Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 02:06 AM JST

PDB ID	:	7VNM
EMDB ID	:	EMD-32042
Title	:	Rba sphaeroides PufY-KO RC-LH1 monomer
Authors	:	Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.
Deposited on	:	2021-10-11
Resolution	:	2.86 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:

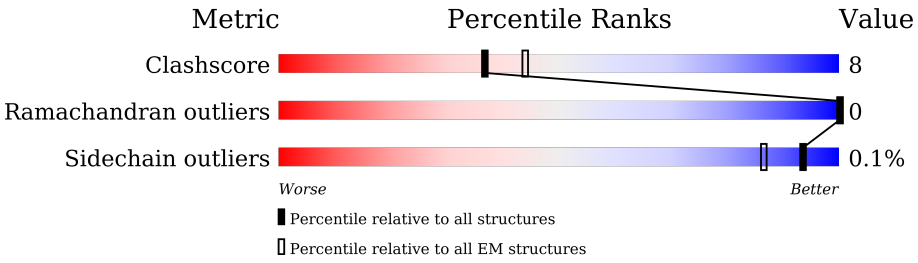
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.86 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	L	282	83% 17%
2	M	308	86% 13%
3	H	260	87% 8% 5%
4	1	58	74% 55% 19% 26%
4	7	58	9% 66% 14% 21%
4	9	58	81% 12% 7%
4	A	58	79% 14% 7%
4	D	58	83% 10% 7%

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Mol	Chain	Length	Quality of chain
4	F	58	91% 7%
4	I	58	79% 14% 7%
4	K	58	5% 78% 16% 7%
4	O	58	5% 81% 12% 7%
4	Q	58	5% 83% 10% 7%
4	S	58	7% 78% 16% 7%
4	U	58	26% 74% 19% 7%
4	W	58	64% 79% 14% 7%
5	0	49	80% 10% 10%
5	2	49	65% 57% 8% 35%
5	8	49	8% 73% 16% 10%
5	B	49	6% 73% 18% 8%
5	C	49	73% 57% 18% 22%
5	E	49	76% 12% 12%
5	G	49	78% 10% 12%
5	J	49	8% 82% 6% 12%
5	N	49	14% 78% 10% 12%
5	P	49	12% 78% 10% 12%
5	R	49	14% 73% 14% 12%
5	T	49	20% 82% 6% 12%
5	V	49	22% 67% 14% 18%
6	X	82	20% 50% 13% 37%

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
12	SPO	0	101	-	X	-	-
12	SPO	0	102	-	X	-	-
12	SPO	8	101	-	X	-	-
12	SPO	9	102	-	X	-	-
12	SPO	A	603	-	X	-	-
12	SPO	D	102	-	X	-	-
12	SPO	D	103	-	X	-	-
12	SPO	D	104	-	X	-	-
12	SPO	E	102	-	X	-	-
12	SPO	F	103	-	X	-	-
12	SPO	I	103	-	X	-	-
12	SPO	I	104	-	X	-	-
12	SPO	K	102	-	X	-	-
12	SPO	K	103	-	X	-	-
12	SPO	M	405	-	X	-	-
12	SPO	P	101	-	X	-	-
12	SPO	P	102	-	X	-	-
12	SPO	Q	102	-	X	-	-
12	SPO	R	101	-	X	-	-
12	SPO	R	103	-	X	-	-
12	SPO	S	103	-	X	-	-
12	SPO	U	103	-	X	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 20588 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	247	Total	C	N	O	S	0	0
			1875	1202	318	345	10		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	D	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	F	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	I	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	K	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	O	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	Q	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	U	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	W	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	7	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
4	9	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	1	43	Total	C	N	O	S	0	0
			351	235	59	56	1		

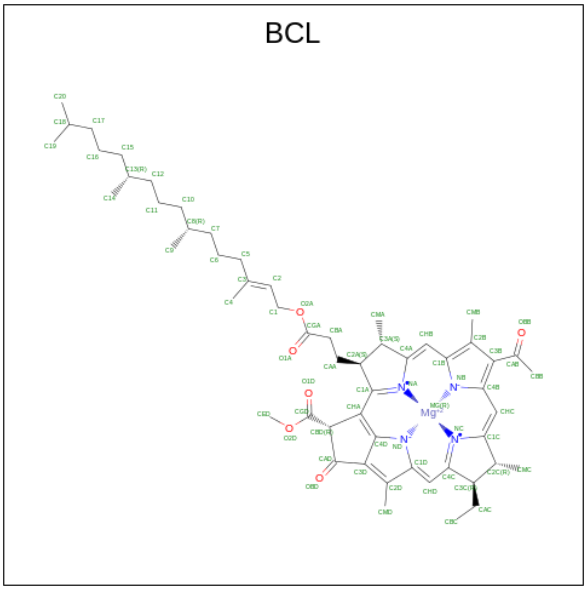
- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	P	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	R	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	T	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	V	40	Total	C	N	O	S	0	0
			327	219	52	55	1		
5	C	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	8	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	0	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	2	32	Total	C	N	O	S	0	0
			270	186	43	40	1		

- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	52	Total	C	N	O	S	0	0
			406	270	71	62	3		

- 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	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	M	1	Total	C	Mg	N	O	0
			129	107	2	8	12	
7	M	1	Total	C	Mg	N	O	0
			129	107	2	8	12	
7	A	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	A	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	D	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	F	1	Total	C	Mg	N	O	0
			132	110	2	8	12	

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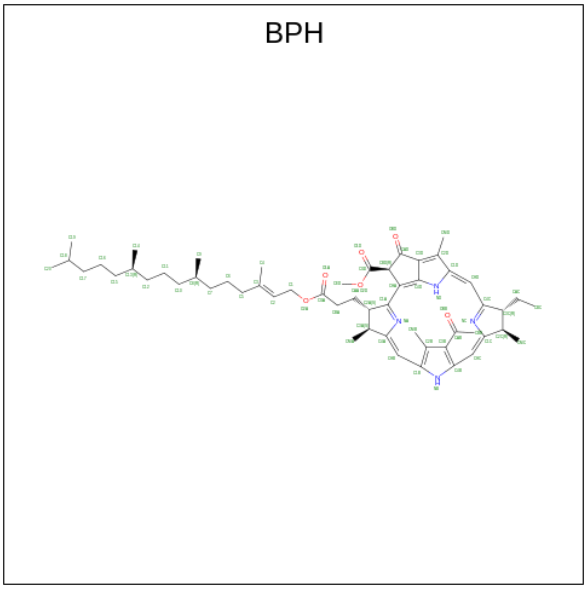
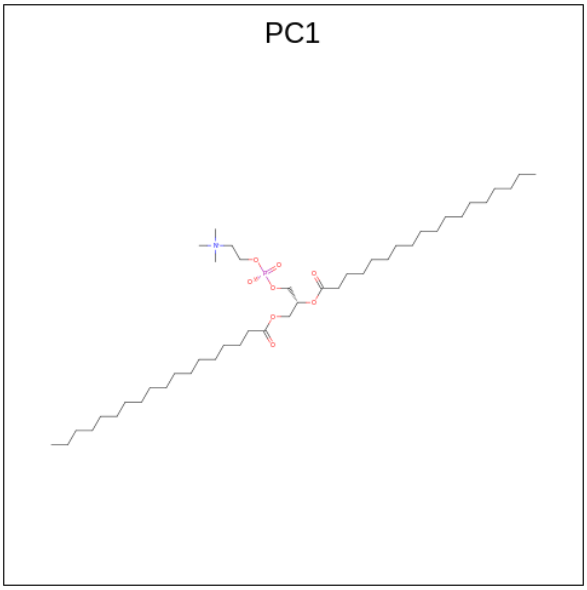
Mol	Chain	Residues	Atoms					AltConf
7	F	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	I	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	I	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	O	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	S	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	U	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	U	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	9	1	Total	C	Mg	N	O	0
			127	105	2	8	12	
7	9	1	Total	C	Mg	N	O	0
			127	105	2	8	12	
7	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



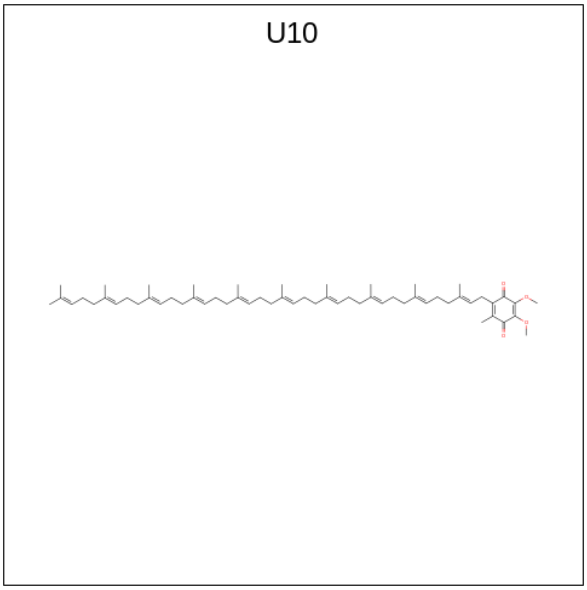
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	N	O	0
			117	97	8	12	
8	L	1	Total	C	N	O	0
			117	97	8	12	

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
9	H	1	Total	C	N	O	P	0
			118	88	3	24	3	
9	H	1	Total	C	N	O	P	0
			118	88	3	24	3	
9	H	1	Total	C	N	O	P	0
			118	88	3	24	3	
9	A	1	Total	C	N	O	P	0
			77	57	2	16	2	
9	A	1	Total	C	N	O	P	0
			77	57	2	16	2	
9	X	1	Total	C	N	O	P	0
			36	26	1	8	1	

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

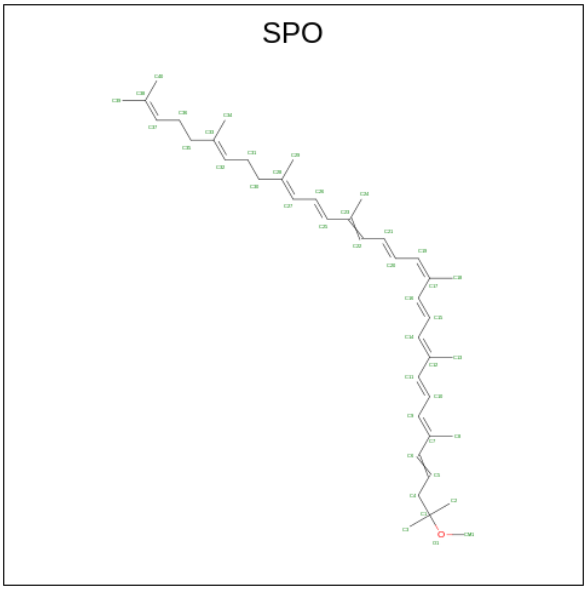


Mol	Chain	Residues	Atoms			AltConf
10	L	1	Total	C	O	0
			43	39	4	
10	M	1	Total	C	O	0
			48	44	4	

- Molecule 11 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
12	M	1	Total C O 42 41 1	0
12	A	1	Total C O 42 41 1	0
12	D	1	Total C O 126 123 3	0
12	D	1	Total C O 126 123 3	0
12	D	1	Total C O 126 123 3	0
12	E	1	Total C O 42 41 1	0
12	F	1	Total C O 42 41 1	0
12	I	1	Total C O 84 82 2	0
12	I	1	Total C O 84 82 2	0
12	K	1	Total C O 84 82 2	0

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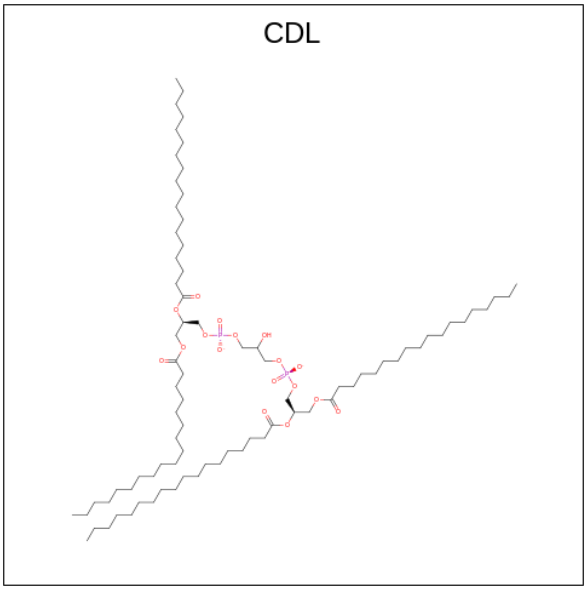
Mol	Chain	Residues	Atoms			AltConf
12	K	1	Total	C	O	0
			84	82	2	
12	P	1	Total	C	O	0
			84	82	2	
12	P	1	Total	C	O	0
			84	82	2	
12	Q	1	Total	C	O	0
			42	41	1	
12	R	1	Total	C	O	0
			84	82	2	
12	R	1	Total	C	O	0
			84	82	2	
12	S	1	Total	C	O	0
			42	41	1	
12	U	1	Total	C	O	0
			42	41	1	
12	8	1	Total	C	O	0
			39	38	1	
12	9	1	Total	C	O	0
			42	41	1	
12	0	1	Total	C	O	0
			84	82	2	
12	0	1	Total	C	O	0
			84	82	2	

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

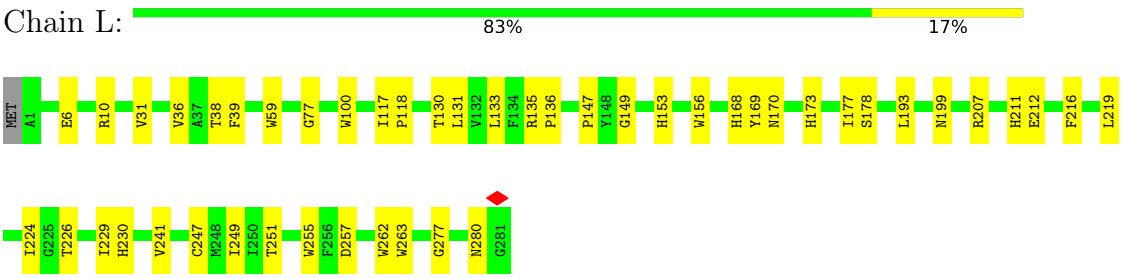


Mol	Chain	Residues	Atoms				AltConf
13	M	1	Total	C	O	P	0
			100	81	17	2	

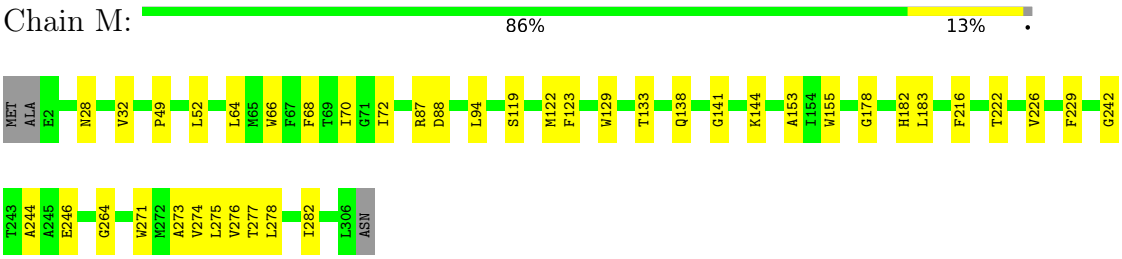
3 Residue-property plots (i)

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.

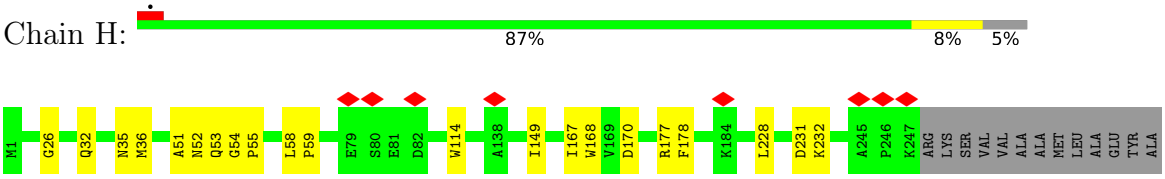
• Molecule 1: Reaction center protein L chain



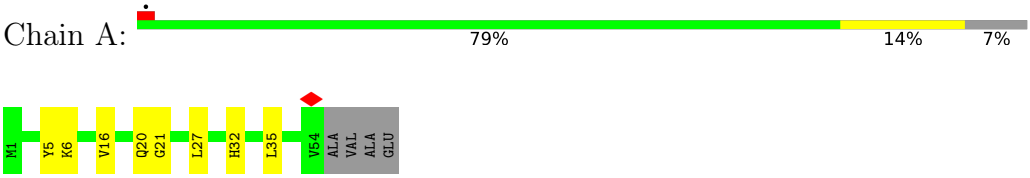
• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain

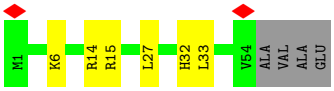


• Molecule 4: Light-harvesting protein B-875 alpha chain



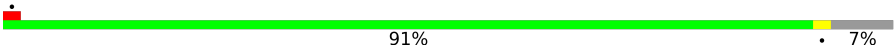
• Molecule 4: Light-harvesting protein B-875 alpha chain

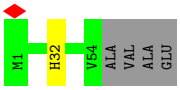
Chain D:



• Molecule 4: Light-harvesting protein B-875 alpha chain

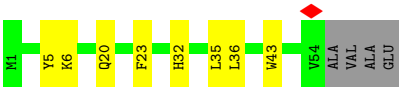
Chain F:





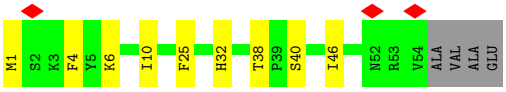
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I:



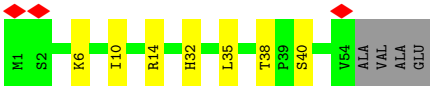
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain K:



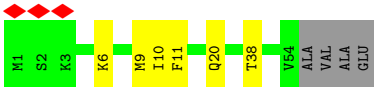
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain O:



• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain Q:

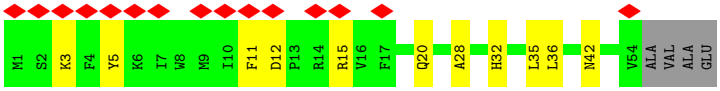


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain S:

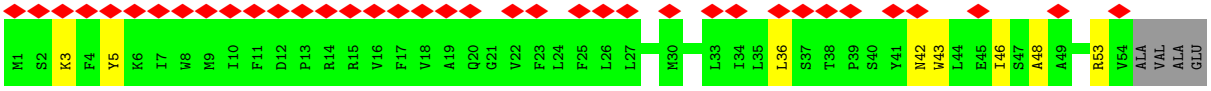
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain U:



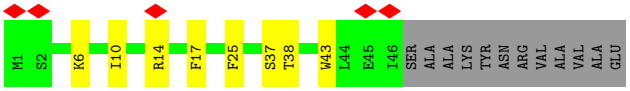
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain W:



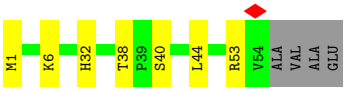
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 7:



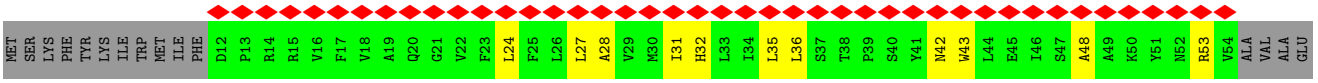
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 9:



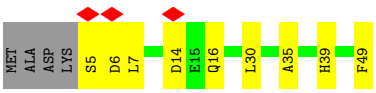
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 1:



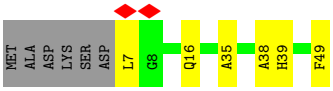
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain B:



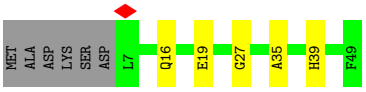
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain E:



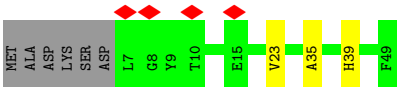
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain G:



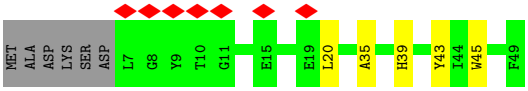
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain J:



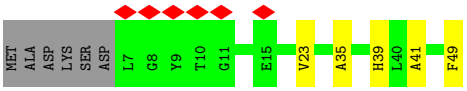
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain N:



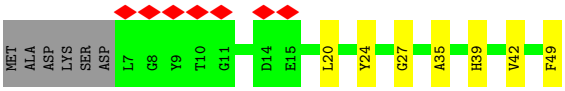
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain P:



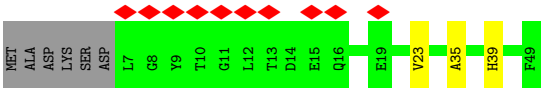
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain R:



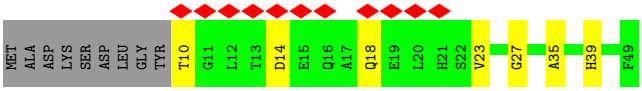
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain T:



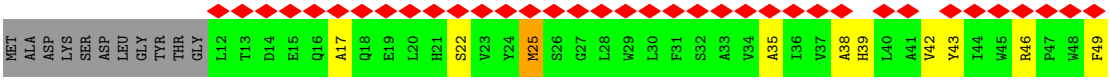
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain V:



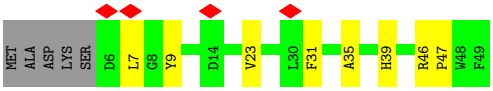
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain C:



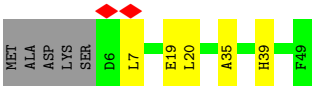
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain 8:



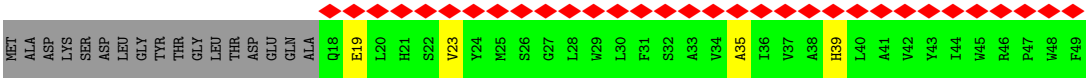
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain 0:



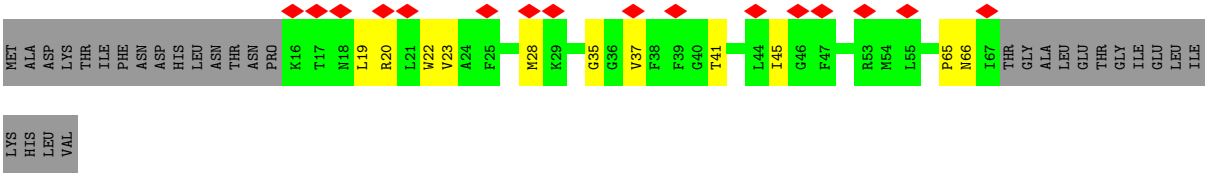
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain 2:



• Molecule 6: Intrinsic membrane protein PufX

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56391	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 ($e^-/Å^2$)	51.527	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	0.194	Depositor
Minimum map value	-0.106	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, PC1, CDL, FE2, BCL, U10, 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	L	0.35	0/2320	0.45	0/3175
2	M	0.35	0/2524	0.44	0/3446
3	H	0.31	0/1925	0.47	0/2620
4	1	0.26	0/360	0.38	0/490
4	7	0.33	0/405	0.39	0/549
4	9	0.34	0/469	0.40	0/635
4	A	0.34	0/469	0.40	0/635
4	D	0.34	0/469	0.40	0/635
4	F	0.35	0/469	0.39	0/635
4	I	0.33	0/469	0.41	0/635
4	K	0.32	0/469	0.40	0/635
4	O	0.36	0/469	0.40	0/635
4	Q	0.34	0/469	0.39	0/635
4	S	0.31	0/469	0.40	0/635
4	U	0.31	0/469	0.39	0/635
4	W	0.26	0/469	0.36	0/635
5	0	0.33	0/372	0.40	0/510
5	2	0.23	0/282	0.31	0/387
5	8	0.32	0/372	0.38	0/510
5	B	0.33	0/378	0.43	0/518
5	C	0.27	0/328	0.40	0/450
5	E	0.31	0/364	0.40	0/499
5	G	0.31	0/364	0.38	0/499
5	J	0.31	0/364	0.39	0/499
5	N	0.31	0/364	0.39	0/499
5	P	0.32	0/364	0.38	0/499
5	R	0.34	0/364	0.43	0/499
5	T	0.31	0/364	0.40	0/499
5	V	0.31	0/339	0.38	0/465
6	X	0.27	0/417	0.40	0/563
All	All	0.33	0/17729	0.42	0/24161

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	41	0
2	M	2431	0	2345	28	0
3	H	1875	0	1877	20	0
4	1	351	0	366	7	0
4	7	392	0	412	9	0
4	9	455	0	477	7	0
4	A	455	0	477	8	0
4	D	455	0	477	11	0
4	F	455	0	477	1	0
4	I	455	0	477	6	0
4	K	455	0	477	7	0
4	O	455	0	477	8	0
4	Q	455	0	477	6	0
4	S	455	0	477	8	0
4	U	455	0	477	10	0
4	W	455	0	477	8	0
5	0	359	0	340	4	0
5	2	270	0	262	4	0
5	8	359	0	340	8	0
5	B	365	0	345	9	0
5	C	316	0	303	10	0
5	E	351	0	336	9	0
5	G	351	0	336	4	0
5	J	351	0	336	2	0
5	N	351	0	336	4	0
5	P	351	0	336	4	0
5	R	351	0	336	7	0
5	T	351	0	336	3	0
5	V	327	0	313	6	0
6	X	406	0	420	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1	66	0	74	3	0
7	2	46	0	35	0	0
7	7	61	0	61	6	0
7	8	66	0	74	3	0
7	9	127	0	135	6	0
7	A	132	0	148	12	0
7	C	66	0	74	3	0
7	D	66	0	74	2	0
7	E	66	0	74	6	0
7	F	132	0	148	4	0
7	I	132	0	148	7	0
7	K	66	0	74	2	0
7	L	132	0	148	4	0
7	M	129	0	139	4	0
7	N	66	0	74	7	0
7	O	132	0	148	8	0
7	Q	66	0	74	4	0
7	R	66	0	74	4	0
7	S	132	0	148	10	0
7	U	132	0	148	14	0
7	W	66	0	74	6	0
8	L	117	0	120	3	0
9	A	77	0	105	9	0
9	H	118	0	161	10	0
9	L	35	0	44	2	0
9	X	36	0	46	0	0
10	L	43	0	55	6	0
10	M	48	0	63	2	0
11	M	1	0	0	0	0
12	0	84	0	120	5	0
12	8	39	0	53	3	0
12	9	42	0	60	4	0
12	A	42	0	60	3	0
12	D	126	0	180	17	0
12	E	42	0	60	3	0
12	F	42	0	60	3	0
12	I	84	0	120	6	0
12	K	84	0	120	9	0
12	M	42	0	60	4	0
12	P	84	0	120	10	0
12	Q	42	0	60	6	0
12	R	84	0	120	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	S	42	0	60	7	0
12	U	42	0	60	5	0
13	M	100	0	156	9	0
All	All	20588	0	21318	347	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:53:GLN:N	9:H:1103:PC1:O14	2.08	0.86
5:R:27:GLY:HA3	12:R:101:SPO:H27	1.59	0.83
12:D:104:SPO:H27	5:G:27:GLY:HA3	1.58	0.82
1:L:193:LEU:HD21	1:L:212:GLU:HB3	1.60	0.81
7:A:602:BCL:H72	9:A:604:PC1:H2B2	1.64	0.77
4:K:6:LYS:HB2	12:K:103:SPO:H341	1.65	0.77
2:M:153:ALA:HA	2:M:277:THR:HG21	1.65	0.76
9:L:303:PC1:H232	4:D:33:LEU:HD13	1.68	0.76
1:L:193:LEU:HD22	1:L:216:PHE:HE2	1.52	0.75
3:H:52:ASN:HD22	9:A:601:PC1:H143	1.51	0.74
4:1:28:ALA:O	4:1:32:HIS:ND1	2.20	0.74
4:7:14:ARG:HG2	6:X:22:TRP:HZ2	1.53	0.74
12:Q:102:SPO:H342	5:T:23:VAL:HG11	1.70	0.74
4:7:6:LYS:NZ	5:0:19:GLU:OE2	2.21	0.74
3:H:54:GLY:O	4:D:15:ARG:NH1	2.22	0.73
1:L:277:GLY:O	2:M:87:ARG:NH1	2.25	0.70
4:O:10:ILE:HD11	12:R:101:SPO:H403	1.75	0.69
4:Q:20:GLN:OE1	5:R:24:TYR:OH	2.10	0.69
5:C:42:VAL:HG11	7:C:101:BCL:HBC1	1.75	0.69
2:M:64:LEU:HD21	4:S:26:LEU:HD21	1.73	0.68
5:2:35:ALA:O	5:2:39:HIS:ND1	2.21	0.68
12:S:103:SPO:H9	7:W:101:BCL:H3A	1.76	0.68
3:H:51:ALA:O	4:D:14:ARG:NH1	2.26	0.68
7:U:101:BCL:H162	12:U:103:SPO:H352	1.76	0.68
13:M:406:CDL:H791	3:H:26:GLY:HA3	1.76	0.66
5:C:43:TYR:HE1	5:C:49:PHE:HB2	1.61	0.66
12:P:102:SPO:H82	12:P:102:SPO:H42	1.78	0.66
12:S:103:SPO:H27	5:V:27:GLY:HA3	1.79	0.65
12:S:103:SPO:H182	7:W:101:BCL:H91	1.77	0.65
12:I:104:SPO:H6	7:O:101:BCL:HMB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:54:GLY:HA3	9:H:1102:PC1:H133	1.79	0.65
7:K:101:BCL:HED3	12:K:102:SPO:H25	1.79	0.64
4:Q:38:THR:HG21	4:S:44:LEU:HD13	1.79	0.64
4:1:48:ALA:HA	4:1:53:ARG:HD2	1.80	0.64
4:U:20:GLN:HE22	12:U:103:SPO:H391	1.63	0.64
5:B:7:LEU:HD12	5:E:16:GLN:HB3	1.80	0.64
4:D:6:LYS:HD3	12:D:104:SPO:H402	1.79	0.64
5:G:35:ALA:O	5:G:39:HIS:ND1	2.21	0.63
12:D:102:SPO:H6	7:F:101:BCL:HMB2	1.79	0.63
3:H:149:ILE:HD11	3:H:167:ILE:HG13	1.79	0.63
5:R:35:ALA:O	5:R:39:HIS:ND1	2.21	0.63
3:H:54:GLY:HA2	9:A:601:PC1:H141	1.82	0.62
4:S:6:LYS:HB2	12:S:103:SPO:H341	1.80	0.62
7:N:101:BCL:H202	12:P:101:SPO:H9	1.82	0.62
4:A:20:GLN:HE21	12:0:101:SPO:H393	1.65	0.62
5:8:35:ALA:O	5:8:39:HIS:ND1	2.21	0.61
4:U:36:LEU:O	4:U:42:ASN:ND2	2.27	0.61
4:1:24:LEU:HB2	7:1:101:BCL:H42	1.82	0.61
4:O:6:LYS:HB3	12:R:101:SPO:H341	1.81	0.61
5:0:35:ALA:O	5:0:39:HIS:ND1	2.21	0.61
1:L:133:LEU:HD21	6:X:45:ILE:HD11	1.82	0.60
7:N:101:BCL:H52	12:P:101:SPO:H241	1.83	0.60
8:L:306:BPH:HBC3	8:L:306:BPH:HHD	1.83	0.60
2:M:32:VAL:HG12	2:M:49:PRO:HD3	1.83	0.60
5:8:23:VAL:HG21	6:X:19:LEU:HD23	1.83	0.59
5:B:35:ALA:O	5:B:39:HIS:ND1	2.21	0.59
12:Q:102:SPO:H6	7:U:101:BCL:HMB2	1.83	0.59
5:R:49:PHE:HB3	12:R:103:SPO:C6	2.32	0.59
5:J:35:ALA:O	5:J:39:HIS:ND1	2.21	0.59
4:W:36:LEU:O	4:W:42:ASN:ND2	2.35	0.59
7:A:605:BCL:H203	12:D:103:SPO:H81	1.85	0.59
4:A:6:LYS:HB3	12:D:102:SPO:H402	1.83	0.59
1:L:59:TRP:HB2	9:L:303:PC1:H112	1.84	0.59
4:D:32:HIS:CE1	7:E:101:BCL:HMD1	2.37	0.59
4:1:36:LEU:O	4:1:42:ASN:ND2	2.36	0.58
5:P:35:ALA:O	5:P:39:HIS:ND1	2.21	0.58
1:L:247:CYS:O	1:L:251:THR:OG1	2.21	0.58
4:D:6:LYS:HB3	12:D:104:SPO:H402	1.85	0.58
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.85	0.58
4:D:6:LYS:HB2	12:D:104:SPO:H341	1.84	0.58
7:I:101:BCL:HED3	12:I:103:SPO:H25	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:38:THR:OG1	4:9:40:SER:O	2.15	0.58
1:L:149:GLY:O	1:L:153:HIS:ND1	2.35	0.57
1:L:178:SER:HB2	10:L:304:U10:H262	1.84	0.57
9:H:1103:PC1:H262	4:A:16:VAL:HG22	1.85	0.57
12:R:101:SPO:H6	7:S:101:BCL:HMB2	1.86	0.57
5:V:35:ALA:O	5:V:39:HIS:ND1	2.21	0.57
12:P:101:SPO:H82	12:P:101:SPO:H31	1.86	0.57
5:T:35:ALA:O	5:T:39:HIS:ND1	2.21	0.57
10:L:304:U10:H102	10:L:304:U10:H1M1	1.86	0.57
5:C:22:SER:HA	5:C:25:MET:HE2	1.86	0.57
1:L:226:THR:O	1:L:230:HIS:ND1	2.35	0.57
1:L:130:THR:HG23	1:L:249:ILE:HD13	1.85	0.56
1:L:193:LEU:HD22	1:L:216:PHE:CE2	2.39	0.56
4:A:21:GLY:HA3	9:A:604:PC1:H2A1	1.88	0.56
4:I:5:TYR:CE1	4:I:6:LYS:HD3	2.41	0.56
5:C:35:ALA:O	5:C:39:HIS:ND1	2.33	0.56
12:0:102:SPO:H41	12:0:102:SPO:H83	1.88	0.56
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.38	0.56
5:E:49:PHE:CE2	7:E:101:BCL:H171	2.41	0.55
12:8:101:SPO:H6	7:9:101:BCL:HMB2	1.88	0.55
5:E:35:ALA:O	5:E:39:HIS:ND1	2.21	0.55
4:K:38:THR:OG1	4:K:40:SER:O	2.19	0.55
1:L:207:ARG:HH21	2:M:141:GLY:HA3	1.72	0.54
4:S:32:HIS:CE1	7:S:102:BCL:HMD1	2.42	0.54
1:L:207:ARG:HD2	1:L:211:HIS:CD2	2.43	0.54
3:H:58:LEU:HD12	3:H:59:PRO:HD2	1.88	0.54
12:D:102:SPO:H293	12:D:103:SPO:H37	1.89	0.54
5:N:35:ALA:O	5:N:39:HIS:ND1	2.21	0.54
2:M:264:GLY:HA3	3:H:35:ASN:ND2	2.23	0.54
12:E:102:SPO:H42	12:E:102:SPO:H83	1.89	0.54
1:L:168:HIS:CD2	2:M:183:LEU:HB3	2.43	0.54
13:M:406:CDL:H712	13:M:406:CDL:CB5	2.37	0.53
4:U:3:LYS:HA	4:U:5:TYR:CE2	2.42	0.53
6:X:19:LEU:O	6:X:23:VAL:HG23	2.08	0.53
4:O:32:HIS:CE1	7:O:102:BCL:HMD1	2.44	0.53
5:E:7:LEU:HD23	5:G:16:GLN:HB3	1.91	0.53
12:I:103:SPO:H82	12:I:103:SPO:H23	1.90	0.53
4:O:38:THR:OG1	4:O:40:SER:O	2.17	0.53
2:M:123:PHE:HB2	12:M:405:SPO:H32	1.91	0.52
12:D:103:SPO:H183	5:E:38:ALA:HB1	1.91	0.52
12:D:104:SPO:H401	5:E:7:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:53:GLN:HG3	9:H:1103:PC1:H132	1.90	0.52
5:E:49:PHE:HE2	7:E:101:BCL:H171	1.75	0.52
12:P:102:SPO:H25	7:Q:101:BCL:CMA	2.40	0.52
12:9:102:SPO:H361	5:0:20:LEU:HG	1.91	0.52
12:S:103:SPO:H342	5:V:23:VAL:HG11	1.92	0.52
4:A:32:HIS:CE1	7:A:605:BCL:HMD1	2.45	0.52
1:L:6:GLU:OE1	1:L:10:ARG:NH1	2.42	0.51
3:H:55:PRO:C	4:D:15:ARG:HH12	2.14	0.51
5:P:41:ALA:HB1	12:P:101:SPO:C11	2.41	0.51
4:W:46:ILE:HG21	5:C:46:ARG:HH12	1.75	0.51
12:K:103:SPO:H6	7:Q:101:BCL:HMB2	1.91	0.51
4:U:32:HIS:CE1	7:U:102:BCL:HMD1	2.45	0.51
4:Q:10:ILE:HD11	12:Q:102:SPO:H37	1.93	0.51
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.76	0.50
1:L:224:ILE:HG22	10:L:304:U10:H8	1.93	0.50
1:L:36:VAL:HA	10:M:404:U10:H403	1.93	0.50
1:L:6:GLU:HG2	1:L:10:ARG:HD2	1.94	0.50
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.94	0.50
5:B:30:LEU:HD22	4:9:1:MET:SD	2.51	0.50
8:L:302:BPH:H141	7:M:401:BCL:HBB3	1.94	0.49
1:L:31:VAL:HB	10:M:404:U10:H361	1.95	0.49
4:F:32:HIS:CE1	7:F:102:BCL:HMD1	2.48	0.49
12:R:103:SPO:H361	7:S:101:BCL:H151	1.94	0.49
12:P:102:SPO:H25	7:Q:101:BCL:HMA3	1.94	0.49
5:P:49:PHE:HB3	12:P:102:SPO:H82	1.94	0.49
12:R:103:SPO:H25	7:S:101:BCL:HED3	1.95	0.49
4:I:35:LEU:HD11	7:I:102:BCL:HHD	1.95	0.49
4:9:32:HIS:CE1	7:9:103:BCL:HMD1	2.48	0.49
2:M:273:ALA:O	2:M:276:VAL:HG12	2.13	0.48
12:Q:102:SPO:H16	7:S:102:BCL:H12	1.95	0.48
7:A:605:BCL:H162	7:A:605:BCL:H192	1.63	0.48
7:R:102:BCL:HMA1	7:S:101:BCL:HMA1	1.95	0.48
7:A:602:BCL:HBA2	12:9:102:SPO:H10	1.96	0.48
5:8:7:LEU:HD23	5:8:9:TYR:CE2	2.48	0.48
7:A:605:BCL:H52	12:D:103:SPO:H241	1.95	0.48
7:C:101:BCL:HMB2	7:C:101:BCL:H62	1.95	0.48
4:Q:11:PHE:HE2	4:S:17:PHE:HD2	1.61	0.48
9:A:601:PC1:H221	9:A:601:PC1:H251	1.45	0.48
7:A:602:BCL:HMB2	12:9:102:SPO:H6	1.95	0.48
4:U:5:TYR:HE1	5:V:14:ASP:OD1	1.97	0.48
3:H:53:GLN:H	9:H:1103:PC1:P	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:8:47:PRO:O	4:9:53:ARG:NH1	2.39	0.48
4:1:35:LEU:HD13	7:1:101:BCL:HAC2	1.96	0.48
3:H:170:ASP:HB2	3:H:177:ARG:HG3	1.95	0.48
5:B:7:LEU:HD23	5:B:7:LEU:O	2.14	0.47
2:M:178:GLY:O	2:M:182:HIS:ND1	2.47	0.47
3:H:55:PRO:O	4:D:15:ARG:NH2	2.31	0.47
6:X:41:THR:O	6:X:45:ILE:HG12	2.14	0.47
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.49	0.47
12:P:102:SPO:H131	5:R:42:VAL:HG22	1.97	0.47
5:C:39:HIS:HB3	7:C:101:BCL:H122	1.94	0.47
5:8:23:VAL:HG13	6:X:20:ARG:HG2	1.96	0.47
1:L:147:PRO:HD3	6:X:66:ASN:OD1	2.15	0.47
7:I:102:BCL:H141	7:I:102:BCL:H162	1.68	0.47
12:M:405:SPO:H392	12:M:405:SPO:H362	1.65	0.47
12:S:103:SPO:H131	7:W:101:BCL:H92	1.97	0.47
4:7:10:ILE:HD11	12:9:102:SPO:H37	1.97	0.47
4:1:43:TRP:CE3	7:1:101:BCL:HBC2	2.50	0.47
1:L:156:TRP:CD1	6:X:65:PRO:HB2	2.50	0.47
9:H:1101:PC1:H292	9:H:1101:PC1:H2C1	1.56	0.47
4:Q:6:LYS:HA	4:Q:9:MET:HG3	1.96	0.47
12:R:101:SPO:H342	12:R:101:SPO:H311	1.72	0.47
7:R:102:BCL:H162	7:R:102:BCL:H192	1.67	0.47
4:W:46:ILE:HG21	5:C:46:ARG:NH1	2.29	0.47
3:H:52:ASN:HA	9:H:1103:PC1:O12	2.15	0.46
12:K:103:SPO:H342	5:P:23:VAL:HG11	1.96	0.46
7:7:101:BCL:H2	5:8:31:PHE:HE1	1.79	0.46
4:O:35:LEU:HD11	7:O:102:BCL:HHD	1.97	0.46
7:8:102:BCL:H162	7:8:102:BCL:H141	1.49	0.46
7:L:301:BCL:CGA	7:M:401:BCL:HBC1	2.45	0.46
4:K:10:ILE:HB	4:O:14:ARG:HG2	1.98	0.46
5:R:20:LEU:HA	12:R:101:SPO:H37	1.96	0.46
4:7:25:PHE:CZ	6:X:35:GLY:HA2	2.50	0.46
12:8:101:SPO:H342	12:8:101:SPO:H312	1.58	0.46
12:F:103:SPO:C34	5:J:23:VAL:HG11	2.45	0.46
4:7:14:ARG:HG2	6:X:22:TRP:CZ2	2.42	0.46
7:A:605:BCL:H162	7:A:605:BCL:H141	1.65	0.46
5:B:49:PHE:CZ	12:D:103:SPO:H132	2.50	0.46
12:0:102:SPO:H393	12:0:102:SPO:H362	1.72	0.46
2:M:271:TRP:HZ2	13:M:406:CDL:H711	1.81	0.46
4:O:6:LYS:HD3	12:R:101:SPO:H393	1.98	0.46
2:M:242:GLY:O	2:M:246:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:101:BCL:O1D	12:D:103:SPO:H22	2.15	0.45
4:O:6:LYS:HG2	12:R:101:SPO:H402	1.98	0.45
7:7:101:BCL:H3A	7:7:101:BCL:HBA2	1.70	0.45
4:I:36:LEU:HD13	4:I:43:TRP:CH2	2.51	0.45
5:C:38:ALA:O	5:C:42:VAL:HG23	2.16	0.45
5:2:19:GLU:O	5:2:23:VAL:HG13	2.17	0.45
3:H:32:GLN:O	3:H:36:MET:HG3	2.16	0.45
4:Q:6:LYS:HB2	12:Q:102:SPO:H352	1.99	0.45
7:R:102:BCL:H162	7:R:102:BCL:H141	1.69	0.45
12:S:103:SPO:H343	12:S:103:SPO:H311	1.70	0.45
7:7:101:BCL:H2	5:8:31:PHE:CE1	2.52	0.45
2:M:70:ILE:HG12	2:M:94:LEU:HD12	1.99	0.45
4:W:5:TYR:HD2	5:C:17:ALA:HB3	1.80	0.45
4:7:38:THR:HG21	4:9:44:LEU:HD13	1.99	0.45
12:A:603:SPO:H393	4:9:6:LYS:HD3	1.99	0.45
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.99	0.45
7:E:101:BCL:H141	7:E:101:BCL:H172	1.99	0.45
4:I:23:PHE:HE1	4:K:25:PHE:CE1	2.35	0.45
12:K:103:SPO:H341	12:K:103:SPO:H361	1.72	0.45
7:U:101:BCL:HHC	7:U:101:BCL:OBB	2.17	0.45
10:L:304:U10:H18	10:L:304:U10:H221	1.65	0.45
2:M:222:THR:O	2:M:226:VAL:HG22	2.17	0.45
1:L:178:SER:CB	10:L:304:U10:H262	2.47	0.44
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.52	0.44
2:M:278:LEU:HD21	13:M:406:CDL:H581	1.99	0.44
7:U:102:BCL:H141	7:U:102:BCL:H193	1.97	0.44
4:W:3:LYS:HB2	5:2:23:VAL:HG12	1.99	0.44
1:L:77:GLY:HA3	4:7:37:SER:HB2	1.99	0.44
5:B:6:ASP:OD1	5:B:7:LEU:N	2.51	0.44
12:I:104:SPO:H403	5:N:20:LEU:HD12	1.99	0.44
4:1:27:LEU:O	4:1:31:ILE:HG13	2.18	0.44
9:H:1102:PC1:H152	9:A:601:PC1:H151	1.98	0.44
7:W:101:BCL:HHC	7:W:101:BCL:OBB	2.17	0.44
2:M:271:TRP:HA	2:M:274:VAL:HG22	1.99	0.44
12:I:104:SPO:H10	7:O:101:BCL:H3A	1.99	0.44
4:U:11:PHE:C	5:V:10:THR:HG21	2.38	0.44
5:8:46:ARG:NH2	4:9:53:ARG:HD3	2.33	0.44
7:9:101:BCL:O1D	12:0:102:SPO:H22	2.18	0.44
4:A:27:LEU:HD11	12:A:603:SPO:H9	2.00	0.44
1:L:199:ASN:HB3	13:M:406:CDL:HB21	1.99	0.44
1:L:39:PHE:HZ	9:A:604:PC1:H2G1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:228:LEU:HG	3:H:232:LYS:HE2	2.00	0.44
5:B:5:SER:OG	5:B:6:ASP:N	2.48	0.44
4:D:27:LEU:HD11	12:D:102:SPO:H9	2.00	0.43
12:K:103:SPO:H20	12:K:103:SPO:H181	1.76	0.43
7:N:101:BCL:H192	7:N:101:BCL:H162	1.68	0.43
5:R:49:PHE:HB3	12:R:103:SPO:H6	1.97	0.43
7:U:101:BCL:O1D	12:U:103:SPO:H22	2.18	0.43
5:B:16:GLN:HB3	5:0:7:LEU:HD12	2.00	0.43
1:L:255:TRP:NE1	1:L:257:ASP:O	2.51	0.43
2:M:275:LEU:HD23	2:M:275:LEU:HA	1.88	0.43
4:7:43:TRP:HZ2	7:7:101:BCL:HBB2	1.83	0.43
4:K:32:HIS:CE1	7:N:101:BCL:HMD1	2.53	0.43
1:L:241:VAL:HG21	8:L:302:BPH:HBC3	2.00	0.43
4:U:35:LEU:HD11	7:U:102:BCL:HHD	2.00	0.43
12:0:101:SPO:H311	12:0:101:SPO:H342	1.80	0.43
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.99	0.43
4:I:32:HIS:CE1	7:I:102:BCL:HMD1	2.53	0.43
7:N:101:BCL:HMB1	7:N:101:BCL:HBB2	2.01	0.43
4:W:43:TRP:CD2	7:W:101:BCL:H2C	2.53	0.43
7:L:305:BCL:H101	7:L:305:BCL:H13	1.63	0.43
12:D:104:SPO:H311	12:D:104:SPO:H342	1.73	0.43
5:N:43:TYR:CZ	7:N:101:BCL:H203	2.54	0.43
12:D:104:SPO:C40	5:E:7:LEU:HD11	2.48	0.43
7:E:101:BCL:H192	7:E:101:BCL:H161	1.80	0.43
12:E:102:SPO:H293	12:E:102:SPO:H26	1.79	0.43
12:P:102:SPO:H22	12:P:102:SPO:H181	1.99	0.43
4:U:5:TYR:CD2	5:V:18:GLN:HG2	2.54	0.43
7:U:102:BCL:H141	7:U:102:BCL:H162	1.90	0.43
1:L:168:HIS:HB3	1:L:173:HIS:CE1	2.53	0.43
7:E:101:BCL:HMB1	7:E:101:BCL:HBB2	2.01	0.43
7:I:102:BCL:H52	12:K:102:SPO:C24	2.49	0.43
12:K:102:SPO:H311	12:K:102:SPO:H342	1.67	0.43
7:U:102:BCL:HBB3	7:W:101:BCL:C1C	2.49	0.43
1:L:207:ARG:HD2	1:L:211:HIS:CG	2.53	0.42
13:M:406:CDL:H391	13:M:406:CDL:H421	1.50	0.42
3:H:114:TRP:HB2	3:H:231:ASP:HB3	2.00	0.42
12:F:103:SPO:H341	12:F:103:SPO:H362	1.80	0.42
7:O:102:BCL:HBB2	7:O:102:BCL:HMB1	2.01	0.42
12:Q:102:SPO:H342	5:T:23:VAL:CG1	2.45	0.42
4:U:28:ALA:HB2	7:U:102:BCL:HED2	2.01	0.42
4:W:48:ALA:HA	4:W:53:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:282:ILE:HD11	13:M:406:CDL:H271	2.01	0.42
7:F:102:BCL:HMB1	7:F:102:BCL:HBB2	2.01	0.42
4:I:20:GLN:HE21	12:I:103:SPO:H393	1.83	0.42
2:M:119:SER:HB3	12:M:405:SPO:H342	2.02	0.42
7:I:102:BCL:H162	7:I:102:BCL:H192	1.81	0.42
7:I:102:BCL:HMB1	7:I:102:BCL:HBB2	2.01	0.42
4:K:46:ILE:HD11	5:N:45:TRP:CH2	2.55	0.42
7:S:102:BCL:HMB1	7:S:102:BCL:HBB2	2.01	0.42
7:8:102:BCL:HMB1	7:8:102:BCL:HBB2	2.01	0.42
7:9:103:BCL:HMB1	7:9:103:BCL:HBB2	2.01	0.42
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.01	0.42
9:A:601:PC1:H112	9:A:601:PC1:H153	1.83	0.42
4:D:6:LYS:NZ	5:G:19:GLU:OE2	2.44	0.42
12:E:102:SPO:H181	12:E:102:SPO:H20	1.67	0.42
4:W:3:LYS:HB2	5:2:23:VAL:CG1	2.49	0.42
7:7:101:BCL:H102	12:8:101:SPO:H293	2.01	0.42
9:H:1101:PC1:H31	9:H:1101:PC1:H111	2.00	0.42
12:A:603:SPO:H27	12:A:603:SPO:H311	1.77	0.42
12:F:103:SPO:H291	12:F:103:SPO:H311	1.89	0.42
4:K:1:MET:HA	4:K:4:PHE:CZ	2.55	0.42
4:S:3:LYS:HD2	4:S:6:LYS:NZ	2.35	0.42
7:U:102:BCL:HMB1	7:U:102:BCL:HBB2	2.01	0.42
7:A:605:BCL:HMB1	7:A:605:BCL:HBB2	2.01	0.42
12:K:102:SPO:H15	12:K:102:SPO:H131	1.68	0.42
7:O:102:BCL:H192	7:O:102:BCL:H162	1.72	0.42
7:Q:101:BCL:OBB	7:Q:101:BCL:HHC	2.19	0.42
4:U:12:ASP:HB3	4:U:15:ARG:HD3	2.02	0.42
7:9:101:BCL:OBB	7:9:101:BCL:HHC	2.20	0.41
6:X:37:VAL:O	6:X:41:THR:HG23	2.19	0.41
7:L:305:BCL:HMB1	7:L:305:BCL:HBB2	2.02	0.41
2:M:28:ASN:HB3	2:M:52:LEU:O	2.20	0.41
7:R:102:BCL:HMB1	7:R:102:BCL:HBB2	2.01	0.41
7:S:102:BCL:HBB3	7:U:101:BCL:C1C	2.51	0.41
7:S:102:BCL:HBB3	7:U:101:BCL:CHC	2.50	0.41
7:8:102:BCL:H162	7:8:102:BCL:H192	1.80	0.41
1:L:131:LEU:HD23	1:L:131:LEU:HA	1.88	0.41
4:A:5:TYR:HE1	5:B:14:ASP:OD1	2.02	0.41
7:K:101:BCL:HHC	7:K:101:BCL:OBB	2.20	0.41
7:M:401:BCL:HBB2	7:M:401:BCL:HMB1	2.02	0.41
12:M:405:SPO:H131	12:M:405:SPO:H15	1.73	0.41
7:F:101:BCL:HHC	7:F:101:BCL:OBB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:35:LEU:HD11	7:S:102:BCL:HHD	2.02	0.41
10:L:304:U10:H101	10:L:304:U10:H122	1.69	0.41
2:M:155:TRP:HB2	13:M:406:CDL:H211	2.01	0.41
7:O:101:BCL:OBB	7:O:101:BCL:HHC	2.21	0.41
1:L:226:THR:O	1:L:229:ILE:HG22	2.20	0.41
7:M:403:BCL:HHC	7:M:403:BCL:OBB	2.20	0.41
9:H:1102:PC1:H142	9:H:1102:PC1:H112	1.82	0.41
7:U:102:BCL:H193	7:U:102:BCL:H162	1.77	0.41
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.03	0.41
2:M:68:PHE:O	2:M:72:ILE:HG12	2.21	0.41
5:E:7:LEU:HD12	5:E:7:LEU:O	2.21	0.41
12:U:103:SPO:H291	12:U:103:SPO:H311	1.80	0.41
2:M:129:TRP:O	2:M:133:THR:HG23	2.21	0.41
4:A:35:LEU:HD11	7:A:605:BCL:HHD	2.03	0.40
7:A:602:BCL:HMA1	7:9:103:BCL:HMA1	2.03	0.40
4:S:48:ALA:HA	4:S:53:ARG:HG3	2.02	0.40
2:M:138:GLN:HA	2:M:144:LYS:HZ2	1.86	0.40
12:D:102:SPO:H27	12:D:102:SPO:H311	1.77	0.40
5:C:25:MET:HE2	5:C:25:MET:HB2	1.90	0.40
4:7:17:PHE:CE2	6:X:23:VAL:HG13	2.56	0.40
13:M:406:CDL:H111	13:M:406:CDL:HA4	1.97	0.40
9:A:604:PC1:H282	9:A:604:PC1:H2B1	1.67	0.40
12:U:103:SPO:H311	12:U:103:SPO:H343	1.86	0.40
7:D:101:BCL:HHC	7:D:101:BCL:OBB	2.21	0.40
7:N:101:BCL:HMA1	7:O:101:BCL:HMA1	2.02	0.40
7:7:101:BCL:H92	6:X:28:MET:SD	2.62	0.40
1:L:168:HIS:ND1	7:L:301:BCL:HMC2	2.37	0.40
1:L:169:TYR:O	1:L:263:TRP:NE1	2.39	0.40
1:L:255:TRP:CZ2	1:L:262:TRP:HB2	2.57	0.40
7:A:602:BCL:HHC	7:A:602:BCL:OBB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/282 (99%)	269 (96%)	10 (4%)	0	100	100
2	M	303/308 (98%)	298 (98%)	5 (2%)	0	100	100
3	H	245/260 (94%)	241 (98%)	4 (2%)	0	100	100
4	1	41/58 (71%)	41 (100%)	0	0	100	100
4	7	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
4	9	52/58 (90%)	52 (100%)	0	0	100	100
4	A	52/58 (90%)	52 (100%)	0	0	100	100
4	D	52/58 (90%)	52 (100%)	0	0	100	100
4	F	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	I	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	K	52/58 (90%)	52 (100%)	0	0	100	100
4	O	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	Q	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	S	52/58 (90%)	52 (100%)	0	0	100	100
4	U	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	W	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
5	0	42/49 (86%)	42 (100%)	0	0	100	100
5	2	30/49 (61%)	29 (97%)	1 (3%)	0	100	100
5	8	42/49 (86%)	42 (100%)	0	0	100	100
5	B	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
5	C	36/49 (74%)	36 (100%)	0	0	100	100
5	E	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	G	41/49 (84%)	41 (100%)	0	0	100	100
5	J	41/49 (84%)	41 (100%)	0	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	41 (100%)	0	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	41/49 (84%)	41 (100%)	0	0	100	100
5	V	38/49 (78%)	38 (100%)	0	0	100	100
6	X	50/82 (61%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2052/2323 (88%)	2021 (98%)	31 (2%)	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	L	220/221 (100%)	220 (100%)	0	100 100
2	M	239/241 (99%)	238 (100%)	1 (0%)	91 96
3	H	199/208 (96%)	199 (100%)	0	100 100
4	1	38/51 (74%)	38 (100%)	0	100 100
4	7	43/51 (84%)	43 (100%)	0	100 100
4	9	49/51 (96%)	49 (100%)	0	100 100
4	A	49/51 (96%)	49 (100%)	0	100 100
4	D	49/51 (96%)	49 (100%)	0	100 100
4	F	49/51 (96%)	49 (100%)	0	100 100
4	I	49/51 (96%)	49 (100%)	0	100 100
4	K	49/51 (96%)	49 (100%)	0	100 100
4	O	49/51 (96%)	49 (100%)	0	100 100
4	Q	49/51 (96%)	49 (100%)	0	100 100
4	S	49/51 (96%)	49 (100%)	0	100 100
4	U	49/51 (96%)	49 (100%)	0	100 100
4	W	49/51 (96%)	49 (100%)	0	100 100
5	0	36/40 (90%)	36 (100%)	0	100 100
5	2	27/40 (68%)	27 (100%)	0	100 100
5	8	36/40 (90%)	36 (100%)	0	100 100
5	B	37/40 (92%)	37 (100%)	0	100 100
5	C	32/40 (80%)	31 (97%)	1 (3%)	40 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	35/40 (88%)	35 (100%)	0	100	100
5	G	35/40 (88%)	35 (100%)	0	100	100
5	J	35/40 (88%)	35 (100%)	0	100	100
5	N	35/40 (88%)	35 (100%)	0	100	100
5	P	35/40 (88%)	35 (100%)	0	100	100
5	R	35/40 (88%)	35 (100%)	0	100	100
5	T	35/40 (88%)	35 (100%)	0	100	100
5	V	33/40 (82%)	33 (100%)	0	100	100
6	X	40/66 (61%)	40 (100%)	0	100	100
All	All	1764/1919 (92%)	1762 (100%)	2 (0%)	93	98

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

Mol	Chain	Res	Type
2	M	216	PHE
5	C	25	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	L	173	HIS
2	M	11	GLN
4	U	20	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 1 is monoatomic - leaving 64 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	BCL	2	101	-	38,54,74	1.46	4 (10%)	45,91,115	1.70	10 (22%)
7	BCL	F	102	-	58,74,74	1.21	4 (6%)	69,115,115	1.47	13 (18%)
7	BCL	L	305	-	58,74,74	1.14	4 (6%)	69,115,115	1.60	15 (21%)
9	PC1	H	1101	-	46,46,53	1.13	3 (6%)	52,54,61	0.98	4 (7%)
9	PC1	H	1102	-	38,38,53	1.24	3 (7%)	44,46,61	1.00	3 (6%)
7	BCL	U	101	-	58,74,74	1.21	4 (6%)	69,115,115	1.46	11 (15%)
12	SPO	F	103	-	40,41,41	6.09	17 (42%)	47,50,50	4.83	29 (61%)
12	SPO	8	101	-	37,38,41	6.25	17 (45%)	43,46,50	4.99	28 (65%)
7	BCL	M	401	-	55,71,74	1.16	4 (7%)	65,111,115	1.37	11 (16%)
7	BCL	Q	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.46	11 (15%)
7	BCL	8	102	-	58,74,74	1.21	4 (6%)	69,115,115	1.45	14 (20%)
8	BPH	L	306	-	41,60,70	1.05	2 (4%)	40,89,101	1.20	5 (12%)
12	SPO	P	102	-	40,41,41	6.57	17 (42%)	47,50,50	4.85	23 (48%)
7	BCL	O	101	-	58,74,74	1.23	4 (6%)	69,115,115	1.45	11 (15%)
12	SPO	9	102	-	40,41,41	6.15	17 (42%)	47,50,50	4.46	29 (61%)
7	BCL	9	103	-	53,69,74	1.25	4 (7%)	63,109,115	1.44	12 (19%)
9	PC1	A	604	-	44,44,53	1.18	4 (9%)	50,52,61	1.23	4 (8%)
12	SPO	0	101	-	40,41,41	6.13	17 (42%)	47,50,50	4.71	32 (68%)
7	BCL	C	101	-	58,74,74	1.20	3 (5%)	69,115,115	1.61	13 (18%)
7	BCL	9	101	-	58,74,74	1.24	4 (6%)	69,115,115	1.55	13 (18%)
7	BCL	R	102	-	58,74,74	1.20	4 (6%)	69,115,115	1.42	12 (17%)
12	SPO	D	104	-	40,41,41	6.03	17 (42%)	47,50,50	4.95	31 (65%)
10	U10	L	304	-	43,43,63	2.66	13 (30%)	52,55,79	1.76	12 (23%)
7	BCL	F	101	-	58,74,74	1.28	5 (8%)	69,115,115	1.46	12 (17%)
12	SPO	K	102	-	40,41,41	6.18	17 (42%)	47,50,50	4.91	28 (59%)
9	PC1	X	1501	-	35,35,53	1.30	5 (14%)	41,43,61	1.21	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	SPO	I	104	-	40,41,41	5.84	17 (42%)	47,50,50	4.85	34 (72%)
12	SPO	K	103	-	40,41,41	5.86	17 (42%)	47,50,50	4.99	30 (63%)
12	SPO	P	101	-	40,41,41	6.04	18 (45%)	47,50,50	5.38	31 (65%)
9	PC1	L	303	-	34,34,53	1.35	5 (14%)	40,42,61	1.28	5 (12%)
7	BCL	L	301	-	58,74,74	1.20	4 (6%)	69,115,115	1.43	10 (14%)
7	BCL	N	101	-	58,74,74	1.20	4 (6%)	69,115,115	1.45	14 (20%)
12	SPO	A	603	-	40,41,41	5.70	16 (40%)	47,50,50	5.18	27 (57%)
7	BCL	E	101	-	58,74,74	1.22	4 (6%)	69,115,115	1.45	13 (18%)
7	BCL	S	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.47	10 (14%)
7	BCL	A	602	-	58,74,74	1.22	5 (8%)	69,115,115	1.43	11 (15%)
7	BCL	M	403	-	58,74,74	1.18	4 (6%)	69,115,115	1.43	11 (15%)
12	SPO	D	102	-	40,41,41	5.70	16 (40%)	47,50,50	5.18	27 (57%)
12	SPO	Q	102	-	40,41,41	6.01	17 (42%)	47,50,50	4.83	31 (65%)
7	BCL	W	101	-	58,74,74	1.18	3 (5%)	69,115,115	1.41	12 (17%)
7	BCL	D	101	-	58,74,74	1.22	5 (8%)	69,115,115	1.43	11 (15%)
7	BCL	O	102	-	58,74,74	1.20	4 (6%)	69,115,115	1.42	12 (17%)
7	BCL	I	101	-	58,74,74	1.23	4 (6%)	69,115,115	1.45	10 (14%)
7	BCL	U	102	-	58,74,74	1.20	4 (6%)	69,115,115	1.41	12 (17%)
7	BCL	1	101	-	58,74,74	1.20	5 (8%)	69,115,115	1.42	11 (15%)
12	SPO	R	103	-	40,41,41	6.23	17 (42%)	47,50,50	4.70	29 (61%)
7	BCL	A	605	-	58,74,74	1.20	4 (6%)	69,115,115	1.42	12 (17%)
10	U10	M	404	-	48,48,63	2.67	14 (29%)	58,61,79	1.63	12 (20%)
7	BCL	7	101	-	53,69,74	1.27	3 (5%)	63,109,115	1.39	10 (15%)
12	SPO	S	103	-	40,41,41	6.11	17 (42%)	47,50,50	4.85	31 (65%)
12	SPO	M	405	-	40,41,41	5.93	17 (42%)	47,50,50	4.87	30 (63%)
12	SPO	D	103	-	40,41,41	5.96	17 (42%)	47,50,50	5.45	28 (59%)
12	SPO	E	102	-	40,41,41	6.07	17 (42%)	47,50,50	5.63	30 (63%)
12	SPO	I	103	-	40,41,41	6.27	17 (42%)	47,50,50	4.65	29 (61%)
12	SPO	R	101	-	40,41,41	6.08	17 (42%)	47,50,50	4.68	28 (59%)
8	BPH	L	302	-	48,67,70	0.96	2 (4%)	48,97,101	1.20	6 (12%)
12	SPO	U	103	-	40,41,41	6.05	17 (42%)	47,50,50	5.32	30 (63%)
12	SPO	0	102	-	40,41,41	6.06	17 (42%)	47,50,50	5.15	28 (59%)
7	BCL	I	102	-	58,74,74	1.20	4 (6%)	69,115,115	1.41	12 (17%)
13	CDL	M	406	-	99,99,99	1.09	7 (7%)	105,111,111	0.85	4 (3%)
7	BCL	S	102	-	58,74,74	1.21	4 (6%)	69,115,115	1.43	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	PC1	H	1103	-	31,31,53	1.34	4 (12%)	37,39,61	1.40	4 (10%)
9	PC1	A	601	-	31,31,53	1.31	3 (9%)	37,39,61	1.11	3 (8%)
7	BCL	K	101	-	58,74,74	1.22	4 (6%)	69,115,115	1.44	11 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	2	101	-	-	6/13/113/137	-
7	BCL	F	102	-	-	7/37/137/137	-
7	BCL	L	305	-	-	7/37/137/137	-
9	PC1	H	1101	-	-	25/50/50/57	-
9	PC1	H	1102	-	-	25/42/42/57	-
7	BCL	U	101	-	-	3/37/137/137	-
12	SPO	F	103	-	-	21/47/47/47	-
12	SPO	8	101	-	-	19/44/44/47	-
7	BCL	M	401	-	-	1/34/134/137	-
7	BCL	Q	101	-	-	0/37/137/137	-
7	BCL	8	102	-	-	8/37/137/137	-
8	BPH	L	306	-	-	4/25/93/105	0/5/6/6
12	SPO	P	102	-	-	25/47/47/47	-
7	BCL	O	101	-	-	6/37/137/137	-
12	SPO	9	102	-	-	17/47/47/47	-
7	BCL	9	103	-	-	6/31/131/137	-
9	PC1	A	604	-	-	25/48/48/57	-
12	SPO	0	101	-	-	21/47/47/47	-
7	BCL	C	101	-	-	13/37/137/137	-
7	BCL	9	101	-	-	4/37/137/137	-
7	BCL	R	102	-	-	6/37/137/137	-
12	SPO	D	104	-	-	22/47/47/47	-
10	U10	L	304	-	-	10/39/63/87	0/1/1/1
7	BCL	F	101	-	-	2/37/137/137	-
12	SPO	K	102	-	-	24/47/47/47	-
9	PC1	X	1501	-	-	14/39/39/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SPO	I	104	-	-	24/47/47/47	-
12	SPO	K	103	-	-	28/47/47/47	-
12	SPO	P	101	-	-	26/47/47/47	-
9	PC1	L	303	-	-	12/38/38/57	-
7	BCL	L	301	-	-	2/37/137/137	-
7	BCL	N	101	-	-	9/37/137/137	-
12	SPO	A	603	-	-	20/47/47/47	-
7	BCL	E	101	-	-	10/37/137/137	-
7	BCL	S	101	-	-	7/37/137/137	-
7	BCL	A	602	-	-	0/37/137/137	-
7	BCL	M	403	-	-	2/37/137/137	-
12	SPO	D	102	-	-	20/47/47/47	-
12	SPO	Q	102	-	-	22/47/47/47	-
7	BCL	W	101	-	-	6/37/137/137	-
7	BCL	D	101	-	-	0/37/137/137	-
7	BCL	O	102	-	-	6/37/137/137	-
7	BCL	I	101	-	-	0/37/137/137	-
7	BCL	U	102	-	-	7/37/137/137	-
7	BCL	1	101	-	-	0/37/137/137	-
12	SPO	R	103	-	-	18/47/47/47	-
7	BCL	A	605	-	-	6/37/137/137	-
10	U10	M	404	-	-	9/45/69/87	0/1/1/1
7	BCL	7	101	-	-	13/31/131/137	-
12	SPO	S	103	-	-	23/47/47/47	-
12	SPO	M	405	-	-	27/47/47/47	-
12	SPO	D	103	-	-	28/47/47/47	-
12	SPO	E	102	-	-	24/47/47/47	-
12	SPO	I	103	-	-	23/47/47/47	-
12	SPO	R	101	-	-	23/47/47/47	-
8	BPH	L	302	-	-	4/34/102/105	0/5/6/6
12	SPO	U	103	-	-	22/47/47/47	-
12	SPO	0	102	-	-	26/47/47/47	-
7	BCL	I	102	-	-	6/37/137/137	-
13	CDL	M	406	-	-	44/110/110/110	-
7	BCL	S	102	-	-	8/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	H	1103	-	-	18/35/35/57	-
9	PC1	A	601	-	-	19/35/35/57	-
7	BCL	K	101	-	-	0/37/137/137	-

All (559) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	102	SPO	C27-C28	19.86	1.54	1.34
12	E	102	SPO	C27-C28	19.80	1.54	1.34
12	P	102	SPO	C27-C28	19.73	1.54	1.34
12	R	103	SPO	C27-C28	19.67	1.54	1.34
12	I	103	SPO	C27-C28	19.67	1.54	1.34
12	8	101	SPO	C27-C28	19.56	1.54	1.34
12	0	102	SPO	C27-C28	19.52	1.54	1.34
12	D	103	SPO	C27-C28	19.44	1.54	1.34
12	F	103	SPO	C27-C28	19.35	1.54	1.34
12	9	102	SPO	C27-C28	19.27	1.54	1.34
12	P	101	SPO	C27-C28	19.26	1.54	1.34
12	I	104	SPO	C27-C28	19.18	1.54	1.34
12	R	101	SPO	C27-C28	19.09	1.53	1.34
12	K	103	SPO	C27-C28	19.04	1.53	1.34
12	S	103	SPO	C27-C28	18.98	1.53	1.34
12	0	101	SPO	C27-C28	18.96	1.53	1.34
12	A	603	SPO	C27-C28	18.89	1.53	1.34
12	D	102	SPO	C27-C28	18.89	1.53	1.34
12	U	103	SPO	C27-C28	18.88	1.53	1.34
12	M	405	SPO	C27-C28	18.83	1.53	1.34
12	Q	102	SPO	C27-C28	18.77	1.53	1.34
12	D	104	SPO	C27-C28	18.42	1.53	1.34
12	P	102	SPO	C14-C12	17.09	1.58	1.35
12	I	103	SPO	C14-C12	16.15	1.57	1.35
12	Q	102	SPO	C14-C12	16.14	1.57	1.35
12	R	103	SPO	C14-C12	16.02	1.57	1.35
12	D	104	SPO	C14-C12	15.93	1.56	1.35
12	E	102	SPO	C14-C12	15.76	1.56	1.35
12	P	102	SPO	C9-C7	15.64	1.56	1.35
12	R	101	SPO	C14-C12	15.56	1.56	1.35
12	8	101	SPO	C14-C12	15.56	1.56	1.35
12	K	103	SPO	C14-C12	15.52	1.56	1.35
12	9	102	SPO	C14-C12	15.43	1.56	1.35
12	P	101	SPO	C14-C12	15.43	1.56	1.35
12	S	103	SPO	C14-C12	15.39	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	0	101	SPO	C14-C12	15.38	1.56	1.35
12	I	104	SPO	C14-C12	15.31	1.56	1.35
12	F	103	SPO	C14-C12	15.15	1.55	1.35
12	P	102	SPO	C22-C23	15.06	1.55	1.35
12	M	405	SPO	C14-C12	15.02	1.55	1.35
12	P	102	SPO	C19-C17	15.00	1.55	1.35
12	0	102	SPO	C14-C12	14.84	1.55	1.35
12	9	102	SPO	C19-C17	14.73	1.55	1.35
12	K	102	SPO	C14-C12	14.70	1.55	1.35
12	D	103	SPO	C19-C17	14.67	1.55	1.35
12	U	103	SPO	C14-C12	14.64	1.55	1.35
12	K	102	SPO	C19-C17	14.64	1.55	1.35
12	S	103	SPO	C19-C17	14.58	1.55	1.35
12	U	103	SPO	C19-C17	14.56	1.55	1.35
12	8	101	SPO	C19-C17	14.50	1.55	1.35
12	F	103	SPO	C19-C17	14.43	1.54	1.35
12	K	102	SPO	C22-C23	14.37	1.54	1.35
12	P	101	SPO	C9-C7	14.36	1.54	1.35
12	I	103	SPO	C19-C17	14.31	1.54	1.35
12	0	101	SPO	C19-C17	14.30	1.54	1.35
12	0	102	SPO	C22-C23	14.29	1.54	1.35
12	D	104	SPO	C19-C17	14.28	1.54	1.35
12	I	103	SPO	C22-C23	14.23	1.54	1.35
12	9	102	SPO	C22-C23	14.23	1.54	1.35
12	D	103	SPO	C14-C12	14.20	1.54	1.35
12	R	101	SPO	C19-C17	14.20	1.54	1.35
12	0	101	SPO	C9-C7	14.08	1.54	1.35
12	R	101	SPO	C22-C23	14.08	1.54	1.35
12	R	103	SPO	C19-C17	14.06	1.54	1.35
12	R	103	SPO	C22-C23	14.06	1.54	1.35
12	S	103	SPO	C22-C23	14.03	1.54	1.35
12	Q	102	SPO	C19-C17	13.99	1.54	1.35
12	D	104	SPO	C22-C23	13.96	1.54	1.35
12	I	103	SPO	C9-C7	13.96	1.54	1.35
12	U	103	SPO	C22-C23	13.95	1.54	1.35
12	8	101	SPO	C22-C23	13.90	1.54	1.35
12	M	405	SPO	C22-C23	13.80	1.54	1.35
12	A	603	SPO	C14-C12	13.78	1.54	1.35
12	D	102	SPO	C14-C12	13.78	1.54	1.35
12	0	101	SPO	C22-C23	13.77	1.54	1.35
12	R	103	SPO	C9-C7	13.75	1.54	1.35
12	0	102	SPO	C19-C17	13.69	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	103	SPO	C22-C23	13.58	1.53	1.35
12	E	102	SPO	C9-C7	13.57	1.53	1.35
12	M	405	SPO	C19-C17	13.50	1.53	1.35
12	F	103	SPO	C22-C23	13.46	1.53	1.35
12	K	103	SPO	C19-C17	13.42	1.53	1.35
12	F	103	SPO	C9-C7	13.39	1.53	1.35
12	E	102	SPO	C19-C17	13.35	1.53	1.35
12	E	102	SPO	C22-C23	13.33	1.53	1.35
12	I	104	SPO	C19-C17	13.28	1.53	1.35
12	P	101	SPO	C19-C17	13.20	1.53	1.35
12	S	103	SPO	C9-C7	13.14	1.53	1.35
12	8	101	SPO	C9-C7	13.08	1.53	1.35
12	Q	102	SPO	C22-C23	13.04	1.53	1.35
12	D	104	SPO	C9-C7	13.01	1.53	1.35
12	D	102	SPO	C19-C17	13.01	1.53	1.35
12	A	603	SPO	C19-C17	13.01	1.53	1.35
12	9	102	SPO	C9-C7	13.00	1.53	1.35
12	K	103	SPO	C22-C23	12.98	1.53	1.35
12	U	103	SPO	C9-C7	12.92	1.52	1.35
12	Q	102	SPO	C9-C7	12.91	1.52	1.35
12	I	104	SPO	C22-C23	12.91	1.52	1.35
12	P	101	SPO	C22-C23	12.91	1.52	1.35
12	A	603	SPO	C22-C23	12.88	1.52	1.35
12	D	102	SPO	C22-C23	12.87	1.52	1.35
12	K	102	SPO	C9-C7	12.86	1.52	1.35
12	M	405	SPO	C9-C7	12.85	1.52	1.35
12	0	102	SPO	C9-C7	12.83	1.52	1.35
12	D	102	SPO	C9-C7	12.69	1.52	1.35
12	A	603	SPO	C9-C7	12.69	1.52	1.35
12	R	101	SPO	C9-C7	12.61	1.52	1.35
12	K	103	SPO	C9-C7	12.17	1.51	1.35
12	D	103	SPO	C9-C7	12.17	1.51	1.35
12	I	104	SPO	C9-C7	11.95	1.51	1.35
12	F	103	SPO	C32-C33	9.21	1.55	1.33
12	M	405	SPO	C32-C33	9.04	1.54	1.33
12	I	103	SPO	C32-C33	9.01	1.54	1.33
12	U	103	SPO	C32-C33	9.00	1.54	1.33
12	P	101	SPO	C32-C33	8.98	1.54	1.33
12	R	101	SPO	C32-C33	8.96	1.54	1.33
12	R	103	SPO	C32-C33	8.94	1.54	1.33
12	P	102	SPO	C32-C33	8.93	1.54	1.33
12	K	102	SPO	C32-C33	8.90	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	0	101	SPO	C32-C33	8.87	1.54	1.33
12	0	102	SPO	C32-C33	8.86	1.54	1.33
12	S	103	SPO	C32-C33	8.83	1.54	1.33
12	D	103	SPO	C32-C33	8.81	1.54	1.33
12	D	104	SPO	C32-C33	8.70	1.53	1.33
12	8	101	SPO	C32-C33	8.69	1.53	1.33
12	9	102	SPO	C32-C33	8.66	1.53	1.33
12	K	103	SPO	C32-C33	8.62	1.53	1.33
12	Q	102	SPO	C32-C33	8.61	1.53	1.33
12	I	104	SPO	C32-C33	8.54	1.53	1.33
12	E	102	SPO	C32-C33	8.47	1.53	1.33
12	A	603	SPO	C32-C33	8.07	1.52	1.33
12	D	102	SPO	C32-C33	8.07	1.52	1.33
12	R	101	SPO	C37-C38	7.64	1.54	1.32
12	0	101	SPO	C37-C38	7.63	1.54	1.32
12	Q	102	SPO	C37-C38	7.62	1.54	1.32
12	D	103	SPO	C37-C38	7.57	1.54	1.32
12	P	102	SPO	C37-C38	7.53	1.54	1.32
12	P	101	SPO	C37-C38	7.52	1.54	1.32
12	I	103	SPO	C37-C38	7.48	1.53	1.32
12	S	103	SPO	C37-C38	7.47	1.53	1.32
12	E	102	SPO	C37-C38	7.45	1.53	1.32
12	I	104	SPO	C37-C38	7.45	1.53	1.32
12	R	103	SPO	C37-C38	7.45	1.53	1.32
12	F	103	SPO	C37-C38	7.44	1.53	1.32
12	M	405	SPO	C37-C38	7.44	1.53	1.32
12	U	103	SPO	C37-C38	7.43	1.53	1.32
12	9	102	SPO	C37-C38	7.43	1.53	1.32
12	K	102	SPO	C37-C38	7.43	1.53	1.32
12	K	103	SPO	C37-C38	7.40	1.53	1.32
12	0	102	SPO	C37-C38	7.38	1.53	1.32
12	D	102	SPO	C37-C38	7.35	1.53	1.32
12	A	603	SPO	C37-C38	7.35	1.53	1.32
12	D	104	SPO	C37-C38	7.34	1.53	1.32
10	L	304	U10	C18-C19	6.00	1.47	1.33
10	M	404	U10	C8-C9	5.97	1.47	1.33
10	L	304	U10	C13-C14	5.93	1.47	1.33
10	L	304	U10	C23-C24	5.92	1.47	1.33
10	L	304	U10	C28-C29	5.90	1.47	1.33
10	M	404	U10	C28-C29	5.88	1.47	1.33
10	M	404	U10	C18-C19	5.84	1.47	1.33
10	M	404	U10	C33-C34	5.83	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	304	U10	C8-C9	5.81	1.46	1.33
10	M	404	U10	C13-C14	5.80	1.46	1.33
10	M	404	U10	C23-C24	5.71	1.46	1.33
10	M	404	U10	O4-C4	-5.54	1.23	1.36
10	L	304	U10	O4-C4	-5.51	1.23	1.36
10	M	404	U10	O3-C3	-5.39	1.23	1.36
10	M	404	U10	C38-C39	5.27	1.47	1.32
10	L	304	U10	C33-C34	5.22	1.47	1.32
10	L	304	U10	O3-C3	-5.20	1.24	1.36
12	I	103	SPO	C11-C12	5.07	1.56	1.45
12	P	102	SPO	C11-C12	5.00	1.56	1.45
7	2	101	BCL	C1B-NB	4.92	1.39	1.35
12	K	102	SPO	C16-C17	4.87	1.56	1.45
7	C	101	BCL	C1B-NB	4.87	1.39	1.35
7	1	101	BCL	C1B-NB	4.86	1.39	1.35
12	0	102	SPO	C11-C12	4.86	1.56	1.45
12	P	102	SPO	C10-C9	4.85	1.58	1.43
12	R	103	SPO	C11-C12	4.84	1.56	1.45
12	P	102	SPO	C16-C17	4.83	1.56	1.45
12	P	102	SPO	C15-C14	4.82	1.58	1.43
7	I	101	BCL	MG-NA	4.81	2.17	2.06
12	9	102	SPO	C11-C12	4.81	1.56	1.45
12	K	102	SPO	C15-C14	4.78	1.58	1.43
7	9	101	BCL	MG-NA	4.75	2.17	2.06
12	U	103	SPO	C16-C17	4.72	1.56	1.45
7	K	101	BCL	MG-NA	4.72	2.17	2.06
7	A	602	BCL	MG-NA	4.72	2.17	2.06
7	D	101	BCL	MG-NA	4.71	2.17	2.06
12	S	103	SPO	C16-C17	4.71	1.56	1.45
12	D	104	SPO	C11-C12	4.70	1.56	1.45
7	2	101	BCL	MG-NA	4.70	2.17	2.06
7	F	101	BCL	MG-NA	4.70	2.17	2.06
7	7	101	BCL	C1B-NB	4.69	1.39	1.35
12	S	103	SPO	C20-C19	4.69	1.58	1.43
12	P	102	SPO	C6-C7	4.68	1.56	1.45
7	S	101	BCL	MG-NA	4.68	2.17	2.06
12	8	101	SPO	C16-C17	4.64	1.55	1.45
12	P	102	SPO	C20-C19	4.62	1.57	1.43
12	8	101	SPO	C11-C12	4.62	1.55	1.45
7	U	101	BCL	MG-NA	4.61	2.17	2.06
7	9	103	BCL	C1B-NB	4.60	1.39	1.35
7	8	102	BCL	C1B-NB	4.60	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	605	BCL	C1B-NB	4.59	1.39	1.35
7	O	102	BCL	C1B-NB	4.59	1.39	1.35
7	R	102	BCL	C1B-NB	4.59	1.39	1.35
7	E	101	BCL	C1B-NB	4.59	1.39	1.35
7	S	102	BCL	C1B-NB	4.59	1.39	1.35
12	Q	102	SPO	C11-C12	4.59	1.55	1.45
7	N	101	BCL	C1B-NB	4.59	1.39	1.35
7	U	102	BCL	C1B-NB	4.59	1.39	1.35
7	E	101	BCL	MG-NA	4.59	2.17	2.06
7	F	102	BCL	C1B-NB	4.58	1.39	1.35
7	U	102	BCL	MG-NA	4.58	2.17	2.06
7	I	102	BCL	MG-NA	4.58	2.17	2.06
7	9	103	BCL	MG-NA	4.58	2.17	2.06
7	8	102	BCL	MG-NA	4.58	2.17	2.06
7	A	605	BCL	MG-NA	4.58	2.17	2.06
7	F	102	BCL	MG-NA	4.58	2.17	2.06
7	N	101	BCL	MG-NA	4.58	2.17	2.06
7	S	102	BCL	MG-NA	4.58	2.17	2.06
7	I	102	BCL	C1B-NB	4.58	1.39	1.35
7	O	102	BCL	MG-NA	4.58	2.17	2.06
12	I	103	SPO	C15-C14	4.58	1.57	1.43
7	R	102	BCL	MG-NA	4.58	2.17	2.06
7	O	101	BCL	MG-NA	4.57	2.17	2.06
12	P	101	SPO	C11-C12	4.57	1.55	1.45
12	F	103	SPO	C20-C19	4.56	1.57	1.43
12	U	103	SPO	C15-C14	4.56	1.57	1.43
7	L	301	BCL	C1B-NB	4.55	1.39	1.35
12	9	102	SPO	C16-C17	4.55	1.55	1.45
7	Q	101	BCL	MG-NA	4.54	2.17	2.06
7	W	101	BCL	MG-NA	4.53	2.17	2.06
12	0	101	SPO	C6-C7	4.53	1.55	1.45
12	F	103	SPO	C16-C17	4.53	1.55	1.45
7	1	101	BCL	MG-NA	4.51	2.17	2.06
7	M	403	BCL	MG-NA	4.50	2.17	2.06
12	0	102	SPO	C10-C9	4.50	1.57	1.43
12	E	102	SPO	C11-C12	4.46	1.55	1.45
7	F	101	BCL	C1B-NB	4.46	1.39	1.35
7	W	101	BCL	C1B-NB	4.46	1.39	1.35
7	M	401	BCL	C1B-NB	4.45	1.39	1.35
7	7	101	BCL	MG-NA	4.45	2.16	2.06
12	M	405	SPO	C11-C12	4.45	1.55	1.45
12	R	101	SPO	C11-C12	4.44	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	103	SPO	C15-C14	4.44	1.57	1.43
12	0	101	SPO	C20-C19	4.42	1.57	1.43
12	D	104	SPO	C15-C14	4.40	1.57	1.43
12	R	101	SPO	C15-C14	4.40	1.57	1.43
7	L	301	BCL	MG-NA	4.39	2.16	2.06
12	U	103	SPO	C20-C19	4.39	1.57	1.43
12	0	102	SPO	C15-C14	4.38	1.57	1.43
7	C	101	BCL	MG-NA	4.37	2.16	2.06
12	0	101	SPO	C15-C14	4.37	1.57	1.43
7	I	101	BCL	C1B-NB	4.37	1.39	1.35
12	K	102	SPO	C20-C19	4.37	1.57	1.43
12	9	102	SPO	C20-C19	4.36	1.57	1.43
7	L	305	BCL	C1B-NB	4.36	1.39	1.35
7	9	101	BCL	C1B-NB	4.36	1.39	1.35
7	K	101	BCL	C1B-NB	4.35	1.39	1.35
12	P	102	SPO	C21-C22	4.33	1.56	1.43
7	U	101	BCL	C1B-NB	4.33	1.39	1.35
12	R	101	SPO	C21-C22	4.32	1.56	1.43
12	Q	102	SPO	C15-C14	4.31	1.56	1.43
12	K	102	SPO	C11-C12	4.30	1.55	1.45
12	U	103	SPO	C10-C9	4.29	1.56	1.43
12	0	101	SPO	C16-C17	4.29	1.55	1.45
12	D	104	SPO	C20-C19	4.29	1.56	1.43
7	M	401	BCL	MG-NA	4.28	2.16	2.06
7	L	305	BCL	MG-NA	4.28	2.16	2.06
12	K	102	SPO	C25-C23	4.28	1.55	1.45
12	Q	102	SPO	C16-C17	4.28	1.55	1.45
12	R	103	SPO	C4-C5	4.27	1.56	1.50
12	R	101	SPO	C20-C19	4.26	1.56	1.43
12	U	103	SPO	C11-C12	4.26	1.55	1.45
12	K	103	SPO	C15-C14	4.26	1.56	1.43
12	9	102	SPO	C15-C14	4.25	1.56	1.43
12	E	102	SPO	C6-C7	4.25	1.55	1.45
12	0	102	SPO	C6-C7	4.23	1.55	1.45
12	F	103	SPO	C11-C12	4.23	1.55	1.45
12	I	104	SPO	C15-C14	4.23	1.56	1.43
12	E	102	SPO	C20-C19	4.21	1.56	1.43
12	I	103	SPO	C20-C19	4.21	1.56	1.43
7	Q	101	BCL	C1B-NB	4.20	1.39	1.35
12	D	104	SPO	C16-C17	4.20	1.55	1.45
12	I	103	SPO	C10-C9	4.19	1.56	1.43
12	I	103	SPO	C16-C17	4.18	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	104	SPO	C11-C12	4.18	1.54	1.45
7	M	403	BCL	C1B-NB	4.17	1.38	1.35
7	O	101	BCL	C1B-NB	4.16	1.38	1.35
7	A	602	BCL	C1B-NB	4.15	1.38	1.35
7	D	101	BCL	C1B-NB	4.15	1.38	1.35
8	L	306	BPH	CBD-CGD	-4.15	1.46	1.52
7	S	101	BCL	C1B-NB	4.14	1.38	1.35
12	0	101	SPO	C11-C12	4.14	1.54	1.45
12	S	103	SPO	C15-C14	4.14	1.56	1.43
12	P	101	SPO	C20-C19	4.13	1.56	1.43
12	K	103	SPO	C11-C12	4.12	1.54	1.45
12	R	103	SPO	C10-C9	4.12	1.56	1.43
12	D	103	SPO	C20-C19	4.12	1.56	1.43
12	Q	102	SPO	C20-C19	4.11	1.56	1.43
12	9	102	SPO	C21-C22	4.11	1.56	1.43
12	0	101	SPO	C21-C22	4.10	1.56	1.43
12	F	103	SPO	C15-C14	4.09	1.56	1.43
12	8	101	SPO	C20-C19	4.09	1.56	1.43
12	P	101	SPO	C15-C14	4.09	1.56	1.43
12	R	103	SPO	C21-C22	4.07	1.56	1.43
12	9	102	SPO	C26-C27	4.07	1.56	1.43
12	K	102	SPO	C21-C22	4.06	1.56	1.43
12	K	102	SPO	C6-C7	4.06	1.54	1.45
12	D	103	SPO	C15-C14	4.06	1.56	1.43
12	K	102	SPO	C26-C27	4.05	1.56	1.43
12	K	102	SPO	C10-C9	4.04	1.56	1.43
12	E	102	SPO	C15-C14	4.03	1.55	1.43
12	I	104	SPO	C16-C17	4.03	1.54	1.45
12	R	103	SPO	C16-C17	4.03	1.54	1.45
12	R	103	SPO	C6-C7	4.02	1.54	1.45
12	0	101	SPO	C10-C9	4.01	1.55	1.43
12	K	103	SPO	C20-C19	4.00	1.55	1.43
12	8	101	SPO	C21-C22	4.00	1.55	1.43
12	D	102	SPO	C15-C14	3.99	1.55	1.43
12	A	603	SPO	C15-C14	3.99	1.55	1.43
12	S	103	SPO	C10-C9	3.99	1.55	1.43
12	0	102	SPO	C21-C22	3.98	1.55	1.43
12	P	101	SPO	C6-C7	3.98	1.54	1.45
12	I	103	SPO	C26-C27	3.98	1.55	1.43
12	9	102	SPO	C25-C23	3.97	1.54	1.45
12	D	103	SPO	C16-C17	3.96	1.54	1.45
12	R	101	SPO	C26-C27	3.96	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	103	SPO	C11-C12	3.95	1.54	1.45
12	0	101	SPO	C26-C27	3.95	1.55	1.43
12	0	102	SPO	C20-C19	3.95	1.55	1.43
12	D	102	SPO	C6-C7	3.95	1.54	1.45
12	A	603	SPO	C6-C7	3.94	1.54	1.45
12	I	103	SPO	C21-C22	3.94	1.55	1.43
12	M	405	SPO	C20-C19	3.94	1.55	1.43
12	0	102	SPO	C26-C27	3.94	1.55	1.43
12	D	104	SPO	C21-C22	3.93	1.55	1.43
12	Q	102	SPO	C10-C9	3.93	1.55	1.43
12	I	104	SPO	C26-C27	3.92	1.55	1.43
12	F	103	SPO	C26-C27	3.92	1.55	1.43
13	M	406	CDL	OB6-CB5	3.92	1.45	1.34
12	A	603	SPO	C10-C9	3.91	1.55	1.43
12	U	103	SPO	C26-C27	3.91	1.55	1.43
12	S	103	SPO	C26-C27	3.91	1.55	1.43
12	D	102	SPO	C10-C9	3.91	1.55	1.43
12	R	101	SPO	C16-C17	3.87	1.54	1.45
12	D	103	SPO	C6-C7	3.87	1.54	1.45
12	I	103	SPO	C6-C7	3.85	1.54	1.45
12	9	102	SPO	C10-C9	3.85	1.55	1.43
12	R	103	SPO	C25-C23	3.84	1.54	1.45
12	R	103	SPO	C20-C19	3.84	1.55	1.43
12	Q	102	SPO	C26-C27	3.84	1.55	1.43
12	I	103	SPO	C25-C23	3.83	1.54	1.45
12	E	102	SPO	C26-C27	3.83	1.55	1.43
12	S	103	SPO	C21-C22	3.83	1.55	1.43
12	M	405	SPO	C21-C22	3.83	1.55	1.43
8	L	302	BPH	CBD-CGD	-3.82	1.47	1.52
12	8	101	SPO	C10-C9	3.82	1.55	1.43
12	M	405	SPO	C15-C14	3.81	1.55	1.43
12	M	405	SPO	C10-C9	3.81	1.55	1.43
12	A	603	SPO	C21-C22	3.81	1.55	1.43
12	D	102	SPO	C21-C22	3.80	1.55	1.43
12	F	103	SPO	C10-C9	3.80	1.55	1.43
12	R	103	SPO	C26-C27	3.80	1.55	1.43
12	D	102	SPO	C20-C19	3.79	1.55	1.43
12	E	102	SPO	C10-C9	3.79	1.55	1.43
12	A	603	SPO	C20-C19	3.79	1.55	1.43
12	P	102	SPO	C26-C27	3.78	1.55	1.43
12	E	102	SPO	C4-C5	3.77	1.56	1.50
12	P	101	SPO	C26-C27	3.75	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	102	SPO	C25-C23	3.74	1.54	1.45
12	A	603	SPO	C25-C23	3.74	1.54	1.45
12	K	103	SPO	C16-C17	3.74	1.54	1.45
12	D	104	SPO	C26-C27	3.74	1.55	1.43
12	R	101	SPO	C25-C23	3.73	1.54	1.45
12	D	103	SPO	C26-C27	3.72	1.55	1.43
12	F	103	SPO	C21-C22	3.72	1.55	1.43
12	U	103	SPO	C6-C7	3.72	1.53	1.45
12	D	103	SPO	C21-C22	3.72	1.55	1.43
12	8	101	SPO	C15-C14	3.72	1.55	1.43
12	E	102	SPO	C21-C22	3.72	1.55	1.43
12	U	103	SPO	C21-C22	3.72	1.55	1.43
12	8	101	SPO	C25-C23	3.70	1.53	1.45
12	P	101	SPO	C10-C9	3.69	1.54	1.43
12	D	103	SPO	C11-C12	3.66	1.53	1.45
12	D	104	SPO	C10-C9	3.65	1.54	1.43
12	I	104	SPO	C20-C19	3.64	1.54	1.43
12	9	102	SPO	C6-C7	3.64	1.53	1.45
12	S	103	SPO	C6-C7	3.63	1.53	1.45
12	K	103	SPO	C10-C9	3.60	1.54	1.43
12	0	102	SPO	C16-C17	3.59	1.53	1.45
12	D	103	SPO	C10-C9	3.57	1.54	1.43
12	P	101	SPO	C21-C22	3.57	1.54	1.43
12	K	103	SPO	C26-C27	3.57	1.54	1.43
12	S	103	SPO	C25-C23	3.56	1.53	1.45
9	L	303	PC1	O31-C31	3.55	1.43	1.33
12	R	101	SPO	C10-C9	3.53	1.54	1.43
12	M	405	SPO	C26-C27	3.53	1.54	1.43
12	P	101	SPO	C16-C17	3.52	1.53	1.45
12	8	101	SPO	C4-C5	3.52	1.55	1.50
12	Q	102	SPO	C6-C7	3.51	1.53	1.45
12	I	104	SPO	C10-C9	3.50	1.54	1.43
12	M	405	SPO	C4-C5	3.50	1.55	1.50
12	F	103	SPO	C6-C7	3.50	1.53	1.45
12	U	103	SPO	C4-C5	3.50	1.55	1.50
12	0	101	SPO	C25-C23	3.49	1.53	1.45
12	I	104	SPO	C21-C22	3.47	1.54	1.43
12	R	101	SPO	C6-C7	3.47	1.53	1.45
12	D	104	SPO	C6-C7	3.45	1.53	1.45
12	U	103	SPO	C25-C23	3.42	1.53	1.45
12	M	405	SPO	C16-C17	3.41	1.53	1.45
12	R	101	SPO	C4-C5	3.41	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	404	U10	C4-C5	-3.41	1.39	1.48
12	8	101	SPO	C26-C27	3.39	1.53	1.43
12	0	102	SPO	C25-C23	3.38	1.53	1.45
12	K	103	SPO	C21-C22	3.38	1.53	1.43
12	P	102	SPO	C25-C23	3.37	1.53	1.45
12	K	102	SPO	C4-C5	3.36	1.55	1.50
12	M	405	SPO	C6-C7	3.34	1.53	1.45
12	Q	102	SPO	C21-C22	3.32	1.53	1.43
12	K	103	SPO	C6-C7	3.31	1.53	1.45
12	F	103	SPO	C25-C23	3.31	1.53	1.45
12	P	101	SPO	C25-C23	3.30	1.53	1.45
12	D	103	SPO	C25-C23	3.29	1.53	1.45
12	D	104	SPO	C25-C23	3.28	1.53	1.45
12	E	102	SPO	C25-C23	3.28	1.53	1.45
12	S	103	SPO	C4-C5	3.26	1.55	1.50
12	D	103	SPO	C4-C5	3.25	1.55	1.50
10	L	304	U10	C4-C5	-3.24	1.39	1.48
10	M	404	U10	C3-C2	-3.24	1.39	1.48
12	9	102	SPO	C4-C5	3.24	1.55	1.50
7	I	101	BCL	MG-NC	3.23	2.14	2.06
9	H	1102	PC1	O31-C31	3.23	1.42	1.33
12	8	101	SPO	C6-C7	3.23	1.52	1.45
7	9	101	BCL	MG-NC	3.23	2.13	2.06
7	K	101	BCL	MG-NC	3.23	2.13	2.06
12	I	104	SPO	C4-C5	3.22	1.55	1.50
7	2	101	BCL	MG-NC	3.21	2.13	2.06
7	7	101	BCL	MG-NC	3.20	2.13	2.06
9	X	1501	PC1	O31-C31	3.18	1.42	1.33
12	I	103	SPO	C4-C5	3.18	1.55	1.50
7	F	101	BCL	MG-NC	3.17	2.13	2.06
13	M	406	CDL	OA8-CA7	3.17	1.42	1.33
12	E	102	SPO	C16-C17	3.15	1.52	1.45
7	U	101	BCL	MG-NC	3.15	2.13	2.06
7	D	101	BCL	MG-NC	3.15	2.13	2.06
7	A	602	BCL	MG-NC	3.15	2.13	2.06
12	A	603	SPO	C16-C17	3.14	1.52	1.45
7	S	101	BCL	MG-NC	3.14	2.13	2.06
12	D	102	SPO	C16-C17	3.14	1.52	1.45
12	K	103	SPO	C25-C23	3.14	1.52	1.45
12	K	103	SPO	C4-C5	3.13	1.55	1.50
7	O	101	BCL	MG-NC	3.13	2.13	2.06
12	Q	102	SPO	C4-C5	3.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	603	SPO	C26-C27	3.11	1.53	1.43
12	D	102	SPO	C26-C27	3.11	1.53	1.43
12	P	101	SPO	C4-C5	3.10	1.55	1.50
7	9	101	BCL	O1A-CGA	-3.08	1.13	1.22
12	D	102	SPO	C11-C12	3.07	1.52	1.45
12	A	603	SPO	C11-C12	3.07	1.52	1.45
13	M	406	CDL	OA6-CA4	-3.06	1.38	1.46
12	I	104	SPO	C6-C7	3.05	1.52	1.45
9	H	1101	PC1	O31-C31	3.04	1.42	1.33
12	0	102	SPO	C4-C5	3.04	1.55	1.50
9	A	601	PC1	O31-C31	3.04	1.42	1.33
12	I	104	SPO	C25-C23	3.02	1.52	1.45
7	E	101	BCL	MG-NC	3.01	2.13	2.06
7	F	102	BCL	MG-NC	3.01	2.13	2.06
7	O	102	BCL	MG-NC	3.01	2.13	2.06
7	8	102	BCL	MG-NC	3.01	2.13	2.06
7	R	102	BCL	MG-NC	3.01	2.13	2.06
7	9	103	BCL	MG-NC	3.01	2.13	2.06
7	N	101	BCL	MG-NC	3.01	2.13	2.06
7	A	605	BCL	MG-NC	3.01	2.13	2.06
7	S	102	BCL	MG-NC	3.01	2.13	2.06
7	U	102	BCL	MG-NC	3.01	2.13	2.06
7	I	102	BCL	MG-NC	3.01	2.13	2.06
12	P	102	SPO	C4-C5	3.00	1.54	1.50
10	L	304	U10	C3-C2	-3.00	1.40	1.48
7	W	101	BCL	MG-NC	2.99	2.13	2.06
7	O	101	BCL	O1A-CGA	-2.99	1.13	1.22
7	Q	101	BCL	MG-NC	2.98	2.13	2.06
13	M	406	CDL	OB8-CB7	2.98	1.42	1.33
7	I	101	BCL	O1A-CGA	-2.96	1.13	1.22
9	H	1103	PC1	O31-C31	2.96	1.42	1.33
9	A	604	PC1	O31-C31	2.96	1.42	1.33
12	0	101	SPO	C4-C5	2.96	1.54	1.50
7	1	101	BCL	MG-NC	2.94	2.13	2.06
12	Q	102	SPO	C25-C23	2.92	1.52	1.45
12	F	103	SPO	C4-C5	2.91	1.54	1.50
7	L	301	BCL	MG-NC	2.90	2.13	2.06
7	K	101	BCL	O1A-CGA	-2.89	1.14	1.22
10	L	304	U10	C6-C5	-2.86	1.38	1.46
9	H	1102	PC1	O21-C21	2.85	1.42	1.34
7	L	301	BCL	O1A-CGA	-2.85	1.14	1.22
9	X	1501	PC1	O21-C21	2.85	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	PC1	O21-C21	2.81	1.42	1.34
9	H	1103	PC1	O21-C21	2.81	1.42	1.34
9	A	604	PC1	O21-C21	2.81	1.42	1.34
12	M	405	SPO	C25-C23	2.81	1.52	1.45
10	M	404	U10	C6-C5	-2.80	1.38	1.46
7	C	101	BCL	MG-NC	2.79	2.12	2.06
9	A	601	PC1	O21-C2	-2.79	1.39	1.46
7	L	305	BCL	MG-NC	2.77	2.12	2.06
7	M	401	BCL	MG-NC	2.77	2.12	2.06
9	H	1101	PC1	O21-C2	-2.73	1.39	1.46
7	M	403	BCL	MG-NC	2.72	2.12	2.06
7	Q	101	BCL	O1A-CGA	-2.71	1.14	1.22
9	L	303	PC1	O21-C21	2.69	1.41	1.34
9	L	303	PC1	O21-C2	-2.69	1.39	1.46
12	D	104	SPO	C4-C5	2.67	1.54	1.50
9	H	1101	PC1	O21-C21	2.67	1.41	1.34
7	F	101	BCL	O1A-CGA	-2.65	1.14	1.22
7	L	305	BCL	O1A-CGA	-2.63	1.14	1.22
9	X	1501	PC1	O21-C2	-2.61	1.40	1.46
7	M	403	BCL	O1A-CGA	-2.60	1.14	1.22
13	M	406	CDL	C51-CB5	2.48	1.57	1.50
7	S	101	BCL	O1A-CGA	-2.46	1.15	1.22
9	H	1102	PC1	O21-C2	-2.45	1.40	1.46
7	F	101	BCL	O2A-CGA	-2.44	1.26	1.33
9	L	303	PC1	C12-C11	2.38	1.58	1.51
7	D	101	BCL	O1A-CGA	-2.38	1.15	1.22
7	A	602	BCL	O1A-CGA	-2.37	1.15	1.22
10	M	404	U10	C6-C1	2.37	1.39	1.35
12	P	101	SPO	C8-C7	2.34	1.55	1.50
13	M	406	CDL	OA6-CA5	2.33	1.40	1.34
10	M	404	U10	C1-C2	-2.28	1.39	1.47
9	H	1103	PC1	O21-C2	-2.27	1.40	1.46
9	A	604	PC1	O21-C2	-2.27	1.40	1.46
10	L	304	U10	C1-C2	-2.26	1.39	1.47
9	A	604	PC1	P-O13	2.22	1.68	1.59
9	H	1103	PC1	P-O13	2.22	1.68	1.59
7	2	101	BCL	OBD-CAD	2.18	1.25	1.22
7	A	602	BCL	O2A-CGA	-2.18	1.26	1.33
7	D	101	BCL	O2A-CGA	-2.18	1.27	1.33
12	8	101	SPO	C30-C28	2.14	1.55	1.51
9	X	1501	PC1	C12-C11	2.13	1.58	1.51
8	L	306	BPH	O1A-CGA	-2.13	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	304	U10	C6-C1	2.13	1.39	1.35
7	M	401	BCL	O1A-CGA	-2.13	1.16	1.22
7	1	101	BCL	OBD-CAD	2.11	1.25	1.22
8	L	302	BPH	O1A-CGA	-2.07	1.16	1.22
13	M	406	CDL	PA1-OA5	2.07	1.67	1.59
7	U	101	BCL	O1A-CGA	-2.07	1.16	1.22
9	X	1501	PC1	P-O13	2.07	1.67	1.59
7	1	101	BCL	C4B-NB	2.06	1.37	1.35
7	N	101	BCL	O1A-CGA	-2.04	1.16	1.22
7	E	101	BCL	O1A-CGA	-2.04	1.16	1.22
7	F	102	BCL	O1A-CGA	-2.04	1.16	1.22
7	S	102	BCL	O1A-CGA	-2.04	1.16	1.22
7	A	605	BCL	O1A-CGA	-2.04	1.16	1.22
7	I	102	BCL	O1A-CGA	-2.04	1.16	1.22
7	8	102	BCL	O1A-CGA	-2.04	1.16	1.22
7	O	102	BCL	O1A-CGA	-2.04	1.16	1.22
7	R	102	BCL	O1A-CGA	-2.04	1.16	1.22
7	U	102	BCL	O1A-CGA	-2.03	1.16	1.22
7	9	103	BCL	O1A-CGA	-2.03	1.16	1.22
9	L	303	PC1	P-O13	2.01	1.67	1.59

All (1062) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	0	102	SPO	C8-C7-C9	-14.15	103.10	122.92
12	E	102	SPO	C20-C19-C17	-13.42	108.16	127.31
12	P	102	SPO	C18-C17-C19	-13.41	104.14	122.92
12	D	103	SPO	C15-C14-C12	-13.25	108.41	127.31
12	P	102	SPO	C13-C12-C14	-13.23	104.40	122.92
12	0	102	SPO	C15-C14-C12	-12.45	109.54	127.31
12	U	103	SPO	C15-C14-C12	-12.40	109.61	127.31
12	K	102	SPO	C13-C12-C14	-12.14	105.91	122.92
12	E	102	SPO	C8-C7-C9	-12.13	105.94	122.92
12	E	102	SPO	C15-C14-C12	-12.07	110.08	127.31
12	P	101	SPO	C10-C9-C7	-12.00	110.19	127.31
12	D	103	SPO	C8-C7-C9	-12.00	106.12	122.92
12	P	101	SPO	C18-C17-C19	-11.80	106.39	122.92
12	K	102	SPO	C8-C7-C9	-11.70	106.53	122.92
12	U	103	SPO	C13-C12-C14	-11.69	106.54	122.92
12	D	103	SPO	C20-C19-C17	-11.51	110.88	127.31
12	I	104	SPO	C10-C9-C7	-11.51	110.88	127.31
12	P	101	SPO	C6-C7-C9	-11.47	101.33	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	405	SPO	C15-C14-C12	-11.47	110.94	127.31
12	R	101	SPO	C15-C14-C12	-11.44	110.98	127.31
12	P	101	SPO	C13-C12-C14	-11.08	107.40	122.92
12	E	102	SPO	C10-C9-C7	-10.98	111.64	127.31
12	P	101	SPO	C20-C19-C17	-10.90	111.75	127.31
12	I	103	SPO	C8-C7-C9	-10.86	107.71	122.92
12	E	102	SPO	C24-C23-C22	-10.79	107.81	122.92
12	Q	102	SPO	C20-C19-C17	-10.75	111.97	127.31
12	I	103	SPO	C13-C12-C14	-10.66	107.99	122.92
12	D	103	SPO	C10-C9-C7	-10.64	112.13	127.31
12	K	103	SPO	C10-C9-C7	-10.60	112.17	127.31
12	0	101	SPO	C13-C12-C14	-10.60	108.08	122.92
12	U	103	SPO	C10-C9-C7	-10.59	112.20	127.31
12	8	101	SPO	C10-C9-C7	-10.52	112.30	127.31
12	D	102	SPO	C24-C23-C22	-10.48	108.25	122.92
12	A	603	SPO	C24-C23-C22	-10.47	108.25	122.92
12	D	104	SPO	C13-C12-C14	-10.43	108.32	122.92
12	D	102	SPO	C18-C17-C19	-10.42	108.33	122.92
12	A	603	SPO	C18-C17-C19	-10.42	108.33	122.92
12	F	103	SPO	C18-C17-C19	-10.33	108.45	122.92
12	0	101	SPO	C18-C17-C19	-10.27	108.53	122.92
12	P	101	SPO	C21-C22-C23	-10.26	112.67	127.31
12	S	103	SPO	C8-C7-C9	-10.24	108.58	122.92
12	R	103	SPO	C15-C14-C12	-10.03	113.00	127.31
12	P	102	SPO	C20-C19-C17	-9.98	113.06	127.31
12	0	101	SPO	C11-C12-C14	-9.96	103.66	118.94
12	K	103	SPO	C20-C19-C17	-9.88	113.21	127.31
12	S	103	SPO	C20-C19-C17	-9.87	113.22	127.31
12	U	103	SPO	C8-C7-C9	-9.85	109.12	122.92
12	S	103	SPO	C10-C9-C7	-9.81	113.31	127.31
12	D	104	SPO	C10-C9-C7	-9.76	113.38	127.31
12	M	405	SPO	C10-C9-C7	-9.75	113.39	127.31
12	E	102	SPO	C18-C17-C19	-9.69	109.35	122.92
12	P	102	SPO	C8-C7-C9	-9.69	109.36	122.92
12	K	103	SPO	C18-C17-C19	-9.68	109.36	122.92
12	K	102	SPO	C15-C14-C12	-9.63	113.57	127.31
12	A	603	SPO	C10-C9-C7	-9.59	113.62	127.31
12	D	102	SPO	C10-C9-C7	-9.59	113.62	127.31
12	K	102	SPO	C18-C17-C19	-9.55	109.55	122.92
12	P	102	SPO	C24-C23-C22	-9.53	109.57	122.92
12	K	103	SPO	C8-C7-C9	-9.47	109.66	122.92
12	U	103	SPO	C13-C12-C11	-9.46	103.16	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Q	102	SPO	C15-C14-C12	-9.43	113.85	127.31
12	R	103	SPO	C8-C7-C9	-9.41	109.75	122.92
12	R	101	SPO	C24-C23-C22	-9.34	109.84	122.92
12	D	103	SPO	C13-C12-C14	-9.33	109.86	122.92
12	8	101	SPO	C24-C23-C22	-9.20	110.04	122.92
12	D	102	SPO	C11-C12-C14	-9.17	104.87	118.94
12	A	603	SPO	C11-C12-C14	-9.17	104.88	118.94
12	0	102	SPO	C13-C12-C14	-9.13	110.14	122.92
12	M	405	SPO	C20-C19-C17	-9.12	114.29	127.31
12	D	104	SPO	C8-C7-C9	-9.10	110.17	122.92
12	D	104	SPO	C18-C17-C19	-9.10	110.18	122.92
12	I	103	SPO	C10-C9-C7	-9.05	114.39	127.31
12	F	103	SPO	C13-C12-C14	-9.01	110.30	122.92
12	S	103	SPO	C18-C17-C19	-8.98	110.34	122.92
12	I	104	SPO	C18-C17-C19	-8.83	110.56	122.92
12	P	101	SPO	C18-C17-C16	-8.82	104.19	118.08
12	0	101	SPO	C24-C23-C22	-8.80	110.59	122.92
12	D	104	SPO	C24-C23-C22	-8.79	110.60	122.92
12	E	102	SPO	C21-C22-C23	-8.79	114.76	127.31
12	F	103	SPO	C8-C7-C9	-8.79	110.61	122.92
12	R	103	SPO	C18-C17-C19	-8.77	110.63	122.92
12	I	104	SPO	C21-C22-C23	-8.75	114.82	127.31
12	A	603	SPO	C21-C22-C23	-8.75	114.82	127.31
12	D	102	SPO	C21-C22-C23	-8.75	114.83	127.31
12	K	103	SPO	C15-C14-C12	-8.74	114.83	127.31
12	F	103	SPO	C10-C9-C7	-8.73	114.85	127.31
12	M	405	SPO	C21-C22-C23	-8.69	114.91	127.31
12	P	102	SPO	C21-C22-C23	-8.63	114.99	127.31
12	A	603	SPO	C20-C19-C17	-8.63	115.00	127.31
12	D	102	SPO	C20-C19-C17	-8.62	115.00	127.31
12	P	101	SPO	C24-C23-C22	-8.57	110.92	122.92
12	K	103	SPO	C21-C22-C23	-8.56	115.10	127.31
12	R	103	SPO	C13-C12-C14	-8.56	110.94	122.92
12	U	103	SPO	C20-C19-C17	-8.55	115.11	127.31
12	I	103	SPO	C18-C17-C19	-8.53	110.97	122.92
12	R	101	SPO	C8-C7-C9	-8.52	110.98	122.92
12	D	103	SPO	C25-C23-C22	-8.49	105.91	118.94
12	9	102	SPO	C8-C7-C9	-8.49	111.03	122.92
12	R	101	SPO	C13-C12-C14	-8.47	111.06	122.92
12	R	103	SPO	C21-C22-C23	-8.46	115.23	127.31
12	M	405	SPO	C13-C12-C14	-8.45	111.08	122.92
12	9	102	SPO	C21-C22-C23	-8.41	115.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	603	SPO	C8-C7-C9	-8.41	111.15	122.92
12	D	102	SPO	C8-C7-C9	-8.40	111.15	122.92
12	E	102	SPO	C13-C12-C14	-8.40	111.15	122.92
12	I	104	SPO	C8-C7-C9	-8.40	111.15	122.92
12	S	103	SPO	C24-C23-C22	-8.40	111.16	122.92
12	M	405	SPO	C8-C7-C9	-8.39	111.17	122.92
12	D	103	SPO	C21-C22-C23	-8.39	115.34	127.31
12	F	103	SPO	C6-C7-C9	-8.36	106.11	118.94
12	F	103	SPO	C20-C19-C17	-8.31	115.44	127.31
12	R	101	SPO	C21-C22-C23	-8.28	115.49	127.31
12	P	102	SPO	C10-C9-C7	-8.26	115.52	127.31
12	K	102	SPO	C10-C9-C7	-8.25	115.53	127.31
12	0	102	SPO	C9-C10-C11	8.25	148.97	123.22
12	8	101	SPO	C8-C7-C9	-8.25	111.37	122.92
12	9	102	SPO	C18-C17-C19	-8.24	111.38	122.92
12	U	103	SPO	C18-C17-C19	-8.23	111.39	122.92
12	9	102	SPO	C13-C12-C14	-8.22	111.40	122.92
12	R	101	SPO	C20-C19-C17	-8.22	115.58	127.31
12	D	104	SPO	C6-C7-C9	-8.21	106.35	118.94
12	Q	102	SPO	C25-C23-C22	-8.18	106.39	118.94
12	Q	102	SPO	C8-C7-C9	-8.17	111.48	122.92
12	F	103	SPO	C11-C12-C14	-8.16	106.43	118.94
12	0	101	SPO	C21-C22-C23	-8.13	115.71	127.31
12	K	102	SPO	C21-C22-C23	-8.10	115.75	127.31
12	R	101	SPO	C6-C7-C9	-8.09	106.53	118.94
12	S	103	SPO	C21-C22-C23	-8.07	115.79	127.31
12	Q	102	SPO	C18-C17-C19	-8.07	111.61	122.92
12	D	102	SPO	C15-C14-C12	-8.01	115.88	127.31
12	A	603	SPO	C15-C14-C12	-8.01	115.88	127.31
12	K	102	SPO	C6-C7-C9	-7.98	106.70	118.94
12	S	103	SPO	C8-C7-C6	-7.95	105.55	118.08
12	D	104	SPO	C15-C14-C12	-7.95	115.97	127.31
12	M	405	SPO	C25-C23-C22	-7.93	106.78	118.94
12	D	103	SPO	C11-C12-C14	-7.93	106.78	118.94
12	F	103	SPO	C24-C23-C22	-7.90	111.86	122.92
12	D	103	SPO	C13-C12-C11	-7.82	105.76	118.08
12	R	103	SPO	C24-C23-C22	-7.80	112.00	122.92
12	8	101	SPO	C25-C23-C22	-7.79	106.99	118.94
12	Q	102	SPO	C13-C12-C14	-7.77	112.04	122.92
12	D	103	SPO	C24-C23-C22	-7.75	112.07	122.92
12	0	101	SPO	C8-C7-C9	-7.71	112.12	122.92
12	9	102	SPO	C24-C23-C22	-7.68	112.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	104	SPO	C24-C23-C22	-7.67	112.18	122.92
12	8	101	SPO	C31-C32-C33	-7.60	109.35	127.66
12	Q	102	SPO	C6-C7-C9	-7.60	107.28	118.94
12	I	103	SPO	C24-C23-C22	-7.56	112.33	122.92
12	8	101	SPO	C18-C17-C19	-7.55	112.34	122.92
12	D	104	SPO	C21-C22-C23	-7.53	116.57	127.31
12	U	103	SPO	C24-C23-C22	-7.48	112.44	122.92
12	A	603	SPO	C13-C12-C14	-7.46	112.47	122.92
12	D	102	SPO	C13-C12-C14	-7.46	112.47	122.92
12	I	103	SPO	C21-C22-C23	-7.45	116.68	127.31
12	P	102	SPO	C24-C23-C25	-7.43	106.37	118.08
12	0	102	SPO	C18-C17-C19	-7.43	112.52	122.92
12	R	101	SPO	C18-C17-C19	-7.40	112.56	122.92
12	I	103	SPO	C15-C14-C12	-7.38	116.78	127.31
12	0	102	SPO	C21-C22-C23	-7.34	116.83	127.31
12	U	103	SPO	C21-C22-C23	-7.32	116.87	127.31
12	8	101	SPO	C20-C19-C17	-7.31	116.88	127.31
12	M	405	SPO	C18-C17-C19	-7.29	112.71	122.92
12	I	104	SPO	C15-C14-C12	-7.29	116.91	127.31
12	8	101	SPO	C15-C14-C12	-7.29	116.91	127.31
12	0	102	SPO	C24-C23-C25	-7.24	106.67	118.08
12	E	102	SPO	C31-C32-C33	-7.22	110.27	127.66
12	8	101	SPO	C24-C23-C25	-7.18	106.77	118.08
12	I	104	SPO	C11-C12-C14	-7.17	107.94	118.94
12	K	103	SPO	C31-C32-C33	-7.11	110.53	127.66
12	0	101	SPO	C20-C19-C17	-7.08	117.20	127.31
12	I	104	SPO	C6-C7-C9	-7.07	108.09	118.94
12	D	103	SPO	C35-C33-C32	-7.06	106.82	121.12
12	P	101	SPO	C25-C23-C22	-7.03	108.15	118.94
12	R	103	SPO	C25-C23-C22	-7.02	108.17	118.94
12	Q	102	SPO	C24-C23-C22	-7.02	113.09	122.92
12	D	104	SPO	C11-C12-C14	-6.98	108.23	118.94
12	K	103	SPO	C11-C12-C14	-6.97	108.25	118.94
12	0	102	SPO	C5-C6-C7	6.95	136.40	125.89
12	R	103	SPO	C10-C9-C7	-6.93	117.42	127.31
12	9	102	SPO	C31-C32-C33	-6.92	110.99	127.66
12	E	102	SPO	C18-C17-C16	-6.89	107.22	118.08
12	S	103	SPO	C24-C23-C25	-6.88	107.23	118.08
12	D	104	SPO	C35-C33-C32	-6.87	107.20	121.12
12	0	102	SPO	C6-C7-C9	-6.87	108.40	118.94
12	S	103	SPO	C31-C32-C33	-6.87	111.12	127.66
12	I	104	SPO	C20-C19-C17	-6.82	117.57	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	0	102	SPO	C24-C23-C22	-6.81	113.38	122.92
12	A	603	SPO	C34-C33-C32	-6.81	106.21	123.68
12	D	102	SPO	C34-C33-C32	-6.81	106.21	123.68
12	8	101	SPO	C21-C22-C23	-6.78	117.64	127.31
12	I	104	SPO	C25-C23-C22	-6.77	108.55	118.94
12	K	103	SPO	C24-C23-C22	-6.75	113.46	122.92
12	I	104	SPO	C35-C33-C32	-6.75	107.47	121.12
12	K	102	SPO	C20-C19-C17	-6.74	117.69	127.31
12	0	101	SPO	C24-C23-C25	-6.73	107.47	118.08
12	F	103	SPO	C34-C33-C32	-6.73	106.42	123.68
12	Q	102	SPO	C10-C9-C7	-6.69	117.76	127.31
12	S	103	SPO	C6-C7-C9	-6.68	108.69	118.94
12	K	102	SPO	C24-C23-C22	-6.64	113.62	122.92
12	D	103	SPO	C18-C17-C19	-6.64	113.62	122.92
12	F	103	SPO	C15-C14-C12	-6.63	117.85	127.31
12	K	102	SPO	C13-C12-C11	-6.62	107.64	118.08
12	K	103	SPO	C13-C12-C14	-6.62	113.65	122.92
12	8	101	SPO	C18-C17-C16	-6.59	107.70	118.08
12	D	104	SPO	C20-C19-C17	-6.57	117.93	127.31
12	9	102	SPO	C20-C19-C17	-6.57	117.94	127.31
12	0	101	SPO	C31-C32-C33	-6.56	111.85	127.66
12	I	104	SPO	C13-C12-C14	-6.56	113.74	122.92
12	I	103	SPO	C31-C32-C33	-6.55	111.88	127.66
12	9	102	SPO	C15-C14-C12	-6.55	117.97	127.31
12	0	102	SPO	C20-C19-C17	-6.55	117.97	127.31
12	F	103	SPO	C25-C23-C22	-6.53	108.92	118.94
12	D	104	SPO	C24-C23-C25	-6.53	107.79	118.08
12	A	603	SPO	C6-C7-C9	-6.51	108.95	118.94
12	D	102	SPO	C6-C7-C9	-6.51	108.95	118.94
12	8	101	SPO	C6-C7-C9	-6.50	108.96	118.94
12	A	603	SPO	C25-C23-C22	-6.48	108.99	118.94
12	D	102	SPO	C25-C23-C22	-6.48	109.00	118.94
12	9	102	SPO	C6-C7-C9	-6.48	109.00	118.94
12	P	102	SPO	C34-C33-C32	-6.45	107.12	123.68
12	R	101	SPO	C10-C9-C7	-6.40	118.18	127.31
12	K	103	SPO	C6-C7-C9	-6.38	109.16	118.94
12	0	102	SPO	C10-C11-C12	6.37	144.30	126.42
12	K	103	SPO	C25-C23-C22	-6.36	109.18	118.94
12	F	103	SPO	C21-C22-C23	-6.36	118.23	127.31
12	K	103	SPO	C24-C23-C25	-6.35	108.07	118.08
12	8	101	SPO	C11-C12-C14	-6.34	109.22	118.94
12	E	102	SPO	C6-C7-C9	-6.32	109.25	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	405	SPO	C24-C23-C22	-6.31	114.09	122.92
12	R	103	SPO	C8-C7-C6	-6.25	108.23	118.08
12	9	102	SPO	C18-C17-C16	-6.24	108.24	118.08
12	U	103	SPO	C31-C32-C33	-6.23	112.66	127.66
12	0	102	SPO	C35-C33-C32	-6.20	108.57	121.12
12	I	103	SPO	C20-C19-C17	-6.20	118.46	127.31
12	K	102	SPO	C31-C32-C33	-6.19	112.75	127.66
12	A	603	SPO	C35-C33-C32	-6.19	108.59	121.12
12	D	102	SPO	C35-C33-C32	-6.19	108.59	121.12
12	Q	102	SPO	C18-C17-C16	-6.19	108.33	118.08
12	Q	102	SPO	C31-C32-C33	-6.13	112.90	127.66
12	D	104	SPO	C31-C32-C33	-6.13	112.91	127.66
12	9	102	SPO	C10-C9-C7	-6.12	118.58	127.31
12	Q	102	SPO	C34-C33-C32	-6.11	107.99	123.68
12	M	405	SPO	C6-C7-C9	-6.10	109.58	118.94
12	0	102	SPO	C18-C17-C16	-6.08	108.49	118.08
12	I	103	SPO	C11-C12-C14	-6.06	109.64	118.94
12	S	103	SPO	C15-C14-C12	-6.06	118.66	127.31
12	U	103	SPO	C24-C23-C25	-6.05	108.54	118.08
12	R	101	SPO	C24-C23-C25	-6.02	108.60	118.08
12	F	103	SPO	C31-C32-C33	-6.00	113.21	127.66
12	A	603	SPO	C18-C17-C16	-6.00	108.62	118.08
12	U	103	SPO	C36-C37-C38	-6.00	107.25	127.75
12	D	102	SPO	C18-C17-C16	-6.00	108.63	118.08
12	P	101	SPO	C24-C23-C25	-5.99	108.64	118.08
12	8	101	SPO	C35-C33-C32	-5.99	109.00	121.12
12	U	103	SPO	C16-C17-C19	-5.98	109.77	118.94
12	R	101	SPO	C31-C32-C33	-5.97	113.28	127.66
12	D	103	SPO	C18-C17-C16	-5.95	108.70	118.08
12	S	103	SPO	C11-C12-C14	-5.94	109.82	118.94
12	R	103	SPO	C20-C19-C17	-5.94	118.84	127.31
12	Q	102	SPO	C21-C22-C23	-5.93	118.85	127.31
12	8	101	SPO	C13-C12-C11	-5.93	108.74	118.08
12	R	103	SPO	C13-C12-C11	-5.91	108.77	118.08
12	R	101	SPO	C35-C33-C32	-5.85	109.28	121.12
12	D	103	SPO	C6-C7-C9	-5.83	109.99	118.94
12	E	102	SPO	C35-C33-C32	-5.82	109.35	121.12
12	S	103	SPO	C13-C12-C14	-5.81	114.78	122.92
12	K	103	SPO	C34-C33-C32	-5.81	108.76	123.68
12	0	102	SPO	C16-C17-C19	-5.80	110.05	118.94
12	U	103	SPO	C25-C23-C22	-5.79	110.05	118.94
12	Q	102	SPO	C24-C23-C25	-5.79	108.96	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	8	101	SPO	C30-C28-C27	-5.78	104.47	121.98
12	I	103	SPO	C6-C7-C9	-5.78	110.07	118.94
12	I	104	SPO	C30-C28-C27	-5.78	104.49	121.98
12	Q	102	SPO	C11-C12-C14	-5.76	110.11	118.94
12	M	405	SPO	C31-C32-C33	-5.75	113.82	127.66
12	M	405	SPO	C35-C33-C32	-5.75	109.49	121.12
12	P	101	SPO	C35-C33-C32	-5.70	109.59	121.12
12	E	102	SPO	C5-C6-C7	5.68	134.47	125.89
12	E	102	SPO	C34-C33-C32	-5.68	109.11	123.68
12	F	103	SPO	C18-C17-C16	-5.66	109.16	118.08
12	9	102	SPO	C24-C23-C25	-5.64	109.19	118.08
12	U	103	SPO	C6-C7-C9	-5.62	110.32	118.94
12	0	101	SPO	C35-C33-C32	-5.61	109.76	121.12
12	0	101	SPO	C6-C7-C9	-5.61	110.34	118.94
12	F	103	SPO	C30-C28-C27	-5.61	105.00	121.98
12	I	104	SPO	C16-C17-C19	-5.57	110.39	118.94
12	A	603	SPO	C16-C17-C19	-5.57	110.40	118.94
12	D	102	SPO	C16-C17-C19	-5.57	110.40	118.94
12	9	102	SPO	C34-C33-C32	-5.56	109.41	123.68
12	D	102	SPO	C31-C32-C33	-5.56	114.28	127.66
12	A	603	SPO	C31-C32-C33	-5.56	114.28	127.66
12	A	603	SPO	C24-C23-C25	-5.55	109.33	118.08
12	D	102	SPO	C24-C23-C25	-5.55	109.33	118.08
12	P	101	SPO	C31-C32-C33	-5.55	114.30	127.66
12	0	101	SPO	C15-C14-C12	-5.54	119.41	127.31
12	U	103	SPO	C5-C6-C7	-5.54	117.53	125.89
12	M	405	SPO	C16-C17-C19	-5.54	110.45	118.94
12	I	104	SPO	C31-C32-C33	-5.52	114.36	127.66
12	Q	102	SPO	C30-C28-C27	-5.51	105.31	121.98
12	Q	102	SPO	C35-C33-C32	-5.50	109.98	121.12
12	S	103	SPO	C35-C33-C32	-5.50	109.98	121.12
12	P	101	SPO	C15-C14-C12	-5.46	119.52	127.31
7	L	305	BCL	C1-C2-C3	5.46	135.48	126.04
12	9	102	SPO	C35-C33-C32	-5.44	110.10	121.12
12	R	101	SPO	C11-C12-C14	-5.42	110.62	118.94
12	U	103	SPO	C34-C33-C32	-5.40	109.82	123.68
12	U	103	SPO	C34-C33-C35	-5.40	106.18	115.27
12	K	103	SPO	C35-C33-C32	-5.39	110.21	121.12
12	R	103	SPO	C31-C32-C33	-5.38	114.70	127.66
12	R	103	SPO	C18-C17-C16	-5.38	109.60	118.08
12	A	603	SPO	C8-C7-C6	-5.34	109.67	118.08
12	D	102	SPO	C8-C7-C6	-5.34	109.67	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	0	102	SPO	C31-C32-C33	-5.33	114.81	127.66
9	H	1103	PC1	O21-C21-C22	5.33	122.98	111.50
9	A	604	PC1	O21-C21-C22	5.33	122.98	111.50
12	M	405	SPO	C18-C17-C16	-5.32	109.69	118.08
12	M	405	SPO	C24-C23-C25	-5.32	109.70	118.08
12	9	102	SPO	C11-C12-C14	-5.31	110.79	118.94
12	K	102	SPO	C35-C33-C32	-5.31	110.37	121.12
12	K	103	SPO	C13-C12-C11	-5.31	109.71	118.08
12	D	102	SPO	C13-C12-C11	-5.28	109.75	118.08
12	K	103	SPO	C8-C7-C6	-5.28	109.76	118.08
12	A	603	SPO	C13-C12-C11	-5.28	109.76	118.08
12	R	103	SPO	C34-C33-C32	-5.28	110.14	123.68
12	E	102	SPO	C13-C12-C11	-5.27	109.78	118.08
12	I	104	SPO	C24-C23-C25	-5.26	109.79	118.08
12	0	102	SPO	C25-C23-C22	-5.26	110.87	118.94
12	I	104	SPO	C34-C33-C32	-5.25	110.21	123.68
12	I	103	SPO	C25-C23-C22	-5.24	110.90	118.94
12	8	101	SPO	C34-C33-C32	-5.24	110.24	123.68
12	D	103	SPO	C34-C33-C32	-5.24	110.24	123.68
12	I	103	SPO	C34-C33-C32	-5.24	110.24	123.68
12	D	104	SPO	C18-C17-C16	-5.23	109.83	118.08
12	K	102	SPO	C25-C23-C22	-5.23	110.92	118.94
12	8	101	SPO	C8-C7-C6	-5.22	109.85	118.08
12	R	103	SPO	C35-C33-C32	-5.19	110.62	121.12
12	D	103	SPO	C8-C7-C6	-5.18	109.92	118.08
12	I	104	SPO	C8-C7-C6	-5.18	109.92	118.08
12	U	103	SPO	C8-C7-C6	-5.15	109.96	118.08
12	S	103	SPO	C34-C33-C32	-5.15	110.47	123.68
12	I	103	SPO	C39-C38-C37	-5.14	107.80	122.65
12	K	102	SPO	C34-C33-C32	-5.12	110.54	123.68
12	D	103	SPO	C31-C32-C33	-5.09	115.40	127.66
12	P	101	SPO	C34-C33-C32	-5.08	110.64	123.68
12	M	405	SPO	C30-C28-C27	-5.07	106.64	121.98
12	8	101	SPO	C13-C12-C14	-5.06	115.83	122.92
12	0	101	SPO	C34-C33-C32	-5.06	110.71	123.68
12	R	101	SPO	C34-C33-C32	-5.04	110.76	123.68
12	P	101	SPO	C8-C7-C9	-5.03	115.88	122.92
12	0	101	SPO	C18-C17-C16	-4.99	110.21	118.08
12	S	103	SPO	C36-C37-C38	-4.98	110.72	127.75
12	D	104	SPO	C39-C38-C37	-4.98	108.25	122.65
12	D	104	SPO	C34-C33-C32	-4.97	110.92	123.68
12	P	102	SPO	C31-C32-C33	-4.97	115.70	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	103	SPO	C36-C37-C38	-4.96	110.79	127.75
7	2	101	BCL	CAD-C3D-C4D	-4.96	105.70	108.47
12	0	101	SPO	C9-C10-C11	4.96	138.69	123.22
12	R	101	SPO	C18-C17-C16	-4.95	110.28	118.08
12	M	405	SPO	C8-C7-C6	-4.94	110.30	118.08
12	F	103	SPO	C8-C7-C6	-4.94	110.30	118.08
12	Q	102	SPO	C13-C12-C11	-4.94	110.30	118.08
12	D	102	SPO	C36-C37-C38	-4.93	110.89	127.75
12	A	603	SPO	C36-C37-C38	-4.93	110.89	127.75
12	I	104	SPO	C13-C12-C11	-4.93	110.31	118.08
12	D	102	SPO	C29-C28-C30	-4.93	106.98	115.27
12	A	603	SPO	C29-C28-C30	-4.93	106.98	115.27
12	0	102	SPO	C34-C33-C32	-4.92	111.06	123.68
12	U	103	SPO	C29-C28-C27	-4.91	109.91	122.59
12	K	102	SPO	C30-C28-C27	-4.91	107.13	121.98
12	9	102	SPO	C25-C23-C22	-4.90	111.42	118.94
12	0	101	SPO	C39-C38-C37	-4.89	108.51	122.65
12	I	103	SPO	C24-C23-C25	-4.89	110.37	118.08
12	M	405	SPO	C29-C28-C27	-4.89	109.98	122.59
12	F	103	SPO	C24-C23-C25	-4.89	110.38	118.08
12	9	102	SPO	C16-C17-C19	-4.86	111.48	118.94
12	D	103	SPO	C40-C38-C37	-4.85	108.62	122.65
12	D	103	SPO	C24-C23-C25	-4.85	110.44	118.08
12	R	103	SPO	C16-C17-C19	-4.85	111.50	118.94
12	K	102	SPO	C40-C38-C37	-4.85	108.64	122.65
12	E	102	SPO	C24-C23-C25	-4.84	110.45	118.08
12	P	102	SPO	C29-C28-C27	-4.84	110.10	122.59
12	M	405	SPO	C36-C37-C38	-4.84	111.22	127.75
12	S	103	SPO	C25-C23-C22	-4.84	111.52	118.94
12	A	603	SPO	C30-C28-C27	-4.83	107.35	121.98
12	D	102	SPO	C30-C28-C27	-4.83	107.36	121.98
12	Q	102	SPO	C29-C28-C27	-4.83	110.14	122.59
12	E	102	SPO	C30-C28-C27	-4.81	107.41	121.98
12	9	102	SPO	C36-C37-C38	-4.81	111.31	127.75
12	D	104	SPO	C29-C28-C27	-4.81	110.18	122.59
12	I	103	SPO	C35-C33-C32	-4.81	111.39	121.12
12	0	102	SPO	C30-C28-C27	-4.80	107.45	121.98
12	P	102	SPO	C35-C33-C32	-4.80	111.41	121.12
12	E	102	SPO	C25-C23-C22	-4.79	111.59	118.94
12	R	103	SPO	C36-C37-C38	-4.76	111.48	127.75
12	R	103	SPO	C30-C28-C27	-4.73	107.67	121.98
10	L	304	U10	C7-C8-C9	-4.72	118.93	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	103	SPO	C16-C17-C19	-4.71	111.71	118.94
12	S	103	SPO	C29-C28-C27	-4.71	110.44	122.59
12	U	103	SPO	C40-C38-C37	-4.70	109.05	122.65
12	E	102	SPO	C36-C37-C38	-4.70	111.67	127.75
12	0	101	SPO	C25-C23-C22	-4.70	111.72	118.94
12	D	103	SPO	C29-C28-C27	-4.70	110.48	122.59
12	M	405	SPO	C11-C12-C14	-4.69	111.74	118.94
12	D	104	SPO	C8-C7-C6	-4.65	110.75	118.08
12	E	102	SPO	C10-C11-C12	-4.64	113.37	126.42
12	0	101	SPO	C29-C28-C27	-4.63	110.64	122.59
12	E	102	SPO	C40-C38-C37	-4.63	109.27	122.65
12	I	103	SPO	C29-C28-C27	-4.62	110.67	122.59
12	D	104	SPO	C25-C23-C22	-4.61	111.86	118.94
12	K	103	SPO	C30-C28-C27	-4.60	108.06	121.98
12	E	102	SPO	C29-C28-C27	-4.59	110.74	122.59
12	I	103	SPO	C30-C28-C27	-4.59	108.10	121.98
12	R	101	SPO	C29-C28-C27	-4.58	110.77	122.59
12	P	102	SPO	C13-C12-C11	-4.58	110.86	118.08
12	D	104	SPO	C16-C17-C19	-4.58	111.91	118.94
12	D	103	SPO	C16-C17-C19	-4.57	111.93	118.94
7	S	101	BCL	CMB-C2B-C1B	-4.57	121.44	128.46
12	F	103	SPO	C39-C38-C37	-4.56	109.45	122.65
12	D	102	SPO	C29-C28-C27	-4.56	110.82	122.59
12	A	603	SPO	C29-C28-C27	-4.56	110.82	122.59
12	K	102	SPO	C36-C37-C38	-4.56	112.17	127.75
12	9	102	SPO	C29-C28-C30	-4.53	107.64	115.27
12	0	102	SPO	C40-C38-C37	-4.53	109.55	122.65
12	D	103	SPO	C30-C28-C27	-4.53	108.28	121.98
12	Q	102	SPO	C8-C7-C6	-4.52	110.95	118.08
12	P	102	SPO	C40-C38-C37	-4.52	109.59	122.65
12	9	102	SPO	C29-C28-C27	-4.50	110.97	122.59
12	0	102	SPO	C36-C37-C38	-4.49	112.40	127.75
7	Q	101	BCL	CMB-C2B-C1B	-4.49	121.56	128.46
12	R	103	SPO	C39-C38-C37	-4.49	109.67	122.65
7	U	101	BCL	CMB-C2B-C1B	-4.48	121.58	128.46
12	K	103	SPO	C29-C28-C27	-4.48	111.04	122.59
7	9	101	BCL	CMB-C2B-C1B	-4.48	121.58	128.46
12	P	101	SPO	C30-C28-C27	-4.48	108.43	121.98
12	R	101	SPO	C39-C38-C37	-4.47	109.73	122.65
7	W	101	BCL	CMB-C2B-C1B	-4.46	121.60	128.46
12	I	104	SPO	C40-C38-C37	-4.46	109.75	122.65
12	P	101	SPO	C40-C38-C37	-4.46	109.75	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	403	BCL	CMB-C2B-C1B	-4.45	121.62	128.46
12	S	103	SPO	C40-C38-C37	-4.45	109.78	122.65
12	P	102	SPO	C30-C28-C27	-4.45	108.51	121.98
12	P	102	SPO	C18-C17-C16	-4.44	111.08	118.08
12	S	103	SPO	C16-C17-C19	-4.44	112.13	118.94
12	D	102	SPO	C34-C33-C35	-4.43	107.81	115.27
12	A	603	SPO	C34-C33-C35	-4.43	107.82	115.27
12	P	101	SPO	C36-C37-C38	-4.43	112.61	127.75
12	R	103	SPO	C11-C12-C14	-4.43	112.14	118.94
7	D	101	BCL	CMB-C2B-C1B	-4.43	121.66	128.46
12	R	103	SPO	C24-C23-C25	-4.42	111.11	118.08
7	A	602	BCL	CMB-C2B-C1B	-4.42	121.66	128.46
12	E	102	SPO	C39-C38-C37	-4.42	109.86	122.65
12	K	103	SPO	C16-C17-C19	-4.41	112.17	118.94
12	D	104	SPO	C36-C37-C38	-4.41	112.68	127.75
12	Q	102	SPO	C39-C38-C37	-4.40	109.92	122.65
12	F	103	SPO	C29-C28-C27	-4.40	111.25	122.59
7	O	101	BCL	CMB-C2B-C1B	-4.38	121.72	128.46
12	8	101	SPO	C16-C17-C19	-4.37	112.23	118.94
12	S	103	SPO	C30-C28-C27	-4.37	108.76	121.98
7	K	101	BCL	CMB-C2B-C1B	-4.36	121.77	128.46
7	F	101	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
12	D	104	SPO	C30-C28-C27	-4.34	108.83	121.98
9	L	303	PC1	O21-C21-C22	4.34	120.86	111.50
12	I	104	SPO	C39-C38-C37	-4.34	110.11	122.65
7	L	301	BCL	CMB-C2B-C1B	-4.32	121.83	128.46
12	R	103	SPO	C29-C28-C27	-4.30	111.48	122.59
12	M	405	SPO	C13-C12-C11	-4.30	111.30	118.08
7	1	101	BCL	CMB-C2B-C1B	-4.30	121.86	128.46
7	I	101	BCL	CMB-C2B-C1B	-4.29	121.86	128.46
12	9	102	SPO	C8-C7-C6	-4.29	111.32	118.08
12	K	103	SPO	C18-C17-C16	-4.28	111.34	118.08
12	R	101	SPO	C16-C17-C19	-4.27	112.39	118.94
12	K	102	SPO	C29-C28-C27	-4.25	111.62	122.59
12	I	103	SPO	C36-C37-C38	-4.25	113.23	127.75
12	D	104	SPO	C9-C10-C11	-4.25	109.97	123.22
12	0	101	SPO	C30-C28-C27	-4.22	109.19	121.98
12	K	103	SPO	C39-C38-C37	-4.22	110.45	122.65
12	P	101	SPO	C20-C21-C22	-4.19	114.88	123.47
12	I	104	SPO	C29-C28-C27	-4.18	111.80	122.59
12	K	103	SPO	C40-C38-C37	-4.18	110.57	122.65
12	I	104	SPO	C36-C37-C38	-4.17	113.50	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	103	SPO	C34-C33-C35	-4.17	108.26	115.27
12	8	101	SPO	C29-C28-C27	-4.16	111.85	122.59
12	P	101	SPO	C29-C28-C30	-4.16	108.27	115.27
12	8	101	SPO	C21-C20-C19	-4.16	114.95	123.47
12	0	102	SPO	C39-C38-C37	-4.14	110.68	122.65
12	R	101	SPO	C30-C28-C27	-4.13	109.48	121.98
7	C	101	BCL	C4A-NA-C1A	4.12	108.56	106.71
12	R	103	SPO	C6-C7-C9	-4.12	112.62	118.94
12	M	405	SPO	C40-C38-C37	-4.11	110.75	122.65
12	P	101	SPO	C29-C28-C27	-4.11	111.98	122.59
7	F	102	BCL	C16-C15-C13	4.10	129.16	115.92
12	E	102	SPO	C11-C12-C14	-4.09	112.67	118.94
12	F	103	SPO	C34-C33-C35	-4.08	108.40	115.27
12	F	103	SPO	C40-C38-C37	-4.08	110.85	122.65
12	D	104	SPO	C40-C38-C37	-4.08	110.86	122.65
7	M	401	BCL	CMB-C2B-C1B	-4.08	122.20	128.46
12	U	103	SPO	C30-C28-C27	-4.07	109.65	121.98
7	L	305	BCL	CMB-C2B-C1B	-4.07	122.21	128.46
12	K	102	SPO	C24-C23-C25	-4.07	111.67	118.08
7	K	101	BCL	C4A-NA-C1A	4.06	108.53	106.71
7	C	101	BCL	CMB-C2B-C1B	-4.06	122.23	128.46
12	F	103	SPO	C9-C10-C11	-4.05	110.59	123.22
12	0	101	SPO	C36-C37-C38	-4.04	113.95	127.75
12	U	103	SPO	C18-C17-C16	-4.03	111.73	118.08
7	U	101	BCL	C4A-NA-C1A	4.02	108.52	106.71
12	A	603	SPO	C39-C38-C37	-4.01	111.06	122.65
12	D	102	SPO	C39-C38-C37	-4.01	111.07	122.65
7	A	602	BCL	C4A-NA-C1A	4.00	108.51	106.71
7	D	101	BCL	C4A-NA-C1A	4.00	108.50	106.71
12	R	103	SPO	C40-C38-C37	-3.98	111.15	122.65
12	R	101	SPO	C8-C7-C6	-3.97	111.82	118.08
12	0	102	SPO	C29-C28-C27	-3.95	112.40	122.59
7	L	301	BCL	CAD-C3D-C4D	-3.95	106.27	108.47
12	M	405	SPO	C34-C33-C32	-3.94	113.56	123.68
9	H	1101	PC1	O21-C21-C22	3.94	120.00	111.50
12	9	102	SPO	C30-C28-C27	-3.93	110.08	121.98
7	O	101	BCL	C4A-NA-C1A	3.93	108.47	106.71
12	9	102	SPO	C39-C38-C37	-3.92	111.31	122.65
12	K	102	SPO	C18-C17-C16	-3.91	111.92	118.08
12	0	101	SPO	C16-C17-C19	-3.90	112.95	118.94
12	Q	102	SPO	C36-C37-C38	-3.90	114.42	127.75
7	O	102	BCL	CMB-C2B-C1B	-3.90	122.47	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	8	102	BCL	CMB-C2B-C1B	-3.90	122.47	128.46
7	9	103	BCL	CMB-C2B-C1B	-3.90	122.47	128.46
7	A	605	BCL	CMB-C2B-C1B	-3.90	122.48	128.46
7	I	102	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
7	N	101	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
7	S	102	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
7	F	102	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
7	E	101	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
7	R	102	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
7	U	102	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
12	R	101	SPO	C13-C12-C11	-3.89	111.95	118.08
12	9	102	SPO	C40-C38-C37	-3.87	111.45	122.65
7	C	101	BCL	CAD-C3D-C4D	-3.87	106.31	108.47
7	Q	101	BCL	C4A-NA-C1A	3.86	108.44	106.71
12	S	103	SPO	C18-C17-C16	-3.86	112.00	118.08
12	S	103	SPO	C39-C38-C37	-3.85	111.53	122.65
12	Q	102	SPO	C16-C17-C19	-3.84	113.05	118.94
7	I	101	BCL	C4A-NA-C1A	3.82	108.42	106.71
7	S	101	BCL	C4A-NA-C1A	3.82	108.42	106.71
12	K	103	SPO	C2-C1-C4	-3.82	104.99	110.86
12	A	603	SPO	C40-C38-C37	-3.82	111.61	122.65
12	D	102	SPO	C40-C38-C37	-3.82	111.61	122.65
12	U	103	SPO	C39-C38-C37	-3.81	111.62	122.65
12	D	103	SPO	C36-C37-C38	-3.81	114.72	127.75
12	E	102	SPO	C15-C16-C17	-3.80	115.73	126.42
12	Q	102	SPO	C20-C21-C22	-3.80	115.68	123.47
12	U	103	SPO	C35-C33-C32	-3.80	113.43	121.12
12	I	103	SPO	C18-C17-C16	-3.80	112.09	118.08
7	M	403	BCL	C4A-NA-C1A	3.80	108.41	106.71
7	2	101	BCL	C4A-NA-C1A	3.79	108.41	106.71
7	F	101	BCL	C4A-NA-C1A	3.77	108.40	106.71
12	F	103	SPO	C36-C37-C38	-3.77	114.86	127.75
12	I	103	SPO	C8-C7-C6	-3.77	112.14	118.08
12	Q	102	SPO	C40-C38-C37	-3.76	111.78	122.65
7	1	101	BCL	CAD-C3D-C4D	-3.75	106.38	108.47
7	9	101	BCL	C4A-NA-C1A	3.74	108.39	106.71
12	E	102	SPO	C2-C1-C4	-3.73	105.13	110.86
7	C	101	BCL	C1C-NC-C4C	3.73	108.38	106.71
12	R	101	SPO	C25-C23-C22	-3.73	113.22	118.94
12	0	101	SPO	C34-C33-C35	-3.73	109.00	115.27
12	R	101	SPO	C40-C38-C37	-3.69	112.00	122.65
13	M	406	CDL	OA6-CA5-C11	3.68	119.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	R	103	SPO	C34-C33-C35	-3.67	109.09	115.27
12	0	101	SPO	C29-C28-C30	-3.66	109.11	115.27
12	R	101	SPO	C36-C37-C38	-3.64	115.29	127.75
7	W	101	BCL	CAD-C3D-C4D	-3.64	106.44	108.47
12	P	101	SPO	C39-C38-C37	-3.64	112.13	122.65
7	S	101	BCL	OBD-CAD-CBD	-3.62	120.72	125.89
7	9	101	BCL	OBD-CAD-CBD	-3.61	120.73	125.89
10	M	404	U10	C25-C24-C26	3.61	121.34	115.27
7	A	602	BCL	OBD-CAD-CBD	-3.60	120.75	125.89
7	D	101	BCL	OBD-CAD-CBD	-3.60	120.75	125.89
12	I	104	SPO	C2-C1-C4	-3.60	105.33	110.86
12	S	103	SPO	C13-C12-C11	-3.59	112.42	118.08
12	P	102	SPO	C36-C37-C38	-3.56	115.58	127.75
12	0	102	SPO	C11-C12-C14	-3.56	113.48	118.94
12	Q	102	SPO	C34-C33-C35	-3.55	109.30	115.27
7	Q	101	BCL	OBD-CAD-CBD	-3.55	120.83	125.89
12	0	102	SPO	C8-C7-C6	-3.54	112.50	118.08
7	7	101	BCL	OBD-CAD-CBD	-3.53	120.84	125.89
7	O	101	BCL	OBD-CAD-CBD	-3.53	120.85	125.89
7	U	101	BCL	OBD-CAD-CBD	-3.52	120.86	125.89
12	E	102	SPO	C20-C21-C22	-3.51	116.28	123.47
13	M	406	CDL	OB6-CB5-C51	3.51	119.07	111.50
12	P	102	SPO	C5-C6-C7	3.50	131.18	125.89
7	K	101	BCL	OBD-CAD-CBD	-3.50	120.89	125.89
7	9	101	BCL	CAD-C3D-C4D	-3.50	106.52	108.47
12	8	101	SPO	C20-C21-C22	-3.50	116.31	123.47
12	M	405	SPO	C39-C38-C37	-3.50	112.55	122.65
9	A	601	PC1	O21-C21-C22	3.49	119.03	111.50
12	A	603	SPO	C3-C1-C4	-3.49	105.50	110.86
12	D	102	SPO	C3-C1-C4	-3.49	105.50	110.86
7	I	101	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
12	K	102	SPO	C8-C7-C6	-3.49	112.58	118.08
12	K	102	SPO	C34-C33-C35	-3.48	109.42	115.27
9	X	1501	PC1	C13-N-C12	3.48	124.16	109.92
9	X	1501	PC1	O21-C21-C22	3.48	118.99	111.50
12	0	102	SPO	C29-C28-C30	-3.48	109.42	115.27
12	P	101	SPO	C15-C16-C17	-3.47	116.67	126.42
7	L	301	BCL	OBD-CAD-CBD	-3.47	120.94	125.89
7	2	101	BCL	CMB-C2B-C1B	-3.47	123.14	128.46
7	F	101	BCL	OBD-CAD-CBD	-3.46	120.95	125.89
7	M	403	BCL	CAD-C3D-C4D	-3.46	106.54	108.47
7	C	101	BCL	OBD-CAD-CBD	-3.45	120.96	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	101	SPO	C8-C7-C6	-3.44	112.65	118.08
12	K	102	SPO	C9-C10-C11	-3.44	112.48	123.22
7	F	102	BCL	OBD-CAD-CBD	-3.44	120.99	125.89
7	N	101	BCL	OBD-CAD-CBD	-3.43	120.99	125.89
7	O	102	BCL	OBD-CAD-CBD	-3.43	120.99	125.89
10	L	304	U10	C12-C13-C14	-3.43	119.39	127.66
7	E	101	BCL	OBD-CAD-CBD	-3.43	120.99	125.89
7	I	102	BCL	OBD-CAD-CBD	-3.43	120.99	125.89
7	A	605	BCL	OBD-CAD-CBD	-3.43	120.99	125.89
7	R	102	BCL	OBD-CAD-CBD	-3.43	120.99	125.89
7	8	102	BCL	OBD-CAD-CBD	-3.43	120.99	125.89
7	S	102	BCL	OBD-CAD-CBD	-3.43	120.99	125.89
7	9	103	BCL	OBD-CAD-CBD	-3.43	121.00	125.89
7	U	102	BCL	OBD-CAD-CBD	-3.43	121.00	125.89
7	M	401	BCL	OBD-CAD-CBD	-3.42	121.01	125.89
12	K	102	SPO	C39-C38-C37	-3.42	112.77	122.65
7	L	305	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
10	M	404	U10	C27-C28-C29	-3.37	119.55	127.66
7	S	101	BCL	CMB-C2B-C3B	3.37	130.98	124.68
7	L	305	BCL	CAD-C3D-C4D	-3.37	106.59	108.47
7	1	101	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
7	W	101	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
7	I	101	BCL	CAD-C3D-C4D	-3.30	106.63	108.47
12	I	103	SPO	C40-C38-C37	-3.30	113.12	122.65
7	U	101	BCL	CMB-C2B-C3B	3.29	130.84	124.68
7	2	101	BCL	CHA-C1A-NA	-3.28	118.89	126.40
7	S	101	BCL	CAD-C3D-C4D	-3.28	106.64	108.47
12	R	103	SPO	C5-C6-C7	-3.25	120.98	125.89
7	M	403	BCL	OBD-CAD-CBD	-3.25	121.25	125.89
7	9	101	BCL	CMB-C2B-C3B	3.25	130.76	124.68
7	Q	101	BCL	CMB-C2B-C3B	3.24	130.74	124.68
7	F	102	BCL	CAD-C3D-C4D	-3.23	106.67	108.47
7	R	102	BCL	CAD-C3D-C4D	-3.23	106.67	108.47
7	I	102	BCL	CAD-C3D-C4D	-3.23	106.67	108.47
7	O	102	BCL	CAD-C3D-C4D	-3.23	106.67	108.47
7	A	605	BCL	CAD-C3D-C4D	-3.22	106.67	108.47
9	H	1102	PC1	O31-C31-C32	3.22	122.02	111.91
7	U	102	BCL	CAD-C3D-C4D	-3.22	106.67	108.47
7	8	102	BCL	CAD-C3D-C4D	-3.22	106.67	108.47
7	9	103	BCL	CAD-C3D-C4D	-3.22	106.68	108.47
7	E	101	BCL	CAD-C3D-C4D	-3.22	106.68	108.47
7	S	102	BCL	CAD-C3D-C4D	-3.22	106.68	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	102	SPO	C39-C38-C37	-3.21	113.36	122.65
7	N	101	BCL	CAD-C3D-C4D	-3.21	106.68	108.47
10	L	304	U10	C30-C29-C31	3.21	120.67	115.27
12	9	102	SPO	C13-C12-C11	-3.20	113.03	118.08
7	L	305	BCL	C4A-NA-C1A	3.20	108.15	106.71
7	O	101	BCL	CMB-C2B-C3B	3.20	130.67	124.68
7	M	403	BCL	CMB-C2B-C3B	3.19	130.65	124.68
12	U	103	SPO	C29-C28-C30	-3.19	109.90	115.27
12	F	103	SPO	C16-C17-C19	-3.19	114.05	118.94
12	M	405	SPO	C34-C33-C35	-3.19	109.91	115.27
12	P	101	SPO	C3-C1-C4	-3.18	105.97	110.86
12	P	101	SPO	C16-C17-C19	-3.18	114.06	118.94
7	W	101	BCL	CMB-C2B-C3B	3.18	130.63	124.68
7	A	602	BCL	CMB-C2B-C3B	3.18	130.62	124.68
7	1	101	BCL	C4A-NA-C1A	3.18	108.13	106.71
7	D	101	BCL	CMB-C2B-C3B	3.18	130.62	124.68
8	L	302	BPH	OBD-CAD-CBD	-3.17	121.17	125.82
12	K	102	SPO	C10-C11-C12	3.17	135.31	126.42
7	F	101	BCL	CMB-C2B-C3B	3.16	130.60	124.68
10	L	304	U10	C27-C28-C29	-3.16	120.04	127.66
12	D	104	SPO	C3-C1-C4	-3.16	106.00	110.86
7	7	101	BCL	CMB-C2B-C1B	-3.16	123.61	128.46
12	0	101	SPO	C40-C38-C37	-3.15	113.54	122.65
12	8	101	SPO	C2-C1-C4	-3.15	106.02	110.86
12	P	101	SPO	C13-C12-C11	-3.15	113.11	118.08
7	L	301	BCL	CMB-C2B-C3B	3.13	130.53	124.68
12	I	104	SPO	C27-C26-C25	-3.12	113.47	123.22
7	M	403	BCL	CHA-C1A-NA	-3.12	119.26	126.40
7	K	101	BCL	CMB-C2B-C3B	3.12	130.51	124.68
12	F	103	SPO	C3-C1-C4	-3.12	106.07	110.86
7	S	101	BCL	CHA-C1A-NA	-3.11	119.27	126.40
12	R	103	SPO	C21-C20-C19	-3.11	117.10	123.47
8	L	306	BPH	OBD-CAD-CBD	-3.11	121.26	125.82
10	M	404	U10	C32-C33-C34	-3.11	120.17	127.66
7	F	101	BCL	CAD-C3D-C4D	-3.10	106.74	108.47
7	2	101	BCL	OBD-CAD-CBD	-3.10	121.46	125.89
7	I	101	BCL	CMB-C2B-C3B	3.10	130.48	124.68
7	Q	101	BCL	CAD-C3D-C4D	-3.09	106.75	108.47
7	C	101	BCL	CHA-C1A-NA	-3.09	119.33	126.40
7	9	101	BCL	CHA-C1A-NA	-3.09	119.33	126.40
7	1	101	BCL	CMB-C2B-C3B	3.08	130.45	124.68
7	K	101	BCL	CAD-C3D-C4D	-3.06	106.76	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	302	BPH	CMB-C2B-C3B	3.05	130.39	124.68
7	C	101	BCL	CMB-C2B-C3B	3.05	130.39	124.68
13	M	406	CDL	OB8-CB7-C71	3.05	121.48	111.91
7	O	101	BCL	CAD-C3D-C4D	-3.05	106.77	108.47
12	I	103	SPO	C13-C12-C11	-3.04	113.28	118.08
7	7	101	BCL	CAD-C3D-C4D	-3.04	106.77	108.47
7	D	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
7	A	602	BCL	CHA-C1A-NA	-3.03	119.46	126.40
7	7	101	BCL	CHA-C1A-NA	-3.03	119.47	126.40
7	I	101	BCL	CHA-C1A-NA	-3.02	119.47	126.40
7	M	401	BCL	CHA-C1A-NA	-3.02	119.48	126.40
12	E	102	SPO	C34-C33-C35	-3.02	110.20	115.27
7	O	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
12	D	104	SPO	C1-C4-C5	-3.01	105.08	113.06
7	U	101	BCL	CAD-C3D-C4D	-3.01	106.79	108.47
12	K	102	SPO	C16-C17-C19	-3.00	114.33	118.94
12	S	103	SPO	C9-C10-C11	-2.99	113.87	123.22
7	1	101	BCL	CHA-C1A-NA	-2.99	119.54	126.40
7	Q	101	BCL	CHA-C1A-NA	-2.99	119.55	126.40
12	Q	102	SPO	C15-C16-C17	-2.99	118.02	126.42
7	9	101	BCL	C1-C2-C3	-2.98	120.88	126.04
7	F	101	BCL	CHA-C1A-NA	-2.98	119.56	126.40
7	D	101	BCL	CAD-C3D-C4D	-2.98	106.81	108.47
7	A	602	BCL	CAD-C3D-C4D	-2.98	106.81	108.47
9	A	604	PC1	O31-C31-C32	2.97	121.24	111.91
9	H	1103	PC1	O31-C31-C32	2.97	121.23	111.91
7	E	101	BCL	CHA-C1A-NA	-2.97	119.59	126.40
7	N	101	BCL	CHA-C1A-NA	-2.97	119.59	126.40
7	S	102	BCL	CHA-C1A-NA	-2.97	119.59	126.40
7	I	102	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	9	103	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	O	102	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	R	102	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	F	102	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	8	102	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	A	605	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	U	102	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	L	301	BCL	CHA-C1A-NA	-2.97	119.60	126.40
7	U	101	BCL	CHA-C1A-NA	-2.96	119.61	126.40
12	D	104	SPO	C29-C28-C30	-2.95	110.31	115.27
7	L	305	BCL	CMB-C2B-C3B	2.95	130.20	124.68
7	L	301	BCL	C2A-C1A-CHA	2.95	129.01	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	302	BPH	C11-C10-C8	-2.95	106.40	115.92
7	O	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	E	101	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	F	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	S	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	9	103	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	A	605	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	I	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	U	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	8	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	R	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	N	101	BCL	C4A-NA-C1A	2.93	108.02	106.71
12	Q	102	SPO	C27-C26-C25	-2.93	114.08	123.22
7	M	401	BCL	CMB-C2B-C3B	2.92	130.14	124.68
12	P	101	SPO	C34-C33-C35	-2.92	110.37	115.27
12	8	101	SPO	C31-C30-C28	2.91	122.56	112.98
7	E	101	BCL	C16-C15-C13	2.91	125.33	115.92
7	L	305	BCL	CHA-C1A-NA	-2.91	119.73	126.40
7	K	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
7	M	401	BCL	CAD-C3D-C4D	-2.91	106.85	108.47
10	L	304	U10	C25-C24-C26	2.90	120.16	115.27
12	F	103	SPO	C35-C33-C32	-2.89	115.27	121.12
9	H	1102	PC1	O21-C21-C22	2.89	117.72	111.50
12	0	101	SPO	C10-C9-C7	-2.88	123.20	127.31
7	O	102	BCL	CMB-C2B-C3B	2.87	130.05	124.68
7	N	101	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	9	103	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	I	102	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	E	101	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	8	102	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	A	605	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	S	102	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	F	102	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	R	102	BCL	CMB-C2B-C3B	2.87	130.04	124.68
7	U	102	BCL	CMB-C2B-C3B	2.87	130.04	124.68
10	M	404	U10	C35-C34-C36	2.86	120.09	115.27
8	L	306	BPH	O2D-CGD-CBD	2.85	114.61	111.00
12	E	102	SPO	C16-C17-C19	-2.85	114.57	118.94
10	L	304	U10	C22-C23-C24	-2.85	120.80	127.66
7	W	101	BCL	CHA-C1A-NA	-2.85	119.88	126.40
10	L	304	U10	C15-C14-C16	2.85	120.06	115.27
10	M	404	U10	C30-C29-C31	2.83	120.03	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	404	U10	C17-C18-C19	-2.82	120.87	127.66
12	D	103	SPO	C39-C38-C37	-2.82	114.51	122.65
9	L	303	PC1	O31-C31-C32	2.82	120.75	111.91
7	7	101	BCL	C2A-C1A-CHA	2.80	128.76	123.86
12	0	101	SPO	C8-C7-C6	-2.78	113.69	118.08
12	R	101	SPO	C29-C28-C30	-2.78	110.60	115.27
10	M	404	U10	C12-C13-C14	-2.78	120.97	127.66
12	P	101	SPO	C5-C6-C7	2.77	130.08	125.89
12	M	405	SPO	C2-C1-C4	-2.77	106.61	110.86
12	I	104	SPO	C5-C6-C7	-2.77	121.71	125.89
7	U	101	BCL	C2A-C1A-CHA	2.77	128.70	123.86
12	E	102	SPO	C26-C25-C23	-2.76	118.67	126.42
12	9	102	SPO	C2-C1-C4	-2.75	106.63	110.86
12	U	103	SPO	C20-C21-C22	-2.75	117.84	123.47
10	L	304	U10	C20-C19-C21	2.75	119.89	115.27
7	Q	101	BCL	C2A-C1A-CHA	2.74	128.65	123.86
10	M	404	U10	C15-C14-C16	2.73	119.87	115.27
7	M	403	BCL	C2A-C1A-CHA	2.72	128.62	123.86
12	R	101	SPO	C34-C33-C35	-2.71	110.72	115.27
7	2	101	BCL	C2A-C1A-CHA	2.71	128.59	123.86
7	C	101	BCL	C2A-C1A-CHA	2.69	128.56	123.86
12	I	104	SPO	C18-C17-C16	-2.69	113.84	118.08
7	O	101	BCL	C2A-C1A-CHA	2.68	128.55	123.86
10	M	404	U10	C22-C23-C24	-2.68	121.21	127.66
10	M	404	U10	C20-C19-C21	2.68	119.78	115.27
7	F	101	BCL	C2A-C1A-CHA	2.68	128.54	123.86
12	Q	102	SPO	C2-C1-C4	-2.67	106.75	110.86
7	1	101	BCL	C2A-C1A-CHA	2.67	128.53	123.86
9	A	601	PC1	C13-N-C12	2.66	120.80	109.92
7	7	101	BCL	C11-C10-C8	-2.64	107.38	115.92
7	9	101	BCL	CMD-C2D-C3D	2.64	129.62	124.68
7	N	101	BCL	C17-C16-C15	2.64	125.35	113.24
7	K	101	BCL	C2A-C1A-CHA	2.63	128.46	123.86
7	2	101	BCL	C1C-NC-C4C	2.63	107.89	106.71
12	S	103	SPO	C34-C33-C35	-2.63	110.85	115.27
12	S	103	SPO	C29-C28-C30	-2.62	110.87	115.27
7	I	101	BCL	C2A-C1A-CHA	2.61	128.42	123.86
12	D	103	SPO	C21-C20-C19	-2.61	118.13	123.47
12	U	103	SPO	C10-C11-C12	2.61	133.74	126.42
7	M	401	BCL	C1-C2-C3	-2.61	121.53	126.04
7	D	101	BCL	C2A-C1A-CHA	2.60	128.40	123.86
7	A	602	BCL	C2A-C1A-CHA	2.60	128.40	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	601	PC1	O31-C31-C32	2.59	120.05	111.91
10	L	304	U10	C17-C18-C19	-2.58	121.44	127.66
7	9	103	BCL	C2A-C1A-CHA	2.58	128.38	123.86
7	E	101	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	8	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	N	101	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	S	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	R	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	I	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
12	F	103	SPO	C13-C12-C11	-2.58	114.01	118.08
13	M	406	CDL	OA8-CA7-C31	2.58	120.00	111.91
7	F	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	U	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	O	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
7	A	605	BCL	C2A-C1A-CHA	2.58	128.37	123.86
12	S	103	SPO	C5-C6-C7	-2.58	122.00	125.89
12	0	101	SPO	C3-C1-C4	-2.57	106.90	110.86
7	S	101	BCL	C2A-C1A-CHA	2.57	128.36	123.86
7	8	102	BCL	C16-C15-C13	-2.57	107.62	115.92
12	D	103	SPO	C5-C6-C7	-2.57	122.01	125.89
10	M	404	U10	C10-C9-C11	2.56	119.58	115.27
7	M	401	BCL	C4A-NA-C1A	2.56	107.86	106.71
7	S	102	BCL	C16-C15-C13	-2.55	107.67	115.92
10	L	304	U10	C1M-C1-C6	-2.55	120.24	124.40
7	K	101	BCL	OBB-CAB-CBB	-2.55	114.43	120.17
7	L	305	BCL	C2A-C1A-CHA	2.55	128.32	123.86
7	E	101	BCL	O2A-C1-C2	-2.55	101.94	108.64
7	N	101	BCL	O2A-C1-C2	-2.55	101.94	108.64
7	R	102	BCL	O2A-C1-C2	-2.55	101.94	108.64
7	U	102	BCL	O2A-C1-C2	-2.55	101.94	108.64
7	9	103	BCL	O2A-C1-C2	-2.55	101.94	108.64
7	S	102	BCL	O2A-C1-C2	-2.54	101.95	108.64
7	O	102	BCL	O2A-C1-C2	-2.54	101.95	108.64
7	8	102	BCL	O2A-C1-C2	-2.54	101.95	108.64
7	F	102	BCL	O2A-C1-C2	-2.54	101.95	108.64
7	A	605	BCL	O2A-C1-C2	-2.54	101.95	108.64
7	I	102	BCL	O2A-C1-C2	-2.54	101.95	108.64
7	M	403	BCL	OBB-CAB-CBB	-2.54	114.45	120.17
8	L	306	BPH	CMB-C2B-C3B	2.54	129.43	124.68
7	R	102	BCL	CMD-C2D-C3D	2.54	129.43	124.68
7	S	102	BCL	CMD-C2D-C3D	2.54	129.43	124.68
7	C	101	BCL	C17-C16-C15	2.54	124.91	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	0	101	SPO	C10-C11-C12	2.54	133.55	126.42
7	O	102	BCL	CMD-C2D-C3D	2.54	129.43	124.68
7	U	102	BCL	CMD-C2D-C3D	2.54	129.43	124.68
7	I	102	BCL	CMD-C2D-C3D	2.54	129.43	124.68
7	F	102	BCL	CMD-C2D-C3D	2.54	129.42	124.68
7	E	101	BCL	CMD-C2D-C3D	2.54	129.42	124.68
7	N	101	BCL	CMD-C2D-C3D	2.54	129.42	124.68
7	A	605	BCL	CMD-C2D-C3D	2.54	129.42	124.68
7	9	103	BCL	CMD-C2D-C3D	2.54	129.42	124.68
7	W	101	BCL	OBB-CAB-CBB	-2.53	114.47	120.17
7	8	102	BCL	CMD-C2D-C3D	2.53	129.42	124.68
12	R	103	SPO	C3-C1-C4	-2.53	106.97	110.86
7	9	101	BCL	OBB-CAB-CBB	-2.52	114.49	120.17
7	W	101	BCL	C4A-NA-C1A	2.52	107.84	106.71
7	9	101	BCL	C2A-C1A-CHA	2.52	128.26	123.86
7	Q	101	BCL	OBB-CAB-CBB	-2.51	114.51	120.17
9	X	1501	PC1	O13-P-O14	2.51	118.89	109.07
9	L	303	PC1	O13-P-O14	2.51	118.86	109.07
9	H	1101	PC1	C3-C2-C1	-2.51	105.86	111.79
8	L	306	BPH	C1-C2-C3	-2.50	121.71	126.04
12	I	104	SPO	C34-C33-C35	-2.50	111.06	115.27
12	D	104	SPO	C34-C33-C35	-2.50	111.07	115.27
12	F	103	SPO	C1-C4-C5	-2.49	106.45	113.06
7	2	101	BCL	CMB-C2B-C3B	2.49	129.34	124.68
7	L	305	BCL	C1C-NC-C4C	2.48	107.82	106.71
7	W	101	BCL	C4B-C3B-CAB	-2.48	122.34	127.13
12	M	405	SPO	C27-C26-C25	-2.48	115.49	123.22
12	K	103	SPO	C21-C20-C19	-2.47	118.41	123.47
12	M	405	SPO	C14-C15-C16	-2.46	115.54	123.22
9	L	303	PC1	C2-O21-C21	-2.45	111.76	117.79
7	I	101	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
7	W	101	BCL	C2A-C1A-CHA	2.45	128.14	123.86
12	P	101	SPO	C11-C12-C14	-2.45	115.19	118.94
7	I	101	BCL	CMD-C2D-C3D	2.45	129.25	124.68
7	O	101	BCL	CMD-C2D-C3D	2.45	129.25	124.68
7	S	101	BCL	OBB-CAB-CBB	-2.44	114.67	120.17
12	9	102	SPO	C26-C25-C23	-2.44	119.56	126.42
9	X	1501	PC1	O31-C31-C32	2.44	119.57	111.91
7	L	301	BCL	OBB-CAB-CBB	-2.44	114.69	120.17
7	L	305	BCL	CAA-CBA-CGA	2.43	120.37	113.25
7	Q	101	BCL	CMD-C2D-C3D	2.43	129.22	124.68
12	R	101	SPO	C26-C25-C23	-2.43	119.59	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	306	BPH	CMD-C2D-C3D	2.42	129.21	124.68
7	7	101	BCL	C4A-NA-C1A	2.42	107.80	106.71
7	F	101	BCL	CMD-C2D-C3D	2.42	129.21	124.68
7	M	401	BCL	C2A-C1A-CHA	2.42	128.09	123.86
12	Q	102	SPO	C21-C20-C19	-2.42	118.52	123.47
7	O	101	BCL	OBB-CAB-CBB	-2.42	114.73	120.17
7	Q	101	BCL	C1C-NC-C4C	2.41	107.79	106.71
12	9	102	SPO	C20-C21-C22	-2.41	118.53	123.47
7	U	101	BCL	CMD-C2D-C3D	2.41	129.19	124.68
8	L	302	BPH	OBB-CAB-CBB	-2.41	114.75	120.17
7	L	305	BCL	CMD-C2D-C3D	2.41	129.18	124.68
12	K	102	SPO	C29-C28-C30	-2.40	111.23	115.27
7	D	101	BCL	OBB-CAB-CBB	-2.40	114.76	120.17
7	A	602	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
7	A	602	BCL	CMD-C2D-C3D	2.40	129.17	124.68
7	D	101	BCL	CMD-C2D-C3D	2.40	129.17	124.68
12	0	101	SPO	C2-C1-C4	-2.39	107.18	110.86
12	0	102	SPO	C34-C33-C35	-2.39	111.25	115.27
12	U	103	SPO	C11-C12-C14	-2.39	115.28	118.94
7	U	101	BCL	OBB-CAB-CBB	-2.38	114.81	120.17
7	M	401	BCL	CMD-C2D-C3D	2.38	129.13	124.68
7	S	101	BCL	CMD-C2D-C3D	2.38	129.13	124.68
7	W	101	BCL	CMD-C2D-C3D	2.38	129.13	124.68
7	K	101	BCL	CMD-C2D-C3D	2.38	129.12	124.68
12	9	102	SPO	C34-C33-C35	-2.36	111.30	115.27
10	L	304	U10	C36-C34-C35	2.36	119.82	114.60
7	E	101	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
7	U	102	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
7	F	102	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
7	9	103	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
7	I	102	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
7	8	102	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
7	N	101	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
7	O	102	BCL	C4B-C3B-CAB	-2.36	122.58	127.13
7	A	605	BCL	C4B-C3B-CAB	-2.35	122.58	127.13
7	S	102	BCL	C4B-C3B-CAB	-2.35	122.58	127.13
7	R	102	BCL	C4B-C3B-CAB	-2.35	122.58	127.13
7	M	401	BCL	C4B-C3B-CAB	-2.35	122.59	127.13
12	K	102	SPO	C2-C1-C4	-2.34	107.27	110.86
12	0	101	SPO	C20-C21-C22	-2.34	118.68	123.47
12	0	102	SPO	C13-C12-C11	-2.33	114.40	118.08
7	C	101	BCL	C4B-C3B-CAB	-2.33	122.63	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	1101	PC1	O31-C31-C32	2.33	119.21	111.91
7	1	101	BCL	C4B-C3B-CAB	-2.32	122.65	127.13
7	L	301	BCL	C4A-NA-C1A	2.32	107.75	106.71
7	7	101	BCL	CMD-C2D-C3D	2.31	129.01	124.68
12	I	104	SPO	C20-C21-C22	-2.31	118.74	123.47
7	U	101	BCL	C4B-C3B-CAB	-2.31	122.67	127.13
7	F	101	BCL	OBB-CAB-CBB	-2.30	115.00	120.17
12	0	101	SPO	C40-C38-C39	-2.30	109.53	114.60
7	L	301	BCL	CMD-C2D-C3D	2.30	128.97	124.68
7	F	101	BCL	C1C-NC-C4C	2.30	107.74	106.71
10	L	304	U10	C12-C11-C9	-2.29	105.44	112.98
7	S	101	BCL	C1C-NC-C4C	2.29	107.73	106.71
7	L	305	BCL	OBB-CAB-CBB	-2.28	115.03	120.17
9	H	1103	PC1	C13-N-C12	2.28	119.25	109.92
9	A	604	PC1	C13-N-C12	2.28	119.24	109.92
8	L	302	BPH	CMD-C2D-C3D	2.28	128.94	124.68
12	I	104	SPO	C3-C1-C4	-2.27	107.37	110.86
12	K	103	SPO	C5-C6-C7	-2.27	122.47	125.89
7	L	305	BCL	C16-C15-C13	-2.25	108.65	115.92
7	C	101	BCL	CMD-C2D-C3D	2.25	128.89	124.68
12	F	103	SPO	C20-C21-C22	-2.25	118.88	123.47
10	M	404	U10	C41-C39-C40	2.24	119.56	114.60
9	H	1102	PC1	C13-N-C12	2.24	119.10	109.92
12	I	104	SPO	C21-C20-C19	-2.24	118.89	123.47
7	2	101	BCL	CMD-C2D-C3D	2.24	128.87	124.68
7	1	101	BCL	OBB-CAB-CBB	-2.24	115.13	120.17
12	M	405	SPO	C3-C1-C4	-2.24	107.42	110.86
12	I	103	SPO	C5-C6-C7	-2.24	122.51	125.89
7	F	101	BCL	C1-C2-C3	-2.23	122.19	126.04
7	7	101	BCL	CMB-C2B-C3B	2.23	128.84	124.68
9	A	604	PC1	C3-C2-C1	-2.22	106.53	111.79
9	H	1103	PC1	C3-C2-C1	-2.22	106.53	111.79
12	8	101	SPO	C26-C25-C23	-2.22	120.18	126.42
7	L	301	BCL	C1C-NC-C4C	2.22	107.70	106.71
7	E	101	BCL	C1C-NC-C4C	2.21	107.70	106.71
7	8	102	BCL	C1C-NC-C4C	2.21	107.70	106.71
7	M	403	BCL	C4B-C3B-CAB	-2.20	122.87	127.13
7	A	605	BCL	C1C-NC-C4C	2.20	107.69	106.71
7	F	102	BCL	C1C-NC-C4C	2.20	107.69	106.71
12	U	103	SPO	C9-C10-C11	-2.20	116.35	123.22
7	N	101	BCL	C1C-NC-C4C	2.20	107.69	106.71
7	U	102	BCL	C1C-NC-C4C	2.20	107.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	9	103	BCL	C1C-NC-C4C	2.20	107.69	106.71
7	1	101	BCL	C1C-NC-C4C	2.20	107.69	106.71
7	1	101	BCL	CMD-C2D-C3D	2.19	128.78	124.68
7	M	403	BCL	CMD-C2D-C3D	2.19	128.78	124.68
7	O	102	BCL	C1C-NC-C4C	2.19	107.69	106.71
12	K	103	SPO	C27-C26-C25	-2.19	116.38	123.22
7	R	102	BCL	C1C-NC-C4C	2.19	107.69	106.71
7	S	102	BCL	C1C-NC-C4C	2.19	107.69	106.71
12	D	104	SPO	C13-C12-C11	-2.19	114.63	118.08
12	D	104	SPO	C40-C38-C39	-2.18	109.78	114.60
12	M	405	SPO	C21-C20-C19	-2.18	119.00	123.47
7	I	102	BCL	C1C-NC-C4C	2.18	107.69	106.71
7	L	305	BCL	C11-C12-C13	-2.18	108.87	115.92
12	I	104	SPO	C29-C28-C30	-2.18	111.60	115.27
7	U	101	BCL	C17-C16-C15	2.18	123.25	113.24
7	C	101	BCL	C11-C10-C8	2.18	122.96	115.92
12	S	103	SPO	C26-C25-C23	-2.18	120.30	126.42
12	D	104	SPO	C26-C25-C23	-2.17	120.33	126.42
7	A	602	BCL	C1C-NC-C4C	2.16	107.68	106.71
7	D	101	BCL	C1C-NC-C4C	2.16	107.68	106.71
12	K	103	SPO	C34-C33-C35	-2.16	111.64	115.27
12	I	103	SPO	C29-C28-C30	-2.16	111.64	115.27
7	K	101	BCL	C1C-NC-C4C	2.16	107.67	106.71
12	P	102	SPO	C6-C7-C9	-2.15	115.64	118.94
7	Q	101	BCL	C4B-C3B-CAB	-2.14	122.98	127.13
7	L	305	BCL	C4B-C3B-CAB	-2.14	122.99	127.13
12	R	101	SPO	C2-C1-C4	-2.14	107.57	110.86
7	K	101	BCL	C4B-C3B-CAB	-2.14	123.00	127.13
7	7	101	BCL	C1-C2-C3	-2.13	122.35	126.04
7	9	101	BCL	C1C-NC-C4C	2.13	107.66	106.71
12	S	103	SPO	C10-C11-C12	-2.13	120.44	126.42
7	F	101	BCL	C4B-C3B-CAB	-2.13	123.02	127.13
12	8	101	SPO	C14-C15-C16	-2.13	116.58	123.22
7	C	101	BCL	C6-C5-C3	2.12	119.02	113.45
7	O	101	BCL	C1C-NC-C4C	2.12	107.66	106.71
7	9	101	BCL	C4B-C3B-CAB	-2.12	123.04	127.13
7	2	101	BCL	CAA-CBA-CGA	2.12	118.12	112.51
9	L	303	PC1	C13-N-C12	2.11	118.53	109.92
12	I	103	SPO	C2-C1-C4	-2.11	107.62	110.86
7	O	101	BCL	C4B-C3B-CAB	-2.10	123.07	127.13
12	I	104	SPO	C9-C10-C11	-2.09	116.69	123.22
7	8	102	BCL	C17-C16-C15	2.08	122.81	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	103	SPO	C20-C21-C22	-2.08	119.22	123.47
9	H	1101	PC1	C13-N-C12	2.07	118.41	109.92
7	W	101	BCL	C6-C7-C8	-2.07	109.22	115.92
12	P	102	SPO	C9-C10-C11	-2.07	116.76	123.22
12	I	104	SPO	C14-C15-C16	-2.07	116.76	123.22
7	9	101	BCL	O2A-CGA-O1A	-2.07	118.37	123.59
7	M	401	BCL	OBB-CAB-CBB	-2.06	115.54	120.17
12	Q	102	SPO	C40-C38-C39	-2.06	110.06	114.60
12	I	103	SPO	C21-C20-C19	-2.05	119.27	123.47
12	8	101	SPO	C3-C1-C4	-2.05	107.71	110.86
12	P	102	SPO	C26-C25-C23	-2.05	120.67	126.42
7	I	101	BCL	C1C-NC-C4C	2.05	107.63	106.71
12	D	103	SPO	C27-C26-C25	-2.05	116.83	123.22
12	P	101	SPO	C10-C11-C12	-2.04	120.68	126.42
7	N	101	BCL	C16-C17-C18	-2.04	106.36	115.98
12	R	103	SPO	C29-C28-C30	-2.03	111.86	115.27
12	P	102	SPO	C16-C17-C19	-2.03	115.83	118.94
7	A	605	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	8	102	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	9	103	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	U	102	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	E	101	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	I	102	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	M	403	BCL	C11-C10-C8	-2.03	109.37	115.92
7	F	102	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	N	101	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	S	102	BCL	OBB-CAB-CBB	-2.03	115.61	120.17
7	A	602	BCL	C4B-C3B-CAB	-2.02	123.22	127.13
7	O	102	BCL	OBB-CAB-CBB	-2.02	115.61	120.17
7	R	102	BCL	OBB-CAB-CBB	-2.02	115.61	120.17
12	S	103	SPO	C2-C1-C4	-2.02	107.75	110.86
7	D	101	BCL	C4B-C3B-CAB	-2.02	123.22	127.13
12	D	103	SPO	C15-C16-C17	-2.02	120.74	126.42
8	L	302	BPH	O2D-CGD-CBD	2.01	113.55	111.00
7	W	101	BCL	C1C-NC-C4C	2.00	107.61	106.71
12	0	101	SPO	C14-C15-C16	-2.00	116.97	123.22

There are no chirality outliers.

All (863) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	305	BCL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	A	605	BCL	C1A-C2A-CAA-CBA
7	E	101	BCL	C1A-C2A-CAA-CBA
7	F	102	BCL	C1A-C2A-CAA-CBA
7	I	102	BCL	C1A-C2A-CAA-CBA
7	N	101	BCL	C1A-C2A-CAA-CBA
7	O	102	BCL	C1A-C2A-CAA-CBA
7	R	102	BCL	C1A-C2A-CAA-CBA
7	S	102	BCL	C1A-C2A-CAA-CBA
7	U	102	BCL	C1A-C2A-CAA-CBA
7	W	101	BCL	CHA-CBD-CGD-O1D
7	W	101	BCL	CHA-CBD-CGD-O2D
7	7	101	BCL	C2C-C3C-CAC-CBC
7	7	101	BCL	C4C-C3C-CAC-CBC
7	8	102	BCL	C1A-C2A-CAA-CBA
7	9	103	BCL	C1A-C2A-CAA-CBA
8	L	306	BPH	C2-C3-C5-C6
8	L	306	BPH	C4-C3-C5-C6
9	L	303	PC1	O21-C2-C3-O31
9	H	1101	PC1	C11-O13-P-O14
9	H	1101	PC1	C12-C11-O13-P
9	H	1101	PC1	O13-C11-C12-N
9	H	1102	PC1	C11-O13-P-O11
9	H	1102	PC1	O32-C31-O31-C3
9	H	1102	PC1	C32-C31-O31-C3
9	H	1103	PC1	C11-O13-P-O12
9	H	1103	PC1	C11-O13-P-O14
9	H	1103	PC1	C1-O11-P-O12
9	H	1103	PC1	C1-O11-P-O14
9	H	1103	PC1	O13-C11-C12-N
9	H	1103	PC1	C2-C1-O11-P
9	A	601	PC1	C11-O13-P-O14
9	A	601	PC1	C11-O13-P-O11
9	A	601	PC1	C12-C11-O13-P
9	A	604	PC1	C11-O13-P-O12
9	A	604	PC1	C11-O13-P-O14
9	A	604	PC1	C1-O11-P-O12
9	A	604	PC1	C1-O11-P-O14
9	A	604	PC1	O13-C11-C12-N
9	A	604	PC1	C2-C1-O11-P
9	X	1501	PC1	C1-O11-P-O14
12	M	405	SPO	O1-C1-C4-C5
12	M	405	SPO	C2-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
12	M	405	SPO	C3-C1-C4-C5
12	M	405	SPO	C5-C6-C7-C8
12	M	405	SPO	C8-C7-C9-C10
12	M	405	SPO	C13-C12-C14-C15
12	M	405	SPO	C18-C17-C19-C20
12	M	405	SPO	C21-C22-C23-C24
12	M	405	SPO	C26-C27-C28-C29
12	M	405	SPO	C31-C32-C33-C34
12	A	603	SPO	C8-C7-C9-C10
12	A	603	SPO	C10-C11-C12-C14
12	A	603	SPO	C13-C12-C14-C15
12	A	603	SPO	C15-C16-C17-C18
12	A	603	SPO	C15-C16-C17-C19
12	A	603	SPO	C18-C17-C19-C20
12	A	603	SPO	C21-C22-C23-C24
12	A	603	SPO	C26-C27-C28-C30
12	A	603	SPO	C32-C33-C35-C36
12	D	102	SPO	C8-C7-C9-C10
12	D	102	SPO	C10-C11-C12-C14
12	D	102	SPO	C13-C12-C14-C15
12	D	102	SPO	C15-C16-C17-C18
12	D	102	SPO	C15-C16-C17-C19
12	D	102	SPO	C18-C17-C19-C20
12	D	102	SPO	C21-C22-C23-C24
12	D	102	SPO	C26-C27-C28-C30
12	D	102	SPO	C32-C33-C35-C36
12	D	103	SPO	C6-C7-C9-C10
12	D	103	SPO	C8-C7-C9-C10
12	D	103	SPO	C13-C12-C14-C15
12	D	103	SPO	C15-C16-C17-C18
12	D	103	SPO	C18-C17-C19-C20
12	D	103	SPO	C21-C22-C23-C24
12	D	103	SPO	C24-C23-C25-C26
12	D	103	SPO	C26-C27-C28-C29
12	D	103	SPO	C31-C32-C33-C34
12	D	103	SPO	C32-C33-C35-C36
12	D	103	SPO	C33-C35-C36-C37
12	D	104	SPO	C5-C6-C7-C8
12	D	104	SPO	C6-C7-C9-C10
12	D	104	SPO	C11-C12-C14-C15
12	D	104	SPO	C18-C17-C19-C20
12	D	104	SPO	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
12	D	104	SPO	C24-C23-C25-C26
12	D	104	SPO	C26-C27-C28-C29
12	D	104	SPO	C31-C32-C33-C34
12	D	104	SPO	C32-C33-C35-C36
12	E	102	SPO	C5-C6-C7-C8
12	E	102	SPO	C8-C7-C9-C10
12	E	102	SPO	C11-C12-C14-C15
12	E	102	SPO	C18-C17-C19-C20
12	E	102	SPO	C21-C22-C23-C25
12	E	102	SPO	C26-C27-C28-C29
12	E	102	SPO	C26-C27-C28-C30
12	E	102	SPO	C31-C32-C33-C34
12	E	102	SPO	C33-C35-C36-C37
12	E	102	SPO	C35-C36-C37-C38
12	E	102	SPO	C36-C37-C38-C39
12	F	103	SPO	C6-C7-C9-C10
12	F	103	SPO	C11-C12-C14-C15
12	F	103	SPO	C15-C16-C17-C18
12	F	103	SPO	C18-C17-C19-C20
12	F	103	SPO	C21-C22-C23-C24
12	F	103	SPO	C24-C23-C25-C26
12	F	103	SPO	C26-C27-C28-C29
12	F	103	SPO	C29-C28-C30-C31
12	F	103	SPO	C28-C30-C31-C32
12	F	103	SPO	C30-C31-C32-C33
12	F	103	SPO	C31-C32-C33-C35
12	F	103	SPO	C33-C35-C36-C37
12	I	103	SPO	C5-C6-C7-C8
12	I	103	SPO	C5-C6-C7-C9
12	I	103	SPO	C6-C7-C9-C10
12	I	103	SPO	C8-C7-C9-C10
12	I	103	SPO	C10-C11-C12-C13
12	I	103	SPO	C10-C11-C12-C14
12	I	103	SPO	C11-C12-C14-C15
12	I	103	SPO	C15-C16-C17-C18
12	I	103	SPO	C18-C17-C19-C20
12	I	103	SPO	C21-C22-C23-C24
12	I	103	SPO	C22-C23-C25-C26
12	I	103	SPO	C26-C27-C28-C29
12	I	103	SPO	C31-C32-C33-C34
12	I	103	SPO	C36-C37-C38-C40
12	I	104	SPO	O1-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
12	I	104	SPO	C3-C1-C4-C5
12	I	104	SPO	C5-C6-C7-C9
12	I	104	SPO	C6-C7-C9-C10
12	I	104	SPO	C8-C7-C9-C10
12	I	104	SPO	C13-C12-C14-C15
12	I	104	SPO	C18-C17-C19-C20
12	I	104	SPO	C26-C27-C28-C29
12	I	104	SPO	C31-C32-C33-C34
12	I	104	SPO	C33-C35-C36-C37
12	K	102	SPO	O1-C1-C4-C5
12	K	102	SPO	C2-C1-C4-C5
12	K	102	SPO	C3-C1-C4-C5
12	K	102	SPO	C1-C4-C5-C6
12	K	102	SPO	C5-C6-C7-C9
12	K	102	SPO	C8-C7-C9-C10
12	K	102	SPO	C10-C11-C12-C13
12	K	102	SPO	C13-C12-C14-C15
12	K	102	SPO	C15-C16-C17-C18
12	K	102	SPO	C18-C17-C19-C20
12	K	102	SPO	C21-C22-C23-C24
12	K	102	SPO	C26-C27-C28-C29
12	K	103	SPO	C6-C7-C9-C10
12	K	103	SPO	C8-C7-C9-C10
12	K	103	SPO	C13-C12-C14-C15
12	K	103	SPO	C21-C22-C23-C24
12	K	103	SPO	C22-C23-C25-C26
12	K	103	SPO	C25-C26-C27-C28
12	K	103	SPO	C26-C27-C28-C29
12	K	103	SPO	C26-C27-C28-C30
12	K	103	SPO	C28-C30-C31-C32
12	K	103	SPO	C31-C32-C33-C35
12	K	103	SPO	C32-C33-C35-C36
12	K	103	SPO	C33-C35-C36-C37
12	P	101	SPO	O1-C1-C4-C5
12	P	101	SPO	C2-C1-C4-C5
12	P	101	SPO	C3-C1-C4-C5
12	P	101	SPO	C5-C6-C7-C8
12	P	101	SPO	C5-C6-C7-C9
12	P	101	SPO	C8-C7-C9-C10
12	P	101	SPO	C13-C12-C14-C15
12	P	101	SPO	C12-C14-C15-C16
12	P	101	SPO	C18-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
12	P	101	SPO	C21-C22-C23-C24
12	P	101	SPO	C26-C27-C28-C29
12	P	101	SPO	C27-C28-C30-C31
12	P	101	SPO	C31-C32-C33-C34
12	P	102	SPO	C8-C7-C9-C10
12	P	102	SPO	C10-C11-C12-C14
12	P	102	SPO	C11-C12-C14-C15
12	P	102	SPO	C15-C16-C17-C19
12	P	102	SPO	C16-C17-C19-C20
12	P	102	SPO	C18-C17-C19-C20
12	P	102	SPO	C21-C22-C23-C25
12	P	102	SPO	C26-C27-C28-C29
12	P	102	SPO	C26-C27-C28-C30
12	P	102	SPO	C32-C33-C35-C36
12	Q	102	SPO	C8-C7-C9-C10
12	Q	102	SPO	C10-C11-C12-C14
12	Q	102	SPO	C11-C12-C14-C15
12	Q	102	SPO	C13-C12-C14-C15
12	Q	102	SPO	C18-C17-C19-C20
12	Q	102	SPO	C21-C22-C23-C24
12	Q	102	SPO	C26-C27-C28-C29
12	Q	102	SPO	C27-C28-C30-C31
12	Q	102	SPO	C31-C32-C33-C35
12	Q	102	SPO	C33-C35-C36-C37
12	R	101	SPO	C5-C6-C7-C9
12	R	101	SPO	C8-C7-C9-C10
12	R	101	SPO	C10-C11-C12-C14
12	R	101	SPO	C13-C12-C14-C15
12	R	101	SPO	C18-C17-C19-C20
12	R	101	SPO	C26-C27-C28-C29
12	R	101	SPO	C31-C32-C33-C34
12	R	101	SPO	C32-C33-C35-C36
12	R	101	SPO	C33-C35-C36-C37
12	R	103	SPO	C6-C7-C9-C10
12	R	103	SPO	C11-C10-C9-C7
12	R	103	SPO	C13-C12-C14-C15
12	R	103	SPO	C15-C16-C17-C18
12	R	103	SPO	C18-C17-C19-C20
12	R	103	SPO	C21-C22-C23-C24
12	R	103	SPO	C24-C23-C25-C26
12	R	103	SPO	C26-C27-C28-C29
12	R	103	SPO	C26-C27-C28-C30

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Mol	Chain	Res	Type	Atoms
12	R	103	SPO	C31-C32-C33-C34
12	S	103	SPO	C5-C6-C7-C8
12	S	103	SPO	C5-C6-C7-C9
12	S	103	SPO	C6-C7-C9-C10
12	S	103	SPO	C8-C7-C9-C10
12	S	103	SPO	C13-C12-C14-C15
12	S	103	SPO	C15-C16-C17-C18
12	S	103	SPO	C18-C17-C19-C20
12	S	103	SPO	C21-C22-C23-C24
12	S	103	SPO	C25-C26-C27-C28
12	S	103	SPO	C26-C27-C28-C29
12	S	103	SPO	C31-C32-C33-C34
12	S	103	SPO	C32-C33-C35-C36
12	S	103	SPO	C36-C37-C38-C39
12	S	103	SPO	C36-C37-C38-C40
12	U	103	SPO	C5-C6-C7-C9
12	U	103	SPO	C6-C7-C9-C10
12	U	103	SPO	C10-C11-C12-C13
12	U	103	SPO	C10-C11-C12-C14
12	U	103	SPO	C13-C12-C14-C15
12	U	103	SPO	C15-C16-C17-C18
12	U	103	SPO	C18-C17-C19-C20
12	U	103	SPO	C21-C22-C23-C24
12	U	103	SPO	C26-C27-C28-C29
12	U	103	SPO	C27-C28-C30-C31
12	U	103	SPO	C31-C32-C33-C34
12	U	103	SPO	C36-C37-C38-C39
12	U	103	SPO	C36-C37-C38-C40
12	8	101	SPO	C5-C6-C7-C9
12	8	101	SPO	C6-C7-C9-C10
12	8	101	SPO	C8-C7-C9-C10
12	8	101	SPO	C15-C16-C17-C18
12	8	101	SPO	C18-C17-C19-C20
12	8	101	SPO	C21-C22-C23-C24
12	8	101	SPO	C22-C23-C25-C26
12	8	101	SPO	C24-C23-C25-C26
12	8	101	SPO	C26-C27-C28-C30
12	8	101	SPO	C29-C28-C30-C31
12	8	101	SPO	C32-C33-C35-C36
12	9	102	SPO	C8-C7-C9-C10
12	9	102	SPO	C10-C11-C12-C14
12	9	102	SPO	C13-C12-C14-C15

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Mol	Chain	Res	Type	Atoms
12	9	102	SPO	C15-C16-C17-C18
12	9	102	SPO	C15-C16-C17-C19
12	9	102	SPO	C18-C17-C19-C20
12	9	102	SPO	C21-C22-C23-C24
12	9	102	SPO	C24-C23-C25-C26
12	9	102	SPO	C26-C27-C28-C29
12	9	102	SPO	C31-C32-C33-C34
12	0	101	SPO	C1-C4-C5-C6
12	0	101	SPO	C5-C6-C7-C8
12	0	101	SPO	C11-C10-C9-C7
12	0	101	SPO	C10-C11-C12-C13
12	0	101	SPO	C11-C12-C14-C15
12	0	101	SPO	C15-C16-C17-C18
12	0	101	SPO	C18-C17-C19-C20
12	0	101	SPO	C21-C22-C23-C24
12	0	101	SPO	C26-C27-C28-C29
12	0	101	SPO	C31-C32-C33-C34
12	0	102	SPO	C3-C1-O1-CM1
12	0	102	SPO	C5-C6-C7-C8
12	0	102	SPO	C5-C6-C7-C9
12	0	102	SPO	C6-C7-C9-C10
12	0	102	SPO	C8-C7-C9-C10
12	0	102	SPO	C13-C12-C14-C15
12	0	102	SPO	C18-C17-C19-C20
12	0	102	SPO	C21-C22-C23-C24
12	0	102	SPO	C26-C27-C28-C29
12	0	102	SPO	C31-C32-C33-C34
12	0	102	SPO	C32-C33-C35-C36
13	M	406	CDL	CA2-C1-CB2-OB2
13	M	406	CDL	CA2-OA2-PA1-OA5
13	M	406	CDL	CA3-OA5-PA1-OA3
13	M	406	CDL	OA7-CA5-OA6-CA4
13	M	406	CDL	C11-CA5-OA6-CA4
13	M	406	CDL	CB2-OB2-PB2-OB5
13	M	406	CDL	CB3-OB5-PB2-OB2
13	M	406	CDL	CB3-OB5-PB2-OB3
13	M	406	CDL	CB3-OB5-PB2-OB4
13	M	406	CDL	OB9-CB7-OB8-CB6
13	M	406	CDL	C71-CB7-OB8-CB6
9	A	601	PC1	O32-C31-O31-C3
12	E	102	SPO	C36-C37-C38-C40
12	K	103	SPO	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
12	P	102	SPO	C36-C37-C38-C40
12	0	101	SPO	C36-C37-C38-C40
9	A	601	PC1	C32-C31-O31-C3
12	K	102	SPO	C36-C37-C38-C39
12	Q	102	SPO	C36-C37-C38-C40
12	R	101	SPO	C36-C37-C38-C39
12	R	103	SPO	C36-C37-C38-C40
12	P	101	SPO	C29-C28-C30-C31
12	S	103	SPO	C34-C33-C35-C36
12	M	405	SPO	C32-C33-C35-C36
12	D	104	SPO	C27-C28-C30-C31
12	F	103	SPO	C32-C33-C35-C36
12	I	104	SPO	C27-C28-C30-C31
12	I	104	SPO	C32-C33-C35-C36
12	K	103	SPO	C27-C28-C30-C31
12	P	101	SPO	C32-C33-C35-C36
12	P	102	SPO	C27-C28-C30-C31
12	R	101	SPO	C27-C28-C30-C31
12	0	101	SPO	C27-C28-C30-C31
12	0	102	SPO	C27-C28-C30-C31
9	H	1101	PC1	C2-C3-O31-C31
9	H	1101	PC1	C22-C23-C24-C25
12	M	405	SPO	C36-C37-C38-C40
12	F	103	SPO	C36-C37-C38-C40
12	A	603	SPO	C31-C32-C33-C34
12	D	102	SPO	C31-C32-C33-C34
12	P	102	SPO	C31-C32-C33-C34
12	E	102	SPO	C12-C14-C15-C16
12	P	102	SPO	C12-C14-C15-C16
12	R	101	SPO	C25-C26-C27-C28
12	0	102	SPO	C11-C10-C9-C7
9	H	1101	PC1	C29-C2A-C2B-C2C
13	M	406	CDL	O1-C1-CB2-OB2
9	A	601	PC1	C22-C23-C24-C25
13	M	406	CDL	C82-C83-C84-C85
12	Q	102	SPO	C35-C36-C37-C38
12	A	603	SPO	C36-C37-C38-C40
12	D	102	SPO	C36-C37-C38-C40
12	D	104	SPO	C36-C37-C38-C40
12	P	101	SPO	C36-C37-C38-C39
12	9	102	SPO	C36-C37-C38-C39
9	A	604	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
12	D	103	SPO	C36-C37-C38-C39
12	I	104	SPO	C36-C37-C38-C40
12	M	405	SPO	C29-C28-C30-C31
12	D	103	SPO	C27-C28-C30-C31
12	E	102	SPO	C27-C28-C30-C31
12	I	103	SPO	C27-C28-C30-C31
12	K	102	SPO	C27-C28-C30-C31
12	R	103	SPO	C27-C28-C30-C31
12	R	103	SPO	C32-C33-C35-C36
12	S	103	SPO	C27-C28-C30-C31
12	9	102	SPO	C32-C33-C35-C36
12	I	103	SPO	C33-C35-C36-C37
12	K	102	SPO	C33-C35-C36-C37
12	P	101	SPO	C33-C35-C36-C37
12	R	103	SPO	C28-C30-C31-C32
12	9	102	SPO	C28-C30-C31-C32
12	0	101	SPO	C33-C35-C36-C37
12	0	102	SPO	C36-C37-C38-C39
12	P	102	SPO	C31-C32-C33-C35
9	X	1501	PC1	O32-C31-O31-C3
13	M	406	CDL	C11-C12-C13-C14
9	X	1501	PC1	C32-C31-O31-C3
12	D	103	SPO	C20-C21-C22-C23
12	S	103	SPO	C12-C14-C15-C16
9	A	604	PC1	C2E-C2F-C2G-C2H
13	M	406	CDL	C39-C40-C41-C42
7	L	305	BCL	C6-C7-C8-C9
7	N	101	BCL	C14-C13-C15-C16
7	C	101	BCL	C11-C10-C8-C9
12	M	405	SPO	C15-C16-C17-C18
12	M	405	SPO	C24-C23-C25-C26
12	D	104	SPO	C15-C16-C17-C18
12	E	102	SPO	C10-C11-C12-C13
12	E	102	SPO	C15-C16-C17-C18
12	E	102	SPO	C24-C23-C25-C26
12	F	103	SPO	C5-C6-C7-C8
12	F	103	SPO	C10-C11-C12-C13
12	I	104	SPO	C24-C23-C25-C26
12	K	102	SPO	C5-C6-C7-C8
12	K	103	SPO	C10-C11-C12-C13
12	P	101	SPO	C10-C11-C12-C13
12	P	101	SPO	C24-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
12	P	102	SPO	C5-C6-C7-C8
12	P	102	SPO	C15-C16-C17-C18
12	P	102	SPO	C24-C23-C25-C26
12	Q	102	SPO	C15-C16-C17-C18
12	Q	102	SPO	C24-C23-C25-C26
12	R	101	SPO	C15-C16-C17-C18
12	R	101	SPO	C24-C23-C25-C26
12	S	103	SPO	C10-C11-C12-C13
12	0	102	SPO	C15-C16-C17-C18
12	D	103	SPO	C5-C6-C7-C9
12	D	103	SPO	C10-C11-C12-C14
12	K	102	SPO	C10-C11-C12-C14
12	K	102	SPO	C22-C23-C25-C26
12	K	103	SPO	C5-C6-C7-C9
12	P	102	SPO	C5-C6-C7-C9
12	Q	102	SPO	C5-C6-C7-C9
12	R	103	SPO	C10-C11-C12-C14
12	9	102	SPO	C5-C6-C7-C9
12	0	101	SPO	C10-C11-C12-C14
9	L	303	PC1	C31-C32-C33-C34
9	L	303	PC1	C21-C22-C23-C24
9	H	1103	PC1	C31-C32-C33-C34
9	A	604	PC1	C31-C32-C33-C34
7	N	101	BCL	C13-C15-C16-C17
12	K	102	SPO	C31-C32-C33-C34
9	A	601	PC1	C21-C22-C23-C24
9	A	601	PC1	C31-C32-C33-C34
9	L	303	PC1	C22-C23-C24-C25
7	F	101	BCL	C10-C11-C12-C13
7	W	101	BCL	C11-C10-C8-C7
12	M	405	SPO	C20-C21-C22-C23
12	D	104	SPO	C25-C26-C27-C28
12	P	101	SPO	C11-C10-C9-C7
12	P	102	SPO	C17-C19-C20-C21
7	7	101	BCL	C10-C11-C12-C13
12	I	104	SPO	C28-C30-C31-C32
9	H	1103	PC1	C11-O13-P-O11
9	H	1103	PC1	C1-O11-P-O13
9	A	604	PC1	C11-O13-P-O11
9	A	604	PC1	C1-O11-P-O13
9	X	1501	PC1	C1-O11-P-O13
12	8	101	SPO	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
12	E	102	SPO	C17-C19-C20-C21
12	F	103	SPO	C8-C7-C9-C10
12	I	103	SPO	C13-C12-C14-C15
12	I	104	SPO	C21-C22-C23-C24
12	K	103	SPO	C18-C17-C19-C20
12	P	102	SPO	C13-C12-C14-C15
12	R	101	SPO	C21-C22-C23-C24
12	U	103	SPO	C8-C7-C9-C10
12	8	101	SPO	C13-C12-C14-C15
12	0	101	SPO	C8-C7-C9-C10
9	H	1101	PC1	C37-C38-C39-C3A
9	H	1102	PC1	C23-C24-C25-C26
9	A	601	PC1	C33-C34-C35-C36
13	M	406	CDL	C20-C21-C22-C23
9	H	1101	PC1	C35-C36-C37-C38
13	M	406	CDL	C80-C81-C82-C83
12	M	405	SPO	C6-C7-C9-C10
12	M	405	SPO	C11-C12-C14-C15
12	A	603	SPO	C6-C7-C9-C10
12	D	102	SPO	C6-C7-C9-C10
12	D	103	SPO	C11-C12-C14-C15
12	D	104	SPO	C21-C22-C23-C25
12	E	102	SPO	C6-C7-C9-C10
12	E	102	SPO	C16-C17-C19-C20
12	I	104	SPO	C21-C22-C23-C25
12	K	102	SPO	C11-C12-C14-C15
12	K	103	SPO	C16-C17-C19-C20
12	K	103	SPO	C21-C22-C23-C25
12	Q	102	SPO	C6-C7-C9-C10
12	R	101	SPO	C11-C12-C14-C15
12	R	101	SPO	C21-C22-C23-C25
12	U	103	SPO	C21-C22-C23-C25
12	8	101	SPO	C11-C12-C14-C15
12	0	101	SPO	C6-C7-C9-C10
12	0	102	SPO	C11-C12-C14-C15
12	0	102	SPO	C16-C17-C19-C20
7	O	101	BCL	C4-C3-C5-C6
7	O	101	BCL	C6-C7-C8-C9
9	H	1101	PC1	C33-C34-C35-C36
13	M	406	CDL	C33-C34-C35-C36
13	M	406	CDL	C73-C74-C75-C76
7	C	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	M	405	SPO	C10-C11-C12-C13
12	A	603	SPO	C24-C23-C25-C26
12	D	102	SPO	C24-C23-C25-C26
12	D	104	SPO	C10-C11-C12-C13
12	I	104	SPO	C10-C11-C12-C13
12	I	104	SPO	C15-C16-C17-C18
12	K	103	SPO	C15-C16-C17-C18
12	P	101	SPO	C15-C16-C17-C18
12	S	103	SPO	C24-C23-C25-C26
12	U	103	SPO	C24-C23-C25-C26
12	8	101	SPO	C10-C11-C12-C13
12	0	101	SPO	C24-C23-C25-C26
12	0	102	SPO	C10-C11-C12-C13
12	0	102	SPO	C24-C23-C25-C26
9	H	1101	PC1	C24-C25-C26-C27
12	A	603	SPO	C5-C6-C7-C9
12	D	102	SPO	C5-C6-C7-C9
12	R	103	SPO	C5-C6-C7-C9
12	S	103	SPO	C15-C16-C17-C19
9	H	1102	PC1	O22-C21-O21-C2
9	H	1102	PC1	C22-C21-O21-C2
9	H	1102	PC1	C37-C38-C39-C3A
10	L	304	U10	C14-C16-C17-C18
12	M	405	SPO	C28-C30-C31-C32
12	Q	102	SPO	C28-C30-C31-C32
9	H	1102	PC1	C32-C33-C34-C35
9	H	1101	PC1	C32-C31-O31-C3
9	H	1102	PC1	C39-C3A-C3B-C3C
9	X	1501	PC1	C35-C36-C37-C38
7	A	605	BCL	C3A-C2A-CAA-CBA
7	E	101	BCL	C3A-C2A-CAA-CBA
7	F	102	BCL	C3A-C2A-CAA-CBA
7	I	102	BCL	C3A-C2A-CAA-CBA
7	N	101	BCL	C3A-C2A-CAA-CBA
7	O	102	BCL	C3A-C2A-CAA-CBA
7	R	102	BCL	C3A-C2A-CAA-CBA
7	S	102	BCL	C3A-C2A-CAA-CBA
7	U	102	BCL	C3A-C2A-CAA-CBA
7	8	102	BCL	C3A-C2A-CAA-CBA
7	9	103	BCL	C3A-C2A-CAA-CBA
9	H	1102	PC1	C38-C39-C3A-C3B
7	S	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	L	304	U10	C15-C14-C16-C17
7	S	101	BCL	C2-C3-C5-C6
10	L	304	U10	C13-C14-C16-C17
9	H	1101	PC1	C32-C33-C34-C35
9	A	601	PC1	O22-C21-O21-C2
10	M	404	U10	C37-C38-C39-C40
9	H	1102	PC1	C33-C34-C35-C36
9	A	601	PC1	C22-C21-O21-C2
12	D	103	SPO	C36-C37-C38-C40
12	I	104	SPO	C36-C37-C38-C39
7	L	305	BCL	C6-C7-C8-C10
7	O	101	BCL	C2-C3-C5-C6
7	O	101	BCL	C6-C7-C8-C10
7	C	101	BCL	C6-C7-C8-C10
8	L	302	BPH	C2-C3-C5-C6
9	H	1101	PC1	O32-C31-O31-C3
9	H	1101	PC1	C2C-C2D-C2E-C2F
9	A	604	PC1	C33-C34-C35-C36
13	M	406	CDL	C32-C33-C34-C35
10	L	304	U10	C19-C21-C22-C23
9	H	1103	PC1	C22-C23-C24-C25
9	A	604	PC1	C22-C23-C24-C25
12	0	102	SPO	C36-C37-C38-C40
13	M	406	CDL	C76-C77-C78-C79
8	L	302	BPH	C4-C3-C5-C6
12	8	101	SPO	C27-C28-C30-C31
7	W	101	BCL	C11-C10-C8-C9
7	C	101	BCL	C6-C7-C8-C9
9	H	1101	PC1	C2A-C2B-C2C-C2D
12	D	103	SPO	C10-C11-C12-C13
12	P	102	SPO	C10-C11-C12-C13
12	0	102	SPO	C10-C11-C12-C14
9	A	604	PC1	C34-C35-C36-C37
13	M	406	CDL	C57-C58-C59-C60
12	M	405	SPO	C1-C4-C5-C6
13	M	406	CDL	C71-C72-C73-C74
7	C	101	BCL	C10-C11-C12-C13
12	R	101	SPO	C36-C37-C38-C40
13	M	406	CDL	C38-C39-C40-C41
12	M	405	SPO	C4-C1-O1-CM1
12	A	603	SPO	C28-C30-C31-C32
12	D	102	SPO	C28-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
12	U	103	SPO	C33-C35-C36-C37
9	H	1102	PC1	C1-C2-O21-C21
12	M	405	SPO	C3-C1-O1-CM1
12	I	104	SPO	C2-C1-O1-CM1
12	I	104	SPO	C3-C1-O1-CM1
12	K	103	SPO	C11-C12-C14-C15
12	P	101	SPO	C6-C7-C9-C10
12	9	102	SPO	C6-C7-C9-C10
12	0	102	SPO	C2-C1-O1-CM1
12	D	103	SPO	C2-C1-C4-C5
12	D	103	SPO	C3-C1-C4-C5
12	I	103	SPO	C2-C1-C4-C5
12	I	103	SPO	C3-C1-C4-C5
12	I	104	SPO	C2-C1-C4-C5
12	K	103	SPO	C2-C1-C4-C5
12	K	103	SPO	C3-C1-C4-C5
12	Q	102	SPO	C2-C1-C4-C5
13	M	406	CDL	C54-C55-C56-C57
7	S	101	BCL	C6-C7-C8-C10
12	A	603	SPO	C27-C28-C30-C31
12	D	102	SPO	C27-C28-C30-C31
7	U	101	BCL	C11-C10-C8-C9
7	7	101	BCL	C6-C7-C8-C9
12	U	103	SPO	C25-C26-C27-C28
10	M	404	U10	C37-C38-C39-C41
12	D	104	SPO	C36-C37-C38-C39
12	D	103	SPO	O1-C1-C4-C5
12	I	103	SPO	O1-C1-C4-C5
12	K	103	SPO	O1-C1-C4-C5
13	M	406	CDL	C37-C38-C39-C40
9	H	1103	PC1	C32-C31-O31-C3
9	A	604	PC1	C32-C31-O31-C3
9	H	1102	PC1	O11-C1-C2-C3
10	M	404	U10	C34-C36-C37-C38
12	9	102	SPO	C27-C28-C30-C31
12	0	101	SPO	C32-C33-C35-C36
12	M	405	SPO	C36-C37-C38-C39
9	A	601	PC1	C2-C1-O11-P
13	M	406	CDL	C1-CA2-OA2-PA1
12	E	102	SPO	C20-C21-C22-C23
9	H	1101	PC1	C21-C22-C23-C24
9	L	303	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
9	H	1103	PC1	C1-C2-C3-O31
9	A	604	PC1	C1-C2-C3-O31
10	M	404	U10	C30-C29-C31-C32
9	H	1101	PC1	C11-O13-P-O11
13	M	406	CDL	C35-C36-C37-C38
9	H	1102	PC1	O11-C1-C2-O21
13	M	406	CDL	OB5-CB3-CB4-OB6
9	H	1103	PC1	C33-C34-C35-C36
10	L	304	U10	C29-C31-C32-C33
12	D	103	SPO	C28-C30-C31-C32
9	A	604	PC1	C35-C36-C37-C38
10	M	404	U10	C28-C29-C31-C32
12	I	103	SPO	C32-C33-C35-C36
7	C	101	BCL	C14-C13-C15-C16
9	A	604	PC1	C29-C2A-C2B-C2C
7	W	101	BCL	C4C-C3C-CAC-CBC
12	M	405	SPO	C5-C6-C7-C9
12	D	104	SPO	C5-C6-C7-C9
9	H	1102	PC1	C25-C26-C27-C28
10	L	304	U10	C20-C19-C21-C22
7	N	101	BCL	C12-C13-C15-C16
7	U	101	BCL	C11-C10-C8-C7
7	C	101	BCL	C11-C10-C8-C7
7	7	101	BCL	C6-C7-C8-C10
7	9	101	BCL	C11-C10-C8-C7
12	E	102	SPO	C32-C33-C35-C36
12	K	102	SPO	C32-C33-C35-C36
12	D	103	SPO	C25-C26-C27-C28
12	D	104	SPO	C20-C21-C22-C23
12	K	102	SPO	C12-C14-C15-C16
12	U	103	SPO	C12-C14-C15-C16
12	8	101	SPO	C25-C26-C27-C28
12	D	104	SPO	C13-C12-C14-C15
12	E	102	SPO	C21-C22-C23-C24
12	F	103	SPO	C13-C12-C14-C15
12	P	102	SPO	C21-C22-C23-C24
13	M	406	CDL	C18-C19-C20-C21
8	L	302	BPH	CAD-CBD-CGD-O2D
9	A	604	PC1	C27-C28-C29-C2A
10	M	404	U10	C35-C34-C36-C37
10	L	304	U10	C5-C4-O4-C4M
9	H	1101	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
9	L	303	PC1	C27-C28-C29-C2A
7	U	101	BCL	C10-C11-C12-C13
9	H	1103	PC1	O32-C31-O31-C3
9	A	604	PC1	O32-C31-O31-C3
12	D	103	SPO	C16-C17-C19-C20
9	H	1101	PC1	O21-C2-C3-O31
9	A	604	PC1	C25-C26-C27-C28
13	M	406	CDL	C62-C63-C64-C65
12	D	103	SPO	C5-C6-C7-C8
9	X	1501	PC1	C22-C23-C24-C25
12	D	104	SPO	C22-C23-C25-C26
7	L	305	BCL	C1A-C2A-CAA-CBA
7	2	101	BCL	C1A-C2A-CAA-CBA
12	R	101	SPO	C12-C14-C15-C16
9	H	1102	PC1	C1-O11-P-O13
12	Q	102	SPO	C29-C28-C30-C31
10	L	304	U10	C18-C19-C21-C22
13	M	406	CDL	C42-C43-C44-C45
9	H	1102	PC1	C1-O11-P-O14
9	A	601	PC1	C1-O11-P-O12
9	X	1501	PC1	C1-O11-P-O12
13	M	406	CDL	OB5-CB3-CB4-CB6
12	U	103	SPO	C28-C30-C31-C32
9	L	303	PC1	C12-C11-O13-P
9	H	1102	PC1	C12-C11-O13-P
12	A	603	SPO	C1-C4-C5-C6
12	D	102	SPO	C1-C4-C5-C6
9	X	1501	PC1	C31-C32-C33-C34
12	D	103	SPO	C34-C33-C35-C36
7	L	305	BCL	C3A-C2A-CAA-CBA
7	E	101	BCL	C12-C13-C15-C16
7	W	101	BCL	C2C-C3C-CAC-CBC
9	H	1103	PC1	C25-C26-C27-C28
9	L	303	PC1	C25-C26-C27-C28
9	H	1102	PC1	O13-C11-C12-N
9	H	1103	PC1	O21-C2-C3-O31
9	A	604	PC1	O21-C2-C3-O31
9	H	1102	PC1	C2-C1-O11-P
7	7	101	BCL	C4-C3-C5-C6
7	S	101	BCL	C6-C7-C8-C9
7	9	101	BCL	C11-C10-C8-C9
12	P	101	SPO	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	0	101	SPO	C9-C10-C11-C12
12	0	102	SPO	C9-C10-C11-C12
9	H	1101	PC1	C28-C29-C2A-C2B
9	A	601	PC1	C35-C36-C37-C38
12	8	101	SPO	C15-C16-C17-C19
13	M	406	CDL	C84-C85-C86-C87
7	9	101	BCL	C4-C3-C5-C6
9	H	1103	PC1	C24-C25-C26-C27
9	A	604	PC1	C24-C25-C26-C27
9	H	1102	PC1	O21-C21-C22-C23
12	R	101	SPO	C34-C33-C35-C36
10	M	404	U10	C33-C34-C36-C37
12	M	405	SPO	C2-C1-O1-CM1
12	S	103	SPO	C28-C30-C31-C32
12	S	103	SPO	C33-C35-C36-C37
7	S	102	BCL	C13-C15-C16-C17
9	L	303	PC1	C1-O11-P-O13
13	M	406	CDL	CA3-OA5-PA1-OA2
12	F	103	SPO	C2-C1-C4-C5
7	E	101	BCL	C14-C13-C15-C16
7	8	102	BCL	C13-C15-C16-C17
12	P	102	SPO	C20-C21-C22-C23
12	U	103	SPO	C17-C19-C20-C21
12	9	102	SPO	C12-C14-C15-C16
13	M	406	CDL	C60-C61-C62-C63
13	M	406	CDL	C79-C80-C81-C82
12	R	101	SPO	C5-C6-C7-C8
12	R	101	SPO	C22-C23-C25-C26
9	H	1101	PC1	C2E-C2F-C2G-C2H
12	K	102	SPO	C31-C32-C33-C35
7	9	101	BCL	C2-C3-C5-C6
12	F	103	SPO	C17-C19-C20-C21
12	Q	102	SPO	C17-C19-C20-C21
12	R	101	SPO	C20-C21-C22-C23
12	D	104	SPO	C28-C30-C31-C32
12	A	603	SPO	C29-C28-C30-C31
12	D	102	SPO	C29-C28-C30-C31
9	X	1501	PC1	C24-C25-C26-C27
7	C	101	BCL	C2-C1-O2A-CGA
7	2	101	BCL	C3A-C2A-CAA-CBA
12	P	101	SPO	C20-C21-C22-C23
12	R	103	SPO	C12-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
7	7	101	BCL	C2-C3-C5-C6
7	8	102	BCL	C14-C13-C15-C16
7	O	101	BCL	C5-C6-C7-C8
12	R	103	SPO	C8-C7-C9-C10
8	L	302	BPH	O2A-C1-C2-C3
12	K	103	SPO	C24-C23-C25-C26
13	M	406	CDL	C43-C44-C45-C46
7	C	101	BCL	C1A-C2A-CAA-CBA
9	X	1501	PC1	C11-C12-N-C14
12	0	101	SPO	C25-C26-C27-C28
9	A	601	PC1	C1-O11-P-O13
7	S	101	BCL	C8-C10-C11-C12
12	Q	102	SPO	C31-C32-C33-C34
7	A	605	BCL	C4-C3-C5-C6
7	E	101	BCL	C4-C3-C5-C6
7	F	102	BCL	C4-C3-C5-C6
7	I	102	BCL	C4-C3-C5-C6
7	N	101	BCL	C4-C3-C5-C6
7	O	102	BCL	C4-C3-C5-C6
7	R	102	BCL	C4-C3-C5-C6
7	S	102	BCL	C4-C3-C5-C6
7	U	102	BCL	C4-C3-C5-C6
7	8	102	BCL	C4-C3-C5-C6
7	9	103	BCL	C4-C3-C5-C6
9	H	1102	PC1	C24-C25-C26-C27
12	P	101	SPO	C11-C12-C14-C15
7	2	101	BCL	CAA-CBA-CGA-O2A
12	I	103	SPO	C25-C26-C27-C28
7	2	101	BCL	CAA-CBA-CGA-O1A
7	M	403	BCL	C10-C11-C12-C13
12	D	104	SPO	C34-C33-C35-C36
12	P	102	SPO	C34-C33-C35-C36
9	A	604	PC1	C28-C29-C2A-C2B
12	Q	102	SPO	C32-C33-C35-C36
12	U	103	SPO	C32-C33-C35-C36
13	M	406	CDL	CB5-C51-C52-C53
7	E	101	BCL	C13-C15-C16-C17
12	M	405	SPO	C17-C19-C20-C21
12	D	103	SPO	C11-C10-C9-C7
7	C	101	BCL	C4-C3-C5-C6
12	8	101	SPO	C34-C33-C35-C36
9	L	303	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
13	M	406	CDL	C53-C54-C55-C56
7	U	102	BCL	C15-C16-C17-C18
7	7	101	BCL	C11-C12-C13-C15
9	A	601	PC1	O11-C1-C2-O21
9	X	1501	PC1	C33-C34-C35-C36
10	M	404	U10	C5-C4-O4-C4M
9	A	601	PC1	O11-C1-C2-C3
12	A	603	SPO	C34-C33-C35-C36
12	D	102	SPO	C34-C33-C35-C36
12	K	103	SPO	C34-C33-C35-C36
9	H	1101	PC1	C2-C1-O11-P
10	M	404	U10	C3-C4-O4-C4M
10	L	304	U10	C30-C29-C31-C32
7	L	305	BCL	C8-C10-C11-C12
7	A	605	BCL	C2-C3-C5-C6
7	E	101	BCL	C2-C3-C5-C6
7	F	102	BCL	C2-C3-C5-C6
7	I	102	BCL	C2-C3-C5-C6
7	N	101	BCL	C2-C3-C5-C6
7	O	102	BCL	C2-C3-C5-C6
7	R	102	BCL	C2-C3-C5-C6
7	S	102	BCL	C2-C3-C5-C6
7	U	102	BCL	C2-C3-C5-C6
7	8	102	BCL	C2-C3-C5-C6
7	9	103	BCL	C2-C3-C5-C6
7	S	102	BCL	C14-C13-C15-C16
7	C	101	BCL	C3A-C2A-CAA-CBA
13	M	406	CDL	C72-C71-CB7-OB8
7	M	401	BCL	CAD-CBD-CGD-O2D
8	L	306	BPH	CAD-CBD-CGD-O2D
12	I	103	SPO	C11-C10-C9-C7
9	H	1101	PC1	C34-C35-C36-C37
7	C	101	BCL	C8-C10-C11-C12
12	0	102	SPO	C34-C33-C35-C36
7	C	101	BCL	C2-C3-C5-C6
10	L	304	U10	C28-C29-C31-C32
12	S	103	SPO	C10-C11-C12-C14
12	0	101	SPO	C5-C6-C7-C9
13	M	406	CDL	OA5-CA3-CA4-OA6
8	L	306	BPH	O2A-C1-C2-C3
7	7	101	BCL	CHA-CBD-CGD-O1D
7	7	101	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
7	2	101	BCL	CHA-CBD-CGD-O1D
7	2	101	BCL	CHA-CBD-CGD-O2D
12	0	102	SPO	C25-C26-C27-C28
7	7	101	BCL	CAA-CBA-CGA-O2A
9	H	1101	PC1	O31-C31-C32-C33
12	K	102	SPO	C6-C7-C9-C10
9	A	601	PC1	O31-C31-C32-C33
7	E	101	BCL	C15-C16-C17-C18
9	L	303	PC1	O21-C21-C22-C23
9	X	1501	PC1	C11-C12-N-C13
9	H	1103	PC1	C21-C22-C23-C24
9	A	604	PC1	C21-C22-C23-C24
12	A	603	SPO	C12-C14-C15-C16
12	D	102	SPO	C12-C14-C15-C16
7	M	403	BCL	C13-C15-C16-C17
9	H	1101	PC1	O32-C31-C32-C33
7	A	605	BCL	CAA-CBA-CGA-O2A
7	E	101	BCL	CAA-CBA-CGA-O2A
7	F	102	BCL	CAA-CBA-CGA-O2A
7	I	102	BCL	CAA-CBA-CGA-O2A
7	N	101	BCL	CAA-CBA-CGA-O2A
7	O	102	BCL	CAA-CBA-CGA-O2A
7	R	102	BCL	CAA-CBA-CGA-O2A
7	S	102	BCL	CAA-CBA-CGA-O2A
7	U	102	BCL	CAA-CBA-CGA-O2A
7	8	102	BCL	CAA-CBA-CGA-O2A
7	9	103	BCL	CAA-CBA-CGA-O2A
7	L	301	BCL	C2A-CAA-CBA-CGA
9	H	1102	PC1	C11-O13-P-O12
9	X	1501	PC1	C11-C12-N-C15
13	M	406	CDL	CB2-OB2-PB2-OB4
9	X	1501	PC1	C38-C39-C3A-C3B
13	M	406	CDL	C72-C71-CB7-OB9
7	7	101	BCL	CAA-CBA-CGA-O1A
7	L	305	BCL	C10-C11-C12-C13
9	L	303	PC1	O22-C21-C22-C23
7	S	101	BCL	C5-C6-C7-C8
7	L	301	BCL	C4-C3-C5-C6
12	K	103	SPO	C35-C36-C37-C38
7	O	101	BCL	CAD-CBD-CGD-O1D
7	7	101	BCL	CAD-CBD-CGD-O1D
7	A	605	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
7	E	101	BCL	CAA-CBA-CGA-O1A
7	F	102	BCL	CAA-CBA-CGA-O1A
7	I	102	BCL	CAA-CBA-CGA-O1A
7	N	101	BCL	CAA-CBA-CGA-O1A
7	O	102	BCL	CAA-CBA-CGA-O1A
7	R	102	BCL	CAA-CBA-CGA-O1A
7	S	102	BCL	CAA-CBA-CGA-O1A
7	U	102	BCL	CAA-CBA-CGA-O1A
7	8	102	BCL	CAA-CBA-CGA-O1A
7	9	103	BCL	CAA-CBA-CGA-O1A
9	H	1102	PC1	O31-C31-C32-C33
7	F	101	BCL	C8-C10-C11-C12
12	F	103	SPO	C1-C4-C5-C6
9	H	1102	PC1	C21-C22-C23-C24
9	A	601	PC1	O32-C31-C32-C33
7	S	101	BCL	C11-C12-C13-C15
12	E	102	SPO	C5-C6-C7-C9
12	I	104	SPO	C22-C23-C25-C26
7	F	102	BCL	C13-C15-C16-C17
12	P	101	SPO	C35-C36-C37-C38
12	K	103	SPO	C29-C28-C30-C31
12	0	102	SPO	C29-C28-C30-C31

There are no ring outliers.

62 monomers are involved in 214 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	102	BCL	2	0
7	L	305	BCL	2	0
9	H	1101	PC1	2	0
9	H	1102	PC1	3	0
7	U	101	BCL	6	0
12	F	103	SPO	3	0
12	8	101	SPO	3	0
7	M	401	BCL	3	0
7	Q	101	BCL	4	0
7	8	102	BCL	3	0
8	L	306	BPH	1	0
12	P	102	SPO	6	0
7	O	101	BCL	4	0
12	9	102	SPO	4	0
7	9	103	BCL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	604	PC1	4	0
12	0	101	SPO	2	0
7	C	101	BCL	3	0
7	9	101	BCL	3	0
7	R	102	BCL	4	0
12	D	104	SPO	7	0
10	L	304	U10	6	0
7	F	101	BCL	2	0
12	K	102	SPO	4	0
12	I	104	SPO	3	0
12	K	103	SPO	5	0
12	P	101	SPO	4	0
9	L	303	PC1	2	0
7	L	301	BCL	2	0
7	N	101	BCL	7	0
12	A	603	SPO	3	0
7	E	101	BCL	6	0
7	S	101	BCL	4	0
7	A	602	BCL	5	0
7	M	403	BCL	1	0
12	D	102	SPO	5	0
12	Q	102	SPO	6	0
7	W	101	BCL	6	0
7	D	101	BCL	2	0
7	O	102	BCL	4	0
7	I	101	BCL	1	0
7	U	102	BCL	8	0
7	1	101	BCL	3	0
12	R	103	SPO	4	0
7	A	605	BCL	7	0
10	M	404	U10	2	0
7	7	101	BCL	6	0
12	S	103	SPO	7	0
12	M	405	SPO	4	0
12	D	103	SPO	6	0
12	E	102	SPO	3	0
12	I	103	SPO	3	0
12	R	101	SPO	8	0
8	L	302	BPH	2	0
12	U	103	SPO	5	0
12	0	102	SPO	3	0
7	I	102	BCL	6	0

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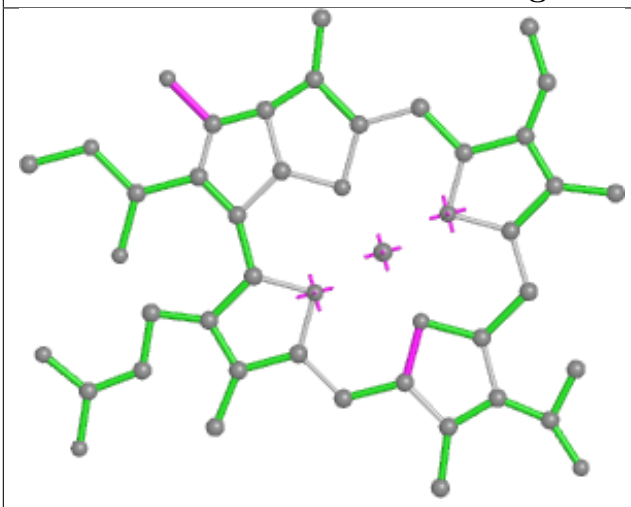
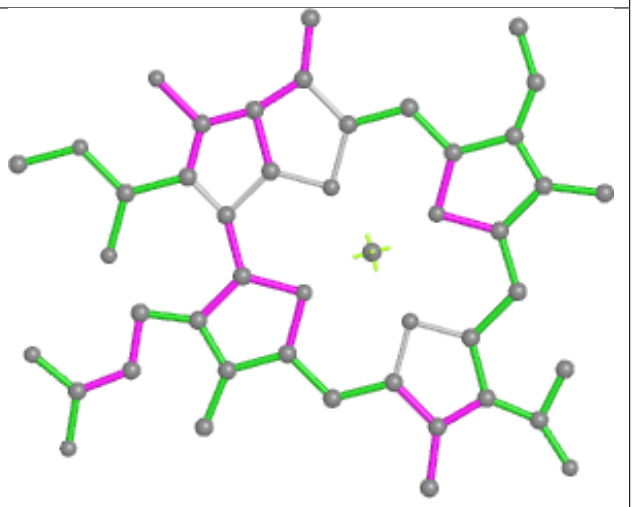
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	406	CDL	9	0
7	S	102	BCL	6	0
9	H	1103	PC1	5	0
9	A	601	PC1	5	0
7	K	101	BCL	2	0

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

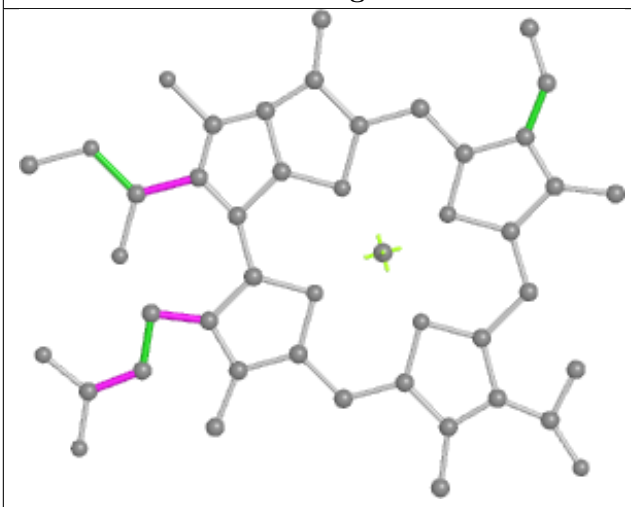
Ligand BCL 2 101



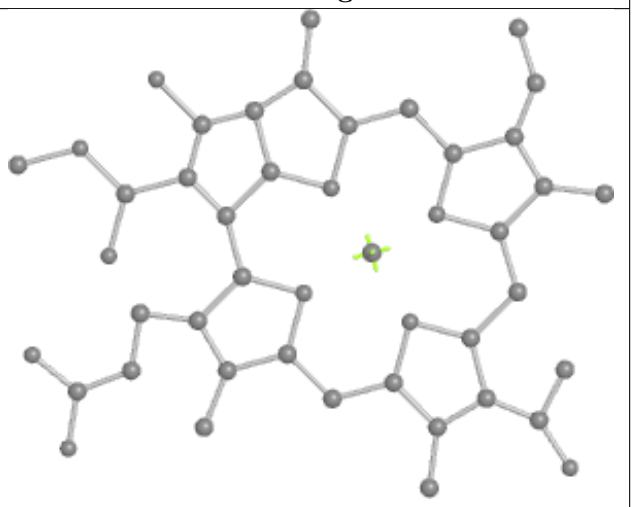
Bond lengths



Bond angles

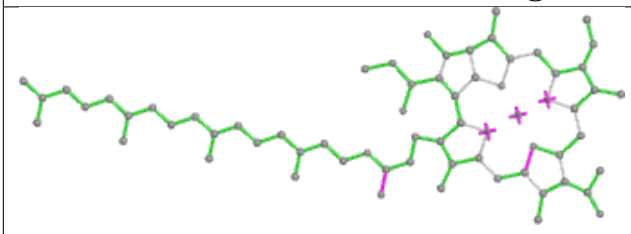


Torsions

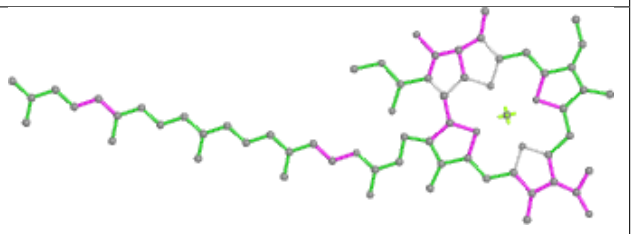


Rings

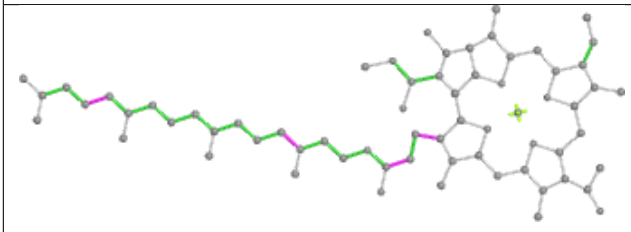
Ligand BCL F 102



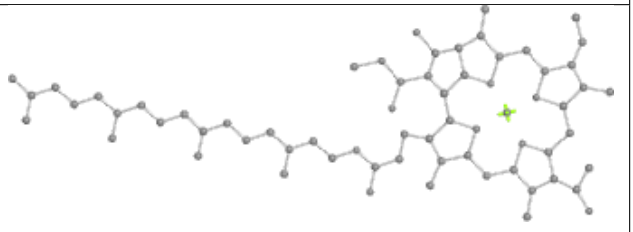
Bond lengths



Bond angles

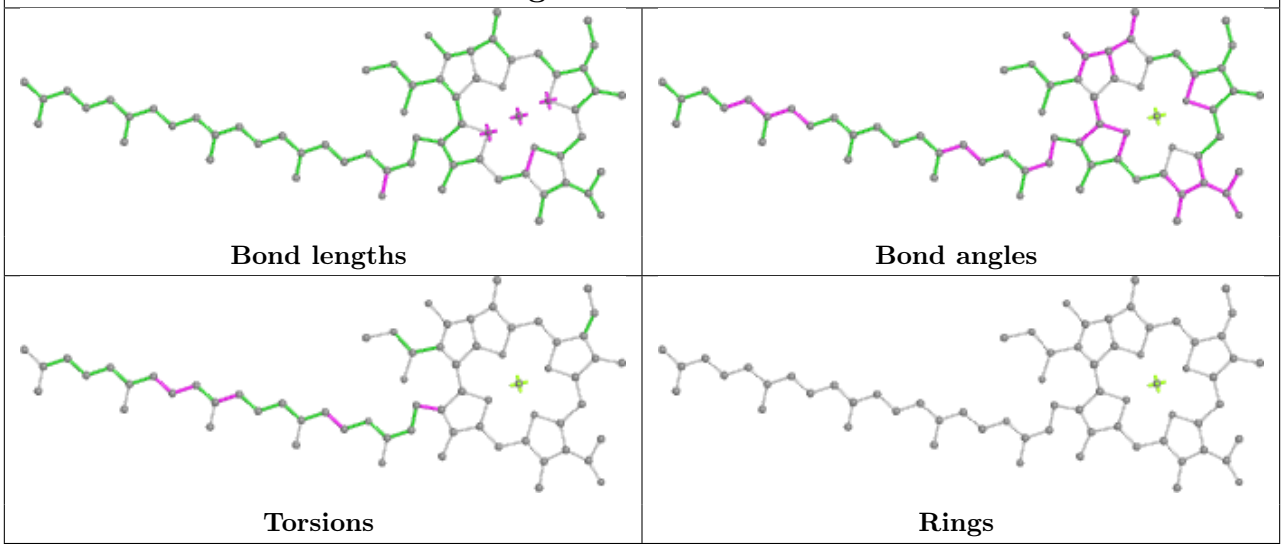


Torsions

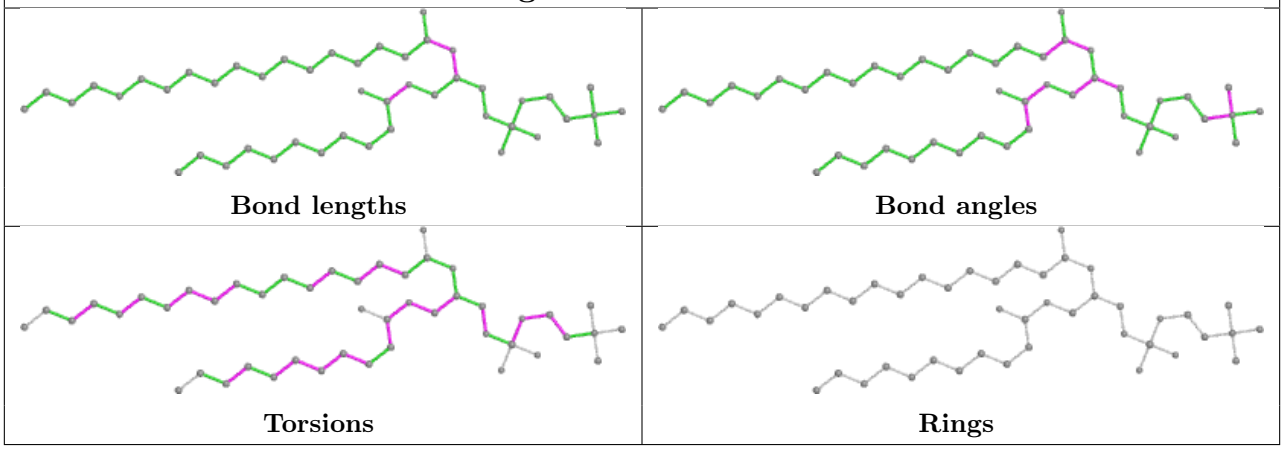


Rings

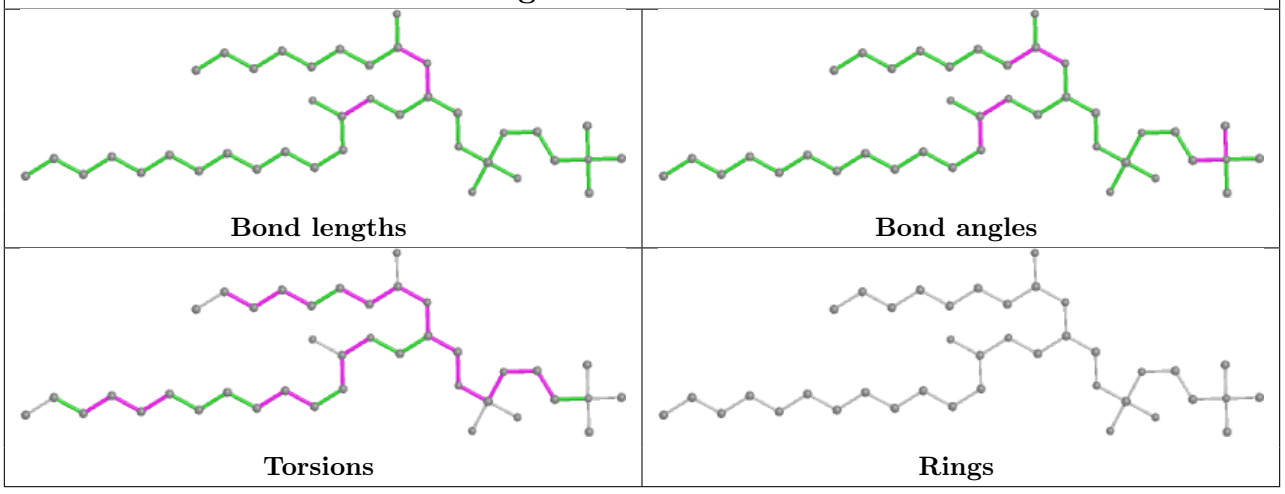
Ligand BCL L 305



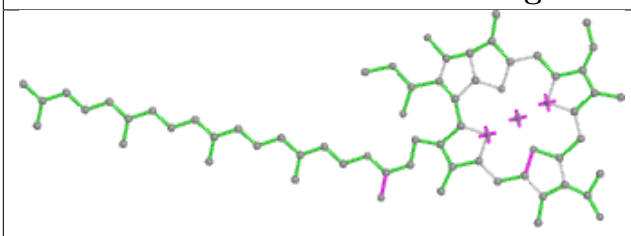
Ligand PC1 H 1101



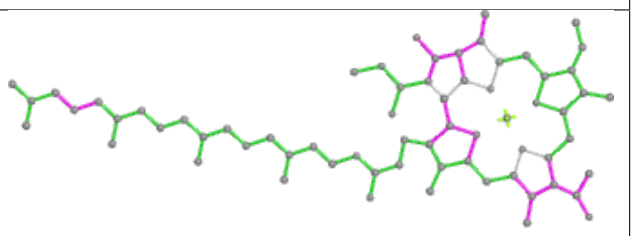
Ligand PC1 H 1102



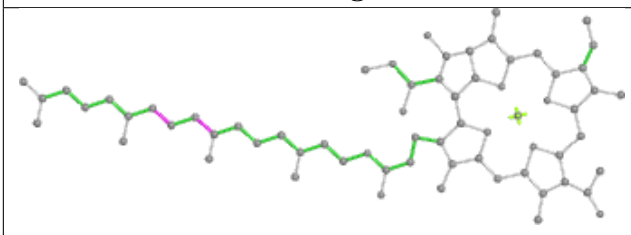
Ligand BCL U 101



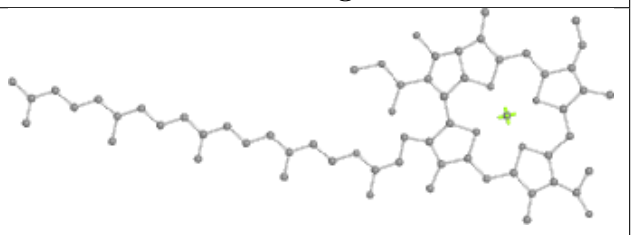
Bond lengths



Bond angles

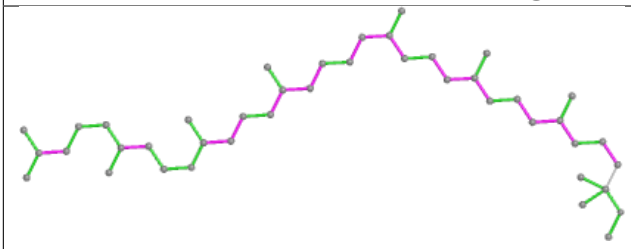


Torsions

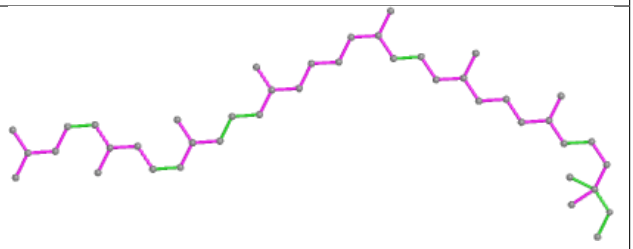


Rings

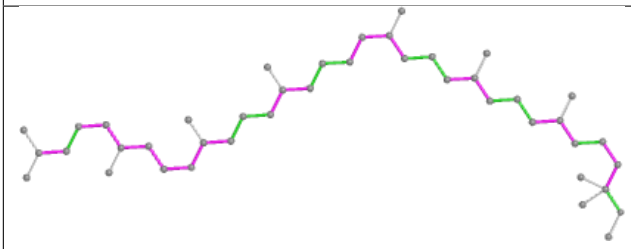
Ligand SPO F 103



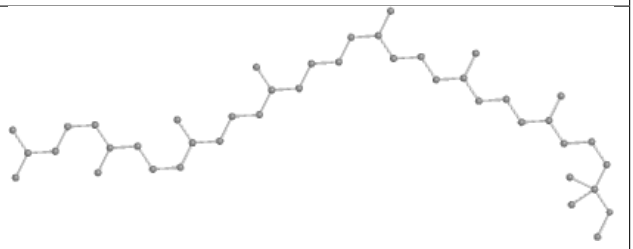
Bond lengths



Bond angles

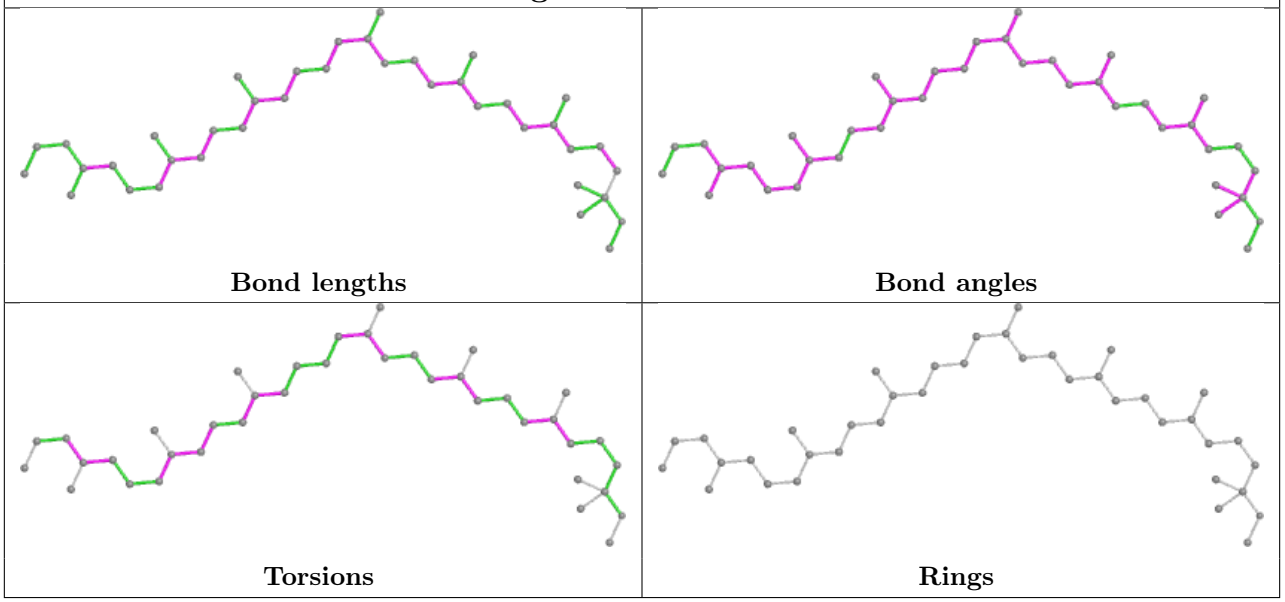


Torsions

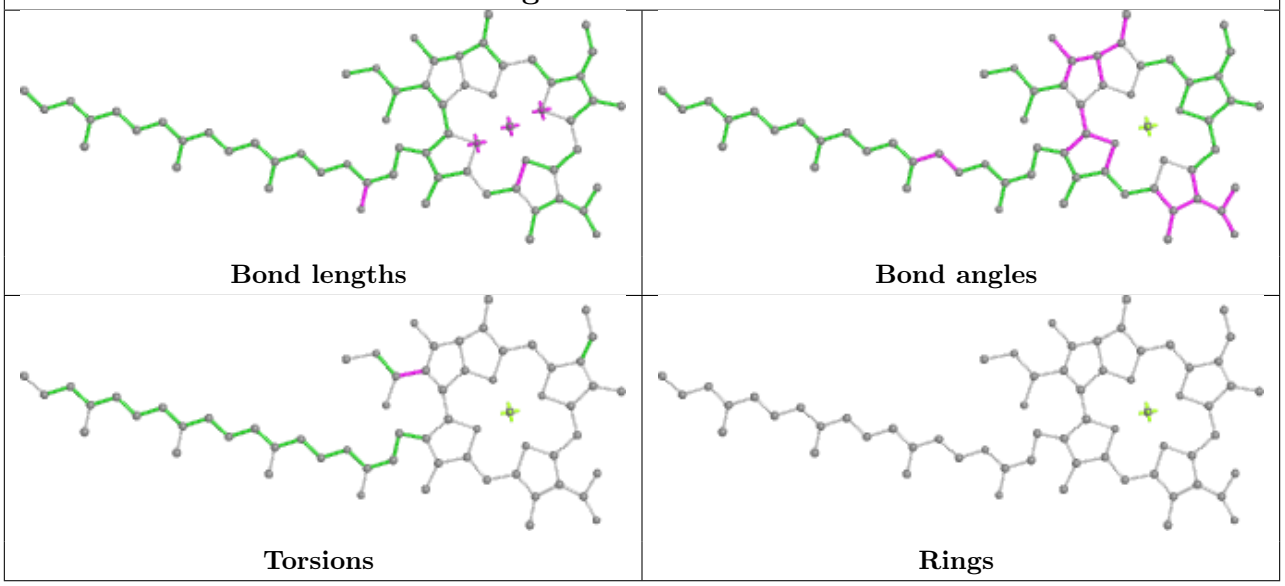


Rings

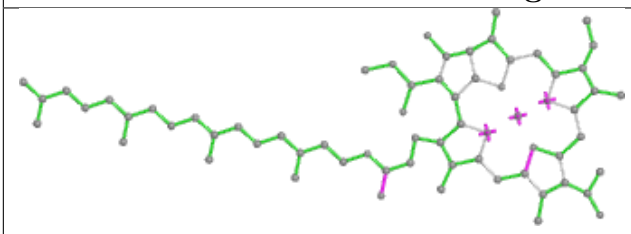
Ligand SPO 8 101



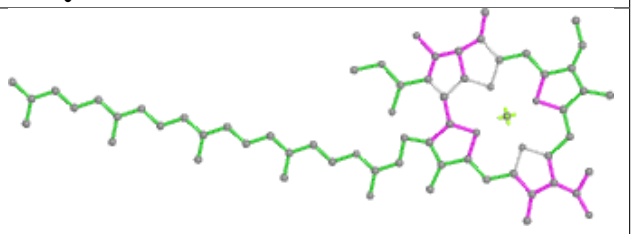
Ligand BCL M 401



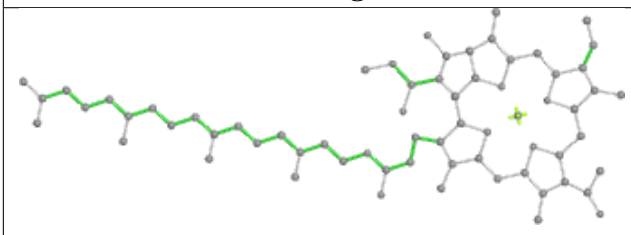
Ligand BCL Q 101



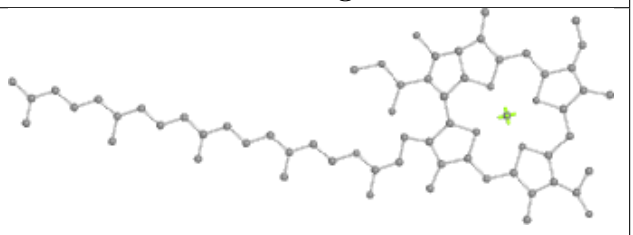
Bond lengths



Bond angles

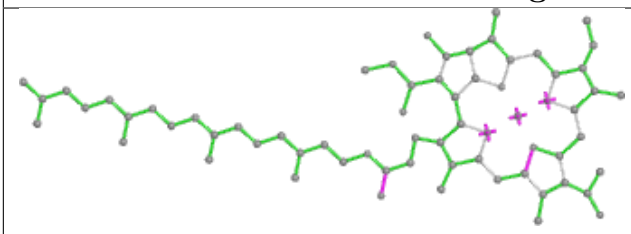


Torsions

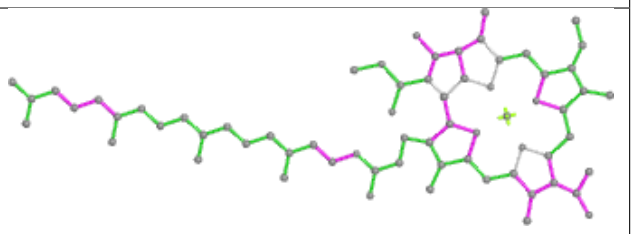


Rings

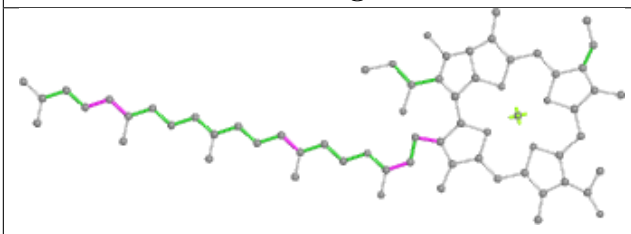
Ligand BCL 8 102



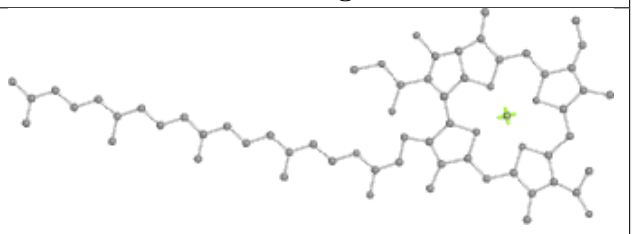
Bond lengths



Bond angles

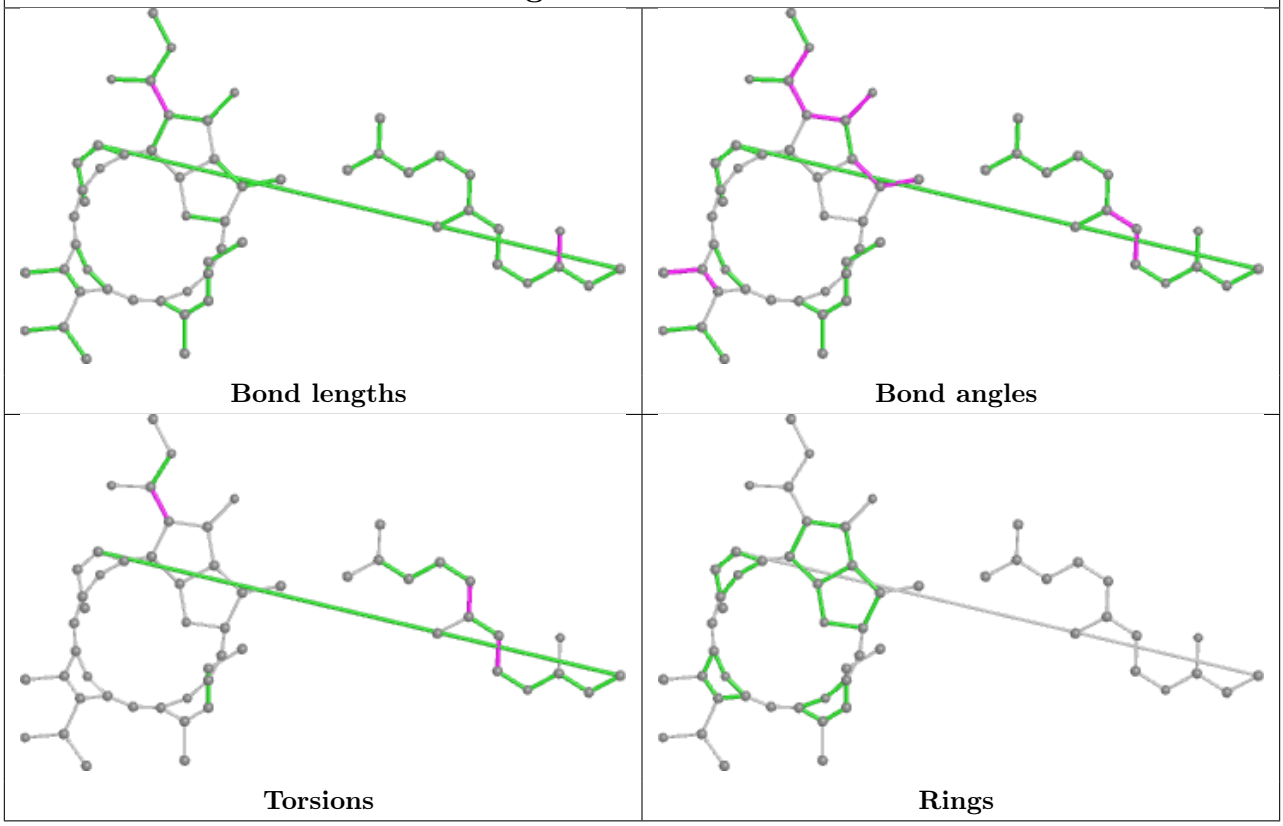


Torsions

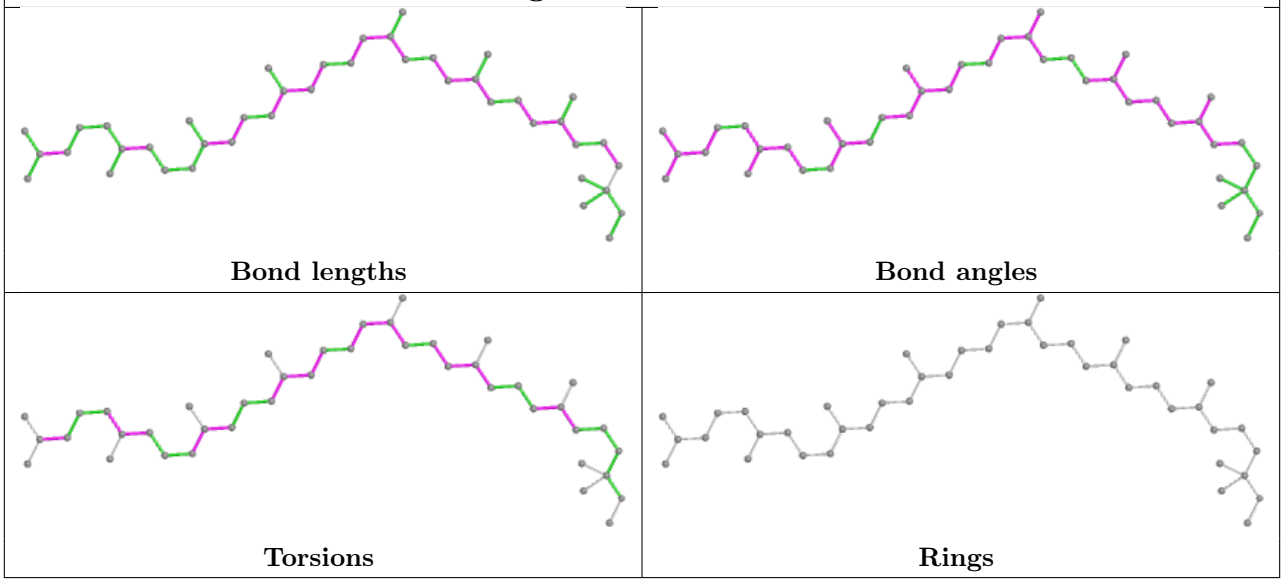


Rings

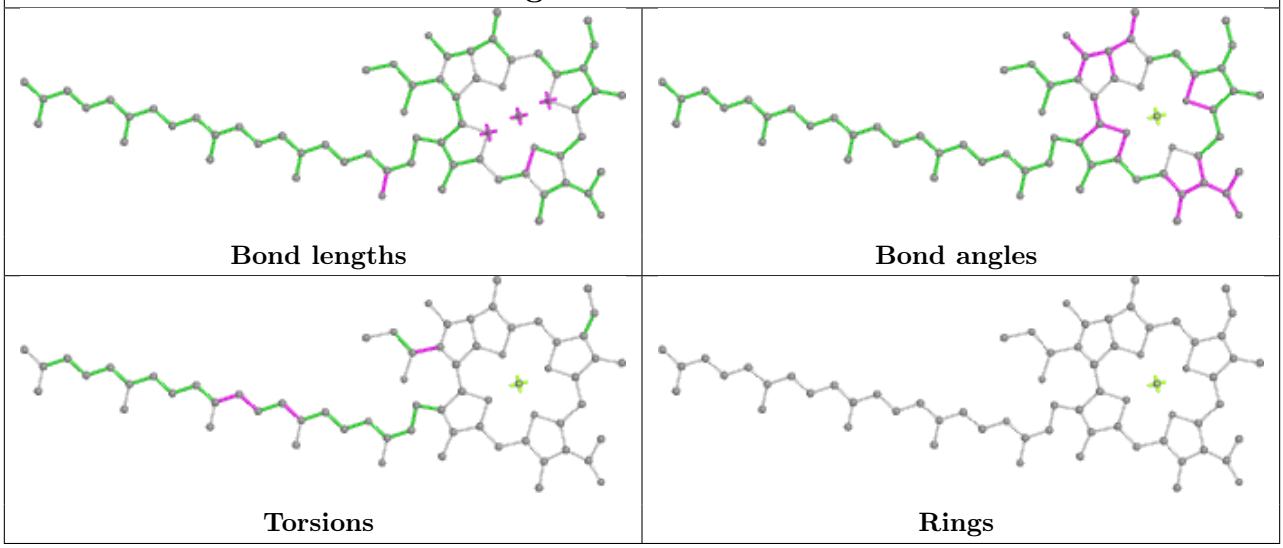
Ligand BPH L 306



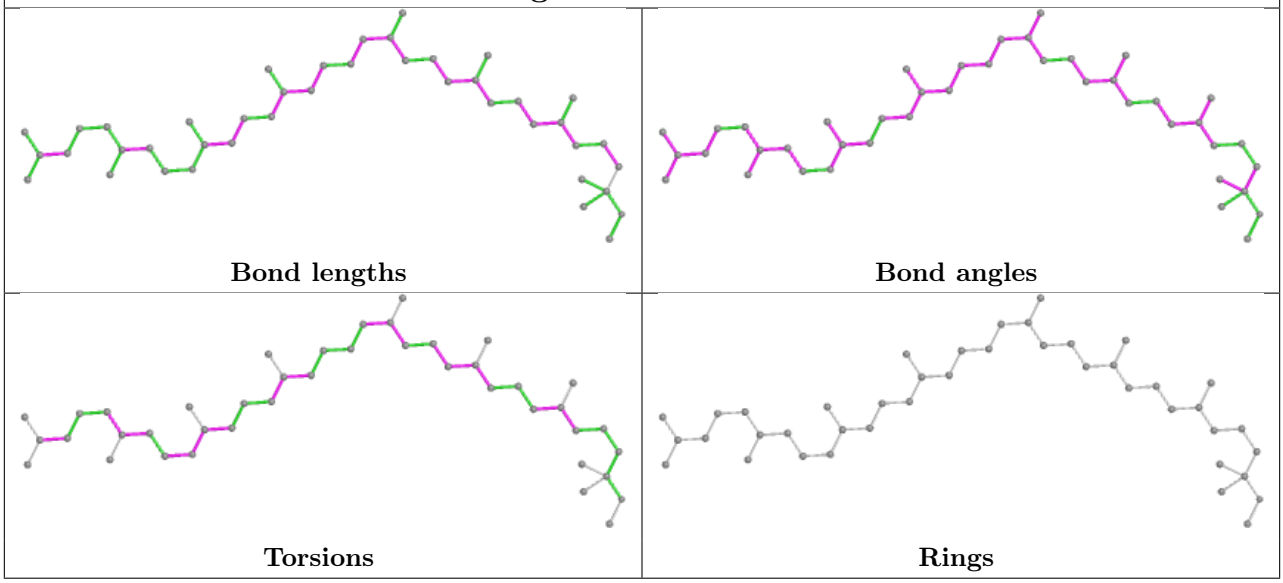
Ligand SPO P 102



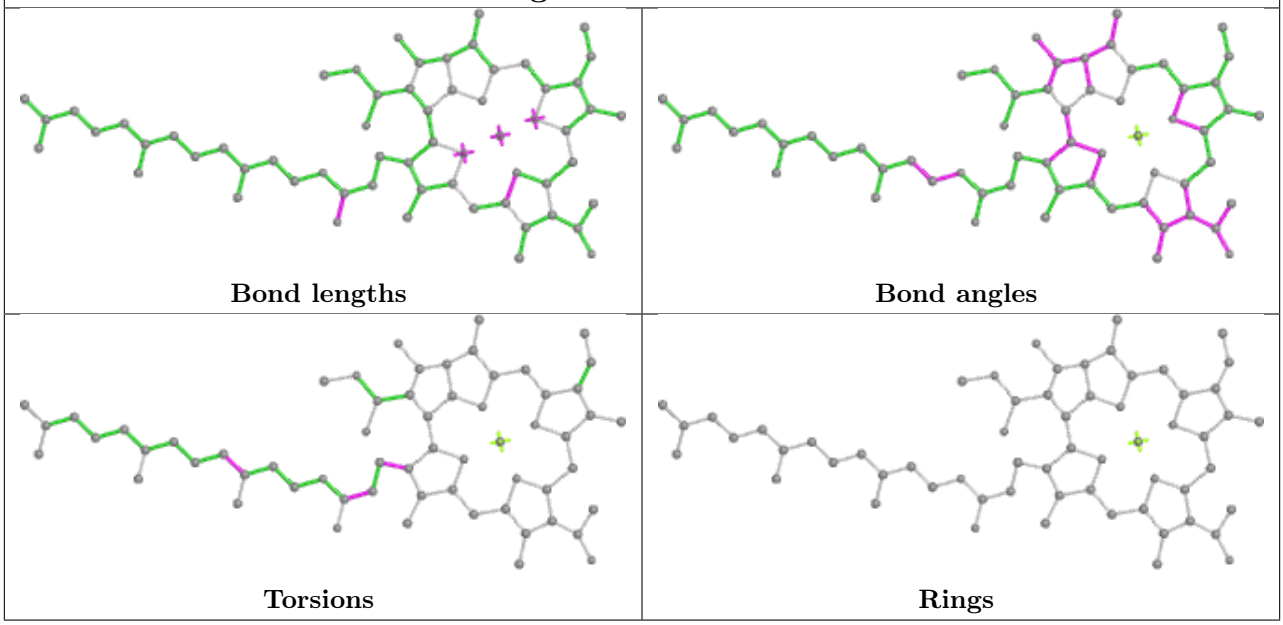
Ligand BCL O 101



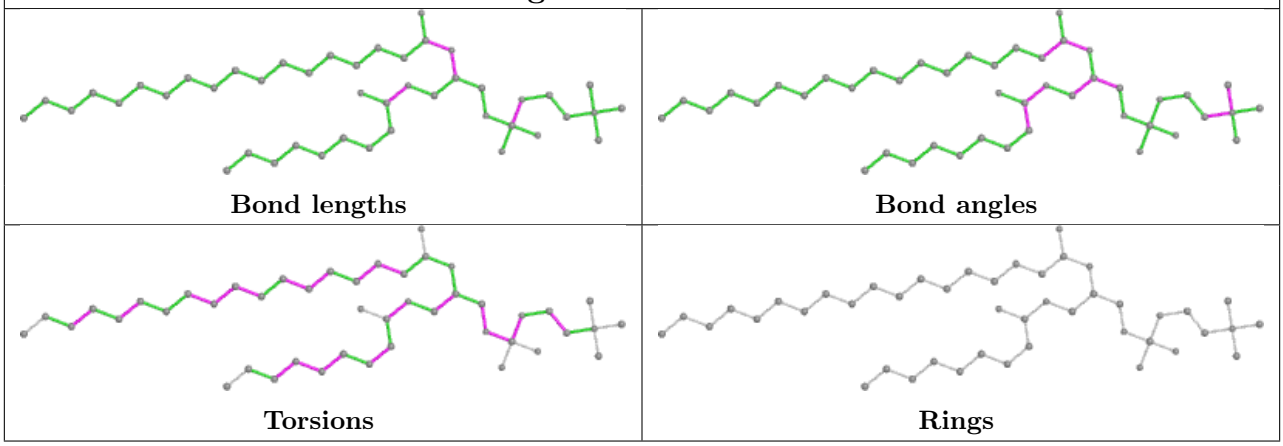
Ligand SPO 9 102



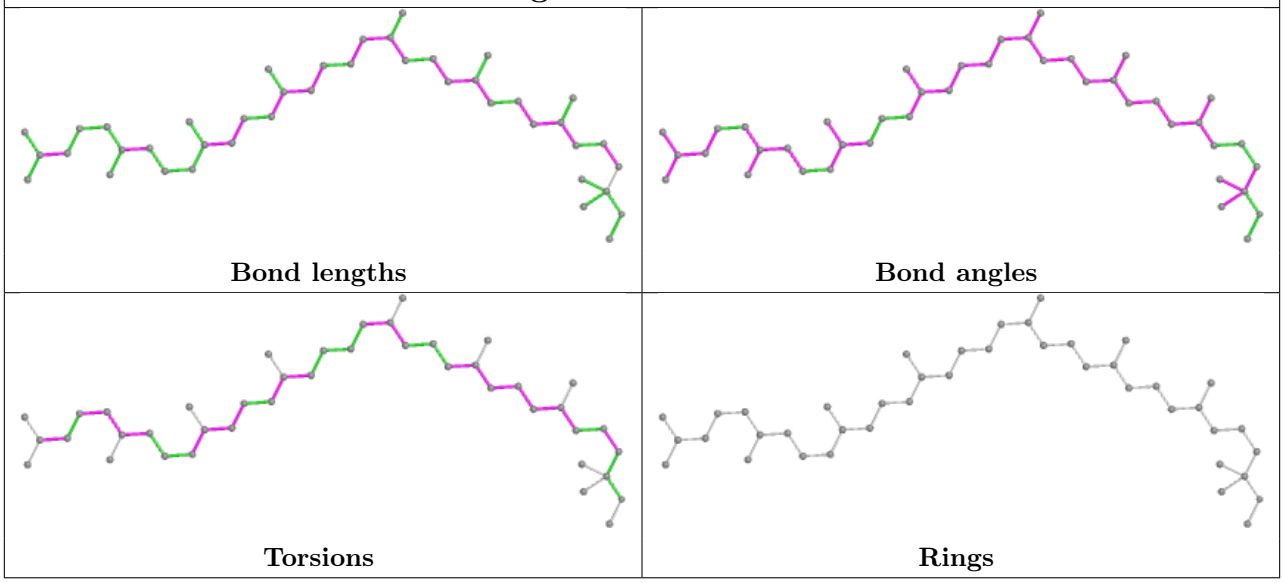
Ligand BCL 9 103



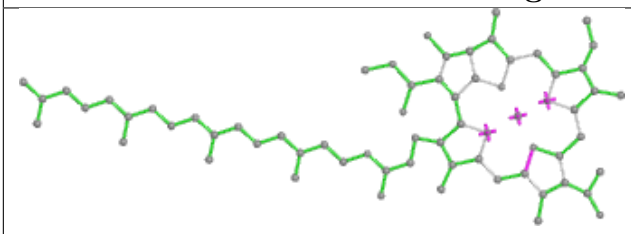
Ligand PC1 A 604



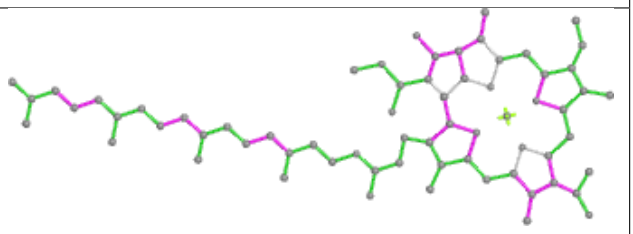
Ligand SPO 0 101



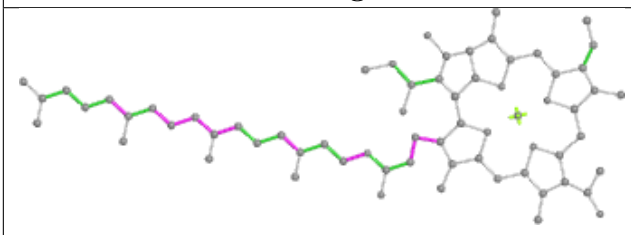
Ligand BCL C 101



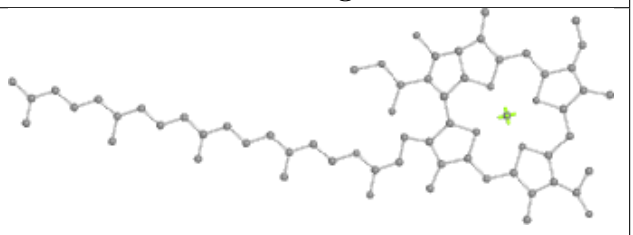
Bond lengths



Bond angles

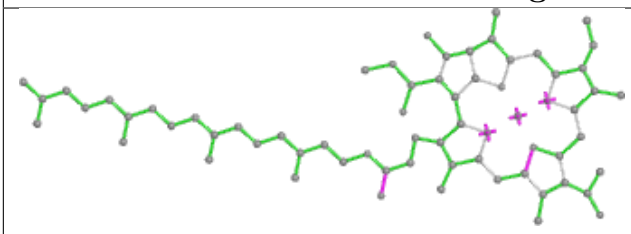


Torsions

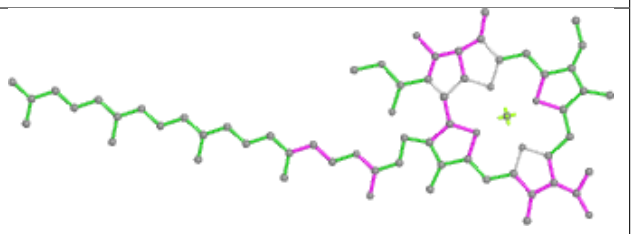


Rings

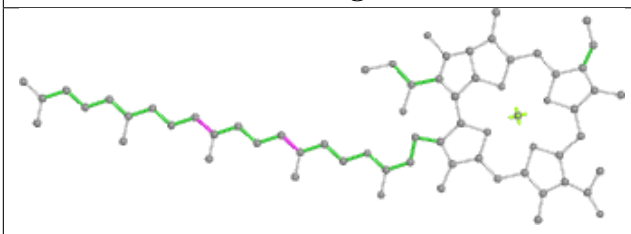
Ligand BCL 9 101



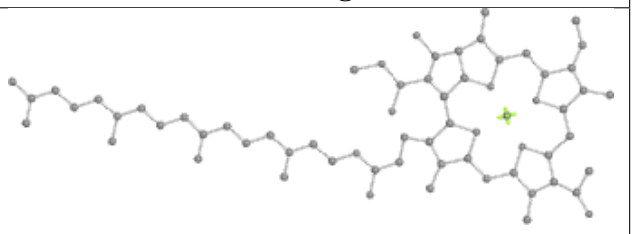
Bond lengths



Bond angles

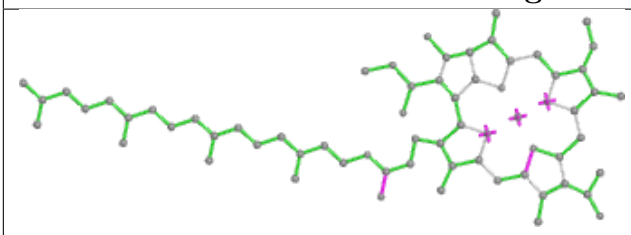


Torsions

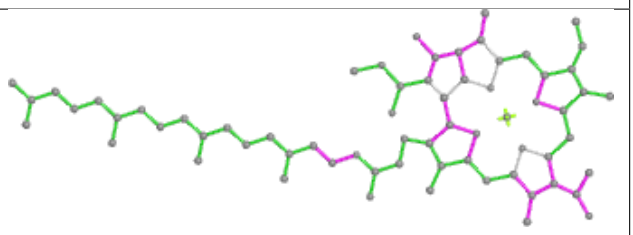


Rings

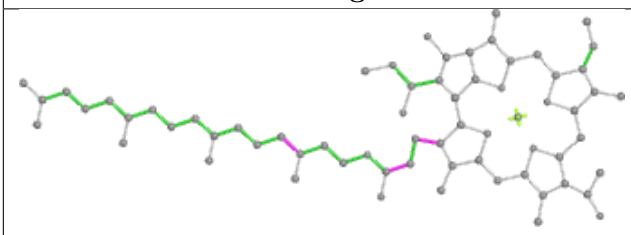
Ligand BCL R 102



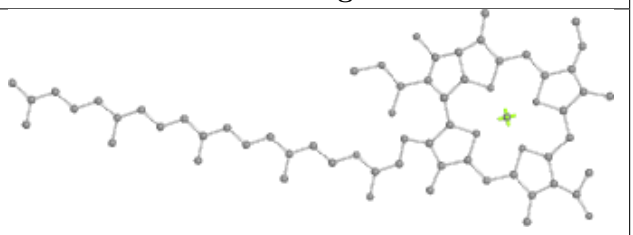
Bond lengths



Bond angles

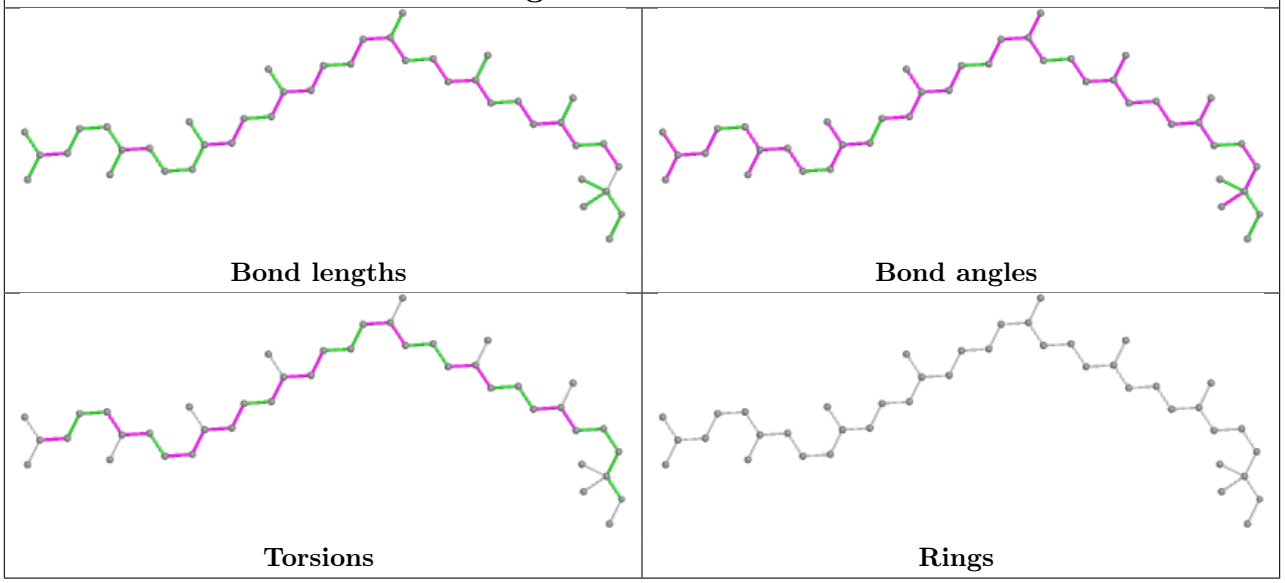


Torsions

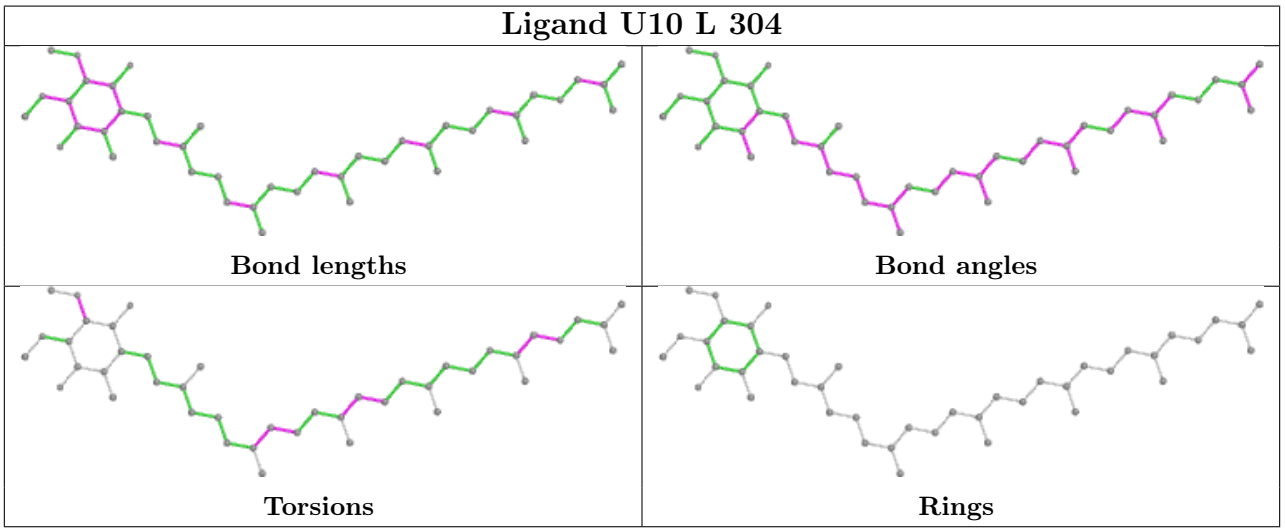


Rings

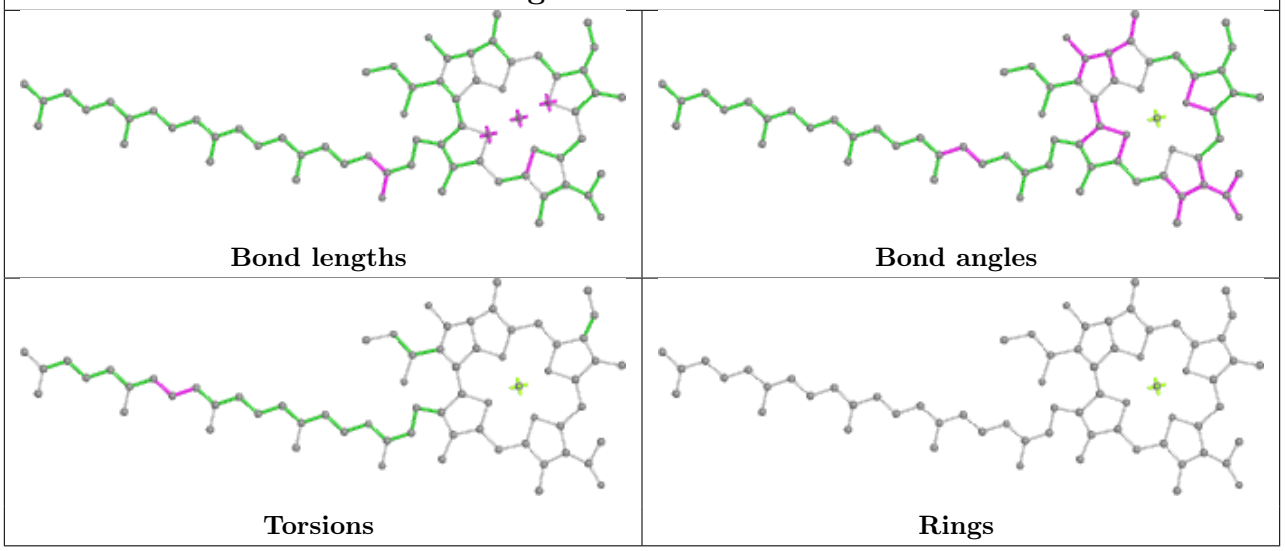
Ligand SPO D 104



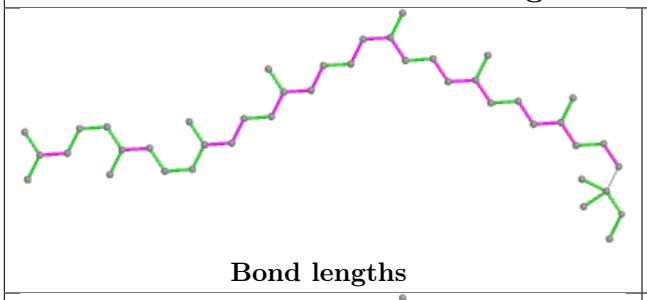
Ligand U10 L 304



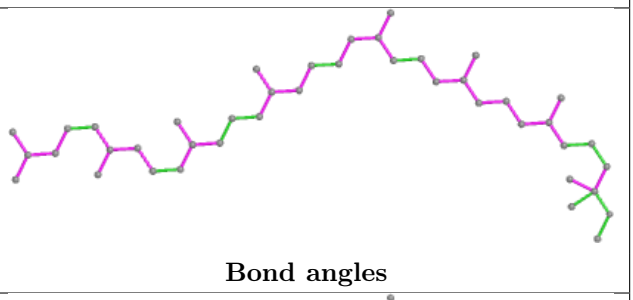
Ligand BCL F 101



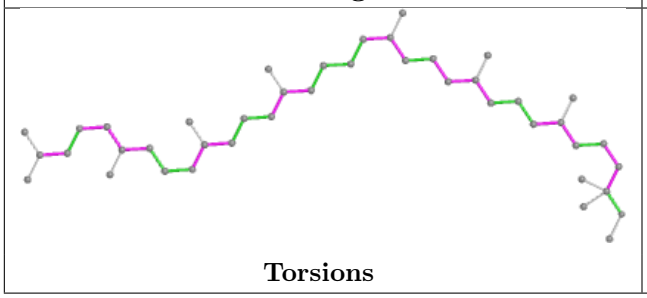
Ligand SPO K 102



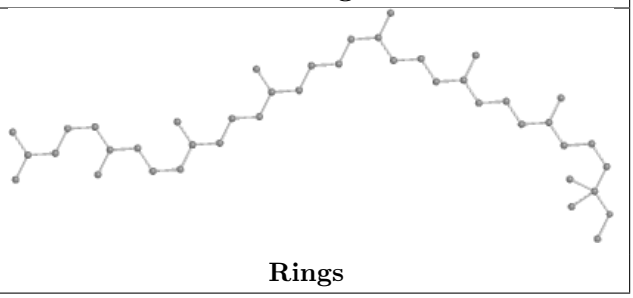
Bond lengths



Bond angles

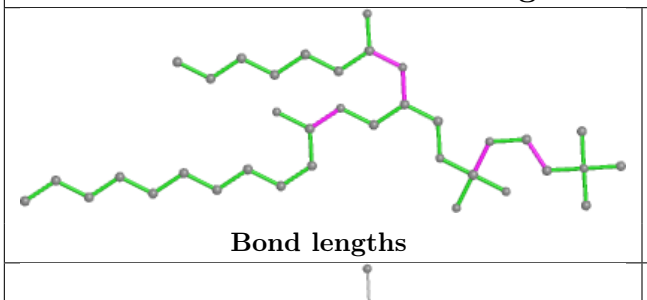


Torsions

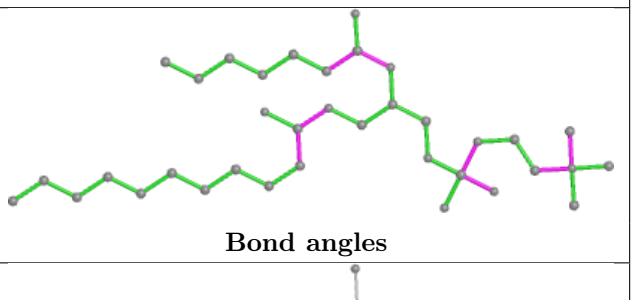


Rings

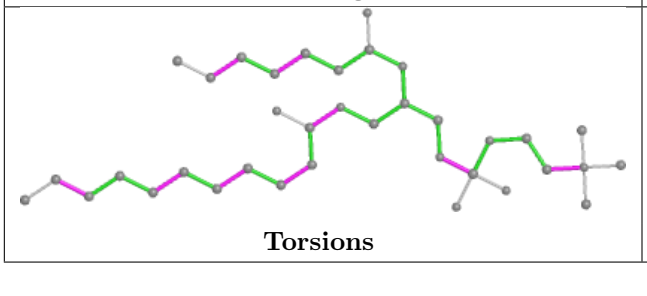
Ligand PC1 X 1501



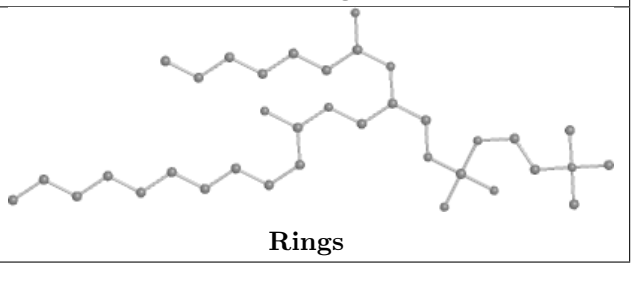
Bond lengths



Bond angles

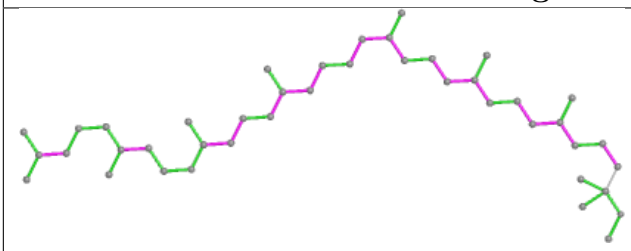


Torsions

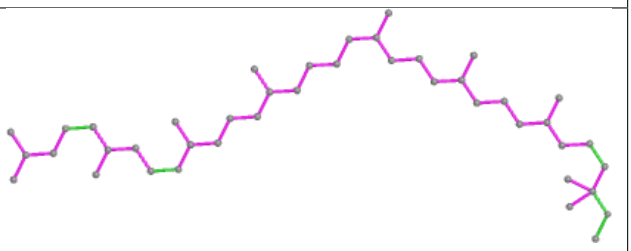


Rings

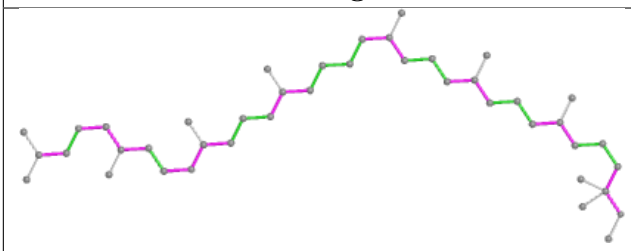
Ligand SPO I 104



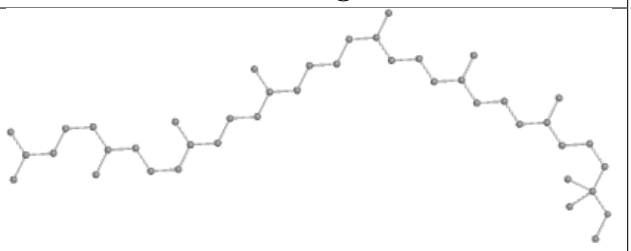
Bond lengths



Bond angles

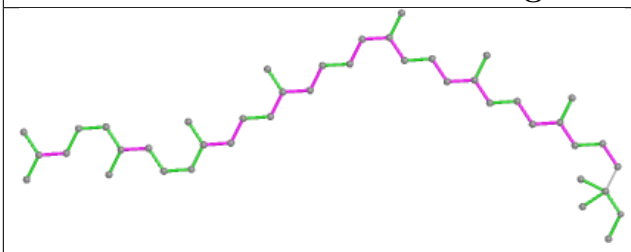


Torsions

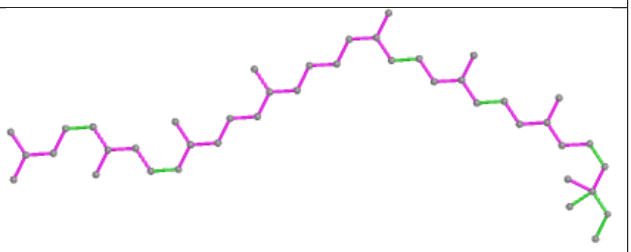


Rings

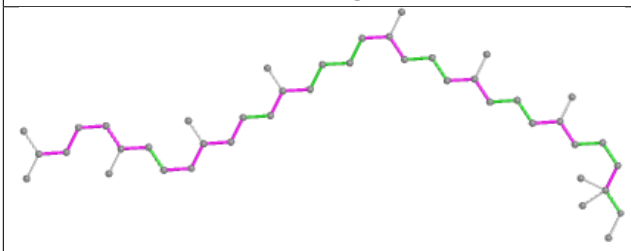
Ligand SPO K 103



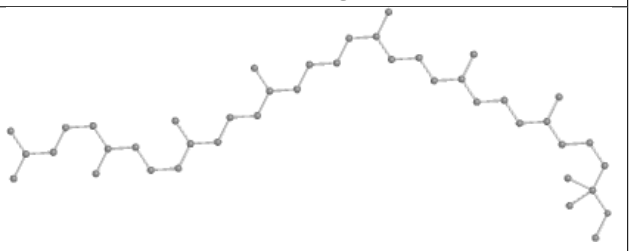
Bond lengths



Bond angles

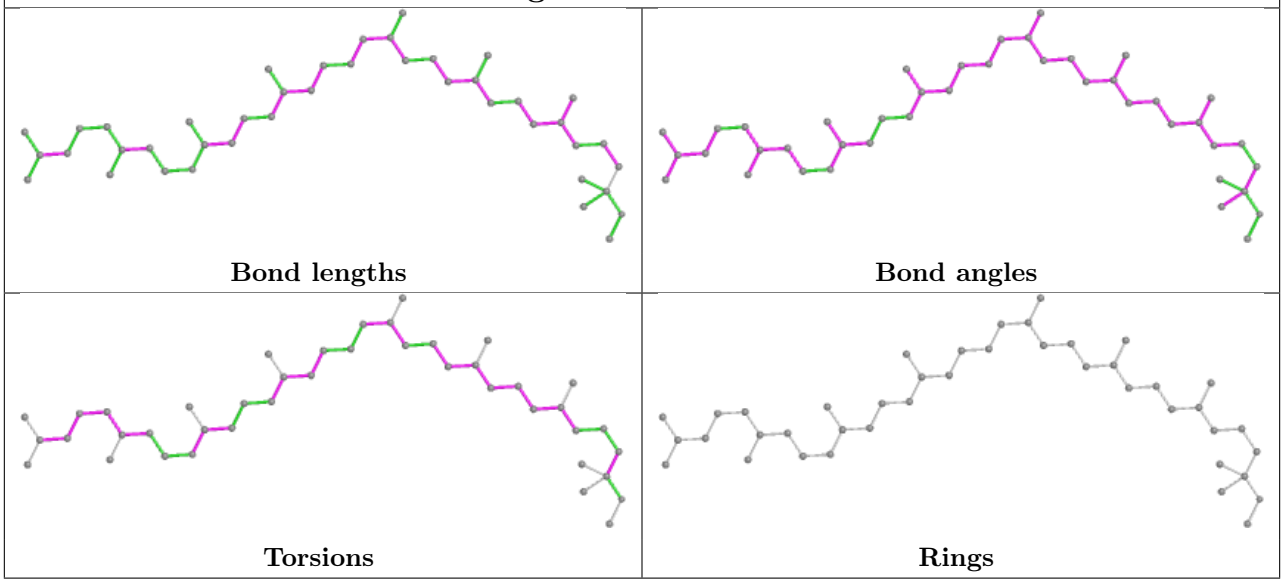


Torsions

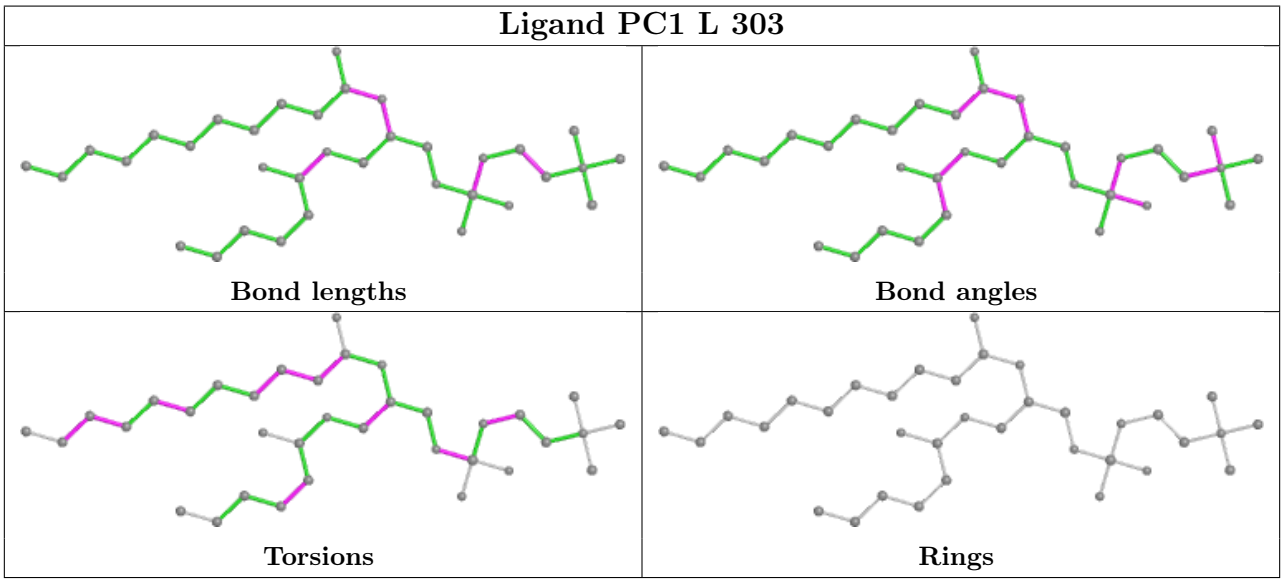


Rings

Ligand SPO P 101



Ligand PC1 L 303



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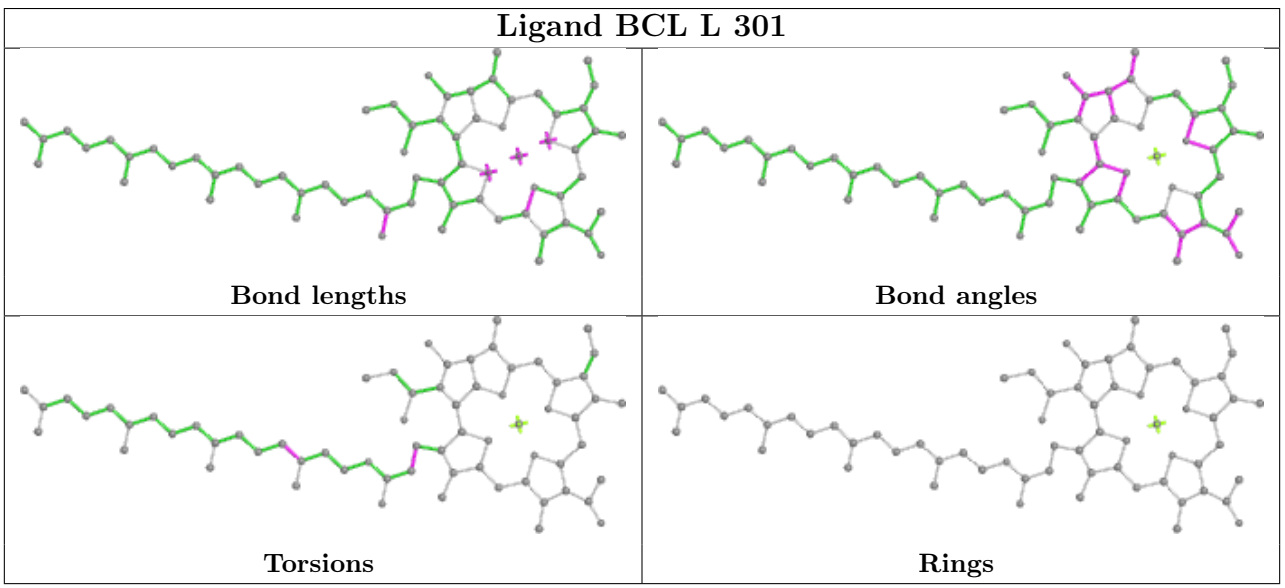

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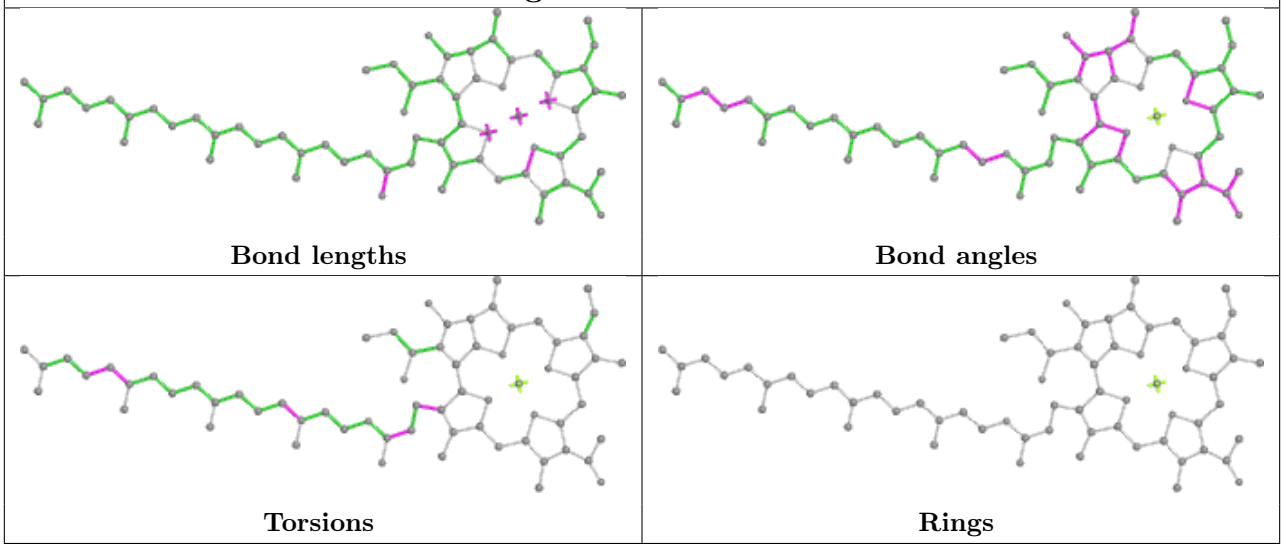
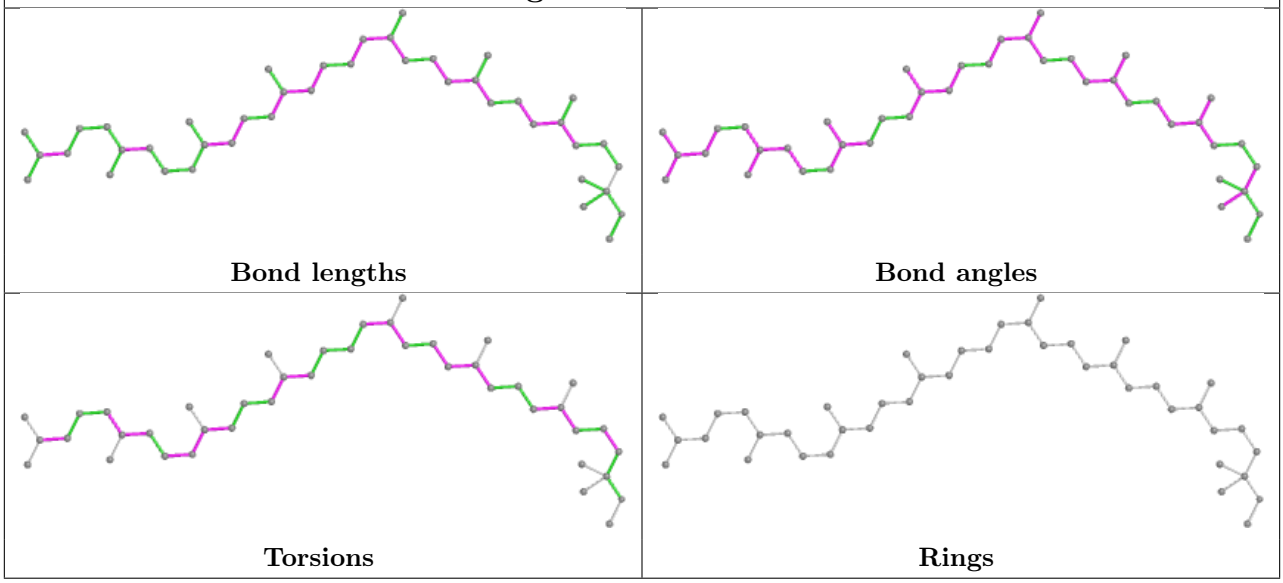


Ligand SPO A 603



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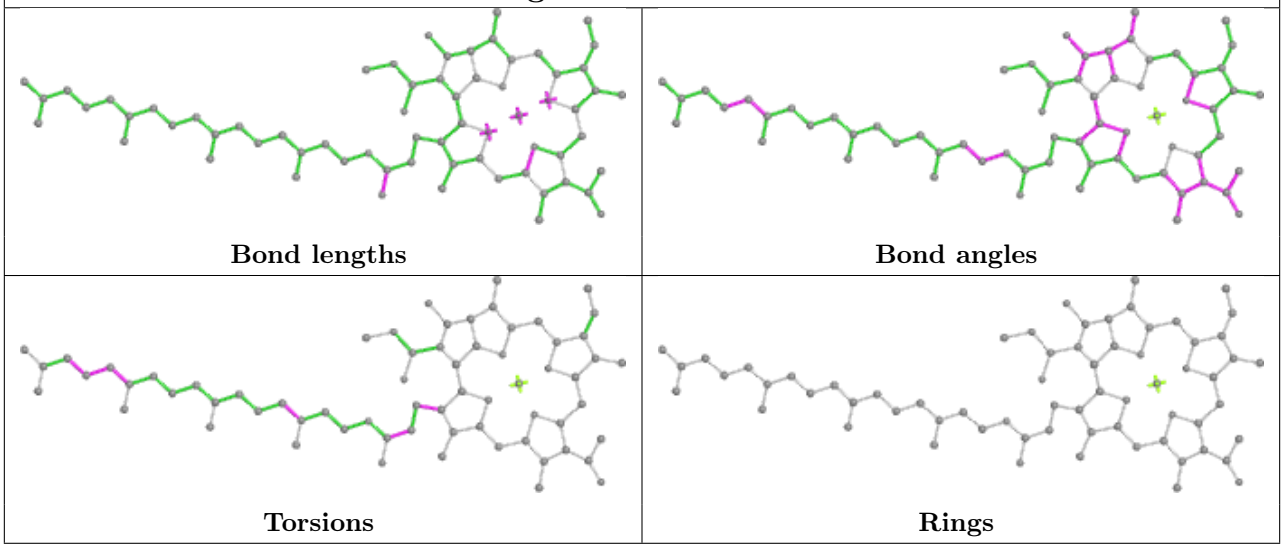

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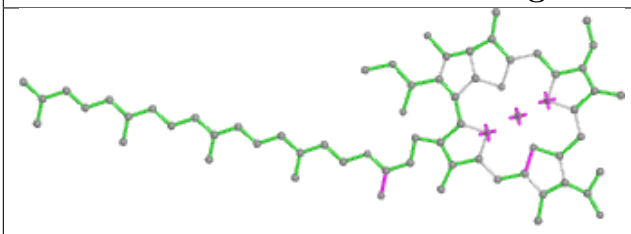
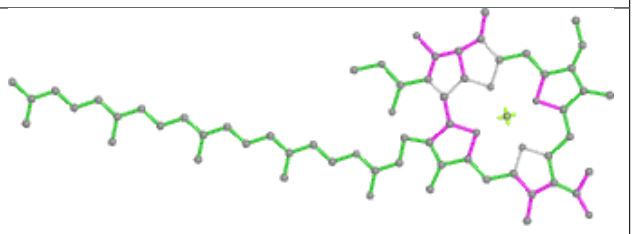
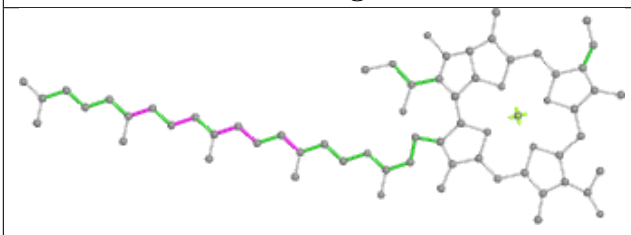


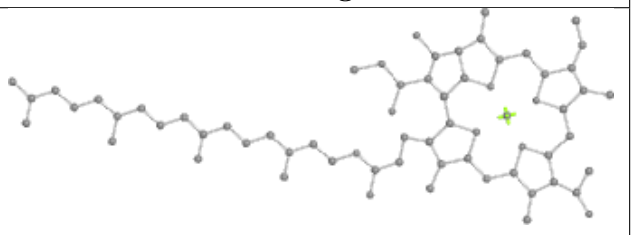
Bond lengths



Bond angles

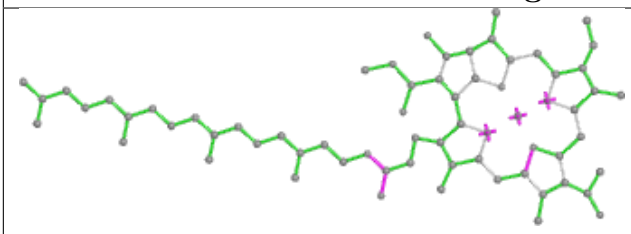


Torsions

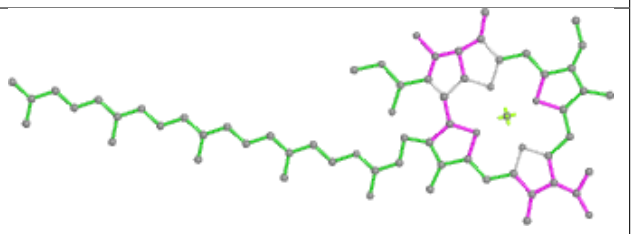


Rings

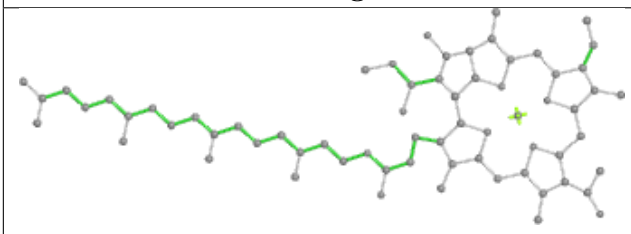
Ligand BCL A 602



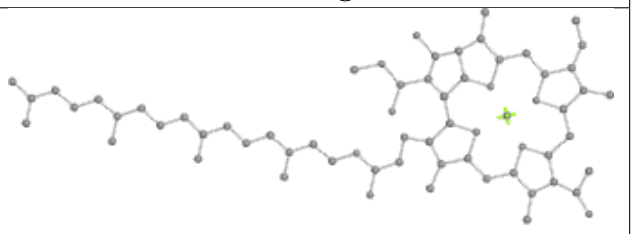
Bond lengths



Bond angles

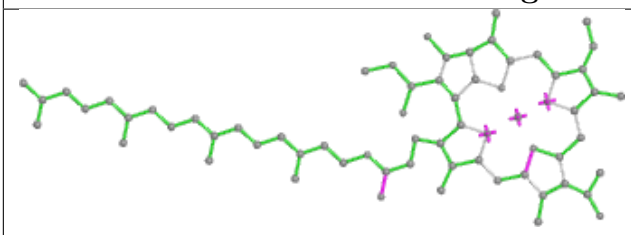


Torsions



Rings

Ligand BCL M 403



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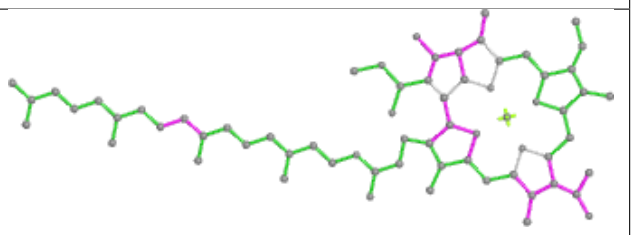
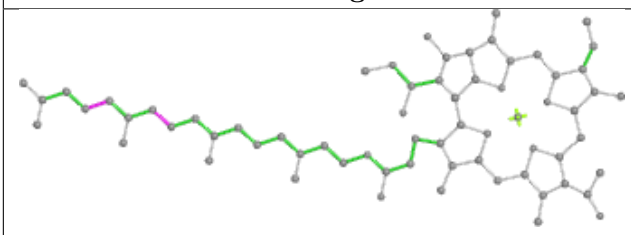


Bond angles



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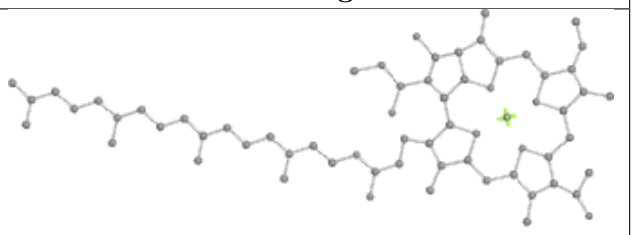
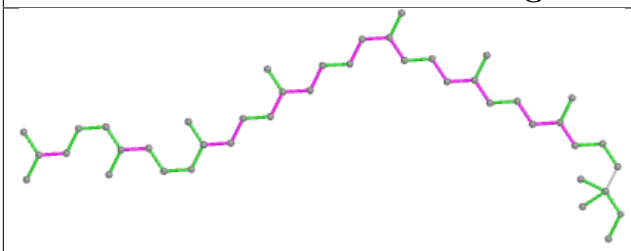


Rings

Ligand SPO D 102



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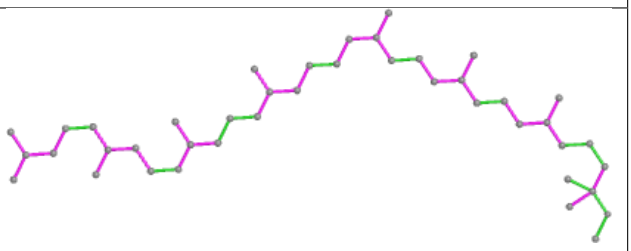

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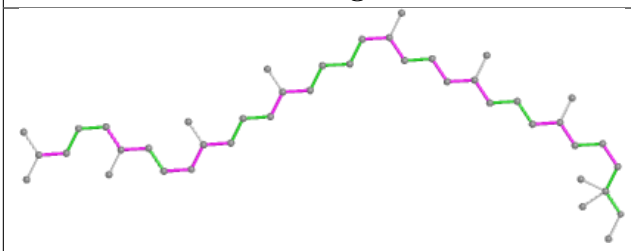

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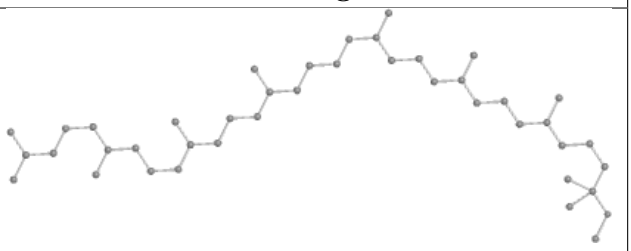
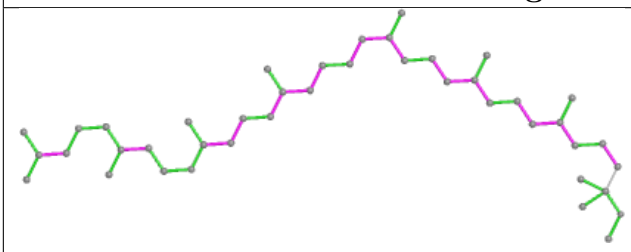
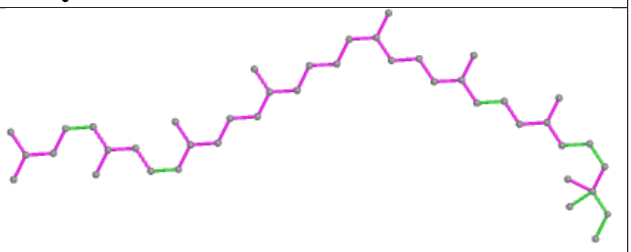


Rings

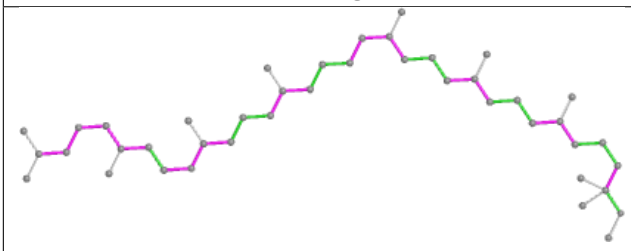
Ligand SPO Q 102



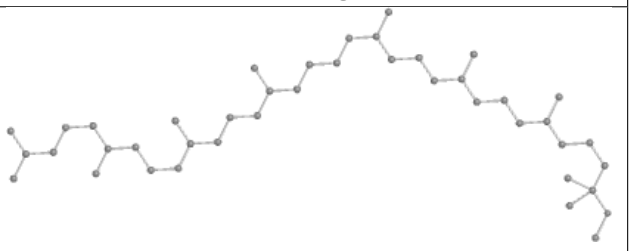
Bond lengths



Bond angles

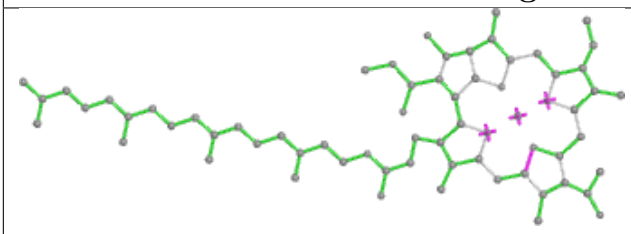


Torsions



Rings

Ligand BCL W 101



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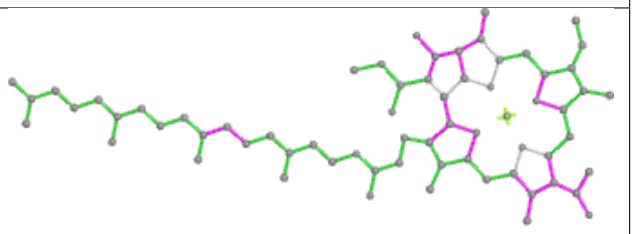
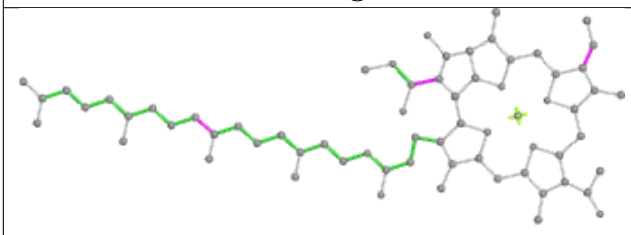


Bond angles



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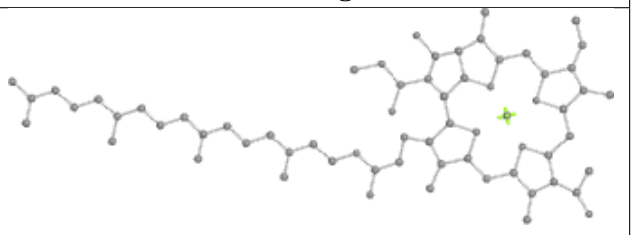
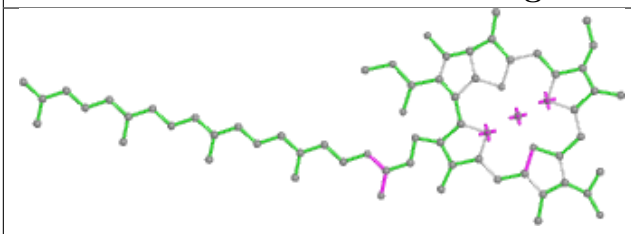


Rings

Ligand BCL D 101



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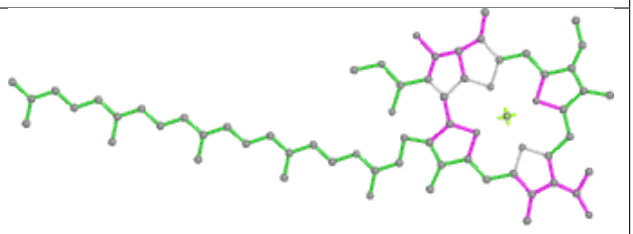
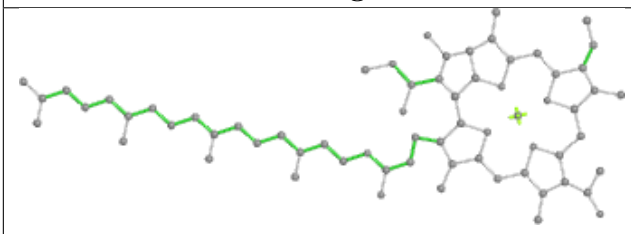


Bond angles



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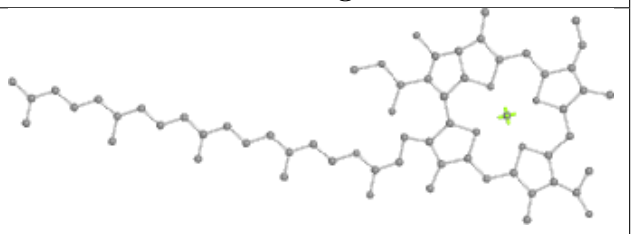
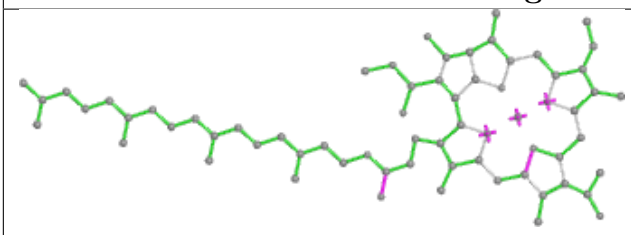


Rings

Ligand BCL O 102



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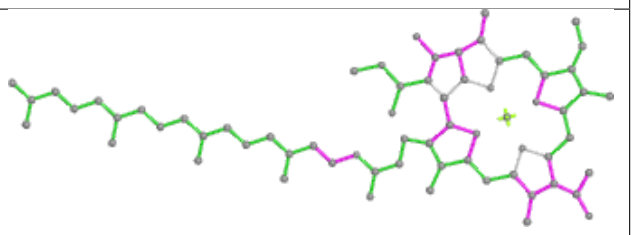
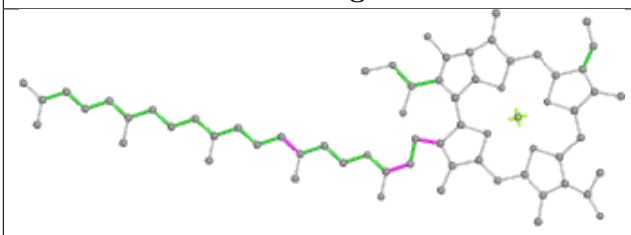


Bond angles



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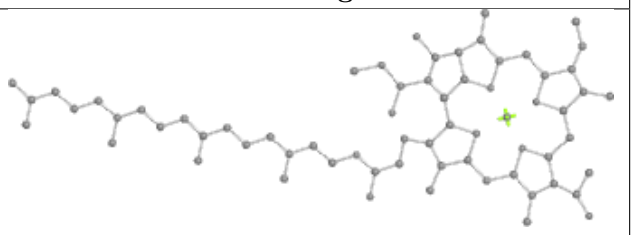
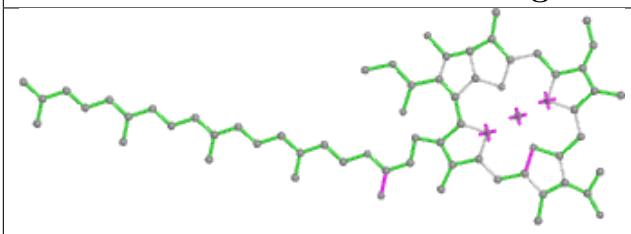


Rings

Ligand BCL I 101



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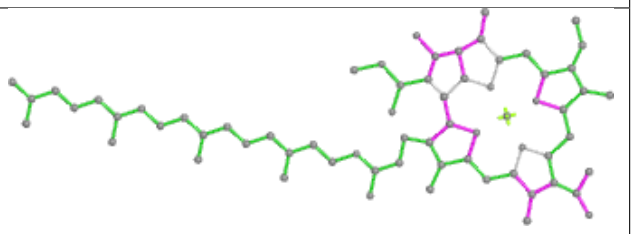

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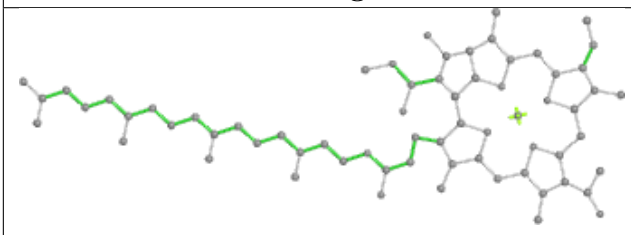

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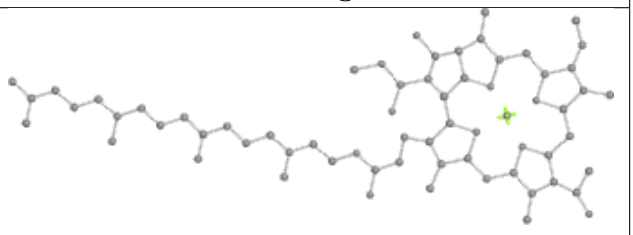
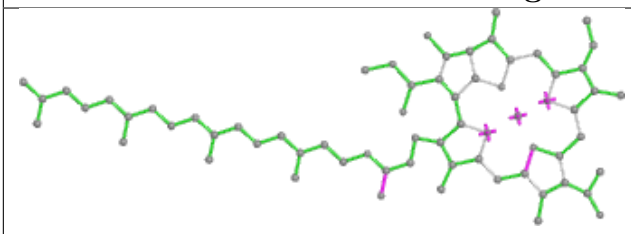
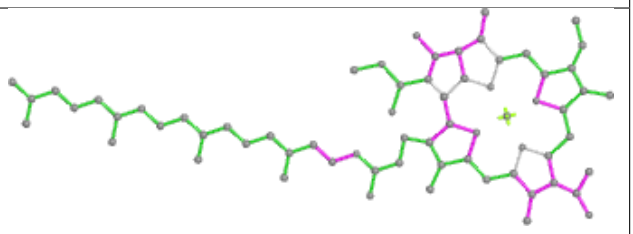


Rings

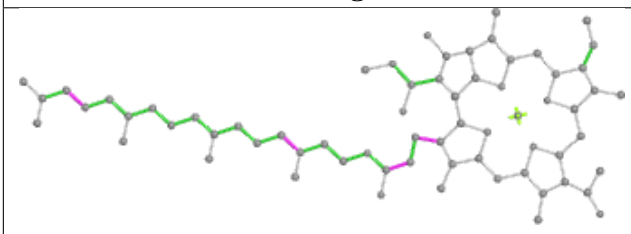
Ligand BCL U 102



Bond lengths



Bond angles



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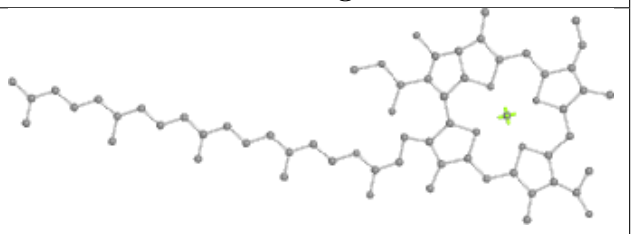
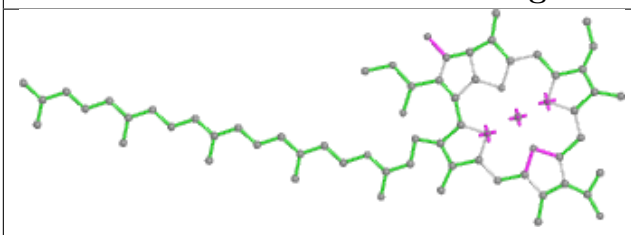
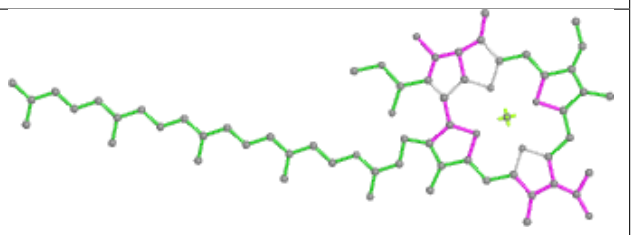


Rings

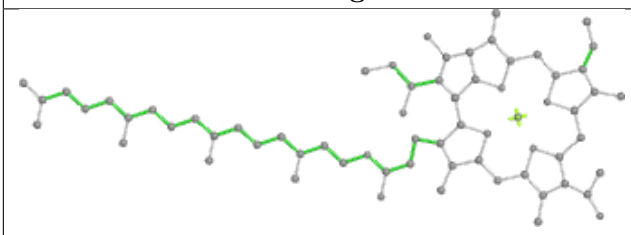
Ligand BCL 1 101



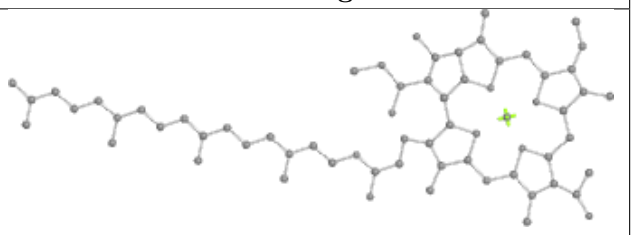
Bond lengths



Bond angles

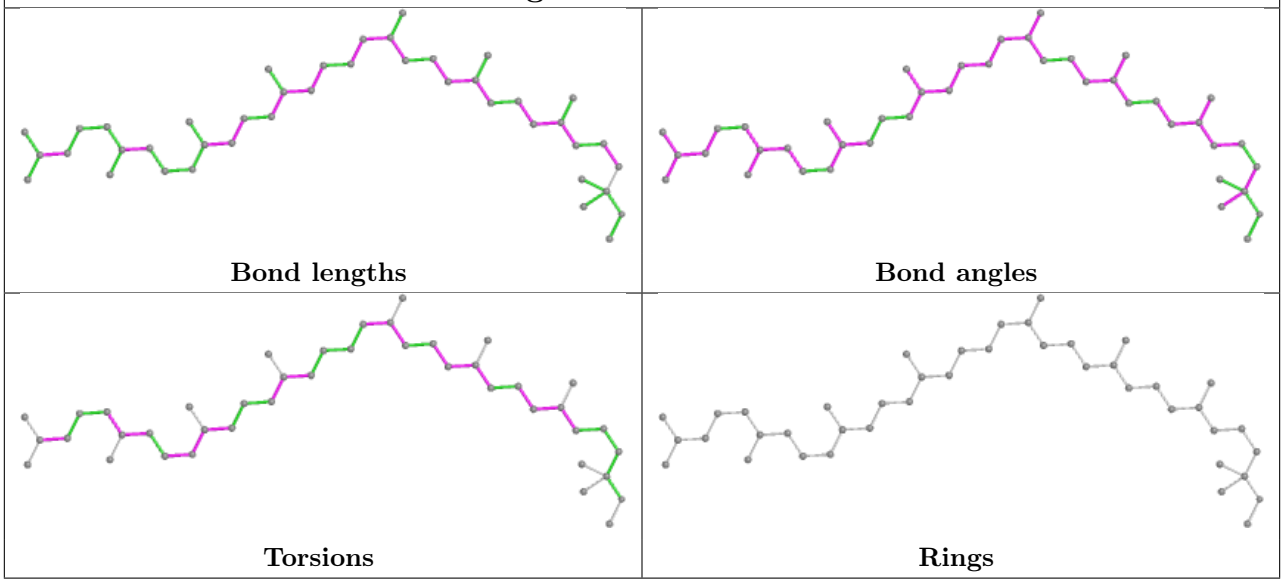


Torsions

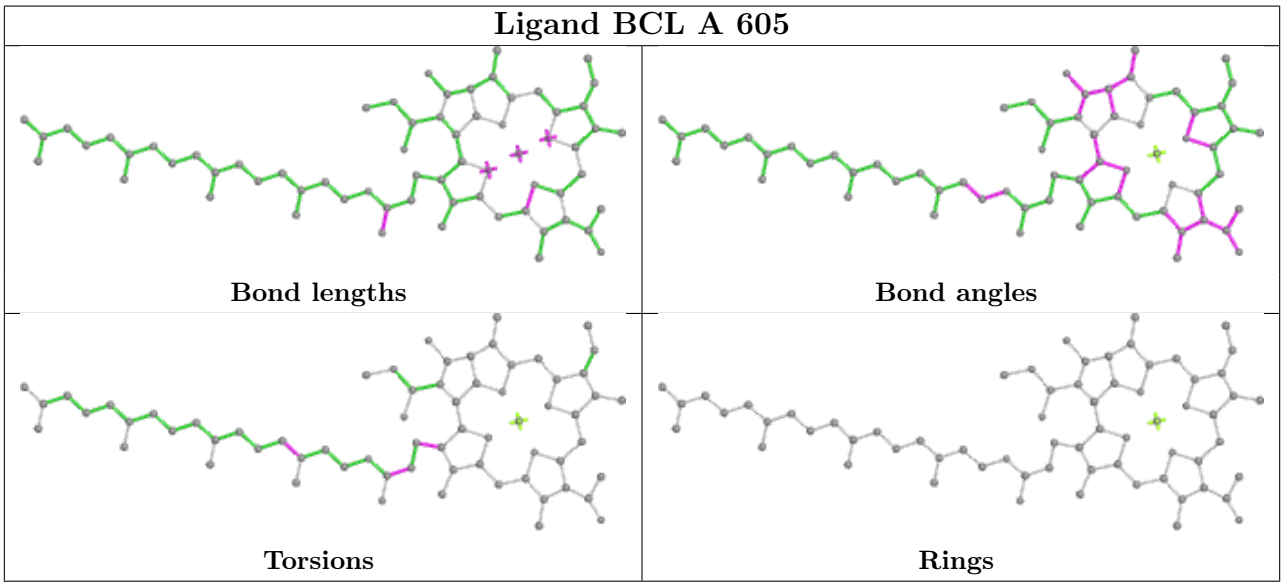


Rings

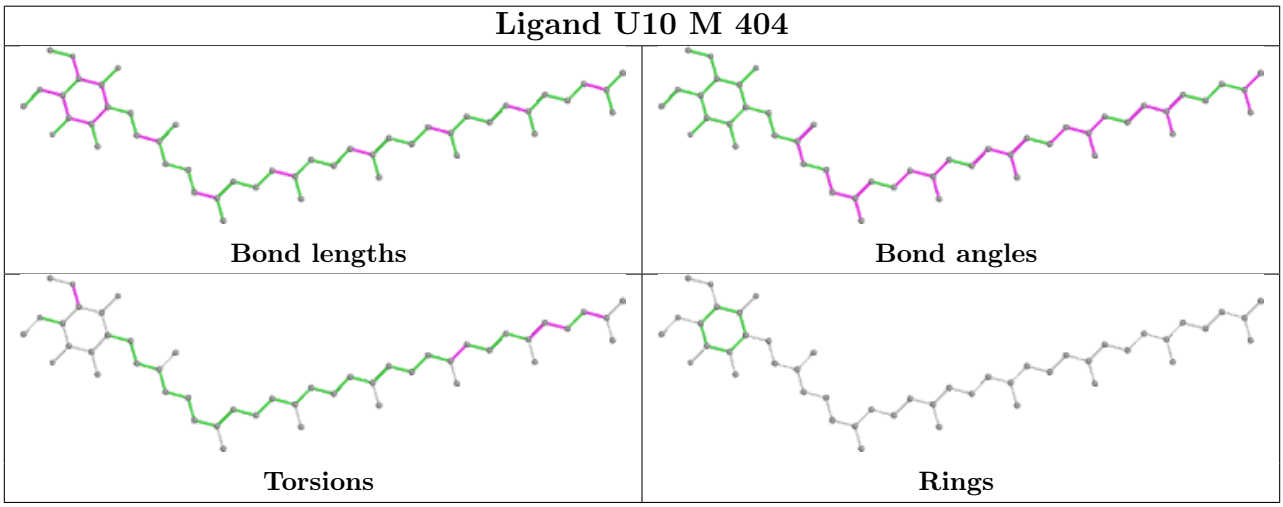
Ligand SPO R 103



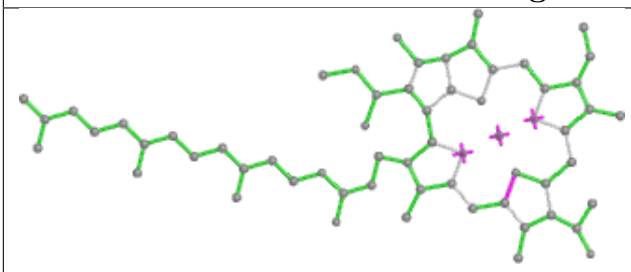
Ligand BCL A 605



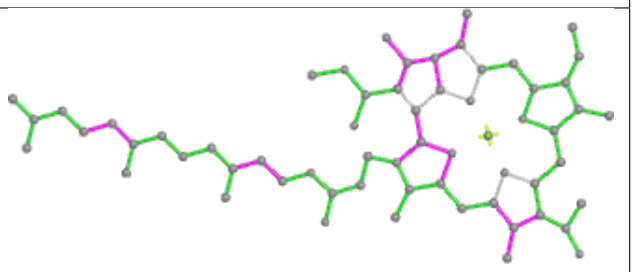
Ligand U10 M 404



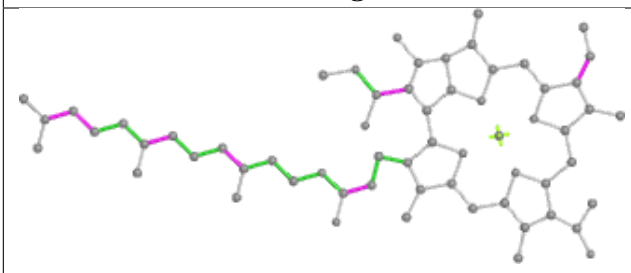
Ligand BCL 7 101



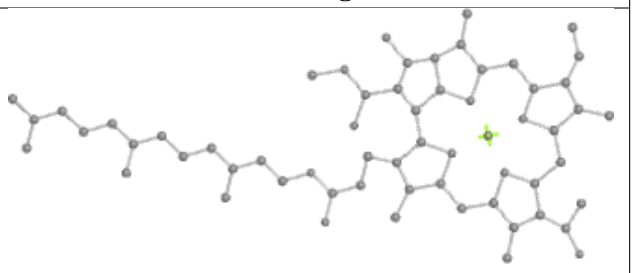
Bond lengths



Bond angles

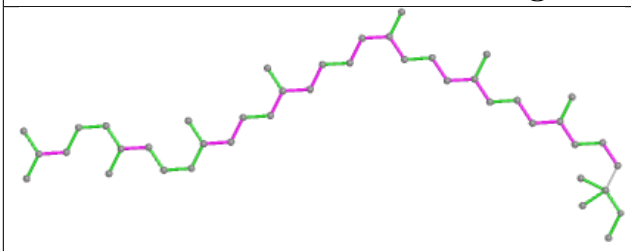


Torsions

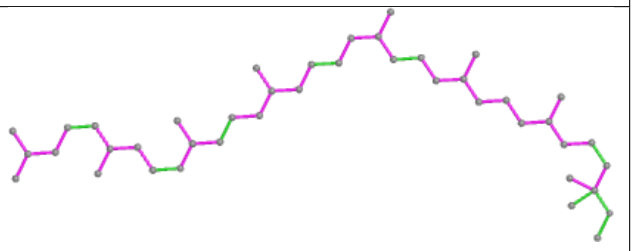


Rings

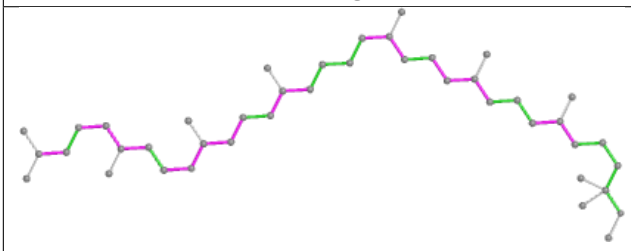
Ligand SPO S 103



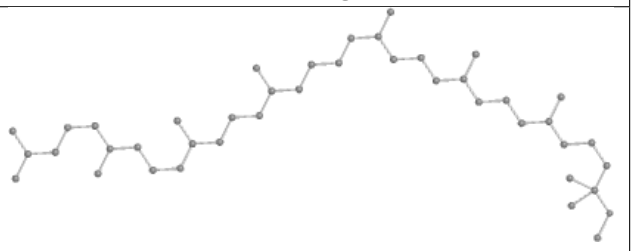
Bond lengths



Bond angles

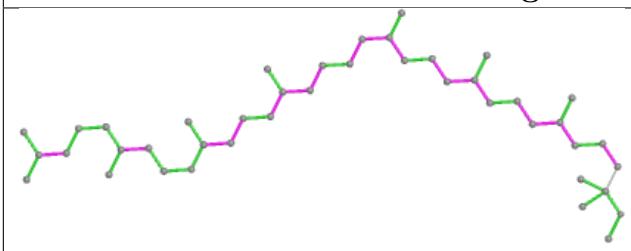


Torsions

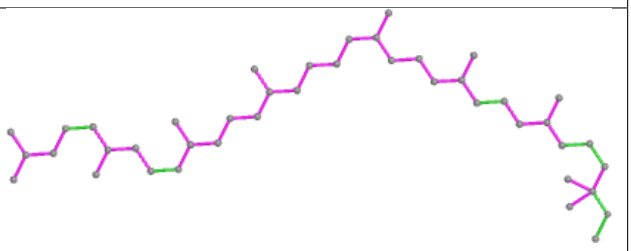


Rings

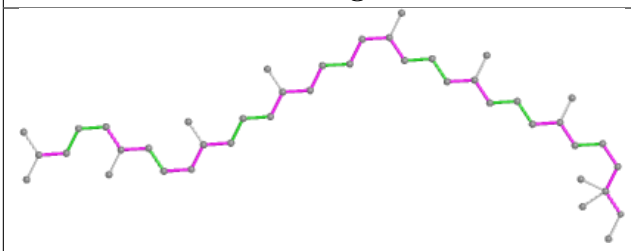
Ligand SPO M 405



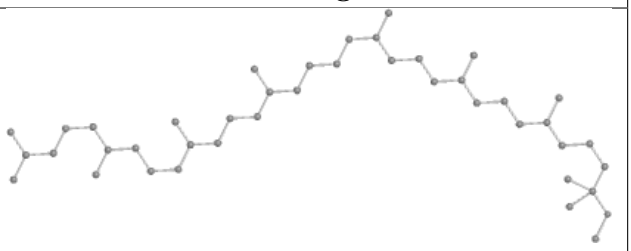
Bond lengths



Bond angles

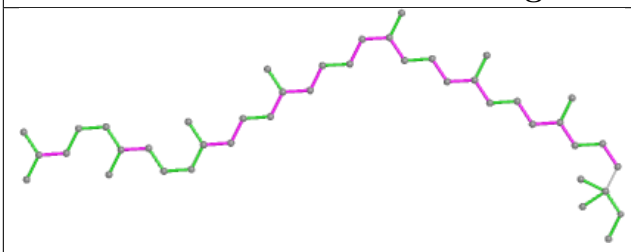


Torsions

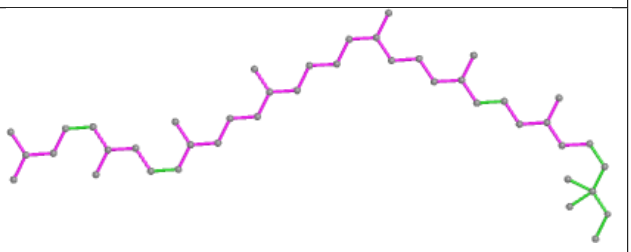


Rings

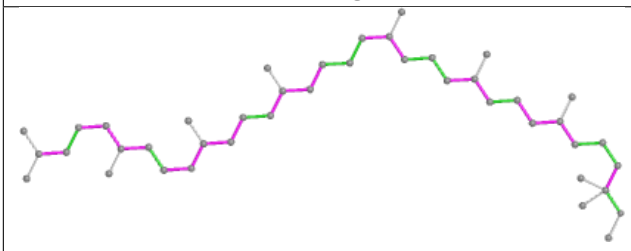
Ligand SPO D 103



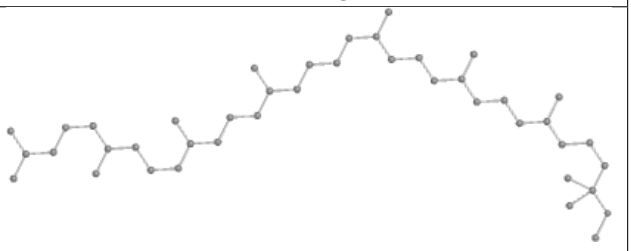
Bond lengths



Bond angles

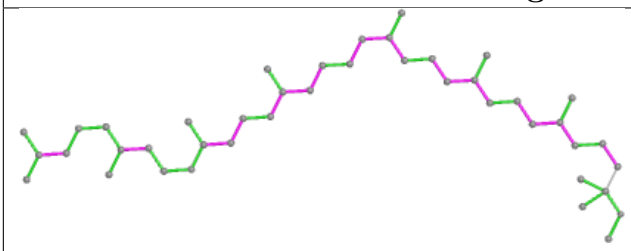


Torsions

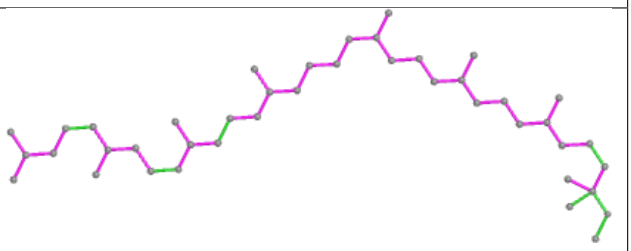


Rings

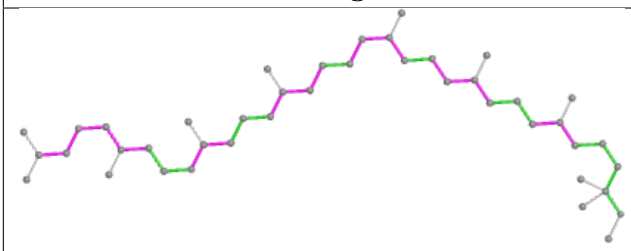
Ligand SPO E 102



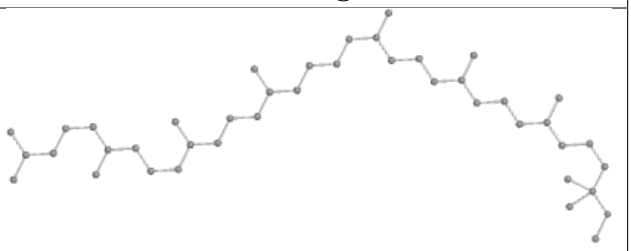
Bond lengths



Bond angles

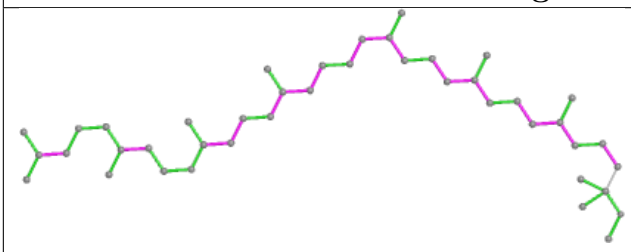


Torsions

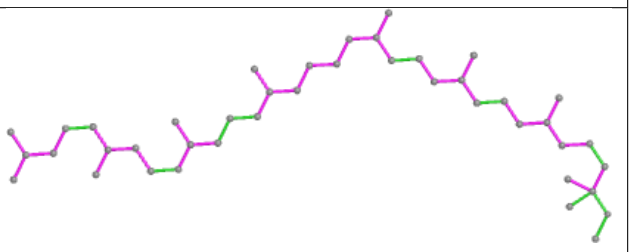


Rings

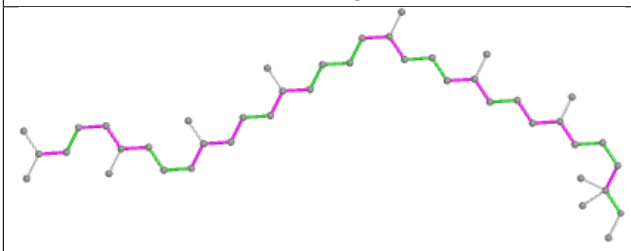
Ligand SPO I 103



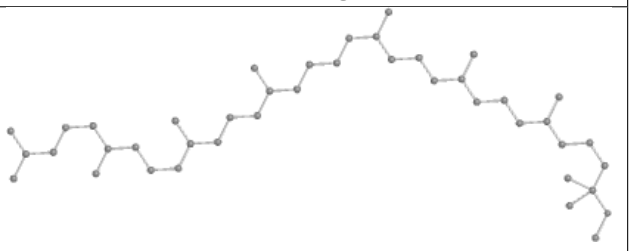
Bond lengths



Bond angles

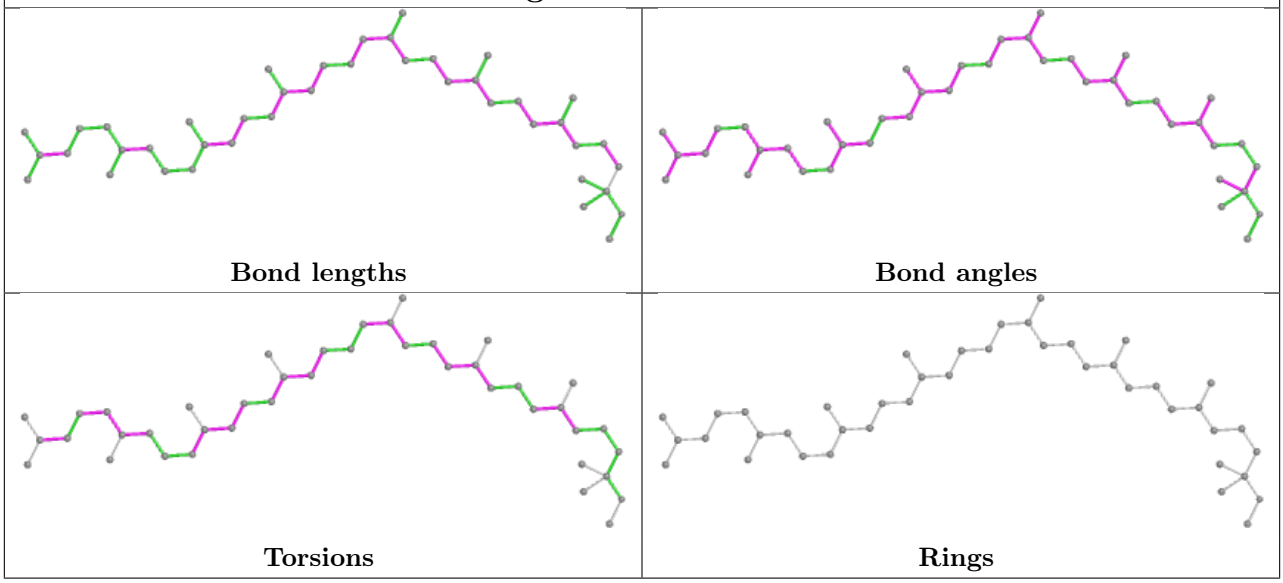


Torsions

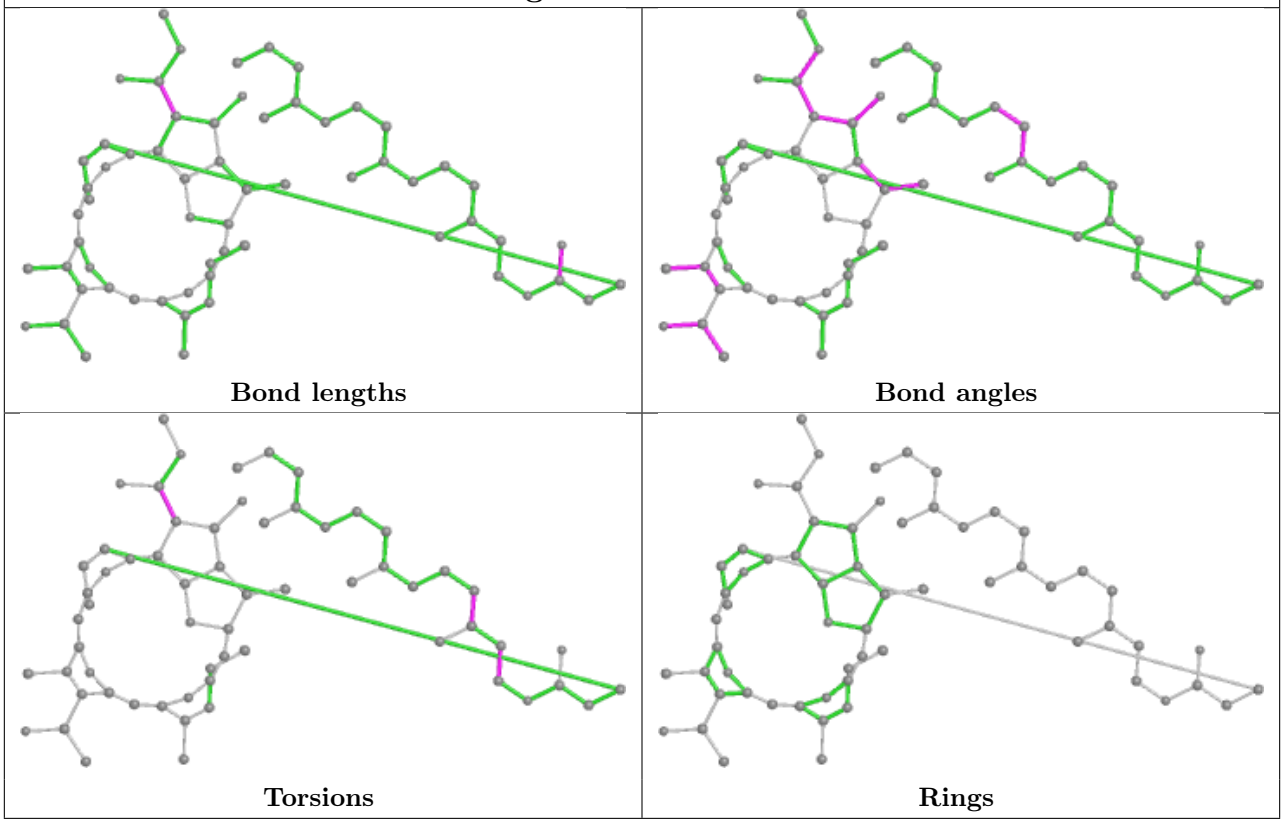


Rings

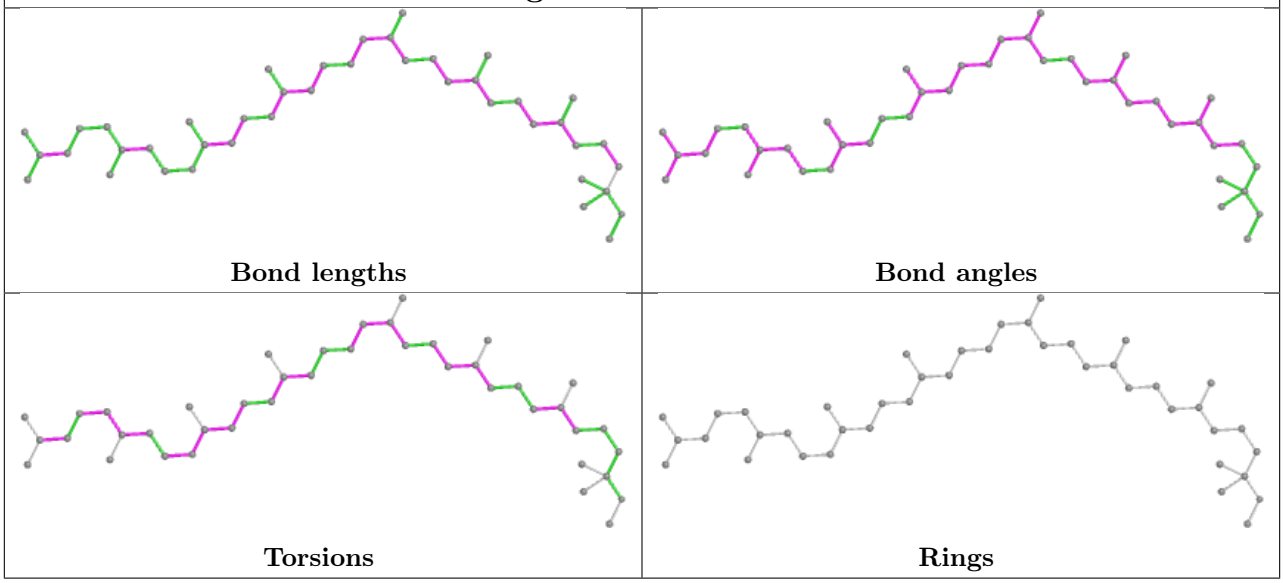
Ligand SPO R 101



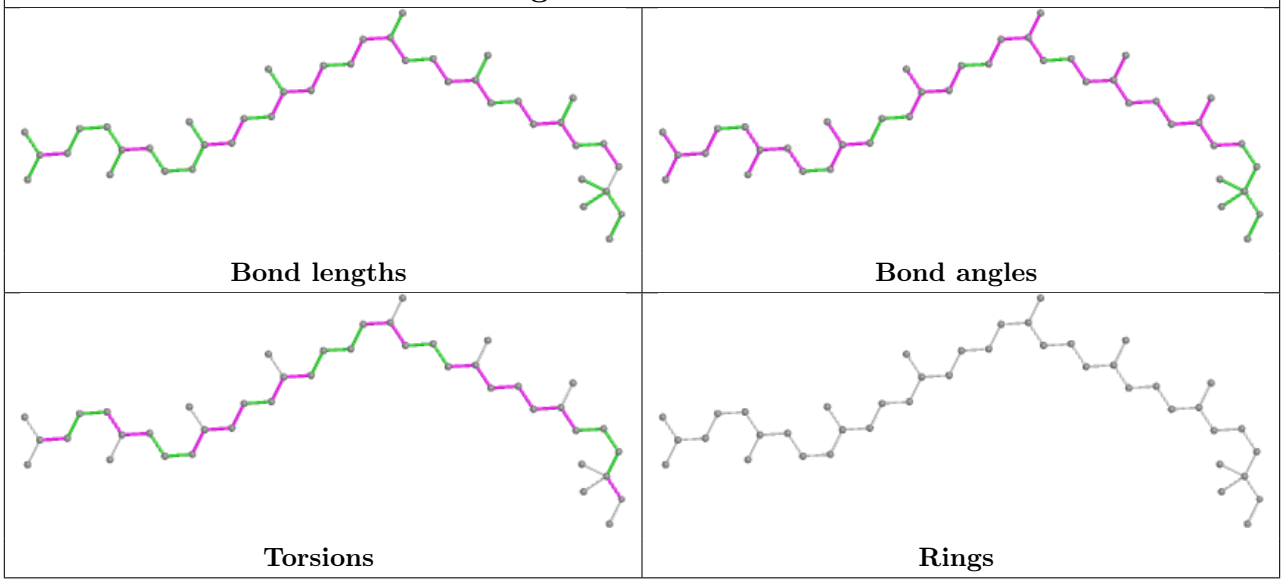
Ligand BPH L 302



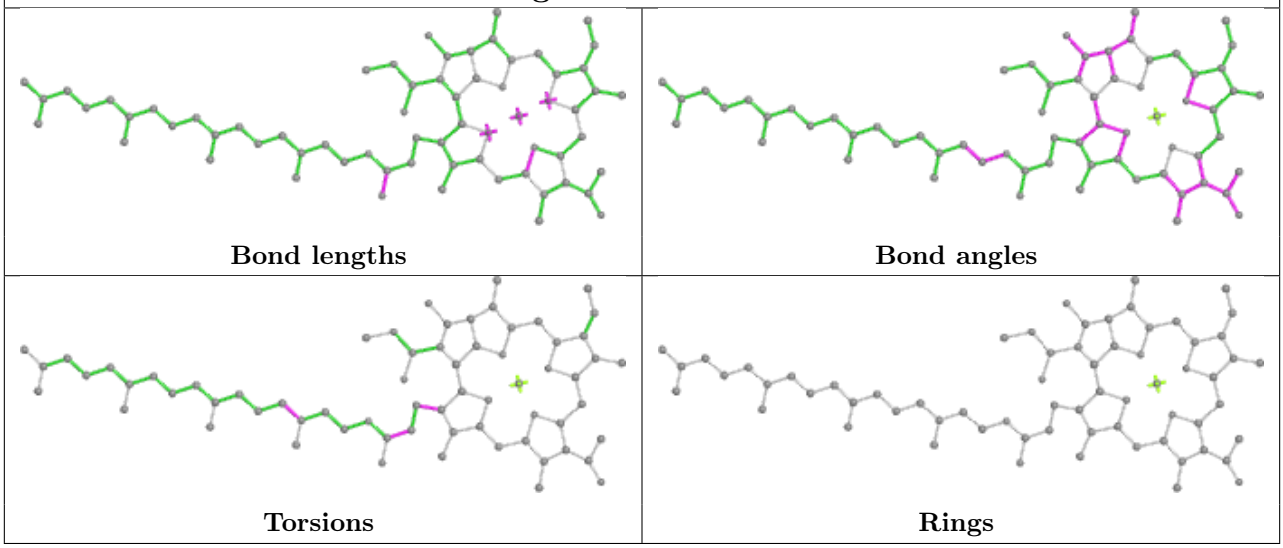
Ligand SPO U 103



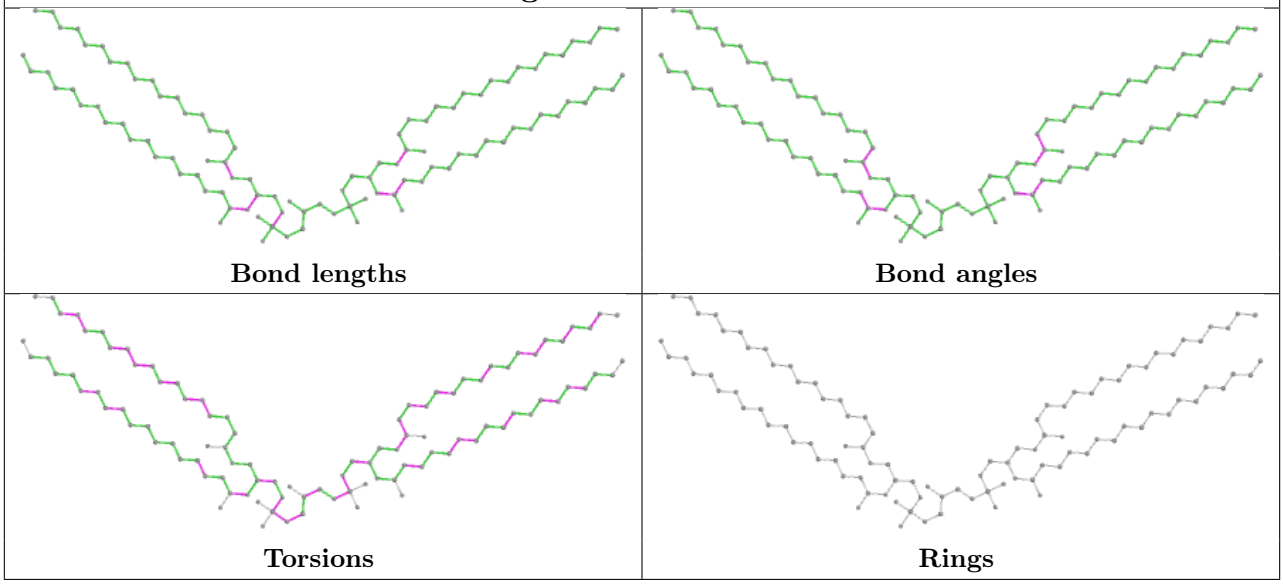
Ligand SPO 0 102



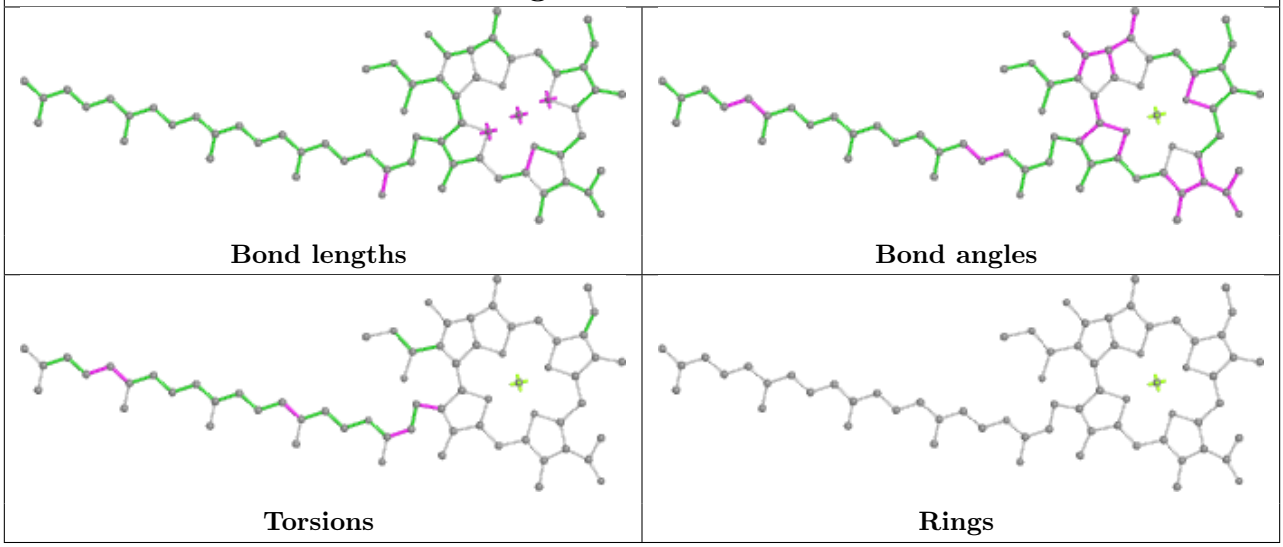
Ligand BCL I 102



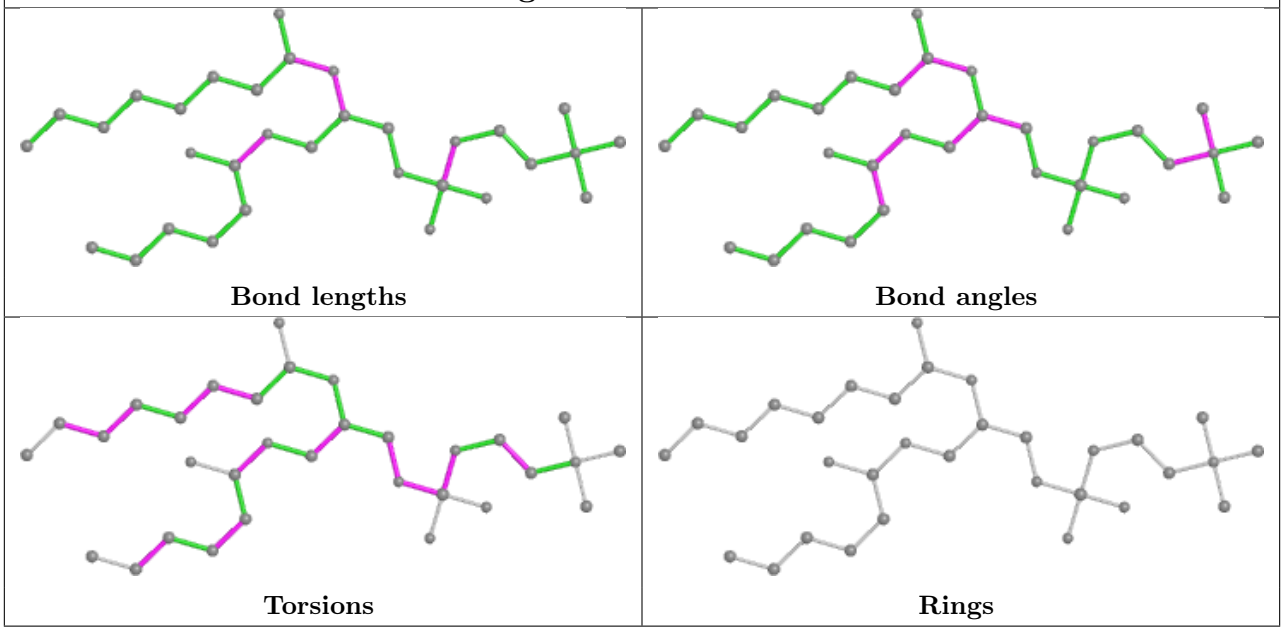
Ligand CDL M 406



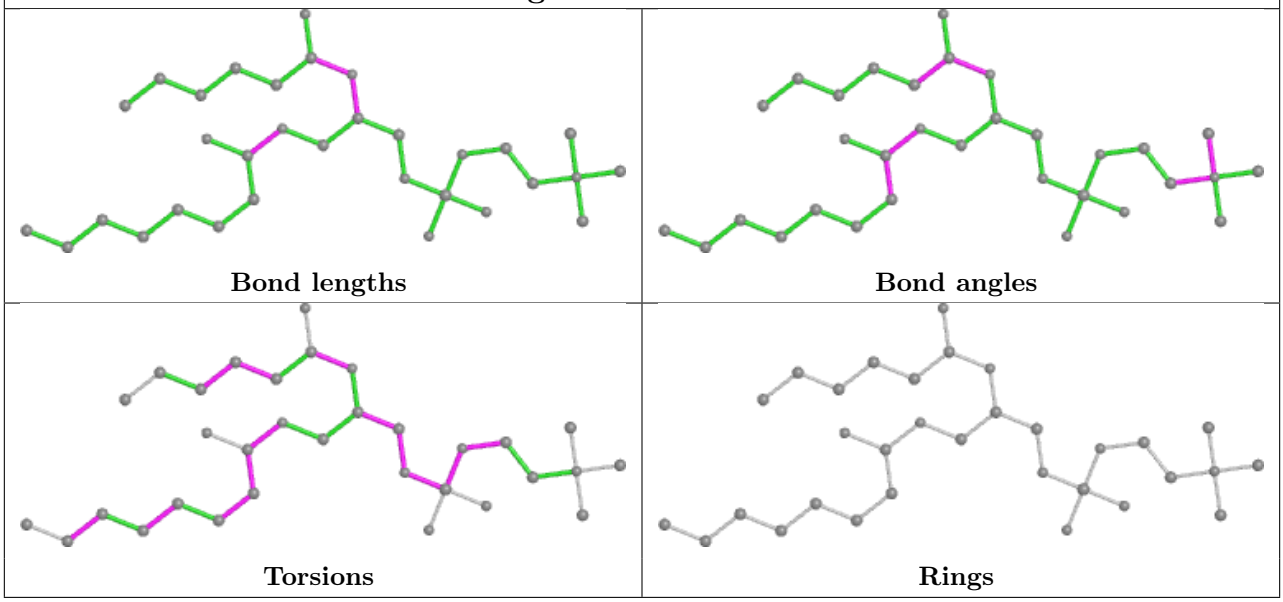
Ligand BCL S 102

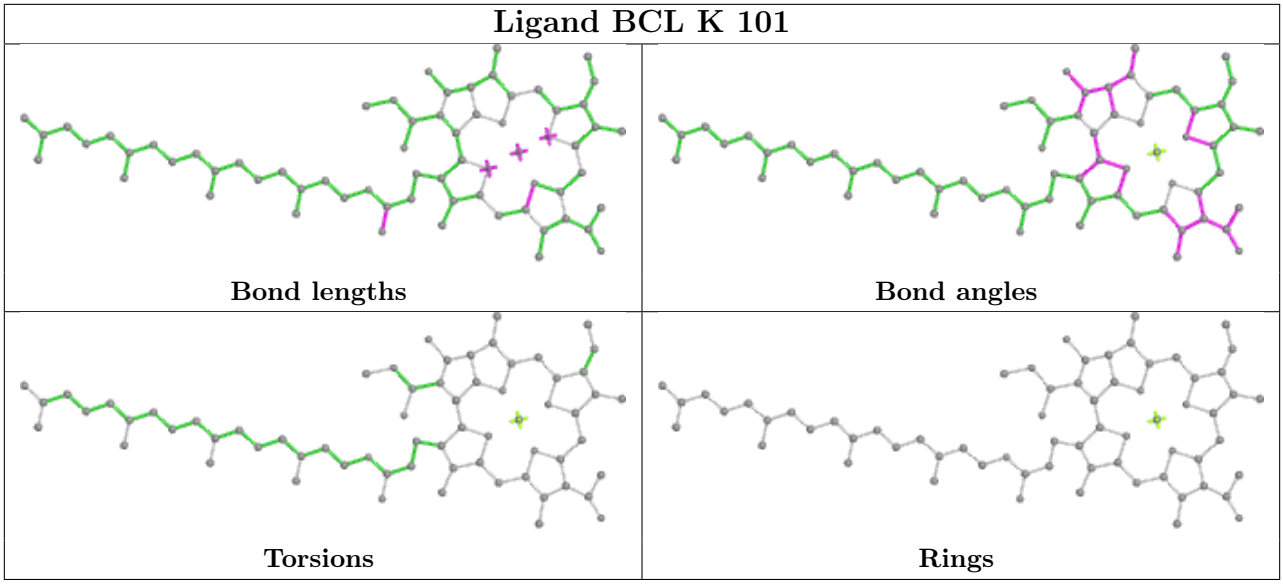


Ligand PC1 H 1103



Ligand PC1 A 601





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.

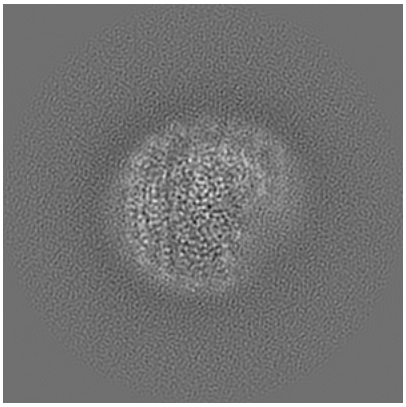
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32042. These allow visual inspection of the internal detail of the map and identification of artifacts.

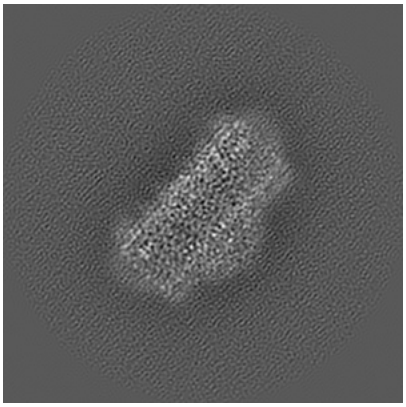
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

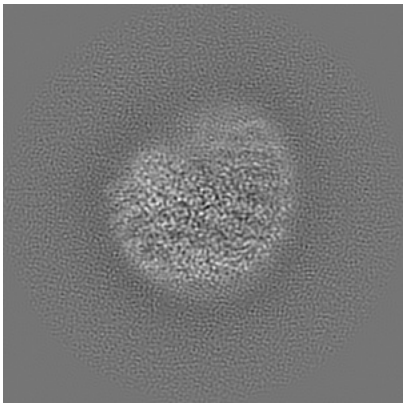
6.1.1 Primary map



X



Y

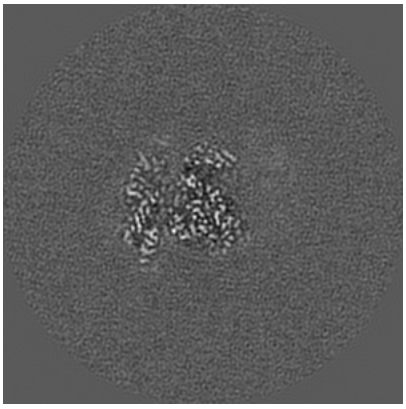


Z

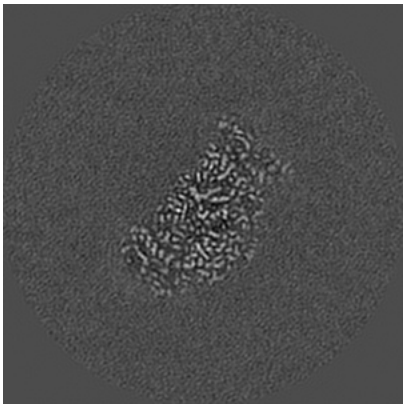
The images above show the map projected in three orthogonal directions.

6.2 Central slices

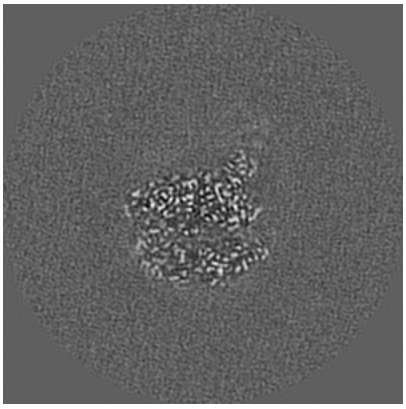
6.2.1 Primary map



X Index: 150



Y Index: 150

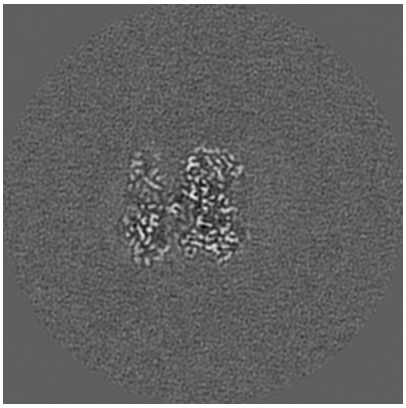


Z Index: 150

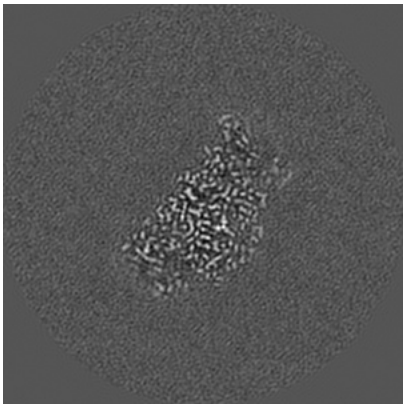
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

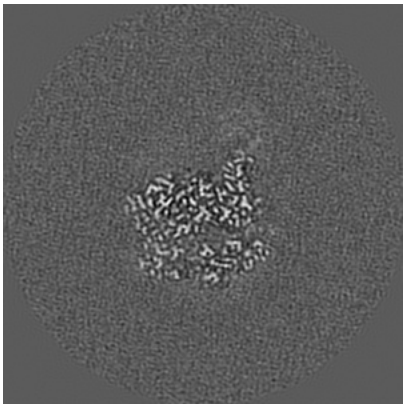
6.3.1 Primary map



X Index: 142



Y Index: 152

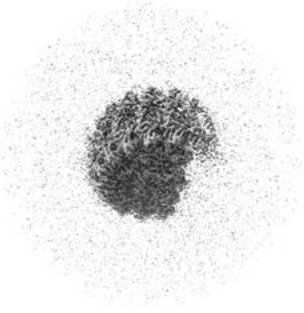


Z Index: 152

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

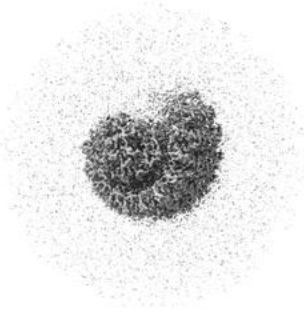
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

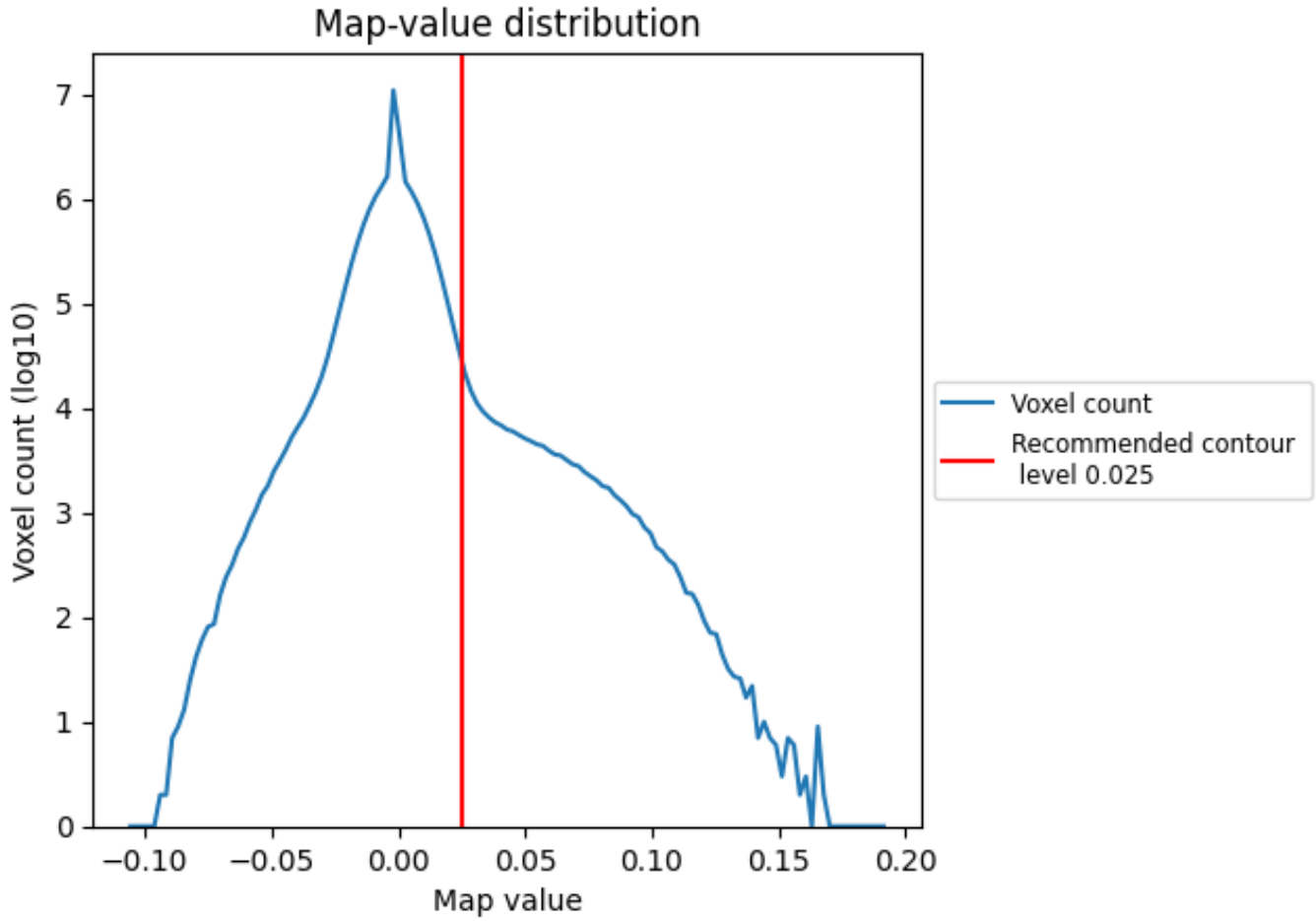
6.5 Mask visualisation (i)

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

7 Map analysis

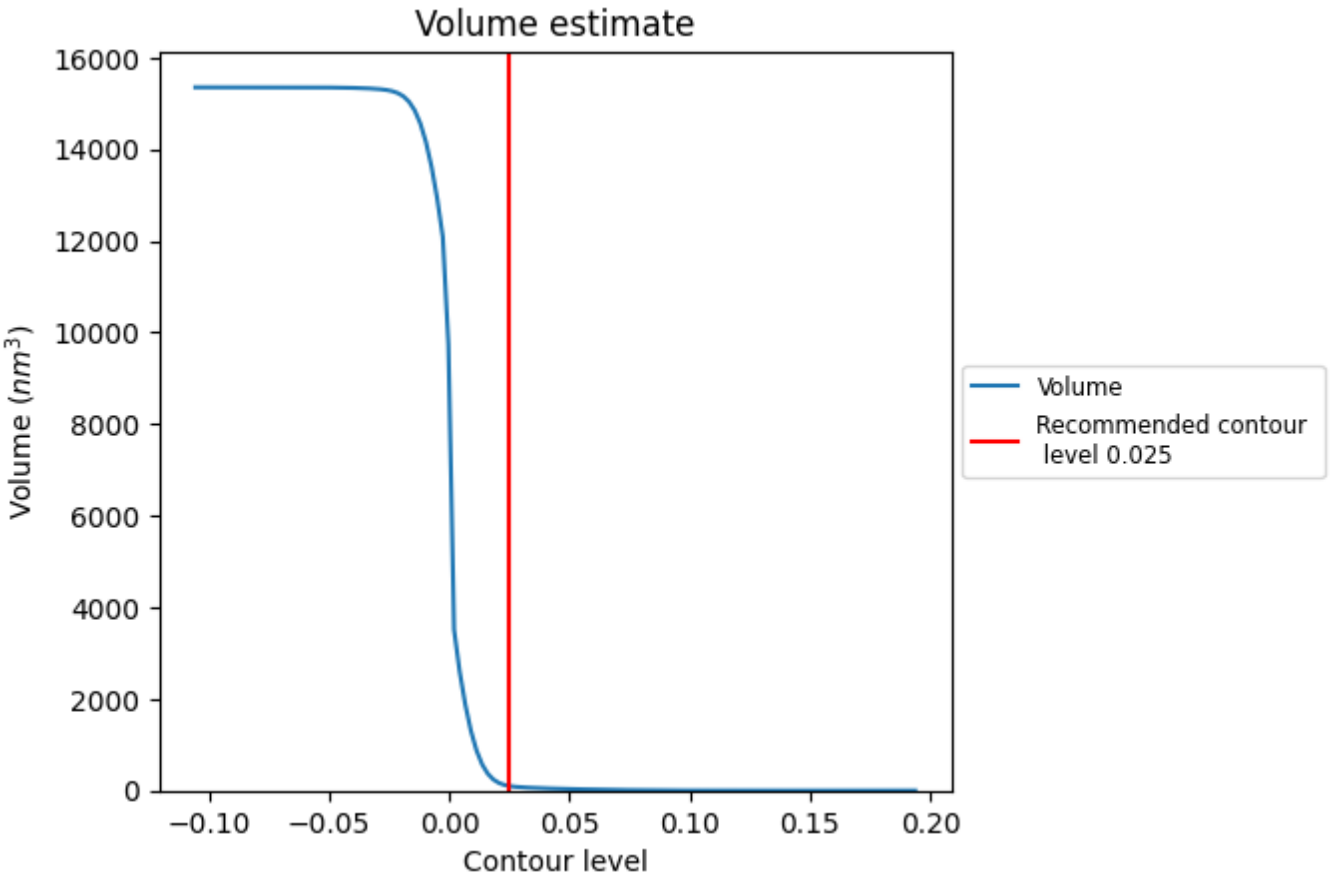
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

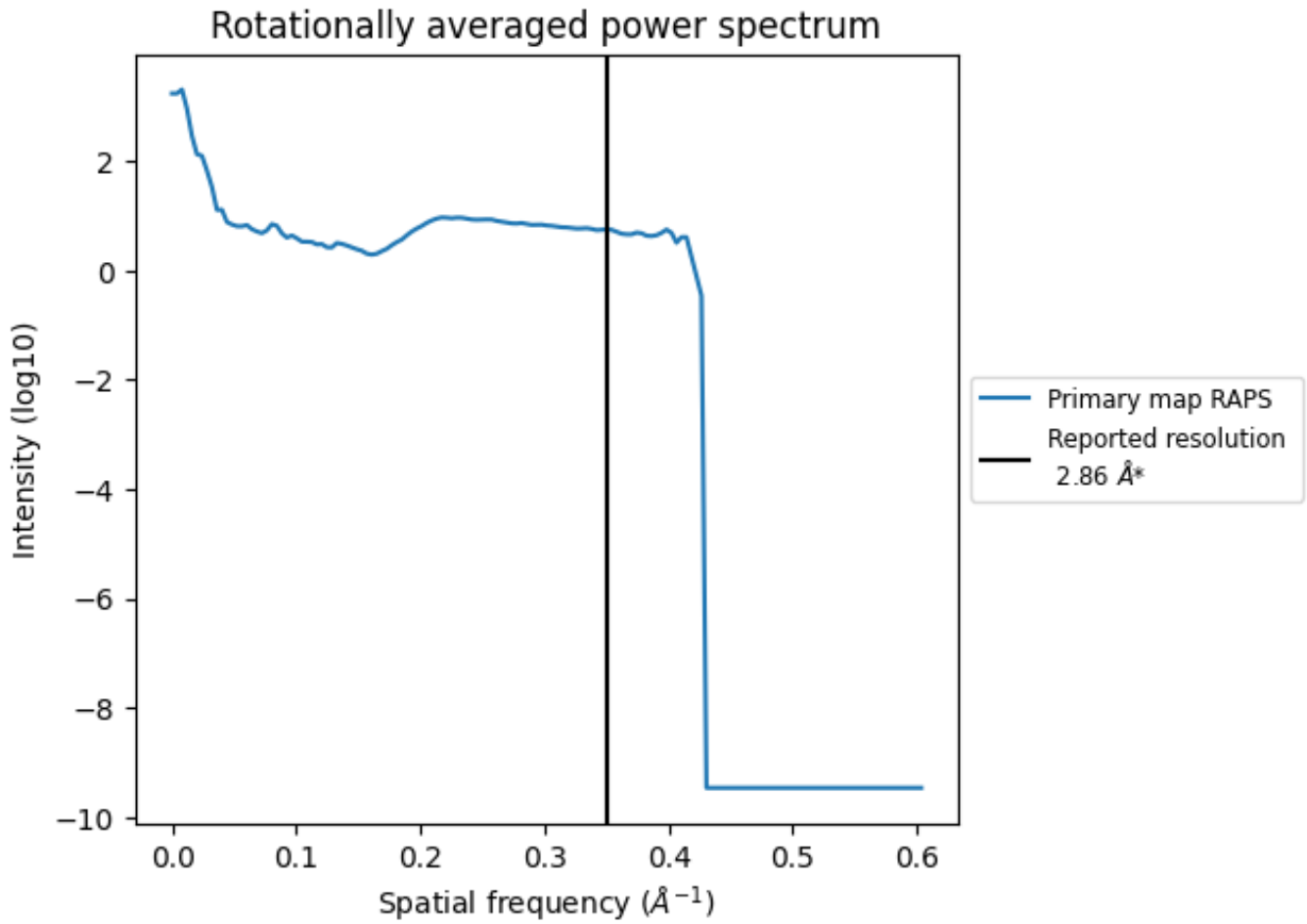
7.2 Volume estimate



The volume at the recommended contour level is 99 nm^3; this corresponds to an approximate mass of 90 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)

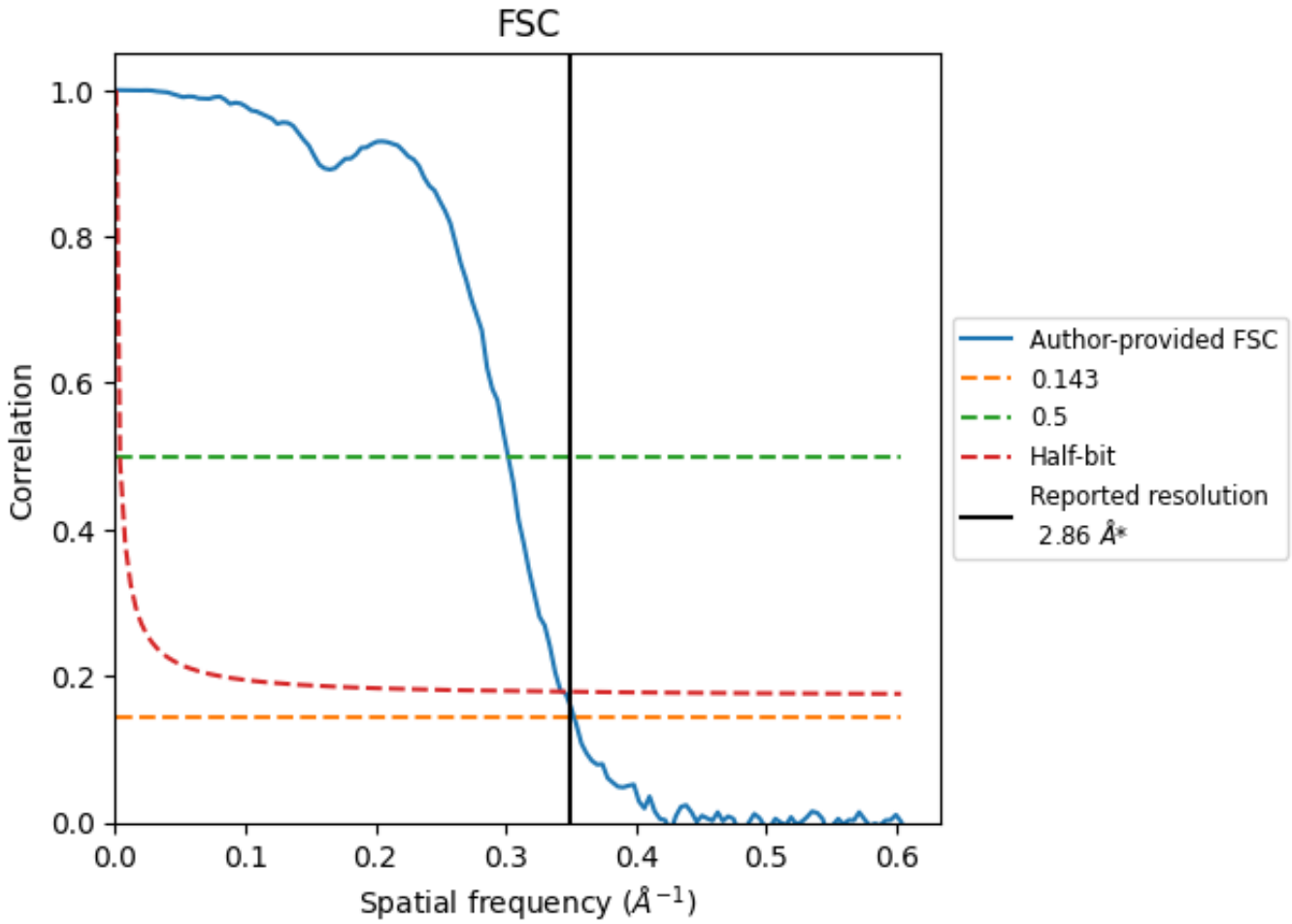


*Reported resolution corresponds to spatial frequency of 0.350 Å^{-1}

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 0.350 Å^{-1}

8.2 Resolution estimates (i)

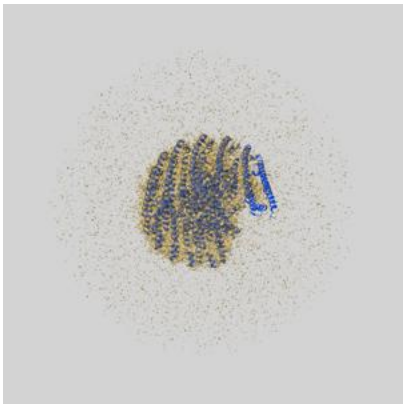
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.84	3.31	2.91
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

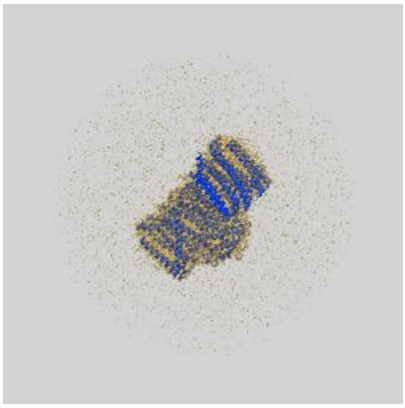
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32042 and PDB model 7VNM. Per-residue inclusion information can be found in section 3 on page 14.

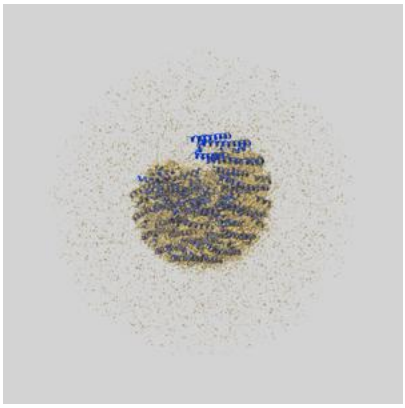
9.1 Map-model overlay



X



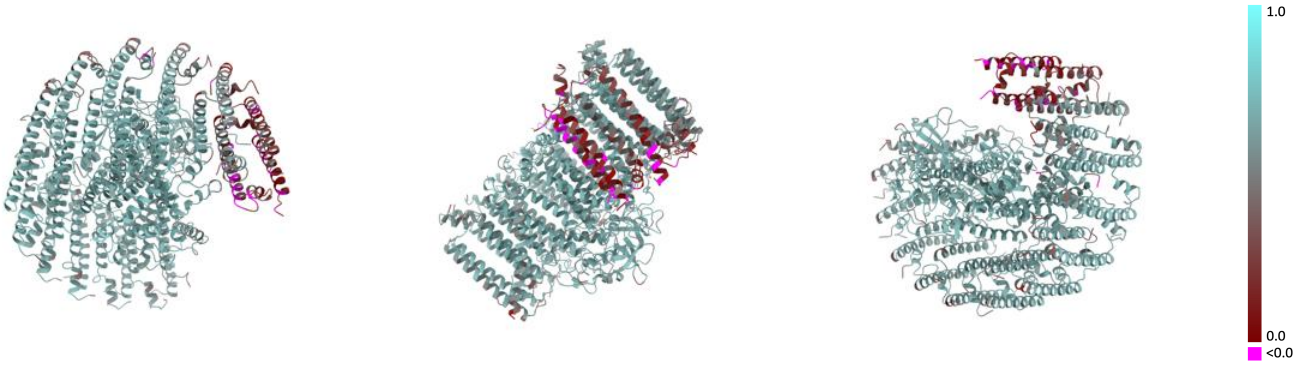
Y



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.

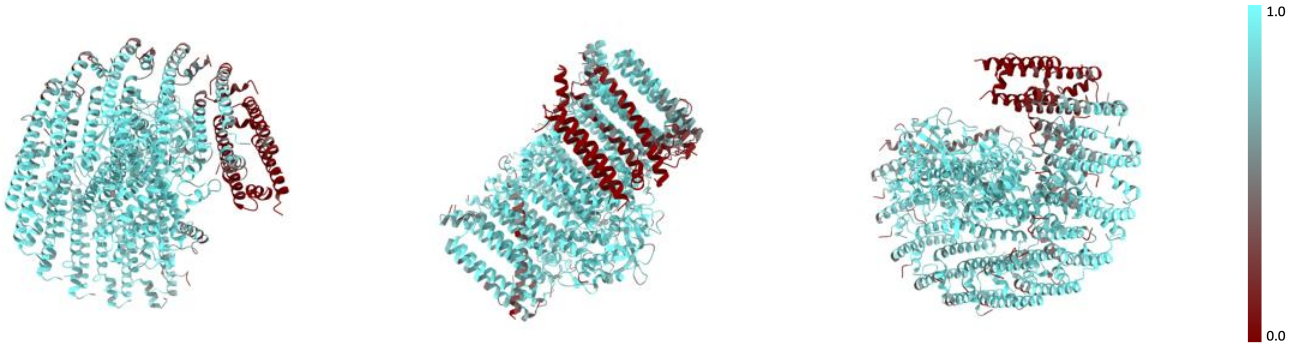
9.2 Q-score mapped to coordinate model (i)



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.

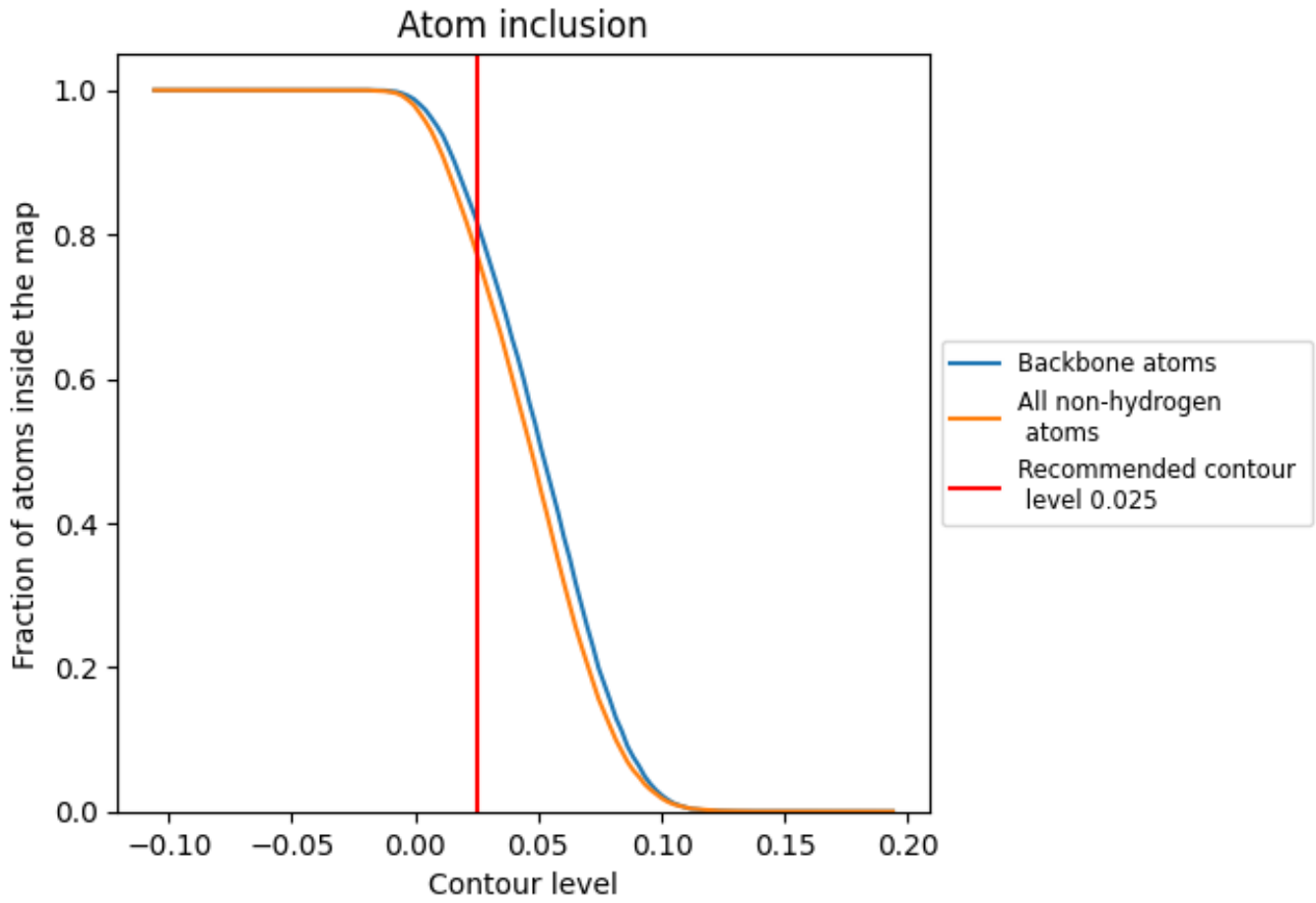
9.3 Atom inclusion mapped to coordinate model (i)



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, 82% of all backbone atoms, 77% 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	0.7738	0.5910
0	0.8391	0.6240
1	0.0173	0.1510
2	0.0131	0.0960
7	0.7483	0.5800
8	0.7323	0.5640
9	0.8760	0.6460
A	0.8688	0.6320
B	0.8599	0.6350
C	0.0755	0.1970
D	0.8671	0.6160
E	0.8233	0.6100
F	0.8820	0.6460
G	0.8601	0.6120
H	0.8314	0.6260
I	0.8681	0.6310
J	0.8251	0.6130
K	0.8254	0.6290
L	0.9240	0.6670
M	0.9372	0.6760
N	0.7753	0.5950
O	0.8380	0.6220
P	0.7026	0.5700
Q	0.8029	0.6120
R	0.7587	0.5800
S	0.7443	0.6090
T	0.6793	0.5510
U	0.6180	0.5350
V	0.5531	0.4740
W	0.2885	0.3800
X	0.4793	0.5260