Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 12:10 PM JST

PDB ID	:	7DDQ / pdb_00007ddq
EMDB ID	:	EMD-30656
Title	:	Structure of RC-LH1-PufX from Rhodobacter veldkampii
Authors	:	Bracun, L.; Yamagata, A.; Shirouzu, M.; Liu, L.N.
Deposited on	:	2020-10-29
Resolution	:	2.84 Å(reported)

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

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

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

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

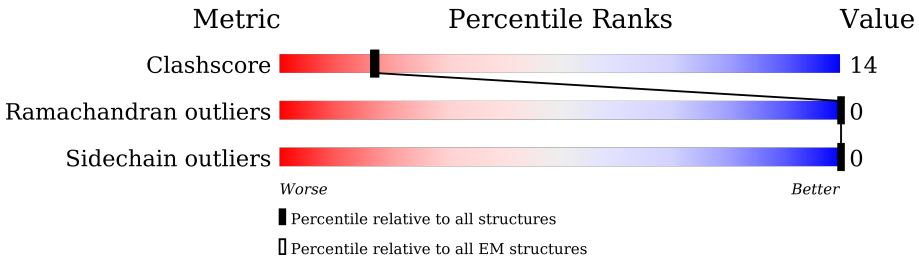
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	a	57	56% 21% 23%
1	b	57	60% 33% 7%
1	d	57	72% 21% 7%
1	e	57	72% 21% 7%
1	f	57	67% 26% 7%
1	g	57	7% 67% 26% 7%
1	i	57	12% 72% 21% 7%
1	j	57	5% 63% 30% 7%

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Mol	Chain	Length	Quality of chain
1	k	57	7% 63% 30% 7%
1	n	57	9% 65% 28% 7%
1	o	57	11% 56% 37% 7%
1	r	57	14% 65% 28% 7%
1	s	57	12% 61% 32% 7%
1	t	57	11% 58% 35% 7%
1	u	57	32% 72% 19% 9%
2	A	48	71% 21% 8%
2	B	48	67% 25% 8%
2	D	48	73% 19% 8%
2	E	48	54% 38% 8%
2	F	48	6% 54% 38% 8%
2	G	48	19% 67% 25% 8%
2	I	48	21% 73% 19% 8%
2	J	48	15% 67% 25% 8%
2	K	48	8% 73% 19% 8%
2	N	48	12% 58% 33% 8%
2	O	48	27% 56% 35% 8%
2	R	48	29% 63% 29% 8%
2	S	48	25% 54% 38% 8%
2	T	48	19% 65% 25% 10%
2	U	48	10% 63% 27% 10%
3	X	83	34% 84% 13%
4	L	276	78% 22%
5	M	308	81% 17%

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Mol	Chain	Length	Quality of chain
6	H	252	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SPO	s	201	-	X	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 22571 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 Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	o	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	t	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	r	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	a	44	Total	C	N	O	S	0	0
			373	258	59	54	2		
1	e	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	b	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	k	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	f	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	u	52	Total	C	N	O	S	0	0
			440	302	71	65	2		
1	s	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	n	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	i	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	j	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	g	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	d	53	Total	C	N	O	S	0	0
			446	305	72	67	2		

- Molecule 2 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	S	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	O	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	U	43	Total	C	N	O	S	0	0
			354	237	57	59	1		
2	D	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	A	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	J	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	E	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	T	43	Total	C	N	O	S	0	0
			354	237	57	59	1		
2	R	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	K	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	G	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	I	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	F	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	B	44	Total	C	N	O	S	0	0
			363	243	58	61	1		

- Molecule 3 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	81	Total	C	N	O	S	0	0
			610	396	100	110	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	275	Total	C	N	O	S	0	0
			2188	1469	350	360	9		

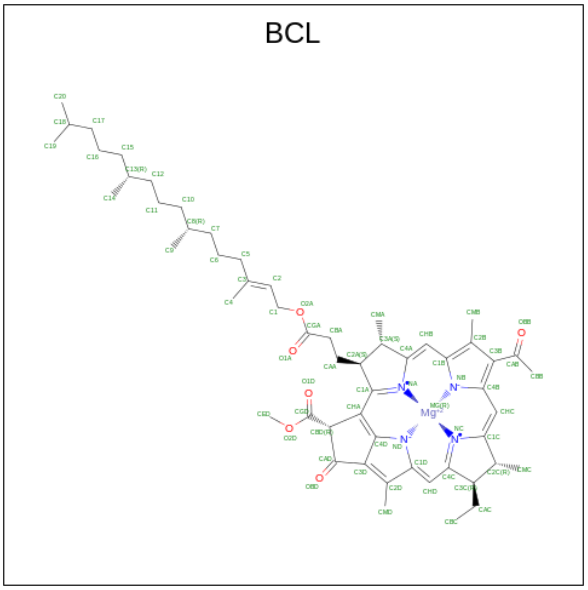
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	305	Total	C	N	O	S	0	0
			2420	1612	393	404	11		

- Molecule 6 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	250	Total	C	N	O	S	0	0
			1907	1223	318	351	15		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
7	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	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	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
7	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	k	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	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	s	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	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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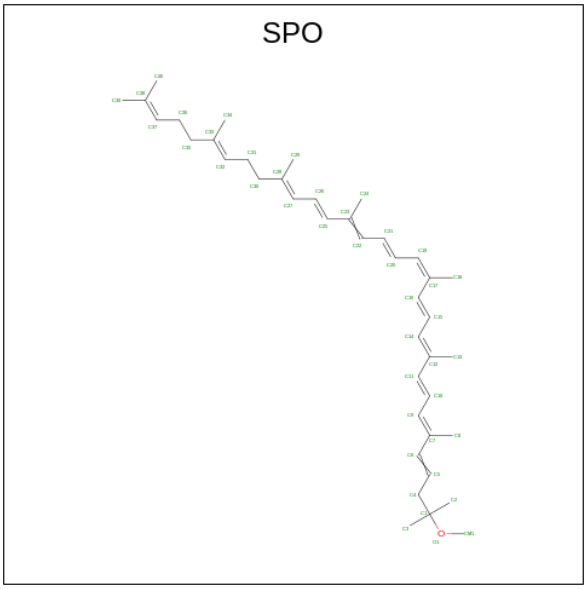
Mol	Chain	Residues	Atoms					AltConf
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			AltConf
8	N	1	Total	C	O	0
			42	41	1	
8	t	1	Total	C	O	0
			42	41	1	
8	r	1	Total	C	O	0
			42	41	1	
8	r	1	Total	C	O	0
			42	41	1	
8	D	1	Total	C	O	0
			42	41	1	
8	k	1	Total	C	O	0
			42	41	1	

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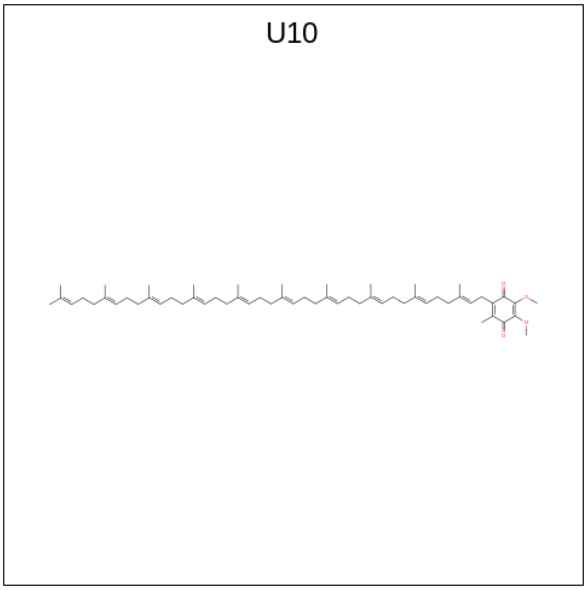
Mol	Chain	Residues	Atoms	AltConf
8	E	1	Total C O 42 41 1	0
8	X	1	Total C O 42 41 1	0
8	s	1	Total C O 42 41 1	0
8	j	1	Total C O 42 41 1	0
8	I	1	Total C O 42 41 1	0
8	M	1	Total C O 42 41 1	0
8	g	1	Total C O 42 41 1	0
8	F	1	Total C O 42 41 1	0
8	B	1	Total C O 42 41 1	0

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms	AltConf
9	a	1	Total C O 48 44 4	0
9	L	1	Total C O 33 29 4	0

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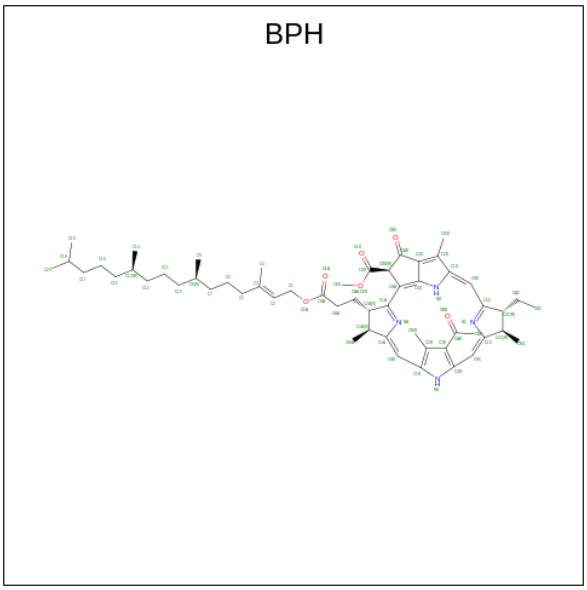
Mol	Chain	Residues	Atoms	AltConf
9	L	1	Total C O 38 34 4	0
9	L	1	Total C O 28 24 4	0
9	M	1	Total C O 48 44 4	0
9	M	1	Total C O 18 14 4	0

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



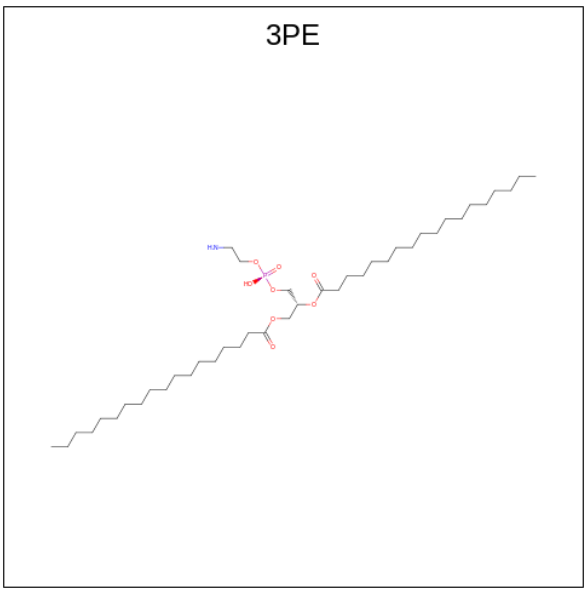
Mol	Chain	Residues	Atoms	AltConf
10	L	1	Total C N O 65 55 4 6	0
10	L	1	Total C N O 45 35 4 6	0
10	M	1	Total C N O 65 55 4 6	0

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:

$C_{41}H_{82}NO_8P$).



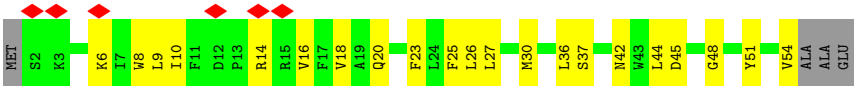
Mol	Chain	Residues	Atoms					AltConf
12	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
12	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
12	d	1	Total	C	N	O	P	0
			43	33	1	8	1	

3 Residue-property plots (i)

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

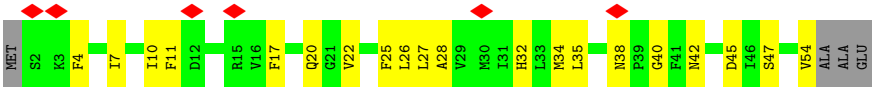
• Molecule 1: Antenna pigment protein alpha chain

Chain o:



• Molecule 1: Antenna pigment protein alpha chain

Chain t:

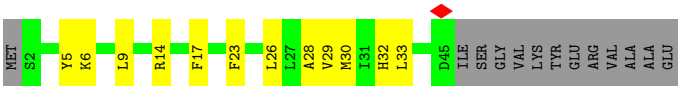


• Molecule 1: Antenna pigment protein alpha chain

Chain r:

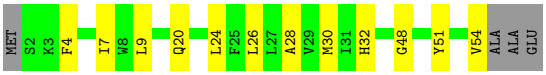
• Molecule 1: Antenna pigment protein alpha chain

Chain a:



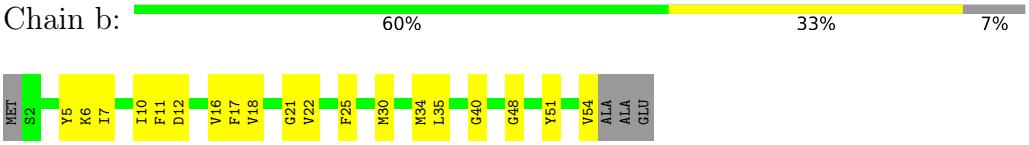
• Molecule 1: Antenna pigment protein alpha chain

Chain e:



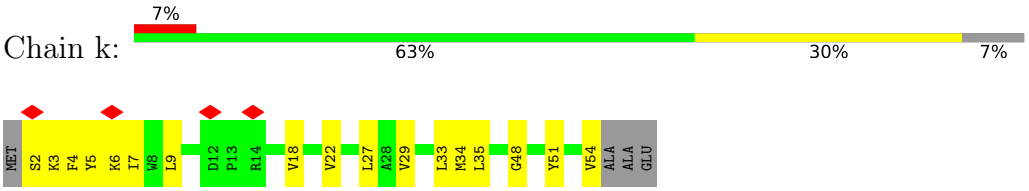
• Molecule 1: Antenna pigment protein alpha chain

Chain b:



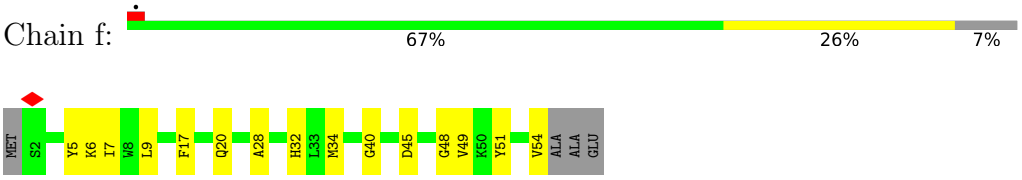
• Molecule 1: Antenna pigment protein alpha chain

Chain k:



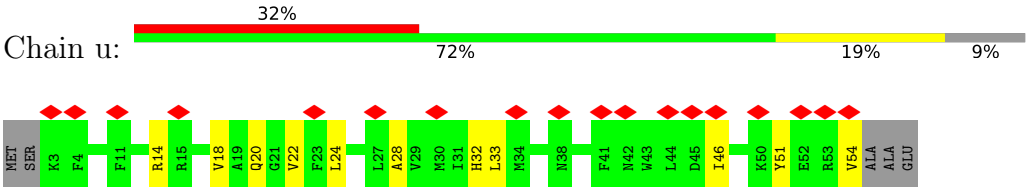
• Molecule 1: Antenna pigment protein alpha chain

Chain f:



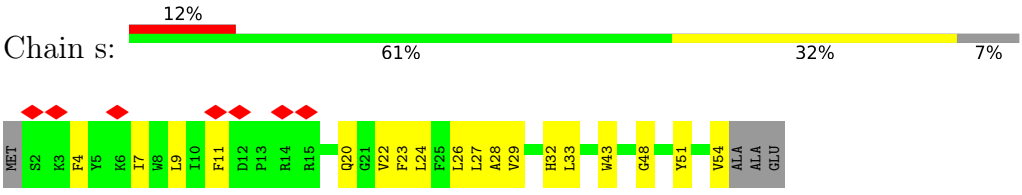
• Molecule 1: Antenna pigment protein alpha chain

Chain u:



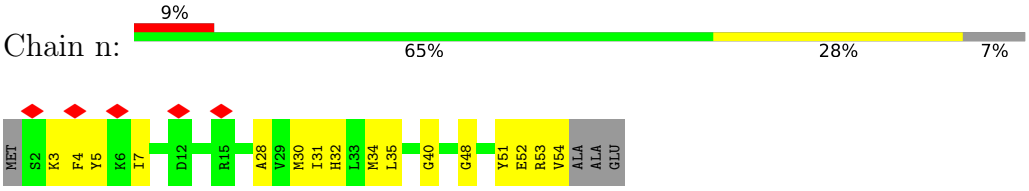
• Molecule 1: Antenna pigment protein alpha chain

Chain s:



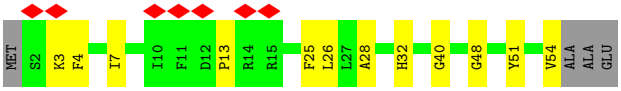
• Molecule 1: Antenna pigment protein alpha chain

Chain n:

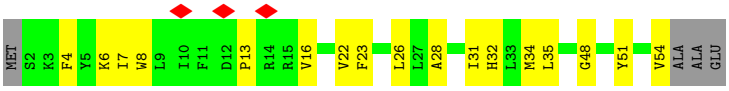


• Molecule 1: Antenna pigment protein alpha chain

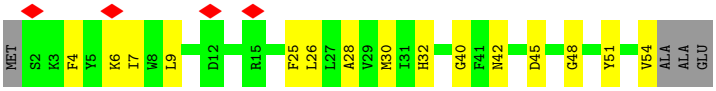
Chain i:



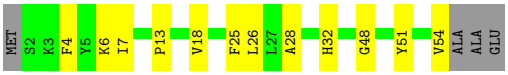
• Molecule 1: Antenna pigment protein alpha chain



• Molecule 1: Antenna pigment protein alpha chain

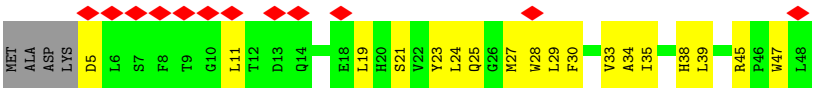


• Molecule 1: Antenna pigment protein alpha chain

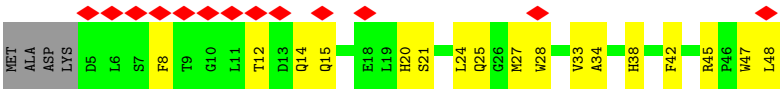


• Molecule 2: Antenna pigment protein beta chain

• Molecule 2: Antenna pigment protein beta chain

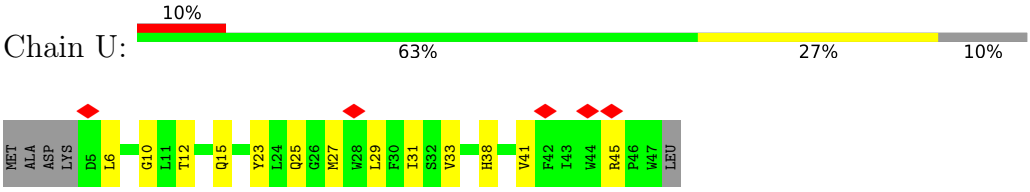


• Molecule 2: Antenna pigment protein beta chain



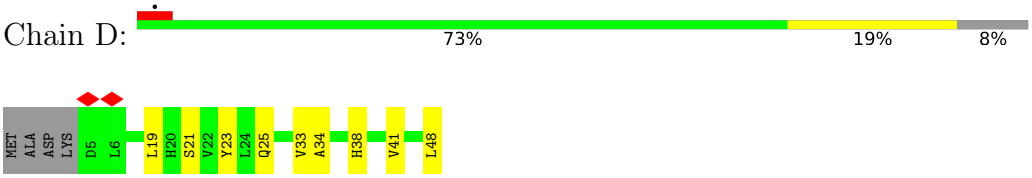
• Molecule 2: Antenna pigment protein beta chain

Chain U:



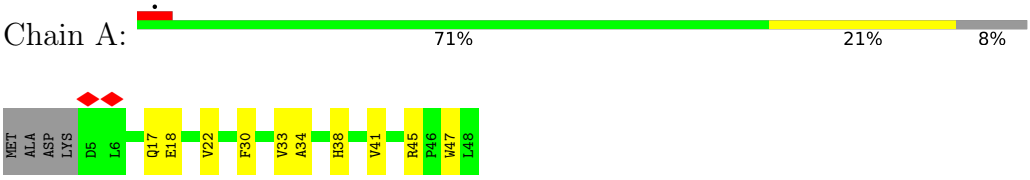
• Molecule 2: Antenna pigment protein beta chain

Chain D:



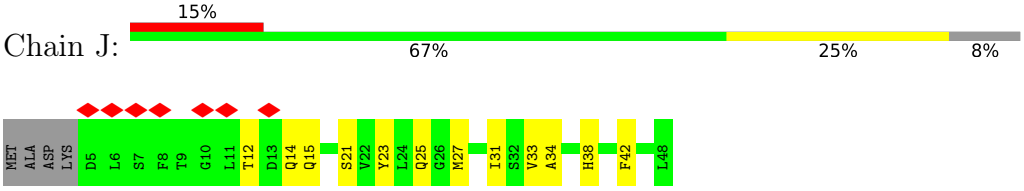
• Molecule 2: Antenna pigment protein beta chain

Chain A:



• Molecule 2: Antenna pigment protein beta chain

Chain J:

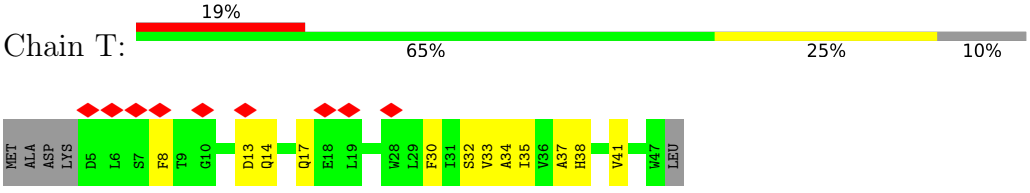


• Molecule 2: Antenna pigment protein beta chain

Chain E:

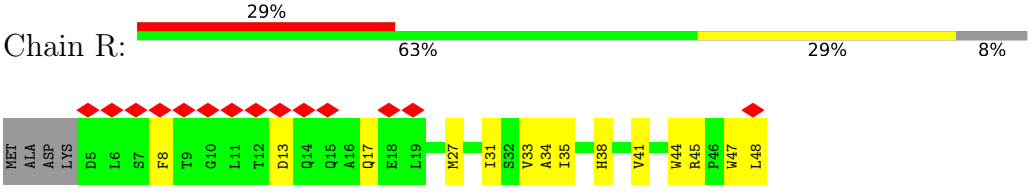
• Molecule 2: Antenna pigment protein beta chain

Chain T:



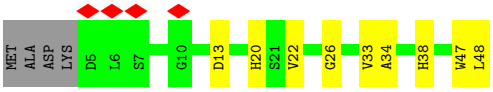
• Molecule 2: Antenna pigment protein beta chain

Chain R:



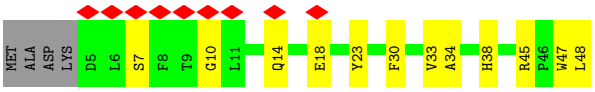
• Molecule 2: Antenna pigment protein beta chain

Chain K:



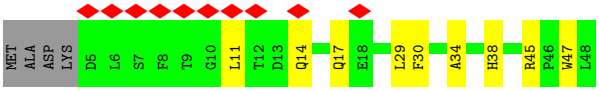
• Molecule 2: Antenna pigment protein beta chain

Chain G:



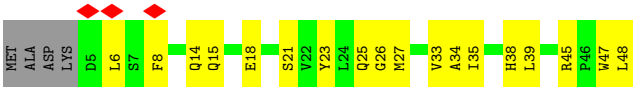
• Molecule 2: Antenna pigment protein beta chain

Chain I:



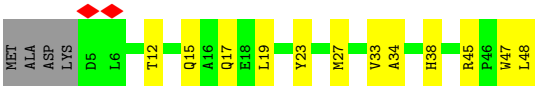
• Molecule 2: Antenna pigment protein beta chain

Chain F:



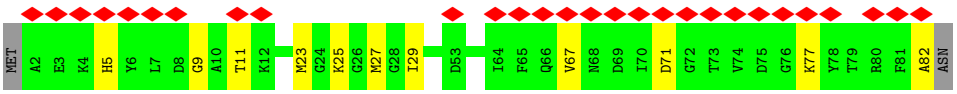
• Molecule 2: Antenna pigment protein beta chain

Chain B:



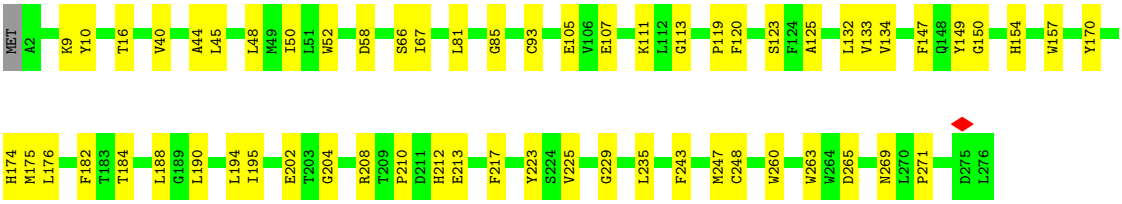
• Molecule 3: PufX

Chain X:

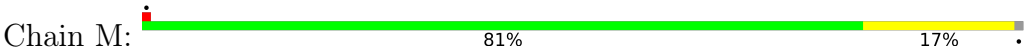


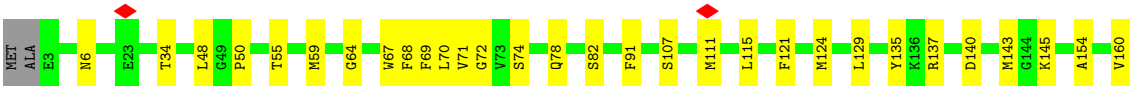
• Molecule 4: Photosynthetic reaction center L subunit

Chain L:

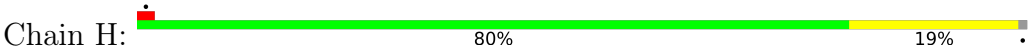


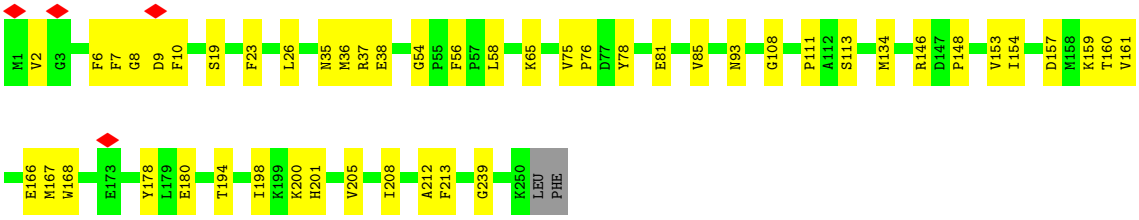
• Molecule 5: Reaction center protein M chain





• Molecule 6: Photosynthetic reaction center subunit H





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184921	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0157	Depositor
Map size (Å)	215.8, 215.8, 215.8	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: U10, FE, BPH, 3PE, BCL, SPO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	a	0.36	0/386	0.60	0/523
1	b	0.31	0/460	0.44	0/622
1	d	0.31	0/460	0.44	0/622
1	e	0.31	0/460	0.43	0/622
1	f	0.29	0/460	0.44	0/622
1	g	0.27	0/460	0.39	0/622
1	i	0.27	0/460	0.46	0/622
1	j	0.27	0/460	0.52	0/622
1	k	0.30	0/460	0.46	0/622
1	n	0.28	0/460	0.38	0/622
1	o	0.28	0/460	0.40	0/622
1	r	0.26	0/460	0.39	0/622
1	s	0.24	0/460	0.38	0/622
1	t	0.23	0/460	0.40	0/622
1	u	0.22	0/454	0.43	0/614
2	A	0.29	0/375	0.41	0/512
2	B	0.31	0/375	0.38	0/512
2	D	0.29	0/375	0.36	0/512
2	E	0.28	0/375	0.37	0/512
2	F	0.26	0/375	0.36	0/512
2	G	0.24	0/375	0.33	0/512
2	I	0.22	0/375	0.33	0/512
2	J	0.25	0/375	0.34	0/512
2	K	0.26	0/375	0.35	0/512
2	N	0.26	0/375	0.36	0/512
2	O	0.24	0/375	0.41	0/512
2	R	0.22	0/375	0.35	0/512
2	S	0.20	0/375	0.36	0/512
2	T	0.21	0/366	0.38	0/501
2	U	0.19	0/366	0.34	0/501
3	X	0.26	0/624	0.50	0/843
4	L	0.35	0/2272	0.48	0/3108

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
5	M	0.38	0/2507	0.50	0/3421
6	H	0.34	0/1959	0.46	0/2664
All	All	0.30	0/19789	0.44	0/26917

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	M	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	M	217	PHE	Sidechain

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	a	373	0	384	9	0
1	b	446	0	462	24	0
1	d	446	0	462	13	0
1	e	446	0	462	10	0
1	f	446	0	462	15	0
1	g	446	0	462	10	0
1	i	446	0	462	9	0
1	j	446	0	462	13	0
1	k	446	0	462	15	0
1	n	446	0	462	14	0
1	o	446	0	462	19	0
1	r	446	0	462	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	s	446	0	462	18	0
1	t	446	0	462	21	0
1	u	440	0	457	9	0
2	A	363	0	355	9	0
2	B	363	0	355	10	0
2	D	363	0	355	9	0
2	E	363	0	355	16	0
2	F	363	0	355	15	0
2	G	363	0	355	9	0
2	I	363	0	355	9	0
2	J	363	0	355	9	0
2	K	363	0	355	8	0
2	N	363	0	355	16	0
2	O	363	0	355	13	0
2	R	363	0	355	14	0
2	S	363	0	355	25	0
2	T	354	0	344	9	0
2	U	354	0	344	14	0
3	X	610	0	601	9	0
4	L	2188	0	2126	46	0
5	M	2420	0	2363	55	0
6	H	1907	0	1880	45	0
7	A	66	0	74	3	0
7	D	66	0	74	2	0
7	E	66	0	74	3	0
7	F	132	0	148	9	0
7	G	66	0	74	2	0
7	I	66	0	74	2	0
7	K	66	0	74	3	0
7	L	66	0	74	3	0
7	M	198	0	222	11	0
7	N	66	0	74	5	0
7	O	66	0	74	3	0
7	R	66	0	74	7	0
7	S	66	0	74	2	0
7	a	66	0	74	2	0
7	b	132	0	148	9	0
7	d	66	0	74	9	0
7	e	66	0	74	5	0
7	g	66	0	74	8	0
7	i	66	0	74	0	0
7	j	132	0	148	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	k	66	0	74	3	0
7	n	66	0	74	5	0
7	o	66	0	74	5	0
7	r	66	0	74	8	0
7	s	66	0	74	5	0
7	t	132	0	148	12	0
7	u	132	0	148	11	0
8	B	42	0	60	11	0
8	D	42	0	60	11	0
8	E	42	0	60	17	0
8	F	42	0	60	12	0
8	I	42	0	60	6	0
8	M	42	0	60	13	0
8	N	42	0	60	12	0
8	X	42	0	60	4	0
8	g	42	0	60	8	0
8	j	42	0	60	7	0
8	k	42	0	60	10	0
8	r	84	0	120	20	0
8	s	42	0	60	16	0
8	t	42	0	60	7	0
9	L	99	0	117	5	0
9	M	66	0	78	6	0
9	a	48	0	63	7	0
10	L	110	0	113	9	0
10	M	65	0	76	12	0
11	M	1	0	0	0	0
12	H	102	0	164	10	0
12	d	43	0	63	2	0
All	All	22571	0	23210	625	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (625) 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)
8:r:102:SPO:H21	7:O:101:BCL:H11	1.53	0.89
8:t:102:SPO:H19	7:t:103:BCL:H11	1.58	0.85
8:t:102:SPO:H37	8:t:102:SPO:H301	1.59	0.84
1:s:24:LEU:HD11	8:s:201:SPO:H27	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:124:MET:HE3	8:M:406:SPO:H351	1.62	0.82
1:o:6:LYS:HA	1:o:9:LEU:HD23	1.61	0.81
2:O:12:THR:OG1	2:O:15:GLN:OE1	2.02	0.78
1:g:51:TYR:HB2	1:g:54:VAL:HA	1.65	0.77
7:d:101:BCL:HHB	8:B:101:SPO:H82	1.67	0.77
5:M:179:GLY:HA3	5:M:182:PRO:HG2	1.67	0.76
5:M:137:ARG:NH2	5:M:140:ASP:OD2	2.18	0.76
1:s:27:LEU:HD11	8:s:201:SPO:H83	1.67	0.76
2:T:13:ASP:OD1	2:T:17:GLN:NE2	2.18	0.75
1:o:36:LEU:HD11	8:N:201:SPO:H41	1.65	0.75
1:a:30:MET:HE3	9:a:102:U10:H18	1.67	0.75
2:A:34:ALA:O	2:A:38:HIS:ND1	2.19	0.74
2:N:31:ILE:HG12	7:N:202:BCL:H12	1.70	0.74
1:o:51:TYR:HB2	1:o:54:VAL:HA	1.70	0.73
1:s:48:GLY:HA2	1:s:54:VAL:HG23	1.70	0.73
2:R:27:MET:O	2:R:31:ILE:HD12	1.89	0.72
5:M:262:THR:HG23	5:M:265:GLY:H	1.53	0.72
5:M:91:PHE:H	9:M:408:U10:H4M1	1.55	0.71
2:E:23:TYR:HA	8:E:201:SPO:H311	1.72	0.71
5:M:262:THR:H	6:H:35:ASN:HD22	1.39	0.71
8:N:201:SPO:H27	8:N:201:SPO:H241	1.72	0.70
1:f:40:GLY:O	2:F:45:ARG:NH1	2.24	0.70
2:R:34:ALA:O	2:R:38:HIS:ND1	2.21	0.70
2:F:34:ALA:O	2:F:38:HIS:ND1	2.24	0.69
1:t:42:ASN:ND2	1:t:45:ASP:OD1	2.25	0.69
8:E:201:SPO:H392	1:d:6:LYS:HB3	1.74	0.69
8:M:406:SPO:H241	8:M:406:SPO:H27	1.75	0.69
4:L:202:GLU:OE1	5:M:145:LYS:NZ	2.25	0.69
5:M:230:LEU:O	5:M:232:GLY:N	2.25	0.69
1:b:25:PHE:HA	7:b:101:BCL:H12	1.75	0.68
1:f:51:TYR:HB2	1:f:54:VAL:HA	1.76	0.68
2:S:34:ALA:O	2:S:38:HIS:ND1	2.21	0.68
1:d:51:TYR:HB2	1:d:54:VAL:HA	1.75	0.68
2:J:27:MET:HG3	8:j:301:SPO:C25	2.24	0.67
2:T:34:ALA:O	2:T:38:HIS:ND1	2.26	0.67
1:j:51:TYR:HB2	1:j:54:VAL:HA	1.76	0.67
1:t:28:ALA:O	1:t:32:HIS:ND1	2.22	0.67
2:I:34:ALA:O	2:I:38:HIS:ND1	2.25	0.67
1:b:34:MET:HE1	8:B:101:SPO:HM13	1.77	0.67
1:i:4:PHE:O	1:i:7:ILE:HG12	1.95	0.67
1:o:44:LEU:HD11	8:N:201:SPO:H32A	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:188:LEU:HD13	5:M:217:PHE:HB2	1.78	0.66
9:a:102:U10:H312	1:b:21:GLY:HA3	1.77	0.66
2:O:34:ALA:O	2:O:38:HIS:ND1	2.21	0.66
1:t:20:GLN:HE21	7:u:101:BCL:H151	1.60	0.66
2:G:34:ALA:O	2:G:38:HIS:ND1	2.25	0.66
1:e:28:ALA:O	1:e:32:HIS:ND1	2.26	0.66
1:o:25:PHE:HB2	7:o:100:BCL:H52	1.77	0.66
5:M:74:SER:O	5:M:78:GLN:HG2	1.95	0.65
7:b:101:BCL:CGD	7:b:101:BCL:HAA1	2.26	0.65
8:k:102:SPO:H311	2:K:26:GLY:HA3	1.78	0.65
8:k:102:SPO:H392	2:K:22:VAL:HG11	1.77	0.65
8:D:201:SPO:H343	1:b:7:ILE:HG23	1.78	0.65
1:n:30:MET:O	1:n:34:MET:HG3	1.96	0.65
8:k:102:SPO:H391	1:j:6:LYS:HB2	1.79	0.65
4:L:113:GLY:H	6:H:111:PRO:HB3	1.62	0.64
2:U:27:MET:O	2:U:31:ILE:HG12	1.97	0.64
2:E:34:ALA:O	2:E:38:HIS:ND1	2.29	0.64
9:a:102:U10:H3M2	4:L:81:LEU:HD13	1.80	0.64
9:a:102:U10:H311	1:b:18:VAL:HA	1.80	0.64
1:j:28:ALA:O	1:j:32:HIS:ND1	2.31	0.64
2:N:12:THR:H	2:N:15:GLN:HE21	1.47	0.63
7:t:101:BCL:HMB2	8:s:201:SPO:H82	1.81	0.63
8:r:102:SPO:H401	1:n:7:ILE:HD13	1.81	0.63
1:j:8:TRP:HZ3	1:j:16:VAL:HG21	1.63	0.63
2:D:34:ALA:O	2:D:38:HIS:ND1	2.28	0.62
7:d:101:BCL:H152	8:B:101:SPO:H131	1.81	0.62
2:N:25:GLN:OE1	1:k:2:SER:OG	2.14	0.62
1:b:51:TYR:HB2	1:b:54:VAL:HA	1.82	0.62
2:O:21:SER:O	2:O:25:GLN:NE2	2.32	0.62
1:k:51:TYR:HB2	1:k:54:VAL:HG22	1.81	0.62
1:d:28:ALA:O	1:d:32:HIS:ND1	2.26	0.62
4:L:50:ILE:HA	4:L:67:ILE:HD11	1.81	0.62
2:R:13:ASP:OD1	2:R:17:GLN:NE2	2.33	0.62
1:d:32:HIS:HB2	8:B:101:SPO:H23	1.81	0.61
1:a:28:ALA:O	1:a:32:HIS:ND1	2.26	0.61
1:s:28:ALA:O	1:s:32:HIS:ND1	2.31	0.61
4:L:204:GLY:O	6:H:65:LYS:NZ	2.25	0.61
7:t:101:BCL:HMB2	8:s:201:SPO:H5	1.83	0.61
2:S:23:TYR:OH	1:s:20:GLN:NE2	2.30	0.61
1:a:14:ARG:HD2	3:X:5:HIS:CG	2.36	0.61
1:r:28:ALA:O	1:r:32:HIS:ND1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:34:ALA:O	2:J:38:HIS:ND1	2.26	0.60
6:H:154:ILE:HG12	6:H:160:THR:HG22	1.84	0.60
1:n:51:TYR:HB2	1:n:54:VAL:HA	1.81	0.60
2:J:12:THR:HB	2:J:15:GLN:HG3	1.82	0.60
1:g:28:ALA:O	1:g:32:HIS:ND1	2.32	0.60
1:t:34:MET:HE2	8:t:102:SPO:H21A	1.84	0.59
1:i:51:TYR:HB2	1:i:54:VAL:HA	1.82	0.59
2:N:45:ARG:NH1	1:n:40:GLY:O	2.34	0.59
4:L:174:HIS:HB2	4:L:248:CYS:SG	2.42	0.59
7:L:301:BCL:H193	9:M:405:U10:H252	1.83	0.59
10:L:302:BPH:HHC	10:L:302:BPH:HBB3	1.84	0.59
10:L:306:BPH:HHC	10:L:306:BPH:HBB3	1.85	0.59
1:u:51:TYR:HB2	1:u:54:VAL:HA	1.85	0.59
2:J:12:THR:HG22	2:J:14:GLN:H	1.67	0.59
1:f:20:GLN:HG2	7:g:101:BCL:H121	1.84	0.59
1:i:3:LYS:HD2	1:i:3:LYS:O	2.02	0.58
7:o:100:BCL:HED1	2:O:33:VAL:HG12	1.84	0.58
1:n:4:PHE:O	1:n:7:ILE:HG12	2.04	0.58
2:G:23:TYR:CE1	8:g:102:SPO:H26	2.38	0.58
2:B:34:ALA:O	2:B:38:HIS:ND1	2.28	0.58
1:s:51:TYR:HB2	1:s:54:VAL:HA	1.84	0.58
1:u:20:GLN:O	1:u:24:LEU:HG	2.04	0.58
8:r:103:SPO:C37	8:r:103:SPO:H311	2.34	0.58
2:U:45:ARG:HH22	1:u:46:ILE:HG21	1.68	0.58
1:g:26:LEU:O	1:g:30:MET:HG2	2.02	0.58
5:M:64:GLY:HA3	10:M:403:BPH:H5C1	1.86	0.58
1:d:18:VAL:HG11	12:d:102:3PE:H222	1.84	0.58
8:r:102:SPO:H25	2:O:27:MET:HA	1.86	0.58
8:r:103:SPO:H241	8:r:103:SPO:C27	2.34	0.58
1:b:48:GLY:HA2	1:b:54:VAL:HG23	1.86	0.58
2:E:27:MET:SD	2:E:31:ILE:HD12	2.44	0.58
5:M:202:PHE:HD1	5:M:280:THR:HG23	1.68	0.58
1:s:22:VAL:O	1:s:26:LEU:HG	2.04	0.57
7:F:103:BCL:H3A	7:F:103:BCL:H52	1.85	0.57
7:o:100:BCL:H171	8:r:102:SPO:H342	1.84	0.57
1:r:48:GLY:HA2	1:r:54:VAL:HG23	1.85	0.57
1:n:48:GLY:HA2	1:n:54:VAL:HG23	1.86	0.57
1:r:32:HIS:CG	8:r:102:SPO:H6	2.40	0.57
4:L:45:LEU:HD22	4:L:93:CYS:SG	2.45	0.57
2:E:21:SER:O	2:E:25:GLN:HG3	2.05	0.57
8:E:201:SPO:H362	1:d:6:LYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:33:VAL:HG12	7:u:101:BCL:HED1	1.87	0.57
1:i:48:GLY:HA2	1:i:54:VAL:HG23	1.87	0.57
6:H:153:VAL:HG13	6:H:161:VAL:HG23	1.86	0.57
1:o:8:TRP:HZ3	1:o:16:VAL:HG21	1.70	0.56
2:U:6:LEU:HD23	6:H:154:ILE:HD11	1.87	0.56
1:e:48:GLY:HA2	1:e:54:VAL:HG23	1.87	0.56
4:L:9:LYS:NZ	6:H:81:GLU:OE1	2.29	0.56
5:M:74:SER:HB2	5:M:115:LEU:HD23	1.87	0.56
1:t:47:SER:HB3	2:S:47:TRP:O	2.06	0.56
9:a:102:U10:H33	7:b:101:BCL:H13	1.87	0.56
2:N:34:ALA:O	2:N:38:HIS:ND1	2.32	0.56
1:e:20:GLN:HE21	7:F:101:BCL:H121	1.69	0.56
1:e:51:TYR:OH	2:D:48:LEU:O	2.19	0.56
2:A:18:GLU:HG2	3:X:11:THR:HG23	1.87	0.56
5:M:262:THR:HG22	6:H:35:ASN:HD22	1.70	0.56
2:A:30:PHE:HE2	7:A:101:BCL:HBA1	1.70	0.56
2:I:14:GLN:HA	2:I:17:GLN:NE2	2.20	0.56
10:L:302:BPH:HHC	10:L:302:BPH:CBB	2.36	0.56
1:k:3:LYS:HB2	1:k:5:TYR:CE1	2.41	0.56
2:F:23:TYR:HD1	8:F:102:SPO:H352	1.70	0.56
5:M:199:TYR:CZ	5:M:305:LYS:HD2	2.40	0.55
1:f:28:ALA:O	1:f:32:HIS:ND1	2.34	0.55
2:T:37:ALA:O	2:T:41:VAL:HG23	2.06	0.55
5:M:262:THR:H	6:H:35:ASN:ND2	2.04	0.55
4:L:125:ALA:HB2	10:L:302:BPH:HAC1	1.89	0.55
2:N:21:SER:O	2:N:25:GLN:HG3	2.07	0.55
5:M:244:THR:HG21	6:H:113:SER:O	2.07	0.55
1:t:54:VAL:HG23	2:S:45:ARG:HH11	1.72	0.55
9:M:405:U10:H221	12:H:302:3PE:H352	1.89	0.55
2:F:26:GLY:HA3	8:F:102:SPO:H393	1.89	0.55
8:D:201:SPO:H27	8:D:201:SPO:H241	1.88	0.55
5:M:69:PHE:HB2	10:M:403:BPH:H18	1.88	0.55
2:S:27:MET:HA	8:s:201:SPO:H241	1.89	0.54
10:M:403:BPH:H171	8:M:406:SPO:H23	1.89	0.54
1:b:40:GLY:O	2:B:45:ARG:NH1	2.40	0.54
1:k:33:LEU:HD11	8:j:301:SPO:H31	1.89	0.54
1:o:14:ARG:O	1:o:18:VAL:HG23	2.08	0.54
3:X:25:LYS:O	3:X:29:ILE:HG12	2.07	0.54
2:O:20:HIS:O	2:O:24:LEU:HG	2.08	0.54
10:M:403:BPH:HBB3	10:M:403:BPH:HHC	1.89	0.54
1:f:20:GLN:NE2	7:g:101:BCL:H151	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:184:THR:HG21	5:M:214:THR:HG23	1.88	0.54
3:X:9:GLY:C	3:X:11:THR:H	2.16	0.54
6:H:19:SER:HB3	12:H:301:3PE:H3G1	1.90	0.54
9:a:102:U10:H251	1:b:22:VAL:HG22	1.90	0.53
2:R:47:TRP:CD1	2:R:48:LEU:HG	2.43	0.53
6:H:148:PRO:HG3	6:H:198:ILE:HD13	1.90	0.53
1:d:48:GLY:HA2	1:d:54:VAL:HG23	1.90	0.53
2:U:38:HIS:HA	2:U:41:VAL:HG12	1.90	0.53
7:t:101:BCL:H151	1:s:20:GLN:HE21	1.74	0.53
8:D:201:SPO:H343	1:b:7:ILE:CG2	2.38	0.53
2:O:42:PHE:HE1	2:O:48:LEU:HD23	1.74	0.53
1:b:12:ASP:CB	6:H:93:ASN:HD22	2.22	0.53
2:K:47:TRP:CD1	2:K:48:LEU:HD12	2.44	0.53
1:t:54:VAL:HB	2:S:45:ARG:HD2	1.90	0.53
2:U:12:THR:OG1	2:U:15:GLN:HG3	2.09	0.53
2:U:31:ILE:HD12	7:u:102:BCL:H11	1.90	0.53
1:s:4:PHE:O	1:s:7:ILE:HG12	2.09	0.53
1:i:28:ALA:O	1:i:32:HIS:ND1	2.33	0.53
7:M:401:BCL:H111	12:H:302:3PE:H3C2	1.90	0.53
1:b:12:ASP:HB2	6:H:93:ASN:HD22	1.74	0.53
4:L:16:THR:HA	4:L:107:GLU:HG2	1.91	0.52
1:a:6:LYS:HA	1:a:9:LEU:HD23	1.90	0.52
1:a:17:PHE:HD1	3:X:23:MET:HE3	1.74	0.52
2:O:47:TRP:CD1	2:O:48:LEU:HD22	2.45	0.52
2:U:45:ARG:HH12	1:u:46:ILE:HD13	1.74	0.52
1:f:17:PHE:CD2	8:F:102:SPO:H351	2.44	0.52
1:f:20:GLN:HE21	7:g:101:BCL:H151	1.74	0.52
2:K:34:ALA:O	2:K:38:HIS:ND1	2.33	0.52
7:M:402:BCL:H43	7:M:407:BCL:HBC3	1.91	0.52
1:t:11:PHE:CE1	1:u:14:ARG:HG2	2.45	0.52
7:t:103:BCL:HBA2	2:T:30:PHE:HE1	1.74	0.52
10:M:403:BPH:HBC3	10:M:403:BPH:HHD	1.91	0.52
2:E:35:ILE:O	2:E:39:LEU:HG	2.09	0.52
4:L:81:LEU:HA	4:L:85:GLY:HA3	1.91	0.52
2:S:30:PHE:HB3	8:s:201:SPO:H242	1.92	0.52
2:N:14:GLN:O	2:N:17:GLN:HB2	2.10	0.51
1:e:9:LEU:HD22	2:E:7:SER:HB3	1.92	0.51
7:e:100:BCL:HED1	2:E:33:VAL:HG12	1.92	0.51
1:k:27:LEU:HD11	8:k:102:SPO:H5	1.92	0.51
4:L:120:PHE:O	4:L:123:SER:OG	2.24	0.51
2:S:27:MET:HE2	8:s:201:SPO:H25	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:17:PHE:HZ	8:B:101:SPO:H342	1.74	0.51
2:J:33:VAL:HG12	7:j:302:BCL:HED1	1.91	0.51
2:N:12:THR:N	2:N:15:GLN:HE21	2.07	0.51
1:i:40:GLY:O	2:I:45:ARG:NH2	2.43	0.51
1:g:48:GLY:HA2	1:g:54:VAL:HG23	1.93	0.51
2:N:30:PHE:HE1	7:N:202:BCL:HBA1	1.74	0.51
2:T:32:SER:HA	2:T:35:ILE:HG12	1.92	0.51
2:F:33:VAL:HG12	7:F:101:BCL:HED1	1.92	0.51
8:F:102:SPO:H402	8:F:102:SPO:H32	1.91	0.51
7:r:101:BCL:HED1	2:R:33:VAL:HG12	1.93	0.51
2:O:47:TRP:NE1	2:O:48:LEU:HD22	2.26	0.51
2:F:35:ILE:O	2:F:39:LEU:HG	2.11	0.51
2:B:12:THR:OG1	2:B:15:GLN:HG3	2.10	0.51
8:E:201:SPO:H9	7:F:101:BCL:HBA2	1.93	0.51
2:U:6:LEU:HD21	6:H:201:HIS:HD2	1.74	0.51
6:H:208:ILE:HG13	6:H:212:ALA:HB3	1.93	0.50
1:j:23:PHE:HZ	8:j:301:SPO:H132	1.77	0.50
4:L:170:TYR:O	4:L:260:TRP:HB3	2.11	0.50
5:M:72:GLY:HA3	8:M:406:SPO:H31	1.94	0.50
7:k:101:BCL:HED1	2:K:33:VAL:HG12	1.93	0.50
7:g:101:BCL:H161	8:g:102:SPO:H361	1.93	0.50
2:U:25:GLN:O	2:U:29:LEU:HG	2.11	0.50
1:k:6:LYS:NZ	2:K:13:ASP:OD2	2.37	0.50
4:L:265:ASP:O	4:L:269:ASN:HB2	2.11	0.50
1:o:37:SER:OG	5:M:82:SER:HA	2.12	0.50
4:L:9:LYS:HB3	6:H:85:VAL:HG11	1.93	0.50
6:H:168:TRP:HB2	6:H:178:TYR:HB2	1.94	0.50
1:e:24:LEU:HD11	8:E:201:SPO:H21	1.93	0.50
4:L:176:LEU:HB2	9:L:304:U10:H112	1.94	0.50
1:d:32:HIS:CB	8:B:101:SPO:H23	2.41	0.50
4:L:210:PRO:HA	4:L:213:GLU:HG2	1.94	0.50
10:L:302:BPH:HMA2	5:M:215:MET:HE1	1.94	0.50
10:L:306:BPH:HMC1	10:M:403:BPH:HMA1	1.93	0.50
1:j:4:PHE:O	1:j:7:ILE:HG12	2.12	0.49
5:M:180:ILE:HG12	8:M:406:SPO:H133	1.93	0.49
2:N:11:LEU:HA	2:N:15:GLN:HE21	1.77	0.49
7:n:100:BCL:H203	2:K:20:HIS:HE1	1.78	0.49
7:t:101:BCL:H151	1:s:20:GLN:NE2	2.27	0.49
5:M:180:ILE:HD11	7:M:407:BCL:H172	1.93	0.49
8:r:103:SPO:H352	8:r:103:SPO:H292	1.94	0.49
1:e:4:PHE:O	1:e:7:ILE:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:205:VAL:HG21	6:H:213:PHE:HZ	1.78	0.49
7:d:101:BCL:H111	8:B:101:SPO:H131	1.93	0.49
7:o:100:BCL:H101	7:o:100:BCL:H142	1.94	0.49
1:t:7:ILE:HD11	7:u:101:BCL:H203	1.94	0.49
2:G:47:TRP:CD1	2:G:48:LEU:HG	2.47	0.49
4:L:40:VAL:HG21	9:M:405:U10:H371	1.93	0.49
5:M:124:MET:HB2	8:M:406:SPO:H312	1.95	0.49
1:o:10:ILE:HG23	2:O:8:PHE:HD2	1.78	0.49
1:k:22:VAL:HG21	5:M:59:MET:HG2	1.95	0.49
2:T:14:GLN:HA	2:T:17:GLN:OE1	2.12	0.49
1:j:31:ILE:HA	1:j:34:MET:HE2	1.94	0.49
1:t:25:PHE:CE2	1:s:23:PHE:HE1	2.31	0.49
8:E:201:SPO:H15	7:E:202:BCL:O1A	2.13	0.49
1:d:25:PHE:HB2	7:d:101:BCL:H52	1.94	0.49
8:D:201:SPO:H392	1:b:6:LYS:HB3	1.95	0.48
2:J:21:SER:O	2:J:25:GLN:HG3	2.13	0.48
2:F:27:MET:HG3	8:F:102:SPO:C21	2.42	0.48
2:S:11:LEU:HD21	2:S:19:LEU:HD12	1.95	0.48
2:E:23:TYR:CA	8:E:201:SPO:H311	2.42	0.48
6:H:8:GLY:O	6:H:9:ASP:HB2	2.13	0.48
2:B:23:TYR:CE1	2:B:27:MET:HE3	2.48	0.48
8:F:102:SPO:H241	8:F:102:SPO:C28	2.43	0.48
7:G:101:BCL:CHB	7:G:101:BCL:H101	2.43	0.48
4:L:111:LYS:O	6:H:111:PRO:HG3	2.14	0.48
1:o:27:LEU:HD11	8:r:102:SPO:H81	1.96	0.48
8:N:201:SPO:HM11	1:n:35:LEU:HG	1.95	0.48
2:I:29:LEU:HD23	8:I:102:SPO:H37	1.94	0.48
5:M:281:GLY:O	7:M:402:BCL:HED3	2.13	0.48
6:H:146:ARG:CZ	6:H:200:LYS:HG3	2.43	0.48
1:b:51:TYR:HB2	1:b:54:VAL:CA	2.44	0.48
1:s:29:VAL:O	1:s:33:LEU:HG	2.14	0.48
4:L:10:TYR:OH	5:M:244:THR:HG22	2.13	0.48
4:L:133:VAL:HG23	4:L:134:VAL:HG23	1.96	0.48
1:f:48:GLY:HA2	1:f:54:VAL:HG23	1.96	0.47
2:E:22:VAL:HG12	8:E:201:SPO:H342	1.96	0.47
8:I:102:SPO:H291	8:I:102:SPO:H393	1.96	0.47
2:S:27:MET:HA	8:s:201:SPO:C24	2.44	0.47
1:r:12:ASP:O	1:r:16:VAL:HG23	2.13	0.47
8:X:201:SPO:H362	8:X:201:SPO:H341	1.45	0.47
5:M:135:TYR:CE2	5:M:145:LYS:HG2	2.49	0.47
2:F:21:SER:O	2:F:25:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:r:103:SPO:H11	7:s:202:BCL:HBA2	1.96	0.47
1:u:18:VAL:O	1:u:22:VAL:HG23	2.15	0.47
2:S:5:ASP:OD1	1:s:9:LEU:HB3	2.15	0.47
8:s:201:SPO:H312	8:s:201:SPO:H291	1.55	0.47
6:H:111:PRO:HB2	6:H:239:GLY:HA2	1.97	0.47
7:t:101:BCL:CMB	8:s:201:SPO:H82	2.43	0.47
1:r:40:GLY:O	2:R:45:ARG:NH1	2.48	0.47
1:f:34:MET:HG3	6:H:7:PHE:CD1	2.49	0.47
1:i:54:VAL:CG1	2:G:45:ARG:HG3	2.44	0.47
7:N:202:BCL:H3A	7:N:202:BCL:H52	1.96	0.47
2:A:47:TRP:HZ2	7:A:101:BCL:H152	1.80	0.47
1:f:6:LYS:HG2	1:f:9:LEU:HD12	1.96	0.47
2:E:27:MET:HG2	8:E:201:SPO:H20	1.97	0.47
10:L:302:BPH:H9C3	7:M:401:BCL:H193	1.96	0.47
1:o:48:GLY:HA2	1:o:54:VAL:HG23	1.96	0.47
2:N:12:THR:HG23	2:N:15:GLN:NE2	2.30	0.47
7:t:101:BCL:HED1	2:T:33:VAL:HG12	1.96	0.47
8:r:102:SPO:H19	7:O:101:BCL:C1	2.45	0.47
3:X:71:ASP:OD2	3:X:71:ASP:N	2.46	0.47
4:L:44:ALA:O	4:L:48:LEU:HB2	2.14	0.47
4:L:208:ARG:HG3	5:M:143:MET:HG2	1.96	0.47
1:t:54:VAL:HB	2:S:45:ARG:CD	2.45	0.47
2:U:23:TYR:OH	1:u:20:GLN:OE1	2.24	0.47
8:E:201:SPO:H241	8:E:201:SPO:H26	1.44	0.47
2:D:21:SER:O	2:D:25:GLN:HG3	2.15	0.47
1:k:48:GLY:HA2	1:k:54:VAL:HG23	1.96	0.47
8:E:201:SPO:H362	1:d:6:LYS:CB	2.45	0.47
8:s:201:SPO:HM13	8:s:201:SPO:H23	1.51	0.47
8:I:102:SPO:H241	8:I:102:SPO:H26	1.71	0.47
7:g:101:BCL:H51	7:g:101:BCL:H11	1.70	0.47
1:f:5:TYR:OH	1:f:6:LYS:HE2	2.15	0.46
5:M:68:PHE:CE2	8:M:406:SPO:H82	2.50	0.46
5:M:265:GLY:HA3	6:H:35:ASN:ND2	2.30	0.46
12:H:301:3PE:H322	12:H:301:3PE:H31	1.79	0.46
1:o:42:ASN:HD22	1:o:45:ASP:HB2	1.79	0.46
8:r:103:SPO:H22	2:R:27:MET:HG3	1.97	0.46
8:E:201:SPO:C15	7:E:202:BCL:H11	2.45	0.46
2:K:48:LEU:HD22	7:K:101:BCL:H171	1.97	0.46
1:r:7:ILE:HA	1:r:10:ILE:HD13	1.96	0.46
1:n:3:LYS:HD3	1:n:5:TYR:HE1	1.80	0.46
2:G:7:SER:HB3	2:G:10:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:271:PRO:HD3	9:L:305:U10:H8	1.97	0.46
6:H:134:MET:SD	6:H:167:MET:HE3	2.55	0.46
1:t:17:PHE:HD2	1:s:11:PHE:CZ	2.33	0.46
1:e:26:LEU:O	1:e:30:MET:HG2	2.16	0.46
1:g:42:ASN:ND2	1:g:45:ASP:OD2	2.49	0.46
2:S:30:PHE:HE2	7:S:101:BCL:HBA2	1.81	0.46
1:b:54:VAL:CG1	2:A:45:ARG:HD3	2.46	0.46
4:L:150:GLY:O	4:L:154:HIS:ND1	2.49	0.46
4:L:182:PHE:CD2	10:M:403:BPH:HBB1	2.51	0.46
4:L:194:LEU:HD21	4:L:213:GLU:HB2	1.98	0.46
8:M:406:SPO:H311	8:M:406:SPO:H291	1.77	0.46
6:H:157:ASP:O	6:H:159:LYS:N	2.48	0.46
2:B:19:LEU:HG	8:B:101:SPO:H341	1.98	0.46
2:B:23:TYR:HE1	2:B:27:MET:HE3	1.81	0.46
2:B:47:TRP:CD1	2:B:48:LEU:HD22	2.51	0.46
8:F:102:SPO:H32	8:F:102:SPO:C38	2.46	0.46
2:S:25:GLN:O	2:S:29:LEU:HG	2.15	0.46
8:M:406:SPO:H21A	8:M:406:SPO:H5	1.42	0.46
4:L:105:GLU:HB3	4:L:119:PRO:HG3	1.97	0.46
1:g:6:LYS:HA	1:g:9:LEU:HD23	1.98	0.46
1:o:42:ASN:ND2	1:o:45:ASP:HB2	2.31	0.46
7:N:202:BCL:H141	7:N:202:BCL:H192	1.98	0.46
2:N:48:LEU:HD12	7:N:202:BCL:H162	1.97	0.45
2:S:33:VAL:HG12	7:s:202:BCL:HED1	1.99	0.45
2:N:11:LEU:HA	2:N:15:GLN:NE2	2.31	0.45
5:M:160:VAL:HA	5:M:164:PHE:HB2	1.97	0.45
1:j:35:LEU:HD11	7:j:303:BCL:HHD	1.99	0.45
1:t:35:LEU:HD11	7:t:103:BCL:HHD	1.98	0.45
5:M:111:MET:HE3	5:M:111:MET:HA	1.98	0.45
2:N:33:VAL:HG12	7:n:100:BCL:HED1	1.98	0.45
8:N:201:SPO:H21	8:N:201:SPO:H25	1.80	0.45
1:r:51:TYR:HB2	1:r:54:VAL:HA	1.98	0.45
1:b:5:TYR:CE2	2:B:17:GLN:HG3	2.51	0.45
1:b:35:LEU:HD11	7:b:102:BCL:HHD	1.99	0.45
5:M:257:MET:HB2	9:M:405:U10:H23	1.98	0.45
7:K:101:BCL:H112	7:K:101:BCL:C2B	2.46	0.45
1:k:6:LYS:HA	1:k:9:LEU:HD23	1.97	0.45
1:f:54:VAL:HG11	2:E:45:ARG:HB3	1.98	0.45
2:E:12:THR:OG1	2:E:15:GLN:HG3	2.17	0.45
8:j:301:SPO:H361	8:j:301:SPO:H341	1.81	0.45
1:f:45:ASP:O	1:f:49:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:301:BCL:CGA	7:M:401:BCL:HBC1	2.47	0.45
7:r:101:BCL:HHD	2:R:41:VAL:HG21	1.99	0.45
8:s:201:SPO:HM12	8:s:201:SPO:H32A	1.49	0.45
2:I:30:PHE:HA	8:I:102:SPO:H342	1.97	0.45
4:L:223:TYR:HE2	4:L:225:VAL:HG22	1.82	0.45
6:H:108:GLY:O	6:H:113:SER:HA	2.17	0.45
1:g:4:PHE:O	1:g:7:ILE:HG12	2.17	0.45
1:o:6:LYS:O	1:o:9:LEU:HB2	2.16	0.45
7:k:101:BCL:H62	7:k:101:BCL:H41	1.73	0.45
2:J:27:MET:HG2	2:J:31:ILE:CD1	2.47	0.45
7:u:102:BCL:H171	7:u:102:BCL:H13	1.60	0.45
4:L:223:TYR:CE2	4:L:225:VAL:HG22	2.52	0.45
5:M:162:SER:HB2	8:M:406:SPO:C27	2.47	0.45
1:g:25:PHE:HB2	7:g:101:BCL:H51	1.99	0.45
8:N:201:SPO:HM12	1:n:31:ILE:HG23	1.99	0.44
1:t:17:PHE:HD2	1:s:11:PHE:HZ	1.64	0.44
5:M:34:THR:HG22	5:M:50:PRO:HD3	1.99	0.44
5:M:107:SER:O	5:M:107:SER:OG	2.28	0.44
8:N:201:SPO:H23	1:n:31:ILE:HA	1.99	0.44
7:t:103:BCL:C1B	7:t:103:BCL:H101	2.47	0.44
8:D:201:SPO:H393	1:b:10:ILE:HD11	1.98	0.44
7:k:101:BCL:HHC	7:k:101:BCL:OBB	2.16	0.44
4:L:182:PHE:HB3	10:M:403:BPH:HBB2	1.99	0.44
8:X:201:SPO:H291	8:X:201:SPO:H312	1.51	0.44
5:M:121:PHE:CD1	8:M:406:SPO:H393	2.53	0.44
8:t:102:SPO:H22A	8:t:102:SPO:HM12	1.69	0.44
2:D:23:TYR:CE1	8:D:201:SPO:H25	2.52	0.44
2:R:47:TRP:CE2	7:R:101:BCL:H2C	2.53	0.44
7:F:101:BCL:H141	7:F:101:BCL:H162	1.73	0.44
1:i:13:PRO:HG2	2:I:11:LEU:HD11	1.99	0.44
7:I:101:BCL:H62	7:I:101:BCL:H41	1.86	0.44
4:L:175:MET:SD	7:M:407:BCL:HED3	2.57	0.44
6:H:7:PHE:HB2	6:H:10:PHE:HB3	1.99	0.44
7:t:101:BCL:H121	1:s:20:GLN:HG3	1.98	0.44
9:M:405:U10:H201	12:H:302:3PE:H371	1.99	0.44
2:F:6:LEU:HD11	2:F:8:PHE:CE1	2.53	0.44
7:o:100:BCL:H151	8:N:201:SPO:H22	1.99	0.44
2:S:21:SER:O	2:S:25:GLN:HG3	2.18	0.44
1:u:28:ALA:O	1:u:32:HIS:ND1	2.45	0.44
8:D:201:SPO:H10	8:D:201:SPO:H81	1.88	0.44
4:L:195:ILE:HG21	5:M:267:HIS:ND1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:6:PHE:N	6:H:10:PHE:O	2.51	0.44
7:d:101:BCL:H62	7:d:101:BCL:H41	1.41	0.44
1:a:29:VAL:O	1:a:33:LEU:HG	2.18	0.43
1:j:54:VAL:HG11	2:I:45:ARG:HB3	2.00	0.43
5:M:293:GLU:OE1	6:H:2:VAL:HG11	2.18	0.43
1:o:16:VAL:O	1:o:20:GLN:HG3	2.18	0.43
8:r:102:SPO:H81	8:r:102:SPO:H10	1.58	0.43
2:G:45:ARG:NH1	1:g:40:GLY:O	2.44	0.43
8:j:301:SPO:H22	8:j:301:SPO:H26	1.80	0.43
7:j:303:BCL:H72	7:j:303:BCL:CHB	2.48	0.43
5:M:154:ALA:HB2	10:M:403:BPH:HAC1	2.00	0.43
1:o:23:PHE:HE2	8:r:102:SPO:H182	1.83	0.43
2:S:23:TYR:HE1	2:S:27:MET:HE3	1.84	0.43
1:r:13:PRO:O	1:r:17:PHE:HD2	2.00	0.43
5:M:262:THR:HG22	6:H:35:ASN:ND2	2.32	0.43
12:H:301:3PE:H342	12:H:301:3PE:H371	1.45	0.43
2:N:48:LEU:HD23	2:N:48:LEU:HA	1.87	0.43
8:N:201:SPO:HM12	8:N:201:SPO:H22A	1.40	0.43
8:N:201:SPO:H21A	8:N:201:SPO:H5	1.23	0.43
1:r:12:ASP:OD1	1:r:13:PRO:HD2	2.17	0.43
1:k:4:PHE:O	1:k:7:ILE:HG12	2.18	0.43
8:k:102:SPO:H33	1:n:32:HIS:HB2	2.00	0.43
8:s:201:SPO:H15	8:s:201:SPO:H19	1.42	0.43
1:g:32:HIS:CG	8:F:102:SPO:H42	2.54	0.43
1:o:27:LEU:HD11	8:r:102:SPO:C8	2.49	0.43
1:r:43:TRP:CE3	7:r:101:BCL:HBC2	2.53	0.43
7:L:301:BCL:HHC	7:L:301:BCL:OBB	2.18	0.43
5:M:67:TRP:O	5:M:71:VAL:HG23	2.18	0.43
8:N:201:SPO:H241	8:N:201:SPO:C27	2.44	0.43
1:t:4:PHE:O	1:t:7:ILE:HG12	2.19	0.43
2:D:19:LEU:HD21	1:d:13:PRO:HG3	2.01	0.43
8:k:102:SPO:H10	7:n:100:BCL:H3A	1.99	0.43
8:I:102:SPO:HM13	8:I:102:SPO:H23	1.60	0.43
6:H:58:LEU:HD23	6:H:78:TYR:HE1	1.84	0.43
1:i:25:PHE:HD2	1:i:26:LEU:HD12	1.83	0.43
2:F:47:TRP:CD1	2:F:48:LEU:HD22	2.54	0.43
7:e:100:BCL:H141	7:e:100:BCL:H162	1.56	0.43
2:T:8:PHE:HZ	6:H:201:HIS:ND1	2.16	0.43
12:H:302:3PE:H3E2	12:H:302:3PE:H3H2	1.51	0.43
7:b:101:BCL:HED1	2:B:33:VAL:HG12	2.00	0.43
8:t:102:SPO:H11	7:u:101:BCL:H3A	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:17:PHE:CG	8:F:102:SPO:H351	2.53	0.43
7:R:101:BCL:H71	7:R:101:BCL:H112	1.89	0.43
4:L:66:SER:HA	4:L:149:TYR:O	2.19	0.43
1:e:20:GLN:NE2	7:F:101:BCL:H151	2.34	0.42
7:u:102:BCL:H162	7:u:102:BCL:H192	1.71	0.42
3:X:77:LYS:HD2	3:X:82:ALA:O	2.18	0.42
8:g:102:SPO:H32	8:g:102:SPO:H241	2.00	0.42
1:r:34:MET:HE2	1:r:34:MET:HB3	1.85	0.42
7:r:101:BCL:H18	8:r:103:SPO:H403	2.02	0.42
7:a:101:BCL:H61	2:A:33:VAL:HG11	1.99	0.42
8:D:201:SPO:HM12	8:D:201:SPO:H22A	1.85	0.42
7:b:101:BCL:OBB	7:b:101:BCL:HHC	2.19	0.42
1:k:29:VAL:HG11	5:M:121:PHE:CE2	2.54	0.42
2:G:33:VAL:HG12	7:g:101:BCL:HED1	2.01	0.42
7:F:101:BCL:H51	7:F:101:BCL:H11	1.76	0.42
2:S:23:TYR:CE1	2:S:27:MET:HE3	2.55	0.42
8:r:103:SPO:HM12	1:s:32:HIS:HB3	2.01	0.42
7:e:100:BCL:HHC	7:e:100:BCL:OBB	2.19	0.42
2:F:26:GLY:C	8:F:102:SPO:H27	2.44	0.42
2:B:27:MET:HB2	8:B:101:SPO:H243	2.01	0.42
1:k:18:VAL:HG11	5:M:55:THR:HG23	2.02	0.42
7:u:102:BCL:H91	7:u:102:BCL:H193	2.01	0.42
8:M:406:SPO:H341	8:M:406:SPO:H362	1.49	0.42
6:H:26:LEU:HB2	12:H:301:3PE:H382	2.00	0.42
7:s:202:BCL:H162	7:s:202:BCL:H192	1.76	0.42
6:H:54:GLY:HA3	12:H:302:3PE:HN3	1.83	0.42
8:r:103:SPO:H15	8:r:103:SPO:H131	1.93	0.42
7:a:101:BCL:HHD	2:A:41:VAL:HG21	2.02	0.42
7:u:102:BCL:H62	7:u:102:BCL:H41	1.89	0.42
3:X:67:VAL:HG23	4:L:58:ASP:HB2	2.01	0.42
7:s:202:BCL:OBB	7:s:202:BCL:HHC	2.19	0.42
2:R:47:TRP:CD2	7:R:101:BCL:H2C	2.55	0.42
6:H:205:VAL:HG21	6:H:213:PHE:CZ	2.55	0.42
8:F:102:SPO:H20	8:F:102:SPO:H181	1.67	0.42
2:S:24:LEU:O	2:S:28:TRP:CD1	2.73	0.42
2:S:30:PHE:HB3	8:s:201:SPO:C24	2.49	0.42
1:e:24:LEU:CD1	8:E:201:SPO:H21	2.48	0.42
8:E:201:SPO:HM12	8:E:201:SPO:H22A	1.77	0.42
1:j:13:PRO:HA	1:j:16:VAL:HG22	2.01	0.42
4:L:190:LEU:HD22	4:L:217:PHE:HZ	1.84	0.42
5:M:59:MET:HB3	5:M:129:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:102:SPO:HM12	8:g:102:SPO:H32A	1.48	0.42
8:N:201:SPO:H33	8:N:201:SPO:HM13	1.46	0.42
1:t:10:ILE:HD11	2:U:15:GLN:OE1	2.19	0.42
7:r:101:BCL:H61	7:r:101:BCL:H41	1.83	0.42
8:r:103:SPO:H352	8:r:103:SPO:C29	2.49	0.42
1:a:23:PHE:HB2	7:b:101:BCL:H162	2.02	0.42
7:e:100:BCL:HED1	2:E:33:VAL:CG1	2.50	0.42
2:D:38:HIS:CE1	7:D:202:BCL:H91	2.55	0.42
2:R:47:TRP:HZ2	7:R:101:BCL:H143	1.84	0.42
5:M:6:ASN:ND2	6:H:194:THR:HG22	2.35	0.42
2:O:24:LEU:O	2:O:28:TRP:CD1	2.73	0.42
2:D:33:VAL:HG12	7:d:101:BCL:HED1	2.02	0.42
1:k:34:MET:HE1	8:k:102:SPO:O1	2.20	0.42
7:d:101:BCL:H152	7:d:101:BCL:H111	1.66	0.42
2:U:6:LEU:HD21	6:H:201:HIS:CD2	2.53	0.41
2:D:41:VAL:HG21	7:d:101:BCL:HHD	2.02	0.41
1:b:11:PHE:HB3	1:b:16:VAL:HG21	2.02	0.41
1:b:30:MET:O	1:b:34:MET:HG3	2.20	0.41
7:b:101:BCL:H61	7:b:101:BCL:H41	1.92	0.41
2:R:31:ILE:O	2:R:35:ILE:HG13	2.19	0.41
1:t:34:MET:HE3	1:t:34:MET:HB3	2.00	0.41
8:r:103:SPO:HM12	8:r:103:SPO:H32A	1.51	0.41
7:O:101:BCL:C1B	7:O:101:BCL:H112	2.51	0.41
1:j:22:VAL:O	1:j:26:LEU:HG	2.19	0.41
9:L:304:U10:H222	9:L:304:U10:H201	1.82	0.41
8:t:102:SPO:HM13	1:u:33:LEU:HD21	2.02	0.41
7:r:101:BCL:HBC3	2:R:44:TRP:CZ3	2.56	0.41
2:O:14:GLN:HG2	2:O:15:GLN:N	2.35	0.41
2:G:14:GLN:O	2:G:18:GLU:HG3	2.20	0.41
4:L:243:PHE:O	4:L:247:MET:HG2	2.20	0.41
8:g:102:SPO:H31	8:g:102:SPO:H5	1.25	0.41
2:F:33:VAL:CG1	7:F:101:BCL:HED1	2.49	0.41
7:t:103:BCL:H72	7:t:103:BCL:CHB	2.50	0.41
2:S:11:LEU:HD12	2:R:8:PHE:HZ	1.85	0.41
1:a:26:LEU:HD23	1:a:26:LEU:HA	1.92	0.41
7:R:101:BCL:H101	7:R:101:BCL:CHB	2.51	0.41
4:L:263:TRP:HE1	9:L:304:U10:H252	1.85	0.41
5:M:229:ARG:H	5:M:229:ARG:HG3	1.70	0.41
6:H:36:MET:HE1	6:H:56:PHE:O	2.21	0.41
1:d:26:LEU:HD23	1:d:26:LEU:HA	1.87	0.41
1:t:22:VAL:O	1:t:26:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5:TYR:CE1	2:A:17:GLN:HG3	2.54	0.41
1:b:11:PHE:HB3	1:b:16:VAL:CG2	2.51	0.41
7:b:101:BCL:H51	7:b:101:BCL:H11	1.80	0.41
7:u:102:BCL:H51	7:u:102:BCL:HAA1	2.02	0.41
1:n:28:ALA:O	1:n:32:HIS:ND1	2.34	0.41
2:G:30:PHE:CG	8:g:102:SPO:H22	2.55	0.41
7:G:101:BCL:H112	7:G:101:BCL:H71	1.69	0.41
8:M:406:SPO:H21	8:M:406:SPO:H25	1.86	0.41
2:S:23:TYR:HA	8:s:201:SPO:H342	2.02	0.41
2:J:23:TYR:HA	8:j:301:SPO:H343	2.01	0.41
2:E:19:LEU:CD1	8:E:201:SPO:H352	2.51	0.41
7:n:100:BCL:H61	7:n:100:BCL:H41	1.72	0.41
7:j:303:BCL:C2B	7:j:303:BCL:H112	2.51	0.41
4:L:147:PHE:HB3	4:L:157:TRP:CD2	2.55	0.41
4:L:225:VAL:HG12	4:L:229:GLY:HA3	2.02	0.41
2:F:14:GLN:NE2	2:F:15:GLN:HG3	2.35	0.41
8:F:102:SPO:H32A	8:F:102:SPO:HM12	1.84	0.41
1:o:20:GLN:HE21	7:r:101:BCL:H121	1.85	0.41
2:S:35:ILE:O	2:S:39:LEU:HD23	2.21	0.41
7:u:102:BCL:H62	7:u:102:BCL:H92	1.83	0.41
1:s:43:TRP:CD2	7:s:202:BCL:H2C	2.55	0.41
8:s:201:SPO:H10	8:s:201:SPO:H81	1.62	0.41
1:j:48:GLY:HA2	1:j:54:VAL:HG23	2.02	0.41
5:M:70:LEU:HD22	5:M:115:LEU:HD11	2.02	0.41
5:M:242:ARG:NH1	6:H:38:GLU:OE2	2.54	0.41
7:M:402:BCL:H102	7:M:407:BCL:HBB2	2.02	0.41
2:N:24:LEU:HD12	2:N:27:MET:HE2	2.02	0.41
9:a:102:U10:H1M3	9:a:102:U10:H71	1.89	0.41
1:b:34:MET:HE1	8:B:101:SPO:CM1	2.47	0.41
9:L:303:U10:H172	9:L:303:U10:H151	1.75	0.41
5:M:179:GLY:CA	5:M:182:PRO:HG2	2.43	0.41
7:M:402:BCL:H203	7:M:407:BCL:H142	2.02	0.41
1:d:4:PHE:O	1:d:7:ILE:HG12	2.20	0.41
8:B:101:SPO:H341	8:B:101:SPO:H362	1.84	0.41
1:t:27:LEU:HD11	8:t:102:SPO:C8	2.51	0.41
1:t:54:VAL:HG23	2:S:45:ARG:NH1	2.34	0.41
8:D:201:SPO:H301	8:D:201:SPO:H26	1.60	0.41
8:k:102:SPO:H33	1:n:32:HIS:CB	2.51	0.41
2:E:30:PHE:CG	8:E:201:SPO:H22	2.56	0.41
3:X:27:MET:HE3	3:X:27:MET:HB2	1.87	0.41
8:X:201:SPO:H33	8:X:201:SPO:H5	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:235:LEU:HD23	5:M:225:LEU:HD12	2.03	0.41
10:L:302:BPH:H141	7:M:401:BCL:HBB3	2.03	0.41
10:L:306:BPH:HMA1	5:M:48:LEU:HB3	2.03	0.41
2:F:47:TRP:CE2	7:F:103:BCL:H2C	2.56	0.41
1:r:11:PHE:HB3	1:r:16:VAL:CG2	2.50	0.41
1:r:54:VAL:HG11	2:O:45:ARG:HB3	2.02	0.41
7:e:100:BCL:HBB2	8:D:201:SPO:H22A	2.03	0.41
7:R:101:BCL:H111	7:R:101:BCL:H152	1.93	0.41
6:H:75:VAL:HA	6:H:76:PRO:C	2.46	0.41
8:D:201:SPO:H341	8:D:201:SPO:H361	1.42	0.40
2:A:22:VAL:HG12	8:X:201:SPO:H293	2.04	0.40
1:k:33:LEU:HD23	1:k:33:LEU:HA	1.94	0.40
1:f:7:ILE:HG21	8:g:102:SPO:H401	2.02	0.40
8:E:201:SPO:H5	8:E:201:SPO:H31	1.66	0.40
2:I:47:TRP:CD2	7:I:101:BCL:H2C	2.56	0.40
7:g:101:BCL:OBB	7:g:101:BCL:HHC	2.21	0.40
8:g:102:SPO:H23	8:g:102:SPO:HM13	1.58	0.40
7:d:101:BCL:H62	7:d:101:BCL:H102	1.85	0.40
7:j:302:BCL:OBB	7:j:302:BCL:HHC	2.22	0.40
4:L:132:LEU:HD23	4:L:132:LEU:HA	1.91	0.40
6:H:166:GLU:HB3	6:H:180:GLU:HB3	2.03	0.40
12:d:102:3PE:H341	12:d:102:3PE:H371	1.91	0.40
2:S:39:LEU:HD13	7:S:101:BCL:H201	2.02	0.40
2:U:10:GLY:HA3	2:T:8:PHE:CE1	2.56	0.40
7:A:101:BCL:H3A	7:A:101:BCL:H52	2.03	0.40
1:k:35:LEU:HD11	7:K:101:BCL:HHD	2.03	0.40
8:k:102:SPO:H22A	7:n:100:BCL:HBB2	2.02	0.40
2:J:42:PHE:CG	7:j:303:BCL:H18	2.56	0.40
2:I:29:LEU:HD23	8:I:102:SPO:C37	2.52	0.40
5:M:68:PHE:HD2	10:M:403:BPH:H161	1.86	0.40
10:M:403:BPH:C2B	7:M:407:BCL:H2	2.51	0.40
10:M:403:BPH:H162	10:M:403:BPH:H121	1.79	0.40
6:H:23:PHE:CD1	12:H:301:3PE:H381	2.56	0.40
1:r:11:PHE:HB3	1:r:16:VAL:HG21	2.03	0.40
1:r:35:LEU:HD11	7:R:101:BCL:HHD	2.03	0.40
2:D:38:HIS:ND1	7:D:202:BCL:H91	2.36	0.40
1:b:34:MET:HE3	4:L:52:TRP:CZ3	2.56	0.40
1:j:34:MET:SD	8:j:301:SPO:H23	2.61	0.40
4:L:208:ARG:HD3	4:L:212:HIS:CD2	2.57	0.40
6:H:37:ARG:HG2	6:H:76:PRO:HD3	2.03	0.40
1:o:26:LEU:O	1:o:30:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:38:ASN:C	1:t:40:GLY:H	2.29	0.40
7:r:101:BCL:OBB	7:r:101:BCL:HHC	2.22	0.40
8:k:102:SPO:H341	8:k:102:SPO:H361	1.91	0.40
2:E:47:TRP:CE2	7:E:202:BCL:H2C	2.57	0.40
1:n:52:GLU:O	1:n:53:ARG:HB2	2.22	0.40
2:F:14:GLN:O	2:F:18:GLU:HG3	2.22	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	a	42/57 (74%)	41 (98%)	1 (2%)	0	100	100
1	b	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	d	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
1	e	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	f	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	g	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
1	i	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	j	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	k	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	n	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	o	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	r	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	s	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	t	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	u	50/57 (88%)	45 (90%)	5 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	42/48 (88%)	42 (100%)	0	0	100	100
2	B	42/48 (88%)	42 (100%)	0	0	100	100
2	D	42/48 (88%)	42 (100%)	0	0	100	100
2	E	42/48 (88%)	42 (100%)	0	0	100	100
2	F	42/48 (88%)	42 (100%)	0	0	100	100
2	G	42/48 (88%)	42 (100%)	0	0	100	100
2	I	42/48 (88%)	42 (100%)	0	0	100	100
2	J	42/48 (88%)	42 (100%)	0	0	100	100
2	K	42/48 (88%)	42 (100%)	0	0	100	100
2	N	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
2	O	42/48 (88%)	42 (100%)	0	0	100	100
2	R	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
2	S	42/48 (88%)	42 (100%)	0	0	100	100
2	T	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
2	U	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
3	X	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
4	L	273/276 (99%)	265 (97%)	8 (3%)	0	100	100
5	M	303/308 (98%)	291 (96%)	12 (4%)	0	100	100
6	H	248/252 (98%)	233 (94%)	15 (6%)	0	100	100
All	All	2286/2494 (92%)	2179 (95%)	107 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	40/50 (80%)	40 (100%)	0	100	100
1	b	48/50 (96%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	48/50 (96%)	48 (100%)	0	100	100
1	e	48/50 (96%)	48 (100%)	0	100	100
1	f	48/50 (96%)	48 (100%)	0	100	100
1	g	48/50 (96%)	48 (100%)	0	100	100
1	i	48/50 (96%)	48 (100%)	0	100	100
1	j	48/50 (96%)	48 (100%)	0	100	100
1	k	48/50 (96%)	48 (100%)	0	100	100
1	n	48/50 (96%)	48 (100%)	0	100	100
1	o	48/50 (96%)	48 (100%)	0	100	100
1	r	48/50 (96%)	48 (100%)	0	100	100
1	s	48/50 (96%)	48 (100%)	0	100	100
1	t	48/50 (96%)	48 (100%)	0	100	100
1	u	47/50 (94%)	47 (100%)	0	100	100
2	A	38/41 (93%)	38 (100%)	0	100	100
2	B	38/41 (93%)	38 (100%)	0	100	100
2	D	38/41 (93%)	38 (100%)	0	100	100
2	E	38/41 (93%)	38 (100%)	0	100	100
2	F	38/41 (93%)	38 (100%)	0	100	100
2	G	38/41 (93%)	38 (100%)	0	100	100
2	I	38/41 (93%)	38 (100%)	0	100	100
2	J	38/41 (93%)	38 (100%)	0	100	100
2	K	38/41 (93%)	38 (100%)	0	100	100
2	N	38/41 (93%)	38 (100%)	0	100	100
2	O	38/41 (93%)	38 (100%)	0	100	100
2	R	38/41 (93%)	38 (100%)	0	100	100
2	S	38/41 (93%)	38 (100%)	0	100	100
2	T	37/41 (90%)	37 (100%)	0	100	100
2	U	37/41 (90%)	37 (100%)	0	100	100
3	X	60/62 (97%)	60 (100%)	0	100	100
4	L	219/220 (100%)	219 (100%)	0	100	100
5	M	241/243 (99%)	241 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	H	202/204 (99%)	202 (100%)	0	100	100
All	All	2001/2094 (96%)	2001 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	o	38	ASN
2	N	15	GLN
1	t	20	GLN
1	t	42	ASN
1	r	20	GLN
1	r	38	ASN
2	O	25	GLN
1	a	42	ASN
2	U	14	GLN
1	e	20	GLN
2	D	14	GLN
2	A	17	GLN
3	X	5	HIS
1	s	20	GLN
2	R	14	GLN
1	n	38	ASN
1	j	20	GLN
2	I	14	GLN
2	I	17	GLN
4	L	68	ASN
4	L	160	ASN
4	L	200	ASN
5	M	78	GLN
6	H	5	ASN
6	H	32	GLN
6	H	35	ASN
6	H	61	GLN
6	H	93	ASN
1	g	20	GLN
2	F	17	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 1 is monoatomic - leaving 61 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SPO	X	201	-	40,41,41	2.23	12 (30%)	47,50,50	3.47	17 (36%)
7	BCL	I	101	-	64,74,74	1.19	5 (7%)	78,115,115	1.54	12 (15%)
9	U10	a	102	-	48,48,63	2.70	13 (27%)	58,61,79	1.71	16 (27%)
7	BCL	F	101	-	64,74,74	1.30	9 (14%)	78,115,115	1.72	15 (19%)
7	BCL	N	202	-	64,74,74	1.21	5 (7%)	78,115,115	1.77	15 (19%)
7	BCL	u	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.74	11 (14%)
7	BCL	K	101	-	64,74,74	1.21	6 (9%)	78,115,115	1.56	13 (16%)
7	BCL	F	103	-	64,74,74	1.20	7 (10%)	78,115,115	1.71	15 (19%)
8	SPO	g	102	-	40,41,41	2.40	12 (30%)	47,50,50	5.01	24 (51%)
8	SPO	s	201	-	40,41,41	2.31	12 (30%)	47,50,50	5.51	25 (53%)
8	SPO	I	102	-	40,41,41	2.33	12 (30%)	47,50,50	4.92	19 (40%)
12	3PE	H	302	-	50,50,50	0.95	2 (4%)	53,55,55	1.16	3 (5%)
7	BCL	e	100	-	64,74,74	1.29	8 (12%)	78,115,115	1.80	16 (20%)
7	BCL	n	100	-	64,74,74	1.22	7 (10%)	78,115,115	1.70	16 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BCL	d	101	-	64,74,74	1.25	8 (12%)	78,115,115	1.70	14 (17%)
7	BCL	g	101	-	64,74,74	1.25	7 (10%)	78,115,115	1.64	14 (17%)
9	U10	L	304	-	38,38,63	2.69	12 (31%)	46,49,79	1.71	13 (28%)
7	BCL	t	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.64	14 (17%)
7	BCL	u	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.62	15 (19%)
7	BCL	o	100	-	64,74,74	1.30	8 (12%)	78,115,115	1.71	11 (14%)
8	SPO	M	406	-	40,41,41	2.26	13 (32%)	47,50,50	4.07	20 (42%)
7	BCL	i	100	-	64,74,74	1.26	8 (12%)	78,115,115	1.62	14 (17%)
7	BCL	j	303	-	64,74,74	1.23	6 (9%)	78,115,115	1.58	13 (16%)
8	SPO	E	201	-	40,41,41	2.24	10 (25%)	47,50,50	5.37	24 (51%)
8	SPO	r	103	-	40,41,41	2.35	12 (30%)	47,50,50	5.14	16 (34%)
9	U10	L	305	-	28,28,63	2.68	10 (35%)	34,37,79	1.45	5 (14%)
7	BCL	j	302	-	64,74,74	1.21	7 (10%)	78,115,115	1.66	15 (19%)
7	BCL	A	101	-	64,74,74	1.27	7 (10%)	78,115,115	1.58	12 (15%)
7	BCL	L	301	-	64,74,74	1.24	7 (10%)	78,115,115	1.55	12 (15%)
9	U10	L	303	-	33,33,63	2.76	10 (30%)	40,43,79	1.64	9 (22%)
7	BCL	G	101	-	64,74,74	1.17	6 (9%)	78,115,115	1.54	13 (16%)
7	BCL	M	407	-	64,74,74	1.30	8 (12%)	78,115,115	1.49	11 (14%)
8	SPO	B	101	-	40,41,41	2.20	11 (27%)	47,50,50	3.96	21 (44%)
12	3PE	d	102	-	42,42,50	1.00	2 (4%)	45,47,55	2.33	7 (15%)
8	SPO	N	201	-	40,41,41	2.21	12 (30%)	47,50,50	5.19	22 (46%)
7	BCL	M	402	-	64,74,74	1.19	5 (7%)	78,115,115	1.82	15 (19%)
10	BPH	M	403	-	51,70,70	1.05	3 (5%)	52,101,101	1.32	4 (7%)
7	BCL	r	101	-	64,74,74	1.24	6 (9%)	78,115,115	1.65	14 (17%)
12	3PE	H	301	-	50,50,50	0.93	3 (6%)	53,55,55	1.15	2 (3%)
8	SPO	t	102	-	40,41,41	2.37	12 (30%)	47,50,50	4.36	24 (51%)
8	SPO	F	102	-	40,41,41	2.26	12 (30%)	47,50,50	3.91	18 (38%)
8	SPO	D	201	-	40,41,41	2.19	11 (27%)	47,50,50	5.18	18 (38%)
7	BCL	b	102	-	64,74,74	1.18	7 (10%)	78,115,115	1.56	12 (15%)
7	BCL	k	101	-	64,74,74	1.22	8 (12%)	78,115,115	1.64	15 (19%)
7	BCL	b	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.88	19 (24%)
8	SPO	j	301	-	40,41,41	2.21	12 (30%)	47,50,50	4.04	18 (38%)
7	BCL	t	103	-	64,74,74	1.25	6 (9%)	78,115,115	1.47	11 (14%)
7	BCL	s	202	-	64,74,74	1.22	6 (9%)	78,115,115	1.60	12 (15%)
7	BCL	M	401	-	64,74,74	1.21	7 (10%)	78,115,115	1.58	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BPH	L	302	-	51,70,70	0.91	3 (5%)	52,101,101	1.12	6 (11%)
7	BCL	a	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.67	13 (16%)
7	BCL	D	202	-	64,74,74	1.22	7 (10%)	78,115,115	1.57	13 (16%)
7	BCL	R	101	-	64,74,74	1.19	6 (9%)	78,115,115	1.47	11 (14%)
9	U10	M	408	-	18,18,63	2.86	8 (44%)	22,25,79	1.49	3 (13%)
10	BPH	L	306	-	31,50,70	1.02	1 (3%)	28,77,101	1.37	5 (17%)
8	SPO	r	102	-	40,41,41	2.29	12 (30%)	47,50,50	5.28	24 (51%)
9	U10	M	405	-	48,48,63	2.70	14 (29%)	58,61,79	1.72	14 (24%)
7	BCL	O	101	-	64,74,74	1.18	5 (7%)	78,115,115	1.55	11 (14%)
8	SPO	k	102	-	40,41,41	2.24	12 (30%)	47,50,50	5.30	21 (44%)
7	BCL	S	101	-	64,74,74	1.20	6 (9%)	78,115,115	1.55	11 (14%)
7	BCL	E	202	-	64,74,74	1.18	7 (10%)	78,115,115	1.65	12 (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
8	SPO	X	201	-	-	14/47/47/47	-
7	BCL	I	101	-	-	10/37/137/137	-
9	U10	a	102	-	-	12/45/69/87	0/1/1/1
7	BCL	F	101	-	-	3/37/137/137	-
7	BCL	N	202	-	-	7/37/137/137	-
7	BCL	u	102	-	-	8/37/137/137	-
7	BCL	K	101	-	-	8/37/137/137	-
7	BCL	F	103	-	-	7/37/137/137	-
8	SPO	g	102	-	-	19/47/47/47	-
8	SPO	s	201	-	-	21/47/47/47	-
8	SPO	I	102	-	-	13/47/47/47	-
12	3PE	H	302	-	-	31/54/54/54	-
7	BCL	e	100	-	-	3/37/137/137	-
7	BCL	n	100	-	-	6/37/137/137	-
7	BCL	d	101	-	-	4/37/137/137	-
7	BCL	g	101	-	-	1/37/137/137	-
9	U10	L	304	-	-	15/33/57/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	t	101	-	-	4/37/137/137	-
7	BCL	u	101	-	-	3/37/137/137	-
7	BCL	o	100	-	-	10/37/137/137	-
8	SPO	M	406	-	-	21/47/47/47	-
7	BCL	i	100	-	-	3/37/137/137	-
7	BCL	j	303	-	-	9/37/137/137	-
8	SPO	E	201	-	-	17/47/47/47	-
8	SPO	r	103	-	-	18/47/47/47	-
9	U10	L	305	-	-	9/21/45/87	0/1/1/1
7	BCL	j	302	-	-	4/37/137/137	-
7	BCL	A	101	-	-	10/37/137/137	-
7	BCL	L	301	-	-	5/37/137/137	-
9	U10	L	303	-	-	12/27/51/87	0/1/1/1
7	BCL	G	101	-	-	8/37/137/137	-
7	BCL	M	407	-	-	5/37/137/137	-
8	SPO	B	101	-	-	14/47/47/47	-
12	3PE	d	102	-	-	19/46/46/54	-
8	SPO	N	201	-	-	16/47/47/47	-
7	BCL	M	402	-	-	7/37/137/137	-
10	BPH	M	403	-	-	8/37/105/105	0/5/6/6
7	BCL	r	101	-	-	5/37/137/137	-
12	3PE	H	301	-	-	26/54/54/54	-
8	SPO	t	102	-	-	13/47/47/47	-
8	SPO	F	102	-	-	17/47/47/47	-
8	SPO	D	201	-	-	15/47/47/47	-
7	BCL	b	102	-	-	5/37/137/137	-
7	BCL	k	101	-	-	3/37/137/137	-
7	BCL	b	101	-	-	10/37/137/137	-
8	SPO	j	301	-	-	19/47/47/47	-
7	BCL	t	103	-	-	6/37/137/137	-
7	BCL	s	202	-	-	4/37/137/137	-
7	BCL	M	401	-	-	2/37/137/137	-
10	BPH	L	302	-	-	4/37/105/105	0/5/6/6
7	BCL	a	101	-	-	5/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	D	202	-	-	6/37/137/137	-
7	BCL	R	101	-	-	10/37/137/137	-
9	U10	M	408	-	-	6/9/33/87	0/1/1/1
10	BPH	L	306	-	-	2/13/81/105	0/5/6/6
8	SPO	r	102	-	-	16/47/47/47	-
9	U10	M	405	-	-	12/45/69/87	0/1/1/1
7	BCL	O	101	-	-	11/37/137/137	-
8	SPO	k	102	-	-	21/47/47/47	-
7	BCL	S	101	-	-	4/37/137/137	-
7	BCL	E	202	-	-	5/37/137/137	-

All (481) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	303	U10	C8-C9	6.23	1.47	1.33
9	L	303	U10	C13-C14	6.17	1.47	1.33
9	L	304	U10	C13-C14	6.14	1.47	1.33
9	M	405	U10	C8-C9	6.05	1.47	1.33
9	L	303	U10	C18-C19	6.02	1.47	1.33
9	L	304	U10	C23-C24	6.00	1.47	1.33
9	L	305	U10	C13-C14	5.98	1.47	1.33
9	M	405	U10	C23-C24	5.98	1.47	1.33
9	M	405	U10	C33-C34	5.96	1.47	1.33
9	L	305	U10	C8-C9	5.94	1.47	1.33
9	a	102	U10	C18-C19	5.94	1.47	1.33
9	L	304	U10	C8-C9	5.93	1.47	1.33
9	M	408	U10	O4-C4	-5.84	1.22	1.36
9	a	102	U10	C13-C14	5.84	1.47	1.33
9	a	102	U10	O4-C4	-5.81	1.22	1.36
9	a	102	U10	C23-C24	5.79	1.46	1.33
9	L	304	U10	C18-C19	5.78	1.46	1.33
9	a	102	U10	C33-C34	5.77	1.46	1.33
9	a	102	U10	C28-C29	5.76	1.46	1.33
9	M	405	U10	O3-C3	-5.76	1.22	1.36
9	a	102	U10	C8-C9	5.72	1.46	1.33
9	L	303	U10	O4-C4	-5.71	1.22	1.36
9	a	102	U10	O3-C3	-5.70	1.22	1.36
9	M	405	U10	C28-C29	5.67	1.46	1.33
9	M	405	U10	C18-C19	5.61	1.46	1.33
9	M	405	U10	C13-C14	5.60	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	408	U10	O3-C3	-5.58	1.23	1.36
9	L	304	U10	O3-C3	-5.54	1.23	1.36
9	L	303	U10	O3-C3	-5.41	1.23	1.36
9	L	304	U10	O4-C4	-5.37	1.23	1.36
9	L	305	U10	O4-C4	-5.36	1.23	1.36
9	M	405	U10	O4-C4	-5.35	1.23	1.36
9	L	305	U10	O3-C3	-5.34	1.23	1.36
9	L	304	U10	C28-C29	5.32	1.47	1.32
9	L	303	U10	C23-C24	5.23	1.47	1.32
9	M	408	U10	C8-C9	5.22	1.47	1.32
9	a	102	U10	C38-C39	5.22	1.47	1.32
9	M	405	U10	C38-C39	5.16	1.47	1.32
9	L	305	U10	C18-C19	5.12	1.47	1.32
8	r	103	SPO	C25-C23	5.03	1.56	1.45
8	g	102	SPO	C16-C17	4.96	1.56	1.45
8	E	201	SPO	C16-C17	4.85	1.56	1.45
8	N	201	SPO	C25-C23	4.81	1.56	1.45
8	I	102	SPO	C16-C17	4.80	1.56	1.45
8	M	406	SPO	C16-C17	4.80	1.56	1.45
8	t	102	SPO	C16-C17	4.76	1.56	1.45
8	t	102	SPO	C11-C12	4.70	1.56	1.45
8	M	406	SPO	C25-C23	4.70	1.56	1.45
8	F	102	SPO	C25-C23	4.69	1.56	1.45
8	g	102	SPO	C11-C12	4.68	1.56	1.45
8	B	101	SPO	C16-C17	4.66	1.56	1.45
7	t	103	BCL	C1B-NB	4.66	1.39	1.35
7	u	102	BCL	MG-NA	4.65	2.17	2.06
8	B	101	SPO	C11-C12	4.62	1.55	1.45
8	X	201	SPO	C16-C17	4.61	1.55	1.45
8	r	103	SPO	C16-C17	4.60	1.55	1.45
8	s	201	SPO	C25-C23	4.59	1.55	1.45
7	t	103	BCL	MG-NA	4.57	2.17	2.06
8	E	201	SPO	C11-C12	4.57	1.55	1.45
7	u	102	BCL	C1B-NB	4.56	1.39	1.35
8	r	102	SPO	C16-C17	4.56	1.55	1.45
7	u	101	BCL	C1B-NB	4.55	1.39	1.35
8	k	102	SPO	C25-C23	4.55	1.55	1.45
7	M	407	BCL	MG-NA	4.49	2.16	2.06
7	u	101	BCL	MG-NA	4.46	2.16	2.06
7	k	101	BCL	MG-NA	4.44	2.16	2.06
7	M	401	BCL	C1B-NB	4.43	1.39	1.35
7	M	407	BCL	C1B-NB	4.43	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	201	SPO	C16-C17	4.41	1.55	1.45
8	E	201	SPO	C15-C14	4.40	1.57	1.43
8	D	201	SPO	C25-C23	4.40	1.55	1.45
7	a	101	BCL	MG-NA	4.39	2.16	2.06
7	S	101	BCL	C1B-NB	4.39	1.39	1.35
8	t	102	SPO	C25-C23	4.39	1.55	1.45
8	I	102	SPO	C25-C23	4.39	1.55	1.45
8	t	102	SPO	C6-C7	4.38	1.55	1.45
7	j	303	BCL	MG-NA	4.38	2.16	2.06
7	I	101	BCL	C1B-NB	4.36	1.39	1.35
7	N	202	BCL	MG-NA	4.35	2.16	2.06
7	F	103	BCL	MG-NA	4.34	2.16	2.06
8	s	201	SPO	C16-C17	4.34	1.55	1.45
8	M	406	SPO	C15-C14	4.33	1.56	1.43
7	t	101	BCL	MG-NA	4.33	2.16	2.06
8	r	103	SPO	C11-C12	4.33	1.55	1.45
7	A	101	BCL	MG-NA	4.32	2.16	2.06
8	I	102	SPO	C6-C7	4.32	1.55	1.45
7	D	202	BCL	C1B-NB	4.31	1.39	1.35
7	E	202	BCL	MG-NA	4.31	2.16	2.06
7	s	202	BCL	C1B-NB	4.31	1.39	1.35
8	j	301	SPO	C25-C23	4.29	1.55	1.45
7	a	101	BCL	C1B-NB	4.29	1.39	1.35
8	X	201	SPO	C25-C23	4.28	1.55	1.45
8	F	102	SPO	C16-C17	4.28	1.55	1.45
8	k	102	SPO	C11-C12	4.28	1.55	1.45
8	s	201	SPO	C11-C12	4.28	1.55	1.45
7	b	101	BCL	MG-NA	4.27	2.16	2.06
7	r	101	BCL	MG-NA	4.27	2.16	2.06
7	I	101	BCL	MG-NA	4.27	2.16	2.06
7	O	101	BCL	C1B-NB	4.26	1.39	1.35
7	t	101	BCL	C1B-NB	4.26	1.39	1.35
8	k	102	SPO	C16-C17	4.24	1.55	1.45
7	r	101	BCL	C1B-NB	4.24	1.39	1.35
7	d	101	BCL	MG-NA	4.23	2.16	2.06
8	I	102	SPO	C11-C12	4.23	1.55	1.45
7	R	101	BCL	C1B-NB	4.21	1.39	1.35
7	j	303	BCL	C1B-NB	4.21	1.39	1.35
8	D	201	SPO	C11-C12	4.21	1.55	1.45
8	X	201	SPO	C11-C12	4.20	1.55	1.45
8	g	102	SPO	C15-C14	4.20	1.56	1.43
8	r	102	SPO	C11-C12	4.20	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	101	BCL	MG-NA	4.19	2.16	2.06
8	g	102	SPO	C25-C23	4.19	1.54	1.45
8	g	102	SPO	C6-C7	4.18	1.54	1.45
8	E	201	SPO	C20-C19	4.17	1.56	1.43
7	E	202	BCL	C1B-NB	4.17	1.38	1.35
7	K	101	BCL	MG-NA	4.17	2.16	2.06
8	k	102	SPO	C6-C7	4.15	1.54	1.45
7	S	101	BCL	MG-NA	4.14	2.16	2.06
7	G	101	BCL	MG-NA	4.14	2.16	2.06
8	X	201	SPO	C6-C7	4.14	1.54	1.45
7	j	302	BCL	MG-NA	4.14	2.16	2.06
8	r	102	SPO	C25-C23	4.13	1.54	1.45
7	e	100	BCL	MG-NA	4.13	2.16	2.06
8	t	102	SPO	C10-C9	4.13	1.56	1.43
7	n	100	BCL	MG-NA	4.12	2.16	2.06
7	b	102	BCL	MG-NA	4.12	2.16	2.06
7	F	101	BCL	MG-NA	4.12	2.16	2.06
7	K	101	BCL	C1B-NB	4.11	1.38	1.35
7	M	401	BCL	MG-NA	4.11	2.16	2.06
7	i	100	BCL	MG-NA	4.10	2.16	2.06
8	r	103	SPO	C6-C7	4.08	1.54	1.45
8	F	102	SPO	C11-C12	4.07	1.54	1.45
8	r	103	SPO	C26-C27	4.07	1.56	1.43
8	g	102	SPO	C26-C27	4.07	1.56	1.43
7	s	202	BCL	MG-NA	4.07	2.15	2.06
8	s	201	SPO	C6-C7	4.07	1.54	1.45
8	g	102	SPO	C20-C19	4.07	1.56	1.43
7	G	101	BCL	C1B-NB	4.06	1.38	1.35
7	M	402	BCL	MG-NA	4.04	2.15	2.06
8	t	102	SPO	C26-C27	4.04	1.56	1.43
7	g	101	BCL	MG-NA	4.04	2.15	2.06
7	N	202	BCL	C1B-NB	4.04	1.38	1.35
8	j	301	SPO	C6-C7	4.03	1.54	1.45
8	t	102	SPO	C15-C14	4.03	1.55	1.43
8	g	102	SPO	C21-C22	4.02	1.55	1.43
8	D	201	SPO	C6-C7	4.00	1.54	1.45
8	B	101	SPO	C6-C7	4.00	1.54	1.45
7	O	101	BCL	MG-NA	4.00	2.15	2.06
8	M	406	SPO	C11-C12	4.00	1.54	1.45
10	M	403	BPH	CBD-CGD	-3.99	1.47	1.52
8	s	201	SPO	C4-C5	3.98	1.56	1.50
7	i	100	BCL	C1B-NB	3.98	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	201	SPO	C6-C7	3.97	1.54	1.45
8	X	201	SPO	C15-C14	3.96	1.55	1.43
7	F	103	BCL	C1B-NB	3.95	1.38	1.35
8	I	102	SPO	C15-C14	3.95	1.55	1.43
8	r	102	SPO	C15-C14	3.95	1.55	1.43
8	r	102	SPO	C21-C22	3.94	1.55	1.43
7	A	101	BCL	C1B-NB	3.94	1.38	1.35
8	E	201	SPO	C21-C22	3.93	1.55	1.43
8	N	201	SPO	C11-C12	3.93	1.54	1.45
8	F	102	SPO	C26-C27	3.93	1.55	1.43
7	k	101	BCL	C1B-NB	3.92	1.38	1.35
7	o	100	BCL	MG-NA	3.92	2.15	2.06
7	g	101	BCL	C1B-NB	3.91	1.38	1.35
7	D	202	BCL	MG-NA	3.91	2.15	2.06
8	g	102	SPO	C10-C9	3.90	1.55	1.43
7	j	302	BCL	C1B-NB	3.90	1.38	1.35
7	b	101	BCL	C1B-NB	3.90	1.38	1.35
9	a	102	U10	C4-C5	-3.89	1.37	1.48
8	r	102	SPO	C10-C9	3.89	1.55	1.43
8	B	101	SPO	C10-C9	3.89	1.55	1.43
8	r	103	SPO	C15-C14	3.88	1.55	1.43
8	F	102	SPO	C10-C9	3.88	1.55	1.43
7	b	102	BCL	C1B-NB	3.88	1.38	1.35
8	r	102	SPO	C26-C27	3.88	1.55	1.43
8	r	102	SPO	C6-C7	3.88	1.54	1.45
8	I	102	SPO	C26-C27	3.87	1.55	1.43
8	k	102	SPO	C10-C9	3.87	1.55	1.43
8	t	102	SPO	C21-C22	3.87	1.55	1.43
7	L	301	BCL	MG-NA	3.86	2.15	2.06
8	F	102	SPO	C6-C7	3.85	1.54	1.45
8	N	201	SPO	C16-C17	3.85	1.54	1.45
8	j	301	SPO	C16-C17	3.83	1.54	1.45
8	j	301	SPO	C10-C9	3.83	1.55	1.43
8	s	201	SPO	C26-C27	3.83	1.55	1.43
8	s	201	SPO	C10-C9	3.82	1.55	1.43
8	N	201	SPO	C10-C9	3.82	1.55	1.43
8	I	102	SPO	C10-C9	3.82	1.55	1.43
8	D	201	SPO	C15-C14	3.81	1.55	1.43
7	e	100	BCL	C1B-NB	3.81	1.38	1.35
8	r	103	SPO	C10-C9	3.81	1.55	1.43
7	n	100	BCL	C1B-NB	3.80	1.38	1.35
8	E	201	SPO	C25-C23	3.79	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	k	102	SPO	C26-C27	3.79	1.55	1.43
8	j	301	SPO	C26-C27	3.78	1.55	1.43
8	g	102	SPO	C4-C5	3.78	1.56	1.50
7	o	100	BCL	C1B-NB	3.78	1.38	1.35
8	M	406	SPO	C20-C19	3.77	1.55	1.43
8	D	201	SPO	C10-C9	3.77	1.55	1.43
8	I	102	SPO	C21-C22	3.77	1.55	1.43
8	s	201	SPO	C15-C14	3.77	1.55	1.43
8	j	301	SPO	C21-C22	3.76	1.55	1.43
7	L	301	BCL	O1A-CGA	-3.75	1.11	1.22
8	B	101	SPO	C21-C22	3.75	1.55	1.43
8	E	201	SPO	C10-C9	3.74	1.55	1.43
8	X	201	SPO	C20-C19	3.72	1.55	1.43
8	B	101	SPO	C26-C27	3.72	1.55	1.43
8	j	301	SPO	C11-C12	3.72	1.53	1.45
8	B	101	SPO	C15-C14	3.72	1.55	1.43
8	k	102	SPO	C15-C14	3.72	1.55	1.43
8	B	101	SPO	C25-C23	3.71	1.53	1.45
8	I	102	SPO	C4-C5	3.71	1.56	1.50
7	L	301	BCL	C1B-NB	3.71	1.38	1.35
8	t	102	SPO	C20-C19	3.71	1.54	1.43
7	F	101	BCL	C1B-NB	3.68	1.38	1.35
8	M	406	SPO	C10-C9	3.68	1.54	1.43
8	X	201	SPO	C26-C27	3.68	1.54	1.43
8	r	102	SPO	C20-C19	3.67	1.54	1.43
8	N	201	SPO	C26-C27	3.66	1.54	1.43
9	L	303	U10	C3-C2	-3.66	1.38	1.48
8	I	102	SPO	C20-C19	3.65	1.54	1.43
8	B	101	SPO	C20-C19	3.63	1.54	1.43
7	d	101	BCL	C1B-NB	3.63	1.38	1.35
8	r	103	SPO	C20-C19	3.62	1.54	1.43
8	r	103	SPO	C21-C22	3.62	1.54	1.43
9	M	405	U10	C3-C2	-3.62	1.38	1.48
8	j	301	SPO	C20-C19	3.62	1.54	1.43
8	M	406	SPO	C26-C27	3.61	1.54	1.43
9	a	102	U10	C3-C2	-3.61	1.38	1.48
8	N	201	SPO	C21-C22	3.60	1.54	1.43
8	X	201	SPO	C10-C9	3.59	1.54	1.43
8	F	102	SPO	C15-C14	3.58	1.54	1.43
8	D	201	SPO	C20-C19	3.57	1.54	1.43
8	s	201	SPO	C21-C22	3.57	1.54	1.43
8	E	201	SPO	C26-C27	3.56	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	X	201	SPO	C21-C22	3.55	1.54	1.43
8	N	201	SPO	C4-C5	3.55	1.55	1.50
10	L	306	BPH	CBD-CGD	-3.55	1.47	1.52
8	F	102	SPO	C21-C22	3.55	1.54	1.43
8	F	102	SPO	C20-C19	3.55	1.54	1.43
8	E	201	SPO	C6-C7	3.55	1.53	1.45
8	j	301	SPO	C15-C14	3.55	1.54	1.43
9	M	408	U10	C4-C5	-3.54	1.38	1.48
8	k	102	SPO	C20-C19	3.54	1.54	1.43
8	D	201	SPO	C21-C22	3.54	1.54	1.43
8	D	201	SPO	C26-C27	3.53	1.54	1.43
8	M	406	SPO	C6-C7	3.51	1.53	1.45
9	M	405	U10	C4-C5	-3.50	1.38	1.48
8	t	102	SPO	C4-C5	3.50	1.55	1.50
8	k	102	SPO	C21-C22	3.49	1.54	1.43
9	M	408	U10	C3-C2	-3.48	1.38	1.48
9	L	304	U10	C4-C5	-3.47	1.38	1.48
7	M	402	BCL	C1B-NB	3.45	1.38	1.35
7	b	101	BCL	O1A-CGA	-3.45	1.12	1.22
10	L	302	BPH	CBD-CGD	-3.44	1.47	1.52
7	M	402	BCL	O1A-CGA	-3.43	1.12	1.22
8	N	201	SPO	C20-C19	3.42	1.54	1.43
8	M	406	SPO	C21-C22	3.39	1.54	1.43
8	N	201	SPO	C15-C14	3.39	1.53	1.43
8	r	103	SPO	C4-C5	3.36	1.55	1.50
8	r	102	SPO	C4-C5	3.36	1.55	1.50
8	s	201	SPO	C20-C19	3.35	1.53	1.43
8	X	201	SPO	C4-C5	3.30	1.55	1.50
8	B	101	SPO	C4-C5	3.28	1.55	1.50
7	t	103	BCL	MG-NC	3.22	2.13	2.06
8	k	102	SPO	C4-C5	3.21	1.55	1.50
12	d	102	3PE	O21-C2	-3.21	1.38	1.46
8	E	201	SPO	C4-C5	3.21	1.55	1.50
8	j	301	SPO	C4-C5	3.19	1.55	1.50
8	F	102	SPO	C4-C5	3.18	1.55	1.50
9	L	305	U10	C3-C2	-3.16	1.39	1.48
7	F	101	BCL	O1A-CGA	-3.16	1.13	1.22
9	L	305	U10	C4-C5	-3.13	1.39	1.48
8	D	201	SPO	C4-C5	3.09	1.55	1.50
7	o	100	BCL	O1A-CGA	-3.08	1.13	1.22
7	u	102	BCL	MG-NC	3.08	2.13	2.06
9	L	303	U10	C4-C5	-3.06	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	406	SPO	C4-C5	3.04	1.55	1.50
9	L	304	U10	C3-C2	-3.02	1.40	1.48
7	n	100	BCL	O1A-CGA	-3.01	1.13	1.22
12	H	302	3PE	O21-C2	-2.99	1.39	1.46
7	o	100	BCL	C3C-C4C	-2.98	1.47	1.51
9	M	405	U10	C6-C5	-2.98	1.38	1.46
7	u	101	BCL	MG-NC	2.96	2.13	2.06
7	M	407	BCL	MG-NC	2.95	2.13	2.06
9	M	408	U10	C6-C5	-2.92	1.38	1.46
7	e	100	BCL	O2A-CGA	-2.89	1.24	1.33
7	D	202	BCL	C3D-C4D	-2.87	1.37	1.44
7	e	100	BCL	O1A-CGA	-2.86	1.14	1.22
7	d	101	BCL	C3C-C4C	-2.85	1.48	1.51
7	r	101	BCL	O1A-CGA	-2.84	1.14	1.22
7	M	402	BCL	C3D-C4D	-2.84	1.37	1.44
7	j	303	BCL	C3D-C4D	-2.84	1.37	1.44
9	L	303	U10	C6-C5	-2.81	1.38	1.46
7	t	101	BCL	MG-NC	2.81	2.12	2.06
7	i	100	BCL	O1A-CGA	-2.80	1.14	1.22
7	d	101	BCL	O1A-CGA	-2.80	1.14	1.22
7	K	101	BCL	C1D-C2D	-2.79	1.39	1.45
7	F	101	BCL	O2A-CGA	-2.79	1.25	1.33
9	a	102	U10	C6-C5	-2.78	1.38	1.46
7	M	401	BCL	MG-NC	2.77	2.12	2.06
7	N	202	BCL	C3D-C4D	-2.76	1.37	1.44
7	N	202	BCL	C1D-C2D	-2.75	1.39	1.45
7	a	101	BCL	MG-NC	2.75	2.12	2.06
7	b	102	BCL	C3D-C4D	-2.74	1.38	1.44
9	L	305	U10	C6-C5	-2.74	1.39	1.46
7	j	303	BCL	MG-NC	2.74	2.12	2.06
7	A	101	BCL	C3D-C4D	-2.73	1.38	1.44
10	M	403	BPH	O1A-CGA	-2.73	1.14	1.22
7	R	101	BCL	MG-NC	2.73	2.12	2.06
7	M	407	BCL	C3D-C4D	-2.73	1.38	1.44
7	K	101	BCL	C3D-C4D	-2.72	1.38	1.44
7	k	101	BCL	O1A-CGA	-2.71	1.14	1.22
7	F	103	BCL	C3D-C4D	-2.71	1.38	1.44
9	M	405	U10	C1-C2	-2.71	1.37	1.47
7	E	202	BCL	C3D-C4D	-2.71	1.38	1.44
7	I	101	BCL	C3D-C4D	-2.70	1.38	1.44
7	b	101	BCL	C1D-C2D	-2.69	1.40	1.45
7	g	101	BCL	O1A-CGA	-2.69	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	303	U10	C1-C2	-2.69	1.37	1.47
7	G	101	BCL	C3D-C4D	-2.68	1.38	1.44
7	O	101	BCL	C3D-C4D	-2.68	1.38	1.44
7	F	101	BCL	C3D-C4D	-2.67	1.38	1.44
7	M	401	BCL	CHD-C1D	2.66	1.43	1.38
7	o	100	BCL	C3D-C4D	-2.66	1.38	1.44
7	N	202	BCL	MG-NC	2.65	2.12	2.06
7	G	101	BCL	MG-NC	2.64	2.12	2.06
7	e	100	BCL	C3D-C4D	-2.63	1.38	1.44
7	A	101	BCL	C3C-C4C	-2.63	1.48	1.51
7	r	101	BCL	MG-NC	2.62	2.12	2.06
7	j	302	BCL	C3D-C4D	-2.62	1.38	1.44
7	S	101	BCL	MG-NC	2.61	2.12	2.06
7	d	101	BCL	C1D-C2D	-2.61	1.40	1.45
7	e	100	BCL	C1D-C2D	-2.61	1.40	1.45
7	k	101	BCL	MG-NC	2.61	2.12	2.06
7	i	100	BCL	C3D-C4D	-2.61	1.38	1.44
7	L	301	BCL	C3D-C4D	-2.60	1.38	1.44
7	M	401	BCL	O1A-CGA	-2.60	1.14	1.22
7	n	100	BCL	O2A-CGA	-2.60	1.25	1.33
12	H	302	3PE	O31-C31	2.59	1.40	1.33
8	r	102	SPO	C35-C33	2.58	1.56	1.51
9	L	304	U10	C6-C5	-2.57	1.39	1.46
8	F	102	SPO	C30-C28	2.57	1.56	1.51
7	s	202	BCL	MG-NC	2.57	2.12	2.06
7	g	101	BCL	C3D-C4D	-2.57	1.38	1.44
7	O	101	BCL	MG-NC	2.56	2.12	2.06
12	d	102	3PE	O31-C31	2.56	1.40	1.33
7	a	101	BCL	C3D-C4D	-2.56	1.38	1.44
7	d	101	BCL	O2A-CGA	-2.56	1.25	1.33
7	R	101	BCL	C3D-C4D	-2.54	1.38	1.44
7	A	101	BCL	O1A-CGA	-2.54	1.15	1.22
7	A	101	BCL	MG-NC	2.54	2.12	2.06
7	A	101	BCL	C1D-C2D	-2.54	1.40	1.45
8	t	102	SPO	C30-C28	2.53	1.56	1.51
7	b	101	BCL	MG-NC	2.53	2.12	2.06
7	e	100	BCL	MG-NC	2.53	2.12	2.06
7	S	101	BCL	C3D-C4D	-2.53	1.38	1.44
7	b	101	BCL	C3D-C4D	-2.53	1.38	1.44
7	t	103	BCL	C3D-C4D	-2.53	1.38	1.44
7	e	100	BCL	C3C-C4C	-2.52	1.48	1.51
7	s	202	BCL	O1A-CGA	-2.51	1.15	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	k	101	BCL	C3D-C4D	-2.50	1.38	1.44
8	g	102	SPO	C30-C28	2.50	1.56	1.51
9	L	305	U10	C1-C2	-2.50	1.38	1.47
7	g	101	BCL	MG-NC	2.50	2.12	2.06
7	d	101	BCL	C3D-C4D	-2.50	1.38	1.44
12	H	301	3PE	O21-C2	-2.49	1.40	1.46
7	i	100	BCL	MG-NC	2.49	2.12	2.06
7	n	100	BCL	C3D-C4D	-2.49	1.38	1.44
9	M	408	U10	C1-C2	-2.49	1.38	1.47
7	I	101	BCL	MG-NC	2.48	2.12	2.06
7	o	100	BCL	C1D-C2D	-2.48	1.40	1.45
7	F	103	BCL	MG-NC	2.47	2.12	2.06
8	I	102	SPO	C30-C28	2.47	1.56	1.51
8	r	102	SPO	C30-C28	2.47	1.56	1.51
7	t	103	BCL	C1D-C2D	-2.46	1.40	1.45
7	M	407	BCL	C1D-C2D	-2.46	1.40	1.45
7	g	101	BCL	O2A-CGA	-2.46	1.26	1.33
7	F	101	BCL	MG-NC	2.46	2.12	2.06
7	F	103	BCL	C1D-C2D	-2.45	1.40	1.45
7	j	302	BCL	C3C-C4C	-2.45	1.48	1.51
7	E	202	BCL	O1A-CGA	-2.45	1.15	1.22
7	i	100	BCL	O2A-CGA	-2.44	1.26	1.33
8	F	102	SPO	C35-C33	2.43	1.56	1.51
7	r	101	BCL	C3D-C4D	-2.43	1.38	1.44
8	j	301	SPO	C30-C28	2.43	1.56	1.51
8	r	103	SPO	C35-C33	2.41	1.56	1.51
8	M	406	SPO	C30-C28	2.41	1.56	1.51
7	n	100	BCL	MG-NC	2.41	2.12	2.06
8	M	406	SPO	C9-C7	-2.41	1.32	1.35
7	D	202	BCL	O1A-CGA	-2.41	1.15	1.22
7	K	101	BCL	MG-NC	2.40	2.12	2.06
7	b	102	BCL	MG-NC	2.40	2.12	2.06
8	s	201	SPO	C30-C28	2.40	1.56	1.51
7	M	402	BCL	CHD-C1D	2.39	1.43	1.38
7	M	401	BCL	C3D-C4D	-2.37	1.38	1.44
9	M	405	U10	C6-C1	2.37	1.39	1.35
7	L	301	BCL	C1D-C2D	-2.37	1.40	1.45
9	L	304	U10	C1-C2	-2.37	1.38	1.47
7	M	407	BCL	CHD-C1D	2.37	1.43	1.38
7	o	100	BCL	MG-NC	2.37	2.11	2.06
7	E	202	BCL	MG-NC	2.36	2.11	2.06
8	g	102	SPO	C35-C33	2.36	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	305	U10	C6-C1	2.35	1.39	1.35
7	n	100	BCL	C1D-C2D	-2.35	1.40	1.45
12	H	301	3PE	O31-C31	2.35	1.40	1.33
7	j	302	BCL	MG-NC	2.35	2.11	2.06
7	d	101	BCL	MG-NC	2.35	2.11	2.06
8	t	102	SPO	C35-C33	2.34	1.56	1.51
10	L	302	BPH	C2C-C3C	-2.33	1.52	1.54
9	M	408	U10	C6-C1	2.32	1.39	1.35
7	u	101	BCL	CHD-C1D	2.31	1.42	1.38
7	i	100	BCL	C3C-C4C	-2.31	1.48	1.51
7	b	102	BCL	O1A-CGA	-2.31	1.15	1.22
7	M	407	BCL	O1A-CGA	-2.30	1.15	1.22
8	r	103	SPO	C30-C28	2.30	1.56	1.51
7	t	101	BCL	C3D-C4D	-2.30	1.39	1.44
8	k	102	SPO	C30-C28	2.29	1.56	1.51
8	s	201	SPO	C35-C33	2.29	1.56	1.51
7	s	202	BCL	C3D-C4D	-2.29	1.39	1.44
8	B	101	SPO	C35-C33	2.28	1.56	1.51
8	I	102	SPO	C35-C33	2.26	1.56	1.51
7	D	202	BCL	MG-NC	2.26	2.11	2.06
7	b	102	BCL	C1D-C2D	-2.25	1.40	1.45
12	H	301	3PE	O21-C21	2.25	1.40	1.34
7	D	202	BCL	C1D-C2D	-2.24	1.40	1.45
7	F	101	BCL	C1D-C2D	-2.23	1.40	1.45
7	k	101	BCL	O2A-CGA	-2.23	1.26	1.33
9	a	102	U10	C1-C2	-2.21	1.39	1.47
8	N	201	SPO	C30-C28	2.21	1.55	1.51
7	s	202	BCL	C1D-C2D	-2.20	1.41	1.45
7	j	302	BCL	C1D-C2D	-2.20	1.41	1.45
7	k	101	BCL	C1D-C2D	-2.20	1.41	1.45
7	K	101	BCL	C3C-C4C	-2.20	1.48	1.51
7	F	103	BCL	O1A-CGA	-2.19	1.16	1.22
7	M	407	BCL	O2A-CGA	-2.19	1.26	1.33
7	j	303	BCL	C1D-C2D	-2.19	1.41	1.45
8	j	301	SPO	C35-C33	2.19	1.55	1.51
7	j	303	BCL	CHD-C1D	2.18	1.42	1.38
7	a	101	BCL	C1D-C2D	-2.18	1.41	1.45
8	k	102	SPO	C35-C33	2.18	1.55	1.51
7	r	101	BCL	C1D-C2D	-2.18	1.41	1.45
10	M	403	BPH	O2A-CGA	-2.18	1.26	1.33
7	i	100	BCL	C1D-C2D	-2.17	1.41	1.45
7	b	102	BCL	C3C-C4C	-2.17	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	101	BCL	O1A-CGA	-2.17	1.16	1.22
7	u	102	BCL	C3D-C4D	-2.17	1.39	1.44
7	t	101	BCL	CHD-C1D	2.16	1.42	1.38
7	E	202	BCL	CHD-C1D	2.16	1.42	1.38
7	a	101	BCL	O1A-CGA	-2.16	1.16	1.22
8	D	201	SPO	C30-C28	2.16	1.55	1.51
7	g	101	BCL	C1D-C2D	-2.15	1.41	1.45
7	u	102	BCL	CHD-C1D	2.14	1.42	1.38
7	F	101	BCL	CHD-C1D	2.13	1.42	1.38
9	L	304	U10	C6-C1	2.13	1.39	1.35
7	R	101	BCL	C1D-C2D	-2.13	1.41	1.45
7	R	101	BCL	O1A-CGA	-2.12	1.16	1.22
7	j	302	BCL	O1A-CGA	-2.12	1.16	1.22
7	o	100	BCL	O2A-CGA	-2.12	1.27	1.33
7	u	101	BCL	O1A-CGA	-2.12	1.16	1.22
7	I	101	BCL	C1D-C2D	-2.11	1.41	1.45
8	N	201	SPO	C35-C33	2.11	1.55	1.51
8	X	201	SPO	C30-C28	2.10	1.55	1.51
7	M	401	BCL	C1D-C2D	-2.10	1.41	1.45
7	G	101	BCL	CHD-C1D	2.08	1.42	1.38
7	G	101	BCL	C1D-C2D	-2.08	1.41	1.45
7	L	301	BCL	MG-NC	2.08	2.11	2.06
7	F	101	BCL	C3C-C4C	-2.06	1.49	1.51
7	S	101	BCL	C1D-C2D	-2.06	1.41	1.45
8	X	201	SPO	C35-C33	2.05	1.55	1.51
7	O	101	BCL	CHD-C1D	2.05	1.42	1.38
7	F	103	BCL	CHD-C1D	2.05	1.42	1.38
7	L	301	BCL	O2A-CGA	-2.05	1.27	1.33
10	L	302	BPH	C1C-C2C	-2.05	1.47	1.51
7	t	103	BCL	CHD-C1D	2.04	1.42	1.38
7	k	101	BCL	CHD-C1D	2.04	1.42	1.38
8	M	406	SPO	C35-C33	2.04	1.55	1.51
7	u	101	BCL	C3D-C4D	-2.03	1.39	1.44
7	D	202	BCL	CHD-C1D	2.01	1.42	1.38
7	E	202	BCL	C1D-C2D	-2.00	1.41	1.45

All (850) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	201	SPO	C3-C1-C4	-23.58	74.66	110.86
8	r	102	SPO	C2-C1-C4	-22.57	76.21	110.86
8	g	102	SPO	C2-C1-C4	-22.55	76.24	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	201	SPO	C2-C1-C4	-21.70	77.55	110.86
8	k	102	SPO	C3-C1-C4	-21.57	77.74	110.86
8	r	103	SPO	C3-C1-C4	-21.37	78.05	110.86
8	I	102	SPO	C2-C1-C4	-20.80	78.92	110.86
8	k	102	SPO	C2-C1-C4	-20.65	79.15	110.86
8	D	201	SPO	C3-C1-C4	-20.64	79.17	110.86
8	D	201	SPO	C2-C1-C4	-20.58	79.26	110.86
8	s	201	SPO	C3-C1-C4	-19.82	80.43	110.86
8	E	201	SPO	C3-C1-C4	-19.63	80.73	110.86
8	r	103	SPO	C2-C1-C4	-19.49	80.93	110.86
8	I	102	SPO	C3-C1-C4	-18.19	82.93	110.86
8	s	201	SPO	C2-C1-C4	-18.18	82.94	110.86
8	r	102	SPO	C3-C1-C4	-17.28	84.32	110.86
8	M	406	SPO	C3-C1-C2	16.99	142.32	110.37
8	t	102	SPO	C3-C1-C2	16.77	141.91	110.37
8	F	102	SPO	C3-C1-C2	16.11	140.67	110.37
8	X	201	SPO	C3-C1-C2	16.05	140.56	110.37
8	g	102	SPO	C3-C1-C4	-15.92	86.41	110.86
8	N	201	SPO	C2-C1-C4	-15.60	86.91	110.86
8	j	301	SPO	C3-C1-C2	15.23	139.01	110.37
8	s	201	SPO	C3-C1-C2	14.66	137.95	110.37
8	B	101	SPO	C3-C1-C2	13.95	136.61	110.37
8	r	103	SPO	C3-C1-C2	13.83	136.38	110.37
8	N	201	SPO	C3-C1-C2	13.54	135.83	110.37
8	I	102	SPO	C3-C1-C2	13.40	135.57	110.37
8	r	102	SPO	C3-C1-C2	12.41	133.71	110.37
8	g	102	SPO	C3-C1-C2	12.36	133.61	110.37
8	j	301	SPO	C2-C1-C4	-11.21	93.65	110.86
8	F	102	SPO	C3-C1-C4	-10.88	94.15	110.86
8	B	101	SPO	C2-C1-C4	-10.57	94.64	110.86
8	s	201	SPO	C10-C9-C7	-10.43	112.42	127.31
8	t	102	SPO	C3-C1-C4	-10.20	95.20	110.86
8	t	102	SPO	C2-C1-C4	-10.17	95.24	110.86
8	D	201	SPO	C3-C1-C2	10.13	129.43	110.37
8	X	201	SPO	C2-C1-C4	-10.07	95.40	110.86
8	D	201	SPO	C5-C6-C7	-9.95	110.85	125.89
8	s	201	SPO	C15-C14-C12	-9.70	113.46	127.31
8	j	301	SPO	C5-C6-C7	-9.67	111.28	125.89
8	E	201	SPO	C3-C1-C2	9.55	128.33	110.37
8	M	406	SPO	C5-C6-C7	-9.53	111.49	125.89
8	t	102	SPO	C21-C22-C23	-9.51	113.74	127.31
8	j	301	SPO	C3-C1-C4	-9.51	96.26	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	k	102	SPO	C3-C1-C2	9.45	128.15	110.37
8	M	406	SPO	C2-C1-C4	-9.44	96.36	110.86
8	F	102	SPO	C2-C1-C4	-9.21	96.72	110.86
8	k	102	SPO	C5-C6-C7	-8.82	112.56	125.89
8	r	102	SPO	C10-C9-C7	-8.22	115.58	127.31
8	j	301	SPO	C15-C14-C12	-8.17	115.65	127.31
8	E	201	SPO	C5-C6-C7	-8.16	113.56	125.89
8	M	406	SPO	C3-C1-C4	-8.02	98.55	110.86
8	r	102	SPO	C5-C6-C7	-7.96	113.86	125.89
8	B	101	SPO	C3-C1-C4	-7.79	98.90	110.86
8	X	201	SPO	C3-C1-C4	-7.75	98.96	110.86
8	B	101	SPO	C11-C12-C14	7.45	130.38	118.94
8	s	201	SPO	C5-C6-C7	-7.17	115.05	125.89
12	d	102	3PE	O11-P-O14	-7.13	81.21	109.07
8	F	102	SPO	C20-C19-C17	-7.09	117.19	127.31
8	t	102	SPO	C15-C14-C12	-7.05	117.24	127.31
8	N	201	SPO	C20-C19-C17	-6.95	117.39	127.31
8	k	102	SPO	C20-C19-C17	-6.93	117.42	127.31
7	u	102	BCL	C1-C2-C3	6.82	137.84	126.04
12	d	102	3PE	O12-P-O11	-6.82	76.07	107.75
8	B	101	SPO	C21-C22-C23	-6.73	117.71	127.31
8	F	102	SPO	C15-C14-C12	-6.58	117.93	127.31
8	E	201	SPO	C20-C19-C17	-6.54	117.98	127.31
12	d	102	3PE	O13-P-O14	-6.50	83.67	109.07
8	B	101	SPO	C13-C12-C14	-6.37	114.00	122.92
7	b	101	BCL	C1-O2A-CGA	6.37	133.14	116.44
8	B	101	SPO	C10-C11-C12	-6.35	108.57	126.42
8	B	101	SPO	C20-C19-C17	-6.20	118.47	127.31
8	r	103	SPO	C24-C23-C22	-6.05	114.44	122.92
12	d	102	3PE	O12-P-O13	-6.05	79.66	107.75
7	M	401	BCL	CHD-C1D-ND	-6.03	118.91	124.45
7	M	402	BCL	CHD-C1D-ND	-5.87	119.06	124.45
7	j	302	BCL	CHD-C1D-ND	-5.81	119.12	124.45
7	o	100	BCL	C1-C2-C3	-5.77	116.07	126.04
8	I	102	SPO	C20-C19-C17	-5.73	119.14	127.31
7	u	101	BCL	CHD-C1D-ND	-5.72	119.19	124.45
8	t	102	SPO	C5-C6-C7	-5.71	117.26	125.89
8	g	102	SPO	C5-C6-C7	-5.67	117.32	125.89
7	M	402	BCL	C4D-CHA-C1A	5.67	128.15	121.25
8	M	406	SPO	C10-C9-C7	-5.64	119.26	127.31
7	M	402	BCL	C16-C15-C13	5.61	134.05	115.92
7	F	101	BCL	CHD-C1D-ND	-5.59	119.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	d	101	BCL	CHD-C1D-ND	-5.54	119.36	124.45
7	E	202	BCL	C4D-CHA-C1A	5.52	127.96	121.25
7	n	100	BCL	CHD-C1D-ND	-5.50	119.40	124.45
7	a	101	BCL	C4D-CHA-C1A	5.45	127.89	121.25
8	k	102	SPO	C21-C22-C23	-5.44	119.55	127.31
7	t	101	BCL	CHD-C1D-ND	-5.42	119.47	124.45
7	K	101	BCL	C4D-CHA-C1A	5.40	127.82	121.25
7	s	202	BCL	CHD-C1D-ND	-5.39	119.50	124.45
7	k	101	BCL	CHD-C1D-ND	-5.37	119.52	124.45
7	E	202	BCL	CHD-C1D-ND	-5.36	119.53	124.45
7	L	301	BCL	CHD-C1D-ND	-5.36	119.53	124.45
7	u	102	BCL	CHD-C1D-ND	-5.34	119.55	124.45
7	F	103	BCL	C4D-CHA-C1A	5.33	127.74	121.25
8	t	102	SPO	C26-C25-C23	-5.33	111.44	126.42
7	O	101	BCL	C4D-CHA-C1A	5.32	127.72	121.25
7	b	102	BCL	C4D-CHA-C1A	5.32	127.72	121.25
7	o	100	BCL	C4D-CHA-C1A	5.30	127.70	121.25
7	r	101	BCL	CHD-C1D-ND	-5.30	119.58	124.45
7	j	303	BCL	C4D-CHA-C1A	5.30	127.70	121.25
7	I	101	BCL	C4D-CHA-C1A	5.30	127.69	121.25
7	o	100	BCL	CHD-C1D-ND	-5.29	119.59	124.45
7	e	100	BCL	CHD-C1D-ND	-5.29	119.60	124.45
8	E	201	SPO	C6-C7-C9	5.28	127.05	118.94
7	t	103	BCL	C4D-CHA-C1A	5.28	127.67	121.25
7	O	101	BCL	CHD-C1D-ND	-5.28	119.60	124.45
7	i	100	BCL	CHD-C1D-ND	-5.27	119.61	124.45
7	R	101	BCL	CHD-C1D-ND	-5.26	119.62	124.45
7	g	101	BCL	CHD-C1D-ND	-5.25	119.63	124.45
8	F	102	SPO	C21-C22-C23	-5.25	119.81	127.31
7	R	101	BCL	C4D-CHA-C1A	5.24	127.63	121.25
7	L	301	BCL	C4D-CHA-C1A	5.24	127.62	121.25
7	N	202	BCL	C4D-CHA-C1A	5.23	127.61	121.25
8	r	102	SPO	C15-C14-C12	-5.22	119.86	127.31
7	n	100	BCL	C4D-CHA-C1A	5.21	127.59	121.25
7	a	101	BCL	CHD-C1D-ND	-5.20	119.67	124.45
7	u	102	BCL	C4D-CHA-C1A	5.19	127.56	121.25
7	A	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
7	D	202	BCL	C4D-CHA-C1A	5.18	127.55	121.25
7	S	101	BCL	CHD-C1D-ND	-5.18	119.70	124.45
8	N	201	SPO	C21-C22-C23	-5.17	119.93	127.31
7	G	101	BCL	C4D-CHA-C1A	5.17	127.55	121.25
7	D	202	BCL	CHD-C1D-ND	-5.16	119.71	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	101	BCL	C4D-CHA-C1A	5.13	127.50	121.25
7	b	102	BCL	CHD-C1D-ND	-5.13	119.74	124.45
7	t	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
7	G	101	BCL	CHD-C1D-ND	-5.11	119.76	124.45
8	M	406	SPO	C21-C20-C19	-5.10	113.02	123.47
7	j	302	BCL	C4D-CHA-C1A	5.10	127.46	121.25
7	b	101	BCL	C4D-CHA-C1A	5.09	127.45	121.25
7	I	101	BCL	CHD-C1D-ND	-5.09	119.78	124.45
7	g	101	BCL	C4D-CHA-C1A	5.09	127.44	121.25
7	F	103	BCL	CHD-C1D-ND	-5.08	119.78	124.45
7	b	101	BCL	CHD-C1D-ND	-5.07	119.79	124.45
9	L	303	U10	C7-C8-C9	-5.07	118.34	126.79
7	F	101	BCL	C4D-CHA-C1A	5.07	127.42	121.25
8	t	102	SPO	C10-C9-C7	-5.05	120.10	127.31
8	s	201	SPO	C15-C16-C17	-5.03	112.29	126.42
7	d	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
7	k	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
7	e	100	BCL	C4D-CHA-C1A	4.98	127.31	121.25
7	j	303	BCL	CHD-C1D-ND	-4.98	119.88	124.45
7	r	101	BCL	C4D-CHA-C1A	4.97	127.29	121.25
7	u	101	BCL	C4D-CHA-C1A	4.97	127.29	121.25
8	D	201	SPO	C20-C19-C17	-4.95	120.24	127.31
8	g	102	SPO	C21-C20-C19	-4.93	113.37	123.47
7	M	401	BCL	C4D-CHA-C1A	4.92	127.23	121.25
8	E	201	SPO	C26-C25-C23	-4.91	112.62	126.42
7	d	101	BCL	CMB-C2B-C1B	-4.91	120.92	128.46
7	A	101	BCL	CHD-C1D-ND	-4.84	120.01	124.45
7	N	202	BCL	CHD-C1D-ND	-4.83	120.02	124.45
7	K	101	BCL	CHD-C1D-ND	-4.82	120.02	124.45
7	i	100	BCL	C4D-CHA-C1A	4.77	127.06	121.25
8	E	201	SPO	C31-C32-C33	-4.75	116.22	127.66
7	N	202	BCL	C1-O2A-CGA	4.75	128.90	116.44
7	o	100	BCL	CMB-C2B-C1B	-4.73	121.19	128.46
8	B	101	SPO	C15-C14-C12	4.70	134.02	127.31
7	s	202	BCL	C4D-CHA-C1A	4.70	126.97	121.25
7	M	407	BCL	C4D-CHA-C1A	4.68	126.94	121.25
7	t	103	BCL	CHD-C1D-ND	-4.67	120.16	124.45
7	i	100	BCL	CMB-C2B-C1B	-4.66	121.31	128.46
8	s	201	SPO	C10-C11-C12	-4.64	113.38	126.42
7	F	101	BCL	CMB-C2B-C1B	-4.63	121.34	128.46
8	N	201	SPO	C24-C23-C25	4.60	125.33	118.08
7	n	100	BCL	CMB-C2B-C1B	-4.57	121.45	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	101	BCL	CMB-C2B-C1B	-4.55	121.47	128.46
7	D	202	BCL	CMB-C2B-C1B	-4.55	121.47	128.46
7	b	101	BCL	CMB-C2B-C1B	-4.55	121.47	128.46
8	M	406	SPO	C9-C10-C11	-4.54	109.04	123.22
7	M	407	BCL	CHD-C1D-ND	-4.50	120.32	124.45
7	M	407	BCL	CMB-C2B-C1B	-4.49	121.57	128.46
8	N	201	SPO	C24-C23-C22	-4.48	116.64	122.92
7	j	302	BCL	CMB-C2B-C1B	-4.47	121.60	128.46
8	g	102	SPO	C25-C23-C22	4.45	125.77	118.94
8	s	201	SPO	C8-C7-C9	-4.45	116.70	122.92
7	e	100	BCL	CMB-C2B-C1B	-4.45	121.63	128.46
8	r	103	SPO	C5-C6-C7	-4.42	119.21	125.89
8	D	201	SPO	C10-C9-C7	-4.41	121.01	127.31
8	E	201	SPO	C25-C23-C22	4.40	125.69	118.94
8	M	406	SPO	C24-C23-C22	-4.39	116.78	122.92
8	j	301	SPO	C14-C15-C16	-4.39	109.53	123.22
8	D	201	SPO	O1-C1-C2	-4.38	78.82	108.97
7	s	202	BCL	CMB-C2B-C1B	-4.38	121.73	128.46
7	E	202	BCL	C1-C2-C3	4.37	133.60	126.04
7	u	102	BCL	C4A-NA-C1A	4.37	108.67	106.71
8	g	102	SPO	O1-C1-C2	-4.37	78.95	108.97
7	r	101	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
8	E	201	SPO	O1-C1-C2	-4.36	78.97	108.97
8	t	102	SPO	C20-C19-C17	-4.36	121.09	127.31
8	r	103	SPO	C10-C9-C7	-4.33	121.13	127.31
8	t	102	SPO	C21-C20-C19	-4.33	114.61	123.47
8	j	301	SPO	C20-C19-C17	-4.32	121.15	127.31
7	N	202	BCL	C16-C15-C13	4.31	129.85	115.92
8	E	201	SPO	C16-C17-C19	4.31	125.55	118.94
8	k	102	SPO	O1-C1-C2	-4.29	79.47	108.97
8	E	201	SPO	C9-C10-C11	-4.28	109.87	123.22
12	H	302	3PE	O21-C21-C22	4.26	120.69	111.50
8	k	102	SPO	C15-C14-C12	-4.26	121.23	127.31
7	t	101	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
7	j	303	BCL	CMB-C2B-C1B	-4.22	121.97	128.46
7	k	101	BCL	CMB-C2B-C1B	-4.22	121.97	128.46
7	F	103	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
8	s	201	SPO	C24-C23-C22	-4.22	117.01	122.92
7	O	101	BCL	CMB-C2B-C1B	-4.21	121.99	128.46
7	F	103	BCL	C11-C10-C8	-4.21	102.30	115.92
7	e	100	BCL	C17-C16-C15	4.20	132.56	113.24
7	E	202	BCL	CMB-C2B-C1B	-4.20	122.01	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	101	BCL	CMB-C2B-C1B	-4.20	122.02	128.46
7	M	401	BCL	C1D-ND-C4D	-4.19	103.36	106.33
7	I	101	BCL	CMB-C2B-C1B	-4.18	122.03	128.46
7	L	301	BCL	CMB-C2B-C1B	-4.17	122.06	128.46
8	F	102	SPO	C24-C23-C22	-4.16	117.09	122.92
9	M	405	U10	C20-C19-C21	4.15	122.26	115.27
7	M	402	BCL	CMB-C2B-C1B	-4.12	122.12	128.46
8	t	102	SPO	C25-C23-C22	4.12	125.26	118.94
8	k	102	SPO	O1-C1-C3	-4.12	80.67	108.97
7	M	402	BCL	C4A-NA-C1A	4.11	108.56	106.71
8	X	201	SPO	C5-C6-C7	-4.11	119.68	125.89
7	A	101	BCL	CMB-C2B-C1B	-4.10	122.16	128.46
7	N	202	BCL	CMB-C2B-C1B	-4.10	122.16	128.46
8	r	102	SPO	O1-C1-C2	-4.10	80.76	108.97
8	D	201	SPO	O1-C1-C3	-4.10	80.79	108.97
7	e	100	BCL	C4A-NA-C1A	4.09	108.54	106.71
8	E	201	SPO	O1-C1-C3	-4.07	81.01	108.97
8	M	406	SPO	C21-C22-C23	-4.06	121.52	127.31
7	S	101	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
7	G	101	BCL	CMB-C2B-C1B	-4.04	122.26	128.46
12	H	301	3PE	O21-C21-C22	4.03	120.18	111.50
8	g	102	SPO	C24-C23-C22	-4.01	117.30	122.92
7	u	101	BCL	C1D-ND-C4D	-3.99	103.50	106.33
7	b	102	BCL	CMB-C2B-C1B	-3.99	122.33	128.46
8	D	201	SPO	C24-C23-C25	3.99	124.36	118.08
7	K	101	BCL	CMB-C2B-C1B	-3.98	122.34	128.46
8	E	201	SPO	C15-C16-C17	-3.95	115.32	126.42
8	r	102	SPO	C6-C7-C9	3.95	125.00	118.94
8	r	103	SPO	O1-C1-C3	-3.94	81.88	108.97
8	M	406	SPO	C15-C14-C12	-3.92	121.71	127.31
10	M	403	BPH	C1-C2-C3	3.91	132.80	126.04
8	r	102	SPO	C15-C16-C17	-3.90	115.45	126.42
8	r	102	SPO	O1-C1-C3	-3.90	82.16	108.97
8	N	201	SPO	O1-C1-C3	-3.89	82.22	108.97
8	N	201	SPO	O1-C1-C2	-3.88	82.28	108.97
7	d	101	BCL	C1D-ND-C4D	-3.87	103.59	106.33
7	k	101	BCL	C4A-NA-C1A	3.86	108.44	106.71
8	I	102	SPO	O1-C1-C2	-3.86	82.45	108.97
8	s	201	SPO	O1-C1-C3	-3.84	82.58	108.97
8	M	406	SPO	C24-C23-C25	3.84	124.12	118.08
7	s	202	BCL	C1D-ND-C4D	-3.83	103.61	106.33
9	L	304	U10	C22-C23-C24	-3.83	118.43	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	g	102	SPO	C20-C21-C22	3.83	131.32	123.47
8	g	102	SPO	C15-C16-C17	-3.83	115.66	126.42
7	b	101	BCL	O2D-CGD-CBD	3.83	118.07	111.27
8	t	102	SPO	C24-C23-C22	-3.83	117.56	122.92
8	r	103	SPO	C24-C23-C25	3.82	124.10	118.08
7	t	103	BCL	CMB-C2B-C1B	-3.81	122.60	128.46
8	B	101	SPO	C26-C25-C23	-3.81	115.71	126.42
7	N	202	BCL	C17-C16-C15	3.80	130.70	113.24
7	o	100	BCL	C1D-ND-C4D	-3.80	103.64	106.33
7	u	101	BCL	CMB-C2B-C1B	-3.79	122.63	128.46
7	j	302	BCL	C1D-ND-C4D	-3.78	103.65	106.33
8	s	201	SPO	O1-C1-C2	-3.77	83.06	108.97
8	t	102	SPO	C13-C12-C14	-3.77	117.65	122.92
7	M	401	BCL	CMB-C2B-C1B	-3.76	122.68	128.46
7	A	101	BCL	C4A-NA-C1A	3.75	108.39	106.71
8	r	102	SPO	C21-C20-C19	-3.75	115.80	123.47
7	t	101	BCL	C1D-ND-C4D	-3.75	103.67	106.33
7	F	101	BCL	C1D-ND-C4D	-3.74	103.68	106.33
7	R	101	BCL	CMB-C2B-C1B	-3.74	122.72	128.46
10	M	403	BPH	C17-C16-C15	3.73	130.37	113.24
7	r	101	BCL	C1D-ND-C4D	-3.71	103.70	106.33
7	a	101	BCL	C16-C15-C13	3.70	127.89	115.92
7	e	100	BCL	C1D-ND-C4D	-3.69	103.71	106.33
8	g	102	SPO	C21-C22-C23	3.67	132.55	127.31
8	I	102	SPO	C21-C22-C23	-3.67	122.07	127.31
8	X	201	SPO	C20-C19-C17	-3.67	122.07	127.31
8	j	301	SPO	C21-C20-C19	-3.66	115.97	123.47
7	u	102	BCL	C1D-ND-C4D	-3.65	103.74	106.33
7	i	100	BCL	C1D-ND-C4D	-3.65	103.74	106.33
8	r	103	SPO	C20-C21-C22	-3.65	116.00	123.47
8	k	102	SPO	C31-C32-C33	-3.63	118.93	127.66
7	n	100	BCL	C1D-ND-C4D	-3.63	103.76	106.33
9	L	304	U10	C7-C8-C9	-3.62	120.76	126.79
7	K	101	BCL	C4A-NA-C1A	3.62	108.33	106.71
7	b	102	BCL	C4A-NA-C1A	3.62	108.33	106.71
8	E	201	SPO	C8-C7-C9	-3.60	117.88	122.92
8	s	201	SPO	C6-C7-C9	3.60	124.46	118.94
7	g	101	BCL	C1D-ND-C4D	-3.60	103.78	106.33
7	E	202	BCL	C4A-NA-C1A	3.59	108.32	106.71
7	k	101	BCL	C1D-ND-C4D	-3.57	103.80	106.33
8	r	103	SPO	O1-C1-C2	-3.57	84.41	108.97
8	D	201	SPO	C31-C32-C33	-3.57	119.06	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	d	102	3PE	O21-C21-C22	3.57	119.19	111.50
12	d	102	3PE	O12-P-O14	3.55	129.81	112.24
7	g	101	BCL	C4A-NA-C1A	3.55	108.30	106.71
8	s	201	SPO	C25-C23-C22	3.55	124.39	118.94
8	F	102	SPO	C10-C9-C7	-3.55	122.25	127.31
9	L	304	U10	C25-C24-C26	3.54	121.23	115.27
9	a	102	U10	C27-C28-C29	-3.53	119.16	127.66
9	L	304	U10	C17-C18-C19	-3.52	119.19	127.66
7	F	103	BCL	C4A-NA-C1A	3.51	108.28	106.71
9	M	405	U10	C35-C34-C36	3.51	121.18	115.27
7	d	101	BCL	C4A-NA-C1A	3.51	108.28	106.71
8	E	201	SPO	C21-C20-C19	-3.49	116.33	123.47
8	I	102	SPO	O1-C1-C3	-3.48	85.04	108.97
7	F	101	BCL	C4A-NA-C1A	3.47	108.27	106.71
8	I	102	SPO	C5-C6-C7	-3.46	120.66	125.89
8	F	102	SPO	C24-C23-C25	3.46	123.52	118.08
8	r	103	SPO	C15-C14-C12	-3.43	122.42	127.31
7	a	101	BCL	C4A-NA-C1A	3.42	108.25	106.71
7	O	101	BCL	C1C-NC-C4C	3.42	108.24	106.71
7	i	100	BCL	CMB-C2B-C3B	3.42	131.07	124.68
8	k	102	SPO	C14-C15-C16	-3.40	112.62	123.22
9	M	405	U10	C12-C13-C14	-3.40	119.48	127.66
7	u	102	BCL	CMB-C2B-C1B	-3.39	123.25	128.46
8	M	406	SPO	C13-C12-C11	-3.39	112.74	118.08
8	E	201	SPO	C34-C33-C35	3.37	120.94	115.27
8	D	201	SPO	C20-C21-C22	-3.37	116.58	123.47
7	d	101	BCL	CMB-C2B-C3B	3.37	130.97	124.68
7	M	402	BCL	C1D-ND-C4D	-3.36	103.95	106.33
7	I	101	BCL	C1D-ND-C4D	-3.35	103.95	106.33
8	I	102	SPO	C26-C25-C23	-3.35	117.01	126.42
8	D	201	SPO	C25-C23-C22	-3.34	113.82	118.94
7	o	100	BCL	CMB-C2B-C3B	3.33	130.91	124.68
7	D	202	BCL	CMB-C2B-C3B	3.33	130.90	124.68
7	a	101	BCL	C1D-ND-C4D	-3.32	103.97	106.33
7	b	101	BCL	CHA-C1A-NA	-3.32	118.79	126.40
7	S	101	BCL	C1D-ND-C4D	-3.31	103.98	106.33
10	L	302	BPH	OBD-CAD-CBD	-3.30	120.98	125.82
7	F	101	BCL	CMB-C2B-C3B	3.30	130.85	124.68
8	N	201	SPO	C14-C15-C16	-3.29	112.94	123.22
8	k	102	SPO	C24-C23-C22	-3.29	118.31	122.92
7	b	101	BCL	CMB-C2B-C3B	3.29	130.84	124.68
7	M	407	BCL	CMB-C2B-C3B	3.29	130.84	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	201	SPO	C13-C12-C11	3.29	123.26	118.08
7	g	101	BCL	CMB-C2B-C3B	3.28	130.82	124.68
8	r	102	SPO	C10-C11-C12	-3.28	117.19	126.42
7	M	402	BCL	C1-O2A-CGA	3.28	125.05	116.44
8	M	406	SPO	C11-C12-C14	3.27	123.97	118.94
7	j	303	BCL	C1D-ND-C4D	-3.27	104.01	106.33
8	g	102	SPO	O1-C1-C3	-3.27	86.49	108.97
7	r	101	BCL	C4A-NA-C1A	3.27	108.17	106.71
9	a	102	U10	C1M-C1-C6	-3.26	119.08	124.40
8	N	201	SPO	C31-C32-C33	-3.25	119.83	127.66
7	A	101	BCL	C1D-ND-C4D	-3.24	104.03	106.33
7	n	100	BCL	C4A-NA-C1A	3.24	108.16	106.71
7	j	302	BCL	CMB-C2B-C3B	3.23	130.72	124.68
7	N	202	BCL	C1D-ND-C4D	-3.22	104.04	106.33
8	B	101	SPO	C29-C28-C30	3.22	120.69	115.27
7	t	103	BCL	CHA-C1A-NA	-3.22	119.03	126.40
10	L	306	BPH	O2D-CGD-CBD	3.21	115.07	111.00
7	n	100	BCL	CMB-C2B-C3B	3.20	130.67	124.68
7	r	101	BCL	CMB-C2B-C3B	3.20	130.67	124.68
9	a	102	U10	C17-C18-C19	-3.20	119.95	127.66
9	a	102	U10	C15-C14-C16	3.20	120.65	115.27
7	b	101	BCL	C16-C15-C13	3.19	126.24	115.92
7	S	101	BCL	C4A-NA-C1A	3.19	108.14	106.71
7	d	101	BCL	O2D-CGD-CBD	3.19	116.93	111.27
7	G	101	BCL	C1D-ND-C4D	-3.18	104.08	106.33
7	t	101	BCL	C4A-NA-C1A	3.17	108.13	106.71
7	D	202	BCL	C1D-ND-C4D	-3.17	104.08	106.33
7	s	202	BCL	CMB-C2B-C3B	3.17	130.61	124.68
7	M	407	BCL	CHA-C1A-NA	-3.16	119.16	126.40
7	D	202	BCL	C4A-NA-C1A	3.16	108.13	106.71
7	e	100	BCL	CMB-C2B-C3B	3.16	130.59	124.68
8	g	102	SPO	C15-C14-C12	3.16	131.81	127.31
8	N	201	SPO	C34-C33-C35	3.16	120.58	115.27
7	R	101	BCL	C1D-ND-C4D	-3.15	104.09	106.33
7	t	101	BCL	CHA-C1A-NA	-3.15	119.19	126.40
7	i	100	BCL	C1C-NC-C4C	3.15	108.12	106.71
7	b	102	BCL	C1D-ND-C4D	-3.14	104.10	106.33
8	g	102	SPO	C29-C28-C30	3.14	120.56	115.27
10	M	403	BPH	OBD-CAD-CBD	-3.14	121.21	125.82
7	b	101	BCL	C1D-ND-C4D	-3.14	104.11	106.33
8	B	101	SPO	C18-C17-C19	-3.13	118.53	122.92
7	L	301	BCL	C1D-ND-C4D	-3.13	104.11	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	405	U10	C17-C18-C19	-3.12	120.14	127.66
7	O	101	BCL	CMB-C2B-C3B	3.12	130.52	124.68
7	u	101	BCL	CHA-C1A-NA	-3.12	119.26	126.40
9	M	405	U10	C27-C28-C29	-3.12	120.16	127.66
8	r	102	SPO	C26-C25-C23	-3.11	117.67	126.42
7	M	402	BCL	CHA-C1A-NA	-3.11	119.27	126.40
8	g	102	SPO	C11-C12-C14	-3.10	114.18	118.94
9	a	102	U10	C10-C9-C11	3.10	120.49	115.27
7	L	301	BCL	CMB-C2B-C3B	3.10	130.48	124.68
8	N	201	SPO	C11-C12-C14	-3.09	114.20	118.94
7	o	100	BCL	CHA-C1A-NA	-3.09	119.32	126.40
8	B	101	SPO	C14-C15-C16	-3.09	113.58	123.22
7	A	101	BCL	CMB-C2B-C3B	3.08	130.44	124.68
8	r	102	SPO	C29-C28-C30	3.08	120.45	115.27
7	j	303	BCL	CMB-C2B-C3B	3.08	130.44	124.68
8	s	201	SPO	C13-C12-C14	-3.08	118.61	122.92
7	F	103	BCL	C1D-ND-C4D	-3.07	104.15	106.33
7	E	202	BCL	C1D-ND-C4D	-3.06	104.16	106.33
7	G	101	BCL	C1C-NC-C4C	3.06	108.08	106.71
7	t	103	BCL	C1D-ND-C4D	-3.06	104.16	106.33
7	N	202	BCL	CHA-C1A-NA	-3.05	119.41	126.40
8	k	102	SPO	C13-C12-C11	3.05	122.88	118.08
7	N	202	BCL	C4A-NA-C1A	3.04	108.07	106.71
7	r	101	BCL	C1C-NC-C4C	3.04	108.07	106.71
7	O	101	BCL	C1D-ND-C4D	-3.04	104.18	106.33
7	E	202	BCL	CMB-C2B-C3B	3.03	130.36	124.68
9	a	102	U10	C20-C19-C21	3.03	120.38	115.27
8	N	201	SPO	C29-C28-C30	3.03	120.37	115.27
7	d	101	BCL	CHA-C1A-NA	-3.03	119.47	126.40
9	M	405	U10	C22-C23-C24	-3.03	120.37	127.66
7	M	407	BCL	C2A-C1A-CHA	3.03	129.15	123.86
7	M	407	BCL	C1C-NC-C4C	3.03	108.07	106.71
7	o	100	BCL	C1C-NC-C4C	3.02	108.06	106.71
7	M	402	BCL	CMB-C2B-C3B	3.02	130.33	124.68
7	F	103	BCL	CMB-C2B-C3B	3.02	130.33	124.68
7	a	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
7	n	100	BCL	CHA-C1A-NA	-3.02	119.49	126.40
7	I	101	BCL	CMB-C2B-C3B	3.01	130.32	124.68
7	M	401	BCL	CHA-C1A-NA	-3.01	119.50	126.40
7	j	302	BCL	CHA-C1A-NA	-3.01	119.51	126.40
7	e	100	BCL	CED-O2D-CGD	-3.01	109.14	115.94
8	k	102	SPO	C34-C33-C35	3.01	120.33	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	301	BCL	C4A-NA-C1A	3.01	108.06	106.71
8	t	102	SPO	C34-C33-C35	3.00	120.33	115.27
8	s	201	SPO	C18-C17-C16	3.00	122.81	118.08
7	G	101	BCL	CHA-C1A-NA	-3.00	119.53	126.40
8	N	201	SPO	C5-C6-C7	-3.00	121.36	125.89
7	e	100	BCL	C1C-NC-C4C	3.00	108.05	106.71
7	k	101	BCL	CMB-C2B-C3B	3.00	130.28	124.68
7	j	302	BCL	C4A-NA-C1A	3.00	108.05	106.71
8	D	201	SPO	C14-C15-C16	-2.99	113.89	123.22
7	t	101	BCL	CMB-C2B-C3B	2.99	130.27	124.68
7	F	103	BCL	CHA-C1A-NA	-2.99	119.56	126.40
8	r	103	SPO	C29-C28-C30	2.99	120.30	115.27
8	k	102	SPO	C24-C23-C25	2.98	122.78	118.08
7	r	101	BCL	CHA-C1A-NA	-2.98	119.56	126.40
7	K	101	BCL	CMB-C2B-C3B	2.98	130.26	124.68
8	X	201	SPO	C31-C32-C33	-2.98	120.48	127.66
7	j	303	BCL	CHA-C1A-NA	-2.98	119.57	126.40
7	L	301	BCL	CHA-C1A-NA	-2.98	119.57	126.40
7	S	101	BCL	CMB-C2B-C3B	2.98	130.25	124.68
8	E	201	SPO	C20-C21-C22	2.98	129.57	123.47
7	j	302	BCL	O2D-CGD-CBD	2.98	116.56	111.27
7	G	101	BCL	CMB-C2B-C3B	2.97	130.24	124.68
7	i	100	BCL	CHA-C1A-NA	-2.97	119.60	126.40
9	M	408	U10	C6-C1-C2	2.97	121.53	119.18
7	M	407	BCL	C1D-ND-C4D	-2.97	104.23	106.33
8	j	301	SPO	C31-C32-C33	-2.97	120.52	127.66
7	k	101	BCL	O2D-CGD-CBD	2.97	116.54	111.27
7	K	101	BCL	C1D-ND-C4D	-2.96	104.23	106.33
8	B	101	SPO	C9-C10-C11	2.96	132.46	123.22
7	N	202	BCL	CMB-C2B-C3B	2.96	130.22	124.68
8	B	101	SPO	C25-C23-C22	2.96	123.48	118.94
8	j	301	SPO	C29-C28-C30	2.96	120.25	115.27
7	j	303	BCL	C4A-NA-C1A	2.96	108.04	106.71
8	k	102	SPO	C29-C28-C30	2.96	120.25	115.27
7	s	202	BCL	C4A-NA-C1A	2.95	108.03	106.71
7	g	101	BCL	CHA-C1A-NA	-2.95	119.65	126.40
7	a	101	BCL	CMB-C2B-C3B	2.94	130.19	124.68
7	a	101	BCL	C1C-NC-C4C	2.94	108.03	106.71
7	S	101	BCL	CHA-C1A-NA	-2.94	119.67	126.40
7	b	102	BCL	CMB-C2B-C3B	2.94	130.17	124.68
7	b	102	BCL	CHA-C1A-NA	-2.93	119.68	126.40
7	E	202	BCL	CHA-C1A-NA	-2.93	119.68	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
7	u	102	BCL	C4B-C3B-CAB	-2.93	121.48	127.13
7	s	202	BCL	CHA-C1A-NA	-2.92	119.70	126.40
9	a	102	U10	C30-C29-C31	2.92	120.19	115.27
12	H	301	3PE	O31-C31-C32	2.91	121.05	111.91
8	r	102	SPO	C8-C7-C9	-2.91	118.84	122.92
7	O	101	BCL	CHA-C1A-NA	-2.91	119.74	126.40
9	L	304	U10	C15-C14-C16	2.91	120.16	115.27
7	e	100	BCL	CHA-C1A-NA	-2.90	119.75	126.40
7	R	101	BCL	CHA-C1A-NA	-2.90	119.75	126.40
7	I	101	BCL	CHA-C1A-NA	-2.90	119.77	126.40
7	k	101	BCL	CHA-C1A-NA	-2.89	119.78	126.40
7	F	101	BCL	O2D-CGD-CBD	2.89	116.40	111.27
9	L	303	U10	C6-C1-C2	2.89	121.46	119.18
7	j	303	BCL	C1C-NC-C4C	2.88	108.00	106.71
7	r	101	BCL	C11-C10-C8	-2.88	106.61	115.92
8	E	201	SPO	C10-C9-C7	2.88	131.42	127.31
7	F	101	BCL	CHA-C1A-NA	-2.88	119.81	126.40
9	L	305	U10	C12-C13-C14	-2.88	120.73	127.66
7	b	101	BCL	CED-O2D-CGD	-2.88	109.43	115.94
8	F	102	SPO	C15-C16-C17	-2.88	118.34	126.42
8	I	102	SPO	C29-C28-C30	2.88	120.11	115.27
9	M	405	U10	C30-C29-C31	2.87	120.10	115.27
7	I	101	BCL	C4A-NA-C1A	2.87	108.00	106.71
7	u	102	BCL	CHA-C1A-NA	-2.86	119.84	126.40
7	u	101	BCL	C2A-C1A-CHA	2.86	128.87	123.86
9	L	304	U10	C20-C19-C21	2.86	120.08	115.27
7	K	101	BCL	C1-C2-C3	2.86	130.98	126.04
8	E	201	SPO	C24-C23-C22	-2.85	118.93	122.92
8	D	201	SPO	C29-C28-C30	2.85	120.07	115.27
7	M	401	BCL	C2A-C1A-CHA	2.85	128.84	123.86
7	A	101	BCL	CHA-C1A-NA	-2.85	119.88	126.40
7	F	101	BCL	C1C-NC-C4C	2.85	107.99	106.71
12	H	302	3PE	O31-C31-C32	2.85	120.84	111.91
8	g	102	SPO	C31-C32-C33	-2.84	120.81	127.66
7	o	100	BCL	C2A-C1A-CHA	2.84	128.83	123.86
9	a	102	U10	C12-C13-C14	-2.84	120.83	127.66
7	F	101	BCL	CED-O2D-CGD	-2.84	109.52	115.94
8	B	101	SPO	C20-C21-C22	-2.83	117.67	123.47
7	e	100	BCL	O2D-CGD-CBD	2.82	116.29	111.27
7	G	101	BCL	C2A-C1A-CHA	2.82	128.79	123.86
9	M	405	U10	C25-C24-C26	2.82	120.01	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	306	BPH	OBD-CAD-CBD	-2.81	121.69	125.82
8	N	201	SPO	C20-C21-C22	-2.80	117.73	123.47
8	j	301	SPO	C34-C33-C35	2.80	119.98	115.27
8	s	201	SPO	C16-C17-C19	-2.80	114.64	118.94
7	j	303	BCL	C1-C2-C3	2.80	130.89	126.04
7	i	100	BCL	O2D-CGD-CBD	2.80	116.24	111.27
7	D	202	BCL	CHA-C1A-NA	-2.79	120.00	126.40
7	t	101	BCL	C2A-C1A-CHA	2.79	128.74	123.86
8	M	406	SPO	C8-C7-C9	-2.79	119.01	122.92
8	B	101	SPO	C34-C33-C32	-2.79	116.52	123.68
7	t	103	BCL	CMB-C2B-C3B	2.78	129.89	124.68
8	B	101	SPO	C24-C23-C22	-2.77	119.04	122.92
7	s	202	BCL	C2A-C1A-CHA	2.77	128.71	123.86
7	n	100	BCL	O2D-CGD-CBD	2.77	116.19	111.27
7	g	101	BCL	CED-O2D-CGD	-2.77	109.67	115.94
9	L	303	U10	C17-C18-C19	-2.76	121.00	127.66
7	e	100	BCL	O2D-CGD-O1D	-2.76	118.45	123.84
8	s	201	SPO	C11-C12-C14	2.75	123.16	118.94
7	u	101	BCL	C4A-NA-C1A	2.75	107.94	106.71
7	u	101	BCL	C17-C16-C15	2.75	125.88	113.24
7	L	301	BCL	C1C-NC-C4C	2.75	107.94	106.71
7	M	401	BCL	CMB-C2B-C3B	2.74	129.81	124.68
7	s	202	BCL	O2D-CGD-CBD	2.73	116.12	111.27
7	R	101	BCL	CMB-C2B-C3B	2.73	129.79	124.68
8	r	102	SPO	C25-C23-C22	-2.73	114.75	118.94
9	a	102	U10	C35-C34-C36	2.73	119.86	115.27
8	B	101	SPO	C34-C33-C35	2.72	119.85	115.27
7	b	101	BCL	C2A-C1A-CHA	2.72	128.62	123.86
9	L	303	U10	C20-C19-C21	2.72	119.85	115.27
7	d	101	BCL	OBB-CAB-CBB	-2.72	114.05	120.17
7	u	101	BCL	CMB-C2B-C3B	2.72	129.76	124.68
8	X	201	SPO	C10-C9-C7	-2.71	123.44	127.31
8	r	103	SPO	C10-C11-C12	-2.70	118.83	126.42
7	b	102	BCL	C4B-C3B-CAB	-2.69	121.92	127.13
9	M	405	U10	C10-C9-C11	2.69	119.80	115.27
8	M	406	SPO	C6-C7-C9	2.68	123.06	118.94
9	L	303	U10	C15-C14-C16	2.68	119.78	115.27
7	E	202	BCL	C1C-NC-C4C	2.68	107.91	106.71
8	I	102	SPO	C34-C33-C35	2.67	119.77	115.27
7	n	100	BCL	OBB-CAB-CBB	-2.67	114.15	120.17
8	X	201	SPO	C27-C26-C25	-2.67	114.88	123.22
7	b	101	BCL	O2D-CGD-O1D	-2.67	118.61	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	103	BCL	C6-C7-C8	2.67	124.55	115.92
7	e	100	BCL	OBB-CAB-CBB	-2.67	114.16	120.17
8	X	201	SPO	C9-C10-C11	-2.67	114.89	123.22
7	F	101	BCL	O2D-CGD-O1D	-2.67	118.62	123.84
7	A	101	BCL	C1C-NC-C4C	2.67	107.91	106.71
8	E	201	SPO	C18-C17-C19	-2.67	119.19	122.92
9	L	305	U10	C21-C19-C20	2.66	120.48	114.60
7	e	100	BCL	C2A-C1A-CHA	2.66	128.51	123.86
7	b	102	BCL	C1C-NC-C4C	2.66	107.90	106.71
7	M	402	BCL	OBB-CAB-CBB	-2.66	114.19	120.17
8	M	406	SPO	C29-C28-C30	2.66	119.74	115.27
7	F	101	BCL	C17-C16-C15	2.65	125.42	113.24
9	L	305	U10	C10-C9-C11	2.65	119.73	115.27
7	b	101	BCL	C4A-NA-C1A	2.65	107.90	106.71
8	F	102	SPO	C31-C32-C33	-2.64	121.31	127.66
9	L	303	U10	O5-C5-C6	-2.63	116.93	121.55
9	M	405	U10	C15-C14-C16	2.63	119.69	115.27
9	L	304	U10	C12-C13-C14	-2.62	121.34	127.66
7	g	101	BCL	C2A-C1A-CHA	2.62	128.45	123.86
7	a	101	BCL	C1-C2-C3	2.62	130.58	126.04
10	L	302	BPH	OBB-CAB-CBB	-2.62	114.27	120.17
8	r	102	SPO	C20-C19-C17	-2.61	123.58	127.31
8	r	103	SPO	C20-C19-C17	-2.61	123.58	127.31
12	d	102	3PE	O31-C31-C32	2.61	120.10	111.91
8	j	301	SPO	C8-C7-C6	2.61	122.19	118.08
7	k	101	BCL	OBB-CAB-CBB	-2.61	114.30	120.17
8	k	102	SPO	C18-C17-C19	-2.60	119.27	122.92
7	d	101	BCL	CED-O2D-CGD	-2.60	110.05	115.94
7	n	100	BCL	C11-C10-C8	-2.60	107.51	115.92
8	M	406	SPO	C31-C32-C33	-2.60	121.40	127.66
7	k	101	BCL	CED-O2D-CGD	-2.60	110.06	115.94
7	d	101	BCL	C2A-C1A-CHA	2.59	128.39	123.86
8	F	102	SPO	C29-C28-C30	2.59	119.63	115.27
8	g	102	SPO	C13-C12-C11	2.59	122.16	118.08
9	a	102	U10	C25-C24-C26	2.59	119.62	115.27
7	n	100	BCL	C2A-C1A-CHA	2.58	128.38	123.86
7	L	301	BCL	C2A-C1A-CHA	2.58	128.37	123.86
8	F	102	SPO	C36-C37-C38	-2.58	118.93	127.75
8	X	201	SPO	C34-C33-C35	2.58	119.61	115.27
8	r	102	SPO	C21-C22-C23	2.58	130.99	127.31
8	F	102	SPO	C34-C33-C35	2.58	119.60	115.27
8	t	102	SPO	C27-C26-C25	2.57	131.25	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	101	BCL	C2A-C1A-CHA	2.57	128.36	123.86
7	F	101	BCL	C1-C2-C3	-2.57	121.60	126.04
7	b	101	BCL	OBB-CAB-CBB	-2.57	114.39	120.17
7	R	101	BCL	C4A-NA-C1A	2.57	107.86	106.71
7	R	101	BCL	C2A-C1A-CHA	2.57	128.35	123.86
7	F	103	BCL	C1-C2-C3	2.57	130.48	126.04
7	O	101	BCL	C2A-C1A-CHA	2.57	128.35	123.86
8	N	201	SPO	C1-C4-C5	2.57	119.86	113.06
7	S	101	BCL	C4B-C3B-CAB	-2.57	122.17	127.13
8	t	102	SPO	C40-C38-C39	2.56	120.27	114.60
7	M	407	BCL	OBB-CAB-CBB	-2.56	114.40	120.17
8	g	102	SPO	C34-C33-C35	2.56	119.58	115.27
7	S	101	BCL	C1C-NC-C4C	2.56	107.86	106.71
9	M	408	U10	C7-C6-C5	-2.56	115.40	118.48
8	D	201	SPO	C9-C10-C11	-2.55	115.26	123.22
7	M	402	BCL	C2A-C1A-CHA	2.55	128.31	123.86
7	I	101	BCL	C1-C2-C3	2.55	130.45	126.04
7	F	101	BCL	C2A-C1A-CHA	2.54	128.31	123.86
7	n	100	BCL	C1C-NC-C4C	2.54	107.85	106.71
9	L	304	U10	C1M-C1-C6	-2.54	120.26	124.40
7	u	101	BCL	C1C-NC-C4C	2.54	107.85	106.71
9	a	102	U10	C41-C39-C40	2.54	120.21	114.60
9	L	304	U10	C10-C9-C11	2.54	119.54	115.27
8	s	201	SPO	C20-C19-C17	-2.54	123.69	127.31
7	s	202	BCL	C4B-C3B-CAB	-2.53	122.23	127.13
7	k	101	BCL	O2D-CGD-O1D	-2.53	118.89	123.84
8	k	102	SPO	C40-C38-C39	2.53	120.19	114.60
7	s	202	BCL	OBB-CAB-CBB	-2.53	114.49	120.17
7	g	101	BCL	C1C-NC-C4C	2.52	107.84	106.71
7	r	101	BCL	C2A-C1A-CHA	2.52	128.27	123.86
7	r	101	BCL	O2D-CGD-CBD	2.52	115.74	111.27
7	t	101	BCL	O2D-CGD-CBD	2.51	115.73	111.27
9	M	405	U10	C41-C39-C40	2.51	120.14	114.60
7	A	101	BCL	CBA-CAA-C2A	-2.50	106.47	113.86
7	k	101	BCL	C2A-C1A-CHA	2.50	128.23	123.86
8	N	201	SPO	C40-C38-C39	2.50	120.12	114.60
7	N	202	BCL	O2A-CGA-O1A	2.50	129.90	123.59
7	D	202	BCL	C1-C2-C3	2.49	130.35	126.04
7	A	101	BCL	C2A-C1A-CHA	2.49	128.21	123.86
9	L	305	U10	C15-C14-C16	2.49	119.46	115.27
7	e	100	BCL	C16-C15-C13	-2.48	107.89	115.92
8	X	201	SPO	C21-C22-C23	-2.48	123.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401	BCL	C1-O2A-CGA	2.48	122.95	116.44
8	j	301	SPO	C10-C9-C7	-2.48	123.77	127.31
7	N	202	BCL	C2A-C1A-CHA	2.48	128.20	123.86
7	g	101	BCL	O2D-CGD-CBD	2.48	115.67	111.27
7	I	101	BCL	C2A-C1A-CHA	2.48	128.19	123.86
7	i	100	BCL	C4A-NA-C1A	2.48	107.82	106.71
8	g	102	SPO	C9-C10-C11	-2.47	115.50	123.22
8	j	301	SPO	C40-C38-C39	2.47	120.07	114.60
7	g	101	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
10	L	302	BPH	O2D-CGD-CBD	2.47	114.12	111.00
7	t	103	BCL	C4A-NA-C1A	2.47	107.81	106.71
7	d	101	BCL	O2D-CGD-O1D	-2.47	119.02	123.84
7	K	101	BCL	C2A-C1A-CHA	2.47	128.17	123.86
7	u	102	BCL	CMB-C2B-C3B	2.46	129.29	124.68
7	F	101	BCL	OBB-CAB-CBB	-2.46	114.63	120.17
8	g	102	SPO	C40-C38-C39	2.45	120.03	114.60
9	a	102	U10	C32-C33-C34	-2.45	121.75	127.66
7	t	103	BCL	C2A-C1A-CHA	2.45	128.15	123.86
7	i	100	BCL	OBB-CAB-CBB	-2.45	114.65	120.17
8	I	102	SPO	C20-C21-C22	-2.45	118.46	123.47
7	r	101	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
7	N	202	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
8	t	102	SPO	C29-C28-C30	2.45	119.39	115.27
8	t	102	SPO	C31-C32-C33	-2.45	121.77	127.66
8	r	102	SPO	C34-C33-C35	2.44	119.38	115.27
8	j	301	SPO	C9-C10-C11	-2.44	115.60	123.22
7	d	101	BCL	C1C-NC-C4C	2.44	107.80	106.71
9	L	303	U10	C26-C24-C25	2.43	119.97	114.60
9	M	405	U10	C32-C33-C34	-2.43	121.80	127.66
8	s	201	SPO	C40-C38-C39	2.43	119.97	114.60
8	X	201	SPO	C40-C38-C39	2.43	119.97	114.60
7	F	103	BCL	C1C-NC-C4C	2.42	107.80	106.71
7	L	301	BCL	OBB-CAB-CBB	-2.42	114.71	120.17
7	j	302	BCL	C2A-C1A-CHA	2.42	128.09	123.86
10	L	302	BPH	CMB-C2B-C3B	2.42	129.20	124.68
7	n	100	BCL	CED-O2D-CGD	-2.42	110.47	115.94
7	i	100	BCL	C2A-C1A-CHA	2.42	128.08	123.86
8	k	102	SPO	C21-C20-C19	-2.41	118.54	123.47
7	j	303	BCL	C2A-C1A-CHA	2.41	128.07	123.86
8	E	201	SPO	C29-C28-C30	2.40	119.31	115.27
7	i	100	BCL	CED-O2D-CGD	-2.40	110.50	115.94
7	b	101	BCL	CAA-C2A-C1A	2.40	119.85	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	u	101	BCL	C4B-C3B-CAB	-2.40	122.49	127.13
9	M	408	U10	C11-C9-C10	2.40	119.91	114.60
7	I	101	BCL	C1C-NC-C4C	2.40	107.78	106.71
7	t	101	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
7	b	101	BCL	C1-C2-C3	-2.40	121.90	126.04
7	M	407	BCL	C4A-NA-C1A	2.40	107.78	106.71
10	L	306	BPH	CMD-C2D-C3D	2.40	129.16	124.68
7	u	102	BCL	C2A-C1A-CHA	2.39	128.05	123.86
7	F	103	BCL	C2A-C1A-CHA	2.39	128.04	123.86
7	k	101	BCL	C6-C7-C8	-2.39	108.19	115.92
7	j	302	BCL	OBB-CAB-CBB	-2.39	114.79	120.17
8	t	102	SPO	C10-C11-C12	-2.39	119.71	126.42
7	I	101	BCL	OBB-CAB-CBB	-2.39	114.80	120.17
7	k	101	BCL	C4B-C3B-CAB	-2.39	122.52	127.13
7	n	100	BCL	O2D-CGD-O1D	-2.38	119.18	123.84
8	I	102	SPO	C18-C17-C19	-2.38	119.59	122.92
7	r	101	BCL	O2D-CGD-O1D	-2.38	119.19	123.84
7	o	100	BCL	OBB-CAB-CBB	-2.38	114.82	120.17
8	r	103	SPO	C40-C38-C39	2.37	119.85	114.60
7	D	202	BCL	C2A-C1A-CHA	2.37	128.01	123.86
7	u	101	BCL	O2D-CGD-CBD	2.37	115.48	111.27
7	E	202	BCL	OBB-CAB-CBB	-2.37	114.85	120.17
7	j	302	BCL	C16-C15-C13	2.36	123.55	115.92
7	b	102	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
7	t	101	BCL	C1C-NC-C4C	2.36	107.77	106.71
8	X	201	SPO	C14-C15-C16	-2.36	115.86	123.22
8	s	201	SPO	C36-C37-C38	-2.35	119.72	127.75
7	D	202	BCL	C1C-NC-C4C	2.34	107.76	106.71
7	D	202	BCL	OBB-CAB-CBB	-2.34	114.90	120.17
8	F	102	SPO	C40-C38-C39	2.34	119.77	114.60
8	N	201	SPO	C6-C7-C9	-2.34	115.35	118.94
10	L	306	BPH	CMB-C2B-C3B	2.34	129.05	124.68
9	M	405	U10	C4M-O4-C4	2.34	124.74	116.47
9	L	305	U10	C7-C8-C9	-2.33	122.91	126.79
7	t	103	BCL	C1C-NC-C4C	2.32	107.75	106.71
7	j	303	BCL	OBB-CAB-CBB	-2.32	114.94	120.17
7	O	101	BCL	C4A-NA-C1A	2.32	107.75	106.71
7	g	101	BCL	O2D-CGD-O1D	-2.32	119.31	123.84
8	r	102	SPO	C40-C38-C39	2.31	119.71	114.60
8	F	102	SPO	C18-C17-C19	-2.31	119.68	122.92
8	r	102	SPO	C11-C12-C14	2.31	122.49	118.94
7	N	202	BCL	C1C-NC-C4C	2.31	107.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	402	BCL	CED-O2D-CGD	2.31	121.16	115.94
7	O	101	BCL	C1-C2-C3	2.31	130.03	126.04
7	j	302	BCL	CED-O2D-CGD	-2.31	110.72	115.94
7	u	101	BCL	OBB-CAB-CBB	-2.30	114.99	120.17
9	L	303	U10	C12-C13-C14	-2.30	122.12	127.66
7	I	101	BCL	C4B-C3B-CAB	-2.30	122.69	127.13
7	R	101	BCL	C4B-C3B-CAB	-2.30	122.69	127.13
7	E	202	BCL	C2A-C1A-CHA	2.30	127.88	123.86
8	I	102	SPO	C24-C23-C22	-2.29	119.71	122.92
7	F	103	BCL	OBB-CAB-CBB	-2.29	115.02	120.17
7	D	202	BCL	O2D-CGD-O1D	-2.28	119.37	123.84
10	L	306	BPH	CBA-CAA-C2A	2.28	120.48	113.81
7	K	101	BCL	C4B-C3B-CAB	-2.28	122.72	127.13
7	i	100	BCL	O2D-CGD-O1D	-2.28	119.38	123.84
7	M	401	BCL	C11-C12-C13	-2.28	108.56	115.92
7	M	401	BCL	OBB-CAB-CBB	-2.27	115.06	120.17
8	D	201	SPO	C26-C25-C23	2.27	132.79	126.42
7	S	101	BCL	C2A-C1A-CHA	2.27	127.82	123.86
8	I	102	SPO	C13-C12-C11	2.27	121.65	118.08
9	L	304	U10	C31-C29-C30	2.27	119.61	114.60
8	g	102	SPO	C8-C7-C6	2.26	121.64	118.08
8	X	201	SPO	O1-C1-C3	-2.26	93.41	108.97
10	L	302	BPH	CMD-C2D-C3D	2.26	128.91	124.68
7	j	302	BCL	C4B-C3B-CAB	-2.26	122.76	127.13
7	e	100	BCL	C4B-C3B-CAB	-2.26	122.77	127.13
7	G	101	BCL	C4A-NA-C1A	2.26	107.72	106.71
9	a	102	U10	C7-C8-C9	-2.26	123.03	126.79
7	G	101	BCL	C4B-C3B-CAB	-2.26	122.77	127.13
7	O	101	BCL	OBB-CAB-CBB	-2.25	115.10	120.17
10	L	302	BPH	CAC-C3C-C2C	-2.25	108.63	114.26
7	j	303	BCL	C4B-C3B-CAB	-2.25	122.78	127.13
8	I	102	SPO	C8-C7-C6	2.25	121.62	118.08
8	F	102	SPO	C13-C12-C11	2.24	121.61	118.08
8	t	102	SPO	C18-C17-C19	-2.24	119.78	122.92
7	b	101	BCL	C4B-C3B-CAB	-2.23	122.81	127.13
7	d	101	BCL	C2D-C1D-ND	2.23	111.75	110.10
9	L	303	U10	C22-C23-C24	-2.22	120.15	127.75
7	L	301	BCL	C4B-C3B-CAB	-2.22	122.83	127.13
7	K	101	BCL	OBB-CAB-CBB	-2.22	115.17	120.17
8	g	102	SPO	C36-C37-C38	-2.22	120.16	127.75
7	R	101	BCL	OBB-CAB-CBB	-2.22	115.17	120.17
8	t	102	SPO	C6-C7-C9	2.22	122.34	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	101	BCL	O2D-CGD-O1D	-2.21	119.52	123.84
8	N	201	SPO	C36-C37-C38	-2.21	120.20	127.75
9	a	102	U10	C37-C38-C39	-2.21	120.21	127.75
10	M	403	BPH	CMD-C2D-C3D	2.20	128.80	124.68
8	j	301	SPO	C20-C21-C22	2.20	127.99	123.47
7	M	402	BCL	C6-C7-C8	-2.20	108.80	115.92
8	D	201	SPO	C13-C12-C11	2.20	121.54	118.08
7	a	101	BCL	OBB-CAB-CBB	-2.19	115.23	120.17
7	G	101	BCL	OBB-CAB-CBB	-2.19	115.23	120.17
7	K	101	BCL	C1C-NC-C4C	2.18	107.69	106.71
7	G	101	BCL	O2D-CGD-O1D	-2.17	119.59	123.84
7	k	101	BCL	C1C-NC-C4C	2.17	107.68	106.71
8	j	301	SPO	C36-C37-C38	-2.17	120.35	127.75
8	X	201	SPO	C36-C37-C38	-2.16	120.37	127.75
9	L	304	U10	C25-C24-C23	-2.16	118.15	123.68
7	M	401	BCL	C1-C2-C3	-2.15	122.32	126.04
9	L	304	U10	C20-C19-C18	-2.15	118.17	123.68
7	M	402	BCL	C4B-C3B-CAB	-2.14	122.99	127.13
7	b	102	BCL	C2A-C1A-CHA	2.14	127.60	123.86
7	t	103	BCL	OBB-CAB-CBB	-2.14	115.35	120.17
8	t	102	SPO	C1-C4-C5	-2.14	107.38	113.06
7	b	102	BCL	OBB-CAB-CBB	-2.14	115.35	120.17
8	t	102	SPO	C11-C12-C14	2.14	122.22	118.94
7	R	101	BCL	O2D-CGD-O1D	-2.14	119.66	123.84
7	t	103	BCL	C4B-C3B-CAB	-2.14	123.00	127.13
8	j	301	SPO	C13-C12-C14	-2.14	119.93	122.92
7	i	100	BCL	C4B-C3B-CAB	-2.13	123.01	127.13
9	M	405	U10	O5-C5-C6	-2.13	117.82	121.55
9	L	304	U10	C27-C28-C29	-2.13	120.47	127.75
8	r	102	SPO	C29-C28-C27	-2.13	117.11	122.59
8	E	201	SPO	C14-C15-C16	2.13	129.85	123.22
8	I	102	SPO	C14-C15-C16	-2.12	116.59	123.22
8	M	406	SPO	C40-C38-C39	2.12	119.30	114.60
12	H	302	3PE	C2-O21-C21	-2.12	112.56	117.79
7	n	100	BCL	C2D-C1D-ND	2.12	111.67	110.10
7	j	302	BCL	O2D-CGD-O1D	-2.12	119.70	123.84
7	L	301	BCL	CED-O2D-CGD	2.11	120.71	115.94
8	E	201	SPO	C34-C33-C32	-2.11	118.27	123.68
7	t	101	BCL	C4B-C3B-CAB	-2.11	123.06	127.13
8	g	102	SPO	C26-C25-C23	-2.11	120.49	126.42
9	a	102	U10	O5-C5-C4	-2.11	116.46	120.93
7	G	101	BCL	C16-C15-C13	-2.10	109.11	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	202	BCL	C4B-C3B-CAB	-2.10	123.07	127.13
7	b	101	BCL	C1C-NC-C4C	2.10	107.65	106.71
7	A	101	BCL	O2D-CGD-O1D	-2.10	119.74	123.84
7	g	101	BCL	C4B-C3B-CAB	-2.10	123.08	127.13
7	M	401	BCL	C4A-NA-C1A	2.09	107.65	106.71
7	j	303	BCL	C4-C3-C5	-2.09	111.75	115.27
8	X	201	SPO	C20-C21-C22	-2.09	119.20	123.47
7	A	101	BCL	OBB-CAB-CBB	-2.09	115.47	120.17
8	t	102	SPO	C8-C7-C9	-2.08	120.00	122.92
8	M	406	SPO	C36-C37-C38	-2.07	120.68	127.75
7	j	302	BCL	C1C-NC-C4C	2.07	107.64	106.71
8	r	103	SPO	C13-C12-C11	2.07	121.33	118.08
7	S	101	BCL	OBB-CAB-CBB	-2.07	115.52	120.17
8	X	201	SPO	C29-C28-C30	2.06	118.74	115.27
7	a	101	BCL	C11-C10-C8	-2.06	109.26	115.92
8	s	201	SPO	C1-C4-C5	2.06	118.52	113.06
8	I	102	SPO	C40-C38-C39	2.06	119.15	114.60
8	k	102	SPO	C36-C37-C38	-2.06	120.72	127.75
8	r	102	SPO	C20-C21-C22	2.05	127.68	123.47
7	r	101	BCL	C2D-C1D-ND	2.05	111.62	110.10
8	s	201	SPO	C34-C33-C35	2.05	118.72	115.27
7	t	101	BCL	C6-C5-C3	2.04	118.81	113.45
7	E	202	BCL	C4B-C3B-CAB	-2.04	123.18	127.13
8	k	102	SPO	C10-C11-C12	-2.04	120.68	126.42
7	M	402	BCL	CHD-C1D-C2D	2.04	129.76	125.48
8	s	201	SPO	C29-C28-C30	2.04	118.70	115.27
7	t	101	BCL	O2D-CGD-O1D	-2.04	119.86	123.84
8	s	201	SPO	C26-C25-C23	-2.03	120.70	126.42
8	r	102	SPO	C34-C33-C32	-2.03	118.46	123.68
8	M	406	SPO	C1-C4-C5	-2.03	107.69	113.06
8	I	102	SPO	C9-C10-C11	-2.03	116.89	123.22
7	b	101	BCL	C17-C16-C15	-2.03	103.93	113.24
8	F	102	SPO	C13-C12-C14	-2.03	120.09	122.92
7	s	202	BCL	C6-C7-C8	2.02	122.45	115.92
8	N	201	SPO	C10-C11-C12	-2.02	120.74	126.42
7	F	103	BCL	C4B-C3B-CAB	-2.02	123.23	127.13
8	g	102	SPO	C6-C7-C9	-2.02	115.85	118.94
7	M	407	BCL	C4B-C3B-CAB	-2.01	123.24	127.13
9	a	102	U10	C22-C23-C24	-2.01	122.82	127.66
7	o	100	BCL	C6-C5-C3	2.01	118.73	113.45
7	u	101	BCL	C4D-C3D-CAD	-2.01	105.73	108.10
7	n	100	BCL	C4B-C3B-CAB	-2.01	123.25	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	103	BCL	O2D-CGD-O1D	-2.01	119.92	123.84
8	B	101	SPO	C30-C31-C32	-2.01	105.29	111.88
8	B	101	SPO	C18-C17-C16	2.01	121.24	118.08
7	u	102	BCL	OBB-CAB-CBB	-2.01	115.66	120.17
7	D	202	BCL	C4B-C3B-CAB	-2.00	123.26	127.13
8	D	201	SPO	C27-C26-C25	2.00	129.47	123.22
7	u	101	BCL	C2D-C1D-ND	2.00	111.58	110.10

There are no chirality outliers.

All (611) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	202	BCL	C2-C1-O2A-CGA
7	O	101	BCL	O2A-C1-C2-C3
7	b	101	BCL	C2-C1-O2A-CGA
7	u	102	BCL	C1A-C2A-CAA-CBA
7	u	102	BCL	O2A-C1-C2-C3
7	R	101	BCL	C1A-C2A-CAA-CBA
7	n	100	BCL	C2-C3-C5-C6
7	n	100	BCL	C4-C3-C5-C6
7	G	101	BCL	C1A-C2A-CAA-CBA
8	N	201	SPO	C4-C1-O1-CM1
8	N	201	SPO	O1-C1-C4-C5
8	N	201	SPO	C2-C1-C4-C5
8	N	201	SPO	C1-C4-C5-C6
8	N	201	SPO	C5-C6-C7-C8
8	N	201	SPO	C5-C6-C7-C9
8	N	201	SPO	C11-C10-C9-C7
8	N	201	SPO	C10-C11-C12-C13
8	N	201	SPO	C27-C28-C30-C31
8	N	201	SPO	C29-C28-C30-C31
8	t	102	SPO	C3-C1-C4-C5
8	t	102	SPO	C15-C16-C17-C18
8	t	102	SPO	C15-C16-C17-C19
8	t	102	SPO	C22-C23-C25-C26
8	t	102	SPO	C24-C23-C25-C26
8	t	102	SPO	C25-C26-C27-C28
8	t	102	SPO	C33-C35-C36-C37
8	r	102	SPO	C3-C1-O1-CM1
8	r	102	SPO	O1-C1-C4-C5
8	r	102	SPO	C10-C11-C12-C13
8	r	102	SPO	C10-C11-C12-C14

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Mol	Chain	Res	Type	Atoms
8	r	102	SPO	C12-C14-C15-C16
8	r	102	SPO	C20-C21-C22-C23
8	r	102	SPO	C22-C23-C25-C26
8	r	102	SPO	C24-C23-C25-C26
8	r	103	SPO	C4-C1-O1-CM1
8	r	103	SPO	C3-C1-C4-C5
8	r	103	SPO	C5-C6-C7-C8
8	r	103	SPO	C5-C6-C7-C9
8	r	103	SPO	C10-C11-C12-C13
8	r	103	SPO	C10-C11-C12-C14
8	D	201	SPO	C2-C1-C4-C5
8	D	201	SPO	C3-C1-C4-C5
8	D	201	SPO	C1-C4-C5-C6
8	D	201	SPO	C5-C6-C7-C8
8	D	201	SPO	C5-C6-C7-C9
8	k	102	SPO	C2-C1-C4-C5
8	k	102	SPO	C3-C1-C4-C5
8	k	102	SPO	C1-C4-C5-C6
8	k	102	SPO	C5-C6-C7-C8
8	k	102	SPO	C5-C6-C7-C9
8	k	102	SPO	C11-C10-C9-C7
8	k	102	SPO	C10-C11-C12-C13
8	k	102	SPO	C10-C11-C12-C14
8	k	102	SPO	C15-C16-C17-C18
8	k	102	SPO	C15-C16-C17-C19
8	k	102	SPO	C22-C23-C25-C26
8	k	102	SPO	C24-C23-C25-C26
8	E	201	SPO	C15-C16-C17-C18
8	E	201	SPO	C15-C16-C17-C19
8	E	201	SPO	C20-C21-C22-C23
8	E	201	SPO	C33-C35-C36-C37
8	X	201	SPO	C4-C1-O1-CM1
8	X	201	SPO	C3-C1-C4-C5
8	X	201	SPO	C1-C4-C5-C6
8	X	201	SPO	C10-C11-C12-C13
8	X	201	SPO	C27-C28-C30-C31
8	X	201	SPO	C29-C28-C30-C31
8	X	201	SPO	C33-C35-C36-C37
8	s	201	SPO	C4-C1-O1-CM1
8	s	201	SPO	O1-C1-C4-C5
8	s	201	SPO	C5-C6-C7-C8
8	s	201	SPO	C5-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
8	s	201	SPO	C17-C19-C20-C21
8	s	201	SPO	C27-C28-C30-C31
8	s	201	SPO	C29-C28-C30-C31
8	j	301	SPO	C4-C1-O1-CM1
8	j	301	SPO	C2-C1-C4-C5
8	j	301	SPO	C3-C1-C4-C5
8	j	301	SPO	C22-C23-C25-C26
8	j	301	SPO	C24-C23-C25-C26
8	j	301	SPO	C32-C33-C35-C36
8	j	301	SPO	C34-C33-C35-C36
8	I	102	SPO	C4-C1-O1-CM1
8	I	102	SPO	O1-C1-C4-C5
8	I	102	SPO	C1-C4-C5-C6
8	I	102	SPO	C5-C6-C7-C8
8	I	102	SPO	C5-C6-C7-C9
8	I	102	SPO	C10-C11-C12-C13
8	I	102	SPO	C10-C11-C12-C14
8	I	102	SPO	C15-C16-C17-C18
8	I	102	SPO	C15-C16-C17-C19
8	M	406	SPO	C4-C1-O1-CM1
8	M	406	SPO	C1-C4-C5-C6
8	M	406	SPO	C12-C14-C15-C16
8	M	406	SPO	C15-C16-C17-C18
8	M	406	SPO	C15-C16-C17-C19
8	M	406	SPO	C27-C28-C30-C31
8	M	406	SPO	C29-C28-C30-C31
8	g	102	SPO	C4-C1-O1-CM1
8	g	102	SPO	O1-C1-C4-C5
8	g	102	SPO	C5-C6-C7-C8
8	g	102	SPO	C5-C6-C7-C9
8	g	102	SPO	C15-C16-C17-C18
8	g	102	SPO	C15-C16-C17-C19
8	F	102	SPO	C4-C1-O1-CM1
8	F	102	SPO	C11-C10-C9-C7
8	F	102	SPO	C12-C14-C15-C16
8	B	101	SPO	C5-C6-C7-C8
8	B	101	SPO	C5-C6-C7-C9
8	B	101	SPO	C15-C16-C17-C18
8	B	101	SPO	C15-C16-C17-C19
8	B	101	SPO	C27-C28-C30-C31
8	B	101	SPO	C29-C28-C30-C31
8	B	101	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
8	B	101	SPO	C34-C33-C35-C36
9	a	102	U10	C32-C33-C34-C35
9	a	102	U10	C34-C36-C37-C38
9	L	303	U10	C9-C11-C12-C13
9	L	303	U10	C12-C13-C14-C15
9	L	303	U10	C12-C13-C14-C16
9	L	304	U10	C7-C8-C9-C10
9	L	304	U10	C7-C8-C9-C11
9	L	304	U10	C14-C16-C17-C18
9	L	304	U10	C22-C23-C24-C25
9	L	304	U10	C22-C23-C24-C26
9	L	304	U10	C25-C24-C26-C27
9	L	304	U10	C27-C28-C29-C30
9	L	305	U10	C12-C13-C14-C15
9	L	305	U10	C12-C13-C14-C16
9	L	305	U10	C14-C16-C17-C18
9	M	405	U10	C22-C23-C24-C25
9	M	405	U10	C22-C23-C24-C26
12	H	301	3PE	O32-C31-O31-C3
12	H	301	3PE	C32-C31-O31-C3
12	H	302	3PE	O13-C11-C12-N
12	H	302	3PE	O11-C1-C2-O21
12	d	102	3PE	C1-O11-P-O13
12	d	102	3PE	C11-O13-P-O11
12	d	102	3PE	C11-O13-P-O14
12	d	102	3PE	O22-C21-O21-C2
12	d	102	3PE	C22-C21-O21-C2
9	L	304	U10	C27-C28-C29-C31
9	M	408	U10	C7-C8-C9-C11
7	d	101	BCL	C3-C5-C6-C7
9	L	305	U10	C17-C18-C19-C21
9	M	408	U10	C7-C8-C9-C10
12	H	302	3PE	O32-C31-O31-C3
7	b	101	BCL	C4-C3-C5-C6
7	k	101	BCL	C4-C3-C5-C6
7	G	101	BCL	C4-C3-C5-C6
7	I	101	BCL	C4-C3-C5-C6
9	M	405	U10	C35-C34-C36-C37
7	t	103	BCL	C2A-CAA-CBA-CGA
7	O	101	BCL	C2A-CAA-CBA-CGA
7	E	202	BCL	C2A-CAA-CBA-CGA
7	F	103	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	M	405	U10	C17-C18-C19-C20
9	a	102	U10	C32-C33-C34-C36
9	M	405	U10	C17-C18-C19-C21
8	r	103	SPO	C25-C26-C27-C28
8	E	201	SPO	C17-C19-C20-C21
8	s	201	SPO	C12-C14-C15-C16
8	s	201	SPO	C20-C21-C22-C23
8	j	301	SPO	C11-C10-C9-C7
8	j	301	SPO	C20-C21-C22-C23
8	I	102	SPO	C17-C19-C20-C21
8	g	102	SPO	C12-C14-C15-C16
8	g	102	SPO	C20-C21-C22-C23
8	F	102	SPO	C25-C26-C27-C28
12	H	302	3PE	C32-C31-O31-C3
9	L	305	U10	C17-C18-C19-C20
7	o	100	BCL	C4-C3-C5-C6
7	j	302	BCL	C4-C3-C5-C6
7	d	101	BCL	C4-C3-C5-C6
8	D	201	SPO	C34-C33-C35-C36
8	X	201	SPO	C34-C33-C35-C36
8	M	406	SPO	C34-C33-C35-C36
7	o	100	BCL	C2-C3-C5-C6
7	k	101	BCL	C2-C3-C5-C6
7	G	101	BCL	C2-C3-C5-C6
7	j	302	BCL	C2-C3-C5-C6
7	d	101	BCL	C2-C3-C5-C6
8	D	201	SPO	C32-C33-C35-C36
8	X	201	SPO	C32-C33-C35-C36
8	M	406	SPO	C32-C33-C35-C36
9	L	304	U10	C23-C24-C26-C27
7	S	101	BCL	C2A-CAA-CBA-CGA
7	A	101	BCL	C2A-CAA-CBA-CGA
8	D	201	SPO	C28-C30-C31-C32
8	D	201	SPO	C33-C35-C36-C37
8	k	102	SPO	C28-C30-C31-C32
8	k	102	SPO	C33-C35-C36-C37
8	X	201	SPO	C28-C30-C31-C32
8	M	406	SPO	C33-C35-C36-C37
9	L	303	U10	C14-C16-C17-C18
9	M	405	U10	C19-C21-C22-C23
12	H	301	3PE	C28-C29-C2A-C2B
8	t	102	SPO	C11-C10-C9-C7

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Mol	Chain	Res	Type	Atoms
8	t	102	SPO	C12-C14-C15-C16
8	t	102	SPO	C17-C19-C20-C21
8	r	102	SPO	C25-C26-C27-C28
9	M	405	U10	C33-C34-C36-C37
7	r	101	BCL	C11-C12-C13-C14
7	O	101	BCL	C6-C7-C8-C9
7	K	101	BCL	C6-C7-C8-C9
7	i	100	BCL	C11-C12-C13-C14
7	j	303	BCL	C6-C7-C8-C9
10	M	403	BPH	C11-C12-C13-C14
8	r	102	SPO	C15-C16-C17-C18
8	r	103	SPO	C15-C16-C17-C18
8	X	201	SPO	C5-C6-C7-C8
8	s	201	SPO	C15-C16-C17-C18
8	M	406	SPO	C10-C11-C12-C13
8	g	102	SPO	C10-C11-C12-C13
8	g	102	SPO	C24-C23-C25-C26
8	N	201	SPO	C10-C11-C12-C14
8	X	201	SPO	C5-C6-C7-C9
8	s	201	SPO	C15-C16-C17-C19
8	j	301	SPO	C5-C6-C7-C9
8	M	406	SPO	C10-C11-C12-C14
8	g	102	SPO	C10-C11-C12-C14
8	g	102	SPO	C22-C23-C25-C26
12	H	301	3PE	C34-C35-C36-C37
7	O	101	BCL	C10-C11-C12-C13
7	L	301	BCL	C15-C16-C17-C18
9	L	304	U10	C17-C18-C19-C20
7	M	402	BCL	C15-C16-C17-C18
8	r	103	SPO	C11-C10-C9-C7
8	k	102	SPO	C12-C14-C15-C16
8	B	101	SPO	C11-C10-C9-C7
8	s	201	SPO	C28-C30-C31-C32
8	g	102	SPO	C28-C30-C31-C32
9	a	102	U10	C14-C16-C17-C18
7	M	402	BCL	C5-C6-C7-C8
12	H	302	3PE	C38-C39-C3A-C3B
12	d	102	3PE	C2D-C2E-C2F-C2G
7	a	101	BCL	C13-C15-C16-C17
7	F	101	BCL	C4-C3-C5-C6
9	L	304	U10	C20-C19-C21-C22
7	o	100	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
7	b	102	BCL	C2A-CAA-CBA-CGA
10	L	306	BPH	C2A-CAA-CBA-CGA
8	r	103	SPO	C17-C19-C20-C21
8	s	201	SPO	C25-C26-C27-C28
8	j	301	SPO	C12-C14-C15-C16
8	I	102	SPO	C11-C10-C9-C7
8	g	102	SPO	C25-C26-C27-C28
12	H	302	3PE	C3E-C3F-C3G-C3H
7	j	303	BCL	C10-C11-C12-C13
12	H	301	3PE	C2B-C2C-C2D-C2E
12	H	302	3PE	C37-C38-C39-C3A
12	H	301	3PE	C32-C33-C34-C35
12	H	301	3PE	C35-C36-C37-C38
12	H	301	3PE	C37-C38-C39-C3A
12	H	302	3PE	C3C-C3D-C3E-C3F
12	H	302	3PE	C3D-C3E-C3F-C3G
12	d	102	3PE	C35-C36-C37-C38
12	H	302	3PE	O21-C2-C3-O31
8	F	102	SPO	C34-C33-C35-C36
12	H	302	3PE	C35-C36-C37-C38
7	I	101	BCL	C2-C3-C5-C6
7	s	202	BCL	C11-C10-C8-C9
7	n	100	BCL	C11-C12-C13-C14
12	d	102	3PE	C2B-C2C-C2D-C2E
7	M	401	BCL	C13-C15-C16-C17
7	R	101	BCL	C2A-CAA-CBA-CGA
8	s	201	SPO	C24-C23-C25-C26
8	j	301	SPO	C5-C6-C7-C8
8	j	301	SPO	C10-C11-C12-C13
12	d	102	3PE	C27-C28-C29-C2A
8	X	201	SPO	C10-C11-C12-C14
8	s	201	SPO	C22-C23-C25-C26
8	j	301	SPO	C10-C11-C12-C14
12	H	301	3PE	C2A-C2B-C2C-C2D
9	a	102	U10	C24-C26-C27-C28
12	H	301	3PE	C33-C34-C35-C36
12	H	302	3PE	C24-C25-C26-C27
12	d	102	3PE	C32-C31-O31-C3
12	H	301	3PE	C26-C27-C28-C29
7	o	100	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	C3A-C2A-CAA-CBA
7	D	202	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	u	102	BCL	C3A-C2A-CAA-CBA
7	R	101	BCL	C3A-C2A-CAA-CBA
7	G	101	BCL	C3A-C2A-CAA-CBA
7	j	303	BCL	C3A-C2A-CAA-CBA
10	L	302	BPH	C5-C6-C7-C8
8	s	201	SPO	C11-C10-C9-C7
12	H	301	3PE	C24-C25-C26-C27
12	H	302	3PE	C33-C34-C35-C36
12	d	102	3PE	C26-C27-C28-C29
7	D	202	BCL	O2A-C1-C2-C3
7	E	202	BCL	O2A-C1-C2-C3
7	j	303	BCL	O2A-C1-C2-C3
7	F	103	BCL	O2A-C1-C2-C3
7	b	101	BCL	C2-C3-C5-C6
8	F	102	SPO	C32-C33-C35-C36
9	L	303	U10	C12-C11-C9-C8
12	H	302	3PE	C2A-C2B-C2C-C2D
7	M	402	BCL	C2-C1-O2A-CGA
12	H	302	3PE	C23-C24-C25-C26
12	H	302	3PE	C28-C29-C2A-C2B
12	H	301	3PE	C39-C3A-C3B-C3C
7	R	101	BCL	C4-C3-C5-C6
9	L	303	U10	C12-C11-C9-C10
10	L	302	BPH	C4-C3-C5-C6
7	t	103	BCL	C12-C13-C15-C16
7	b	101	BCL	C11-C12-C13-C15
7	s	202	BCL	C11-C10-C8-C7
10	L	302	BPH	C2-C3-C5-C6
10	M	403	BPH	C11-C12-C13-C15
10	M	403	BPH	C12-C13-C15-C16
12	d	102	3PE	O32-C31-O31-C3
7	t	103	BCL	C13-C15-C16-C17
7	o	100	BCL	C8-C10-C11-C12
7	K	101	BCL	C10-C11-C12-C13
12	H	302	3PE	C39-C3A-C3B-C3C
12	H	302	3PE	C22-C21-O21-C2
7	u	102	BCL	C4-C3-C5-C6
7	F	101	BCL	C2-C3-C5-C6
9	L	304	U10	C18-C19-C21-C22
12	H	302	3PE	C25-C26-C27-C28
7	t	103	BCL	C14-C13-C15-C16
7	b	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	L	301	BCL	C2A-CAA-CBA-CGA
8	F	102	SPO	C10-C11-C12-C13
8	r	102	SPO	C15-C16-C17-C19
8	F	102	SPO	C10-C11-C12-C14
7	o	100	BCL	C1A-C2A-CAA-CBA
7	D	202	BCL	C1A-C2A-CAA-CBA
7	j	303	BCL	C1A-C2A-CAA-CBA
7	M	407	BCL	C8-C10-C11-C12
12	H	302	3PE	C21-C22-C23-C24
9	M	408	U10	C6-C7-C8-C9
12	H	302	3PE	O11-C1-C2-C3
8	r	102	SPO	C1-C4-C5-C6
8	j	301	SPO	C1-C4-C5-C6
12	d	102	3PE	C28-C29-C2A-C2B
7	s	202	BCL	C10-C11-C12-C13
12	H	302	3PE	C22-C23-C24-C25
9	a	102	U10	C1-C6-C7-C8
12	H	301	3PE	C3D-C3E-C3F-C3G
9	M	405	U10	C30-C29-C31-C32
9	L	303	U10	C5-C6-C7-C8
9	M	408	U10	C5-C6-C7-C8
8	r	102	SPO	C2-C1-O1-CM1
8	D	201	SPO	C2-C1-O1-CM1
8	D	201	SPO	C3-C1-O1-CM1
8	k	102	SPO	C2-C1-O1-CM1
8	k	102	SPO	C3-C1-O1-CM1
8	E	201	SPO	C2-C1-O1-CM1
8	E	201	SPO	C3-C1-O1-CM1
8	X	201	SPO	C3-C1-O1-CM1
8	M	406	SPO	C2-C1-O1-CM1
8	M	406	SPO	C3-C1-O1-CM1
8	F	102	SPO	C2-C1-O1-CM1
8	B	101	SPO	C3-C1-O1-CM1
12	H	302	3PE	O22-C21-O21-C2
8	E	201	SPO	C2-C1-C4-C5
8	M	406	SPO	C3-C1-C4-C5
12	H	301	3PE	C2E-C2F-C2G-C2H
7	N	202	BCL	C11-C10-C8-C7
7	R	101	BCL	C12-C13-C15-C16
7	I	101	BCL	C11-C10-C8-C7
7	u	102	BCL	C13-C15-C16-C17
8	t	102	SPO	O1-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
8	r	103	SPO	O1-C1-C4-C5
8	E	201	SPO	O1-C1-C4-C5
8	M	406	SPO	O1-C1-C4-C5
7	a	101	BCL	C10-C11-C12-C13
7	b	101	BCL	C8-C10-C11-C12
7	I	101	BCL	C15-C16-C17-C18
7	D	202	BCL	C10-C11-C12-C13
8	t	102	SPO	C28-C30-C31-C32
8	r	103	SPO	C33-C35-C36-C37
8	B	101	SPO	C33-C35-C36-C37
9	L	304	U10	C24-C26-C27-C28
7	r	101	BCL	C4-C3-C5-C6
9	a	102	U10	C35-C34-C36-C37
9	M	405	U10	C28-C29-C31-C32
7	I	101	BCL	C3A-C2A-CAA-CBA
12	H	302	3PE	C1-C2-C3-O31
7	t	103	BCL	O2A-C1-C2-C3
7	R	101	BCL	O2A-C1-C2-C3
7	I	101	BCL	O2A-C1-C2-C3
8	D	201	SPO	C29-C28-C30-C31
9	L	303	U10	C15-C14-C16-C17
12	d	102	3PE	C36-C37-C38-C39
8	E	201	SPO	C12-C14-C15-C16
7	M	407	BCL	C14-C13-C15-C16
7	L	301	BCL	C4C-C3C-CAC-CBC
7	M	401	BCL	C4C-C3C-CAC-CBC
8	r	103	SPO	C15-C16-C17-C19
12	H	301	3PE	O22-C21-O21-C2
7	G	101	BCL	C3-C5-C6-C7
7	t	101	BCL	C11-C10-C8-C7
9	a	102	U10	C33-C34-C36-C37
8	N	201	SPO	C17-C19-C20-C21
8	k	102	SPO	C17-C19-C20-C21
8	k	102	SPO	C25-C26-C27-C28
8	M	406	SPO	C17-C19-C20-C21
7	j	303	BCL	C2A-CAA-CBA-CGA
12	H	301	3PE	C3B-C3C-C3D-C3E
12	H	301	3PE	C31-C32-C33-C34
7	e	100	BCL	CAD-CBD-CGD-O2D
7	b	101	BCL	CAD-CBD-CGD-O2D
7	k	101	BCL	CAD-CBD-CGD-O2D
7	u	101	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
10	M	403	BPH	CAD-CBD-CGD-O2D
12	H	301	3PE	C3-C2-O21-C21
12	H	301	3PE	C22-C21-O21-C2
12	d	102	3PE	O11-C1-C2-O21
12	d	102	3PE	C29-C2A-C2B-C2C
7	E	202	BCL	C11-C12-C13-C14
8	E	201	SPO	C10-C11-C12-C13
8	j	301	SPO	C15-C16-C17-C18
8	F	102	SPO	C5-C6-C7-C8
8	F	102	SPO	C24-C23-C25-C26
8	E	201	SPO	C10-C11-C12-C14
8	F	102	SPO	C5-C6-C7-C9
7	N	202	BCL	C1A-C2A-CAA-CBA
7	O	101	BCL	C1A-C2A-CAA-CBA
7	b	101	BCL	C1A-C2A-CAA-CBA
7	A	101	BCL	C1A-C2A-CAA-CBA
7	I	101	BCL	C1A-C2A-CAA-CBA
12	H	302	3PE	C11-O13-P-O11
9	a	102	U10	C12-C11-C9-C10
7	u	102	BCL	C2-C3-C5-C6
7	R	101	BCL	C2-C3-C5-C6
9	L	303	U10	C13-C14-C16-C17
12	d	102	3PE	C34-C35-C36-C37
10	L	306	BPH	CAD-CBD-CGD-O1D
12	H	302	3PE	C12-C11-O13-P
7	n	100	BCL	C5-C6-C7-C8
7	F	103	BCL	C8-C10-C11-C12
7	j	303	BCL	C3-C5-C6-C7
8	F	102	SPO	C1-C4-C5-C6
12	H	301	3PE	C3E-C3F-C3G-C3H
7	r	101	BCL	C11-C12-C13-C15
7	i	100	BCL	C11-C12-C13-C15
12	H	301	3PE	C1-C2-C3-O31
12	H	301	3PE	O21-C2-C3-O31
7	G	101	BCL	C8-C10-C11-C12
7	t	101	BCL	C11-C10-C8-C9
7	e	100	BCL	C11-C12-C13-C14
7	R	101	BCL	C14-C13-C15-C16
7	i	100	BCL	C14-C13-C15-C16
8	N	201	SPO	C23-C25-C26-C27
8	r	103	SPO	C23-C25-C26-C27
8	D	201	SPO	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
8	k	102	SPO	C23-C25-C26-C27
8	s	201	SPO	C23-C25-C26-C27
8	M	406	SPO	C23-C25-C26-C27
8	g	102	SPO	C23-C25-C26-C27
8	F	102	SPO	C23-C25-C26-C27
12	H	302	3PE	C3B-C3C-C3D-C3E
9	L	304	U10	C5-C4-O4-C4M
12	H	301	3PE	C23-C24-C25-C26
7	K	101	BCL	C2A-CAA-CBA-CGA
7	L	301	BCL	C2-C1-O2A-CGA
9	L	304	U10	C17-C18-C19-C21
7	r	101	BCL	C2-C3-C5-C6
9	a	102	U10	C12-C11-C9-C8
7	D	202	BCL	C2A-CAA-CBA-CGA
8	s	201	SPO	C33-C35-C36-C37
8	j	301	SPO	C3-C1-O1-CM1
8	B	101	SPO	C2-C1-O1-CM1
8	s	201	SPO	C3-C1-C4-C5
8	r	103	SPO	C20-C21-C22-C23
9	L	303	U10	C11-C12-C13-C14
8	D	201	SPO	C27-C28-C30-C31
8	F	102	SPO	C20-C21-C22-C23
8	j	301	SPO	C28-C30-C31-C32
7	A	101	BCL	C10-C11-C12-C13
12	H	301	3PE	C38-C39-C3A-C3B
7	u	101	BCL	C2-C1-O2A-CGA
7	D	202	BCL	C5-C6-C7-C8
7	a	101	BCL	C15-C16-C17-C18
12	H	302	3PE	C31-C32-C33-C34
7	b	101	BCL	C3A-C2A-CAA-CBA
9	L	303	U10	C5-C4-O4-C4M
9	L	305	U10	C5-C4-O4-C4M
7	M	402	BCL	CAA-CBA-CGA-O2A
8	M	406	SPO	C11-C10-C9-C7
7	o	100	BCL	C6-C7-C8-C9
7	S	101	BCL	C6-C7-C8-C9
7	A	101	BCL	C14-C13-C15-C16
7	u	102	BCL	C11-C10-C8-C9
8	N	201	SPO	C21-C22-C23-C24
8	r	103	SPO	C21-C22-C23-C24
8	E	201	SPO	C8-C7-C9-C10
8	E	201	SPO	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	s	201	SPO	C21-C22-C23-C24
8	I	102	SPO	C21-C22-C23-C24
8	M	406	SPO	C21-C22-C23-C24
8	g	102	SPO	C21-C22-C23-C24
8	F	102	SPO	C21-C22-C23-C24
8	B	101	SPO	C13-C12-C14-C15
7	K	101	BCL	O2A-C1-C2-C3
10	L	302	BPH	O2A-C1-C2-C3
7	K	101	BCL	C1A-C2A-CAA-CBA
7	o	100	BCL	C11-C12-C13-C15
7	b	102	BCL	C11-C10-C8-C7
7	E	202	BCL	C11-C10-C8-C7
7	I	101	BCL	C5-C6-C7-C8
7	O	101	BCL	C5-C6-C7-C8
9	M	405	U10	C5-C4-O4-C4M
9	M	408	U10	C5-C4-O4-C4M
8	N	201	SPO	C21-C22-C23-C25
8	r	103	SPO	C21-C22-C23-C25
8	E	201	SPO	C6-C7-C9-C10
8	E	201	SPO	C21-C22-C23-C25
8	s	201	SPO	C21-C22-C23-C25
8	I	102	SPO	C21-C22-C23-C25
8	M	406	SPO	C21-C22-C23-C25
8	g	102	SPO	C21-C22-C23-C25
8	F	102	SPO	C21-C22-C23-C25
8	B	101	SPO	C11-C12-C14-C15
8	D	201	SPO	C12-C14-C15-C16
8	g	102	SPO	C17-C19-C20-C21
8	r	103	SPO	C1-C4-C5-C6
8	E	201	SPO	C1-C4-C5-C6
7	O	101	BCL	C4-C3-C5-C6
7	I	101	BCL	C2-C1-O2A-CGA
12	H	302	3PE	C2D-C2E-C2F-C2G
12	H	301	3PE	C3C-C3D-C3E-C3F
12	H	302	3PE	C27-C28-C29-C2A
7	N	202	BCL	C15-C16-C17-C18
7	e	100	BCL	C4-C3-C5-C6
7	A	101	BCL	C4-C3-C5-C6
9	L	305	U10	C12-C11-C9-C10
7	M	407	BCL	C12-C13-C15-C16
9	M	405	U10	C3-C4-O4-C4M
9	M	408	U10	C3-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
12	d	102	3PE	O31-C31-C32-C33
7	N	202	BCL	C4-C3-C5-C6
8	t	102	SPO	C29-C28-C30-C31
7	o	100	BCL	C11-C12-C13-C14
10	M	403	BPH	C14-C13-C15-C16
7	j	303	BCL	C13-C15-C16-C17
7	N	202	BCL	C3A-C2A-CAA-CBA
7	A	101	BCL	C3A-C2A-CAA-CBA
7	K	101	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	CAA-CBA-CGA-O2A
7	t	101	BCL	CAD-CBD-CGD-O2D
7	s	202	BCL	CAD-CBD-CGD-O2D
7	n	100	BCL	CAD-CBD-CGD-O2D
7	M	402	BCL	CAD-CBD-CGD-O2D
7	M	407	BCL	CAD-CBD-CGD-O2D
7	F	101	BCL	CAD-CBD-CGD-O2D
7	d	101	BCL	CAD-CBD-CGD-O2D
7	t	101	BCL	C2-C1-O2A-CGA
10	M	403	BPH	C2-C1-O2A-CGA
8	k	102	SPO	C34-C33-C35-C36
9	a	102	U10	C30-C29-C31-C32
9	a	102	U10	C5-C4-O4-C4M
7	b	102	BCL	O2A-C1-C2-C3
7	A	101	BCL	O2A-C1-C2-C3
7	N	202	BCL	C2A-CAA-CBA-CGA
10	M	403	BPH	C2A-CAA-CBA-CGA
7	u	101	BCL	CHA-CBD-CGD-O2D
7	A	101	BCL	CAA-CBA-CGA-O2A
12	H	302	3PE	C29-C2A-C2B-C2C
7	r	101	BCL	C8-C10-C11-C12
7	a	101	BCL	CAA-CBA-CGA-O2A
7	F	103	BCL	C4-C3-C5-C6
7	O	101	BCL	C6-C7-C8-C10
7	j	303	BCL	C6-C7-C8-C10
9	L	305	U10	C12-C11-C9-C8
7	b	102	BCL	CAA-CBA-CGA-O2A
8	r	102	SPO	C28-C30-C31-C32
8	N	201	SPO	C25-C26-C27-C28
8	g	102	SPO	C11-C10-C9-C7
9	L	303	U10	C3-C4-O4-C4M
9	L	305	U10	C3-C4-O4-C4M
12	d	102	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
7	F	103	BCL	C10-C11-C12-C13
10	M	403	BPH	C2C-C3C-CAC-CBC
7	M	402	BCL	C13-C15-C16-C17
8	r	102	SPO	C29-C28-C30-C31
8	j	301	SPO	C15-C16-C17-C19
7	t	103	BCL	C1A-C2A-CAA-CBA
7	S	101	BCL	C1A-C2A-CAA-CBA
7	E	202	BCL	C1A-C2A-CAA-CBA
7	b	102	BCL	CAA-CBA-CGA-O1A
7	u	102	BCL	C16-C17-C18-C19
7	A	101	BCL	CAA-CBA-CGA-O1A
7	O	101	BCL	CAA-CBA-CGA-O1A
7	n	100	BCL	C14-C13-C15-C16
7	G	101	BCL	C14-C13-C15-C16
7	j	302	BCL	C11-C10-C8-C9
7	I	101	BCL	C11-C10-C8-C9
7	M	407	BCL	C11-C12-C13-C14
7	F	103	BCL	CAA-CBA-CGA-O2A
7	R	101	BCL	C8-C10-C11-C12
7	R	101	BCL	CAA-CBA-CGA-O2A
8	r	102	SPO	C30-C31-C32-C33
7	M	402	BCL	C4-C3-C5-C6
7	b	101	BCL	C12-C13-C15-C16
7	A	101	BCL	C12-C13-C15-C16
7	K	101	BCL	C6-C7-C8-C10
7	K	101	BCL	C11-C10-C8-C7
7	j	302	BCL	C11-C10-C8-C7
7	L	301	BCL	C2C-C3C-CAC-CBC
7	g	101	BCL	C6-C7-C8-C10
7	o	100	BCL	CAA-CBA-CGA-O2A
7	S	101	BCL	C13-C15-C16-C17
7	a	101	BCL	CAA-CBA-CGA-O1A
7	F	103	BCL	CAA-CBA-CGA-O1A
9	M	405	U10	C29-C31-C32-C33
7	G	101	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

60 monomers are involved in 316 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	X	201	SPO	4	0
7	I	101	BCL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	102	U10	7	0
7	F	101	BCL	7	0
7	N	202	BCL	5	0
7	u	102	BCL	7	0
7	K	101	BCL	3	0
7	F	103	BCL	2	0
8	g	102	SPO	8	0
8	s	201	SPO	16	0
8	I	102	SPO	6	0
12	H	302	3PE	5	0
7	e	100	BCL	5	0
7	n	100	BCL	5	0
7	d	101	BCL	9	0
7	g	101	BCL	8	0
9	L	304	U10	3	0
7	t	101	BCL	7	0
7	u	101	BCL	4	0
7	o	100	BCL	5	0
8	M	406	SPO	13	0
7	j	303	BCL	4	0
8	E	201	SPO	17	0
8	r	103	SPO	10	0
9	L	305	U10	1	0
7	j	302	BCL	2	0
7	A	101	BCL	3	0
7	L	301	BCL	3	0
9	L	303	U10	1	0
7	G	101	BCL	2	0
7	M	407	BCL	6	0
8	B	101	SPO	11	0
12	d	102	3PE	2	0
8	N	201	SPO	12	0
7	M	402	BCL	4	0
10	M	403	BPH	12	0
7	r	101	BCL	8	0
12	H	301	3PE	5	0
8	t	102	SPO	7	0
8	F	102	SPO	12	0
8	D	201	SPO	11	0
7	b	102	BCL	1	0
7	k	101	BCL	3	0
7	b	101	BCL	8	0

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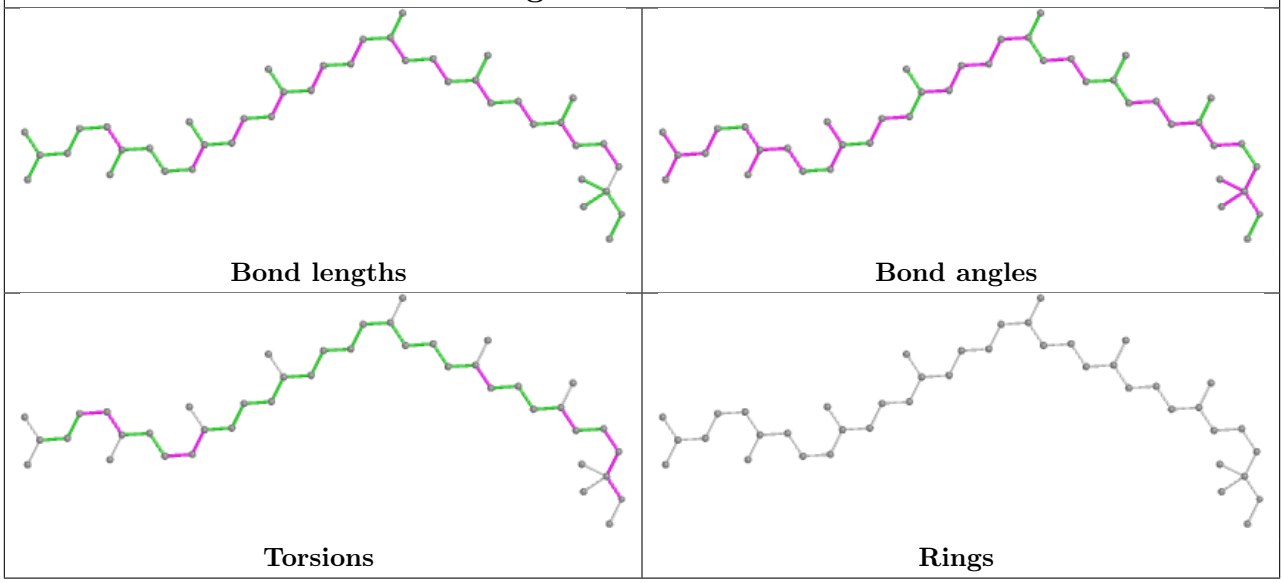
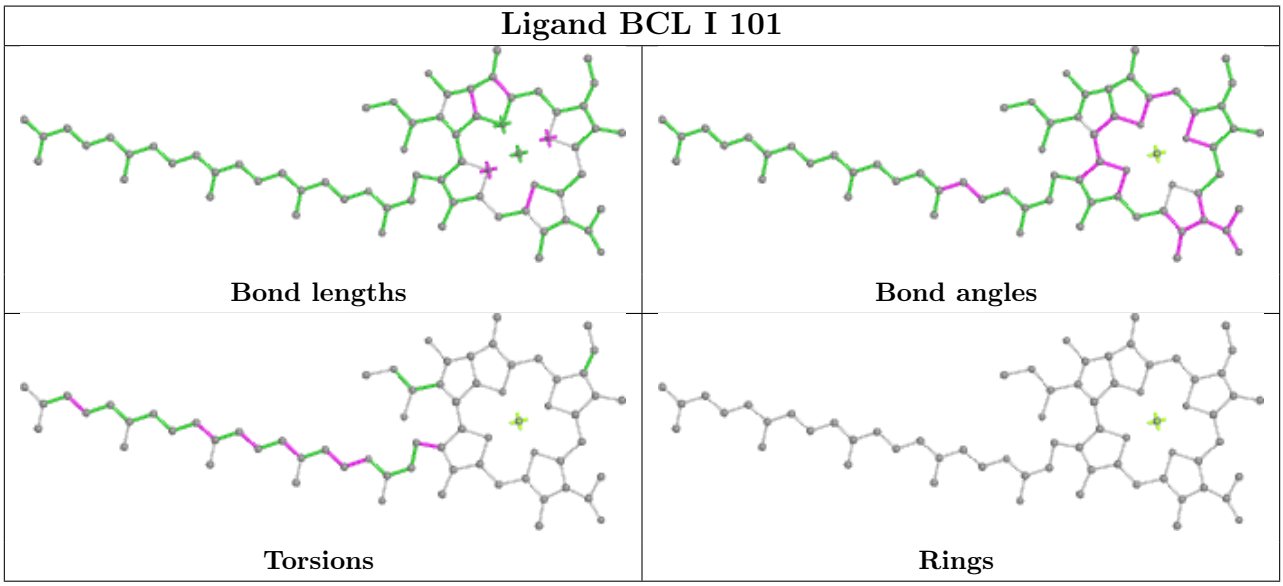
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	j	301	SPO	7	0
7	t	103	BCL	5	0
7	s	202	BCL	5	0
7	M	401	BCL	4	0
10	L	302	BPH	6	0
7	a	101	BCL	2	0
7	D	202	BCL	2	0
7	R	101	BCL	7	0
9	M	408	U10	1	0
10	L	306	BPH	3	0
8	r	102	SPO	10	0
9	M	405	U10	5	0
7	O	101	BCL	3	0
8	k	102	SPO	10	0
7	S	101	BCL	2	0
7	E	202	BCL	3	0

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.

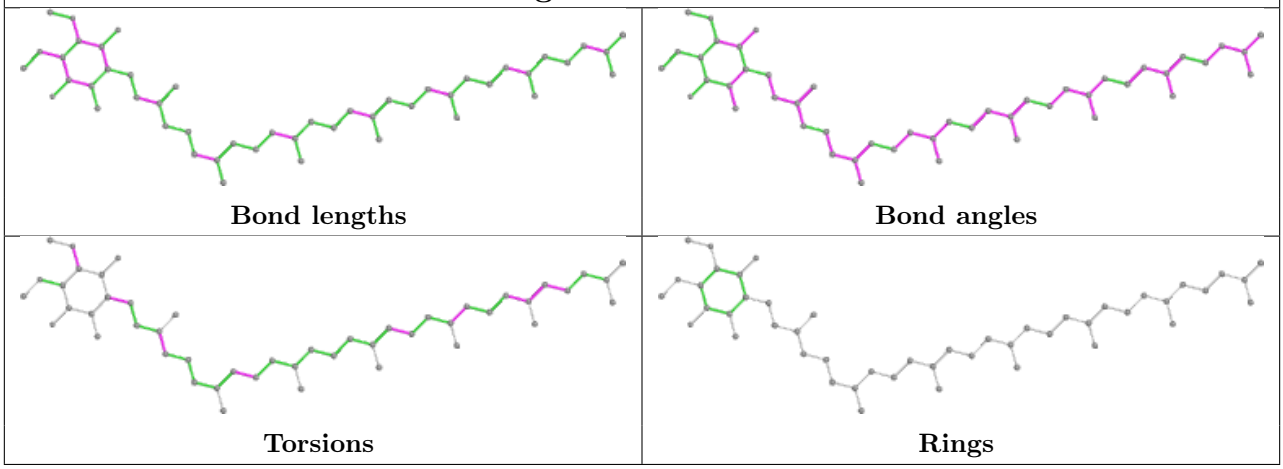
Ligand SPO X 201



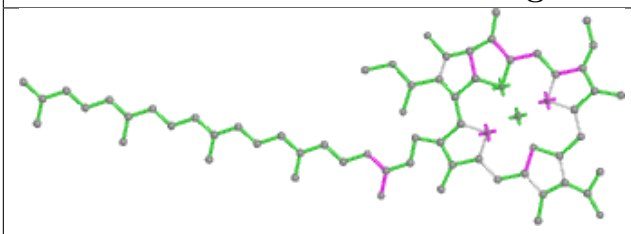
Ligand BCL I 101



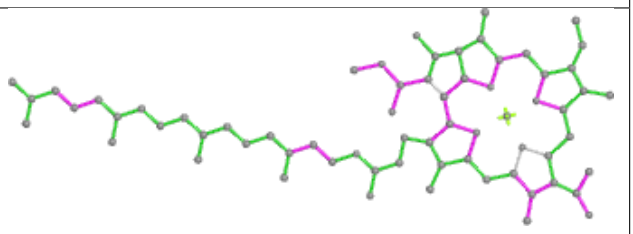
Ligand U10 a 102



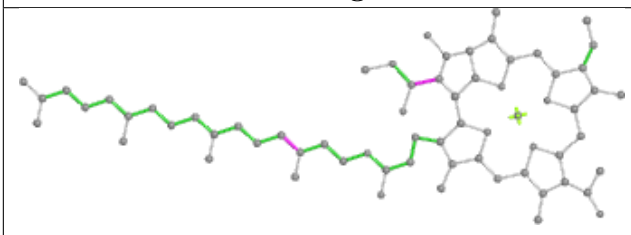
Ligand BCL F 101



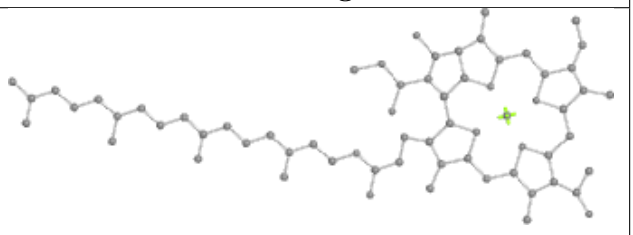
Bond lengths



Bond angles

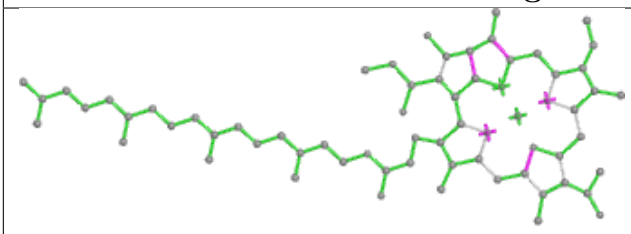


Torsions

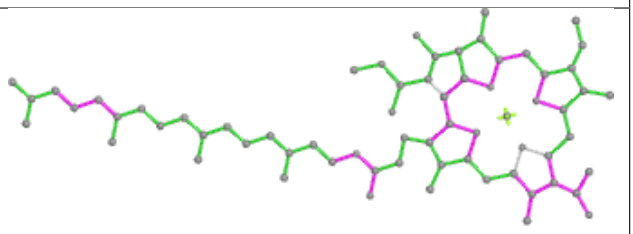


Rings

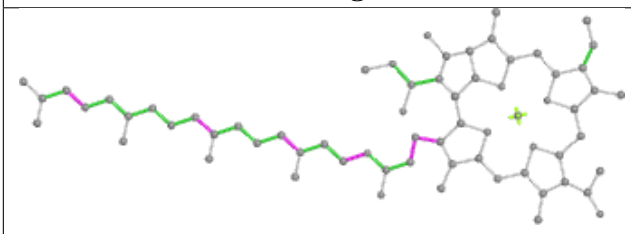
Ligand BCL N 202



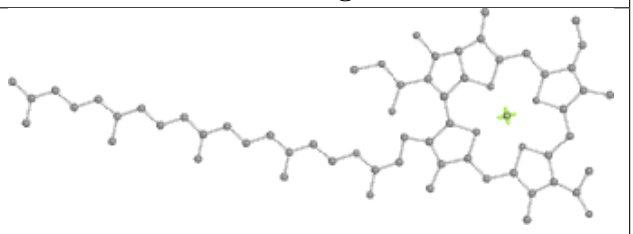
Bond lengths



Bond angles

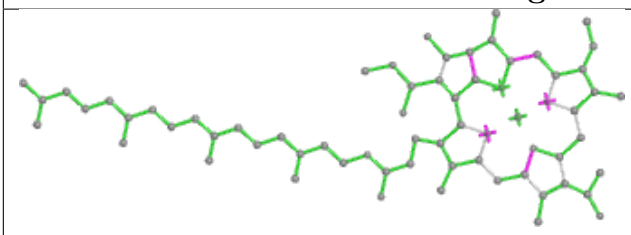


Torsions

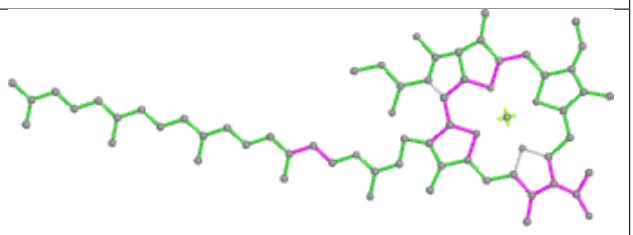


Rings

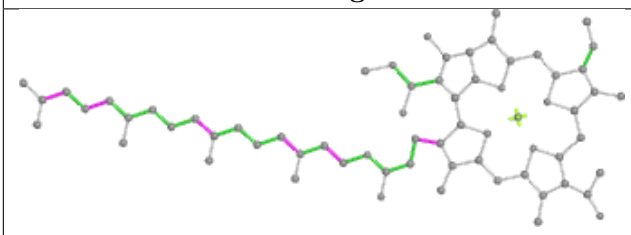
Ligand BCL u 102



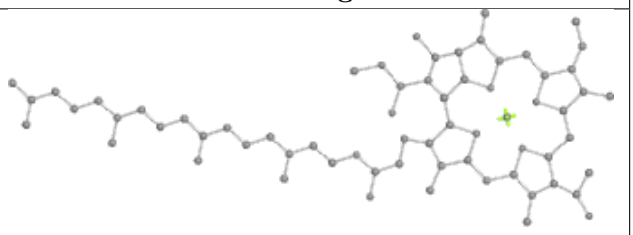
Bond lengths



Bond angles

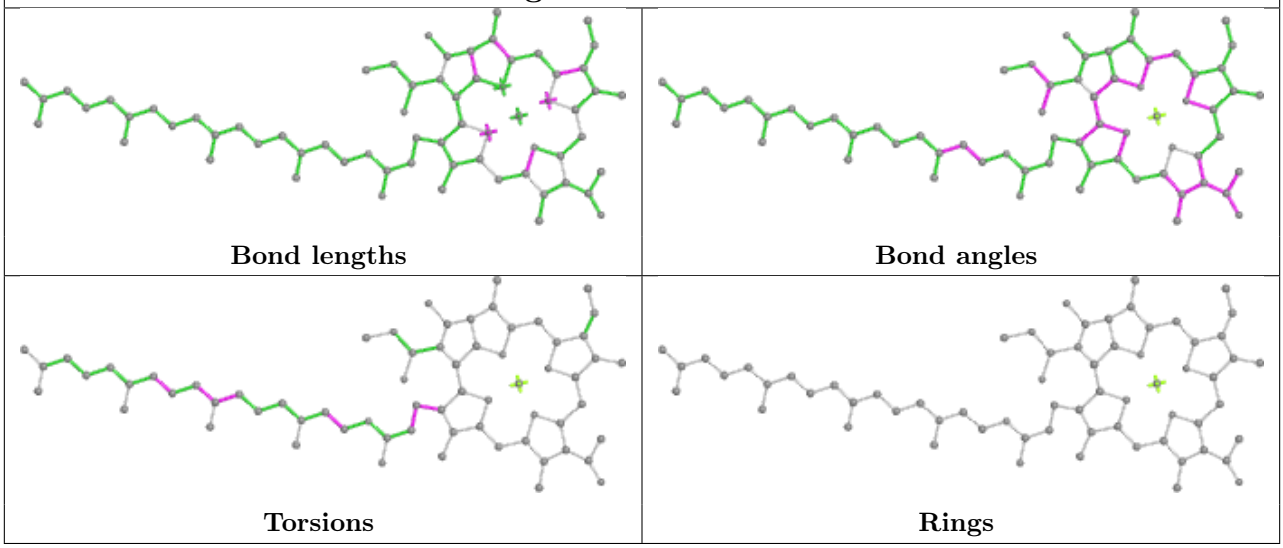


Torsions

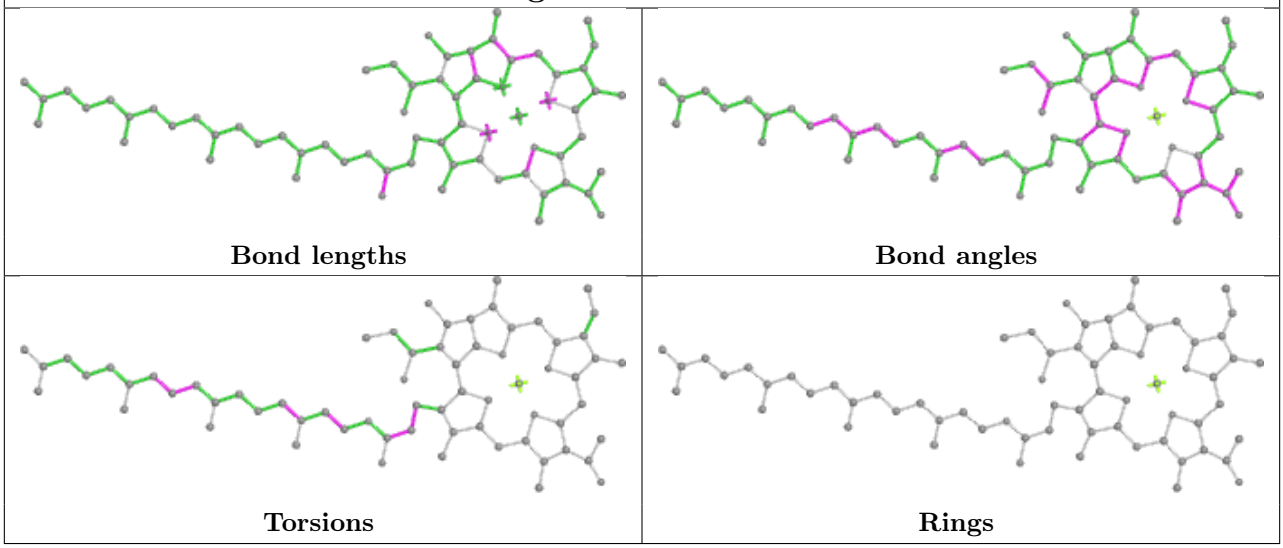


Rings

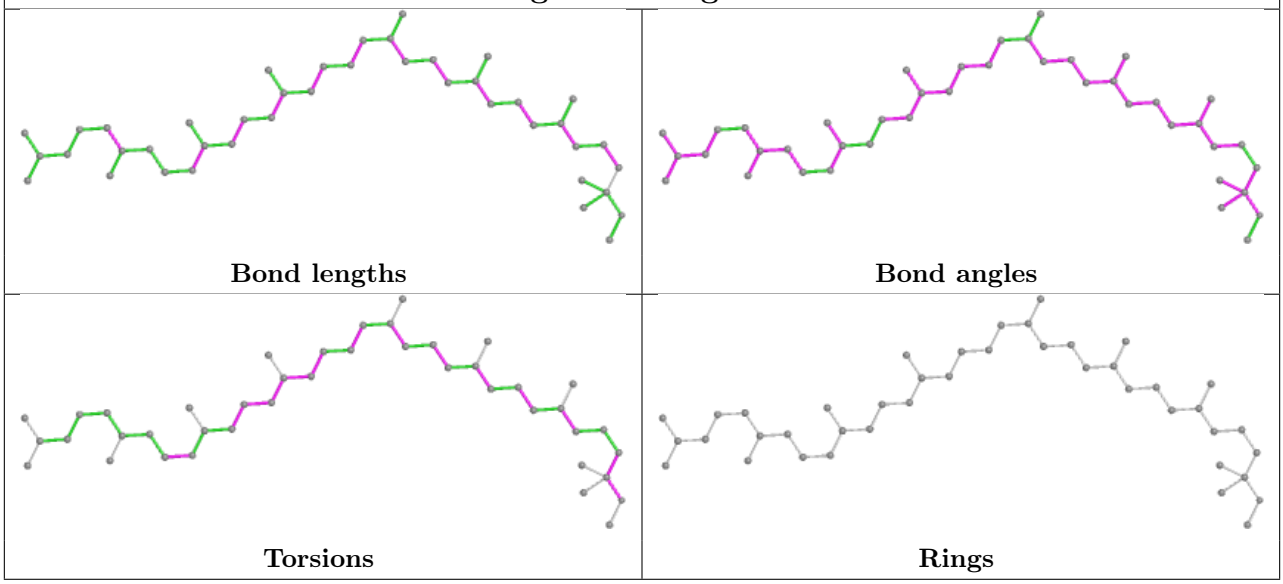
Ligand BCL K 101



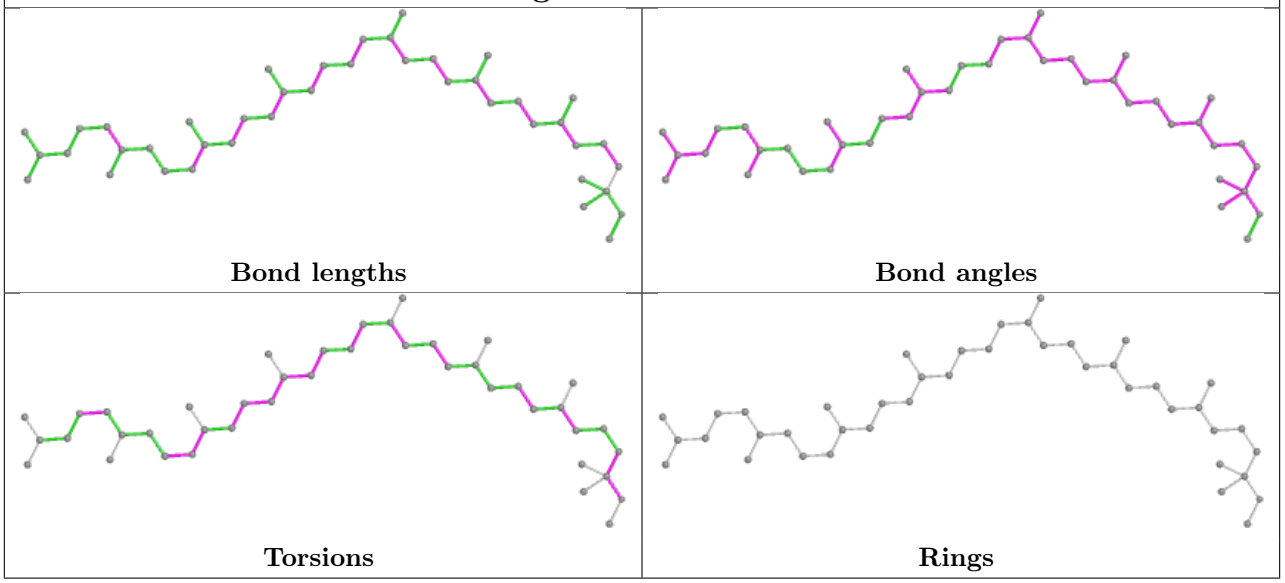
Ligand BCL F 103



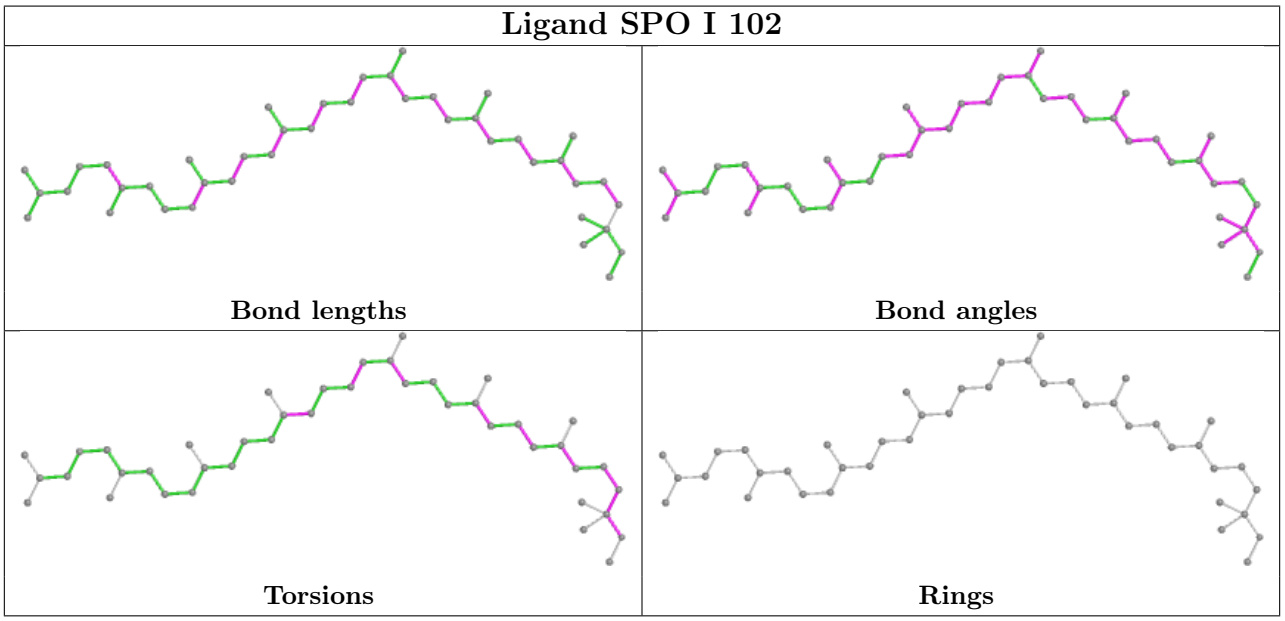
Ligand SPO g 102



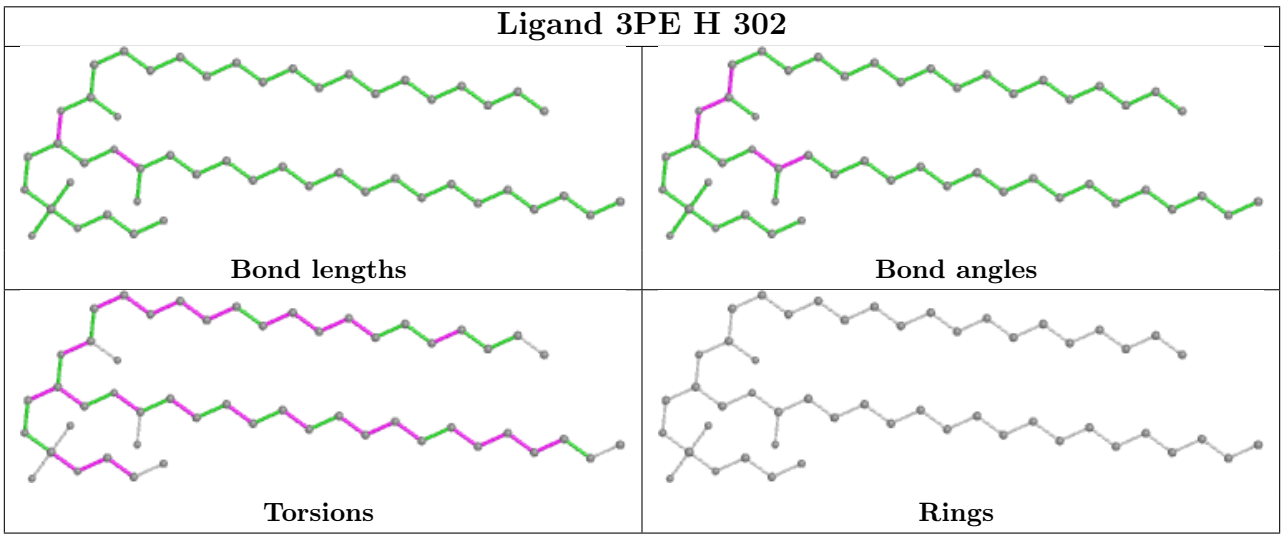
Ligand SPO s 201



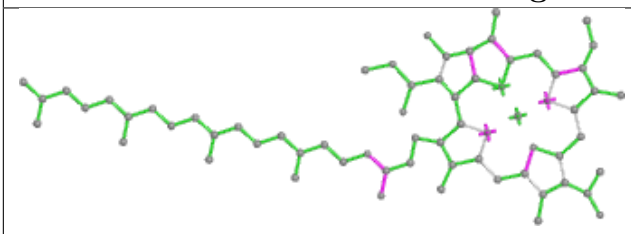
Ligand SPO I 102



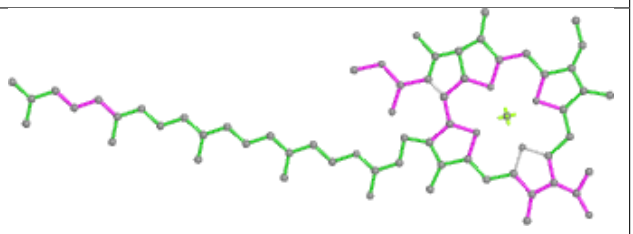
Ligand 3PE H 302



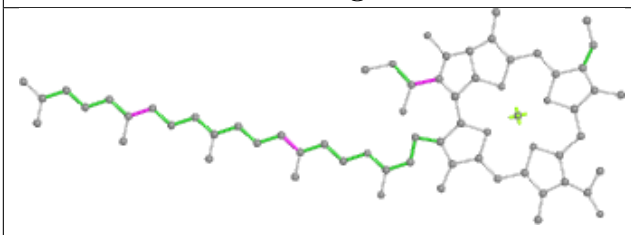
Ligand BCL e 100



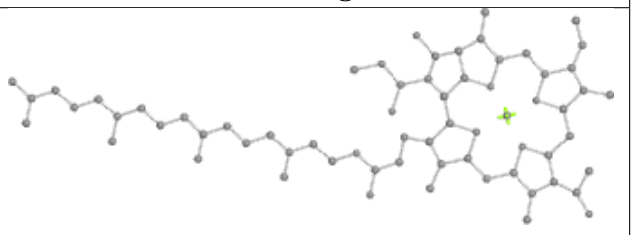
Bond lengths



Bond angles

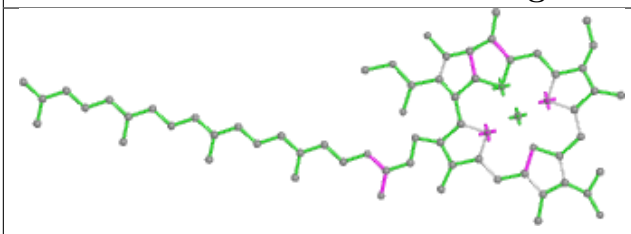


Torsions



Rings

Ligand BCL n 100



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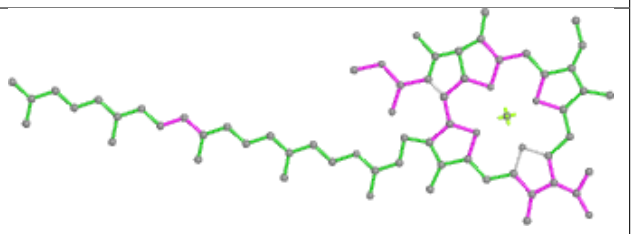
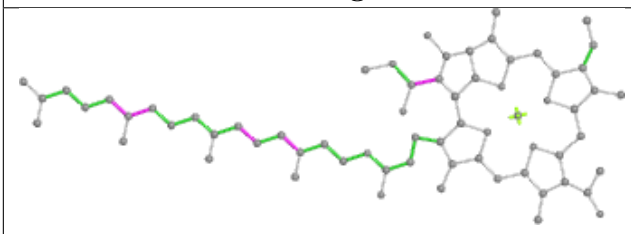
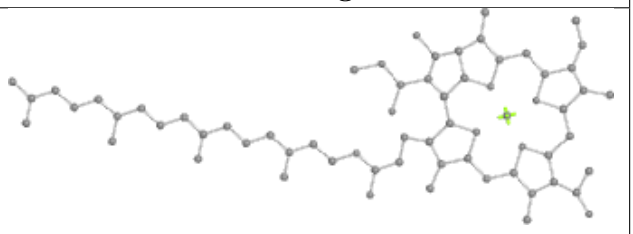


Bond angles

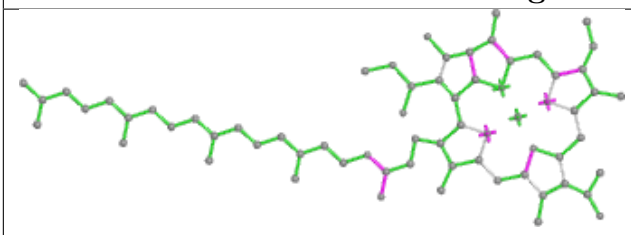


Torsions

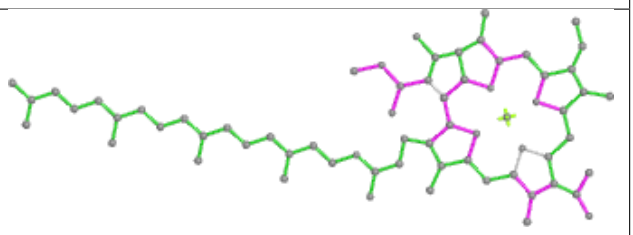


Rings

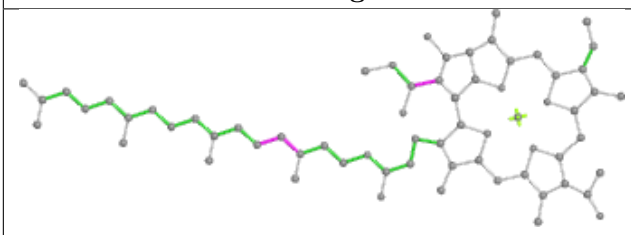
Ligand BCL d 101



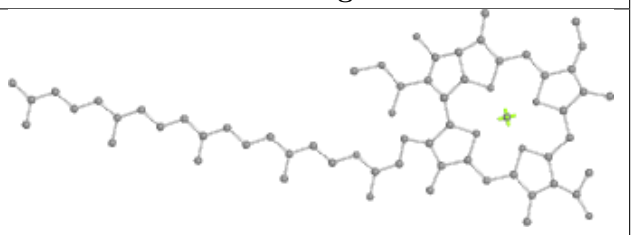
Bond lengths



Bond angles

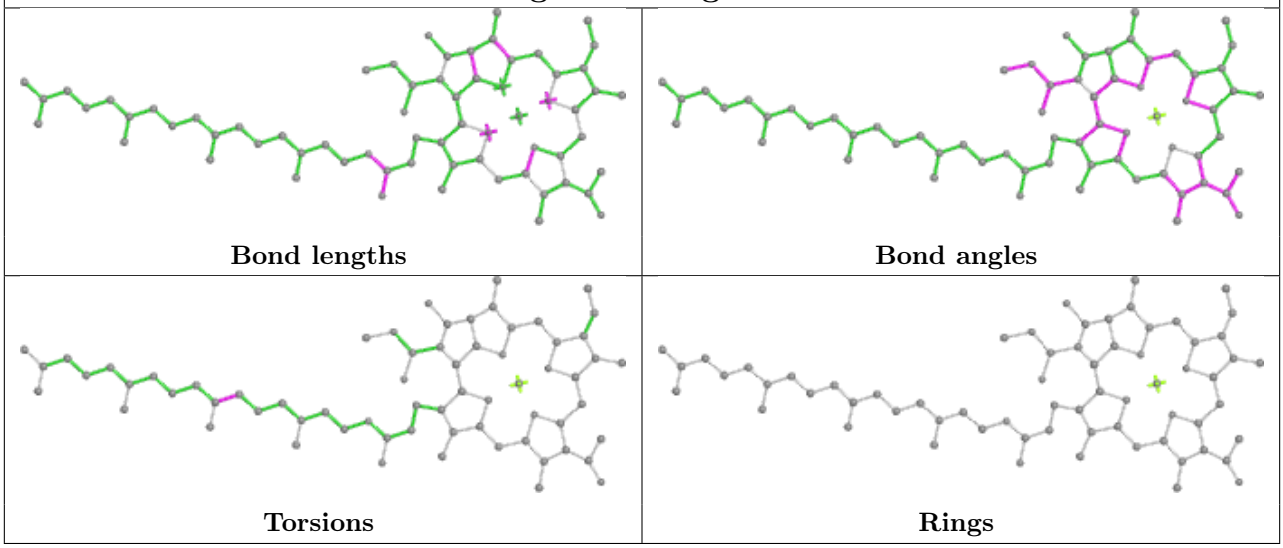


Torsions

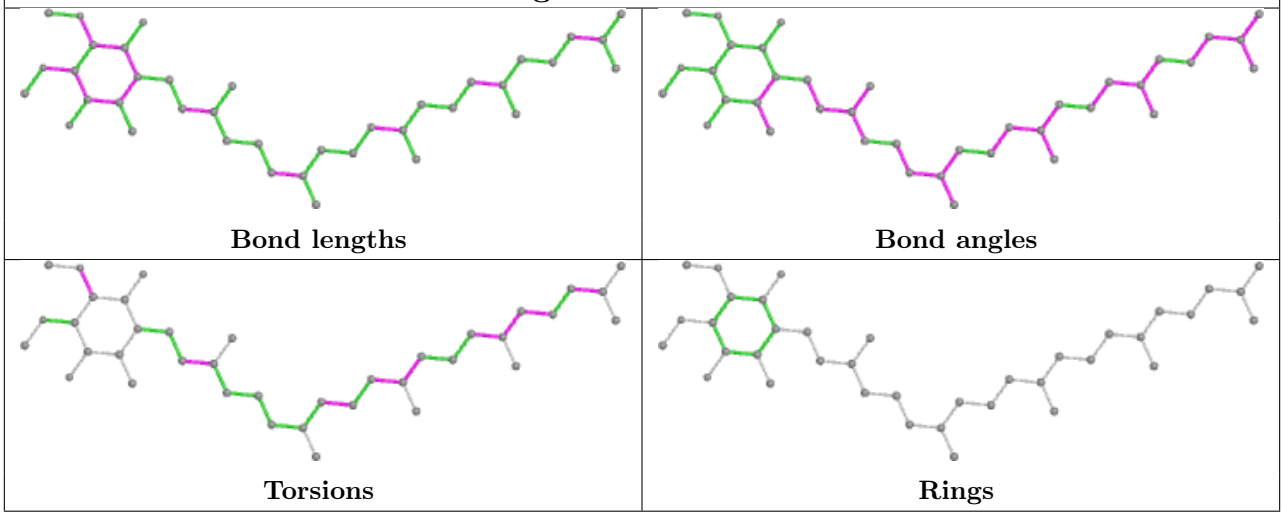


Rings

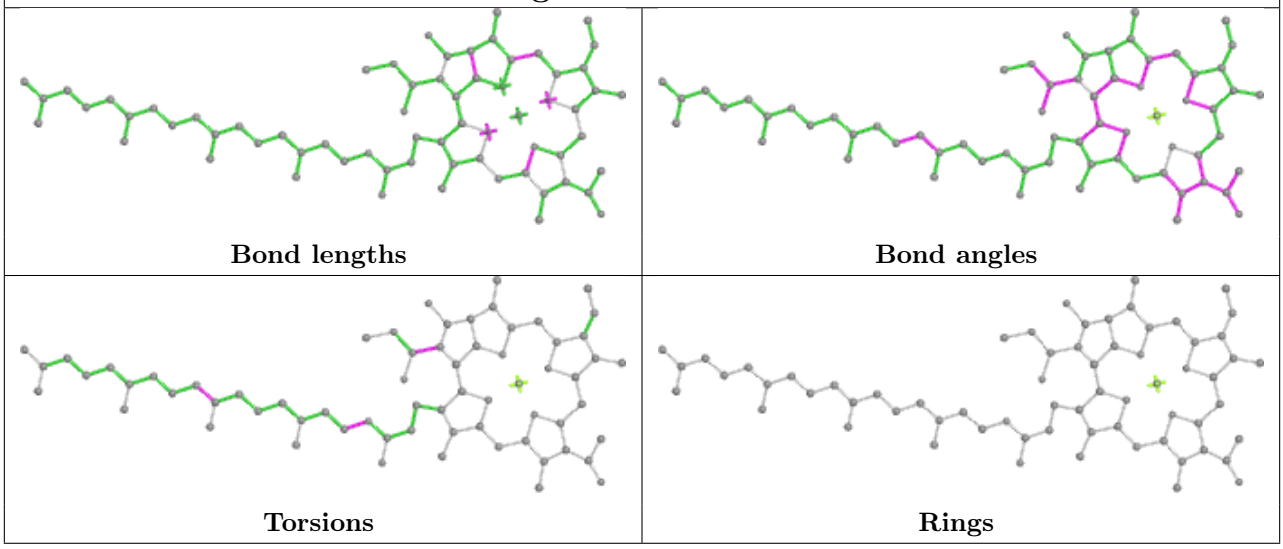
Ligand BCL g 101



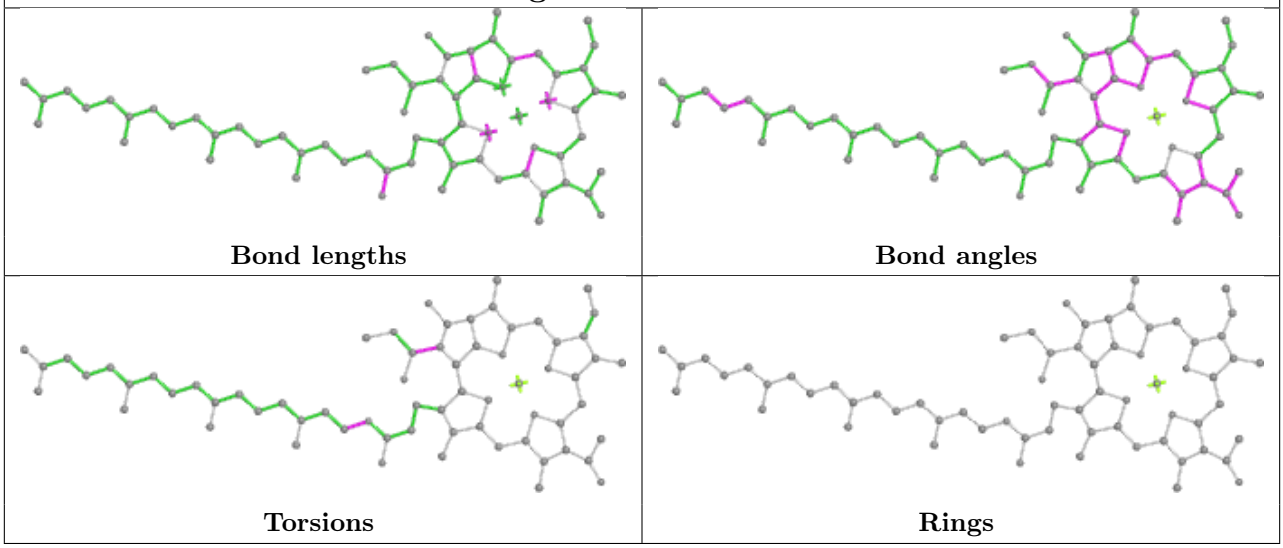
Ligand U10 L 304



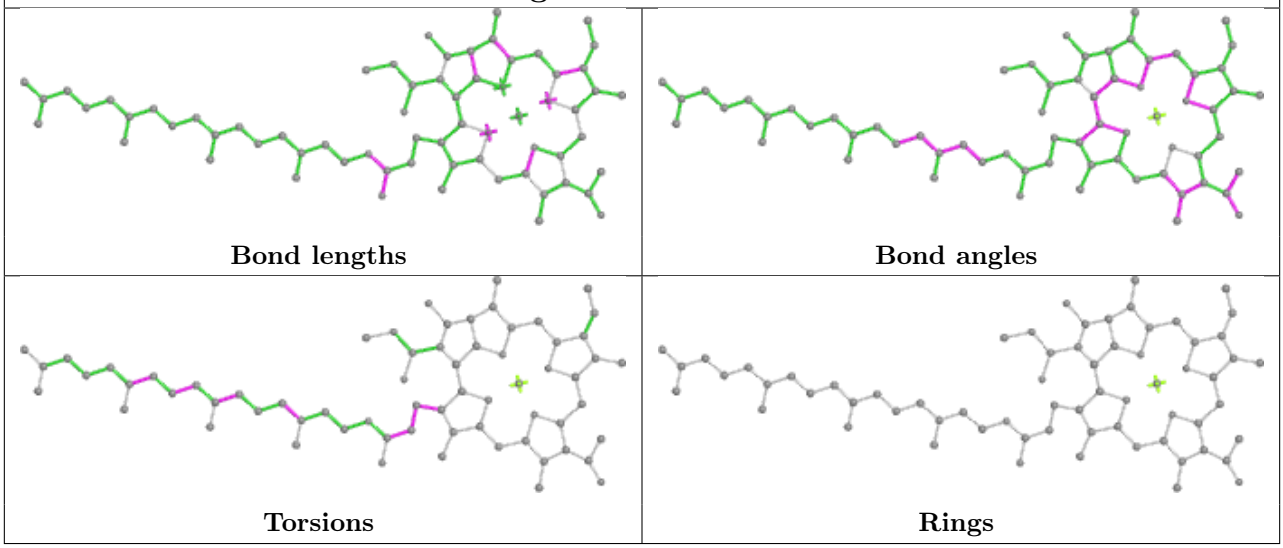
Ligand BCL t 101



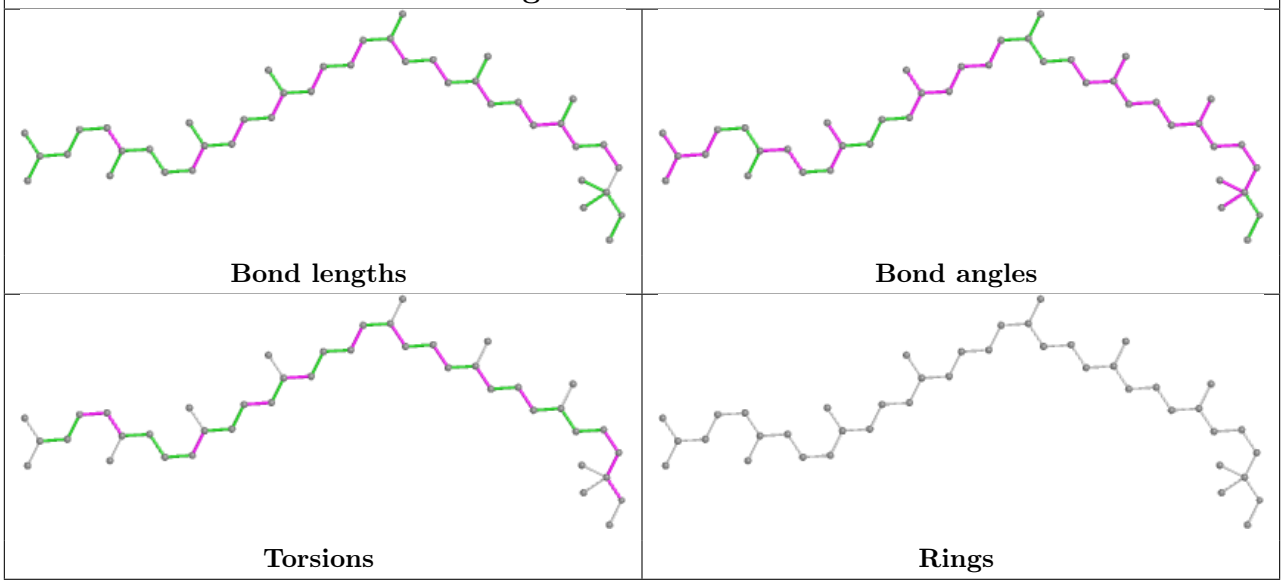
Ligand BCL u 101



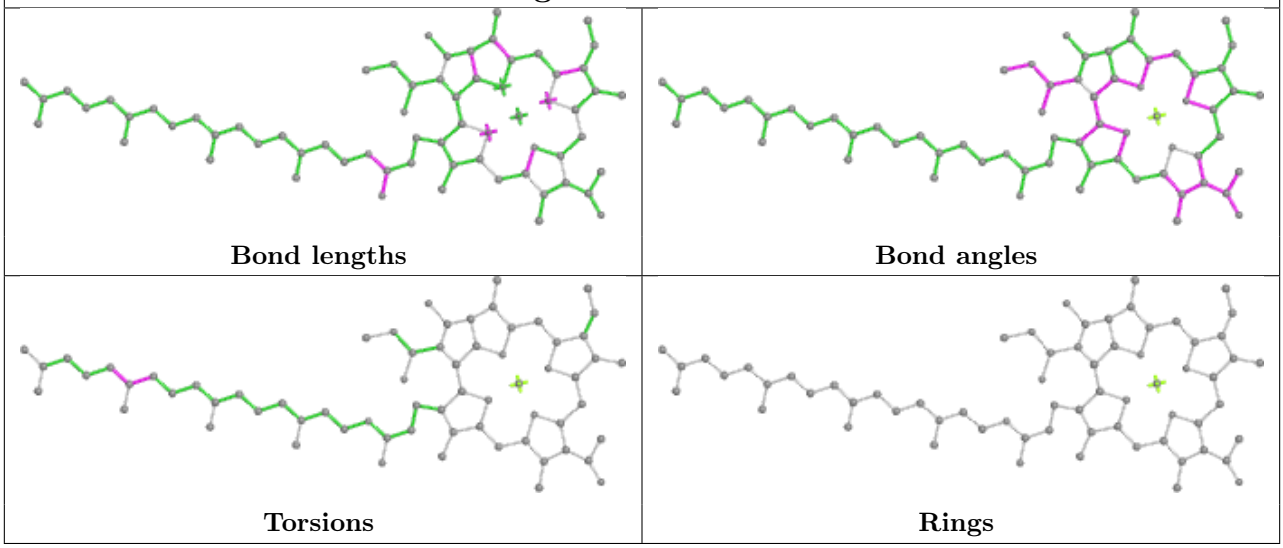
Ligand BCL o 100



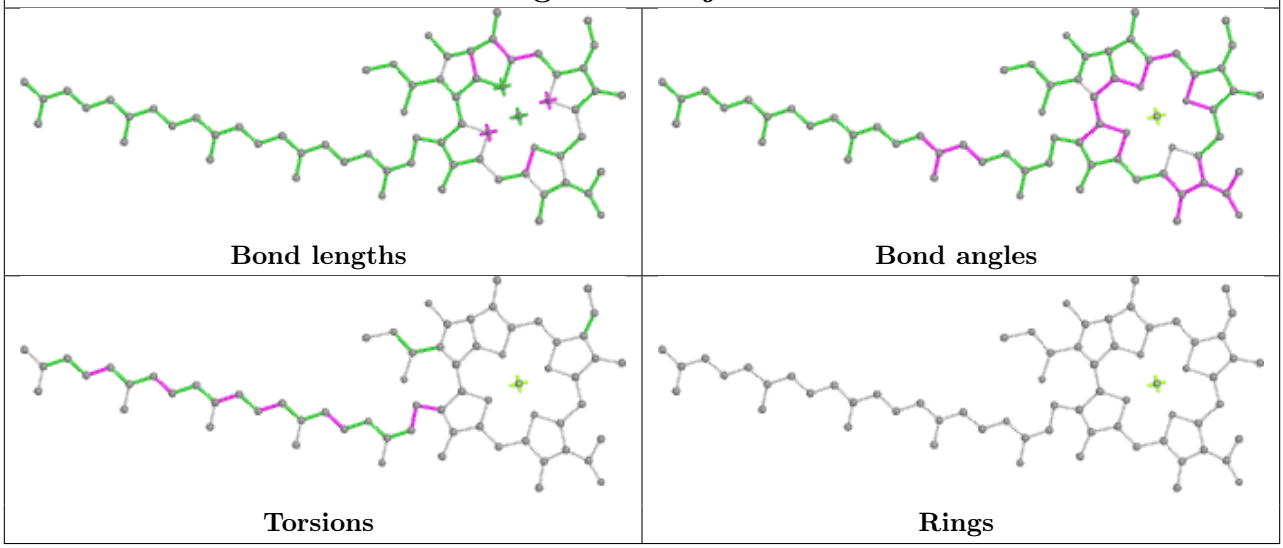
Ligand SPO M 406



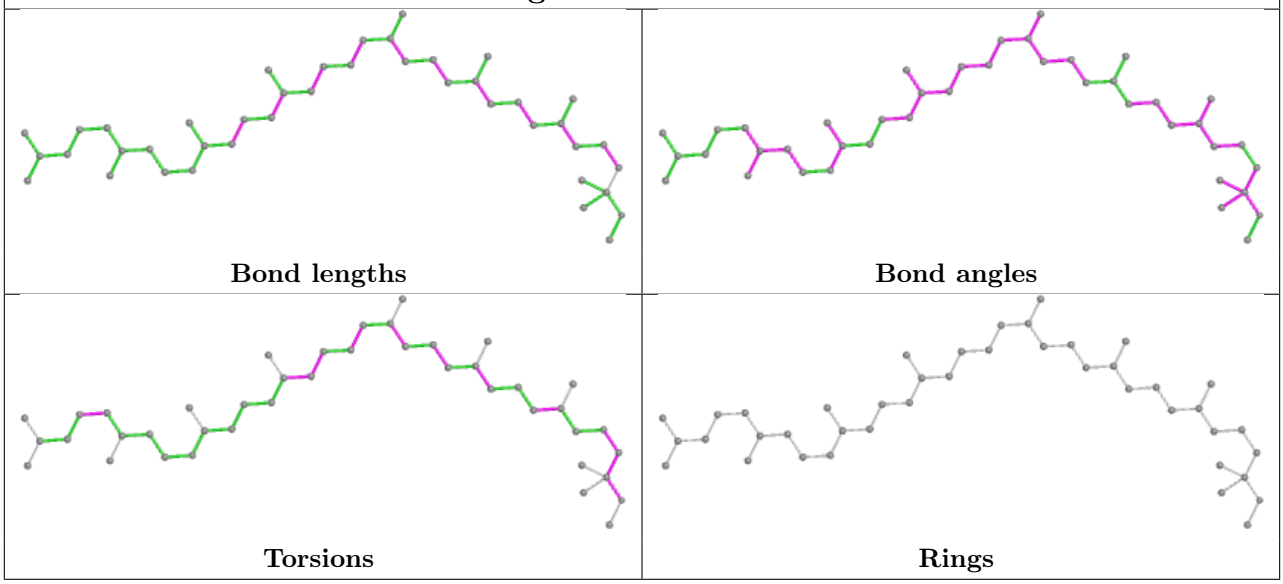
Ligand BCL i 100



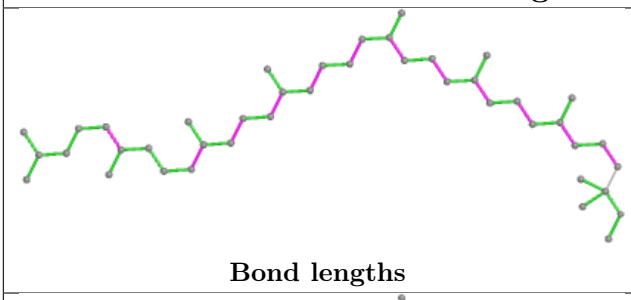
Ligand BCL j 303



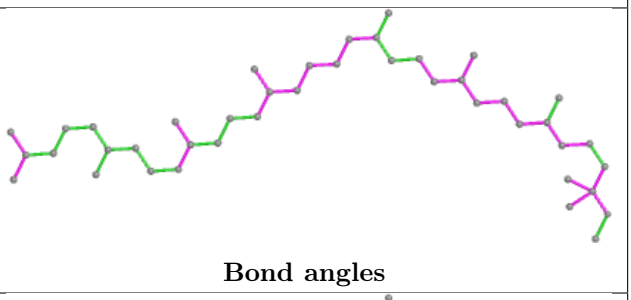
Ligand SPO E 201



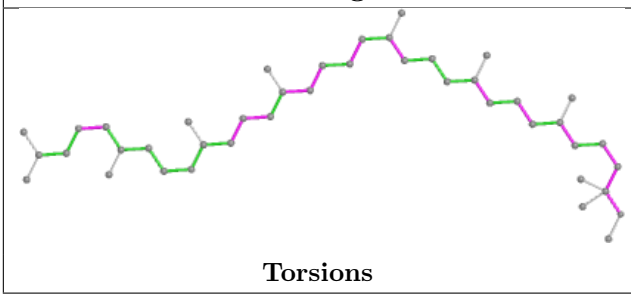
Ligand SPO r 103



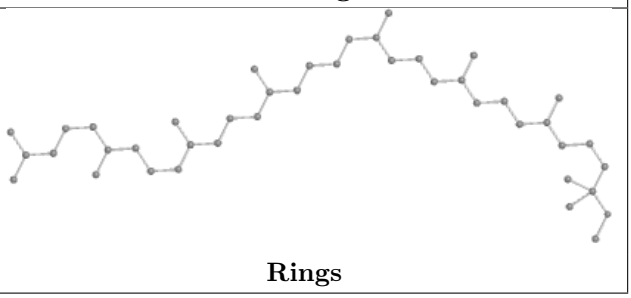
Bond lengths



Bond angles

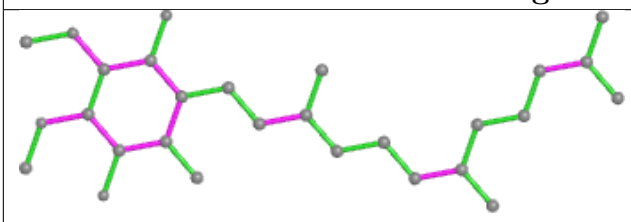


Torsions

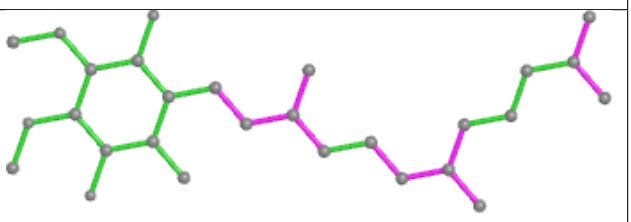


Rings

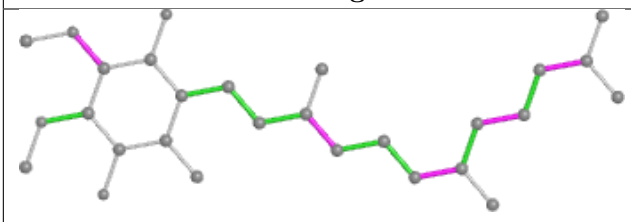
Ligand U10 L 305



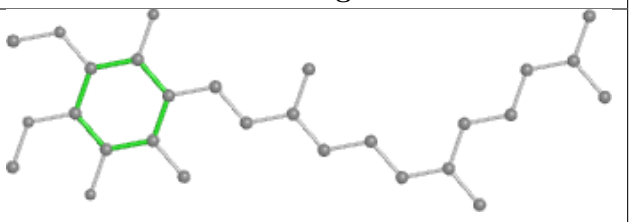
Bond lengths



Bond angles

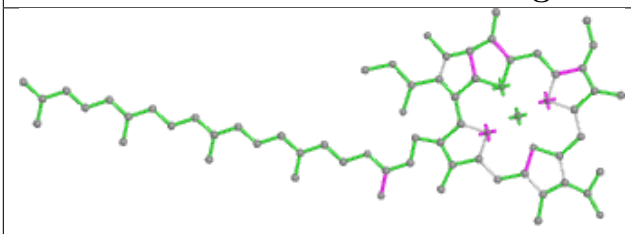


Torsions

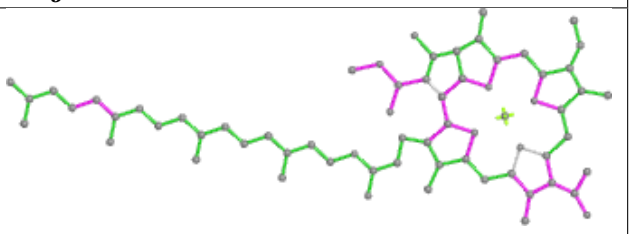


Rings

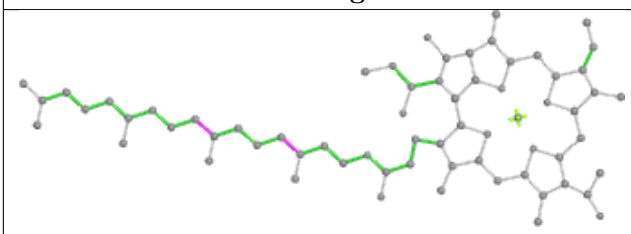
Ligand BCL j 302



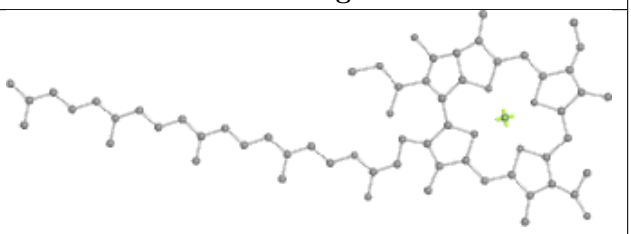
Bond lengths



Bond angles

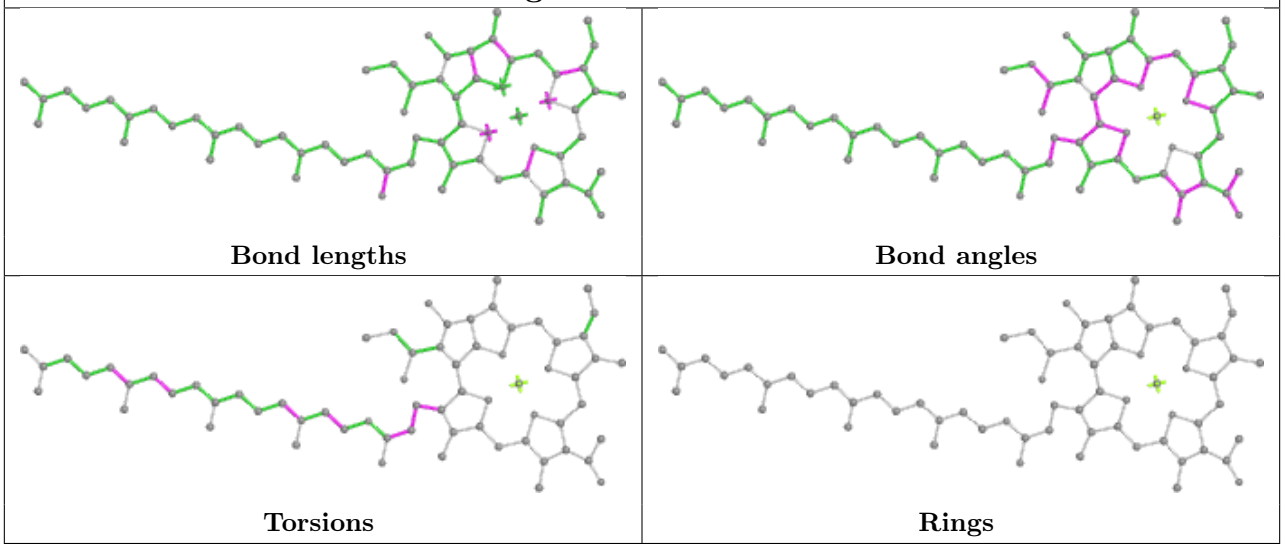


Torsions

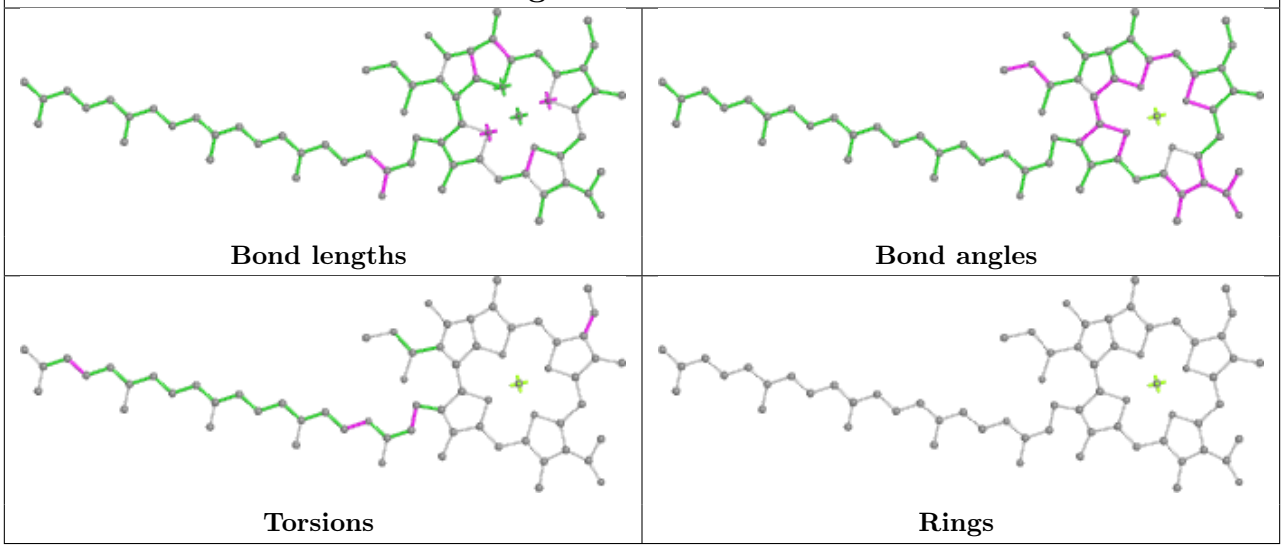


Rings

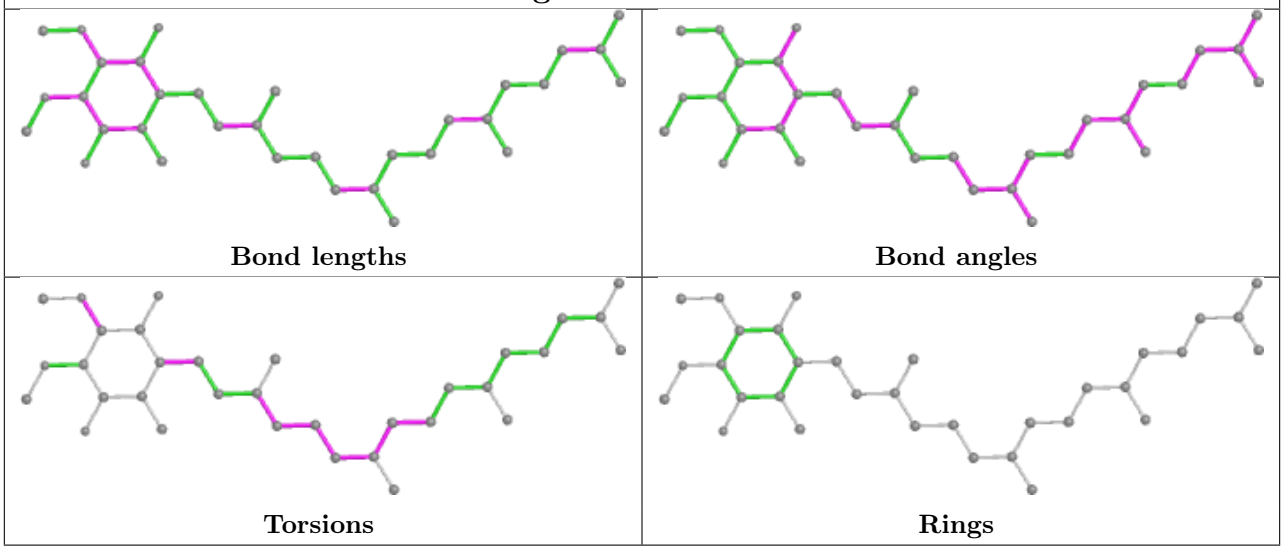
Ligand BCL A 101



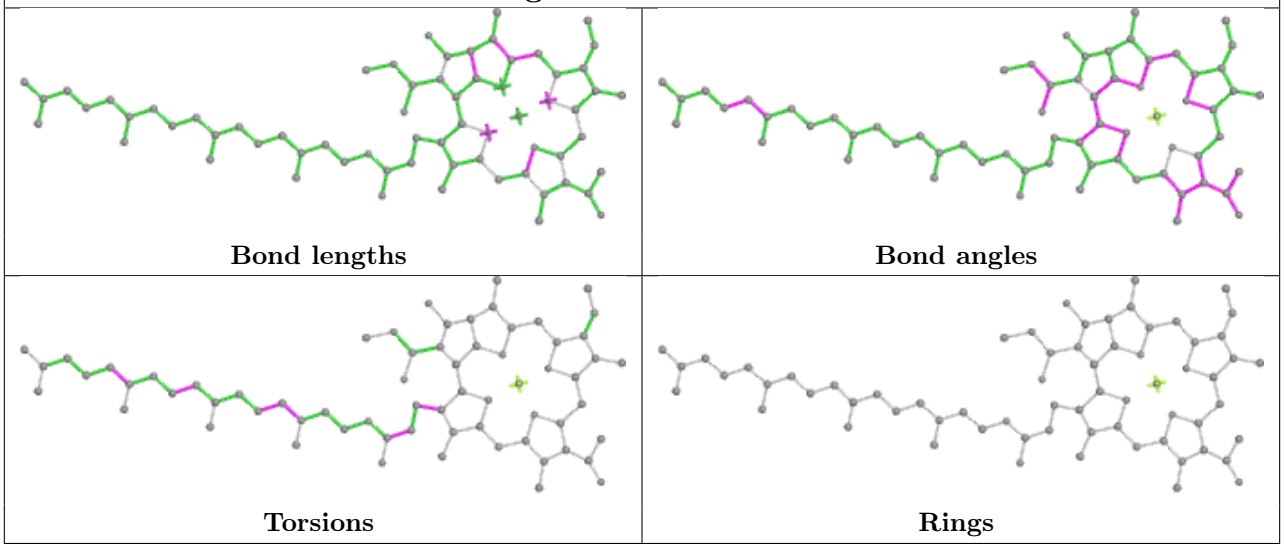
Ligand BCL L 301



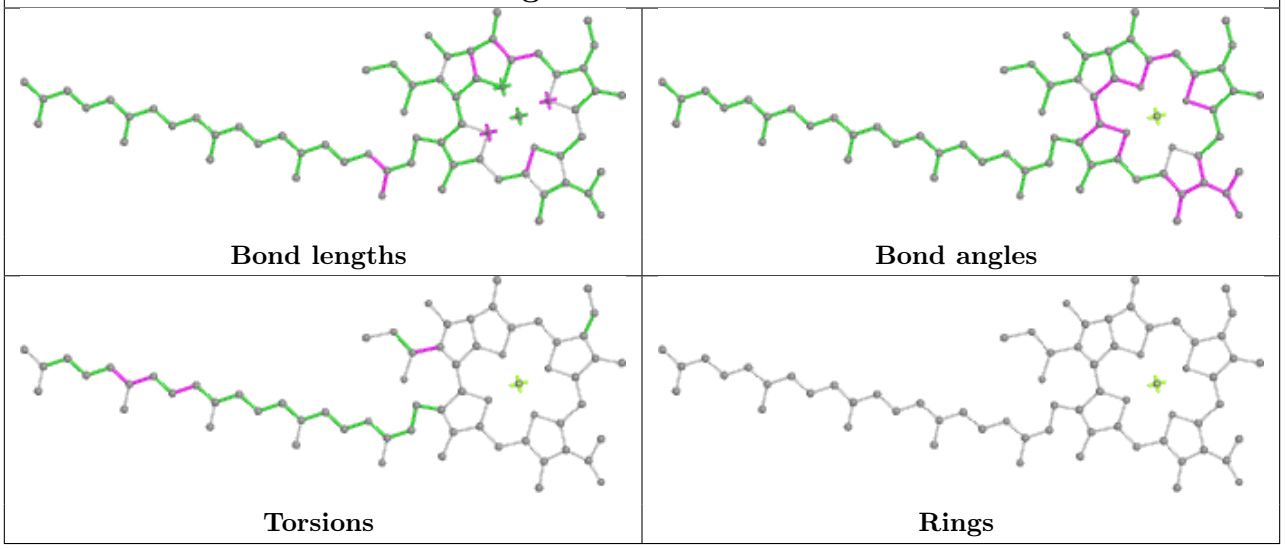
Ligand U10 L 303



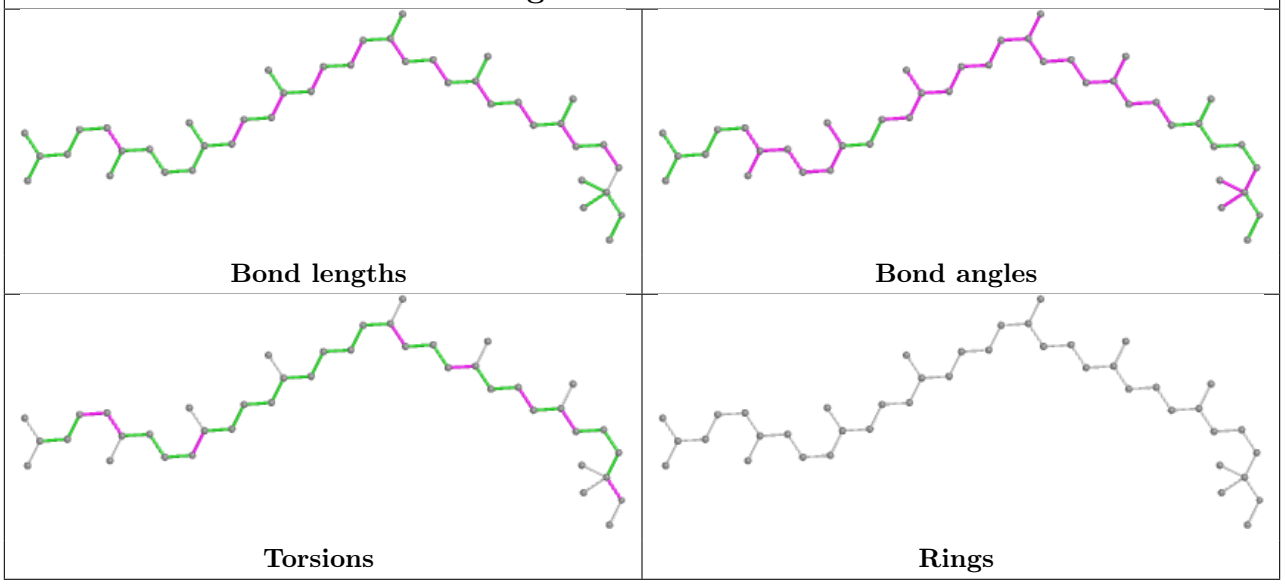
Ligand BCL G 101



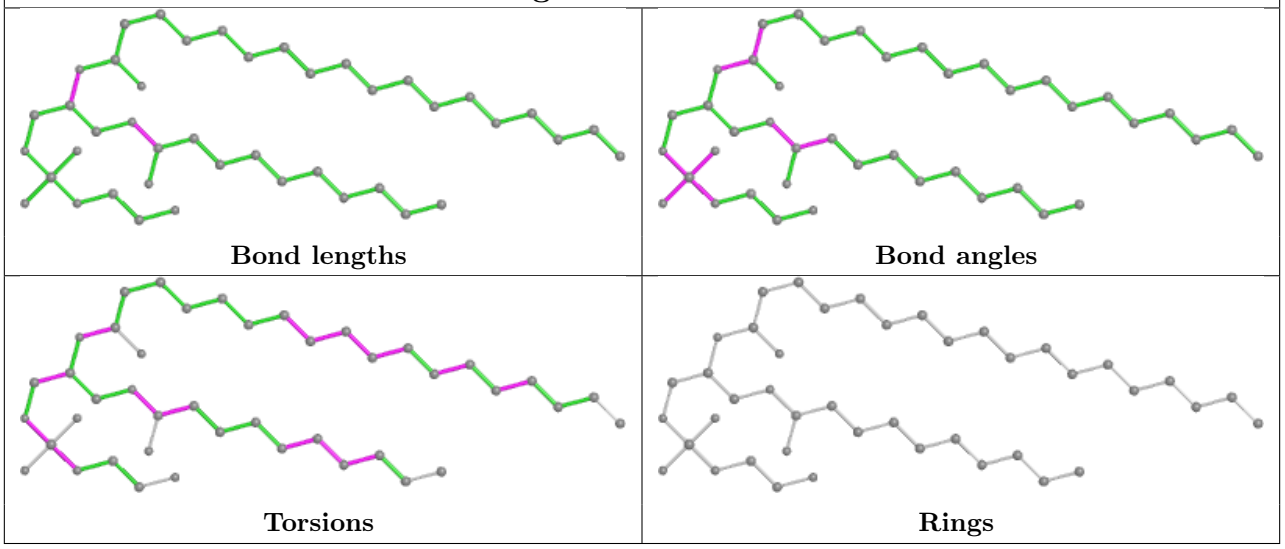
Ligand BCL M 407



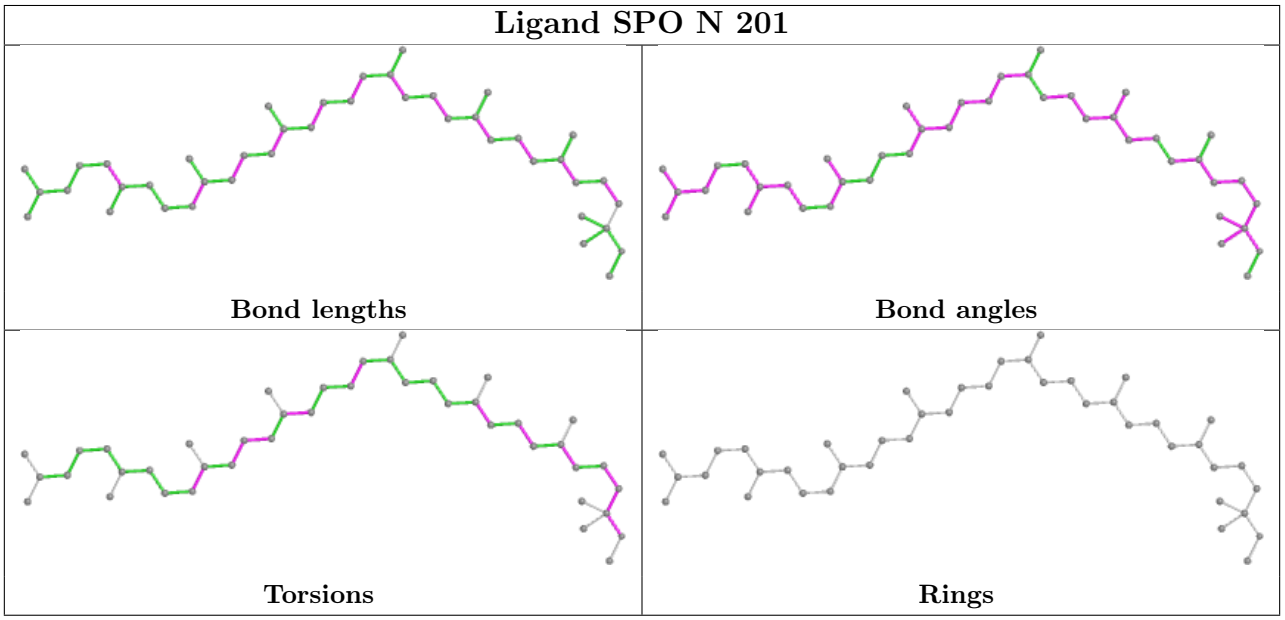
Ligand SPO B 101



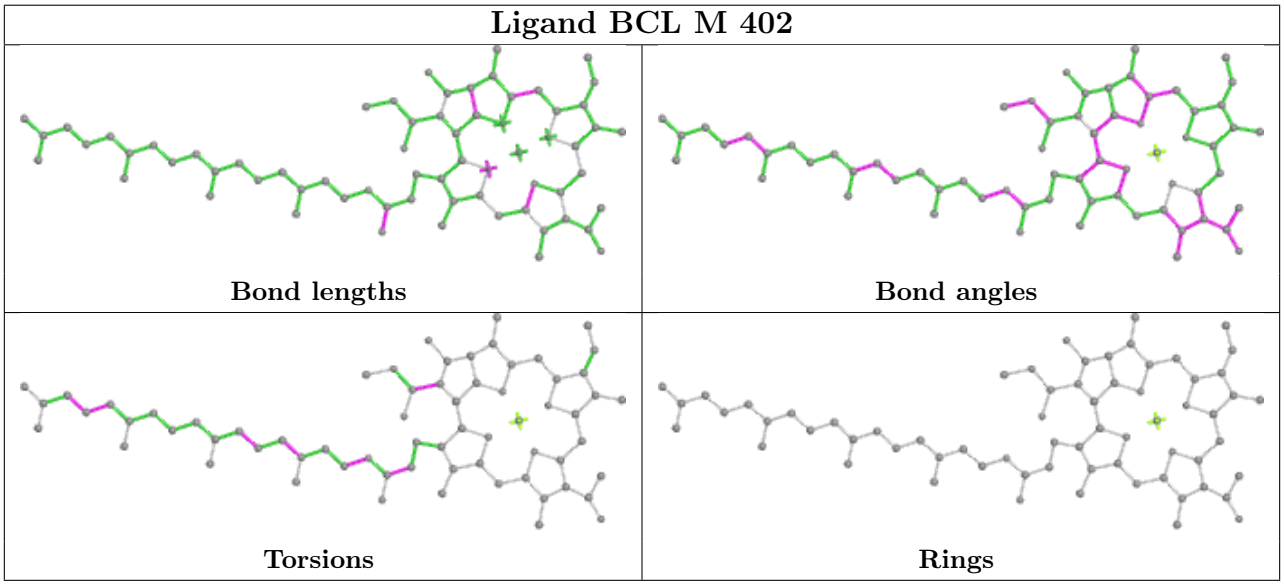
Ligand 3PE d 102



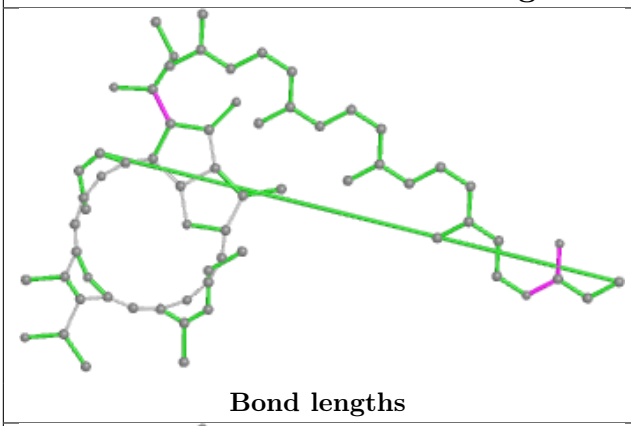
Ligand SPO N 201



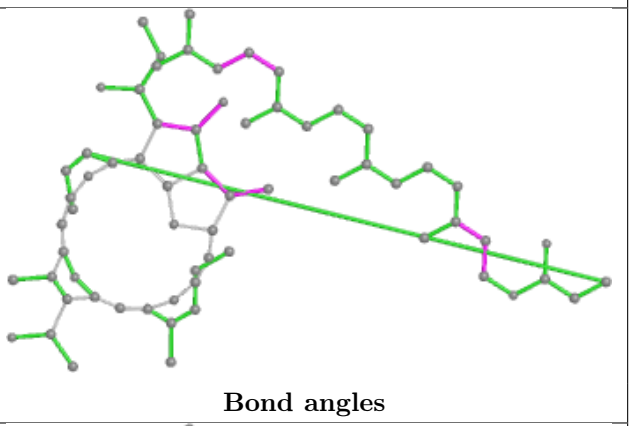
Ligand BCL M 402



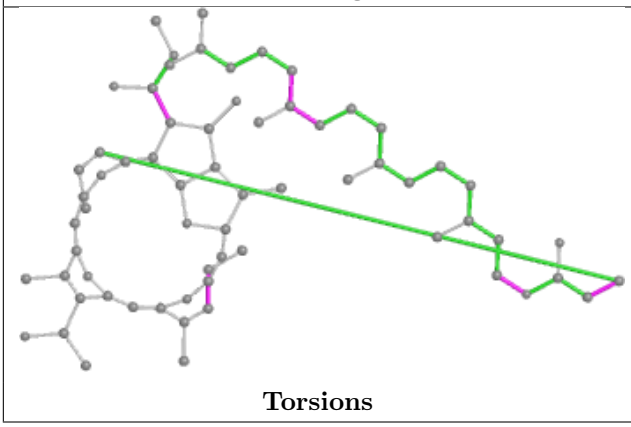
Ligand BPH M 403



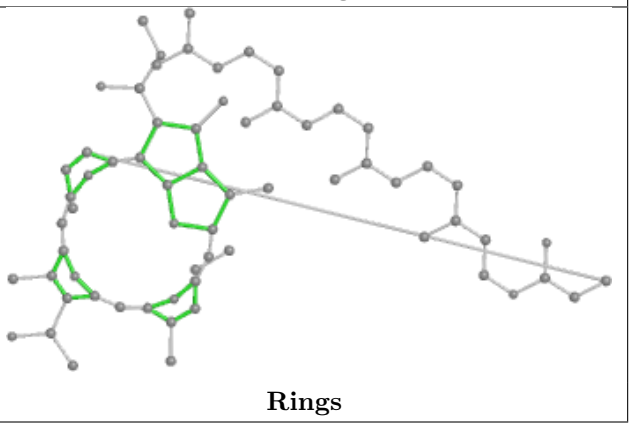
Bond lengths



Bond angles

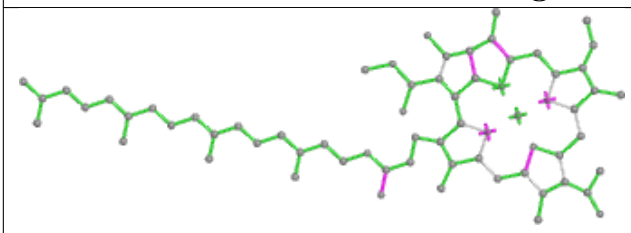


Torsions

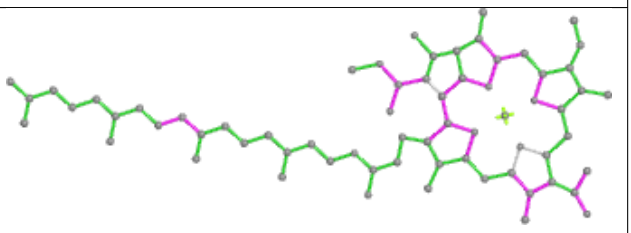


Rings

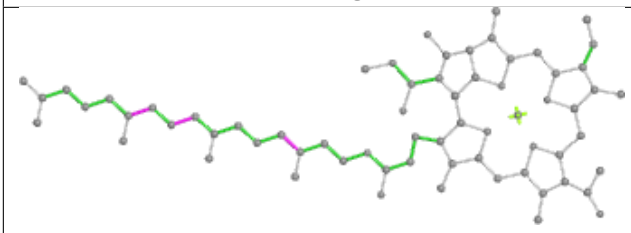
Ligand BCL r 101



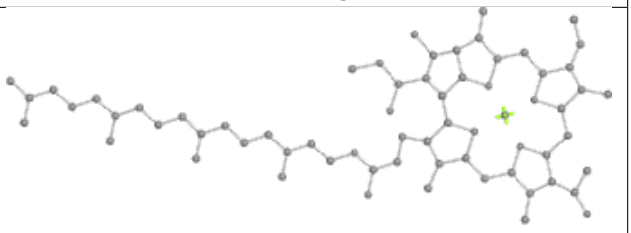
Bond lengths



Bond angles

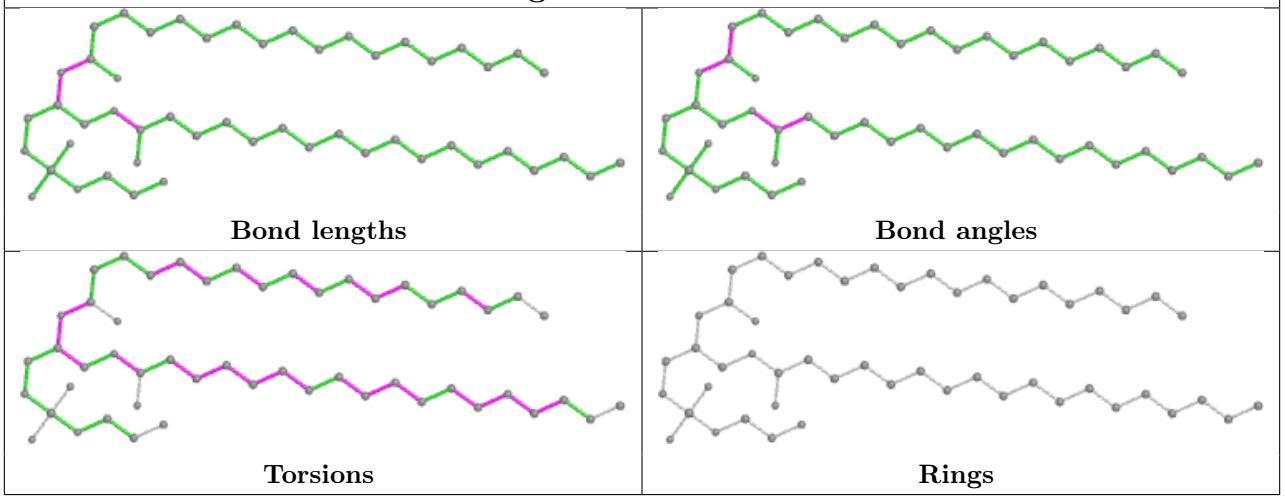


Torsions

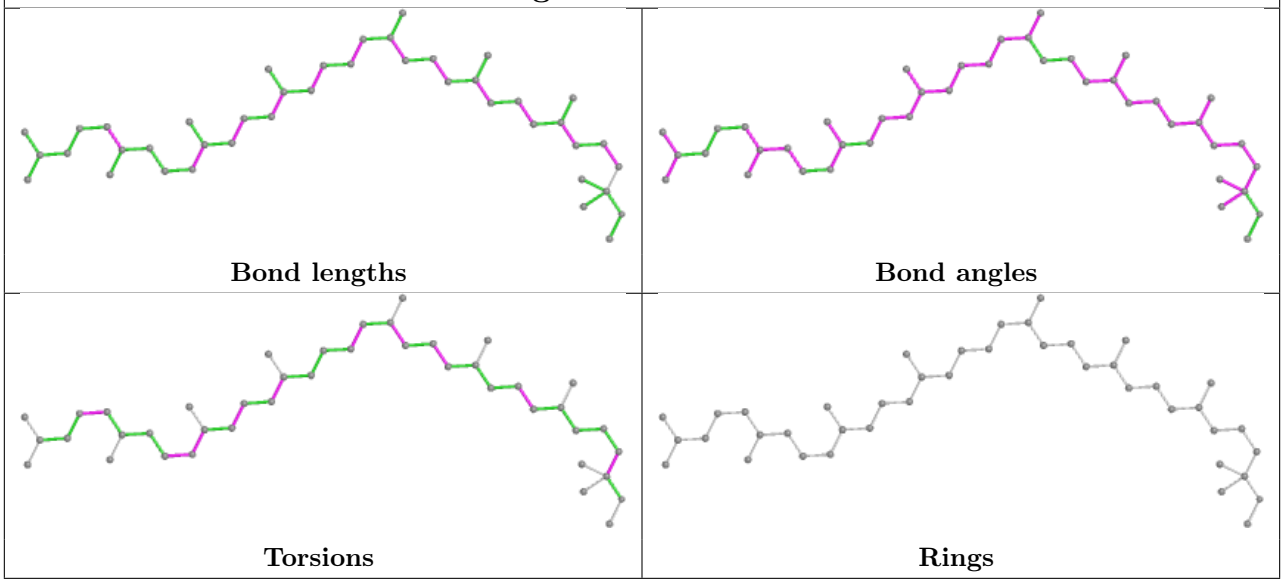


Rings

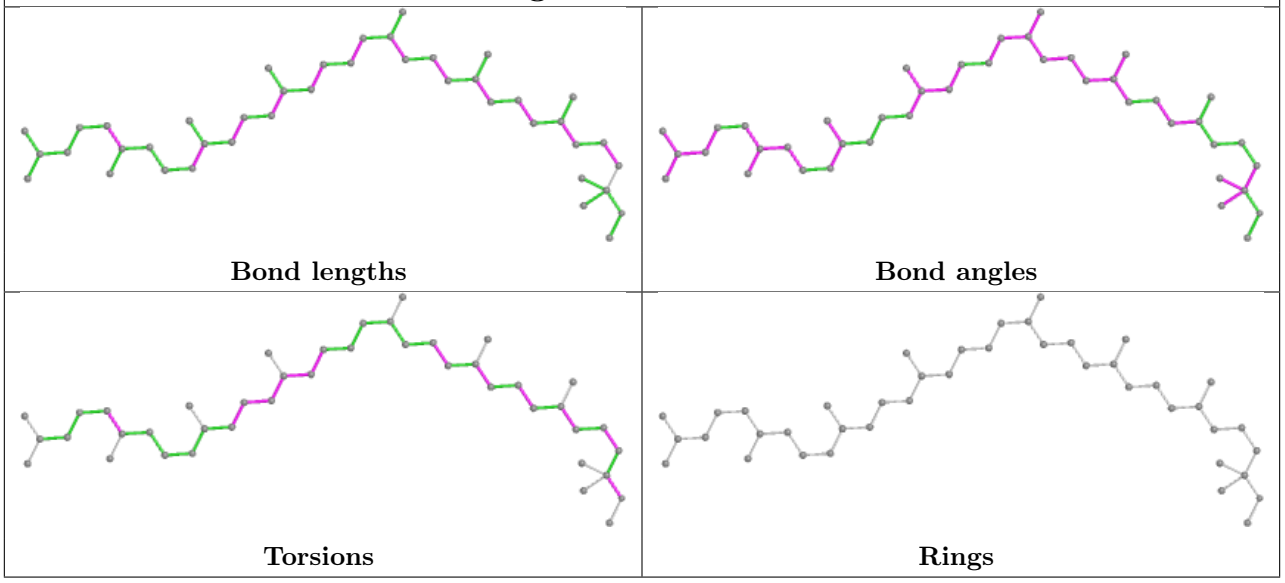
Ligand 3PE H 301



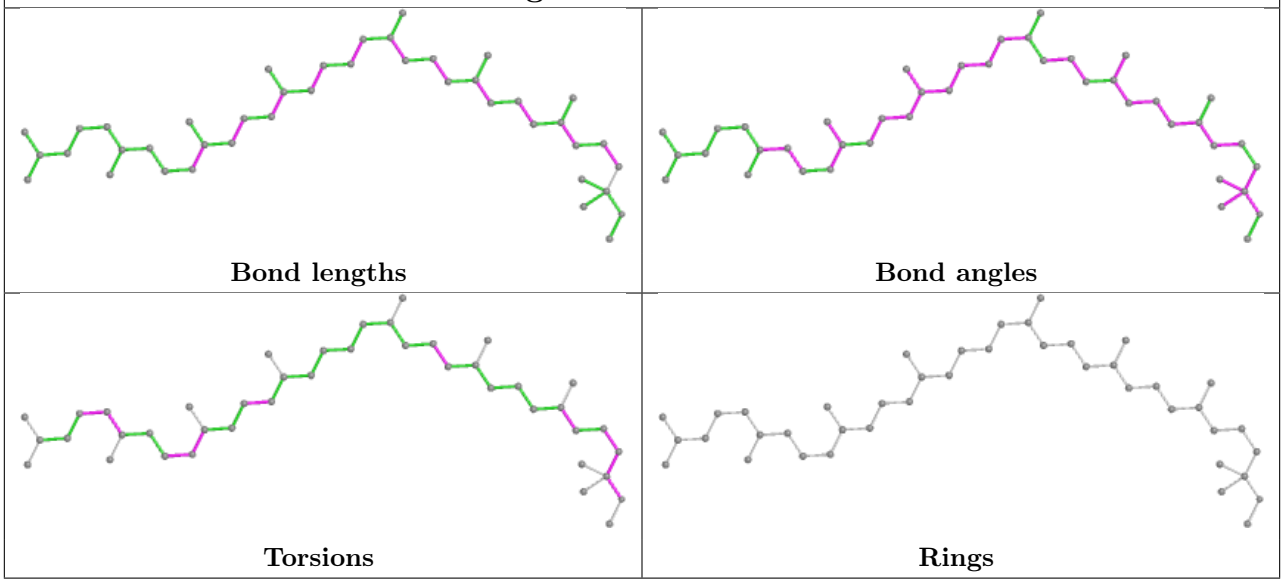
Ligand SPO t 102



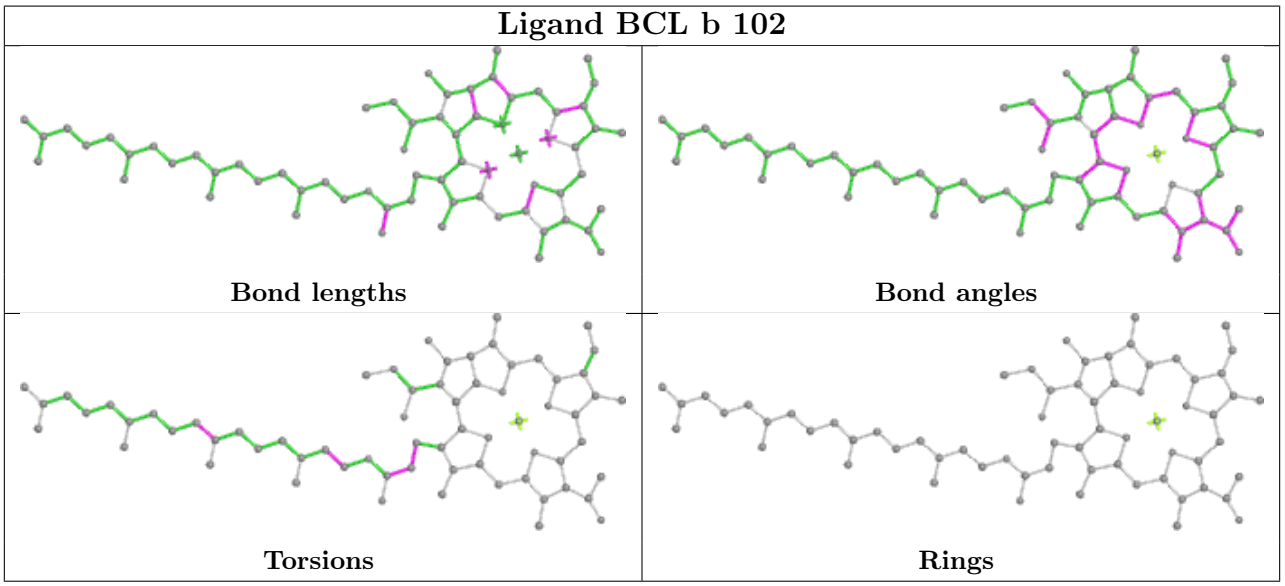
Ligand SPO F 102



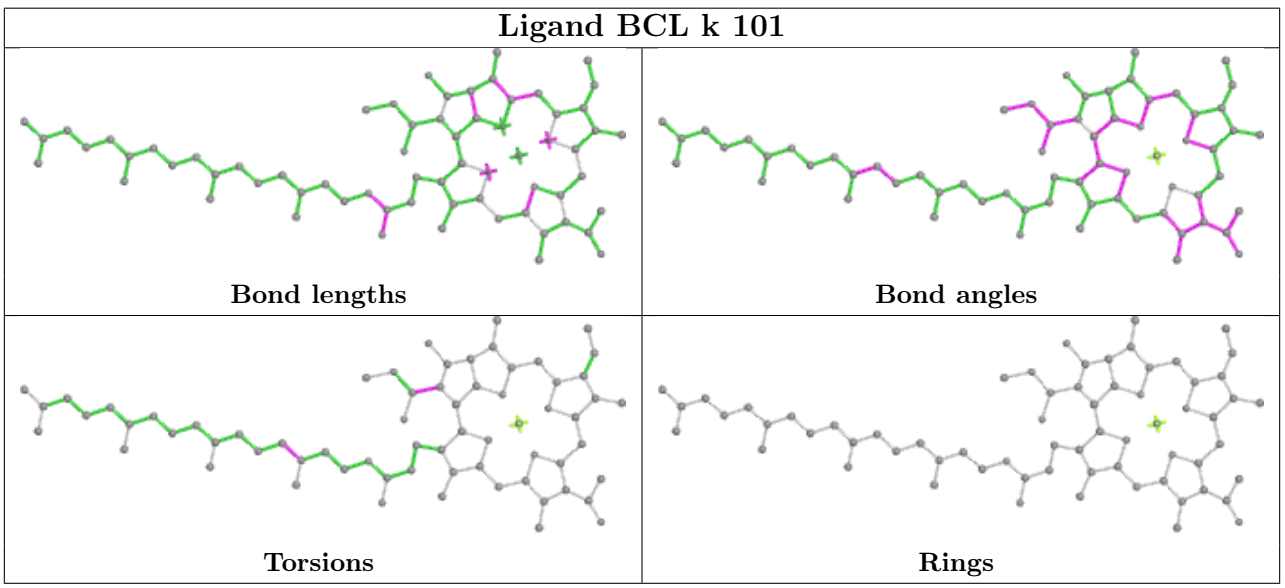
Ligand SPO D 201



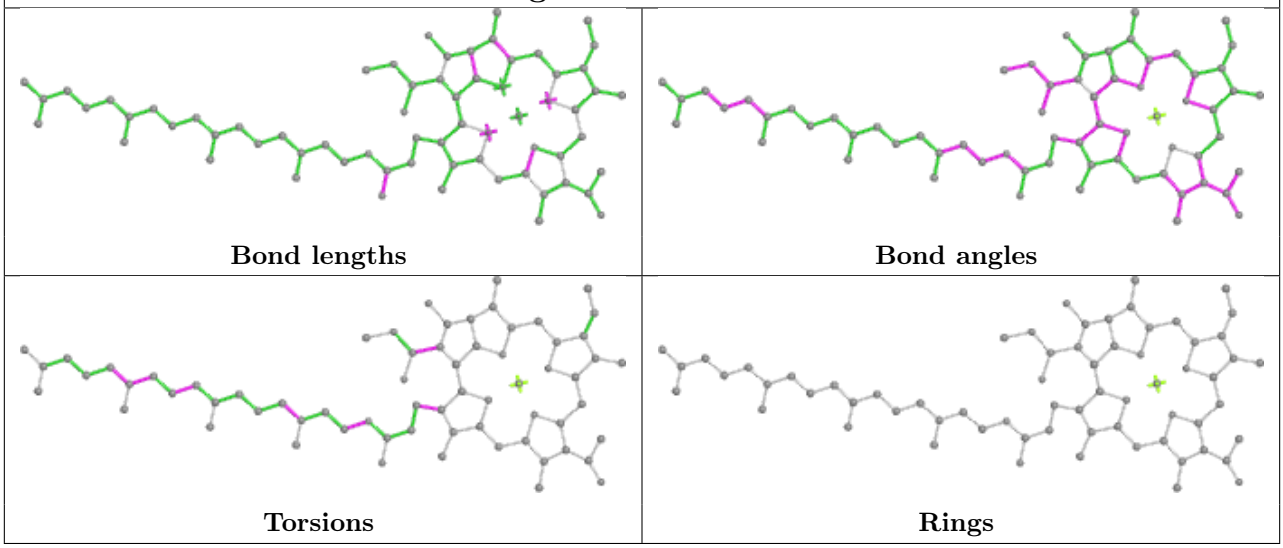
Ligand BCL b 102



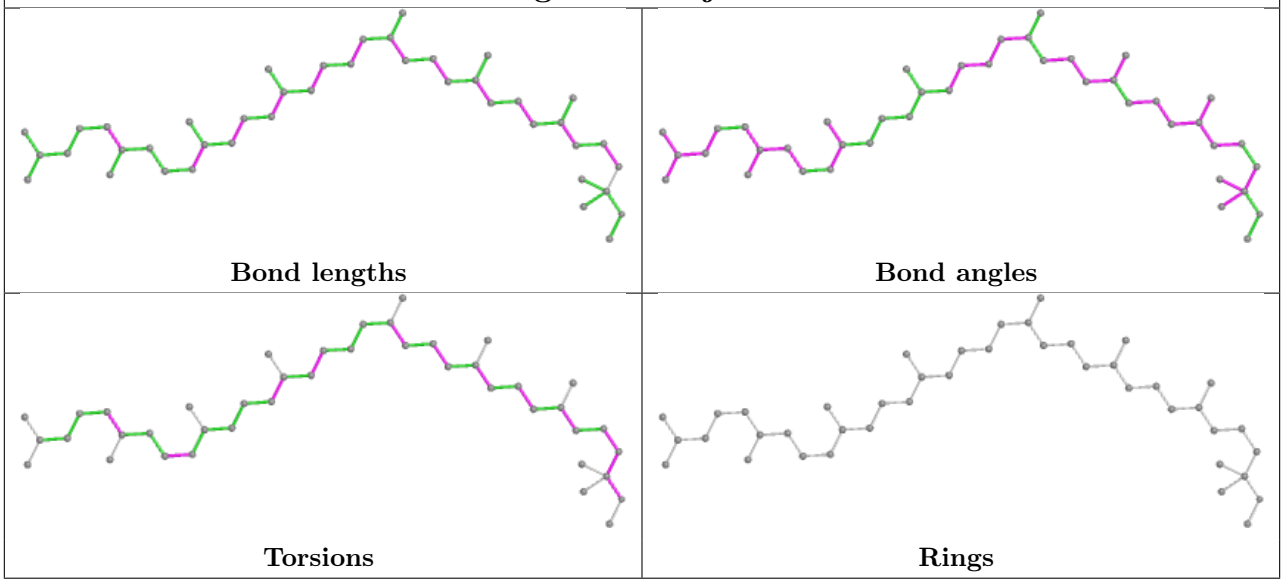
Ligand BCL k 101



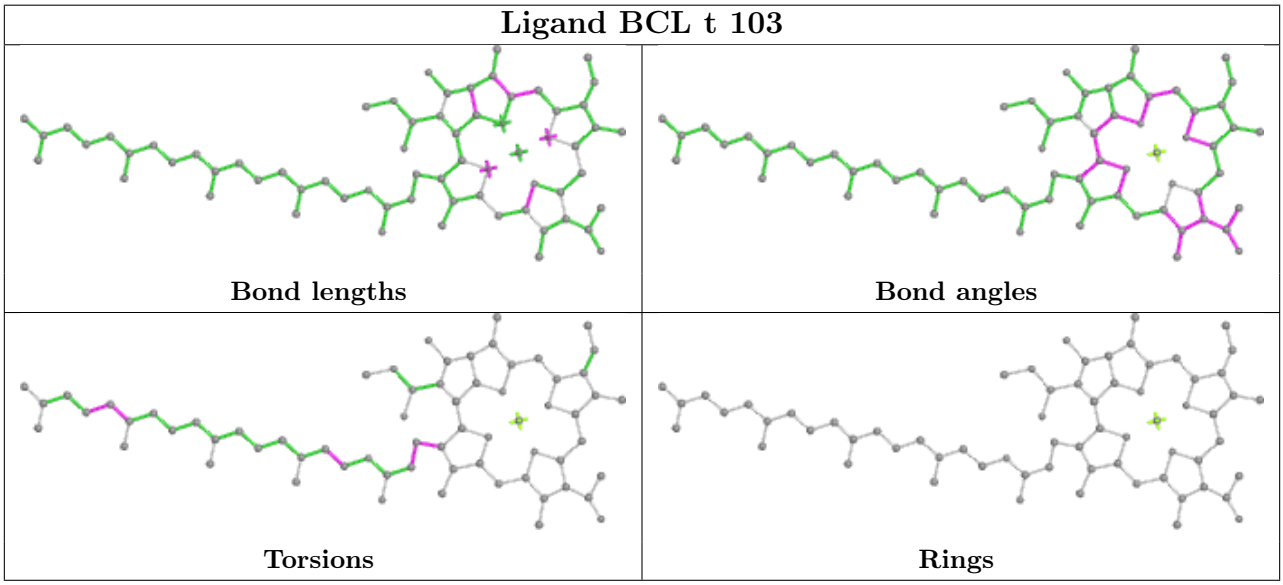
Ligand BCL b 101

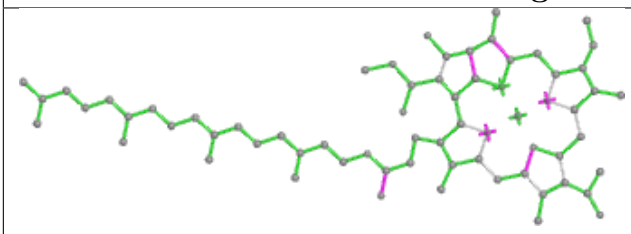
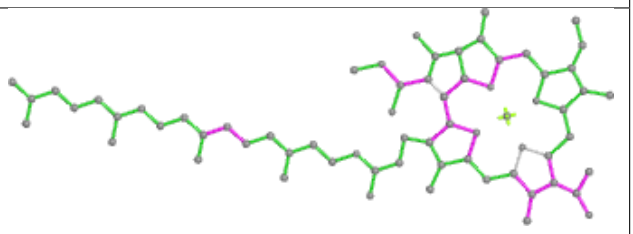
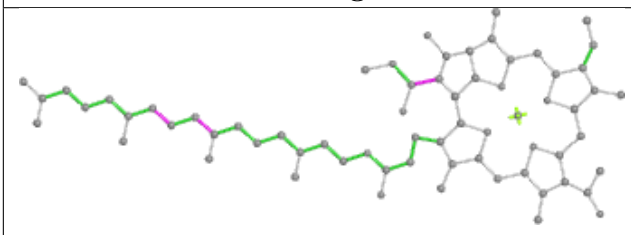
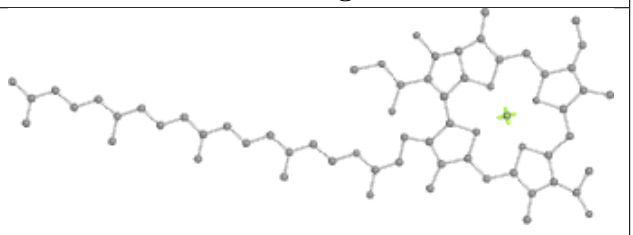


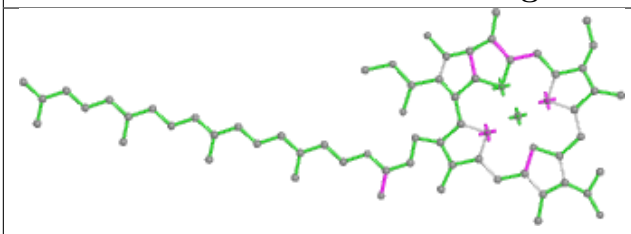
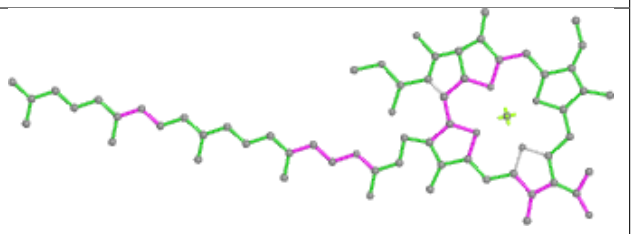
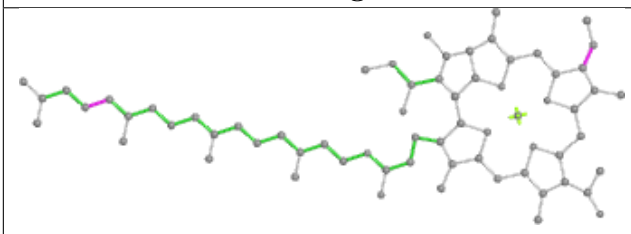
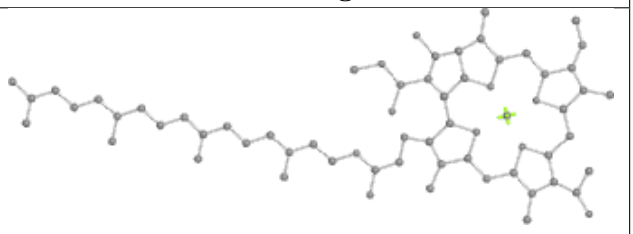
Ligand SPO j 301



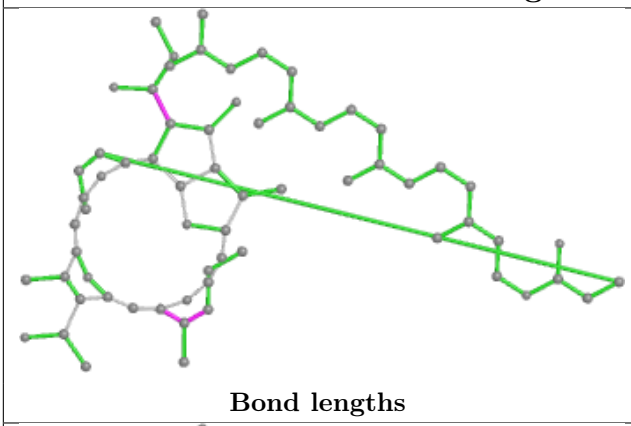
Ligand BCL t 103



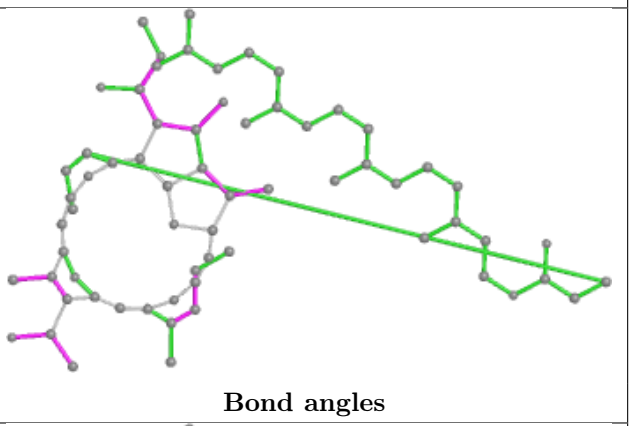
Ligand BCL s 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL M 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

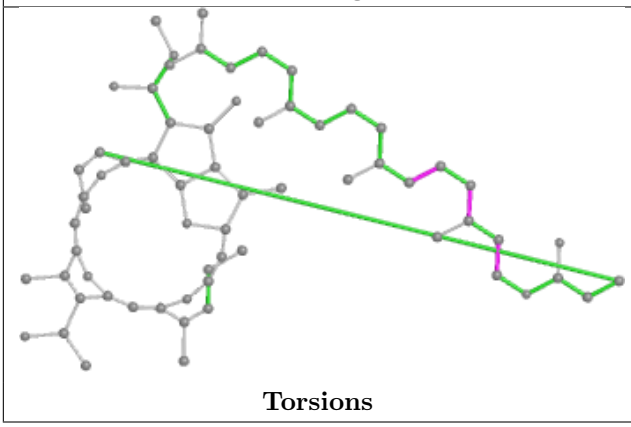
Ligand BPH L 302



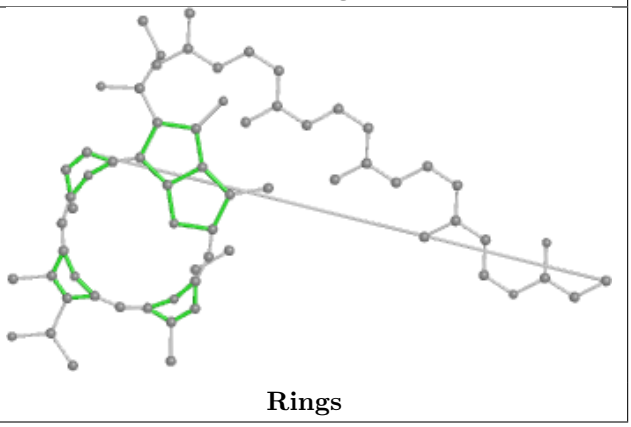
Bond lengths



Bond angles

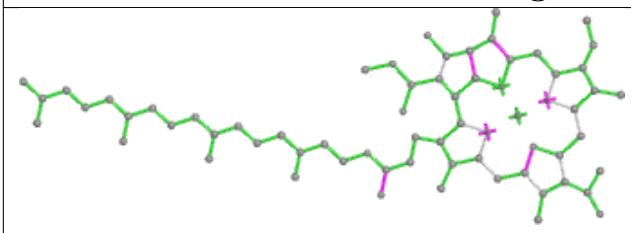


Torsions

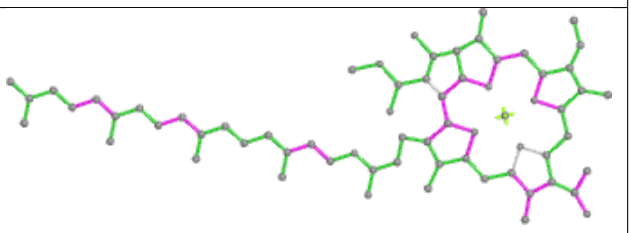


Rings

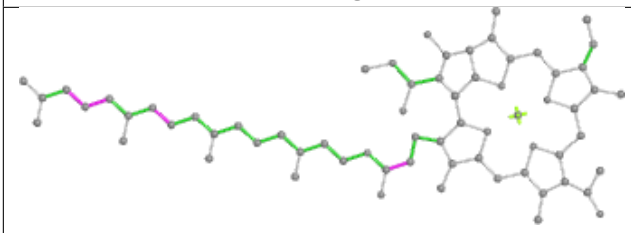
Ligand BCL a 101



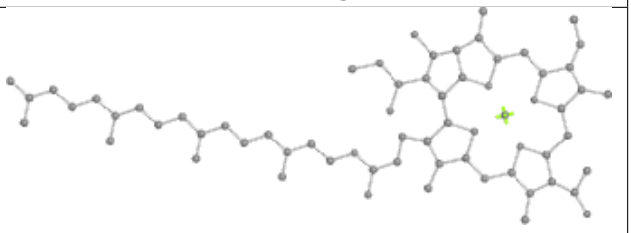
Bond lengths



Bond angles

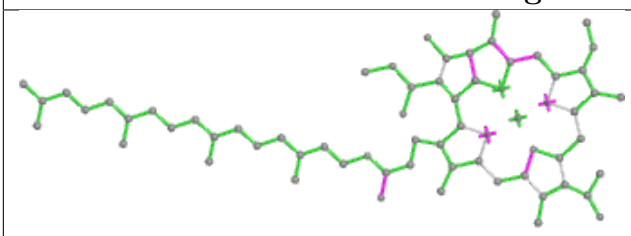


Torsions

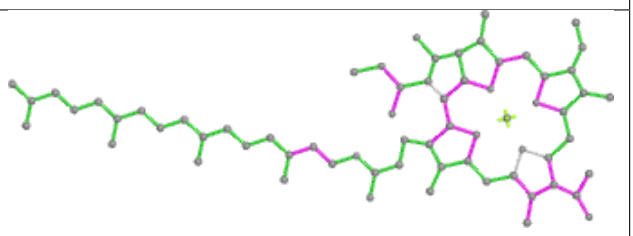


Rings

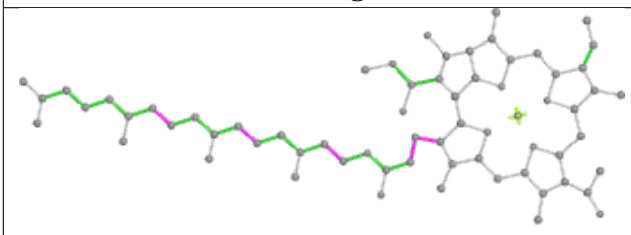
Ligand BCL D 202



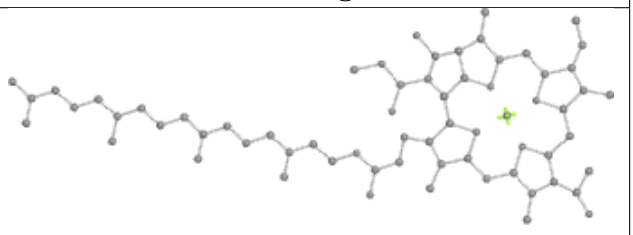
Bond lengths



Bond angles

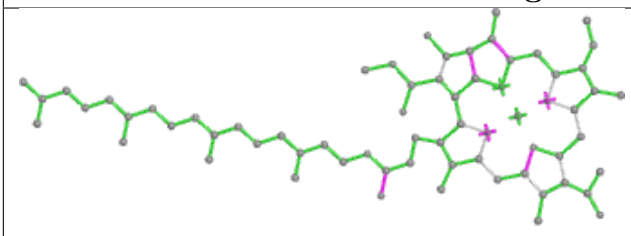


Torsions

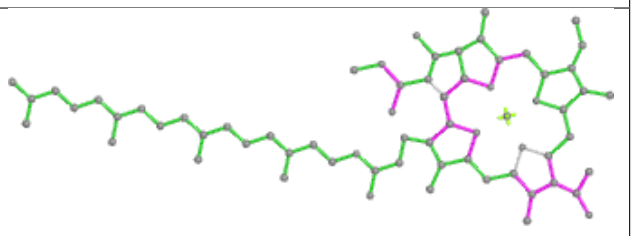


Rings

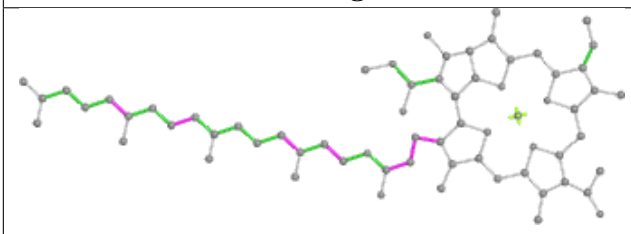
Ligand BCL R 101



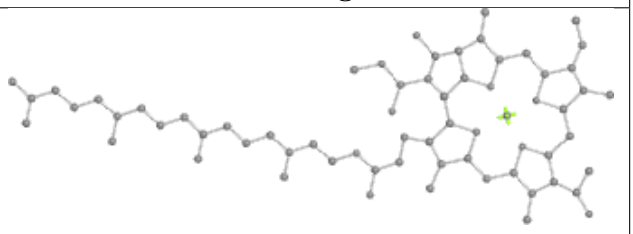
Bond lengths



Bond angles

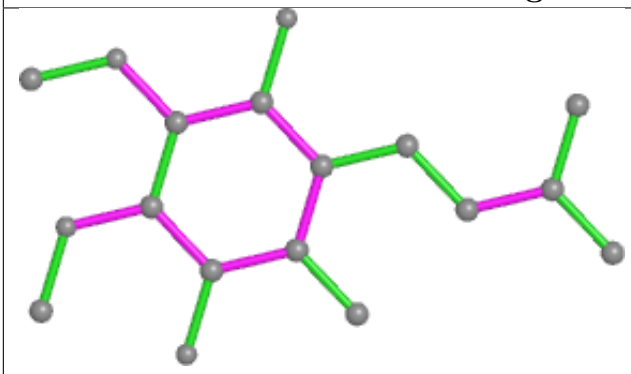


Torsions

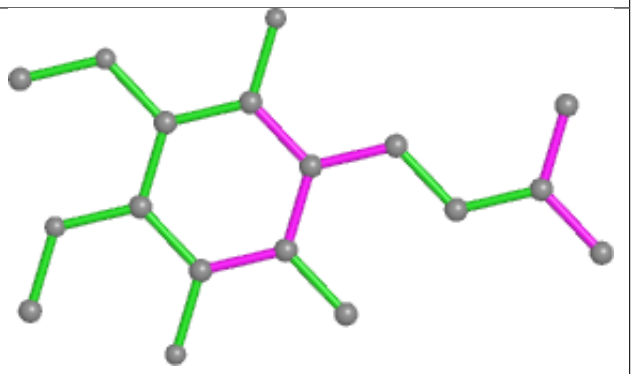


Rings

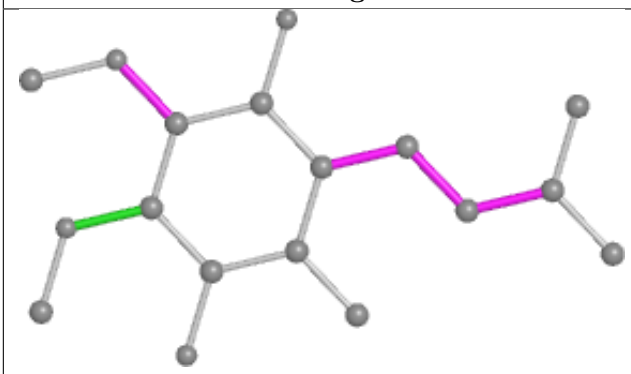
Ligand U10 M 408



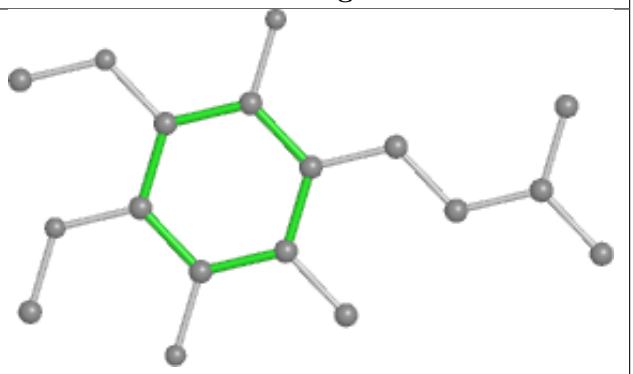
Bond lengths



Bond angles

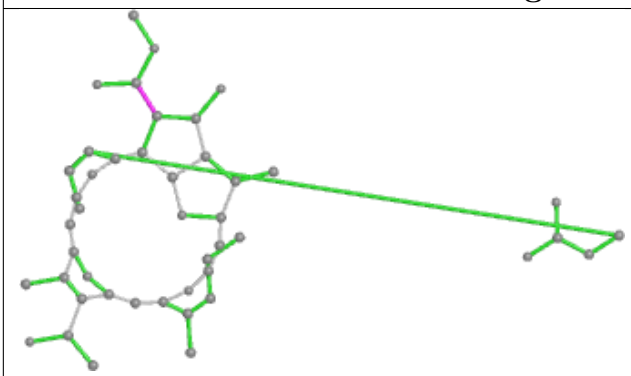


Torsions

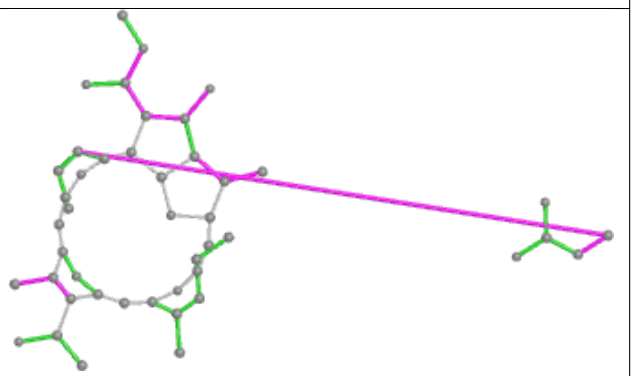


Rings

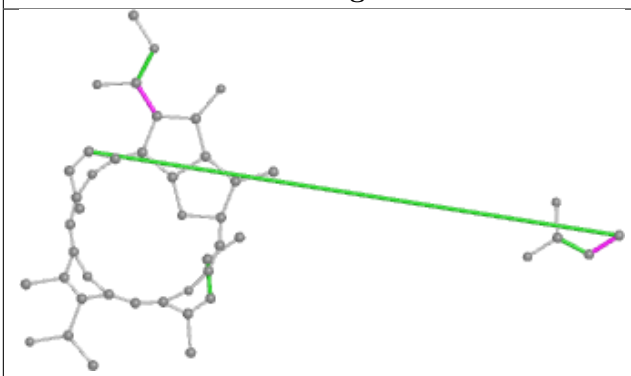
Ligand BPH L 306



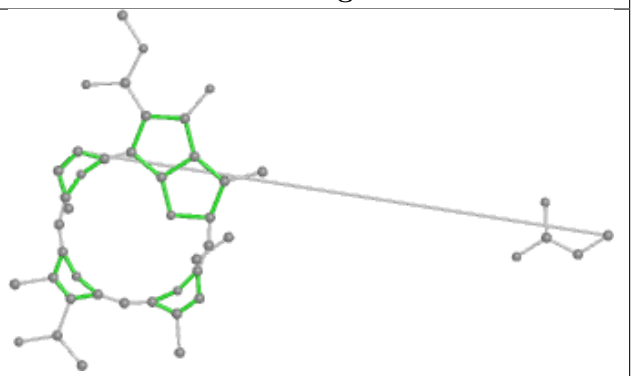
Bond lengths



Bond angles

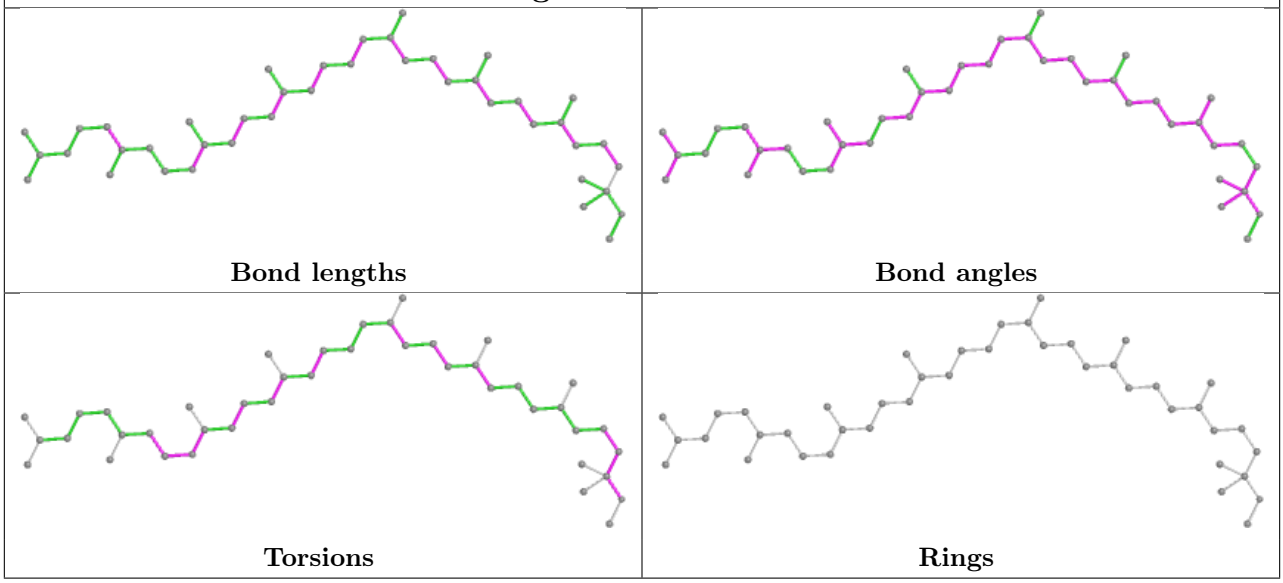


Torsions

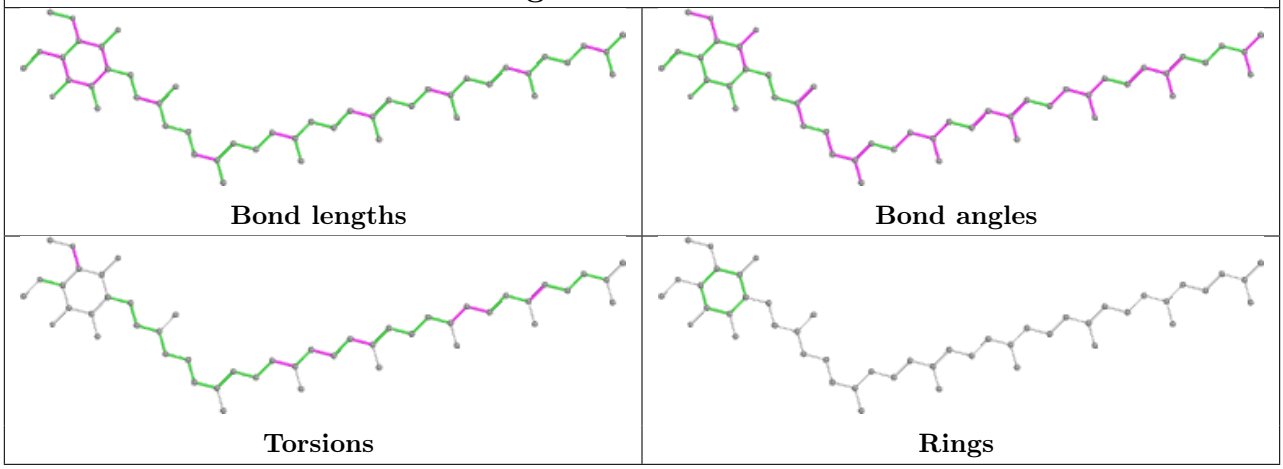


Rings

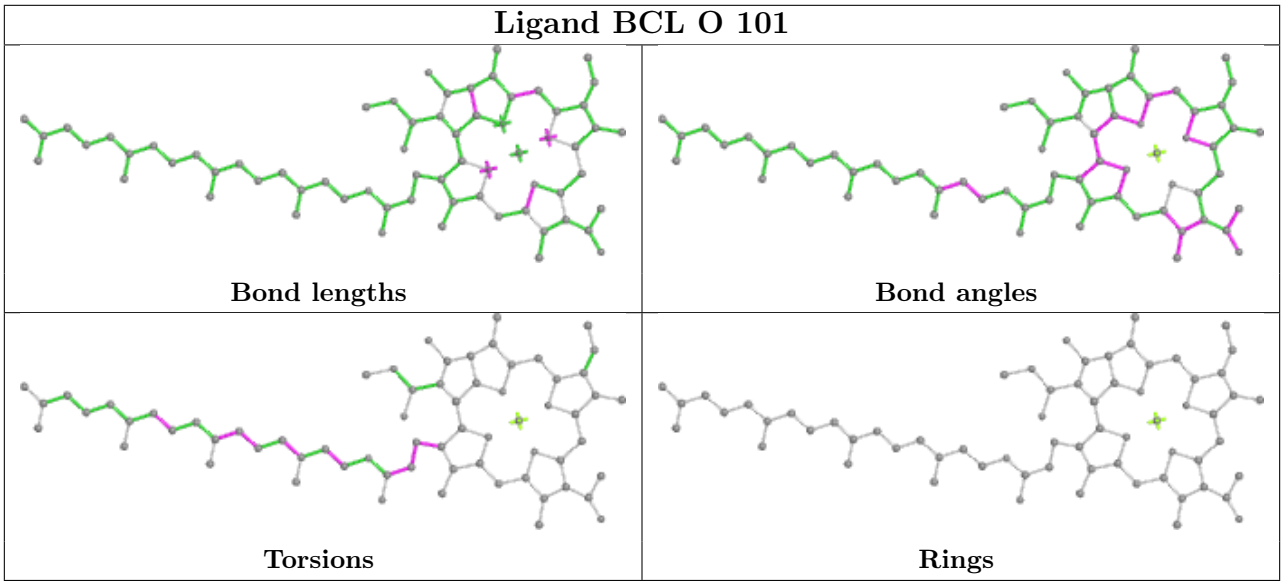
Ligand SPO r 102



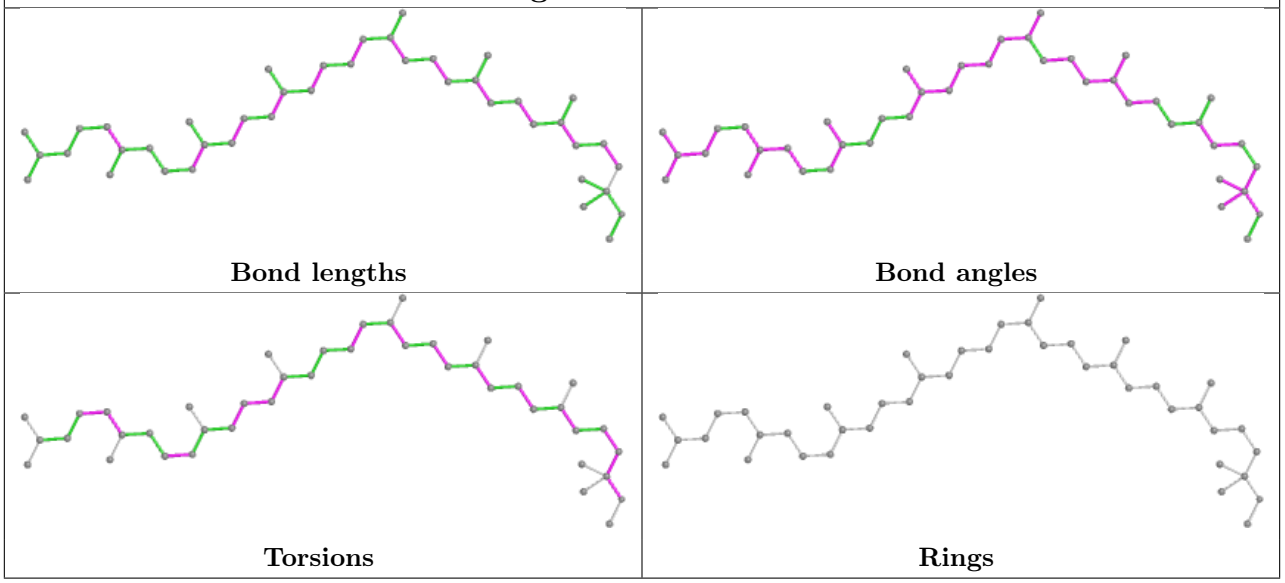
Ligand U10 M 405



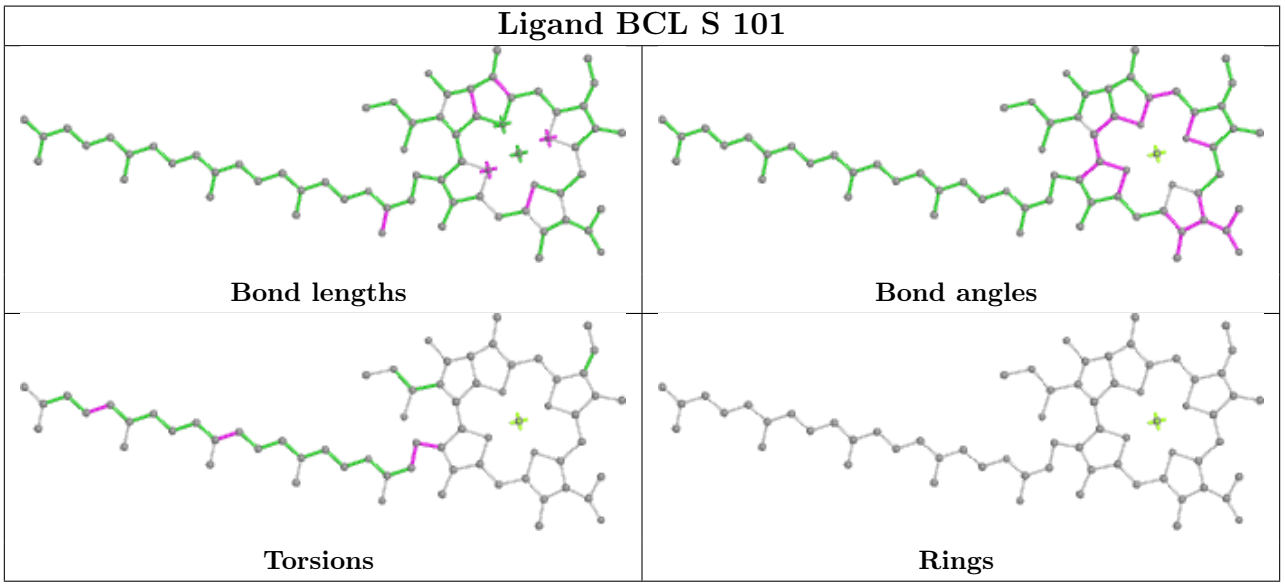
Ligand BCL O 101



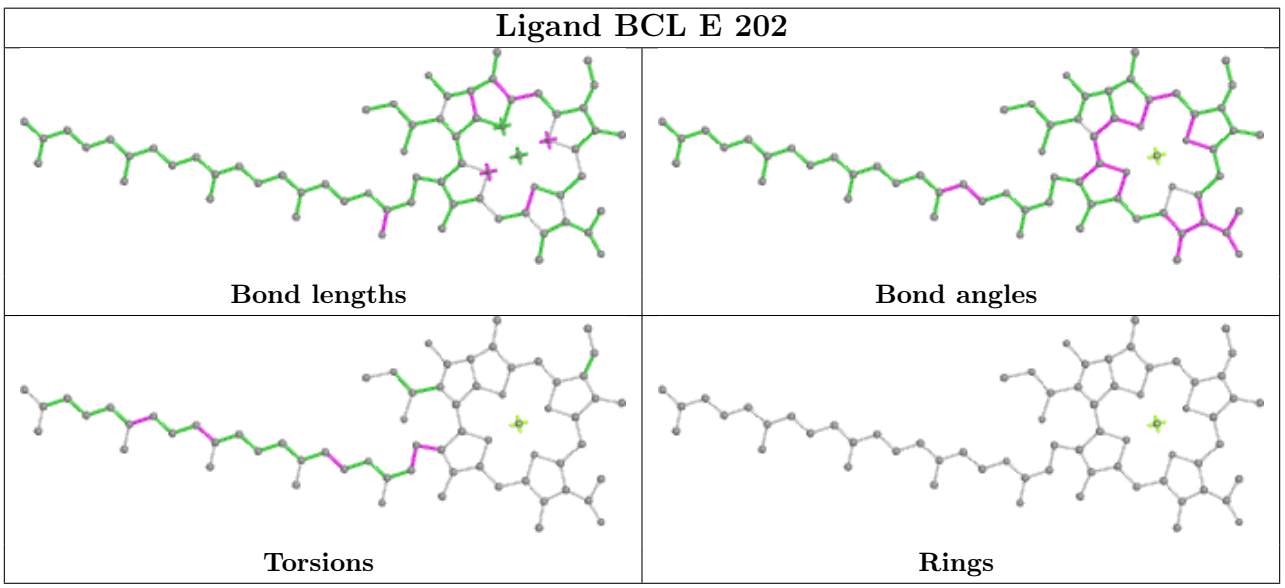
Ligand SPO k 102



Ligand BCL S 101



Ligand BCL E 202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

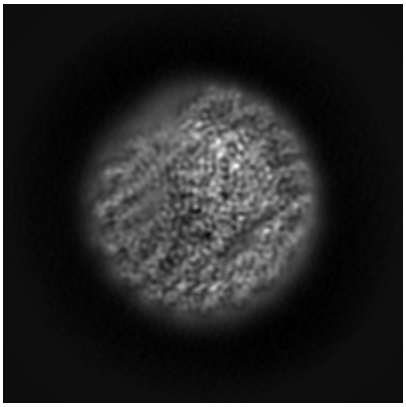
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30656. These allow visual inspection of the internal detail of the map and identification of artifacts.

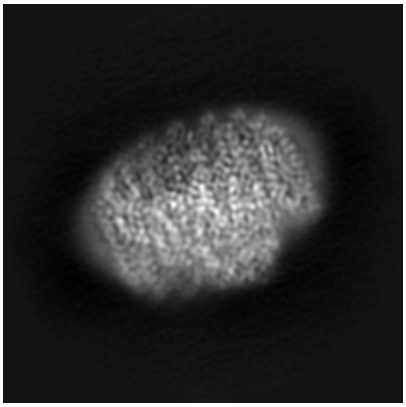
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

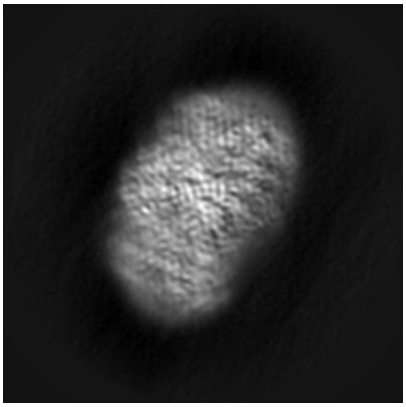
6.1.1 Primary map



X



Y

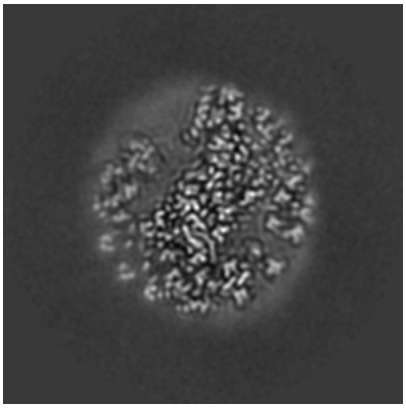


Z

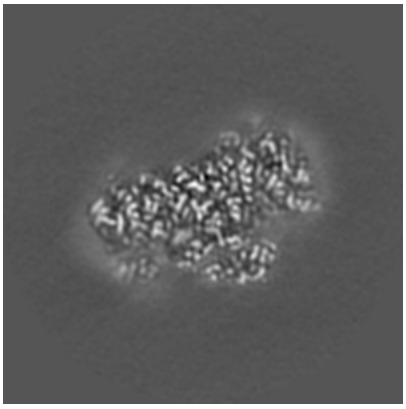
The images above show the map projected in three orthogonal directions.

6.2 Central slices

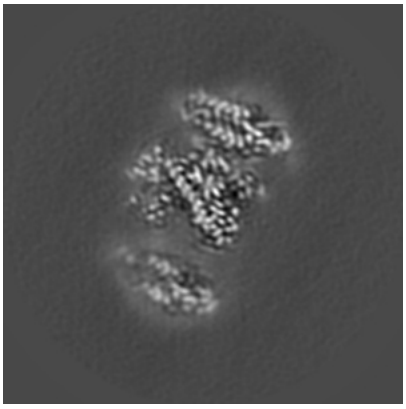
6.2.1 Primary map



X Index: 130



Y Index: 130

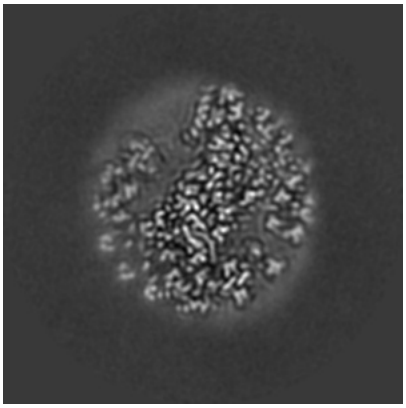


Z Index: 130

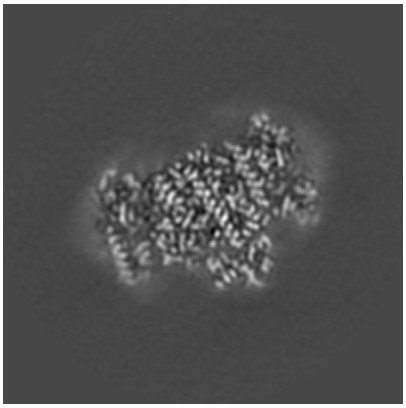
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

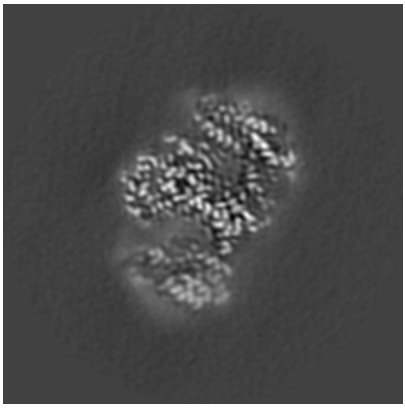
6.3.1 Primary map



X Index: 130



Y Index: 140

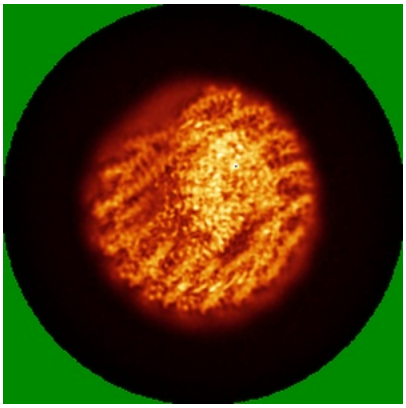


Z Index: 150

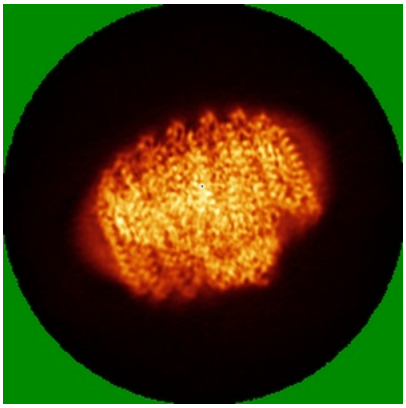
The images above show the largest variance slices of the map in three orthogonal directions.

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

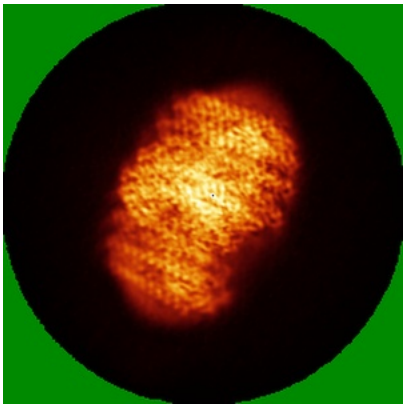
6.4.1 Primary map



X



Y

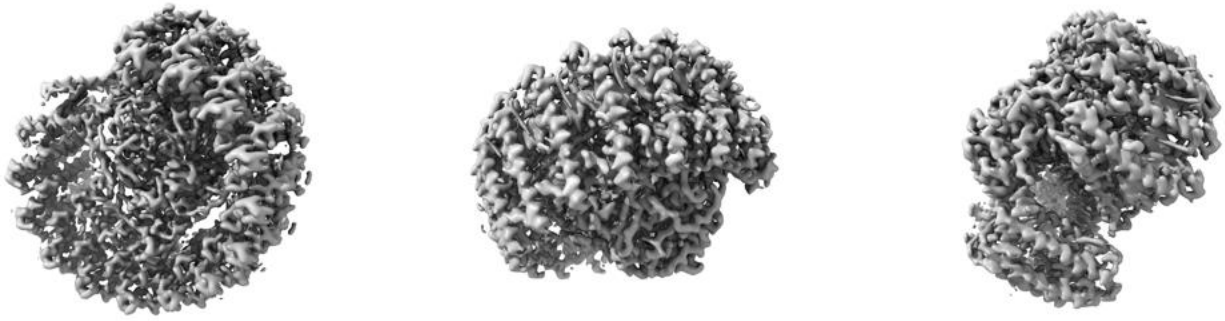


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

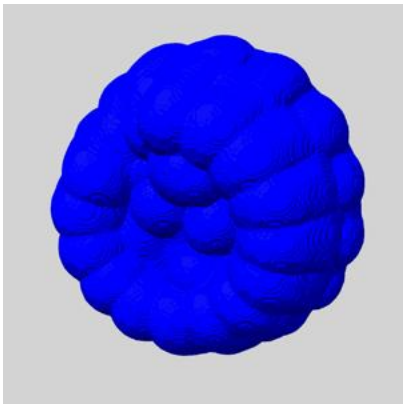
6.6 Mask visualisation (i)

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

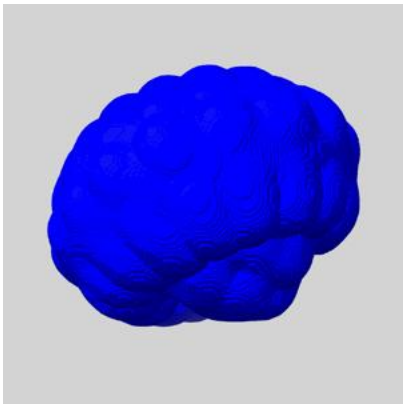
A mask typically either:

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

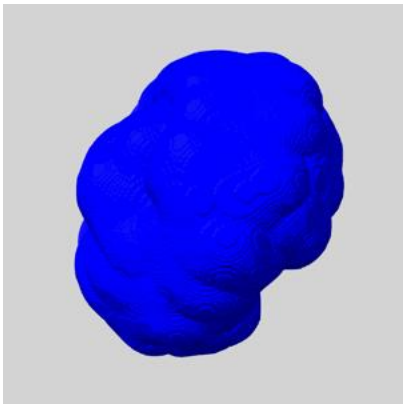
6.6.1 emd_30656_msk_1.map (i)



X



Y

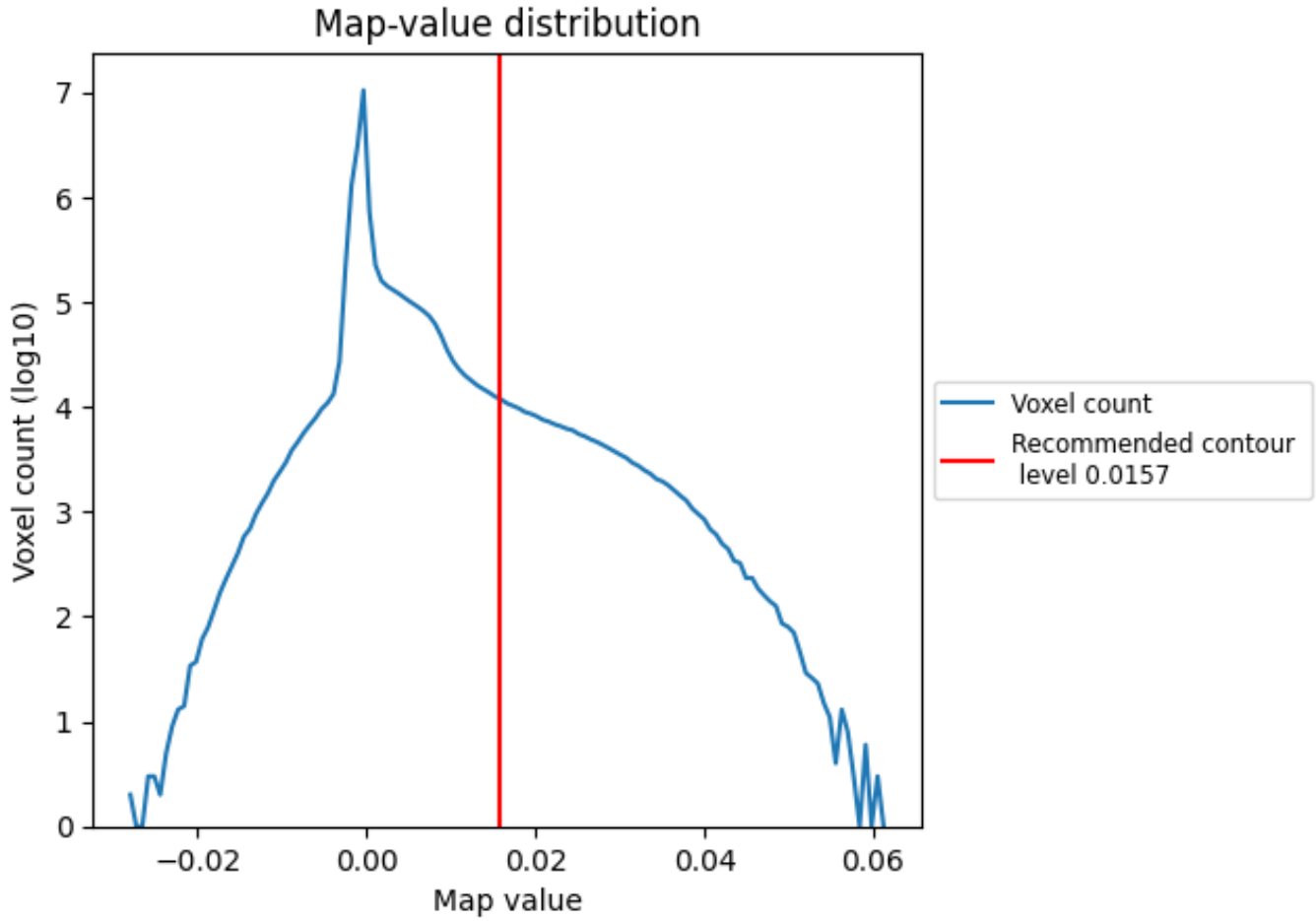


Z

7 Map analysis

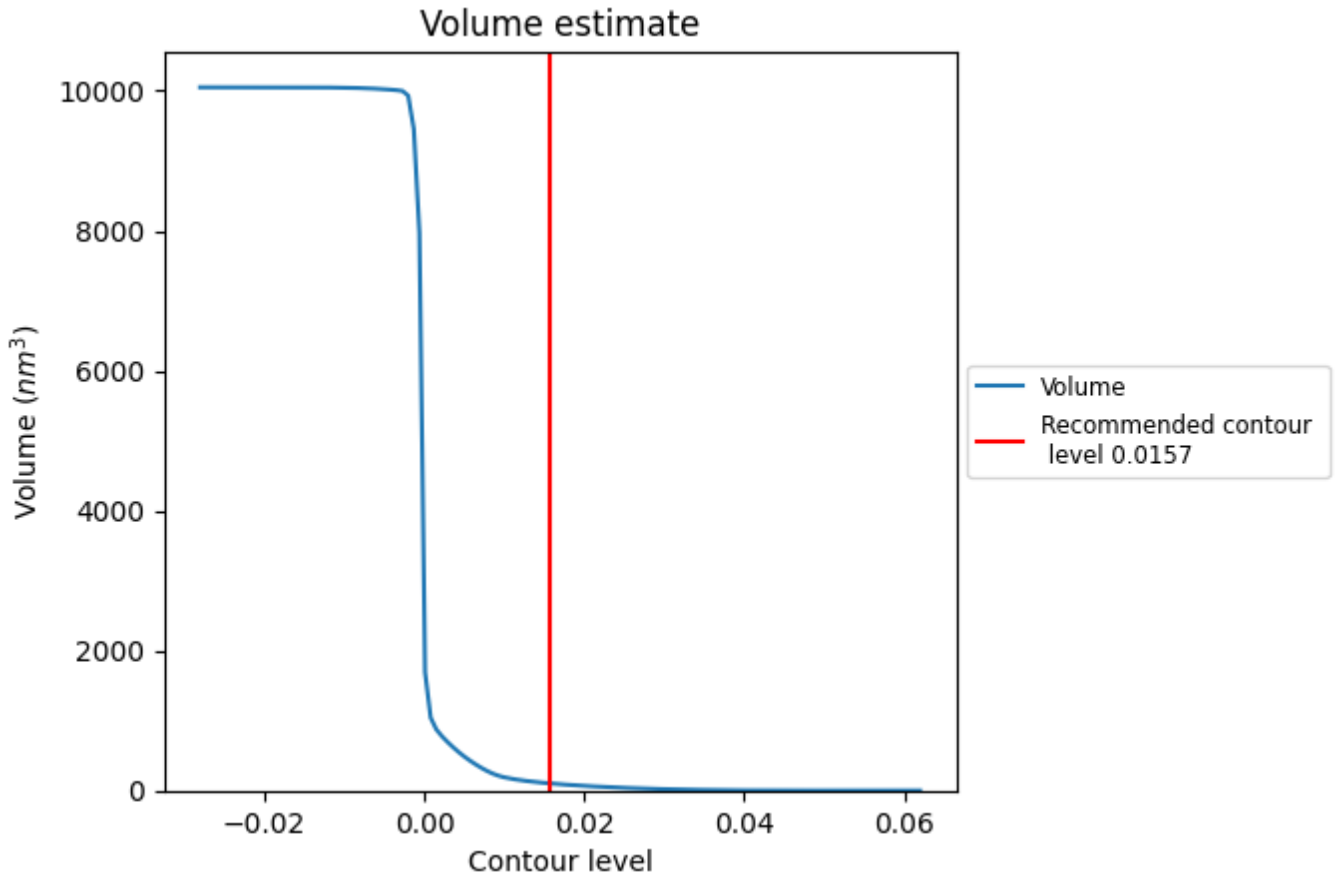
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

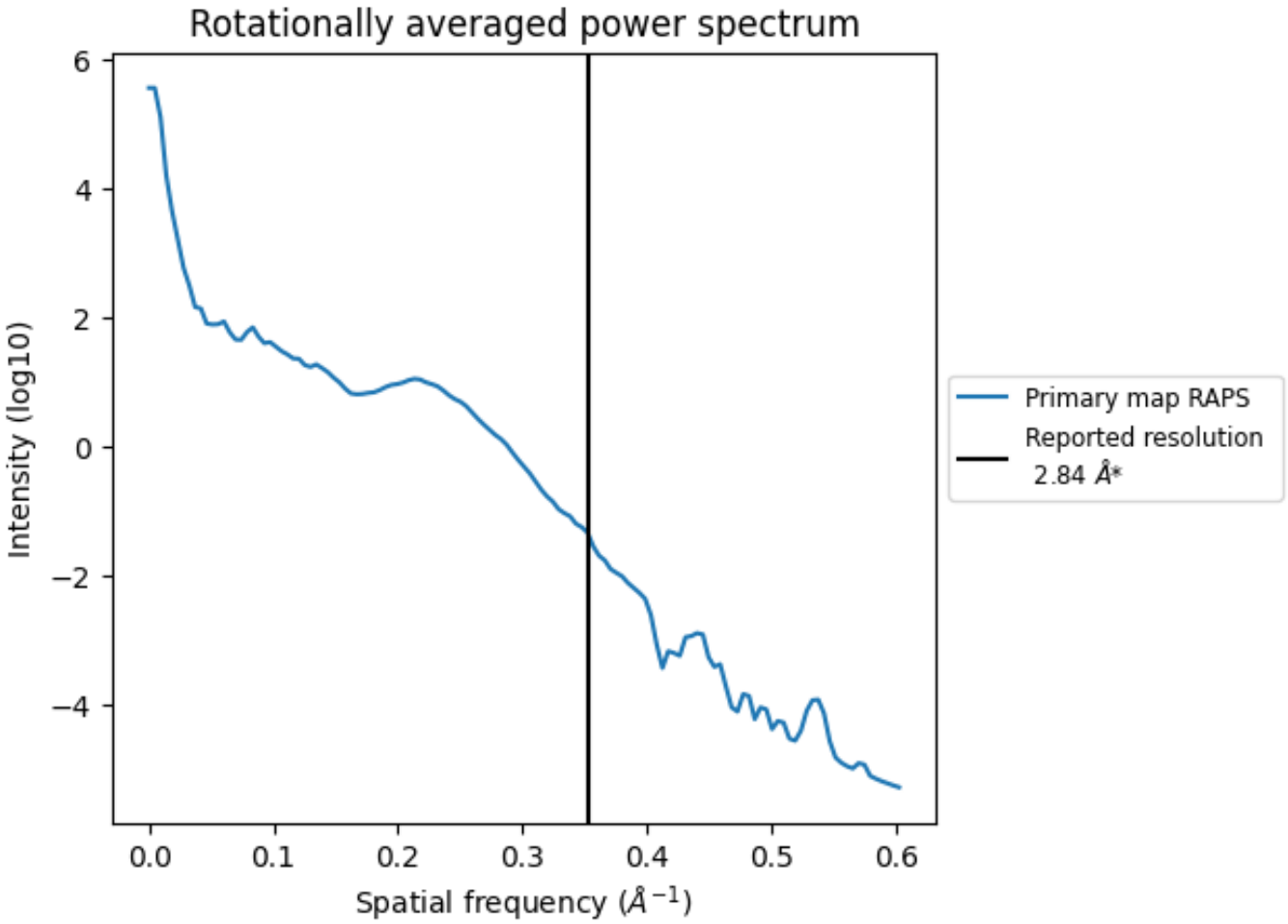
7.2 Volume estimate



The volume at the recommended contour level is 102 nm^3; this corresponds to an approximate mass of 93 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)

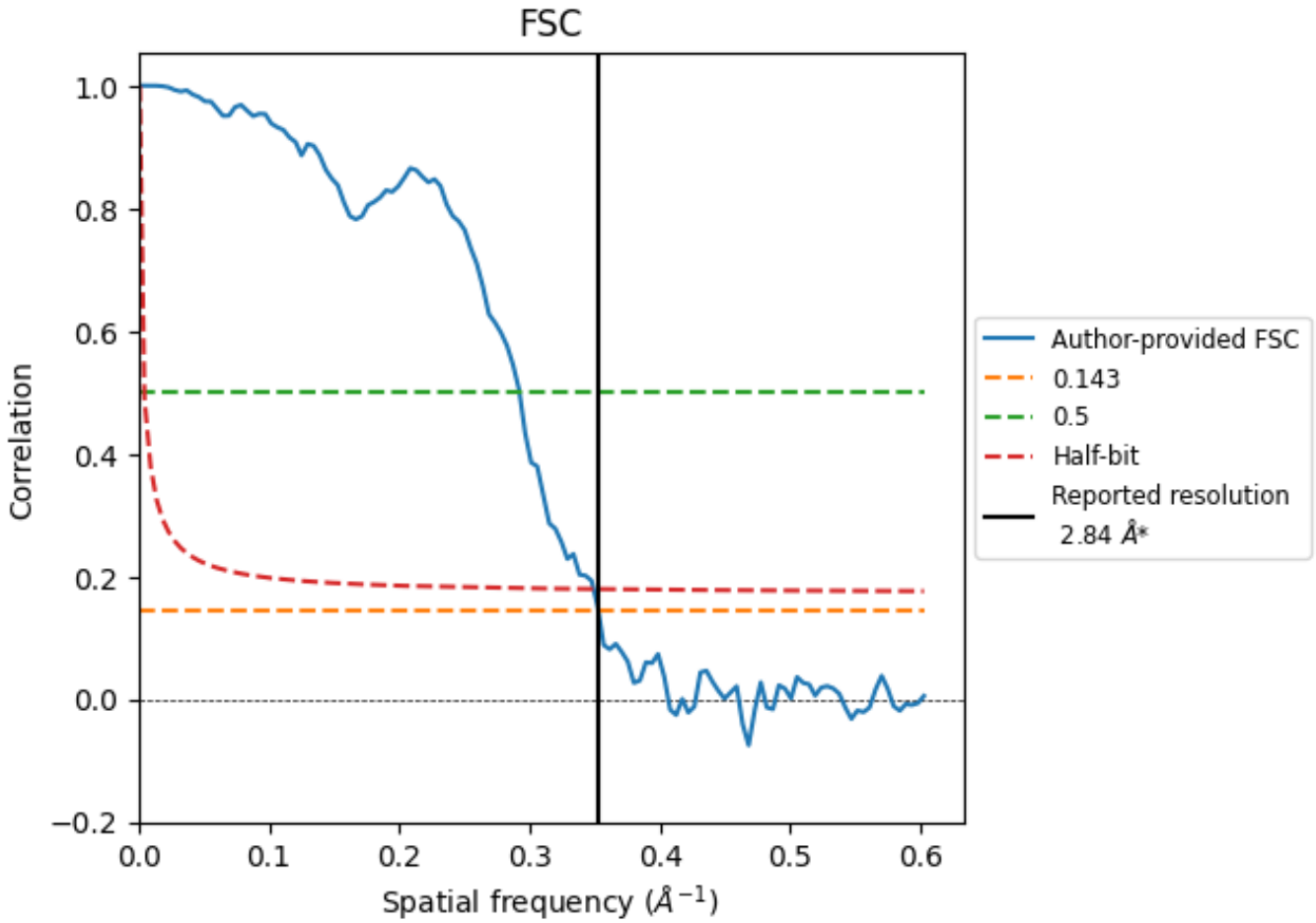


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

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 0.352 Å^{-1}

8.2 Resolution estimates (i)

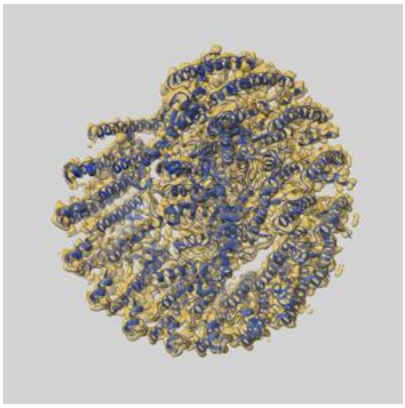
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.83	3.42	2.86
Unmasked-calculated*	-	-	-

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

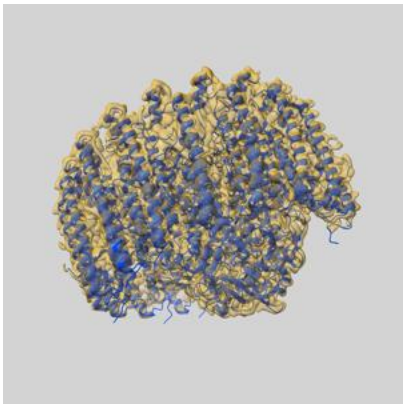
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30656 and PDB model 7DDQ. Per-residue inclusion information can be found in section 3 on page 13.

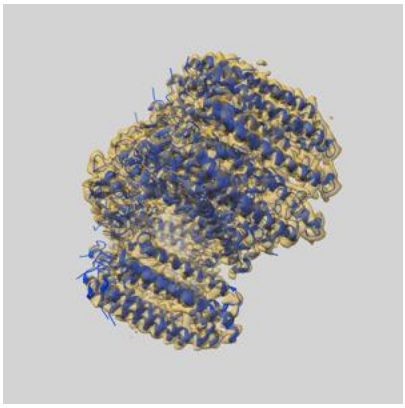
9.1 Map-model overlay



X



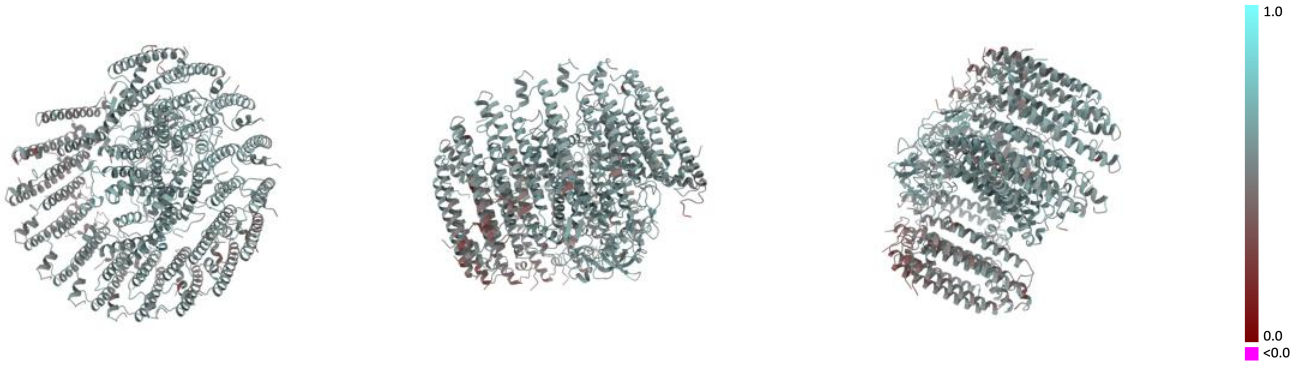
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

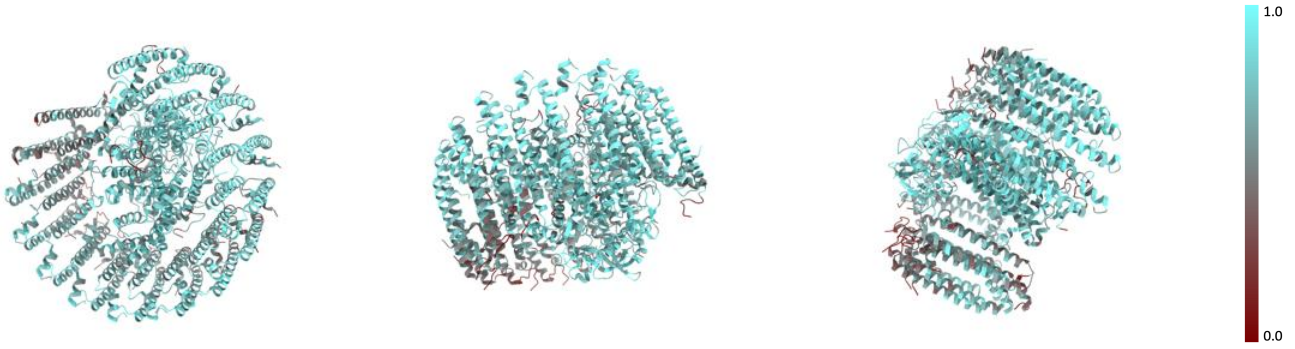
9.2 Q-score mapped to coordinate model



X Y Z

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

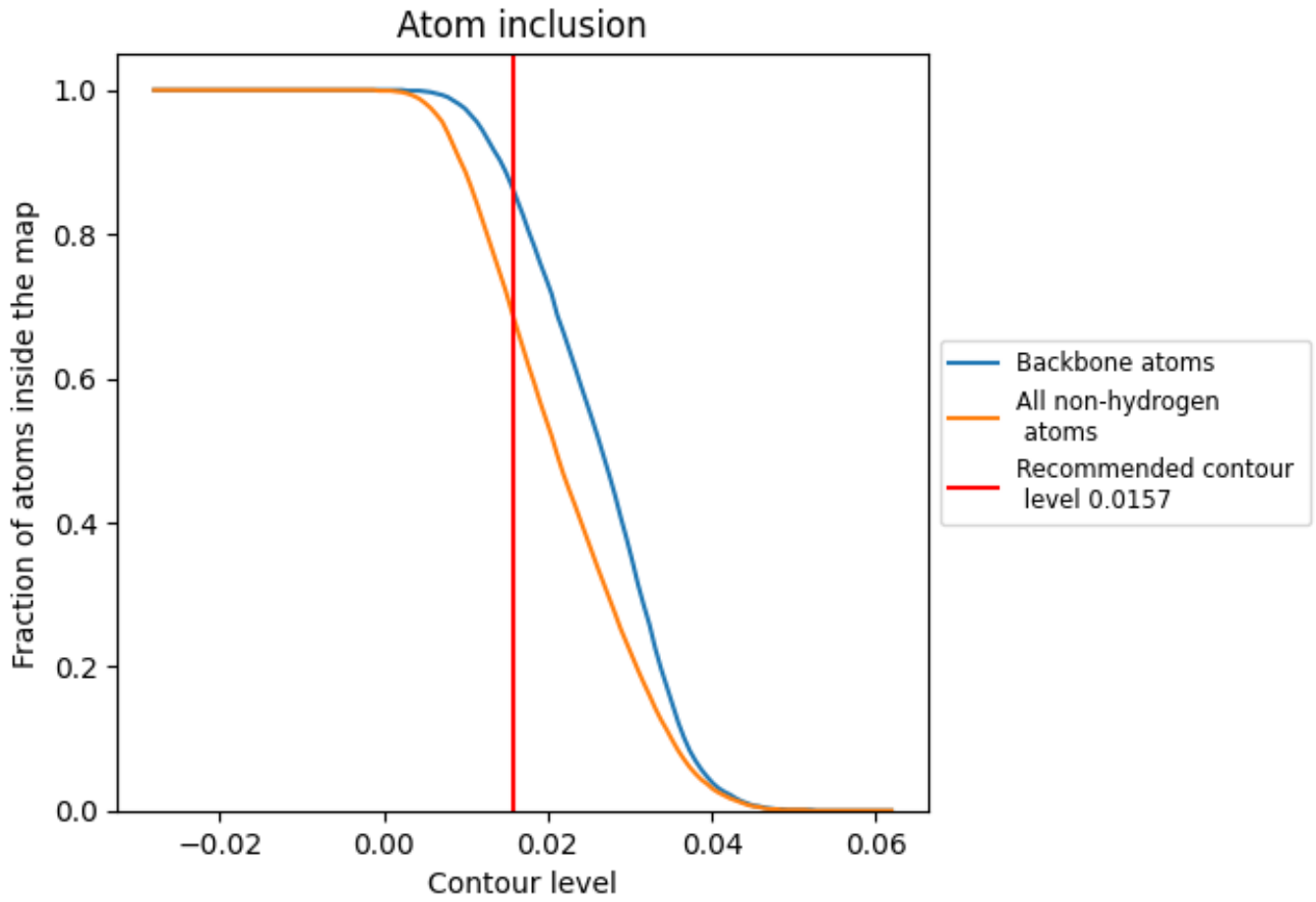
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0157).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 69% 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 (0.0157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6900	0.5380
A	0.7260	0.5420
B	0.7720	0.5540
D	0.7330	0.5600
E	0.6700	0.5270
F	0.6420	0.5260
G	0.6420	0.5080
H	0.7990	0.5740
I	0.5510	0.4670
J	0.6300	0.4970
K	0.6710	0.5240
L	0.8110	0.5900
M	0.8100	0.5890
N	0.5900	0.4990
O	0.5700	0.4800
R	0.5230	0.4660
S	0.5460	0.4510
T	0.5630	0.4640
U	0.5720	0.4900
X	0.5120	0.5240
a	0.7100	0.5580
b	0.7610	0.5710
d	0.7570	0.5680
e	0.7630	0.5680
f	0.7500	0.5520
g	0.6540	0.5190
i	0.6410	0.5110
j	0.6180	0.5120
k	0.6650	0.5340
n	0.6870	0.5380
o	0.6510	0.5120
r	0.5430	0.4730
s	0.5480	0.4870
t	0.5400	0.4910
u	0.5070	0.4940