Full wwPDB EM Validation Report ⓘ

Jul 15, 2024 – 01:02 pm BST

PDB ID	:	8B64
EMDB ID	:	EMD-15862
Title	:	Cryo-EM structure of RC-LH1-PufX photosynthetic core complex from Rba. capsulatus
Authors	:	Bracun, L.; Yamagata, A.; Shirouzu, M.; Liu, L.N.
Deposited on	:	2022-09-26
Resolution	:	2.59 Å(reported)

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

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

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

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

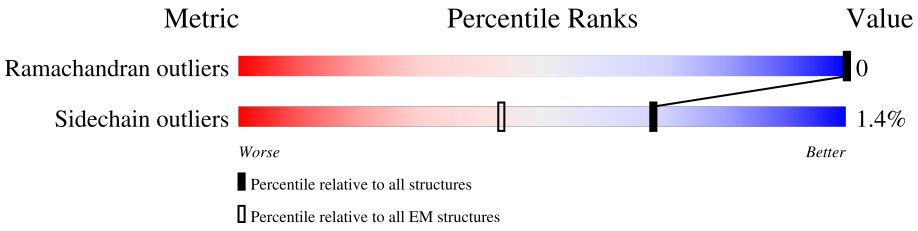
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.59 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	58	76% 24%
1	b	58	90% 7%
1	d	58	91% 7%
1	e	58	93% 7%
1	f	58	93% 7%
1	g	58	93% 7%
1	i	58	91% 9%
1	j	58	93% 7%
1	k	58	90% 9%

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Mol	Chain	Length	Quality of chain
1	n	58	10% 93% 7%
1	o	58	16% 86% 14%
1	r	58	16% 74% 26%
1	s	58	40% 74% 26%
1	t	58	72% 74% 26%
1	u	58	67% 66% 33%
2	A	49	88% 10%
2	B	49	90% 10%
2	D	49	90% 10%
2	E	49	86% 10%
2	F	49	86% 14%
2	G	49	6% 84% 14%
2	I	49	6% 86% 14%
2	J	49	86% 12%
2	K	49	86% 12%
2	N	49	8% 84% 14%
2	O	49	22% 86% 14%
2	R	49	43% 78% 22%
2	S	49	65% 73% 24%
2	T	49	71% 76% 24%
2	U	49	53% 53% 47%
3	X	78	79% 19%
4	L	282	99%
5	M	307	98%
6	H	254	95%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SPO	A	201	-	X	-	-
8	SPO	B	101	-	X	-	-
8	SPO	D	102	-	X	-	-
8	SPO	E	201	-	X	-	-
8	SPO	E	202	-	X	-	-
8	SPO	E	203	-	X	-	-
8	SPO	F	101	-	X	-	-
8	SPO	G	201	-	X	-	-
8	SPO	I	102	-	X	-	-
8	SPO	J	101	-	X	-	-
8	SPO	K	101	-	X	-	-
8	SPO	K	103	-	X	-	-
8	SPO	M	404	-	X	-	-
8	SPO	N	201	-	X	-	-
8	SPO	O	102	-	X	-	-
8	SPO	R	101	-	X	-	-
8	SPO	S	201	-	X	-	-
8	SPO	S	202	-	X	-	-
8	SPO	b	103	-	X	-	-
8	SPO	d	102	-	X	-	-
8	SPO	f	102	-	X	-	-
8	SPO	i	102	-	X	-	-
8	SPO	j	102	-	X	-	-
8	SPO	k	102	-	X	-	-
8	SPO	o	102	-	X	-	-
8	SPO	r	102	-	X	-	-
8	SPO	t	102	-	X	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 21678 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 Light-harvesting protein B-870 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	44	Total	C	N	O	S	0	0
			372	261	58	52	1		
1	e	54	Total	C	N	O	S	0	0
			445	308	71	65	1		
1	b	54	Total	C	N	O	S	0	0
			445	308	71	65	1		
1	d	54	Total	C	N	O	S	0	0
			445	308	71	65	1		
1	t	43	Total	C	N	O		0	0
			342	233	57	52			
1	s	43	Total	C	N	O		0	0
			342	233	57	52			
1	u	39	Total	C	N	O		0	0
			309	213	50	46			
1	r	43	Total	C	N	O		0	0
			342	233	57	52			
1	o	50	Total	C	N	O		0	0
			411	285	66	60			
1	n	54	Total	C	N	O	S	0	0
			445	308	71	65	1		
1	k	53	Total	C	N	O		0	0
			437	303	70	64			
1	j	54	Total	C	N	O	S	0	0
			445	308	71	65	1		
1	i	53	Total	C	N	O		0	0
			437	303	70	64			
1	g	54	Total	C	N	O	S	0	0
			445	308	71	65	1		
1	f	54	Total	C	N	O	S	0	0
			445	308	71	65	1		

- Molecule 2 is a protein called LH1 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	44	Total	C	N	O	S	0	0
			347	229	55	61	2		
2	A	44	Total	C	N	O	S	0	0
			347	229	55	61	2		
2	E	44	Total	C	N	O	S	0	0
			347	229	55	61	2		
2	B	44	Total	C	N	O	S	0	0
			347	229	55	61	2		
2	S	37	Total	C	N	O	S	0	0
			295	195	48	50	2		
2	T	37	Total	C	N	O	S	0	0
			295	195	48	50	2		
2	U	26	Total	C	N	O	S	0	0
			195	133	31	29	2		
2	O	42	Total	C	N	O	S	0	0
			331	219	53	57	2		
2	R	38	Total	C	N	O	S	0	0
			303	201	49	51	2		
2	K	43	Total	C	N	O	S	0	0
			339	225	54	58	2		
2	N	42	Total	C	N	O	S	0	0
			331	219	53	57	2		
2	I	42	Total	C	N	O	S	0	0
			331	219	53	57	2		
2	J	43	Total	C	N	O	S	0	0
			339	225	54	58	2		
2	F	42	Total	C	N	O	S	0	0
			331	219	53	57	2		
2	G	42	Total	C	N	O	S	0	0
			331	219	53	57	2		

- Molecule 3 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	63	Total	C	N	O	S	0	0
			490	325	77	84	4		

- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	281	Total	C	N	O	S	0	0
			2227	1491	353	366	17		

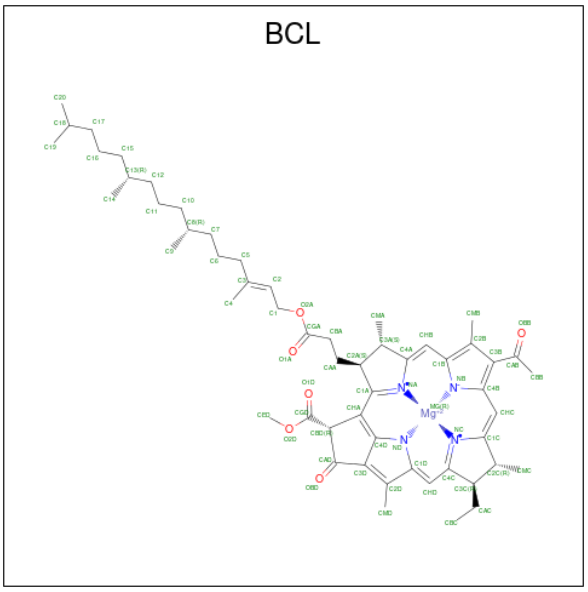
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	304	Total	C	N	O	S	0	0
			2422	1613	393	403	13		

- Molecule 6 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	245	Total	C	N	O	S	0	0
			1943	1239	327	367	10		

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



Mol	Chain	Residues	Atoms					AltConf
7	a	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
7	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	t	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	T	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	r	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
7	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	k	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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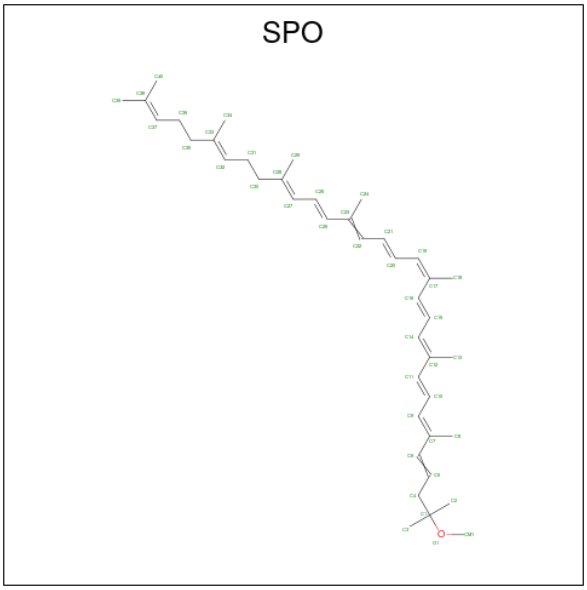
Mol	Chain	Residues	Atoms					AltConf
7	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C		0
			35	35		
8	b	1	Total	C	O	0
			42	41	1	
8	A	1	Total	C	O	0
			42	41	1	
8	E	1	Total	C	O	0
			42	41	1	
8	E	1	Total	C		0
			35	35		

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Mol	Chain	Residues	Atoms	AltConf
8	E	1	Total C 35 35	0
8	M	1	Total C O 42 41 1	0
8	d	1	Total C O 42 41 1	0
8	B	1	Total C 35 35	0
8	t	1	Total C O 42 41 1	0
8	S	1	Total C O 42 41 1	0
8	S	1	Total C 35 35	0
8	r	1	Total C O 42 41 1	0
8	O	1	Total C 35 35	0
8	R	1	Total C 35 35	0
8	o	1	Total C O 42 41 1	0
8	K	1	Total C 35 35	0
8	K	1	Total C 35 35	0
8	N	1	Total C O 42 41 1	0
8	k	1	Total C O 42 41 1	0
8	j	1	Total C O 42 41 1	0
8	I	1	Total C 35 35	0
8	J	1	Total C 35 35	0
8	i	1	Total C O 42 41 1	0
8	F	1	Total C 35 35	0
8	G	1	Total C O 42 41 1	0

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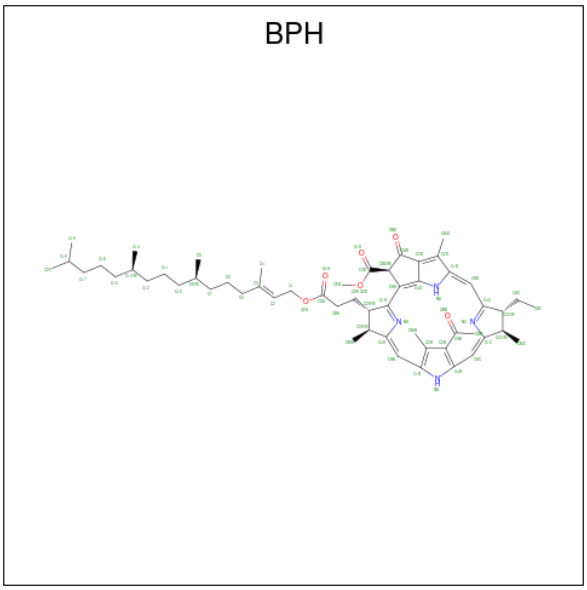
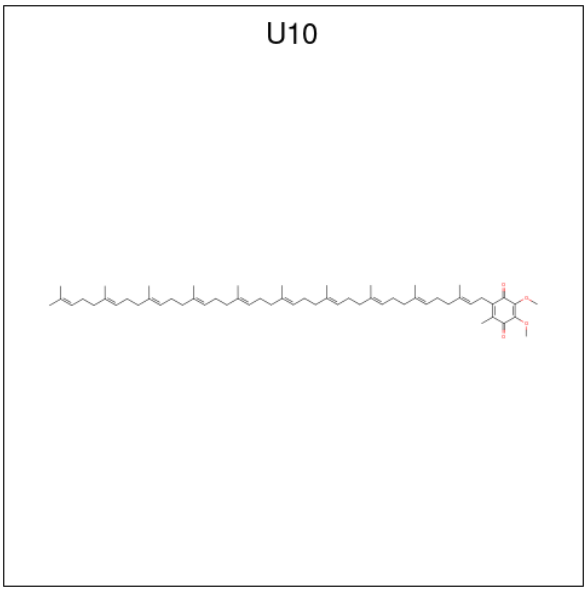
Mol	Chain	Residues	Atoms			AltConf
8	f	1	Total	C	O	0
			42	41	1	

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



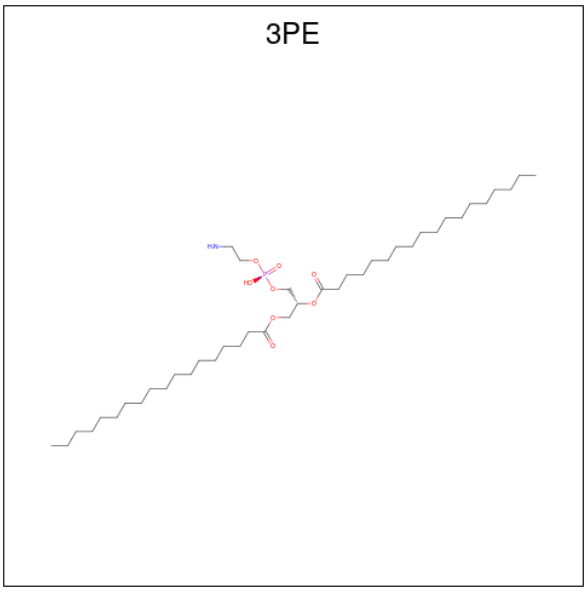
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 10 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
10	L	1	Total C O 33 29 4	0
10	L	1	Total C O 23 19 4	0
10	L	1	Total C O 18 14 4	0
10	M	1	Total C O 48 44 4	0

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			41	31	1	8	1	
11	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	H	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	H	1	Total	C	N	O	P	0
			45	35	1	8	1	
11	d	1	Total	C	N	O	P	0
			37	27	1	8	1	
11	d	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

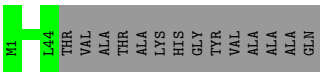
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Fe	0
			1	1	

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.

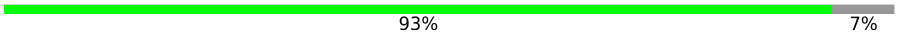
• Molecule 1: Light-harvesting protein B-870 alpha chain

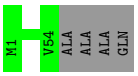
Chain a:



• Molecule 1: Light-harvesting protein B-870 alpha chain

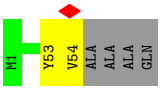
Chain e:





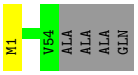
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain b:



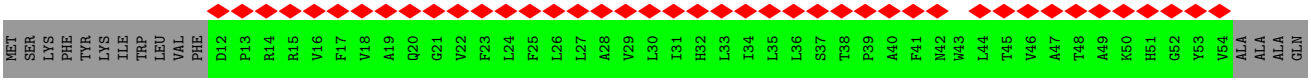
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain d:



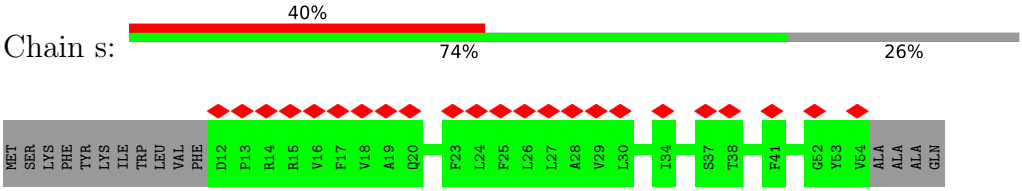
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain t:



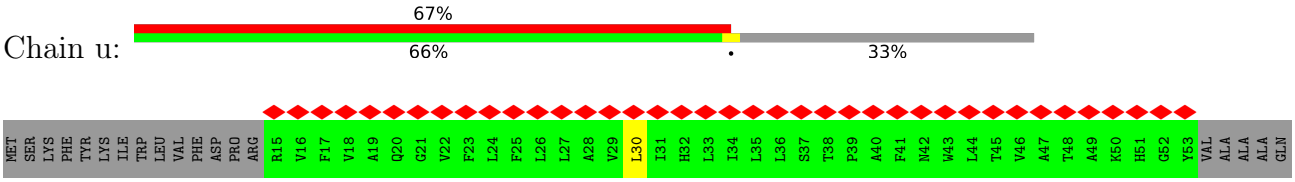
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain s:



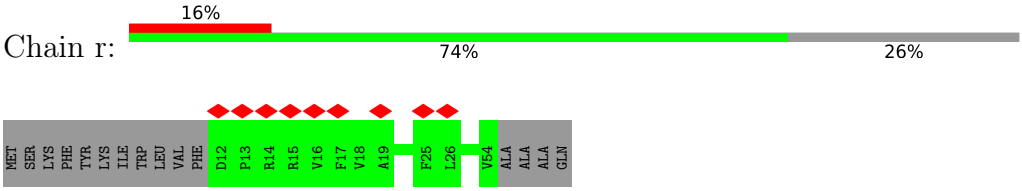
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain u:



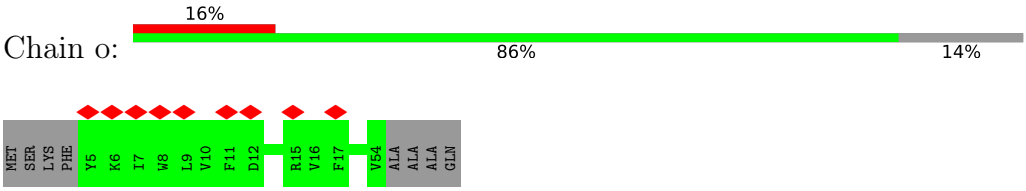
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain r:



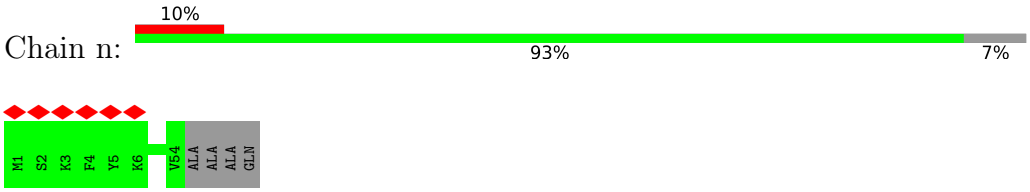
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain o:



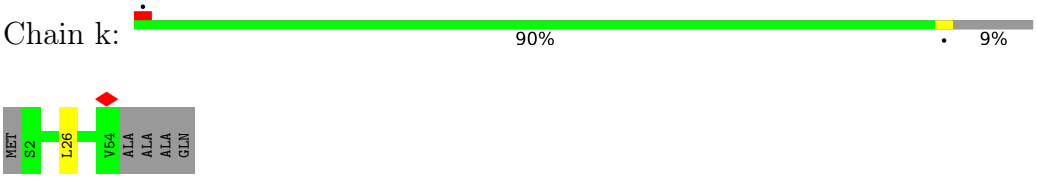
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain n:



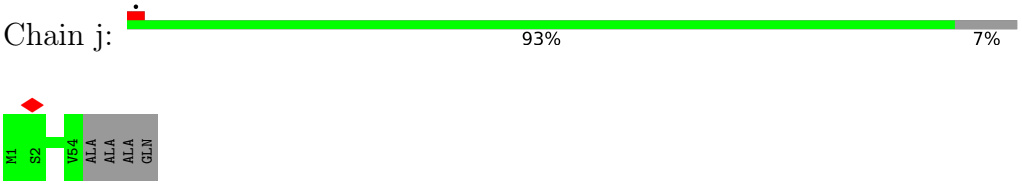
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain k:



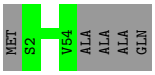
• Molecule 1: Light-harvesting protein B-870 alpha chain

Chain j:



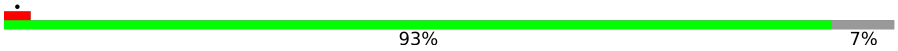
• Molecule 1: Light-harvesting protein B-870 alpha chain

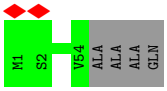
Chain i:



• Molecule 1: Light-harvesting protein B-870 alpha chain

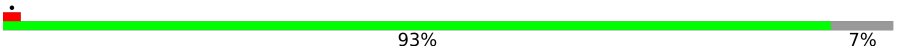
Chain g:

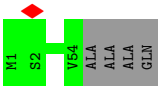




• Molecule 1: Light-harvesting protein B-870 alpha chain

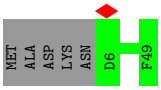
Chain f:





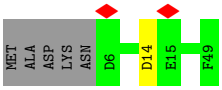
• Molecule 2: LH1 beta chain

Chain D:



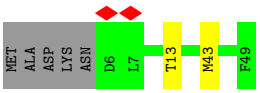
• Molecule 2: LH1 beta chain

Chain A:



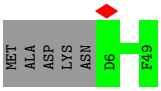
• Molecule 2: LH1 beta chain

Chain E:



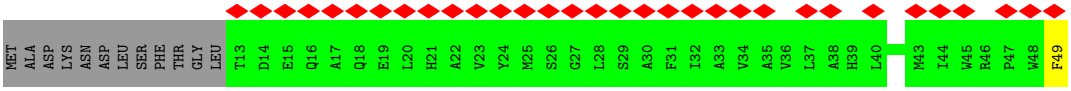
• Molecule 2: LH1 beta chain

Chain B:



• Molecule 2: LH1 beta chain

Chain S:

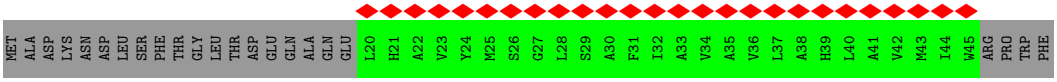


• Molecule 2: LH1 beta chain

Chain T:

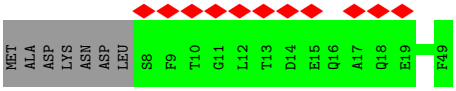
• Molecule 2: LH1 beta chain

Chain U:



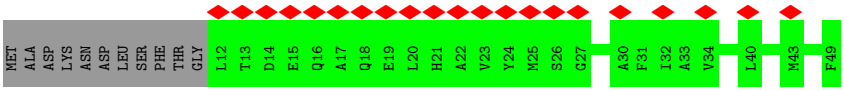
• Molecule 2: LH1 beta chain

Chain O:



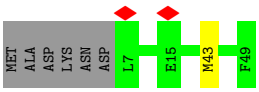
• Molecule 2: LH1 beta chain

Chain R:



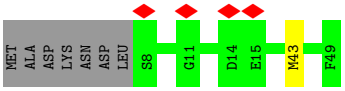
• Molecule 2: LH1 beta chain

Chain K:



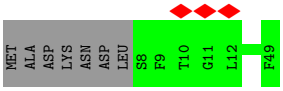
• Molecule 2: LH1 beta chain

Chain N:



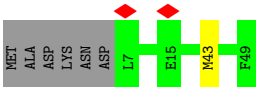
• Molecule 2: LH1 beta chain

Chain I:



• Molecule 2: LH1 beta chain

Chain J:

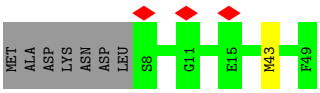


• Molecule 2: LH1 beta chain

Chain F:

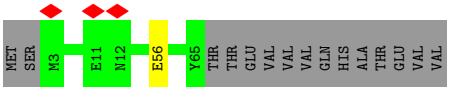
• Molecule 2: LH1 beta chain

Chain G:



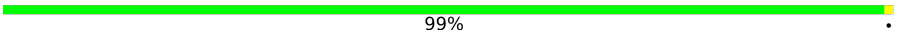
• Molecule 3: Intrinsic membrane protein PufX

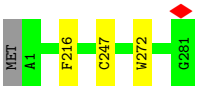
Chain X:



• Molecule 4: Reaction center protein L chain

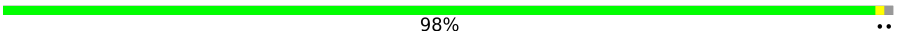
Chain L:





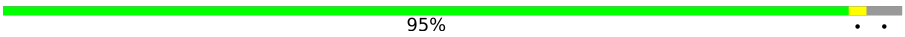
• Molecule 5: Reaction center protein M chain

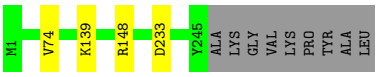
Chain M:



• Molecule 6: Reaction center protein H chain

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181054	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.32	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	248.54999, 248.54999, 248.54999	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, FE, U10, BCL, 3PE, BPH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.26	0/385	0.39	0/524
1	b	0.25	0/460	0.41	0/627
1	d	0.25	0/460	0.38	0/627
1	e	0.25	0/460	0.39	0/627
1	f	0.25	0/460	0.39	0/627
1	g	0.25	0/460	0.38	0/627
1	i	0.25	0/452	0.38	0/617
1	j	0.25	0/460	0.40	0/627
1	k	0.26	0/452	0.39	0/617
1	n	0.25	0/460	0.39	0/627
1	o	0.25	0/425	0.39	0/582
1	r	0.24	0/352	0.41	0/482
1	s	0.24	0/352	0.40	0/482
1	t	0.24	0/352	0.39	0/482
1	u	0.24	0/318	0.37	0/435
2	A	0.25	0/357	0.39	0/486
2	B	0.26	0/357	0.43	0/486
2	D	0.24	0/357	0.38	0/486
2	E	0.26	0/357	0.41	0/486
2	F	0.25	0/341	0.41	0/464
2	G	0.26	0/341	0.40	0/464
2	I	0.25	0/341	0.38	0/464
2	J	0.25	0/349	0.40	0/475
2	K	0.24	0/349	0.40	0/475
2	N	0.27	0/341	0.39	0/464
2	O	0.25	0/341	0.39	0/464
2	R	0.24	0/312	0.38	0/425
2	S	0.24	0/304	0.39	0/414
2	T	0.24	0/304	0.36	0/414
2	U	0.23	0/200	0.32	0/273
3	X	0.26	0/506	0.42	0/682
4	L	0.26	0/2313	0.44	0/3161

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
5	M	0.25	0/2514	0.44	0/3435
6	H	0.25	0/1993	0.48	0/2709
All	All	0.25	0/18585	0.42	0/25337

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)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	42/58 (72%)	42 (100%)	0	0	100	100
1	b	52/58 (90%)	52 (100%)	0	0	100	100
1	d	52/58 (90%)	52 (100%)	0	0	100	100
1	e	52/58 (90%)	52 (100%)	0	0	100	100
1	f	52/58 (90%)	52 (100%)	0	0	100	100
1	g	52/58 (90%)	52 (100%)	0	0	100	100
1	i	51/58 (88%)	51 (100%)	0	0	100	100
1	j	52/58 (90%)	52 (100%)	0	0	100	100
1	k	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
1	n	52/58 (90%)	52 (100%)	0	0	100	100
1	o	48/58 (83%)	48 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	r	41/58 (71%)	41 (100%)	0	0	100	100
1	s	41/58 (71%)	41 (100%)	0	0	100	100
1	t	41/58 (71%)	41 (100%)	0	0	100	100
1	u	37/58 (64%)	36 (97%)	1 (3%)	0	100	100
2	A	42/49 (86%)	42 (100%)	0	0	100	100
2	B	42/49 (86%)	42 (100%)	0	0	100	100
2	D	42/49 (86%)	42 (100%)	0	0	100	100
2	E	42/49 (86%)	42 (100%)	0	0	100	100
2	F	40/49 (82%)	40 (100%)	0	0	100	100
2	G	40/49 (82%)	40 (100%)	0	0	100	100
2	I	40/49 (82%)	40 (100%)	0	0	100	100
2	J	41/49 (84%)	41 (100%)	0	0	100	100
2	K	41/49 (84%)	41 (100%)	0	0	100	100
2	N	40/49 (82%)	40 (100%)	0	0	100	100
2	O	40/49 (82%)	40 (100%)	0	0	100	100
2	R	36/49 (74%)	36 (100%)	0	0	100	100
2	S	35/49 (71%)	35 (100%)	0	0	100	100
2	T	35/49 (71%)	35 (100%)	0	0	100	100
2	U	24/49 (49%)	24 (100%)	0	0	100	100
3	X	61/78 (78%)	59 (97%)	2 (3%)	0	100	100
4	L	279/282 (99%)	274 (98%)	5 (2%)	0	100	100
5	M	302/307 (98%)	296 (98%)	6 (2%)	0	100	100
6	H	243/254 (96%)	240 (99%)	3 (1%)	0	100	100
All	All	2181/2526 (86%)	2163 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	a	40/48 (83%)	40 (100%)	0	100	100
1	b	47/48 (98%)	45 (96%)	2 (4%)	29	52
1	d	47/48 (98%)	46 (98%)	1 (2%)	53	75
1	e	47/48 (98%)	47 (100%)	0	100	100
1	f	47/48 (98%)	47 (100%)	0	100	100
1	g	47/48 (98%)	47 (100%)	0	100	100
1	i	46/48 (96%)	46 (100%)	0	100	100
1	j	47/48 (98%)	47 (100%)	0	100	100
1	k	46/48 (96%)	45 (98%)	1 (2%)	52	74
1	n	47/48 (98%)	47 (100%)	0	100	100
1	o	43/48 (90%)	43 (100%)	0	100	100
1	r	36/48 (75%)	36 (100%)	0	100	100
1	s	36/48 (75%)	36 (100%)	0	100	100
1	t	36/48 (75%)	36 (100%)	0	100	100
1	u	32/48 (67%)	31 (97%)	1 (3%)	40	64
2	A	35/39 (90%)	34 (97%)	1 (3%)	42	66
2	B	35/39 (90%)	35 (100%)	0	100	100
2	D	35/39 (90%)	35 (100%)	0	100	100
2	E	35/39 (90%)	33 (94%)	2 (6%)	20	39
2	F	33/39 (85%)	33 (100%)	0	100	100
2	G	33/39 (85%)	32 (97%)	1 (3%)	41	65
2	I	33/39 (85%)	33 (100%)	0	100	100
2	J	34/39 (87%)	33 (97%)	1 (3%)	42	66
2	K	34/39 (87%)	33 (97%)	1 (3%)	42	66
2	N	33/39 (85%)	32 (97%)	1 (3%)	41	65
2	O	33/39 (85%)	33 (100%)	0	100	100
2	R	30/39 (77%)	30 (100%)	0	100	100
2	S	29/39 (74%)	28 (97%)	1 (3%)	37	60
2	T	29/39 (74%)	29 (100%)	0	100	100
2	U	19/39 (49%)	19 (100%)	0	100	100
3	X	49/63 (78%)	48 (98%)	1 (2%)	55	76
4	L	225/226 (100%)	222 (99%)	3 (1%)	69	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	M	236/239 (99%)	232 (98%)	4 (2%)	60 79
6	H	213/219 (97%)	209 (98%)	4 (2%)	57 77
All	All	1847/2052 (90%)	1822 (99%)	25 (1%)	68 84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	53	TYR
1	b	54	VAL
2	A	14	ASP
2	E	13	THR
2	E	43	MET
3	X	56	GLU
4	L	216	PHE
4	L	247	CYS
4	L	272	TRP
5	M	35	PHE
5	M	214	PHE
5	M	237	VAL
5	M	274	VAL
6	H	74	VAL
6	H	139	LYS
6	H	148	ARG
6	H	233	ASP
1	d	1	MET
2	S	49	PHE
1	u	30	LEU
2	K	43	MET
2	N	43	MET
1	k	26	LEU
2	J	43	MET
2	G	43	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	r	42	ASN
2	R	16	GLN
2	J	16	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 75 ligands modelled in this entry, 1 is monoatomic - leaving 74 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SPO	E	202	-	34,34,41	3.49	20 (58%)	39,40,50	11.27	30 (76%)
8	SPO	d	102	-	40,41,41	3.44	21 (52%)	47,50,50	11.31	31 (65%)
11	3PE	M	409	-	50,50,50	1.33	5 (10%)	53,55,55	1.10	2 (3%)
8	SPO	S	202	-	34,34,41	3.42	20 (58%)	39,40,50	11.42	32 (82%)
7	BCL	g	101	-	64,74,74	1.27	5 (7%)	78,115,115	1.54	11 (14%)
7	BCL	U	102	-	44,54,74	1.46	4 (9%)	54,91,115	1.71	10 (18%)
11	3PE	L	306	-	40,40,50	1.46	5 (12%)	43,45,55	1.20	2 (4%)
8	SPO	f	102	-	40,41,41	3.44	21 (52%)	47,50,50	11.34	32 (68%)
7	BCL	e	101	-	64,74,74	1.28	6 (9%)	78,115,115	1.70	16 (20%)
7	BCL	b	102	-	64,74,74	1.27	4 (6%)	78,115,115	1.45	10 (12%)
7	BCL	s	101	-	44,54,74	1.50	5 (11%)	54,91,115	1.67	8 (14%)
8	SPO	j	102	-	40,41,41	3.44	21 (52%)	47,50,50	10.99	32 (68%)
10	U10	M	403	-	48,48,63	2.72	19 (39%)	58,61,79	11.29	29 (50%)
8	SPO	E	201	-	40,41,41	3.41	21 (52%)	47,50,50	11.11	32 (68%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	3PE	d	104	-	34,34,50	1.42	5 (14%)	37,39,55	1.11	2 (5%)
7	BCL	r	101	-	49,59,74	1.42	6 (12%)	60,97,115	1.70	10 (16%)
7	BCL	n	102	-	64,74,74	1.26	4 (6%)	78,115,115	1.47	12 (15%)
8	SPO	S	201	-	40,41,41	3.46	21 (52%)	47,50,50	11.67	32 (68%)
11	3PE	H	302	-	44,44,50	1.34	5 (11%)	47,49,55	1.15	2 (4%)
11	3PE	M	406	-	50,50,50	1.33	5 (10%)	53,55,55	1.08	2 (3%)
7	BCL	e	102	-	64,74,74	1.26	4 (6%)	78,115,115	1.45	9 (11%)
10	U10	L	304	-	23,23,63	3.16	8 (34%)	28,31,79	6.41	9 (32%)
9	BPH	L	302	-	51,70,70	0.83	1 (1%)	52,101,101	1.02	6 (11%)
8	SPO	E	203	-	34,34,41	3.57	20 (58%)	39,40,50	11.69	31 (79%)
8	SPO	N	201	-	40,41,41	3.46	21 (52%)	47,50,50	11.09	31 (65%)
7	BCL	b	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.61	12 (15%)
7	BCL	o	101	-	64,74,74	1.27	5 (7%)	78,115,115	1.53	11 (14%)
7	BCL	s	102	-	44,54,74	1.47	5 (11%)	54,91,115	1.76	10 (18%)
8	SPO	k	102	-	40,41,41	3.44	21 (52%)	47,50,50	10.82	33 (70%)
7	BCL	k	101	-	64,74,74	1.26	6 (9%)	78,115,115	1.54	10 (12%)
7	BCL	f	101	-	64,74,74	1.26	6 (9%)	78,115,115	1.50	10 (12%)
8	SPO	M	404	-	40,41,41	3.46	21 (52%)	47,50,50	11.10	31 (65%)
7	BCL	L	301	-	64,74,74	1.25	4 (6%)	78,115,115	1.47	11 (14%)
8	SPO	G	201	-	40,41,41	3.43	22 (55%)	47,50,50	11.08	31 (65%)
7	BCL	n	101	-	64,74,74	1.25	5 (7%)	78,115,115	1.53	11 (14%)
8	SPO	I	102	-	34,34,41	3.52	20 (58%)	39,40,50	11.82	31 (79%)
8	SPO	i	102	-	40,41,41	3.42	21 (52%)	47,50,50	11.38	32 (68%)
8	SPO	D	102	-	34,34,41	3.52	20 (58%)	39,40,50	11.32	31 (79%)
7	BCL	I	101	-	64,74,74	1.27	4 (6%)	78,115,115	1.47	10 (12%)
8	SPO	O	102	-	34,34,41	3.48	20 (58%)	39,40,50	11.86	30 (76%)
7	BCL	D	101	-	64,74,74	1.26	4 (6%)	78,115,115	1.45	11 (14%)
7	BCL	O	101	-	64,74,74	1.26	4 (6%)	78,115,115	1.49	10 (12%)
8	SPO	B	101	-	34,34,41	3.52	20 (58%)	39,40,50	11.08	30 (76%)
7	BCL	d	101	-	64,74,74	1.25	4 (6%)	78,115,115	1.57	11 (14%)
7	BCL	t	101	-	44,54,74	1.47	5 (11%)	54,91,115	1.66	8 (14%)
8	SPO	b	103	-	40,41,41	3.41	21 (52%)	47,50,50	10.88	32 (68%)
11	3PE	d	103	-	36,36,50	1.43	5 (13%)	39,41,55	1.17	2 (5%)
8	SPO	R	101	-	34,34,41	3.47	20 (58%)	39,40,50	11.72	30 (76%)
11	3PE	H	301	-	42,42,50	1.43	5 (11%)	45,47,55	1.12	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SPO	r	102	-	40,41,41	3.40	21 (52%)	47,50,50	11.01	32 (68%)
7	BCL	U	101	-	44,54,74	1.47	4 (9%)	54,91,115	1.62	9 (16%)
7	BCL	M	405	-	64,74,74	1.23	4 (6%)	78,115,115	1.51	11 (14%)
7	BCL	a	100	-	49,59,74	1.43	5 (10%)	60,97,115	1.64	9 (15%)
7	BCL	i	101	-	64,74,74	1.27	5 (7%)	78,115,115	1.52	10 (12%)
7	BCL	A	202	-	64,74,74	1.25	5 (7%)	78,115,115	1.48	11 (14%)
8	SPO	A	201	-	40,41,41	3.46	21 (52%)	47,50,50	11.62	31 (65%)
7	BCL	J	102	-	64,74,74	1.28	5 (7%)	78,115,115	1.47	11 (14%)
8	SPO	J	101	-	34,34,41	3.44	20 (58%)	39,40,50	11.34	31 (79%)
7	BCL	K	102	-	64,74,74	1.25	4 (6%)	78,115,115	1.47	10 (12%)
8	SPO	o	102	-	40,41,41	3.45	21 (52%)	47,50,50	11.70	32 (68%)
8	SPO	K	101	-	34,34,41	3.59	20 (58%)	39,40,50	11.06	30 (76%)
7	BCL	g	102	-	64,74,74	1.27	4 (6%)	78,115,115	1.45	10 (12%)
8	SPO	t	102	-	40,41,41	3.40	21 (52%)	47,50,50	11.19	32 (68%)
9	BPH	M	408	-	51,70,70	0.88	2 (3%)	52,101,101	1.09	6 (11%)
7	BCL	T	101	-	44,54,74	1.48	5 (11%)	54,91,115	1.73	10 (18%)
10	U10	L	305	-	18,18,63	3.32	8 (44%)	22,25,79	5.92	6 (27%)
7	BCL	j	101	-	64,74,74	1.26	6 (9%)	78,115,115	1.50	10 (12%)
7	BCL	M	407	-	64,74,74	1.27	6 (9%)	78,115,115	1.76	15 (19%)
7	BCL	F	102	-	64,74,74	1.27	4 (6%)	78,115,115	1.46	10 (12%)
8	SPO	F	101	-	34,34,41	3.48	20 (58%)	39,40,50	12.25	31 (79%)
7	BCL	r	103	-	44,54,74	1.50	5 (11%)	54,91,115	1.63	8 (14%)
10	U10	L	303	-	33,33,63	2.84	12 (36%)	40,43,79	9.69	17 (42%)
8	SPO	K	103	-	34,34,41	3.49	20 (58%)	39,40,50	11.85	30 (76%)
7	BCL	M	401	-	64,74,74	1.24	5 (7%)	78,115,115	1.49	11 (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
8	SPO	E	202	-	-	10/37/37/47	-
8	SPO	d	102	-	-	14/47/47/47	-
11	3PE	M	409	-	-	40/54/54/54	-
8	SPO	S	202	-	-	13/37/37/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	g	101	-	-	4/37/137/137	-
7	BCL	U	102	-	-	3/13/113/137	-
11	3PE	L	306	-	-	25/44/44/54	-
8	SPO	f	102	-	-	13/47/47/47	-
7	BCL	e	101	-	-	0/37/137/137	-
7	BCL	b	102	-	-	8/37/137/137	-
7	BCL	s	101	-	-	4/13/113/137	-
8	SPO	j	102	-	-	18/47/47/47	-
10	U10	M	403	-	-	7/45/69/87	0/1/1/1
8	SPO	E	201	-	-	13/47/47/47	-
11	3PE	d	104	-	-	21/38/38/54	-
7	BCL	r	101	-	-	0/19/119/137	-
7	BCL	n	102	-	-	9/37/137/137	-
8	SPO	S	201	-	-	15/47/47/47	-
11	3PE	H	302	-	-	25/48/48/54	-
11	3PE	M	406	-	-	29/54/54/54	-
7	BCL	e	102	-	-	8/37/137/137	-
10	U10	L	304	-	-	0/15/39/87	0/1/1/1
9	BPH	L	302	-	-	6/37/105/105	0/5/6/6
8	SPO	E	203	-	-	11/37/37/47	-
8	SPO	N	201	-	-	10/47/47/47	-
7	BCL	b	101	-	-	5/37/137/137	-
7	BCL	o	101	-	-	4/37/137/137	-
7	BCL	s	102	-	-	0/13/113/137	-
8	SPO	k	102	-	-	13/47/47/47	-
7	BCL	k	101	-	-	4/37/137/137	-
7	BCL	f	101	-	-	4/37/137/137	-
8	SPO	M	404	-	-	16/47/47/47	-
7	BCL	L	301	-	-	2/37/137/137	-
8	SPO	G	201	-	-	15/47/47/47	-
7	BCL	n	101	-	-	5/37/137/137	-
8	SPO	I	102	-	-	11/37/37/47	-
8	SPO	i	102	-	-	16/47/47/47	-
8	SPO	D	102	-	-	12/37/37/47	-
7	BCL	I	101	-	-	5/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SPO	O	102	-	-	11/37/37/47	-
7	BCL	D	101	-	-	6/37/137/137	-
7	BCL	O	101	-	-	5/37/137/137	-
8	SPO	B	101	-	-	14/37/37/47	-
7	BCL	d	101	-	-	2/37/137/137	-
7	BCL	t	101	-	-	1/13/113/137	-
8	SPO	b	103	-	-	14/47/47/47	-
11	3PE	d	103	-	-	20/40/40/54	-
8	SPO	R	101	-	-	11/37/37/47	-
11	3PE	H	301	-	-	19/46/46/54	-
8	SPO	r	102	-	-	16/47/47/47	-
7	BCL	U	101	-	-	4/13/113/137	-
7	BCL	M	405	-	-	1/37/137/137	-
7	BCL	a	100	-	-	2/19/119/137	-
7	BCL	i	101	-	-	4/37/137/137	-
7	BCL	A	202	-	-	11/37/137/137	-
8	SPO	A	201	-	-	18/47/47/47	-
7	BCL	J	102	-	-	10/37/137/137	-
8	SPO	J	101	-	-	11/37/37/47	-
7	BCL	K	102	-	-	5/37/137/137	-
8	SPO	o	102	-	-	12/47/47/47	-
8	SPO	K	101	-	-	10/37/37/47	-
7	BCL	g	102	-	-	9/37/137/137	-
8	SPO	t	102	-	-	15/47/47/47	-
9	BPH	M	408	-	-	6/37/105/105	0/5/6/6
7	BCL	T	101	-	-	3/13/113/137	-
10	U10	L	305	-	-	1/9/33/87	0/1/1/1
7	BCL	j	101	-	-	5/37/137/137	-
7	BCL	M	407	-	-	9/37/137/137	-
7	BCL	F	102	-	-	4/37/137/137	-
8	SPO	F	101	-	-	12/37/37/47	-
7	BCL	r	103	-	-	4/13/113/137	-
10	U10	L	303	-	-	4/27/51/87	0/1/1/1
8	SPO	K	103	-	-	13/37/37/47	-
7	BCL	M	401	-	-	2/37/137/137	-

All (803) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403	U10	C6-C1	10.26	1.54	1.35
10	L	304	U10	C6-C1	10.25	1.53	1.35
10	L	303	U10	C6-C1	10.21	1.53	1.35
10	L	305	U10	C6-C1	10.12	1.53	1.35
8	M	404	SPO	C25-C23	8.41	1.64	1.45
8	K	101	SPO	C25-C23	8.19	1.63	1.45
8	E	203	SPO	C25-C23	7.99	1.63	1.45
8	I	102	SPO	C25-C23	7.85	1.62	1.45
8	B	101	SPO	C25-C23	7.84	1.62	1.45
8	D	102	SPO	C25-C23	7.82	1.62	1.45
8	k	102	SPO	C25-C23	7.81	1.62	1.45
8	k	102	SPO	C16-C17	7.78	1.62	1.45
8	E	202	SPO	C25-C23	7.78	1.62	1.45
8	j	102	SPO	C25-C23	7.77	1.62	1.45
8	N	201	SPO	C25-C23	7.77	1.62	1.45
8	d	102	SPO	C16-C17	7.76	1.62	1.45
8	A	201	SPO	C25-C23	7.74	1.62	1.45
8	R	101	SPO	C25-C23	7.70	1.62	1.45
8	r	102	SPO	C25-C23	7.70	1.62	1.45
8	K	103	SPO	C25-C23	7.69	1.62	1.45
8	o	102	SPO	C25-C23	7.69	1.62	1.45
8	K	101	SPO	C16-C17	7.68	1.62	1.45
8	F	101	SPO	C25-C23	7.68	1.62	1.45
8	G	201	SPO	C25-C23	7.67	1.62	1.45
8	f	102	SPO	C16-C17	7.66	1.62	1.45
8	O	102	SPO	C25-C23	7.66	1.62	1.45
8	d	102	SPO	C25-C23	7.66	1.62	1.45
8	t	102	SPO	C25-C23	7.66	1.62	1.45
8	b	103	SPO	C25-C23	7.65	1.62	1.45
8	f	102	SPO	C25-C23	7.64	1.62	1.45
8	i	102	SPO	C25-C23	7.64	1.62	1.45
8	S	201	SPO	C25-C23	7.63	1.62	1.45
8	D	102	SPO	C16-C17	7.63	1.62	1.45
8	E	201	SPO	C25-C23	7.63	1.62	1.45
8	A	201	SPO	C16-C17	7.62	1.62	1.45
8	B	101	SPO	C16-C17	7.62	1.62	1.45
8	S	201	SPO	C16-C17	7.61	1.62	1.45
8	E	202	SPO	C16-C17	7.60	1.62	1.45
8	J	101	SPO	C25-C23	7.59	1.62	1.45
8	R	101	SPO	C16-C17	7.59	1.62	1.45
8	N	201	SPO	C16-C17	7.59	1.62	1.45
8	o	102	SPO	C16-C17	7.58	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	102	SPO	C16-C17	7.58	1.62	1.45
8	O	102	SPO	C16-C17	7.58	1.62	1.45
8	b	103	SPO	C16-C17	7.57	1.62	1.45
8	E	203	SPO	C16-C17	7.57	1.62	1.45
8	r	102	SPO	C16-C17	7.55	1.62	1.45
8	K	103	SPO	C16-C17	7.54	1.62	1.45
8	M	404	SPO	C16-C17	7.54	1.62	1.45
8	G	201	SPO	C16-C17	7.53	1.62	1.45
8	t	102	SPO	C16-C17	7.53	1.62	1.45
8	E	201	SPO	C16-C17	7.52	1.62	1.45
8	j	102	SPO	C16-C17	7.51	1.62	1.45
8	I	102	SPO	C16-C17	7.51	1.62	1.45
8	F	101	SPO	C16-C17	7.48	1.62	1.45
8	J	101	SPO	C16-C17	7.42	1.61	1.45
8	S	202	SPO	C16-C17	7.40	1.61	1.45
8	S	202	SPO	C25-C23	7.39	1.61	1.45
8	d	102	SPO	C11-C12	6.04	1.58	1.45
8	k	102	SPO	C11-C12	6.02	1.58	1.45
8	N	201	SPO	C35-C33	5.98	1.63	1.51
8	S	201	SPO	C11-C12	5.93	1.58	1.45
8	G	201	SPO	C35-C33	5.93	1.63	1.51
8	o	102	SPO	C11-C12	5.92	1.58	1.45
8	N	201	SPO	C11-C12	5.91	1.58	1.45
8	f	102	SPO	C11-C12	5.91	1.58	1.45
8	j	102	SPO	C11-C12	5.88	1.58	1.45
8	i	102	SPO	C11-C12	5.86	1.58	1.45
8	b	103	SPO	C11-C12	5.86	1.58	1.45
8	E	201	SPO	C11-C12	5.84	1.58	1.45
8	B	101	SPO	C35-C33	5.84	1.63	1.51
8	A	201	SPO	C11-C12	5.83	1.58	1.45
8	G	201	SPO	C11-C12	5.83	1.58	1.45
8	K	101	SPO	C11-C12	5.81	1.58	1.45
8	j	102	SPO	C35-C33	5.79	1.63	1.51
8	E	201	SPO	C35-C33	5.79	1.63	1.51
8	b	103	SPO	C35-C33	5.79	1.63	1.51
8	M	404	SPO	C11-C12	5.76	1.58	1.45
8	r	102	SPO	C35-C33	5.74	1.63	1.51
8	E	203	SPO	C11-C12	5.70	1.58	1.45
8	t	102	SPO	C35-C33	5.67	1.63	1.51
8	t	102	SPO	C11-C12	5.67	1.58	1.45
8	r	102	SPO	C11-C12	5.66	1.58	1.45
8	r	102	SPO	C6-C7	5.65	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	201	SPO	C35-C33	5.65	1.63	1.51
8	O	102	SPO	C11-C12	5.65	1.58	1.45
8	D	102	SPO	C35-C33	5.64	1.63	1.51
8	D	102	SPO	C11-C12	5.63	1.58	1.45
8	S	201	SPO	C35-C33	5.62	1.63	1.51
8	E	202	SPO	C35-C33	5.62	1.63	1.51
8	E	203	SPO	C35-C33	5.62	1.63	1.51
8	k	102	SPO	C20-C19	5.61	1.60	1.43
8	R	101	SPO	C35-C33	5.61	1.62	1.51
8	B	101	SPO	C11-C12	5.60	1.58	1.45
8	o	102	SPO	C35-C33	5.59	1.62	1.51
8	S	201	SPO	C6-C7	5.58	1.57	1.45
8	A	201	SPO	C6-C7	5.57	1.57	1.45
8	K	101	SPO	C35-C33	5.57	1.62	1.51
8	I	102	SPO	C35-C33	5.56	1.62	1.51
8	J	101	SPO	C35-C33	5.56	1.62	1.51
8	d	102	SPO	C20-C19	5.56	1.60	1.43
8	j	102	SPO	C6-C7	5.56	1.57	1.45
8	E	202	SPO	C11-C12	5.56	1.57	1.45
8	t	102	SPO	C6-C7	5.55	1.57	1.45
8	N	201	SPO	C6-C7	5.55	1.57	1.45
8	i	102	SPO	C6-C7	5.55	1.57	1.45
8	f	102	SPO	C35-C33	5.55	1.62	1.51
8	K	103	SPO	C35-C33	5.54	1.62	1.51
8	K	103	SPO	C11-C12	5.54	1.57	1.45
8	o	102	SPO	C6-C7	5.54	1.57	1.45
8	O	102	SPO	C35-C33	5.53	1.62	1.51
8	K	101	SPO	C20-C19	5.53	1.60	1.43
8	k	102	SPO	C6-C7	5.52	1.57	1.45
8	E	203	SPO	C20-C19	5.52	1.60	1.43
8	E	201	SPO	C6-C7	5.52	1.57	1.45
8	N	201	SPO	C20-C19	5.51	1.60	1.43
8	F	101	SPO	C35-C33	5.51	1.62	1.51
8	b	103	SPO	C6-C7	5.51	1.57	1.45
8	o	102	SPO	C20-C19	5.50	1.60	1.43
8	b	103	SPO	C20-C19	5.50	1.60	1.43
8	F	101	SPO	C11-C12	5.49	1.57	1.45
8	S	201	SPO	C20-C19	5.49	1.60	1.43
8	R	101	SPO	C11-C12	5.49	1.57	1.45
8	i	102	SPO	C35-C33	5.49	1.62	1.51
8	f	102	SPO	C6-C7	5.49	1.57	1.45
8	G	201	SPO	C6-C7	5.49	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	102	SPO	C20-C19	5.49	1.60	1.43
8	M	404	SPO	C6-C7	5.48	1.57	1.45
8	J	101	SPO	C11-C12	5.48	1.57	1.45
8	A	201	SPO	C20-C19	5.48	1.60	1.43
8	k	102	SPO	C35-C33	5.48	1.62	1.51
8	I	102	SPO	C11-C12	5.47	1.57	1.45
8	d	102	SPO	C6-C7	5.47	1.57	1.45
8	i	102	SPO	C20-C19	5.46	1.60	1.43
8	j	102	SPO	C20-C19	5.45	1.60	1.43
8	E	201	SPO	C20-C19	5.45	1.60	1.43
8	S	202	SPO	C35-C33	5.44	1.62	1.51
8	t	102	SPO	C20-C19	5.44	1.60	1.43
8	G	201	SPO	C20-C19	5.43	1.60	1.43
8	I	102	SPO	C20-C19	5.42	1.60	1.43
8	M	404	SPO	C35-C33	5.42	1.62	1.51
8	F	101	SPO	C20-C19	5.41	1.60	1.43
8	d	102	SPO	C35-C33	5.41	1.62	1.51
8	D	102	SPO	C20-C19	5.41	1.60	1.43
8	r	102	SPO	C20-C19	5.40	1.60	1.43
8	M	404	SPO	C20-C19	5.39	1.60	1.43
8	E	202	SPO	C20-C19	5.37	1.60	1.43
8	S	202	SPO	C11-C12	5.37	1.57	1.45
8	R	101	SPO	C20-C19	5.36	1.60	1.43
8	B	101	SPO	C20-C19	5.36	1.60	1.43
8	K	103	SPO	C20-C19	5.35	1.60	1.43
8	O	102	SPO	C20-C19	5.35	1.60	1.43
8	B	101	SPO	C30-C28	5.34	1.62	1.51
8	N	201	SPO	C30-C28	5.32	1.62	1.51
8	S	202	SPO	C20-C19	5.31	1.59	1.43
8	J	101	SPO	C20-C19	5.29	1.59	1.43
8	G	201	SPO	C30-C28	5.25	1.62	1.51
8	K	101	SPO	C30-C28	5.22	1.62	1.51
8	D	102	SPO	C30-C28	5.20	1.62	1.51
8	j	102	SPO	C30-C28	5.20	1.62	1.51
8	E	203	SPO	C30-C28	5.17	1.62	1.51
7	r	103	BCL	C1B-NB	5.16	1.39	1.35
8	o	102	SPO	C30-C28	5.13	1.62	1.51
8	S	201	SPO	C30-C28	5.13	1.61	1.51
8	M	404	SPO	C30-C28	5.10	1.61	1.51
8	E	202	SPO	C30-C28	5.10	1.61	1.51
8	E	201	SPO	C30-C28	5.09	1.61	1.51
8	r	102	SPO	C30-C28	5.08	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	102	SPO	C30-C28	5.07	1.61	1.51
8	t	102	SPO	C30-C28	5.07	1.61	1.51
7	J	102	BCL	C1B-NB	5.07	1.39	1.35
7	s	101	BCL	C1B-NB	5.07	1.39	1.35
8	S	201	SPO	C26-C27	5.06	1.59	1.43
8	K	103	SPO	C30-C28	5.06	1.61	1.51
8	A	201	SPO	C15-C14	5.05	1.59	1.43
7	D	101	BCL	C1B-NB	5.03	1.39	1.35
7	F	102	BCL	C1B-NB	5.03	1.39	1.35
8	A	201	SPO	C30-C28	5.02	1.61	1.51
8	o	102	SPO	C26-C27	5.02	1.59	1.43
7	T	101	BCL	C1B-NB	5.02	1.39	1.35
8	S	202	SPO	C30-C28	5.02	1.61	1.51
8	K	101	SPO	C26-C27	5.02	1.59	1.43
8	d	102	SPO	C15-C14	5.01	1.59	1.43
7	I	101	BCL	C1B-NB	4.99	1.39	1.35
8	f	102	SPO	C30-C28	4.99	1.61	1.51
7	b	101	BCL	MG-NA	4.99	2.18	2.06
7	n	102	BCL	C1B-NB	4.98	1.39	1.35
7	A	202	BCL	C1B-NB	4.98	1.39	1.35
8	J	101	SPO	C30-C28	4.98	1.61	1.51
7	s	102	BCL	MG-NA	4.98	2.18	2.06
8	A	201	SPO	C26-C27	4.97	1.58	1.43
8	f	102	SPO	C15-C14	4.97	1.58	1.43
8	E	203	SPO	C26-C27	4.97	1.58	1.43
7	O	101	BCL	C1B-NB	4.97	1.39	1.35
8	I	102	SPO	C26-C27	4.97	1.58	1.43
7	g	102	BCL	C1B-NB	4.97	1.39	1.35
7	e	102	BCL	C1B-NB	4.97	1.39	1.35
7	b	102	BCL	C1B-NB	4.97	1.39	1.35
8	k	102	SPO	C15-C14	4.96	1.58	1.43
7	U	102	BCL	C1B-NB	4.96	1.39	1.35
8	G	201	SPO	C26-C27	4.96	1.58	1.43
8	N	201	SPO	C26-C27	4.96	1.58	1.43
7	U	101	BCL	C1B-NB	4.95	1.39	1.35
7	d	101	BCL	MG-NA	4.95	2.18	2.06
7	e	101	BCL	MG-NA	4.95	2.18	2.06
7	g	101	BCL	MG-NA	4.95	2.18	2.06
8	i	102	SPO	C15-C14	4.95	1.58	1.43
7	K	102	BCL	C1B-NB	4.94	1.39	1.35
8	D	102	SPO	C26-C27	4.94	1.58	1.43
7	j	101	BCL	MG-NA	4.94	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	103	SPO	C15-C14	4.94	1.58	1.43
7	M	407	BCL	MG-NA	4.94	2.18	2.06
8	k	102	SPO	C30-C28	4.93	1.61	1.51
7	o	101	BCL	MG-NA	4.93	2.18	2.06
8	O	102	SPO	C30-C28	4.93	1.61	1.51
7	k	101	BCL	MG-NA	4.93	2.18	2.06
8	f	102	SPO	C26-C27	4.93	1.58	1.43
8	j	102	SPO	C26-C27	4.93	1.58	1.43
8	i	102	SPO	C26-C27	4.92	1.58	1.43
8	t	102	SPO	C26-C27	4.92	1.58	1.43
8	R	101	SPO	C30-C28	4.92	1.61	1.51
7	f	101	BCL	MG-NA	4.92	2.17	2.06
10	L	303	U10	C16-C14	4.91	1.61	1.51
8	i	102	SPO	C30-C28	4.91	1.61	1.51
8	E	202	SPO	C26-C27	4.91	1.58	1.43
8	R	101	SPO	C26-C27	4.91	1.58	1.43
8	o	102	SPO	C15-C14	4.90	1.58	1.43
8	S	201	SPO	C15-C14	4.90	1.58	1.43
8	M	404	SPO	C15-C14	4.90	1.58	1.43
8	B	101	SPO	C26-C27	4.90	1.58	1.43
8	k	102	SPO	C26-C27	4.90	1.58	1.43
8	E	201	SPO	C15-C14	4.90	1.58	1.43
8	G	201	SPO	C15-C14	4.90	1.58	1.43
8	b	103	SPO	C26-C27	4.89	1.58	1.43
8	r	102	SPO	C26-C27	4.89	1.58	1.43
8	K	103	SPO	C26-C27	4.89	1.58	1.43
8	E	201	SPO	C26-C27	4.89	1.58	1.43
10	M	403	U10	C16-C14	4.89	1.61	1.51
8	d	102	SPO	C26-C27	4.89	1.58	1.43
7	M	405	BCL	C1B-NB	4.88	1.39	1.35
8	N	201	SPO	C15-C14	4.88	1.58	1.43
7	a	100	BCL	C1B-NB	4.88	1.39	1.35
8	F	101	SPO	C26-C27	4.88	1.58	1.43
8	E	203	SPO	C15-C14	4.88	1.58	1.43
7	i	101	BCL	MG-NA	4.88	2.17	2.06
7	r	101	BCL	MG-NA	4.88	2.17	2.06
8	F	101	SPO	C30-C28	4.87	1.61	1.51
8	j	102	SPO	C15-C14	4.87	1.58	1.43
8	F	101	SPO	C15-C14	4.87	1.58	1.43
8	K	101	SPO	C15-C14	4.87	1.58	1.43
8	M	404	SPO	C26-C27	4.86	1.58	1.43
7	t	101	BCL	MG-NA	4.86	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	301	BCL	C1B-NB	4.86	1.39	1.35
8	O	102	SPO	C26-C27	4.86	1.58	1.43
7	n	101	BCL	MG-NA	4.86	2.17	2.06
8	J	101	SPO	C26-C27	4.85	1.58	1.43
7	F	102	BCL	MG-NA	4.85	2.17	2.06
7	s	101	BCL	MG-NA	4.84	2.17	2.06
8	d	102	SPO	C30-C28	4.83	1.61	1.51
8	S	202	SPO	C26-C27	4.82	1.58	1.43
8	b	103	SPO	C30-C28	4.82	1.61	1.51
7	g	102	BCL	MG-NA	4.82	2.17	2.06
7	b	102	BCL	MG-NA	4.82	2.17	2.06
7	M	401	BCL	C1B-NB	4.81	1.39	1.35
7	t	101	BCL	C1B-NB	4.81	1.39	1.35
7	O	101	BCL	MG-NA	4.81	2.17	2.06
8	D	102	SPO	C15-C14	4.81	1.58	1.43
8	t	102	SPO	C15-C14	4.81	1.58	1.43
7	J	102	BCL	MG-NA	4.80	2.17	2.06
8	K	103	SPO	C15-C14	4.79	1.58	1.43
7	M	407	BCL	C1B-NB	4.79	1.39	1.35
7	r	103	BCL	MG-NA	4.79	2.17	2.06
7	r	101	BCL	C1B-NB	4.78	1.39	1.35
7	a	100	BCL	MG-NA	4.78	2.17	2.06
7	o	101	BCL	C1B-NB	4.78	1.39	1.35
7	e	101	BCL	C1B-NB	4.78	1.39	1.35
7	I	101	BCL	MG-NA	4.78	2.17	2.06
8	R	101	SPO	C15-C14	4.77	1.58	1.43
7	e	102	BCL	MG-NA	4.77	2.17	2.06
7	n	102	BCL	MG-NA	4.77	2.17	2.06
7	T	101	BCL	MG-NA	4.77	2.17	2.06
8	O	102	SPO	C15-C14	4.77	1.58	1.43
8	J	101	SPO	C15-C14	4.77	1.58	1.43
7	i	101	BCL	C1B-NB	4.77	1.39	1.35
7	g	101	BCL	C1B-NB	4.77	1.39	1.35
7	K	102	BCL	MG-NA	4.76	2.17	2.06
8	r	102	SPO	C15-C14	4.76	1.58	1.43
8	S	202	SPO	C15-C14	4.76	1.58	1.43
7	U	101	BCL	MG-NA	4.76	2.17	2.06
8	A	201	SPO	C10-C9	4.75	1.58	1.43
8	E	202	SPO	C15-C14	4.75	1.58	1.43
8	I	102	SPO	C15-C14	4.75	1.58	1.43
7	n	101	BCL	C1B-NB	4.74	1.39	1.35
7	j	101	BCL	C1B-NB	4.73	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	102	SPO	C10-C9	4.73	1.58	1.43
8	B	101	SPO	C15-C14	4.73	1.58	1.43
7	A	202	BCL	MG-NA	4.70	2.17	2.06
7	k	101	BCL	C1B-NB	4.70	1.39	1.35
8	S	201	SPO	C10-C9	4.69	1.58	1.43
7	b	101	BCL	C1B-NB	4.69	1.39	1.35
7	s	102	BCL	C1B-NB	4.68	1.39	1.35
7	d	101	BCL	C1B-NB	4.68	1.39	1.35
8	d	102	SPO	C10-C9	4.68	1.58	1.43
7	f	101	BCL	C1B-NB	4.67	1.39	1.35
7	U	102	BCL	MG-NA	4.67	2.17	2.06
7	D	101	BCL	MG-NA	4.67	2.17	2.06
7	L	301	BCL	MG-NA	4.66	2.17	2.06
8	k	102	SPO	C21-C22	4.65	1.57	1.43
8	i	102	SPO	C10-C9	4.65	1.57	1.43
8	o	102	SPO	C10-C9	4.65	1.57	1.43
8	E	201	SPO	C10-C9	4.65	1.57	1.43
8	M	404	SPO	C10-C9	4.64	1.57	1.43
8	K	101	SPO	C21-C22	4.64	1.57	1.43
8	d	102	SPO	C21-C22	4.63	1.57	1.43
8	k	102	SPO	C10-C9	4.63	1.57	1.43
7	M	401	BCL	MG-NA	4.62	2.17	2.06
8	N	201	SPO	C21-C22	4.61	1.57	1.43
8	A	201	SPO	C21-C22	4.61	1.57	1.43
10	L	305	U10	C4-C3	4.60	1.55	1.36
8	S	201	SPO	C21-C22	4.60	1.57	1.43
8	b	103	SPO	C10-C9	4.60	1.57	1.43
8	G	201	SPO	C10-C9	4.60	1.57	1.43
8	t	102	SPO	C10-C9	4.60	1.57	1.43
8	i	102	SPO	C21-C22	4.60	1.57	1.43
8	K	101	SPO	C10-C9	4.59	1.57	1.43
8	N	201	SPO	C10-C9	4.59	1.57	1.43
8	E	203	SPO	C21-C22	4.59	1.57	1.43
7	M	405	BCL	MG-NA	4.58	2.17	2.06
8	o	102	SPO	C21-C22	4.57	1.57	1.43
8	b	103	SPO	C21-C22	4.57	1.57	1.43
8	f	102	SPO	C21-C22	4.56	1.57	1.43
8	t	102	SPO	C21-C22	4.56	1.57	1.43
8	j	102	SPO	C21-C22	4.56	1.57	1.43
8	r	102	SPO	C10-C9	4.54	1.57	1.43
8	E	201	SPO	C21-C22	4.53	1.57	1.43
8	I	102	SPO	C21-C22	4.53	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	j	102	SPO	C10-C9	4.52	1.57	1.43
8	I	102	SPO	C10-C9	4.52	1.57	1.43
8	G	201	SPO	C21-C22	4.52	1.57	1.43
8	D	102	SPO	C21-C22	4.51	1.57	1.43
8	r	102	SPO	C21-C22	4.50	1.57	1.43
8	E	202	SPO	C21-C22	4.49	1.57	1.43
8	F	101	SPO	C21-C22	4.48	1.57	1.43
8	F	101	SPO	C10-C9	4.47	1.57	1.43
8	R	101	SPO	C21-C22	4.46	1.57	1.43
10	M	403	U10	C31-C29	4.46	1.60	1.51
8	B	101	SPO	C21-C22	4.45	1.57	1.43
8	O	102	SPO	C21-C22	4.44	1.57	1.43
8	K	103	SPO	C21-C22	4.44	1.57	1.43
8	S	202	SPO	C21-C22	4.42	1.57	1.43
8	E	203	SPO	C10-C9	4.42	1.57	1.43
10	M	403	U10	C4-C3	4.40	1.54	1.36
8	J	101	SPO	C21-C22	4.39	1.57	1.43
8	S	202	SPO	C10-C9	4.39	1.57	1.43
8	K	103	SPO	C10-C9	4.35	1.56	1.43
8	J	101	SPO	C10-C9	4.34	1.56	1.43
8	R	101	SPO	C10-C9	4.34	1.56	1.43
8	O	102	SPO	C10-C9	4.33	1.56	1.43
8	D	102	SPO	C10-C9	4.33	1.56	1.43
10	L	304	U10	C4-C3	4.30	1.53	1.36
8	E	202	SPO	C10-C9	4.29	1.56	1.43
8	B	101	SPO	C10-C9	4.29	1.56	1.43
10	L	303	U10	C4-C3	4.28	1.53	1.36
8	M	404	SPO	C21-C22	4.28	1.56	1.43
8	A	201	SPO	C27-C28	4.21	1.38	1.34
8	M	404	SPO	C27-C28	4.17	1.38	1.34
8	o	102	SPO	C27-C28	4.16	1.38	1.34
8	K	101	SPO	C27-C28	4.16	1.38	1.34
10	L	304	U10	C16-C14	4.10	1.61	1.50
8	E	203	SPO	C27-C28	4.10	1.38	1.34
8	f	102	SPO	C27-C28	4.07	1.38	1.34
8	S	201	SPO	C27-C28	4.07	1.38	1.34
8	D	102	SPO	C27-C28	4.06	1.38	1.34
8	k	102	SPO	C27-C28	4.06	1.38	1.34
8	j	102	SPO	C27-C28	4.05	1.38	1.34
8	i	102	SPO	C27-C28	4.04	1.38	1.34
8	I	102	SPO	C27-C28	4.03	1.38	1.34
8	d	102	SPO	C27-C28	4.01	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	201	SPO	C27-C28	4.00	1.38	1.34
8	b	103	SPO	C27-C28	4.00	1.38	1.34
8	r	102	SPO	C27-C28	3.96	1.38	1.34
8	K	103	SPO	C27-C28	3.96	1.38	1.34
10	L	304	U10	C7-C8	3.94	1.56	1.50
8	G	201	SPO	C27-C28	3.93	1.38	1.34
8	E	202	SPO	C27-C28	3.90	1.38	1.34
8	E	201	SPO	C27-C28	3.90	1.38	1.34
8	t	102	SPO	C27-C28	3.85	1.38	1.34
8	B	101	SPO	C27-C28	3.85	1.38	1.34
8	O	102	SPO	C27-C28	3.83	1.38	1.34
10	M	403	U10	C11-C9	3.79	1.59	1.51
8	A	201	SPO	C4-C5	3.78	1.56	1.50
8	R	101	SPO	C27-C28	3.78	1.38	1.34
10	M	403	U10	C26-C24	3.78	1.59	1.51
8	N	201	SPO	C4-C5	3.77	1.56	1.50
8	J	101	SPO	C27-C28	3.77	1.38	1.34
8	r	102	SPO	C4-C5	3.76	1.56	1.50
8	S	201	SPO	C4-C5	3.76	1.56	1.50
8	S	202	SPO	C27-C28	3.75	1.38	1.34
8	i	102	SPO	C4-C5	3.75	1.56	1.50
8	k	102	SPO	C4-C5	3.73	1.56	1.50
8	M	404	SPO	C4-C5	3.73	1.56	1.50
8	d	102	SPO	C4-C5	3.72	1.56	1.50
8	o	102	SPO	C4-C5	3.71	1.56	1.50
10	L	304	U10	C11-C9	3.69	1.59	1.51
8	F	101	SPO	C27-C28	3.69	1.38	1.34
8	b	103	SPO	C4-C5	3.68	1.56	1.50
8	f	102	SPO	C4-C5	3.68	1.56	1.50
8	j	102	SPO	C4-C5	3.65	1.55	1.50
8	t	102	SPO	C4-C5	3.64	1.55	1.50
9	M	408	BPH	CBD-CGD	-3.60	1.47	1.52
8	G	201	SPO	C4-C5	3.59	1.55	1.50
8	E	201	SPO	C4-C5	3.57	1.55	1.50
9	L	302	BPH	CBD-CGD	-3.55	1.47	1.52
7	b	101	BCL	MG-NC	3.48	2.14	2.06
7	F	102	BCL	MG-NC	3.46	2.14	2.06
7	r	103	BCL	MG-NC	3.45	2.14	2.06
7	s	102	BCL	MG-NC	3.43	2.14	2.06
11	H	301	3PE	O31-C31	3.43	1.43	1.33
11	M	406	3PE	O31-C31	3.43	1.43	1.33
7	e	101	BCL	MG-NC	3.43	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	102	BCL	MG-NC	3.43	2.14	2.06
10	M	403	U10	C36-C34	3.42	1.58	1.51
7	g	102	BCL	MG-NC	3.42	2.14	2.06
7	b	102	BCL	MG-NC	3.41	2.14	2.06
10	L	305	U10	C7-C8	3.41	1.55	1.50
11	d	104	3PE	O31-C31	3.41	1.43	1.33
11	M	409	3PE	O31-C31	3.41	1.43	1.33
7	g	101	BCL	MG-NC	3.41	2.14	2.06
7	e	102	BCL	MG-NC	3.40	2.14	2.06
7	a	100	BCL	MG-NC	3.40	2.14	2.06
7	T	101	BCL	MG-NC	3.40	2.14	2.06
11	d	103	3PE	O31-C31	3.39	1.43	1.33
11	H	302	3PE	O31-C31	3.38	1.43	1.33
7	s	101	BCL	MG-NC	3.38	2.14	2.06
7	I	101	BCL	MG-NC	3.38	2.14	2.06
10	L	303	U10	C7-C8	3.38	1.55	1.50
7	n	102	BCL	MG-NC	3.37	2.14	2.06
7	U	101	BCL	MG-NC	3.37	2.14	2.06
7	O	101	BCL	MG-NC	3.37	2.14	2.06
7	A	202	BCL	MG-NC	3.35	2.14	2.06
10	M	403	U10	C7-C8	3.35	1.55	1.50
7	o	101	BCL	MG-NC	3.34	2.14	2.06
7	d	101	BCL	MG-NC	3.33	2.14	2.06
7	n	101	BCL	MG-NC	3.33	2.14	2.06
10	L	303	U10	C11-C9	3.32	1.58	1.51
7	K	102	BCL	MG-NC	3.31	2.14	2.06
11	L	306	3PE	O31-C31	3.31	1.43	1.33
7	D	101	BCL	MG-NC	3.28	2.14	2.06
7	j	101	BCL	MG-NC	3.27	2.14	2.06
7	i	101	BCL	MG-NC	3.25	2.14	2.06
10	M	403	U10	C21-C19	3.25	1.58	1.51
7	U	102	BCL	MG-NC	3.23	2.13	2.06
7	k	101	BCL	MG-NC	3.23	2.13	2.06
7	f	101	BCL	MG-NC	3.22	2.13	2.06
7	L	301	BCL	MG-NC	3.22	2.13	2.06
7	r	101	BCL	MG-NC	3.20	2.13	2.06
8	I	102	SPO	C32-C33	3.20	1.40	1.33
7	M	407	BCL	MG-NC	3.20	2.13	2.06
8	S	201	SPO	C32-C33	3.19	1.40	1.33
8	E	203	SPO	C32-C33	3.19	1.40	1.33
7	M	405	BCL	MG-NC	3.18	2.13	2.06
8	o	102	SPO	C32-C33	3.17	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	102	SPO	C32-C33	3.17	1.40	1.33
7	t	101	BCL	MG-NC	3.15	2.13	2.06
8	A	201	SPO	C14-C12	3.15	1.40	1.35
7	M	401	BCL	MG-NC	3.14	2.13	2.06
8	K	103	SPO	C32-C33	3.14	1.40	1.33
8	i	102	SPO	C32-C33	3.13	1.40	1.33
8	F	101	SPO	C32-C33	3.13	1.40	1.33
8	O	102	SPO	C32-C33	3.11	1.40	1.33
11	M	406	3PE	O21-C21	3.11	1.43	1.34
8	M	404	SPO	C32-C33	3.09	1.40	1.33
8	d	102	SPO	C32-C33	3.09	1.40	1.33
8	S	201	SPO	C31-C32	3.08	1.60	1.50
8	E	203	SPO	C31-C32	3.07	1.60	1.50
8	o	102	SPO	C31-C32	3.07	1.60	1.50
10	L	303	U10	C21-C19	3.06	1.57	1.51
10	L	305	U10	C7-C6	3.06	1.56	1.51
8	I	102	SPO	C31-C32	3.05	1.60	1.50
8	f	102	SPO	C31-C32	3.05	1.60	1.50
8	K	103	SPO	C31-C32	3.04	1.60	1.50
10	M	403	U10	C41-C39	3.02	1.58	1.50
8	O	102	SPO	C31-C32	3.01	1.60	1.50
8	i	102	SPO	C31-C32	3.01	1.60	1.50
8	M	404	SPO	C31-C32	3.00	1.60	1.50
8	d	102	SPO	C31-C32	3.00	1.60	1.50
8	F	101	SPO	C31-C32	3.00	1.60	1.50
10	L	304	U10	C7-C6	2.99	1.56	1.51
11	H	302	3PE	O21-C21	2.99	1.42	1.34
10	M	403	U10	C7-C6	2.98	1.56	1.51
8	f	102	SPO	C14-C12	2.97	1.39	1.35
11	d	103	3PE	O21-C21	2.97	1.42	1.34
10	L	303	U10	C26-C24	2.97	1.58	1.50
8	M	404	SPO	C14-C12	2.95	1.39	1.35
8	k	102	SPO	C14-C12	2.95	1.39	1.35
11	M	409	3PE	O21-C21	2.94	1.42	1.34
11	L	306	3PE	O21-C21	2.94	1.42	1.34
8	d	102	SPO	C14-C12	2.93	1.39	1.35
8	N	201	SPO	C31-C32	2.93	1.60	1.50
11	d	104	3PE	O21-C21	2.92	1.42	1.34
8	b	103	SPO	C14-C12	2.92	1.39	1.35
10	L	305	U10	C11-C9	2.90	1.58	1.50
8	A	201	SPO	C13-C12	2.89	1.56	1.50
10	L	303	U10	C7-C6	2.89	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	101	SPO	C18-C17	2.89	1.56	1.50
8	D	102	SPO	C31-C32	2.88	1.59	1.50
8	A	201	SPO	C31-C32	2.88	1.59	1.50
8	S	202	SPO	C13-C12	2.88	1.56	1.50
8	G	201	SPO	C31-C32	2.87	1.59	1.50
11	H	301	3PE	O21-C21	2.87	1.42	1.34
8	b	103	SPO	C31-C32	2.87	1.59	1.50
8	t	102	SPO	C13-C12	2.86	1.56	1.50
8	K	101	SPO	C31-C32	2.86	1.59	1.50
8	G	201	SPO	C14-C12	2.85	1.39	1.35
8	r	102	SPO	C31-C32	2.85	1.59	1.50
8	j	102	SPO	C14-C12	2.85	1.39	1.35
8	B	101	SPO	C13-C12	2.85	1.56	1.50
8	j	102	SPO	C31-C32	2.85	1.59	1.50
8	S	201	SPO	C13-C12	2.85	1.56	1.50
8	S	202	SPO	C31-C32	2.84	1.59	1.50
8	k	102	SPO	C31-C32	2.84	1.59	1.50
8	t	102	SPO	C31-C32	2.84	1.59	1.50
8	i	102	SPO	C14-C12	2.84	1.39	1.35
8	R	101	SPO	C18-C17	2.83	1.56	1.50
8	M	404	SPO	C13-C12	2.83	1.56	1.50
8	f	102	SPO	C13-C12	2.82	1.56	1.50
8	o	102	SPO	C13-C12	2.82	1.56	1.50
8	E	201	SPO	C31-C32	2.82	1.59	1.50
8	b	103	SPO	C13-C12	2.82	1.56	1.50
8	S	201	SPO	C14-C12	2.82	1.39	1.35
8	E	201	SPO	C14-C12	2.82	1.39	1.35
11	H	301	3PE	O21-C2	-2.82	1.39	1.46
8	E	203	SPO	C13-C12	2.81	1.56	1.50
8	k	102	SPO	C13-C12	2.80	1.56	1.50
8	j	102	SPO	C13-C12	2.80	1.56	1.50
8	K	103	SPO	C18-C17	2.80	1.56	1.50
8	o	102	SPO	C14-C12	2.79	1.39	1.35
8	J	101	SPO	C13-C12	2.79	1.56	1.50
8	E	201	SPO	C13-C12	2.79	1.56	1.50
8	d	102	SPO	C13-C12	2.79	1.56	1.50
11	d	104	3PE	O21-C2	-2.79	1.39	1.46
8	E	202	SPO	C31-C32	2.79	1.59	1.50
8	D	102	SPO	C18-C17	2.79	1.56	1.50
8	i	102	SPO	C13-C12	2.79	1.56	1.50
8	R	101	SPO	C31-C32	2.78	1.59	1.50
8	R	101	SPO	C13-C12	2.78	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	102	SPO	C13-C12	2.78	1.56	1.50
8	O	102	SPO	C18-C17	2.78	1.56	1.50
8	N	201	SPO	C14-C12	2.78	1.39	1.35
8	E	202	SPO	C18-C17	2.77	1.56	1.50
8	D	102	SPO	C13-C12	2.77	1.56	1.50
8	N	201	SPO	C13-C12	2.77	1.56	1.50
11	d	103	3PE	O21-C2	-2.77	1.39	1.46
8	E	202	SPO	C13-C12	2.77	1.56	1.50
8	N	201	SPO	C32-C33	2.77	1.39	1.33
8	K	101	SPO	C6-C7	2.76	1.57	1.50
8	K	103	SPO	C13-C12	2.76	1.56	1.50
8	G	201	SPO	C13-C12	2.76	1.56	1.50
8	J	101	SPO	C31-C32	2.76	1.59	1.50
8	K	101	SPO	C13-C12	2.76	1.56	1.50
8	r	102	SPO	C18-C17	2.75	1.56	1.50
11	M	409	3PE	O21-C2	-2.75	1.39	1.46
8	F	101	SPO	C13-C12	2.75	1.56	1.50
8	A	201	SPO	C8-C7	2.75	1.56	1.50
8	B	101	SPO	C31-C32	2.75	1.59	1.50
8	O	102	SPO	C6-C7	2.74	1.57	1.50
8	S	202	SPO	C18-C17	2.74	1.56	1.50
8	M	404	SPO	C8-C7	2.73	1.56	1.50
8	S	201	SPO	C18-C17	2.73	1.56	1.50
8	J	101	SPO	C18-C17	2.73	1.56	1.50
8	G	201	SPO	C32-C33	2.73	1.39	1.33
8	E	203	SPO	C6-C7	2.73	1.57	1.50
8	D	102	SPO	C32-C33	2.72	1.39	1.33
11	L	306	3PE	O21-C2	-2.72	1.39	1.46
8	K	101	SPO	C14-C12	2.72	1.39	1.35
8	D	102	SPO	C6-C7	2.71	1.57	1.50
8	I	102	SPO	C6-C7	2.71	1.57	1.50
8	t	102	SPO	C32-C33	2.71	1.39	1.33
8	R	101	SPO	C6-C7	2.70	1.57	1.50
8	E	202	SPO	C6-C7	2.70	1.57	1.50
8	K	101	SPO	C18-C17	2.70	1.56	1.50
8	F	101	SPO	C6-C7	2.70	1.57	1.50
8	r	102	SPO	C13-C12	2.70	1.56	1.50
8	K	103	SPO	C6-C7	2.70	1.57	1.50
8	B	101	SPO	C6-C7	2.70	1.57	1.50
8	f	102	SPO	C18-C17	2.69	1.56	1.50
8	S	202	SPO	C6-C7	2.69	1.57	1.50
8	t	102	SPO	C18-C17	2.69	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	101	SPO	C32-C33	2.69	1.39	1.33
8	J	101	SPO	C6-C7	2.69	1.57	1.50
11	H	302	3PE	O21-C2	-2.68	1.39	1.46
8	E	203	SPO	C14-C12	2.68	1.39	1.35
8	b	103	SPO	C18-C17	2.68	1.56	1.50
8	E	201	SPO	C18-C17	2.68	1.56	1.50
8	i	102	SPO	C8-C7	2.68	1.56	1.50
8	f	102	SPO	C8-C7	2.68	1.56	1.50
8	M	404	SPO	C18-C17	2.68	1.56	1.50
8	d	102	SPO	C8-C7	2.67	1.56	1.50
8	I	102	SPO	C18-C17	2.67	1.56	1.50
8	G	201	SPO	C18-C17	2.66	1.56	1.50
8	t	102	SPO	C8-C7	2.66	1.56	1.50
8	j	102	SPO	C18-C17	2.66	1.56	1.50
8	b	103	SPO	C32-C33	2.66	1.39	1.33
8	A	201	SPO	C18-C17	2.65	1.56	1.50
8	i	102	SPO	C18-C17	2.65	1.56	1.50
8	o	102	SPO	C18-C17	2.65	1.56	1.50
8	d	102	SPO	C18-C17	2.65	1.56	1.50
8	r	102	SPO	C32-C33	2.65	1.39	1.33
8	t	102	SPO	C14-C12	2.64	1.39	1.35
8	j	102	SPO	C32-C33	2.64	1.39	1.33
8	F	101	SPO	C18-C17	2.64	1.56	1.50
8	I	102	SPO	C13-C12	2.63	1.56	1.50
8	k	102	SPO	C18-C17	2.63	1.56	1.50
8	E	201	SPO	C32-C33	2.63	1.39	1.33
7	t	101	BCL	CHD-C1D	2.63	1.43	1.38
8	E	202	SPO	C32-C33	2.63	1.39	1.33
8	B	101	SPO	C32-C33	2.63	1.39	1.33
8	G	201	SPO	C8-C7	2.62	1.56	1.50
8	b	103	SPO	C8-C7	2.62	1.56	1.50
8	k	102	SPO	C32-C33	2.61	1.39	1.33
8	S	201	SPO	C8-C7	2.60	1.56	1.50
10	L	304	U10	C6-C5	2.60	1.53	1.46
8	J	101	SPO	C32-C33	2.60	1.39	1.33
8	E	201	SPO	C8-C7	2.60	1.56	1.50
8	R	101	SPO	C32-C33	2.59	1.39	1.33
8	o	102	SPO	C8-C7	2.58	1.56	1.50
8	N	201	SPO	C8-C7	2.57	1.56	1.50
8	E	203	SPO	C18-C17	2.57	1.56	1.50
8	j	102	SPO	C8-C7	2.57	1.56	1.50
8	N	201	SPO	C30-C31	2.56	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	103	SPO	C14-C12	2.56	1.39	1.35
8	N	201	SPO	C18-C17	2.56	1.56	1.50
8	r	102	SPO	C8-C7	2.56	1.56	1.50
7	U	102	BCL	CHD-C1D	2.56	1.43	1.38
8	D	102	SPO	C14-C12	2.54	1.39	1.35
8	k	102	SPO	C8-C7	2.54	1.56	1.50
8	F	101	SPO	C14-C12	2.54	1.39	1.35
8	G	201	SPO	C30-C31	2.52	1.62	1.53
10	L	305	U10	C6-C5	2.52	1.53	1.46
8	S	202	SPO	C32-C33	2.51	1.39	1.33
8	j	102	SPO	C30-C31	2.50	1.62	1.53
7	j	101	BCL	CHD-C1D	2.50	1.43	1.38
7	a	100	BCL	CHD-C1D	2.50	1.43	1.38
7	o	101	BCL	CHD-C1D	2.49	1.43	1.38
8	E	201	SPO	C30-C31	2.49	1.62	1.53
10	M	403	U10	C6-C5	2.49	1.53	1.46
8	J	101	SPO	C14-C12	2.48	1.39	1.35
8	B	101	SPO	C14-C12	2.47	1.39	1.35
7	f	101	BCL	CHD-C1D	2.47	1.43	1.38
8	r	102	SPO	C30-C31	2.47	1.61	1.53
8	t	102	SPO	C30-C31	2.47	1.61	1.53
7	r	101	BCL	CHD-C1D	2.46	1.43	1.38
8	S	202	SPO	C14-C12	2.46	1.39	1.35
10	L	303	U10	C6-C5	2.45	1.53	1.46
7	L	301	BCL	CHD-C1D	2.45	1.43	1.38
8	S	201	SPO	C30-C31	2.45	1.61	1.53
8	O	102	SPO	C14-C12	2.44	1.39	1.35
7	i	101	BCL	CHD-C1D	2.44	1.43	1.38
8	E	202	SPO	C14-C12	2.43	1.39	1.35
7	M	401	BCL	CHD-C1D	2.43	1.43	1.38
8	B	101	SPO	C30-C31	2.42	1.61	1.53
8	E	202	SPO	C30-C31	2.42	1.61	1.53
8	o	102	SPO	C30-C31	2.42	1.61	1.53
8	D	102	SPO	C30-C31	2.41	1.61	1.53
11	M	406	3PE	O21-C2	-2.41	1.40	1.46
7	M	407	BCL	CHD-C1D	2.40	1.43	1.38
8	r	102	SPO	C14-C12	2.40	1.39	1.35
8	A	201	SPO	C30-C31	2.40	1.61	1.53
8	K	101	SPO	C30-C31	2.39	1.61	1.53
11	M	406	3PE	C32-C31	2.39	1.57	1.50
7	b	102	BCL	CHD-C1D	2.39	1.43	1.38
8	R	101	SPO	C30-C31	2.39	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	102	BCL	CHD-C1D	2.38	1.43	1.38
8	E	203	SPO	C24-C23	2.38	1.55	1.50
8	R	101	SPO	C14-C12	2.37	1.38	1.35
8	E	203	SPO	C30-C31	2.36	1.61	1.53
7	I	101	BCL	CHD-C1D	2.36	1.43	1.38
7	k	101	BCL	CHD-C1D	2.36	1.43	1.38
8	I	102	SPO	C30-C31	2.35	1.61	1.53
7	b	101	BCL	CHD-C1D	2.35	1.43	1.38
7	T	101	BCL	CHD-C1D	2.35	1.43	1.38
8	J	101	SPO	C30-C31	2.35	1.61	1.53
11	d	103	3PE	C32-C31	2.35	1.57	1.50
8	F	101	SPO	C30-C31	2.34	1.61	1.53
8	I	102	SPO	C14-C12	2.34	1.38	1.35
8	K	101	SPO	C24-C23	2.34	1.55	1.50
8	M	404	SPO	C30-C31	2.34	1.61	1.53
7	D	101	BCL	CHD-C1D	2.34	1.42	1.38
11	L	306	3PE	C32-C31	2.34	1.57	1.50
8	K	103	SPO	C30-C31	2.32	1.61	1.53
8	A	201	SPO	C32-C33	2.32	1.38	1.33
7	A	202	BCL	CHD-C1D	2.32	1.42	1.38
7	M	405	BCL	CHD-C1D	2.32	1.42	1.38
7	d	101	BCL	CHD-C1D	2.32	1.42	1.38
8	M	404	SPO	C24-C23	2.32	1.55	1.50
11	d	104	3PE	C22-C21	2.31	1.57	1.50
8	I	102	SPO	C8-C7	2.31	1.56	1.50
10	L	305	U10	O4-C4	2.31	1.42	1.36
8	f	102	SPO	C30-C31	2.30	1.61	1.53
8	S	202	SPO	C30-C31	2.30	1.61	1.53
7	F	102	BCL	CHD-C1D	2.29	1.42	1.38
11	L	306	3PE	C22-C21	2.29	1.57	1.50
8	O	102	SPO	C30-C31	2.29	1.61	1.53
11	M	409	3PE	C22-C21	2.29	1.57	1.50
8	A	201	SPO	C24-C23	2.29	1.55	1.50
11	M	406	3PE	C22-C21	2.29	1.57	1.50
7	K	102	BCL	CHD-C1D	2.28	1.42	1.38
7	e	102	BCL	CHD-C1D	2.28	1.42	1.38
8	t	102	SPO	C24-C23	2.28	1.55	1.50
8	F	101	SPO	C24-C23	2.28	1.55	1.50
11	M	409	3PE	C32-C31	2.28	1.57	1.50
7	J	102	BCL	CHD-C1D	2.28	1.42	1.38
11	H	302	3PE	C32-C31	2.28	1.57	1.50
7	n	102	BCL	CHD-C1D	2.27	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	302	3PE	C22-C21	2.27	1.57	1.50
7	U	101	BCL	CHD-C1D	2.27	1.42	1.38
11	d	104	3PE	C32-C31	2.27	1.57	1.50
7	O	101	BCL	CHD-C1D	2.27	1.42	1.38
7	s	102	BCL	CHD-C1D	2.27	1.42	1.38
7	g	101	BCL	CHD-C1D	2.26	1.42	1.38
7	e	101	BCL	CHD-C1D	2.25	1.42	1.38
8	N	201	SPO	C24-C23	2.25	1.55	1.50
8	k	102	SPO	C30-C31	2.25	1.61	1.53
11	H	301	3PE	C32-C31	2.25	1.57	1.50
8	r	102	SPO	C24-C23	2.25	1.55	1.50
8	k	102	SPO	C24-C23	2.25	1.55	1.50
8	I	102	SPO	C24-C23	2.25	1.55	1.50
8	i	102	SPO	C30-C31	2.25	1.61	1.53
11	d	103	3PE	C22-C21	2.25	1.57	1.50
8	K	101	SPO	C8-C7	2.24	1.56	1.50
11	H	301	3PE	C22-C21	2.24	1.57	1.50
7	r	103	BCL	CHD-C1D	2.24	1.42	1.38
8	E	201	SPO	C24-C23	2.23	1.55	1.50
8	B	101	SPO	C24-C23	2.23	1.55	1.50
8	b	103	SPO	C30-C31	2.22	1.61	1.53
7	s	101	BCL	CHD-C1D	2.22	1.42	1.38
8	j	102	SPO	C24-C23	2.22	1.55	1.50
8	d	102	SPO	C30-C31	2.22	1.61	1.53
8	d	102	SPO	C24-C23	2.21	1.55	1.50
8	i	102	SPO	C24-C23	2.21	1.55	1.50
8	b	103	SPO	C24-C23	2.21	1.55	1.50
8	G	201	SPO	C24-C23	2.21	1.55	1.50
8	J	101	SPO	C8-C7	2.21	1.56	1.50
8	o	102	SPO	C24-C23	2.20	1.55	1.50
8	S	202	SPO	C8-C7	2.20	1.56	1.50
8	S	202	SPO	C24-C23	2.20	1.55	1.50
8	S	201	SPO	C24-C23	2.19	1.55	1.50
10	L	305	U10	O3-C3	2.19	1.42	1.36
7	n	101	BCL	CHD-C1D	2.19	1.42	1.38
8	K	103	SPO	C8-C7	2.19	1.56	1.50
7	i	101	BCL	C4B-NB	2.19	1.37	1.35
8	D	102	SPO	C8-C7	2.18	1.56	1.50
8	K	103	SPO	C24-C23	2.18	1.55	1.50
8	E	202	SPO	C8-C7	2.18	1.56	1.50
8	D	102	SPO	C24-C23	2.17	1.55	1.50
8	f	102	SPO	C24-C23	2.17	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	203	SPO	C8-C7	2.17	1.56	1.50
7	M	407	BCL	C1D-ND	2.17	1.40	1.37
8	F	101	SPO	C8-C7	2.16	1.56	1.50
10	M	403	U10	O3-C3	2.16	1.42	1.36
8	R	101	SPO	C8-C7	2.16	1.56	1.50
8	O	102	SPO	C8-C7	2.16	1.56	1.50
7	s	101	BCL	C4B-NB	2.16	1.37	1.35
8	B	101	SPO	C8-C7	2.15	1.56	1.50
8	O	102	SPO	C24-C23	2.14	1.55	1.50
8	R	101	SPO	C24-C23	2.13	1.55	1.50
8	J	101	SPO	C24-C23	2.12	1.55	1.50
10	M	403	U10	C40-C39	2.12	1.56	1.50
7	a	100	BCL	C1D-ND	2.11	1.40	1.37
7	f	101	BCL	C1D-ND	2.11	1.40	1.37
10	M	403	U10	C27-C28	2.10	1.57	1.50
7	M	407	BCL	C4B-NB	2.10	1.37	1.35
7	j	101	BCL	C4B-NB	2.08	1.37	1.35
7	r	101	BCL	C1D-ND	2.08	1.40	1.37
7	k	101	BCL	C1D-ND	2.08	1.40	1.37
8	E	202	SPO	C24-C23	2.08	1.55	1.50
7	j	101	BCL	C1D-ND	2.07	1.40	1.37
7	r	101	BCL	C4B-NB	2.07	1.37	1.35
10	M	403	U10	C12-C13	2.07	1.57	1.50
10	L	303	U10	O3-C3	2.07	1.41	1.36
8	G	201	SPO	C36-C37	2.06	1.57	1.50
7	T	101	BCL	C1D-ND	2.06	1.40	1.37
10	L	303	U10	C20-C19	2.05	1.55	1.50
7	o	101	BCL	C1D-ND	2.05	1.40	1.37
10	M	403	U10	C35-C34	2.04	1.55	1.50
10	M	403	U10	O5-C5	-2.04	1.18	1.23
7	e	101	BCL	C4B-NB	2.04	1.37	1.35
7	e	101	BCL	C1D-ND	2.04	1.40	1.37
7	f	101	BCL	C4B-NB	2.03	1.37	1.35
9	M	408	BPH	OBD-CAD	2.03	1.25	1.22
7	k	101	BCL	C4B-NB	2.03	1.37	1.35
7	r	103	BCL	C4B-NB	2.02	1.37	1.35
7	J	102	BCL	C3D-C4D	-2.02	1.39	1.44
7	M	401	BCL	C1D-ND	2.02	1.40	1.37
10	L	303	U10	O5-C5	-2.01	1.19	1.23
7	A	202	BCL	C3D-C4D	-2.01	1.39	1.44
7	s	102	BCL	C1D-ND	2.01	1.40	1.37
7	g	101	BCL	C1D-ND	2.01	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403	U10	O4-C4	2.01	1.41	1.36
7	n	101	BCL	C1D-ND	2.01	1.40	1.37
10	L	304	U10	O3-C3	2.00	1.41	1.36
7	b	101	BCL	C4B-NB	2.00	1.37	1.35
7	t	101	BCL	C1D-ND	2.00	1.40	1.37

All (1286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	201	SPO	C24-C23-C22	32.20	168.02	122.92
8	t	102	SPO	C24-C23-C22	32.19	168.01	122.92
8	i	102	SPO	C24-C23-C22	32.04	167.80	122.92
8	S	202	SPO	C24-C23-C22	31.90	167.62	122.92
8	o	102	SPO	C24-C23-C22	31.85	167.54	122.92
8	G	201	SPO	C24-C23-C22	31.81	167.48	122.92
8	d	102	SPO	C24-C23-C22	31.78	167.44	122.92
8	E	201	SPO	C24-C23-C22	31.74	167.39	122.92
8	b	103	SPO	C24-C23-C22	31.66	167.27	122.92
8	f	102	SPO	C24-C23-C22	31.58	167.16	122.92
8	j	102	SPO	C24-C23-C22	31.53	167.09	122.92
8	F	101	SPO	C24-C23-C22	31.44	166.97	122.92
8	N	201	SPO	C24-C23-C22	31.41	166.92	122.92
8	k	102	SPO	C24-C23-C22	31.40	166.91	122.92
8	M	404	SPO	C34-C33-C35	-31.32	62.59	115.27
8	A	201	SPO	C24-C23-C22	31.21	166.65	122.92
8	r	102	SPO	C24-C23-C22	31.17	166.59	122.92
8	d	102	SPO	C34-C33-C35	-30.95	63.20	115.27
8	i	102	SPO	C34-C33-C35	-30.89	63.31	115.27
8	O	102	SPO	C24-C23-C22	30.88	166.17	122.92
8	J	101	SPO	C24-C23-C22	30.81	166.09	122.92
8	K	103	SPO	C24-C23-C22	30.78	166.04	122.92
8	I	102	SPO	C34-C33-C35	-30.73	63.58	115.27
8	K	103	SPO	C34-C33-C35	-30.72	63.59	115.27
8	O	102	SPO	C34-C33-C35	-30.72	63.59	115.27
8	R	101	SPO	C24-C23-C22	30.70	165.92	122.92
8	F	101	SPO	C34-C33-C35	-30.69	63.64	115.27
8	I	102	SPO	C24-C23-C22	30.68	165.90	122.92
8	f	102	SPO	C34-C33-C35	-30.56	63.86	115.27
8	D	102	SPO	C24-C23-C22	30.44	165.57	122.92
8	E	203	SPO	C34-C33-C35	-30.36	64.20	115.27
8	o	102	SPO	C34-C33-C35	-30.32	64.26	115.27
8	S	201	SPO	C34-C33-C35	-30.28	64.33	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	101	SPO	C24-C23-C22	30.21	165.25	122.92
8	E	202	SPO	C24-C23-C22	30.17	165.18	122.92
8	E	203	SPO	C24-C23-C22	30.17	165.18	122.92
8	K	101	SPO	C24-C23-C22	29.60	164.38	122.92
8	M	404	SPO	C24-C23-C22	28.95	163.47	122.92
8	A	201	SPO	C29-C28-C30	-28.45	67.41	115.27
8	A	201	SPO	C34-C33-C35	-28.14	67.94	115.27
10	M	403	U10	C35-C34-C36	-28.07	68.05	115.27
8	F	101	SPO	C29-C28-C30	-27.81	68.49	115.27
10	L	303	U10	C20-C19-C21	-27.77	68.56	115.27
10	M	403	U10	C20-C19-C21	-27.63	68.79	115.27
10	M	403	U10	C25-C24-C26	-27.61	68.82	115.27
8	S	201	SPO	C29-C28-C30	-27.57	68.89	115.27
8	o	102	SPO	C29-C28-C30	-27.53	68.97	115.27
8	R	101	SPO	C29-C28-C30	-27.37	69.24	115.27
8	t	102	SPO	C29-C28-C30	-27.23	69.47	115.27
8	r	102	SPO	C29-C28-C30	-27.15	69.60	115.27
8	G	201	SPO	C29-C28-C30	-27.01	69.83	115.27
8	E	201	SPO	C29-C28-C30	-27.00	69.85	115.27
8	N	201	SPO	C29-C28-C30	-27.00	69.86	115.27
8	j	102	SPO	C29-C28-C30	-26.89	70.03	115.27
10	M	403	U10	C10-C9-C11	-26.77	70.23	115.27
8	D	102	SPO	C35-C33-C32	23.85	169.39	121.12
8	K	101	SPO	C35-C33-C32	23.67	169.01	121.12
8	k	102	SPO	C35-C33-C32	23.64	168.96	121.12
8	S	202	SPO	C35-C33-C32	23.30	168.27	121.12
10	L	303	U10	C16-C14-C13	23.28	168.22	121.12
10	M	403	U10	C31-C29-C28	23.21	168.08	121.12
8	J	101	SPO	C35-C33-C32	23.08	167.82	121.12
8	R	101	SPO	C35-C33-C32	23.08	167.81	121.12
8	E	202	SPO	C35-C33-C32	23.07	167.80	121.12
10	M	403	U10	C16-C14-C13	23.02	167.70	121.12
8	t	102	SPO	C35-C33-C32	23.00	167.66	121.12
8	b	103	SPO	C35-C33-C32	22.95	167.57	121.12
8	r	102	SPO	C35-C33-C32	22.88	167.42	121.12
8	B	101	SPO	C35-C33-C32	22.78	167.21	121.12
8	E	201	SPO	C35-C33-C32	22.71	167.08	121.12
8	j	102	SPO	C35-C33-C32	22.69	167.02	121.12
8	G	201	SPO	C35-C33-C32	22.66	166.97	121.12
8	N	201	SPO	C35-C33-C32	22.58	166.82	121.12
8	d	102	SPO	C24-C23-C25	-22.13	83.21	118.08
8	S	201	SPO	C24-C23-C25	-22.04	83.36	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	o	102	SPO	C24-C23-C25	-21.84	83.66	118.08
8	S	202	SPO	C24-C23-C25	-21.79	83.74	118.08
8	i	102	SPO	C24-C23-C25	-21.71	83.87	118.08
8	f	102	SPO	C24-C23-C25	-21.64	83.98	118.08
8	b	103	SPO	C24-C23-C25	-21.60	84.04	118.08
8	I	102	SPO	C24-C23-C25	-21.54	84.14	118.08
8	k	102	SPO	C24-C23-C25	-21.50	84.20	118.08
8	A	201	SPO	C24-C23-C25	-21.47	84.26	118.08
8	E	202	SPO	C24-C23-C25	-21.40	84.36	118.08
8	N	201	SPO	C24-C23-C25	-21.39	84.37	118.08
8	G	201	SPO	C24-C23-C25	-21.30	84.52	118.08
8	r	102	SPO	C24-C23-C25	-21.27	84.56	118.08
8	E	201	SPO	C24-C23-C25	-21.22	84.64	118.08
8	O	102	SPO	C24-C23-C25	-21.21	84.66	118.08
10	L	305	U10	C11-C9-C10	-21.20	67.78	114.60
10	L	303	U10	C26-C24-C25	-21.19	67.81	114.60
8	J	101	SPO	C24-C23-C25	-21.08	84.87	118.08
8	D	102	SPO	C24-C23-C25	-21.05	84.91	118.08
8	K	103	SPO	C24-C23-C25	-20.99	85.01	118.08
8	j	102	SPO	C24-C23-C25	-20.89	85.16	118.08
8	R	101	SPO	C24-C23-C25	-20.85	85.23	118.08
8	t	102	SPO	C24-C23-C25	-20.83	85.26	118.08
8	F	101	SPO	C24-C23-C25	-20.74	85.40	118.08
8	K	101	SPO	C24-C23-C25	-20.32	86.06	118.08
8	B	101	SPO	C24-C23-C25	-20.18	86.29	118.08
8	E	203	SPO	C24-C23-C25	-20.13	86.36	118.08
8	M	404	SPO	C20-C21-C22	-19.29	83.96	123.47
8	D	102	SPO	C34-C33-C35	-18.96	83.38	115.27
8	k	102	SPO	C34-C33-C35	-18.84	83.58	115.27
8	M	404	SPO	C24-C23-C25	-18.82	88.42	118.08
8	K	101	SPO	C34-C33-C35	-18.79	83.66	115.27
8	d	102	SPO	C5-C6-C7	18.70	154.15	125.89
8	M	404	SPO	C5-C6-C7	18.66	154.08	125.89
8	i	102	SPO	C5-C6-C7	18.62	154.02	125.89
8	k	102	SPO	C5-C6-C7	18.50	153.85	125.89
10	L	303	U10	C15-C14-C16	-18.45	84.23	115.27
10	M	403	U10	C30-C29-C31	-18.45	84.24	115.27
8	S	201	SPO	C35-C33-C32	18.39	158.33	121.12
8	S	202	SPO	C34-C33-C35	-18.37	84.37	115.27
8	E	203	SPO	C35-C33-C32	18.37	158.29	121.12
8	o	102	SPO	C35-C33-C32	18.36	158.27	121.12
8	b	103	SPO	C29-C28-C27	18.33	169.89	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	201	SPO	C5-C6-C7	18.31	153.56	125.89
8	f	102	SPO	C35-C33-C32	18.28	158.10	121.12
8	d	102	SPO	C29-C28-C27	18.25	169.70	122.59
8	i	102	SPO	C29-C28-C27	18.22	169.61	122.59
10	M	403	U10	C15-C14-C16	-18.20	84.65	115.27
8	F	101	SPO	C35-C33-C32	18.20	157.94	121.12
8	O	102	SPO	C35-C33-C32	18.15	157.85	121.12
8	I	102	SPO	C35-C33-C32	18.15	157.85	121.12
8	k	102	SPO	C29-C28-C27	18.14	169.42	122.59
8	K	103	SPO	C35-C33-C32	18.11	157.76	121.12
8	o	102	SPO	C5-C6-C7	18.11	153.25	125.89
8	J	101	SPO	C34-C33-C35	-18.11	84.81	115.27
8	f	102	SPO	C29-C28-C27	18.07	169.23	122.59
8	t	102	SPO	C34-C33-C35	-18.07	84.88	115.27
8	f	102	SPO	C5-C6-C7	18.04	153.15	125.89
8	i	102	SPO	C35-C33-C32	18.02	157.57	121.12
8	d	102	SPO	C35-C33-C32	17.99	157.52	121.12
8	E	202	SPO	C34-C33-C35	-17.98	85.02	115.27
8	O	102	SPO	C29-C28-C27	17.95	168.93	122.59
8	b	103	SPO	C29-C28-C30	-17.94	85.09	115.27
8	R	101	SPO	C34-C33-C35	-17.94	85.10	115.27
10	L	303	U10	C10-C9-C8	17.92	169.64	123.68
8	S	201	SPO	C5-C6-C7	17.92	152.96	125.89
8	A	201	SPO	C5-C6-C7	17.86	152.89	125.89
8	J	101	SPO	C29-C28-C27	17.86	168.70	122.59
8	b	103	SPO	C5-C6-C7	17.85	152.87	125.89
8	E	202	SPO	C21-C22-C23	-17.81	101.89	127.31
8	I	102	SPO	C29-C28-C27	17.79	168.51	122.59
8	M	404	SPO	C35-C33-C32	17.76	157.06	121.12
8	K	103	SPO	C29-C28-C27	17.76	168.43	122.59
8	S	202	SPO	C29-C28-C27	17.76	168.42	122.59
8	E	203	SPO	C29-C28-C27	17.76	168.42	122.59
8	r	102	SPO	C34-C33-C35	-17.75	85.42	115.27
10	L	304	U10	C10-C9-C11	-17.69	85.51	115.27
8	E	202	SPO	C29-C28-C27	17.61	168.06	122.59
8	D	102	SPO	C29-C28-C27	17.60	168.03	122.59
10	M	403	U10	C11-C9-C8	-17.57	85.56	121.12
8	M	404	SPO	C29-C28-C27	17.56	167.92	122.59
8	K	101	SPO	C29-C28-C27	17.53	167.84	122.59
10	L	303	U10	C21-C19-C18	-17.50	85.70	121.12
8	d	102	SPO	C29-C28-C30	-17.46	85.90	115.27
8	b	103	SPO	C34-C33-C35	-17.45	85.92	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	102	SPO	C29-C28-C30	-17.43	85.96	115.27
10	M	403	U10	C26-C24-C23	-17.38	85.95	121.12
8	J	101	SPO	C21-C22-C23	-17.32	102.59	127.31
8	E	201	SPO	C34-C33-C35	-17.31	86.15	115.27
8	k	102	SPO	C29-C28-C30	-17.28	86.21	115.27
8	j	102	SPO	C34-C33-C35	-17.28	86.21	115.27
8	I	102	SPO	C29-C28-C30	-17.26	86.23	115.27
8	f	102	SPO	C29-C28-C30	-17.26	86.24	115.27
8	G	201	SPO	C34-C33-C35	-17.21	86.32	115.27
8	B	101	SPO	C29-C28-C27	17.21	167.01	122.59
8	N	201	SPO	C34-C33-C35	-17.17	86.39	115.27
10	L	303	U10	C10-C9-C11	-17.16	86.40	115.27
8	B	101	SPO	C34-C33-C35	-17.13	86.45	115.27
10	M	403	U10	C36-C34-C33	-17.09	86.53	121.12
10	M	403	U10	C21-C19-C18	-17.08	86.55	121.12
8	O	102	SPO	C29-C28-C30	-17.04	86.61	115.27
8	E	201	SPO	C5-C6-C7	16.96	151.52	125.89
8	B	101	SPO	C21-C22-C23	-16.95	103.11	127.31
8	K	103	SPO	C29-C28-C30	-16.94	86.78	115.27
10	L	304	U10	C10-C9-C8	16.88	166.97	123.68
8	K	103	SPO	C21-C22-C23	-16.80	103.33	127.31
8	D	102	SPO	C21-C22-C23	-16.80	103.33	127.31
8	D	102	SPO	C29-C28-C30	-16.78	87.05	115.27
8	E	203	SPO	C29-C28-C30	-16.76	87.08	115.27
8	R	101	SPO	C21-C22-C23	-16.76	103.40	127.31
8	J	101	SPO	C29-C28-C30	-16.75	87.10	115.27
8	O	102	SPO	C21-C22-C23	-16.72	103.45	127.31
8	E	202	SPO	C29-C28-C30	-16.72	87.15	115.27
8	t	102	SPO	C5-C6-C7	16.66	151.06	125.89
8	K	101	SPO	C29-C28-C30	-16.56	87.41	115.27
8	K	101	SPO	C21-C22-C23	-16.49	103.78	127.31
8	M	404	SPO	C29-C28-C30	-16.49	87.54	115.27
8	S	202	SPO	C29-C28-C30	-16.45	87.60	115.27
8	A	201	SPO	C13-C12-C11	-16.39	92.26	118.08
8	G	201	SPO	C5-C6-C7	16.33	150.57	125.89
8	I	102	SPO	C21-C22-C23	-16.23	104.15	127.31
8	A	201	SPO	C35-C33-C32	16.19	153.89	121.12
8	E	203	SPO	C21-C22-C23	-16.18	104.22	127.31
8	S	202	SPO	C21-C22-C23	-16.11	104.32	127.31
8	r	102	SPO	C5-C6-C7	16.01	150.09	125.89
8	I	102	SPO	C13-C12-C11	-16.00	92.87	118.08
8	r	102	SPO	C21-C22-C23	-15.94	104.57	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	403	U10	C40-C39-C38	15.83	168.40	122.65
10	L	304	U10	C16-C14-C13	15.75	168.17	122.65
8	K	101	SPO	C13-C12-C11	-15.70	93.33	118.08
8	F	101	SPO	C13-C12-C11	-15.68	93.38	118.08
8	f	102	SPO	C13-C12-C11	-15.65	93.41	118.08
8	E	203	SPO	C13-C12-C11	-15.65	93.42	118.08
8	j	102	SPO	C5-C6-C7	15.62	149.49	125.89
8	M	404	SPO	C13-C12-C11	-15.61	93.48	118.08
8	K	103	SPO	C13-C12-C11	-15.60	93.50	118.08
8	J	101	SPO	C13-C12-C11	-15.51	93.64	118.08
8	S	202	SPO	C13-C12-C11	-15.46	93.73	118.08
8	E	202	SPO	C13-C12-C11	-15.45	93.73	118.08
8	D	102	SPO	C13-C12-C11	-15.44	93.74	118.08
8	G	201	SPO	C13-C12-C11	-15.36	93.87	118.08
8	f	102	SPO	C8-C7-C6	-15.33	93.92	118.08
8	B	101	SPO	C29-C28-C30	-15.33	89.48	115.27
8	A	201	SPO	C8-C7-C6	-15.32	93.94	118.08
8	O	102	SPO	C13-C12-C11	-15.28	94.00	118.08
8	M	404	SPO	C8-C7-C6	-15.28	94.01	118.08
8	i	102	SPO	C13-C12-C11	-15.22	94.09	118.08
8	E	201	SPO	C13-C12-C11	-15.20	94.14	118.08
8	b	103	SPO	C13-C12-C11	-15.18	94.16	118.08
8	t	102	SPO	C20-C21-C22	-15.17	92.41	123.47
8	R	101	SPO	C13-C12-C11	-15.13	94.24	118.08
8	B	101	SPO	C13-C12-C11	-15.12	94.26	118.08
8	S	201	SPO	C8-C7-C6	-15.08	94.32	118.08
8	E	201	SPO	C8-C7-C6	-15.07	94.33	118.08
8	S	201	SPO	C13-C12-C11	-15.07	94.34	118.08
8	o	102	SPO	C8-C7-C6	-15.04	94.38	118.08
8	o	102	SPO	C13-C12-C11	-15.03	94.39	118.08
8	F	101	SPO	C21-C22-C23	-15.03	105.87	127.31
8	f	102	SPO	C21-C22-C23	-15.01	105.89	127.31
8	d	102	SPO	C13-C12-C11	-15.01	94.43	118.08
8	d	102	SPO	C8-C7-C6	-14.98	94.48	118.08
8	r	102	SPO	C10-C11-C12	-14.95	84.40	126.42
8	j	102	SPO	C13-C12-C11	-14.93	94.55	118.08
8	b	103	SPO	C8-C7-C6	-14.90	94.61	118.08
8	k	102	SPO	C13-C12-C11	-14.86	94.67	118.08
8	N	201	SPO	C13-C12-C11	-14.83	94.71	118.08
8	A	201	SPO	C21-C22-C23	-14.79	106.20	127.31
8	t	102	SPO	C8-C7-C6	-14.79	94.77	118.08
8	k	102	SPO	C8-C7-C6	-14.75	94.84	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	b	103	SPO	C21-C22-C23	-14.74	106.27	127.31
8	A	201	SPO	C34-C33-C32	-14.71	85.95	123.68
8	i	102	SPO	C8-C7-C6	-14.70	94.92	118.08
8	M	404	SPO	C18-C17-C16	-14.70	94.92	118.08
8	d	102	SPO	C21-C22-C23	-14.69	106.35	127.31
8	G	201	SPO	C8-C7-C6	-14.68	94.95	118.08
8	r	102	SPO	C20-C21-C22	-14.58	93.60	123.47
8	i	102	SPO	C20-C21-C22	-14.57	93.63	123.47
8	f	102	SPO	C20-C21-C22	-14.56	93.64	123.47
8	b	103	SPO	C20-C21-C22	-14.56	93.66	123.47
8	F	101	SPO	C10-C11-C12	-14.51	85.65	126.42
8	N	201	SPO	C8-C7-C6	-14.49	95.25	118.08
8	t	102	SPO	C18-C17-C16	-14.48	95.26	118.08
8	N	201	SPO	C21-C22-C23	-14.45	106.68	127.31
8	o	102	SPO	C20-C21-C22	-14.42	93.94	123.47
8	k	102	SPO	C21-C22-C23	-14.32	106.88	127.31
8	B	101	SPO	C20-C21-C22	-14.31	94.17	123.47
8	j	102	SPO	C20-C21-C22	-14.30	94.17	123.47
8	G	201	SPO	C21-C22-C23	-14.26	106.96	127.31
8	o	102	SPO	C21-C22-C23	-14.23	107.00	127.31
8	E	201	SPO	C21-C22-C23	-14.23	107.00	127.31
8	b	103	SPO	C18-C17-C16	-14.23	95.66	118.08
8	j	102	SPO	C8-C7-C6	-14.16	95.76	118.08
8	t	102	SPO	C13-C12-C11	-14.15	95.78	118.08
8	G	201	SPO	C20-C21-C22	-14.14	94.50	123.47
8	o	102	SPO	C18-C17-C16	-14.13	95.81	118.08
8	k	102	SPO	C18-C17-C16	-14.12	95.83	118.08
8	i	102	SPO	C18-C17-C16	-14.11	95.84	118.08
8	S	201	SPO	C20-C21-C22	-14.11	94.57	123.47
8	N	201	SPO	C18-C17-C16	-14.09	95.87	118.08
8	A	201	SPO	C18-C17-C16	-14.08	95.89	118.08
8	E	201	SPO	C20-C21-C22	-14.07	94.66	123.47
8	t	102	SPO	C10-C11-C12	-14.07	86.90	126.42
8	R	101	SPO	C10-C11-C12	-14.05	86.95	126.42
8	j	102	SPO	C10-C11-C12	-14.03	87.01	126.42
8	R	101	SPO	C20-C21-C22	-13.99	94.82	123.47
8	E	203	SPO	C18-C17-C16	-13.98	96.05	118.08
8	r	102	SPO	C8-C7-C6	-13.95	96.10	118.08
8	S	202	SPO	C20-C21-C22	-13.94	94.92	123.47
8	i	102	SPO	C21-C22-C23	-13.93	107.42	127.31
8	k	102	SPO	C10-C11-C12	-13.92	87.32	126.42
8	M	404	SPO	C10-C11-C12	-13.89	87.41	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	j	102	SPO	C21-C22-C23	-13.88	107.50	127.31
8	N	201	SPO	C10-C11-C12	-13.88	87.43	126.42
10	M	403	U10	C41-C39-C40	-13.87	83.96	114.60
8	S	202	SPO	C10-C11-C12	-13.87	87.44	126.42
8	K	103	SPO	C20-C21-C22	-13.86	95.09	123.47
10	L	304	U10	C16-C14-C15	-13.83	84.05	114.60
8	f	102	SPO	C18-C17-C16	-13.81	96.32	118.08
8	b	103	SPO	C10-C11-C12	-13.79	87.66	126.42
8	j	102	SPO	C18-C17-C16	-13.79	96.34	118.08
8	d	102	SPO	C10-C11-C12	-13.78	87.71	126.42
8	G	201	SPO	C10-C11-C12	-13.74	87.81	126.42
8	E	201	SPO	C10-C11-C12	-13.73	87.86	126.42
8	J	101	SPO	C10-C11-C12	-13.70	87.94	126.42
8	I	102	SPO	C10-C11-C12	-13.69	87.95	126.42
8	k	102	SPO	C20-C21-C22	-13.69	95.43	123.47
8	E	201	SPO	C18-C17-C16	-13.66	96.55	118.08
8	o	102	SPO	C10-C11-C12	-13.66	88.03	126.42
8	J	101	SPO	C20-C21-C22	-13.65	95.51	123.47
8	O	102	SPO	C20-C21-C22	-13.65	95.51	123.47
8	G	201	SPO	C18-C17-C16	-13.64	96.59	118.08
8	i	102	SPO	C10-C11-C12	-13.62	88.16	126.42
8	S	201	SPO	C21-C22-C23	-13.62	107.88	127.31
8	N	201	SPO	C20-C21-C22	-13.62	95.58	123.47
8	d	102	SPO	C18-C17-C16	-13.60	96.66	118.08
8	S	201	SPO	C10-C11-C12	-13.59	88.24	126.42
8	I	102	SPO	C20-C21-C22	-13.54	95.74	123.47
8	r	102	SPO	C13-C12-C11	-13.53	96.76	118.08
8	B	101	SPO	C10-C11-C12	-13.51	88.47	126.42
8	K	101	SPO	C10-C11-C12	-13.48	88.54	126.42
8	K	101	SPO	C18-C17-C16	-13.43	96.92	118.08
8	E	203	SPO	C20-C21-C22	-13.41	96.01	123.47
8	I	102	SPO	C18-C17-C16	-13.36	97.02	118.08
8	F	101	SPO	C18-C17-C16	-13.35	97.04	118.08
8	S	201	SPO	C18-C17-C16	-13.35	97.04	118.08
8	D	102	SPO	C10-C11-C12	-13.30	89.04	126.42
8	f	102	SPO	C10-C11-C12	-13.30	89.05	126.42
8	K	103	SPO	C10-C11-C12	-13.30	89.06	126.42
8	E	202	SPO	C10-C11-C12	-13.28	89.10	126.42
8	A	201	SPO	C10-C11-C12	-13.23	89.26	126.42
8	O	102	SPO	C10-C11-C12	-13.22	89.27	126.42
8	D	102	SPO	C20-C21-C22	-13.20	96.43	123.47
8	E	203	SPO	C10-C11-C12	-13.18	89.40	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	j	102	SPO	C29-C28-C27	13.11	156.43	122.59
8	A	201	SPO	C29-C28-C27	13.09	156.39	122.59
8	d	102	SPO	C20-C21-C22	-13.06	96.71	123.47
8	N	201	SPO	C29-C28-C27	13.03	156.24	122.59
8	G	201	SPO	C29-C28-C27	13.01	156.19	122.59
8	t	102	SPO	C21-C22-C23	-13.01	108.75	127.31
8	A	201	SPO	C20-C21-C22	-12.98	96.88	123.47
8	E	202	SPO	C20-C21-C22	-12.97	96.91	123.47
10	L	303	U10	C26-C24-C23	-12.92	85.29	122.65
8	r	102	SPO	C29-C28-C27	12.90	155.88	122.59
8	E	201	SPO	C29-C28-C27	12.89	155.86	122.59
8	r	102	SPO	C18-C17-C16	-12.86	97.81	118.08
8	o	102	SPO	C29-C28-C27	12.82	155.69	122.59
10	L	305	U10	C11-C9-C8	-12.81	85.64	122.65
8	M	404	SPO	C15-C16-C17	-12.80	90.44	126.42
8	J	101	SPO	C18-C17-C16	-12.80	97.91	118.08
8	j	102	SPO	C15-C16-C17	-12.77	90.53	126.42
8	D	102	SPO	C18-C17-C16	-12.72	98.04	118.08
8	t	102	SPO	C29-C28-C27	12.71	155.40	122.59
8	F	101	SPO	C20-C21-C22	-12.70	97.46	123.47
8	S	201	SPO	C29-C28-C27	12.70	155.37	122.59
8	S	202	SPO	C18-C17-C16	-12.70	98.07	118.08
8	K	103	SPO	C18-C17-C16	-12.64	98.16	118.08
8	O	102	SPO	C18-C17-C16	-12.51	98.36	118.08
8	E	202	SPO	C18-C17-C16	-12.50	98.38	118.08
10	M	403	U10	C10-C9-C8	12.50	155.74	123.68
8	I	102	SPO	C15-C16-C17	-12.48	91.36	126.42
8	K	101	SPO	C20-C21-C22	-12.47	97.93	123.47
8	R	101	SPO	C29-C28-C27	12.45	154.73	122.59
8	A	201	SPO	C15-C16-C17	-12.44	91.46	126.42
8	t	102	SPO	C15-C16-C17	-12.43	91.49	126.42
8	G	201	SPO	C15-C16-C17	-12.37	91.66	126.42
10	M	403	U10	C20-C19-C18	12.34	155.33	123.68
8	E	201	SPO	C15-C16-C17	-12.33	91.79	126.42
8	F	101	SPO	C29-C28-C27	12.31	154.36	122.59
8	R	101	SPO	C18-C17-C16	-12.28	98.72	118.08
8	S	202	SPO	C15-C16-C17	-12.27	91.95	126.42
8	o	102	SPO	C15-C16-C17	-12.25	92.01	126.42
8	f	102	SPO	C15-C16-C17	-12.21	92.11	126.42
8	B	101	SPO	C18-C17-C16	-12.19	98.87	118.08
8	i	102	SPO	C15-C16-C17	-12.17	92.22	126.42
8	J	101	SPO	C15-C16-C17	-12.17	92.23	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	403	U10	C25-C24-C23	12.12	154.77	123.68
8	b	103	SPO	C15-C16-C17	-12.10	92.42	126.42
8	K	103	SPO	C15-C16-C17	-12.07	92.51	126.42
8	R	101	SPO	C30-C28-C27	-12.05	85.51	121.98
10	M	403	U10	C35-C34-C33	12.04	154.57	123.68
8	N	201	SPO	C15-C16-C17	-12.04	92.59	126.42
8	F	101	SPO	C30-C28-C27	-11.93	85.88	121.98
10	L	303	U10	C20-C19-C18	11.92	154.25	123.68
8	E	203	SPO	C15-C16-C17	-11.91	92.95	126.42
8	t	102	SPO	C30-C28-C27	-11.90	85.95	121.98
8	E	201	SPO	C30-C28-C27	-11.88	86.03	121.98
8	S	201	SPO	C15-C16-C17	-11.83	93.18	126.42
8	S	201	SPO	C27-C26-C25	-11.82	86.33	123.22
8	R	101	SPO	C15-C16-C17	-11.80	93.27	126.42
8	O	102	SPO	C15-C16-C17	-11.80	93.28	126.42
8	r	102	SPO	C30-C28-C27	-11.79	86.29	121.98
8	F	101	SPO	C15-C16-C17	-11.77	93.36	126.42
8	G	201	SPO	C30-C28-C27	-11.76	86.38	121.98
8	N	201	SPO	C30-C28-C27	-11.75	86.40	121.98
8	j	102	SPO	C30-C28-C27	-11.75	86.42	121.98
8	S	201	SPO	C30-C28-C27	-11.72	86.49	121.98
8	E	202	SPO	C15-C16-C17	-11.70	93.55	126.42
8	D	102	SPO	C15-C16-C17	-11.69	93.56	126.42
8	o	102	SPO	C30-C28-C27	-11.64	86.73	121.98
8	d	102	SPO	C27-C26-C25	-11.59	87.06	123.22
8	S	201	SPO	C34-C33-C32	-11.57	94.00	123.68
8	o	102	SPO	C34-C33-C32	-11.56	94.01	123.68
8	E	203	SPO	C34-C33-C32	-11.53	94.09	123.68
8	K	101	SPO	C15-C16-C17	-11.53	94.04	126.42
8	K	103	SPO	C34-C33-C32	-11.50	94.17	123.68
8	f	102	SPO	C34-C33-C32	-11.47	94.25	123.68
8	O	102	SPO	C34-C33-C32	-11.47	94.26	123.68
8	i	102	SPO	C34-C33-C32	-11.46	94.27	123.68
8	I	102	SPO	C34-C33-C32	-11.46	94.28	123.68
8	F	101	SPO	C34-C33-C32	-11.45	94.30	123.68
8	B	101	SPO	C15-C16-C17	-11.45	94.25	126.42
8	d	102	SPO	C34-C33-C32	-11.44	94.32	123.68
8	M	404	SPO	C34-C33-C32	-11.38	94.48	123.68
8	i	102	SPO	C27-C26-C25	-11.36	87.75	123.22
8	f	102	SPO	C27-C26-C25	-11.36	87.77	123.22
8	o	102	SPO	C27-C26-C25	-11.32	87.90	123.22
8	b	103	SPO	C27-C26-C25	-11.23	88.18	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	101	SPO	C10-C9-C7	-11.22	111.22	127.30
8	k	102	SPO	C27-C26-C25	-11.19	88.28	123.22
8	r	102	SPO	C15-C16-C17	-11.15	95.10	126.42
8	k	102	SPO	C15-C16-C17	-11.14	95.11	126.42
8	S	202	SPO	C27-C26-C25	-11.12	88.51	123.22
8	M	404	SPO	C20-C19-C17	-10.98	111.64	127.31
8	J	101	SPO	C27-C26-C25	-10.92	89.13	123.22
8	O	102	SPO	C27-C26-C25	-10.90	89.21	123.22
8	A	201	SPO	C30-C28-C27	-10.89	89.01	121.98
8	K	103	SPO	C27-C26-C25	-10.89	89.23	123.22
8	E	202	SPO	C10-C9-C7	-10.78	111.84	127.30
8	d	102	SPO	C15-C16-C17	-10.75	96.21	126.42
10	L	305	U10	C10-C9-C8	10.65	153.41	122.65
8	B	101	SPO	C27-C26-C25	-10.63	90.05	123.22
8	M	404	SPO	C8-C7-C9	10.62	137.80	122.92
8	O	102	SPO	C10-C9-C7	-10.61	112.09	127.30
8	E	203	SPO	C27-C26-C25	-10.59	90.16	123.22
8	A	201	SPO	C8-C7-C9	10.57	137.73	122.92
8	R	101	SPO	C27-C26-C25	-10.57	90.23	123.22
8	D	102	SPO	C27-C26-C25	-10.54	90.34	123.22
10	L	303	U10	C25-C24-C23	10.54	153.10	122.65
8	D	102	SPO	C10-C9-C7	-10.46	112.30	127.30
8	E	202	SPO	C27-C26-C25	-10.43	90.68	123.22
8	K	103	SPO	C10-C9-C7	-10.39	112.40	127.30
8	I	102	SPO	C27-C26-C25	-10.36	90.89	123.22
8	r	102	SPO	C27-C26-C25	-10.33	90.98	123.22
8	K	101	SPO	C27-C26-C25	-10.27	91.16	123.22
8	f	102	SPO	C8-C7-C9	10.25	137.28	122.92
8	d	102	SPO	C8-C7-C9	10.24	137.27	122.92
8	t	102	SPO	C27-C26-C25	-10.24	91.26	123.22
8	F	101	SPO	C21-C20-C19	-10.14	102.70	123.47
8	N	201	SPO	C27-C26-C25	-10.07	91.80	123.22
8	i	102	SPO	C8-C7-C9	9.99	136.91	122.92
8	F	101	SPO	C27-C26-C25	-9.98	92.08	123.22
8	E	201	SPO	C8-C7-C9	9.95	136.87	122.92
8	E	202	SPO	C21-C20-C19	-9.93	103.13	123.47
8	G	201	SPO	C27-C26-C25	-9.93	92.23	123.22
8	J	101	SPO	C21-C20-C19	-9.92	103.16	123.47
8	I	102	SPO	C8-C7-C6	-9.87	92.80	114.60
8	R	101	SPO	C10-C9-C7	-9.85	113.18	127.30
8	j	102	SPO	C27-C26-C25	-9.79	92.67	123.22
8	G	201	SPO	C8-C7-C9	9.78	136.62	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	o	102	SPO	C8-C7-C9	9.77	136.61	122.92
8	E	201	SPO	C27-C26-C25	-9.76	92.76	123.22
8	b	103	SPO	C8-C7-C9	9.73	136.56	122.92
10	L	303	U10	C7-C8-C9	-9.71	110.63	126.79
8	k	102	SPO	C8-C7-C9	9.68	136.48	122.92
8	K	101	SPO	C11-C12-C14	9.66	133.76	118.94
8	S	202	SPO	C21-C20-C19	-9.55	103.92	123.47
8	S	201	SPO	C8-C7-C9	9.54	136.28	122.92
8	M	404	SPO	C16-C17-C19	9.53	133.57	118.94
8	J	101	SPO	C10-C9-C7	-9.51	113.67	127.30
8	O	102	SPO	C21-C20-C19	-9.50	104.02	123.47
8	K	101	SPO	C21-C20-C19	-9.49	104.03	123.47
8	t	102	SPO	C8-C7-C9	9.49	136.21	122.92
8	D	102	SPO	C11-C12-C14	9.42	133.39	118.94
8	I	102	SPO	C11-C12-C14	9.39	133.35	118.94
8	D	102	SPO	C21-C20-C19	-9.38	104.25	123.47
8	j	102	SPO	C8-C7-C9	9.37	136.05	122.92
8	I	102	SPO	C21-C20-C19	-9.36	104.30	123.47
8	E	203	SPO	C11-C12-C14	9.33	133.26	118.94
8	K	103	SPO	C21-C20-C19	-9.33	104.37	123.47
8	O	102	SPO	C11-C12-C14	9.32	133.24	118.94
8	E	202	SPO	C11-C12-C14	9.31	133.22	118.94
10	M	403	U10	C7-C8-C9	-9.25	111.39	126.79
8	K	101	SPO	C8-C7-C6	-9.25	94.18	114.60
8	F	101	SPO	C8-C7-C6	-9.24	94.19	114.60
8	t	102	SPO	C20-C19-C17	-9.24	114.13	127.31
8	N	201	SPO	C8-C7-C9	9.20	135.82	122.92
8	S	202	SPO	C10-C9-C7	-9.19	114.13	127.30
8	R	101	SPO	C21-C20-C19	-9.17	104.68	123.47
8	K	103	SPO	C11-C12-C14	9.17	133.01	118.94
8	M	404	SPO	C27-C26-C25	-9.17	94.60	123.22
8	E	202	SPO	C15-C14-C12	-9.04	114.41	127.31
8	I	102	SPO	C15-C14-C12	-9.03	114.42	127.31
8	A	201	SPO	C21-C20-C19	-9.00	105.03	123.47
8	D	102	SPO	C15-C14-C12	-8.98	114.49	127.31
8	S	201	SPO	C11-C12-C14	8.94	132.67	118.94
8	S	202	SPO	C8-C7-C6	-8.89	94.97	114.60
8	A	201	SPO	C27-C26-C25	-8.89	95.49	123.22
8	R	101	SPO	C15-C14-C12	-8.86	114.67	127.31
8	B	101	SPO	C11-C12-C14	8.85	132.52	118.94
8	A	201	SPO	C13-C12-C14	8.85	135.32	122.92
8	R	101	SPO	C11-C12-C14	8.84	132.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	101	SPO	C11-C12-C14	8.83	132.49	118.94
8	K	103	SPO	C8-C7-C6	-8.82	95.11	114.60
8	F	101	SPO	C11-C12-C14	8.81	132.47	118.94
8	E	203	SPO	C8-C7-C6	-8.81	95.14	114.60
8	d	102	SPO	C21-C20-C19	-8.81	105.43	123.47
8	J	101	SPO	C8-C7-C6	-8.80	95.17	114.60
8	B	101	SPO	C21-C20-C19	-8.79	105.47	123.47
8	A	201	SPO	C11-C12-C14	8.78	132.42	118.94
8	t	102	SPO	C16-C17-C19	8.77	132.41	118.94
8	E	202	SPO	C8-C7-C6	-8.77	95.23	114.60
8	D	102	SPO	C8-C7-C6	-8.76	95.25	114.60
8	d	102	SPO	C11-C12-C14	8.74	132.35	118.94
8	O	102	SPO	C15-C14-C12	-8.73	114.85	127.31
8	N	201	SPO	C11-C12-C14	8.72	132.32	118.94
8	G	201	SPO	C11-C12-C14	8.70	132.29	118.94
8	R	101	SPO	C8-C7-C6	-8.69	95.40	114.60
8	M	404	SPO	C13-C12-C14	8.68	135.08	122.92
8	B	101	SPO	C8-C7-C6	-8.68	95.43	114.60
8	O	102	SPO	C8-C7-C6	-8.66	95.47	114.60
8	f	102	SPO	C11-C12-C14	8.66	132.22	118.94
8	E	203	SPO	C21-C20-C19	-8.62	105.81	123.47
8	b	103	SPO	C20-C19-C17	-8.62	115.00	127.31
8	o	102	SPO	C11-C12-C14	8.61	132.16	118.94
8	b	103	SPO	C16-C17-C19	8.56	132.08	118.94
8	B	101	SPO	C15-C14-C12	-8.54	115.13	127.31
8	k	102	SPO	C11-C12-C14	8.51	131.99	118.94
10	L	303	U10	C11-C9-C8	-8.48	103.95	121.12
8	r	102	SPO	C8-C7-C9	8.46	134.77	122.92
8	E	201	SPO	C11-C12-C14	8.45	131.91	118.94
8	i	102	SPO	C11-C12-C14	8.44	131.89	118.94
8	G	201	SPO	C21-C20-C19	-8.42	106.22	123.47
8	r	102	SPO	C21-C20-C19	-8.42	106.23	123.47
8	b	103	SPO	C11-C12-C14	8.37	131.79	118.94
8	N	201	SPO	C21-C20-C19	-8.34	106.39	123.47
8	E	201	SPO	C21-C20-C19	-8.34	106.40	123.47
8	S	202	SPO	C11-C12-C14	8.32	131.71	118.94
8	S	202	SPO	C13-C12-C14	8.31	134.57	122.92
8	A	201	SPO	C16-C17-C19	8.28	131.65	118.94
8	j	102	SPO	C11-C12-C14	8.21	131.55	118.94
8	K	103	SPO	C15-C14-C12	-8.21	115.59	127.31
8	J	101	SPO	C15-C14-C12	-8.20	115.60	127.31
8	f	102	SPO	C13-C12-C14	8.17	134.36	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	404	SPO	C11-C12-C14	8.15	131.44	118.94
8	K	101	SPO	C15-C14-C12	-8.14	115.69	127.31
8	j	102	SPO	C21-C20-C19	-8.12	106.84	123.47
8	S	201	SPO	C21-C20-C19	-8.09	106.90	123.47
8	i	102	SPO	C16-C17-C19	8.07	131.33	118.94
8	E	203	SPO	C10-C9-C7	-8.04	115.77	127.30
8	o	102	SPO	C16-C17-C19	8.03	131.27	118.94
8	F	101	SPO	C13-C12-C14	8.02	134.16	122.92
8	F	101	SPO	C18-C17-C19	8.02	134.15	122.92
8	i	102	SPO	C20-C19-C17	-8.01	115.88	127.31
8	S	202	SPO	C15-C14-C12	-8.00	115.89	127.31
8	S	202	SPO	C18-C17-C19	7.97	134.09	122.92
8	J	101	SPO	C18-C17-C19	7.97	134.08	122.92
8	t	102	SPO	C25-C23-C22	-7.96	106.73	118.94
8	b	103	SPO	C13-C12-C14	7.94	134.04	122.92
8	A	201	SPO	C20-C19-C17	-7.92	116.00	127.31
8	i	102	SPO	C13-C12-C14	7.91	134.00	122.92
8	E	201	SPO	C13-C12-C14	7.87	133.95	122.92
8	t	102	SPO	C13-C12-C14	7.87	133.95	122.92
8	f	102	SPO	C16-C17-C19	7.87	131.02	118.94
8	k	102	SPO	C16-C17-C19	7.86	131.00	118.94
8	o	102	SPO	C21-C20-C19	-7.85	107.40	123.47
8	j	102	SPO	C13-C12-C14	7.83	133.89	122.92
8	J	101	SPO	C13-C12-C14	7.82	133.88	122.92
8	G	201	SPO	C13-C12-C14	7.79	133.83	122.92
8	o	102	SPO	C20-C19-C17	-7.78	116.20	127.31
8	k	102	SPO	C21-C20-C19	-7.78	107.54	123.47
8	I	102	SPO	C18-C17-C19	7.77	133.81	122.92
8	N	201	SPO	C16-C17-C19	7.74	130.82	118.94
8	I	102	SPO	C13-C12-C14	7.74	133.76	122.92
8	i	102	SPO	C21-C20-C19	-7.71	107.69	123.47
8	E	203	SPO	C15-C14-C12	-7.70	116.32	127.31
8	f	102	SPO	C21-C20-C19	-7.67	107.75	123.47
8	K	101	SPO	C18-C17-C19	7.66	133.66	122.92
8	S	201	SPO	C18-C17-C19	7.66	133.65	122.92
8	f	102	SPO	C20-C19-C17	-7.63	116.41	127.31
8	F	101	SPO	C15-C14-C12	-7.62	116.43	127.31
8	K	103	SPO	C18-C17-C19	7.61	133.59	122.92
8	r	102	SPO	C18-C17-C19	7.61	133.58	122.92
8	r	102	SPO	C13-C12-C14	7.59	133.56	122.92
8	E	203	SPO	C18-C17-C19	7.59	133.56	122.92
8	b	103	SPO	C21-C20-C19	-7.59	107.94	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	101	SPO	C18-C17-C19	7.56	133.51	122.92
8	K	103	SPO	C13-C12-C14	7.54	133.49	122.92
8	o	102	SPO	C13-C12-C14	7.51	133.45	122.92
8	E	201	SPO	C20-C19-C17	-7.51	116.59	127.31
8	j	102	SPO	C20-C19-C17	-7.49	116.62	127.31
8	j	102	SPO	C16-C17-C19	7.48	130.42	118.94
8	G	201	SPO	C18-C17-C19	7.48	133.40	122.92
8	E	201	SPO	C16-C17-C19	7.44	130.35	118.94
8	k	102	SPO	C13-C12-C14	7.44	133.34	122.92
8	E	203	SPO	C16-C17-C19	7.43	130.34	118.94
8	E	202	SPO	C18-C17-C19	7.41	133.31	122.92
10	M	403	U10	C17-C18-C19	-7.41	109.81	127.66
8	E	203	SPO	C13-C12-C14	7.40	133.28	122.92
8	F	101	SPO	C25-C23-C22	-7.40	107.59	118.94
8	d	102	SPO	C18-C17-C19	7.38	133.26	122.92
8	t	102	SPO	C11-C12-C14	7.38	130.27	118.94
8	R	101	SPO	C13-C12-C14	7.38	133.26	122.92
8	D	102	SPO	C18-C17-C19	7.37	133.25	122.92
8	N	201	SPO	C18-C17-C19	7.36	133.23	122.92
8	d	102	SPO	C13-C12-C14	7.35	133.22	122.92
8	B	101	SPO	C13-C12-C14	7.35	133.22	122.92
8	j	102	SPO	C18-C17-C19	7.32	133.18	122.92
8	j	102	SPO	C25-C23-C22	-7.31	107.72	118.94
8	O	102	SPO	C18-C17-C19	7.30	133.16	122.92
8	t	102	SPO	C21-C20-C19	-7.29	108.55	123.47
8	k	102	SPO	C18-C17-C19	7.24	133.06	122.92
8	E	202	SPO	C13-C12-C14	7.22	133.04	122.92
8	E	201	SPO	C18-C17-C19	7.22	133.03	122.92
8	S	201	SPO	C13-C12-C14	7.19	132.99	122.92
8	d	102	SPO	C16-C17-C19	7.18	129.96	118.94
8	G	201	SPO	C16-C17-C19	7.17	129.95	118.94
8	N	201	SPO	C13-C12-C14	7.17	132.97	122.92
8	E	201	SPO	C25-C23-C22	-7.16	107.96	118.94
8	G	201	SPO	C25-C23-C22	-7.13	108.00	118.94
8	K	101	SPO	C13-C12-C14	7.10	132.87	122.92
8	D	102	SPO	C13-C12-C14	7.10	132.87	122.92
8	R	101	SPO	C18-C17-C19	7.10	132.87	122.92
8	o	102	SPO	C18-C17-C19	7.09	132.86	122.92
8	M	404	SPO	C25-C23-C22	-7.09	108.07	118.94
8	O	102	SPO	C13-C12-C14	7.02	132.76	122.92
8	i	102	SPO	C18-C17-C19	7.00	132.73	122.92
8	r	102	SPO	C11-C12-C14	6.99	129.67	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	201	SPO	C20-C19-C17	-6.99	117.34	127.31
8	i	102	SPO	C25-C23-C22	-6.93	108.30	118.94
8	f	102	SPO	C18-C17-C19	6.90	132.59	122.92
8	S	201	SPO	C15-C14-C12	-6.88	117.49	127.31
10	M	403	U10	C32-C33-C34	-6.87	111.11	127.66
8	E	203	SPO	C25-C23-C22	-6.85	108.42	118.94
8	B	101	SPO	C34-C33-C32	-6.85	106.10	123.68
8	B	101	SPO	C25-C23-C22	-6.84	108.44	118.94
8	S	201	SPO	C6-C7-C9	6.81	129.40	118.94
10	L	303	U10	C17-C18-C19	-6.81	111.25	127.66
8	K	101	SPO	C16-C17-C19	6.79	129.36	118.94
10	L	304	U10	C11-C9-C8	-6.79	107.38	121.12
8	N	201	SPO	C20-C19-C17	-6.77	117.64	127.31
8	b	103	SPO	C34-C33-C32	-6.76	106.33	123.68
8	A	201	SPO	C18-C17-C19	6.76	132.39	122.92
8	r	102	SPO	C15-C14-C12	-6.73	117.70	127.31
8	S	201	SPO	C25-C23-C22	-6.73	108.61	118.94
8	S	201	SPO	C16-C17-C19	6.72	129.25	118.94
8	S	202	SPO	C25-C23-C22	-6.71	108.64	118.94
8	N	201	SPO	C15-C14-C12	-6.70	117.75	127.31
8	b	103	SPO	C25-C23-C22	-6.70	108.67	118.94
8	G	201	SPO	C34-C33-C32	-6.69	106.51	123.68
8	N	201	SPO	C25-C23-C22	-6.69	108.67	118.94
8	t	102	SPO	C18-C17-C19	6.68	132.28	122.92
8	N	201	SPO	C34-C33-C32	-6.68	106.54	123.68
8	I	102	SPO	C16-C17-C19	6.66	129.15	118.94
8	j	102	SPO	C34-C33-C32	-6.65	106.61	123.68
8	E	201	SPO	C34-C33-C32	-6.65	106.61	123.68
8	r	102	SPO	C6-C7-C9	6.64	129.12	118.94
8	o	102	SPO	C25-C23-C22	-6.61	108.80	118.94
8	A	201	SPO	C26-C25-C23	-6.60	107.86	126.42
8	b	103	SPO	C18-C17-C19	6.60	132.17	122.92
8	R	101	SPO	C25-C23-C22	-6.59	108.83	118.94
8	k	102	SPO	C25-C23-C22	-6.59	108.83	118.94
8	f	102	SPO	C25-C23-C22	-6.59	108.83	118.94
8	F	101	SPO	C10-C9-C7	-6.58	117.86	127.30
8	r	102	SPO	C25-C23-C22	-6.58	108.84	118.94
8	E	202	SPO	C34-C33-C32	-6.58	106.81	123.68
8	D	102	SPO	C34-C33-C32	-6.57	106.81	123.68
8	t	102	SPO	C6-C7-C9	6.57	129.02	118.94
8	R	101	SPO	C20-C19-C17	-6.56	117.94	127.31
8	o	102	SPO	C6-C7-C9	6.56	129.01	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	103	SPO	C25-C23-C22	-6.55	108.89	118.94
8	R	101	SPO	C34-C33-C32	-6.54	106.91	123.68
8	r	102	SPO	C20-C19-C17	-6.53	117.98	127.31
8	r	102	SPO	C34-C33-C32	-6.51	106.97	123.68
8	N	201	SPO	C6-C7-C9	6.51	128.93	118.94
8	K	101	SPO	C34-C33-C32	-6.48	107.05	123.68
8	J	101	SPO	C25-C23-C22	-6.47	109.02	118.94
8	t	102	SPO	C15-C14-C12	-6.45	118.11	127.31
8	k	102	SPO	C20-C19-C17	-6.45	118.11	127.31
8	J	101	SPO	C34-C33-C32	-6.45	107.13	123.68
8	b	103	SPO	C6-C7-C9	6.45	128.83	118.94
8	A	201	SPO	C25-C23-C22	-6.43	109.08	118.94
8	E	201	SPO	C6-C7-C9	6.42	128.80	118.94
8	f	102	SPO	C6-C7-C9	6.42	128.80	118.94
8	F	101	SPO	C16-C17-C19	6.39	128.75	118.94
8	S	202	SPO	C34-C33-C32	-6.39	107.29	123.68
8	t	102	SPO	C34-C33-C32	-6.39	107.30	123.68
8	O	102	SPO	C25-C23-C22	-6.38	109.15	118.94
8	O	102	SPO	C20-C19-C17	-6.38	118.20	127.31
10	L	303	U10	C15-C14-C13	-6.37	107.33	123.68
8	k	102	SPO	C6-C7-C9	6.35	128.68	118.94
8	D	102	SPO	C16-C17-C19	6.34	128.67	118.94
8	k	102	SPO	C34-C33-C32	-6.34	107.43	123.68
8	A	201	SPO	C31-C32-C33	-6.29	112.51	127.66
10	M	403	U10	C30-C29-C28	-6.28	107.58	123.68
8	r	102	SPO	C16-C17-C19	6.28	128.57	118.94
8	d	102	SPO	C25-C23-C22	-6.26	109.33	118.94
10	M	403	U10	C15-C14-C13	-6.25	107.64	123.68
8	E	201	SPO	C26-C25-C23	-6.25	108.87	126.42
8	E	203	SPO	C20-C19-C17	-6.23	118.41	127.31
8	S	201	SPO	C20-C19-C17	-6.22	118.43	127.31
8	O	102	SPO	C16-C17-C19	6.20	128.46	118.94
8	G	201	SPO	C6-C7-C9	6.18	128.43	118.94
8	D	102	SPO	C25-C23-C22	-6.17	109.47	118.94
8	R	101	SPO	C16-C17-C19	6.16	128.39	118.94
8	K	101	SPO	C25-C23-C22	-6.15	109.50	118.94
8	B	101	SPO	C30-C28-C27	-6.14	103.39	121.98
8	A	201	SPO	C6-C7-C9	6.12	128.33	118.94
8	E	202	SPO	C16-C17-C19	6.08	128.27	118.94
8	M	404	SPO	C18-C17-C19	6.08	131.44	122.92
8	d	102	SPO	C6-C7-C9	6.07	128.25	118.94
8	G	201	SPO	C15-C14-C12	-6.06	118.67	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	403	U10	C22-C23-C24	-6.06	113.08	127.66
8	K	103	SPO	C16-C17-C19	6.05	128.23	118.94
8	K	103	SPO	C20-C19-C17	-6.03	118.70	127.31
8	M	404	SPO	C6-C7-C9	6.03	128.19	118.94
8	j	102	SPO	C6-C7-C9	6.03	128.19	118.94
8	D	102	SPO	C20-C19-C17	-6.02	118.71	127.31
8	i	102	SPO	C6-C7-C9	6.01	128.17	118.94
8	S	202	SPO	C30-C28-C27	-6.00	103.83	121.98
8	G	201	SPO	C26-C25-C23	-5.94	109.72	126.42
8	J	101	SPO	C30-C28-C27	-5.93	104.02	121.98
7	M	407	BCL	C1-O2A-CGA	5.91	131.94	116.44
8	J	101	SPO	C16-C17-C19	5.89	127.98	118.94
8	I	102	SPO	C25-C23-C22	-5.88	109.92	118.94
8	t	102	SPO	C26-C25-C23	-5.87	109.92	126.42
8	k	102	SPO	C30-C28-C27	-5.87	104.20	121.98
7	U	102	BCL	CHD-C1D-ND	-5.85	119.07	124.45
8	d	102	SPO	C20-C19-C17	-5.85	118.96	127.31
8	E	202	SPO	C20-C19-C17	-5.85	118.96	127.31
8	E	203	SPO	C30-C28-C27	-5.84	104.31	121.98
8	d	102	SPO	C30-C28-C27	-5.84	104.31	121.98
8	i	102	SPO	C30-C28-C27	-5.84	104.31	121.98
8	S	202	SPO	C20-C19-C17	-5.83	118.99	127.31
8	F	101	SPO	C26-C25-C23	-5.83	110.05	126.42
8	O	102	SPO	C30-C28-C27	-5.82	104.35	121.98
8	f	102	SPO	C30-C28-C27	-5.81	104.39	121.98
8	o	102	SPO	C15-C14-C12	-5.80	119.03	127.31
8	j	102	SPO	C26-C25-C23	-5.80	110.13	126.42
8	S	202	SPO	C16-C17-C19	5.79	127.82	118.94
8	M	404	SPO	C30-C28-C27	-5.78	104.48	121.98
8	K	101	SPO	C30-C28-C27	-5.75	104.57	121.98
8	E	202	SPO	C30-C28-C27	-5.74	104.61	121.98
8	K	103	SPO	C30-C28-C27	-5.73	104.62	121.98
8	D	102	SPO	C30-C28-C27	-5.70	104.74	121.98
8	I	102	SPO	C20-C19-C17	-5.68	119.20	127.31
8	J	101	SPO	C20-C19-C17	-5.64	119.26	127.31
8	B	101	SPO	C16-C17-C19	5.64	127.59	118.94
8	E	201	SPO	C15-C14-C12	-5.63	119.28	127.31
8	b	103	SPO	C30-C28-C27	-5.62	104.97	121.98
8	I	102	SPO	C30-C28-C27	-5.58	105.10	121.98
8	E	202	SPO	C25-C23-C22	-5.55	110.42	118.94
8	N	201	SPO	C26-C25-C23	-5.54	110.84	126.42
8	B	101	SPO	C20-C19-C17	-5.50	119.46	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	202	SPO	C26-C25-C23	-5.45	111.11	126.42
8	r	102	SPO	C26-C25-C23	-5.45	111.11	126.42
8	K	101	SPO	C20-C19-C17	-5.44	119.55	127.31
8	F	101	SPO	C20-C19-C17	-5.44	119.55	127.31
7	M	401	BCL	CHD-C1D-ND	-5.41	119.48	124.45
7	M	407	BCL	C4D-CHA-C1A	5.40	127.82	121.25
7	t	101	BCL	CHD-C1D-ND	-5.36	119.53	124.45
8	r	102	SPO	C14-C15-C16	-5.32	106.60	123.22
8	J	101	SPO	C26-C25-C23	-5.32	111.48	126.42
7	s	101	BCL	C4D-CHA-C1A	5.31	127.71	121.25
8	d	102	SPO	C15-C14-C12	-5.30	119.75	127.31
7	o	101	BCL	C4D-CHA-C1A	5.30	127.69	121.25
8	k	102	SPO	C15-C14-C12	-5.28	119.78	127.31
8	j	102	SPO	C15-C14-C12	-5.27	119.79	127.31
7	r	101	BCL	C4D-CHA-C1A	5.27	127.66	121.25
7	k	101	BCL	C4D-CHA-C1A	5.26	127.65	121.25
7	g	102	BCL	C4D-CHA-C1A	5.26	127.65	121.25
8	b	103	SPO	C15-C14-C12	-5.25	119.81	127.31
8	i	102	SPO	C15-C14-C12	-5.25	119.81	127.31
7	K	102	BCL	C4D-CHA-C1A	5.24	127.63	121.25
8	M	404	SPO	C21-C22-C23	-5.24	119.83	127.31
7	r	103	BCL	C4D-CHA-C1A	5.24	127.62	121.25
7	e	101	BCL	C4D-CHA-C1A	5.23	127.62	121.25
7	F	102	BCL	C4D-CHA-C1A	5.22	127.60	121.25
7	d	101	BCL	CHD-C1D-ND	-5.22	119.66	124.45
7	g	101	BCL	C4D-CHA-C1A	5.21	127.59	121.25
7	I	101	BCL	C4D-CHA-C1A	5.21	127.59	121.25
7	T	101	BCL	CHD-C1D-ND	-5.21	119.67	124.45
7	b	101	BCL	C4D-CHA-C1A	5.20	127.58	121.25
7	a	100	BCL	C4D-CHA-C1A	5.20	127.58	121.25
7	r	101	BCL	CHD-C1D-ND	-5.20	119.68	124.45
10	M	403	U10	C41-C39-C38	-5.19	107.64	122.65
7	M	401	BCL	C4D-CHA-C1A	5.19	127.56	121.25
7	O	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
7	j	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
7	J	102	BCL	C4D-CHA-C1A	5.17	127.55	121.25
7	j	101	BCL	CHD-C1D-ND	-5.17	119.70	124.45
7	a	100	BCL	CHD-C1D-ND	-5.17	119.70	124.45
7	T	101	BCL	C4D-CHA-C1A	5.17	127.53	121.25
7	D	101	BCL	C4D-CHA-C1A	5.16	127.53	121.25
7	b	102	BCL	C4D-CHA-C1A	5.16	127.53	121.25
7	t	101	BCL	C4D-CHA-C1A	5.16	127.53	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	s	102	BCL	C4D-CHA-C1A	5.15	127.52	121.25
10	L	304	U10	C15-C14-C13	-5.14	107.78	122.65
7	A	202	BCL	C4D-CHA-C1A	5.14	127.51	121.25
7	b	101	BCL	CHD-C1D-ND	-5.13	119.74	124.45
7	L	301	BCL	C4D-CHA-C1A	5.12	127.48	121.25
7	d	101	BCL	C4D-CHA-C1A	5.12	127.47	121.25
7	n	101	BCL	C4D-CHA-C1A	5.11	127.47	121.25
7	o	101	BCL	CHD-C1D-ND	-5.11	119.76	124.45
7	n	102	BCL	C4D-CHA-C1A	5.11	127.46	121.25
8	E	202	SPO	C26-C25-C23	-5.11	112.07	126.42
7	k	101	BCL	CHD-C1D-ND	-5.10	119.76	124.45
7	e	102	BCL	C4D-CHA-C1A	5.10	127.46	121.25
7	f	101	BCL	C4D-CHA-C1A	5.10	127.45	121.25
10	L	305	U10	C7-C8-C9	-5.08	111.33	127.26
7	L	301	BCL	CHD-C1D-ND	-5.08	119.79	124.45
7	A	202	BCL	CHD-C1D-ND	-5.07	119.79	124.45
8	O	102	SPO	C26-C25-C23	-5.05	112.22	126.42
7	e	101	BCL	CHD-C1D-ND	-5.05	119.81	124.45
7	g	101	BCL	CHD-C1D-ND	-5.05	119.81	124.45
7	U	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
7	i	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
7	f	101	BCL	CHD-C1D-ND	-5.03	119.83	124.45
7	M	407	BCL	CHD-C1D-ND	-5.01	119.85	124.45
7	s	102	BCL	CHD-C1D-ND	-5.01	119.85	124.45
7	n	101	BCL	CHD-C1D-ND	-5.01	119.85	124.45
7	M	405	BCL	CHD-C1D-ND	-4.98	119.88	124.45
8	D	102	SPO	C26-C25-C23	-4.95	112.51	126.42
7	i	101	BCL	CHD-C1D-ND	-4.95	119.91	124.45
7	O	101	BCL	CHD-C1D-ND	-4.94	119.91	124.45
7	J	102	BCL	CHD-C1D-ND	-4.93	119.92	124.45
8	K	103	SPO	C26-C25-C23	-4.93	112.56	126.42
7	r	103	BCL	CHD-C1D-ND	-4.93	119.92	124.45
7	F	102	BCL	CHD-C1D-ND	-4.93	119.93	124.45
7	D	101	BCL	CHD-C1D-ND	-4.91	119.94	124.45
7	U	101	BCL	CHD-C1D-ND	-4.90	119.95	124.45
7	U	102	BCL	C4D-CHA-C1A	4.90	127.21	121.25
7	K	102	BCL	CHD-C1D-ND	-4.87	119.98	124.45
7	n	102	BCL	CHD-C1D-ND	-4.86	119.98	124.45
7	g	102	BCL	CHD-C1D-ND	-4.86	119.98	124.45
7	b	102	BCL	CHD-C1D-ND	-4.86	119.99	124.45
7	e	102	BCL	CHD-C1D-ND	-4.86	119.99	124.45
7	M	405	BCL	C4D-CHA-C1A	4.84	127.14	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	101	BCL	CHD-C1D-ND	-4.84	120.01	124.45
8	I	102	SPO	C26-C25-C23	-4.83	112.85	126.42
7	s	101	BCL	CHD-C1D-ND	-4.82	120.02	124.45
7	M	407	BCL	C1-C2-C3	-4.75	117.82	126.04
8	R	101	SPO	C26-C25-C23	-4.74	113.11	126.42
8	r	102	SPO	C10-C9-C7	-4.69	120.62	127.31
8	B	101	SPO	C26-C25-C23	-4.66	113.33	126.42
8	f	102	SPO	C15-C14-C12	-4.60	120.75	127.31
10	L	303	U10	C22-C23-C24	-4.58	112.09	127.75
8	b	103	SPO	C26-C25-C23	-4.57	113.57	126.42
11	L	306	3PE	O21-C21-C22	4.56	121.32	111.50
8	i	102	SPO	C26-C25-C23	-4.47	113.85	126.42
8	E	202	SPO	C14-C15-C16	-4.47	109.27	123.22
8	M	404	SPO	C21-C20-C19	-4.41	114.44	123.47
8	B	101	SPO	C14-C15-C16	-4.41	109.47	123.22
8	d	102	SPO	C14-C15-C16	-4.38	109.54	123.22
8	o	102	SPO	C26-C25-C23	-4.38	114.11	126.42
7	n	101	BCL	CMB-C2B-C1B	-4.38	121.74	128.46
8	f	102	SPO	C26-C25-C23	-4.35	114.18	126.42
8	k	102	SPO	C14-C15-C16	-4.33	109.69	123.22
8	J	101	SPO	C14-C15-C16	-4.31	109.76	123.22
7	d	101	BCL	CMB-C2B-C1B	-4.29	121.86	128.46
7	b	101	BCL	CMB-C2B-C1B	-4.28	121.88	128.46
8	F	101	SPO	C14-C15-C16	-4.28	109.86	123.22
7	e	101	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
7	k	101	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
8	D	102	SPO	C14-C15-C16	-4.27	109.90	123.22
8	O	102	SPO	C14-C15-C16	-4.26	109.92	123.22
8	S	202	SPO	C14-C15-C16	-4.25	109.95	123.22
8	R	101	SPO	C14-C15-C16	-4.24	109.97	123.22
11	d	103	3PE	O21-C21-C22	4.22	120.60	111.50
8	M	404	SPO	C26-C25-C23	-4.22	114.57	126.42
8	k	102	SPO	C26-C25-C23	-4.20	114.61	126.42
8	S	201	SPO	C14-C15-C16	-4.20	110.11	123.22
8	N	201	SPO	C14-C15-C16	-4.19	110.15	123.22
8	M	404	SPO	C15-C14-C12	-4.18	121.34	127.31
7	i	101	BCL	CMB-C2B-C1B	-4.18	122.04	128.46
8	E	203	SPO	C26-C25-C23	-4.17	114.69	126.42
8	B	101	SPO	C31-C32-C33	-4.15	117.67	127.66
8	A	201	SPO	C15-C14-C12	-4.15	121.39	127.31
8	t	102	SPO	C14-C15-C16	-4.14	110.28	123.22
8	d	102	SPO	C26-C25-C23	-4.14	114.79	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	301	BCL	CMB-C2B-C1B	-4.14	122.11	128.46
8	K	103	SPO	C14-C15-C16	-4.12	110.35	123.22
7	j	101	BCL	CMB-C2B-C1B	-4.12	122.13	128.46
7	f	101	BCL	CMB-C2B-C1B	-4.12	122.13	128.46
7	g	101	BCL	CMB-C2B-C1B	-4.12	122.14	128.46
7	r	101	BCL	CMB-C2B-C1B	-4.10	122.17	128.46
7	M	405	BCL	CMB-C2B-C1B	-4.09	122.17	128.46
8	E	203	SPO	C14-C15-C16	-4.09	110.46	123.22
8	K	101	SPO	C26-C25-C23	-4.07	114.98	126.42
8	K	101	SPO	C14-C15-C16	-4.06	110.55	123.22
7	s	102	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
7	g	101	BCL	C4A-NA-C1A	4.04	108.52	106.71
11	M	409	3PE	O21-C21-C22	4.02	120.16	111.50
7	j	101	BCL	C4A-NA-C1A	4.00	108.50	106.71
10	L	304	U10	C7-C8-C9	-3.98	120.17	126.79
7	o	101	BCL	CMB-C2B-C1B	-3.97	122.37	128.46
7	i	101	BCL	C4A-NA-C1A	3.96	108.49	106.71
8	t	102	SPO	C10-C9-C7	-3.95	121.67	127.31
8	I	102	SPO	C14-C15-C16	-3.94	110.93	123.22
7	d	101	BCL	C4A-NA-C1A	3.93	108.47	106.71
11	H	302	3PE	O21-C21-C22	3.92	119.96	111.50
7	e	101	BCL	C4A-NA-C1A	3.92	108.47	106.71
7	M	401	BCL	C1D-ND-C4D	-3.92	103.55	106.33
8	D	102	SPO	C31-C32-C33	-3.91	118.25	127.66
11	H	301	3PE	O21-C21-C22	3.89	119.88	111.50
8	k	102	SPO	C31-C32-C33	-3.86	118.37	127.66
11	d	104	3PE	O21-C21-C22	3.85	119.80	111.50
8	o	102	SPO	C14-C15-C16	-3.84	111.22	123.22
7	M	407	BCL	CMB-C2B-C1B	-3.83	122.57	128.46
8	E	202	SPO	C9-C10-C11	-3.83	111.27	123.22
7	k	101	BCL	C4A-NA-C1A	3.83	108.43	106.71
8	K	101	SPO	C31-C32-C33	-3.82	118.46	127.66
7	D	101	BCL	CMB-C2B-C1B	-3.82	122.59	128.46
11	M	406	3PE	O21-C21-C22	3.81	119.72	111.50
8	S	201	SPO	C26-C25-C23	-3.81	115.72	126.42
7	o	101	BCL	C4A-NA-C1A	3.76	108.39	106.71
8	O	102	SPO	C9-C10-C11	-3.75	111.50	123.22
8	E	201	SPO	C14-C15-C16	-3.75	111.51	123.22
10	L	303	U10	C12-C13-C14	-3.75	118.63	127.66
7	e	102	BCL	CMB-C2B-C1B	-3.75	122.70	128.46
8	I	102	SPO	C10-C9-C7	-3.74	121.93	127.30
7	M	401	BCL	CMB-C2B-C1B	-3.74	122.71	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	102	BCL	CMB-C2B-C1B	-3.73	122.72	128.46
7	A	202	BCL	CMB-C2B-C1B	-3.73	122.73	128.46
8	E	202	SPO	C31-C32-C33	-3.73	118.68	127.66
7	I	101	BCL	CMB-C2B-C1B	-3.73	122.73	128.46
8	b	103	SPO	C14-C15-C16	-3.73	111.58	123.22
7	F	102	BCL	CMB-C2B-C1B	-3.72	122.75	128.46
8	G	201	SPO	C14-C15-C16	-3.72	111.61	123.22
7	r	101	BCL	C4A-NA-C1A	3.70	108.37	106.71
7	n	101	BCL	C4A-NA-C1A	3.69	108.37	106.71
8	i	102	SPO	C14-C15-C16	-3.68	111.74	123.22
8	b	103	SPO	C31-C32-C33	-3.68	118.80	127.66
8	S	202	SPO	C31-C32-C33	-3.68	118.80	127.66
8	B	101	SPO	C9-C10-C11	-3.68	111.74	123.22
7	T	101	BCL	C1D-ND-C4D	-3.68	103.72	106.33
7	O	101	BCL	CMB-C2B-C1B	-3.67	122.82	128.46
7	a	100	BCL	C1D-ND-C4D	-3.67	103.73	106.33
7	f	101	BCL	C4A-NA-C1A	3.67	108.35	106.71
8	R	101	SPO	C31-C32-C33	-3.66	118.84	127.66
8	J	101	SPO	C31-C32-C33	-3.65	118.86	127.66
7	U	102	BCL	CMB-C2B-C1B	-3.65	122.85	128.46
7	t	101	BCL	C4A-NA-C1A	3.63	108.34	106.71
7	b	101	BCL	C4A-NA-C1A	3.63	108.34	106.71
7	r	101	BCL	C1D-ND-C4D	-3.63	103.76	106.33
7	g	101	BCL	C1D-ND-C4D	-3.63	103.76	106.33
7	s	101	BCL	CMB-C2B-C1B	-3.62	122.90	128.46
8	K	103	SPO	C9-C10-C11	-3.62	111.93	123.22
7	b	102	BCL	CMB-C2B-C1B	-3.62	122.91	128.46
7	T	101	BCL	CMB-C2B-C1B	-3.61	122.91	128.46
7	J	102	BCL	CMB-C2B-C1B	-3.60	122.92	128.46
7	U	102	BCL	C4A-NA-C1A	3.59	108.32	106.71
8	N	201	SPO	C10-C9-C7	-3.59	122.18	127.31
7	j	101	BCL	C1D-ND-C4D	-3.57	103.80	106.33
7	k	101	BCL	C1D-ND-C4D	-3.57	103.80	106.33
8	D	102	SPO	C9-C10-C11	-3.56	112.12	123.22
7	n	102	BCL	CMB-C2B-C1B	-3.55	123.00	128.46
7	n	101	BCL	C1D-ND-C4D	-3.54	103.82	106.33
7	s	102	BCL	C1D-ND-C4D	-3.54	103.82	106.33
7	d	101	BCL	C1D-ND-C4D	-3.54	103.82	106.33
7	s	102	BCL	C4A-NA-C1A	3.53	108.29	106.71
8	K	101	SPO	C10-C9-C7	-3.53	122.25	127.30
7	e	101	BCL	C16-C15-C13	-3.52	104.54	115.92
7	g	102	BCL	CMB-C2B-C1B	-3.49	123.11	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	101	SPO	C9-C10-C11	-3.48	112.36	123.22
7	b	101	BCL	C1D-ND-C4D	-3.47	103.87	106.33
8	j	102	SPO	C14-C15-C16	-3.46	112.41	123.22
8	S	201	SPO	C10-C9-C7	-3.45	122.39	127.31
7	e	101	BCL	C1D-ND-C4D	-3.43	103.89	106.33
7	a	100	BCL	C4A-NA-C1A	3.43	108.25	106.71
8	t	102	SPO	C31-C32-C33	-3.43	119.40	127.66
7	M	407	BCL	CHA-C1A-NA	-3.43	118.55	126.40
7	i	101	BCL	C1D-ND-C4D	-3.42	103.91	106.33
8	J	101	SPO	C9-C10-C11	-3.41	112.58	123.22
7	o	101	BCL	C1D-ND-C4D	-3.41	103.92	106.33
10	M	403	U10	C12-C13-C14	-3.40	119.47	127.66
7	t	101	BCL	CMB-C2B-C1B	-3.39	123.25	128.46
8	r	102	SPO	C31-C32-C33	-3.38	119.52	127.66
8	E	201	SPO	C31-C32-C33	-3.38	119.53	127.66
7	M	407	BCL	C1D-ND-C4D	-3.37	103.94	106.33
7	f	101	BCL	C1D-ND-C4D	-3.36	103.94	106.33
10	M	403	U10	C27-C28-C29	-3.36	119.56	127.66
8	f	102	SPO	C14-C15-C16	-3.35	112.75	123.22
8	j	102	SPO	C31-C32-C33	-3.35	119.60	127.66
8	S	202	SPO	C9-C10-C11	-3.34	112.79	123.22
7	L	301	BCL	C1D-ND-C4D	-3.31	103.98	106.33
7	t	101	BCL	C1D-ND-C4D	-3.31	103.98	106.33
8	G	201	SPO	C31-C32-C33	-3.30	119.71	127.66
7	a	100	BCL	CMB-C2B-C1B	-3.29	123.40	128.46
7	e	102	BCL	C1D-ND-C4D	-3.29	104.00	106.33
7	M	405	BCL	C1D-ND-C4D	-3.29	104.00	106.33
7	A	202	BCL	C1D-ND-C4D	-3.26	104.02	106.33
7	U	101	BCL	CHA-C1A-NA	-3.25	118.96	126.40
8	E	203	SPO	C9-C10-C11	-3.25	113.09	123.22
7	U	101	BCL	C1D-ND-C4D	-3.24	104.03	106.33
7	b	101	BCL	C1-C2-C3	-3.23	120.45	126.04
8	j	102	SPO	C10-C9-C7	-3.22	122.71	127.31
7	b	102	BCL	C1D-ND-C4D	-3.21	104.06	106.33
7	D	101	BCL	C1D-ND-C4D	-3.21	104.06	106.33
7	K	102	BCL	C1D-ND-C4D	-3.19	104.07	106.33
7	s	101	BCL	C1D-ND-C4D	-3.19	104.07	106.33
7	I	101	BCL	C1D-ND-C4D	-3.19	104.07	106.33
7	n	101	BCL	CMB-C2B-C3B	3.19	130.64	124.68
7	r	103	BCL	C1D-ND-C4D	-3.19	104.07	106.33
7	O	101	BCL	C1D-ND-C4D	-3.18	104.08	106.33
7	U	101	BCL	CMB-C2B-C1B	-3.18	123.58	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	102	BCL	C1D-ND-C4D	-3.17	104.08	106.33
9	M	408	BPH	OBD-CAD-CBD	-3.16	121.18	125.82
7	n	102	BCL	C1D-ND-C4D	-3.16	104.09	106.33
9	L	302	BPH	OBD-CAD-CBD	-3.16	121.19	125.82
7	U	102	BCL	C1D-ND-C4D	-3.14	104.10	106.33
7	J	102	BCL	C1D-ND-C4D	-3.14	104.11	106.33
7	g	102	BCL	C4A-NA-C1A	3.14	108.12	106.71
7	s	102	BCL	CHA-C1A-NA	-3.14	119.21	126.40
8	N	201	SPO	C31-C32-C33	-3.13	120.11	127.66
7	d	101	BCL	CMB-C2B-C3B	3.13	130.54	124.68
7	g	102	BCL	C1D-ND-C4D	-3.13	104.11	106.33
7	s	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
7	M	405	BCL	CHA-C1A-NA	-3.11	119.27	126.40
7	e	101	BCL	CMB-C2B-C3B	3.11	130.50	124.68
7	b	101	BCL	CMB-C2B-C3B	3.10	130.48	124.68
8	b	103	SPO	C10-C9-C7	-3.09	122.90	127.31
7	k	101	BCL	CMB-C2B-C3B	3.09	130.46	124.68
7	r	103	BCL	CMB-C2B-C1B	-3.08	123.72	128.46
7	T	101	BCL	CHA-C1A-NA	-3.08	119.35	126.40
7	M	405	BCL	C4A-NA-C1A	3.07	108.09	106.71
7	k	101	BCL	CHA-C1A-NA	-3.07	119.38	126.40
8	G	201	SPO	C10-C9-C7	-3.06	122.94	127.31
7	b	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
7	g	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
7	f	101	BCL	CHA-C1A-NA	-3.04	119.43	126.40
7	K	102	BCL	CHA-C1A-NA	-3.04	119.44	126.40
7	M	405	BCL	CMB-C2B-C3B	3.03	130.35	124.68
7	i	101	BCL	CMB-C2B-C3B	3.03	130.34	124.68
7	M	401	BCL	C4A-NA-C1A	3.02	108.06	106.71
7	o	101	BCL	CHA-C1A-NA	-3.01	119.49	126.40
7	I	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	j	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	g	101	BCL	CMB-C2B-C3B	3.01	130.32	124.68
7	n	102	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	f	101	BCL	CMB-C2B-C3B	3.01	130.31	124.68
7	L	301	BCL	CMB-C2B-C3B	3.01	130.31	124.68
7	d	101	BCL	CHA-C1A-NA	-3.01	119.51	126.40
7	b	102	BCL	C4A-NA-C1A	3.01	108.06	106.71
7	J	102	BCL	CHA-C1A-NA	-3.00	119.52	126.40
7	g	102	BCL	CHA-C1A-NA	-3.00	119.52	126.40
7	M	401	BCL	CHA-C1A-NA	-3.00	119.53	126.40
7	e	102	BCL	CHA-C1A-NA	-2.99	119.54	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	102	BCL	CHA-C1A-NA	-2.99	119.55	126.40
7	a	100	BCL	CHA-C1A-NA	-2.99	119.56	126.40
7	e	101	BCL	CHA-C1A-NA	-2.99	119.56	126.40
7	b	102	BCL	CHA-C1A-NA	-2.99	119.56	126.40
7	A	202	BCL	CHA-C1A-NA	-2.98	119.57	126.40
7	j	101	BCL	CMB-C2B-C3B	2.98	130.26	124.68
7	r	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
7	O	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
7	r	103	BCL	CHA-C1A-NA	-2.98	119.58	126.40
7	s	102	BCL	CMB-C2B-C3B	2.97	130.24	124.68
7	D	101	BCL	CHA-C1A-NA	-2.97	119.59	126.40
7	n	101	BCL	CHA-C1A-NA	-2.97	119.61	126.40
7	K	102	BCL	C4A-NA-C1A	2.96	108.04	106.71
7	I	101	BCL	C4A-NA-C1A	2.96	108.04	106.71
7	L	301	BCL	CHA-C1A-NA	-2.96	119.61	126.40
7	O	101	BCL	C4A-NA-C1A	2.95	108.03	106.71
7	r	101	BCL	CMB-C2B-C3B	2.95	130.19	124.68
7	r	103	BCL	C4A-NA-C1A	2.92	108.02	106.71
7	o	101	BCL	CMB-C2B-C3B	2.91	130.12	124.68
7	i	101	BCL	CHA-C1A-NA	-2.91	119.74	126.40
7	t	101	BCL	CHA-C1A-NA	-2.89	119.78	126.40
7	F	102	BCL	C4A-NA-C1A	2.89	108.00	106.71
7	M	405	BCL	C2A-C1A-CHA	2.87	128.88	123.86
8	o	102	SPO	C10-C9-C7	-2.84	123.25	127.31
7	L	301	BCL	C2A-C1A-CHA	2.84	128.82	123.86
7	D	101	BCL	CMB-C2B-C3B	2.83	129.97	124.68
7	J	102	BCL	C4A-NA-C1A	2.82	107.97	106.71
7	e	102	BCL	C4A-NA-C1A	2.82	107.97	106.71
7	U	102	BCL	CHA-C1A-NA	-2.81	119.95	126.40
7	T	101	BCL	C4A-NA-C1A	2.79	107.96	106.71
7	n	102	BCL	C4A-NA-C1A	2.78	107.96	106.71
7	a	100	BCL	C2A-C1A-CHA	2.78	128.72	123.86
10	L	303	U10	C1M-C1-C6	-2.77	119.87	124.40
8	M	404	SPO	C14-C15-C16	-2.77	114.57	123.22
7	I	101	BCL	CMB-C2B-C3B	2.76	129.85	124.68
7	A	202	BCL	CMB-C2B-C3B	2.75	129.83	124.68
8	I	102	SPO	C8-C7-C9	2.74	137.34	122.73
7	M	401	BCL	CMB-C2B-C3B	2.74	129.81	124.68
7	r	101	BCL	C2A-C1A-CHA	2.74	128.65	123.86
7	e	102	BCL	CMB-C2B-C3B	2.73	129.79	124.68
7	e	101	BCL	C1-C2-C3	-2.73	121.33	126.04
11	M	406	3PE	O31-C31-C32	2.72	120.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	102	BCL	CMB-C2B-C3B	2.72	129.76	124.68
7	O	101	BCL	CMB-C2B-C3B	2.71	129.75	124.68
10	L	305	U10	C1M-C1-C6	-2.71	119.99	124.40
7	U	102	BCL	CMB-C2B-C3B	2.70	129.74	124.68
7	K	102	BCL	CMB-C2B-C3B	2.70	129.73	124.68
10	M	403	U10	C37-C38-C39	-2.69	118.55	127.75
7	I	101	BCL	C2A-C1A-CHA	2.68	128.55	123.86
7	M	407	BCL	C4A-NA-C1A	2.68	107.91	106.71
7	b	102	BCL	CMB-C2B-C3B	2.67	129.67	124.68
7	J	102	BCL	CMB-C2B-C3B	2.66	129.66	124.68
7	D	101	BCL	C4A-NA-C1A	2.66	107.90	106.71
7	M	405	BCL	C1C-NC-C4C	2.65	107.90	106.71
7	T	101	BCL	CMB-C2B-C3B	2.65	129.64	124.68
7	s	101	BCL	CMB-C2B-C3B	2.65	129.63	124.68
7	b	102	BCL	C2A-C1A-CHA	2.65	128.48	123.86
7	A	202	BCL	C4A-NA-C1A	2.64	107.89	106.71
7	t	101	BCL	C2A-C1A-CHA	2.63	128.45	123.86
7	n	102	BCL	CMB-C2B-C3B	2.62	129.59	124.68
7	e	102	BCL	C2A-C1A-CHA	2.62	128.44	123.86
8	E	201	SPO	C10-C9-C7	-2.62	123.58	127.31
7	e	101	BCL	C17-C16-C15	2.61	125.25	113.24
7	U	102	BCL	C2A-C1A-CHA	2.61	128.43	123.86
7	n	102	BCL	C2A-C1A-CHA	2.61	128.42	123.86
7	M	407	BCL	OBB-CAB-CBB	-2.61	114.31	120.17
7	M	401	BCL	C2A-C1A-CHA	2.59	128.39	123.86
7	D	101	BCL	C2A-C1A-CHA	2.59	128.39	123.86
7	i	101	BCL	C2A-C1A-CHA	2.59	128.39	123.86
8	A	201	SPO	C14-C15-C16	-2.58	115.15	123.22
7	o	101	BCL	C1-C2-C3	-2.58	121.57	126.04
8	k	102	SPO	C10-C9-C7	-2.58	123.63	127.31
11	d	103	3PE	O31-C31-C32	2.58	120.00	111.91
7	s	101	BCL	C4A-NA-C1A	2.57	107.86	106.71
7	U	101	BCL	C4A-NA-C1A	2.57	107.86	106.71
7	O	101	BCL	C2A-C1A-CHA	2.57	128.35	123.86
7	k	101	BCL	C2A-C1A-CHA	2.56	128.34	123.86
7	n	102	BCL	C11-C10-C8	-2.56	107.65	115.92
7	J	102	BCL	C2A-C1A-CHA	2.56	128.33	123.86
7	g	102	BCL	CMB-C2B-C3B	2.56	129.46	124.68
7	F	102	BCL	C2A-C1A-CHA	2.55	128.32	123.86
7	g	101	BCL	C2A-C1A-CHA	2.54	128.31	123.86
11	H	302	3PE	O31-C31-C32	2.54	119.87	111.91
7	n	101	BCL	C2A-C1A-CHA	2.54	128.29	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	o	101	BCL	C2A-C1A-CHA	2.54	128.29	123.86
7	g	102	BCL	C2A-C1A-CHA	2.53	128.28	123.86
7	f	101	BCL	C2A-C1A-CHA	2.53	128.28	123.86
7	M	407	BCL	CMB-C2B-C3B	2.53	129.41	124.68
11	M	409	3PE	O31-C31-C32	2.52	119.82	111.91
8	K	101	SPO	C8-C7-C9	2.52	136.16	122.73
7	U	101	BCL	C1C-NC-C4C	2.52	107.84	106.71
7	j	101	BCL	C2A-C1A-CHA	2.51	128.25	123.86
7	M	407	BCL	C2A-C1A-CHA	2.51	128.25	123.86
9	L	302	BPH	CMB-C2B-C3B	2.51	129.37	124.68
10	L	304	U10	C12-C13-C14	-2.51	119.18	127.75
9	M	408	BPH	C6-C5-C3	2.50	120.01	113.45
7	e	101	BCL	OBB-CAB-CBB	-2.49	114.56	120.17
7	U	101	BCL	C2A-C1A-CHA	2.48	128.19	123.86
7	k	101	BCL	OBB-CAB-CBB	-2.47	114.60	120.17
7	d	101	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
7	b	101	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
7	T	101	BCL	C2A-C1A-CHA	2.47	128.18	123.86
7	e	101	BCL	C6-C7-C8	-2.47	107.95	115.92
7	d	101	BCL	C2A-C1A-CHA	2.46	128.17	123.86
11	d	104	3PE	O31-C31-C32	2.46	119.64	111.91
8	f	102	SPO	C10-C9-C7	-2.46	123.80	127.31
8	k	102	SPO	C36-C37-C38	-2.46	119.33	127.75
7	K	102	BCL	C2A-C1A-CHA	2.46	128.16	123.86
10	M	403	U10	C1M-C1-C6	-2.46	120.39	124.40
11	H	301	3PE	O31-C31-C32	2.46	119.62	111.91
7	e	101	BCL	C2A-C1A-CHA	2.46	128.16	123.86
8	S	202	SPO	C40-C38-C39	2.44	120.00	114.60
7	t	101	BCL	CMB-C2B-C3B	2.44	129.25	124.68
7	r	103	BCL	C2A-C1A-CHA	2.44	128.12	123.86
8	i	102	SPO	C40-C38-C39	2.44	119.98	114.60
7	i	101	BCL	OBB-CAB-CBB	-2.43	114.69	120.17
7	s	102	BCL	C2A-C1A-CHA	2.43	128.11	123.86
9	L	302	BPH	OBB-CAB-CBB	-2.43	114.70	120.17
7	n	101	BCL	OBB-CAB-CBB	-2.43	114.71	120.17
11	L	306	3PE	O31-C31-C32	2.42	119.50	111.91
7	e	102	BCL	C1C-NC-C4C	2.42	107.79	106.71
7	M	405	BCL	OBB-CAB-CBB	-2.42	114.73	120.17
8	d	102	SPO	C40-C38-C39	2.40	119.90	114.60
8	M	404	SPO	C40-C38-C39	2.38	119.86	114.60
9	M	408	BPH	C1-C2-C3	-2.38	121.92	126.04
7	F	102	BCL	C1C-NC-C4C	2.38	107.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	100	BCL	CMB-C2B-C3B	2.38	129.12	124.68
8	i	102	SPO	C10-C9-C7	-2.37	123.92	127.31
7	M	407	BCL	C16-C15-C13	2.37	123.57	115.92
7	A	202	BCL	C17-C16-C15	2.37	124.11	113.24
7	O	101	BCL	C1C-NC-C4C	2.36	107.77	106.71
8	F	101	SPO	C9-C10-C11	-2.36	115.85	123.22
7	b	101	BCL	C2A-C1A-CHA	2.36	127.98	123.86
8	K	101	SPO	C40-C38-C39	2.36	119.81	114.60
8	E	202	SPO	C40-C38-C39	2.35	119.79	114.60
7	A	202	BCL	C2A-C1A-CHA	2.35	127.96	123.86
9	L	302	BPH	CMD-C2D-C3D	2.34	129.06	124.68
7	M	405	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
7	A	202	BCL	C1C-NC-C4C	2.34	107.76	106.71
9	M	408	BPH	CMD-C2D-C3D	2.33	129.04	124.68
8	F	101	SPO	C40-C38-C39	2.33	119.75	114.60
7	L	301	BCL	C4A-NA-C1A	2.33	107.75	106.71
8	t	102	SPO	C40-C38-C39	2.33	119.75	114.60
8	R	101	SPO	C40-C38-C39	2.32	119.72	114.60
8	F	101	SPO	C8-C7-C9	2.31	135.06	122.73
8	A	201	SPO	C40-C38-C39	2.31	119.71	114.60
7	n	101	BCL	C1C-NC-C4C	2.31	107.74	106.71
10	L	305	U10	C7-C6-C5	2.30	121.25	118.48
8	B	101	SPO	C40-C38-C39	2.30	119.68	114.60
8	o	102	SPO	C40-C38-C39	2.30	119.68	114.60
7	i	101	BCL	C4B-C3B-CAB	-2.30	122.69	127.13
7	f	101	BCL	C4B-C3B-CAB	-2.29	122.70	127.13
7	L	301	BCL	OBB-CAB-CBB	-2.29	115.01	120.17
8	k	102	SPO	C40-C38-C39	2.28	119.64	114.60
7	s	101	BCL	C1C-NC-C4C	2.28	107.73	106.71
8	J	101	SPO	C40-C38-C39	2.28	119.64	114.60
7	j	101	BCL	OBB-CAB-CBB	-2.28	115.05	120.17
7	s	102	BCL	C4B-C3B-CAB	-2.27	122.74	127.13
7	f	101	BCL	OBB-CAB-CBB	-2.27	115.06	120.17
7	U	101	BCL	CMB-C2B-C3B	2.27	128.92	124.68
7	M	407	BCL	CAA-CBA-CGA	2.26	119.87	113.25
8	S	201	SPO	C40-C38-C39	2.26	119.59	114.60
7	J	102	BCL	C16-C15-C13	-2.26	108.62	115.92
7	n	102	BCL	C17-C16-C15	2.26	123.61	113.24
7	b	101	BCL	C4B-C3B-CAB	-2.26	122.77	127.13
8	K	103	SPO	C40-C38-C39	2.25	119.58	114.60
8	i	102	SPO	C36-C37-C38	-2.25	120.06	127.75
8	b	103	SPO	C40-C38-C39	2.25	119.57	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	r	103	BCL	CMB-C2B-C3B	2.23	128.86	124.68
7	O	101	BCL	C4B-C3B-CAB	-2.23	122.82	127.13
7	d	101	BCL	C1C-NC-C4C	2.22	107.71	106.71
7	T	101	BCL	C1C-NC-C4C	2.22	107.70	106.71
7	g	102	BCL	C1C-NC-C4C	2.22	107.70	106.71
8	I	102	SPO	C40-C38-C39	2.22	119.50	114.60
7	A	202	BCL	C4B-C3B-CAB	-2.22	122.84	127.13
7	g	101	BCL	C4B-C3B-CAB	-2.21	122.85	127.13
7	g	101	BCL	OBB-CAB-CBB	-2.21	115.19	120.17
8	S	202	SPO	C36-C37-C38	-2.21	120.20	127.75
7	k	101	BCL	C4B-C3B-CAB	-2.21	122.86	127.13
7	L	301	BCL	C4B-C3B-CAB	-2.21	122.87	127.13
8	D	102	SPO	C40-C38-C39	2.20	119.47	114.60
8	o	102	SPO	C36-C37-C38	-2.20	120.23	127.75
7	I	101	BCL	C1C-NC-C4C	2.20	107.69	106.71
8	I	102	SPO	C36-C37-C38	-2.20	120.24	127.75
7	e	101	BCL	C4B-C3B-CAB	-2.20	122.89	127.13
7	J	102	BCL	C1C-NC-C4C	2.19	107.69	106.71
7	s	102	BCL	OBB-CAB-CBB	-2.19	115.23	120.17
8	K	103	SPO	C36-C37-C38	-2.19	120.27	127.75
7	o	101	BCL	C4B-C3B-CAB	-2.19	122.90	127.13
7	g	101	BCL	C1-C2-C3	-2.19	122.26	126.04
7	b	102	BCL	C1C-NC-C4C	2.18	107.69	106.71
7	U	102	BCL	CHD-C4C-NC	-2.18	122.66	125.08
7	F	102	BCL	C4B-C3B-CAB	-2.18	122.92	127.13
7	K	102	BCL	C1C-NC-C4C	2.17	107.68	106.71
7	r	101	BCL	OBB-CAB-CBB	-2.17	115.29	120.17
7	n	101	BCL	C4B-C3B-CAB	-2.16	122.95	127.13
7	n	102	BCL	C1C-NC-C4C	2.16	107.68	106.71
7	r	101	BCL	C4B-C3B-CAB	-2.16	122.95	127.13
8	M	404	SPO	C36-C37-C38	-2.16	120.36	127.75
8	E	201	SPO	C40-C38-C39	2.16	119.37	114.60
7	D	101	BCL	C4B-C3B-CAB	-2.16	122.96	127.13
7	e	101	BCL	CAA-CBA-CGA	-2.15	106.97	113.25
8	E	203	SPO	C40-C38-C39	2.15	119.34	114.60
9	L	302	BPH	C11-C10-C8	-2.14	108.99	115.92
8	f	102	SPO	C40-C38-C39	2.14	119.32	114.60
7	n	102	BCL	C4B-C3B-CAB	-2.13	123.01	127.13
7	b	102	BCL	C4B-C3B-CAB	-2.13	123.02	127.13
7	T	101	BCL	C4B-C3B-CAB	-2.12	123.04	127.13
7	d	101	BCL	C4B-C3B-CAB	-2.12	123.04	127.13
8	O	102	SPO	C40-C38-C39	2.11	119.27	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	101	BCL	C1C-NC-C4C	2.11	107.66	106.71
7	J	102	BCL	C4B-C3B-CAB	-2.10	123.06	127.13
8	S	201	SPO	C36-C37-C38	-2.10	120.57	127.75
8	f	102	SPO	C36-C37-C38	-2.10	120.57	127.75
9	M	408	BPH	O2D-CGD-CBD	2.10	113.65	111.00
7	e	101	BCL	C1C-NC-C4C	2.10	107.65	106.71
7	M	401	BCL	C4B-C3B-CAB	-2.09	123.09	127.13
7	M	401	BCL	C1-C2-C3	-2.08	122.44	126.04
9	M	408	BPH	CMB-C2B-C3B	2.08	128.57	124.68
7	o	101	BCL	OBB-CAB-CBB	-2.07	115.51	120.17
7	K	102	BCL	C4B-C3B-CAB	-2.07	123.13	127.13
8	E	203	SPO	C8-C7-C9	2.07	133.75	122.73
7	b	101	BCL	C1C-NC-C4C	2.07	107.64	106.71
7	L	301	BCL	C1C-NC-C4C	2.06	107.63	106.71
7	M	401	BCL	C2D-C1D-ND	2.06	111.62	110.10
8	r	102	SPO	C40-C38-C39	2.06	119.15	114.60
9	L	302	BPH	O2D-CGD-CBD	2.06	113.60	111.00
7	I	101	BCL	C4B-C3B-CAB	-2.06	123.16	127.13
7	U	102	BCL	C4B-C3B-CAB	-2.06	123.16	127.13
7	j	101	BCL	C4B-C3B-CAB	-2.05	123.18	127.13
8	O	102	SPO	C36-C37-C38	-2.04	120.78	127.75
7	a	100	BCL	C1C-NC-C4C	2.04	107.62	106.71
8	j	102	SPO	C40-C38-C39	2.03	119.10	114.60
8	S	202	SPO	C8-C7-C9	2.03	133.56	122.73
7	M	407	BCL	O2A-CGA-O1A	2.03	128.70	123.59
8	F	101	SPO	C36-C37-C38	-2.02	120.85	127.75
8	d	102	SPO	C36-C37-C38	-2.02	120.86	127.75
7	M	407	BCL	O2A-CGA-CBA	-2.01	105.58	111.91
8	I	102	SPO	C9-C10-C11	-2.01	116.94	123.22
7	g	102	BCL	C4B-C3B-CAB	-2.01	123.25	127.13
7	D	101	BCL	OBB-CAB-CBB	-2.01	115.66	120.17
8	D	102	SPO	C36-C37-C38	-2.00	120.90	127.75
8	E	203	SPO	C36-C37-C38	-2.00	120.90	127.75
8	J	101	SPO	C8-C7-C9	2.00	133.39	122.73
10	L	304	U10	C1M-C1-C6	-2.00	121.14	124.40

There are no chirality outliers.

All (712) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	a	100	BCL	C2C-C3C-CAC-CBC
7	a	100	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	b	101	BCL	C4-C3-C5-C6
7	A	202	BCL	C1A-C2A-CAA-CBA
7	A	202	BCL	C3A-C2A-CAA-CBA
7	M	407	BCL	C1A-C2A-CAA-CBA
7	M	407	BCL	C2-C1-O2A-CGA
7	n	102	BCL	C2-C3-C5-C6
7	n	102	BCL	C4-C3-C5-C6
8	D	102	SPO	C12-C14-C15-C16
8	b	103	SPO	C5-C6-C7-C8
8	b	103	SPO	C5-C6-C7-C9
8	b	103	SPO	C12-C14-C15-C16
8	b	103	SPO	C25-C26-C27-C28
8	b	103	SPO	C28-C30-C31-C32
8	A	201	SPO	C5-C6-C7-C8
8	A	201	SPO	C5-C6-C7-C9
8	A	201	SPO	C10-C11-C12-C13
8	A	201	SPO	C10-C11-C12-C14
8	A	201	SPO	C28-C30-C31-C32
8	A	201	SPO	C33-C35-C36-C37
8	E	201	SPO	C12-C14-C15-C16
8	E	201	SPO	C15-C16-C17-C18
8	E	201	SPO	C15-C16-C17-C19
8	E	201	SPO	C33-C35-C36-C37
8	E	202	SPO	C28-C30-C31-C32
8	E	203	SPO	C11-C10-C9-C7
8	E	203	SPO	C12-C14-C15-C16
8	E	203	SPO	C15-C16-C17-C18
8	E	203	SPO	C15-C16-C17-C19
8	E	203	SPO	C32-C33-C35-C36
8	M	404	SPO	O1-C1-C4-C5
8	M	404	SPO	C2-C1-C4-C5
8	M	404	SPO	C3-C1-C4-C5
8	M	404	SPO	C22-C23-C25-C26
8	M	404	SPO	C24-C23-C25-C26
8	d	102	SPO	C11-C10-C9-C7
8	d	102	SPO	C10-C11-C12-C13
8	d	102	SPO	C10-C11-C12-C14
8	d	102	SPO	C12-C14-C15-C16
8	d	102	SPO	C15-C16-C17-C18
8	d	102	SPO	C15-C16-C17-C19
8	B	101	SPO	C12-C14-C15-C16
8	t	102	SPO	O1-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
8	t	102	SPO	C12-C14-C15-C16
8	S	201	SPO	C5-C6-C7-C8
8	S	201	SPO	C5-C6-C7-C9
8	S	201	SPO	C10-C11-C12-C13
8	S	201	SPO	C10-C11-C12-C14
8	S	201	SPO	C12-C14-C15-C16
8	S	201	SPO	C15-C16-C17-C18
8	S	201	SPO	C15-C16-C17-C19
8	S	201	SPO	C22-C23-C25-C26
8	S	201	SPO	C24-C23-C25-C26
8	S	201	SPO	C32-C33-C35-C36
8	S	201	SPO	C33-C35-C36-C37
8	S	202	SPO	C11-C10-C9-C7
8	S	202	SPO	C12-C14-C15-C16
8	S	202	SPO	C15-C16-C17-C18
8	S	202	SPO	C15-C16-C17-C19
8	S	202	SPO	C22-C23-C25-C26
8	S	202	SPO	C24-C23-C25-C26
8	r	102	SPO	C11-C10-C9-C7
8	r	102	SPO	C15-C16-C17-C18
8	r	102	SPO	C15-C16-C17-C19
8	O	102	SPO	C12-C14-C15-C16
8	R	101	SPO	C12-C14-C15-C16
8	R	101	SPO	C25-C26-C27-C28
8	R	101	SPO	C33-C35-C36-C37
8	o	102	SPO	C10-C11-C12-C13
8	o	102	SPO	C10-C11-C12-C14
8	o	102	SPO	C12-C14-C15-C16
8	o	102	SPO	C15-C16-C17-C18
8	o	102	SPO	C15-C16-C17-C19
8	o	102	SPO	C22-C23-C25-C26
8	o	102	SPO	C24-C23-C25-C26
8	o	102	SPO	C33-C35-C36-C37
8	K	101	SPO	C12-C14-C15-C16
8	K	101	SPO	C15-C16-C17-C18
8	K	101	SPO	C15-C16-C17-C19
8	K	101	SPO	C33-C35-C36-C37
8	K	103	SPO	C12-C14-C15-C16
8	K	103	SPO	C15-C16-C17-C18
8	K	103	SPO	C15-C16-C17-C19
8	K	103	SPO	C32-C33-C35-C36
8	K	103	SPO	C33-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
8	N	201	SPO	C12-C14-C15-C16
8	N	201	SPO	C15-C16-C17-C18
8	N	201	SPO	C15-C16-C17-C19
8	k	102	SPO	C12-C14-C15-C16
8	k	102	SPO	C15-C16-C17-C18
8	k	102	SPO	C15-C16-C17-C19
8	k	102	SPO	C25-C26-C27-C28
8	j	102	SPO	C2-C1-C4-C5
8	j	102	SPO	C3-C1-C4-C5
8	j	102	SPO	C12-C14-C15-C16
8	j	102	SPO	C15-C16-C17-C18
8	j	102	SPO	C15-C16-C17-C19
8	j	102	SPO	C33-C35-C36-C37
8	I	102	SPO	C10-C11-C12-C13
8	I	102	SPO	C10-C11-C12-C14
8	I	102	SPO	C12-C14-C15-C16
8	I	102	SPO	C15-C16-C17-C18
8	I	102	SPO	C15-C16-C17-C19
8	J	101	SPO	C12-C14-C15-C16
8	J	101	SPO	C15-C16-C17-C18
8	J	101	SPO	C15-C16-C17-C19
8	i	102	SPO	C5-C6-C7-C8
8	i	102	SPO	C5-C6-C7-C9
8	i	102	SPO	C12-C14-C15-C16
8	F	101	SPO	C11-C10-C9-C7
8	F	101	SPO	C12-C14-C15-C16
8	F	101	SPO	C15-C16-C17-C18
8	F	101	SPO	C15-C16-C17-C19
8	F	101	SPO	C33-C35-C36-C37
8	G	201	SPO	C5-C6-C7-C8
8	G	201	SPO	C5-C6-C7-C9
8	G	201	SPO	C12-C14-C15-C16
8	G	201	SPO	C15-C16-C17-C18
8	G	201	SPO	C15-C16-C17-C19
8	G	201	SPO	C22-C23-C25-C26
8	G	201	SPO	C24-C23-C25-C26
8	f	102	SPO	C10-C11-C12-C13
8	f	102	SPO	C10-C11-C12-C14
8	f	102	SPO	C12-C14-C15-C16
8	f	102	SPO	C15-C16-C17-C19
8	f	102	SPO	C25-C26-C27-C28
9	L	302	BPH	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	L	302	BPH	C2C-C3C-CAC-CBC
9	M	408	BPH	C4-C3-C5-C6
10	L	303	U10	C16-C17-C18-C19
10	M	403	U10	C21-C22-C23-C24
11	L	306	3PE	C1-O11-P-O12
11	L	306	3PE	C1-O11-P-O13
11	L	306	3PE	C11-O13-P-O11
11	L	306	3PE	C11-O13-P-O12
11	L	306	3PE	O13-C11-C12-N
11	M	406	3PE	C11-O13-P-O12
11	M	406	3PE	C11-O13-P-O14
11	M	406	3PE	C22-C21-O21-C2
11	M	409	3PE	C1-O11-P-O14
11	M	409	3PE	C11-O13-P-O14
11	M	409	3PE	O13-C11-C12-N
11	H	301	3PE	O13-C11-C12-N
11	H	302	3PE	C12-C11-O13-P
11	H	302	3PE	O13-C11-C12-N
11	d	103	3PE	C1-O11-P-O12
11	d	103	3PE	C1-O11-P-O14
11	d	103	3PE	O13-C11-C12-N
11	d	103	3PE	O22-C21-O21-C2
11	d	103	3PE	C22-C21-O21-C2
11	L	306	3PE	O32-C31-O31-C3
11	M	406	3PE	O22-C21-O21-C2
7	b	102	BCL	C4-C3-C5-C6
7	n	101	BCL	C4-C3-C5-C6
7	b	101	BCL	C2-C3-C5-C6
7	T	101	BCL	C2A-CAA-CBA-CGA
7	s	101	BCL	C2A-CAA-CBA-CGA
7	U	102	BCL	C2A-CAA-CBA-CGA
11	L	306	3PE	C32-C31-O31-C3
8	A	201	SPO	C11-C10-C9-C7
8	E	202	SPO	C12-C14-C15-C16
8	M	404	SPO	C11-C10-C9-C7
8	M	404	SPO	C12-C14-C15-C16
8	d	102	SPO	C25-C26-C27-C28
8	B	101	SPO	C25-C26-C27-C28
8	S	202	SPO	C25-C26-C27-C28
8	r	102	SPO	C20-C21-C22-C23
8	K	103	SPO	C25-C26-C27-C28
8	j	102	SPO	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
8	J	101	SPO	C11-C10-C9-C7
11	H	302	3PE	C22-C21-O21-C2
7	b	102	BCL	C2-C3-C5-C6
8	M	404	SPO	C32-C33-C35-C36
9	M	408	BPH	C2-C3-C5-C6
8	D	102	SPO	C33-C35-C36-C37
8	E	201	SPO	C28-C30-C31-C32
8	d	102	SPO	C28-C30-C31-C32
8	S	202	SPO	C33-C35-C36-C37
8	R	101	SPO	C28-C30-C31-C32
8	J	101	SPO	C28-C30-C31-C32
8	i	102	SPO	C28-C30-C31-C32
8	i	102	SPO	C33-C35-C36-C37
8	G	201	SPO	C28-C30-C31-C32
10	L	303	U10	C9-C11-C12-C13
11	M	406	3PE	C32-C33-C34-C35
11	H	302	3PE	O22-C21-O21-C2
8	A	201	SPO	C25-C26-C27-C28
8	O	102	SPO	C11-C10-C9-C7
8	R	101	SPO	C11-C10-C9-C7
8	K	103	SPO	C11-C10-C9-C7
8	i	102	SPO	C25-C26-C27-C28
11	d	104	3PE	O21-C2-C3-O31
11	d	103	3PE	C24-C25-C26-C27
7	d	101	BCL	C4-C3-C5-C6
7	j	101	BCL	C4-C3-C5-C6
7	J	102	BCL	C4-C3-C5-C6
7	n	101	BCL	C2-C3-C5-C6
7	g	102	BCL	C2A-CAA-CBA-CGA
8	D	102	SPO	C10-C11-C12-C13
8	D	102	SPO	C15-C16-C17-C18
8	b	103	SPO	C10-C11-C12-C13
8	b	103	SPO	C24-C23-C25-C26
8	A	201	SPO	C24-C23-C25-C26
8	E	201	SPO	C5-C6-C7-C8
8	E	201	SPO	C10-C11-C12-C13
8	E	201	SPO	C24-C23-C25-C26
8	E	202	SPO	C10-C11-C12-C13
8	E	202	SPO	C15-C16-C17-C18
8	E	203	SPO	C10-C11-C12-C13
8	E	203	SPO	C24-C23-C25-C26
8	M	404	SPO	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
8	M	404	SPO	C15-C16-C17-C18
8	d	102	SPO	C24-C23-C25-C26
8	B	101	SPO	C10-C11-C12-C13
8	B	101	SPO	C15-C16-C17-C18
8	t	102	SPO	C5-C6-C7-C8
8	t	102	SPO	C24-C23-C25-C26
8	r	102	SPO	C5-C6-C7-C8
8	r	102	SPO	C10-C11-C12-C13
8	r	102	SPO	C24-C23-C25-C26
8	O	102	SPO	C10-C11-C12-C13
8	O	102	SPO	C15-C16-C17-C18
8	R	101	SPO	C10-C11-C12-C13
8	R	101	SPO	C15-C16-C17-C18
8	K	101	SPO	C10-C11-C12-C13
8	K	101	SPO	C24-C23-C25-C26
8	K	103	SPO	C10-C11-C12-C13
8	N	201	SPO	C10-C11-C12-C13
8	N	201	SPO	C24-C23-C25-C26
8	k	102	SPO	C10-C11-C12-C13
8	j	102	SPO	C10-C11-C12-C13
8	j	102	SPO	C24-C23-C25-C26
8	J	101	SPO	C24-C23-C25-C26
8	i	102	SPO	C10-C11-C12-C13
8	i	102	SPO	C24-C23-C25-C26
8	F	101	SPO	C10-C11-C12-C13
8	F	101	SPO	C24-C23-C25-C26
8	G	201	SPO	C10-C11-C12-C13
8	f	102	SPO	C15-C16-C17-C18
8	D	102	SPO	C10-C11-C12-C14
8	D	102	SPO	C15-C16-C17-C19
8	b	103	SPO	C10-C11-C12-C14
8	b	103	SPO	C22-C23-C25-C26
8	A	201	SPO	C22-C23-C25-C26
8	E	201	SPO	C5-C6-C7-C9
8	E	201	SPO	C10-C11-C12-C14
8	E	201	SPO	C22-C23-C25-C26
8	E	202	SPO	C10-C11-C12-C14
8	E	202	SPO	C15-C16-C17-C19
8	E	203	SPO	C10-C11-C12-C14
8	E	203	SPO	C22-C23-C25-C26
8	M	404	SPO	C10-C11-C12-C14
8	M	404	SPO	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
8	d	102	SPO	C22-C23-C25-C26
8	B	101	SPO	C10-C11-C12-C14
8	B	101	SPO	C15-C16-C17-C19
8	t	102	SPO	C5-C6-C7-C9
8	t	102	SPO	C22-C23-C25-C26
8	r	102	SPO	C5-C6-C7-C9
8	r	102	SPO	C22-C23-C25-C26
8	O	102	SPO	C10-C11-C12-C14
8	O	102	SPO	C15-C16-C17-C19
8	O	102	SPO	C22-C23-C25-C26
8	R	101	SPO	C15-C16-C17-C19
8	K	101	SPO	C10-C11-C12-C14
8	K	101	SPO	C22-C23-C25-C26
8	K	103	SPO	C10-C11-C12-C14
8	N	201	SPO	C10-C11-C12-C14
8	N	201	SPO	C22-C23-C25-C26
8	k	102	SPO	C10-C11-C12-C14
8	j	102	SPO	C10-C11-C12-C14
8	j	102	SPO	C22-C23-C25-C26
8	J	101	SPO	C22-C23-C25-C26
8	i	102	SPO	C10-C11-C12-C14
8	i	102	SPO	C22-C23-C25-C26
8	F	101	SPO	C22-C23-C25-C26
8	G	201	SPO	C10-C11-C12-C14
8	f	102	SPO	C22-C23-C25-C26
11	M	409	3PE	C32-C31-O31-C3
11	d	104	3PE	C32-C31-O31-C3
7	e	102	BCL	C15-C16-C17-C18
7	J	102	BCL	C15-C16-C17-C18
7	M	407	BCL	C10-C11-C12-C13
11	M	406	3PE	C21-C22-C23-C24
11	M	409	3PE	C31-C32-C33-C34
11	M	409	3PE	C21-C22-C23-C24
11	H	301	3PE	C21-C22-C23-C24
7	g	101	BCL	C8-C10-C11-C12
11	M	406	3PE	C31-C32-C33-C34
11	d	103	3PE	C21-C22-C23-C24
8	D	102	SPO	C11-C10-C9-C7
8	D	102	SPO	C25-C26-C27-C28
8	E	202	SPO	C11-C10-C9-C7
8	B	101	SPO	C11-C10-C9-C7
8	r	102	SPO	C12-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
8	r	102	SPO	C25-C26-C27-C28
8	o	102	SPO	C25-C26-C27-C28
8	N	201	SPO	C25-C26-C27-C28
8	I	102	SPO	C25-C26-C27-C28
8	J	101	SPO	C25-C26-C27-C28
8	F	101	SPO	C25-C26-C27-C28
7	e	102	BCL	C2A-CAA-CBA-CGA
7	b	102	BCL	C2A-CAA-CBA-CGA
7	O	101	BCL	C2A-CAA-CBA-CGA
7	K	102	BCL	C2A-CAA-CBA-CGA
7	F	102	BCL	C2A-CAA-CBA-CGA
8	b	103	SPO	C33-C35-C36-C37
8	E	203	SPO	C33-C35-C36-C37
8	M	404	SPO	C28-C30-C31-C32
8	B	101	SPO	C33-C35-C36-C37
8	S	202	SPO	C28-C30-C31-C32
8	k	102	SPO	C33-C35-C36-C37
8	G	201	SPO	C33-C35-C36-C37
8	f	102	SPO	C28-C30-C31-C32
8	f	102	SPO	C33-C35-C36-C37
10	M	403	U10	C14-C16-C17-C18
10	M	403	U10	C29-C31-C32-C33
7	j	101	BCL	C13-C15-C16-C17
11	M	409	3PE	O32-C31-O31-C3
11	d	104	3PE	O32-C31-O31-C3
11	H	301	3PE	C3B-C3C-C3D-C3E
11	M	406	3PE	C11-O13-P-O11
11	M	409	3PE	C11-O13-P-O11
11	H	301	3PE	C1-O11-P-O13
11	d	103	3PE	C1-O11-P-O13
11	H	302	3PE	C31-C32-C33-C34
7	D	101	BCL	C2A-CAA-CBA-CGA
11	H	302	3PE	C32-C31-O31-C3
8	E	201	SPO	C25-C26-C27-C28
8	E	202	SPO	C25-C26-C27-C28
8	t	102	SPO	C25-C26-C27-C28
8	S	201	SPO	C25-C26-C27-C28
8	O	102	SPO	C25-C26-C27-C28
8	G	201	SPO	C25-C26-C27-C28
11	L	306	3PE	C37-C38-C39-C3A
11	M	409	3PE	C35-C36-C37-C38
11	d	103	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
7	D	101	BCL	C16-C17-C18-C19
11	H	302	3PE	C22-C23-C24-C25
11	H	302	3PE	C23-C24-C25-C26
11	M	406	3PE	C3-C2-O21-C21
11	M	409	3PE	C24-C25-C26-C27
11	d	104	3PE	C33-C34-C35-C36
8	o	102	SPO	C34-C33-C35-C36
8	K	103	SPO	C34-C33-C35-C36
8	k	102	SPO	C34-C33-C35-C36
11	M	406	3PE	C3E-C3F-C3G-C3H
11	d	104	3PE	C26-C27-C28-C29
7	d	101	BCL	C2-C3-C5-C6
7	n	101	BCL	C6-C7-C8-C9
11	L	306	3PE	C32-C33-C34-C35
11	H	302	3PE	C26-C27-C28-C29
7	n	102	BCL	C2A-CAA-CBA-CGA
8	D	102	SPO	C24-C23-C25-C26
8	E	202	SPO	C24-C23-C25-C26
8	B	101	SPO	C24-C23-C25-C26
8	O	102	SPO	C24-C23-C25-C26
8	R	101	SPO	C24-C23-C25-C26
8	K	103	SPO	C24-C23-C25-C26
8	k	102	SPO	C24-C23-C25-C26
8	I	102	SPO	C24-C23-C25-C26
8	J	101	SPO	C10-C11-C12-C13
8	f	102	SPO	C24-C23-C25-C26
11	d	104	3PE	C25-C26-C27-C28
8	D	102	SPO	C22-C23-C25-C26
8	E	202	SPO	C22-C23-C25-C26
8	B	101	SPO	C22-C23-C25-C26
8	r	102	SPO	C10-C11-C12-C14
8	R	101	SPO	C10-C11-C12-C14
8	R	101	SPO	C22-C23-C25-C26
8	K	103	SPO	C22-C23-C25-C26
8	k	102	SPO	C22-C23-C25-C26
8	I	102	SPO	C22-C23-C25-C26
8	J	101	SPO	C10-C11-C12-C14
8	F	101	SPO	C10-C11-C12-C14
11	L	306	3PE	C22-C21-O21-C2
11	M	409	3PE	C22-C23-C24-C25
11	M	409	3PE	C25-C26-C27-C28
11	H	301	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
11	H	301	3PE	C23-C24-C25-C26
11	H	302	3PE	C24-C25-C26-C27
11	d	103	3PE	C33-C34-C35-C36
11	d	104	3PE	C27-C28-C29-C2A
11	M	406	3PE	O13-C11-C12-N
11	L	306	3PE	C35-C36-C37-C38
11	M	406	3PE	C24-C25-C26-C27
11	M	409	3PE	C38-C39-C3A-C3B
11	M	409	3PE	C26-C27-C28-C29
11	M	406	3PE	C28-C29-C2A-C2B
8	A	201	SPO	C12-C14-C15-C16
8	N	201	SPO	C11-C10-C9-C7
8	j	102	SPO	C11-C10-C9-C7
8	f	102	SPO	C11-C10-C9-C7
11	M	406	3PE	C3B-C3C-C3D-C3E
11	L	306	3PE	O22-C21-O21-C2
7	b	102	BCL	O2A-C1-C2-C3
7	n	102	BCL	O2A-C1-C2-C3
7	J	102	BCL	O2A-C1-C2-C3
11	L	306	3PE	C24-C25-C26-C27
7	J	102	BCL	C2A-CAA-CBA-CGA
11	H	302	3PE	O32-C31-O31-C3
7	L	301	BCL	C15-C16-C17-C18
11	L	306	3PE	C33-C34-C35-C36
11	d	103	3PE	C32-C33-C34-C35
11	L	306	3PE	C3B-C3C-C3D-C3E
7	k	101	BCL	C4-C3-C5-C6
9	L	302	BPH	C4-C3-C5-C6
7	n	101	BCL	C6-C7-C8-C10
8	k	102	SPO	C32-C33-C35-C36
9	L	302	BPH	C2-C3-C5-C6
7	I	101	BCL	C2A-CAA-CBA-CGA
7	j	101	BCL	C8-C10-C11-C12
11	d	104	3PE	C28-C29-C2A-C2B
11	M	409	3PE	C3E-C3F-C3G-C3H
8	B	101	SPO	C28-C30-C31-C32
8	r	102	SPO	C28-C30-C31-C32
11	H	301	3PE	C35-C36-C37-C38
11	H	301	3PE	C22-C21-O21-C2
11	L	306	3PE	C3D-C3E-C3F-C3G
7	g	102	BCL	C13-C15-C16-C17
11	H	301	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
11	M	409	3PE	C37-C38-C39-C3A
11	d	104	3PE	C24-C25-C26-C27
8	E	203	SPO	C34-C33-C35-C36
8	S	201	SPO	C34-C33-C35-C36
7	j	101	BCL	C2-C3-C5-C6
7	J	102	BCL	C2-C3-C5-C6
8	o	102	SPO	C32-C33-C35-C36
11	M	409	3PE	C23-C24-C25-C26
11	d	104	3PE	C29-C2A-C2B-C2C
11	M	406	3PE	C35-C36-C37-C38
11	H	301	3PE	C26-C27-C28-C29
11	d	104	3PE	C32-C33-C34-C35
8	t	102	SPO	C11-C10-C9-C7
8	M	404	SPO	C1-C4-C5-C6
8	r	102	SPO	C1-C4-C5-C6
11	L	306	3PE	C23-C24-C25-C26
8	d	102	SPO	C34-C33-C35-C36
7	b	101	BCL	C2C-C3C-CAC-CBC
11	d	104	3PE	C1-C2-C3-O31
8	r	102	SPO	C33-C35-C36-C37
8	N	201	SPO	C28-C30-C31-C32
8	I	102	SPO	C33-C35-C36-C37
10	M	403	U10	C9-C11-C12-C13
8	K	101	SPO	C11-C10-C9-C7
11	M	406	3PE	C29-C2A-C2B-C2C
8	f	102	SPO	C34-C33-C35-C36
7	k	101	BCL	C2-C3-C5-C6
7	D	101	BCL	C16-C17-C18-C20
11	M	409	3PE	C3B-C3C-C3D-C3E
11	M	406	3PE	C3F-C3G-C3H-C3I
11	d	104	3PE	C2A-C2B-C2C-C2D
7	n	102	BCL	C2-C1-O2A-CGA
11	H	302	3PE	C35-C36-C37-C38
11	M	406	3PE	C2D-C2E-C2F-C2G
11	H	302	3PE	O21-C2-C3-O31
11	M	406	3PE	C22-C23-C24-C25
8	t	102	SPO	C2-C1-C4-C5
7	b	102	BCL	C11-C10-C8-C7
7	i	101	BCL	C11-C10-C8-C7
7	M	407	BCL	C11-C10-C8-C9
7	i	101	BCL	C11-C10-C8-C9
8	j	102	SPO	O1-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
8	G	201	SPO	O1-C1-C4-C5
8	S	202	SPO	C10-C11-C12-C13
8	i	102	SPO	C15-C16-C17-C18
8	S	202	SPO	C10-C11-C12-C14
8	j	102	SPO	C5-C6-C7-C9
8	i	102	SPO	C15-C16-C17-C19
9	M	408	BPH	C10-C11-C12-C13
7	g	101	BCL	C4-C3-C5-C6
7	g	102	BCL	C4-C3-C5-C6
8	I	102	SPO	C34-C33-C35-C36
11	M	409	3PE	C3F-C3G-C3H-C3I
7	M	407	BCL	C3A-C2A-CAA-CBA
11	H	301	3PE	C32-C33-C34-C35
11	M	406	3PE	C1-C2-C3-O31
11	H	302	3PE	C1-C2-C3-O31
7	e	102	BCL	O2A-C1-C2-C3
7	g	102	BCL	O2A-C1-C2-C3
8	F	101	SPO	C34-C33-C35-C36
11	H	302	3PE	C11-O13-P-O11
11	d	103	3PE	O11-C1-C2-O21
8	E	201	SPO	C11-C10-C9-C7
8	S	201	SPO	C11-C10-C9-C7
8	o	102	SPO	C11-C10-C9-C7
8	k	102	SPO	C11-C10-C9-C7
8	I	102	SPO	C11-C10-C9-C7
8	i	102	SPO	C11-C10-C9-C7
8	j	102	SPO	C28-C30-C31-C32
10	M	403	U10	C24-C26-C27-C28
7	o	101	BCL	C6-C7-C8-C9
11	M	406	3PE	C3C-C3D-C3E-C3F
7	M	401	BCL	C13-C15-C16-C17
7	n	102	BCL	C10-C11-C12-C13
7	A	202	BCL	C2A-CAA-CBA-CGA
11	d	103	3PE	C22-C23-C24-C25
11	M	409	3PE	O21-C21-C22-C23
8	t	102	SPO	C15-C16-C17-C18
8	j	102	SPO	C5-C6-C7-C8
7	b	101	BCL	C4C-C3C-CAC-CBC
7	e	102	BCL	C10-C11-C12-C13
11	L	306	3PE	C3F-C3G-C3H-C3I
11	M	406	3PE	O11-C1-C2-C3
11	M	406	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
11	M	406	3PE	C2C-C2D-C2E-C2F
7	M	407	BCL	C11-C10-C8-C7
11	M	409	3PE	C32-C33-C34-C35
8	b	103	SPO	C11-C10-C9-C7
8	B	101	SPO	C20-C21-C22-C23
8	K	103	SPO	C20-C21-C22-C23
8	J	101	SPO	C20-C21-C22-C23
8	G	201	SPO	C11-C10-C9-C7
11	H	301	3PE	C3A-C3B-C3C-C3D
7	M	405	BCL	CAD-CBD-CGD-O2D
7	U	101	BCL	CAD-CBD-CGD-O2D
9	L	302	BPH	CAD-CBD-CGD-O2D
11	H	302	3PE	C1-C2-O21-C21
8	i	102	SPO	C34-C33-C35-C36
11	H	301	3PE	C2-C1-O11-P
8	A	201	SPO	C20-C21-C22-C23
11	M	406	3PE	O21-C2-C3-O31
11	H	302	3PE	C33-C34-C35-C36
7	A	202	BCL	C6-C7-C8-C9
11	L	306	3PE	C3A-C3B-C3C-C3D
8	b	103	SPO	C15-C16-C17-C18
8	A	201	SPO	C15-C16-C17-C18
8	t	102	SPO	C10-C11-C12-C13
9	M	408	BPH	C2C-C3C-CAC-CBC
8	b	103	SPO	C15-C16-C17-C19
8	A	201	SPO	C15-C16-C17-C19
8	t	102	SPO	C10-C11-C12-C14
8	t	102	SPO	C15-C16-C17-C19
7	r	103	BCL	C1A-C2A-CAA-CBA
7	n	101	BCL	C8-C10-C11-C12
11	M	409	3PE	C1-O11-P-O13
11	H	301	3PE	C3F-C3G-C3H-C3I
11	L	306	3PE	C1-O11-P-O14
11	L	306	3PE	C11-O13-P-O14
11	M	409	3PE	C11-O13-P-O12
11	H	301	3PE	C1-O11-P-O14
11	H	302	3PE	C2C-C2D-C2E-C2F
11	L	306	3PE	C12-C11-O13-P
8	j	102	SPO	C1-C4-C5-C6
7	A	202	BCL	C6-C7-C8-C10
11	M	406	3PE	O11-C1-C2-O21
11	d	104	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
11	H	301	3PE	C25-C26-C27-C28
9	M	408	BPH	C4C-C3C-CAC-CBC
7	j	101	BCL	C11-C10-C8-C9
10	L	303	U10	C19-C21-C22-C23
8	d	102	SPO	C5-C6-C7-C8
7	M	407	BCL	C13-C15-C16-C17
7	n	102	BCL	C16-C17-C18-C20
11	M	409	3PE	C3D-C3E-C3F-C3G
10	M	403	U10	C5-C4-O4-C4M
7	A	202	BCL	C2-C1-O2A-CGA
11	L	306	3PE	C21-C22-C23-C24
7	e	102	BCL	C4-C3-C5-C6
8	B	101	SPO	C29-C28-C30-C31
8	S	202	SPO	C34-C33-C35-C36
8	O	102	SPO	C34-C33-C35-C36
11	M	409	3PE	C2E-C2F-C2G-C2H
11	M	409	3PE	C34-C35-C36-C37
11	d	103	3PE	C11-O13-P-O11
11	d	104	3PE	C11-O13-P-O11
8	t	102	SPO	C3-C1-C4-C5
8	G	201	SPO	C2-C1-C4-C5
11	M	409	3PE	C2C-C2D-C2E-C2F
11	M	409	3PE	C29-C2A-C2B-C2C
8	j	102	SPO	C20-C21-C22-C23
7	A	202	BCL	C5-C6-C7-C8
8	r	102	SPO	O1-C1-C4-C5
11	M	406	3PE	C2A-C2B-C2C-C2D
11	d	103	3PE	C2-C1-O11-P
11	H	301	3PE	C22-C23-C24-C25
7	g	101	BCL	C2-C3-C5-C6
7	g	102	BCL	C2-C3-C5-C6
8	B	101	SPO	C27-C28-C30-C31
8	F	101	SPO	C20-C21-C22-C23
8	O	102	SPO	C28-C30-C31-C32
11	L	306	3PE	C36-C37-C38-C39
7	o	101	BCL	C4-C3-C5-C6
7	i	101	BCL	C4-C3-C5-C6
7	g	102	BCL	C15-C16-C17-C18
7	e	102	BCL	C2-C1-O2A-CGA
7	g	102	BCL	C2-C1-O2A-CGA
7	A	202	BCL	C13-C15-C16-C17
11	M	409	3PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
7	g	101	BCL	C11-C10-C8-C9
8	M	404	SPO	C21-C22-C23-C24
11	H	302	3PE	C38-C39-C3A-C3B
7	n	102	BCL	C16-C17-C18-C19
11	H	302	3PE	C32-C33-C34-C35
7	O	101	BCL	C1A-C2A-CAA-CBA
7	J	102	BCL	C1A-C2A-CAA-CBA
7	F	102	BCL	C1A-C2A-CAA-CBA
7	g	102	BCL	C11-C10-C8-C7
10	M	403	U10	C3-C4-O4-C4M
7	b	101	BCL	C5-C6-C7-C8
11	d	103	3PE	C29-C2A-C2B-C2C
10	L	305	U10	C5-C4-O4-C4M
8	M	404	SPO	C21-C22-C23-C25
8	D	102	SPO	C20-C21-C22-C23
8	i	102	SPO	C1-C4-C5-C6
7	f	101	BCL	C4-C3-C5-C6
7	O	101	BCL	C2-C1-O2A-CGA
7	I	101	BCL	C2-C1-O2A-CGA
7	F	102	BCL	C2-C1-O2A-CGA
7	s	101	BCL	CAA-CBA-CGA-O2A
11	M	409	3PE	O22-C21-O21-C2
7	I	101	BCL	C16-C17-C18-C20
11	d	103	3PE	C31-C32-C33-C34
11	M	409	3PE	C39-C3A-C3B-C3C
11	d	103	3PE	O11-C1-C2-C3
8	D	102	SPO	C34-C33-C35-C36
7	J	102	BCL	C11-C10-C8-C7
7	T	101	BCL	CAA-CBA-CGA-O2A
11	M	409	3PE	O21-C2-C3-O31
7	D	101	BCL	C5-C6-C7-C8
11	d	104	3PE	O21-C21-C22-C23
8	b	103	SPO	C29-C28-C30-C31
10	L	303	U10	C20-C19-C21-C22
7	U	101	BCL	CAA-CBA-CGA-O2A
7	r	103	BCL	CAA-CBA-CGA-O2A
8	d	102	SPO	C32-C33-C35-C36
8	S	202	SPO	C32-C33-C35-C36
7	b	102	BCL	C11-C10-C8-C9
11	H	302	3PE	C2B-C2C-C2D-C2E
7	T	101	BCL	CAA-CBA-CGA-O1A
7	s	101	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
7	r	103	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	C3A-C2A-CAA-CBA
7	M	401	BCL	CAD-CBD-CGD-O2D
7	t	101	BCL	CAD-CBD-CGD-O2D
9	M	408	BPH	CAD-CBD-CGD-O2D
7	J	102	BCL	C2-C1-O2A-CGA
11	M	409	3PE	C36-C37-C38-C39
11	H	302	3PE	O31-C31-C32-C33
8	A	201	SPO	C29-C28-C30-C31
8	A	201	SPO	C34-C33-C35-C36
8	K	101	SPO	C34-C33-C35-C36
11	H	302	3PE	C2D-C2E-C2F-C2G
8	d	102	SPO	C5-C6-C7-C9
8	k	102	SPO	C28-C30-C31-C32
7	U	101	BCL	CAA-CBA-CGA-O1A
11	M	409	3PE	O11-C1-C2-O21
7	D	101	BCL	O2A-C1-C2-C3
7	A	202	BCL	O2A-C1-C2-C3
7	O	101	BCL	O2A-C1-C2-C3
7	K	102	BCL	O2A-C1-C2-C3
7	I	101	BCL	O2A-C1-C2-C3
7	F	102	BCL	O2A-C1-C2-C3
9	L	302	BPH	O2A-C1-C2-C3
7	A	202	BCL	CAA-CBA-CGA-O2A
7	M	407	BCL	CAA-CBA-CGA-O2A
11	H	301	3PE	O31-C31-C32-C33
7	U	102	BCL	CHA-CBD-CGD-O1D
7	U	102	BCL	CHA-CBD-CGD-O2D
8	A	201	SPO	C17-C19-C20-C21
7	r	103	BCL	CAA-CBA-CGA-O1A
11	d	104	3PE	O31-C31-C32-C33
11	d	103	3PE	C37-C38-C39-C3A
11	M	409	3PE	O31-C31-C32-C33
11	M	409	3PE	O22-C21-C22-C23
7	k	101	BCL	C12-C13-C15-C16
8	A	201	SPO	C27-C28-C30-C31
8	t	102	SPO	C33-C35-C36-C37
11	M	409	3PE	C28-C29-C2A-C2B
11	M	409	3PE	C22-C21-O21-C2
7	L	301	BCL	C2A-CAA-CBA-CGA
11	H	302	3PE	O32-C31-C32-C33
7	o	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	f	102	SPO	C5-C6-C7-C9
7	e	102	BCL	C1A-C2A-CAA-CBA
7	D	101	BCL	C1A-C2A-CAA-CBA
7	b	102	BCL	C1A-C2A-CAA-CBA
7	s	101	BCL	C1A-C2A-CAA-CBA
7	U	101	BCL	C1A-C2A-CAA-CBA
7	n	102	BCL	C1A-C2A-CAA-CBA
7	K	102	BCL	C1A-C2A-CAA-CBA
7	I	101	BCL	C1A-C2A-CAA-CBA
7	g	102	BCL	C1A-C2A-CAA-CBA
11	L	306	3PE	C39-C3A-C3B-C3C
7	A	202	BCL	CAA-CBA-CGA-O1A
11	d	104	3PE	O22-C21-C22-C23
8	i	102	SPO	C35-C36-C37-C38
11	d	103	3PE	C1-C2-C3-O31
7	M	407	BCL	CAA-CBA-CGA-O1A
7	e	102	BCL	C2-C3-C5-C6
7	i	101	BCL	C2-C3-C5-C6
7	f	101	BCL	C10-C11-C12-C13
11	d	104	3PE	C1-O11-P-O14
7	K	102	BCL	CAA-CBA-CGA-O2A
11	H	301	3PE	O32-C31-C32-C33
8	S	201	SPO	C35-C36-C37-C38
7	J	102	BCL	CAD-CBD-CGD-O1D
7	k	101	BCL	C14-C13-C15-C16
7	f	101	BCL	C14-C13-C15-C16
11	M	406	3PE	O32-C31-C32-C33
11	M	406	3PE	C25-C26-C27-C28
11	M	409	3PE	O32-C31-C32-C33
7	o	101	BCL	C6-C7-C8-C10
7	J	102	BCL	C3A-C2A-CAA-CBA
7	f	101	BCL	C2-C3-C5-C6
11	M	409	3PE	C2B-C2C-C2D-C2E
7	b	102	BCL	CAA-CBA-CGA-O2A
11	H	302	3PE	C2A-C2B-C2C-C2D
11	d	104	3PE	O32-C31-C32-C33
7	K	102	BCL	CAA-CBA-CGA-O1A
11	d	104	3PE	C23-C24-C25-C26

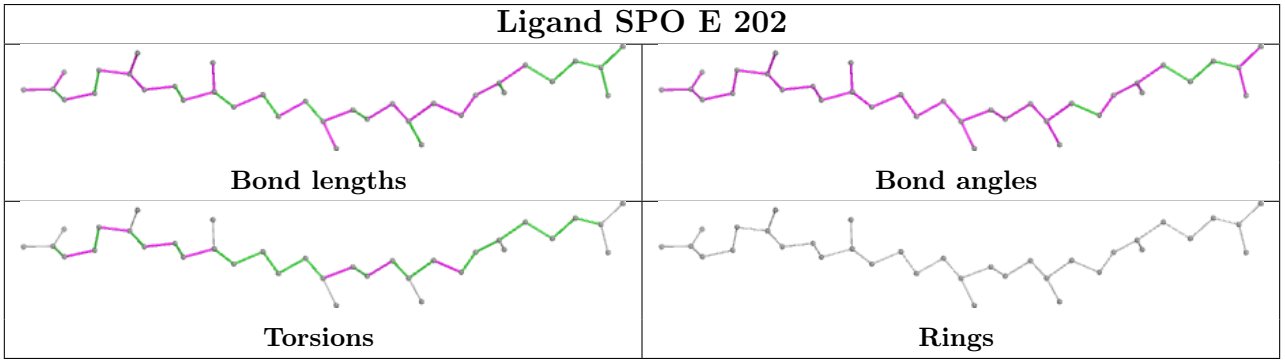
There are no ring outliers.

No monomer is involved in short contacts.

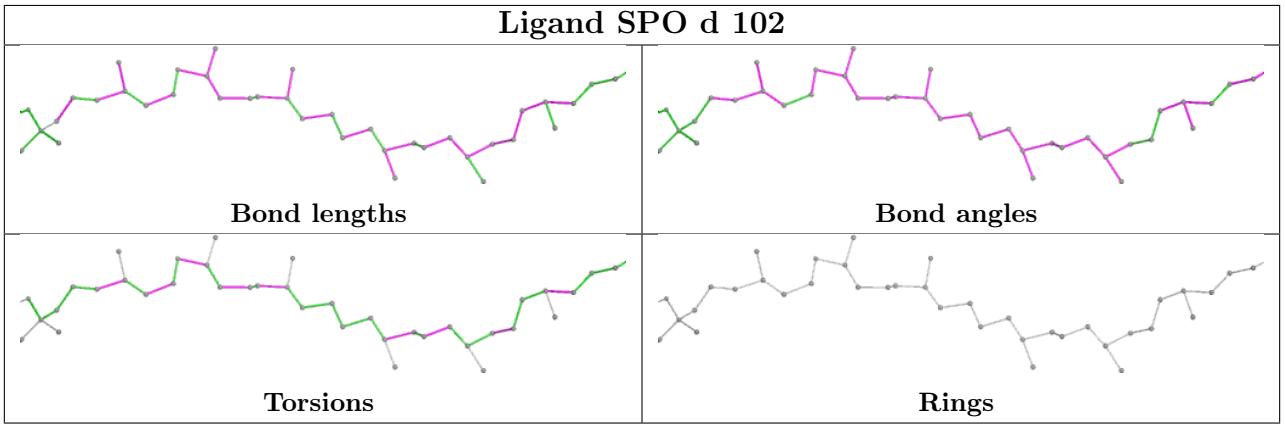
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

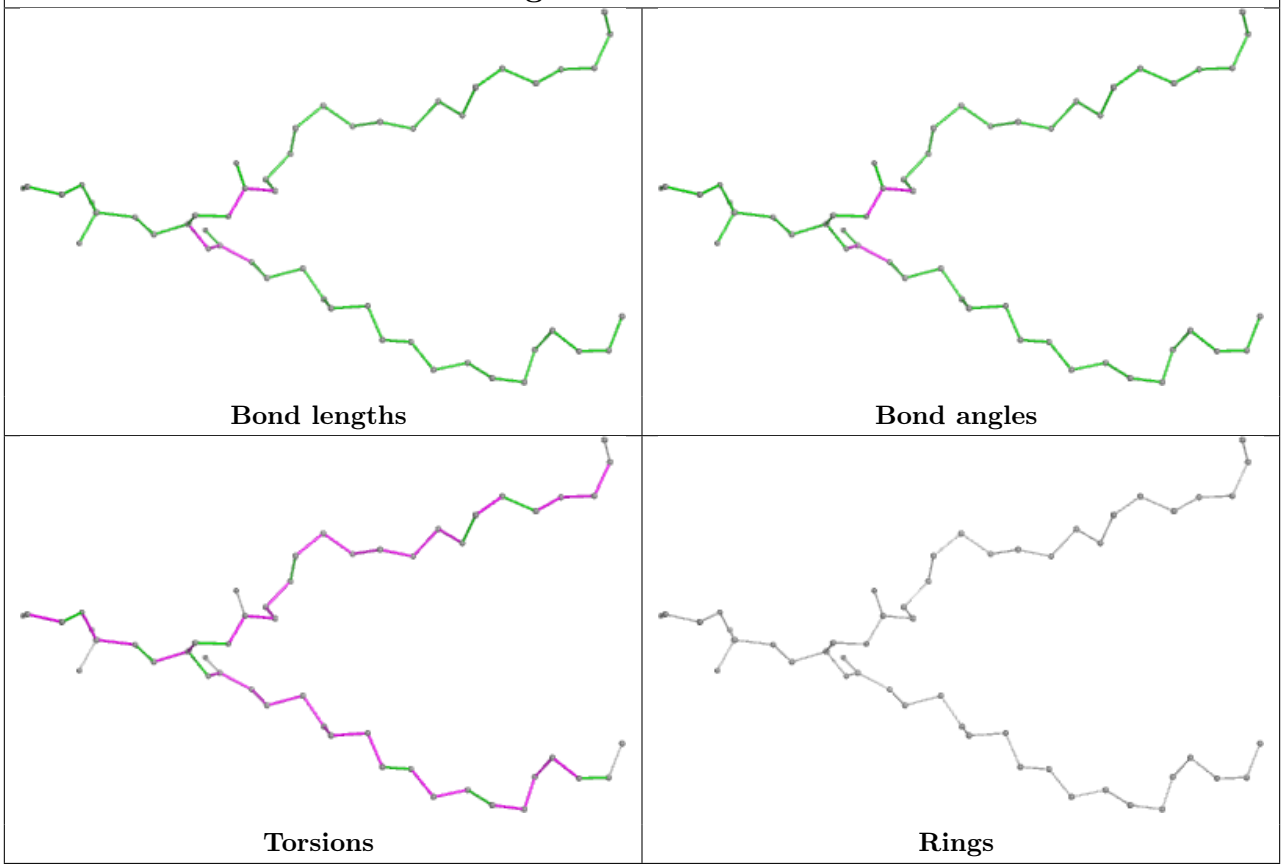
Ligand SPO E 202



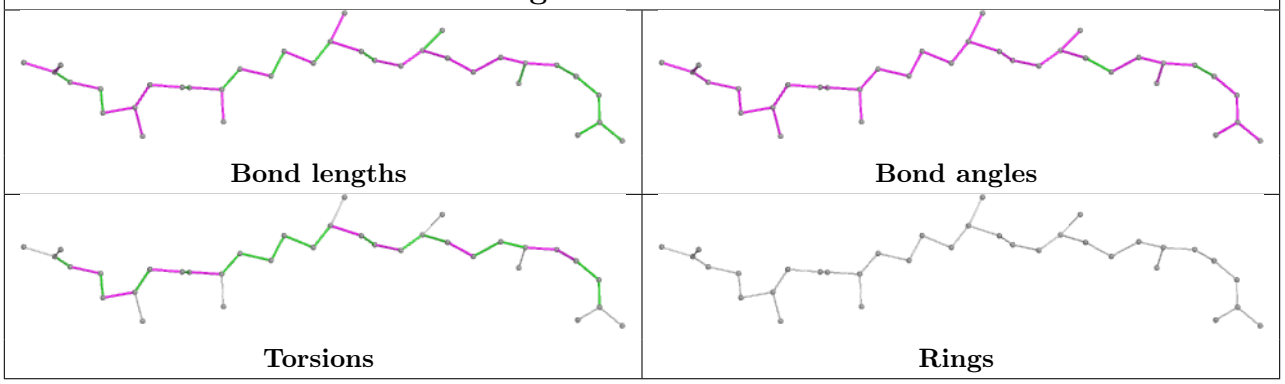
Ligand SPO d 102



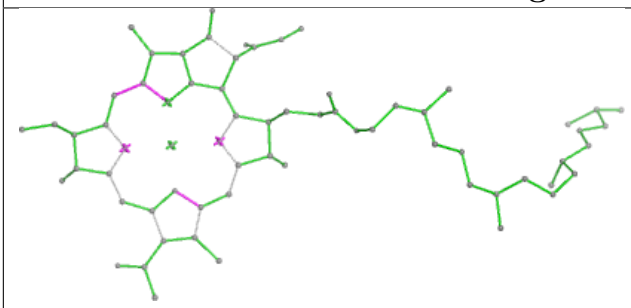
Ligand 3PE M 409



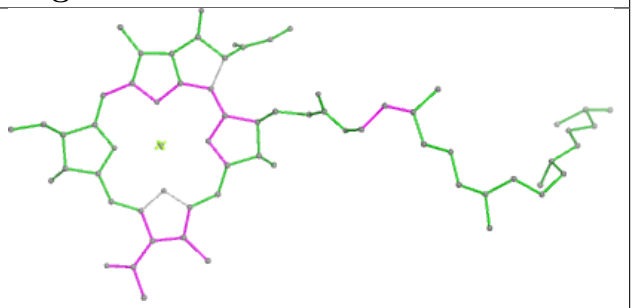
Ligand SPO S 202



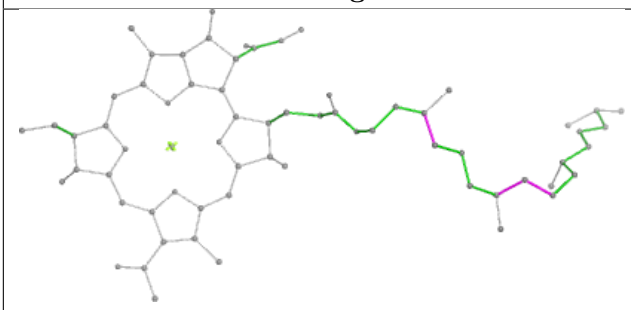
Ligand BCL g 101



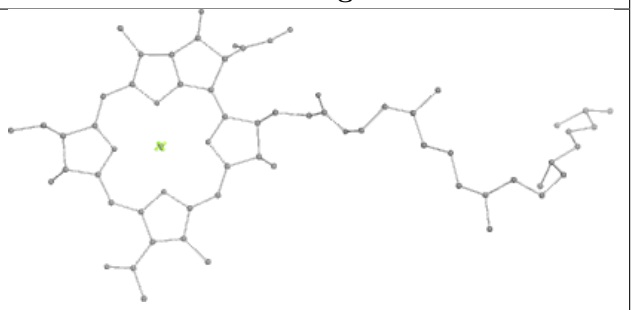
Bond lengths



Bond angles

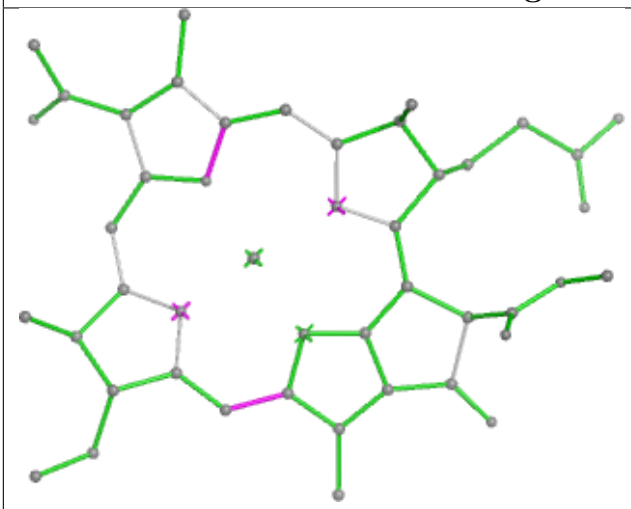


Torsions

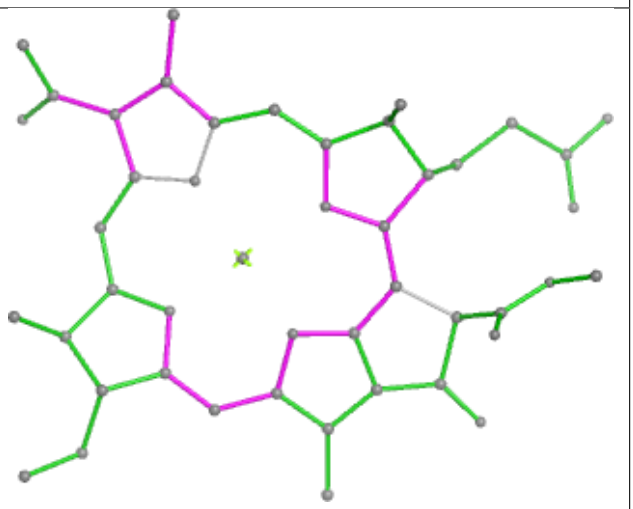


Rings

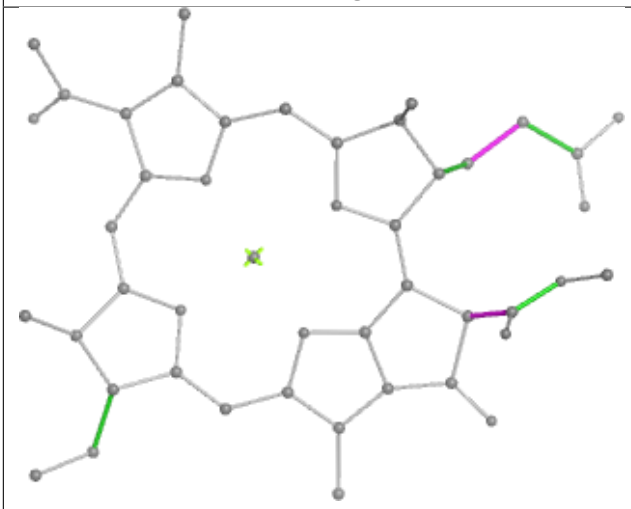
Ligand BCL U 102



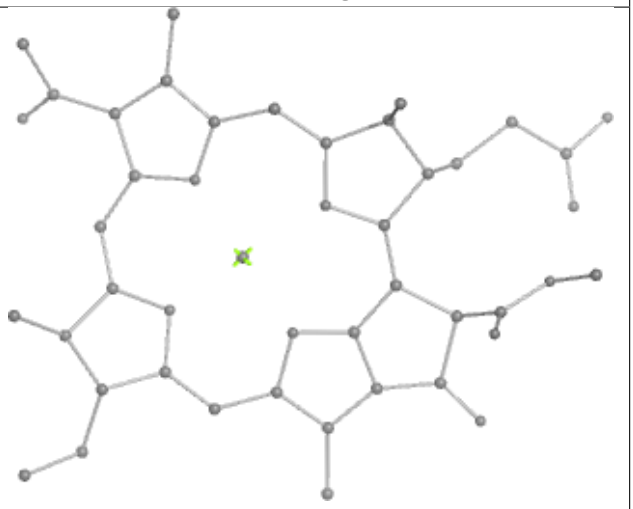
Bond lengths



Bond angles

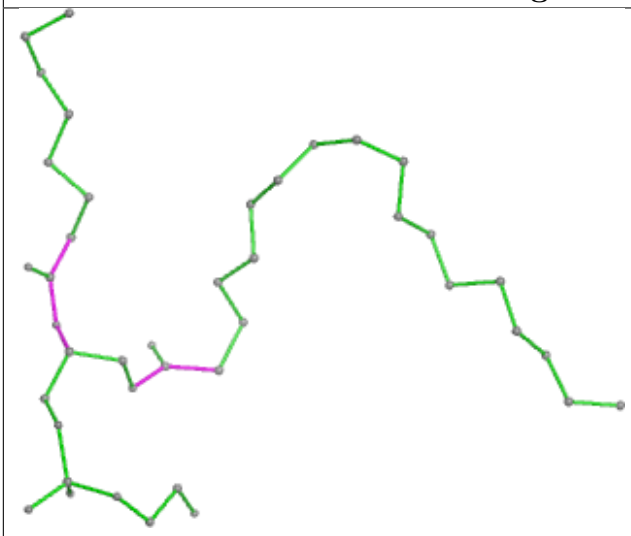


Torsions

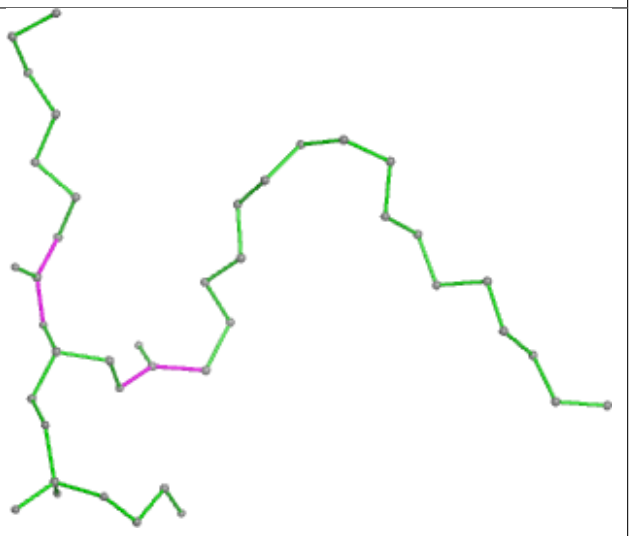


Rings

Ligand 3PE L 306



Bond lengths



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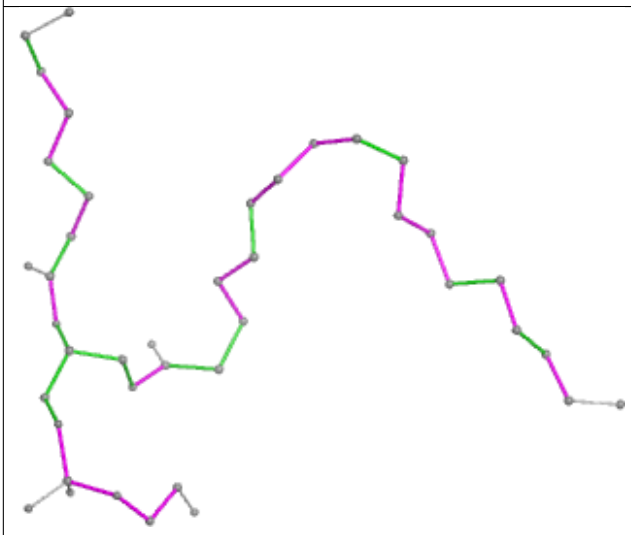
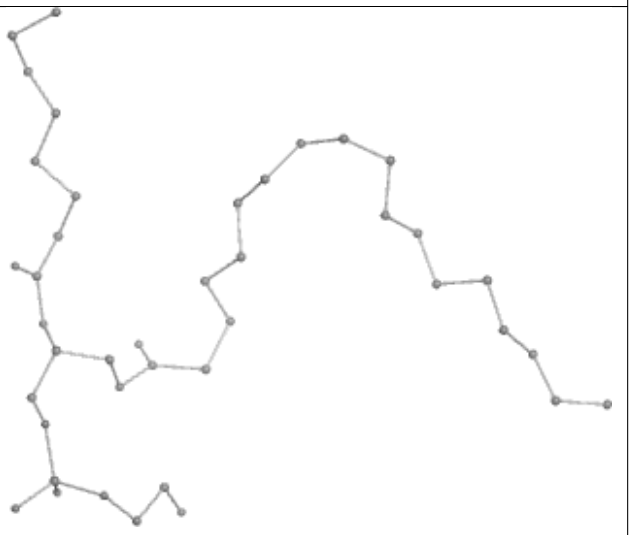
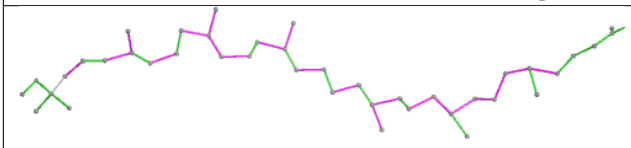


Torsions



Rings

Ligand SPO f 102



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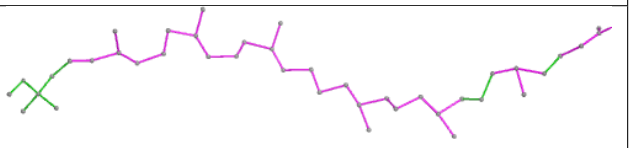

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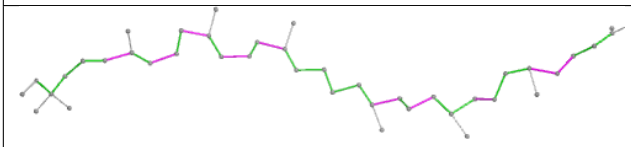

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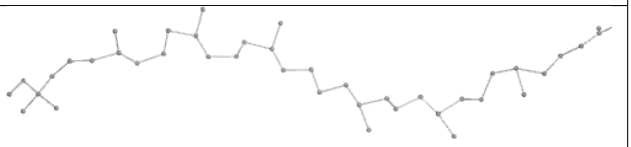
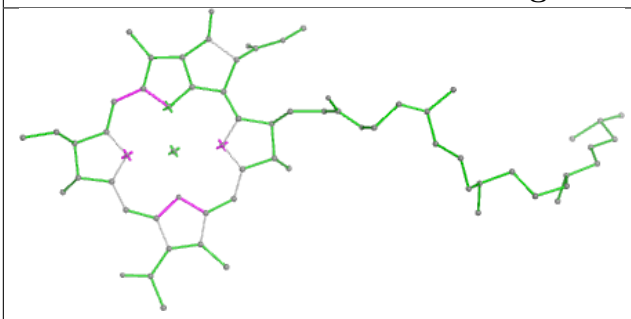


Rings

Ligand BCL e 101



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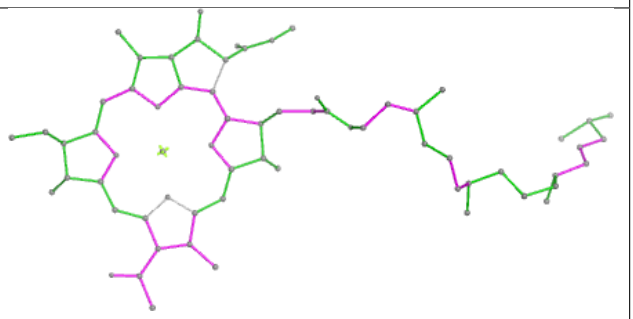

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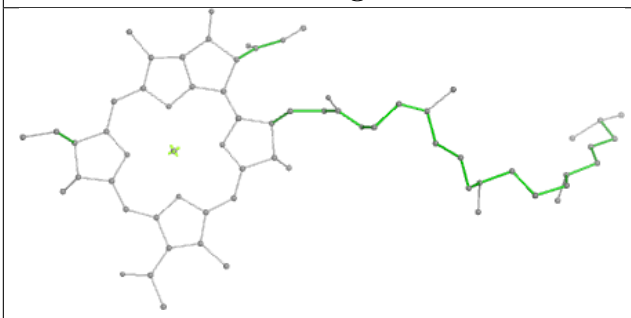

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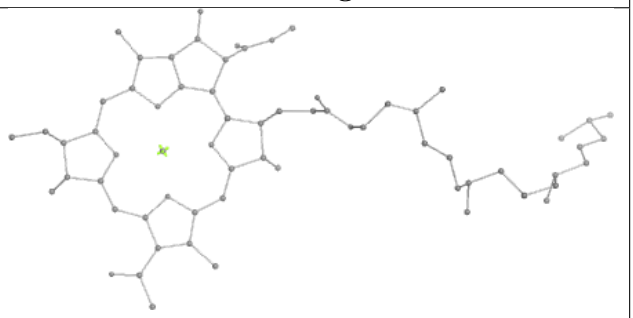
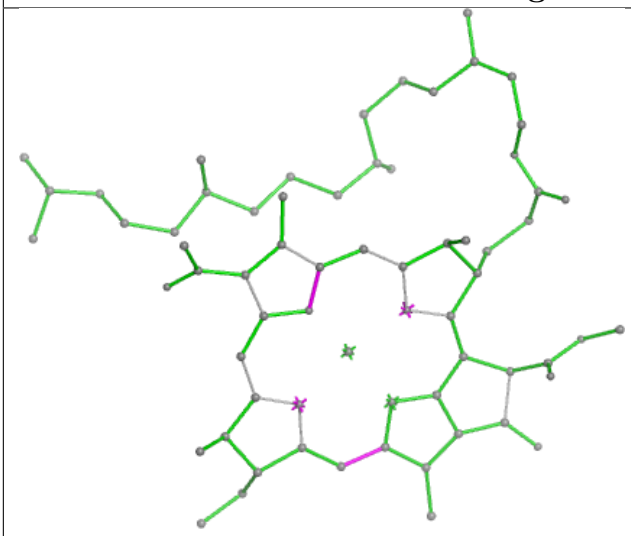


Rings

Ligand BCL b 102



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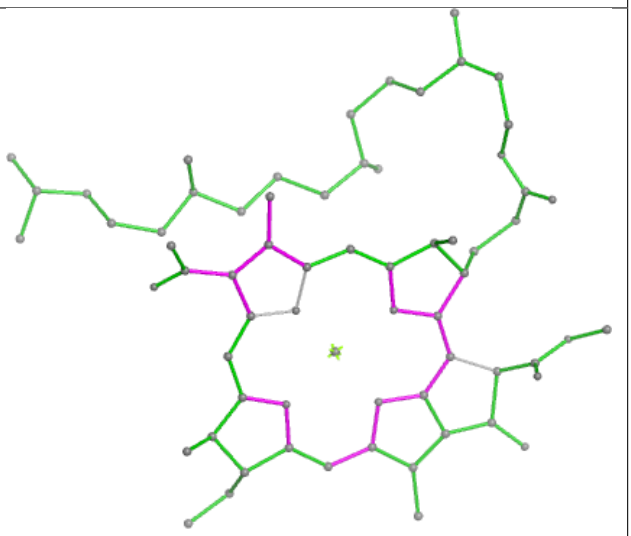

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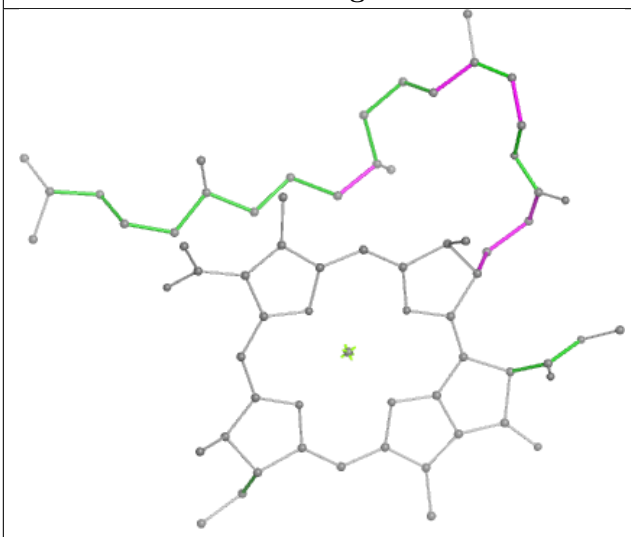

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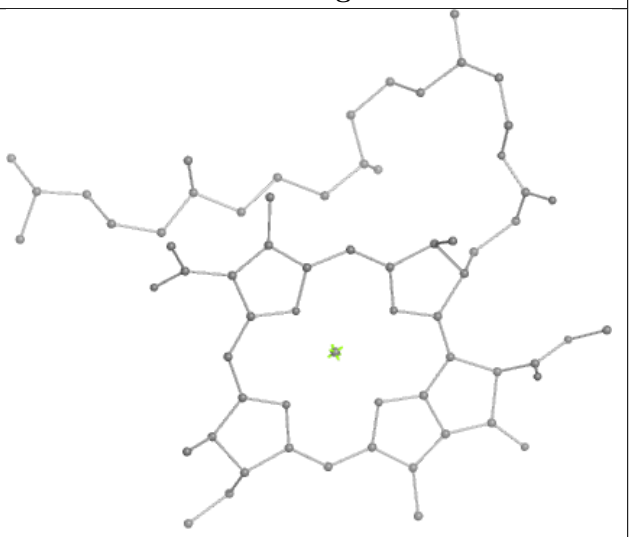
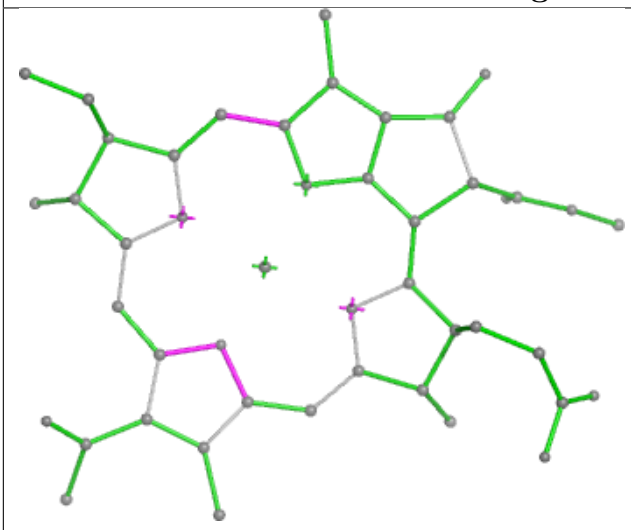


Rings

Ligand BCL s 101



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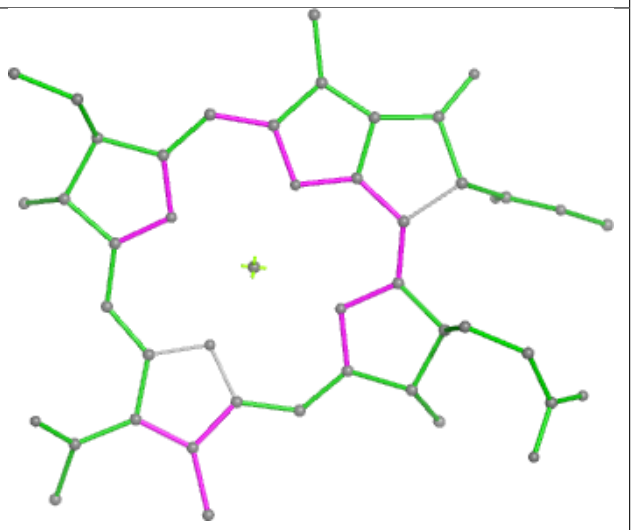

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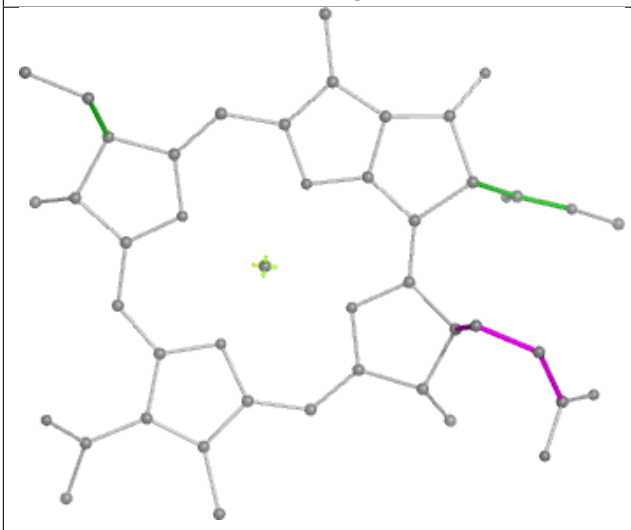

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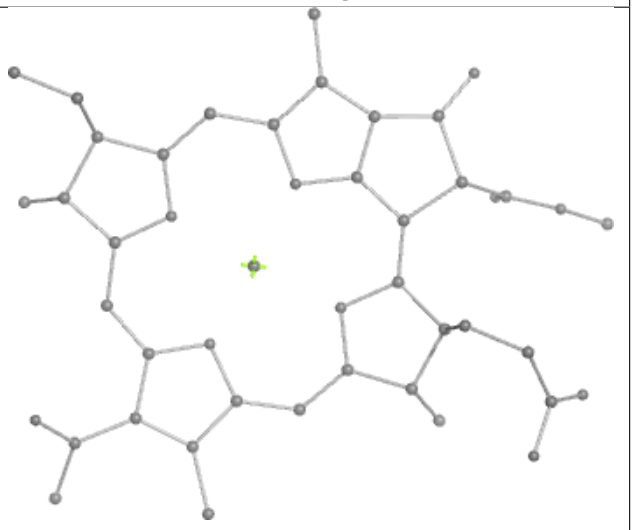
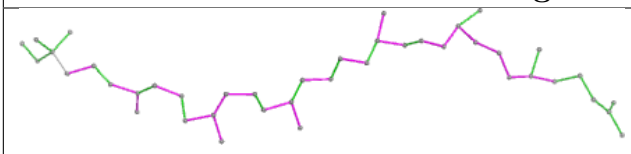


Rings

Ligand SPO j 102



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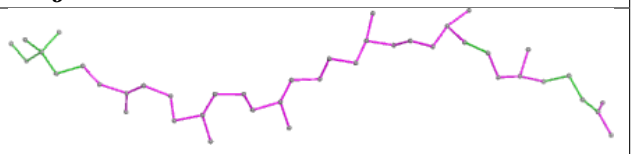

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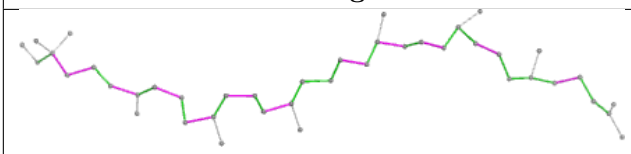
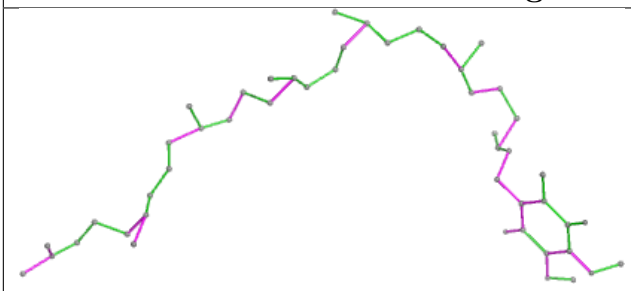


Torsions

Rings

Ligand U10 M 403



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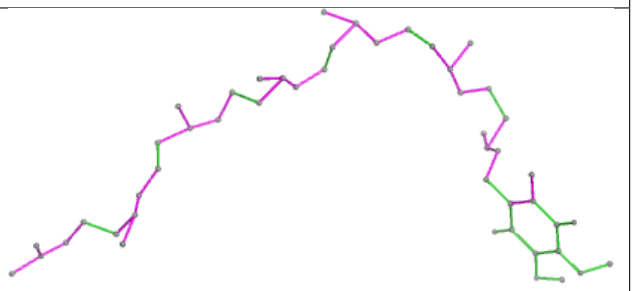

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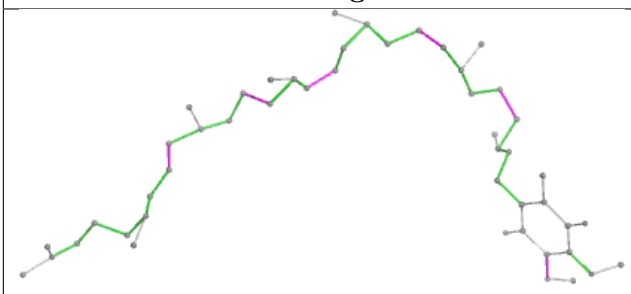

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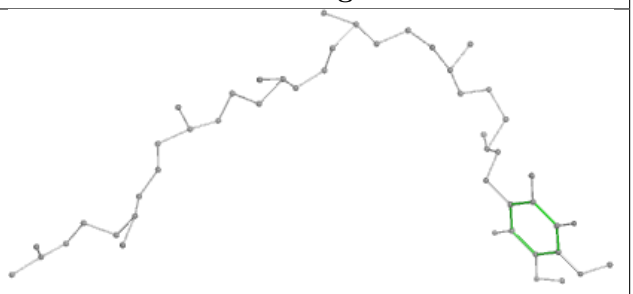
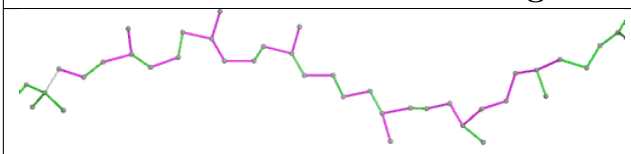


Rings

Ligand SPO E 201



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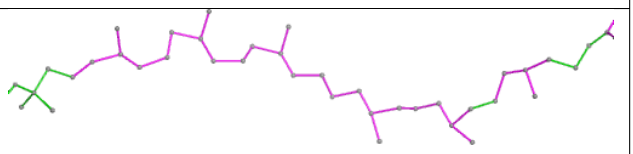
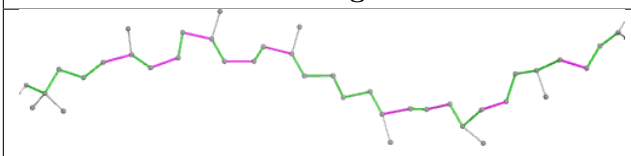


Bond angles



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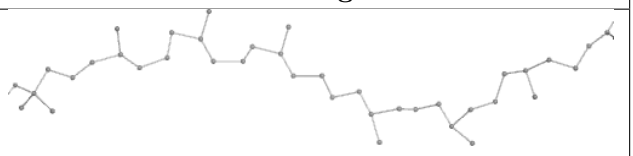
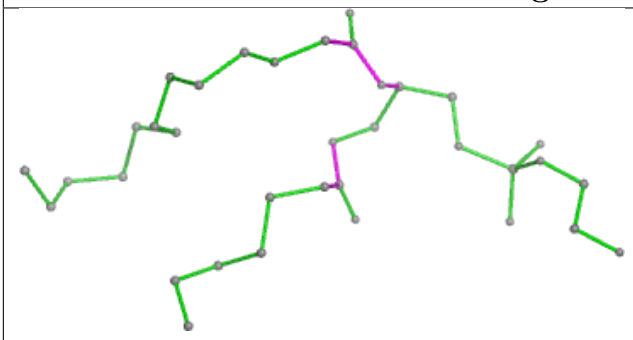


Rings

Ligand 3PE d 104



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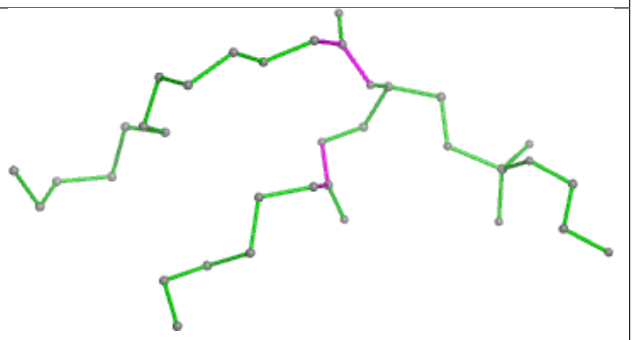
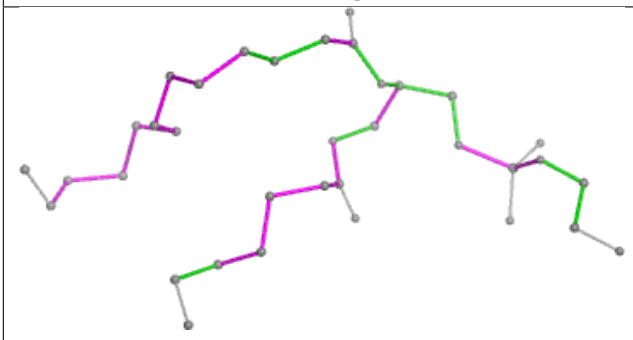


Bond angles



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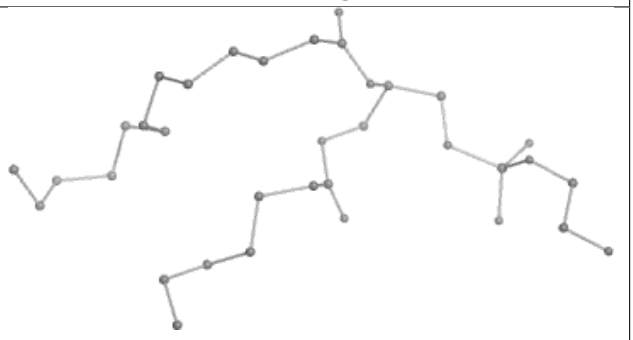
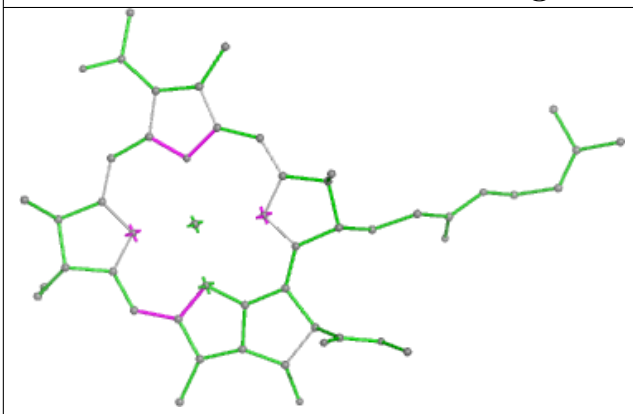


Rings

Ligand BCL r 101



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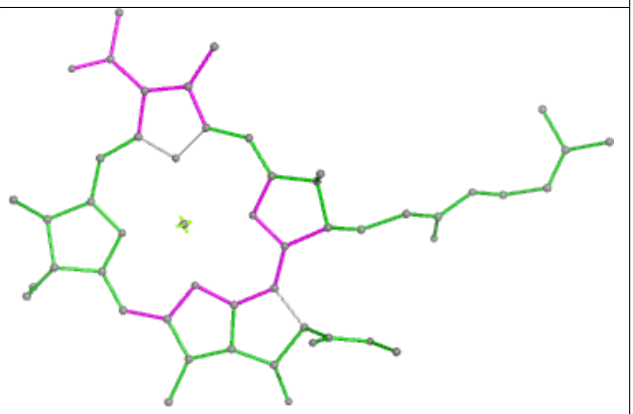
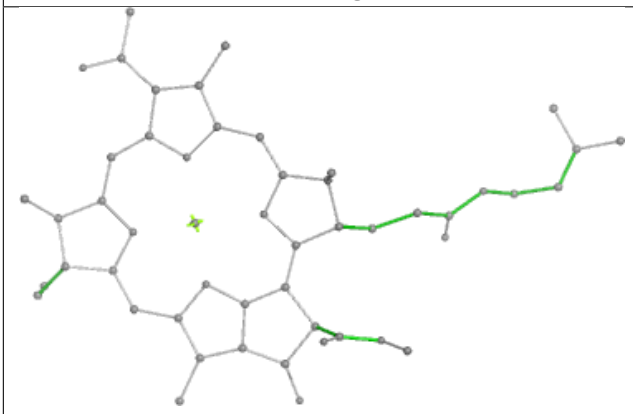


Bond angles



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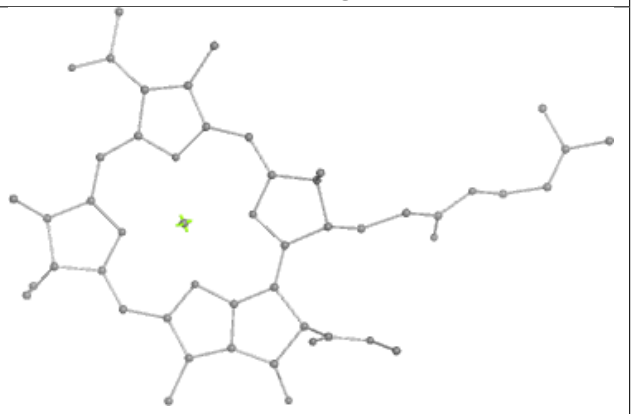
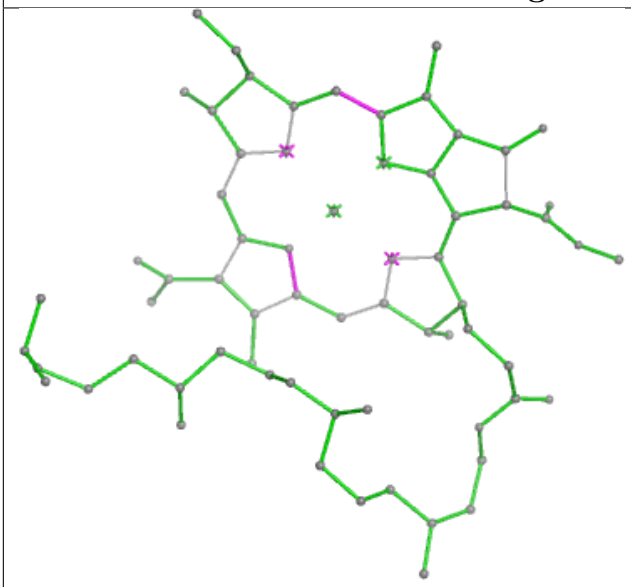


Rings

Ligand BCL n 102



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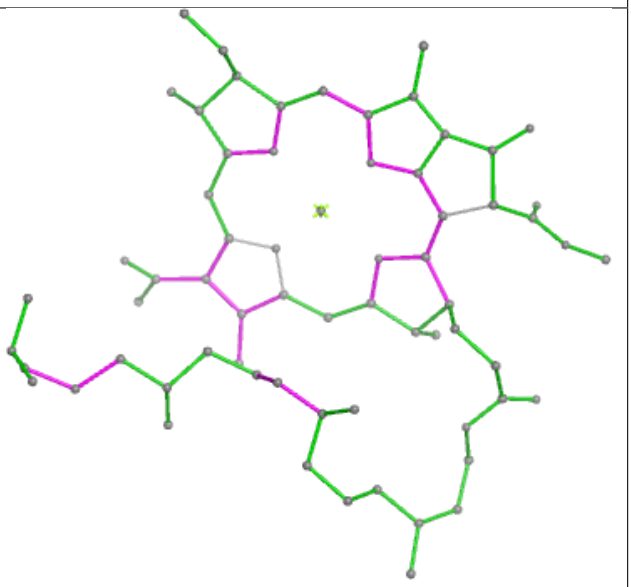

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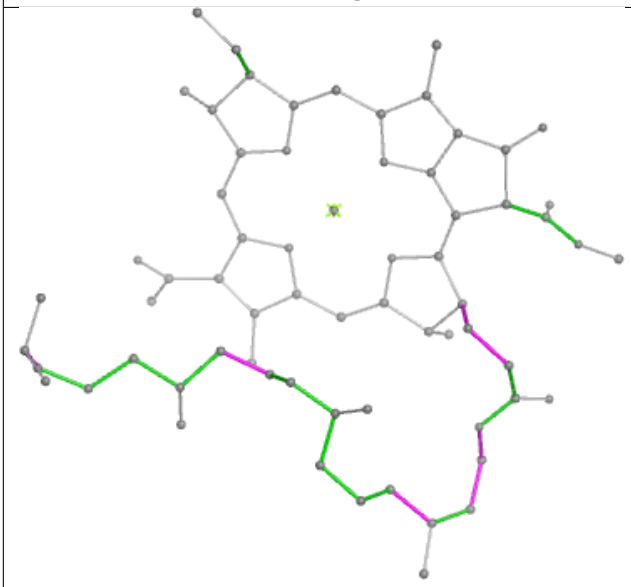

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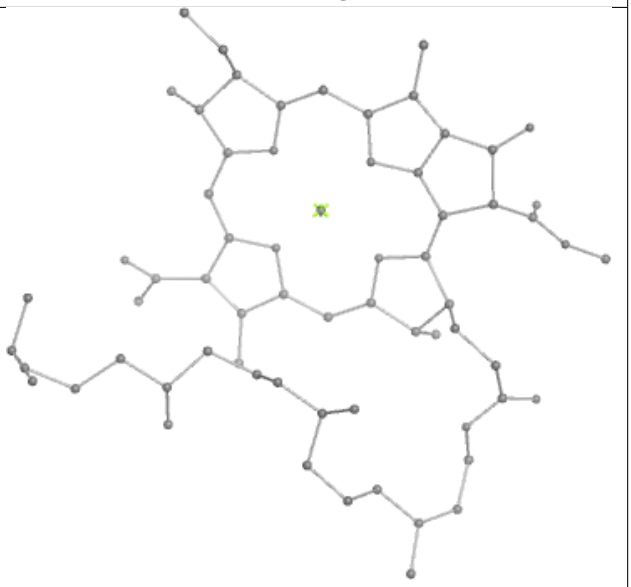
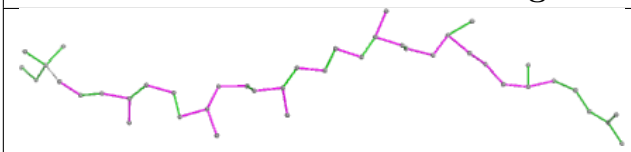


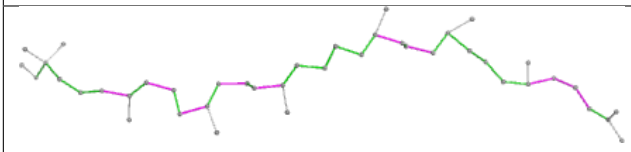
Rings

Ligand SPO S 201



Bond lengths

Bond angles



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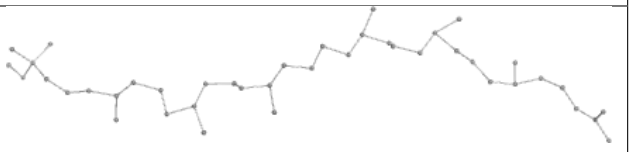
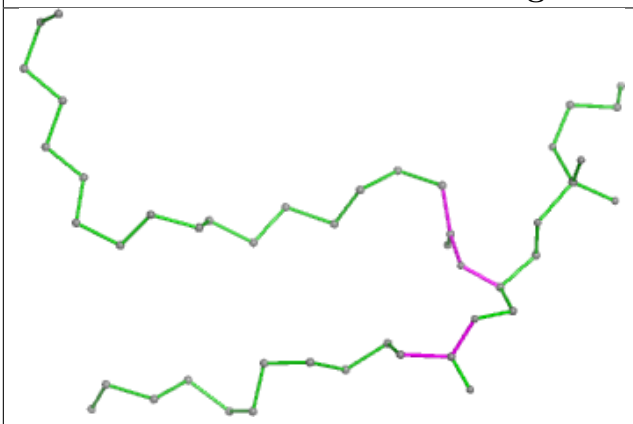


Rings

Ligand 3PE H 302



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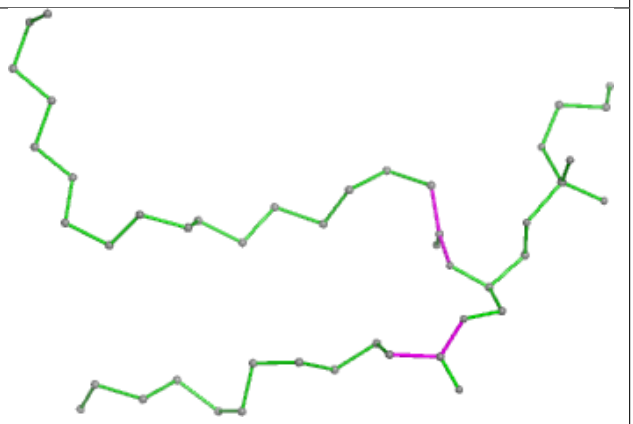
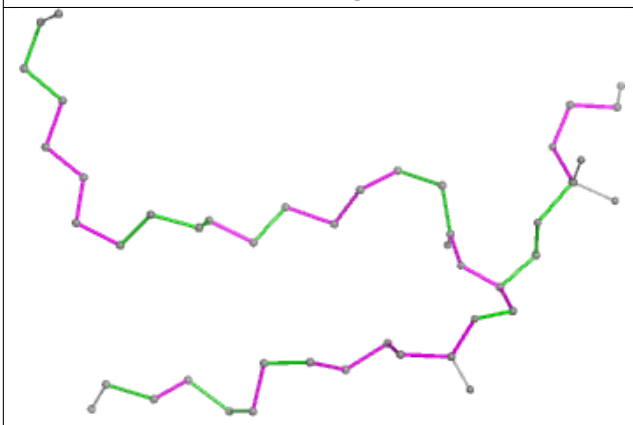
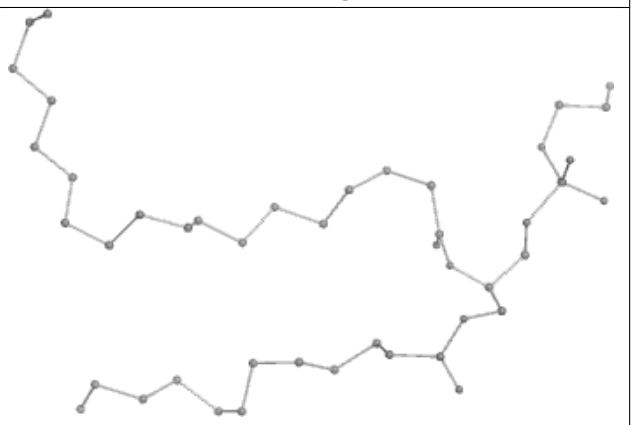


Bond angles

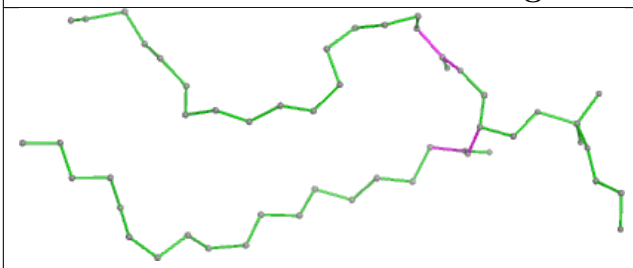


Torsions



Rings

Ligand 3PE M 406



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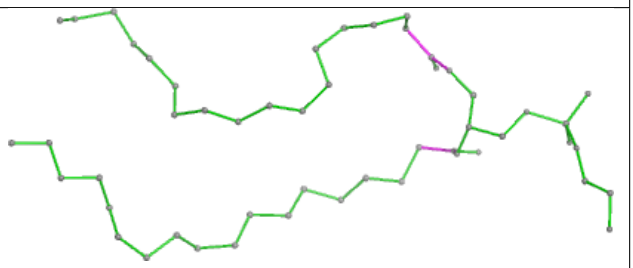
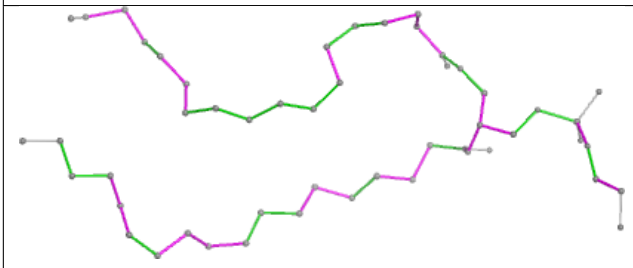
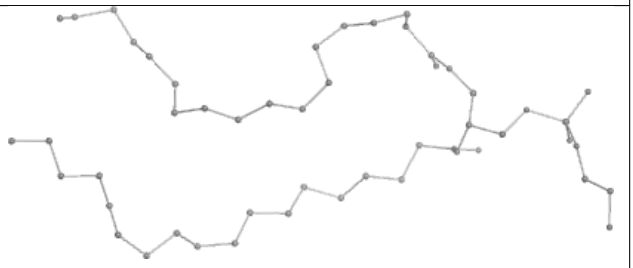


Bond angles

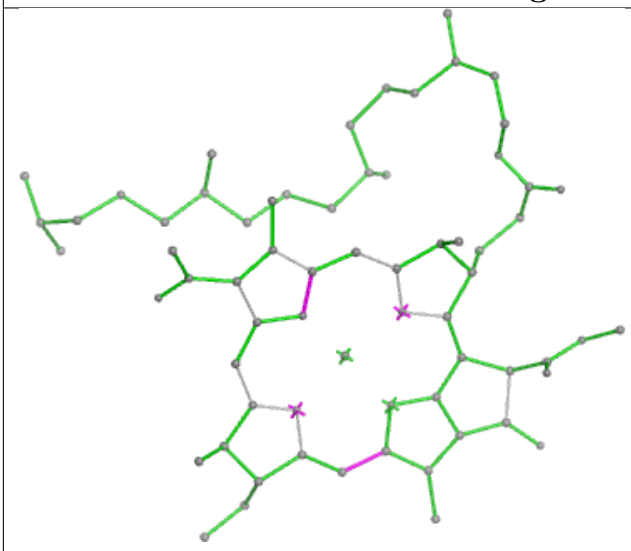


Torsions



Rings

Ligand BCL e 102



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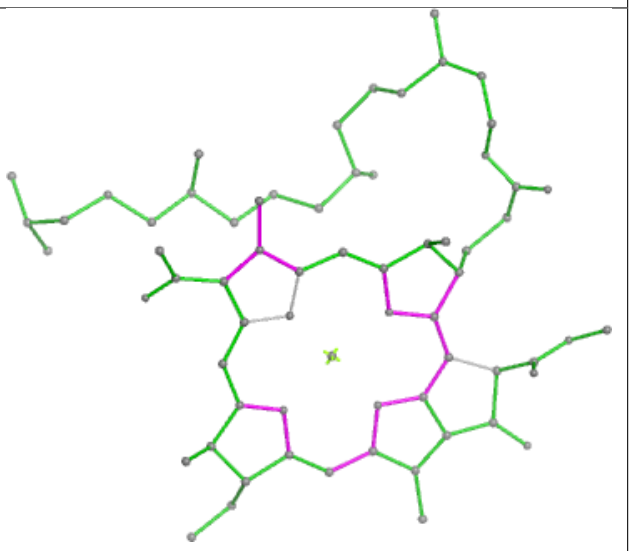
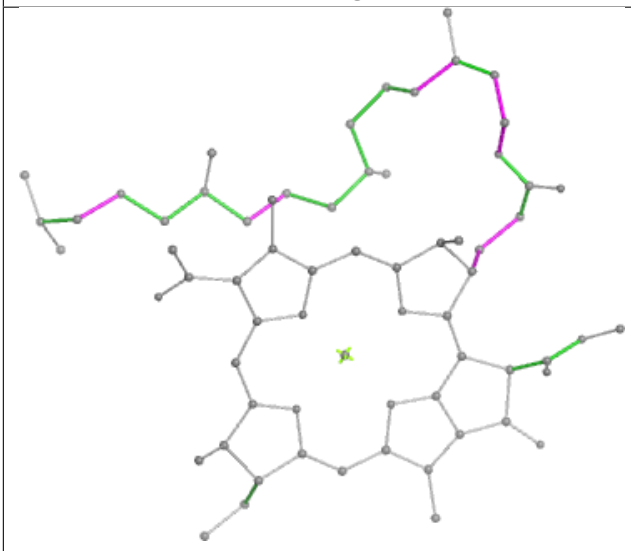


Bond angles



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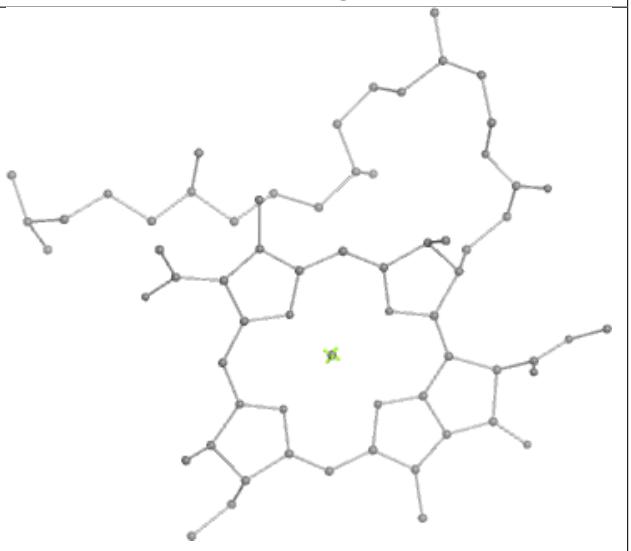
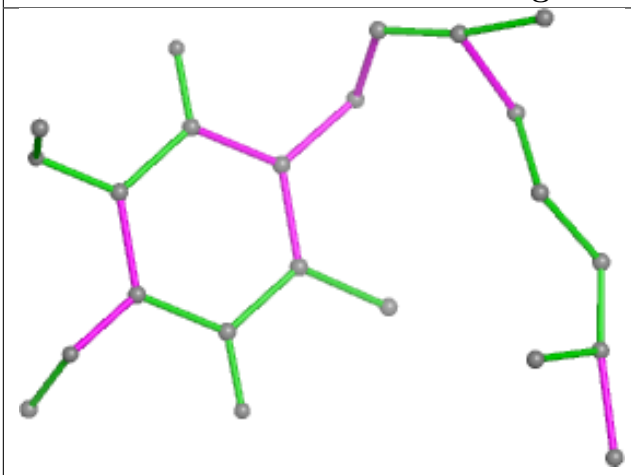
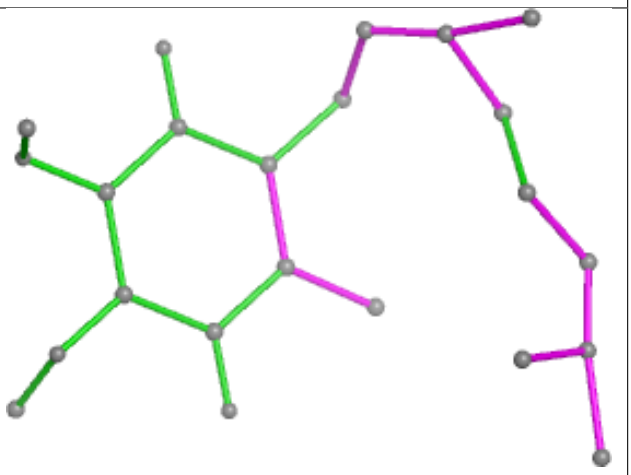


Rings

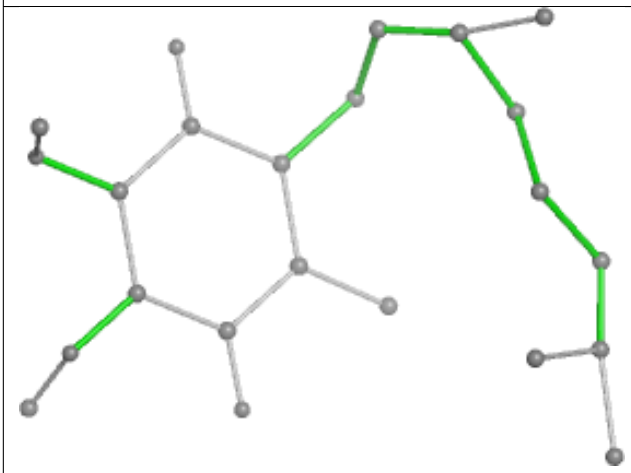
Ligand U10 L 304



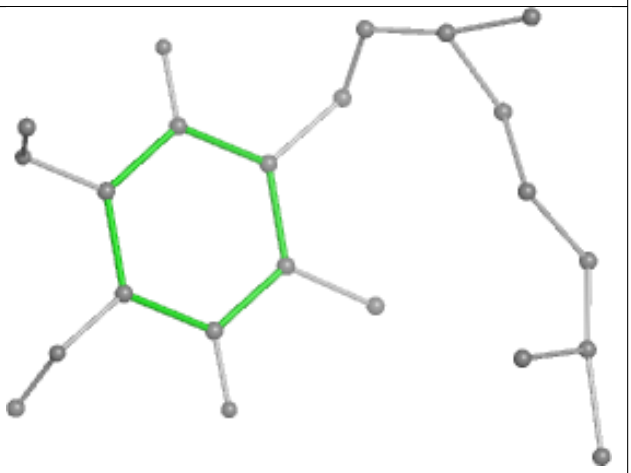
Bond lengths



Bond angles

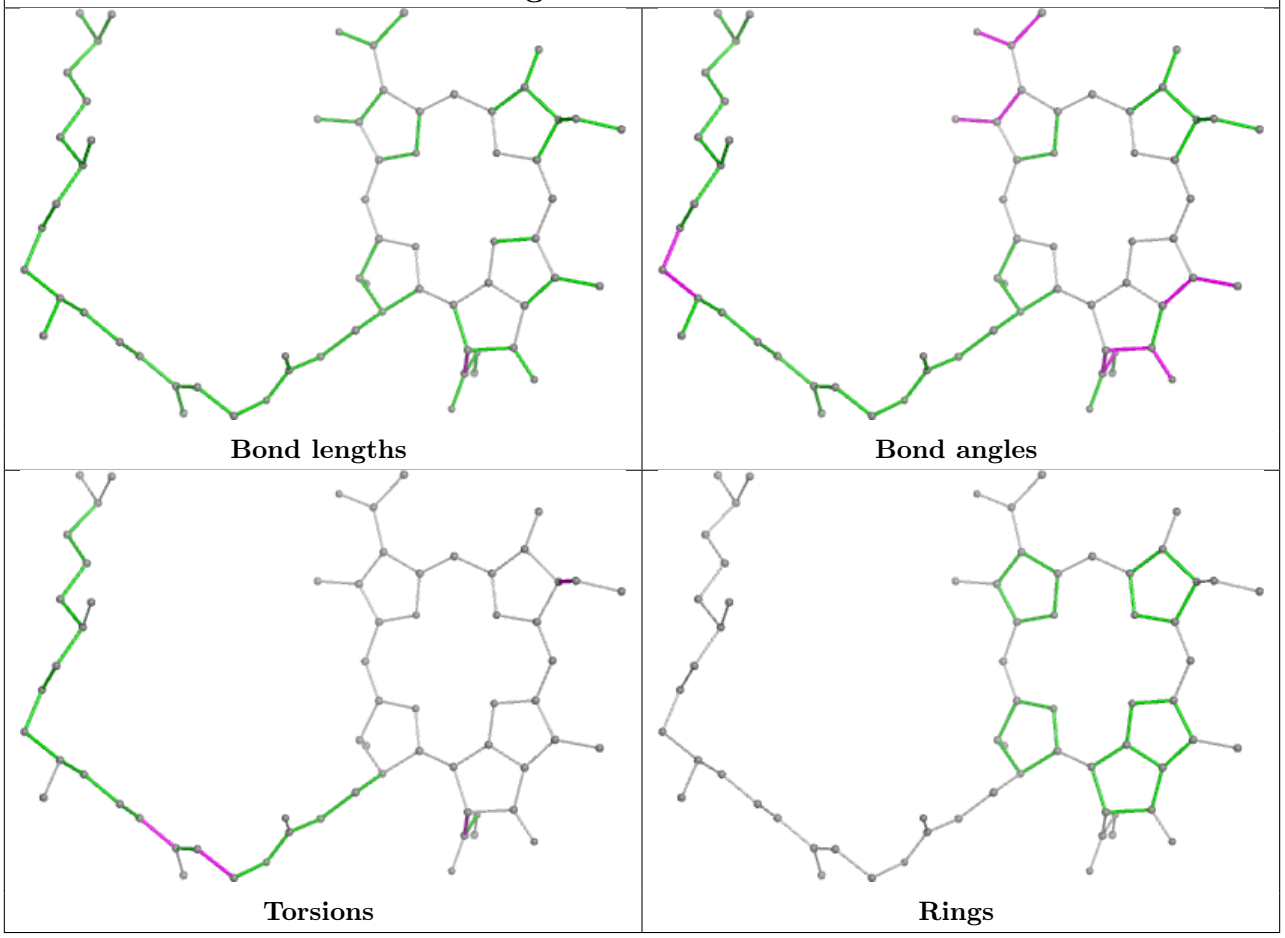


Torsions

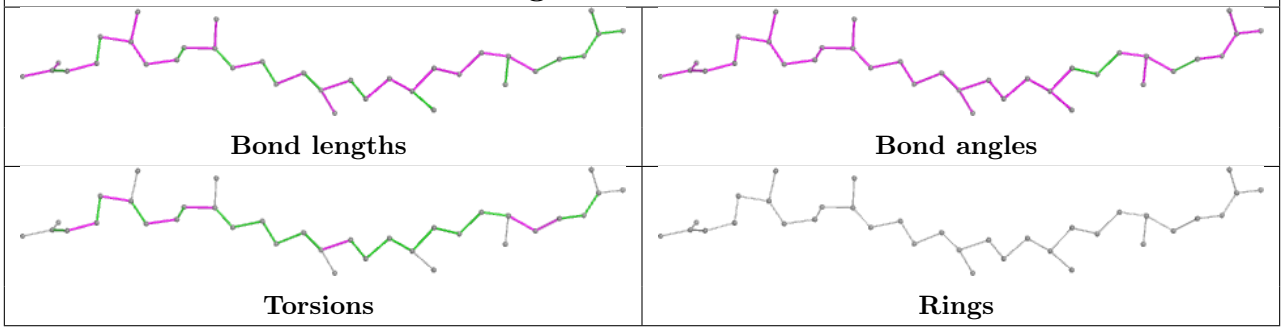


Rings

Ligand BPH L 302



Ligand SPO E 203



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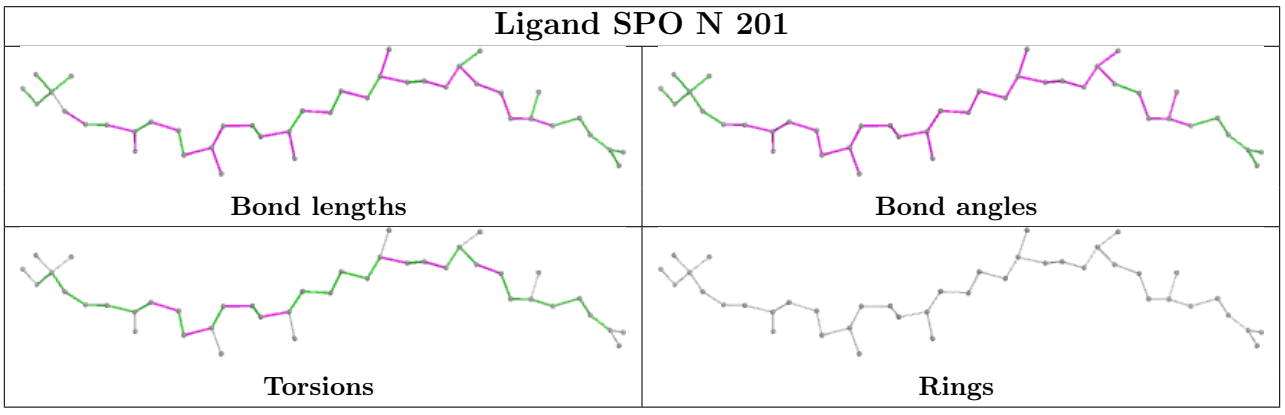
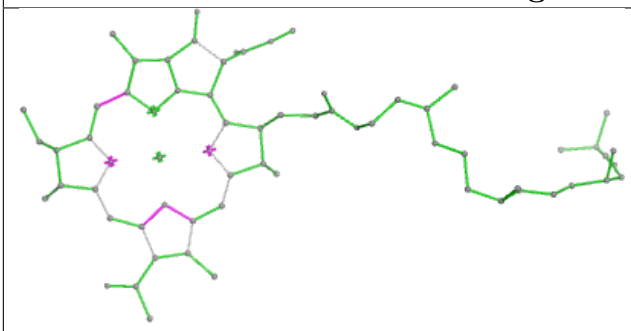
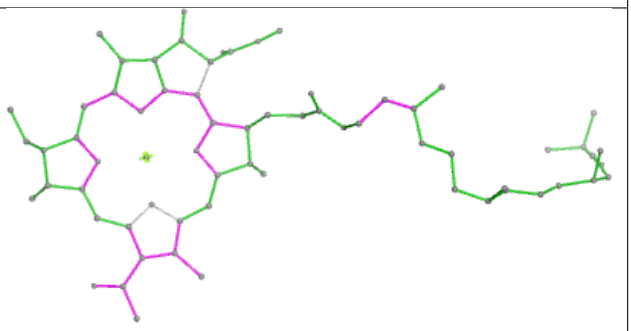


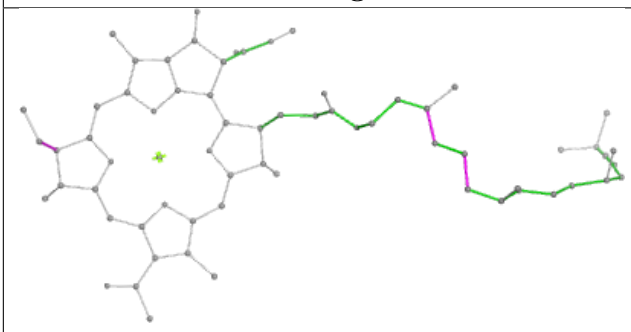
Ligand BCL b 101



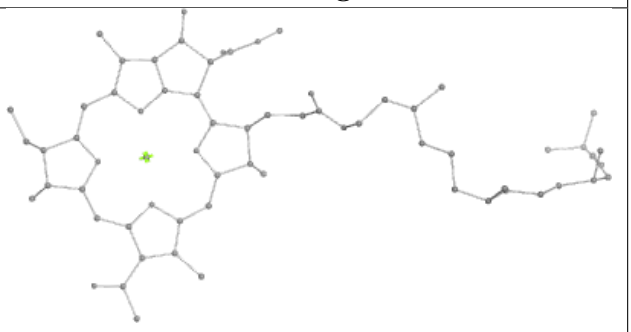
Bond lengths



Bond angles

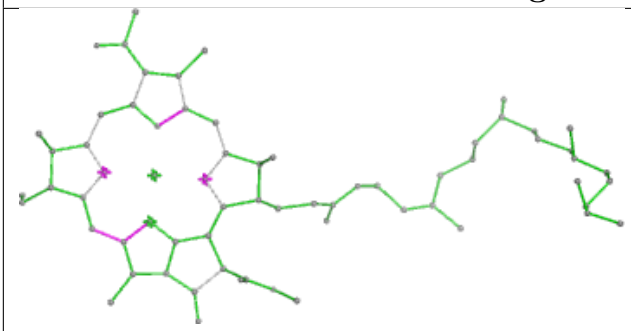


Torsions



Rings

Ligand BCL o 101



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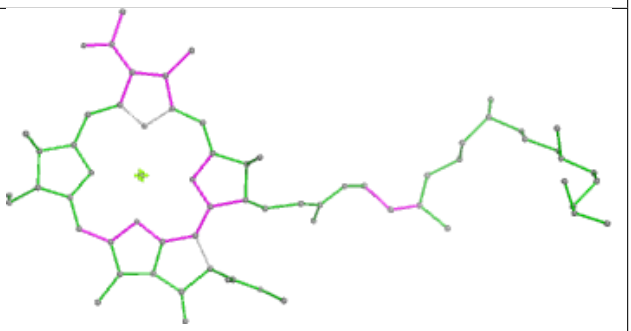
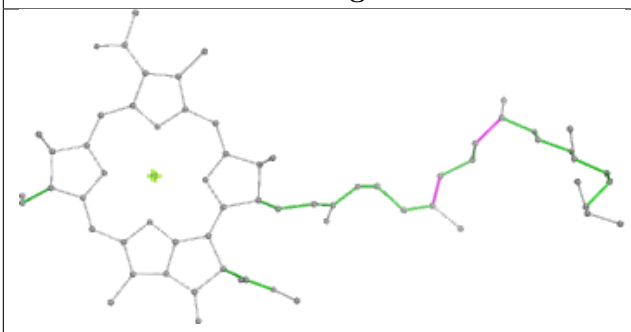
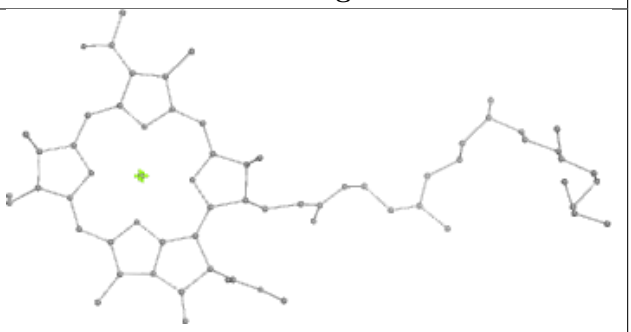


Bond angles

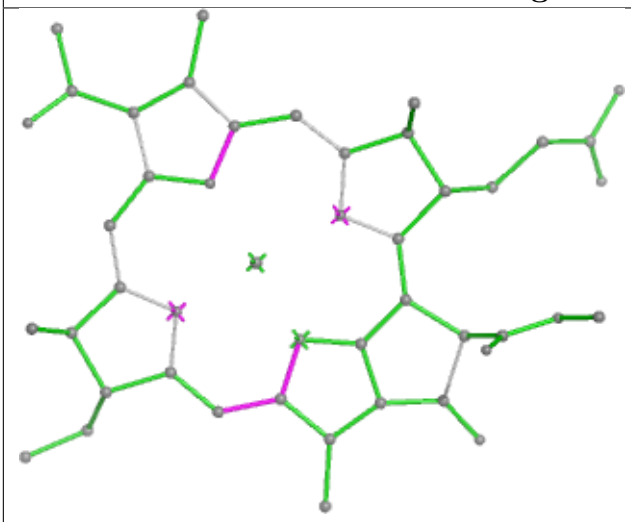


Torsions



Rings

Ligand BCL s 102



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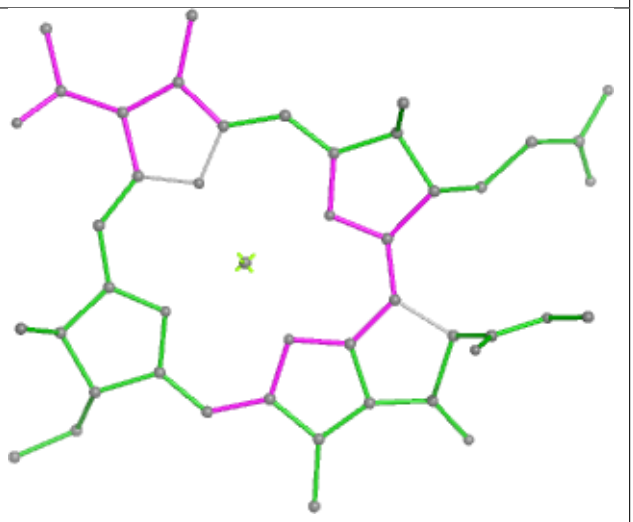
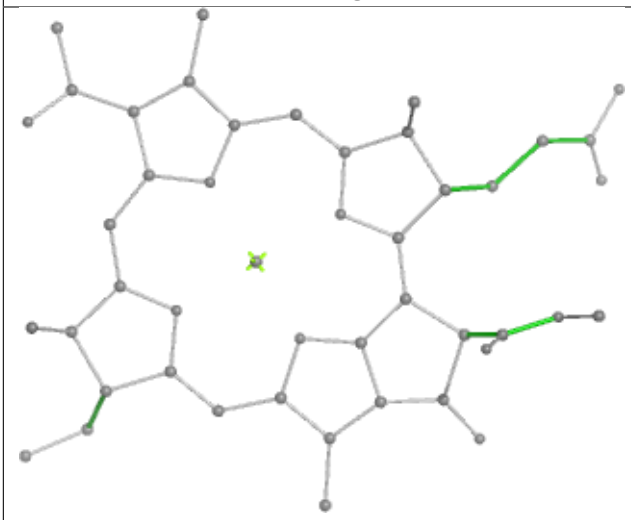


Bond angles



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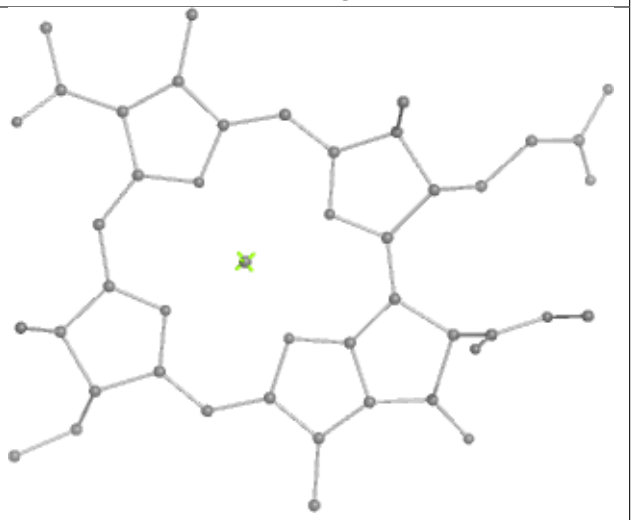
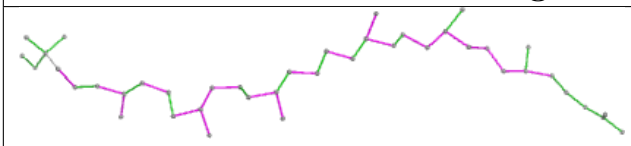


Rings

Ligand SPO k 102



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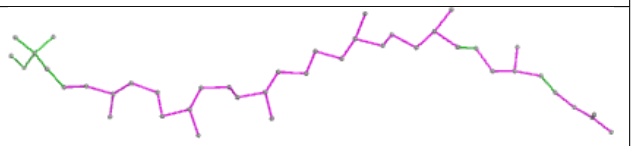
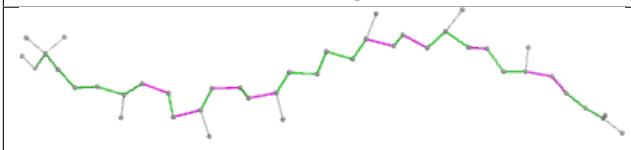
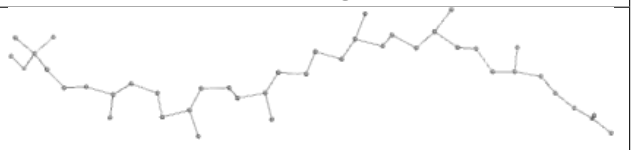


Bond angles

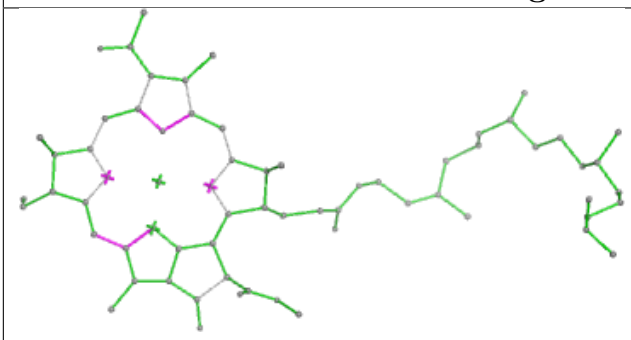


Torsions



Rings

Ligand BCL k 101



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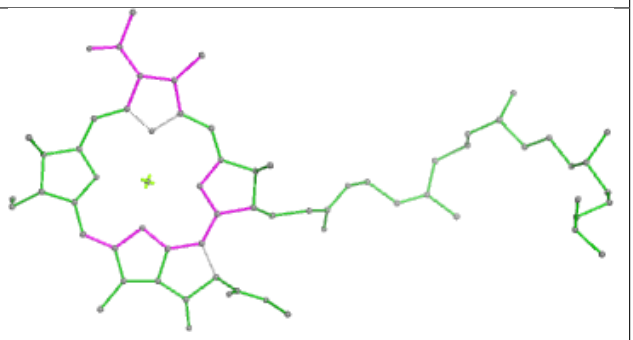
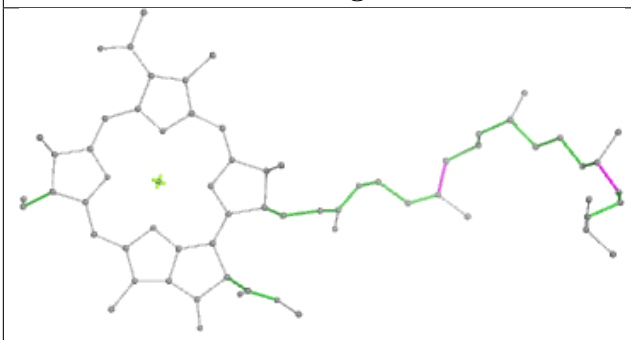
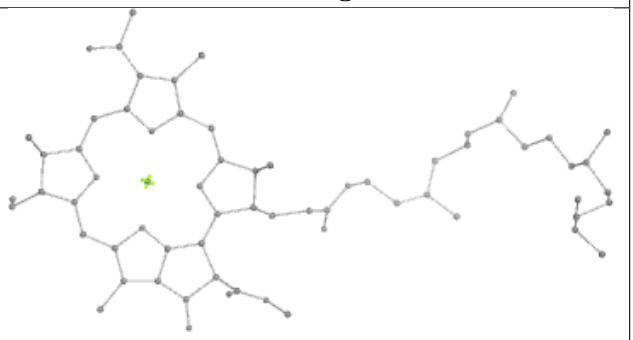


Bond angles

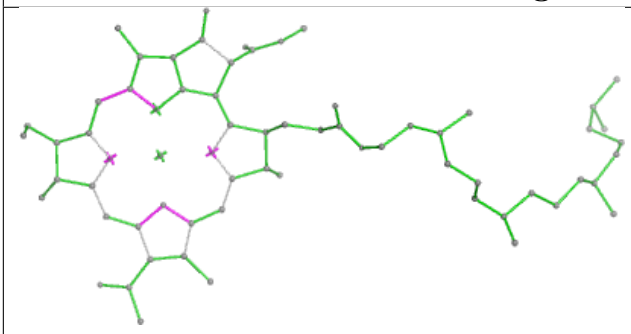


Torsions

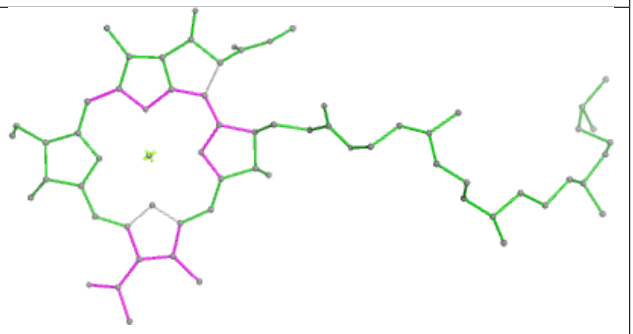


Rings

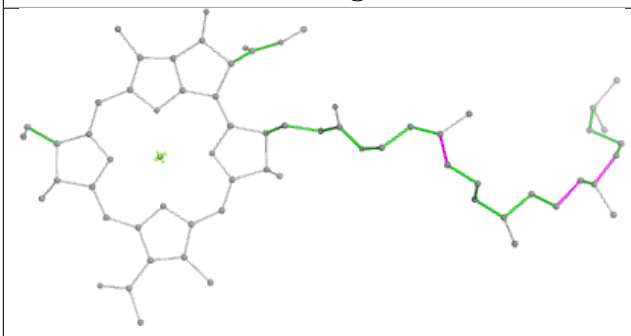
Ligand BCL f 101



Bond lengths



Bond angles



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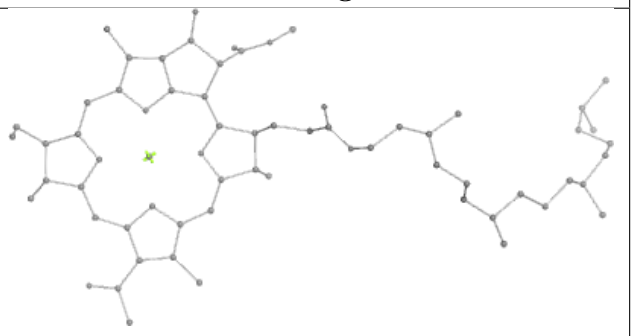
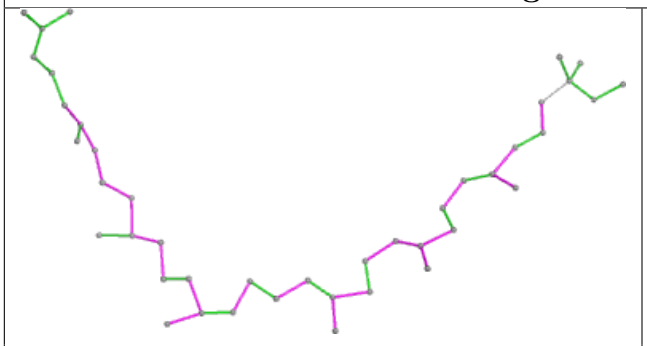
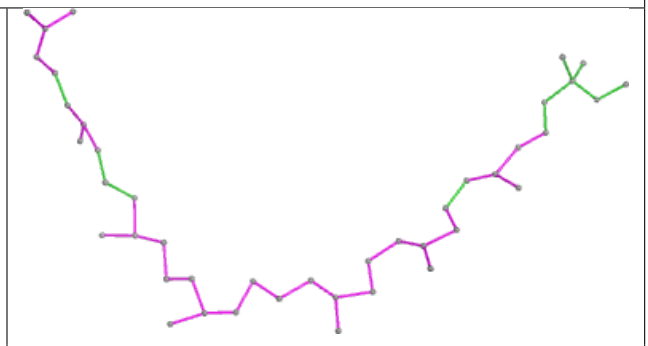


Rings

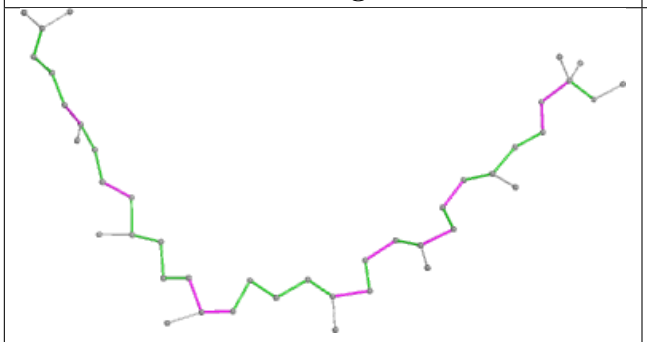
Ligand SPO M 404



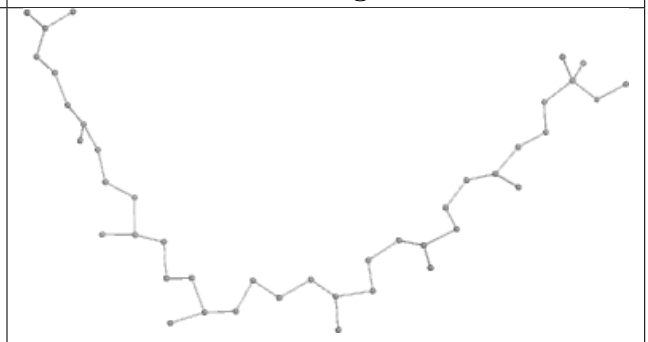
Bond lengths



Bond angles

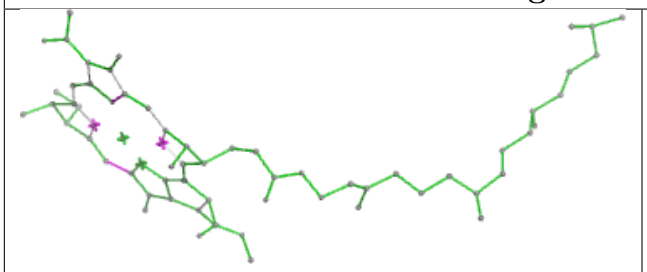


Torsions

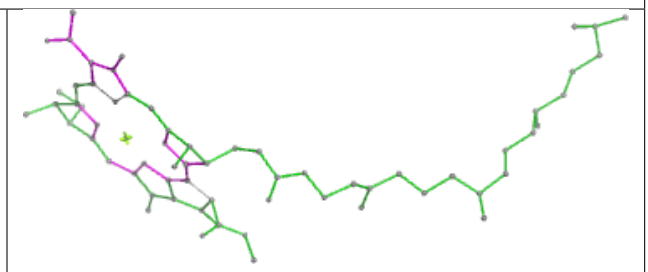


Rings

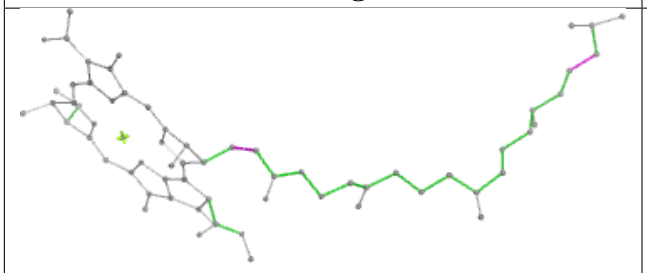
Ligand BCL L 301



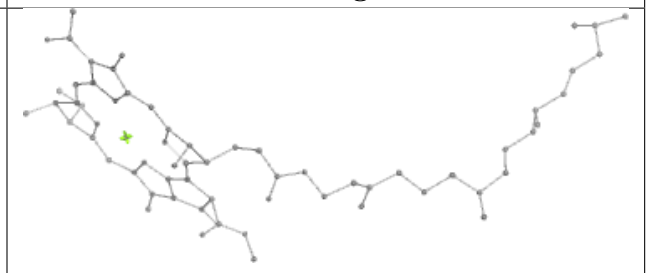
Bond lengths



Bond angles

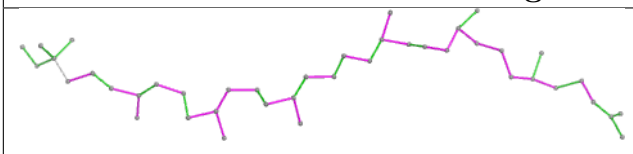


Torsions



Rings

Ligand SPO G 201



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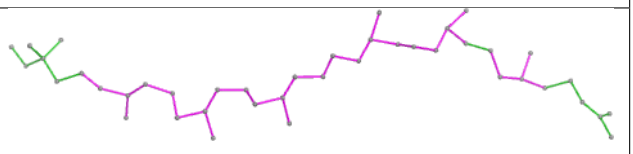
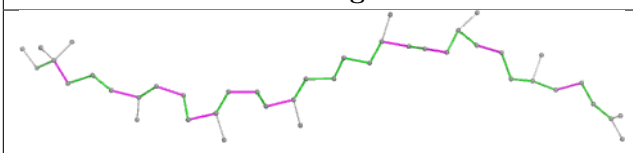


Bond angles



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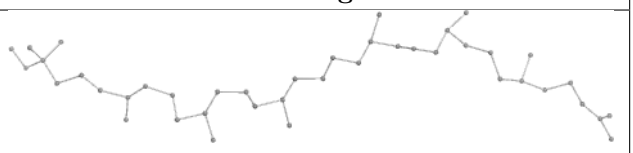
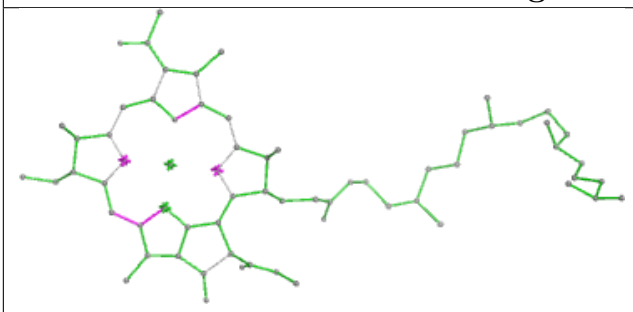


Rings

Ligand BCL n 101



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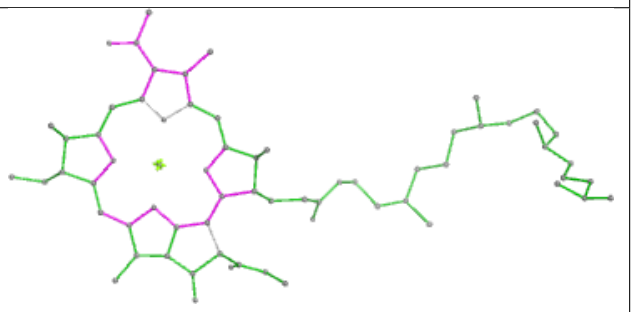
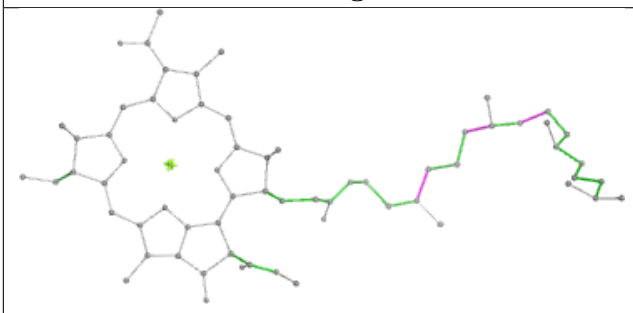


Bond angles



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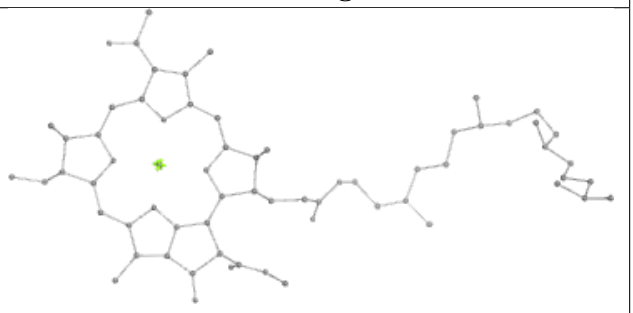
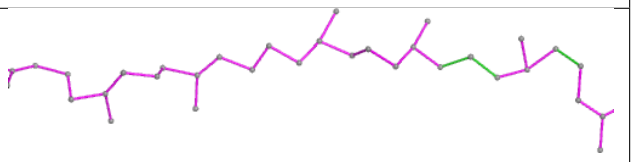


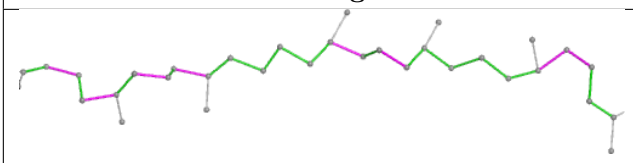
Rings

Ligand SPO I 102

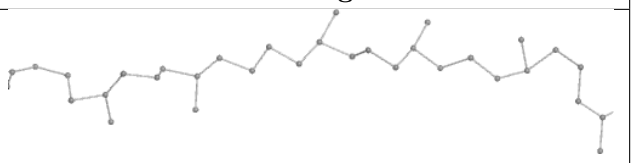
Bond lengths



Bond angles

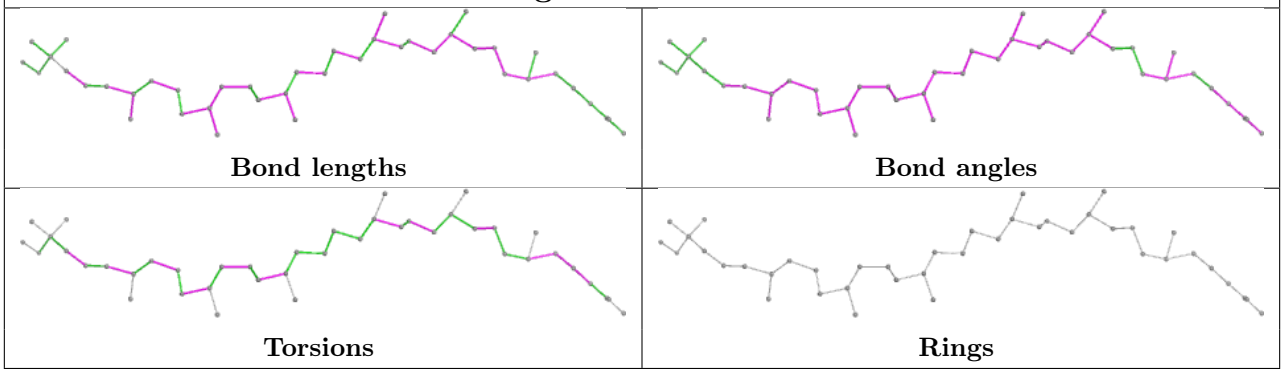


Torsions

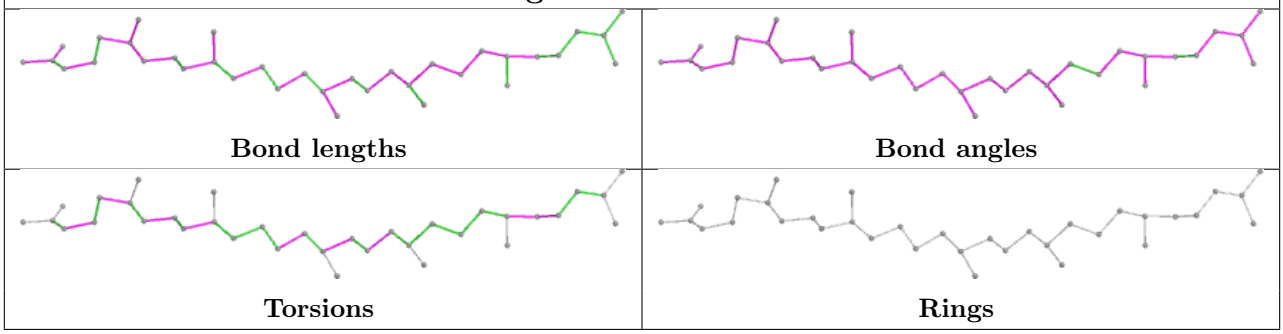


Rings

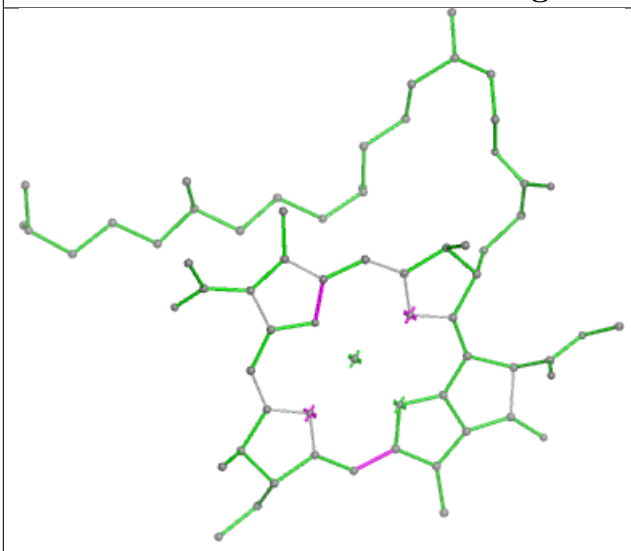
Ligand SPO i 102



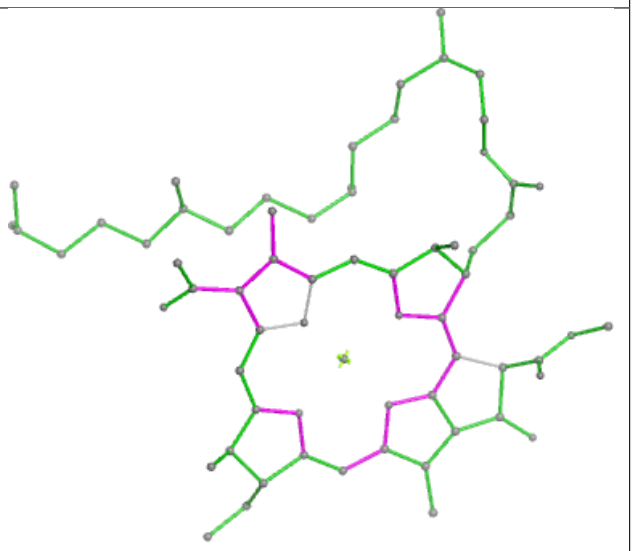
Ligand SPO D 102



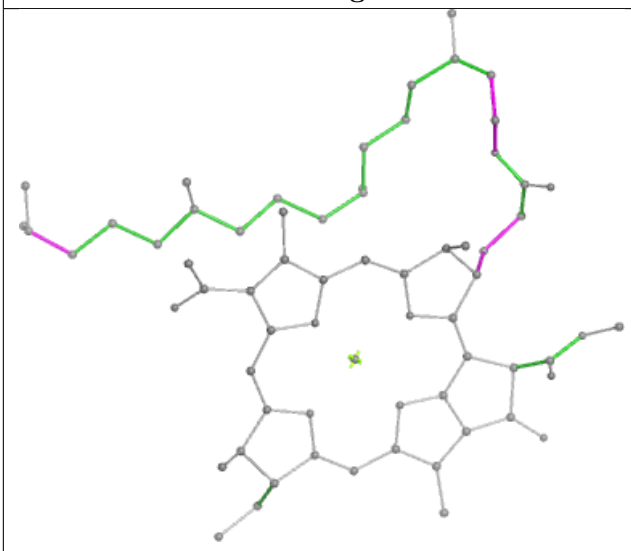
Ligand BCL I 101



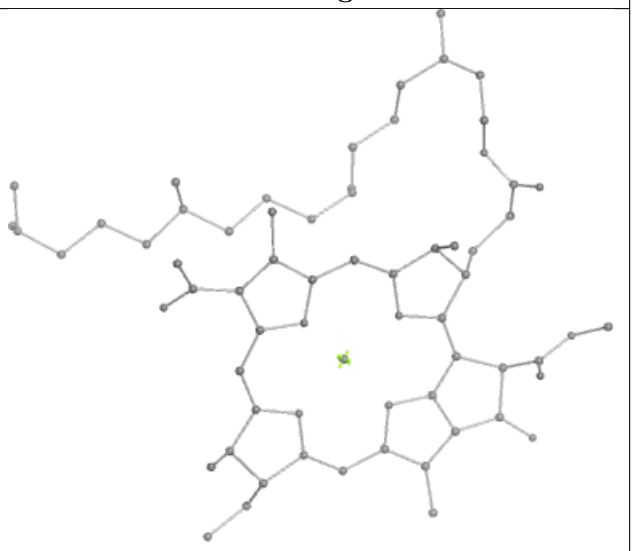
Bond lengths



Bond angles

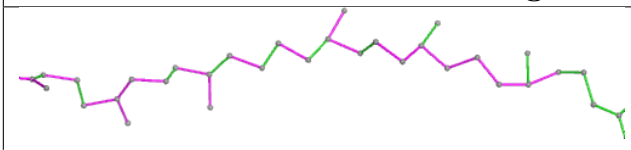


Torsions

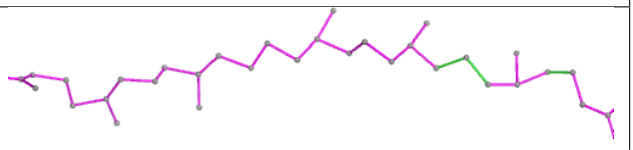


Rings

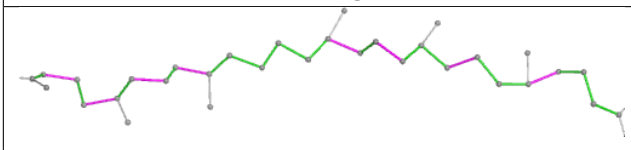
Ligand SPO O 102



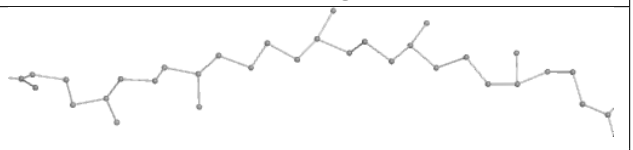
Bond lengths



Bond angles

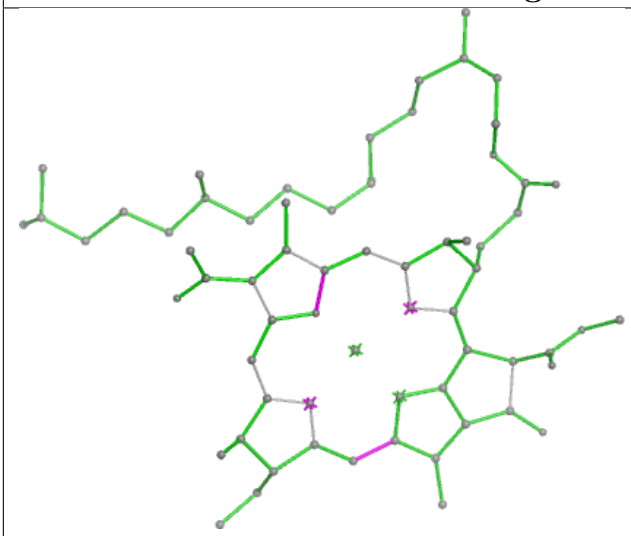


Torsions



Rings

Ligand BCL D 101



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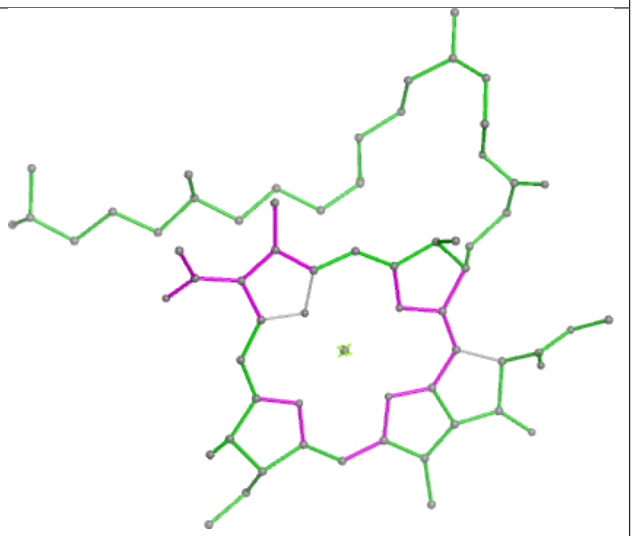

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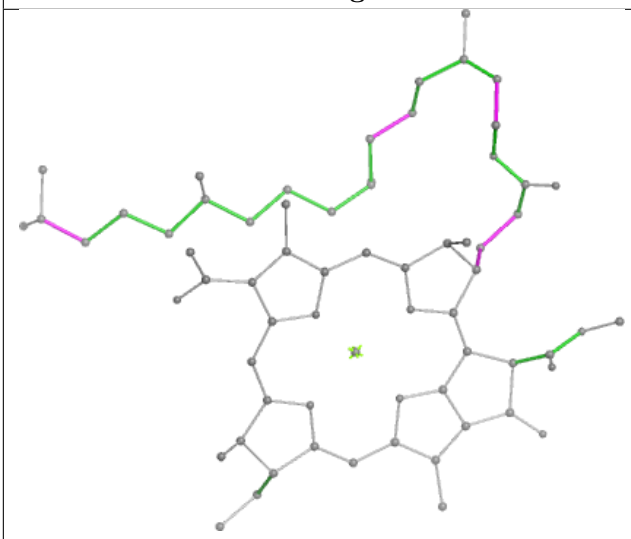

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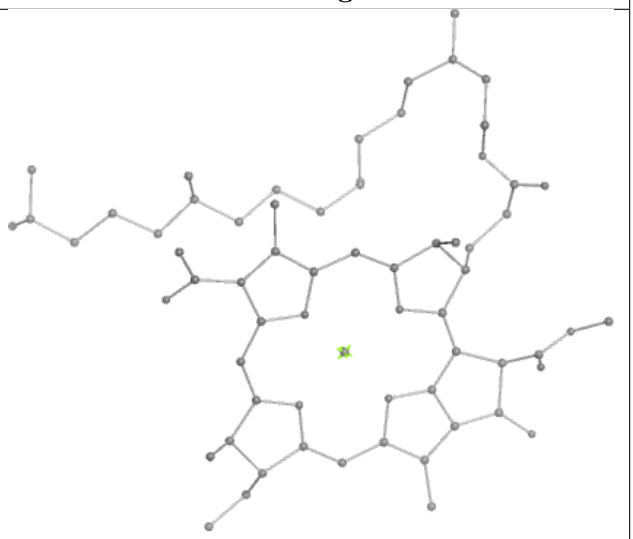

Rings

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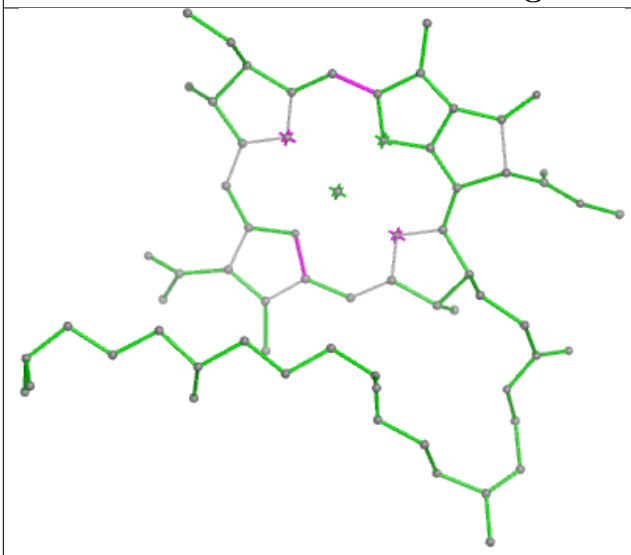

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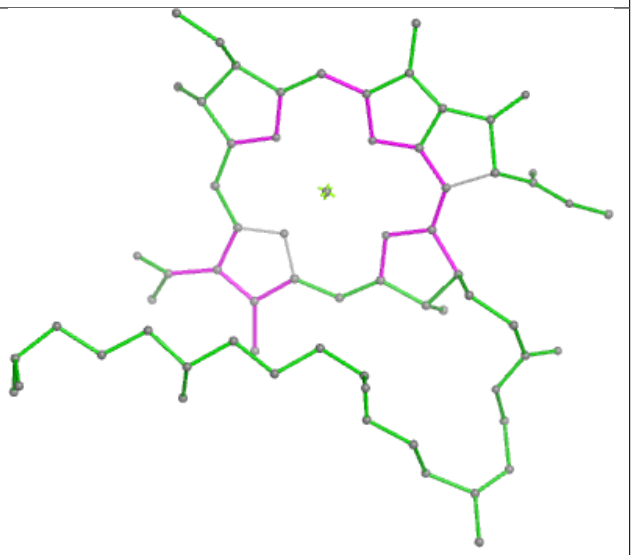

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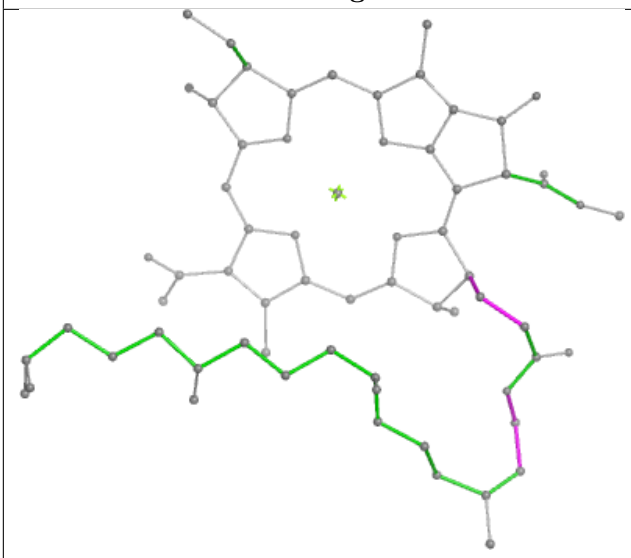

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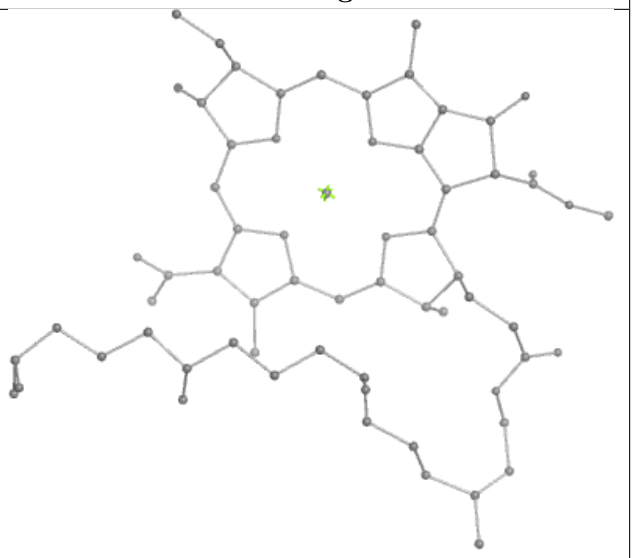
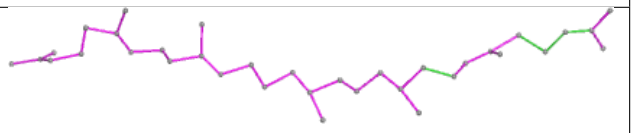


Rings

Ligand SPO B 101

Bond lengths



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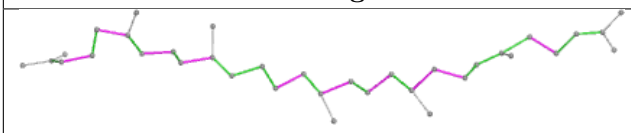

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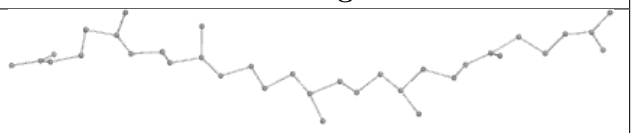
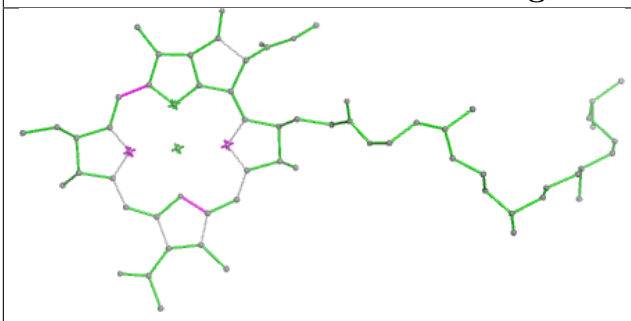


Rings

Ligand BCL d 101



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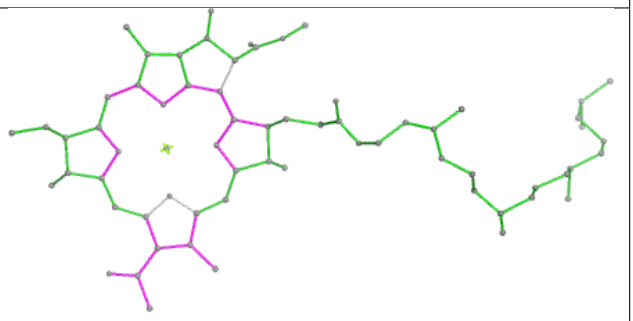

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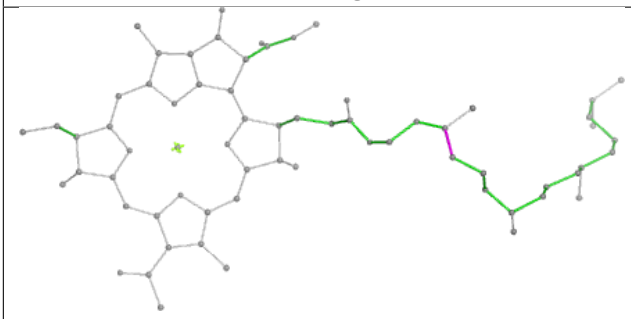

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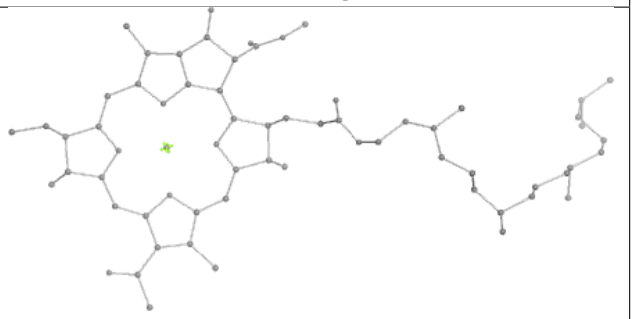
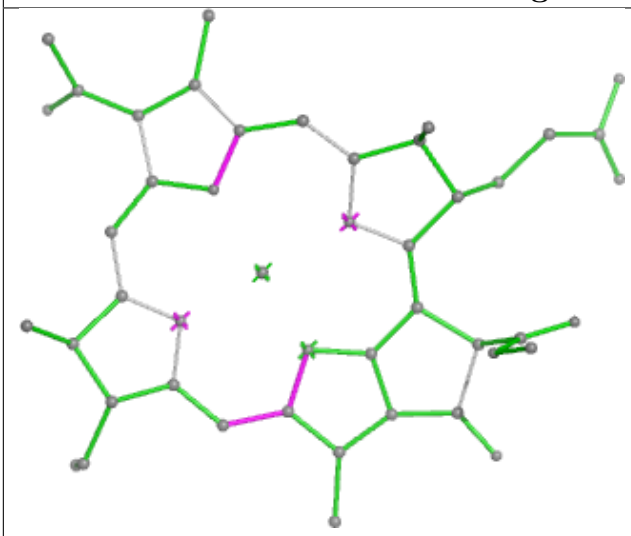


Rings

Ligand BCL t 101



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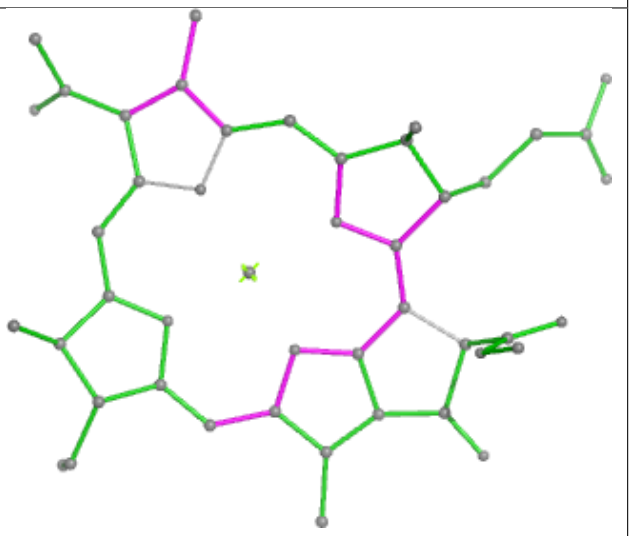

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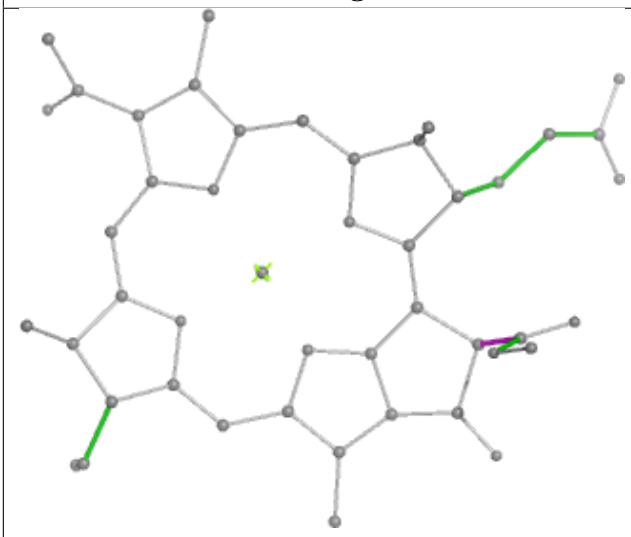

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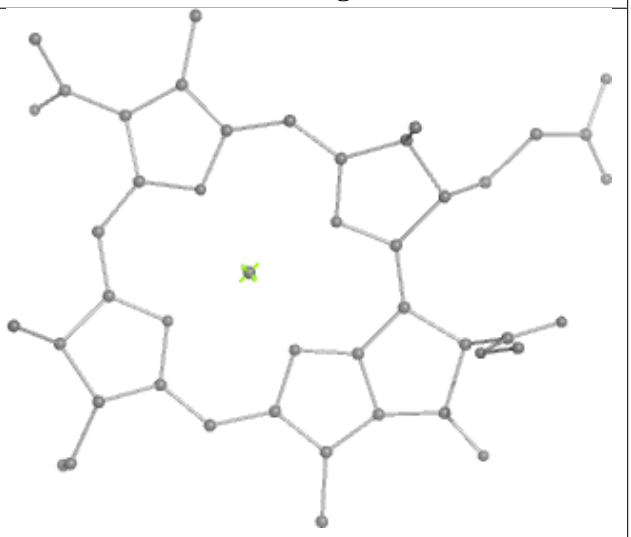

Rings

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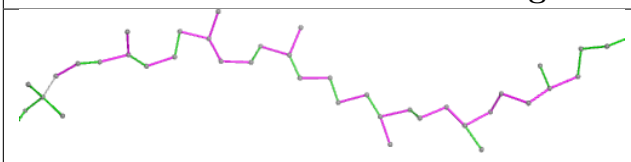

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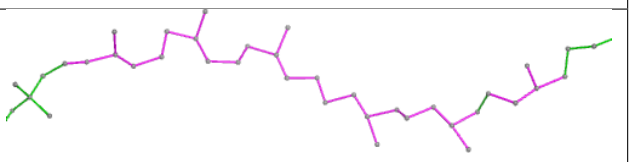

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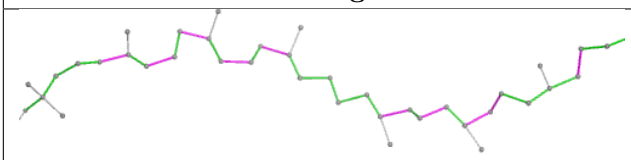

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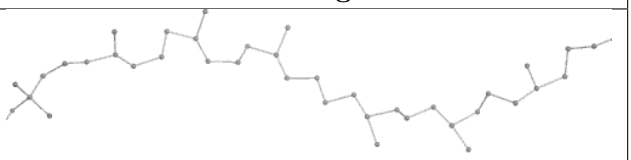
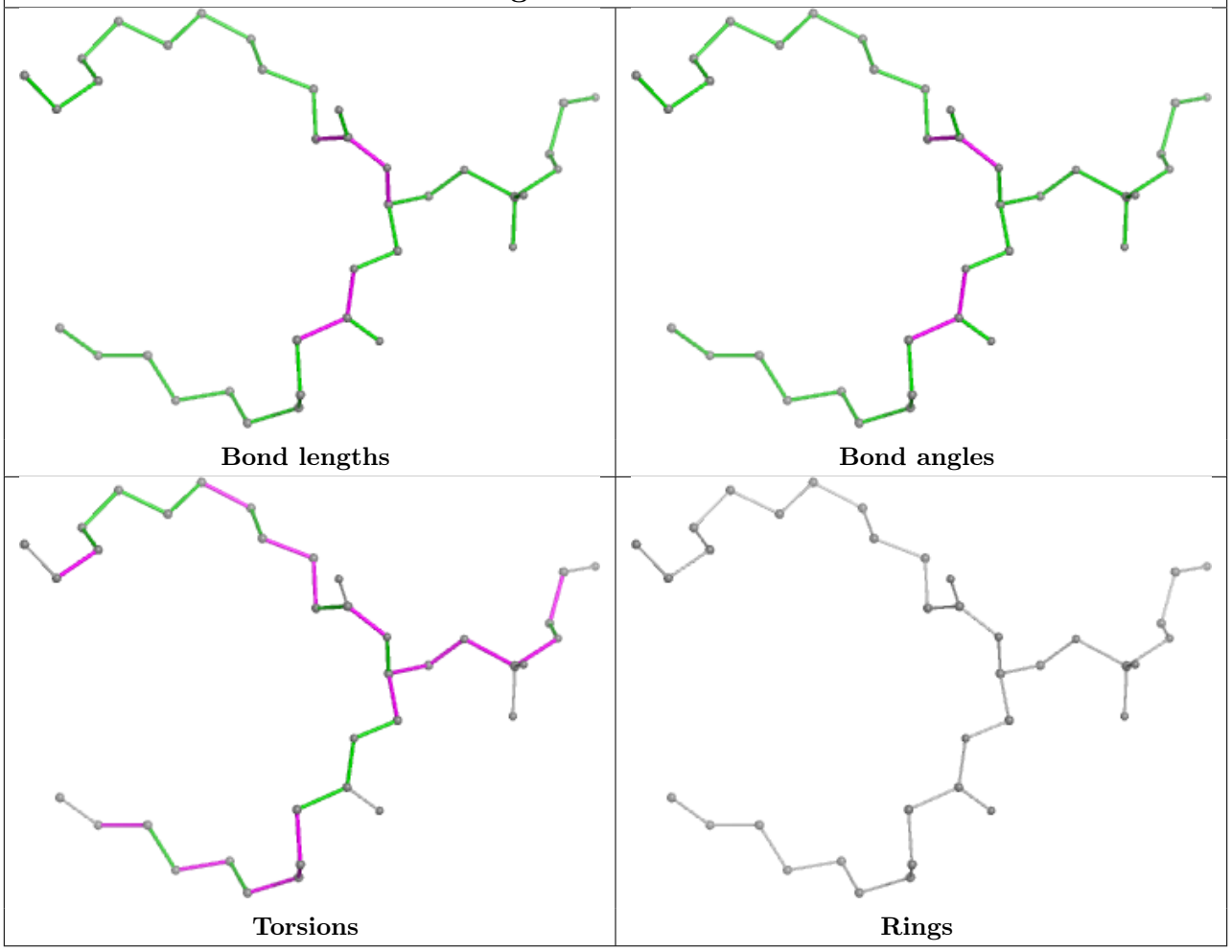


Rings

Ligand 3PE d 103



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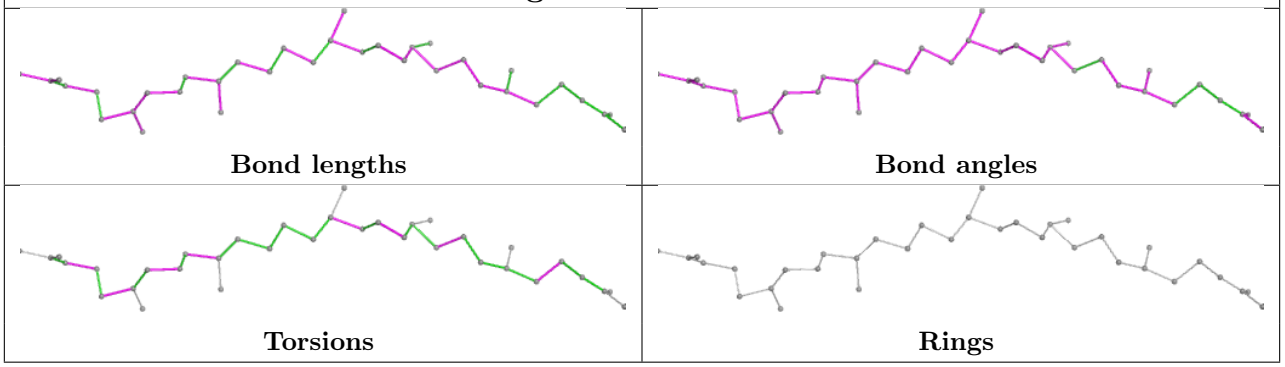

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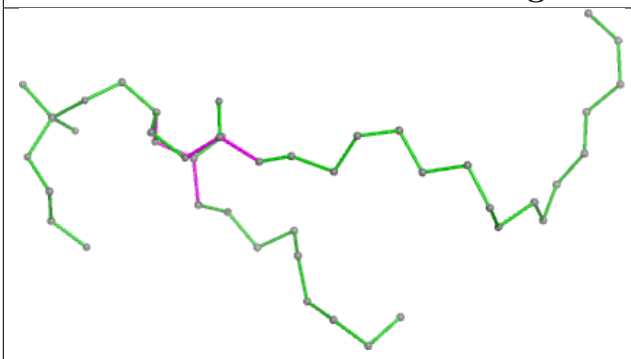

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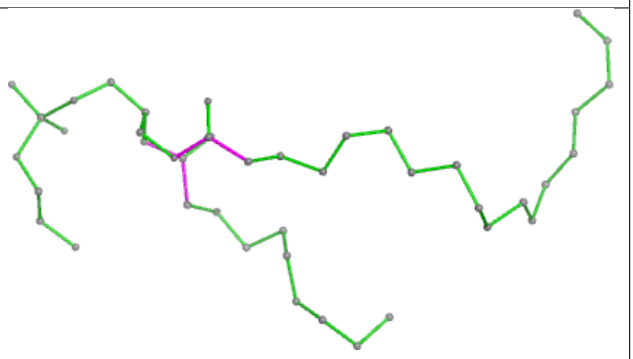
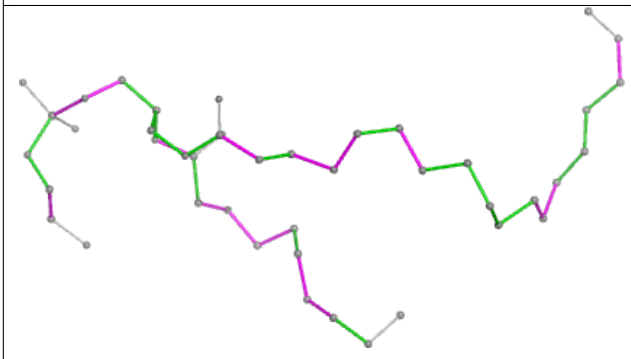


Bond angles



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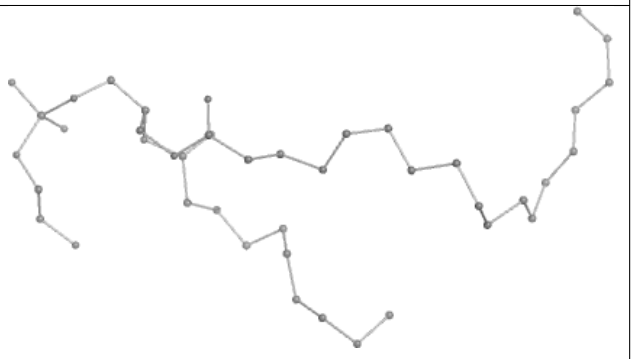

Rings

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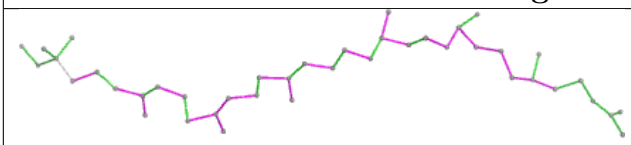

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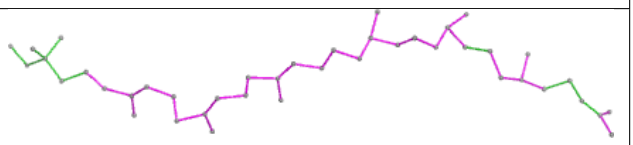

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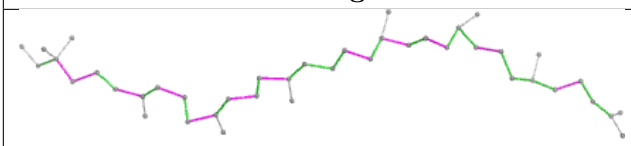

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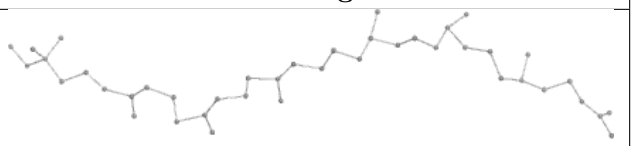
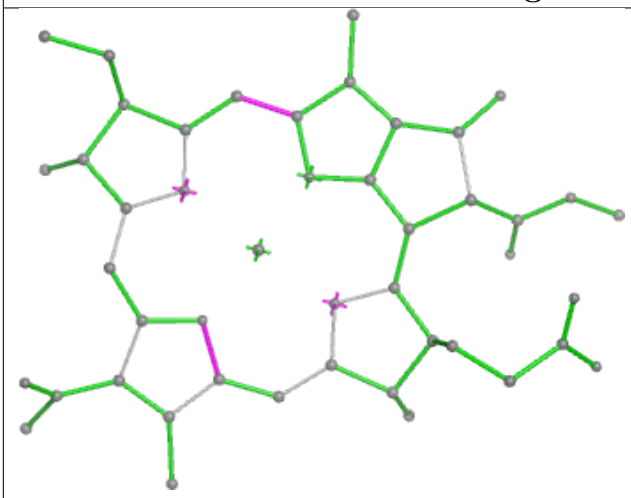


Rings

Ligand BCL U 101



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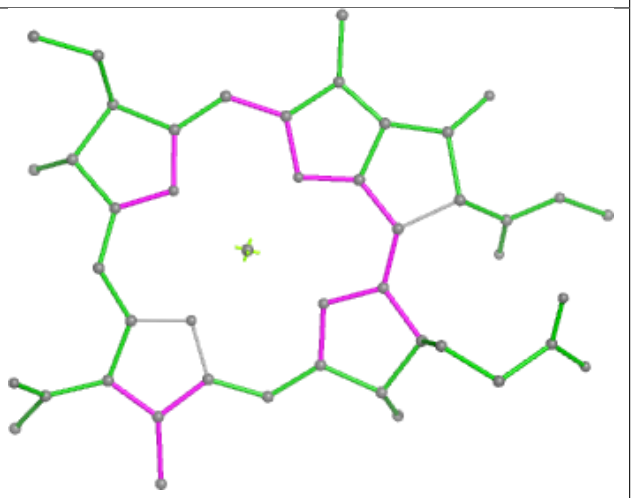

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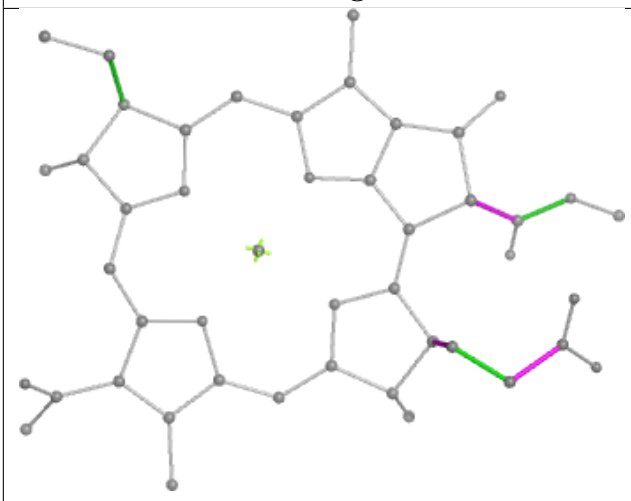

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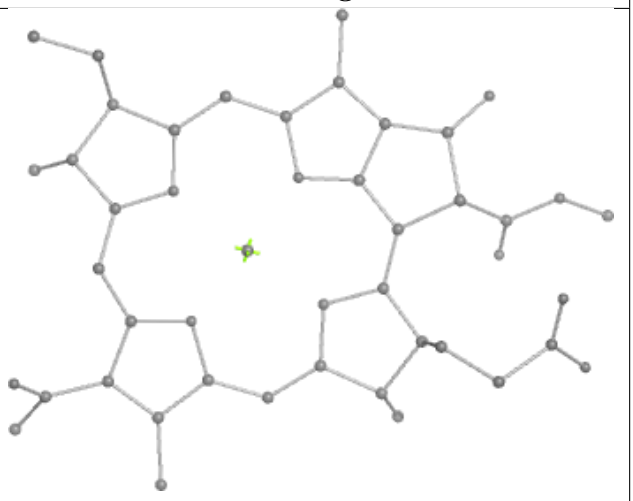
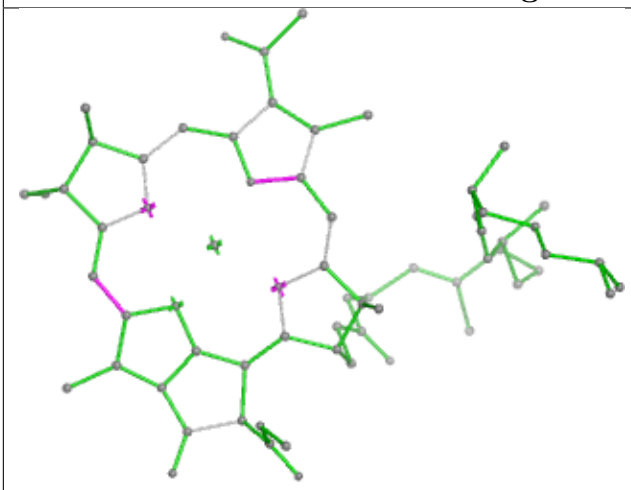


Rings

Ligand BCL M 405



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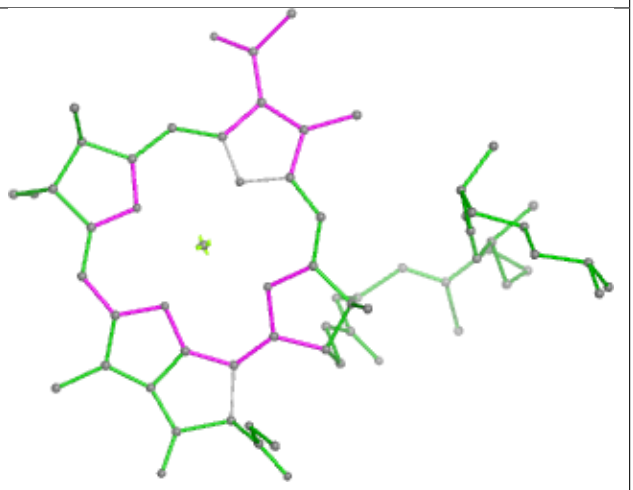
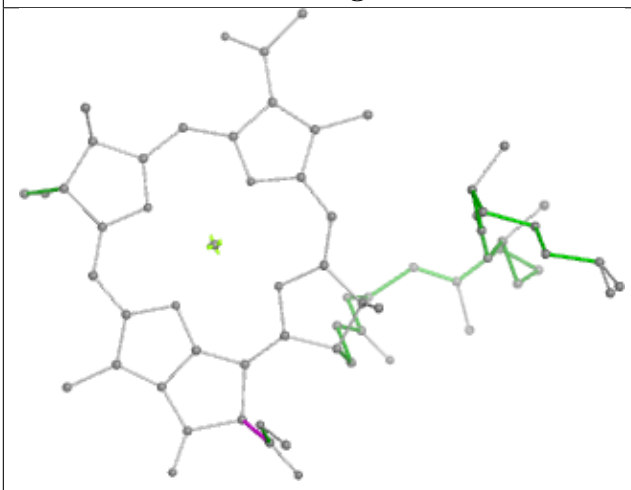


Bond angles



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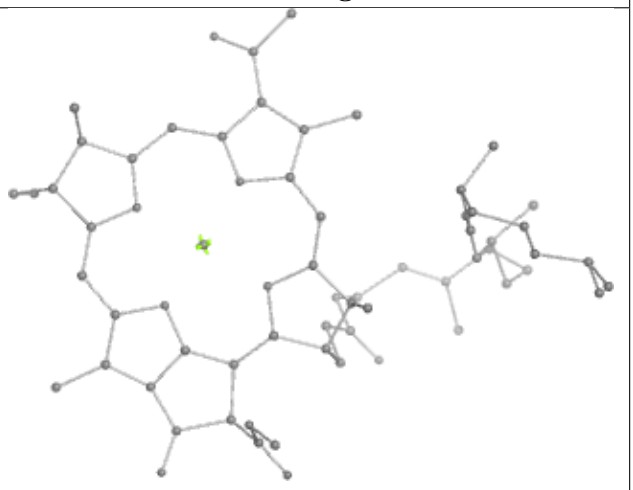
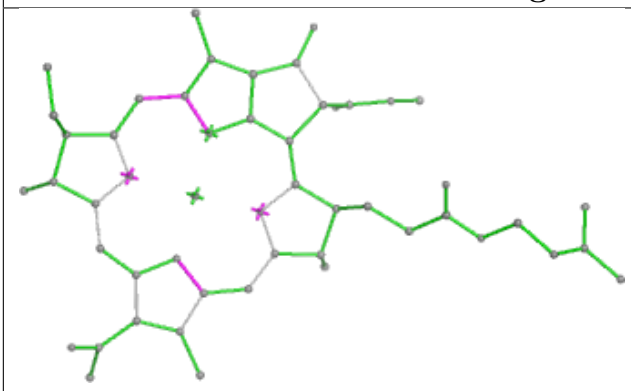


Rings

Ligand BCL a 100



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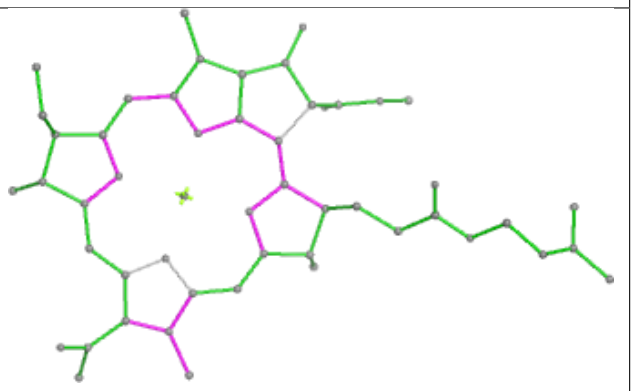
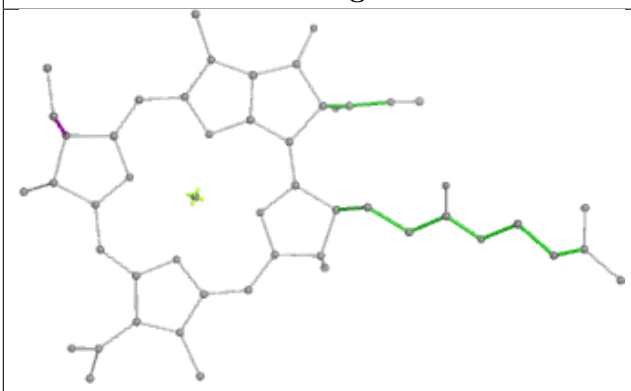


Bond angles



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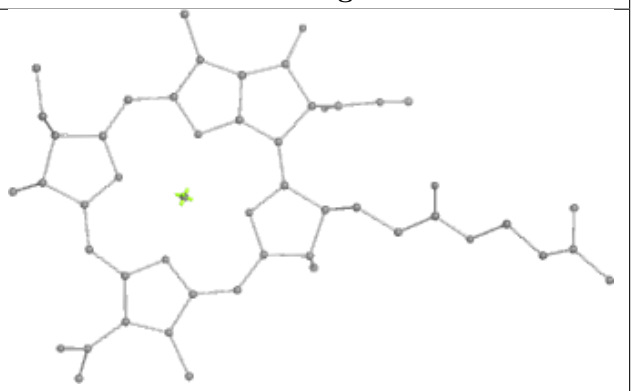
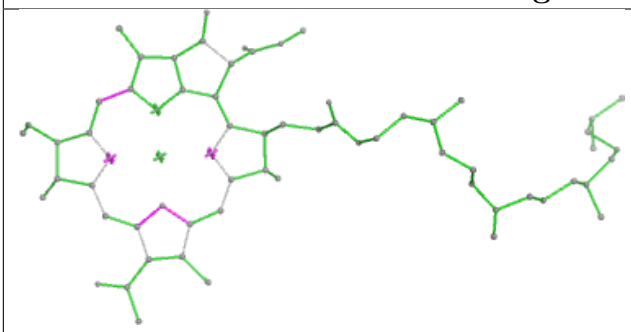


Rings

Ligand BCL i 101



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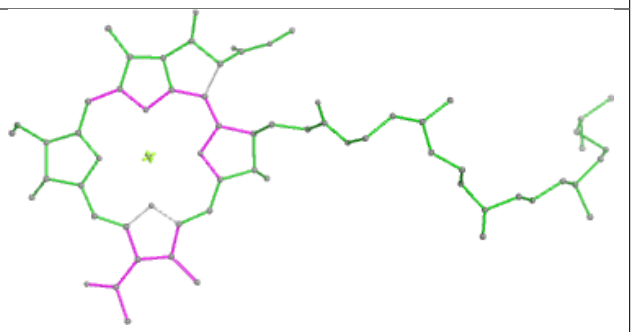
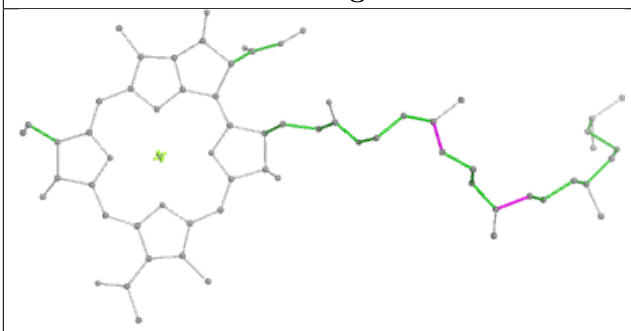


Bond angles



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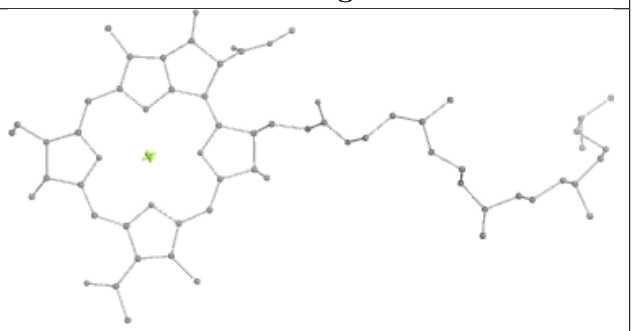
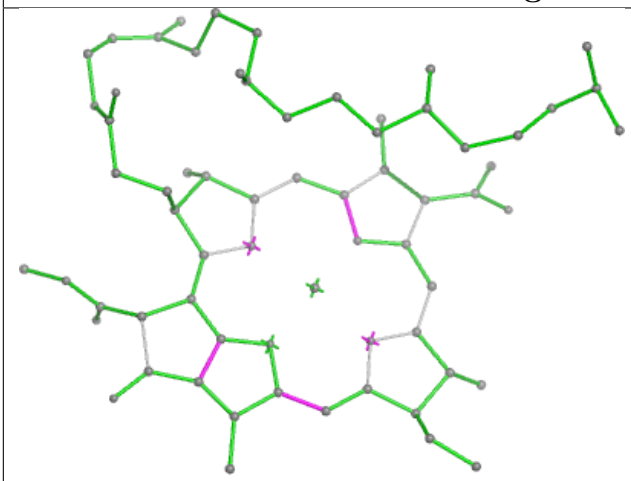


Rings

Ligand BCL A 202



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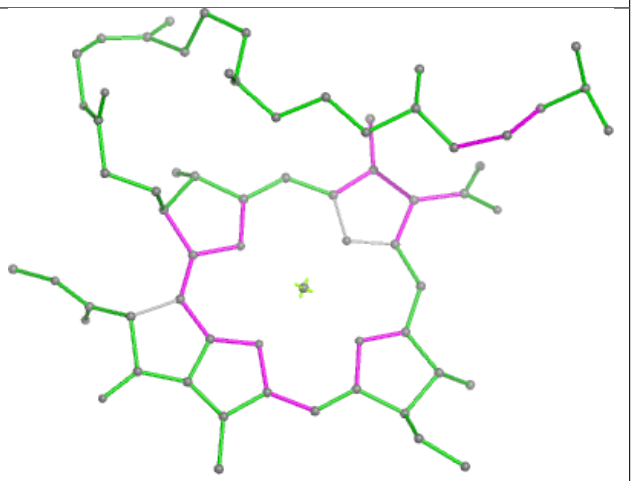
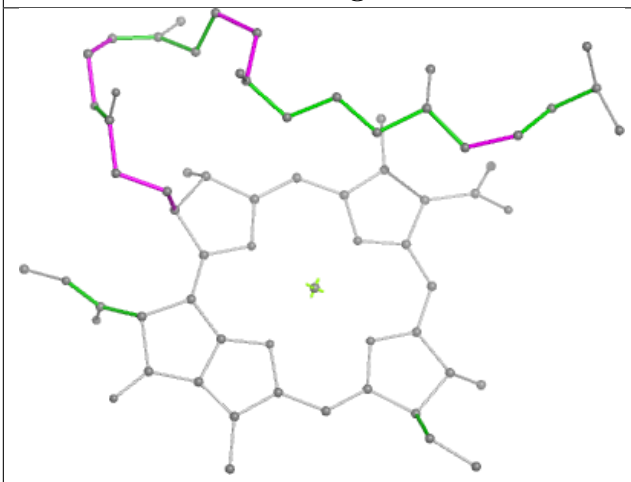


Bond angles



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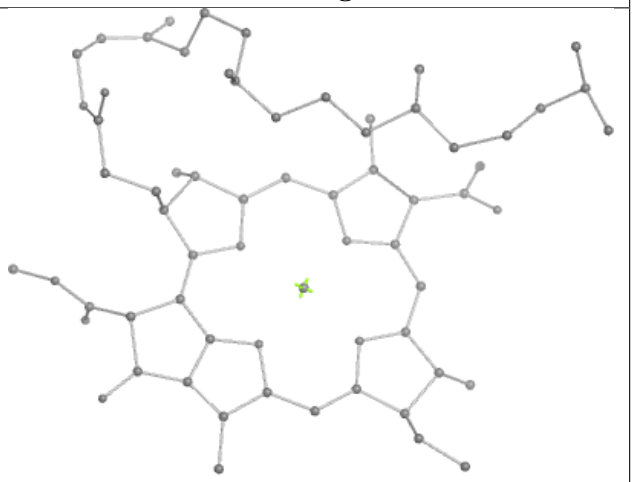
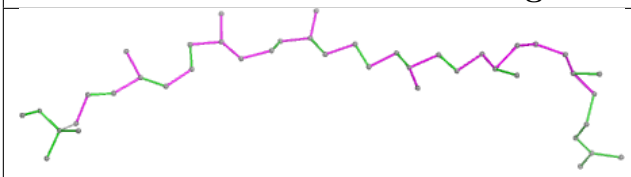


Rings

Ligand SPO A 201



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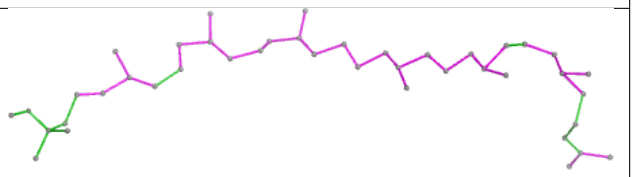
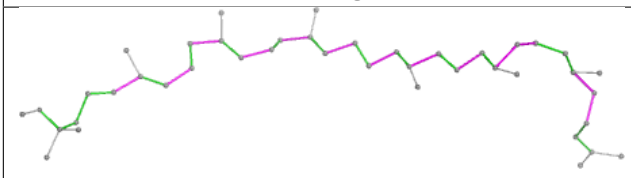
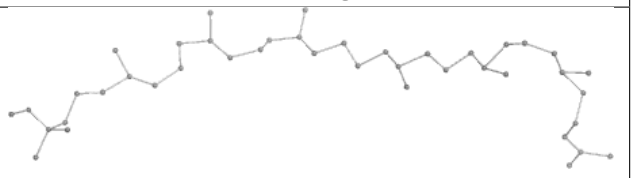


Bond angles

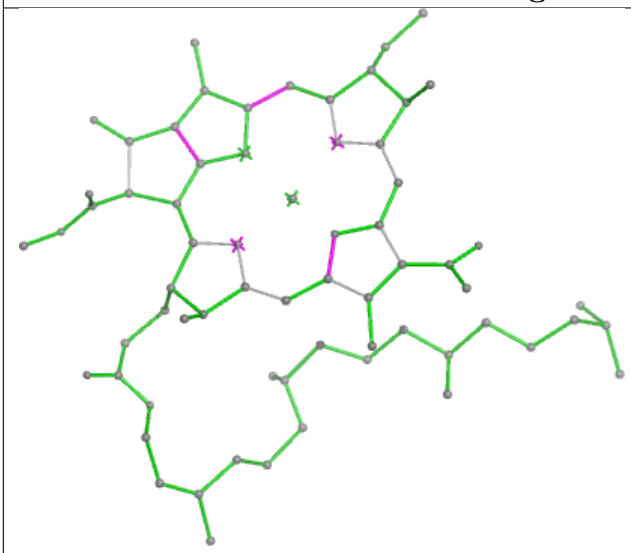


Torsions

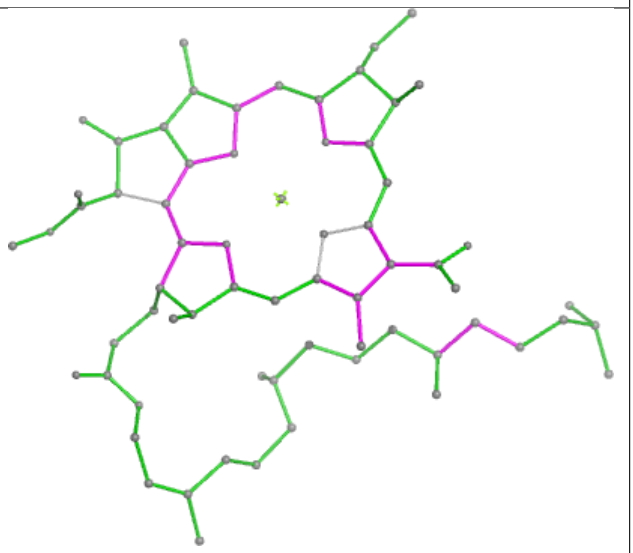


Rings

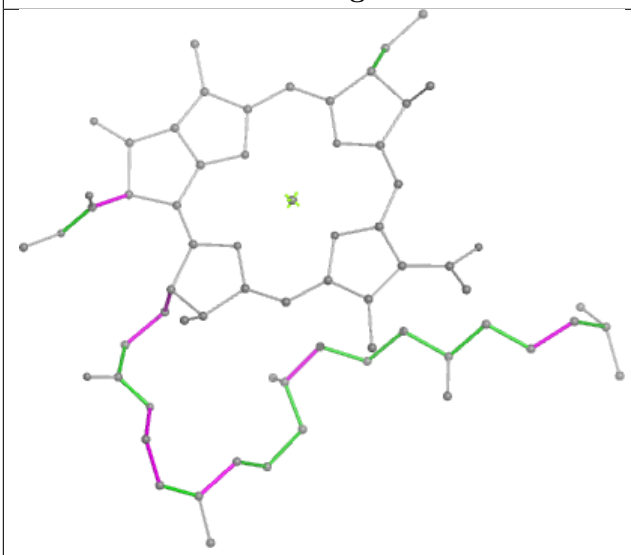
Ligand BCL J 102



Bond lengths



Bond angles



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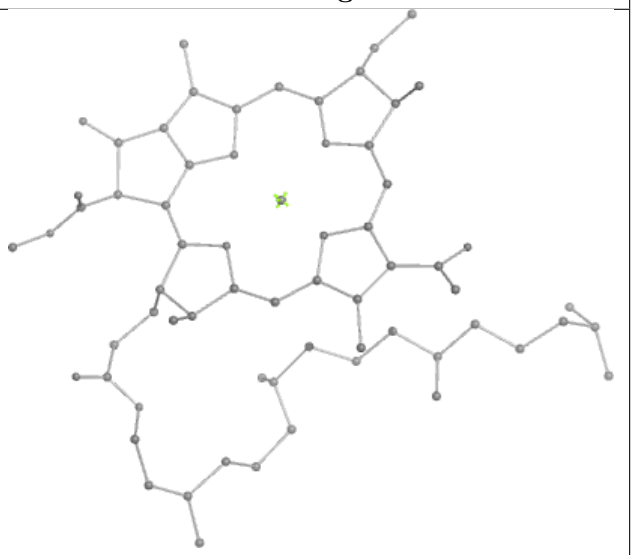
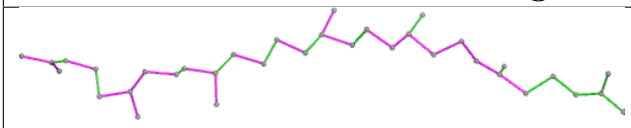


Rings

Ligand SPO J 101



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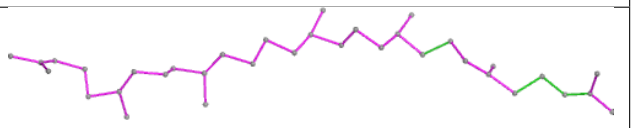
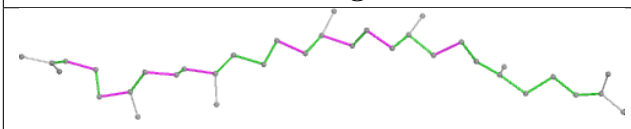


Bond angles



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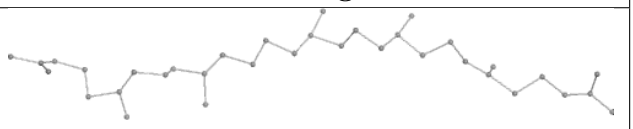
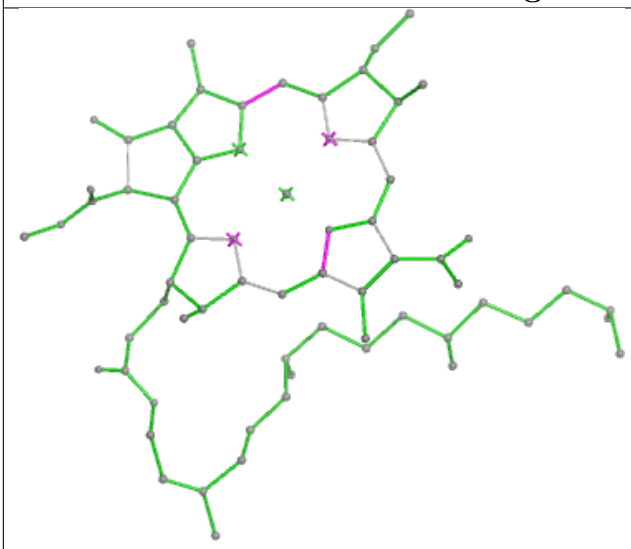


Rings

Ligand BCL K 102



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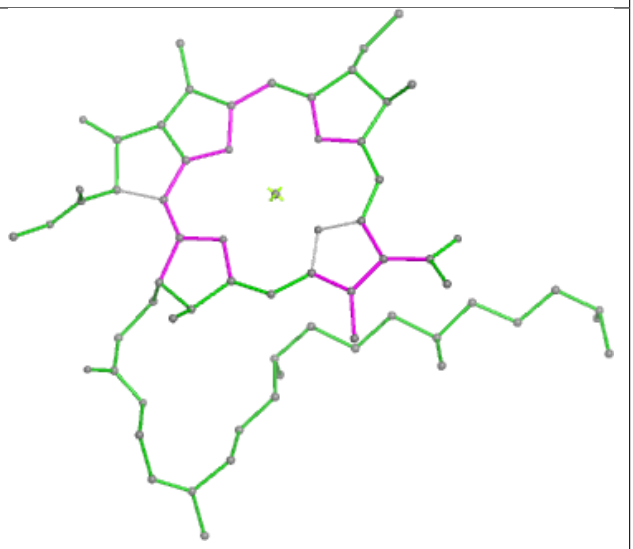

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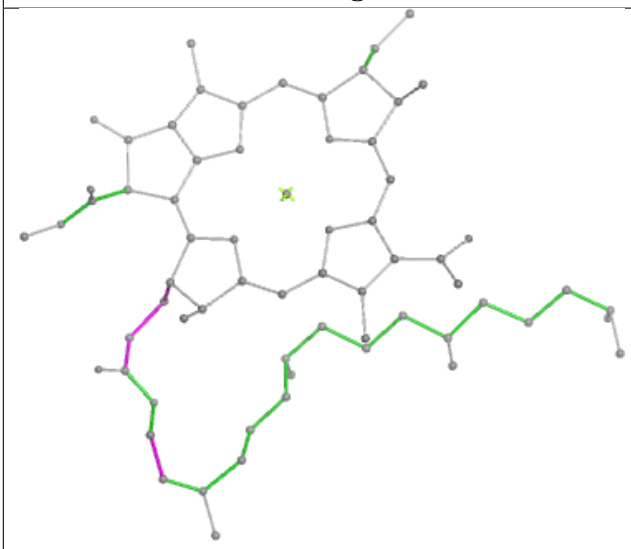

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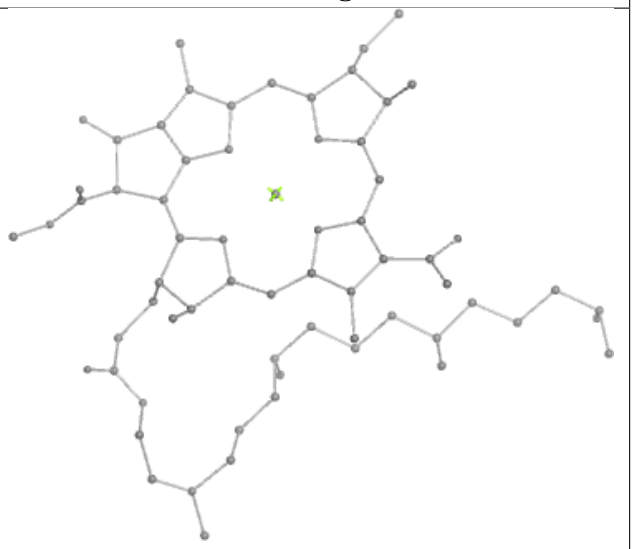
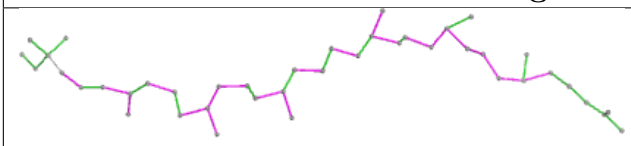


Rings

Ligand SPO o 102



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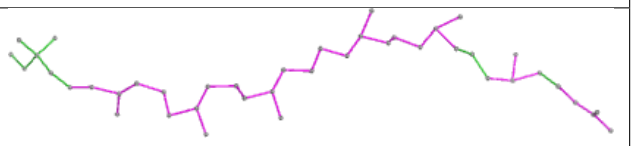

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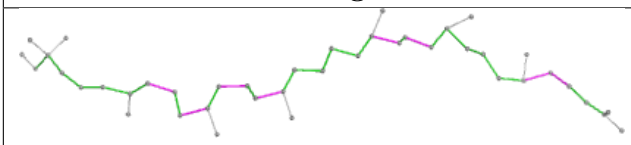

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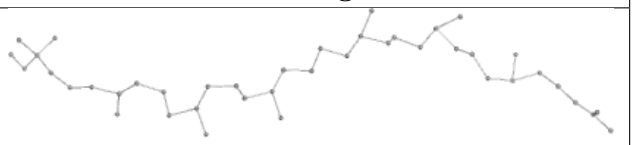
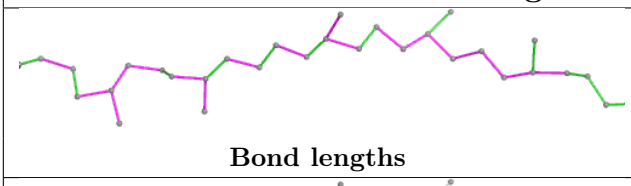


Rings

Ligand SPO K 101



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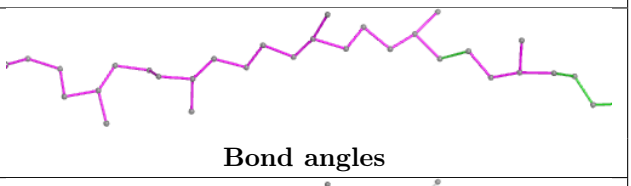

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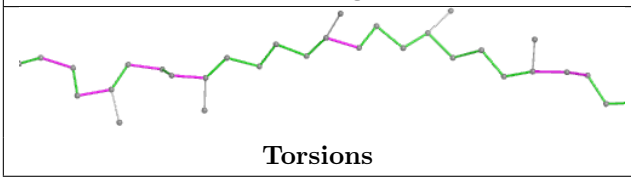

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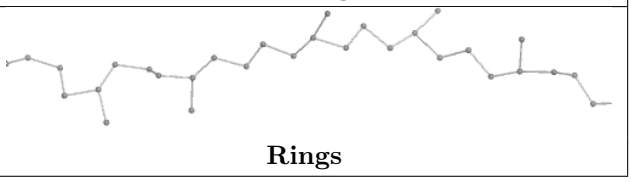
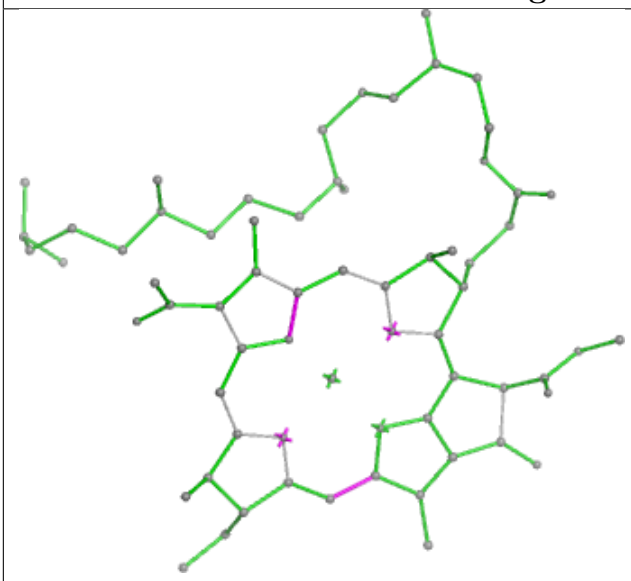


Rings

Ligand BCL g 102



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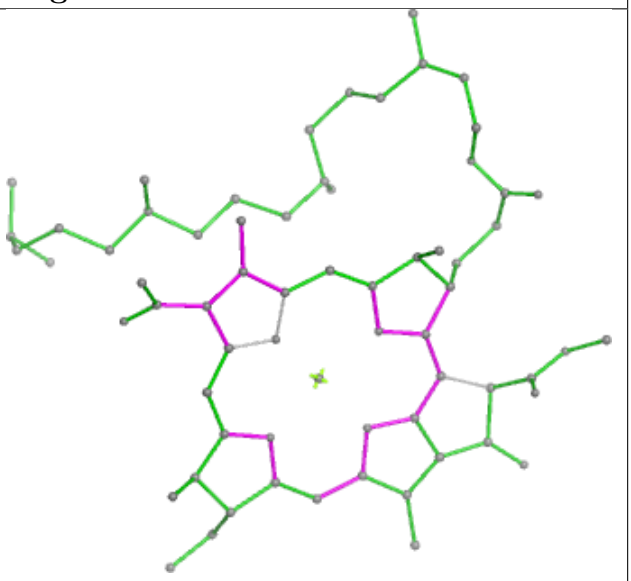

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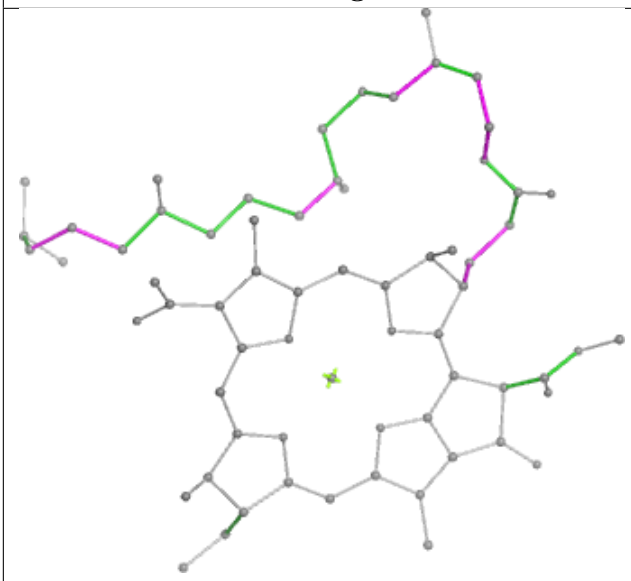

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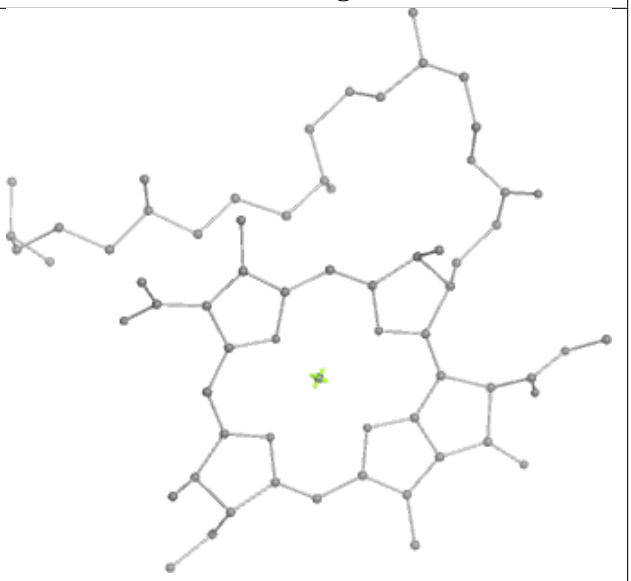
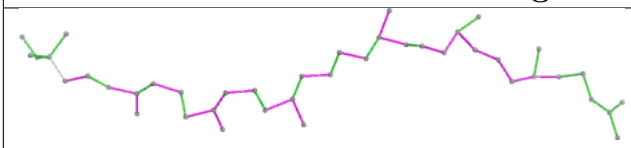


Rings

Ligand SPO t 102



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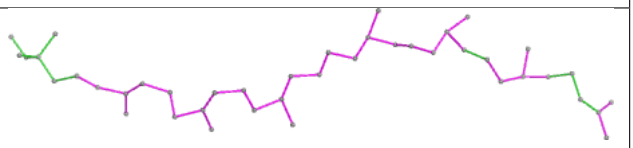

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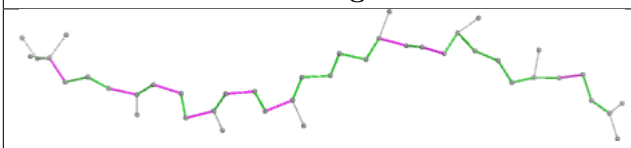

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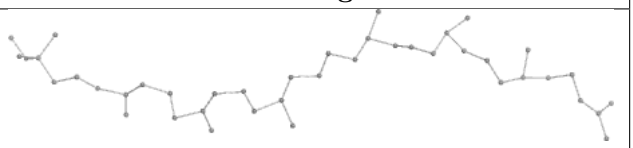
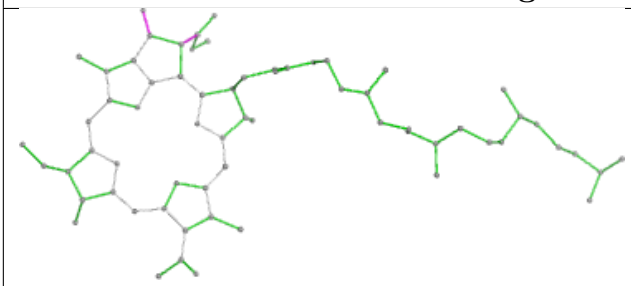


Rings

Ligand BPH M 408



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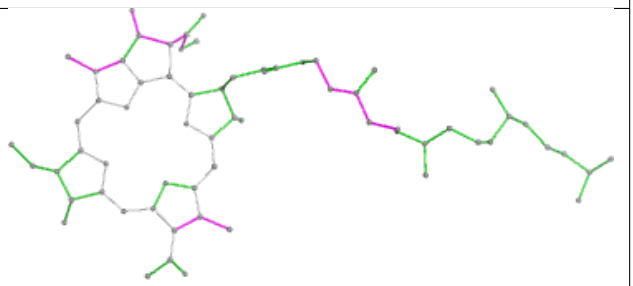

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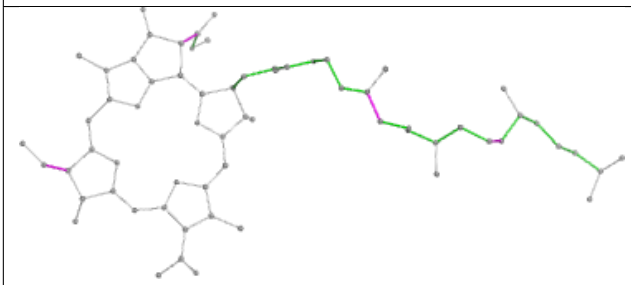

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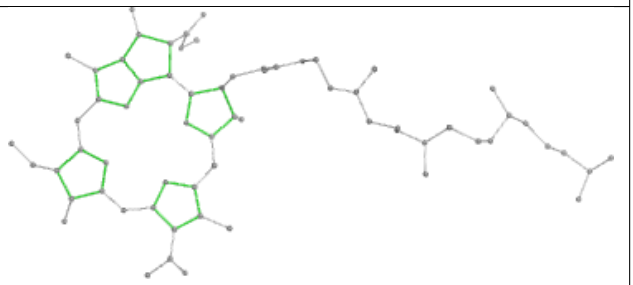
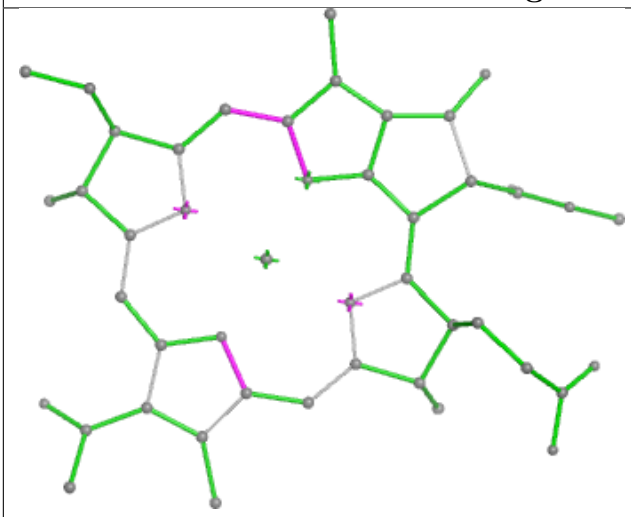


Rings

Ligand BCL T 101



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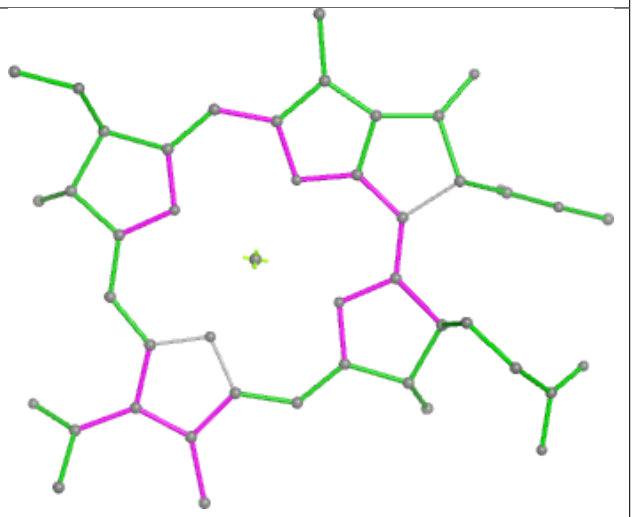
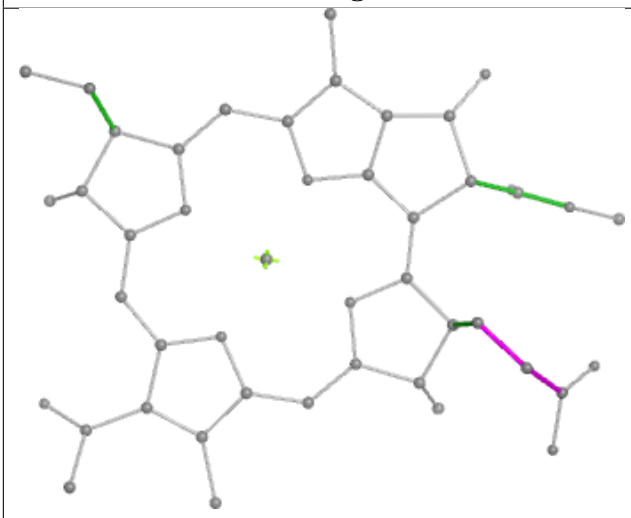


Bond angles



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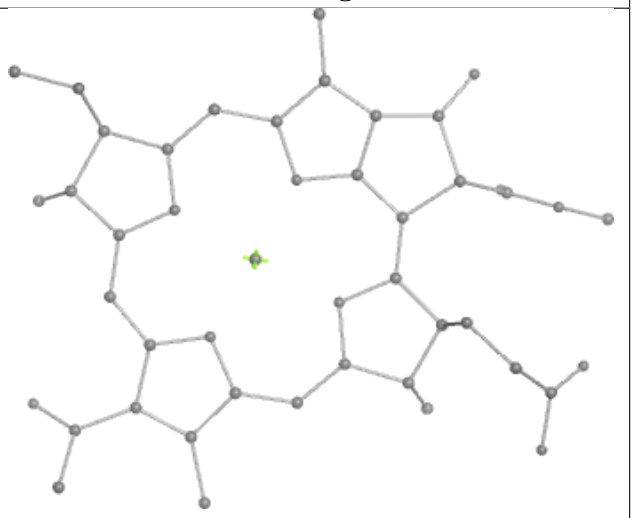
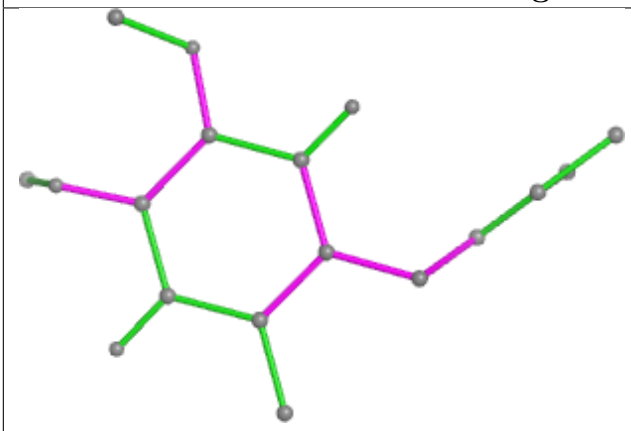


Rings

Ligand U10 L 305



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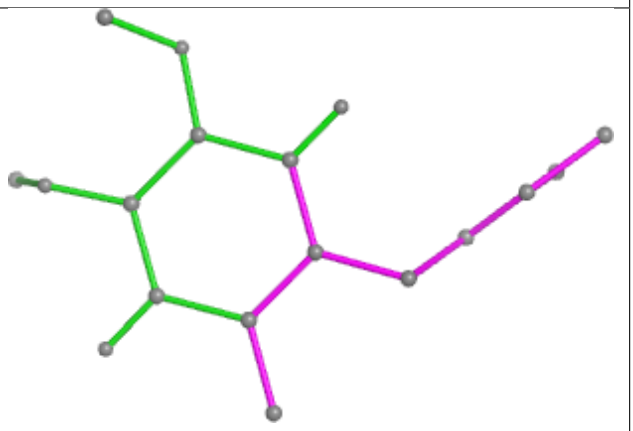
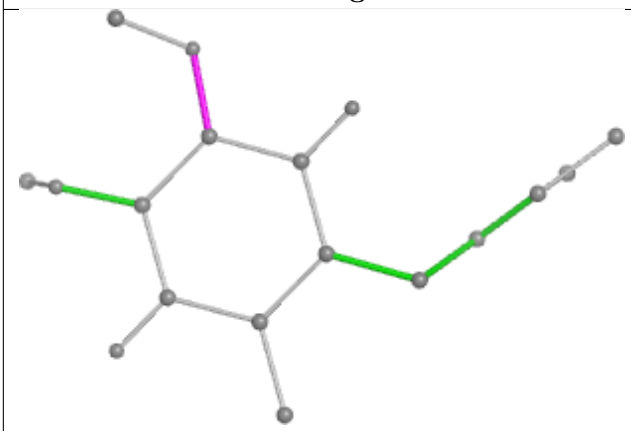


Bond angles



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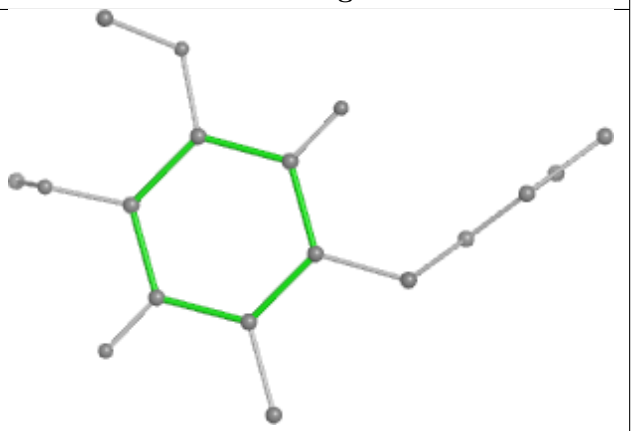
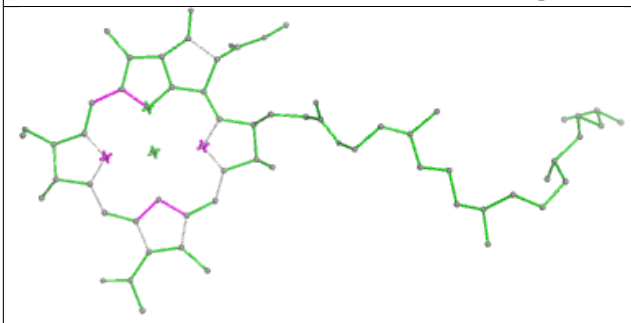


Rings

Ligand BCL j 101



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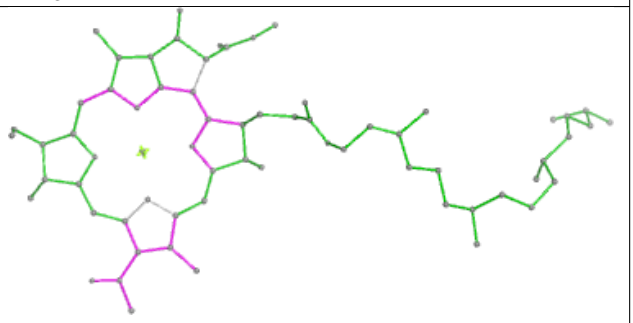

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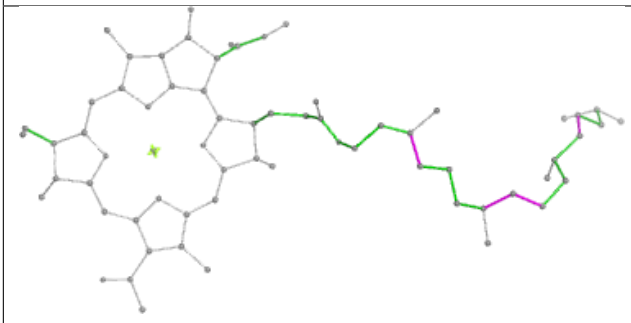

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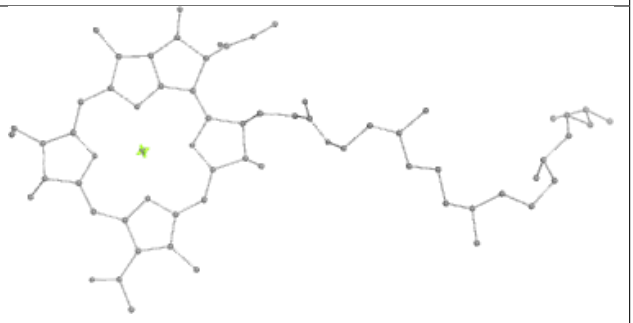
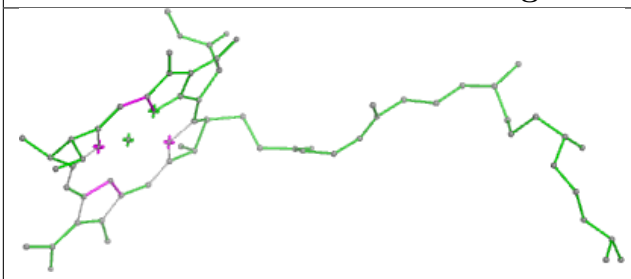


Rings

Ligand BCL M 407



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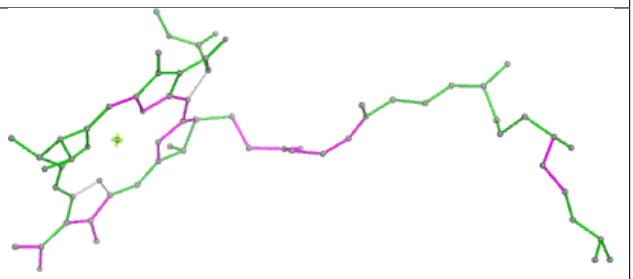
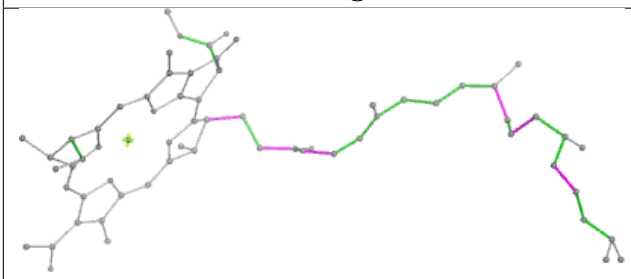


Bond angles



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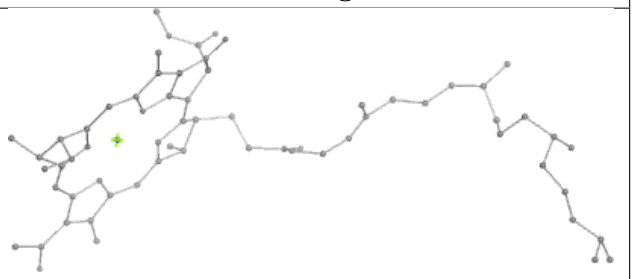
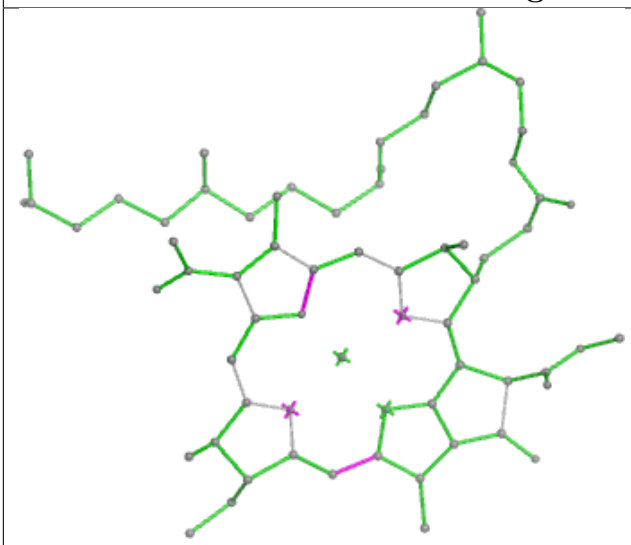


Rings

Ligand BCL F 102



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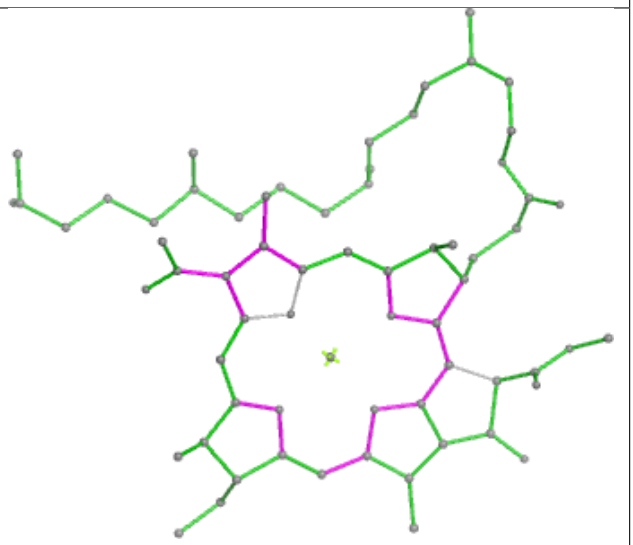
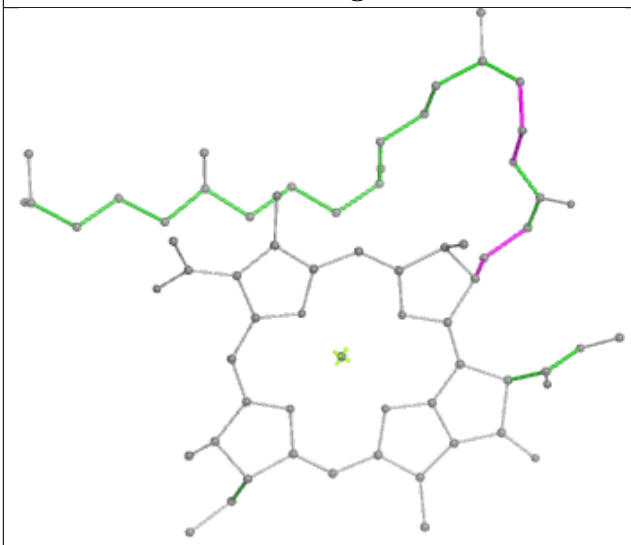


Bond angles



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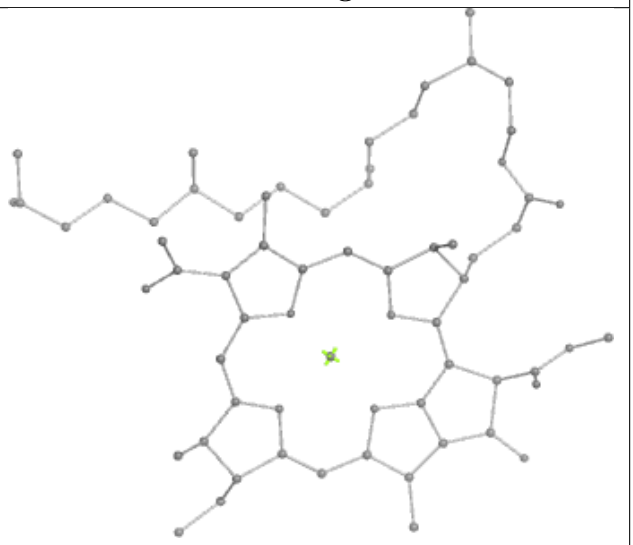
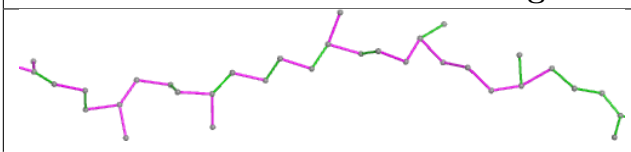


Rings

Ligand SPO F 101



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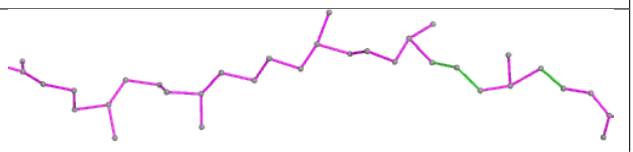
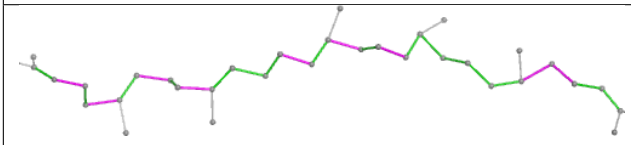


Bond angles



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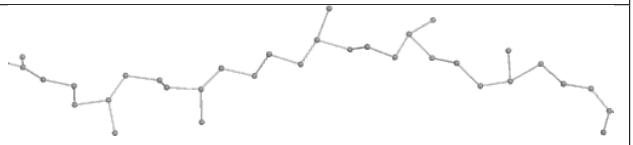
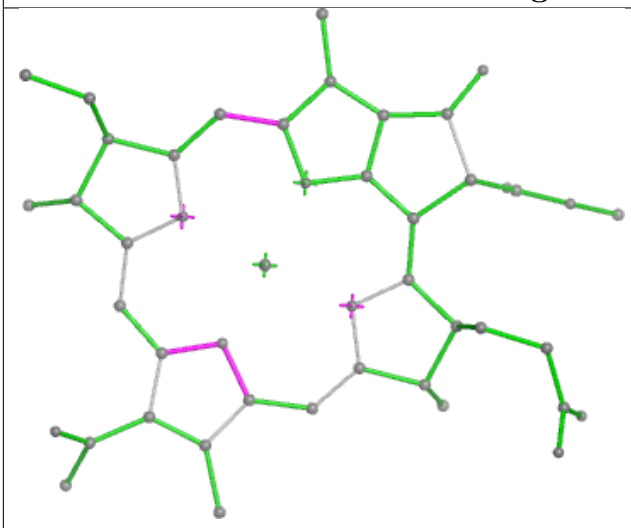
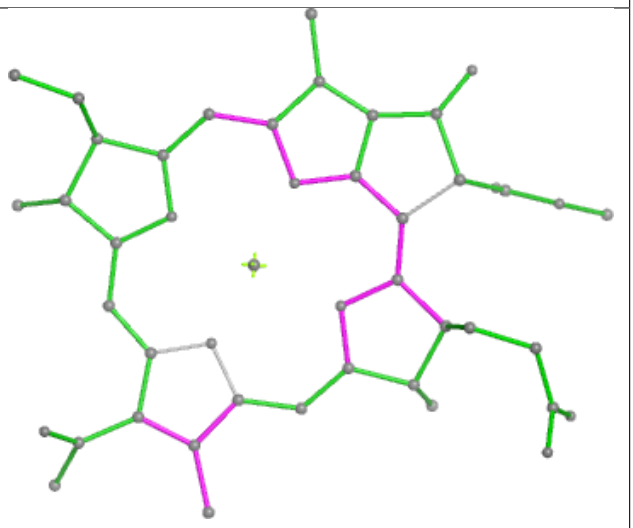


Rings

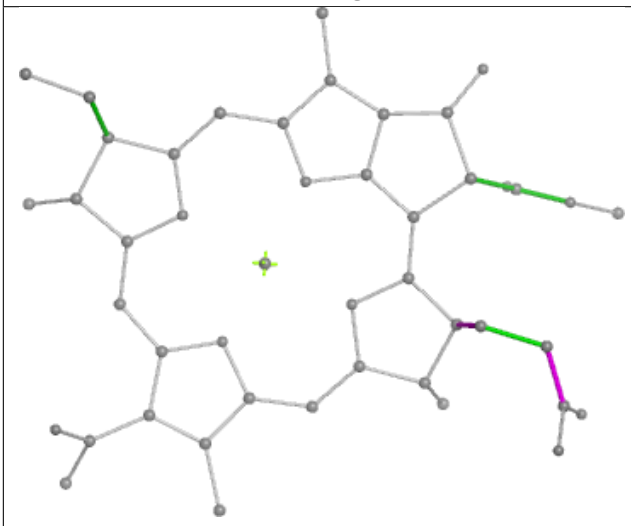
Ligand BCL r 103



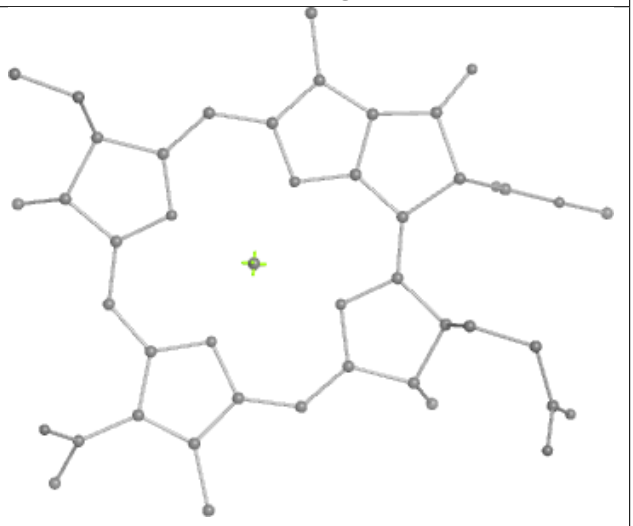
Bond lengths



Bond angles

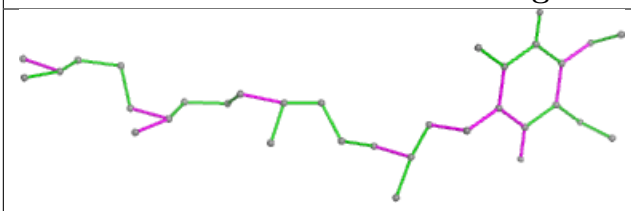


Torsions

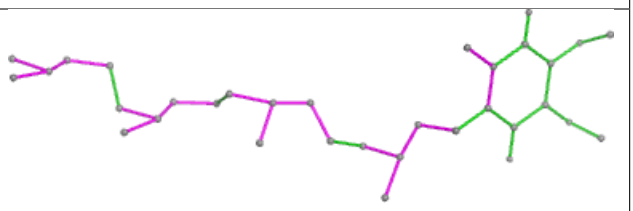


Rings

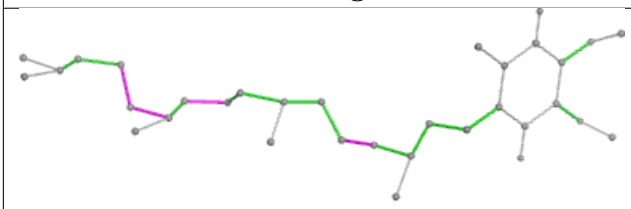
Ligand U10 L 303



Bond lengths

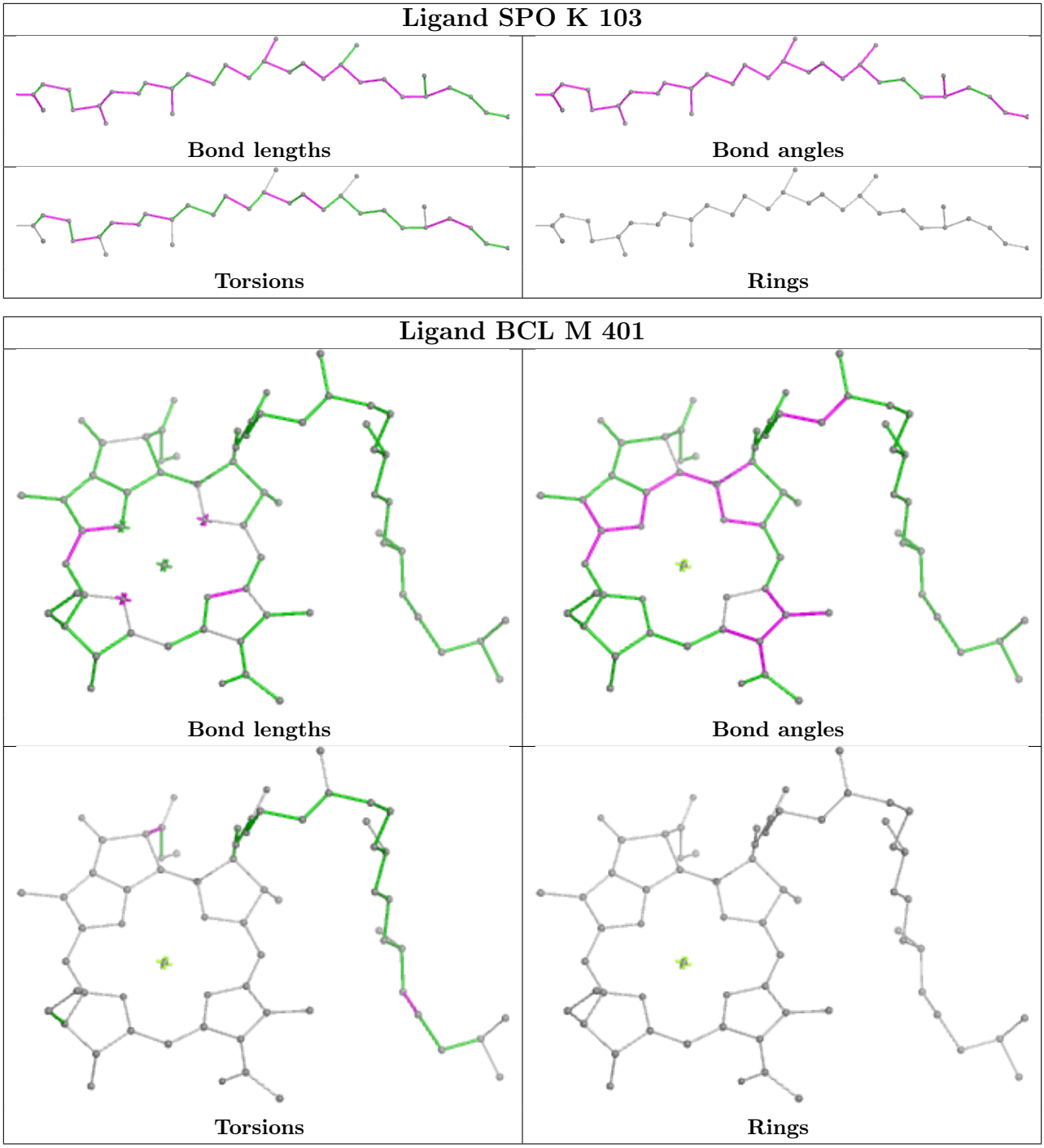


Bond angles



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.

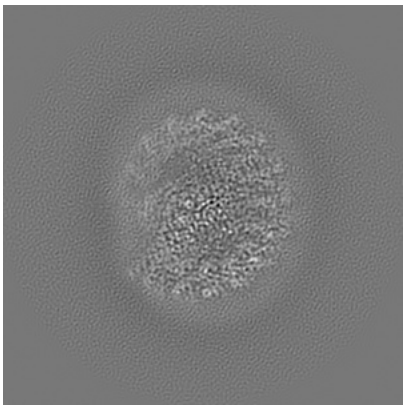
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15862. These allow visual inspection of the internal detail of the map and identification of artifacts.

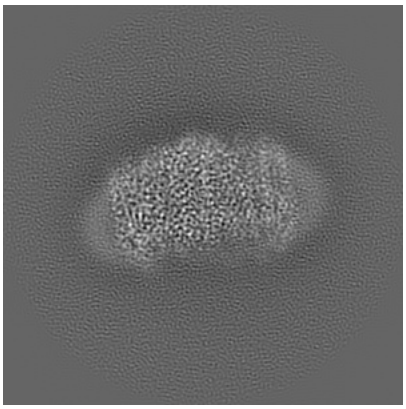
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

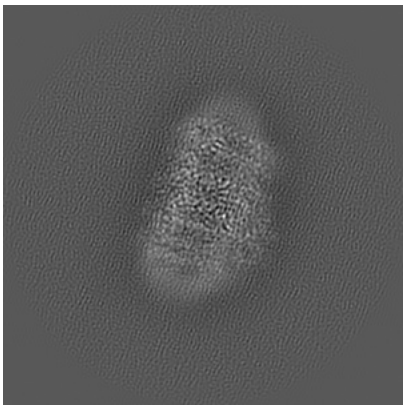
6.1.1 Primary map



X

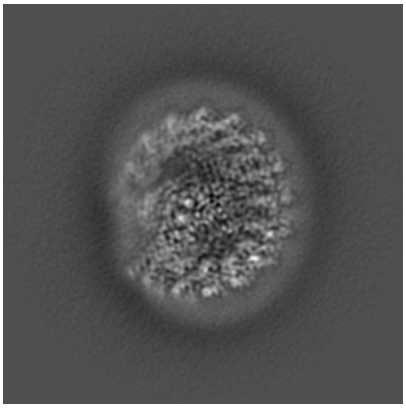


Y

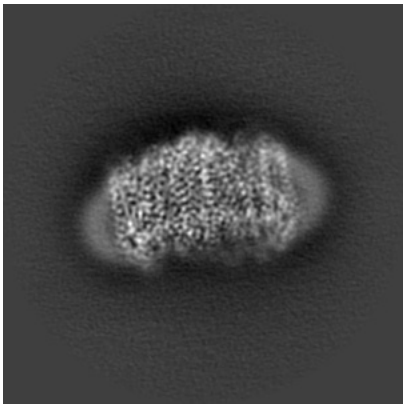


Z

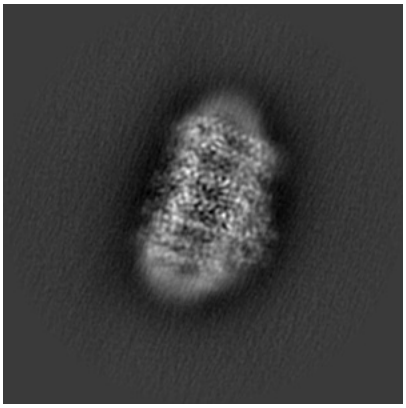
6.1.2 Raw map



X



Y

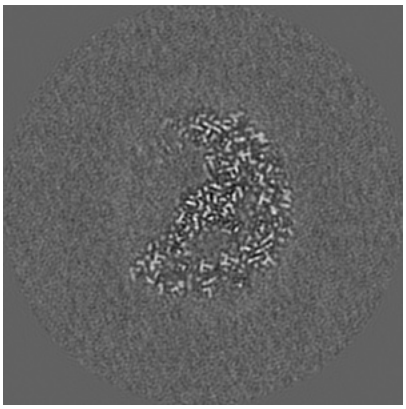


Z

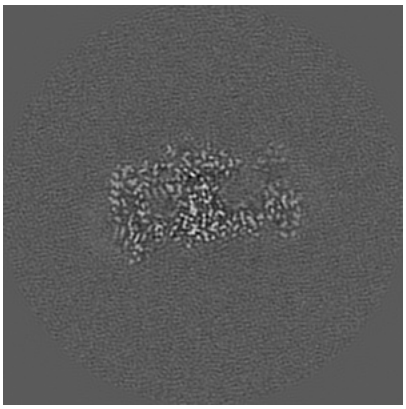
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

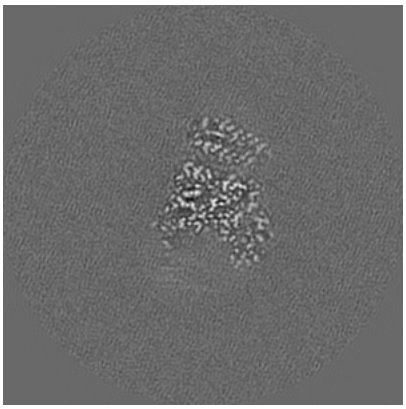
6.2.1 Primary map



X Index: 150

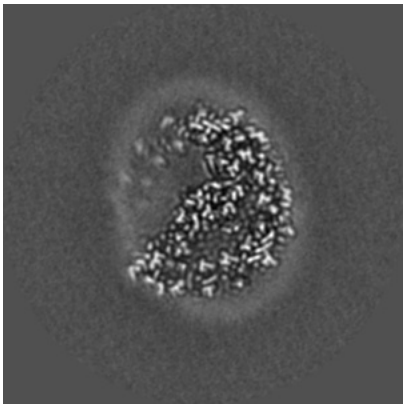


Y Index: 150

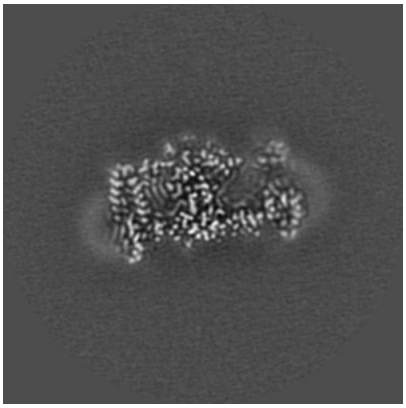


Z Index: 150

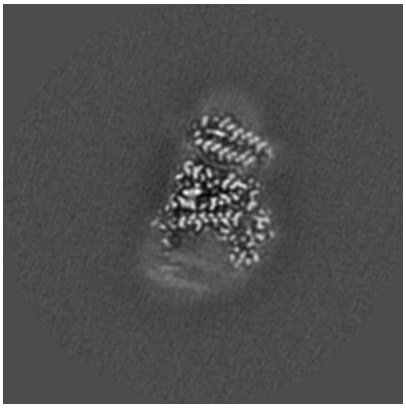
6.2.2 Raw map



X Index: 150



Y Index: 150

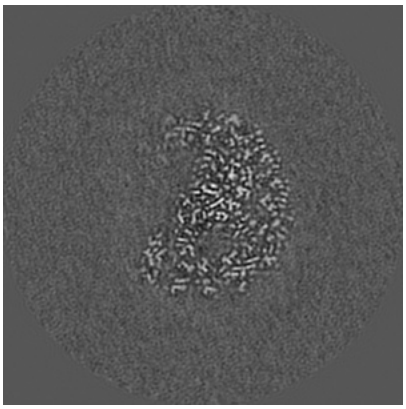


Z Index: 150

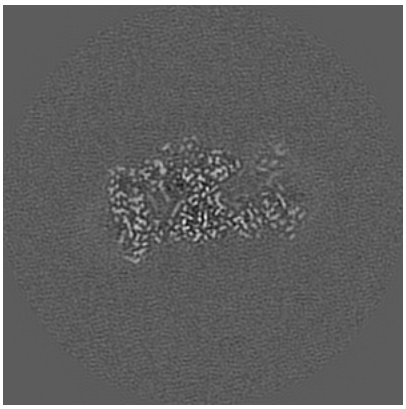
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

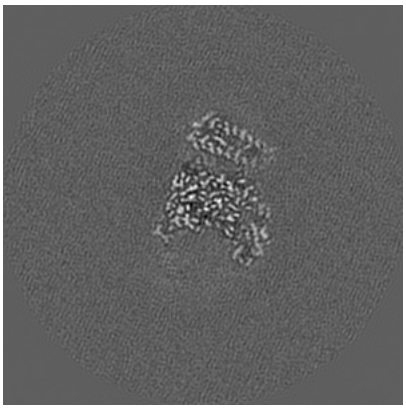
6.3.1 Primary map



X Index: 144

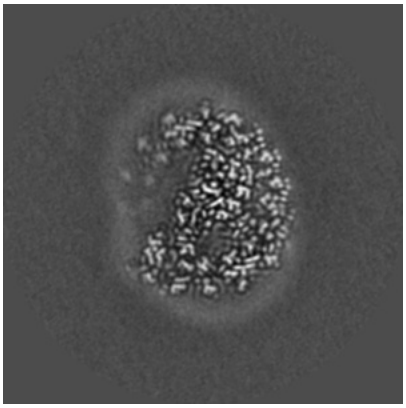


Y Index: 152

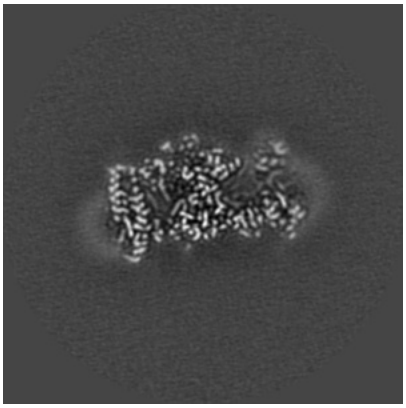


Z Index: 153

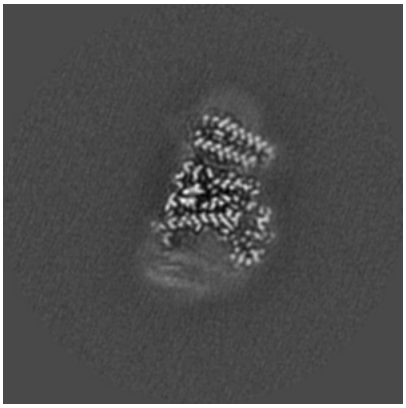
6.3.2 Raw map



X Index: 144



Y Index: 152

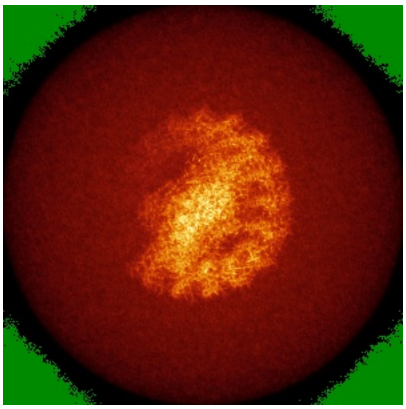


Z Index: 151

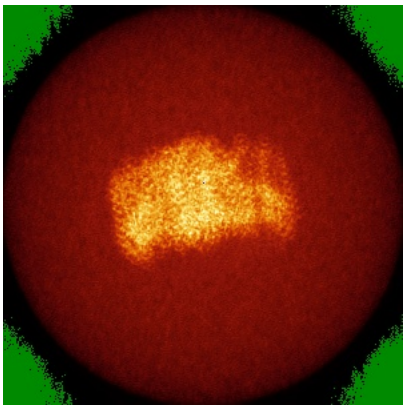
The images above show the largest variance slices of the map in three orthogonal directions.

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

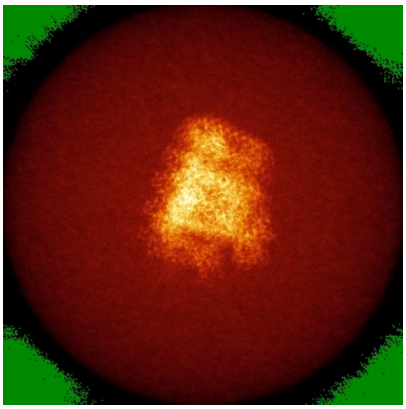
6.4.1 Primary map



X

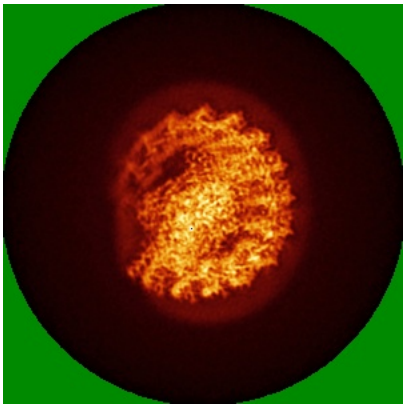


Y

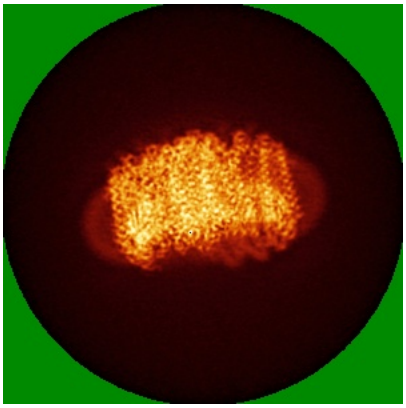


Z

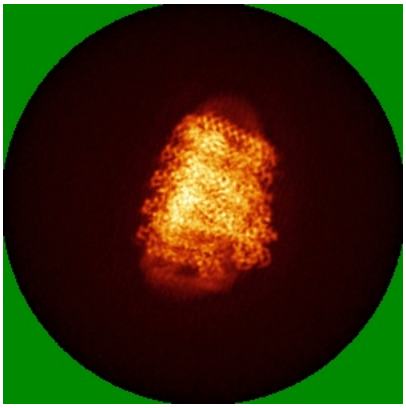
6.4.2 Raw map



X



Y

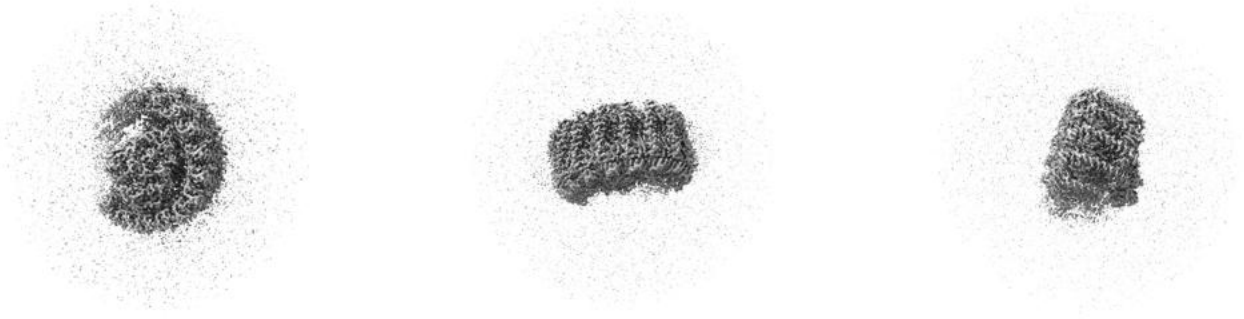


Z

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)

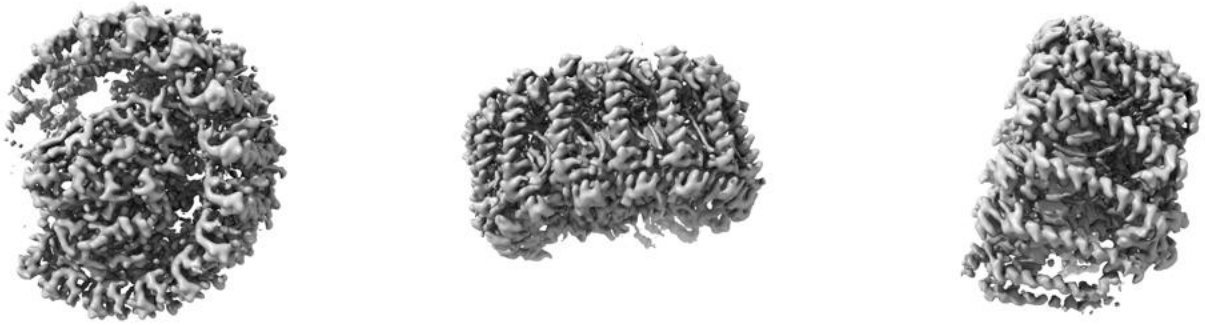
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

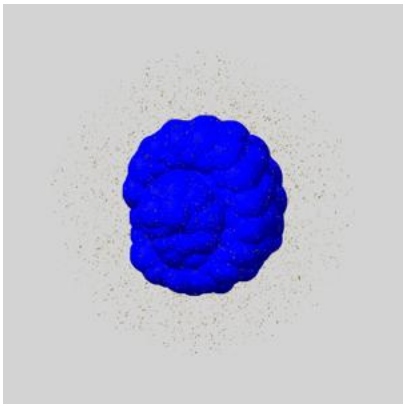
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

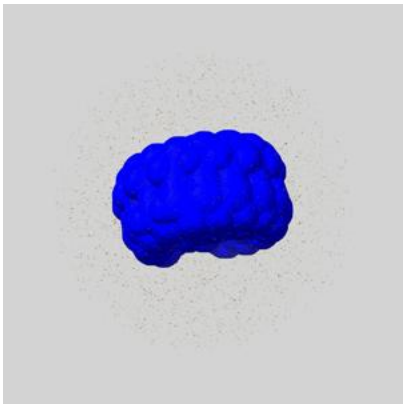
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_15862_msk_1.map



X



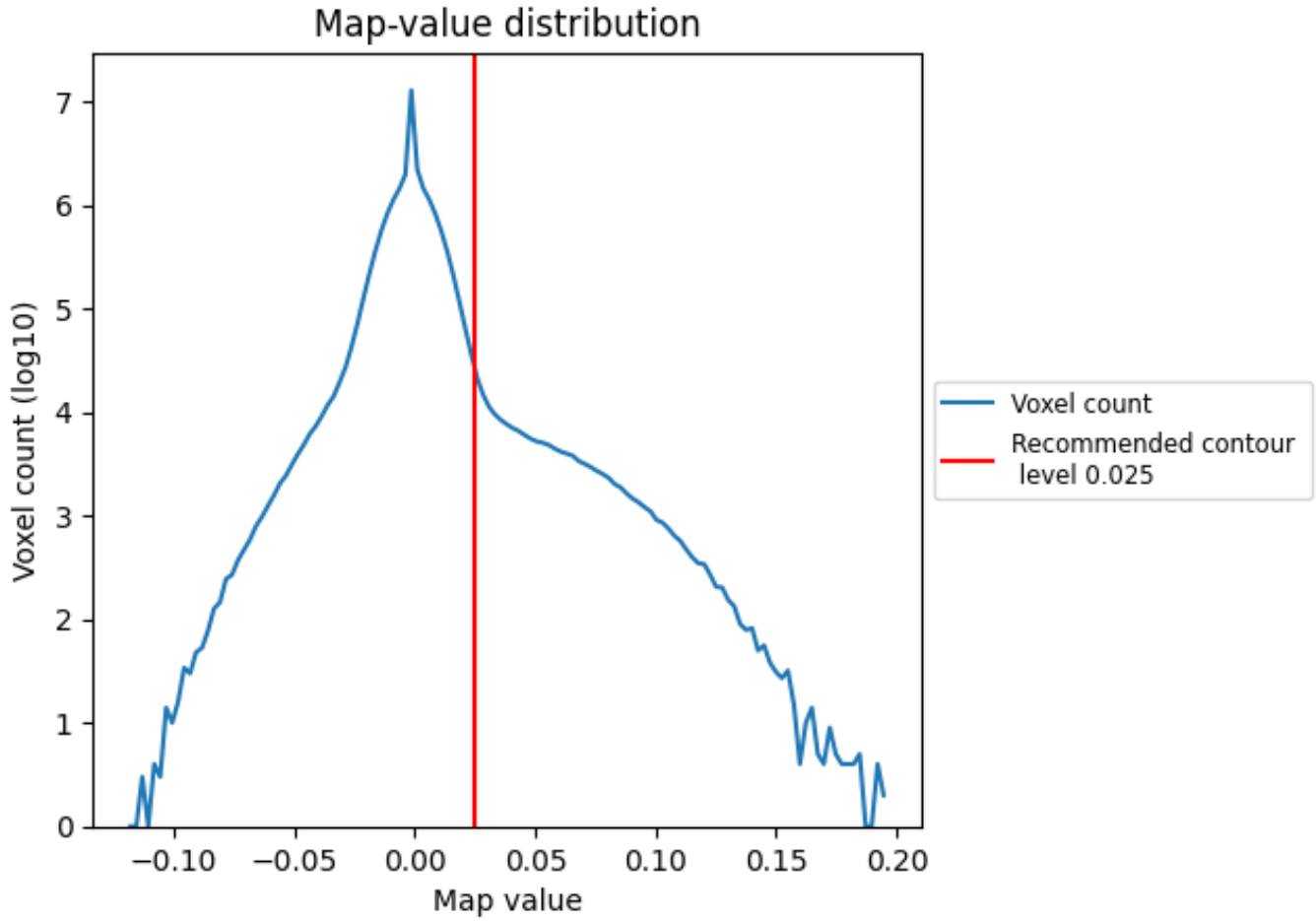
Y

Z

7 Map analysis

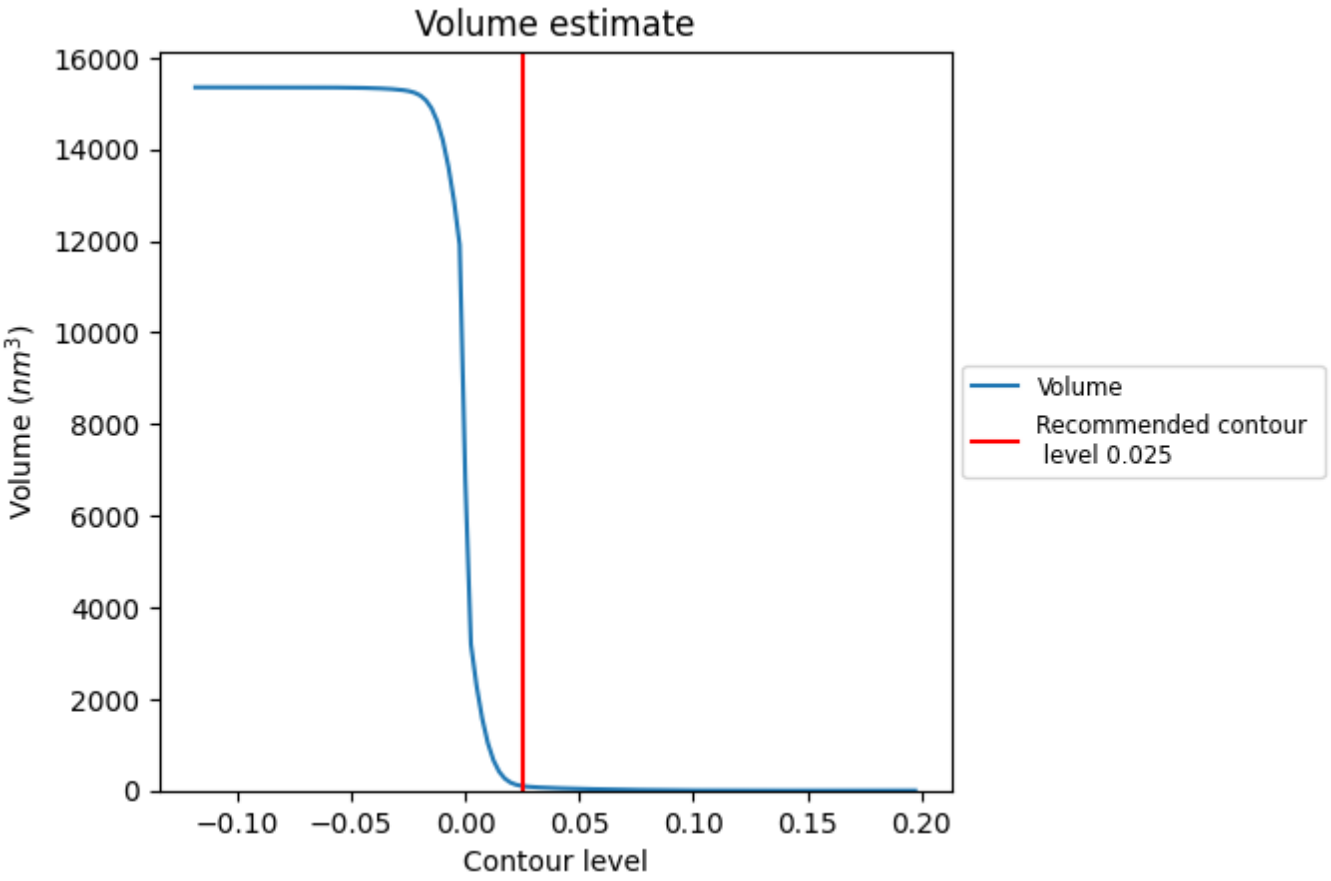
This section contains the results of statistical analysis of the map.

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.

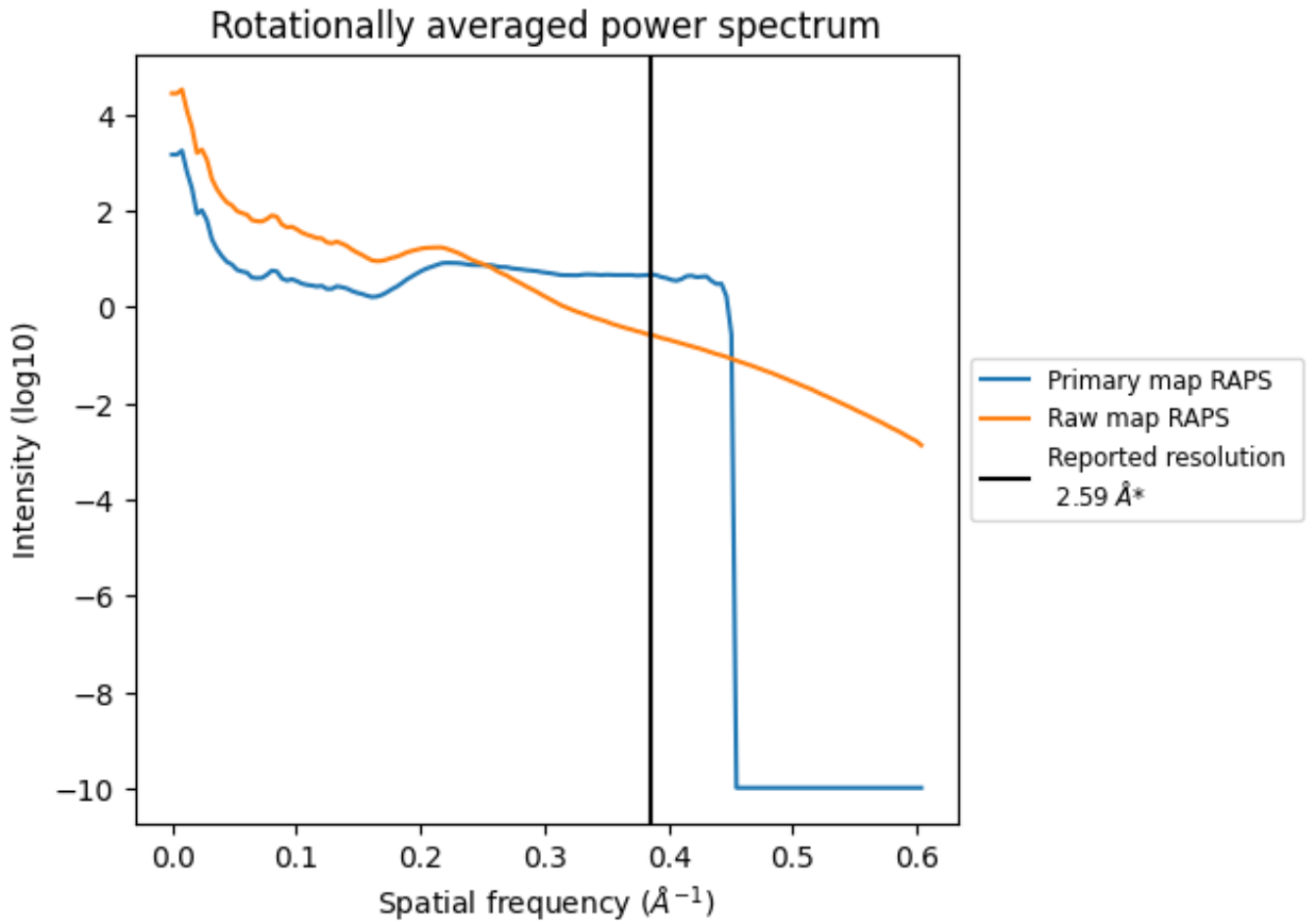
7.2 Volume estimate (i)



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 91 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)

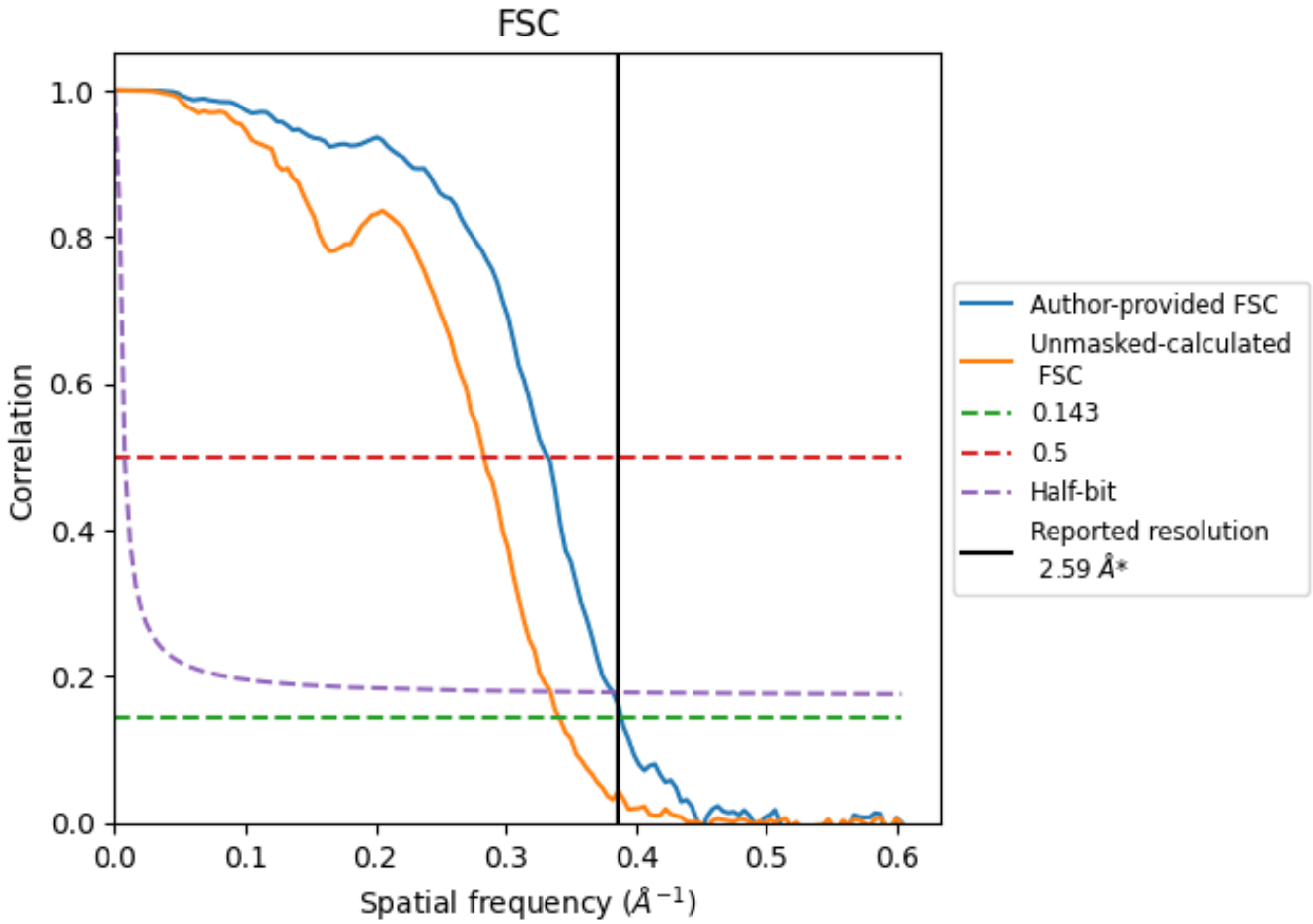


*Reported resolution corresponds to spatial frequency of 0.386 Å^{-1}

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 0.386 Å^{-1}

8.2 Resolution estimates (i)

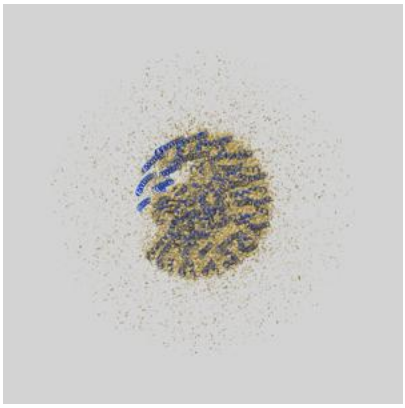
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.57	3.01	2.62
Unmasked-calculated*	2.93	3.53	2.99

*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 2.93 differs from the reported value 2.589 by more than 10 %

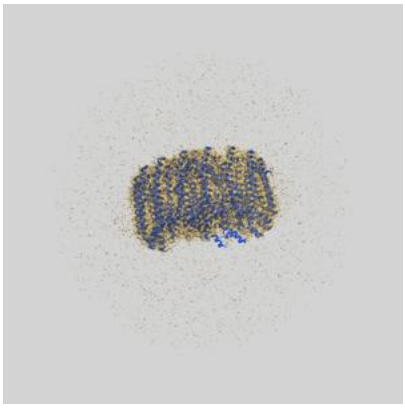
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15862 and PDB model 8B64. Per-residue inclusion information can be found in section 3 on page 14.

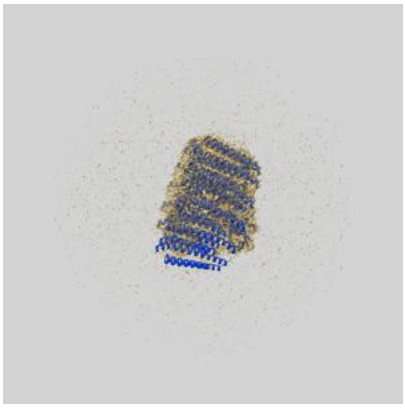
9.1 Map-model overlay



X



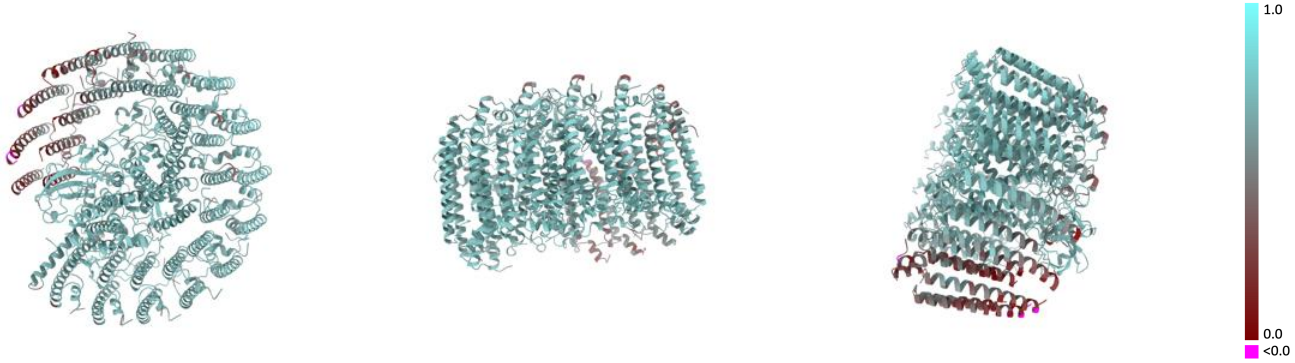
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

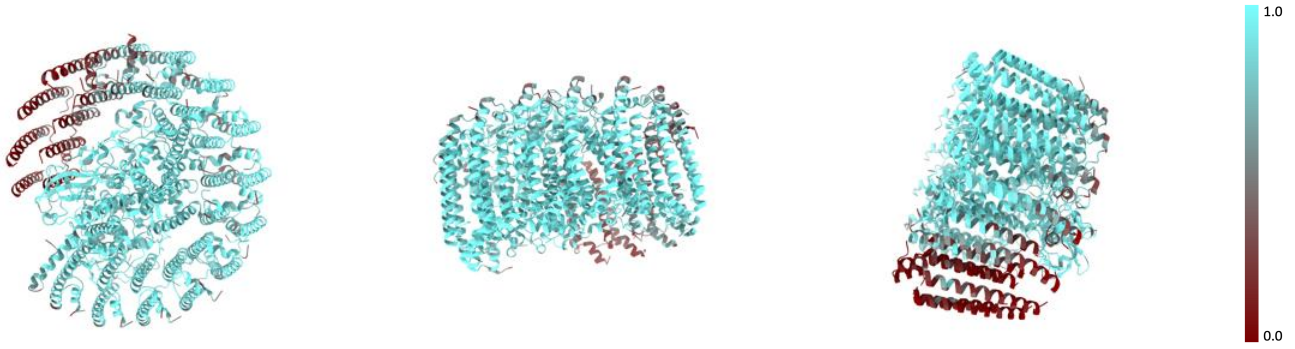
9.2 Q-score mapped to coordinate model (i)



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.

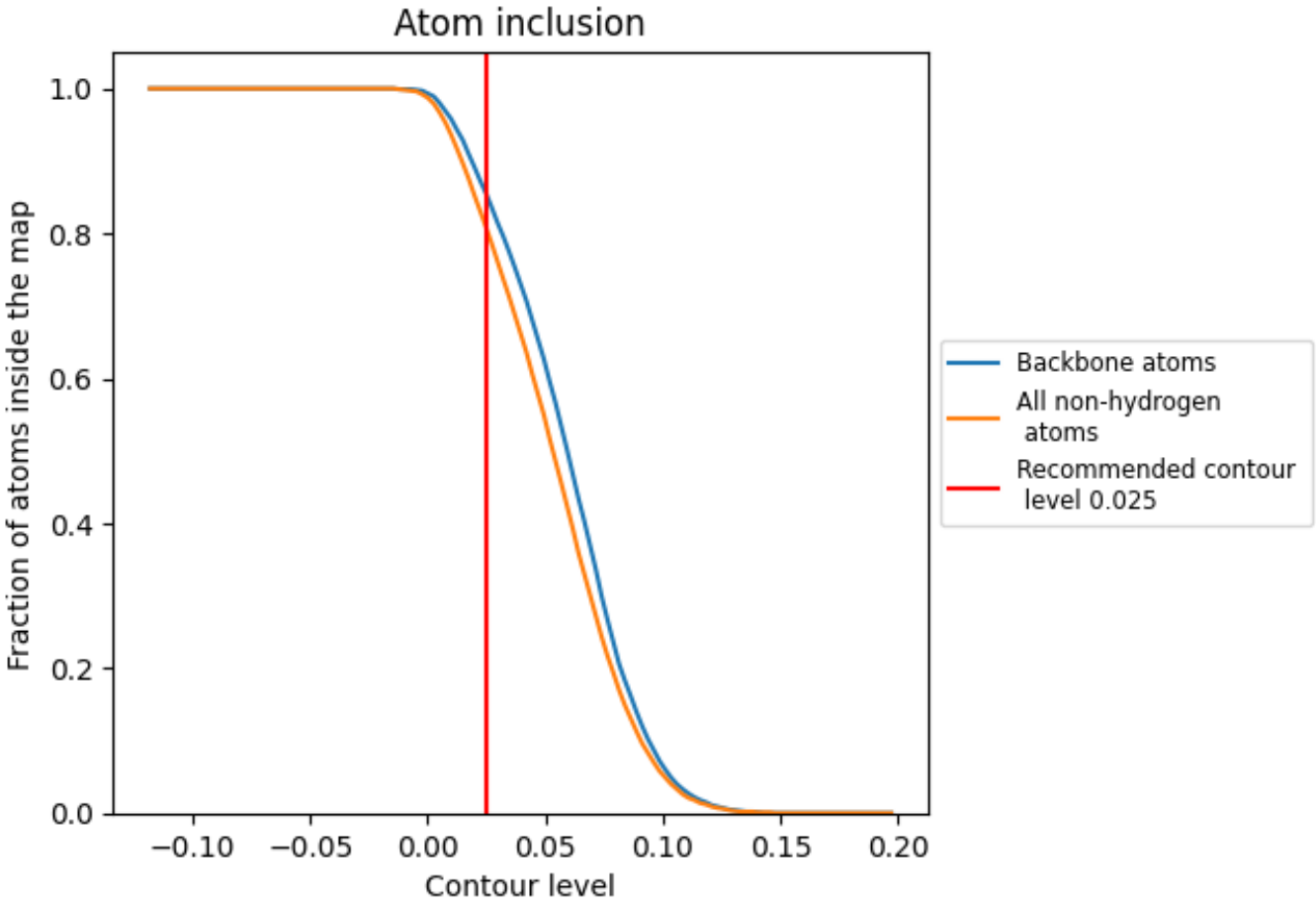
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.6390
A	0.8300	0.6340
B	0.9070	0.6610
D	0.8840	0.6710
E	0.8550	0.6460
F	0.8680	0.6670
G	0.8180	0.6490
H	0.9130	0.6900
I	0.7940	0.6340
J	0.8400	0.6520
K	0.8410	0.6480
L	0.9620	0.7090
M	0.9580	0.7090
N	0.7740	0.6170
O	0.6340	0.5730
R	0.3840	0.4620
S	0.2120	0.3850
T	0.0960	0.3420
U	0.0690	0.3090
X	0.8610	0.6660
a	0.9320	0.6820
b	0.9050	0.6740
d	0.9280	0.6850
e	0.9410	0.6860
f	0.9130	0.6790
g	0.8840	0.6710
i	0.8480	0.6550
j	0.8850	0.6760
k	0.9080	0.6730
n	0.8090	0.6400
o	0.7480	0.6180
r	0.6380	0.5800
s	0.4410	0.5030
t	0.1310	0.3580
u	0.0360	0.2800