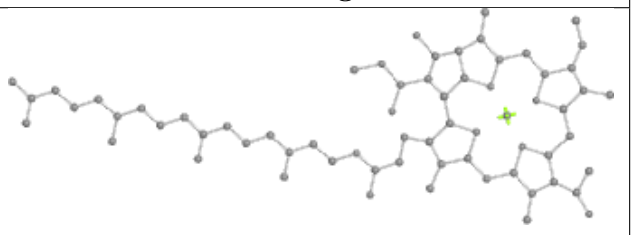
Bond lengths



Bond angles

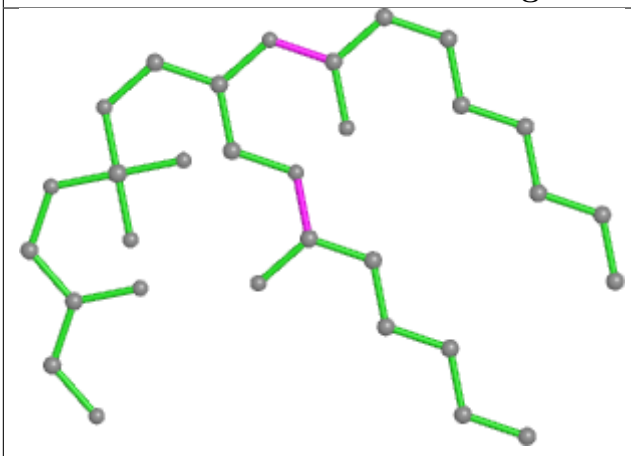


Torsions

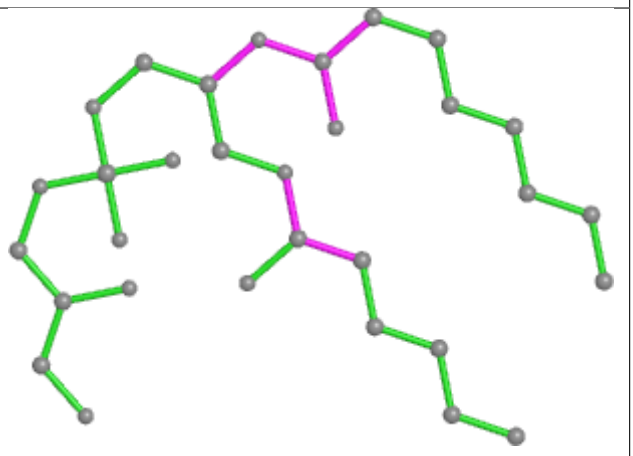


Rings

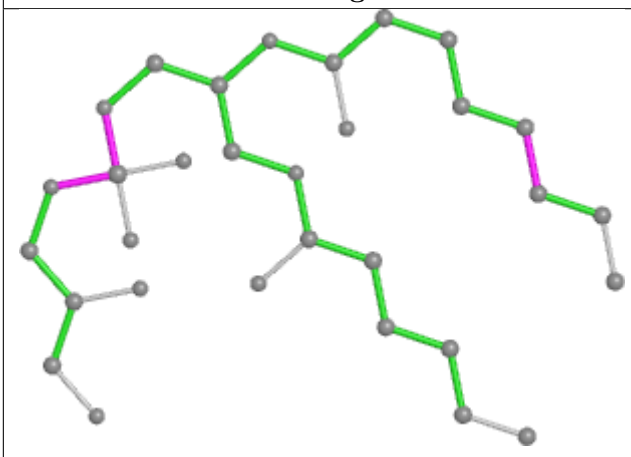
Ligand PGV C 409



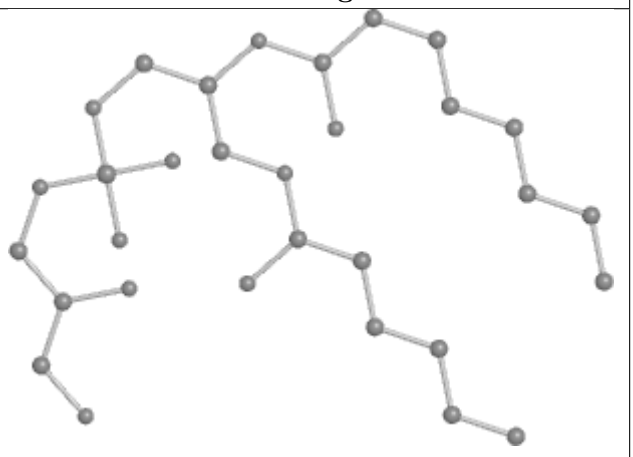
Bond lengths



Bond angles

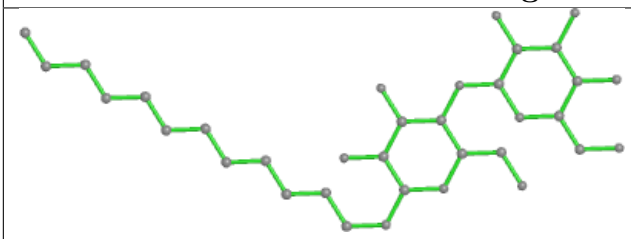


Torsions

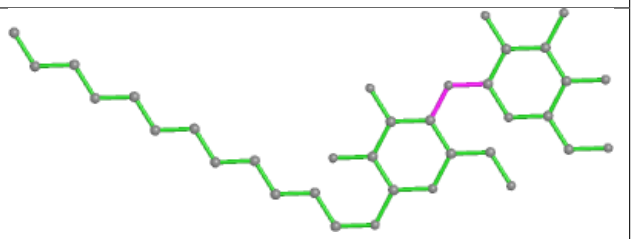


Rings

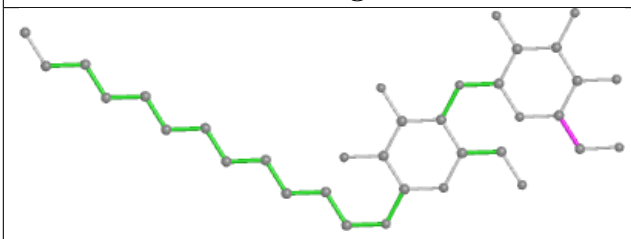
Ligand LMT B 101



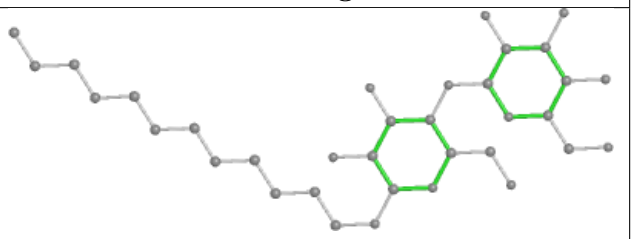
Bond lengths



Bond angles

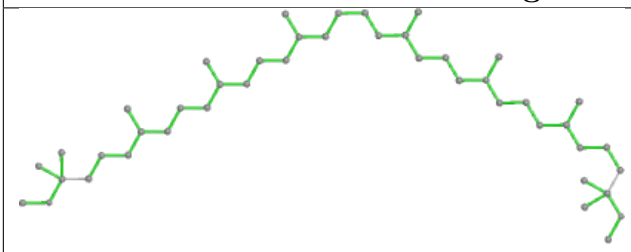


Torsions

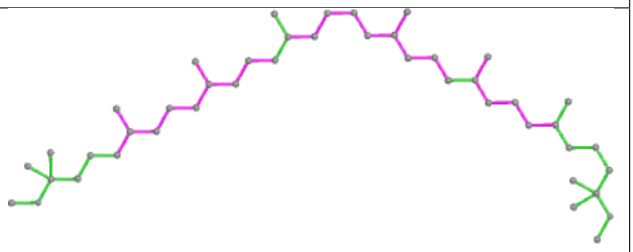


Rings

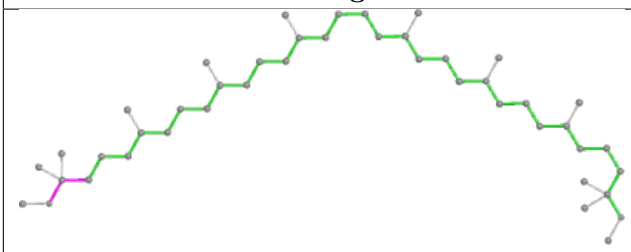
Ligand CRT G 103



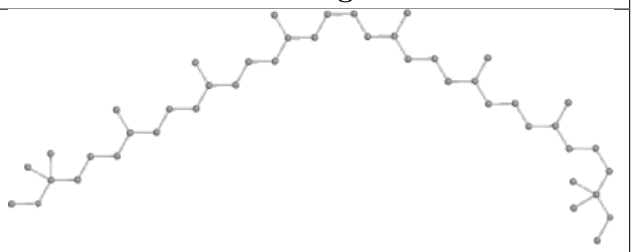
Bond lengths



Bond angles

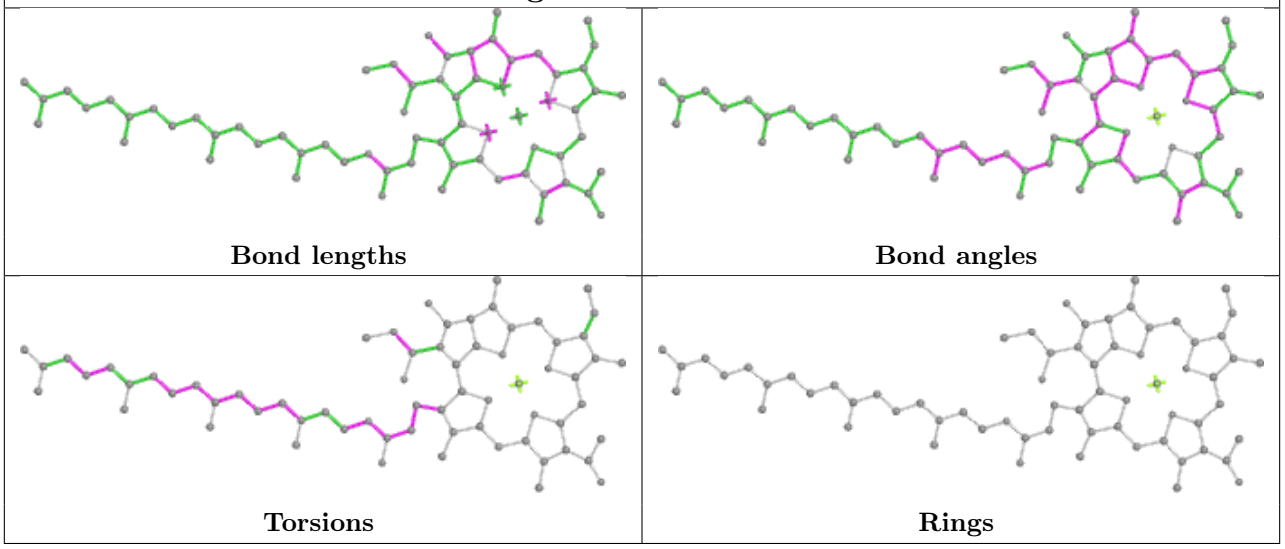


Torsions

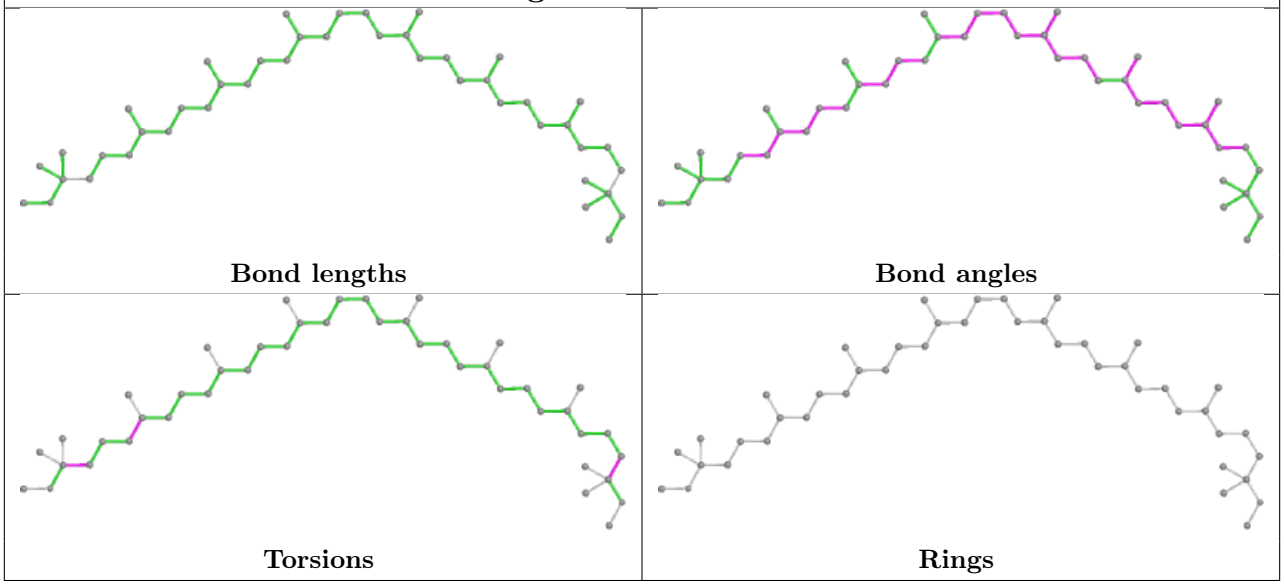


Rings

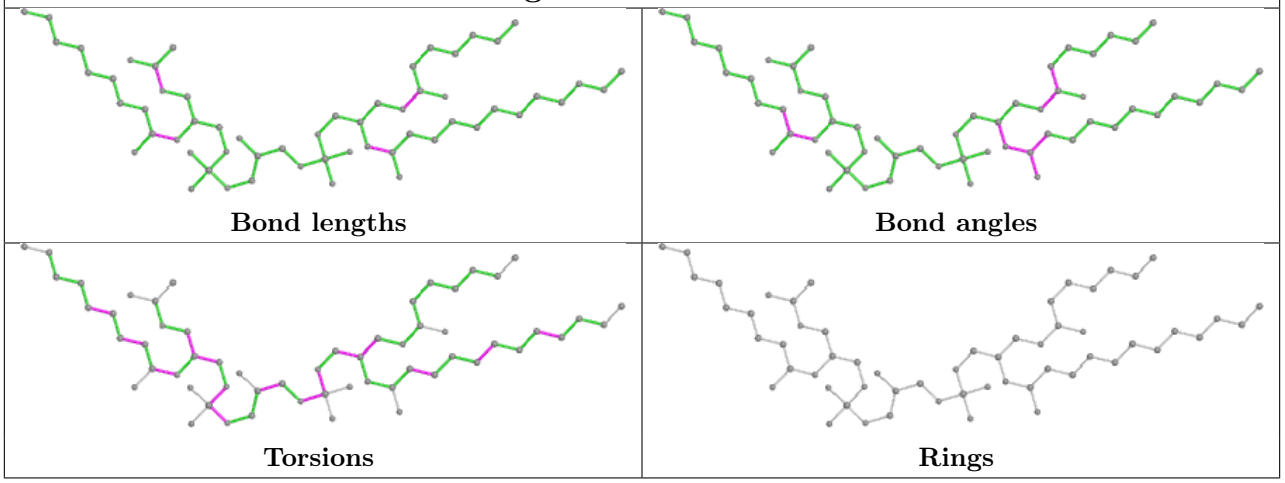
Ligand BCL P 102



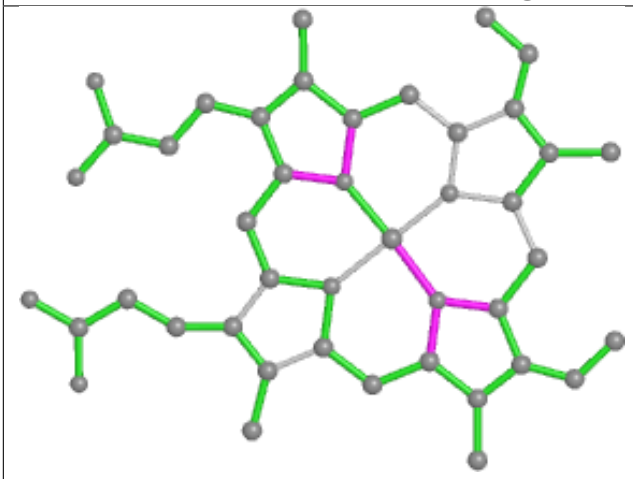
Ligand CRT Z 103



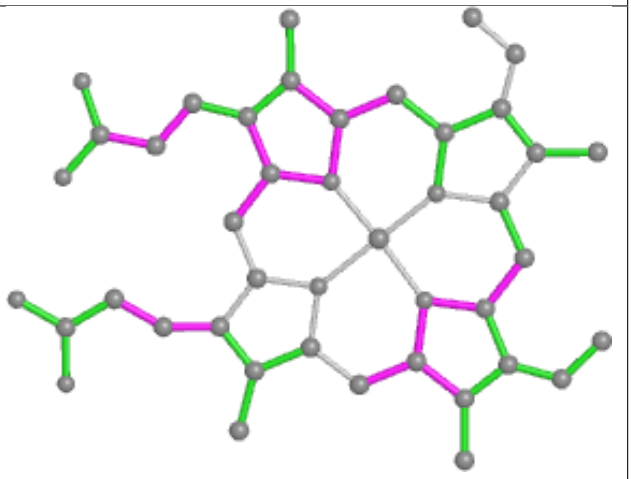
Ligand CDL D 502



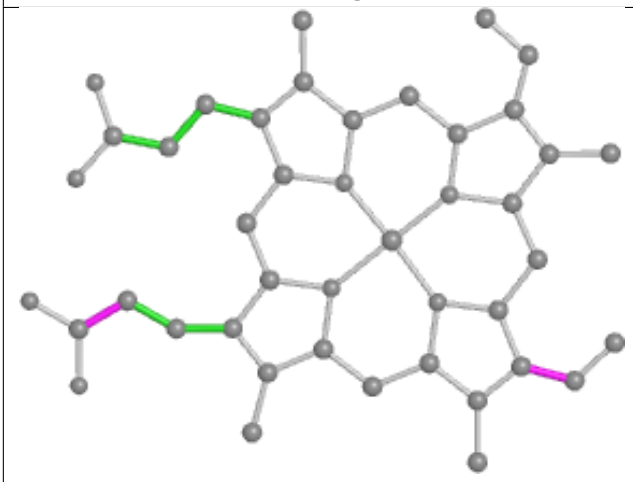
Ligand HEM C 404



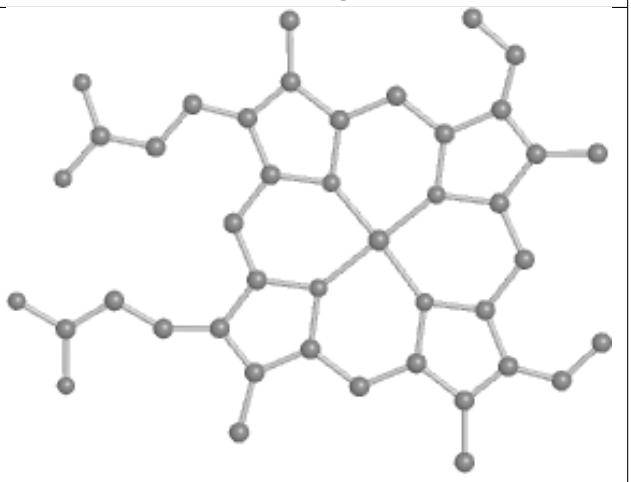
Bond lengths



Bond angles

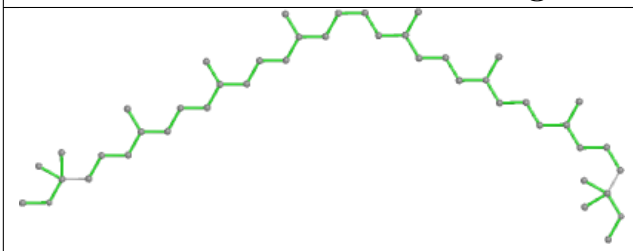


Torsions

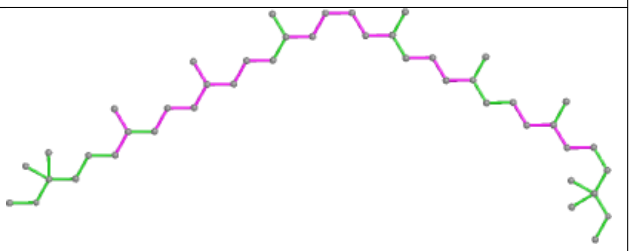


Rings

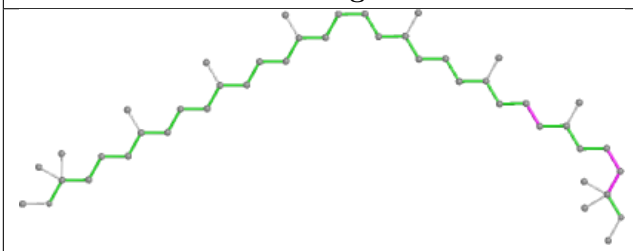
Ligand CRT 8 103



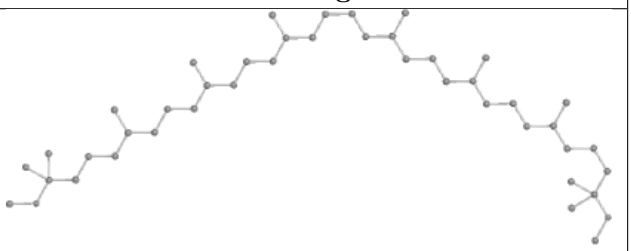
Bond lengths



Bond angles

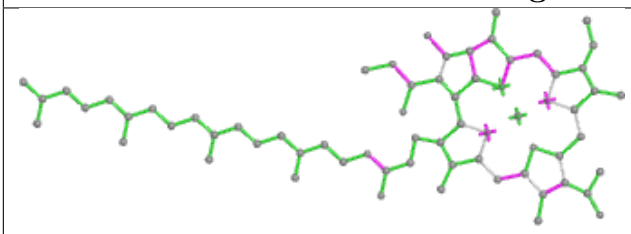


Torsions

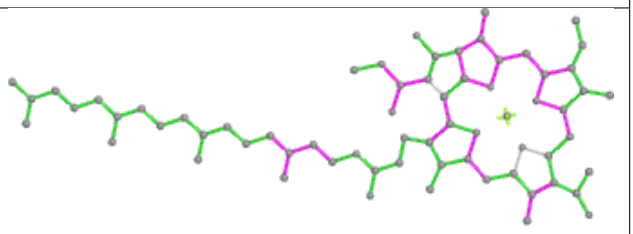


Rings

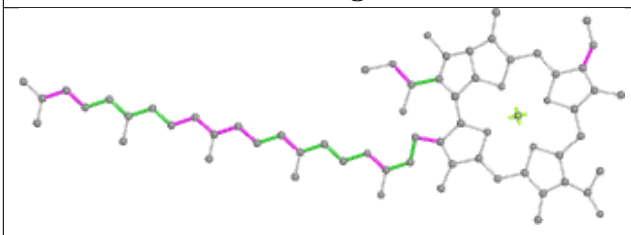
Ligand BCL 0 102



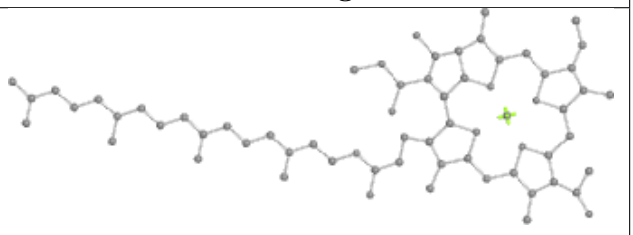
Bond lengths



Bond angles

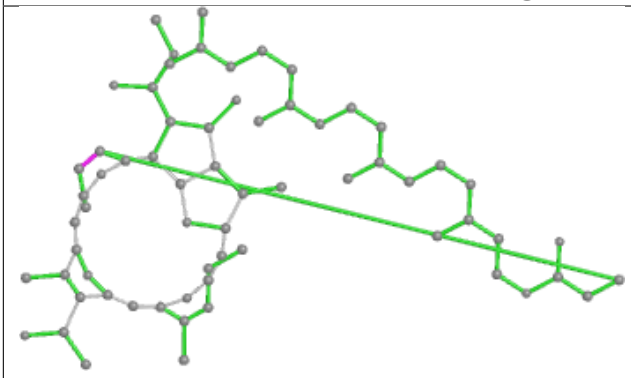


Torsions

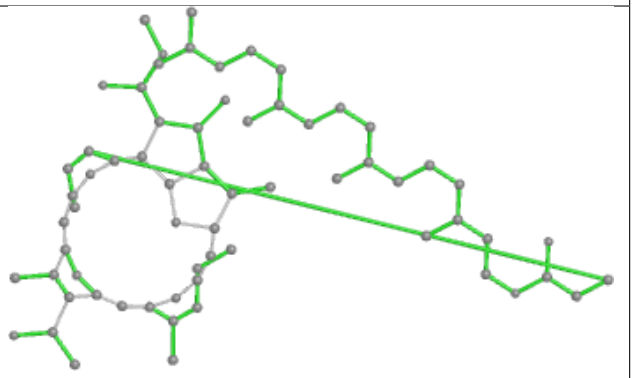


Rings

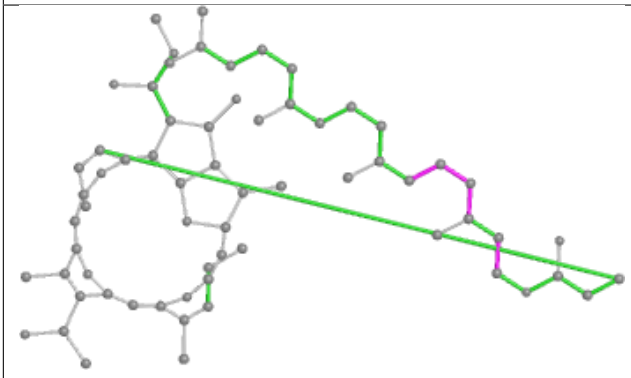
Ligand BPH M 405



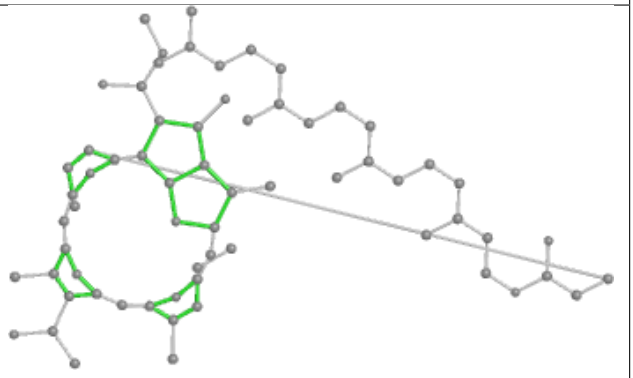
Bond lengths



Bond angles

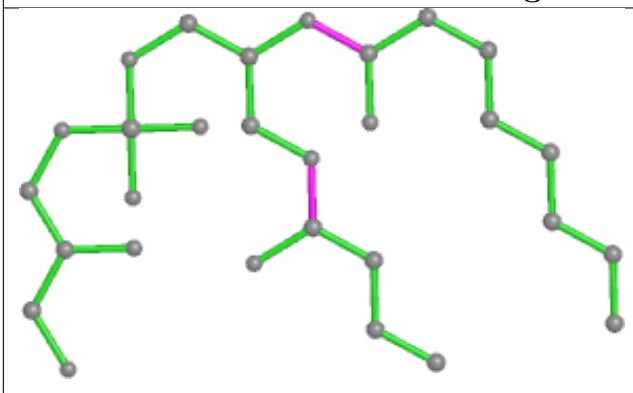


Torsions

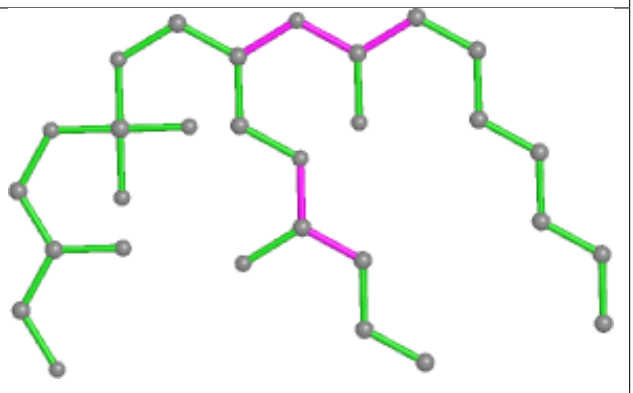


Rings

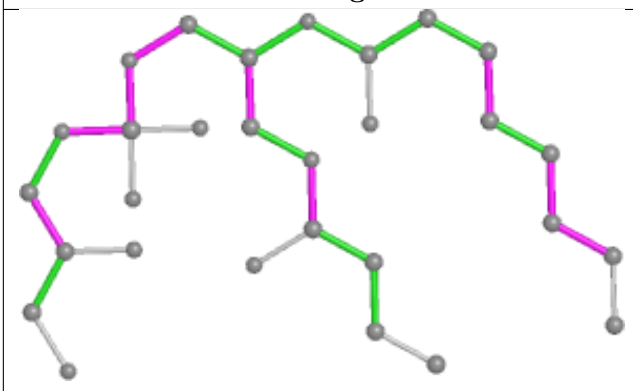
Ligand PGV L 305



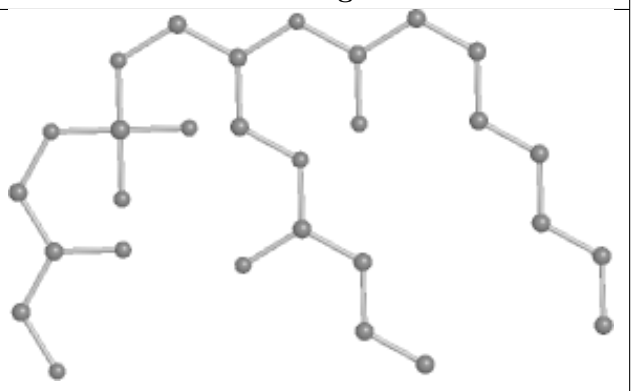
Bond lengths



Bond angles

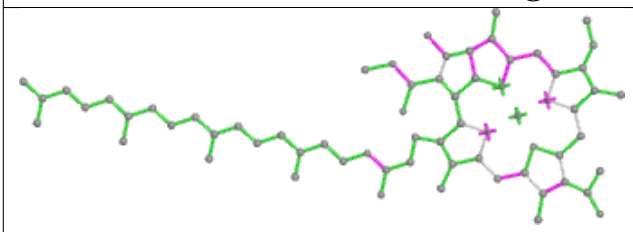


Torsions

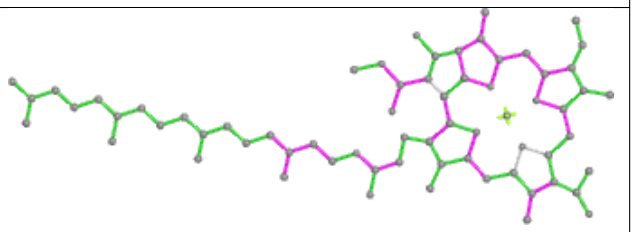


Rings

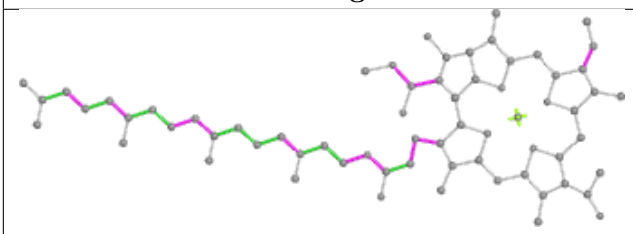
Ligand BCL O 502



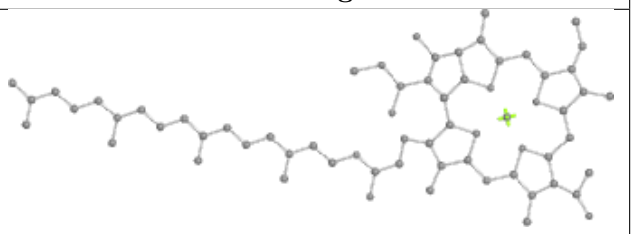
Bond lengths



Bond angles

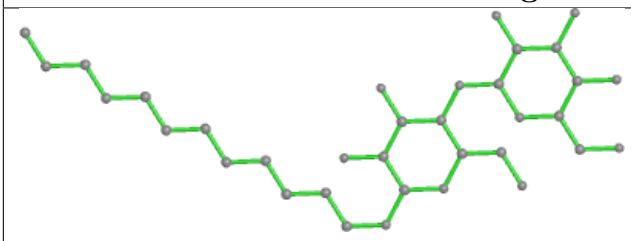


Torsions

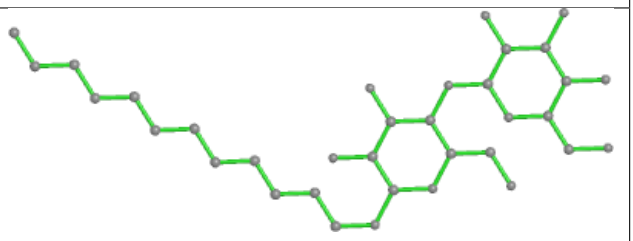


Rings

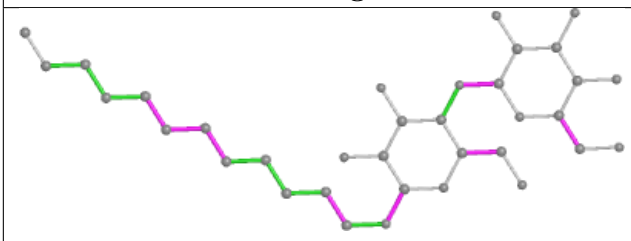
Ligand LMT V 101



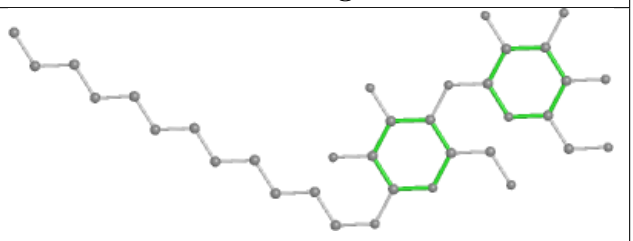
Bond lengths



Bond angles

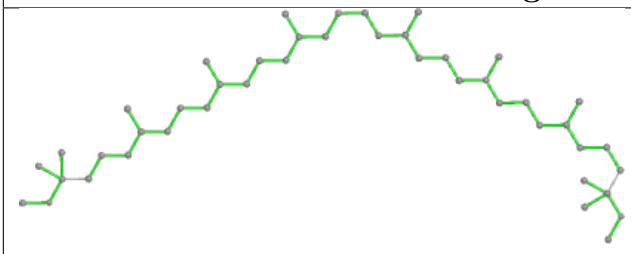


Torsions

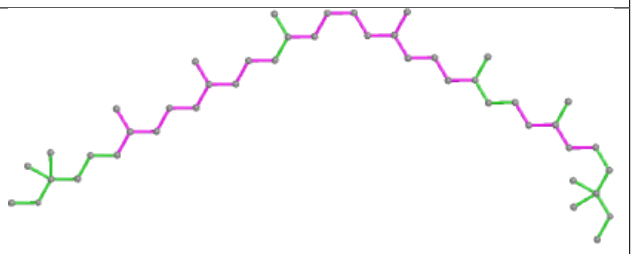


Rings

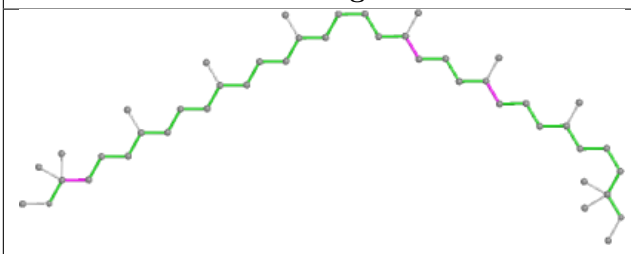
Ligand CRT N 102



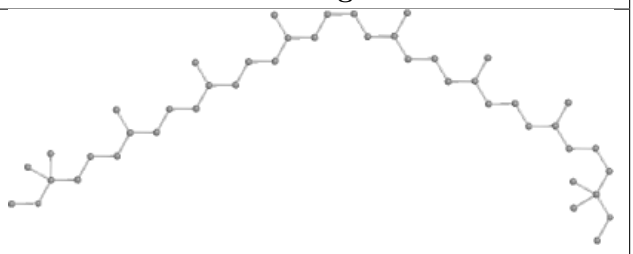
Bond lengths



Bond angles

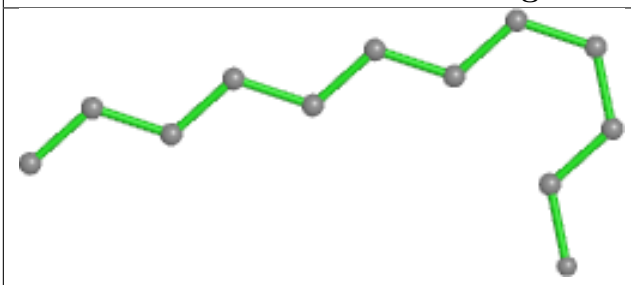


Torsions

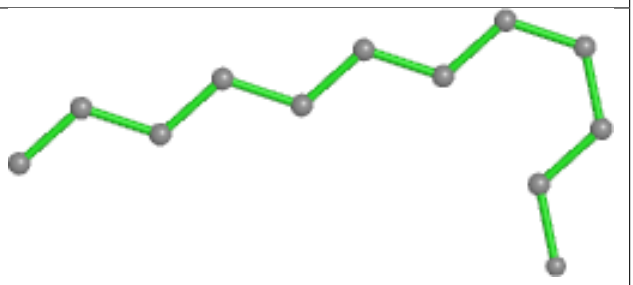


Rings

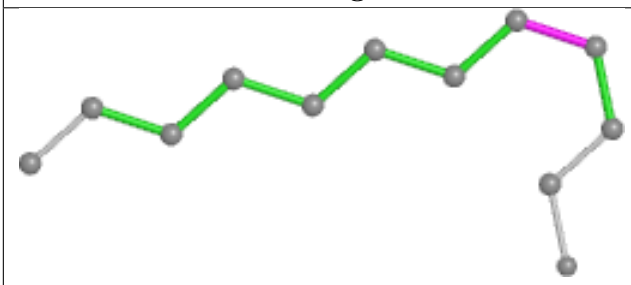
Ligand PLM C 408



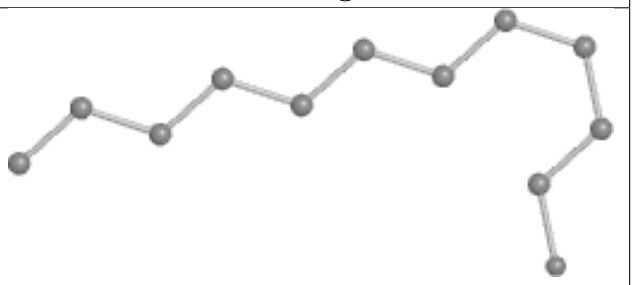
Bond lengths



Bond angles

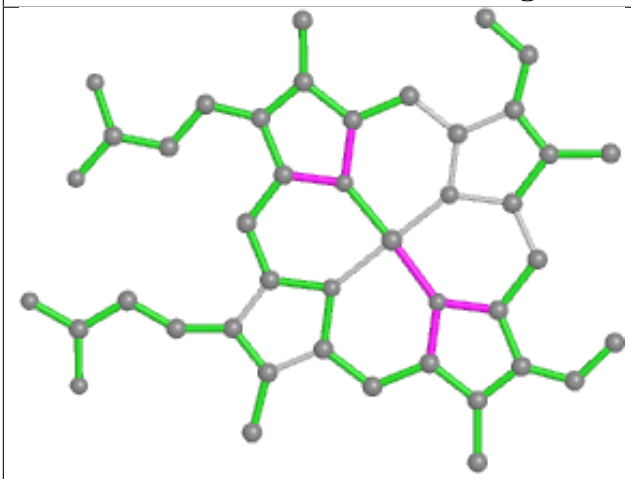


Torsions

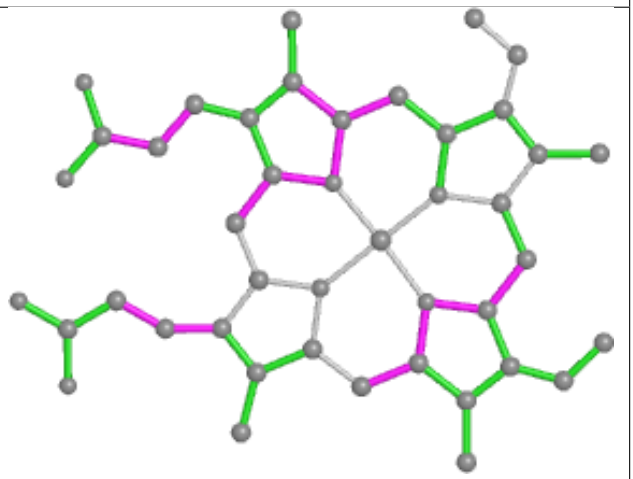


Rings

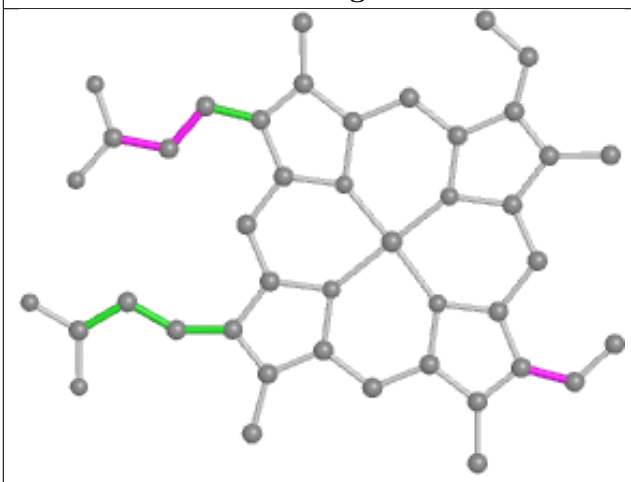
Ligand HEM C 402



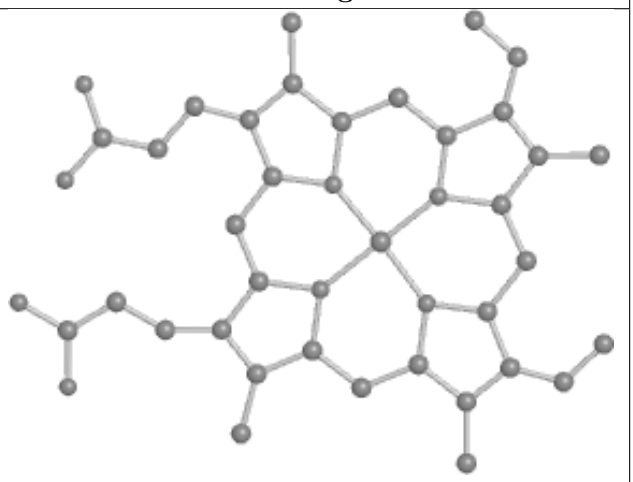
Bond lengths



Bond angles

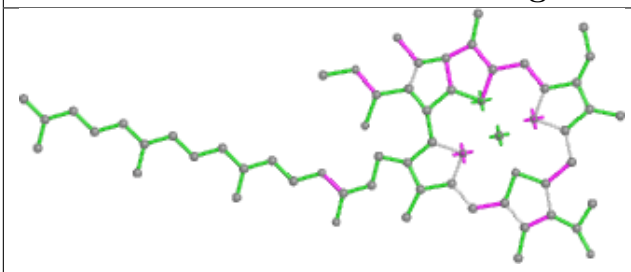


Torsions

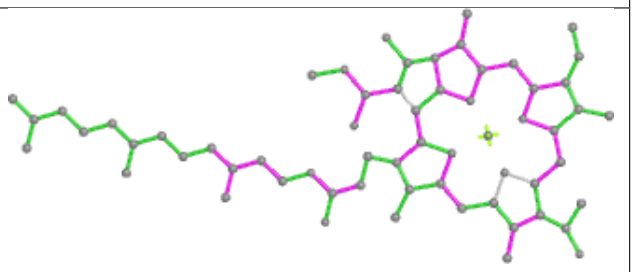


Rings

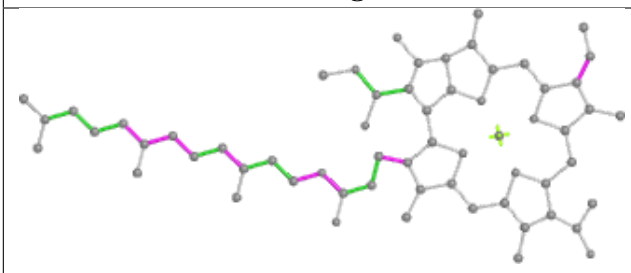
Ligand BCL 7 102



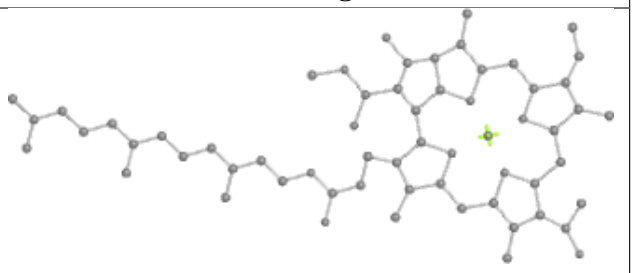
Bond lengths



Bond angles

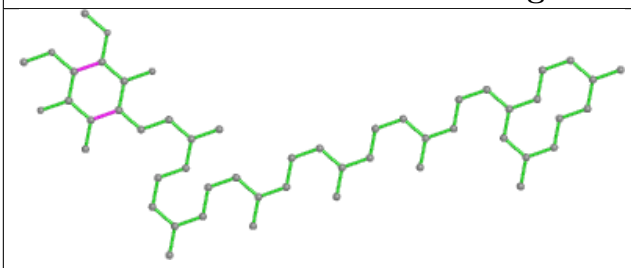


Torsions

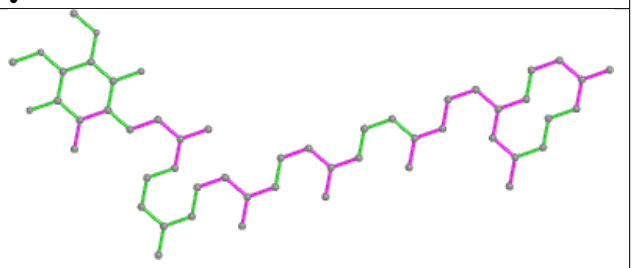


Rings

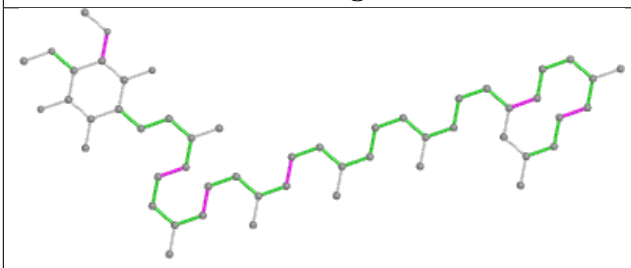
Ligand UQ8 L 308



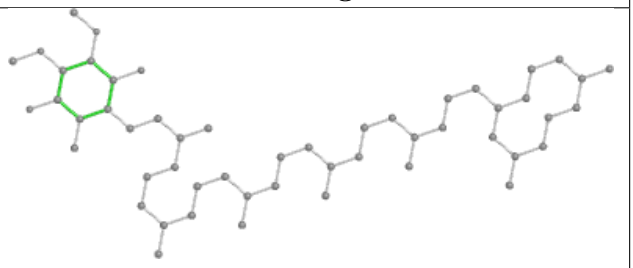
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

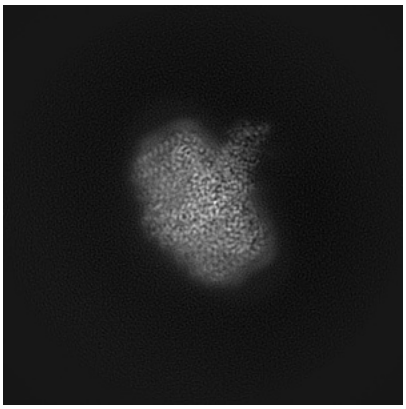
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37466. These allow visual inspection of the internal detail of the map and identification of artifacts.

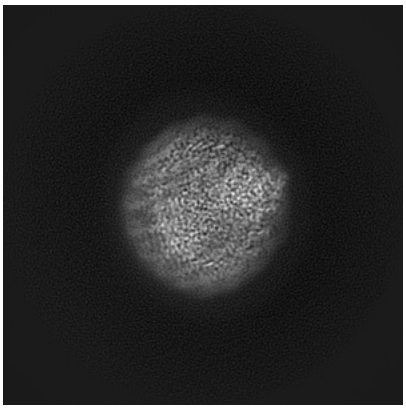
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

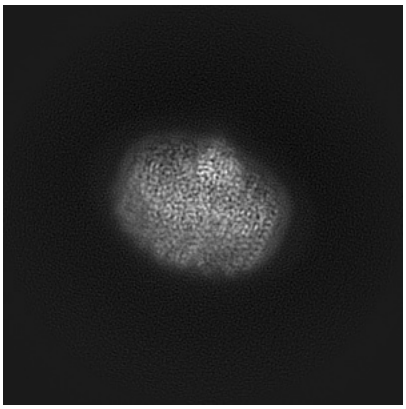
6.1.1 Primary map



X

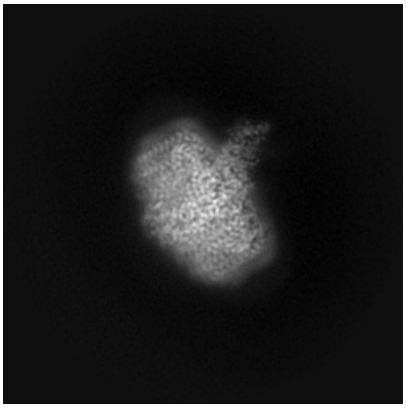


Y

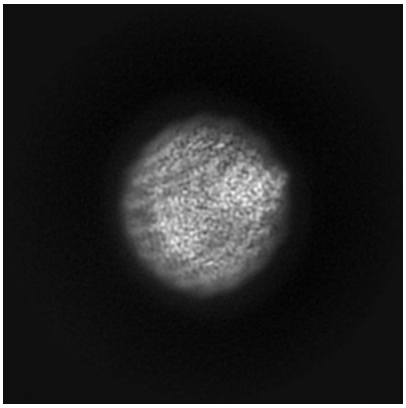


Z

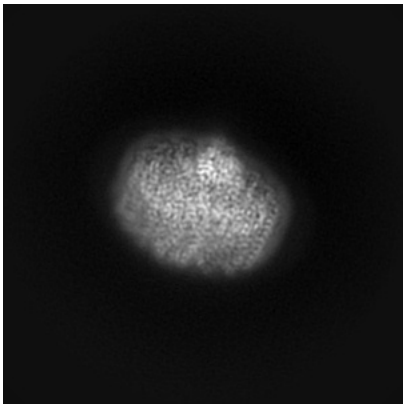
6.1.2 Raw map



X



Y

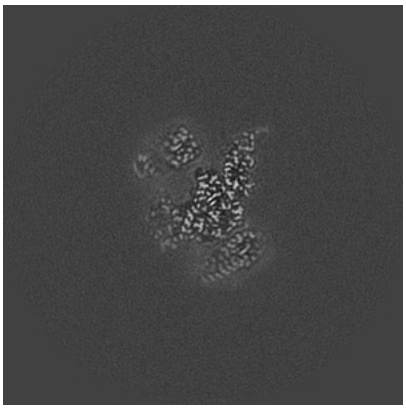


Z

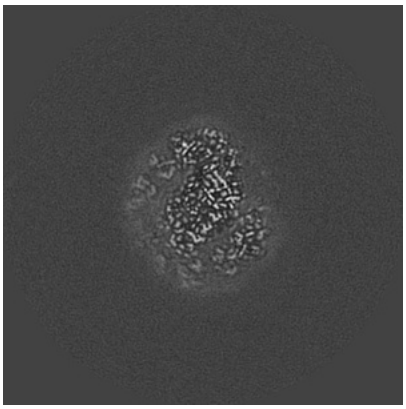
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

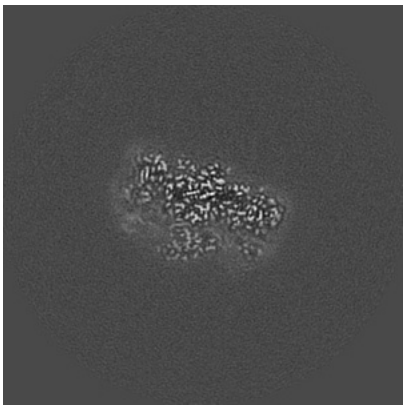
6.2.1 Primary map



X Index: 180

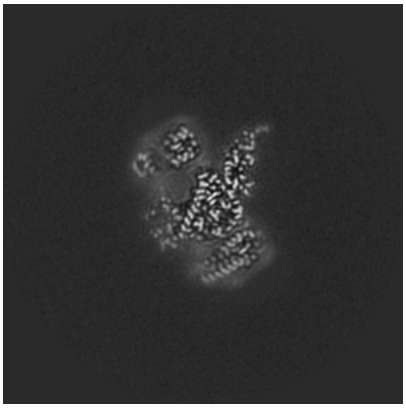


Y Index: 180

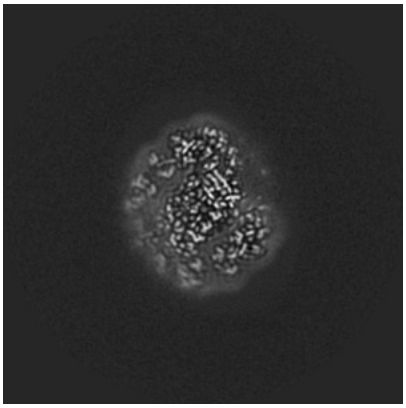


Z Index: 180

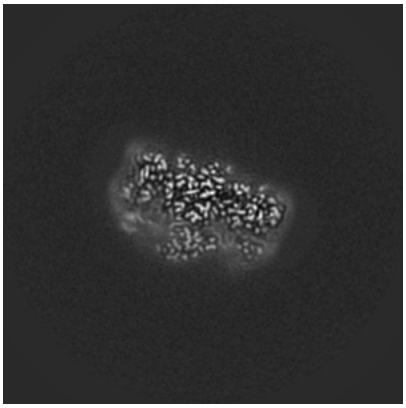
6.2.2 Raw map



X Index: 180



Y Index: 180

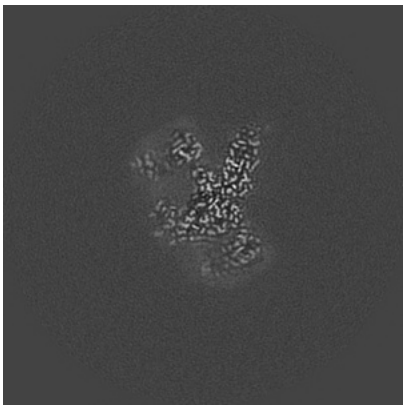


Z Index: 180

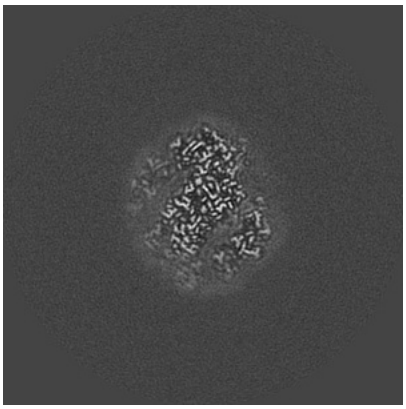
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

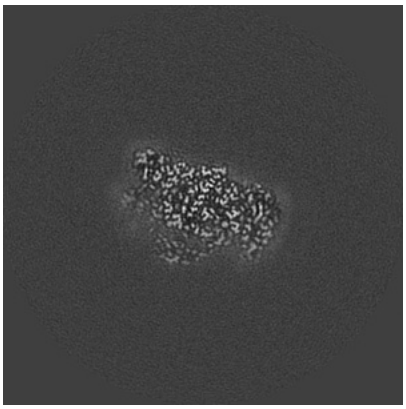
6.3.1 Primary map



X Index: 184

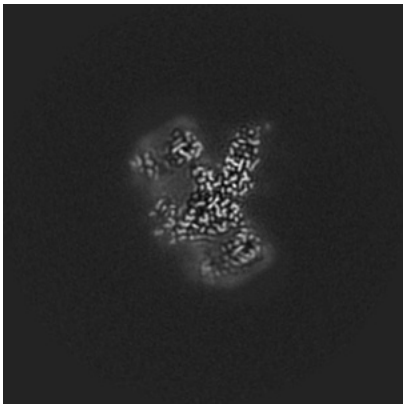


Y Index: 178

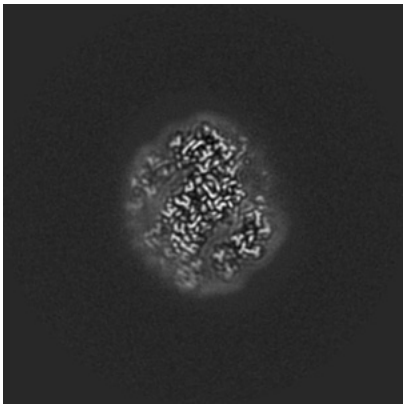


Z Index: 173

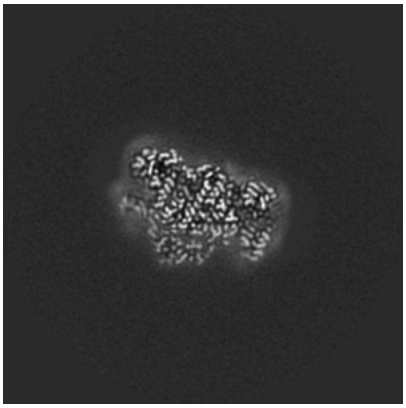
6.3.2 Raw map



X Index: 184



Y Index: 178

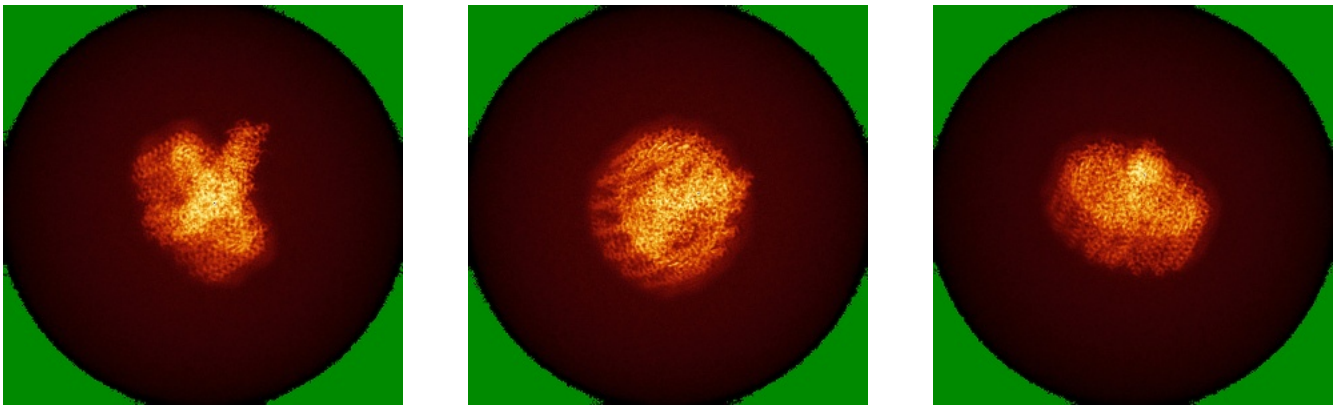


Z Index: 169

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

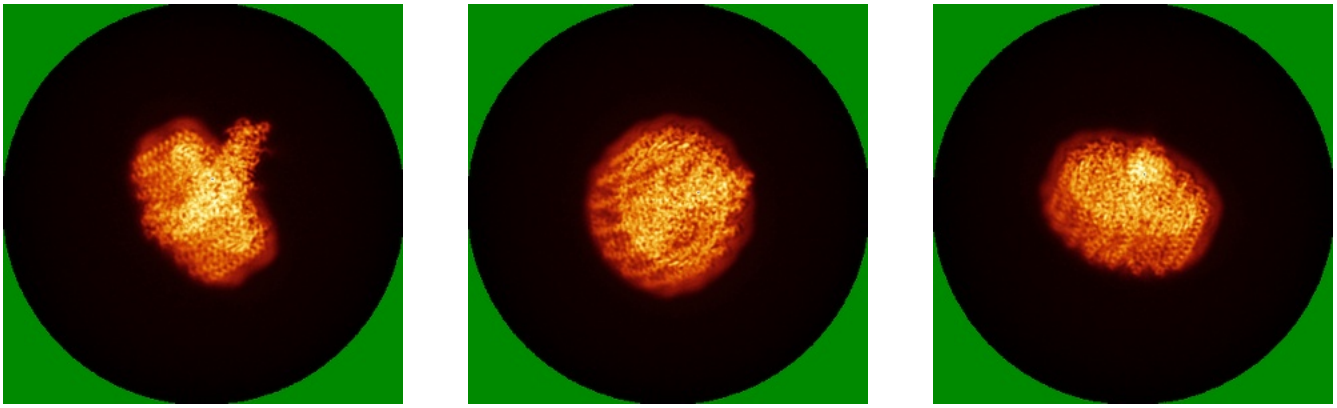
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

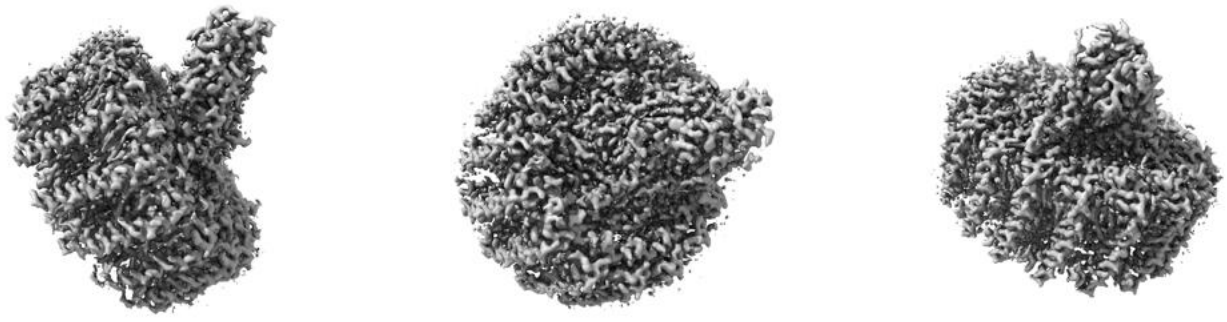


X Y Z

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)

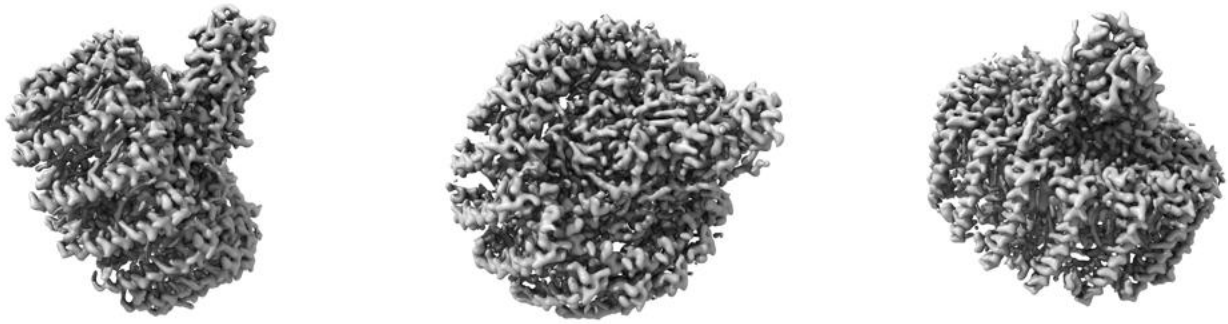
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

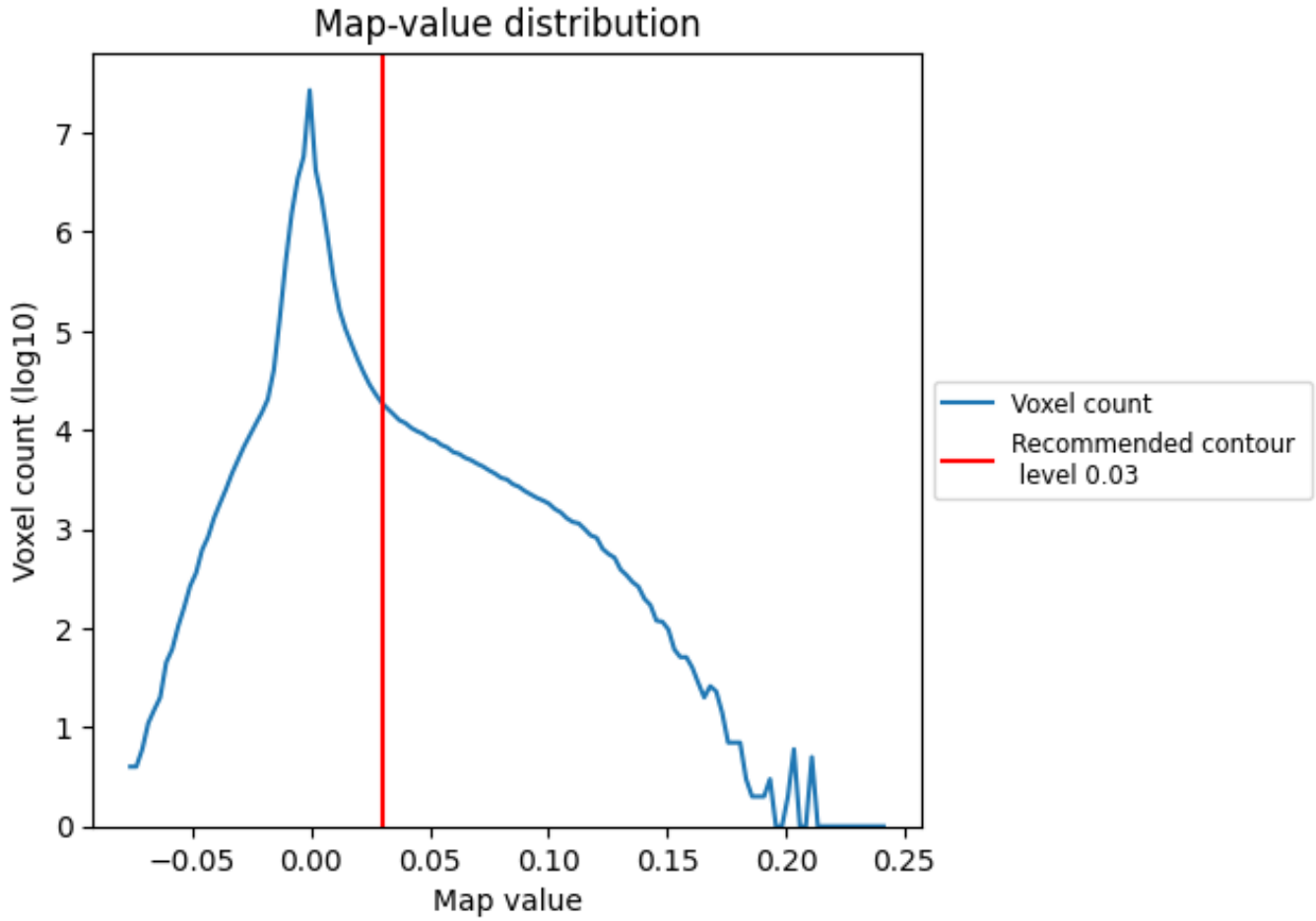
6.6 Mask visualisation (i)

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

7 Map analysis

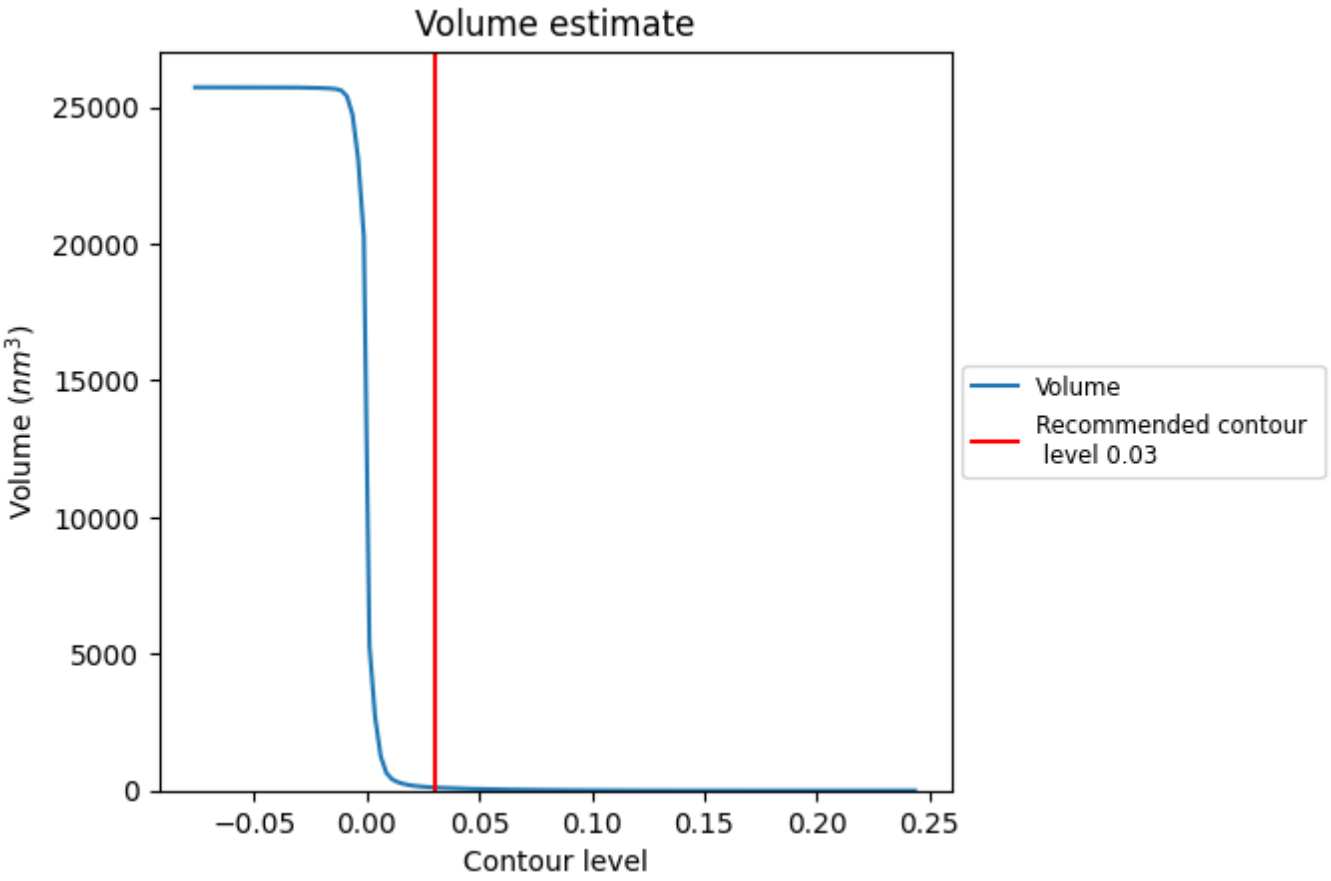
This section contains the results of statistical analysis of the map.

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.

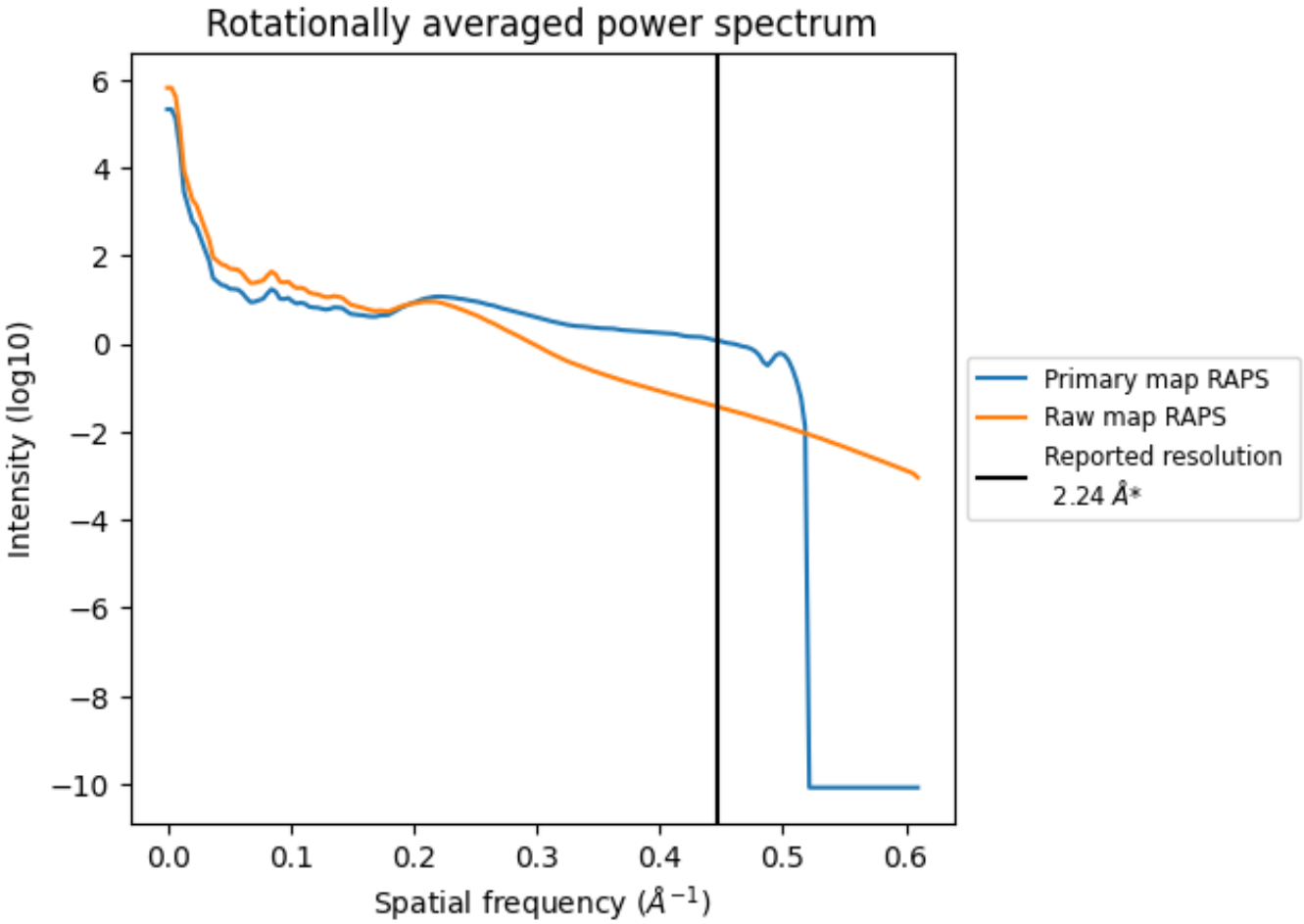
7.2 Volume estimate



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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)

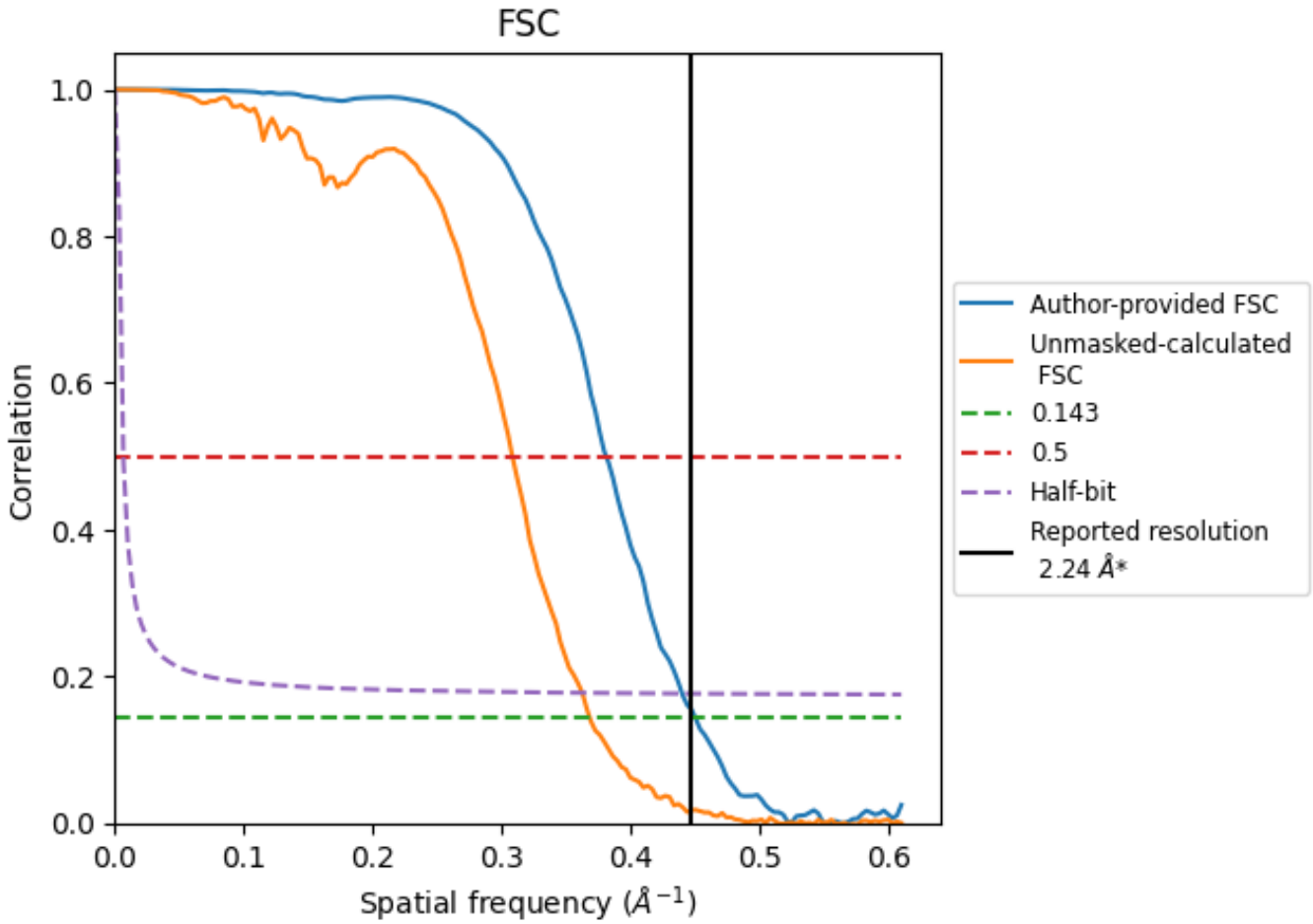


*Reported resolution corresponds to spatial frequency of 0.446 Å^{-1}

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)

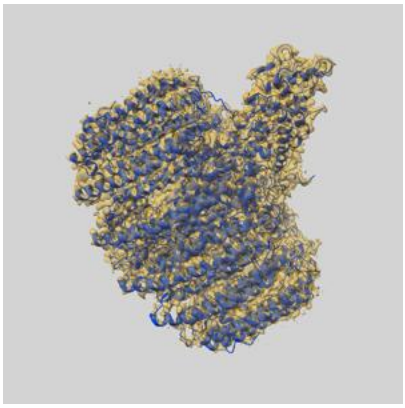
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.22	2.63	2.27
Unmasked-calculated*	2.72	3.24	2.76

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

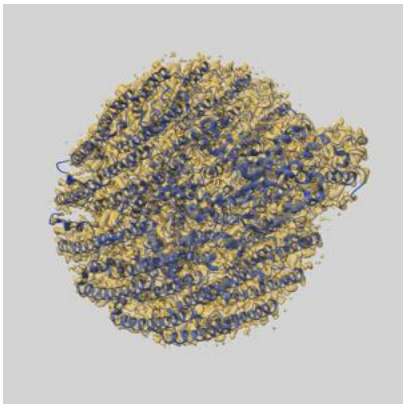
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37466 and PDB model 8WDV. Per-residue inclusion information can be found in section 3 on page 22.

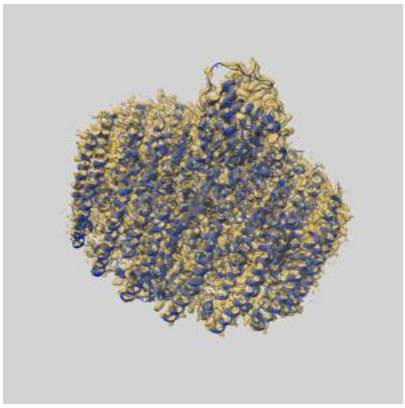
9.1 Map-model overlay



X



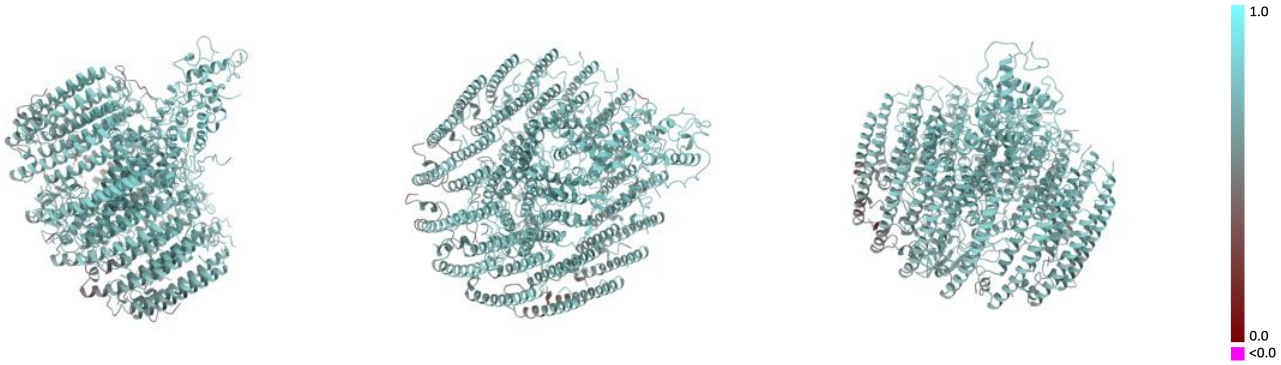
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

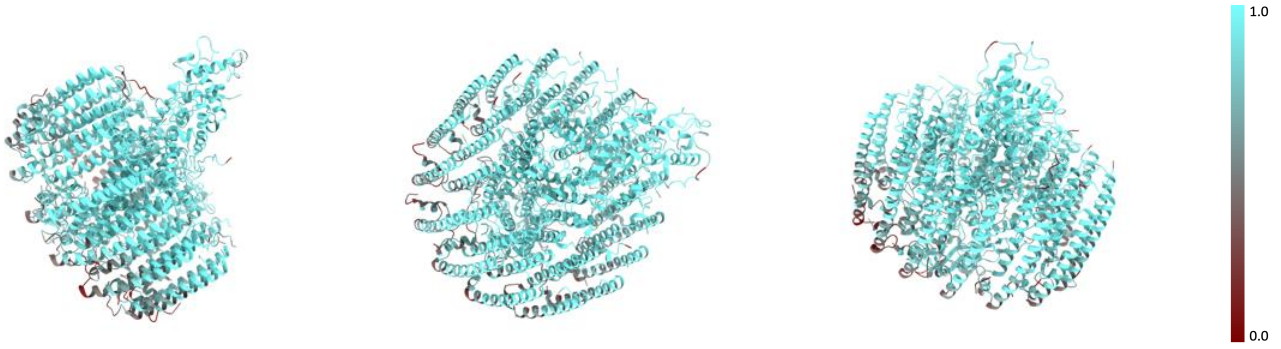
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

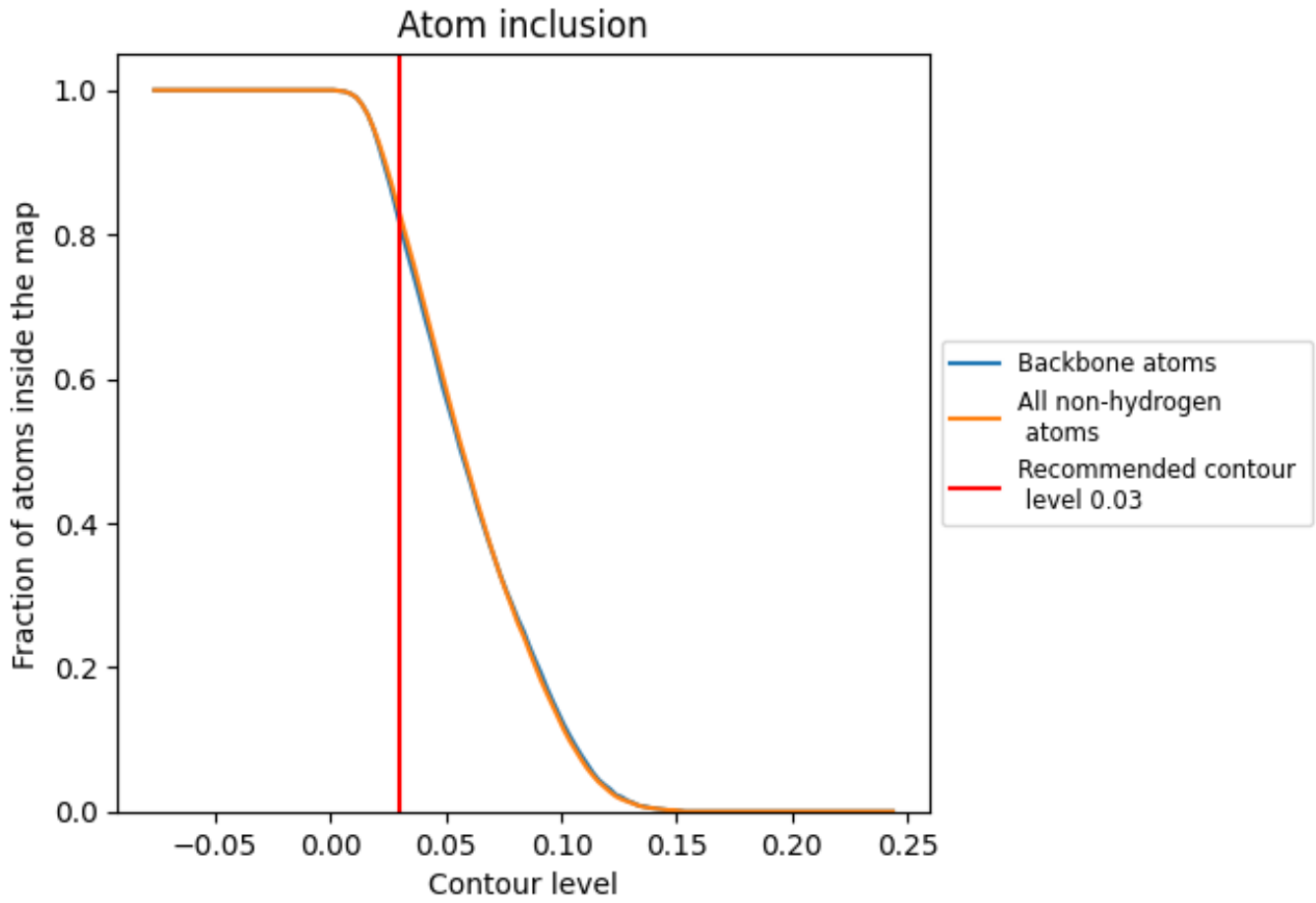
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 83% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8290	0.6580
0	0.7650	0.6280
1	0.8150	0.6430
2	0.6960	0.6040
3	0.8110	0.6480
4	0.6440	0.5770
5	0.7650	0.6040
6	0.6760	0.5750
7	0.7660	0.6160
8	0.7020	0.5920
9	0.8460	0.6580
A	0.8940	0.6750
B	0.7940	0.6350
C	0.9510	0.7090
D	0.7750	0.6370
E	0.7850	0.6330
F	0.7180	0.6200
G	0.6630	0.5930
H	0.7680	0.6550
I	0.8100	0.6400
J	0.7160	0.6030
K	0.7400	0.6140
L	0.9290	0.7070
M	0.9120	0.7000
N	0.7460	0.6180
O	0.8540	0.6600
P	0.7610	0.6250
Q	0.9020	0.6800
R	0.8250	0.6570
S	0.8850	0.6740
T	0.8640	0.6690
U	0.8740	0.6720
V	0.8140	0.6490
W	0.8130	0.6500
X	0.7960	0.6420

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.7380	0.6250
Z	0.7910	0.6290