



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 04:45 AM JST

PDB ID : 9LTI / pdb_00009lti
EMDB ID : EMD-63370
Title : Cryo-EM structure of LH1-RC from Ery. sanguineus
Authors : Yue, X.-Y.; Wang, G.-L.; Yu, L.-J.
Deposited on : 2025-02-06
Resolution : 2.27 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

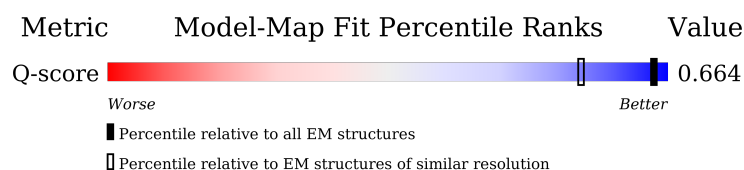
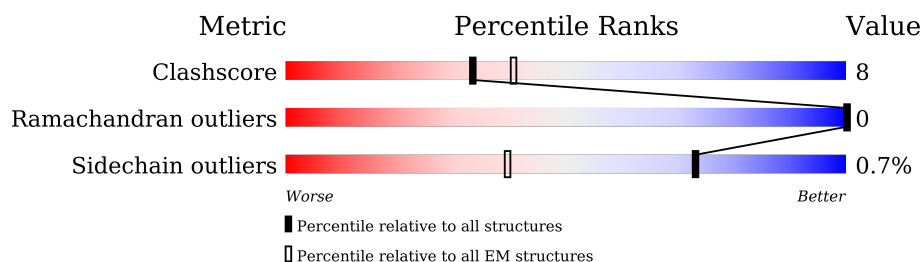
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.27 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.



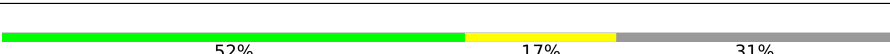
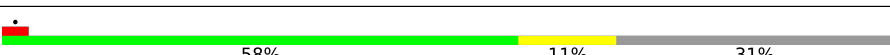
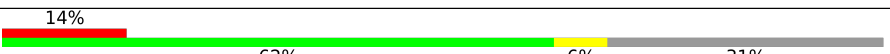
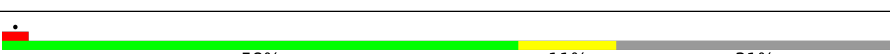
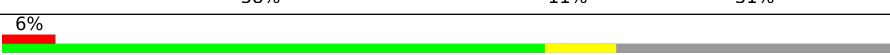
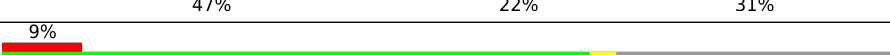
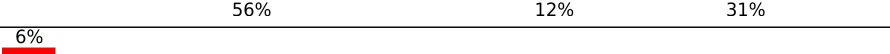
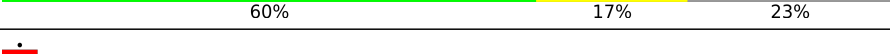
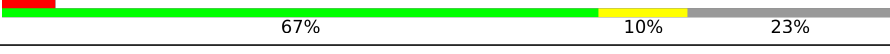
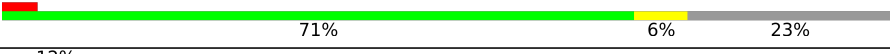
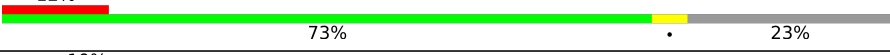
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3593 (1.77 - 2.77)

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 $\leq 5\%$. 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	64	
1	B	64	
1	C	64	
1	D	64	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	64	
1	F	64	
1	G	64	
1	I	64	
1	J	64	
1	K	64	
1	N	64	
1	O	64	
1	P	64	
1	Q	64	
1	R	64	
1	S	64	
2	a	52	
2	b	52	
2	c	52	
2	d	52	
2	e	52	
2	f	52	
2	g	52	
2	i	52	
2	j	52	
2	k	52	
2	n	52	
2	o	52	
2	p	52	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	q	52	
2	r	52	
2	s	52	
3	L	274	
4	H	268	
5	M	323	
6	T	135	

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
9	A1ELD	R	102	-	X	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 22831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Light-harvesting complex 1 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	B	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	C	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	D	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	E	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	F	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	G	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	Q	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	I	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	J	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	K	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	R	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	S	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	N	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	O	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	P	44	Total	C	N	O	S	0	0
			384	260	67	56	1		

- Molecule 2 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	a	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	p	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	o	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	n	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	s	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	r	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	k	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	j	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	c	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	d	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	e	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	f	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	g	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	q	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	i	40	Total	C	N	O	S	0	0
			326	223	49	52	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	273	Total	C	N	O	S	0	0
			2135	1431	340	358	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	265	Total	C	N	O	S	0	0
			2079	1343	347	380	9		

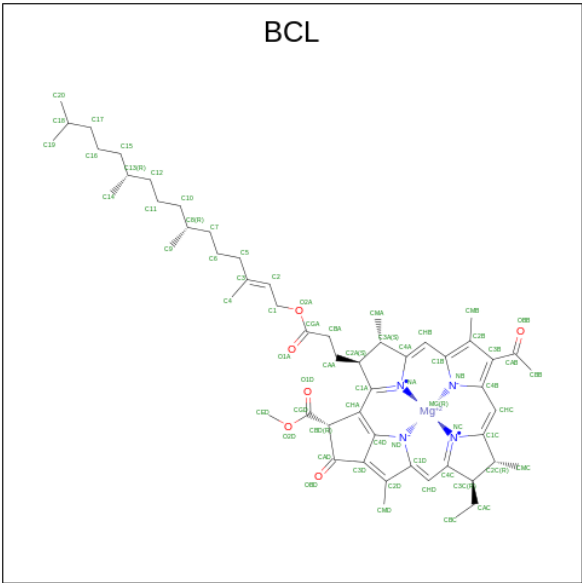
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	320	2543	1689	412	433	9	0	0

- Molecule 6 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	20	120	68	23	28	1	0	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	A	1	66	55	1	4	6	0
7	B	1	66	55	1	4	6	0
7	C	1	66	55	1	4	6	0
7	D	1	66	55	1	4	6	0
7	E	1	66	55	1	4	6	0
7	F	1	66	55	1	4	6	0

Continued on next page...

Continued from previous page...

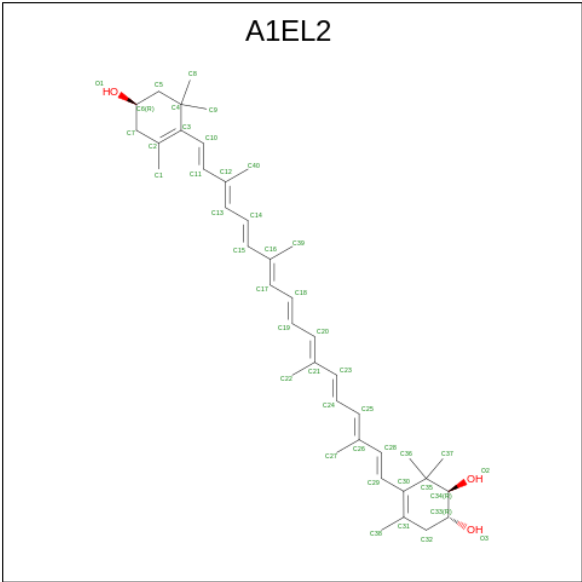
Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	c	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	d	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
7	e	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	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	q	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	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	

- Molecule 8 is (1 {R},2 {R})-3,3,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-4-ene-1,2-diol (CCD ID: A1EL2) (formula: C₄₀H₅₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			43	40	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total 43	C 40	O 3	0
8	C	1	Total 43	C 40	O 3	0
8	D	1	Total 43	C 40	O 3	0
8	E	1	Total 43	C 40	O 3	0
8	F	1	Total 43	C 40	O 3	0
8	G	1	Total 43	C 40	O 3	0
8	Q	1	Total 43	C 40	O 3	0
8	I	1	Total 43	C 40	O 3	0
8	J	1	Total 43	C 40	O 3	0
8	K	1	Total 43	C 40	O 3	0
8	N	1	Total 43	C 40	O 3	0
8	O	1	Total 43	C 40	O 3	0
8	P	1	Total 43	C 40	O 3	0
8	r	1	Total 43	C 40	O 3	0
8	r	1	Total 43	C 40	O 3	0

- Molecule 9 is (2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E},16 {E})-2-[(1 {Z},3 {Z},5 {E})-8-methoxy-4,8-dimethyl-nona-1,3,5-trienyl]-6,11,15-trimethyl-17-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]heptadeca-2,4,6,8,10,12,14,16-octaenal (CCD ID: A1ELD) (formula: C₄₁H₅₆O₃) (labeled as "Ligand of Interest" by depositor).

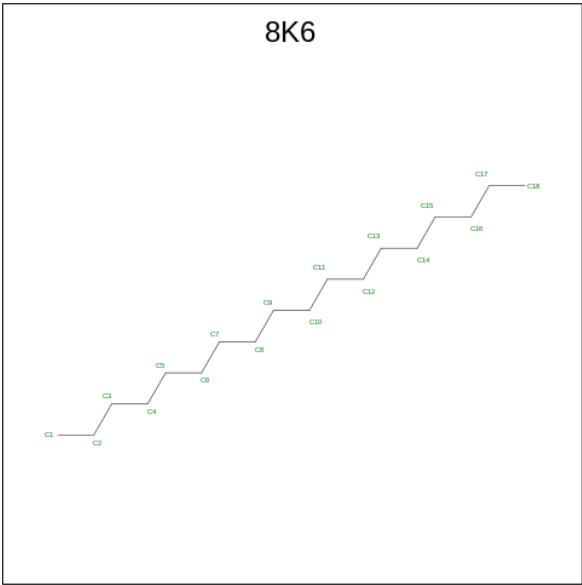


Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
9	g	1	Total	C	O	0
			44	41	3	
9	q	1	Total	C	O	0
			44	41	3	

- Molecule 10 is Octadecane (CCD ID: 8K6) (formula: C₁₈H₃₈).



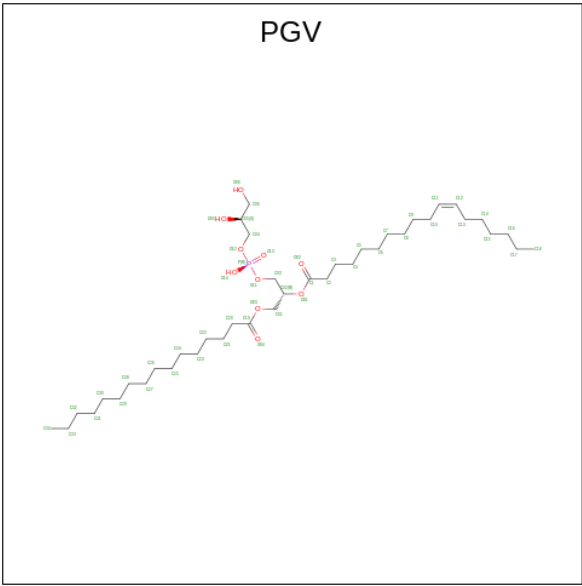
Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	C	0
			9	9	
10	Q	1	Total	C	0
			18	18	
10	Q	1	Total	C	0
			18	18	
10	S	1	Total	C	0
			13	13	
10	f	1	Total	C	0
			14	14	
10	L	1	Total	C	0
			12	12	
10	L	1	Total	C	0
			14	14	
10	L	1	Total	C	0
			10	10	
10	L	1	Total	C	0
			15	15	

Continued on next page...

Continued from previous page...

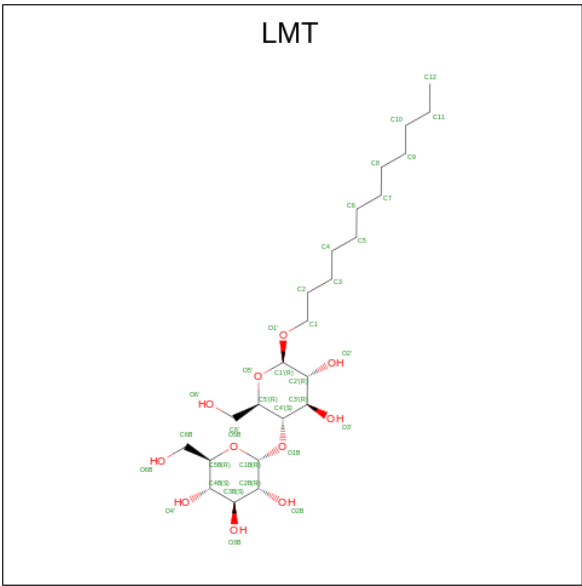
Mol	Chain	Residues	Atoms	AltConf
10	H	1	Total C 18 18	0
10	M	1	Total C 15 15	0

- Molecule 11 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).



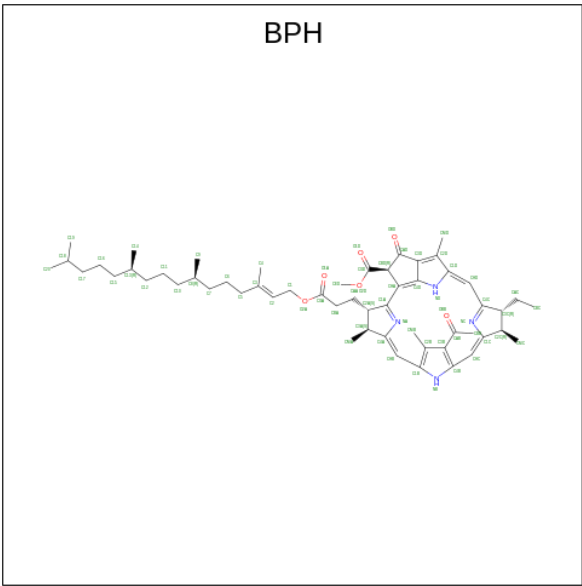
Mol	Chain	Residues	Atoms	AltConf
11	D	1	Total C O P 51 40 10 1	0
11	F	1	Total C O P 51 40 10 1	0
11	G	1	Total C O P 23 14 8 1	0
11	L	1	Total C O P 21 12 8 1	0
11	L	1	Total C O P 29 18 10 1	0
11	M	1	Total C O P 38 29 8 1	0
11	T	1	Total C O 20 16 4	0
11	T	1	Total C O P 30 21 8 1	0

- Molecule 12 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



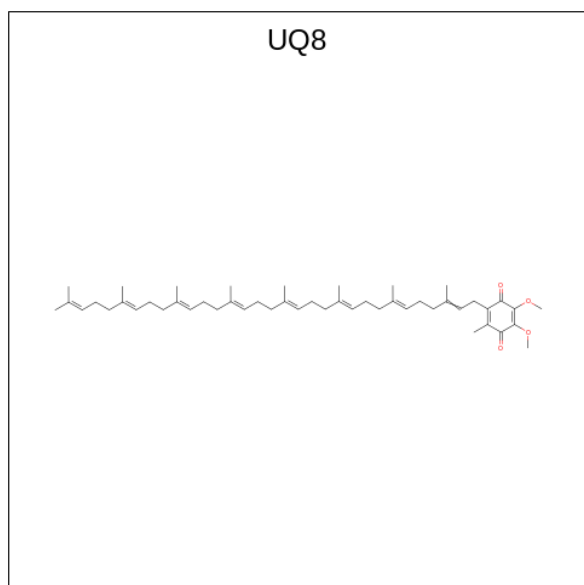
Mol	Chain	Residues	Atoms			AltConf
12	G	1	Total	C	O	0
			30	19	11	
12	N	1	Total	C	O	0
			26	15	11	
12	L	1	Total	C	O	0
			28	17	11	

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄) (labeled as "Ligand of Interest" by depositor).

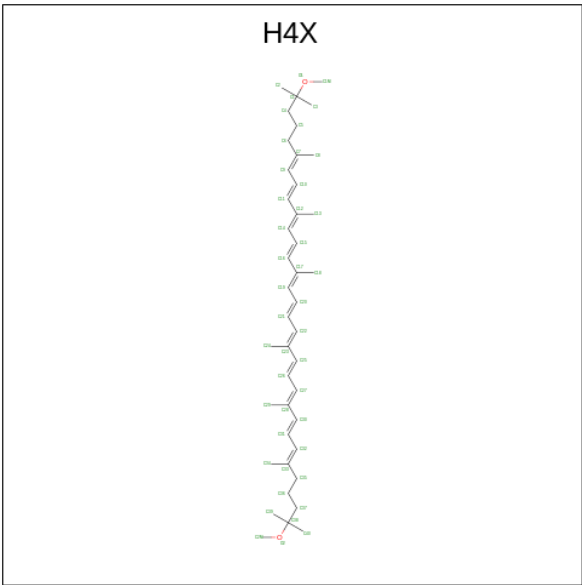


Mol	Chain	Residues	Atoms			AltConf
14	L	1	Total	C	O	0
			19	15	4	
14	L	1	Total	C	O	0
			18	14	4	
14	M	1	Total	C	O	0
			53	49	4	

- Molecule 15 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

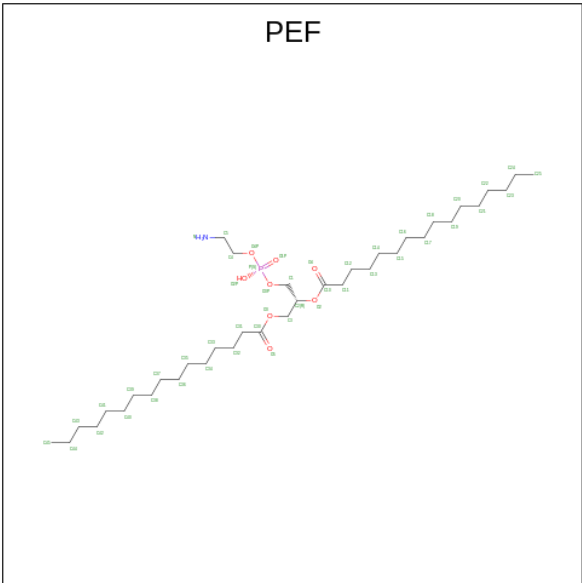
Mol	Chain	Residues	Atoms		AltConf
15	M	1	Total	Fe	0
			1	1	

- Molecule 16 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E},26 {E})-2,31-dimethoxy-2,6,10,14,19,23,27,31-octamethyl-dotriaconta-6,8,10,12,14,16,18,20,22,24,26-undecaene (CCD ID: H4X) (formula: C₄₂H₆₄O₂) (labeled as "Ligand of Interest" by depositor).



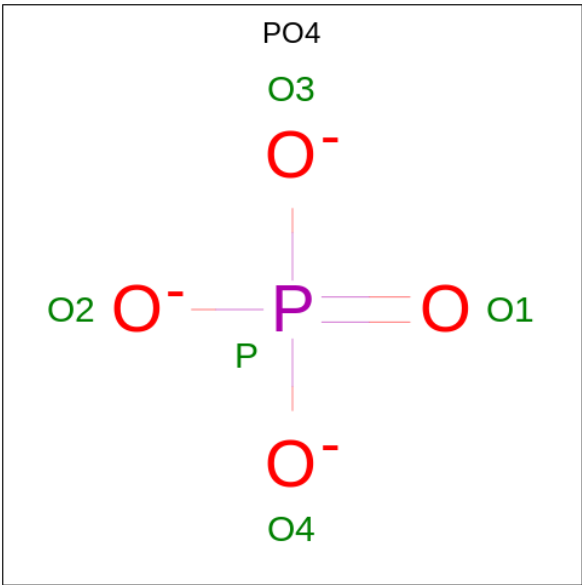
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			44	42	2	

- Molecule 17 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



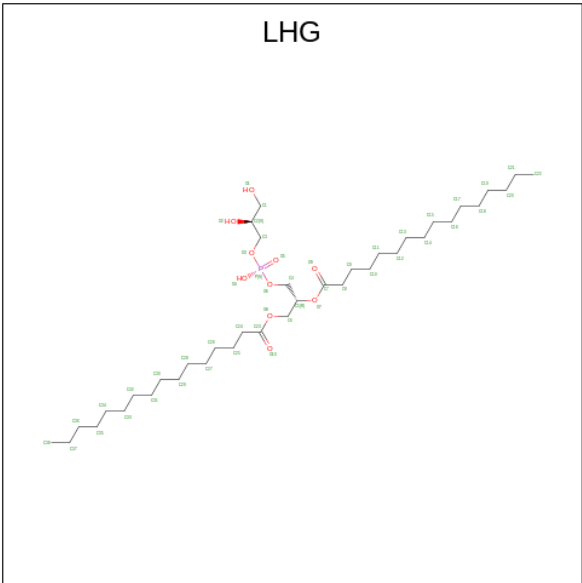
Mol	Chain	Residues	Atoms					AltConf
17	M	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 18 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	O	P	0
			5	4	1	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

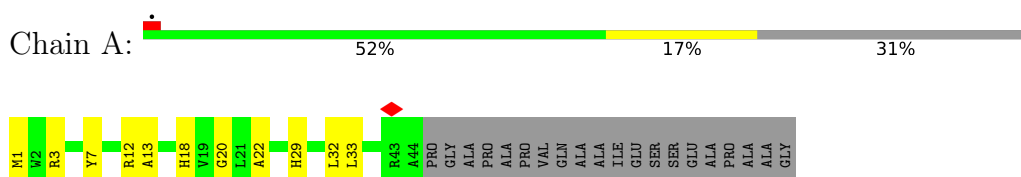


Mol	Chain	Residues	Atoms			AltConf
19	T	1	Total	C	O	0
			10	9	1	

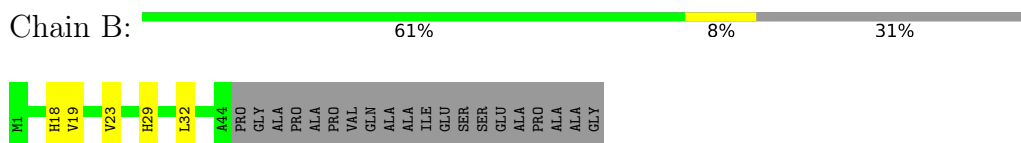
3 Residue-property plots [i](#)

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

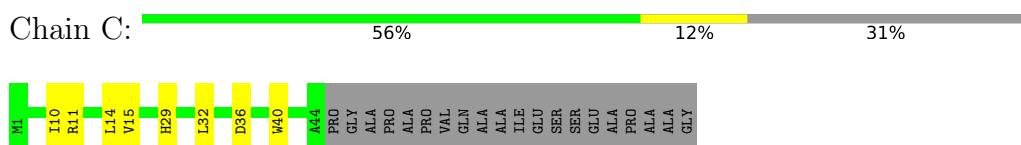
- Molecule 1: Light-harvesting complex 1 alpha chain



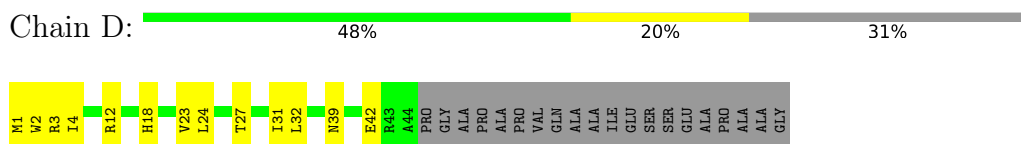
- Molecule 1: Light-harvesting complex 1 alpha chain



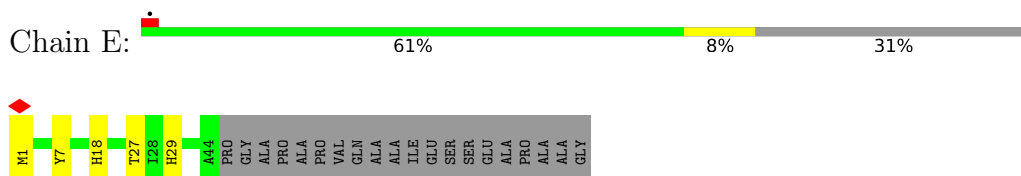
- Molecule 1: Light-harvesting complex 1 alpha chain



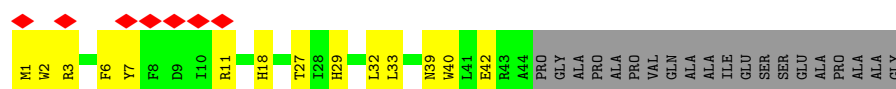
- Molecule 1: Light-harvesting complex 1 alpha chain



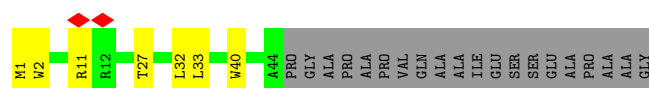
- Molecule 1: Light-harvesting complex 1 alpha chain



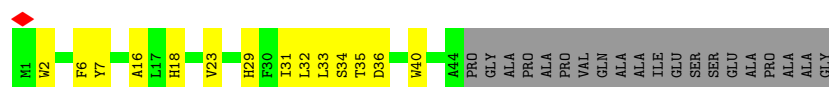
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



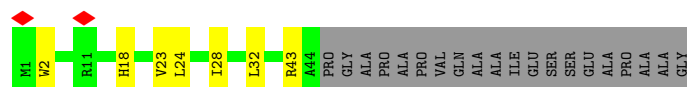
- Molecule 1: Light-harvesting complex 1 alpha chain



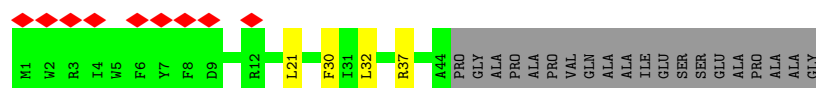
- Molecule 1: Light-harvesting complex 1 alpha chain



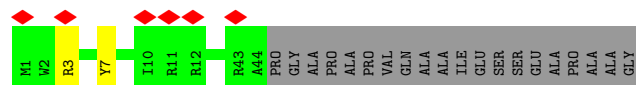
- Molecule 1: Light-harvesting complex 1 alpha chain



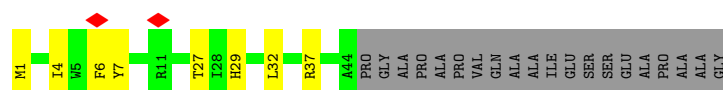
- Molecule 1: Light-harvesting complex 1 alpha chain



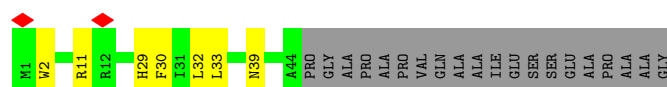
- Molecule 1: Light-harvesting complex 1 alpha chain



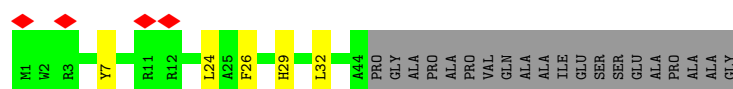
- Molecule 1: Light-harvesting complex 1 alpha chain



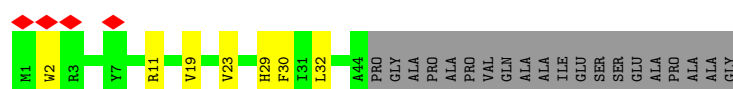
- Molecule 1: Light-harvesting complex 1 alpha chain



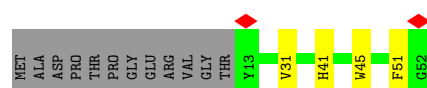
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 2: Antenna complex alpha/beta subunit

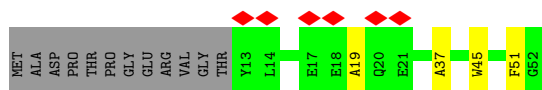


- Molecule 2: Antenna complex alpha/beta subunit

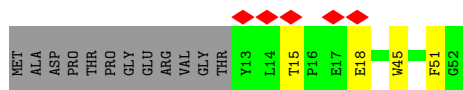


- Molecule 2: Antenna complex alpha/beta subunit

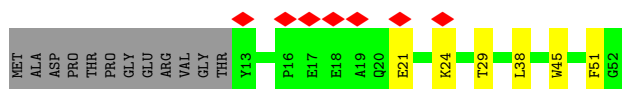




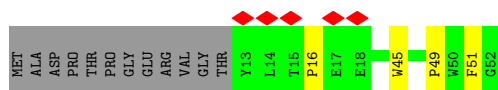
- Molecule 2: Antenna complex alpha/beta subunit



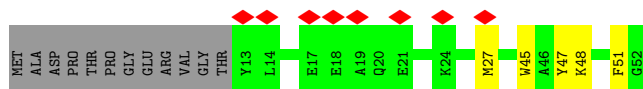
- Molecule 2: Antenna complex alpha/beta subunit



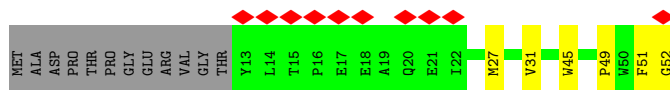
- Molecule 2: Antenna complex alpha/beta subunit



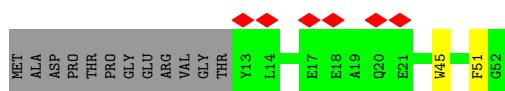
- Molecule 2: Antenna complex alpha/beta subunit



- Molecule 2: Antenna complex alpha/beta subunit



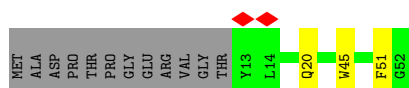
- Molecule 2: Antenna complex alpha/beta subunit



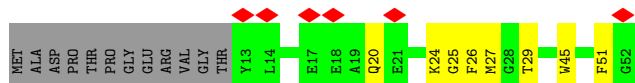
- Molecule 2: Antenna complex alpha/beta subunit



- Molecule 2: Antenna complex alpha/beta subunit



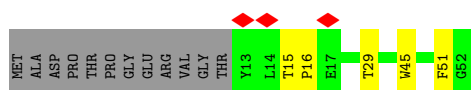
- Molecule 2: Antenna complex alpha/beta subunit



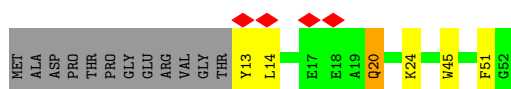
- Molecule 2: Antenna complex alpha/beta subunit



- Molecule 2: Antenna complex alpha/beta subunit



- Molecule 2: Antenna complex alpha/beta subunit



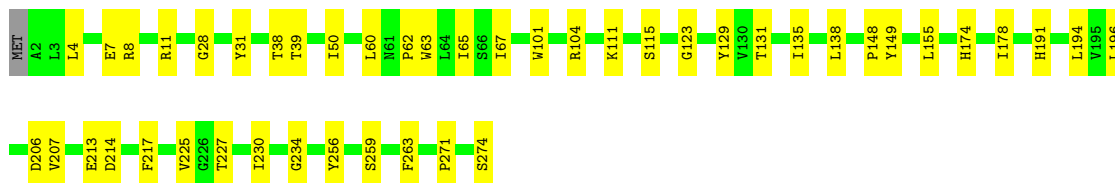
- Molecule 2: Antenna complex alpha/beta subunit





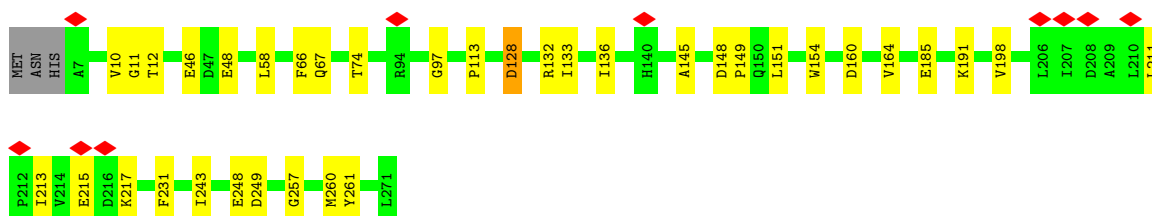
• Molecule 3: Reaction center protein L chain

Chain L: 83% 16%



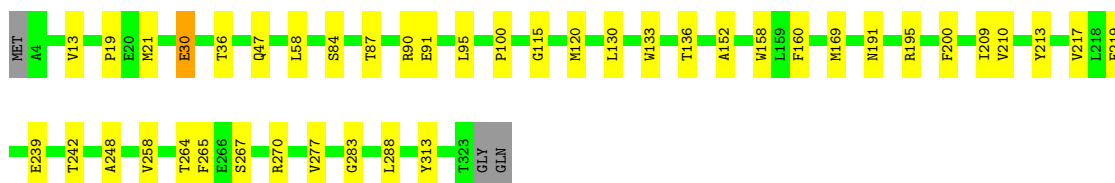
• Molecule 4: Photosynthetic reaction center H subunit

Chain H: 85% 13%



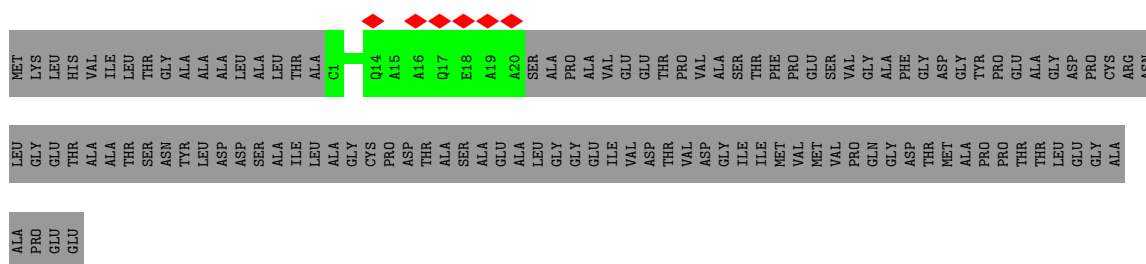
• Molecule 5: Reaction center protein M chain

Chain M: 86% 13%



• Molecule 6: Secreted protein

Chain T: 15% 85%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.532	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0961	Depositor
Map size ($\text{\AA}$)	323.2, 323.2, 323.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, 8K6, FE, A1ELD, BPH, PO4, H4X, BCL, UQ8, PEF, LHG, A1EL2, PGV

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	0.12	0/397	0.26	0/540
1	B	0.10	0/397	0.19	0/540
1	C	0.58	0/397	0.87	0/540
1	D	0.09	0/397	0.20	0/540
1	E	0.09	0/397	0.20	0/540
1	F	0.09	0/397	0.25	0/540
1	G	0.09	0/397	0.19	0/540
1	I	0.09	0/397	0.21	0/540
1	J	0.18	0/397	0.27	0/540
1	K	0.54	0/397	0.72	0/540
1	N	0.09	0/397	0.19	0/540
1	O	0.07	0/397	0.18	0/540
1	P	0.19	0/397	0.32	0/540
1	Q	0.09	0/397	0.20	0/540
1	R	0.10	0/397	0.28	0/540
1	S	0.10	0/397	0.28	0/540
2	a	0.14	0/339	0.27	0/462
2	b	0.12	0/339	0.25	0/462
2	c	0.13	0/339	0.26	0/462
2	d	0.11	0/339	0.21	0/462
2	e	0.12	0/339	0.25	0/462
2	f	0.13	0/339	0.28	0/462
2	g	0.13	0/339	0.28	0/462
2	i	0.10	0/339	0.21	0/462
2	j	0.12	0/339	0.24	0/462
2	k	0.11	0/339	0.25	0/462
2	n	0.12	0/339	0.24	0/462
2	o	0.10	0/339	0.21	0/462
2	p	0.11	0/339	0.23	0/462
2	q	0.12	0/339	0.22	0/462
2	r	0.11	0/339	0.26	0/462
2	s	0.11	0/339	0.20	0/462

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	L	0.14	0/2214	0.30	0/3033
4	H	0.23	0/2139	0.36	1/2912 (0.0%)
5	M	0.13	0/2640	0.27	0/3612
6	T	0.06	0/119	0.17	0/161
All	All	0.18	0/18888	0.31	1/25750 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	198	VAL	N-CA-C	-5.57	107.30	112.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	384	0	389	12	0
1	B	384	0	389	5	0
1	C	384	0	389	8	0
1	D	384	0	389	13	0
1	E	384	0	389	10	0
1	F	384	0	389	16	0
1	G	384	0	389	6	0
1	I	384	0	389	12	0
1	J	384	0	389	10	0
1	K	384	0	389	3	0
1	N	384	0	389	11	0
1	O	384	0	389	5	0
1	P	384	0	389	7	0
1	Q	384	0	389	14	0
1	R	384	0	389	12	0
1	S	384	0	389	7	0
2	a	326	0	317	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	326	0	317	3	0
2	c	326	0	317	8	0
2	d	326	0	317	1	0
2	e	326	0	317	8	0
2	f	326	0	317	10	0
2	g	326	0	317	6	0
2	i	326	0	317	2	0
2	j	326	0	317	1	0
2	k	326	0	317	6	0
2	n	326	0	317	4	0
2	o	326	0	317	2	0
2	p	326	0	317	3	0
2	q	326	0	317	3	0
2	r	326	0	317	9	0
2	s	326	0	317	4	0
3	L	2135	0	2086	43	0
4	H	2079	0	2037	25	0
5	M	2543	0	2434	36	0
6	T	120	0	103	0	0
7	A	66	0	74	2	0
7	B	66	0	74	4	0
7	C	66	0	74	5	0
7	D	66	0	74	0	0
7	E	66	0	74	3	0
7	F	66	0	74	3	0
7	G	66	0	74	1	0
7	I	66	0	74	3	0
7	J	66	0	74	1	0
7	K	66	0	74	1	0
7	L	132	0	148	9	0
7	M	132	0	148	4	0
7	N	66	0	74	3	0
7	O	66	0	74	2	0
7	P	66	0	74	3	0
7	Q	66	0	74	1	0
7	R	66	0	74	2	0
7	S	66	0	74	3	0
7	a	66	0	74	4	0
7	b	66	0	74	8	0
7	c	66	0	74	3	0
7	d	66	0	74	4	0
7	e	66	0	74	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	f	66	0	74	5	0
7	g	66	0	74	2	0
7	i	66	0	74	0	0
7	j	66	0	74	2	0
7	k	66	0	74	3	0
7	n	66	0	74	5	0
7	o	66	0	74	4	0
7	p	66	0	74	3	0
7	q	66	0	74	3	0
7	r	66	0	74	2	0
7	s	66	0	74	3	0
8	A	43	0	0	1	0
8	B	43	0	0	1	0
8	C	43	0	0	0	0
8	D	43	0	0	1	0
8	E	43	0	0	1	0
8	F	43	0	0	1	0
8	G	43	0	0	0	0
8	I	43	0	0	4	0
8	J	43	0	0	3	0
8	K	43	0	0	1	0
8	N	43	0	0	0	0
8	O	43	0	0	0	0
8	P	43	0	0	1	0
8	Q	43	0	0	1	0
8	r	86	0	0	9	0
9	A	44	0	0	0	0
9	B	44	0	0	1	0
9	C	44	0	0	0	0
9	J	44	0	0	0	0
9	O	44	0	0	1	0
9	R	88	0	0	23	0
9	b	44	0	0	0	0
9	d	44	0	0	1	0
9	e	44	0	0	7	0
9	f	44	0	0	7	0
9	g	44	0	0	3	0
9	j	44	0	0	0	0
9	o	44	0	0	1	0
9	q	44	0	0	0	0
9	r	44	0	0	1	0
10	C	9	0	14	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	18	0	38	0	0
10	L	51	0	92	11	0
10	M	15	0	29	1	0
10	Q	36	0	76	8	0
10	S	13	0	25	1	0
10	f	14	0	27	0	0
11	D	51	0	76	8	0
11	F	51	0	76	4	0
11	G	23	0	21	1	0
11	L	50	0	43	4	0
11	M	38	0	50	3	0
11	T	50	0	54	3	0
12	G	30	0	32	0	0
12	L	28	0	29	2	0
12	N	26	0	24	1	0
13	L	130	0	150	6	0
14	L	37	0	32	6	0
14	M	53	0	74	1	0
15	M	1	0	0	0	0
16	M	44	0	0	0	0
17	M	43	0	62	1	0
18	M	5	0	0	0	0
19	T	10	0	14	3	0
All	All	22831	0	21658	370	0

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

All (370) 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)
9:R:102:A1ELD:C35	9:R:102:A1ELD:C36	1.76	1.59
9:R:102:A1ELD:C39	9:R:102:A1ELD:C37	1.80	1.59
9:R:102:A1ELD:C39	1:N:33:LEU:CD1	2.15	1.24
9:R:102:A1ELD:C39	1:N:33:LEU:HD11	1.76	1.14
9:R:102:A1ELD:C39	1:N:33:LEU:HD12	1.80	1.11
1:J:18:HIS:NE2	8:J:102:A1EL2:O1	1.87	1.05
1:R:7:TYR:CE2	9:R:102:A1ELD:C45	2.41	1.03
2:g:29:THR:HG21	9:g:101:A1ELD:C13	1.91	1.00
1:R:3:ARG:HB2	9:R:102:A1ELD:C6	1.98	0.92
2:r:47:TYR:CD1	8:r:102:A1EL2:C29	2.52	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:7:TYR:CD2	9:R:102:A1ELD:C45	2.53	0.91
1:I:18:HIS:NE2	8:I:102:A1EL2:O1	2.06	0.88
8:r:102:A1EL2:C38	2:k:52:GLY:C	2.48	0.87
2:c:13:TYR:CD2	2:c:14:LEU:N	2.43	0.86
1:E:7:TYR:HA	1:F:11:ARG:HH21	1.41	0.85
1:F:18:HIS:NE2	8:F:102:A1EL2:O1	2.09	0.85
1:F:1:MET:HE2	1:F:3:ARG:HG3	1.60	0.84
2:c:13:TYR:CG	2:c:14:LEU:N	2.46	0.83
2:c:13:TYR:CD2	2:c:18:GLU:OE1	2.32	0.82
2:e:29:THR:HG21	9:e:101:A1ELD:C13	2.09	0.82
2:g:29:THR:CG2	9:g:101:A1ELD:C13	2.59	0.80
1:A:18:HIS:NE2	8:A:102:A1EL2:O1	2.15	0.80
1:R:3:ARG:CB	9:R:102:A1ELD:O46	2.31	0.77
9:r:101:A1ELD:O13	8:r:103:A1EL2:C9	2.34	0.76
2:f:29:THR:HG21	9:f:101:A1ELD:C13	2.15	0.75
2:e:29:THR:HG21	9:e:101:A1ELD:C10	2.17	0.74
2:r:47:TYR:CD2	8:r:102:A1EL2:C27	2.69	0.74
10:Q:103:8K6:H51C	5:M:58:LEU:HD21	1.70	0.74
8:r:102:A1EL2:C38	2:k:52:GLY:O	2.35	0.74
1:E:1:MET:SD	9:f:101:A1ELD:C43	2.77	0.73
1:E:7:TYR:HA	1:F:11:ARG:NH2	2.03	0.72
1:A:1:MET:HE1	1:A:3:ARG:HB2	1.70	0.72
2:f:29:THR:HG21	9:f:101:A1ELD:C10	2.20	0.71
2:g:29:THR:HG21	9:g:101:A1ELD:C10	2.20	0.71
3:L:123:GLY:HA3	10:L:312:8K6:H161	1.74	0.69
3:L:227:THR:HA	14:L:304:UQ8:H3MB	1.73	0.69
2:c:13:TYR:CE2	2:c:14:LEU:HB2	2.28	0.69
2:e:29:THR:CG2	9:e:101:A1ELD:C13	2.71	0.68
1:E:1:MET:CE	9:f:101:A1ELD:C43	2.71	0.68
1:R:3:ARG:CB	9:R:102:A1ELD:C6	2.70	0.68
1:I:18:HIS:HE2	8:I:102:A1EL2:C6	2.06	0.68
2:a:13:TYR:HB3	2:a:18:GLU:HG3	1.77	0.67
1:Q:23:VAL:HG21	10:Q:103:8K6:H131	1.77	0.67
1:D:23:VAL:HG22	11:D:103:PGV:H312	1.77	0.66
5:M:191:ASN:O	5:M:195:ARG:HG3	1.95	0.66
2:b:45:TRP:HH2	2:b:51:PHE:HB2	1.60	0.66
2:r:47:TYR:CE2	2:r:48:LYS:HE2	2.30	0.66
1:D:23:VAL:HA	11:D:103:PGV:H291	1.77	0.65
9:R:102:A1ELD:C36	9:R:102:A1ELD:C39	2.68	0.65
1:J:43:ARG:NH1	1:J:43:ARG:HB2	2.11	0.65
1:E:1:MET:HE1	9:f:101:A1ELD:C43	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:15:THR:OG1	2:a:18:GLU:OE2	2.14	0.65
1:R:3:ARG:HB3	9:R:102:A1ELD:O46	1.97	0.64
1:Q:2:TRP:HZ3	1:Q:6:PHE:CZ	2.16	0.64
2:f:29:THR:CG2	9:f:101:A1ELD:C13	2.74	0.64
1:K:37:ARG:NH2	2:k:49:PRO:O	2.31	0.64
1:E:27:THR:HG21	7:F:101:BCL:H202	1.80	0.64
1:F:7:TYR:HB3	1:G:11:ARG:HG2	1.80	0.63
1:J:18:HIS:HE2	8:J:102:A1EL2:C6	2.09	0.63
7:B:101:BCL:H51	9:B:103:A1ELD:C12	2.29	0.63
1:J:18:HIS:CE1	8:J:102:A1EL2:O1	2.52	0.63
1:Q:7:TYR:HB3	1:I:11:ARG:HG2	1.81	0.62
2:f:23:HIS:O	2:f:27:MET:HG2	2.00	0.61
1:J:43:ARG:HB2	1:J:43:ARG:HH11	1.66	0.61
1:N:39:ASN:HD21	12:N:103:LMT:H6'2	1.64	0.61
3:L:274:SER:HB2	5:M:90:ARG:HE	1.65	0.61
13:L:303:BPH:HBB3	13:L:303:BPH:HHC	1.82	0.61
2:c:45:TRP:HH2	2:c:51:PHE:HB2	1.65	0.61
3:L:38:THR:HG22	11:L:308:PGV:H02	1.83	0.60
3:L:138:LEU:HD11	19:T:302:LHG:H251	1.82	0.60
2:d:45:TRP:HH2	2:d:51:PHE:HB2	1.66	0.60
3:L:104:ARG:NH2	5:M:258:VAL:O	2.32	0.60
1:C:15:VAL:HG21	10:L:313:8K6:H91C	1.84	0.60
3:L:225:VAL:H	14:L:304:UQ8:H8	1.66	0.60
1:S:7:TYR:HB3	1:N:11:ARG:HG2	1.84	0.59
1:E:7:TYR:O	1:F:11:ARG:NE	2.35	0.59
1:I:19:VAL:O	1:I:23:VAL:HG23	2.03	0.59
2:k:45:TRP:HH2	2:k:51:PHE:HB2	1.67	0.59
3:L:31:TYR:O	3:L:104:ARG:NH1	2.36	0.59
2:s:45:TRP:HH2	2:s:51:PHE:HB2	1.68	0.58
2:e:45:TRP:HH2	2:e:51:PHE:HB2	1.68	0.58
1:F:27:THR:HG23	11:F:103:PGV:H242	1.84	0.58
2:o:45:TRP:HH2	2:o:51:PHE:HB2	1.69	0.58
4:H:145:ALA:HB3	4:H:148:ASP:HB2	1.86	0.57
2:f:15:THR:HG23	2:f:18:GLU:HB2	1.87	0.57
1:O:7:TYR:HB3	1:P:11:ARG:HG2	1.87	0.57
2:c:13:TYR:CE2	2:c:18:GLU:OE1	2.58	0.57
2:a:14:LEU:HD23	2:a:15:THR:HG23	1.86	0.56
1:I:30:PHE:HB3	5:M:120:MET:HE2	1.87	0.56
4:H:211:LEU:HB3	4:H:213:ILE:HG12	1.87	0.56
7:b:102:BCL:H3A	7:b:102:BCL:H52	1.87	0.56
2:i:45:TRP:HH2	2:i:51:PHE:HB2	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:45:TRP:HH2	2:n:51:PHE:HB2	1.71	0.56
1:K:21:LEU:HD23	7:R:101:BCL:H142	1.86	0.56
1:Q:18:HIS:NE2	8:Q:102:A1EL2:O1	2.36	0.55
2:n:38:LEU:HD22	7:n:101:BCL:H93	1.88	0.55
2:r:47:TYR:CG	8:r:102:A1EL2:C29	2.89	0.55
2:r:47:TYR:CG	8:r:102:A1EL2:C27	2.90	0.55
3:L:28:GLY:H	10:L:313:8K6:H42C	1.72	0.55
7:C:101:BCL:HBC3	2:c:44:MET:HE2	1.89	0.55
3:L:230:ILE:HG21	14:L:304:UQ8:H3MA	1.87	0.55
1:J:18:HIS:HD2	7:J:101:BCL:H41	1.71	0.55
1:N:11:ARG:NE	4:H:215:GLU:OE1	2.39	0.54
1:J:32:LEU:HD11	7:j:102:BCL:HHD	1.90	0.54
5:M:160:PHE:HD1	7:M:403:BCL:HBB1	1.71	0.54
1:Q:16:ALA:HA	10:Q:103:8K6:H71C	1.89	0.54
2:q:45:TRP:HH2	2:q:51:PHE:HB2	1.71	0.54
2:j:45:TRP:HH2	2:j:51:PHE:HB2	1.73	0.54
1:R:3:ARG:HB2	9:R:102:A1ELD:C5	2.38	0.53
3:L:196:LEU:HD21	5:M:270:ARG:HG2	1.90	0.53
10:Q:103:8K6:H151	5:M:130:LEU:HB3	1.91	0.53
2:a:45:TRP:HH2	2:a:51:PHE:HB2	1.73	0.53
9:R:102:A1ELD:C39	9:R:102:A1ELD:C38	2.74	0.53
2:g:45:TRP:HH2	2:g:51:PHE:HB2	1.74	0.53
1:R:3:ARG:HB2	9:R:102:A1ELD:O46	2.01	0.53
2:e:25:GLY:O	2:e:29:THR:HG22	2.07	0.53
1:D:12:ARG:HB3	4:H:58:LEU:HG	1.91	0.52
3:L:206:ASP:OD1	4:H:67:GLN:NE2	2.30	0.52
1:C:10:ILE:CD1	1:C:14:LEU:HD13	2.39	0.52
2:f:45:TRP:HH2	2:f:51:PHE:HB2	1.74	0.52
2:r:47:TYR:HD1	8:r:102:A1EL2:C36	2.23	0.52
1:K:32:LEU:HD11	7:k:101:BCL:HHD	1.92	0.52
5:M:133:TRP:O	5:M:136:THR:HG22	2.10	0.52
2:r:27:MET:HA	2:r:27:MET:HE3	1.91	0.52
9:R:102:A1ELD:C36	1:N:29:HIS:HB3	2.40	0.52
3:L:234:GLY:HA3	5:M:219:PHE:CE1	2.45	0.52
19:T:302:LHG:H271	11:T:303:PGV:H231	1.92	0.52
2:p:45:TRP:HH2	2:p:51:PHE:HB2	1.75	0.51
1:B:18:HIS:NE2	8:B:102:A1EL2:O1	2.38	0.51
1:I:18:HIS:HE2	8:I:102:A1EL2:C5	2.22	0.51
1:D:24:LEU:HD23	7:d:102:BCL:HED3	1.93	0.51
1:I:18:HIS:CE1	8:I:102:A1EL2:O1	2.62	0.51
13:L:303:BPH:NC	5:M:217:VAL:HG22	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:101:BCL:H92	7:a:101:BCL:HBA2	1.92	0.51
10:Q:104:8K6:H182	10:Q:104:8K6:H102	1.93	0.51
1:R:7:TYR:CE2	9:R:102:A1ELD:C7	2.94	0.51
2:a:20:GLN:O	2:a:24:LYS:HG2	2.11	0.51
2:r:45:TRP:HH2	2:r:51:PHE:HB2	1.76	0.51
2:o:15:THR:HG23	2:o:18:GLU:H	1.76	0.51
1:E:7:TYR:O	1:F:11:ARG:CZ	2.59	0.51
1:D:18:HIS:NE2	8:D:102:A1EL2:O1	2.36	0.50
1:C:36:ASP:OD2	10:C:104:8K6:H112	2.11	0.50
1:G:2:TRP:H	1:G:2:TRP:CD1	2.29	0.50
3:L:256:TYR:OH	3:L:259:SER:O	2.25	0.50
1:D:3:ARG:HB3	9:e:101:A1ELD:O46	2.12	0.50
5:M:19:PRO:HB2	5:M:21:MET:CE	2.42	0.50
1:B:32:LEU:HD11	7:b:102:BCL:HHD	1.94	0.49
2:k:27:MET:O	2:k:31:VAL:HG23	2.12	0.49
1:G:1:MET:HE3	1:G:1:MET:HA	1.93	0.49
8:P:102:A1EL2:C9	9:o:101:A1ELD:O13	2.60	0.49
3:L:194:LEU:HD23	14:L:304:UQ8:C3	2.41	0.49
7:L:302:BCL:HAA1	5:M:210:VAL:HG22	1.95	0.49
2:q:20:GLN:O	2:q:24:LYS:HG3	2.13	0.49
5:M:248:ALA:HA	5:M:265:PHE:CE1	2.47	0.49
1:Q:2:TRP:CZ3	1:Q:6:PHE:CE2	3.01	0.49
3:L:207:VAL:HG11	5:M:242:THR:HG21	1.95	0.49
7:B:101:BCL:H151	1:P:23:VAL:HB	1.95	0.48
1:C:10:ILE:HD12	1:C:14:LEU:HD13	1.95	0.48
5:M:100:PRO:HG3	5:M:115:GLY:HA3	1.94	0.48
2:b:45:TRP:CH2	2:b:51:PHE:HB2	2.46	0.48
1:O:24:LEU:HB2	7:P:101:BCL:H122	1.95	0.48
3:L:191:HIS:HA	14:L:304:UQ8:H1M	1.95	0.48
4:H:113:PRO:HB2	4:H:257:GLY:HA2	1.95	0.48
4:H:128:ASP:OD1	4:H:128:ASP:N	2.32	0.48
9:R:102:A1ELD:C35	9:R:102:A1ELD:C37	2.74	0.48
1:N:2:TRP:CD1	1:N:2:TRP:H	2.31	0.47
11:D:103:PGV:H183	3:L:50:ILE:HD12	1.95	0.47
2:g:45:TRP:CH2	2:g:51:PHE:HB2	2.49	0.47
3:L:129:TYR:CD1	7:L:302:BCL:HBB1	2.49	0.47
3:L:148:PRO:HG3	5:M:313:TYR:CE1	2.50	0.47
4:H:185:GLU:HB2	4:H:191:LYS:HD3	1.96	0.47
1:S:32:LEU:HD11	7:s:101:BCL:HHD	1.96	0.47
3:L:131:THR:HA	3:L:135:ILE:HB	1.96	0.47
7:F:101:BCL:H62	7:F:101:BCL:H41	1.64	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:194:LEU:HD21	3:L:213:GLU:HB3	1.97	0.47
4:H:12:THR:HB	17:M:407:PEF:H52	1.96	0.47
4:H:66:PHE:O	4:H:74:THR:HA	2.14	0.47
3:L:263:PHE:HA	12:L:309:LMT:H3'	1.97	0.47
2:f:25:GLY:O	2:f:29:THR:HG22	2.14	0.47
2:f:29:THR:HG21	9:f:101:A1ELD:C9	2.45	0.47
1:G:32:LEU:HD11	7:g:102:BCL:HHD	1.96	0.46
7:s:101:BCL:H2	7:s:101:BCL:H61	1.54	0.46
3:L:39:THR:HG21	3:L:101:TRP:HE3	1.80	0.46
4:H:149:PRO:HB3	4:H:154:TRP:CH2	2.51	0.46
4:H:243:ILE:HG12	4:H:248:GLU:HG3	1.97	0.46
7:L:301:BCL:H2	13:L:303:BPH:HHC	1.97	0.46
1:F:42:GLU:CD	4:H:11:GLY:H	2.24	0.46
3:L:8:ARG:NH2	4:H:46:GLU:OE1	2.48	0.46
3:L:50:ILE:HD13	3:L:67:ILE:HG13	1.98	0.46
5:M:19:PRO:HG3	5:M:36:THR:HG21	1.97	0.46
1:N:32:LEU:HD11	7:n:101:BCL:HHD	1.98	0.46
2:r:47:TYR:CD1	8:r:102:A1EL2:C30	2.99	0.46
1:D:27:THR:HG21	7:E:101:BCL:H202	1.97	0.46
7:O:101:BCL:H61	7:O:101:BCL:H41	1.53	0.46
3:L:256:TYR:HD1	10:L:311:8K6:H131	1.79	0.46
1:F:32:LEU:HD11	7:f:102:BCL:HHD	1.96	0.46
1:F:33:LEU:HG	1:F:40:TRP:CH2	2.51	0.46
4:H:151:LEU:HD11	5:M:13:VAL:HG21	1.97	0.46
1:P:2:TRP:HB2	2:p:19:ALA:HB1	1.98	0.46
7:p:101:BCL:H102	7:p:101:BCL:H61	1.49	0.46
1:A:1:MET:SD	1:A:3:ARG:HG3	2.55	0.46
1:A:32:LEU:HD11	7:a:101:BCL:HHD	1.98	0.46
7:P:101:BCL:H71	7:P:101:BCL:H112	1.59	0.46
7:a:101:BCL:HBA1	7:a:101:BCL:H3A	1.42	0.46
2:e:20:GLN:O	2:e:24:LYS:HG3	2.15	0.46
3:L:155:LEU:HD23	5:M:200:PHE:HB3	1.98	0.46
7:L:302:BCL:H11	7:L:302:BCL:H51	1.78	0.46
5:M:152:ALA:HA	5:M:277:VAL:HG22	1.99	0.46
5:M:213:TYR:O	5:M:217:VAL:HG23	2.15	0.45
1:B:23:VAL:HG21	11:L:308:PGV:H22	1.99	0.45
1:Q:23:VAL:HG12	7:I:101:BCL:H161	1.99	0.45
7:Q:101:BCL:H112	7:Q:101:BCL:H152	1.63	0.45
1:I:12:ARG:NH1	5:M:30:GLU:OE2	2.50	0.45
7:I:101:BCL:H61	7:I:101:BCL:H2	1.68	0.45
3:L:214:ASP:OD1	5:M:47:GLN:NE2	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ALA:HA	10:L:313:8K6:H131	1.96	0.45
1:B:29:HIS:CE1	7:b:102:BCL:HMD3	2.52	0.45
1:D:2:TRP:CD1	1:D:2:TRP:H	2.35	0.45
1:Q:2:TRP:CZ3	1:Q:6:PHE:CZ	3.01	0.45
1:J:23:VAL:HG12	7:K:101:BCL:H13	1.99	0.45
3:L:62:PRO:HA	3:L:65:ILE:HD12	1.99	0.45
5:M:283:GLY:HA2	7:M:401:BCL:HED2	1.99	0.45
11:D:103:PGV:H131	11:D:103:PGV:H102	1.69	0.45
7:S:101:BCL:H162	7:S:101:BCL:H193	1.75	0.45
7:e:102:BCL:H61	7:e:102:BCL:H93	1.78	0.45
7:E:101:BCL:H62	7:E:101:BCL:H41	1.72	0.45
1:O:29:HIS:CE1	7:o:102:BCL:HMD1	2.52	0.45
1:A:20:GLY:HA3	7:C:101:BCL:H102	1.98	0.45
7:B:101:BCL:H171	7:B:101:BCL:H13	1.78	0.45
1:Q:36:ASP:OD1	10:Q:104:8K6:H162	2.16	0.45
7:N:101:BCL:H61	7:N:101:BCL:H2	1.61	0.45
7:n:101:BCL:H92	7:n:101:BCL:H61	1.78	0.45
13:L:305:BPH:HMB2	7:M:403:BCL:H51	1.99	0.45
1:E:18:HIS:NE2	8:E:102:A1EL2:O1	2.43	0.45
1:E:29:HIS:CE1	7:e:102:BCL:HMD1	2.51	0.45
1:S:27:THR:HA	10:S:102:8K6:H92C	1.98	0.45
1:S:37:ARG:NH2	2:s:49:PRO:O	2.47	0.45
2:e:26:PHE:HD2	2:e:27:MET:HE2	1.82	0.45
1:D:1:MET:SD	1:D:3:ARG:NH2	2.86	0.44
11:F:103:PGV:H101	11:F:103:PGV:H272	1.99	0.44
7:P:101:BCL:HED2	2:p:37:ALA:HB2	2.00	0.44
7:r:104:BCL:H2	7:r:104:BCL:H61	1.63	0.44
7:d:102:BCL:H2	7:d:102:BCL:H61	1.72	0.44
13:L:303:BPH:H141	13:L:303:BPH:H161	1.75	0.44
8:K:102:A1EL2:C40	7:j:102:BCL:H52	2.48	0.44
3:L:11:ARG:HH12	10:L:313:8K6:H11C	1.82	0.44
1:D:39:ASN:OD1	1:D:42:GLU:HG2	2.16	0.44
2:a:24:LYS:HA	2:a:24:LYS:HD3	1.88	0.44
7:c:101:BCL:H61	7:c:101:BCL:H2	1.78	0.44
5:M:264:THR:H	5:M:267:SER:HB3	1.82	0.44
1:A:1:MET:HE3	1:A:1:MET:HB3	1.80	0.44
1:D:32:LEU:HD11	7:d:102:BCL:HHD	1.99	0.44
1:Q:32:LEU:HD11	7:q:102:BCL:HHD	2.00	0.44
1:N:29:HIS:CE1	7:n:101:BCL:HMD3	2.52	0.44
7:b:102:BCL:H13	7:b:102:BCL:H172	1.81	0.44
2:s:45:TRP:CH2	2:s:51:PHE:HB2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:102:BCL:H62	7:g:102:BCL:H41	1.53	0.44
11:F:103:PGV:H102	11:F:103:PGV:H131	1.79	0.44
11:F:103:PGV:H11	7:G:101:BCL:H171	2.00	0.44
7:R:101:BCL:H141	7:R:101:BCL:H161	1.63	0.44
2:c:13:TYR:HD2	2:c:15:THR:H	1.63	0.44
10:L:313:8K6:H22C	4:H:97:GLY:CA	2.47	0.44
5:M:158:TRP:CZ2	11:M:408:PGV:H162	2.53	0.44
7:B:101:BCL:HBD	7:B:101:BCL:HBA2	2.00	0.44
9:R:102:A1ELD:C12	7:N:101:BCL:H72	2.48	0.43
1:O:32:LEU:HD11	7:o:102:BCL:HHH	1.99	0.43
7:L:302:BCL:HHH	7:L:302:BCL:HBB2	2.00	0.43
7:M:403:BCL:H51	7:M:403:BCL:H11	1.85	0.43
7:C:101:BCL:H111	7:C:101:BCL:H142	1.73	0.43
1:F:2:TRP:H	1:F:2:TRP:CD1	2.35	0.43
7:L:302:BCL:HMD2	5:M:209:ILE:HD13	2.00	0.43
4:H:217:LYS:HD2	4:H:217:LYS:HA	1.63	0.43
19:T:302:LHG:H242	11:T:303:PGV:H212	2.00	0.43
1:S:1:MET:O	1:S:4:ILE:HG22	2.19	0.43
3:L:60:LEU:HD23	3:L:60:LEU:HA	1.84	0.43
1:G:27:THR:HA	11:G:103:PGV:H241	1.99	0.43
2:n:21:GLU:HA	2:n:24:LYS:HG2	2.00	0.43
1:R:3:ARG:HD2	9:R:102:A1ELD:O46	2.18	0.43
3:L:174:HIS:CE1	3:L:178:ILE:HD11	2.53	0.43
1:Q:33:LEU:HG	1:Q:40:TRP:CH2	2.54	0.43
2:b:41:HIS:CD2	7:b:102:BCL:H122	2.54	0.43
7:d:102:BCL:H141	7:d:102:BCL:H162	1.80	0.43
12:L:309:LMT:O2'	10:L:311:8K6:H132	2.19	0.43
5:M:91:GLU:O	5:M:95:LEU:HG	2.18	0.43
1:I:31:ILE:HG13	5:M:120:MET:HE1	2.00	0.43
9:R:102:A1ELD:C41	1:N:30:PHE:CD1	3.02	0.43
7:k:101:BCL:H2	7:k:101:BCL:H62	1.60	0.43
5:M:288:LEU:HD23	10:M:406:8K6:H12C	2.00	0.43
10:Q:104:8K6:H182	10:Q:104:8K6:H132	2.01	0.43
1:J:2:TRP:CD1	1:J:2:TRP:H	2.36	0.43
2:k:45:TRP:CH2	2:k:51:PHE:HB2	2.50	0.43
7:f:102:BCL:H62	7:f:102:BCL:H41	1.83	0.43
4:H:132:ARG:HH12	5:M:239:GLU:CD	2.26	0.43
5:M:169:MET:HE3	5:M:169:MET:HB3	1.93	0.43
7:S:101:BCL:H2	7:S:101:BCL:H62	1.58	0.42
3:L:217:PHE:CG	14:L:304:UQ8:H7	2.54	0.42
7:b:102:BCL:H72	7:b:102:BCL:H112	1.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:102:BCL:H162	7:f:102:BCL:H122	1.70	0.42
7:q:102:BCL:H111	7:q:102:BCL:H72	1.94	0.42
11:M:408:PGV:H131	11:M:408:PGV:H102	1.78	0.42
5:M:267:SER:HA	5:M:270:ARG:HG3	2.00	0.42
7:C:101:BCL:H112	7:C:101:BCL:H72	1.73	0.42
3:L:271:PRO:HD3	10:L:310:8K6:H111	2.02	0.42
4:H:160:ASP:OD1	4:H:160:ASP:N	2.47	0.42
1:Q:34:SER:HA	10:Q:104:8K6:H121	2.01	0.42
1:P:19:VAL:O	1:P:23:VAL:HG23	2.20	0.42
7:o:102:BCL:H141	7:o:102:BCL:H162	1.83	0.42
7:k:101:BCL:H141	7:k:101:BCL:H162	1.87	0.42
7:n:101:BCL:H162	7:n:101:BCL:H203	1.74	0.42
1:R:7:TYR:HE2	9:R:102:A1ELD:C6	2.32	0.42
7:A:101:BCL:H143	11:L:308:PGV:H031	2.02	0.42
1:C:29:HIS:CE1	7:c:101:BCL:HMD1	2.55	0.42
7:r:104:BCL:H112	7:r:104:BCL:H72	1.89	0.42
3:L:4:LEU:HB2	3:L:7:GLU:HB2	2.01	0.42
3:L:111:LYS:HA	4:H:260:MET:HE1	2.02	0.42
1:Q:31:ILE:O	1:Q:35:THR:HG23	2.20	0.42
4:H:113:PRO:HD2	4:H:261:TYR:CE2	2.54	0.42
1:F:39:ASN:HD21	4:H:10:VAL:HB	1.85	0.42
11:D:103:PGV:H32	3:L:62:PRO:HG2	2.00	0.41
7:N:101:BCL:H112	7:N:101:BCL:H152	1.62	0.41
1:A:12:ARG:HH12	10:L:313:8K6:H31C	1.84	0.41
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.94	0.41
7:E:101:BCL:H51	9:d:101:A1ELD:C12	2.51	0.41
1:F:33:LEU:O	1:F:39:ASN:ND2	2.52	0.41
1:S:29:HIS:CE1	7:s:101:BCL:HMD1	2.56	0.41
1:P:29:HIS:CE1	7:p:101:BCL:HMD1	2.56	0.41
7:b:102:BCL:H52	7:b:102:BCL:H8	1.75	0.41
3:L:8:ARG:NH1	4:H:48:GLU:O	2.54	0.41
3:L:11:ARG:HH12	10:L:313:8K6:C1	2.34	0.41
1:C:40:TRP:HE1	7:C:101:BCL:HBB2	1.85	0.41
1:P:30:PHE:HB3	11:T:303:PGV:H202	2.02	0.41
7:I:101:BCL:H143	7:I:101:BCL:H162	1.94	0.41
7:b:102:BCL:H143	7:b:102:BCL:H111	1.88	0.41
2:f:34:VAL:HG22	7:f:102:BCL:H43	2.02	0.41
1:I:2:TRP:CD1	1:I:2:TRP:H	2.38	0.41
1:O:26:PHE:CZ	7:O:101:BCL:H162	2.55	0.41
9:O:102:A1ELD:C13	2:n:29:THR:HB	2.50	0.41
2:e:29:THR:HG21	9:e:101:A1ELD:C9	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:HD11	7:c:101:BCL:HHD	2.01	0.41
1:A:22:ALA:HB2	7:A:101:BCL:H51	2.03	0.41
1:A:29:HIS:CE1	7:a:101:BCL:HMD1	2.56	0.41
1:D:31:ILE:HA	11:D:103:PGV:H201	2.02	0.41
11:D:103:PGV:H221	11:L:307:PGV:H32	2.03	0.41
1:F:6:PHE:HZ	2:f:16:PRO:HA	1.86	0.41
7:F:101:BCL:H51	9:e:101:A1ELD:C12	2.51	0.41
1:I:1:MET:O	1:I:4:ILE:HG22	2.20	0.41
1:S:6:PHE:HZ	2:s:16:PRO:HA	1.86	0.41
1:P:32:LEU:HD11	7:p:101:BCL:HHD	2.02	0.41
2:g:15:THR:HA	2:g:16:PRO:HD3	1.96	0.41
7:L:302:BCL:H61	14:M:402:UQ8:H20	2.02	0.41
1:A:7:TYR:HB3	1:C:11:ARG:HG2	2.02	0.41
1:B:19:VAL:O	1:B:23:VAL:HG23	2.21	0.41
1:Q:29:HIS:CE1	7:q:102:BCL:HMD1	2.56	0.41
11:D:103:PGV:H61	3:L:63:TRP:CZ2	2.56	0.40
1:I:37:ARG:NH2	2:i:49:PRO:O	2.53	0.40
7:o:102:BCL:HBA1	7:o:102:BCL:H3A	1.71	0.40
2:q:13:TYR:CE2	2:q:14:LEU:HD13	2.56	0.40
4:H:215:GLU:HG3	4:H:217:LYS:HG2	2.03	0.40
4:H:164:VAL:HG21	4:H:231:PHE:CG	2.57	0.40
1:F:29:HIS:CE1	7:f:102:BCL:HMD1	2.57	0.40
7:S:101:BCL:H143	7:S:101:BCL:H111	1.66	0.40
3:L:129:TYR:HD1	7:L:302:BCL:HBB1	1.86	0.40
7:L:301:BCL:H152	13:L:303:BPH:H3A	2.03	0.40
5:M:270:ARG:NH2	11:M:408:PGV:O14	2.54	0.40
1:D:4:ILE:HD12	9:e:101:A1ELD:C45	2.52	0.40
1:G:33:LEU:HG	1:G:40:TRP:CH2	2.57	0.40
1:R:7:TYR:HE2	9:R:102:A1ELD:C7	2.34	0.40
1:J:24:LEU:O	1:J:28:ILE:HG13	2.21	0.40
3:L:67:ILE:HB	3:L:149:TYR:HB2	2.03	0.40
5:M:84:SER:HB3	5:M:87:THR:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	42/64 (66%)	42 (100%)	0	0	100	100
1	B	42/64 (66%)	42 (100%)	0	0	100	100
1	C	42/64 (66%)	42 (100%)	0	0	100	100
1	D	42/64 (66%)	42 (100%)	0	0	100	100
1	E	42/64 (66%)	42 (100%)	0	0	100	100
1	F	42/64 (66%)	42 (100%)	0	0	100	100
1	G	42/64 (66%)	42 (100%)	0	0	100	100
1	I	42/64 (66%)	42 (100%)	0	0	100	100
1	J	42/64 (66%)	42 (100%)	0	0	100	100
1	K	42/64 (66%)	41 (98%)	1 (2%)	0	100	100
1	N	42/64 (66%)	42 (100%)	0	0	100	100
1	O	42/64 (66%)	42 (100%)	0	0	100	100
1	P	42/64 (66%)	42 (100%)	0	0	100	100
1	Q	42/64 (66%)	42 (100%)	0	0	100	100
1	R	42/64 (66%)	42 (100%)	0	0	100	100
1	S	42/64 (66%)	42 (100%)	0	0	100	100
2	a	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	b	38/52 (73%)	38 (100%)	0	0	100	100
2	c	38/52 (73%)	38 (100%)	0	0	100	100
2	d	38/52 (73%)	38 (100%)	0	0	100	100
2	e	38/52 (73%)	38 (100%)	0	0	100	100
2	f	38/52 (73%)	38 (100%)	0	0	100	100
2	g	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	i	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	j	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	k	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	n	38/52 (73%)	38 (100%)	0	0	100	100
2	o	38/52 (73%)	38 (100%)	0	0	100	100
2	p	38/52 (73%)	37 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	q	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	r	38/52 (73%)	38 (100%)	0	0	100	100
2	s	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
3	L	271/274 (99%)	268 (99%)	3 (1%)	0	100	100
4	H	263/268 (98%)	258 (98%)	5 (2%)	0	100	100
5	M	318/323 (98%)	314 (99%)	4 (1%)	0	100	100
6	T	18/135 (13%)	18 (100%)	0	0	100	100
All	All	2150/2856 (75%)	2129 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	38/49 (78%)	38 (100%)	0	100	100
1	B	38/49 (78%)	38 (100%)	0	100	100
1	C	38/49 (78%)	38 (100%)	0	100	100
1	D	38/49 (78%)	38 (100%)	0	100	100
1	E	38/49 (78%)	38 (100%)	0	100	100
1	F	38/49 (78%)	38 (100%)	0	100	100
1	G	38/49 (78%)	38 (100%)	0	100	100
1	I	38/49 (78%)	38 (100%)	0	100	100
1	J	38/49 (78%)	38 (100%)	0	100	100
1	K	38/49 (78%)	37 (97%)	1 (3%)	40	56
1	N	38/49 (78%)	38 (100%)	0	100	100
1	O	38/49 (78%)	38 (100%)	0	100	100
1	P	38/49 (78%)	38 (100%)	0	100	100
1	Q	38/49 (78%)	38 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	38/49 (78%)	38 (100%)	0	100	100
1	S	38/49 (78%)	38 (100%)	0	100	100
2	a	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	b	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	c	31/40 (78%)	31 (100%)	0	100	100
2	d	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	e	31/40 (78%)	31 (100%)	0	100	100
2	f	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	g	31/40 (78%)	31 (100%)	0	100	100
2	i	31/40 (78%)	31 (100%)	0	100	100
2	j	31/40 (78%)	31 (100%)	0	100	100
2	k	31/40 (78%)	31 (100%)	0	100	100
2	n	31/40 (78%)	31 (100%)	0	100	100
2	o	31/40 (78%)	31 (100%)	0	100	100
2	p	31/40 (78%)	31 (100%)	0	100	100
2	q	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	r	31/40 (78%)	31 (100%)	0	100	100
2	s	31/40 (78%)	31 (100%)	0	100	100
3	L	215/216 (100%)	214 (100%)	1 (0%)	81	89
4	H	216/220 (98%)	212 (98%)	4 (2%)	50	66
5	M	250/252 (99%)	249 (100%)	1 (0%)	84	91
6	T	9/94 (10%)	9 (100%)	0	100	100
All	All	1794/2206 (81%)	1782 (99%)	12 (1%)	73	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	30	PHE
2	b	31	VAL
2	a	22	ILE
2	d	20	GLN
2	f	15	THR
2	q	20	GLN
3	L	115	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	128	ASP
4	H	133	ILE
4	H	136	ILE
4	H	249	ASP
5	M	30	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	29	HIS
1	N	29	HIS
1	P	18	HIS
2	a	20	GLN
4	H	204	ASN
5	M	296	ASN
5	M	302	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 100 ligands modelled in this entry, 1 is monoatomic - leaving 99 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	b	102	2	69,74,74	1.82	18 (26%)	83,115,115	2.39	26 (31%)
7	BCL	M	403	5	69,74,74	1.80	18 (26%)	83,115,115	2.61	22 (26%)
10	8K6	C	104	-	8,8,17	0.09	0	7,7,16	0.10	0
10	8K6	f	103	-	13,13,17	0.09	0	12,12,16	0.08	0
8	A1EL2	D	102	-	43,44,44	1.63	8 (18%)	56,62,62	1.53	10 (17%)
9	A1ELD	o	101	-	43,44,44	4.99	31 (72%)	51,58,58	1.86	13 (25%)
7	BCL	B	101	1	69,74,74	1.80	17 (24%)	83,115,115	2.57	26 (31%)
8	A1EL2	B	102	-	43,44,44	1.63	8 (18%)	56,62,62	1.52	10 (17%)
17	PEF	M	407	-	42,42,46	0.28	0	45,47,51	0.32	0
7	BCL	k	101	2	69,74,74	1.78	17 (24%)	83,115,115	2.33	23 (27%)
7	BCL	i	101	2	69,74,74	1.80	17 (24%)	83,115,115	2.52	25 (30%)
8	A1EL2	J	102	-	43,44,44	3.81	29 (67%)	56,62,62	4.38	36 (64%)
10	8K6	M	406	-	14,14,17	0.09	0	13,13,16	0.11	0
14	UQ8	L	304	-	19,19,53	1.01	2 (10%)	23,26,67	0.99	1 (4%)
9	A1ELD	R	103	-	43,44,44	1.74	10 (23%)	51,58,58	1.64	12 (23%)
8	A1EL2	O	103	-	43,44,44	2.90	23 (53%)	56,62,62	1.82	15 (26%)
9	A1ELD	q	101	-	43,44,44	1.70	10 (23%)	51,58,58	1.61	10 (19%)
16	H4X	M	405	-	43,43,43	1.60	8 (18%)	50,54,54	1.27	9 (18%)
11	PGV	M	408	-	37,37,50	1.09	2 (5%)	41,42,56	1.20	4 (9%)
8	A1EL2	K	102	-	43,44,44	1.90	13 (30%)	56,62,62	1.31	7 (12%)
7	BCL	e	102	2	69,74,74	1.81	18 (26%)	83,115,115	2.43	26 (31%)
10	8K6	L	310	-	11,11,17	0.08	0	10,10,16	0.07	0
13	BPH	L	303	-	59,70,70	2.55	15 (25%)	61,101,101	2.17	16 (26%)
7	BCL	c	101	2	69,74,74	1.82	16 (23%)	83,115,115	2.39	22 (26%)
10	8K6	Q	104	-	17,17,17	0.07	0	16,16,16	0.11	0
7	BCL	G	101	1	69,74,74	1.81	19 (27%)	83,115,115	2.61	24 (28%)
11	PGV	D	103	-	50,50,50	0.91	2 (4%)	53,56,56	1.06	4 (7%)
8	A1EL2	C	103	-	43,44,44	1.63	8 (18%)	56,62,62	1.53	9 (16%)
19	LHG	T	302	6	9,9,48	0.28	0	8,8,54	1.12	1 (12%)
12	LMT	L	309	-	29,29,36	1.30	5 (17%)	40,40,47	1.06	1 (2%)
7	BCL	C	101	1	69,74,74	1.80	19 (27%)	83,115,115	2.70	26 (31%)
9	A1ELD	A	103	-	43,44,44	1.66	10 (23%)	51,58,58	1.47	10 (19%)
7	BCL	j	102	2	69,74,74	1.79	16 (23%)	83,115,115	2.44	23 (27%)
7	BCL	R	101	1	69,74,74	1.80	20 (28%)	83,115,115	2.59	22 (26%)
7	BCL	D	101	1	69,74,74	1.82	19 (27%)	83,115,115	2.74	29 (34%)
9	A1ELD	b	101	-	43,44,44	1.83	10 (23%)	51,58,58	1.58	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	PO4	M	409	-	4,4,4	0.96	0	6,6,6	0.43	0
10	8K6	H	301	-	17,17,17	0.08	0	16,16,16	0.06	0
12	LMT	N	103	-	27,27,36	1.35	6 (22%)	37,38,47	0.92	1 (2%)
10	8K6	Q	103	-	17,17,17	0.09	0	16,16,16	0.07	0
7	BCL	L	302	3	69,74,74	1.81	17 (24%)	83,115,115	2.32	23 (27%)
8	A1EL2	I	102	-	43,44,44	2.73	22 (51%)	56,62,62	3.18	29 (51%)
7	BCL	o	102	2	69,74,74	1.79	18 (26%)	83,115,115	2.40	27 (32%)
7	BCL	d	102	2	69,74,74	1.81	16 (23%)	83,115,115	2.50	23 (27%)
7	BCL	L	301	3	69,74,74	1.84	17 (24%)	83,115,115	2.62	23 (27%)
7	BCL	f	102	2	69,74,74	1.78	17 (24%)	83,115,115	2.50	27 (32%)
8	A1EL2	A	102	-	43,44,44	1.62	8 (18%)	56,62,62	1.52	10 (17%)
7	BCL	s	101	2	69,74,74	1.80	17 (24%)	83,115,115	2.40	22 (26%)
9	A1ELD	R	102	-	43,44,44	6.22	37 (86%)	51,58,58	4.71	27 (52%)
10	8K6	L	312	-	9,9,17	0.10	0	8,8,16	0.08	0
10	8K6	S	102	-	12,12,17	0.09	0	11,11,16	0.10	0
8	A1EL2	G	102	-	43,44,44	2.26	18 (41%)	56,62,62	1.40	9 (16%)
9	A1ELD	J	103	-	43,44,44	1.87	13 (30%)	51,58,58	1.55	10 (19%)
11	PGV	G	103	-	22,22,50	1.75	3 (13%)	24,26,56	1.48	3 (12%)
7	BCL	I	101	1	69,74,74	1.80	18 (26%)	83,115,115	2.60	27 (32%)
8	A1EL2	r	103	-	43,44,44	4.76	34 (79%)	56,62,62	2.88	30 (53%)
11	PGV	T	301	-	19,19,50	1.52	2 (10%)	21,21,56	1.59	5 (23%)
7	BCL	n	101	2	69,74,74	1.81	17 (24%)	83,115,115	2.44	26 (31%)
9	A1ELD	C	102	-	43,44,44	1.61	6 (13%)	51,58,58	1.76	11 (21%)
10	8K6	L	313	-	14,14,17	0.10	0	13,13,16	0.12	0
7	BCL	F	101	1	69,74,74	1.92	20 (28%)	83,115,115	2.41	23 (27%)
7	BCL	K	101	1	69,74,74	1.81	18 (26%)	83,115,115	2.60	26 (31%)
7	BCL	A	101	1	69,74,74	1.83	20 (28%)	83,115,115	2.67	26 (31%)
7	BCL	r	104	2	69,74,74	1.80	17 (24%)	83,115,115	2.39	20 (24%)
8	A1EL2	Q	102	-	43,44,44	3.24	25 (58%)	56,62,62	1.43	7 (12%)
13	BPH	L	305	-	59,70,70	0.83	4 (6%)	61,101,101	1.27	4 (6%)
8	A1EL2	r	102	-	43,44,44	2.38	14 (32%)	56,62,62	1.67	13 (23%)
9	A1ELD	e	101	-	43,44,44	2.62	22 (51%)	51,58,58	1.53	10 (19%)
9	A1ELD	B	103	-	43,44,44	2.37	19 (44%)	51,58,58	2.06	16 (31%)
8	A1EL2	P	102	-	43,44,44	3.45	21 (48%)	56,62,62	2.23	26 (46%)
9	A1ELD	r	101	-	43,44,44	1.71	10 (23%)	51,58,58	1.59	12 (23%)
7	BCL	g	102	2	69,74,74	1.80	17 (24%)	83,115,115	2.41	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	A1ELD	j	101	-	43,44,44	1.32	6 (13%)	51,58,58	1.75	11 (21%)
12	LMT	G	104	-	31,31,36	1.27	5 (16%)	42,42,47	0.93	2 (4%)
7	BCL	Q	101	1	69,74,74	1.80	19 (27%)	83,115,115	2.56	23 (27%)
8	A1EL2	E	102	-	43,44,44	1.63	8 (18%)	56,62,62	1.53	10 (17%)
7	BCL	q	102	2	69,74,74	1.81	17 (24%)	83,115,115	2.47	25 (30%)
14	UQ8	L	306	-	18,18,53	1.07	2 (11%)	22,25,67	0.74	0
7	BCL	S	101	1	69,74,74	1.83	17 (24%)	83,115,115	2.65	25 (30%)
7	BCL	p	101	2	69,74,74	1.80	17 (24%)	83,115,115	2.38	23 (27%)
11	PGV	L	307	-	20,20,50	1.25	2 (10%)	24,25,56	1.38	3 (12%)
7	BCL	O	101	1	69,74,74	1.83	19 (27%)	83,115,115	2.64	23 (27%)
10	8K6	L	311	-	13,13,17	0.08	0	12,12,16	0.11	0
8	A1EL2	F	102	-	43,44,44	1.62	8 (18%)	56,62,62	1.52	10 (17%)
11	PGV	F	103	-	50,50,50	0.90	2 (4%)	53,56,56	1.08	4 (7%)
9	A1ELD	g	101	-	43,44,44	1.69	9 (20%)	51,58,58	1.72	11 (21%)
7	BCL	N	101	1	69,74,74	1.82	20 (28%)	83,115,115	2.61	25 (30%)
7	BCL	E	101	1	69,74,74	1.81	18 (26%)	83,115,115	2.55	25 (30%)
9	A1ELD	d	101	-	43,44,44	1.91	14 (32%)	51,58,58	1.46	9 (17%)
7	BCL	M	401	5	69,74,74	1.89	19 (27%)	83,115,115	2.73	27 (32%)
14	UQ8	M	402	-	53,53,53	0.65	2 (3%)	64,67,67	0.56	0
7	BCL	a	101	2	69,74,74	1.77	17 (24%)	83,115,115	2.35	25 (30%)
9	A1ELD	f	101	-	43,44,44	1.67	9 (20%)	51,58,58	1.52	11 (21%)
7	BCL	P	101	1	69,74,74	1.83	19 (27%)	83,115,115	2.64	25 (30%)
8	A1EL2	N	102	-	43,44,44	1.61	8 (18%)	56,62,62	1.49	10 (17%)
11	PGV	T	303	-	29,29,50	1.22	2 (6%)	33,34,56	1.31	4 (12%)
11	PGV	L	308	-	28,28,50	1.23	2 (7%)	31,34,56	1.28	4 (12%)
7	BCL	J	101	1	69,74,74	1.83	18 (26%)	83,115,115	2.65	23 (27%)
9	A1ELD	O	102	-	43,44,44	3.36	21 (48%)	51,58,58	2.74	17 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	b	102	2	-	15/41/137/137	-
7	BCL	M	403	5	-	17/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	8K6	C	104	-	-	3/6/6/15	-
10	8K6	f	103	-	-	0/11/11/15	-
8	A1EL2	D	102	-	-	4/29/72/72	0/2/2/2
9	A1ELD	o	101	-	-	3/42/61/61	0/1/1/1
7	BCL	B	101	1	-	22/41/137/137	-
8	A1EL2	B	102	-	-	4/29/72/72	0/2/2/2
17	PEF	M	407	-	-	4/46/46/50	-
7	BCL	k	101	2	-	17/41/137/137	-
7	BCL	i	101	2	-	17/41/137/137	-
8	A1EL2	J	102	-	-	4/29/72/72	0/2/2/2
10	8K6	M	406	-	-	2/12/12/15	-
14	UQ8	L	304	-	-	7/11/35/75	0/1/1/1
9	A1ELD	R	103	-	-	5/42/61/61	0/1/1/1
8	A1EL2	O	103	-	-	3/29/72/72	0/2/2/2
9	A1ELD	q	101	-	-	5/42/61/61	0/1/1/1
16	H4X	M	405	-	-	2/51/51/51	-
11	PGV	M	408	-	-	12/39/39/55	-
8	A1EL2	K	102	-	-	4/29/72/72	0/2/2/2
7	BCL	e	102	2	-	14/41/137/137	-
10	8K6	L	310	-	-	0/9/9/15	-
13	BPH	L	303	-	-	11/37/105/105	0/5/6/6
7	BCL	c	101	2	-	26/41/137/137	-
10	8K6	Q	104	-	-	4/15/15/15	-
7	BCL	G	101	1	-	19/41/137/137	-
11	PGV	D	103	-	-	12/55/55/55	-
8	A1EL2	C	103	-	-	4/29/72/72	0/2/2/2
19	LHG	T	302	6	-	3/6/7/53	-
12	LMT	L	309	-	-	7/14/54/61	0/2/2/2
7	BCL	C	101	1	-	16/41/137/137	-
9	A1ELD	A	103	-	-	3/42/61/61	0/1/1/1
7	BCL	j	102	2	-	13/41/137/137	-
7	BCL	R	101	1	-	17/41/137/137	-
7	BCL	D	101	1	-	22/41/137/137	-
9	A1ELD	b	101	-	-	3/42/61/61	0/1/1/1
10	8K6	H	301	-	-	1/15/15/15	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	N	103	-	-	3/12/52/61	0/2/2/2
10	8K6	Q	103	-	-	2/15/15/15	-
7	BCL	L	302	3	-	17/41/137/137	-
8	A1EL2	I	102	-	-	4/29/72/72	0/2/2/2
7	BCL	o	102	2	-	19/41/137/137	-
7	BCL	d	102	2	-	16/41/137/137	-
7	BCL	L	301	3	-	9/41/137/137	-
7	BCL	f	102	2	-	17/41/137/137	-
8	A1EL2	A	102	-	-	4/29/72/72	0/2/2/2
7	BCL	s	101	2	-	19/41/137/137	-
9	A1ELD	R	102	-	-	3/42/61/61	0/1/1/1
10	8K6	L	312	-	-	0/7/7/15	-
10	8K6	S	102	-	-	2/10/10/15	-
8	A1EL2	G	102	-	-	4/29/72/72	0/2/2/2
9	A1ELD	J	103	-	-	3/42/61/61	0/1/1/1
11	PGV	G	103	-	-	6/23/23/55	-
7	BCL	I	101	1	-	16/41/137/137	-
8	A1EL2	r	103	-	-	2/29/72/72	0/2/2/2
11	PGV	T	301	-	-	6/20/20/55	-
7	BCL	n	101	2	-	19/41/137/137	-
9	A1ELD	C	102	-	-	3/42/61/61	0/1/1/1
10	8K6	L	313	-	-	0/12/12/15	-
7	BCL	F	101	1	-	16/41/137/137	-
7	BCL	K	101	1	-	16/41/137/137	-
7	BCL	A	101	1	-	11/41/137/137	-
7	BCL	r	104	2	-	18/41/137/137	-
8	A1EL2	Q	102	-	-	4/29/72/72	0/2/2/2
13	BPH	L	305	-	-	16/37/105/105	0/5/6/6
8	A1EL2	r	102	-	-	9/29/72/72	0/2/2/2
9	A1ELD	e	101	-	-	3/42/61/61	0/1/1/1
9	A1ELD	B	103	-	-	3/42/61/61	0/1/1/1
8	A1EL2	P	102	-	-	4/29/72/72	0/2/2/2
9	A1ELD	r	101	-	-	0/42/61/61	0/1/1/1
7	BCL	g	102	2	-	17/41/137/137	-
9	A1ELD	j	101	-	-	3/42/61/61	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	G	104	-	-	4/16/56/61	0/2/2/2
7	BCL	Q	101	1	-	18/41/137/137	-
8	A1EL2	E	102	-	-	4/29/72/72	0/2/2/2
7	BCL	q	102	2	-	17/41/137/137	-
14	UQ8	L	306	-	-	2/9/33/75	0/1/1/1
7	BCL	S	101	1	-	24/41/137/137	-
7	BCL	p	101	2	-	23/41/137/137	-
11	PGV	L	307	-	-	4/21/21/55	-
7	BCL	O	101	1	-	18/41/137/137	-
10	8K6	L	311	-	-	0/11/11/15	-
8	A1EL2	F	102	-	-	4/29/72/72	0/2/2/2
11	PGV	F	103	-	-	9/55/55/55	-
9	A1ELD	g	101	-	-	3/42/61/61	0/1/1/1
7	BCL	N	101	1	-	13/41/137/137	-
7	BCL	E	101	1	-	17/41/137/137	-
9	A1ELD	d	101	-	-	3/42/61/61	0/1/1/1
7	BCL	M	401	5	-	9/41/137/137	-
14	UQ8	M	402	-	-	8/51/75/75	0/1/1/1
7	BCL	a	101	2	-	18/41/137/137	-
9	A1ELD	f	101	-	-	3/42/61/61	0/1/1/1
7	BCL	P	101	1	-	16/41/137/137	-
8	A1EL2	N	102	-	-	2/29/72/72	0/2/2/2
11	PGV	T	303	-	-	9/31/31/55	-
11	PGV	L	308	-	-	12/33/33/55	-
7	BCL	J	101	1	-	14/41/137/137	-
9	A1ELD	O	102	-	-	3/42/61/61	0/1/1/1

All (1201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	102	A1ELD	C36-C35	16.77	1.76	1.50
9	R	102	A1ELD	C39-C37	12.20	1.80	1.52
9	R	102	A1ELD	C5-C4	11.91	1.69	1.51
8	r	103	A1EL2	C33-C34	11.72	1.69	1.52
9	o	101	A1ELD	C13-C10	11.63	1.51	1.35
9	R	102	A1ELD	C2-C3	10.76	1.68	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	o	101	A1ELD	C18-C16	10.66	1.49	1.35
8	J	102	A1EL2	C7-C2	9.71	1.66	1.51
8	r	103	A1EL2	C37-C35	9.38	1.74	1.54
9	R	102	A1ELD	C43-C4	9.29	1.66	1.50
9	O	102	A1ELD	C7-C6	-9.20	1.39	1.52
9	R	102	A1ELD	C34-C32	8.77	1.64	1.45
13	L	303	BPH	C1B-C2B	8.68	1.49	1.39
13	L	303	BPH	C1D-C2D	8.64	1.49	1.39
9	R	102	A1ELD	C5-C6	8.24	1.66	1.52
9	R	102	A1ELD	C7-C6	-8.16	1.40	1.52
8	P	102	A1EL2	C35-C34	-8.16	1.42	1.54
8	J	102	A1EL2	C35-C34	8.03	1.66	1.54
8	r	103	A1EL2	C2-C3	8.00	1.48	1.34
9	o	101	A1ELD	C9-C10	-7.93	1.28	1.45
8	Q	102	A1EL2	C17-C16	7.85	1.46	1.35
8	J	102	A1EL2	C32-C31	7.82	1.63	1.51
9	o	101	A1ELD	C29-C27	-7.79	1.29	1.45
9	R	102	A1ELD	C31-C32	7.70	1.46	1.35
9	O	102	A1ELD	C44-C2	-7.49	1.39	1.53
9	o	101	A1ELD	C5-C4	-7.45	1.39	1.51
9	R	102	A1ELD	O13-C12	7.39	1.39	1.22
8	P	102	A1EL2	C15-C16	-7.36	1.30	1.45
8	Q	102	A1EL2	C20-C21	7.26	1.45	1.35
9	o	101	A1ELD	C34-C32	-7.17	1.30	1.45
8	Q	102	A1EL2	C13-C12	7.13	1.45	1.35
9	o	101	A1ELD	C24-C22	-7.12	1.30	1.45
8	P	102	A1EL2	C32-C31	-7.11	1.40	1.51
9	R	102	A1ELD	C29-C27	6.99	1.60	1.45
9	o	101	A1ELD	C36-C35	-6.97	1.39	1.50
8	P	102	A1EL2	C23-C21	-6.91	1.31	1.45
9	o	101	A1ELD	C45-C2	6.88	1.67	1.53
9	o	101	A1ELD	C21-C22	6.81	1.44	1.35
9	B	103	A1ELD	C7-C6	-6.63	1.42	1.52
8	r	103	A1EL2	C36-C35	-6.53	1.40	1.54
9	o	101	A1ELD	C2-C3	-6.49	1.44	1.53
9	R	102	A1ELD	C45-C2	-6.49	1.41	1.53
8	r	103	A1EL2	C38-C31	6.46	1.61	1.50
8	Q	102	A1EL2	C25-C26	6.43	1.44	1.35
8	P	102	A1EL2	C11-C12	-6.42	1.32	1.45
9	o	101	A1ELD	C15-C16	-6.38	1.32	1.45
8	r	102	A1EL2	C17-C16	6.21	1.44	1.35
9	R	102	A1ELD	C15-C16	6.20	1.59	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	r	103	A1EL2	C15-C16	-6.20	1.32	1.45
9	O	102	A1ELD	C21-C22	-6.18	1.27	1.35
9	O	102	A1ELD	C33-C32	-6.16	1.38	1.50
9	e	101	A1ELD	C21-C22	6.12	1.43	1.35
8	J	102	A1EL2	C8-C4	-6.10	1.41	1.53
8	r	102	A1EL2	C20-C21	6.05	1.43	1.35
8	O	103	A1EL2	C20-C21	6.04	1.43	1.35
8	O	103	A1EL2	C25-C26	6.03	1.43	1.35
8	J	102	A1EL2	C32-C33	-6.03	1.42	1.52
8	O	103	A1EL2	C13-C12	6.01	1.43	1.35
9	R	102	A1ELD	C9-C10	5.99	1.58	1.45
8	r	103	A1EL2	C9-C4	-5.97	1.42	1.53
8	r	103	A1EL2	C35-C34	-5.88	1.45	1.54
9	O	102	A1ELD	C5-C6	5.86	1.62	1.52
8	r	103	A1EL2	C13-C12	-5.86	1.28	1.35
8	r	102	A1EL2	C13-C12	5.85	1.43	1.35
9	O	102	A1ELD	C18-C16	-5.84	1.28	1.35
8	P	102	A1EL2	C28-C26	-5.79	1.33	1.45
8	r	103	A1EL2	C25-C26	-5.78	1.28	1.35
9	e	101	A1ELD	C18-C16	5.77	1.43	1.35
8	O	103	A1EL2	C17-C16	5.76	1.43	1.35
11	G	103	PGV	O01-C1	5.71	1.45	1.33
9	R	102	A1ELD	C4-C3	-5.70	1.24	1.34
8	I	102	A1EL2	C25-C26	5.68	1.43	1.35
13	L	303	BPH	C3B-C2B	5.67	1.49	1.39
8	J	102	A1EL2	C17-C16	-5.63	1.28	1.35
9	o	101	A1ELD	C14-C15	5.62	1.49	1.34
9	R	102	A1ELD	C44-C2	-5.62	1.42	1.53
9	R	102	A1ELD	C30-C31	5.58	1.60	1.43
8	r	103	A1EL2	C7-C6	5.55	1.61	1.52
7	F	101	BCL	C3D-C4D	-5.55	1.31	1.44
8	I	102	A1EL2	C7-C2	5.53	1.59	1.51
8	J	102	A1EL2	C27-C26	-5.52	1.39	1.50
9	O	102	A1ELD	C38-C37	-5.52	1.40	1.52
7	M	401	BCL	O2D-CGD	5.42	1.46	1.33
9	e	101	A1ELD	C13-C10	5.42	1.43	1.35
8	r	103	A1EL2	C23-C21	-5.41	1.34	1.45
13	L	303	BPH	C4D-CHA	5.40	1.48	1.39
7	L	301	BCL	O2D-CGD	5.38	1.46	1.33
8	P	102	A1EL2	C18-C17	-5.34	1.26	1.43
9	R	102	A1ELD	O46-C6	5.31	1.59	1.43
8	Q	102	A1EL2	C28-C26	-5.31	1.34	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	r	103	A1EL2	C20-C21	-5.30	1.28	1.35
9	g	101	A1ELD	C31-C32	5.30	1.42	1.35
9	R	102	A1ELD	C8-C3	5.29	1.63	1.45
9	o	101	A1ELD	C39-C37	-5.28	1.40	1.52
9	J	103	A1ELD	C13-C10	5.27	1.42	1.35
7	F	101	BCL	C4B-NB	-5.26	1.31	1.37
8	r	103	A1EL2	C27-C26	-5.23	1.40	1.50
8	P	102	A1EL2	C19-C20	-5.22	1.27	1.43
8	Q	102	A1EL2	C4-C3	-5.21	1.46	1.53
7	M	401	BCL	C3B-C4B	5.21	1.50	1.41
8	r	103	A1EL2	C17-C16	-5.20	1.28	1.35
13	L	303	BPH	C3D-C2D	5.18	1.48	1.39
9	C	102	A1ELD	C31-C32	5.16	1.42	1.35
7	Q	101	BCL	O2D-CGD	5.08	1.45	1.33
8	r	103	A1EL2	C32-C31	-5.07	1.43	1.51
7	C	101	BCL	O2D-CGD	5.07	1.45	1.33
7	N	101	BCL	O2D-CGD	5.07	1.45	1.33
7	D	101	BCL	C3B-C4B	5.05	1.50	1.41
7	D	101	BCL	O2D-CGD	5.05	1.45	1.33
8	P	102	A1EL2	C7-C2	-5.05	1.43	1.51
7	B	101	BCL	O2D-CGD	5.04	1.45	1.33
8	O	103	A1EL2	C33-C34	5.04	1.59	1.52
8	I	102	A1EL2	C35-C34	5.04	1.61	1.54
7	G	101	BCL	O2D-CGD	5.03	1.45	1.33
8	r	103	A1EL2	C28-C26	-5.02	1.35	1.45
9	o	101	A1ELD	C30-C31	-5.01	1.27	1.43
7	S	101	BCL	O2D-CGD	5.01	1.45	1.33
7	F	101	BCL	O2A-CGA	5.00	1.47	1.33
7	O	101	BCL	O2D-CGD	4.97	1.45	1.33
8	G	102	A1EL2	C17-C16	4.96	1.42	1.35
7	I	101	BCL	O2D-CGD	4.96	1.45	1.33
13	L	303	BPH	O2D-CGD	4.95	1.45	1.33
8	r	103	A1EL2	C8-C4	4.95	1.63	1.53
7	A	101	BCL	O2D-CGD	4.95	1.45	1.33
7	M	403	BCL	O2D-CGD	4.94	1.45	1.33
13	L	303	BPH	C3B-C4B	4.94	1.50	1.41
7	M	403	BCL	C3B-C4B	4.94	1.50	1.41
7	K	101	BCL	O2D-CGD	4.93	1.45	1.33
9	b	101	A1ELD	C13-C10	4.88	1.42	1.35
7	E	101	BCL	O2D-CGD	4.88	1.45	1.33
7	o	102	BCL	O2D-CGD	4.88	1.45	1.33
7	c	101	BCL	O2D-CGD	4.88	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	101	BCL	O2D-CGD	4.87	1.45	1.33
8	O	103	A1EL2	C31-C30	4.86	1.42	1.34
7	R	101	BCL	O2D-CGD	4.85	1.45	1.33
7	L	302	BCL	O2D-CGD	4.83	1.45	1.33
7	s	101	BCL	O2D-CGD	4.83	1.45	1.33
7	s	101	BCL	C3D-C4D	-4.82	1.33	1.44
8	I	102	A1EL2	C32-C33	-4.81	1.44	1.52
7	e	102	BCL	O2D-CGD	4.80	1.44	1.33
7	b	102	BCL	O2D-CGD	4.80	1.44	1.33
7	M	403	BCL	C3D-C4D	-4.78	1.33	1.44
7	r	104	BCL	O2D-CGD	4.78	1.44	1.33
7	L	302	BCL	C3D-C4D	-4.78	1.33	1.44
7	q	102	BCL	C3D-C4D	-4.77	1.33	1.44
7	j	102	BCL	O2D-CGD	4.77	1.44	1.33
7	n	101	BCL	O2D-CGD	4.76	1.44	1.33
7	C	101	BCL	C3B-C4B	4.76	1.50	1.41
7	f	102	BCL	O2D-CGD	4.76	1.44	1.33
7	b	102	BCL	C3D-C4D	-4.76	1.33	1.44
7	e	102	BCL	C3D-C4D	-4.76	1.33	1.44
7	i	101	BCL	C3D-C4D	-4.75	1.33	1.44
7	a	101	BCL	C3D-C4D	-4.75	1.33	1.44
7	g	102	BCL	C3D-C4D	-4.75	1.33	1.44
7	d	102	BCL	O2D-CGD	4.74	1.44	1.33
7	f	102	BCL	C3D-C4D	-4.73	1.33	1.44
7	L	301	BCL	C3B-C4B	4.73	1.49	1.41
8	I	102	A1EL2	C32-C31	4.73	1.58	1.51
9	o	101	A1ELD	C14-C13	-4.72	1.28	1.43
7	p	101	BCL	O2D-CGD	4.72	1.44	1.33
7	a	101	BCL	O2D-CGD	4.72	1.44	1.33
7	q	102	BCL	O2D-CGD	4.72	1.44	1.33
7	r	104	BCL	C3D-C4D	-4.71	1.33	1.44
8	r	103	A1EL2	C11-C12	-4.70	1.35	1.45
7	j	102	BCL	C3D-C4D	-4.70	1.33	1.44
7	c	101	BCL	C3D-C4D	-4.69	1.33	1.44
7	k	101	BCL	O2D-CGD	4.68	1.44	1.33
7	M	401	BCL	C3D-C4D	-4.67	1.33	1.44
7	g	102	BCL	O2D-CGD	4.67	1.44	1.33
7	p	101	BCL	C3D-C4D	-4.67	1.33	1.44
7	J	101	BCL	O2D-CGD	4.66	1.44	1.33
7	n	101	BCL	C3D-C4D	-4.66	1.33	1.44
7	E	101	BCL	C3D-C4D	-4.66	1.33	1.44
7	L	301	BCL	C3D-C4D	-4.66	1.33	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	101	BCL	C3D-C4D	-4.66	1.33	1.44
8	J	102	A1EL2	C2-C3	4.65	1.42	1.34
8	r	103	A1EL2	C18-C17	-4.65	1.29	1.43
7	i	101	BCL	O2D-CGD	4.64	1.44	1.33
9	R	102	A1ELD	C14-C13	4.63	1.57	1.43
7	k	101	BCL	C3D-C4D	-4.63	1.33	1.44
8	r	102	A1EL2	C28-C26	-4.62	1.36	1.45
9	R	102	A1ELD	C7-C2	4.62	1.69	1.54
7	I	101	BCL	C3D-C4D	-4.60	1.33	1.44
7	d	102	BCL	C3D-C4D	-4.60	1.33	1.44
7	R	101	BCL	C3D-C4D	-4.59	1.33	1.44
8	P	102	A1EL2	C14-C13	-4.59	1.29	1.43
7	G	101	BCL	C3D-C4D	-4.58	1.33	1.44
7	S	101	BCL	C3D-C4D	-4.56	1.33	1.44
7	B	101	BCL	C3D-C4D	-4.56	1.33	1.44
7	P	101	BCL	C3D-C4D	-4.55	1.33	1.44
7	A	101	BCL	C3D-C4D	-4.55	1.33	1.44
7	Q	101	BCL	C3D-C4D	-4.54	1.33	1.44
13	L	303	BPH	OBD-CAD	4.53	1.28	1.22
7	K	101	BCL	C3D-C4D	-4.53	1.34	1.44
7	O	101	BCL	C3D-C4D	-4.53	1.34	1.44
7	N	101	BCL	C3B-C4B	4.52	1.49	1.41
7	o	102	BCL	C3D-C4D	-4.50	1.34	1.44
7	D	101	BCL	C3D-C4D	-4.49	1.34	1.44
11	T	301	PGV	O01-C1	4.49	1.47	1.34
8	r	102	A1EL2	C11-C12	-4.48	1.36	1.45
7	N	101	BCL	C3D-C4D	-4.47	1.34	1.44
7	C	101	BCL	C3D-C4D	-4.46	1.34	1.44
9	O	102	A1ELD	C43-C4	4.46	1.58	1.50
7	F	101	BCL	O2D-CGD	4.45	1.44	1.33
7	P	101	BCL	C3B-C4B	4.42	1.49	1.41
9	b	101	A1ELD	C18-C16	4.42	1.41	1.35
8	J	102	A1EL2	O1-C6	4.40	1.56	1.43
7	M	401	BCL	O2A-CGA	4.40	1.46	1.33
8	I	102	A1EL2	C13-C12	4.39	1.41	1.35
7	A	101	BCL	C3B-C4B	4.38	1.49	1.41
7	o	102	BCL	O2A-CGA	4.37	1.46	1.33
9	R	102	A1ELD	C23-C22	4.37	1.59	1.50
9	R	102	A1ELD	C24-C22	4.37	1.55	1.45
7	j	102	BCL	C3B-C4B	4.36	1.49	1.41
9	e	101	A1ELD	C29-C27	-4.36	1.36	1.45
7	M	403	BCL	O2A-CGA	4.35	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	101	BCL	C3B-C4B	4.35	1.49	1.41
7	G	101	BCL	C3B-C4B	4.35	1.49	1.41
9	o	101	A1ELD	C43-C4	-4.35	1.43	1.50
7	L	301	BCL	O2A-CGA	4.35	1.46	1.33
7	I	101	BCL	C3B-C4B	4.33	1.49	1.41
11	G	103	PGV	O03-C19	4.33	1.46	1.33
7	k	101	BCL	O2A-CGA	4.33	1.46	1.33
7	p	101	BCL	C3B-C4B	4.32	1.49	1.41
8	G	102	A1EL2	C13-C12	4.32	1.41	1.35
9	e	101	A1ELD	C9-C10	-4.31	1.36	1.45
8	G	102	A1EL2	C20-C21	4.31	1.41	1.35
9	o	101	A1ELD	C20-C21	-4.30	1.30	1.43
7	o	102	BCL	C3B-C4B	4.29	1.49	1.41
7	i	101	BCL	C3B-C4B	4.29	1.49	1.41
9	o	101	A1ELD	C25-C26	-4.29	1.30	1.43
7	a	101	BCL	O2A-CGA	4.28	1.45	1.33
7	r	104	BCL	C3B-C4B	4.28	1.49	1.41
7	g	102	BCL	O2A-CGA	4.28	1.45	1.33
7	b	102	BCL	O2A-CGA	4.28	1.45	1.33
7	d	102	BCL	C3B-C4B	4.28	1.49	1.41
7	g	102	BCL	C3B-C4B	4.27	1.49	1.41
9	R	103	A1ELD	C13-C10	4.26	1.41	1.35
7	e	102	BCL	O2A-CGA	4.26	1.45	1.33
7	q	102	BCL	C3B-C4B	4.26	1.49	1.41
8	P	102	A1EL2	C24-C25	-4.26	1.30	1.43
9	B	103	A1ELD	C5-C6	4.26	1.59	1.52
7	b	102	BCL	C3B-C4B	4.26	1.49	1.41
9	R	102	A1ELD	C25-C26	4.25	1.56	1.43
8	r	103	A1EL2	C19-C20	-4.25	1.30	1.43
8	Q	102	A1EL2	C23-C21	-4.25	1.36	1.45
7	r	104	BCL	O2A-CGA	4.24	1.45	1.33
13	L	303	BPH	O2A-CGA	4.24	1.45	1.33
11	T	301	PGV	O03-C19	4.24	1.45	1.33
11	L	308	PGV	O01-C1	4.24	1.46	1.34
11	M	408	PGV	O03-C19	4.23	1.45	1.33
7	s	101	BCL	O2A-CGA	4.23	1.45	1.33
9	R	103	A1ELD	C21-C22	4.23	1.41	1.35
7	E	101	BCL	C3B-C4B	4.23	1.49	1.41
7	j	102	BCL	O2A-CGA	4.22	1.45	1.33
9	g	101	A1ELD	C21-C22	4.22	1.41	1.35
7	K	101	BCL	C3B-C4B	4.22	1.48	1.41
8	J	102	A1EL2	C5-C4	4.22	1.68	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	101	BCL	O2A-CGA	4.22	1.45	1.33
8	J	102	A1EL2	C20-C21	-4.21	1.30	1.35
11	D	103	PGV	O03-C19	4.21	1.45	1.33
11	T	303	PGV	O03-C19	4.21	1.45	1.33
7	f	102	BCL	C3B-C4B	4.20	1.48	1.41
7	q	102	BCL	O2A-CGA	4.20	1.45	1.33
7	L	302	BCL	O2A-CGA	4.20	1.45	1.33
11	L	308	PGV	O03-C19	4.19	1.45	1.33
7	s	101	BCL	C3B-C4B	4.19	1.48	1.41
7	S	101	BCL	O2A-CGA	4.18	1.45	1.33
7	c	101	BCL	C3B-C4B	4.18	1.48	1.41
9	R	103	A1ELD	C18-C16	4.18	1.41	1.35
7	N	101	BCL	O2A-CGA	4.17	1.45	1.33
9	f	101	A1ELD	C13-C10	4.17	1.41	1.35
7	i	101	BCL	O2A-CGA	4.16	1.45	1.33
7	O	101	BCL	C3B-C4B	4.15	1.48	1.41
7	c	101	BCL	C1B-NB	-4.15	1.32	1.37
9	b	101	A1ELD	C31-C32	4.14	1.41	1.35
7	E	101	BCL	O2A-CGA	4.14	1.45	1.33
8	I	102	A1EL2	C27-C26	-4.14	1.42	1.50
7	K	101	BCL	O2A-CGA	4.14	1.45	1.33
7	n	101	BCL	O2A-CGA	4.14	1.45	1.33
7	k	101	BCL	C3B-C4B	4.13	1.48	1.41
7	I	101	BCL	O2A-CGA	4.12	1.45	1.33
7	p	101	BCL	O2A-CGA	4.12	1.45	1.33
7	G	101	BCL	O2A-CGA	4.12	1.45	1.33
11	M	408	PGV	O01-C1	4.10	1.45	1.34
11	T	303	PGV	O01-C1	4.10	1.45	1.34
7	e	102	BCL	C3B-C4B	4.10	1.48	1.41
7	J	101	BCL	C3B-C4B	4.10	1.48	1.41
9	d	101	A1ELD	C13-C10	4.09	1.41	1.35
7	J	101	BCL	O2A-CGA	4.09	1.45	1.33
7	d	102	BCL	O2A-CGA	4.09	1.45	1.33
11	F	103	PGV	O03-C19	4.09	1.45	1.33
8	J	102	A1EL2	C31-C30	-4.08	1.27	1.34
7	n	101	BCL	C3B-C4B	4.08	1.48	1.41
7	P	101	BCL	O2A-CGA	4.07	1.45	1.33
8	K	102	A1EL2	C17-C16	4.07	1.41	1.35
7	L	302	BCL	C3B-C4B	4.07	1.48	1.41
11	L	307	PGV	O01-C1	4.07	1.45	1.34
11	D	103	PGV	O01-C1	4.07	1.45	1.34
7	B	101	BCL	O2A-CGA	4.07	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	103	PGV	O01-C1	4.06	1.45	1.34
7	O	101	BCL	O2A-CGA	4.05	1.45	1.33
8	r	103	A1EL2	C1-C2	4.05	1.57	1.50
9	o	101	A1ELD	O13-C12	-4.05	1.12	1.22
9	R	102	A1ELD	C17-C16	4.05	1.59	1.50
8	J	102	A1EL2	C10-C3	4.04	1.59	1.45
9	o	101	A1ELD	C19-C18	-4.04	1.30	1.43
9	r	101	A1ELD	C18-C16	4.04	1.41	1.35
9	o	101	A1ELD	C7-C2	-4.04	1.42	1.54
7	B	101	BCL	C3B-C4B	4.03	1.48	1.41
7	Q	101	BCL	C3B-C4B	4.03	1.48	1.41
7	c	101	BCL	O2A-CGA	4.03	1.45	1.33
7	a	101	BCL	C3B-C4B	4.03	1.48	1.41
9	r	101	A1ELD	C13-C10	4.02	1.41	1.35
9	R	102	A1ELD	C33-C32	-4.02	1.42	1.50
9	b	101	A1ELD	C21-C22	4.02	1.41	1.35
7	f	102	BCL	O2A-CGA	4.01	1.45	1.33
9	B	103	A1ELD	C36-C35	4.01	1.56	1.50
7	M	401	BCL	C1B-NB	-4.00	1.32	1.37
7	A	101	BCL	O2A-CGA	4.00	1.45	1.33
7	D	101	BCL	O2A-CGA	4.00	1.45	1.33
9	r	101	A1ELD	C21-C22	4.00	1.41	1.35
7	c	101	BCL	C1D-ND	-3.99	1.32	1.37
9	q	101	A1ELD	C13-C10	3.98	1.41	1.35
7	Q	101	BCL	O2A-CGA	3.97	1.44	1.33
7	R	101	BCL	C3B-C4B	3.97	1.48	1.41
9	q	101	A1ELD	C21-C22	3.96	1.41	1.35
7	k	101	BCL	C1D-ND	-3.95	1.32	1.37
9	e	101	A1ELD	C34-C32	-3.95	1.37	1.45
9	e	101	A1ELD	C31-C32	3.94	1.41	1.35
9	q	101	A1ELD	C31-C32	3.94	1.41	1.35
7	o	102	BCL	C1D-ND	-3.92	1.33	1.37
9	R	102	A1ELD	C21-C22	-3.91	1.30	1.35
16	M	405	H4X	C27-C28	3.90	1.41	1.35
9	R	103	A1ELD	C31-C32	3.90	1.41	1.35
7	e	102	BCL	C1D-ND	-3.90	1.33	1.37
8	A	102	A1EL2	C17-C16	3.89	1.40	1.35
9	q	101	A1ELD	C18-C16	3.89	1.40	1.35
7	n	101	BCL	C1D-ND	-3.89	1.33	1.37
8	E	102	A1EL2	C17-C16	3.88	1.40	1.35
8	B	102	A1EL2	C17-C16	3.88	1.40	1.35
8	C	103	A1EL2	C17-C16	3.88	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	101	BCL	O2A-CGA	3.88	1.44	1.33
8	F	102	A1EL2	C17-C16	3.88	1.40	1.35
8	r	103	A1EL2	C32-C33	-3.87	1.46	1.52
8	r	102	A1EL2	C25-C26	3.87	1.40	1.35
8	D	102	A1EL2	C17-C16	3.87	1.40	1.35
7	f	102	BCL	C1D-ND	-3.86	1.33	1.37
9	r	101	A1ELD	C31-C32	3.86	1.40	1.35
16	M	405	H4X	C19-C17	3.86	1.40	1.35
8	N	102	A1EL2	C13-C12	3.85	1.40	1.35
9	C	102	A1ELD	C21-C22	3.85	1.40	1.35
9	O	102	A1ELD	C45-C2	3.84	1.61	1.53
16	M	405	H4X	C14-C12	3.84	1.40	1.35
7	b	102	BCL	C1D-ND	-3.83	1.33	1.37
8	N	102	A1EL2	C17-C16	3.82	1.40	1.35
16	M	405	H4X	C22-C23	3.82	1.40	1.35
8	J	102	A1EL2	C11-C12	3.82	1.54	1.45
9	B	103	A1ELD	C44-C2	-3.81	1.46	1.53
7	q	102	BCL	C1D-ND	-3.81	1.33	1.37
9	J	103	A1ELD	C18-C16	3.81	1.40	1.35
8	K	102	A1EL2	C15-C16	-3.81	1.37	1.45
9	O	102	A1ELD	C20-C19	-3.81	1.26	1.36
8	r	103	A1EL2	C4-C3	3.80	1.59	1.53
8	D	102	A1EL2	C13-C12	3.79	1.40	1.35
7	L	302	BCL	C1D-ND	-3.79	1.33	1.37
7	p	101	BCL	C1D-ND	-3.79	1.33	1.37
7	j	102	BCL	C1D-ND	-3.79	1.33	1.37
8	G	102	A1EL2	C25-C26	3.79	1.40	1.35
8	D	102	A1EL2	C25-C26	3.78	1.40	1.35
8	I	102	A1EL2	C40-C12	-3.78	1.43	1.50
7	a	101	BCL	C1D-ND	-3.78	1.33	1.37
8	I	102	A1EL2	C8-C4	-3.77	1.46	1.53
8	A	102	A1EL2	C13-C12	3.77	1.40	1.35
7	s	101	BCL	C1D-ND	-3.77	1.33	1.37
7	r	104	BCL	C1D-ND	-3.77	1.33	1.37
8	E	102	A1EL2	C13-C12	3.76	1.40	1.35
9	o	101	A1ELD	C9-C8	3.76	1.44	1.33
8	r	102	A1EL2	C23-C21	-3.76	1.37	1.45
8	B	102	A1EL2	C20-C21	3.76	1.40	1.35
8	C	103	A1EL2	C20-C21	3.75	1.40	1.35
8	C	103	A1EL2	C25-C26	3.75	1.40	1.35
7	J	101	BCL	C4B-NB	-3.75	1.33	1.37
7	d	102	BCL	C1D-ND	-3.75	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	101	BCL	C4B-NB	-3.74	1.33	1.37
9	A	103	A1ELD	C13-C10	3.74	1.40	1.35
8	F	102	A1EL2	C13-C12	3.74	1.40	1.35
8	B	102	A1EL2	C13-C12	3.74	1.40	1.35
7	g	102	BCL	C1D-ND	-3.73	1.33	1.37
8	A	102	A1EL2	C20-C21	3.73	1.40	1.35
9	A	103	A1ELD	C21-C22	3.73	1.40	1.35
8	N	102	A1EL2	C25-C26	3.72	1.40	1.35
8	C	103	A1EL2	C13-C12	3.72	1.40	1.35
8	K	102	A1EL2	C11-C12	-3.72	1.38	1.45
9	d	101	A1ELD	C9-C10	-3.72	1.38	1.45
8	B	102	A1EL2	C25-C26	3.72	1.40	1.35
9	O	102	A1ELD	C36-C35	3.72	1.56	1.50
9	B	103	A1ELD	C43-C4	3.71	1.57	1.50
8	E	102	A1EL2	C25-C26	3.71	1.40	1.35
8	E	102	A1EL2	C20-C21	3.71	1.40	1.35
8	A	102	A1EL2	C25-C26	3.70	1.40	1.35
8	G	102	A1EL2	C28-C26	-3.70	1.38	1.45
8	r	102	A1EL2	C15-C16	-3.70	1.38	1.45
9	o	101	A1ELD	O46-C6	-3.69	1.32	1.43
9	A	103	A1ELD	C18-C16	3.69	1.40	1.35
8	F	102	A1EL2	C25-C26	3.69	1.40	1.35
8	O	103	A1EL2	C5-C6	-3.69	1.47	1.52
9	O	102	A1ELD	O42-C41	-3.69	1.31	1.43
8	O	103	A1EL2	C11-C12	-3.69	1.38	1.45
8	N	102	A1EL2	C20-C21	3.69	1.40	1.35
8	F	102	A1EL2	C20-C21	3.68	1.40	1.35
7	i	101	BCL	C1D-ND	-3.68	1.33	1.37
8	Q	102	A1EL2	C11-C12	-3.68	1.38	1.45
8	D	102	A1EL2	C20-C21	3.67	1.40	1.35
8	J	102	A1EL2	C29-C30	3.66	1.58	1.45
7	M	403	BCL	C1D-ND	-3.64	1.33	1.37
9	B	103	A1ELD	C38-C37	-3.64	1.44	1.52
8	P	102	A1EL2	C38-C31	3.62	1.56	1.50
9	o	101	A1ELD	C44-C2	3.62	1.60	1.53
8	r	103	A1EL2	C14-C13	-3.61	1.32	1.43
8	G	102	A1EL2	C33-C34	-3.60	1.47	1.52
7	O	101	BCL	CHD-C1D	3.59	1.45	1.38
9	A	103	A1ELD	C31-C32	3.59	1.40	1.35
7	P	101	BCL	CHD-C1D	3.58	1.45	1.38
7	R	101	BCL	C4B-NB	-3.57	1.33	1.37
7	J	101	BCL	CHD-C1D	3.56	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	102	A1EL2	C40-C12	-3.56	1.43	1.50
7	F	101	BCL	CHB-C4A	-3.54	1.29	1.37
7	O	101	BCL	C4B-NB	-3.54	1.33	1.37
8	O	103	A1EL2	C8-C4	3.53	1.60	1.53
7	P	101	BCL	C4B-NB	-3.52	1.33	1.37
9	R	102	A1ELD	C18-C16	-3.51	1.31	1.35
8	I	102	A1EL2	C22-C21	-3.51	1.43	1.50
9	o	101	A1ELD	C20-C19	3.50	1.45	1.36
8	K	102	A1EL2	C20-C21	3.49	1.40	1.35
7	S	101	BCL	C4B-NB	-3.48	1.33	1.37
7	I	101	BCL	C4B-NB	-3.47	1.33	1.37
8	Q	102	A1EL2	C1-C2	-3.47	1.45	1.50
7	K	101	BCL	CHD-C1D	3.46	1.45	1.38
7	M	403	BCL	OBD-CAD	3.46	1.28	1.22
9	d	101	A1ELD	C29-C27	-3.46	1.38	1.45
7	M	401	BCL	C1D-ND	-3.44	1.33	1.37
7	G	101	BCL	CHD-C1D	3.44	1.45	1.38
7	E	101	BCL	C4B-NB	-3.43	1.33	1.37
8	J	102	A1EL2	C36-C35	-3.43	1.46	1.54
7	E	101	BCL	CHD-C1D	3.43	1.45	1.38
7	M	403	BCL	CHC-C4B	3.42	1.47	1.39
9	B	103	A1ELD	C4-C3	-3.42	1.28	1.34
8	I	102	A1EL2	C33-C34	-3.42	1.47	1.52
8	r	103	A1EL2	C22-C21	-3.42	1.43	1.50
7	F	101	BCL	C3B-C4B	3.41	1.47	1.41
8	r	103	A1EL2	C14-C15	-3.41	1.25	1.34
9	R	102	A1ELD	C34-C35	3.40	1.40	1.32
7	B	101	BCL	CHB-C1B	3.40	1.47	1.39
7	B	101	BCL	CHD-C1D	3.40	1.45	1.38
8	Q	102	A1EL2	C14-C15	3.39	1.43	1.34
7	B	101	BCL	C4B-NB	-3.39	1.33	1.37
7	D	101	BCL	CHD-C1D	3.38	1.45	1.38
7	S	101	BCL	CHB-C1B	3.38	1.47	1.39
7	Q	101	BCL	CHD-C1D	3.38	1.44	1.38
9	f	101	A1ELD	C18-C16	3.38	1.40	1.35
7	Q	101	BCL	C4B-NB	-3.37	1.33	1.37
8	r	103	A1EL2	C24-C25	-3.37	1.33	1.43
7	n	101	BCL	C4B-NB	-3.36	1.33	1.37
7	L	301	BCL	CHC-C4B	3.36	1.46	1.39
7	M	401	BCL	CHD-C1D	3.36	1.44	1.38
7	j	102	BCL	CHD-C1D	3.35	1.44	1.38
9	B	103	A1ELD	C2-C3	3.35	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	101	BCL	OBD-CAD	3.35	1.28	1.22
9	e	101	A1ELD	C24-C22	-3.35	1.38	1.45
8	G	102	A1EL2	C23-C21	-3.34	1.38	1.45
13	L	303	BPH	CHA-CBD	-3.34	1.47	1.51
9	R	102	A1ELD	C38-C37	-3.34	1.45	1.52
7	N	101	BCL	C4B-NB	-3.33	1.33	1.37
9	d	101	A1ELD	C18-C16	3.33	1.40	1.35
7	Q	101	BCL	CHB-C1B	3.32	1.46	1.39
7	k	101	BCL	CHB-C1B	3.32	1.46	1.39
7	a	101	BCL	CHB-C1B	3.32	1.46	1.39
9	j	101	A1ELD	C7-C6	-3.32	1.47	1.52
8	r	103	A1EL2	C19-C18	-3.32	1.27	1.36
7	E	101	BCL	CHB-C1B	3.31	1.46	1.39
8	O	103	A1EL2	C28-C26	-3.30	1.38	1.45
9	B	103	A1ELD	C33-C32	-3.30	1.44	1.50
7	N	101	BCL	CHD-C1D	3.30	1.44	1.38
7	J	101	BCL	OBD-CAD	3.30	1.28	1.22
9	O	102	A1ELD	C2-C3	3.29	1.58	1.53
8	I	102	A1EL2	C20-C21	3.29	1.40	1.35
7	p	101	BCL	OBD-CAD	3.29	1.28	1.22
7	j	102	BCL	OBD-CAD	3.28	1.28	1.22
9	B	103	A1ELD	O42-C41	-3.27	1.32	1.43
9	o	101	A1ELD	C8-C3	-3.27	1.33	1.45
7	o	102	BCL	CHB-C1B	3.27	1.46	1.39
7	O	101	BCL	OBD-CAD	3.27	1.28	1.22
7	I	101	BCL	CHD-C1D	3.26	1.44	1.38
9	O	102	A1ELD	C12-C27	-3.26	1.34	1.45
7	L	301	BCL	C4B-NB	-3.26	1.33	1.37
7	C	101	BCL	OBD-CAD	3.25	1.28	1.22
7	j	102	BCL	CHC-C4B	3.25	1.46	1.39
7	R	101	BCL	CHD-C1D	3.25	1.44	1.38
7	K	101	BCL	OBD-CAD	3.25	1.28	1.22
9	e	101	A1ELD	C15-C16	-3.25	1.39	1.45
9	B	103	A1ELD	C24-C22	-3.24	1.39	1.45
7	d	102	BCL	OBD-CAD	3.24	1.28	1.22
8	r	103	A1EL2	C24-C23	-3.24	1.26	1.34
7	L	302	BCL	C4B-NB	-3.24	1.33	1.37
7	g	102	BCL	CHB-C1B	3.23	1.46	1.39
7	n	101	BCL	CHB-C1B	3.22	1.46	1.39
9	d	101	A1ELD	C24-C22	-3.22	1.39	1.45
7	D	101	BCL	OBD-CAD	3.22	1.28	1.22
7	C	101	BCL	CHD-C1D	3.22	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	101	BCL	C1B-NB	-3.22	1.33	1.37
7	k	101	BCL	OBD-CAD	3.22	1.28	1.22
8	J	102	A1EL2	C22-C21	-3.22	1.44	1.50
7	L	302	BCL	CHB-C1B	3.21	1.46	1.39
7	P	101	BCL	OBD-CAD	3.21	1.28	1.22
7	q	102	BCL	C4B-NB	-3.21	1.33	1.37
7	A	101	BCL	CHD-C1D	3.21	1.44	1.38
7	N	101	BCL	OBD-CAD	3.21	1.28	1.22
7	R	101	BCL	OBD-CAD	3.20	1.28	1.22
9	R	102	A1ELD	O42-C41	-3.20	1.33	1.43
8	J	102	A1EL2	C15-C16	3.20	1.52	1.45
7	K	101	BCL	CHB-C1B	3.20	1.46	1.39
7	o	102	BCL	OBD-CAD	3.19	1.28	1.22
7	e	102	BCL	C4B-NB	-3.19	1.33	1.37
7	p	101	BCL	CHC-C4B	3.19	1.46	1.39
7	s	101	BCL	C4B-NB	-3.19	1.33	1.37
7	g	102	BCL	CHC-C4B	3.19	1.46	1.39
7	r	104	BCL	OBD-CAD	3.19	1.28	1.22
7	f	102	BCL	CHB-C1B	3.18	1.46	1.39
7	b	102	BCL	CHB-C1B	3.18	1.46	1.39
9	J	103	A1ELD	C9-C10	-3.18	1.39	1.45
7	a	101	BCL	CHD-C1D	3.18	1.44	1.38
7	e	102	BCL	CHB-C1B	3.18	1.46	1.39
7	F	101	BCL	C3D-C2D	3.17	1.47	1.39
8	P	102	A1EL2	C2-C3	3.17	1.39	1.34
8	Q	102	A1EL2	C7-C6	-3.17	1.46	1.52
7	L	301	BCL	C1B-NB	-3.17	1.33	1.37
7	p	101	BCL	CHD-C1D	3.16	1.44	1.38
7	Q	101	BCL	OBD-CAD	3.16	1.27	1.22
7	L	302	BCL	OBD-CAD	3.16	1.27	1.22
7	M	401	BCL	CHC-C4B	3.16	1.46	1.39
7	A	101	BCL	OBD-CAD	3.16	1.27	1.22
7	g	102	BCL	OBD-CAD	3.16	1.27	1.22
7	L	302	BCL	CHD-C1D	3.16	1.44	1.38
7	g	102	BCL	C4B-NB	-3.15	1.33	1.37
9	g	101	A1ELD	C30-C29	3.15	1.42	1.34
8	J	102	A1EL2	C19-C18	-3.15	1.27	1.36
7	r	104	BCL	CHB-C1B	3.15	1.46	1.39
7	I	101	BCL	CHB-C1B	3.15	1.46	1.39
7	q	102	BCL	CHC-C4B	3.14	1.46	1.39
7	G	101	BCL	C4B-NB	-3.14	1.33	1.37
7	b	102	BCL	C4B-NB	-3.14	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	102	BCL	CHC-C4B	3.14	1.46	1.39
7	k	101	BCL	CHC-C4B	3.14	1.46	1.39
7	r	104	BCL	CHC-C4B	3.14	1.46	1.39
7	c	101	BCL	CHD-C1D	3.13	1.44	1.38
7	p	101	BCL	CHB-C1B	3.13	1.46	1.39
7	K	101	BCL	C4B-NB	-3.13	1.33	1.37
8	K	102	A1EL2	C5-C6	-3.13	1.47	1.52
7	F	101	BCL	CHC-C4B	3.13	1.46	1.39
7	b	102	BCL	OBD-CAD	3.13	1.27	1.22
7	L	301	BCL	CHD-C1D	3.13	1.44	1.38
8	G	102	A1EL2	C5-C6	3.12	1.56	1.52
9	d	101	A1ELD	C34-C32	-3.12	1.39	1.45
7	r	104	BCL	CHD-C1D	3.12	1.44	1.38
7	G	101	BCL	C1B-NB	-3.12	1.33	1.37
9	f	101	A1ELD	C9-C10	-3.12	1.39	1.45
9	R	102	A1ELD	C30-C29	3.12	1.42	1.34
7	f	102	BCL	CHC-C4B	3.11	1.46	1.39
7	G	101	BCL	OBD-CAD	3.11	1.27	1.22
7	d	102	BCL	CHC-C4B	3.11	1.46	1.39
11	G	103	PGV	O01-C02	-3.11	1.43	1.46
8	Q	102	A1EL2	C35-C34	-3.11	1.49	1.54
7	S	101	BCL	CHD-C1D	3.10	1.44	1.38
7	n	101	BCL	OBD-CAD	3.10	1.27	1.22
7	d	102	BCL	C4B-NB	-3.10	1.34	1.37
7	r	104	BCL	C4B-NB	-3.10	1.34	1.37
7	i	101	BCL	CHC-C4B	3.09	1.46	1.39
7	M	403	BCL	CHD-C1D	3.09	1.44	1.38
7	g	102	BCL	CHD-C1D	3.09	1.44	1.38
7	s	101	BCL	CHD-C1D	3.09	1.44	1.38
7	A	101	BCL	C1B-NB	-3.08	1.34	1.37
9	g	101	A1ELD	C18-C16	3.08	1.39	1.35
7	i	101	BCL	CHB-C1B	3.08	1.46	1.39
7	d	102	BCL	CHD-C1D	3.08	1.44	1.38
7	o	102	BCL	CHC-C4B	3.07	1.46	1.39
7	L	301	BCL	CHB-C1B	3.07	1.46	1.39
7	q	102	BCL	CHD-C1D	3.07	1.44	1.38
9	C	102	A1ELD	C30-C29	3.06	1.42	1.34
8	Q	102	A1EL2	C24-C23	3.06	1.42	1.34
7	a	101	BCL	C4B-NB	-3.06	1.34	1.37
7	s	101	BCL	CHC-C4B	3.06	1.46	1.39
7	L	301	BCL	C1D-ND	-3.05	1.34	1.37
9	O	102	A1ELD	C25-C24	-3.05	1.26	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	102	BCL	CHD-C1D	3.05	1.44	1.38
7	j	102	BCL	CHB-C1B	3.04	1.46	1.39
7	p	101	BCL	C4B-NB	-3.04	1.34	1.37
7	f	102	BCL	C4B-NB	-3.04	1.34	1.37
7	N	101	BCL	C1B-NB	-3.04	1.34	1.37
7	S	101	BCL	OBD-CAD	3.04	1.27	1.22
7	s	101	BCL	CHB-C1B	3.04	1.46	1.39
8	Q	102	A1EL2	C19-C18	3.04	1.43	1.36
8	Q	102	A1EL2	C32-C31	-3.04	1.46	1.51
8	Q	102	A1EL2	C24-C25	-3.04	1.34	1.43
7	k	101	BCL	CHD-C1D	3.03	1.44	1.38
8	K	102	A1EL2	C13-C12	3.03	1.39	1.35
9	d	101	A1ELD	C15-C16	-3.03	1.39	1.45
7	d	102	BCL	CHB-C1B	3.03	1.46	1.39
8	G	102	A1EL2	C11-C12	-3.03	1.39	1.45
7	M	401	BCL	CHB-C1B	3.03	1.46	1.39
7	e	102	BCL	CHC-C4B	3.02	1.46	1.39
8	O	103	A1EL2	C27-C26	-3.02	1.44	1.50
7	o	102	BCL	C3D-C2D	3.02	1.47	1.39
7	q	102	BCL	CHB-C1B	3.02	1.46	1.39
7	D	101	BCL	CHB-C1B	3.02	1.46	1.39
7	b	102	BCL	CHD-C1D	3.02	1.44	1.38
7	B	101	BCL	OBD-CAD	3.01	1.27	1.22
7	e	102	BCL	CHD-C1D	3.01	1.44	1.38
9	f	101	A1ELD	C21-C22	3.00	1.39	1.35
7	M	401	BCL	OBD-CAD	3.00	1.27	1.22
7	R	101	BCL	C1D-ND	-3.00	1.34	1.37
7	C	101	BCL	CHC-C4B	2.99	1.46	1.39
9	d	101	A1ELD	C21-C22	2.99	1.39	1.35
7	D	101	BCL	CHC-C4B	2.98	1.46	1.39
7	f	102	BCL	CHD-C1D	2.98	1.44	1.38
7	G	101	BCL	CHB-C1B	2.98	1.46	1.39
7	c	101	BCL	C3D-C2D	2.98	1.47	1.39
7	s	101	BCL	C1B-NB	-2.98	1.34	1.37
7	i	101	BCL	OBD-CAD	2.98	1.27	1.22
7	d	102	BCL	C1B-NB	-2.98	1.34	1.37
7	f	102	BCL	OBD-CAD	2.98	1.27	1.22
7	p	101	BCL	C3D-C2D	2.98	1.47	1.39
7	L	302	BCL	CHC-C4B	2.97	1.46	1.39
7	A	101	BCL	CHB-C1B	2.97	1.46	1.39
7	L	302	BCL	C3D-C2D	2.97	1.47	1.39
8	Q	102	A1EL2	C15-C16	-2.96	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	e	102	BCL	OBD-CAD	2.96	1.27	1.22
7	M	403	BCL	CHB-C1B	2.96	1.46	1.39
7	o	102	BCL	C4B-NB	-2.96	1.34	1.37
7	A	101	BCL	CHC-C1C	-2.96	1.30	1.37
7	i	101	BCL	CHD-C1D	2.95	1.44	1.38
9	O	102	A1ELD	C26-C27	-2.95	1.31	1.41
7	S	101	BCL	C3D-C2D	2.95	1.47	1.39
7	e	102	BCL	C1B-NB	-2.95	1.34	1.37
7	E	101	BCL	C1D-ND	-2.95	1.34	1.37
7	n	101	BCL	CHD-C1D	2.95	1.44	1.38
9	f	101	A1ELD	C31-C32	2.94	1.39	1.35
7	E	101	BCL	C3D-C2D	2.94	1.47	1.39
7	a	101	BCL	C1B-NB	-2.94	1.34	1.37
7	i	101	BCL	C4B-NB	-2.94	1.34	1.37
7	N	101	BCL	C1D-ND	-2.94	1.34	1.37
7	I	101	BCL	C1D-ND	-2.93	1.34	1.37
8	J	102	A1EL2	C33-C34	-2.93	1.48	1.52
7	N	101	BCL	CHB-C1B	2.93	1.46	1.39
7	C	101	BCL	C1B-NB	-2.93	1.34	1.37
7	d	102	BCL	C3D-C2D	2.93	1.47	1.39
7	c	101	BCL	C4B-NB	-2.93	1.34	1.37
7	K	101	BCL	C3D-C2D	2.93	1.47	1.39
9	A	103	A1ELD	C9-C10	-2.92	1.39	1.45
7	G	101	BCL	C3D-C2D	2.92	1.47	1.39
7	B	101	BCL	C1D-ND	-2.92	1.34	1.37
7	a	101	BCL	CHC-C4B	2.92	1.46	1.39
7	q	102	BCL	OBD-CAD	2.91	1.27	1.22
7	P	101	BCL	C1B-NB	-2.91	1.34	1.37
7	r	104	BCL	C1B-NB	-2.91	1.34	1.37
7	f	102	BCL	C3D-C2D	2.91	1.47	1.39
7	S	101	BCL	C1D-ND	-2.91	1.34	1.37
7	n	101	BCL	C3D-C2D	2.91	1.47	1.39
7	O	101	BCL	C3D-C2D	2.91	1.47	1.39
8	J	102	A1EL2	C23-C21	2.91	1.52	1.45
7	S	101	BCL	MG-NA	-2.91	1.99	2.06
7	o	102	BCL	C1B-NB	-2.90	1.34	1.37
7	s	101	BCL	OBD-CAD	2.90	1.27	1.22
7	j	102	BCL	C4B-NB	-2.90	1.34	1.37
7	G	101	BCL	C1D-ND	-2.90	1.34	1.37
9	R	102	A1ELD	C19-C18	2.90	1.52	1.43
7	C	101	BCL	C3D-C2D	2.90	1.47	1.39
7	i	101	BCL	C1B-NB	-2.89	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	101	BCL	C3D-C2D	2.89	1.47	1.39
9	R	102	A1ELD	C9-C8	2.89	1.41	1.33
9	e	101	A1ELD	C30-C31	-2.89	1.34	1.43
7	J	101	BCL	C1B-NB	-2.89	1.34	1.37
7	J	101	BCL	C1D-ND	-2.88	1.34	1.37
7	P	101	BCL	C3D-C2D	2.88	1.47	1.39
7	k	101	BCL	C4B-NB	-2.88	1.34	1.37
7	q	102	BCL	C1B-NB	-2.88	1.34	1.37
7	J	101	BCL	C3D-C2D	2.88	1.47	1.39
7	a	101	BCL	C3D-C2D	2.88	1.47	1.39
7	k	101	BCL	C3D-C2D	2.87	1.47	1.39
7	n	101	BCL	CHC-C4B	2.87	1.45	1.39
9	J	103	A1ELD	C29-C27	-2.87	1.39	1.45
7	D	101	BCL	C1B-NB	-2.87	1.34	1.37
7	n	101	BCL	C1B-NB	-2.87	1.34	1.37
7	r	104	BCL	C3D-C2D	2.87	1.46	1.39
8	O	103	A1EL2	C29-C28	2.87	1.41	1.33
7	B	101	BCL	C3D-C2D	2.87	1.46	1.39
7	C	101	BCL	C1D-ND	-2.87	1.34	1.37
9	C	102	A1ELD	C18-C16	2.86	1.39	1.35
7	R	101	BCL	C1B-NB	-2.86	1.34	1.37
7	f	102	BCL	C1B-NB	-2.86	1.34	1.37
8	P	102	A1EL2	C32-C33	2.86	1.57	1.52
7	Q	101	BCL	C1D-ND	-2.86	1.34	1.37
7	D	101	BCL	C3D-C2D	2.86	1.46	1.39
7	j	102	BCL	C3D-C2D	2.86	1.46	1.39
7	A	101	BCL	C1D-ND	-2.85	1.34	1.37
7	g	102	BCL	C3D-C2D	2.85	1.46	1.39
7	P	101	BCL	CHC-C4B	2.85	1.45	1.39
7	R	101	BCL	C3D-C2D	2.85	1.46	1.39
8	F	102	A1EL2	C11-C12	-2.85	1.39	1.45
7	e	102	BCL	C3D-C2D	2.85	1.46	1.39
7	P	101	BCL	C1D-ND	-2.85	1.34	1.37
8	D	102	A1EL2	C11-C12	-2.84	1.39	1.45
7	q	102	BCL	C3D-C2D	2.84	1.46	1.39
7	C	101	BCL	CHB-C1B	2.84	1.45	1.39
8	E	102	A1EL2	C11-C12	-2.84	1.39	1.45
8	D	102	A1EL2	C28-C26	-2.84	1.39	1.45
7	O	101	BCL	C1B-NB	-2.84	1.34	1.37
9	J	103	A1ELD	C24-C22	-2.84	1.39	1.45
7	B	101	BCL	C1B-NB	-2.84	1.34	1.37
7	c	101	BCL	CHC-C4B	2.83	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	101	BCL	C1B-NB	-2.83	1.34	1.37
8	O	103	A1EL2	C15-C16	-2.83	1.39	1.45
8	C	103	A1EL2	C11-C12	-2.83	1.39	1.45
7	L	302	BCL	MG-NA	-2.83	1.99	2.06
7	I	101	BCL	C3D-C2D	2.83	1.46	1.39
7	g	102	BCL	C1B-NB	-2.83	1.34	1.37
8	C	103	A1EL2	C28-C26	-2.83	1.39	1.45
8	N	102	A1EL2	C11-C12	-2.82	1.39	1.45
7	I	101	BCL	CHC-C4B	2.82	1.45	1.39
7	Q	101	BCL	C3D-C2D	2.82	1.46	1.39
8	A	102	A1EL2	C11-C12	-2.82	1.39	1.45
8	B	102	A1EL2	C11-C12	-2.82	1.39	1.45
7	O	101	BCL	C1D-ND	-2.82	1.34	1.37
9	B	103	A1ELD	C26-C27	-2.81	1.32	1.41
7	D	101	BCL	C1D-ND	-2.81	1.34	1.37
8	E	102	A1EL2	C28-C26	-2.81	1.39	1.45
7	R	101	BCL	CHB-C1B	2.80	1.45	1.39
8	N	102	A1EL2	C28-C26	-2.80	1.39	1.45
7	O	101	BCL	CHC-C4B	2.80	1.45	1.39
7	a	101	BCL	OBD-CAD	2.80	1.27	1.22
8	A	102	A1EL2	C28-C26	-2.80	1.39	1.45
9	O	102	A1ELD	C39-C37	2.80	1.58	1.52
7	p	101	BCL	C1B-NB	-2.79	1.34	1.37
8	F	102	A1EL2	C28-C26	-2.79	1.40	1.45
8	B	102	A1EL2	C28-C26	-2.79	1.40	1.45
7	L	302	BCL	C1B-NB	-2.79	1.34	1.37
9	R	103	A1ELD	C9-C10	-2.78	1.40	1.45
13	L	305	BPH	C4D-ND	-2.78	1.34	1.38
7	A	101	BCL	C3D-C2D	2.78	1.46	1.39
7	c	101	BCL	CHB-C1B	2.78	1.45	1.39
8	O	103	A1EL2	C24-C23	2.77	1.41	1.34
7	L	301	BCL	C3D-C2D	2.77	1.46	1.39
8	r	103	A1EL2	C5-C6	-2.77	1.48	1.52
7	J	101	BCL	CHB-C1B	2.77	1.45	1.39
7	R	101	BCL	CHC-C4B	2.77	1.45	1.39
7	b	102	BCL	C3D-C2D	2.77	1.46	1.39
9	q	101	A1ELD	C9-C10	-2.77	1.40	1.45
7	B	101	BCL	CHC-C4B	2.76	1.45	1.39
9	f	101	A1ELD	C24-C22	-2.76	1.40	1.45
7	M	403	BCL	C3D-C2D	2.76	1.46	1.39
7	G	101	BCL	CHC-C4B	2.76	1.45	1.39
7	O	101	BCL	CHB-C1B	2.76	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	101	A1ELD	C29-C27	-2.75	1.39	1.45
8	O	103	A1EL2	C22-C21	-2.75	1.45	1.50
7	s	101	BCL	C3D-C2D	2.75	1.46	1.39
7	i	101	BCL	C3D-C2D	2.75	1.46	1.39
7	j	102	BCL	C1B-NB	-2.75	1.34	1.37
7	F	101	BCL	CHC-C1C	-2.75	1.31	1.37
7	K	101	BCL	C1D-ND	-2.75	1.34	1.37
7	J	101	BCL	MG-NA	-2.75	1.99	2.06
7	E	101	BCL	CHC-C4B	2.74	1.45	1.39
9	o	101	A1ELD	C11-C10	2.74	1.56	1.50
7	P	101	BCL	CHB-C1B	2.73	1.45	1.39
7	F	101	BCL	CHB-C1B	2.73	1.45	1.39
7	O	101	BCL	MG-NA	-2.73	1.99	2.06
9	b	101	A1ELD	C9-C10	-2.73	1.40	1.45
7	Q	101	BCL	CHC-C4B	2.73	1.45	1.39
7	A	101	BCL	CHC-C4B	2.73	1.45	1.39
8	K	102	A1EL2	C23-C21	-2.73	1.40	1.45
7	N	101	BCL	CHC-C4B	2.72	1.45	1.39
7	F	101	BCL	C3A-C2A	-2.72	1.46	1.54
7	M	403	BCL	C4B-NB	-2.72	1.34	1.37
12	G	104	LMT	O3'-C3'	-2.72	1.36	1.43
9	e	101	A1ELD	C25-C24	2.70	1.41	1.34
7	R	101	BCL	MG-NA	-2.70	1.99	2.06
14	L	306	UQ8	C3-C2	-2.70	1.41	1.48
7	E	101	BCL	MG-NA	-2.69	1.99	2.06
7	J	101	BCL	CHC-C4B	2.69	1.45	1.39
12	N	103	LMT	O3'-C3'	-2.69	1.36	1.43
8	G	102	A1EL2	C15-C16	-2.69	1.40	1.45
8	J	102	A1EL2	C13-C12	-2.68	1.32	1.35
9	r	101	A1ELD	C9-C10	-2.68	1.40	1.45
13	L	305	BPH	C4D-CHA	2.68	1.43	1.39
7	E	101	BCL	OBD-CAD	2.68	1.27	1.22
8	J	102	A1EL2	C14-C13	2.68	1.51	1.43
7	Q	101	BCL	C1B-NB	-2.67	1.34	1.37
7	b	102	BCL	C1B-NB	-2.66	1.34	1.37
7	D	101	BCL	MG-NA	-2.66	2.00	2.06
7	F	101	BCL	CHD-C1D	2.66	1.43	1.38
7	S	101	BCL	CHC-C4B	2.65	1.45	1.39
7	I	101	BCL	OBD-CAD	2.65	1.27	1.22
7	F	101	BCL	MG-NA	-2.65	2.00	2.06
7	I	101	BCL	MG-NA	-2.65	2.00	2.06
9	d	101	A1ELD	C31-C32	2.65	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	101	BCL	CHD-C4C	2.65	1.46	1.39
7	D	101	BCL	CHD-C4C	2.64	1.46	1.39
7	M	401	BCL	C3D-C2D	2.64	1.46	1.39
8	I	102	A1EL2	C39-C16	-2.64	1.45	1.50
7	c	101	BCL	CHB-C4A	-2.63	1.31	1.37
8	r	102	A1EL2	C14-C15	2.63	1.41	1.34
9	R	102	A1ELD	C20-C21	2.63	1.51	1.43
7	M	403	BCL	MG-NA	-2.63	2.00	2.06
7	S	101	BCL	C1B-NB	-2.62	1.34	1.37
7	k	101	BCL	C1B-NB	-2.62	1.34	1.37
9	J	103	A1ELD	C31-C32	2.62	1.39	1.35
9	A	103	A1ELD	C29-C27	-2.61	1.40	1.45
7	P	101	BCL	CHD-C4C	2.61	1.46	1.39
7	D	101	BCL	C1D-C2D	2.60	1.50	1.45
9	e	101	A1ELD	C30-C29	2.60	1.41	1.34
7	C	101	BCL	C3C-C4C	-2.60	1.48	1.51
8	Q	102	A1EL2	C9-C4	2.60	1.58	1.53
12	L	309	LMT	O3'-C3'	-2.60	1.36	1.43
7	i	101	BCL	C3C-C4C	-2.60	1.48	1.51
7	M	401	BCL	CHB-C4A	-2.60	1.31	1.37
8	G	102	A1EL2	O2-C34	2.59	1.47	1.42
7	O	101	BCL	CHD-C4C	2.59	1.46	1.39
8	O	103	A1EL2	C11-C10	2.59	1.40	1.33
7	A	101	BCL	MG-NA	-2.59	2.00	2.06
7	K	101	BCL	CHC-C1C	-2.58	1.31	1.37
7	E	101	BCL	C1D-C2D	2.58	1.50	1.45
7	S	101	BCL	CHC-C1C	-2.58	1.31	1.37
7	E	101	BCL	C1B-NB	-2.58	1.34	1.37
7	J	101	BCL	C1D-C2D	2.57	1.50	1.45
9	r	101	A1ELD	C29-C27	-2.57	1.40	1.45
7	L	302	BCL	CHC-C1C	-2.57	1.31	1.37
7	P	101	BCL	MG-NA	-2.56	2.00	2.06
7	F	101	BCL	MG-ND	-2.56	2.00	2.05
7	M	403	BCL	CHD-C4C	2.56	1.46	1.39
13	L	303	BPH	C2C-C3C	-2.56	1.52	1.54
7	E	101	BCL	CHD-C4C	2.55	1.46	1.39
7	K	101	BCL	CHD-C4C	2.55	1.46	1.39
8	K	102	A1EL2	C28-C26	-2.54	1.40	1.45
7	F	101	BCL	C3C-C4C	-2.54	1.48	1.51
9	B	103	A1ELD	C9-C10	-2.54	1.40	1.45
7	M	401	BCL	C4B-NB	-2.54	1.34	1.37
7	N	101	BCL	MG-NA	-2.54	2.00	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Q	102	A1EL2	C5-C6	2.54	1.56	1.52
7	K	101	BCL	CHC-C4B	2.54	1.45	1.39
9	R	103	A1ELD	C29-C27	-2.54	1.40	1.45
7	B	101	BCL	CHC-C1C	-2.53	1.31	1.37
8	Q	102	A1EL2	C36-C35	2.53	1.59	1.54
7	P	101	BCL	C1D-C2D	2.53	1.50	1.45
9	R	102	A1ELD	C20-C19	-2.53	1.29	1.36
9	o	101	A1ELD	C5-C6	-2.53	1.47	1.52
7	G	101	BCL	CHD-C4C	2.53	1.46	1.39
7	R	101	BCL	CHD-C4C	2.53	1.46	1.39
7	n	101	BCL	MG-NA	-2.52	2.00	2.06
9	q	101	A1ELD	C29-C27	-2.52	1.40	1.45
8	r	102	A1EL2	C14-C13	-2.52	1.35	1.43
8	K	102	A1EL2	C25-C26	2.52	1.39	1.35
8	D	102	A1EL2	C15-C16	-2.52	1.40	1.45
9	J	103	A1ELD	C21-C22	2.52	1.39	1.35
8	B	102	A1EL2	C15-C16	-2.52	1.40	1.45
8	r	102	A1EL2	C24-C23	2.51	1.41	1.34
8	C	103	A1EL2	C15-C16	-2.51	1.40	1.45
9	j	101	A1ELD	C44-C2	-2.51	1.48	1.53
13	L	303	BPH	C4B-NB	-2.51	1.33	1.38
8	K	102	A1EL2	C18-C17	-2.51	1.35	1.43
9	J	103	A1ELD	C34-C32	-2.50	1.40	1.45
7	I	101	BCL	CHD-C4C	2.50	1.46	1.39
8	E	102	A1EL2	C15-C16	-2.50	1.40	1.45
12	L	309	LMT	O2'-C2'	-2.50	1.37	1.43
8	A	102	A1EL2	C15-C16	-2.49	1.40	1.45
8	G	102	A1EL2	C9-C4	2.49	1.58	1.53
7	F	101	BCL	C2C-C3C	-2.49	1.47	1.54
7	C	101	BCL	MG-NA	-2.49	2.00	2.06
13	L	303	BPH	C1D-ND	-2.49	1.33	1.38
9	b	101	A1ELD	C29-C27	-2.49	1.40	1.45
9	b	101	A1ELD	C30-C29	2.49	1.41	1.34
14	L	304	UQ8	C3-C2	-2.49	1.41	1.48
8	O	103	A1EL2	C14-C15	2.49	1.41	1.34
7	O	101	BCL	C1D-C2D	2.48	1.50	1.45
9	J	103	A1ELD	C15-C16	-2.48	1.40	1.45
7	Q	101	BCL	CHC-C1C	-2.48	1.31	1.37
11	L	307	PGV	O03-C19	2.48	1.45	1.33
7	Q	101	BCL	C1D-C2D	2.48	1.50	1.45
7	B	101	BCL	C1D-C2D	2.48	1.50	1.45
7	Q	101	BCL	CHD-C4C	2.47	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	103	A1ELD	C24-C22	-2.47	1.40	1.45
7	N	101	BCL	CHD-C4C	2.47	1.46	1.39
9	A	103	A1ELD	C15-C16	-2.47	1.40	1.45
7	q	102	BCL	C3C-C4C	-2.47	1.48	1.51
8	F	102	A1EL2	C15-C16	-2.47	1.40	1.45
13	L	305	BPH	C3A-C2A	-2.47	1.52	1.54
7	n	101	BCL	C3C-C4C	-2.46	1.48	1.51
7	B	101	BCL	CHD-C4C	2.46	1.46	1.39
7	M	401	BCL	CHC-C1C	-2.46	1.31	1.37
8	Q	102	A1EL2	C19-C20	-2.46	1.35	1.43
8	r	103	A1EL2	C31-C30	2.46	1.38	1.34
8	N	102	A1EL2	C15-C16	-2.45	1.40	1.45
8	K	102	A1EL2	C14-C13	-2.45	1.35	1.43
9	j	101	A1ELD	C33-C32	-2.45	1.45	1.50
14	L	306	UQ8	C4-C5	-2.45	1.41	1.48
7	J	101	BCL	CHC-C1C	-2.45	1.31	1.37
7	B	101	BCL	MG-NA	-2.45	2.00	2.06
8	J	102	A1EL2	C14-C15	-2.45	1.28	1.34
7	E	101	BCL	CHC-C1C	-2.44	1.31	1.37
9	R	103	A1ELD	C30-C29	2.44	1.40	1.34
7	G	101	BCL	CHC-C1C	-2.44	1.31	1.37
14	L	304	UQ8	C4-C5	-2.44	1.41	1.48
7	S	101	BCL	CHD-C4C	2.44	1.46	1.39
9	e	101	A1ELD	C17-C16	-2.44	1.45	1.50
7	C	101	BCL	C4B-NB	-2.44	1.34	1.37
14	M	402	UQ8	C4-C5	-2.44	1.41	1.48
7	Q	101	BCL	C1B-C2B	2.44	1.49	1.43
8	N	102	A1EL2	C23-C21	-2.43	1.40	1.45
9	f	101	A1ELD	C15-C16	-2.43	1.40	1.45
9	g	101	A1ELD	C4-C3	2.43	1.38	1.34
9	j	101	A1ELD	C31-C32	2.43	1.39	1.35
7	C	101	BCL	CHD-C4C	2.43	1.46	1.39
8	r	102	A1EL2	C19-C20	-2.42	1.35	1.43
7	Q	101	BCL	MG-NA	-2.42	2.00	2.06
7	j	102	BCL	CHD-C4C	2.42	1.46	1.39
7	M	401	BCL	C1D-C2D	2.42	1.50	1.45
9	r	101	A1ELD	C30-C29	2.42	1.40	1.34
7	C	101	BCL	C1D-C2D	2.42	1.50	1.45
8	C	103	A1EL2	C23-C21	-2.42	1.40	1.45
7	S	101	BCL	C1D-C2D	2.42	1.50	1.45
7	K	101	BCL	C1D-C2D	2.41	1.50	1.45
7	K	101	BCL	MG-NA	-2.41	2.00	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	r	103	A1EL2	C7-C2	-2.41	1.47	1.51
7	F	101	BCL	C1D-ND	-2.41	1.34	1.37
9	e	101	A1ELD	C14-C15	2.40	1.40	1.34
8	I	102	A1EL2	C38-C31	-2.40	1.47	1.50
7	R	101	BCL	MG-NC	-2.40	2.00	2.06
8	D	102	A1EL2	C23-C21	-2.40	1.40	1.45
7	L	301	BCL	OBD-CAD	2.40	1.26	1.22
7	J	101	BCL	CHB-C4A	-2.40	1.32	1.37
9	q	101	A1ELD	C30-C29	2.40	1.40	1.34
7	s	101	BCL	CHD-C4C	2.39	1.46	1.39
9	g	101	A1ELD	C13-C10	2.39	1.39	1.35
9	B	103	A1ELD	C20-C21	-2.39	1.36	1.43
8	E	102	A1EL2	C23-C21	-2.39	1.40	1.45
12	G	104	LMT	O2'-C2'	-2.39	1.37	1.43
9	b	101	A1ELD	C34-C32	-2.39	1.40	1.45
7	L	301	BCL	CHB-C4A	-2.38	1.32	1.37
8	B	102	A1EL2	C23-C21	-2.38	1.40	1.45
8	A	102	A1EL2	C23-C21	-2.38	1.40	1.45
7	r	104	BCL	CHD-C4C	2.38	1.45	1.39
9	R	102	A1ELD	C11-C10	-2.37	1.46	1.50
7	O	101	BCL	MG-NC	-2.37	2.00	2.06
8	O	103	A1EL2	C32-C33	-2.37	1.48	1.52
8	G	102	A1EL2	C36-C35	2.37	1.59	1.54
7	R	101	BCL	CHC-C1C	-2.37	1.32	1.37
7	g	102	BCL	C3C-C4C	-2.37	1.48	1.51
9	e	101	A1ELD	C14-C13	-2.37	1.36	1.43
9	C	102	A1ELD	C13-C10	2.37	1.38	1.35
7	e	102	BCL	C3C-C4C	-2.37	1.48	1.51
9	R	103	A1ELD	C34-C32	-2.37	1.40	1.45
7	L	302	BCL	CHD-C4C	2.37	1.45	1.39
9	J	103	A1ELD	C33-C32	-2.37	1.46	1.50
7	G	101	BCL	C1D-C2D	2.37	1.50	1.45
8	P	102	A1EL2	C25-C26	-2.36	1.32	1.35
16	M	405	H4X	C11-C12	-2.36	1.40	1.45
12	G	104	LMT	O3B-C3B	-2.36	1.37	1.43
9	B	103	A1ELD	C39-C37	2.36	1.57	1.52
9	o	101	A1ELD	C4-C3	-2.36	1.30	1.34
7	P	101	BCL	CHC-C1C	-2.36	1.32	1.37
9	e	101	A1ELD	C11-C10	-2.36	1.46	1.50
7	E	101	BCL	C1B-C2B	2.36	1.48	1.43
7	S	101	BCL	C1B-C2B	2.35	1.48	1.43
8	F	102	A1EL2	C23-C21	-2.35	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	402	UQ8	C3-C2	-2.35	1.42	1.48
12	L	309	LMT	O2B-C2B	-2.35	1.37	1.43
13	L	305	BPH	C1B-C2B	2.35	1.42	1.39
13	L	303	BPH	C1B-NB	-2.35	1.34	1.38
7	c	101	BCL	C3C-C4C	-2.35	1.48	1.51
7	n	101	BCL	CHC-C1C	-2.34	1.32	1.37
9	r	101	A1ELD	C34-C32	-2.34	1.40	1.45
7	c	101	BCL	CHD-C4C	2.34	1.45	1.39
8	I	102	A1EL2	C17-C16	2.34	1.38	1.35
7	i	101	BCL	MG-NA	-2.34	2.00	2.06
12	G	104	LMT	O2B-C2B	-2.34	1.37	1.43
9	A	103	A1ELD	C34-C32	-2.34	1.40	1.45
7	B	101	BCL	C1B-C2B	2.34	1.48	1.43
7	d	102	BCL	C3C-C4C	-2.34	1.48	1.51
7	I	101	BCL	C1D-C2D	2.33	1.49	1.45
7	N	101	BCL	CHC-C1C	-2.33	1.32	1.37
7	R	101	BCL	C1D-C2D	2.33	1.49	1.45
7	p	101	BCL	C3C-C4C	-2.33	1.48	1.51
16	M	405	H4X	C30-C28	-2.32	1.41	1.45
12	N	103	LMT	O3B-C3B	-2.32	1.37	1.43
8	O	103	A1EL2	C23-C21	-2.32	1.41	1.45
8	I	102	A1EL2	C10-C3	2.32	1.53	1.45
7	I	101	BCL	CHC-C1C	-2.32	1.32	1.37
7	P	101	BCL	CHB-C4A	-2.32	1.32	1.37
7	p	101	BCL	CHD-C4C	2.32	1.45	1.39
12	L	309	LMT	O3B-C3B	-2.32	1.37	1.43
7	a	101	BCL	CHC-C1C	-2.32	1.32	1.37
8	G	102	A1EL2	C7-C6	-2.32	1.48	1.52
7	q	102	BCL	CHD-C4C	2.32	1.45	1.39
7	e	102	BCL	MG-NA	-2.32	2.00	2.06
9	e	101	A1ELD	C20-C19	2.32	1.42	1.36
7	G	101	BCL	MG-NA	-2.32	2.00	2.06
7	M	403	BCL	CHB-C4A	-2.31	1.32	1.37
7	L	302	BCL	MG-NC	-2.31	2.00	2.06
8	P	102	A1EL2	C37-C35	2.31	1.59	1.54
8	O	103	A1EL2	C19-C18	2.31	1.42	1.36
7	N	101	BCL	C1D-C2D	2.31	1.49	1.45
7	b	102	BCL	MG-NA	-2.30	2.00	2.06
12	N	103	LMT	O2B-C2B	-2.30	1.37	1.43
12	N	103	LMT	O2'-C2'	-2.30	1.37	1.43
7	O	101	BCL	CHC-C1C	-2.30	1.32	1.37
8	J	102	A1EL2	C28-C26	2.30	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	301	BCL	CHD-C4C	2.30	1.45	1.39
7	C	101	BCL	CHB-C4A	-2.29	1.32	1.37
9	r	101	A1ELD	C15-C16	-2.29	1.41	1.45
16	M	405	H4X	C16-C17	-2.29	1.41	1.45
7	d	102	BCL	CHB-C4A	-2.29	1.32	1.37
7	P	101	BCL	MG-NC	-2.29	2.00	2.06
7	b	102	BCL	CHC-C1C	-2.29	1.32	1.37
9	r	101	A1ELD	C24-C22	-2.29	1.41	1.45
7	a	101	BCL	CHD-C4C	2.28	1.45	1.39
7	R	101	BCL	CHB-C4A	-2.28	1.32	1.37
7	s	101	BCL	CHB-C4A	-2.28	1.32	1.37
9	q	101	A1ELD	C34-C32	-2.28	1.41	1.45
16	M	405	H4X	C25-C23	-2.28	1.41	1.45
9	q	101	A1ELD	C15-C16	-2.28	1.41	1.45
7	e	102	BCL	CHC-C1C	-2.28	1.32	1.37
7	r	104	BCL	C3C-C4C	-2.28	1.48	1.51
9	e	101	A1ELD	C7-C6	2.28	1.55	1.52
9	O	102	A1ELD	C11-C10	-2.28	1.46	1.50
7	d	102	BCL	CHD-C4C	2.27	1.45	1.39
8	r	102	A1EL2	C29-C28	2.27	1.39	1.33
8	O	103	A1EL2	C9-C4	-2.27	1.49	1.53
8	P	102	A1EL2	C27-C26	2.27	1.55	1.50
7	o	102	BCL	CHD-C4C	2.27	1.45	1.39
8	I	102	A1EL2	C29-C28	2.27	1.39	1.33
7	f	102	BCL	CHC-C1C	-2.26	1.32	1.37
7	R	101	BCL	C1B-C2B	2.26	1.48	1.43
7	J	101	BCL	MG-NC	-2.26	2.00	2.06
7	M	401	BCL	CHD-C4C	2.26	1.45	1.39
7	O	101	BCL	CHB-C4A	-2.26	1.32	1.37
13	L	303	BPH	CBD-CGD	-2.26	1.49	1.52
8	G	102	A1EL2	C4-C3	-2.26	1.50	1.53
9	d	101	A1ELD	C30-C31	-2.26	1.36	1.43
7	A	101	BCL	CHD-C4C	2.25	1.45	1.39
8	J	102	A1EL2	C1-C2	2.25	1.54	1.50
7	g	102	BCL	CHD-C4C	2.25	1.45	1.39
7	a	101	BCL	C3C-C4C	-2.25	1.48	1.51
7	G	101	BCL	CHB-C4A	-2.25	1.32	1.37
7	o	102	BCL	CHC-C1C	-2.24	1.32	1.37
7	f	102	BCL	C3C-C4C	-2.24	1.48	1.51
9	q	101	A1ELD	C24-C22	-2.24	1.41	1.45
9	e	101	A1ELD	C23-C22	-2.24	1.46	1.50
7	i	101	BCL	CHD-C4C	2.24	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	k	101	BCL	C3C-C4C	-2.24	1.48	1.51
7	A	101	BCL	C1B-C2B	2.24	1.48	1.43
8	I	102	A1EL2	C2-C3	2.24	1.38	1.34
7	b	102	BCL	C3C-C4C	-2.24	1.48	1.51
7	M	401	BCL	MG-NC	-2.23	2.01	2.06
7	s	101	BCL	C3C-C4C	-2.23	1.48	1.51
7	A	101	BCL	MG-NC	-2.23	2.01	2.06
7	M	403	BCL	MG-NC	-2.23	2.01	2.06
9	A	103	A1ELD	C30-C29	2.23	1.40	1.34
7	n	101	BCL	CHD-C4C	2.22	1.45	1.39
7	b	102	BCL	C1B-C2B	2.22	1.48	1.43
8	K	102	A1EL2	C19-C20	-2.22	1.36	1.43
9	R	103	A1ELD	C24-C22	-2.22	1.41	1.45
8	G	102	A1EL2	C24-C25	-2.22	1.36	1.43
7	G	101	BCL	MG-NC	-2.22	2.01	2.06
8	G	102	A1EL2	C19-C20	-2.22	1.36	1.43
9	B	103	A1ELD	C13-C10	2.22	1.38	1.35
7	q	102	BCL	MG-NA	-2.22	2.01	2.06
8	Q	102	A1EL2	C29-C28	2.21	1.39	1.33
7	q	102	BCL	CHB-C4A	-2.21	1.32	1.37
7	e	102	BCL	CHD-C4C	2.21	1.45	1.39
8	P	102	A1EL2	C10-C3	-2.21	1.37	1.45
7	D	101	BCL	C3C-C4C	-2.21	1.48	1.51
7	k	101	BCL	CHD-C4C	2.21	1.45	1.39
7	f	102	BCL	CHD-C4C	2.21	1.45	1.39
7	j	102	BCL	CHB-C4A	-2.21	1.32	1.37
7	L	301	BCL	CHC-C1C	-2.20	1.32	1.37
9	j	101	A1ELD	C15-C16	-2.20	1.41	1.45
7	M	403	BCL	C1B-NB	-2.20	1.35	1.37
8	O	103	A1EL2	O3-C33	-2.20	1.38	1.43
9	J	103	A1ELD	C7-C6	-2.19	1.49	1.52
7	F	101	BCL	C4D-ND	-2.19	1.34	1.37
7	D	101	BCL	CHB-C4A	-2.19	1.32	1.37
7	I	101	BCL	C1B-C2B	2.19	1.48	1.43
7	N	101	BCL	CHB-C4A	-2.19	1.32	1.37
9	f	101	A1ELD	C34-C32	-2.19	1.41	1.45
9	B	103	A1ELD	C15-C16	-2.19	1.41	1.45
9	b	101	A1ELD	C24-C22	-2.19	1.41	1.45
7	M	403	BCL	C1B-C2B	2.19	1.48	1.43
7	O	101	BCL	C1B-C2B	2.18	1.48	1.43
7	b	102	BCL	CHD-C4C	2.18	1.45	1.39
7	K	101	BCL	C1B-C2B	2.18	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	p	101	BCL	CHB-C4A	-2.18	1.32	1.37
7	s	101	BCL	CHC-C1C	-2.18	1.32	1.37
7	d	102	BCL	MG-NA	-2.18	2.01	2.06
7	L	301	BCL	MG-NA	-2.17	2.01	2.06
7	r	104	BCL	CHB-C4A	-2.17	1.32	1.37
7	q	102	BCL	CHC-C1C	-2.17	1.32	1.37
9	B	103	A1ELD	C19-C18	-2.17	1.36	1.43
7	L	302	BCL	CHB-C4A	-2.16	1.32	1.37
9	O	102	A1ELD	C14-C15	-2.16	1.29	1.34
7	e	102	BCL	MG-NC	-2.16	2.01	2.06
7	i	101	BCL	CHB-C4A	-2.16	1.32	1.37
12	N	103	LMT	O4'-C4B	-2.15	1.37	1.43
12	L	309	LMT	O4'-C4B	-2.15	1.37	1.43
7	D	101	BCL	MG-NC	-2.15	2.01	2.06
9	g	101	A1ELD	C34-C32	-2.14	1.41	1.45
7	e	102	BCL	CHB-C4A	-2.14	1.32	1.37
9	R	103	A1ELD	C15-C16	-2.14	1.41	1.45
7	g	102	BCL	MG-NA	-2.14	2.01	2.06
7	R	101	BCL	C3C-C4C	-2.14	1.48	1.51
7	A	101	BCL	C1D-C2D	2.14	1.49	1.45
7	M	401	BCL	C3C-C4C	-2.14	1.48	1.51
7	A	101	BCL	CHB-C4A	-2.13	1.32	1.37
7	s	101	BCL	MG-NA	-2.13	2.01	2.06
7	g	102	BCL	CHB-C4A	-2.13	1.32	1.37
7	D	101	BCL	C4B-NB	-2.13	1.35	1.37
12	G	104	LMT	O4'-C4B	-2.12	1.38	1.43
8	I	102	A1EL2	C5-C6	2.12	1.55	1.52
7	C	101	BCL	CHC-C1C	-2.12	1.32	1.37
7	F	101	BCL	C4D-CHA	2.12	1.45	1.38
7	g	102	BCL	CHC-C1C	-2.12	1.32	1.37
7	N	101	BCL	C1B-C2B	2.12	1.48	1.43
9	o	101	A1ELD	C25-C24	2.12	1.40	1.34
7	f	102	BCL	CHB-C4A	-2.11	1.32	1.37
7	j	102	BCL	C3C-C4C	-2.11	1.48	1.51
7	o	102	BCL	C3C-C4C	-2.11	1.48	1.51
7	o	102	BCL	MG-NA	-2.11	2.01	2.06
9	C	102	A1ELD	C4-C3	2.11	1.38	1.34
7	c	101	BCL	CHC-C1C	-2.11	1.32	1.37
7	r	104	BCL	CHC-C1C	-2.10	1.32	1.37
7	D	101	BCL	C1B-C2B	2.10	1.48	1.43
9	d	101	A1ELD	C20-C21	-2.10	1.36	1.43
7	p	101	BCL	CHC-C1C	-2.10	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	d	101	A1ELD	C14-C13	-2.10	1.36	1.43
8	r	103	A1EL2	C11-C10	-2.10	1.26	1.33
8	Q	102	A1EL2	O2-C34	2.10	1.47	1.42
7	I	101	BCL	CHB-C4A	-2.10	1.32	1.37
9	B	103	A1ELD	C21-C22	-2.10	1.33	1.35
9	e	101	A1ELD	C36-C35	-2.09	1.46	1.50
7	r	104	BCL	MG-NA	-2.09	2.01	2.06
7	n	101	BCL	CHB-C4A	-2.09	1.32	1.37
8	I	102	A1EL2	C24-C23	2.09	1.40	1.34
9	g	101	A1ELD	C9-C10	-2.09	1.41	1.45
9	j	101	A1ELD	C36-C35	2.08	1.53	1.50
7	o	102	BCL	C1B-C2B	2.08	1.48	1.43
8	O	103	A1EL2	C7-C6	2.08	1.55	1.52
9	J	103	A1ELD	C9-C8	2.08	1.39	1.33
7	C	101	BCL	MG-NC	-2.08	2.01	2.06
7	Q	101	BCL	MG-NC	-2.08	2.01	2.06
7	i	101	BCL	MG-NC	-2.07	2.01	2.06
7	k	101	BCL	CHC-C1C	-2.07	1.32	1.37
8	J	102	A1EL2	C24-C25	2.07	1.49	1.43
7	M	401	BCL	MG-NA	-2.07	2.01	2.06
9	J	103	A1ELD	C14-C15	2.07	1.39	1.34
7	p	101	BCL	MG-NA	-2.07	2.01	2.06
8	P	102	A1EL2	C22-C21	2.07	1.55	1.50
9	O	102	A1ELD	O42-C37	2.07	1.53	1.41
8	Q	102	A1EL2	C11-C10	2.06	1.39	1.33
7	P	101	BCL	C1B-C2B	2.06	1.48	1.43
8	I	102	A1EL2	C11-C10	2.06	1.39	1.33
7	K	101	BCL	MG-NC	-2.06	2.01	2.06
7	f	102	BCL	MG-NA	-2.05	2.01	2.06
9	O	102	A1ELD	C23-C22	-2.05	1.46	1.50
7	o	102	BCL	CHB-C4A	-2.05	1.32	1.37
7	a	101	BCL	CHB-C4A	-2.05	1.32	1.37
8	r	102	A1EL2	C11-C10	2.05	1.39	1.33
8	P	102	A1EL2	C17-C16	2.04	1.38	1.35
7	k	101	BCL	C1B-C2B	2.04	1.48	1.43
9	b	101	A1ELD	C15-C16	-2.04	1.41	1.45
8	I	102	A1EL2	O2-C34	2.04	1.46	1.42
7	k	101	BCL	CHB-C4A	-2.04	1.32	1.37
7	N	101	BCL	MG-NC	-2.04	2.01	2.06
7	G	101	BCL	C1B-C2B	2.04	1.48	1.43
9	e	101	A1ELD	C20-C21	-2.04	1.37	1.43
7	b	102	BCL	MG-NC	-2.03	2.01	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	102	A1EL2	O2-C34	2.03	1.46	1.42
9	d	101	A1ELD	C19-C18	-2.03	1.37	1.43
7	N	101	BCL	C3C-C4C	-2.03	1.49	1.51
8	Q	102	A1EL2	C18-C17	-2.02	1.37	1.43
8	J	102	A1EL2	C4-C3	2.02	1.56	1.53
9	e	101	A1ELD	C5-C4	-2.02	1.47	1.51
7	Q	101	BCL	C3C-C4C	-2.02	1.49	1.51
7	F	101	BCL	C1B-NB	-2.02	1.35	1.37
7	E	101	BCL	CHB-C4A	-2.02	1.32	1.37
7	j	102	BCL	C1D-C2D	2.02	1.49	1.45
7	M	403	BCL	C1D-C2D	2.02	1.49	1.45
7	L	301	BCL	MG-NC	-2.02	2.01	2.06
7	a	101	BCL	C1B-C2B	2.02	1.48	1.43
8	G	102	A1EL2	C18-C17	-2.01	1.37	1.43
12	N	103	LMT	O1'-C1'	-2.01	1.36	1.40
9	g	101	A1ELD	C25-C24	2.01	1.39	1.34
7	A	101	BCL	C3C-C4C	-2.01	1.49	1.51
9	d	101	A1ELD	C17-C16	-2.01	1.46	1.50
8	K	102	A1EL2	C38-C31	2.00	1.54	1.50

All (1389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	102	A1EL2	C40-C12-C13	-11.90	106.26	122.92
9	R	102	A1ELD	C11-C10-C13	-11.77	106.44	122.92
7	P	101	BCL	C2B-C1B-NB	11.76	118.12	110.23
9	R	102	A1ELD	C33-C32-C31	-11.50	106.82	122.92
7	J	101	BCL	C2B-C1B-NB	11.49	117.93	110.23
7	O	101	BCL	C2B-C1B-NB	11.40	117.88	110.23
7	N	101	BCL	C2B-C1B-NB	11.40	117.87	110.23
7	C	101	BCL	C2B-C1B-NB	11.19	117.73	110.23
7	G	101	BCL	C2B-C1B-NB	11.16	117.71	110.23
8	J	102	A1EL2	C27-C26-C25	-11.13	107.33	122.92
7	L	301	BCL	C2B-C1B-NB	11.09	117.67	110.23
7	A	101	BCL	C2B-C1B-NB	11.03	117.63	110.23
7	d	102	BCL	C2B-C1B-NB	11.03	117.63	110.23
7	j	102	BCL	C2B-C1B-NB	10.91	117.55	110.23
7	R	101	BCL	C2B-C1B-NB	10.90	117.54	110.23
7	q	102	BCL	C2B-C1B-NB	10.86	117.52	110.23
7	D	101	BCL	C2B-C1B-NB	10.82	117.48	110.23
7	s	101	BCL	C2B-C1B-NB	10.81	117.48	110.23
7	I	101	BCL	C2B-C1B-NB	10.60	117.33	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	101	BCL	C2B-C1B-NB	10.59	117.33	110.23
7	p	101	BCL	C2B-C1B-NB	10.55	117.30	110.23
7	g	102	BCL	C2B-C1B-NB	10.51	117.28	110.23
7	F	101	BCL	C2B-C1B-NB	10.43	117.23	110.23
7	r	104	BCL	C2B-C1B-NB	10.43	117.23	110.23
7	f	102	BCL	C2B-C1B-NB	10.40	117.20	110.23
7	o	102	BCL	C2B-C1B-NB	10.40	117.20	110.23
7	b	102	BCL	C2B-C1B-NB	10.40	117.20	110.23
7	e	102	BCL	C2B-C1B-NB	10.36	117.18	110.23
7	M	401	BCL	C2B-C1B-NB	10.36	117.18	110.23
7	E	101	BCL	C2B-C1B-NB	10.35	117.17	110.23
7	n	101	BCL	C2B-C1B-NB	10.28	117.12	110.23
7	M	403	BCL	C2B-C1B-NB	10.22	117.08	110.23
8	J	102	A1EL2	C39-C16-C17	-10.20	108.64	122.92
7	i	101	BCL	C2B-C1B-NB	10.18	117.06	110.23
7	S	101	BCL	C2B-C1B-NB	10.18	117.05	110.23
7	Q	101	BCL	C2B-C1B-NB	10.09	117.00	110.23
7	k	101	BCL	C2B-C1B-NB	10.02	116.95	110.23
8	J	102	A1EL2	C22-C21-C20	-9.96	108.97	122.92
7	a	101	BCL	C2B-C1B-NB	9.91	116.88	110.23
7	B	101	BCL	C2B-C1B-NB	9.68	116.72	110.23
9	R	102	A1ELD	C17-C16-C18	-9.51	109.60	122.92
7	c	101	BCL	C2B-C1B-NB	9.45	116.56	110.23
7	L	302	BCL	C2B-C1B-NB	9.05	116.30	110.23
7	D	101	BCL	CHD-C1D-ND	-8.71	116.45	124.45
7	J	101	BCL	CHD-C1D-ND	-8.45	116.69	124.45
7	S	101	BCL	CHD-C1D-ND	-8.38	116.75	124.45
7	E	101	BCL	CHD-C1D-ND	-8.34	116.79	124.45
7	B	101	BCL	CHD-C1D-ND	-8.31	116.81	124.45
9	R	102	A1ELD	C23-C22-C21	-8.21	111.42	122.92
7	C	101	BCL	CHD-C1D-ND	-8.20	116.92	124.45
7	O	101	BCL	CHD-C1D-ND	-8.16	116.96	124.45
7	I	101	BCL	CHD-C1D-ND	-8.09	117.02	124.45
7	P	101	BCL	CHD-C1D-ND	-8.07	117.04	124.45
7	M	401	BCL	CHD-C1D-ND	-8.07	117.04	124.45
7	G	101	BCL	CHD-C1D-ND	-8.06	117.05	124.45
7	Q	101	BCL	CHD-C1D-ND	-8.02	117.08	124.45
7	M	401	BCL	CMD-C2D-C1D	8.01	138.83	124.71
9	R	102	A1ELD	C34-C32-C31	8.00	131.22	118.94
7	K	101	BCL	CHD-C1D-ND	-7.96	117.14	124.45
7	N	101	BCL	CHD-C1D-ND	-7.93	117.17	124.45
7	R	101	BCL	CHD-C1D-ND	-7.92	117.18	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	101	BCL	CMD-C2D-C1D	7.90	138.63	124.71
8	J	102	A1EL2	C38-C31-C30	-7.86	115.70	124.53
8	I	102	A1EL2	C40-C12-C13	-7.83	111.95	122.92
7	B	101	BCL	CMD-C2D-C1D	7.79	138.45	124.71
7	M	403	BCL	CHD-C1D-ND	-7.79	117.29	124.45
7	J	101	BCL	CMD-C2D-C1D	7.74	138.35	124.71
7	E	101	BCL	CMD-C2D-C1D	7.72	138.33	124.71
7	Q	101	BCL	CMD-C2D-C1D	7.65	138.20	124.71
7	C	101	BCL	CMD-C2D-C1D	7.58	138.06	124.71
7	P	101	BCL	CMD-C2D-C1D	7.58	138.06	124.71
7	K	101	BCL	CMD-C2D-C1D	7.53	137.99	124.71
7	i	101	BCL	CHD-C1D-ND	-7.49	117.57	124.45
8	I	102	A1EL2	C39-C16-C17	-7.48	112.44	122.92
7	I	101	BCL	CMD-C2D-C1D	7.47	137.88	124.71
7	G	101	BCL	CMD-C2D-C1D	7.46	137.85	124.71
7	d	102	BCL	CHD-C1D-ND	-7.45	117.60	124.45
9	R	102	A1ELD	C43-C4-C3	-7.45	116.16	124.53
7	O	101	BCL	CMD-C2D-C1D	7.44	137.82	124.71
7	c	101	BCL	CHD-C1D-ND	-7.41	117.64	124.45
7	A	101	BCL	CHD-C1D-ND	-7.40	117.66	124.45
9	O	102	A1ELD	C33-C32-C31	-7.37	112.59	122.92
7	R	101	BCL	CMD-C2D-C1D	7.36	137.69	124.71
7	q	102	BCL	CHD-C1D-ND	-7.36	117.69	124.45
7	S	101	BCL	CMD-C2D-C1D	7.35	137.67	124.71
7	F	101	BCL	CMD-C2D-C1D	7.32	137.61	124.71
7	L	301	BCL	CHD-C1D-ND	-7.25	117.79	124.45
7	j	102	BCL	CHD-C1D-ND	-7.25	117.79	124.45
9	R	102	A1ELD	C6-C5-C4	7.24	126.28	111.85
7	N	101	BCL	CMD-C2D-C1D	7.24	137.47	124.71
7	L	301	BCL	CMD-C2D-C1D	7.22	137.43	124.71
7	p	101	BCL	CHD-C1D-ND	-7.22	117.82	124.45
7	n	101	BCL	CHD-C1D-ND	-7.21	117.83	124.45
7	s	101	BCL	CHD-C1D-ND	-7.16	117.87	124.45
7	r	104	BCL	CHD-C1D-ND	-7.14	117.89	124.45
7	M	403	BCL	CMD-C2D-C1D	7.11	137.24	124.71
7	A	101	BCL	CMD-C2D-C1D	7.10	137.23	124.71
7	f	102	BCL	CHD-C1D-ND	-7.07	117.96	124.45
7	L	302	BCL	CHD-C1D-ND	-7.03	118.00	124.45
9	R	102	A1ELD	C17-C16-C15	7.02	129.13	118.08
9	B	103	A1ELD	C33-C32-C31	-6.91	113.25	122.92
9	R	102	A1ELD	C8-C9-C10	6.89	136.65	126.23
8	J	102	A1EL2	C35-C30-C31	-6.82	112.42	122.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	102	BCL	CHD-C1D-ND	-6.80	118.21	124.45
9	R	102	A1ELD	C23-C22-C24	6.80	128.78	118.08
7	F	101	BCL	CHD-C1D-ND	-6.77	118.24	124.45
7	b	102	BCL	CHD-C1D-ND	-6.76	118.25	124.45
7	e	102	BCL	CHD-C1D-ND	-6.72	118.27	124.45
9	O	102	A1ELD	C11-C10-C13	-6.72	113.51	122.92
7	a	101	BCL	CHD-C1D-ND	-6.72	118.28	124.45
7	k	101	BCL	CHD-C1D-ND	-6.65	118.34	124.45
8	I	102	A1EL2	C27-C26-C25	-6.59	113.69	122.92
9	O	102	A1ELD	C17-C16-C18	-6.59	113.70	122.92
7	o	102	BCL	CHD-C1D-ND	-6.56	118.43	124.45
8	r	103	A1EL2	O3-C33-C34	6.54	122.75	109.74
13	L	303	BPH	C2B-C1B-NB	6.52	114.03	109.53
9	R	102	A1ELD	C43-C4-C5	6.49	126.38	114.36
8	J	102	A1EL2	C40-C12-C11	6.48	128.28	118.08
8	J	102	A1EL2	C34-C35-C30	6.47	122.03	110.48
7	s	101	BCL	CMD-C2D-C1D	6.47	136.11	124.71
9	O	102	A1ELD	C23-C22-C21	-6.46	113.87	122.92
7	M	401	BCL	CHC-C4B-NB	-6.40	117.48	124.26
8	r	103	A1EL2	C27-C26-C25	-6.38	113.99	122.92
9	R	102	A1ELD	O46-C6-C5	6.37	123.32	109.68
9	R	102	A1ELD	C30-C31-C32	6.31	136.32	127.31
7	j	102	BCL	CMD-C2D-C1D	6.30	135.81	124.71
8	I	102	A1EL2	C22-C21-C20	-6.29	114.11	122.92
7	i	101	BCL	CMD-C2D-C1D	6.26	135.75	124.71
7	A	101	BCL	C2D-C1D-ND	6.22	114.69	110.10
7	d	102	BCL	CMD-C2D-C1D	6.18	135.60	124.71
7	r	104	BCL	CMD-C2D-C1D	6.18	135.60	124.71
7	q	102	BCL	CMD-C2D-C1D	6.13	135.52	124.71
9	R	102	A1ELD	C35-C34-C32	6.10	135.10	125.89
7	D	101	BCL	CHC-C4B-NB	-6.09	117.81	124.26
9	R	102	A1ELD	C11-C10-C9	6.04	127.60	118.08
7	i	101	BCL	C2D-C1D-ND	6.02	114.54	110.10
8	J	102	A1EL2	C39-C16-C15	6.01	127.54	118.08
7	f	102	BCL	CMD-C2D-C1D	5.97	135.24	124.71
7	L	302	BCL	O2D-CGD-CBD	5.93	121.81	111.27
7	C	101	BCL	C2D-C1D-ND	5.92	114.47	110.10
7	L	302	BCL	CMD-C2D-C1D	5.92	135.14	124.71
7	a	101	BCL	CMD-C2D-C1D	5.90	135.11	124.71
7	b	102	BCL	CMD-C2D-C1D	5.89	135.10	124.71
7	D	101	BCL	C2D-C1D-ND	5.89	114.44	110.10
7	M	403	BCL	O2D-CGD-CBD	5.85	121.67	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	101	BCL	CHC-C4B-NB	-5.83	118.08	124.26
7	c	101	BCL	CMD-C2D-C1D	5.81	134.95	124.71
7	M	403	BCL	CHC-C4B-NB	-5.78	118.13	124.26
8	J	102	A1EL2	C28-C26-C25	5.77	127.79	118.94
7	p	101	BCL	CMD-C2D-C1D	5.77	134.88	124.71
7	R	101	BCL	C2D-C1D-ND	5.76	114.35	110.10
7	n	101	BCL	CMD-C2D-C1D	5.76	134.86	124.71
7	B	101	BCL	C2D-C1D-ND	5.75	114.34	110.10
7	L	301	BCL	CED-O2D-CGD	5.75	128.94	115.94
7	I	101	BCL	C2D-C1D-ND	5.73	114.33	110.10
7	F	101	BCL	C3D-C2D-C1D	-5.73	98.02	105.83
13	L	303	BPH	CMC-C2C-C1C	5.73	126.91	114.38
7	g	102	BCL	CMD-C2D-C1D	5.71	134.78	124.71
7	S	101	BCL	C2D-C1D-ND	5.69	114.30	110.10
7	Q	101	BCL	C2D-C1D-ND	5.69	114.30	110.10
7	N	101	BCL	C2D-C1D-ND	5.66	114.28	110.10
7	e	102	BCL	CMD-C2D-C1D	5.66	134.68	124.71
7	d	102	BCL	C2D-C1D-ND	5.65	114.27	110.10
8	r	103	A1EL2	C40-C12-C11	5.64	126.96	118.08
7	C	101	BCL	CHC-C4B-NB	-5.56	118.37	124.26
7	q	102	BCL	C2D-C1D-ND	5.52	114.17	110.10
8	I	102	A1EL2	C19-C18-C17	5.52	134.78	123.47
7	M	401	BCL	O2D-CGD-CBD	5.51	121.06	111.27
9	O	102	A1ELD	C34-C32-C31	5.51	127.40	118.94
7	o	102	BCL	C2D-C1D-ND	5.49	114.15	110.10
8	r	103	A1EL2	C5-C6-C7	5.49	117.82	110.30
7	k	101	BCL	C2D-C1D-ND	5.48	114.14	110.10
7	G	101	BCL	C2D-C1D-ND	5.48	114.14	110.10
7	e	102	BCL	C2D-C1D-ND	5.47	114.14	110.10
7	f	102	BCL	C2D-C1D-ND	5.44	114.11	110.10
13	L	305	BPH	C4D-CHA-CBD	-5.41	106.07	108.52
7	k	101	BCL	CMD-C2D-C1D	5.38	134.19	124.71
7	A	101	BCL	C3D-C2D-C1D	-5.36	98.51	105.83
7	C	101	BCL	C3D-C2D-C1D	-5.35	98.52	105.83
7	n	101	BCL	C2D-C1D-ND	5.34	114.04	110.10
7	B	101	BCL	C3D-C2D-C1D	-5.34	98.54	105.83
7	g	102	BCL	C2D-C1D-ND	5.30	114.01	110.10
7	o	102	BCL	CMD-C2D-C1D	5.30	134.05	124.71
13	L	303	BPH	CAC-C3C-C4C	5.29	125.57	113.73
7	O	101	BCL	C2D-C1D-ND	5.29	114.00	110.10
7	b	102	BCL	C2D-C1D-ND	5.29	114.00	110.10
7	N	101	BCL	CHC-C4B-NB	-5.29	118.66	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	101	BCL	C2D-C1D-ND	5.28	114.00	110.10
7	M	403	BCL	C2D-C1D-ND	5.28	113.99	110.10
7	J	101	BCL	O2D-CGD-CBD	5.26	120.62	111.27
8	r	103	A1EL2	O2-C34-C33	5.26	119.88	109.41
7	Q	101	BCL	C3D-C2D-C1D	-5.25	98.66	105.83
7	I	101	BCL	C3D-C2D-C1D	-5.24	98.68	105.83
7	S	101	BCL	C4A-NA-C1A	5.24	109.06	106.71
7	K	101	BCL	C2D-C1D-ND	5.20	113.94	110.10
7	P	101	BCL	C2D-C1D-ND	5.19	113.93	110.10
8	I	102	A1EL2	C38-C31-C30	-5.19	118.70	124.53
7	R	101	BCL	C3D-C2D-C1D	-5.18	98.76	105.83
7	E	101	BCL	C3D-C2D-C1D	-5.18	98.77	105.83
7	I	101	BCL	CHC-C4B-NB	-5.18	118.78	124.26
7	D	101	BCL	C3D-C2D-C1D	-5.18	98.77	105.83
7	P	101	BCL	CHC-C4B-NB	-5.17	118.78	124.26
7	G	101	BCL	C3D-C2D-C1D	-5.17	98.77	105.83
7	p	101	BCL	C2D-C1D-ND	5.16	113.91	110.10
7	S	101	BCL	CHC-C4B-NB	-5.16	118.79	124.26
7	N	101	BCL	C3D-C2D-C1D	-5.15	98.80	105.83
9	R	102	A1ELD	C2-C3-C4	-5.14	115.37	122.61
9	C	102	A1ELD	C11-C10-C13	-5.14	115.73	122.92
7	i	101	BCL	C3C-C4C-CHD	-5.13	112.42	123.39
7	L	301	BCL	C2D-C1D-ND	5.13	113.88	110.10
7	i	101	BCL	C3D-C2D-C1D	-5.12	98.84	105.83
7	S	101	BCL	C3D-C2D-C1D	-5.12	98.84	105.83
7	E	101	BCL	C2D-C1D-ND	5.12	113.88	110.10
8	J	102	A1EL2	C22-C21-C23	5.12	126.14	118.08
13	L	303	BPH	O2D-CGD-CBD	5.11	117.47	111.00
13	L	303	BPH	C4A-C3A-C2A	-5.10	97.99	102.84
7	c	101	BCL	C2D-C1D-ND	5.09	113.86	110.10
7	i	101	BCL	CHD-C4C-NC	5.09	130.73	125.08
7	K	101	BCL	C3D-C2D-C1D	-5.09	98.89	105.83
7	E	101	BCL	CHC-C4B-NB	-5.08	118.87	124.26
11	G	103	PGV	O01-C1-O02	-5.07	119.12	125.57
7	r	104	BCL	C2D-C1D-ND	5.06	113.84	110.10
7	J	101	BCL	C2D-C1D-ND	5.06	113.83	110.10
9	o	101	A1ELD	C38-C37-C36	5.05	118.61	110.86
7	L	301	BCL	CHC-C4B-NB	-5.04	118.92	124.26
7	G	101	BCL	CHC-C4B-NB	-5.04	118.92	124.26
9	g	101	A1ELD	C11-C10-C13	-5.02	115.89	122.92
7	C	101	BCL	CHD-C4C-NC	5.01	130.64	125.08
7	D	101	BCL	CHD-C4C-NC	5.00	130.63	125.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	305	BPH	CMC-C2C-C1C	-4.99	103.44	114.38
8	O	103	A1EL2	C19-C18-C17	4.99	133.69	123.47
7	O	101	BCL	C3D-C2D-C1D	-4.98	99.03	105.83
7	P	101	BCL	C3D-C2D-C1D	-4.98	99.03	105.83
7	L	301	BCL	O2D-CGD-CBD	4.96	120.08	111.27
7	f	102	BCL	C3D-C2D-C1D	-4.94	99.09	105.83
7	J	101	BCL	C3D-C2D-C1D	-4.94	99.10	105.83
7	J	101	BCL	CHC-C4B-NB	-4.93	119.04	124.26
7	M	401	BCL	CHD-C4C-NC	4.92	130.55	125.08
7	q	102	BCL	C3D-C2D-C1D	-4.92	99.12	105.83
7	n	101	BCL	CHD-C4C-NC	4.90	130.52	125.08
7	M	401	BCL	C3D-C2D-C1D	-4.90	99.15	105.83
7	S	101	BCL	CHD-C4C-NC	4.89	130.51	125.08
9	j	101	A1ELD	C33-C32-C31	-4.89	116.07	122.92
7	K	101	BCL	CHC-C4B-NB	-4.89	119.08	124.26
7	j	102	BCL	C2D-C1D-ND	4.86	113.69	110.10
7	L	301	BCL	C3D-C2D-C1D	-4.85	99.21	105.83
8	I	102	A1EL2	C28-C26-C25	4.84	126.37	118.94
9	R	102	A1ELD	C2-C3-C8	4.83	129.45	115.78
7	F	101	BCL	C2D-C1D-ND	4.82	113.65	110.10
7	s	101	BCL	C2D-C1D-ND	4.79	113.63	110.10
8	Q	102	A1EL2	C19-C18-C17	4.79	133.28	123.47
7	n	101	BCL	C3C-C4C-CHD	-4.78	113.17	123.39
7	O	101	BCL	CHC-C4B-NB	-4.78	119.20	124.26
7	d	102	BCL	C3D-C2D-C1D	-4.77	99.32	105.83
8	J	102	A1EL2	C10-C11-C12	4.76	133.43	126.23
9	j	101	A1ELD	C11-C10-C13	-4.76	116.26	122.92
7	d	102	BCL	CHD-C4C-NC	4.76	130.36	125.08
7	e	102	BCL	C3D-C2D-C1D	-4.75	99.34	105.83
7	a	101	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
7	c	101	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
7	n	101	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
7	r	104	BCL	CHD-C4C-NC	4.73	130.34	125.08
7	s	101	BCL	C3D-C2D-C1D	-4.72	99.38	105.83
7	e	102	BCL	O2D-CGD-CBD	4.71	119.64	111.27
7	q	102	BCL	CHD-C4C-NC	4.71	130.31	125.08
9	R	103	A1ELD	C19-C20-C21	4.71	133.12	123.47
8	I	102	A1EL2	C15-C16-C17	4.70	126.16	118.94
7	F	101	BCL	C3C-C4C-CHD	-4.70	113.35	123.39
7	e	102	BCL	C3C-C4C-CHD	-4.70	113.36	123.39
7	j	102	BCL	O2D-CGD-CBD	4.70	119.61	111.27
7	e	102	BCL	CHD-C4C-NC	4.69	130.28	125.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	101	BCL	C1D-ND-C4D	-4.67	103.02	106.33
7	M	403	BCL	CHD-C4C-NC	4.66	130.25	125.08
7	f	102	BCL	CHD-C4C-NC	4.66	130.25	125.08
9	O	102	A1ELD	C11-C10-C9	4.65	125.40	118.08
7	b	102	BCL	C3C-C4C-CHD	-4.64	113.49	123.39
7	k	101	BCL	CHD-C4C-NC	4.63	130.22	125.08
7	C	101	BCL	C3C-C4C-CHD	-4.63	113.50	123.39
7	A	101	BCL	C1D-ND-C4D	-4.63	103.05	106.33
7	c	101	BCL	CHD-C4C-NC	4.63	130.22	125.08
7	s	101	BCL	CHD-C4C-NC	4.63	130.21	125.08
7	g	102	BCL	C3C-C4C-CHD	-4.62	113.52	123.39
7	M	401	BCL	C2D-C1D-ND	4.62	113.51	110.10
7	r	104	BCL	C3D-C2D-C1D	-4.62	99.53	105.83
7	k	101	BCL	O2D-CGD-CBD	4.61	119.46	111.27
7	g	102	BCL	CHD-C4C-NC	4.61	130.19	125.08
7	S	101	BCL	C3C-C4C-CHD	-4.61	113.55	123.39
7	k	101	BCL	C3C-C4C-CHD	-4.60	113.56	123.39
7	M	403	BCL	C3D-C2D-C1D	-4.60	99.55	105.83
7	f	102	BCL	C3C-C4C-CHD	-4.60	113.57	123.39
7	b	102	BCL	CHD-C4C-NC	4.60	130.18	125.08
7	p	101	BCL	C3D-C2D-C1D	-4.59	99.56	105.83
7	o	102	BCL	C3D-C2D-C1D	-4.59	99.57	105.83
7	M	401	BCL	CED-O2D-CGD	4.58	126.30	115.94
7	d	102	BCL	C3C-C4C-CHD	-4.58	113.61	123.39
7	k	101	BCL	C3D-C2D-C1D	-4.57	99.59	105.83
7	q	102	BCL	C3C-C4C-CHD	-4.57	113.63	123.39
9	R	102	A1ELD	C9-C10-C13	4.56	125.94	118.94
7	b	102	BCL	C3D-C2D-C1D	-4.56	99.60	105.83
7	r	104	BCL	O2D-CGD-CBD	4.56	119.37	111.27
7	g	102	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
7	r	104	BCL	C3C-C4C-CHD	-4.55	113.68	123.39
7	c	101	BCL	CHC-C4B-NB	-4.53	119.46	124.26
7	p	101	BCL	O2D-CGD-CBD	4.53	119.31	111.27
7	N	101	BCL	CHD-C4C-NC	4.52	130.10	125.08
7	D	101	BCL	C3C-C4C-CHD	-4.52	113.74	123.39
7	o	102	BCL	C3C-C4C-CHD	-4.51	113.75	123.39
7	F	101	BCL	CHC-C4B-NB	-4.51	119.48	124.26
8	J	102	A1EL2	C19-C18-C17	4.51	132.72	123.47
7	L	302	BCL	C2D-C1D-ND	4.51	113.43	110.10
8	J	102	A1EL2	C29-C28-C26	4.51	133.04	126.23
8	P	102	A1EL2	C5-C6-C7	4.50	116.46	110.30
7	p	101	BCL	CHD-C4C-NC	4.49	130.06	125.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	c	101	BCL	O2D-CGD-CBD	4.49	119.24	111.27
7	K	101	BCL	CHD-C4C-NC	4.48	130.05	125.08
7	j	102	BCL	C3D-C2D-C1D	-4.48	99.72	105.83
8	I	102	A1EL2	C10-C11-C12	4.47	132.99	126.23
8	r	102	A1EL2	C19-C18-C17	4.46	132.62	123.47
7	M	401	BCL	C1C-NC-C4C	-4.44	104.71	106.71
7	s	101	BCL	C3C-C4C-CHD	-4.44	113.91	123.39
9	o	101	A1ELD	C17-C16-C15	-4.43	111.10	118.08
8	I	102	A1EL2	C23-C21-C20	4.42	125.73	118.94
7	Q	101	BCL	CHC-C4B-NB	-4.42	119.58	124.26
7	L	301	BCL	CHD-C4C-NC	4.41	129.98	125.08
7	j	102	BCL	CHD-C4C-NC	4.41	129.97	125.08
7	R	101	BCL	CHD-C4C-NC	4.39	129.95	125.08
7	F	101	BCL	C1C-NC-C4C	-4.39	104.73	106.71
7	i	101	BCL	C1D-ND-C4D	-4.39	103.22	106.33
7	L	301	BCL	C3C-C4C-CHD	-4.39	114.02	123.39
7	c	101	BCL	C3C-C4C-CHD	-4.38	114.04	123.39
7	I	101	BCL	CHD-C4C-NC	4.37	129.93	125.08
7	a	101	BCL	C3C-C4C-CHD	-4.37	114.06	123.39
7	o	102	BCL	CHD-C4C-NC	4.36	129.91	125.08
7	R	101	BCL	C1D-ND-C4D	-4.35	103.24	106.33
7	p	101	BCL	C3C-C4C-CHD	-4.35	114.10	123.39
9	O	102	A1ELD	C23-C22-C24	4.35	124.93	118.08
7	L	302	BCL	C3D-C2D-C1D	-4.34	99.90	105.83
11	D	103	PGV	O01-C1-C2	4.34	120.86	111.50
8	I	102	A1EL2	C35-C30-C31	-4.34	116.09	122.54
8	J	102	A1EL2	C24-C25-C26	4.34	133.51	127.31
7	d	102	BCL	O2D-CGD-CBD	4.34	118.98	111.27
7	B	101	BCL	CHC-C4B-NB	-4.34	119.66	124.26
7	R	101	BCL	CHC-C4B-NB	-4.34	119.67	124.26
7	M	403	BCL	C3C-C4C-CHD	-4.33	114.13	123.39
9	O	102	A1ELD	C30-C31-C32	4.33	133.48	127.31
7	N	101	BCL	C3C-C4C-CHD	-4.32	114.16	123.39
8	J	102	A1EL2	C27-C26-C28	4.32	124.88	118.08
7	G	101	BCL	CHD-C4C-NC	4.32	129.87	125.08
7	M	403	BCL	C1D-ND-C4D	-4.31	103.27	106.33
7	g	102	BCL	O2D-CGD-CBD	4.31	118.93	111.27
7	Q	101	BCL	CHD-C4C-NC	4.31	129.87	125.08
7	I	101	BCL	C3C-C4C-CHD	-4.31	114.18	123.39
8	I	102	A1EL2	C11-C12-C13	4.31	125.55	118.94
8	r	103	A1EL2	C1-C2-C3	4.30	129.36	124.53
11	L	308	PGV	O01-C1-C2	4.30	120.77	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	102	A1EL2	C19-C18-C17	4.29	132.27	123.47
11	F	103	PGV	O01-C1-C2	4.28	120.73	111.50
7	M	401	BCL	C3C-C4C-CHD	-4.28	114.24	123.39
7	O	101	BCL	CHD-C4C-NC	4.28	129.83	125.08
8	D	102	A1EL2	C27-C26-C25	-4.28	116.93	122.92
8	A	102	A1EL2	C19-C18-C17	4.27	132.22	123.47
8	E	102	A1EL2	C19-C18-C17	4.27	132.22	123.47
8	N	102	A1EL2	C27-C26-C25	-4.26	116.95	122.92
8	C	103	A1EL2	C19-C18-C17	4.26	132.21	123.47
8	B	102	A1EL2	C19-C18-C17	4.26	132.21	123.47
8	C	103	A1EL2	C27-C26-C25	-4.26	116.96	122.92
7	q	102	BCL	O2D-CGD-CBD	4.26	118.83	111.27
8	F	102	A1EL2	C27-C26-C25	-4.25	116.97	122.92
8	D	102	A1EL2	C19-C18-C17	4.25	132.18	123.47
8	E	102	A1EL2	C27-C26-C25	-4.25	116.97	122.92
8	J	102	A1EL2	C11-C12-C13	4.25	125.46	118.94
7	a	101	BCL	CHD-C4C-NC	4.24	129.79	125.08
7	d	102	BCL	CHC-C4B-NB	-4.24	119.77	124.26
8	A	102	A1EL2	C27-C26-C25	-4.24	116.99	122.92
8	P	102	A1EL2	C9-C4-C3	4.23	117.16	110.30
7	i	101	BCL	CHC-C4B-NB	-4.23	119.78	124.26
8	B	102	A1EL2	C27-C26-C25	-4.23	117.00	122.92
7	j	102	BCL	C3C-C4C-CHD	-4.22	114.37	123.39
7	R	101	BCL	C3C-C4C-CHD	-4.22	114.38	123.39
7	I	101	BCL	C1D-ND-C4D	-4.22	103.34	106.33
7	b	102	BCL	O2D-CGD-CBD	4.22	118.77	111.27
7	P	101	BCL	CHD-C4C-NC	4.21	129.75	125.08
9	O	102	A1ELD	C17-C16-C15	4.21	124.71	118.08
7	a	101	BCL	O2D-CGD-CBD	4.21	118.75	111.27
7	o	102	BCL	O2D-CGD-CBD	4.21	118.74	111.27
7	Q	101	BCL	C1D-ND-C4D	-4.20	103.35	106.33
9	e	101	A1ELD	C20-C19-C18	4.20	132.07	123.47
9	R	102	A1ELD	C44-C2-C3	-4.19	103.50	110.30
7	S	101	BCL	C1D-ND-C4D	-4.19	103.36	106.33
7	E	101	BCL	CHD-C4C-NC	4.19	129.73	125.08
8	r	102	A1EL2	C27-C26-C25	-4.18	117.06	122.92
7	q	102	BCL	CHC-C4B-NB	-4.15	119.86	124.26
9	R	102	A1ELD	C14-C13-C10	4.15	133.23	127.31
7	A	101	BCL	CHD-C4C-NC	4.14	129.68	125.08
7	A	101	BCL	C3C-C4C-CHD	-4.14	114.55	123.39
8	r	103	A1EL2	C8-C4-C3	4.13	117.00	110.30
7	Q	101	BCL	C3C-C4C-CHD	-4.13	114.57	123.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	101	BCL	O2D-CGD-CBD	4.12	118.59	111.27
7	C	101	BCL	C1D-ND-C4D	-4.12	103.41	106.33
8	K	102	A1EL2	C27-C26-C25	-4.11	117.16	122.92
7	f	102	BCL	CHC-C4B-NB	-4.11	119.90	124.26
8	P	102	A1EL2	C27-C26-C28	4.11	124.56	118.08
8	r	103	A1EL2	C4-C3-C2	4.11	128.41	122.61
7	g	102	BCL	CHC-C4B-NB	-4.11	119.91	124.26
9	B	103	A1ELD	C11-C10-C13	-4.11	117.17	122.92
7	J	101	BCL	CHD-C4C-NC	4.11	129.64	125.08
7	d	102	BCL	C1D-ND-C4D	-4.10	103.42	106.33
11	M	408	PGV	O01-C1-C2	4.10	120.34	111.50
8	G	102	A1EL2	C19-C18-C17	4.10	131.88	123.47
7	o	102	BCL	CHC-C4B-NB	-4.10	119.92	124.26
7	S	101	BCL	O2D-CGD-CBD	4.10	118.55	111.27
7	F	101	BCL	CHD-C4C-NC	4.10	129.63	125.08
8	r	103	A1EL2	O1-C6-C7	-4.09	100.90	109.68
7	L	302	BCL	CHC-C4B-NB	-4.09	119.93	124.26
7	n	101	BCL	CHC-C4B-NB	-4.08	119.93	124.26
7	B	101	BCL	C3C-C4C-CHD	-4.07	114.69	123.39
9	o	101	A1ELD	C20-C19-C18	4.07	131.81	123.47
7	n	101	BCL	O2D-CGD-CBD	4.07	118.49	111.27
7	G	101	BCL	C3C-C4C-CHD	-4.06	114.71	123.39
7	B	101	BCL	C1D-ND-C4D	-4.06	103.45	106.33
8	r	103	A1EL2	C40-C12-C13	-4.06	117.24	122.92
7	O	101	BCL	C1D-ND-C4D	-4.06	103.45	106.33
8	r	103	A1EL2	O3-C33-C32	-4.05	100.53	109.53
7	s	101	BCL	CHC-C4B-NB	-4.05	119.97	124.26
9	j	101	A1ELD	C11-C10-C9	4.05	124.46	118.08
9	r	101	A1ELD	C11-C10-C13	-4.05	117.25	122.92
7	p	101	BCL	CHC-C4B-NB	-4.04	119.98	124.26
11	L	307	PGV	O01-C1-C2	4.04	120.20	111.50
8	I	102	A1EL2	C14-C13-C12	4.04	133.07	127.31
7	j	102	BCL	CHC-C4B-NB	-4.04	119.98	124.26
11	T	303	PGV	O01-C1-C2	4.03	120.19	111.50
9	R	103	A1ELD	C11-C10-C13	-4.03	117.28	122.92
7	J	101	BCL	C1D-ND-C4D	-4.03	103.47	106.33
7	K	101	BCL	C3C-C4C-CHD	-4.02	114.80	123.39
7	r	104	BCL	CHC-C4B-NB	-4.02	120.00	124.26
8	J	102	A1EL2	C1-C2-C3	-4.01	120.02	124.53
7	D	101	BCL	O2D-CGD-CBD	4.01	118.39	111.27
7	b	102	BCL	C1D-ND-C4D	-4.01	103.49	106.33
7	E	101	BCL	C4A-NA-C1A	4.00	108.51	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	102	BCL	O2D-CGD-CBD	3.99	118.36	111.27
7	B	101	BCL	CHD-C4C-NC	3.99	129.50	125.08
7	k	101	BCL	C1D-ND-C4D	-3.99	103.50	106.33
9	C	102	A1ELD	C17-C16-C18	-3.98	117.35	122.92
8	r	103	A1EL2	C9-C4-C8	-3.98	96.32	108.53
9	R	102	A1ELD	C7-C6-C5	-3.97	104.87	110.30
7	E	101	BCL	C3C-C4C-CHD	-3.97	114.92	123.39
7	A	101	BCL	C4A-NA-C1A	3.96	108.48	106.71
8	J	102	A1EL2	C35-C30-C29	3.96	127.01	115.81
7	N	101	BCL	C1D-ND-C4D	-3.95	103.53	106.33
8	O	103	A1EL2	C27-C26-C25	-3.95	117.39	122.92
9	q	101	A1ELD	C11-C10-C13	-3.94	117.40	122.92
8	N	102	A1EL2	C19-C18-C17	3.94	131.55	123.47
7	P	101	BCL	C1D-ND-C4D	-3.94	103.54	106.33
9	j	101	A1ELD	C23-C22-C21	-3.94	117.41	122.92
8	N	102	A1EL2	C40-C12-C13	-3.93	117.41	122.92
7	g	102	BCL	C1D-ND-C4D	-3.93	103.54	106.33
7	D	101	BCL	CHC-C1C-NC	3.91	129.91	124.51
8	r	103	A1EL2	C38-C31-C30	3.89	128.90	124.53
8	F	102	A1EL2	C40-C12-C13	-3.89	117.47	122.92
7	e	102	BCL	CHC-C4B-NB	-3.89	120.14	124.26
7	Q	101	BCL	C4A-NA-C1A	3.89	108.45	106.71
7	O	101	BCL	C3C-C4C-CHD	-3.88	115.09	123.39
8	E	102	A1EL2	C40-C12-C13	-3.88	117.49	122.92
8	J	102	A1EL2	C23-C21-C20	3.88	124.89	118.94
8	C	103	A1EL2	C40-C12-C13	-3.88	117.49	122.92
7	f	102	BCL	C1-C2-C3	-3.87	119.35	126.04
8	D	102	A1EL2	C40-C12-C13	-3.87	117.51	122.92
7	J	101	BCL	C3C-C4C-CHD	-3.86	115.14	123.39
7	P	101	BCL	C3C-C4C-CHD	-3.86	115.14	123.39
8	B	102	A1EL2	C40-C12-C13	-3.85	117.52	122.92
9	q	101	A1ELD	C33-C32-C31	-3.84	117.54	122.92
7	B	101	BCL	C4A-NA-C1A	3.84	108.43	106.71
7	b	102	BCL	CHC-C4B-NB	-3.84	120.19	124.26
7	G	101	BCL	C1D-ND-C4D	-3.84	103.61	106.33
9	C	102	A1ELD	C23-C22-C21	-3.84	117.55	122.92
8	A	102	A1EL2	C40-C12-C13	-3.84	117.55	122.92
8	r	103	A1EL2	C27-C26-C28	3.84	124.12	118.08
9	B	103	A1ELD	C34-C32-C31	3.83	124.82	118.94
9	A	103	A1ELD	C11-C10-C13	-3.83	117.56	122.92
7	e	102	BCL	C1D-ND-C4D	-3.82	103.62	106.33
8	I	102	A1EL2	C19-C20-C21	3.81	132.75	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	101	BCL	O2D-CGD-CBD	3.81	118.04	111.27
7	O	101	BCL	C4-C3-C5	3.81	121.68	115.27
9	q	101	A1ELD	C34-C32-C31	3.80	124.77	118.94
8	I	102	A1EL2	C24-C25-C26	3.80	132.73	127.31
8	r	103	A1EL2	C1-C2-C7	-3.79	107.33	114.36
7	Q	101	BCL	CHB-C1B-NB	-3.79	120.25	124.26
7	M	403	BCL	CHB-C1B-NB	-3.79	120.25	124.26
8	r	102	A1EL2	C40-C12-C13	-3.78	117.62	122.92
7	G	101	BCL	O2D-CGD-CBD	3.78	117.99	111.27
7	a	101	BCL	CHC-C4B-NB	-3.77	120.26	124.26
9	g	101	A1ELD	C17-C16-C18	-3.77	117.64	122.92
7	q	102	BCL	C1D-ND-C4D	-3.77	103.66	106.33
7	L	302	BCL	C3C-C4C-CHD	-3.76	115.35	123.39
13	L	303	BPH	CBC-CAC-C3C	-3.76	106.20	113.77
9	g	101	A1ELD	C23-C22-C21	-3.76	117.66	122.92
7	P	101	BCL	O2D-CGD-CBD	3.75	117.94	111.27
9	b	101	A1ELD	C11-C10-C13	-3.75	117.67	122.92
8	P	102	A1EL2	C40-C12-C11	3.74	123.97	118.08
9	B	103	A1ELD	C17-C16-C18	-3.74	117.69	122.92
7	P	101	BCL	C4-C3-C5	3.74	121.56	115.27
9	j	101	A1ELD	C17-C16-C18	-3.73	117.70	122.92
13	L	303	BPH	C4D-CHA-CBD	-3.72	106.83	108.52
7	L	302	BCL	CHD-C4C-NC	3.72	129.21	125.08
7	c	101	BCL	C4B-C3B-C2B	-3.72	102.38	108.36
7	C	101	BCL	C4A-NA-C1A	3.71	108.38	106.71
7	O	101	BCL	O2D-CGD-CBD	3.71	117.86	111.27
7	s	101	BCL	O2D-CGD-CBD	3.71	117.86	111.27
9	o	101	A1ELD	C39-C37-C36	-3.70	105.17	110.86
7	n	101	BCL	C4A-NA-C1A	3.70	108.37	106.71
7	o	102	BCL	C1D-ND-C4D	-3.70	103.71	106.33
7	k	101	BCL	CHC-C4B-NB	-3.69	120.35	124.26
7	L	301	BCL	CMB-C2B-C3B	3.69	135.88	125.93
9	f	101	A1ELD	C11-C10-C13	-3.69	117.76	122.92
9	r	101	A1ELD	C19-C20-C21	3.68	131.02	123.47
7	A	101	BCL	CHB-C1B-NB	-3.68	120.36	124.26
8	P	102	A1EL2	C29-C30-C31	-3.68	112.56	121.46
8	J	102	A1EL2	C38-C31-C32	3.67	121.16	114.36
7	M	401	BCL	C4B-C3B-C2B	-3.67	102.46	108.36
9	b	101	A1ELD	C20-C19-C18	3.67	130.98	123.47
9	e	101	A1ELD	C19-C20-C21	3.66	130.98	123.47
7	I	101	BCL	O2D-CGD-CBD	3.66	117.76	111.27
7	K	101	BCL	C4B-C3B-C2B	-3.65	102.48	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	101	A1ELD	C20-C19-C18	3.65	130.95	123.47
7	p	101	BCL	C1D-ND-C4D	-3.65	103.74	106.33
7	C	101	BCL	O2D-CGD-CBD	3.64	117.74	111.27
7	K	101	BCL	CHC-C1C-NC	3.63	129.54	124.51
7	f	102	BCL	O2A-CGA-CBA	3.63	123.31	111.91
7	L	301	BCL	C1D-ND-C4D	-3.63	103.76	106.33
9	J	103	A1ELD	C33-C32-C31	-3.63	117.84	122.92
7	L	301	BCL	O2A-CGA-CBA	3.62	123.28	111.91
9	g	101	A1ELD	C20-C19-C18	3.62	130.90	123.47
9	C	102	A1ELD	C20-C19-C18	3.62	130.90	123.47
7	I	101	BCL	C1-C2-C3	-3.62	119.78	126.04
9	O	102	A1ELD	C35-C34-C32	3.61	131.35	125.89
7	C	101	BCL	CHC-C1C-NC	3.61	129.51	124.51
7	j	102	BCL	C1D-ND-C4D	-3.61	103.77	106.33
13	L	305	BPH	C2B-C1B-NB	-3.61	107.03	109.53
7	K	101	BCL	C1D-ND-C4D	-3.61	103.77	106.33
7	R	101	BCL	C4-C3-C5	3.59	121.30	115.27
7	A	101	BCL	O2D-CGD-CBD	3.58	117.63	111.27
7	r	104	BCL	C1D-ND-C4D	-3.58	103.80	106.33
7	i	101	BCL	C4A-NA-C1A	3.57	108.31	106.71
7	a	101	BCL	C1D-ND-C4D	-3.57	103.80	106.33
7	f	102	BCL	C4-C3-C5	3.56	121.27	115.27
7	M	403	BCL	C3D-C4D-ND	3.55	115.98	110.24
7	D	101	BCL	C4A-NA-C1A	3.55	108.30	106.71
7	J	101	BCL	C4A-NA-C1A	3.54	108.30	106.71
8	r	102	A1EL2	C39-C16-C17	-3.53	117.97	122.92
7	M	403	BCL	CAB-C3B-C2B	-3.53	123.05	128.34
8	I	102	A1EL2	C1-C2-C3	-3.53	120.56	124.53
9	R	103	A1ELD	C23-C22-C21	-3.53	117.98	122.92
7	R	101	BCL	CHB-C4A-NA	3.53	129.39	124.51
8	O	103	A1EL2	C23-C21-C20	3.52	124.35	118.94
9	f	101	A1ELD	C33-C32-C31	-3.52	118.00	122.92
9	q	101	A1ELD	C20-C19-C18	3.52	130.68	123.47
8	G	102	A1EL2	C40-C12-C13	-3.51	118.00	122.92
7	J	101	BCL	O2D-CGD-O1D	-3.50	116.99	123.84
7	B	101	BCL	O2D-CGD-CBD	3.50	117.50	111.27
7	E	101	BCL	C1D-ND-C4D	-3.50	103.85	106.33
7	E	101	BCL	O2D-CGD-CBD	3.50	117.49	111.27
7	n	101	BCL	O2A-CGA-CBA	3.50	122.89	111.91
8	J	102	A1EL2	C14-C13-C12	3.50	132.30	127.31
7	D	101	BCL	C4B-C3B-C2B	-3.49	102.75	108.36
7	K	101	BCL	O2D-CGD-CBD	3.48	117.46	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	102	A1EL2	O3-C33-C34	3.48	116.67	109.74
9	J	103	A1ELD	C20-C19-C18	3.48	130.60	123.47
9	e	101	A1ELD	C15-C16-C18	3.48	124.28	118.94
9	A	103	A1ELD	C20-C19-C18	3.48	130.60	123.47
7	o	102	BCL	C4A-NA-C1A	3.48	108.27	106.71
8	r	103	A1EL2	C22-C21-C20	-3.46	118.07	122.92
7	G	101	BCL	C4B-C3B-C2B	-3.46	102.80	108.36
9	j	101	A1ELD	C34-C32-C31	3.45	124.24	118.94
7	P	101	BCL	CHB-C4A-NA	3.45	129.28	124.51
7	D	101	BCL	CAB-C3B-C2B	-3.44	123.18	128.34
8	O	103	A1EL2	C15-C16-C17	3.44	124.22	118.94
7	f	102	BCL	C1D-ND-C4D	-3.44	103.89	106.33
9	f	101	A1ELD	C20-C19-C18	3.44	130.53	123.47
7	c	101	BCL	O2A-CGA-CBA	3.44	122.70	111.91
7	R	101	BCL	CHB-C1B-NB	-3.44	120.62	124.26
9	B	103	A1ELD	C23-C22-C21	-3.43	118.11	122.92
7	A	101	BCL	CHB-C4A-NA	3.43	129.26	124.51
8	I	102	A1EL2	C34-C35-C30	3.43	116.60	110.48
7	R	101	BCL	O2D-CGD-CBD	3.42	117.35	111.27
8	O	103	A1EL2	C28-C26-C25	3.42	124.19	118.94
7	n	101	BCL	C1D-ND-C4D	-3.42	103.91	106.33
7	N	101	BCL	O2D-CGD-CBD	3.42	117.34	111.27
8	Q	102	A1EL2	C15-C16-C17	3.42	124.18	118.94
7	B	101	BCL	C1-C2-C3	-3.41	120.14	126.04
8	I	102	A1EL2	C18-C19-C20	3.40	130.45	123.47
7	K	101	BCL	C4A-NA-C1A	3.40	108.24	106.71
8	P	102	A1EL2	C4-C3-C2	3.40	127.40	122.61
7	S	101	BCL	C1C-NC-C4C	-3.40	105.18	106.71
9	r	101	A1ELD	C20-C19-C18	3.40	130.43	123.47
7	s	101	BCL	CMB-C2B-C3B	3.40	135.10	125.93
8	P	102	A1EL2	C1-C2-C3	3.39	128.34	124.53
7	N	101	BCL	CHC-C1C-NC	3.39	129.20	124.51
7	N	101	BCL	C4B-C3B-C2B	-3.39	102.91	108.36
7	P	101	BCL	C1-C2-C3	-3.38	120.19	126.04
7	A	101	BCL	C1C-NC-C4C	-3.37	105.19	106.71
7	I	101	BCL	C4A-NA-C1A	3.37	108.22	106.71
7	B	101	BCL	C4-C3-C5	3.37	120.95	115.27
8	P	102	A1EL2	C29-C28-C26	-3.37	121.14	126.23
7	O	101	BCL	CHB-C4A-NA	3.37	129.17	124.51
8	I	102	A1EL2	C29-C28-C26	3.36	131.31	126.23
7	r	104	BCL	CMB-C2B-C3B	3.36	135.00	125.93
9	o	101	A1ELD	C15-C16-C18	3.35	124.09	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	101	BCL	C4A-NA-C1A	3.35	108.21	106.71
8	r	103	A1EL2	C6-C7-C2	-3.34	105.20	111.85
9	q	101	A1ELD	C19-C20-C21	3.34	130.31	123.47
8	K	102	A1EL2	C19-C18-C17	3.33	130.30	123.47
7	J	101	BCL	C3D-C4D-ND	3.33	115.62	110.24
7	E	101	BCL	CHB-C1B-NB	-3.33	120.73	124.26
7	M	403	BCL	CMB-C2B-C1B	3.32	130.43	125.37
8	P	102	A1EL2	C24-C25-C26	-3.32	122.57	127.31
7	J	101	BCL	CHB-C4A-NA	3.32	129.11	124.51
7	A	101	BCL	C4B-C3B-C2B	-3.32	103.01	108.36
9	d	101	A1ELD	C11-C10-C13	-3.32	118.28	122.92
7	O	101	BCL	C1-C2-C3	-3.32	120.31	126.04
9	e	101	A1ELD	C24-C22-C21	3.31	124.02	118.94
7	D	101	BCL	C3D-C4D-ND	3.30	115.58	110.24
7	c	101	BCL	CHC-C1C-NC	3.30	129.07	124.51
9	R	103	A1ELD	C24-C22-C21	3.29	124.00	118.94
7	K	101	BCL	C4-C3-C5	3.29	120.81	115.27
7	S	101	BCL	C4B-C3B-C2B	-3.29	103.06	108.36
9	b	101	A1ELD	C23-C22-C21	-3.28	118.32	122.92
9	B	103	A1ELD	C6-C5-C4	3.28	118.39	111.85
9	b	101	A1ELD	C17-C16-C18	-3.28	118.33	122.92
7	O	101	BCL	CHB-C1B-NB	-3.28	120.79	124.26
7	M	401	BCL	O2A-CGA-CBA	3.27	122.17	111.91
8	r	102	A1EL2	C15-C16-C17	3.27	123.96	118.94
9	B	103	A1ELD	C11-C10-C9	3.27	123.23	118.08
9	R	103	A1ELD	C17-C16-C18	-3.26	118.36	122.92
7	R	101	BCL	C3D-C4D-ND	3.25	115.50	110.24
7	O	101	BCL	C3D-C4D-ND	3.25	115.50	110.24
7	d	102	BCL	C3D-C4D-ND	3.25	115.49	110.24
7	G	101	BCL	CHC-C1C-NC	3.25	129.00	124.51
7	B	101	BCL	C4B-C3B-C2B	-3.24	103.14	108.36
8	C	103	A1EL2	C39-C16-C17	-3.24	118.38	122.92
9	r	101	A1ELD	C17-C16-C18	-3.24	118.38	122.92
11	T	301	PGV	O01-C1-C2	3.24	118.49	111.50
7	b	102	BCL	C3D-C4D-ND	3.24	115.48	110.24
8	r	102	A1EL2	C22-C21-C20	-3.24	118.39	122.92
9	f	101	A1ELD	C17-C16-C18	-3.23	118.39	122.92
7	S	101	BCL	CHC-C1C-NC	3.23	128.98	124.51
8	D	102	A1EL2	C39-C16-C17	-3.23	118.40	122.92
7	N	101	BCL	C4A-NA-C1A	3.22	108.16	106.71
9	r	101	A1ELD	C23-C22-C21	-3.22	118.42	122.92
8	A	102	A1EL2	C39-C16-C17	-3.22	118.42	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	q	102	BCL	CMB-C2B-C3B	3.21	134.61	125.93
9	o	101	A1ELD	C7-C6-C5	-3.21	105.91	110.30
7	s	101	BCL	C1D-ND-C4D	-3.21	104.06	106.33
8	E	102	A1EL2	C39-C16-C17	-3.20	118.44	122.92
8	B	102	A1EL2	C39-C16-C17	-3.20	118.44	122.92
7	R	101	BCL	C4A-NA-C1A	3.20	108.14	106.71
9	o	101	A1ELD	C19-C20-C21	3.20	130.03	123.47
9	g	101	A1ELD	C11-C10-C9	3.19	123.11	118.08
9	q	101	A1ELD	C17-C16-C18	-3.19	118.45	122.92
7	B	101	BCL	CHB-C1B-NB	-3.19	120.88	124.26
13	L	303	BPH	CMC-C2C-C3C	3.19	126.82	113.99
8	J	102	A1EL2	C15-C16-C17	3.18	123.82	118.94
7	P	101	BCL	C3D-C4D-ND	3.18	115.38	110.24
8	F	102	A1EL2	C39-C16-C17	-3.17	118.48	122.92
7	g	102	BCL	C3D-C4D-ND	3.17	115.37	110.24
7	I	101	BCL	C4B-C3B-C2B	-3.17	103.26	108.36
13	L	303	BPH	C1A-C2A-C3A	-3.17	99.82	102.84
7	J	101	BCL	CHC-C1C-NC	3.17	128.89	124.51
7	M	401	BCL	C1D-ND-C4D	-3.17	104.09	106.33
7	j	102	BCL	C3D-C4D-ND	3.17	115.36	110.24
9	q	101	A1ELD	C23-C22-C21	-3.17	118.49	122.92
7	S	101	BCL	C3D-C4D-ND	3.17	115.36	110.24
7	C	101	BCL	O2A-CGA-CBA	3.16	121.84	111.91
7	d	102	BCL	CMB-C2B-C3B	3.16	134.46	125.93
7	M	401	BCL	C4-C3-C5	3.16	120.58	115.27
7	B	101	BCL	C1C-NC-C4C	-3.16	105.29	106.71
8	N	102	A1EL2	C39-C16-C17	-3.16	118.50	122.92
7	c	101	BCL	C1D-ND-C4D	-3.16	104.09	106.33
9	C	102	A1ELD	C11-C10-C9	3.15	123.05	118.08
7	M	401	BCL	C4A-NA-C1A	3.15	108.12	106.71
7	e	102	BCL	CMB-C2B-C3B	3.15	134.44	125.93
7	A	101	BCL	C3D-C4D-ND	3.15	115.33	110.24
7	P	101	BCL	CHC-C1C-NC	3.15	128.86	124.51
7	k	101	BCL	C3D-C4D-ND	3.14	115.32	110.24
9	J	103	A1ELD	C23-C22-C21	-3.14	118.53	122.92
7	I	101	BCL	C3D-C4D-ND	3.13	115.31	110.24
7	c	101	BCL	O2D-CGD-O1D	-3.13	117.72	123.84
12	L	309	LMT	C1'-O5'-C5'	-3.13	107.55	113.69
7	i	101	BCL	C3D-C4D-ND	3.12	115.28	110.24
9	A	103	A1ELD	C33-C32-C31	-3.12	118.56	122.92
7	g	102	BCL	CMB-C2B-C3B	3.12	134.35	125.93
9	A	103	A1ELD	C17-C16-C18	-3.12	118.56	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	101	BCL	CAB-C3B-C2B	-3.12	123.67	128.34
7	L	302	BCL	O1D-CGD-CBD	-3.11	118.12	124.48
9	g	101	A1ELD	C19-C20-C21	3.11	129.85	123.47
7	j	102	BCL	CMB-C2B-C3B	3.11	134.33	125.93
7	G	101	BCL	C1-C2-C3	-3.11	120.67	126.04
7	p	101	BCL	C3D-C4D-ND	3.10	115.26	110.24
7	Q	101	BCL	C3D-C4D-ND	3.10	115.25	110.24
7	o	102	BCL	C3D-C4D-ND	3.10	115.25	110.24
7	p	101	BCL	CMB-C2B-C3B	3.10	134.30	125.93
7	e	102	BCL	C3D-C4D-ND	3.10	115.25	110.24
7	f	102	BCL	CMB-C2B-C3B	3.10	134.29	125.93
9	C	102	A1ELD	C19-C20-C21	3.09	129.81	123.47
9	b	101	A1ELD	C19-C20-C21	3.09	129.81	123.47
9	O	102	A1ELD	C38-C37-C36	-3.09	106.12	110.86
9	f	101	A1ELD	C23-C22-C21	-3.09	118.60	122.92
7	d	102	BCL	C4A-NA-C1A	3.08	108.09	106.71
9	J	103	A1ELD	C17-C16-C18	-3.08	118.61	122.92
13	L	303	BPH	C3D-C4D-ND	3.08	111.91	107.72
7	K	101	BCL	O2A-CGA-CBA	3.07	121.55	111.91
9	d	101	A1ELD	C19-C20-C21	3.07	129.76	123.47
8	N	102	A1EL2	C22-C21-C20	-3.07	118.63	122.92
7	O	101	BCL	CHC-C1C-NC	3.07	128.75	124.51
9	A	103	A1ELD	C23-C22-C21	-3.07	118.63	122.92
7	b	102	BCL	CMB-C2B-C3B	3.06	134.21	125.93
8	P	102	A1EL2	O3-C33-C34	3.06	115.83	109.74
7	N	101	BCL	CMB-C2B-C3B	3.06	134.20	125.93
7	M	403	BCL	O1D-CGD-CBD	-3.06	118.22	124.48
7	N	101	BCL	CHB-C4A-NA	3.06	128.75	124.51
8	O	103	A1EL2	C19-C20-C21	3.06	131.67	127.31
7	c	101	BCL	C1-O2A-CGA	3.06	124.46	116.44
7	b	102	BCL	O2A-CGA-CBA	3.05	121.49	111.91
9	b	101	A1ELD	C33-C32-C31	-3.05	118.65	122.92
9	d	101	A1ELD	C17-C16-C18	-3.05	118.65	122.92
7	r	104	BCL	C3D-C4D-ND	3.05	115.17	110.24
7	c	101	BCL	CED-O2D-CGD	3.05	122.83	115.94
7	n	101	BCL	C1-O2A-CGA	3.05	124.43	116.44
9	J	103	A1ELD	C11-C10-C13	-3.04	118.66	122.92
7	C	101	BCL	CHB-C4A-NA	3.04	128.72	124.51
7	i	101	BCL	C4B-C3B-C2B	-3.04	103.47	108.36
7	C	101	BCL	C4B-C3B-C2B	-3.03	103.48	108.36
7	a	101	BCL	C1-C2-C3	-3.03	120.80	126.04
7	K	101	BCL	CHB-C1B-NB	-3.03	121.05	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	101	BCL	C3D-C4D-ND	3.03	115.14	110.24
7	E	101	BCL	C4B-C3B-C2B	-3.03	103.49	108.36
7	n	101	BCL	CMB-C2B-C3B	3.03	134.11	125.93
7	E	101	BCL	CHC-C1C-NC	3.03	128.70	124.51
7	I	101	BCL	CHC-C1C-NC	3.02	128.69	124.51
7	M	401	BCL	CMB-C2B-C3B	3.02	134.09	125.93
8	G	102	A1EL2	C27-C26-C25	-3.02	118.69	122.92
7	R	101	BCL	CHC-C1C-NC	3.02	128.69	124.51
9	d	101	A1ELD	C23-C22-C21	-3.02	118.69	122.92
7	L	301	BCL	C4B-C3B-C2B	-3.02	103.50	108.36
7	K	101	BCL	C1-O2A-CGA	3.02	124.36	116.44
7	g	102	BCL	C4A-NA-C1A	3.01	108.06	106.71
7	G	101	BCL	C3D-C4D-ND	3.01	115.11	110.24
8	P	102	A1EL2	C38-C31-C30	3.01	127.91	124.53
7	F	101	BCL	C1D-CHD-C4C	-3.01	119.36	126.62
7	L	302	BCL	C3D-C4D-ND	3.01	115.10	110.24
7	N	101	BCL	C3D-C4D-ND	3.00	115.09	110.24
7	c	101	BCL	CMB-C2B-C3B	3.00	134.03	125.93
7	L	302	BCL	C1D-CHD-C4C	-3.00	119.39	126.62
7	Q	101	BCL	CHC-C1C-NC	3.00	128.65	124.51
7	F	101	BCL	O2D-CGD-CBD	2.99	116.58	111.27
7	G	101	BCL	CHB-C4A-NA	2.99	128.65	124.51
7	Q	101	BCL	C4B-C3B-C2B	-2.99	103.55	108.36
7	o	102	BCL	C4B-C3B-C2B	-2.99	103.55	108.36
7	J	101	BCL	CHB-C1B-NB	-2.99	121.09	124.26
7	o	102	BCL	C4-C3-C5	2.98	120.29	115.27
7	M	401	BCL	C3D-C4D-ND	2.98	115.05	110.24
7	E	101	BCL	C3D-C4D-ND	2.97	115.05	110.24
9	C	102	A1ELD	C33-C32-C31	-2.97	118.77	122.92
9	J	103	A1ELD	C34-C32-C31	2.97	123.49	118.94
7	P	101	BCL	CHB-C1B-NB	-2.97	121.12	124.26
7	d	102	BCL	CHB-C4A-NA	2.96	128.61	124.51
7	c	101	BCL	C3D-C4D-ND	2.96	115.03	110.24
8	r	102	A1EL2	C28-C26-C25	2.96	123.48	118.94
7	G	101	BCL	CMB-C2B-C3B	2.96	133.92	125.93
7	a	101	BCL	C4B-C3B-C2B	-2.96	103.60	108.36
11	L	308	PGV	O03-C19-C20	2.95	121.18	111.91
16	M	405	H4X	C29-C28-C27	-2.95	118.79	122.92
7	a	101	BCL	C3D-C4D-ND	2.95	115.01	110.24
7	G	101	BCL	C4-C3-C5	2.95	120.23	115.27
7	s	101	BCL	C4B-C3B-C2B	-2.95	103.61	108.36
7	C	101	BCL	C3D-C4D-ND	2.95	115.01	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	301	PGV	O01-C02-C03	2.95	114.67	107.93
7	L	302	BCL	C1C-NC-C4C	-2.94	105.38	106.71
8	O	103	A1EL2	C18-C19-C20	2.94	129.51	123.47
7	N	101	BCL	CHB-C1B-NB	-2.94	121.14	124.26
7	G	101	BCL	C4A-NA-C1A	2.94	108.03	106.71
7	K	101	BCL	C3D-C4D-ND	2.94	115.00	110.24
8	J	102	A1EL2	O1-C6-C5	2.94	115.64	109.80
11	F	103	PGV	C02-O01-C1	-2.94	110.56	117.79
7	j	102	BCL	C4-C3-C5	2.94	120.21	115.27
9	d	101	A1ELD	C33-C32-C31	-2.94	118.81	122.92
9	O	102	A1ELD	C44-C2-C3	-2.94	105.54	110.30
8	r	103	A1EL2	C39-C16-C15	2.93	122.69	118.08
7	q	102	BCL	C3D-C4D-ND	2.93	114.97	110.24
7	a	101	BCL	C4-C3-C5	2.93	120.19	115.27
7	P	101	BCL	C4B-C3B-C2B	-2.92	103.66	108.36
11	D	103	PGV	C02-O01-C1	-2.92	110.61	117.79
7	M	403	BCL	CHC-C1C-NC	2.91	128.54	124.51
7	a	101	BCL	C4A-NA-C1A	2.91	108.02	106.71
7	M	403	BCL	CBB-CAB-C3B	-2.91	114.21	120.43
9	R	103	A1ELD	C26-C25-C24	2.91	132.30	123.22
7	f	102	BCL	C4B-C3B-C2B	-2.91	103.68	108.36
7	Q	101	BCL	CHB-C4A-NA	2.91	128.53	124.51
7	K	101	BCL	CHB-C4A-NA	2.91	128.53	124.51
7	e	102	BCL	C4B-C3B-C2B	-2.90	103.69	108.36
7	L	301	BCL	O1D-CGD-CBD	-2.90	118.54	124.48
9	A	103	A1ELD	C19-C20-C21	2.90	129.42	123.47
16	M	405	H4X	C18-C17-C19	-2.90	118.86	122.92
7	L	302	BCL	C1D-ND-C4D	-2.90	104.28	106.33
8	J	102	A1EL2	C9-C4-C8	-2.90	99.63	108.53
8	C	103	A1EL2	C22-C21-C20	-2.90	118.87	122.92
9	g	101	A1ELD	C24-C22-C21	2.89	123.38	118.94
7	B	101	BCL	CHB-C4A-NA	2.89	128.51	124.51
7	M	401	BCL	O1D-CGD-CBD	-2.89	118.57	124.48
7	P	101	BCL	CMB-C2B-C3B	2.88	133.72	125.93
7	D	101	BCL	C4-C3-C5	2.88	120.12	115.27
9	f	101	A1ELD	C19-C20-C21	2.88	129.38	123.47
7	M	403	BCL	O2A-CGA-CBA	2.88	120.95	111.91
9	B	103	A1ELD	C23-C22-C24	2.88	122.61	118.08
11	M	408	PGV	O03-C19-C20	2.88	120.94	111.91
8	K	102	A1EL2	C27-C26-C28	2.87	122.61	118.08
7	e	102	BCL	O2A-CGA-CBA	2.87	120.92	111.91
8	P	102	A1EL2	C11-C12-C13	-2.87	114.53	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	103	PGV	O03-C19-C20	2.87	120.91	111.91
7	d	102	BCL	CHC-C1C-NC	2.87	128.48	124.51
7	n	101	BCL	C3D-C4D-ND	2.87	114.88	110.24
7	c	101	BCL	O2A-CGA-O1A	-2.87	116.36	123.59
7	D	101	BCL	CHB-C4A-NA	2.86	128.47	124.51
9	b	101	A1ELD	C15-C16-C18	2.86	123.33	118.94
7	j	102	BCL	O2D-CGD-O1D	-2.86	118.24	123.84
8	O	103	A1EL2	C37-C35-C36	-2.86	103.00	107.81
7	f	102	BCL	C3D-C4D-ND	2.86	114.86	110.24
7	i	101	BCL	CMB-C2B-C3B	2.85	133.64	125.93
9	e	101	A1ELD	C11-C10-C13	-2.85	118.92	122.92
9	C	102	A1ELD	C24-C22-C21	2.85	123.32	118.94
7	f	102	BCL	O2A-CGA-O1A	-2.85	116.40	123.59
8	E	102	A1EL2	C22-C21-C20	-2.85	118.93	122.92
9	o	101	A1ELD	C23-C22-C24	-2.85	113.59	118.08
8	B	102	A1EL2	C22-C21-C20	-2.85	118.93	122.92
8	D	102	A1EL2	C22-C21-C20	-2.85	118.93	122.92
11	T	301	PGV	C02-O01-C1	2.85	121.54	117.88
7	I	101	BCL	CHB-C4A-NA	2.84	128.45	124.51
7	I	101	BCL	CHB-C1B-NB	-2.84	121.25	124.26
7	s	101	BCL	C3D-C4D-ND	2.84	114.83	110.24
7	L	301	BCL	C3D-C4D-ND	2.84	114.83	110.24
8	J	102	A1EL2	C19-C20-C21	2.84	131.36	127.31
7	q	102	BCL	C4-C3-C5	2.84	120.04	115.27
7	a	101	BCL	O2A-CGA-CBA	2.84	120.81	111.91
7	n	101	BCL	C4B-C3B-C2B	-2.84	103.80	108.36
7	r	104	BCL	C4B-C3B-C2B	-2.84	103.80	108.36
7	r	104	BCL	C4-C3-C5	2.84	120.04	115.27
7	J	101	BCL	C4B-C3B-C2B	-2.83	103.80	108.36
9	J	103	A1ELD	C19-C20-C21	2.83	129.27	123.47
7	G	101	BCL	CHB-C1B-NB	-2.83	121.26	124.26
8	K	102	A1EL2	C40-C12-C11	2.83	122.53	118.08
7	b	102	BCL	C4B-C3B-C2B	-2.83	103.81	108.36
7	n	101	BCL	O2A-CGA-O1A	-2.82	116.47	123.59
7	B	101	BCL	CHC-C1C-NC	2.82	128.41	124.51
8	A	102	A1EL2	C22-C21-C20	-2.82	118.97	122.92
7	n	101	BCL	C1C-NC-C4C	-2.82	105.44	106.71
8	F	102	A1EL2	C22-C21-C20	-2.81	118.98	122.92
16	M	405	H4X	C13-C12-C14	-2.81	118.99	122.92
7	e	102	BCL	O2D-CGD-O1D	-2.81	118.34	123.84
7	j	102	BCL	CHC-C1C-NC	2.81	128.40	124.51
8	O	103	A1EL2	C22-C21-C20	-2.81	118.99	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	102	A1EL2	C40-C12-C11	2.81	122.50	118.08
7	c	101	BCL	CHB-C1B-C2B	-2.80	119.32	127.24
7	b	102	BCL	CHB-C4A-NA	2.80	128.39	124.51
8	O	103	A1EL2	C39-C16-C17	-2.80	119.00	122.92
7	F	101	BCL	CMB-C2B-C3B	2.80	133.49	125.93
7	Q	101	BCL	C4-C3-C5	2.79	119.97	115.27
7	g	102	BCL	C4B-C3B-C2B	-2.79	103.87	108.36
7	n	101	BCL	CHC-C1C-NC	2.79	128.37	124.51
7	L	301	BCL	C1D-CHD-C4C	-2.79	119.90	126.62
7	d	102	BCL	C4-C3-C5	2.79	119.96	115.27
7	K	101	BCL	CMB-C2B-C3B	2.79	133.45	125.93
7	o	102	BCL	CMB-C2B-C3B	2.79	133.45	125.93
7	q	102	BCL	CHB-C4A-NA	2.79	128.36	124.51
9	d	101	A1ELD	C15-C16-C18	2.79	123.22	118.94
7	q	102	BCL	C4A-NA-C1A	2.78	107.96	106.71
7	S	101	BCL	CHB-C1B-NB	-2.78	121.32	124.26
7	b	102	BCL	CHB-C1B-NB	-2.78	121.32	124.26
9	O	102	A1ELD	C45-C2-C3	2.77	114.80	110.30
11	T	303	PGV	O03-C19-C20	2.77	120.61	111.91
7	a	101	BCL	CMB-C2B-C3B	2.77	133.41	125.93
7	k	101	BCL	O2A-CGA-CBA	2.77	120.60	111.91
9	g	101	A1ELD	C33-C32-C31	-2.77	119.04	122.92
7	J	101	BCL	CMB-C2B-C3B	2.77	133.40	125.93
8	r	102	A1EL2	C23-C21-C20	2.76	123.18	118.94
8	O	103	A1EL2	C40-C12-C13	-2.76	119.06	122.92
9	C	102	A1ELD	C34-C32-C31	2.76	123.17	118.94
9	r	101	A1ELD	C33-C32-C31	-2.76	119.06	122.92
7	f	102	BCL	C1-O2A-CGA	2.75	123.65	116.44
9	r	101	A1ELD	C15-C16-C18	2.74	123.15	118.94
7	K	101	BCL	C1C-NC-C4C	-2.74	105.47	106.71
9	R	103	A1ELD	C15-C16-C18	2.74	123.14	118.94
11	T	301	PGV	O03-C19-C20	2.74	120.50	111.91
7	j	102	BCL	CHB-C4A-NA	2.74	128.30	124.51
7	q	102	BCL	CHC-C1C-NC	2.73	128.29	124.51
9	R	103	A1ELD	C33-C32-C31	-2.73	119.09	122.92
7	k	101	BCL	CHB-C4A-NA	2.73	128.29	124.51
8	J	102	A1EL2	O3-C33-C32	-2.73	103.46	109.53
9	R	102	A1ELD	C31-C30-C29	2.73	131.74	123.22
7	p	101	BCL	C4B-C3B-C2B	-2.73	103.97	108.36
7	L	302	BCL	CHC-C1C-NC	2.73	128.28	124.51
7	r	104	BCL	CHC-C1C-NC	2.73	128.28	124.51
7	S	101	BCL	CMB-C2B-C3B	2.73	133.29	125.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	103	A1ELD	C20-C19-C18	2.73	129.06	123.47
9	b	101	A1ELD	C34-C32-C31	2.72	123.12	118.94
9	r	101	A1ELD	C24-C22-C21	2.72	123.12	118.94
7	N	101	BCL	CED-O2D-CGD	2.72	122.10	115.94
7	q	102	BCL	C4B-C3B-C2B	-2.72	103.98	108.36
7	S	101	BCL	CHB-C4A-NA	2.72	128.27	124.51
7	s	101	BCL	CHB-C4A-NA	2.71	128.26	124.51
7	O	101	BCL	O2A-CGA-CBA	2.71	120.41	111.91
7	g	102	BCL	O2A-CGA-CBA	2.71	120.41	111.91
7	O	101	BCL	C4B-C3B-C2B	-2.71	104.00	108.36
7	M	401	BCL	CHB-C1B-C2B	-2.71	119.59	127.24
13	L	303	BPH	C4-C3-C5	2.71	119.82	115.27
8	r	102	A1EL2	C35-C30-C31	-2.70	118.52	122.54
8	D	102	A1EL2	C15-C16-C17	2.70	123.09	118.94
7	A	101	BCL	CHC-C1C-NC	2.70	128.24	124.51
7	A	101	BCL	CED-O2D-CGD	2.69	122.02	115.94
9	J	103	A1ELD	C15-C16-C18	2.69	123.07	118.94
7	k	101	BCL	C4B-C3B-C2B	-2.69	104.03	108.36
9	C	102	A1ELD	C15-C16-C18	2.69	123.07	118.94
9	R	103	A1ELD	C9-C10-C13	2.69	123.06	118.94
7	i	101	BCL	CHB-C4A-NA	2.69	128.23	124.51
7	S	101	BCL	C1-C2-C3	-2.68	121.40	126.04
8	C	103	A1EL2	C15-C16-C17	2.68	123.06	118.94
7	A	101	BCL	C1-C2-C3	-2.68	121.41	126.04
7	s	101	BCL	CHC-C1C-NC	2.68	128.22	124.51
8	B	102	A1EL2	C15-C16-C17	2.68	123.05	118.94
7	B	101	BCL	CAA-C2A-C3A	-2.68	105.45	112.78
7	N	101	BCL	CAA-C2A-C3A	-2.68	105.45	112.78
7	F	101	BCL	C1-O2A-CGA	2.68	123.46	116.44
7	d	102	BCL	C4B-C3B-C2B	-2.67	104.06	108.36
7	I	101	BCL	CMB-C2B-C3B	2.67	133.14	125.93
9	g	101	A1ELD	C15-C16-C18	2.67	123.03	118.94
11	F	103	PGV	O03-C19-C20	2.67	120.28	111.91
8	A	102	A1EL2	C15-C16-C17	2.67	123.03	118.94
8	J	102	A1EL2	C37-C35-C36	2.67	112.30	107.81
7	P	101	BCL	C4A-NA-C1A	2.67	107.91	106.71
7	o	102	BCL	CHB-C1B-NB	-2.66	121.44	124.26
8	E	102	A1EL2	C15-C16-C17	2.66	123.03	118.94
9	b	101	A1ELD	C24-C22-C21	2.66	123.03	118.94
7	s	101	BCL	O2A-CGA-CBA	2.66	120.27	111.91
7	r	104	BCL	O2D-CGD-O1D	-2.66	118.64	123.84
9	q	101	A1ELD	C15-C16-C18	2.66	123.02	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	q	102	BCL	O2D-CGD-O1D	-2.66	118.64	123.84
7	M	401	BCL	C1-C2-C3	-2.66	121.45	126.04
9	j	101	A1ELD	C20-C19-C18	2.65	128.91	123.47
7	o	102	BCL	CHB-C4A-NA	2.65	128.18	124.51
7	L	301	BCL	O2A-CGA-O1A	-2.65	116.91	123.59
7	j	102	BCL	C1-C2-C3	-2.65	121.47	126.04
7	P	101	BCL	O2A-CGA-CBA	2.65	120.21	111.91
11	D	103	PGV	O03-C19-C20	2.64	120.21	111.91
8	P	102	A1EL2	C34-C35-C30	2.64	115.20	110.48
7	o	102	BCL	C1-C2-C3	-2.64	121.48	126.04
7	i	101	BCL	C4-C3-C5	2.64	119.71	115.27
7	a	101	BCL	CHC-C1C-NC	2.64	128.16	124.51
8	P	102	A1EL2	C18-C17-C16	-2.63	123.55	127.31
7	e	102	BCL	C1C-NC-C4C	-2.63	105.52	106.71
7	R	101	BCL	C4B-C3B-C2B	-2.63	104.12	108.36
9	o	101	A1ELD	C11-C10-C13	2.63	126.61	122.92
8	F	102	A1EL2	C15-C16-C17	2.63	122.98	118.94
7	n	101	BCL	CHB-C4A-NA	2.63	128.15	124.51
8	J	102	A1EL2	C4-C3-C2	-2.63	118.91	122.61
8	G	102	A1EL2	C39-C16-C17	-2.63	119.24	122.92
7	M	401	BCL	C1D-CHD-C4C	-2.63	120.29	126.62
9	f	101	A1ELD	C34-C32-C31	2.63	122.97	118.94
16	M	405	H4X	C24-C23-C22	-2.62	119.25	122.92
7	A	101	BCL	C1D-CHD-C4C	-2.62	120.29	126.62
7	e	102	BCL	CHC-C1C-NC	2.62	128.14	124.51
9	R	102	A1ELD	C9-C8-C3	2.62	134.57	127.20
8	P	102	A1EL2	O2-C34-C35	-2.62	103.77	108.95
8	K	102	A1EL2	C40-C12-C13	-2.62	119.25	122.92
7	L	302	BCL	C4B-C3B-C2B	-2.62	104.14	108.36
7	Q	101	BCL	CED-O2D-CGD	2.62	121.86	115.94
8	N	102	A1EL2	C15-C16-C17	2.61	122.95	118.94
7	p	101	BCL	O2D-CGD-O1D	-2.61	118.73	123.84
7	f	102	BCL	C4A-NA-C1A	2.61	107.88	106.71
7	E	101	BCL	CHB-C4A-NA	2.61	128.12	124.51
7	E	101	BCL	C1C-NC-C4C	-2.61	105.53	106.71
7	k	101	BCL	CMB-C2B-C3B	2.60	132.96	125.93
9	g	101	A1ELD	C34-C32-C31	2.60	122.93	118.94
8	G	102	A1EL2	C15-C16-C17	2.60	122.93	118.94
7	a	101	BCL	C1C-NC-C4C	-2.60	105.54	106.71
7	N	101	BCL	O2A-CGA-CBA	2.60	120.06	111.91
7	L	302	BCL	C4-C3-C5	2.60	119.64	115.27
7	j	102	BCL	C4B-C3B-C2B	-2.60	104.18	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	102	A1ELD	C8-C3-C4	-2.60	115.17	121.46
9	d	101	A1ELD	C24-C22-C21	2.59	122.92	118.94
9	f	101	A1ELD	C15-C16-C18	2.59	122.92	118.94
7	q	102	BCL	O2A-CGA-CBA	2.59	120.05	111.91
7	C	101	BCL	CED-O2D-CGD	2.59	121.79	115.94
7	A	101	BCL	CMB-C2B-C3B	2.59	132.92	125.93
7	i	101	BCL	CHC-C1C-NC	2.58	128.08	124.51
7	S	101	BCL	C1D-CHD-C4C	-2.58	120.40	126.62
7	D	101	BCL	CHB-C1B-NB	-2.58	121.53	124.26
7	S	101	BCL	O2A-CGA-CBA	2.58	119.99	111.91
8	J	102	A1EL2	C18-C19-C20	2.58	128.75	123.47
7	j	102	BCL	O2A-CGA-CBA	2.57	119.98	111.91
9	q	101	A1ELD	C24-C22-C21	2.57	122.89	118.94
7	f	102	BCL	CHB-C4A-NA	2.57	128.06	124.51
8	r	103	A1EL2	C29-C30-C31	-2.57	115.24	121.46
7	r	104	BCL	O2A-CGA-CBA	2.57	119.96	111.91
7	f	102	BCL	CHC-C1C-NC	2.57	128.06	124.51
7	I	101	BCL	C1C-NC-C4C	-2.56	105.56	106.71
7	o	102	BCL	CHC-C1C-NC	2.56	128.05	124.51
7	k	101	BCL	CHC-C1C-NC	2.55	128.04	124.51
7	g	102	BCL	CHC-C1C-NC	2.55	128.04	124.51
9	O	102	A1ELD	C20-C19-C18	2.54	128.69	123.47
9	B	103	A1ELD	C43-C4-C5	2.54	119.05	114.36
8	I	102	A1EL2	C5-C6-C7	-2.53	106.84	110.30
8	N	102	A1EL2	C18-C19-C20	2.53	128.65	123.47
7	a	101	BCL	CHB-C1B-NB	-2.53	121.58	124.26
9	A	103	A1ELD	C15-C16-C18	2.52	122.81	118.94
8	r	102	A1EL2	C19-C20-C21	2.52	130.91	127.31
8	I	102	A1EL2	O1-C6-C5	2.52	114.81	109.80
7	p	101	BCL	CHC-C1C-NC	2.52	127.99	124.51
8	J	102	A1EL2	C24-C23-C21	2.52	133.48	126.42
7	D	101	BCL	C1-C2-C3	-2.52	121.69	126.04
7	B	101	BCL	CED-O2D-CGD	2.51	121.62	115.94
8	I	102	A1EL2	C35-C30-C29	2.51	122.92	115.81
7	a	101	BCL	O2D-CGD-O1D	-2.51	118.93	123.84
13	L	303	BPH	C3B-C4B-NB	2.51	111.79	108.04
7	M	403	BCL	OBB-CAB-C3B	2.51	125.05	120.41
7	p	101	BCL	C4-C3-C5	2.51	119.49	115.27
8	J	102	A1EL2	C28-C29-C30	2.51	134.24	127.20
8	I	102	A1EL2	C24-C23-C21	2.50	133.44	126.42
7	J	101	BCL	O2A-CGA-CBA	2.50	119.75	111.91
7	g	102	BCL	C1D-CHD-C4C	-2.50	120.59	126.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	101	BCL	C1D-CHD-C4C	-2.50	120.59	126.62
7	M	401	BCL	C1-O2A-CGA	2.50	123.00	116.44
8	P	102	A1EL2	C14-C13-C12	-2.50	123.75	127.31
7	n	101	BCL	C1D-CHD-C4C	-2.49	120.61	126.62
11	T	301	PGV	O01-C02-C01	2.49	111.90	106.13
9	A	103	A1ELD	C11-C10-C9	2.49	122.00	118.08
8	r	103	A1EL2	C22-C21-C23	2.48	121.98	118.08
7	k	101	BCL	O2D-CGD-O1D	-2.48	119.00	123.84
7	s	101	BCL	CHB-C1B-C2B	-2.47	120.25	127.24
11	L	308	PGV	C02-O01-C1	-2.47	111.71	117.79
7	e	102	BCL	CHB-C4A-NA	2.47	127.92	124.51
9	R	102	A1ELD	C33-C32-C34	2.47	121.96	118.08
8	P	102	A1EL2	C35-C30-C29	2.47	122.79	115.81
7	S	101	BCL	C4-C3-C5	2.47	119.42	115.27
7	K	101	BCL	C1D-CHD-C4C	-2.46	120.68	126.62
7	N	101	BCL	C1-O2A-CGA	2.46	122.91	116.44
7	s	101	BCL	C4-C3-C5	2.46	119.41	115.27
7	D	101	BCL	O2A-CGA-CBA	2.46	119.61	111.91
7	e	102	BCL	C1D-CHD-C4C	-2.45	120.72	126.62
7	i	101	BCL	O2D-CGD-O1D	-2.45	119.05	123.84
7	g	102	BCL	CHB-C4A-NA	2.45	127.89	124.51
8	r	103	A1EL2	O2-C34-C35	-2.45	104.12	108.95
7	o	102	BCL	O2D-CGD-O1D	-2.44	119.06	123.84
9	B	103	A1ELD	C33-C32-C34	2.44	121.93	118.08
7	g	102	BCL	O2D-CGD-O1D	-2.44	119.07	123.84
7	N	101	BCL	C1D-CHD-C4C	-2.44	120.74	126.62
7	C	101	BCL	C1D-CHD-C4C	-2.44	120.74	126.62
9	C	102	A1ELD	C8-C9-C10	2.44	129.92	126.23
7	M	401	BCL	CMD-C2D-C3D	-2.44	122.01	127.61
7	o	102	BCL	C1C-NC-C4C	-2.43	105.61	106.71
8	Q	102	A1EL2	C18-C19-C20	2.43	128.46	123.47
7	i	101	BCL	C1D-CHD-C4C	-2.43	120.75	126.62
7	K	101	BCL	O2A-CGA-O1A	-2.43	117.45	123.59
7	A	101	BCL	C4-C3-C5	2.43	119.36	115.27
9	A	103	A1ELD	C34-C32-C31	2.43	122.67	118.94
7	a	101	BCL	CHB-C4A-NA	2.43	127.87	124.51
7	b	102	BCL	O2D-CGD-O1D	-2.43	119.09	123.84
8	G	102	A1EL2	C34-C35-C30	2.42	114.81	110.48
7	L	301	BCL	C1C-NC-C4C	-2.42	105.62	106.71
9	e	101	A1ELD	C17-C16-C18	-2.42	119.54	122.92
7	A	101	BCL	CAA-C2A-C3A	-2.42	106.16	112.78
8	P	102	A1EL2	C10-C11-C12	-2.42	122.58	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	102	BCL	CHB-C1B-NB	-2.42	121.70	124.26
8	O	103	A1EL2	C24-C25-C26	2.41	130.76	127.31
12	N	103	LMT	C1'-O5'-C5'	-2.41	108.95	113.69
8	r	103	A1EL2	C34-C35-C30	2.41	114.79	110.48
7	G	101	BCL	O2A-CGA-CBA	2.41	119.48	111.91
7	B	101	BCL	CMB-C2B-C3B	2.41	132.44	125.93
8	N	102	A1EL2	C23-C21-C20	2.41	122.64	118.94
7	q	102	BCL	CHB-C1B-C2B	-2.41	120.43	127.24
8	P	102	A1EL2	C11-C10-C3	-2.41	120.43	127.20
7	j	102	BCL	CHB-C1B-C2B	-2.41	120.44	127.24
7	L	301	BCL	CHB-C1B-C2B	-2.41	120.44	127.24
9	r	101	A1ELD	C35-C34-C32	2.41	129.53	125.89
7	b	102	BCL	CHC-C1C-NC	2.40	127.83	124.51
9	A	103	A1ELD	C24-C22-C21	2.40	122.62	118.94
7	I	101	BCL	C4-C3-C5	2.40	119.31	115.27
7	i	101	BCL	O2A-CGA-CBA	2.40	119.44	111.91
7	d	102	BCL	CHB-C1B-C2B	-2.40	120.46	127.24
7	r	104	BCL	CHB-C1B-C2B	-2.40	120.47	127.24
9	B	103	A1ELD	C17-C16-C15	2.39	121.85	118.08
7	O	101	BCL	CMB-C2B-C3B	2.39	132.39	125.93
7	C	101	BCL	CHB-C1B-C2B	-2.39	120.48	127.24
7	M	401	BCL	CAB-C3B-C2B	-2.39	124.76	128.34
7	p	101	BCL	CHB-C4A-NA	2.39	127.81	124.51
9	R	102	A1ELD	C39-C37-C38	2.38	114.85	110.37
8	I	102	A1EL2	C18-C17-C16	2.38	130.70	127.31
7	b	102	BCL	C4-C3-C2	-2.38	117.58	123.68
7	A	101	BCL	C11-C10-C8	-2.38	108.24	115.92
11	G	103	PGV	O14-P-O13	2.37	119.97	110.68
7	E	101	BCL	C1D-CHD-C4C	-2.37	120.90	126.62
9	d	101	A1ELD	C34-C32-C31	2.37	122.58	118.94
7	d	102	BCL	O2A-CGA-CBA	2.37	119.34	111.91
12	G	104	LMT	C1'-O5'-C5'	-2.37	109.04	113.69
8	r	102	A1EL2	C4-C3-C2	-2.37	119.28	122.61
7	E	101	BCL	CMB-C2B-C3B	2.37	132.32	125.93
7	C	101	BCL	C1-C2-C3	-2.36	121.95	126.04
7	i	101	BCL	C1-C2-C3	-2.36	121.95	126.04
7	d	102	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
7	Q	101	BCL	C1C-NC-C4C	-2.36	105.64	106.71
7	o	102	BCL	O2A-CGA-CBA	2.36	119.32	111.91
16	M	405	H4X	C21-C22-C23	2.36	130.68	127.31
7	R	101	BCL	C1D-CHD-C4C	-2.36	120.93	126.62
7	b	102	BCL	O2A-CGA-O1A	-2.36	117.64	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	102	A1EL2	C35-C30-C29	2.35	122.47	115.81
8	r	103	A1EL2	C39-C16-C17	-2.35	119.63	122.92
7	n	101	BCL	O2D-CGD-O1D	-2.35	119.24	123.84
8	P	102	A1EL2	C28-C26-C25	-2.35	115.33	118.94
11	L	307	PGV	O14-P-O13	2.35	119.89	110.68
11	T	303	PGV	O14-P-O13	2.35	119.88	110.68
7	I	101	BCL	C1-O2A-CGA	2.35	122.61	116.44
8	r	103	A1EL2	C9-C4-C3	2.35	114.11	110.30
7	F	101	BCL	CHC-C1C-NC	2.35	127.76	124.51
7	p	101	BCL	CHB-C1B-C2B	-2.34	120.61	127.24
8	Q	102	A1EL2	C33-C32-C31	-2.34	107.69	112.97
7	r	104	BCL	CHB-C4A-NA	2.34	127.75	124.51
7	b	102	BCL	C1D-CHD-C4C	-2.34	120.97	126.62
7	C	101	BCL	C4-C3-C5	2.34	119.21	115.27
7	r	104	BCL	C1D-CHD-C4C	-2.34	120.98	126.62
9	B	103	A1ELD	C8-C3-C4	-2.34	115.80	121.46
11	L	307	PGV	C02-O01-C1	-2.34	112.04	117.79
8	P	102	A1EL2	C1-C2-C7	-2.34	110.03	114.36
9	B	103	A1ELD	C2-C3-C8	2.34	122.38	115.78
7	C	101	BCL	CHB-C1B-NB	-2.33	121.79	124.26
7	L	301	BCL	CHB-C4A-NA	2.33	127.74	124.51
7	k	101	BCL	CHB-C1B-NB	-2.33	121.79	124.26
7	K	101	BCL	CED-O2D-CGD	2.33	121.20	115.94
8	r	103	A1EL2	C10-C11-C12	-2.33	122.72	126.23
7	b	102	BCL	C1-O2A-CGA	2.33	122.55	116.44
8	r	102	A1EL2	C40-C12-C11	2.32	121.74	118.08
7	P	101	BCL	CED-O2D-CGD	2.32	121.19	115.94
8	Q	102	A1EL2	C23-C21-C20	2.32	122.50	118.94
7	G	101	BCL	C1D-CHD-C4C	-2.32	121.03	126.62
13	L	303	BPH	O2A-CGA-CBA	2.32	119.18	111.91
7	p	101	BCL	C4A-NA-C1A	2.31	107.74	106.71
7	G	101	BCL	CED-O2D-CGD	2.31	121.16	115.94
7	f	102	BCL	C1D-CHD-C4C	-2.31	121.05	126.62
7	o	102	BCL	C1D-CHD-C4C	-2.31	121.05	126.62
8	G	102	A1EL2	C8-C4-C3	-2.31	106.56	110.30
7	Q	101	BCL	C1-O2A-CGA	2.31	122.50	116.44
7	P	101	BCL	C1D-CHD-C4C	-2.30	121.06	126.62
8	J	102	A1EL2	O2-C34-C33	2.30	113.99	109.41
7	i	101	BCL	C1C-NC-C4C	-2.30	105.67	106.71
8	r	103	A1EL2	C19-C18-C17	2.30	128.18	123.47
9	B	103	A1ELD	C30-C31-C32	2.30	130.59	127.31
7	k	101	BCL	C1D-CHD-C4C	-2.30	121.08	126.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	101	BCL	C16-C15-C13	-2.30	108.50	115.92
7	Q	101	BCL	C1D-CHD-C4C	-2.29	121.09	126.62
7	g	102	BCL	CHB-C1B-C2B	-2.29	120.76	127.24
7	P	101	BCL	CHB-C1B-C2B	-2.29	120.76	127.24
7	k	101	BCL	C4A-NA-C1A	2.29	107.74	106.71
7	I	101	BCL	O2A-CGA-CBA	2.29	119.10	111.91
7	E	101	BCL	C4-C3-C5	2.29	119.12	115.27
7	M	401	BCL	CHB-C4A-NA	2.29	127.68	124.51
16	M	405	H4X	C30-C28-C27	2.29	122.45	118.94
7	f	102	BCL	CHB-C1B-NB	-2.29	121.84	124.26
7	L	301	BCL	CHC-C1C-NC	2.28	127.67	124.51
7	p	101	BCL	C1-C2-C3	-2.28	122.09	126.04
7	E	101	BCL	O2A-CGA-CBA	2.28	119.07	111.91
8	Q	102	A1EL2	C19-C20-C21	2.28	130.57	127.31
7	I	101	BCL	CED-O2D-CGD	2.28	121.10	115.94
7	e	102	BCL	C4-C3-C5	2.28	119.11	115.27
12	G	104	LMT	C3'-C4'-C5'	-2.28	105.69	110.93
9	g	101	A1ELD	C8-C9-C10	2.28	129.68	126.23
9	o	101	A1ELD	C45-C2-C44	2.28	115.52	108.53
9	O	102	A1ELD	C8-C9-C10	2.27	129.67	126.23
11	M	408	PGV	C02-O01-C1	-2.27	112.19	117.79
7	A	101	BCL	O2A-CGA-CBA	2.27	119.03	111.91
8	D	102	A1EL2	C40-C12-C11	2.27	121.65	118.08
8	E	102	A1EL2	C40-C12-C11	2.27	121.65	118.08
7	O	101	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
7	i	101	BCL	CHB-C1B-C2B	-2.27	120.83	127.24
8	C	103	A1EL2	C40-C12-C11	2.27	121.65	118.08
7	n	101	BCL	CHB-C1B-C2B	-2.26	120.84	127.24
7	M	403	BCL	C4B-C3B-C2B	-2.26	104.72	108.36
8	r	103	A1EL2	C14-C13-C12	-2.26	124.08	127.31
7	M	403	BCL	C4-C3-C5	2.26	119.08	115.27
7	a	101	BCL	C1D-CHD-C4C	-2.26	121.17	126.62
8	r	102	A1EL2	C18-C19-C20	2.26	128.11	123.47
7	q	102	BCL	C6-C5-C3	-2.26	107.53	113.45
8	r	103	A1EL2	C18-C17-C16	-2.26	124.08	127.31
8	B	102	A1EL2	C40-C12-C11	2.26	121.64	118.08
8	F	102	A1EL2	C40-C12-C11	2.26	121.64	118.08
9	q	101	A1ELD	C31-C30-C29	2.26	130.26	123.22
7	F	101	BCL	O2A-CGA-CBA	2.26	118.99	111.91
7	F	101	BCL	CHB-C1B-NB	-2.25	121.87	124.26
7	L	301	BCL	CHB-C1B-NB	-2.25	121.87	124.26
7	p	101	BCL	O2A-CGA-CBA	2.25	118.98	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	s	101	BCL	C1D-CHD-C4C	-2.25	121.19	126.62
7	M	403	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
7	E	101	BCL	CED-O2D-CGD	2.25	121.02	115.94
8	A	102	A1EL2	C40-C12-C11	2.25	121.62	118.08
7	F	101	BCL	CHB-C1B-C2B	-2.25	120.89	127.24
7	e	102	BCL	C4A-NA-C1A	2.25	107.72	106.71
9	o	101	A1ELD	C24-C22-C21	2.25	122.39	118.94
7	d	102	BCL	CHB-C1B-NB	-2.25	121.88	124.26
7	n	101	BCL	CBC-CAC-C3C	-2.25	108.47	113.47
9	e	101	A1ELD	C14-C13-C10	2.25	130.51	127.31
7	J	101	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
7	d	102	BCL	C1-C2-C3	-2.24	122.16	126.04
7	L	302	BCL	O2A-CGA-CBA	2.24	118.94	111.91
7	q	102	BCL	C1D-CHD-C4C	-2.24	121.22	126.62
9	f	101	A1ELD	C24-C22-C21	2.24	122.38	118.94
8	Q	102	A1EL2	C40-C12-C13	-2.24	119.79	122.92
9	j	101	A1ELD	C30-C31-C32	2.24	130.50	127.31
7	O	101	BCL	CED-O2D-CGD	2.24	120.99	115.94
7	f	102	BCL	CHB-C1B-C2B	-2.23	120.93	127.24
7	D	101	BCL	C1D-CHD-C4C	-2.23	121.23	126.62
11	M	408	PGV	O14-P-O13	2.23	119.41	110.68
13	L	303	BPH	C1-O2A-CGA	2.23	122.29	116.44
8	I	102	A1EL2	C4-C3-C2	-2.23	119.48	122.61
7	f	102	BCL	O2D-CGD-O1D	-2.22	119.49	123.84
8	O	103	A1EL2	C38-C31-C32	-2.22	110.23	114.36
7	B	101	BCL	C1D-CHD-C4C	-2.22	121.26	126.62
7	i	101	BCL	C6-C5-C3	-2.22	107.63	113.45
7	J	101	BCL	CHB-C1B-C2B	-2.22	120.97	127.24
7	N	101	BCL	CHB-C1B-C2B	-2.21	120.98	127.24
7	D	101	BCL	CHB-C1B-C2B	-2.21	120.99	127.24
9	o	101	A1ELD	C35-C34-C32	-2.21	122.55	125.89
7	S	101	BCL	CAA-CBA-CGA	-2.21	106.80	113.25
7	s	101	BCL	O2D-CGD-O1D	-2.21	119.52	123.84
7	B	101	BCL	O2A-CGA-CBA	2.21	118.83	111.91
19	T	302	LHG	C27-C26-C25	-2.21	103.23	114.42
9	J	103	A1ELD	C24-C22-C21	2.21	122.33	118.94
7	J	101	BCL	CMD-C2D-C3D	-2.20	122.55	127.61
16	M	405	H4X	C16-C17-C19	2.20	122.32	118.94
9	e	101	A1ELD	C20-C21-C22	2.20	130.45	127.31
7	G	101	BCL	CHB-C1B-C2B	-2.20	121.03	127.24
7	I	101	BCL	CAA-C2A-C3A	-2.20	106.76	112.78
7	F	101	BCL	CHB-C4A-NA	2.19	127.55	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	o	102	BCL	O2A-CGA-O1A	-2.19	118.06	123.59
7	j	102	BCL	C4A-NA-C1A	2.19	107.69	106.71
7	p	101	BCL	C1D-CHD-C4C	-2.19	121.35	126.62
7	q	102	BCL	C1-C2-C3	-2.18	122.27	126.04
9	R	103	A1ELD	C30-C31-C32	2.18	130.42	127.31
7	b	102	BCL	C4D-CHA-C1A	-2.18	118.59	121.25
7	g	102	BCL	CHB-C1B-NB	-2.18	121.95	124.26
11	L	308	PGV	O03-C19-O04	-2.18	118.09	123.59
7	N	101	BCL	O2A-CGA-O1A	-2.18	118.09	123.59
7	D	101	BCL	CMD-C2D-C3D	-2.18	122.60	127.61
7	R	101	BCL	CMB-C2B-C3B	2.18	131.81	125.93
9	f	101	A1ELD	C11-C10-C9	2.17	121.50	118.08
7	d	102	BCL	C1D-CHD-C4C	-2.17	121.38	126.62
8	I	102	A1EL2	C14-C15-C16	2.17	132.51	126.42
9	J	103	A1ELD	C7-C6-C5	-2.17	107.33	110.30
7	e	102	BCL	CHB-C1B-C2B	-2.17	121.11	127.24
8	r	103	A1EL2	C11-C10-C3	-2.17	121.12	127.20
7	g	102	BCL	C1-C2-C3	-2.17	122.30	126.04
7	S	101	BCL	O2D-CGD-O1D	-2.17	119.61	123.84
9	b	101	A1ELD	C11-C10-C9	2.16	121.48	118.08
7	M	401	BCL	CHC-C1C-NC	2.16	127.50	124.51
7	e	102	BCL	O2A-CGA-O1A	-2.15	118.15	123.59
13	L	305	BPH	C1A-C2A-C3A	-2.15	100.79	102.84
9	j	101	A1ELD	C23-C22-C24	2.15	121.47	118.08
7	P	101	BCL	O2D-CGD-O1D	-2.15	119.63	123.84
11	T	303	PGV	C02-O01-C1	-2.15	112.50	117.79
9	r	101	A1ELD	C6-C5-C4	-2.15	107.57	111.85
7	f	102	BCL	C1C-NC-C4C	-2.15	105.74	106.71
7	B	101	BCL	CHC-C4B-C3B	-2.14	124.72	132.35
13	L	303	BPH	CMA-C3A-C4A	-2.14	109.68	114.38
7	j	102	BCL	CHB-C1B-NB	-2.14	121.99	124.26
16	M	405	H4X	C11-C12-C14	2.14	122.22	118.94
9	e	101	A1ELD	C8-C9-C10	2.13	129.46	126.23
7	F	101	BCL	O2D-CGD-O1D	-2.13	119.67	123.84
7	F	101	BCL	C4B-C3B-C2B	-2.13	104.93	108.36
7	K	101	BCL	CHC-C4B-C3B	-2.13	124.78	132.35
8	O	103	A1EL2	C33-C32-C31	-2.13	108.18	112.97
9	e	101	A1ELD	C23-C22-C21	-2.13	119.94	122.92
7	c	101	BCL	C1D-CHD-C4C	-2.13	121.49	126.62
7	k	101	BCL	CHB-C1B-C2B	-2.12	121.24	127.24
7	G	101	BCL	C1C-NC-C4C	-2.12	105.75	106.71
7	F	101	BCL	CAA-C2A-C3A	-2.12	106.97	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	n	101	BCL	CHB-C1B-NB	-2.12	122.01	124.26
7	g	102	BCL	C4-C3-C5	2.12	118.83	115.27
7	f	102	BCL	O2A-C1-C2	-2.12	103.08	108.64
7	D	101	BCL	CAA-CBA-CGA	-2.11	107.08	113.25
7	D	101	BCL	O2D-CGD-O1D	-2.11	119.71	123.84
7	R	101	BCL	C4-C3-C2	-2.11	118.26	123.68
7	q	102	BCL	CHB-C1B-NB	-2.11	122.02	124.26
7	E	101	BCL	C11-C10-C8	-2.11	109.10	115.92
7	Q	101	BCL	CHC-C4B-C3B	-2.11	124.85	132.35
8	G	102	A1EL2	C40-C12-C11	2.11	121.40	118.08
9	o	101	A1ELD	C9-C8-C3	-2.11	121.28	127.20
8	I	102	A1EL2	C39-C16-C15	2.11	121.40	118.08
7	N	101	BCL	C1C-NC-C4C	-2.11	105.76	106.71
7	Q	101	BCL	C16-C15-C13	-2.11	109.11	115.92
8	D	102	A1EL2	C23-C21-C20	2.10	122.16	118.94
7	g	102	BCL	CBA-CAA-C2A	-2.10	107.67	113.86
8	O	103	A1EL2	C9-C4-C3	-2.10	106.90	110.30
7	e	102	BCL	C1-O2A-CGA	2.10	121.94	116.44
7	F	101	BCL	C3B-C2B-C1B	-2.09	99.64	106.39
7	s	101	BCL	CBC-CAC-C3C	-2.09	108.81	113.47
7	K	101	BCL	CBC-CAC-C3C	-2.09	108.81	113.47
8	K	102	A1EL2	C34-C35-C30	2.09	114.21	110.48
8	C	103	A1EL2	C23-C21-C20	2.09	122.15	118.94
7	O	101	BCL	CHB-C1B-C2B	-2.09	121.34	127.24
7	o	102	BCL	CHB-C1B-C2B	-2.09	121.34	127.24
8	C	103	A1EL2	C28-C26-C25	2.09	122.14	118.94
8	F	102	A1EL2	C28-C26-C25	2.09	122.14	118.94
9	b	101	A1ELD	C8-C9-C10	2.09	129.39	126.23
7	a	101	BCL	CHC-C4B-C3B	-2.08	124.94	132.35
7	J	101	BCL	C4-C3-C5	2.08	118.77	115.27
7	o	102	BCL	C1-O2A-CGA	2.08	121.90	116.44
9	B	103	A1ELD	C20-C19-C18	2.08	127.73	123.47
11	F	103	PGV	O01-C1-O02	-2.08	118.68	123.70
7	k	101	BCL	C4-C3-C5	2.07	118.76	115.27
8	A	102	A1EL2	C28-C26-C25	2.07	122.12	118.94
16	M	405	H4X	C20-C19-C17	2.07	130.27	127.31
9	f	101	A1ELD	C8-C9-C10	2.07	129.36	126.23
7	C	101	BCL	CAC-C3C-C4C	-2.07	107.99	112.58
8	E	102	A1EL2	C23-C21-C20	2.07	122.11	118.94
7	p	101	BCL	CHB-C1B-NB	-2.07	122.07	124.26
7	b	102	BCL	C4A-NA-C1A	2.07	107.64	106.71
7	D	101	BCL	C1-O2A-CGA	2.07	121.86	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	102	A1EL2	C7-C2-C3	2.07	125.45	120.85
7	C	101	BCL	CAA-C2A-C3A	-2.06	107.12	112.78
7	I	101	BCL	CHB-C1B-C2B	-2.06	121.41	127.24
7	j	102	BCL	C1D-CHD-C4C	-2.06	121.64	126.62
8	P	102	A1EL2	C4-C5-C6	-2.06	108.98	113.64
8	E	102	A1EL2	C28-C26-C25	2.06	122.10	118.94
7	i	101	BCL	CHB-C1B-NB	-2.06	122.08	124.26
14	L	304	UQ8	C7-C6-C5	2.06	120.96	118.48
7	D	101	BCL	C11-C10-C8	-2.06	109.26	115.92
9	j	101	A1ELD	C19-C20-C21	2.06	127.69	123.47
8	P	102	A1EL2	C23-C21-C20	-2.06	115.79	118.94
8	D	102	A1EL2	C28-C26-C25	2.06	122.09	118.94
8	N	102	A1EL2	C40-C12-C11	2.05	121.31	118.08
7	b	102	BCL	CHC-C4B-C3B	-2.05	125.04	132.35
7	c	101	BCL	C4-C3-C5	2.05	118.73	115.27
7	L	302	BCL	C1-O2A-CGA	2.05	121.82	116.44
8	r	103	A1EL2	C11-C12-C13	-2.05	115.80	118.94
7	P	101	BCL	CMD-C2D-C3D	-2.05	122.90	127.61
7	D	101	BCL	CAA-C2A-C3A	-2.05	107.17	112.78
7	E	101	BCL	CMD-C2D-C3D	-2.05	122.91	127.61
7	b	102	BCL	CHB-C1B-C2B	-2.04	121.47	127.24
7	k	101	BCL	CBC-CAC-C3C	-2.04	108.92	113.47
8	N	102	A1EL2	C28-C26-C25	2.04	122.08	118.94
8	K	102	A1EL2	C35-C30-C29	2.04	121.59	115.81
13	L	303	BPH	C1-C2-C3	-2.04	122.51	126.04
9	j	101	A1ELD	C37-C36-C35	2.04	118.46	113.06
8	F	102	A1EL2	C23-C21-C20	2.04	122.07	118.94
8	I	102	A1EL2	C7-C2-C3	2.04	125.39	120.85
7	E	101	BCL	C4-C3-C2	-2.03	118.46	123.68
8	B	102	A1EL2	C28-C26-C25	2.03	122.06	118.94
7	L	302	BCL	C1-C2-C3	-2.03	122.53	126.04
11	D	103	PGV	O01-C1-O02	-2.03	118.79	123.70
7	S	101	BCL	CED-O2D-CGD	2.03	120.53	115.94
8	A	102	A1EL2	C23-C21-C20	2.03	122.05	118.94
8	B	102	A1EL2	C23-C21-C20	2.03	122.05	118.94
7	L	302	BCL	CHB-C1B-C2B	-2.03	121.52	127.24
8	P	102	A1EL2	C8-C4-C3	-2.03	107.01	110.30
7	L	302	BCL	CMB-C2B-C3B	2.02	131.40	125.93
9	r	101	A1ELD	C30-C31-C32	2.02	130.19	127.31
7	a	101	BCL	CHB-C1B-C2B	-2.02	121.53	127.24
7	q	102	BCL	C11-C12-C13	-2.02	109.39	115.92
7	C	101	BCL	CBA-CAA-C2A	-2.02	107.90	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	102	BCL	CHC-C4B-C3B	-2.02	125.16	132.35
8	P	102	A1EL2	C19-C20-C21	-2.02	124.43	127.31
7	g	102	BCL	C1C-NC-C4C	-2.02	105.80	106.71
7	R	101	BCL	CHC-C4B-C3B	-2.02	125.17	132.35
7	D	101	BCL	CED-O2D-CGD	2.02	120.50	115.94
8	J	102	A1EL2	C33-C32-C31	2.02	117.51	112.97
7	s	101	BCL	C4A-NA-C1A	2.02	107.61	106.71
9	r	101	A1ELD	C2-C3-C4	-2.01	119.78	122.61
8	B	102	A1EL2	C34-C35-C30	2.01	114.07	110.48
9	O	102	A1ELD	C19-C20-C21	2.01	127.59	123.47
7	R	101	BCL	O2A-CGA-CBA	2.01	118.22	111.91
8	D	102	A1EL2	C34-C35-C30	2.01	114.07	110.48
8	P	102	A1EL2	C27-C26-C25	-2.01	120.11	122.92
7	n	101	BCL	C11-C10-C8	-2.01	109.43	115.92
8	F	102	A1EL2	C34-C35-C30	2.01	114.06	110.48
7	F	101	BCL	CED-O2D-CGD	2.01	120.48	115.94
7	I	101	BCL	C11-C12-C13	-2.01	109.43	115.92
9	R	103	A1ELD	C34-C32-C31	2.01	122.02	118.94
9	O	102	A1ELD	C6-C5-C4	2.01	115.85	111.85
7	L	302	BCL	C11-C10-C8	-2.00	109.44	115.92
8	E	102	A1EL2	C34-C35-C30	2.00	114.06	110.48
8	A	102	A1EL2	C34-C35-C30	2.00	114.06	110.48
9	B	103	A1ELD	C35-C34-C32	2.00	128.92	125.89
7	B	101	BCL	CMD-C2D-C3D	-2.00	123.01	127.61
7	o	102	BCL	CHC-C4B-C3B	-2.00	125.23	132.35
9	R	102	A1ELD	C20-C19-C18	2.00	127.57	123.47

There are no chirality outliers.

All (876) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	101	BCL	C1A-C2A-CAA-CBA
7	C	101	BCL	C4B-C3B-CAB-CBB
7	D	101	BCL	C1A-C2A-CAA-CBA
7	D	101	BCL	C2B-C3B-CAB-OBB
7	D	101	BCL	C2B-C3B-CAB-CBB
7	D	101	BCL	C4B-C3B-CAB-CBB
7	Q	101	BCL	C3A-C2A-CAA-CBA
7	Q	101	BCL	C4-C3-C5-C6
7	J	101	BCL	CBD-CGD-O2D-CED
7	N	101	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	b	102	BCL	C2C-C3C-CAC-CBC
7	b	102	BCL	C4C-C3C-CAC-CBC
7	b	102	BCL	C11-C10-C8-C7
7	a	101	BCL	C3A-C2A-CAA-CBA
7	a	101	BCL	C2C-C3C-CAC-CBC
7	a	101	BCL	C4C-C3C-CAC-CBC
7	p	101	BCL	C2C-C3C-CAC-CBC
7	p	101	BCL	C4C-C3C-CAC-CBC
7	o	102	BCL	C1A-C2A-CAA-CBA
7	o	102	BCL	C3A-C2A-CAA-CBA
7	o	102	BCL	C2C-C3C-CAC-CBC
7	o	102	BCL	C4C-C3C-CAC-CBC
7	n	101	BCL	C1A-C2A-CAA-CBA
7	n	101	BCL	C3A-C2A-CAA-CBA
7	n	101	BCL	C2C-C3C-CAC-CBC
7	n	101	BCL	C4C-C3C-CAC-CBC
7	s	101	BCL	C2C-C3C-CAC-CBC
7	s	101	BCL	C4C-C3C-CAC-CBC
7	s	101	BCL	C11-C10-C8-C7
7	r	104	BCL	C2C-C3C-CAC-CBC
7	r	104	BCL	C4C-C3C-CAC-CBC
7	k	101	BCL	C2C-C3C-CAC-CBC
7	k	101	BCL	C4C-C3C-CAC-CBC
7	j	102	BCL	C2C-C3C-CAC-CBC
7	j	102	BCL	C4C-C3C-CAC-CBC
7	c	101	BCL	C2C-C3C-CAC-CBC
7	c	101	BCL	C4C-C3C-CAC-CBC
7	c	101	BCL	CHA-CBD-CGD-O1D
7	c	101	BCL	CHA-CBD-CGD-O2D
7	d	102	BCL	C2C-C3C-CAC-CBC
7	d	102	BCL	C4C-C3C-CAC-CBC
7	d	102	BCL	C6-C7-C8-C9
7	e	102	BCL	C2C-C3C-CAC-CBC
7	e	102	BCL	C4C-C3C-CAC-CBC
7	f	102	BCL	C2C-C3C-CAC-CBC
7	f	102	BCL	C4C-C3C-CAC-CBC
7	g	102	BCL	C1A-C2A-CAA-CBA
7	g	102	BCL	C3A-C2A-CAA-CBA
7	g	102	BCL	C2C-C3C-CAC-CBC
7	g	102	BCL	C4C-C3C-CAC-CBC
7	q	102	BCL	C2C-C3C-CAC-CBC
7	q	102	BCL	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	i	101	BCL	C2C-C3C-CAC-CBC
7	i	101	BCL	C4C-C3C-CAC-CBC
7	L	302	BCL	C2B-C3B-CAB-OB
7	L	302	BCL	C2B-C3B-CAB-CB
7	L	302	BCL	C4B-C3B-CAB-OB
7	L	302	BCL	C4B-C3B-CAB-CB
7	L	302	BCL	C4C-C3C-CAC-CBC
7	M	403	BCL	C1A-C2A-CAA-CBA
7	M	403	BCL	C2B-C3B-CAB-OB
7	M	403	BCL	C2B-C3B-CAB-CB
7	M	403	BCL	C4B-C3B-CAB-CB
9	A	103	A1ELD	C2-C3-C8-C9
9	A	103	A1ELD	C34-C35-C36-C37
9	B	103	A1ELD	C2-C3-C8-C9
9	B	103	A1ELD	C34-C35-C36-C37
9	C	102	A1ELD	C2-C3-C8-C9
9	C	102	A1ELD	C34-C35-C36-C37
9	J	103	A1ELD	C2-C3-C8-C9
9	J	103	A1ELD	C34-C35-C36-C37
9	R	102	A1ELD	C2-C3-C8-C9
9	R	102	A1ELD	C34-C35-C36-C37
9	R	103	A1ELD	C13-C10-C9-C8
9	R	103	A1ELD	C21-C22-C24-C25
9	R	103	A1ELD	C23-C22-C24-C25
9	b	101	A1ELD	C2-C3-C8-C9
9	b	101	A1ELD	C34-C35-C36-C37
9	o	101	A1ELD	C2-C3-C8-C9
9	o	101	A1ELD	C34-C35-C36-C37
9	j	101	A1ELD	C2-C3-C8-C9
9	j	101	A1ELD	C34-C35-C36-C37
9	d	101	A1ELD	C2-C3-C8-C9
9	d	101	A1ELD	C34-C35-C36-C37
9	e	101	A1ELD	C34-C35-C36-C37
9	f	101	A1ELD	C2-C3-C8-C9
9	f	101	A1ELD	C34-C35-C36-C37
9	g	101	A1ELD	C34-C35-C36-C37
9	q	101	A1ELD	C2-C3-C8-C9
9	q	101	A1ELD	C31-C32-C34-C35
9	q	101	A1ELD	C33-C32-C34-C35
9	q	101	A1ELD	C34-C35-C36-C37
11	G	103	PGV	O02-C1-O01-C02
11	L	308	PGV	C03-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	L	308	PGV	C03-O11-P-O13
11	L	308	PGV	C03-O11-P-O14
11	L	308	PGV	O03-C01-C02-O01
11	T	301	PGV	O03-C01-C02-C03
11	T	301	PGV	C03-C02-O01-C1
11	T	303	PGV	C03-O11-P-O12
11	T	303	PGV	C03-O11-P-O13
11	T	303	PGV	C03-O11-P-O14
12	G	104	LMT	C2-C1-O1'-C1'
12	N	103	LMT	C2-C1-O1'-C1'
12	L	309	LMT	O5B-C1B-O1B-C4'
12	L	309	LMT	C2-C1-O1'-C1'
13	L	303	BPH	C4C-C3C-CAC-CBC
13	L	303	BPH	C2C-C3C-CAC-CBC
13	L	305	BPH	C4C-C3C-CAC-CBC
13	L	305	BPH	C2C-C3C-CAC-CBC
14	L	304	UQ8	C12-C11-C9-C8
14	M	402	UQ8	C25-C24-C26-C27
14	M	402	UQ8	C23-C24-C26-C27
17	M	407	PEF	C2-C1-O3P-P
7	L	301	BCL	O1D-CGD-O2D-CED
7	P	101	BCL	CBD-CGD-O2D-CED
7	L	301	BCL	CBD-CGD-O2D-CED
7	M	401	BCL	CBD-CGD-O2D-CED
7	N	101	BCL	O1A-CGA-O2A-C1
7	P	101	BCL	O1A-CGA-O2A-C1
7	f	102	BCL	O1A-CGA-O2A-C1
7	J	101	BCL	O1D-CGD-O2D-CED
7	N	101	BCL	CBA-CGA-O2A-C1
7	A	101	BCL	O1A-CGA-O2A-C1
7	E	101	BCL	O1A-CGA-O2A-C1
7	F	101	BCL	O1A-CGA-O2A-C1
7	R	101	BCL	O1A-CGA-O2A-C1
7	b	102	BCL	O1A-CGA-O2A-C1
7	o	102	BCL	O1A-CGA-O2A-C1
7	n	101	BCL	O1A-CGA-O2A-C1
7	e	102	BCL	O1A-CGA-O2A-C1
7	M	401	BCL	O1D-CGD-O2D-CED
7	A	101	BCL	C3-C5-C6-C7
7	D	101	BCL	C3-C5-C6-C7
7	J	101	BCL	C3-C5-C6-C7
7	R	101	BCL	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	N	101	BCL	C3-C5-C6-C7
7	P	101	BCL	C3-C5-C6-C7
7	c	101	BCL	C3-C5-C6-C7
7	e	102	BCL	C3-C5-C6-C7
7	q	102	BCL	C3-C5-C6-C7
7	i	101	BCL	C3-C5-C6-C7
13	L	305	BPH	C3-C5-C6-C7
7	B	101	BCL	CBA-CGA-O2A-C1
7	P	101	BCL	CBA-CGA-O2A-C1
7	b	102	BCL	CBA-CGA-O2A-C1
7	n	101	BCL	CBA-CGA-O2A-C1
7	f	102	BCL	CBA-CGA-O2A-C1
7	g	102	BCL	C4-C3-C5-C6
7	Q	101	BCL	C2-C3-C5-C6
7	O	101	BCL	C2-C3-C5-C6
7	g	102	BCL	C2-C3-C5-C6
7	B	101	BCL	CBD-CGD-O2D-CED
7	g	102	BCL	C2A-CAA-CBA-CGA
7	M	403	BCL	C2A-CAA-CBA-CGA
7	Q	101	BCL	C3-C5-C6-C7
7	S	101	BCL	C3-C5-C6-C7
7	O	101	BCL	C3-C5-C6-C7
7	o	102	BCL	C3-C5-C6-C7
7	A	101	BCL	CBA-CGA-O2A-C1
7	E	101	BCL	CBA-CGA-O2A-C1
7	F	101	BCL	CBA-CGA-O2A-C1
7	R	101	BCL	CBA-CGA-O2A-C1
7	O	101	BCL	CBA-CGA-O2A-C1
7	a	101	BCL	CBA-CGA-O2A-C1
7	o	102	BCL	CBA-CGA-O2A-C1
7	e	102	BCL	CBA-CGA-O2A-C1
7	P	101	BCL	O1D-CGD-O2D-CED
13	L	305	BPH	CBD-CGD-O2D-CED
7	B	101	BCL	O1A-CGA-O2A-C1
7	a	101	BCL	O1A-CGA-O2A-C1
7	c	101	BCL	O1A-CGA-O2A-C1
9	R	103	A1ELD	C24-C25-C26-C27
7	S	101	BCL	CBD-CGD-O2D-CED
7	q	102	BCL	CBD-CGD-O2D-CED
7	s	101	BCL	C3-C5-C6-C7
7	k	101	BCL	C3-C5-C6-C7
7	M	401	BCL	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	O	101	BCL	O1A-CGA-O2A-C1
7	O	101	BCL	CBD-CGD-O2D-CED
7	c	101	BCL	CBA-CGA-O2A-C1
7	M	401	BCL	O1A-CGA-O2A-C1
7	B	101	BCL	C4-C3-C5-C6
7	E	101	BCL	C4-C3-C5-C6
7	F	101	BCL	C4-C3-C5-C6
14	M	402	UQ8	C30-C29-C31-C32
12	G	104	LMT	C4'-C5'-C6'-O6'
7	B	101	BCL	C2-C3-C5-C6
7	E	101	BCL	C2-C3-C5-C6
7	F	101	BCL	C2-C3-C5-C6
14	M	402	UQ8	C28-C29-C31-C32
7	I	101	BCL	C2A-CAA-CBA-CGA
7	J	101	BCL	C2A-CAA-CBA-CGA
7	a	101	BCL	C2A-CAA-CBA-CGA
12	L	309	LMT	C4B-C5B-C6B-O6B
7	J	101	BCL	CBA-CGA-O2A-C1
13	L	305	BPH	CBA-CGA-O2A-C1
7	G	101	BCL	CBD-CGD-O2D-CED
13	L	305	BPH	O1A-CGA-O2A-C1
7	J	101	BCL	O1A-CGA-O2A-C1
7	d	102	BCL	C3-C5-C6-C7
7	Q	101	BCL	CBA-CGA-O2A-C1
7	L	302	BCL	CBA-CGA-O2A-C1
7	F	101	BCL	C8-C10-C11-C12
7	o	102	BCL	CBD-CGD-O2D-CED
7	e	102	BCL	C8-C10-C11-C12
7	g	102	BCL	C5-C6-C7-C8
7	Q	101	BCL	O1A-CGA-O2A-C1
7	I	101	BCL	C11-C12-C13-C14
7	I	101	BCL	C14-C13-C15-C16
7	S	101	BCL	C11-C12-C13-C14
7	S	101	BCL	C14-C13-C15-C16
7	o	102	BCL	C6-C7-C8-C9
7	n	101	BCL	C6-C7-C8-C9
7	n	101	BCL	C11-C12-C13-C14
7	c	101	BCL	C6-C7-C8-C9
7	L	302	BCL	C6-C7-C8-C9
8	r	102	A1EL2	C27-C26-C28-C29
9	R	103	A1ELD	C11-C10-C9-C8
7	L	302	BCL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	101	BCL	C5-C6-C7-C8
7	E	101	BCL	C8-C10-C11-C12
7	S	101	BCL	C10-C11-C12-C13
7	n	101	BCL	C13-C15-C16-C17
7	A	101	BCL	C5-C6-C7-C8
7	A	101	BCL	C13-C15-C16-C17
7	B	101	BCL	C10-C11-C12-C13
7	K	101	BCL	C15-C16-C17-C18
7	R	101	BCL	C5-C6-C7-C8
7	P	101	BCL	C8-C10-C11-C12
7	r	104	BCL	C15-C16-C17-C18
7	i	101	BCL	C5-C6-C7-C8
7	L	302	BCL	CBD-CGD-O2D-CED
12	G	104	LMT	O5'-C5'-C6'-O6'
12	N	103	LMT	O5'-C5'-C6'-O6'
7	B	101	BCL	C8-C10-C11-C12
7	K	101	BCL	C5-C6-C7-C8
7	n	101	BCL	C10-C11-C12-C13
7	s	101	BCL	C15-C16-C17-C18
7	c	101	BCL	C15-C16-C17-C18
7	e	102	BCL	C13-C15-C16-C17
7	L	302	BCL	C15-C16-C17-C18
7	M	403	BCL	C10-C11-C12-C13
13	L	303	BPH	C13-C15-C16-C17
11	F	103	PGV	C1-C2-C3-C4
7	P	101	BCL	C13-C15-C16-C17
7	g	102	BCL	C8-C10-C11-C12
7	p	101	BCL	C3-C5-C6-C7
7	p	101	BCL	C8-C10-C11-C12
7	O	101	BCL	C15-C16-C17-C18
7	B	101	BCL	C12-C13-C15-C16
7	C	101	BCL	C6-C7-C8-C10
7	G	101	BCL	C12-C13-C15-C16
7	Q	101	BCL	C11-C12-C13-C15
7	I	101	BCL	C11-C12-C13-C15
7	N	101	BCL	C11-C12-C13-C15
7	p	101	BCL	C6-C7-C8-C10
7	r	104	BCL	C11-C10-C8-C7
7	i	101	BCL	C11-C10-C8-C7
13	L	303	BPH	C11-C10-C8-C7
7	R	101	BCL	C2A-CAA-CBA-CGA
7	B	101	BCL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	N	101	BCL	C5-C6-C7-C8
7	L	301	BCL	C15-C16-C17-C18
7	f	102	BCL	C8-C10-C11-C12
8	r	102	A1EL2	C21-C23-C24-C25
12	L	309	LMT	O5B-C5B-C6B-O6B
13	L	305	BPH	C13-C15-C16-C17
7	J	101	BCL	C8-C10-C11-C12
7	R	101	BCL	C13-C15-C16-C17
7	n	101	BCL	C15-C16-C17-C18
7	E	101	BCL	C10-C11-C12-C13
7	o	102	BCL	C8-C10-C11-C12
7	f	102	BCL	C10-C11-C12-C13
7	r	104	BCL	C3-C5-C6-C7
7	j	102	BCL	CBA-CGA-O2A-C1
7	C	101	BCL	C10-C11-C12-C13
7	F	101	BCL	C10-C11-C12-C13
7	K	101	BCL	C8-C10-C11-C12
7	s	101	BCL	CBD-CGD-O2D-CED
7	D	101	BCL	C16-C17-C18-C19
7	Q	101	BCL	C16-C17-C18-C19
7	L	302	BCL	C3-C5-C6-C7
7	r	104	BCL	CBA-CGA-O2A-C1
7	r	104	BCL	C16-C17-C18-C19
11	G	103	PGV	C21-C22-C23-C24
7	q	102	BCL	O1D-CGD-O2D-CED
7	q	102	BCL	C13-C15-C16-C17
19	T	302	LHG	C27-C28-C29-C30
7	C	101	BCL	C13-C15-C16-C17
7	j	102	BCL	C8-C10-C11-C12
7	d	102	BCL	C8-C10-C11-C12
7	s	101	BCL	C16-C17-C18-C19
7	c	101	BCL	C16-C17-C18-C20
7	C	101	BCL	C4B-C3B-CAB-OB
7	M	403	BCL	C4B-C3B-CAB-OB
7	S	101	BCL	O1D-CGD-O2D-CED
13	L	305	BPH	O1D-CGD-O2D-CED
7	s	101	BCL	C4-C3-C5-C6
7	r	104	BCL	C4-C3-C5-C6
7	d	102	BCL	C4-C3-C5-C6
11	G	103	PGV	C23-C24-C25-C26
7	d	102	BCL	C2-C3-C5-C6
7	C	101	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	F	101	BCL	C11-C10-C8-C9
7	O	101	BCL	C11-C10-C8-C9
7	o	102	BCL	C11-C10-C8-C9
7	e	102	BCL	C11-C10-C8-C9
7	g	102	BCL	C11-C10-C8-C9
7	C	101	BCL	C3-C5-C6-C7
7	g	102	BCL	C3-C5-C6-C7
7	p	101	BCL	C10-C11-C12-C13
11	T	301	PGV	C1-C2-C3-C4
7	B	101	BCL	C16-C17-C18-C20
7	r	104	BCL	C16-C17-C18-C20
7	R	101	BCL	C10-C11-C12-C13
7	L	301	BCL	C13-C15-C16-C17
7	r	104	BCL	O1A-CGA-O2A-C1
7	s	101	BCL	CBA-CGA-O2A-C1
7	A	101	BCL	C3A-C2A-CAA-CBA
7	D	101	BCL	C3A-C2A-CAA-CBA
7	E	101	BCL	C3A-C2A-CAA-CBA
7	F	101	BCL	C3A-C2A-CAA-CBA
7	I	101	BCL	C3A-C2A-CAA-CBA
7	S	101	BCL	C3A-C2A-CAA-CBA
7	b	102	BCL	C3A-C2A-CAA-CBA
7	p	101	BCL	C3A-C2A-CAA-CBA
7	s	101	BCL	C3A-C2A-CAA-CBA
7	r	104	BCL	C3A-C2A-CAA-CBA
7	k	101	BCL	C3A-C2A-CAA-CBA
7	j	102	BCL	C3A-C2A-CAA-CBA
7	c	101	BCL	C3A-C2A-CAA-CBA
7	d	102	BCL	C3A-C2A-CAA-CBA
7	e	102	BCL	C3A-C2A-CAA-CBA
7	f	102	BCL	C3A-C2A-CAA-CBA
7	q	102	BCL	C3A-C2A-CAA-CBA
7	i	101	BCL	C3A-C2A-CAA-CBA
7	M	403	BCL	C3A-C2A-CAA-CBA
7	C	101	BCL	C2B-C3B-CAB-CBB
7	j	102	BCL	O1A-CGA-O2A-C1
7	O	101	BCL	C16-C17-C18-C19
7	O	101	BCL	C16-C17-C18-C20
7	D	101	BCL	CBD-CGD-O2D-CED
7	J	101	BCL	C4-C3-C5-C6
7	J	101	BCL	C2-C3-C5-C6
7	Q	101	BCL	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	s	101	BCL	O1A-CGA-O2A-C1
7	D	101	BCL	C16-C17-C18-C20
7	n	101	BCL	C3-C5-C6-C7
8	G	102	A1EL2	C11-C10-C3-C4
8	r	102	A1EL2	C11-C10-C3-C2
8	r	102	A1EL2	C11-C10-C3-C4
9	A	103	A1ELD	C4-C3-C8-C9
9	B	103	A1ELD	C4-C3-C8-C9
9	C	102	A1ELD	C4-C3-C8-C9
9	J	103	A1ELD	C4-C3-C8-C9
9	R	102	A1ELD	C4-C3-C8-C9
9	b	101	A1ELD	C4-C3-C8-C9
9	o	101	A1ELD	C4-C3-C8-C9
9	j	101	A1ELD	C4-C3-C8-C9
9	d	101	A1ELD	C4-C3-C8-C9
9	e	101	A1ELD	C2-C3-C8-C9
9	e	101	A1ELD	C4-C3-C8-C9
9	f	101	A1ELD	C4-C3-C8-C9
9	g	101	A1ELD	C2-C3-C8-C9
9	g	101	A1ELD	C4-C3-C8-C9
9	q	101	A1ELD	C4-C3-C8-C9
7	R	101	BCL	C15-C16-C17-C18
7	q	102	BCL	C5-C6-C7-C8
13	L	305	BPH	C5-C6-C7-C8
7	P	101	BCL	C4-C3-C5-C6
7	c	101	BCL	C4-C3-C5-C6
7	F	101	BCL	C11-C10-C8-C7
7	G	101	BCL	C11-C10-C8-C7
7	S	101	BCL	C11-C10-C8-C7
7	S	101	BCL	C11-C12-C13-C15
7	n	101	BCL	C2-C3-C5-C6
7	s	101	BCL	C2-C3-C5-C6
7	r	104	BCL	C2-C3-C5-C6
7	e	102	BCL	C11-C10-C8-C7
7	M	403	BCL	C11-C10-C8-C7
13	L	305	BPH	C12-C13-C15-C16
10	Q	104	8K6	C13-C14-C15-C16
7	R	101	BCL	C16-C17-C18-C20
7	s	101	BCL	C16-C17-C18-C20
7	k	101	BCL	CBA-CGA-O2A-C1
7	q	102	BCL	CBA-CGA-O2A-C1
11	T	301	PGV	C20-C19-O03-C01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	S	101	BCL	C2A-CAA-CBA-CGA
7	S	101	BCL	C15-C16-C17-C18
7	j	102	BCL	C15-C16-C17-C18
7	c	101	BCL	C13-C15-C16-C17
7	d	102	BCL	C10-C11-C12-C13
7	G	101	BCL	O1D-CGD-O2D-CED
7	o	102	BCL	C10-C11-C12-C13
7	i	101	BCL	C15-C16-C17-C18
7	a	101	BCL	C8-C10-C11-C12
11	M	408	PGV	C3-C4-C5-C6
11	M	408	PGV	C4-C5-C6-C7
11	M	408	PGV	O03-C01-C02-O01
7	B	101	BCL	C16-C17-C18-C19
7	c	101	BCL	C16-C17-C18-C19
7	r	104	BCL	C13-C15-C16-C17
7	k	101	BCL	C5-C6-C7-C8
7	n	101	BCL	C4-C3-C5-C6
7	c	101	BCL	C2-C3-C5-C6
7	B	101	BCL	C14-C13-C15-C16
7	E	101	BCL	C11-C10-C8-C9
7	G	101	BCL	C11-C10-C8-C9
7	R	101	BCL	C11-C10-C8-C9
7	p	101	BCL	C11-C10-C8-C9
7	i	101	BCL	C11-C10-C8-C9
7	M	403	BCL	C11-C10-C8-C9
13	L	303	BPH	C11-C10-C8-C9
13	L	305	BPH	C14-C13-C15-C16
7	a	101	BCL	C10-C11-C12-C13
7	B	101	BCL	C2A-CAA-CBA-CGA
7	q	102	BCL	C15-C16-C17-C18
7	k	101	BCL	O1A-CGA-O2A-C1
7	A	101	BCL	C1A-C2A-CAA-CBA
7	E	101	BCL	C1A-C2A-CAA-CBA
7	F	101	BCL	C1A-C2A-CAA-CBA
7	Q	101	BCL	C1A-C2A-CAA-CBA
7	I	101	BCL	C1A-C2A-CAA-CBA
7	S	101	BCL	C1A-C2A-CAA-CBA
7	N	101	BCL	C1A-C2A-CAA-CBA
7	b	102	BCL	C1A-C2A-CAA-CBA
7	a	101	BCL	C1A-C2A-CAA-CBA
7	p	101	BCL	C1A-C2A-CAA-CBA
7	s	101	BCL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	r	104	BCL	C1A-C2A-CAA-CBA
7	k	101	BCL	C1A-C2A-CAA-CBA
7	j	102	BCL	C1A-C2A-CAA-CBA
7	c	101	BCL	C1A-C2A-CAA-CBA
7	d	102	BCL	C1A-C2A-CAA-CBA
7	e	102	BCL	C1A-C2A-CAA-CBA
7	f	102	BCL	C1A-C2A-CAA-CBA
7	q	102	BCL	C1A-C2A-CAA-CBA
7	i	101	BCL	C1A-C2A-CAA-CBA
7	L	302	BCL	C1A-C2A-CAA-CBA
7	J	101	BCL	C15-C16-C17-C18
7	P	101	BCL	C10-C11-C12-C13
7	g	102	BCL	C15-C16-C17-C18
7	O	101	BCL	O1D-CGD-O2D-CED
7	A	101	BCL	C15-C16-C17-C18
11	D	103	PGV	C01-C02-C03-O11
11	F	103	PGV	C19-C20-C21-C22
9	O	102	A1ELD	C34-C35-C36-C37
11	D	103	PGV	C26-C27-C28-C29
7	k	101	BCL	C4-C3-C5-C6
7	c	101	BCL	C8-C10-C11-C12
11	T	301	PGV	O04-C19-O03-C01
7	O	101	BCL	C13-C15-C16-C17
7	o	102	BCL	O1D-CGD-O2D-CED
11	L	308	PGV	O03-C01-C02-C03
7	q	102	BCL	O1A-CGA-O2A-C1
14	L	304	UQ8	C1-C6-C7-C8
10	Q	104	8K6	C5-C6-C7-C8
7	L	302	BCL	O1D-CGD-O2D-CED
10	M	406	8K6	C10-C11-C12-C13
13	L	303	BPH	C3-C5-C6-C7
7	c	101	BCL	CBD-CGD-O2D-CED
7	K	101	BCL	C10-C11-C12-C13
7	p	101	BCL	C5-C6-C7-C8
8	r	102	A1EL2	C24-C25-C26-C27
12	L	309	LMT	O5'-C5'-C6'-O6'
7	K	101	BCL	C16-C17-C18-C20
7	K	101	BCL	CBA-CGA-O2A-C1
14	L	304	UQ8	C5-C6-C7-C8
7	Q	101	BCL	C2A-CAA-CBA-CGA
7	D	101	BCL	O1D-CGD-O2D-CED
7	e	102	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	S	101	BCL	CBA-CGA-O2A-C1
7	d	102	BCL	CBA-CGA-O2A-C1
7	S	101	BCL	C16-C17-C18-C20
7	j	102	BCL	C13-C15-C16-C17
13	L	305	BPH	C8-C10-C11-C12
8	r	102	A1EL2	C24-C25-C26-C28
11	G	103	PGV	O03-C01-C02-O01
7	D	101	BCL	C4B-C3B-CAB-OB
7	b	102	BCL	C8-C10-C11-C12
7	B	101	BCL	C11-C10-C8-C7
7	C	101	BCL	C12-C13-C15-C16
7	D	101	BCL	C11-C10-C8-C7
7	E	101	BCL	C11-C10-C8-C7
7	R	101	BCL	C11-C10-C8-C7
7	b	102	BCL	C12-C13-C15-C16
7	a	101	BCL	C6-C7-C8-C10
7	p	101	BCL	C11-C10-C8-C7
7	f	102	BCL	C11-C12-C13-C15
7	g	102	BCL	C6-C7-C8-C10
7	g	102	BCL	C11-C10-C8-C7
7	q	102	BCL	C11-C10-C8-C7
13	L	305	BPH	C11-C10-C8-C7
7	D	101	BCL	C6-C7-C8-C9
7	D	101	BCL	C11-C10-C8-C9
7	D	101	BCL	C14-C13-C15-C16
7	Q	101	BCL	C11-C12-C13-C14
7	b	102	BCL	C14-C13-C15-C16
7	a	101	BCL	C6-C7-C8-C9
7	r	104	BCL	C11-C10-C8-C9
7	f	102	BCL	C11-C12-C13-C14
7	g	102	BCL	C6-C7-C8-C9
7	i	101	BCL	C6-C7-C8-C9
13	L	305	BPH	C11-C10-C8-C9
7	k	101	BCL	CBD-CGD-O2D-CED
7	P	101	BCL	C2A-CAA-CBA-CGA
7	s	101	BCL	O1D-CGD-O2D-CED
7	S	101	BCL	O1A-CGA-O2A-C1
7	d	102	BCL	O1A-CGA-O2A-C1
7	L	302	BCL	C8-C10-C11-C12
7	I	101	BCL	C5-C6-C7-C8
7	K	101	BCL	O1A-CGA-O2A-C1
11	L	307	PGV	C01-C02-C03-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	T	303	PGV	C1-C2-C3-C4
7	P	101	BCL	C2-C3-C5-C6
7	k	101	BCL	C2-C3-C5-C6
10	Q	103	8K6	C4-C5-C6-C7
7	f	102	BCL	C15-C16-C17-C18
10	H	301	8K6	C4-C5-C6-C7
12	L	309	LMT	C5'-C4'-O1B-C1B
7	B	101	BCL	C3A-C2A-CAA-CBA
7	C	101	BCL	C2B-C3B-CAB-OB
7	M	403	BCL	C16-C17-C18-C20
7	i	101	BCL	CBA-CGA-O2A-C1
7	K	101	BCL	C13-C15-C16-C17
11	M	408	PGV	O03-C01-C02-C03
16	M	405	H4X	C3-C1-C4-C5
16	M	405	H4X	C2-C1-C4-C5
7	j	102	BCL	C10-C11-C12-C13
11	D	103	PGV	O01-C02-C03-O11
11	L	307	PGV	O01-C02-C03-O11
7	K	101	BCL	C16-C17-C18-C19
7	Q	101	BCL	C8-C10-C11-C12
7	R	101	BCL	C16-C17-C18-C19
7	p	101	BCL	C2-C1-O2A-CGA
7	L	301	BCL	C5-C6-C7-C8
7	B	101	BCL	C11-C10-C8-C9
7	C	101	BCL	C11-C12-C13-C14
7	K	101	BCL	C11-C12-C13-C14
7	a	101	BCL	C11-C10-C8-C9
7	q	102	BCL	C6-C7-C8-C9
7	O	101	BCL	C10-C11-C12-C13
7	b	102	BCL	C15-C16-C17-C18
14	L	304	UQ8	C12-C11-C9-C10
7	E	101	BCL	C16-C17-C18-C20
7	S	101	BCL	C16-C17-C18-C19
8	C	103	A1EL2	C11-C10-C3-C2
8	Q	102	A1EL2	C11-C10-C3-C2
8	Q	102	A1EL2	C11-C10-C3-C4
8	I	102	A1EL2	C11-C10-C3-C2
8	I	102	A1EL2	C11-C10-C3-C4
8	J	102	A1EL2	C28-C29-C30-C31
8	N	102	A1EL2	C11-C10-C3-C2
8	N	102	A1EL2	C11-C10-C3-C4
8	P	102	A1EL2	C11-C10-C3-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	P	102	A1EL2	C11-C10-C3-C4
8	r	102	A1EL2	C25-C26-C28-C29
7	c	101	BCL	C10-C11-C12-C13
7	M	403	BCL	C5-C6-C7-C8
11	L	308	PGV	C2-C1-O01-C02
7	D	101	BCL	C6-C7-C8-C10
7	D	101	BCL	C12-C13-C15-C16
7	E	101	BCL	C6-C7-C8-C10
7	F	101	BCL	C6-C7-C8-C10
7	G	101	BCL	C11-C12-C13-C15
7	J	101	BCL	C11-C10-C8-C7
7	K	101	BCL	C11-C12-C13-C15
7	O	101	BCL	C12-C13-C15-C16
7	a	101	BCL	C11-C10-C8-C7
7	n	101	BCL	C11-C12-C13-C15
7	c	101	BCL	C6-C7-C8-C10
7	d	102	BCL	C6-C7-C8-C10
7	f	102	BCL	C11-C10-C8-C7
7	q	102	BCL	C6-C7-C8-C10
7	i	101	BCL	C6-C7-C8-C10
11	L	308	PGV	O02-C1-O01-C02
7	G	101	BCL	C15-C16-C17-C18
7	p	101	BCL	C15-C16-C17-C18
11	G	103	PGV	C22-C23-C24-C25
11	F	103	PGV	C2-C1-O01-C02
7	F	101	BCL	C16-C17-C18-C20
7	q	102	BCL	C16-C17-C18-C19
7	D	101	BCL	CBA-CGA-O2A-C1
11	L	308	PGV	C20-C19-O03-C01
7	L	301	BCL	CAD-CBD-CGD-O2D
7	k	101	BCL	O1D-CGD-O2D-CED
7	s	101	BCL	C5-C6-C7-C8
8	r	102	A1EL2	C26-C28-C29-C30
7	c	101	BCL	O1D-CGD-O2D-CED
7	o	102	BCL	C4-C3-C5-C6
7	n	101	BCL	C5-C6-C7-C8
7	R	101	BCL	C8-C10-C11-C12
7	D	101	BCL	O1A-CGA-O2A-C1
7	i	101	BCL	O1A-CGA-O2A-C1
11	F	103	PGV	C6-C7-C8-C9
12	N	103	LMT	C4'-C5'-C6'-O6'
11	F	103	PGV	O02-C1-O01-C02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	E	101	BCL	C6-C7-C8-C9
7	F	101	BCL	C6-C7-C8-C9
7	b	102	BCL	C11-C10-C8-C9
7	G	101	BCL	C1A-C2A-CAA-CBA
7	M	403	BCL	C16-C17-C18-C19
7	b	102	BCL	C13-C15-C16-C17
7	p	101	BCL	O1A-CGA-O2A-C1
7	M	403	BCL	C15-C16-C17-C18
13	L	303	BPH	C5-C6-C7-C8
11	M	408	PGV	C01-C02-C03-O11
11	T	303	PGV	C01-C02-C03-O11
7	o	102	BCL	C15-C16-C17-C18
7	L	301	BCL	C2A-CAA-CBA-CGA
7	p	101	BCL	CBA-CGA-O2A-C1
7	B	101	BCL	C6-C7-C8-C10
7	G	101	BCL	C6-C7-C8-C10
7	Q	101	BCL	C12-C13-C15-C16
7	I	101	BCL	C12-C13-C15-C16
7	N	101	BCL	C12-C13-C15-C16
7	p	101	BCL	C11-C12-C13-C15
7	o	102	BCL	C6-C7-C8-C10
7	k	101	BCL	C6-C7-C8-C10
7	k	101	BCL	C11-C12-C13-C15
7	L	302	BCL	C6-C7-C8-C10
7	L	302	BCL	C11-C10-C8-C7
7	M	403	BCL	C12-C13-C15-C16
11	M	408	PGV	O01-C02-C03-O11
11	T	303	PGV	O01-C02-C03-O11
11	L	308	PGV	O04-C19-O03-C01
7	F	101	BCL	C3-C5-C6-C7
11	G	103	PGV	O03-C01-C02-C03
19	T	302	LHG	C23-C24-C25-C26
7	o	102	BCL	C13-C15-C16-C17
13	L	303	BPH	CBA-CGA-O2A-C1
7	A	101	BCL	C14-C13-C15-C16
7	G	101	BCL	C11-C12-C13-C14
7	G	101	BCL	C14-C13-C15-C16
7	J	101	BCL	C11-C10-C8-C9
7	N	101	BCL	C11-C12-C13-C14
7	O	101	BCL	C14-C13-C15-C16
7	p	101	BCL	C6-C7-C8-C9
7	s	101	BCL	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	c	101	BCL	C14-C13-C15-C16
7	f	102	BCL	C11-C10-C8-C9
7	L	301	BCL	C11-C10-C8-C9
13	L	303	BPH	O1A-CGA-O2A-C1
7	E	101	BCL	C16-C17-C18-C19
12	G	104	LMT	C3-C4-C5-C6
10	C	104	8K6	C6-C7-C8-C9
7	d	102	BCL	C15-C16-C17-C18
7	I	101	BCL	C4-C3-C5-C6
7	c	101	BCL	C5-C6-C7-C8
7	i	101	BCL	O1D-CGD-O2D-CED
7	J	101	BCL	C2-C1-O2A-CGA
7	c	101	BCL	C2-C1-O2A-CGA
13	L	303	BPH	C2-C1-O2A-CGA
12	L	309	LMT	C3'-C4'-O1B-C1B
7	G	101	BCL	C3-C5-C6-C7
11	T	303	PGV	O03-C19-C20-C21
8	A	102	A1EL2	C11-C10-C3-C2
8	A	102	A1EL2	C11-C10-C3-C4
8	B	102	A1EL2	C11-C10-C3-C2
8	B	102	A1EL2	C11-C10-C3-C4
8	C	103	A1EL2	C11-C10-C3-C4
8	D	102	A1EL2	C11-C10-C3-C2
8	D	102	A1EL2	C11-C10-C3-C4
8	E	102	A1EL2	C11-C10-C3-C2
8	E	102	A1EL2	C11-C10-C3-C4
8	F	102	A1EL2	C11-C10-C3-C2
8	F	102	A1EL2	C11-C10-C3-C4
8	G	102	A1EL2	C11-C10-C3-C2
8	K	102	A1EL2	C11-C10-C3-C2
8	K	102	A1EL2	C11-C10-C3-C4
9	O	102	A1ELD	C2-C3-C8-C9
11	D	103	PGV	C03-O11-P-O12
11	D	103	PGV	C04-O12-P-O11
17	M	407	PEF	C4-O4P-P-O3P
7	q	102	BCL	C16-C17-C18-C20
7	D	101	BCL	C13-C15-C16-C17
7	o	102	BCL	C2-C3-C5-C6
7	o	102	BCL	C11-C10-C8-C7
7	c	101	BCL	C11-C10-C8-C7
7	L	301	BCL	C11-C10-C8-C7
11	F	103	PGV	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	101	BCL	C6-C7-C8-C9
7	k	101	BCL	C11-C12-C13-C14
10	C	104	8K6	C11-C10-C9-C8
14	L	306	UQ8	C2-C3-O3-C3M
7	I	101	BCL	C10-C11-C12-C13
10	S	102	8K6	C7-C8-C9-C10
7	I	101	BCL	C2-C3-C5-C6
7	M	401	BCL	C5-C6-C7-C8
7	i	101	BCL	CBD-CGD-O2D-CED
7	F	101	BCL	C16-C17-C18-C19
7	E	101	BCL	C3-C5-C6-C7
7	F	101	BCL	C5-C6-C7-C8
17	M	407	PEF	C14-C15-C16-C17
7	p	101	BCL	C16-C17-C18-C19
7	R	101	BCL	C4-C3-C5-C6
7	f	102	BCL	C4-C3-C5-C6
7	E	101	BCL	C5-C6-C7-C8
11	F	103	PGV	C7-C8-C9-C10
7	G	101	BCL	C3A-C2A-CAA-CBA
7	M	401	BCL	C3A-C2A-CAA-CBA
7	G	101	BCL	C6-C7-C8-C9
7	Q	101	BCL	C14-C13-C15-C16
7	K	101	BCL	C14-C13-C15-C16
7	P	101	BCL	C6-C7-C8-C9
7	p	101	BCL	C11-C12-C13-C14
7	j	102	BCL	C11-C12-C13-C14
7	i	101	BCL	C14-C13-C15-C16
7	G	101	BCL	C16-C17-C18-C19
7	d	102	BCL	C13-C15-C16-C17
11	T	303	PGV	C21-C22-C23-C24
7	B	101	BCL	C13-C15-C16-C17
11	F	103	PGV	O03-C01-C02-C03
14	L	304	UQ8	C7-C8-C9-C10
7	Q	101	BCL	O2A-C1-C2-C3
10	C	104	8K6	C7-C8-C9-C10
10	Q	104	8K6	C10-C11-C12-C13
7	K	101	BCL	C1A-C2A-CAA-CBA
7	O	101	BCL	C1A-C2A-CAA-CBA
7	Q	101	BCL	C11-C10-C8-C7
7	n	101	BCL	C6-C7-C8-C10
7	a	101	BCL	C15-C16-C17-C18
7	S	101	BCL	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	Q	104	8K6	C6-C7-C8-C9
7	G	101	BCL	C5-C6-C7-C8
7	f	102	BCL	C5-C6-C7-C8
11	D	103	PGV	C25-C26-C27-C28
7	I	101	BCL	C16-C17-C18-C20
7	a	101	BCL	C4-C3-C5-C6
7	r	104	BCL	C5-C6-C7-C8
7	I	101	BCL	C15-C16-C17-C18
8	I	102	A1EL2	C28-C29-C30-C35
8	J	102	A1EL2	C11-C10-C3-C4
8	J	102	A1EL2	C28-C29-C30-C35
8	r	102	A1EL2	C28-C29-C30-C35
8	r	103	A1EL2	C28-C29-C30-C35
9	O	102	A1ELD	C4-C3-C8-C9
11	M	408	PGV	C5-C6-C7-C8
7	C	101	BCL	C4-C3-C5-C6
7	A	101	BCL	C16-C17-C18-C20
14	L	306	UQ8	C5-C4-O4-C4M
7	p	101	BCL	C4-C3-C5-C6
14	M	402	UQ8	C15-C14-C16-C17
7	p	101	BCL	C12-C13-C15-C16
7	j	102	BCL	C11-C12-C13-C15
11	M	408	PGV	O02-C1-O01-C02
7	g	102	BCL	CAA-CBA-CGA-O2A
7	R	101	BCL	CAA-CBA-CGA-O2A
7	b	102	BCL	CAA-CBA-CGA-O2A
7	e	102	BCL	CAA-CBA-CGA-O2A
11	L	307	PGV	O01-C1-C2-C3
7	J	101	BCL	C5-C6-C7-C8
10	S	102	8K6	C5-C6-C7-C8
7	S	101	BCL	CAA-CBA-CGA-O2A
7	N	101	BCL	C14-C13-C15-C16
7	r	104	BCL	C11-C12-C13-C14
7	k	101	BCL	C6-C7-C8-C9
7	L	302	BCL	C11-C10-C8-C9
7	M	403	BCL	C14-C13-C15-C16
7	K	101	BCL	C3A-C2A-CAA-CBA
13	L	305	BPH	C15-C16-C17-C18
11	M	408	PGV	C2-C3-C4-C5
7	M	403	BCL	CAD-CBD-CGD-O2D
7	I	101	BCL	CAA-CBA-CGA-O2A
14	M	402	UQ8	C35-C34-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	a	101	BCL	C2-C3-C5-C6
11	D	103	PGV	C20-C21-C22-C23
7	n	101	BCL	O2A-C1-C2-C3
7	c	101	BCL	O2A-C1-C2-C3
7	P	101	BCL	CHA-CBD-CGD-O1D
7	P	101	BCL	CHA-CBD-CGD-O2D
7	M	401	BCL	CHA-CBD-CGD-O1D
7	a	101	BCL	CAA-CBA-CGA-O2A
11	T	303	PGV	O03-C01-C02-O01
7	S	101	BCL	C13-C15-C16-C17
7	M	401	BCL	CAA-CBA-CGA-O2A
7	A	101	BCL	C12-C13-C15-C16
14	M	402	UQ8	C33-C34-C36-C37
7	G	101	BCL	C16-C17-C18-C20
7	p	101	BCL	C16-C17-C18-C20
11	D	103	PGV	O03-C19-C20-C21
7	Q	101	BCL	C11-C10-C8-C9
7	S	101	BCL	C11-C10-C8-C9
7	p	101	BCL	C14-C13-C15-C16
7	n	101	BCL	C11-C10-C8-C9
7	R	101	BCL	CAA-CBA-CGA-O1A
11	L	308	PGV	C1-C2-C3-C4
14	L	304	UQ8	C5-C4-O4-C4M
11	T	301	PGV	C6-C7-C8-C9
7	g	102	BCL	CAA-CBA-CGA-O1A
7	s	101	BCL	CAA-CBA-CGA-O2A
11	D	103	PGV	O04-C19-C20-C21
7	C	101	BCL	C1A-C2A-CAA-CBA
7	M	401	BCL	C1A-C2A-CAA-CBA
11	M	408	PGV	C2-C1-O01-C02
11	D	103	PGV	C30-C31-C32-C33
7	C	101	BCL	C2-C1-O2A-CGA
7	D	101	BCL	C2-C1-O2A-CGA
7	I	101	BCL	CAA-CBA-CGA-O1A
7	S	101	BCL	CAA-CBA-CGA-O1A
11	L	307	PGV	O02-C1-C2-C3
10	M	406	8K6	C4-C5-C6-C7
11	D	103	PGV	O02-C1-O01-C02
7	N	101	BCL	C10-C11-C12-C13
11	D	103	PGV	C03-O11-P-O13
14	M	402	UQ8	C41-C42-C43-C44
7	e	102	BCL	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	102	A1EL2	C28-C29-C30-C31
8	A	102	A1EL2	C28-C29-C30-C35
8	B	102	A1EL2	C28-C29-C30-C31
8	B	102	A1EL2	C28-C29-C30-C35
8	C	103	A1EL2	C28-C29-C30-C31
8	C	103	A1EL2	C28-C29-C30-C35
8	D	102	A1EL2	C28-C29-C30-C31
8	D	102	A1EL2	C28-C29-C30-C35
8	E	102	A1EL2	C28-C29-C30-C31
8	E	102	A1EL2	C28-C29-C30-C35
8	F	102	A1EL2	C28-C29-C30-C31
8	F	102	A1EL2	C28-C29-C30-C35
8	G	102	A1EL2	C28-C29-C30-C31
8	G	102	A1EL2	C28-C29-C30-C35
8	Q	102	A1EL2	C28-C29-C30-C31
8	Q	102	A1EL2	C28-C29-C30-C35
8	I	102	A1EL2	C28-C29-C30-C31
8	J	102	A1EL2	C11-C10-C3-C2
8	K	102	A1EL2	C28-C29-C30-C31
8	K	102	A1EL2	C28-C29-C30-C35
8	O	103	A1EL2	C11-C10-C3-C4
8	O	103	A1EL2	C28-C29-C30-C31
8	O	103	A1EL2	C28-C29-C30-C35
8	P	102	A1EL2	C28-C29-C30-C31
8	P	102	A1EL2	C28-C29-C30-C35
8	r	103	A1EL2	C28-C29-C30-C31
10	Q	103	8K6	C6-C7-C8-C9
7	k	101	BCL	C15-C16-C17-C18
11	M	408	PGV	O01-C1-C2-C3
7	i	101	BCL	C16-C17-C18-C20
7	b	102	BCL	CAA-CBA-CGA-O1A
7	N	101	BCL	CAA-CBA-CGA-O2A
7	R	101	BCL	C2-C3-C5-C6
7	I	101	BCL	C16-C17-C18-C19
7	E	101	BCL	CAD-CBD-CGD-O1D
7	P	101	BCL	CAD-CBD-CGD-O1D
7	d	102	BCL	CAD-CBD-CGD-O1D
13	L	305	BPH	CAD-CBD-CGD-O1D
7	G	101	BCL	CAA-CBA-CGA-O2A
7	j	102	BCL	C6-C7-C8-C9
11	F	103	PGV	C9-C10-C11-C12
7	B	101	BCL	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	T	302	LHG	C26-C27-C28-C29
11	L	308	PGV	O12-C04-C05-C06
7	f	102	BCL	C3-C5-C6-C7
7	s	101	BCL	C13-C15-C16-C17
7	C	101	BCL	C2C-C3C-CAC-CBC
7	K	101	BCL	C6-C7-C8-C10
7	S	101	BCL	C2-C3-C5-C6
7	S	101	BCL	C12-C13-C15-C16
7	O	101	BCL	C3A-C2A-CAA-CBA
7	P	101	BCL	C11-C10-C8-C7
7	f	102	BCL	C2-C3-C5-C6
13	L	303	BPH	C3A-C2A-CAA-CBA
7	B	101	BCL	CAA-CBA-CGA-O1A
7	G	101	BCL	CAA-CBA-CGA-O1A
7	a	101	BCL	CAA-CBA-CGA-O1A
7	r	104	BCL	CAA-CBA-CGA-O2A
7	S	101	BCL	C5-C6-C7-C8
14	L	304	UQ8	C3-C4-O4-C4M
7	N	101	BCL	CAA-CBA-CGA-O1A
11	L	308	PGV	O12-C04-C05-O05
17	M	407	PEF	O3-C30-C31-C32
11	M	408	PGV	O02-C1-C2-C3
7	O	101	BCL	C2A-CAA-CBA-CGA
7	K	101	BCL	C4-C3-C5-C6
7	D	101	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

79 monomers are involved in 220 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	b	102	BCL	8	0
7	M	403	BCL	3	0
10	C	104	8K6	1	0
8	D	102	A1EL2	1	0
9	o	101	A1ELD	1	0
7	B	101	BCL	4	0
8	B	102	A1EL2	1	0
17	M	407	PEF	1	0
7	k	101	BCL	3	0
8	J	102	A1EL2	3	0
10	M	406	8K6	1	0
14	L	304	UQ8	6	0

Continued on next page...

Continued from previous page...

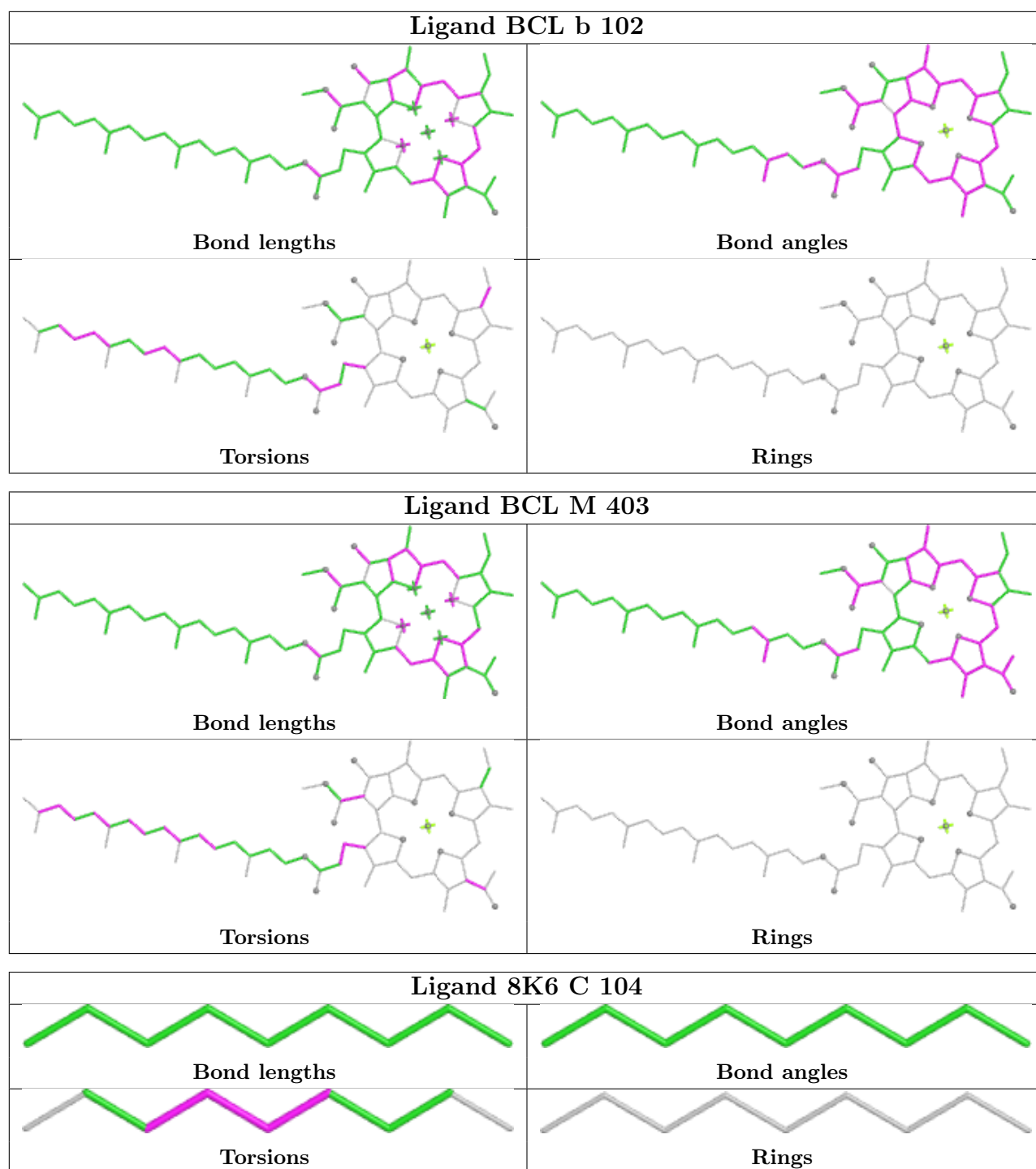
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	408	PGV	3	0
8	K	102	A1EL2	1	0
7	e	102	BCL	2	0
10	L	310	8K6	1	0
13	L	303	BPH	5	0
7	c	101	BCL	3	0
10	Q	104	8K6	4	0
7	G	101	BCL	1	0
11	D	103	PGV	8	0
19	T	302	LHG	3	0
12	L	309	LMT	2	0
7	C	101	BCL	5	0
7	j	102	BCL	2	0
7	R	101	BCL	2	0
12	N	103	LMT	1	0
10	Q	103	8K6	4	0
7	L	302	BCL	7	0
8	I	102	A1EL2	4	0
7	o	102	BCL	4	0
7	d	102	BCL	4	0
7	L	301	BCL	2	0
7	f	102	BCL	5	0
8	A	102	A1EL2	1	0
7	s	101	BCL	3	0
9	R	102	A1ELD	23	0
10	L	312	8K6	1	0
10	S	102	8K6	1	0
11	G	103	PGV	1	0
7	I	101	BCL	3	0
8	r	103	A1EL2	1	0
7	n	101	BCL	5	0
10	L	313	8K6	7	0
7	F	101	BCL	3	0
7	K	101	BCL	1	0
7	A	101	BCL	2	0
7	r	104	BCL	2	0
8	Q	102	A1EL2	1	0
13	L	305	BPH	1	0
8	r	102	A1EL2	8	0
9	e	101	A1ELD	7	0
9	B	103	A1ELD	1	0
8	P	102	A1EL2	1	0

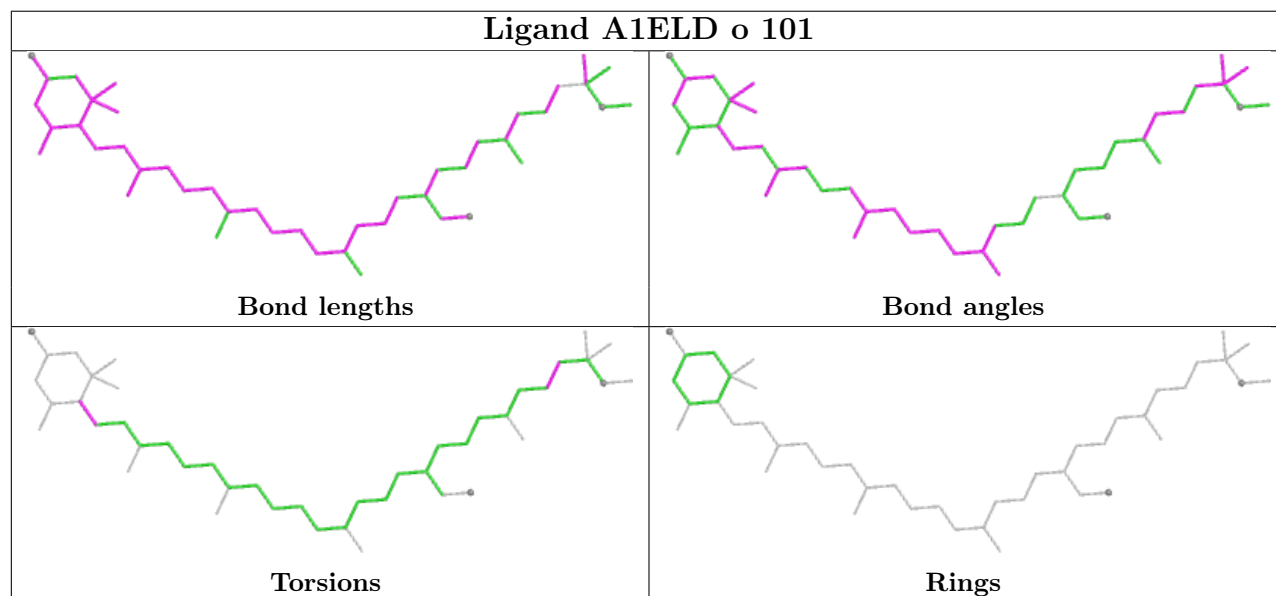
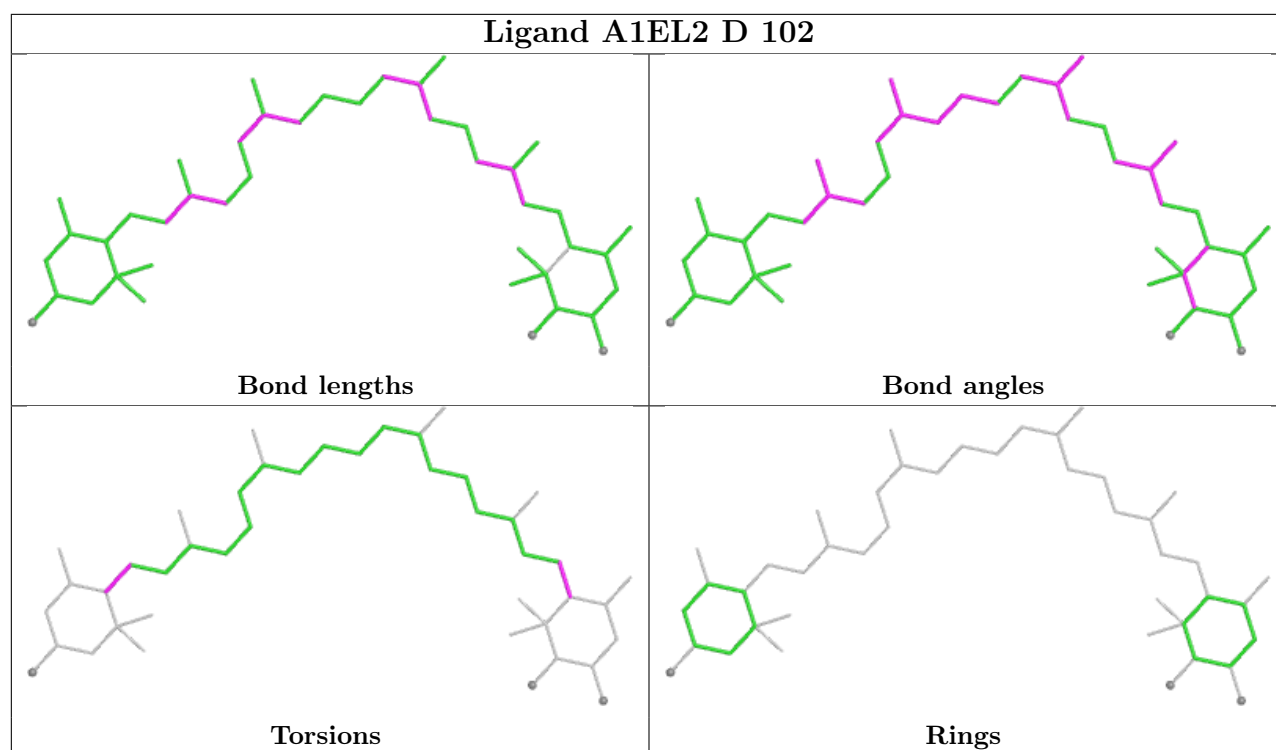
Continued on next page...

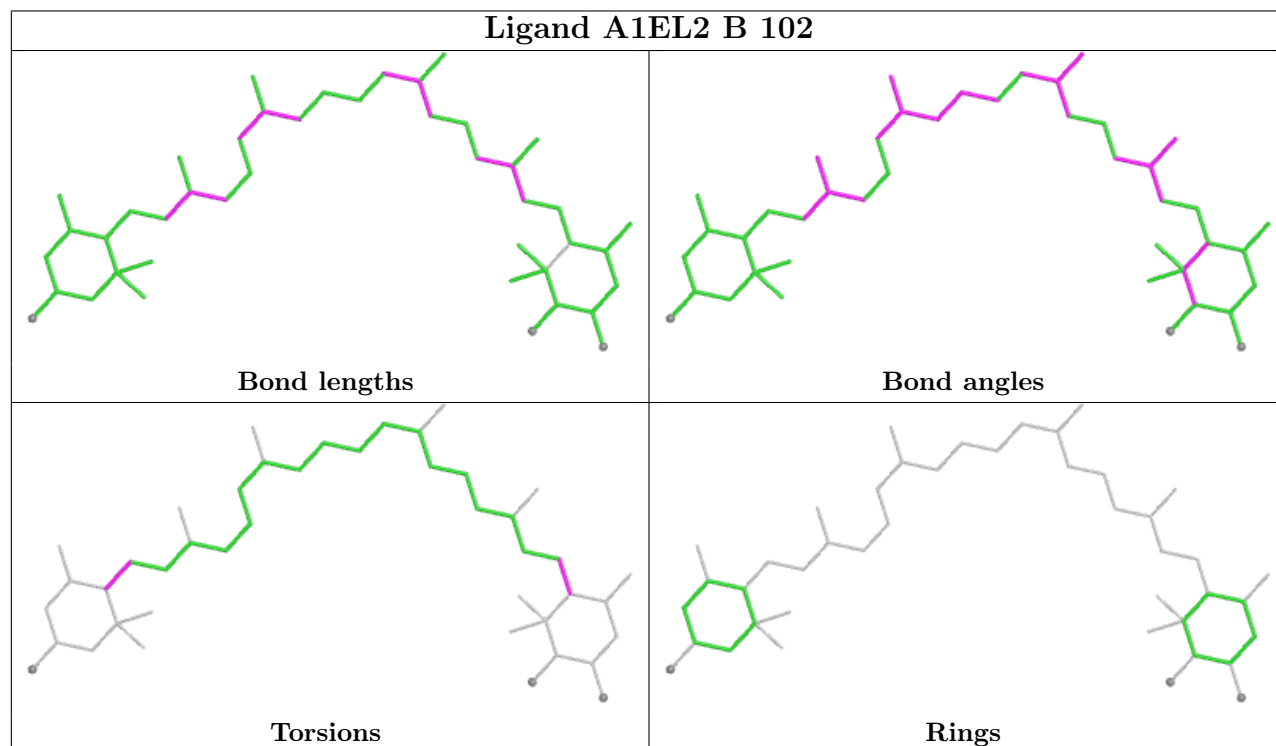
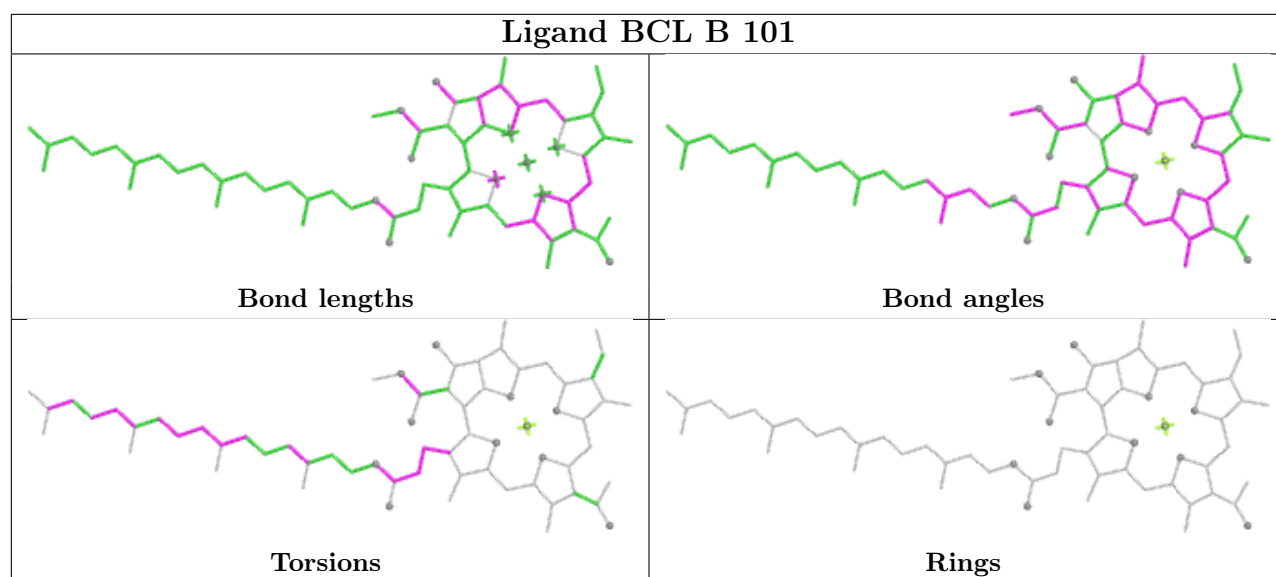
Continued from previous page...

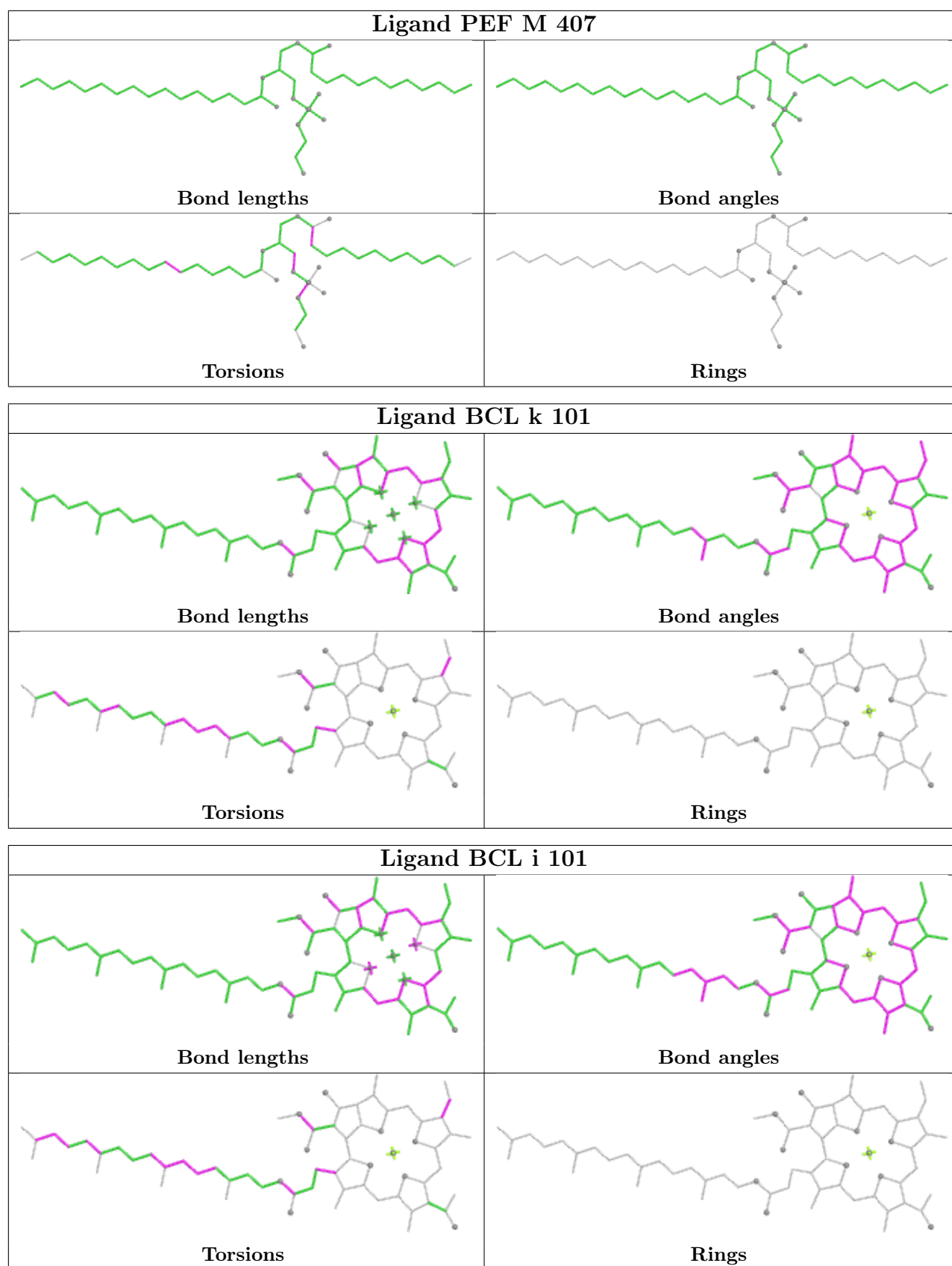
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	r	101	A1ELD	1	0
7	g	102	BCL	2	0
7	Q	101	BCL	1	0
8	E	102	A1EL2	1	0
7	q	102	BCL	3	0
7	S	101	BCL	3	0
7	p	101	BCL	3	0
11	L	307	PGV	1	0
7	O	101	BCL	2	0
10	L	311	8K6	2	0
8	F	102	A1EL2	1	0
11	F	103	PGV	4	0
9	g	101	A1ELD	3	0
7	N	101	BCL	3	0
7	E	101	BCL	3	0
9	d	101	A1ELD	1	0
7	M	401	BCL	1	0
14	M	402	UQ8	1	0
7	a	101	BCL	4	0
9	f	101	A1ELD	7	0
7	P	101	BCL	3	0
11	T	303	PGV	3	0
11	L	308	PGV	3	0
7	J	101	BCL	1	0
9	O	102	A1ELD	1	0

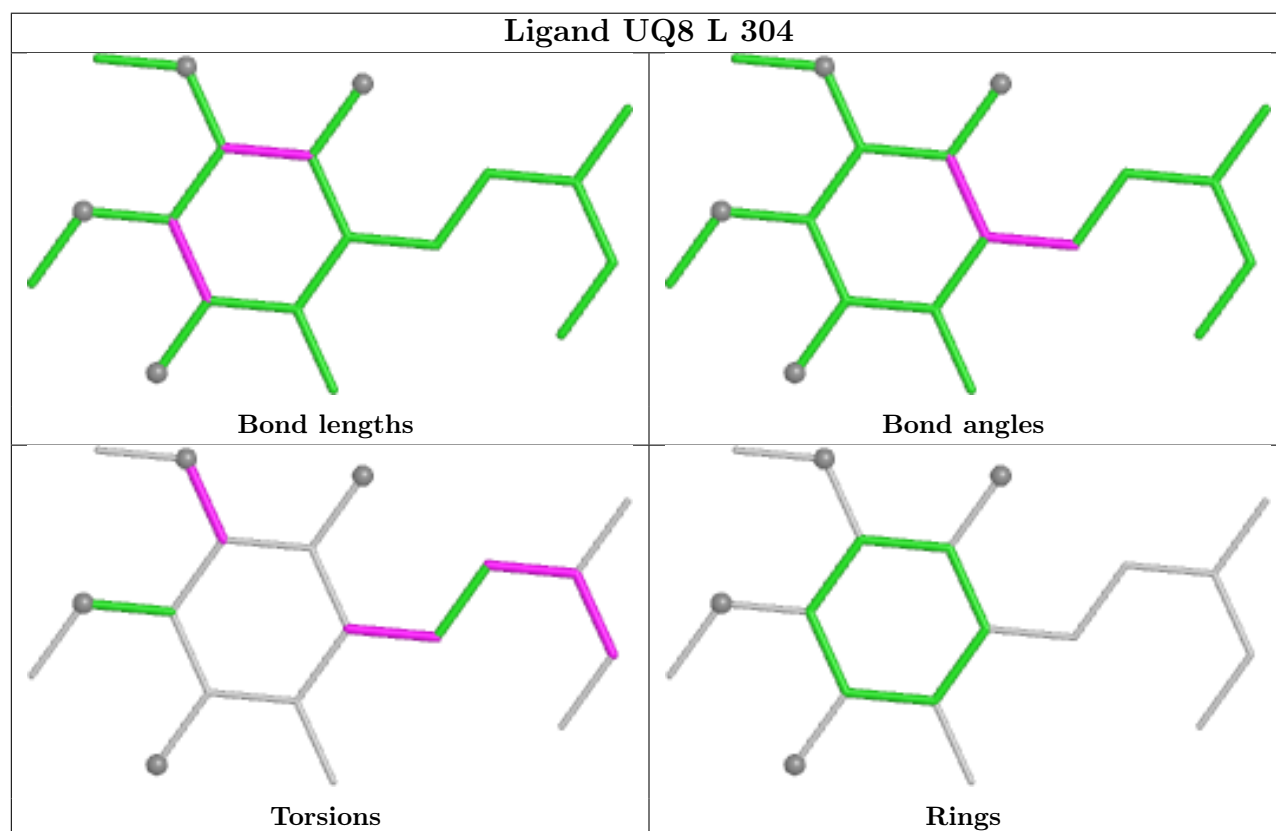
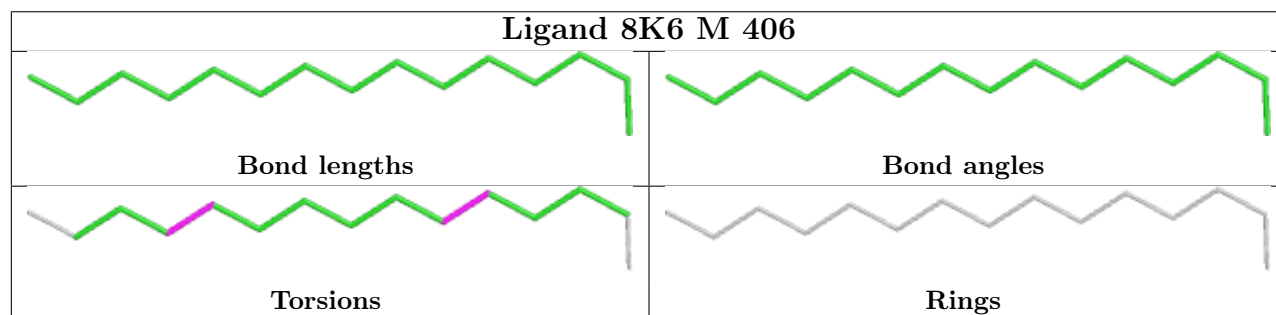
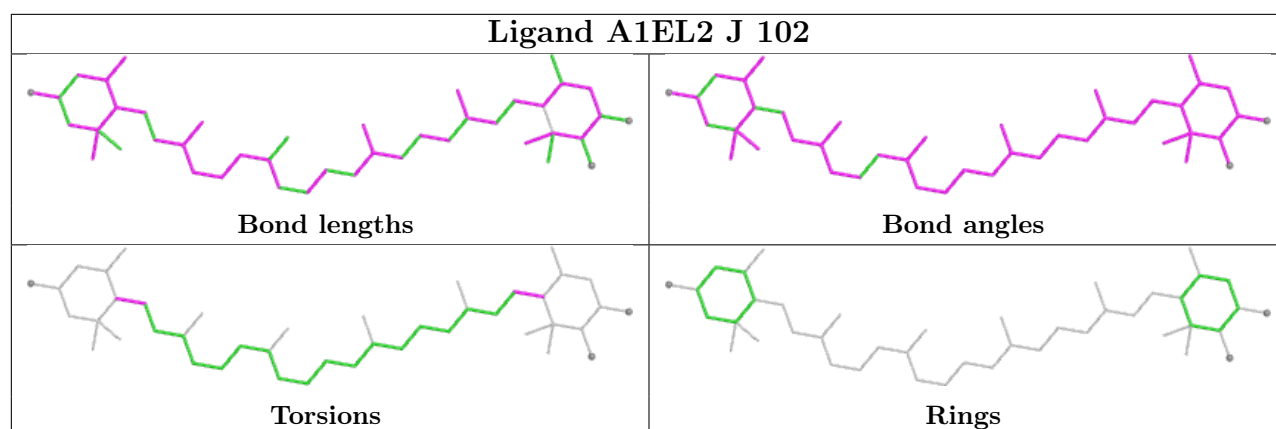
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

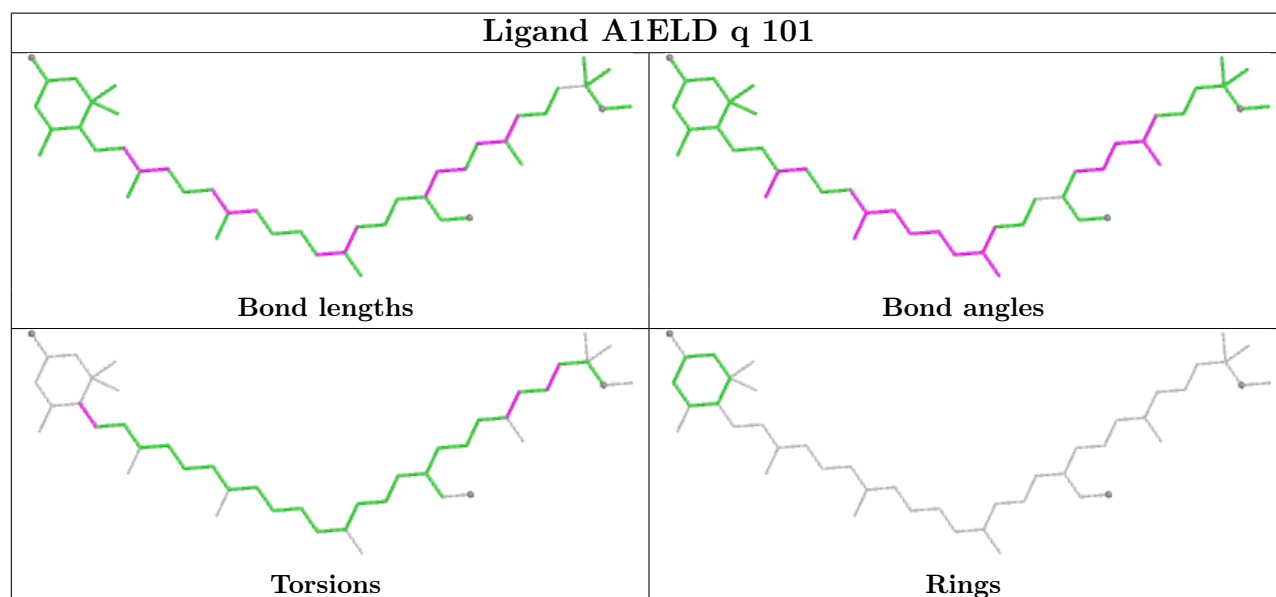
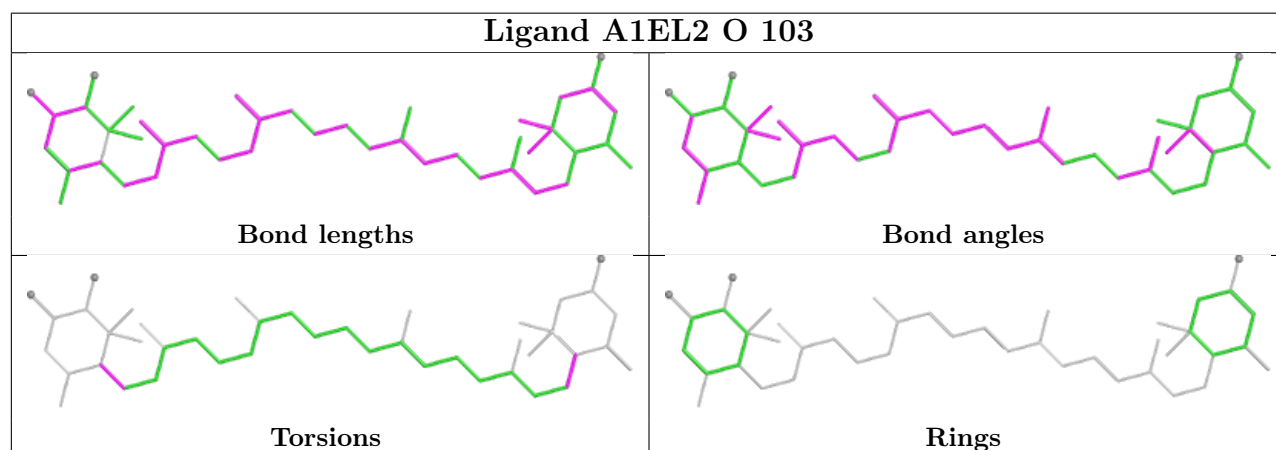
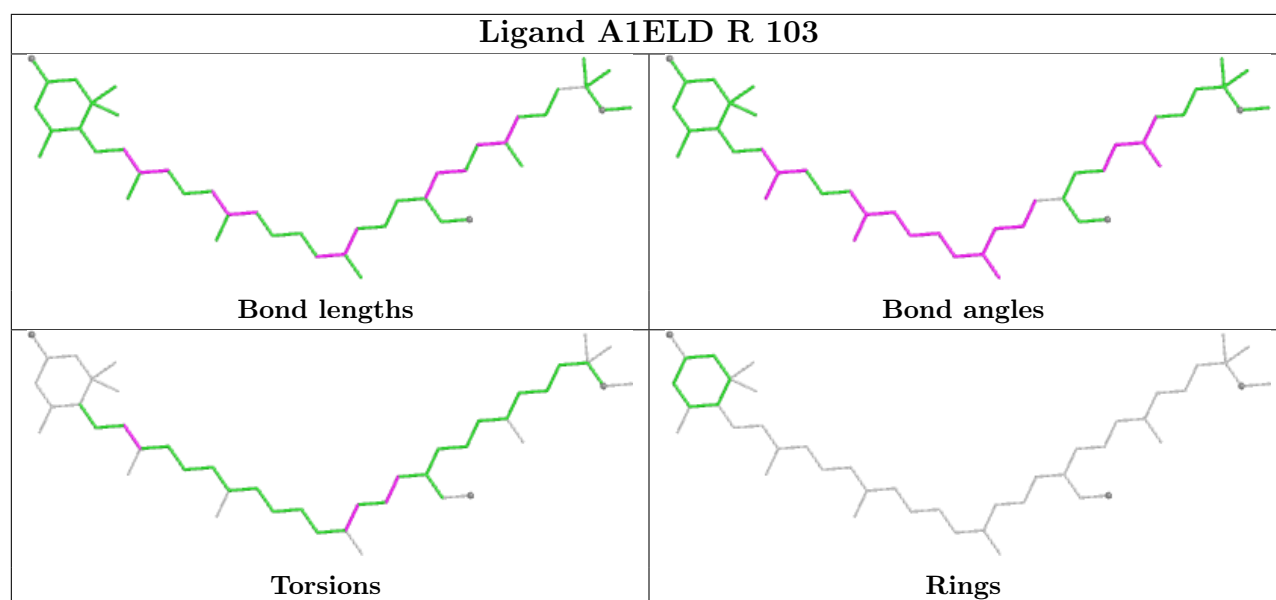


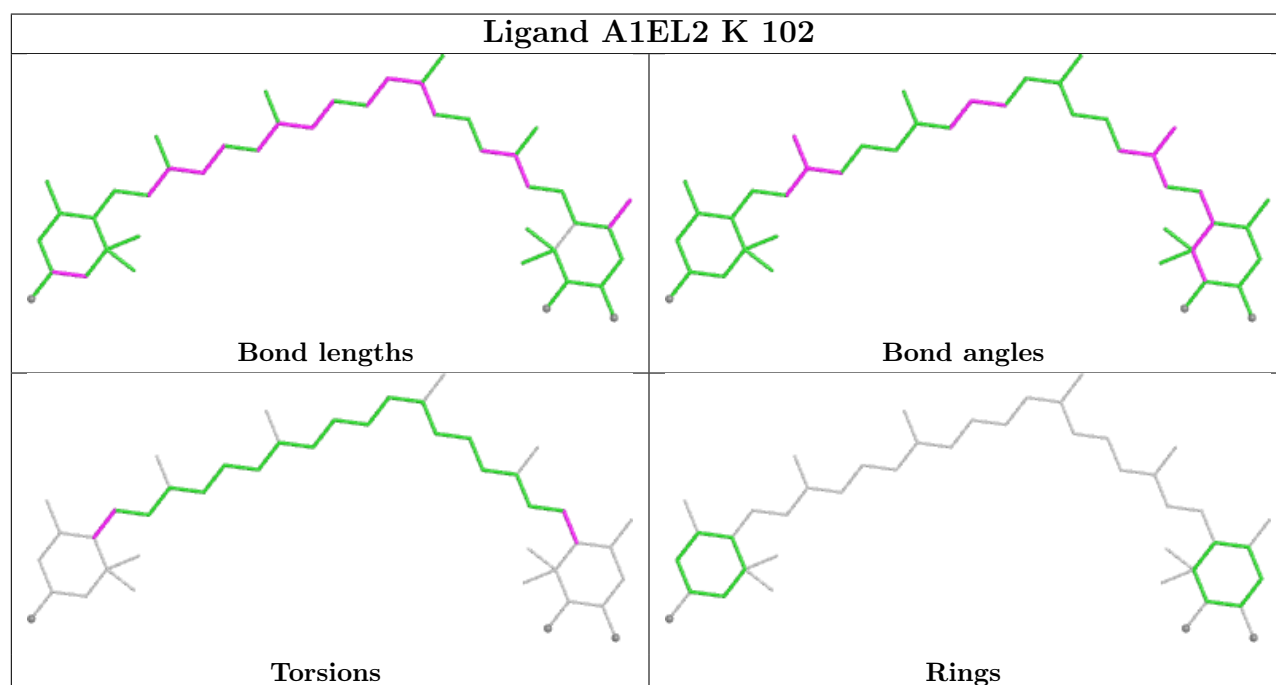
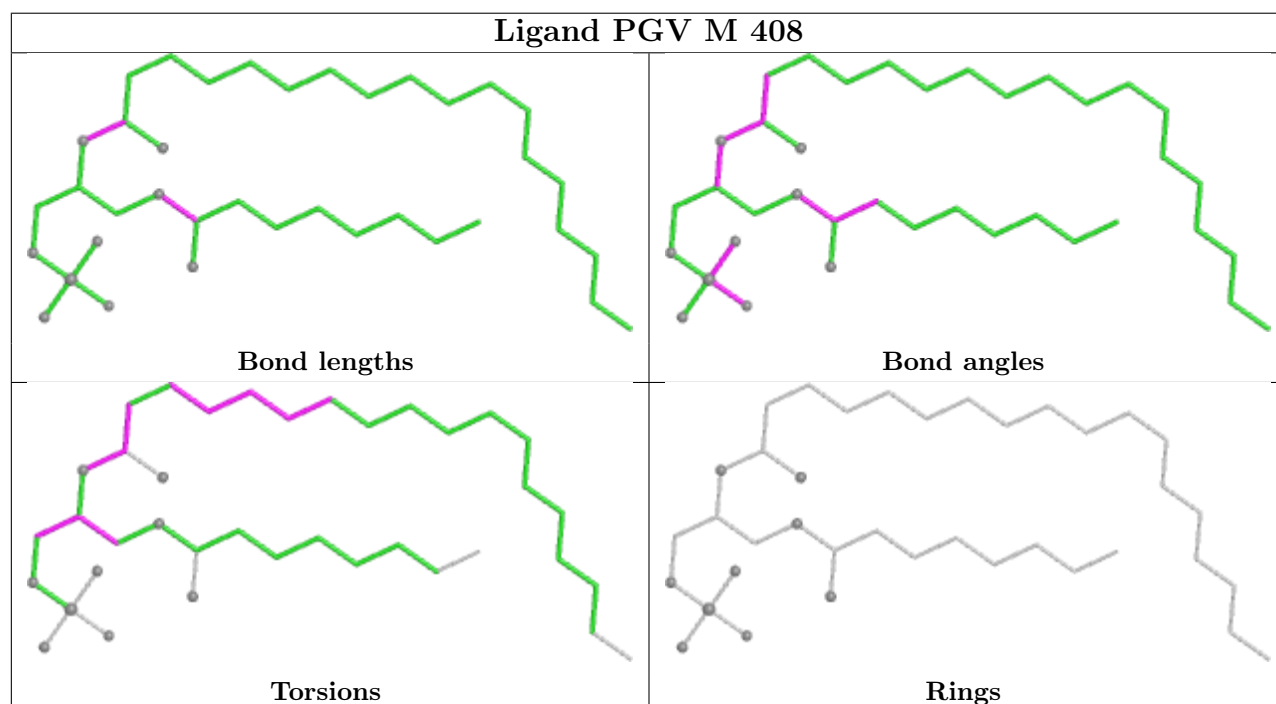
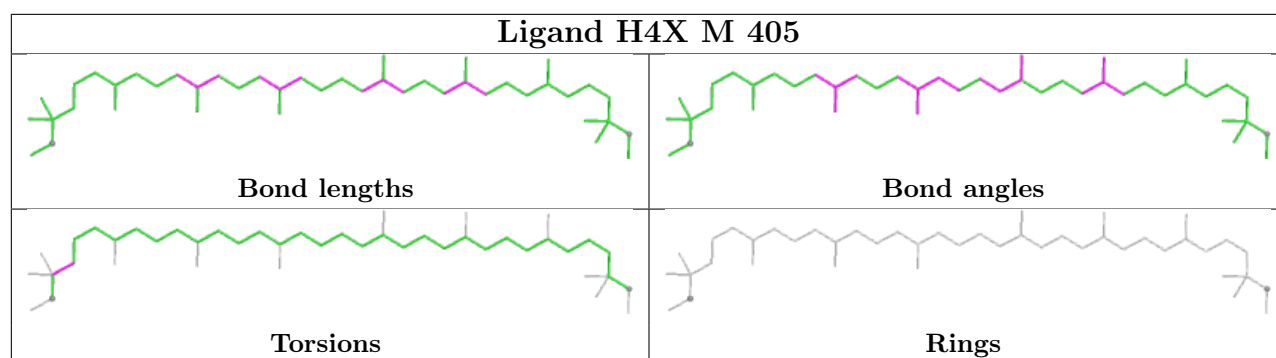


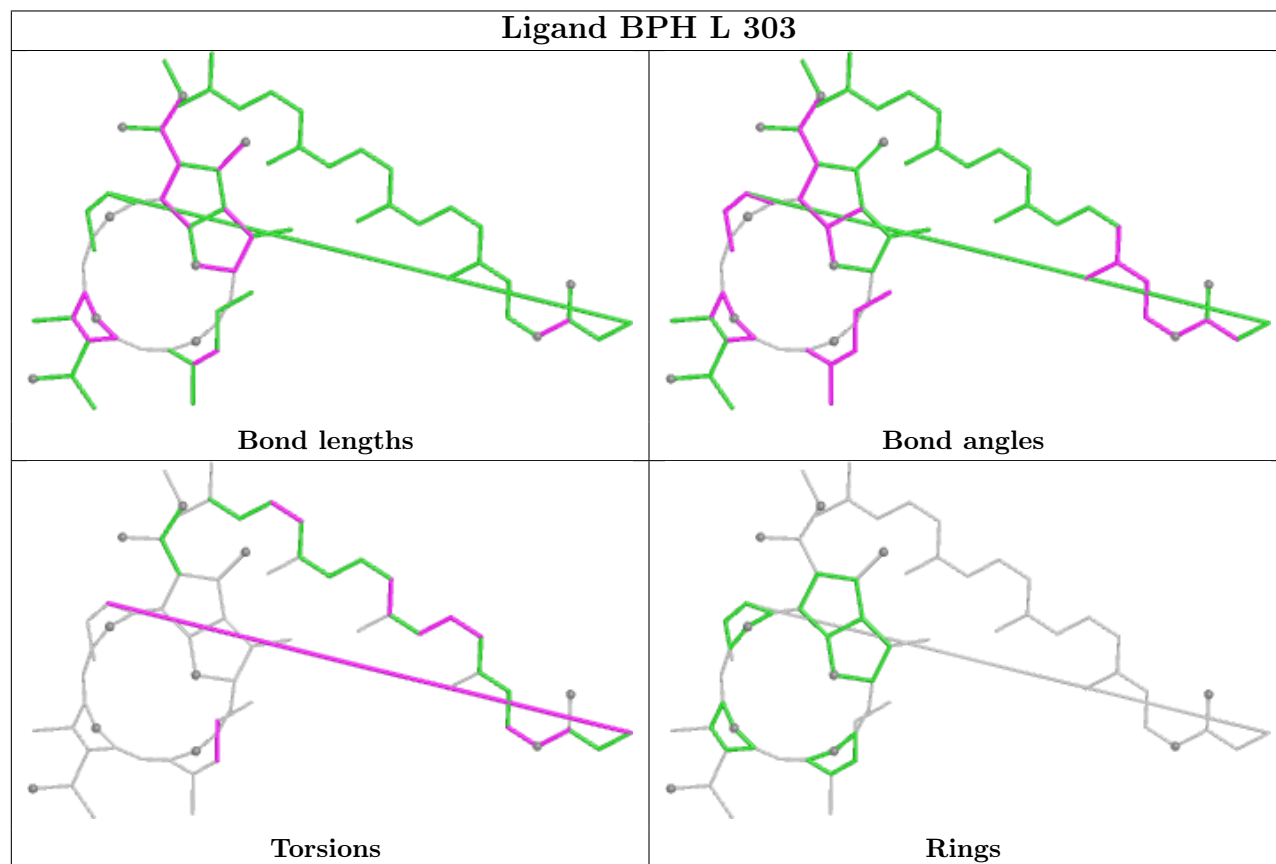
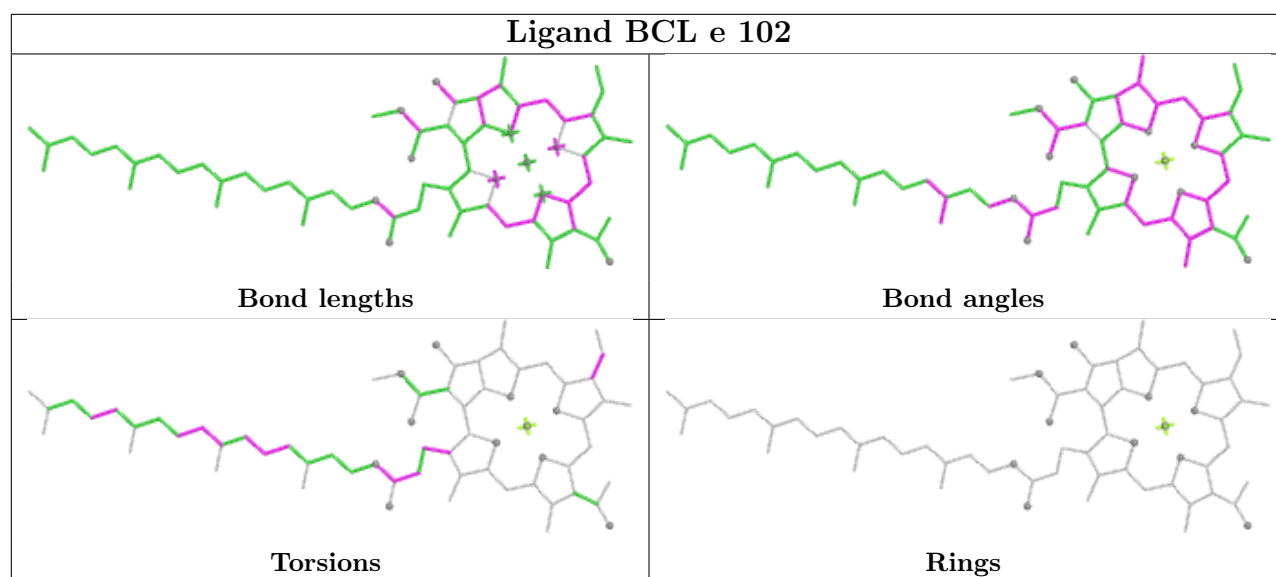


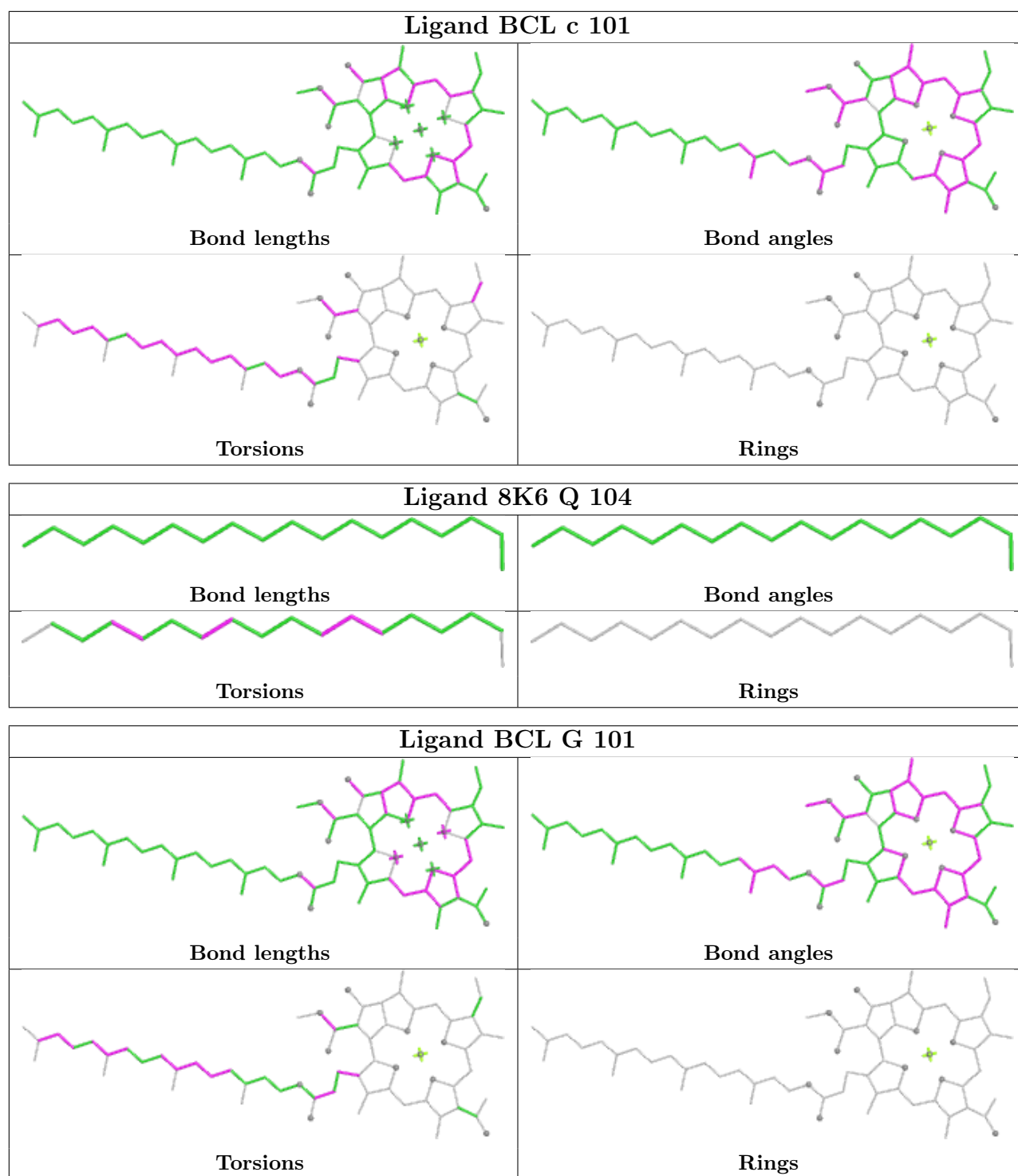


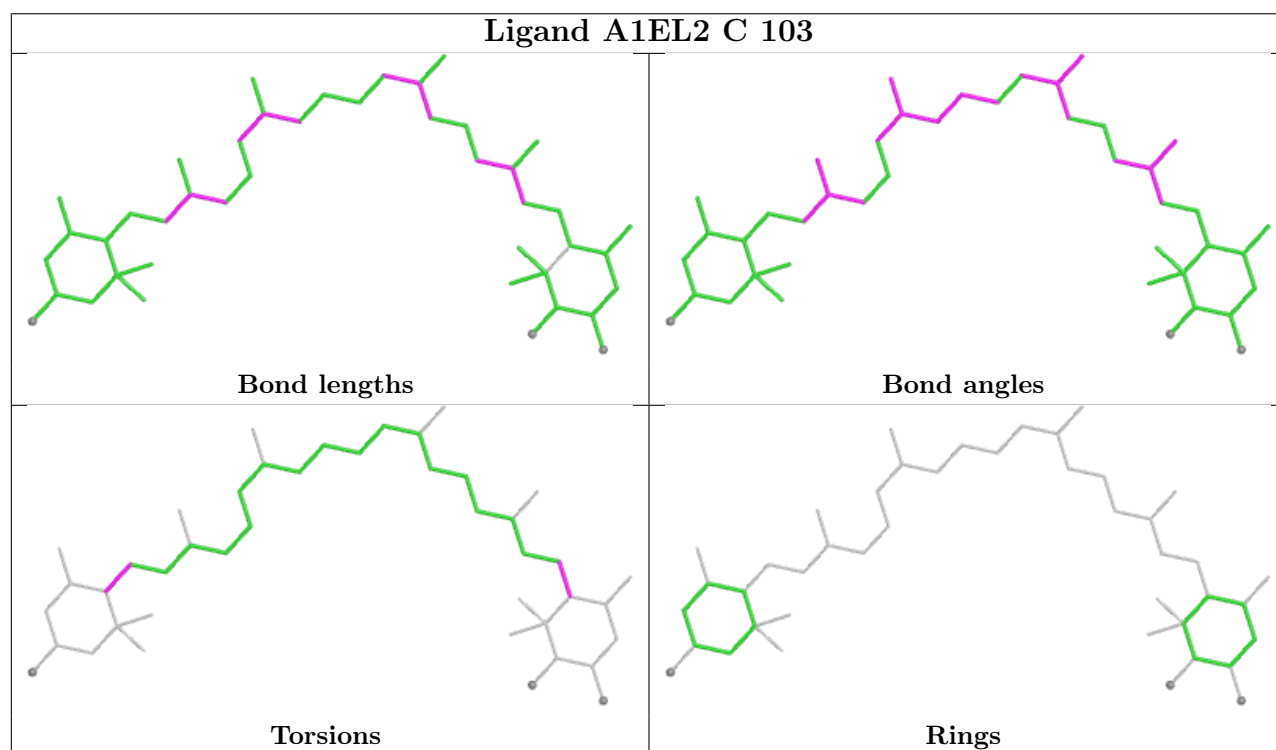
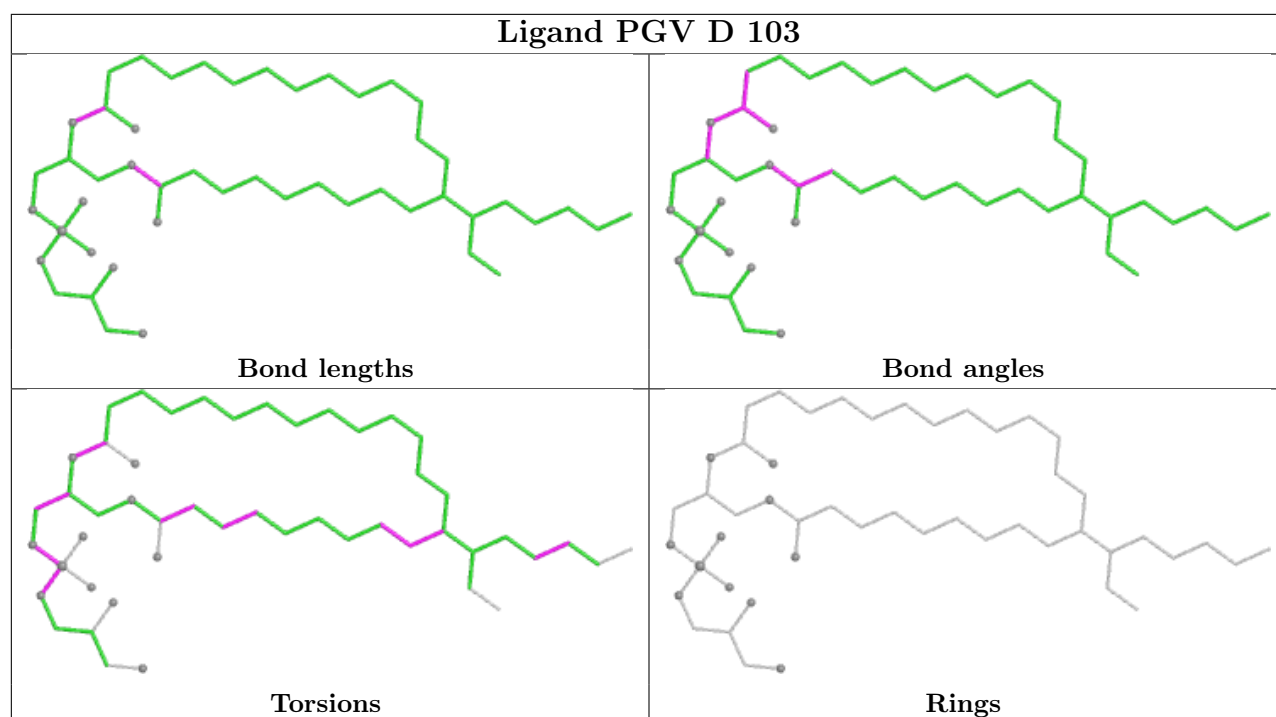


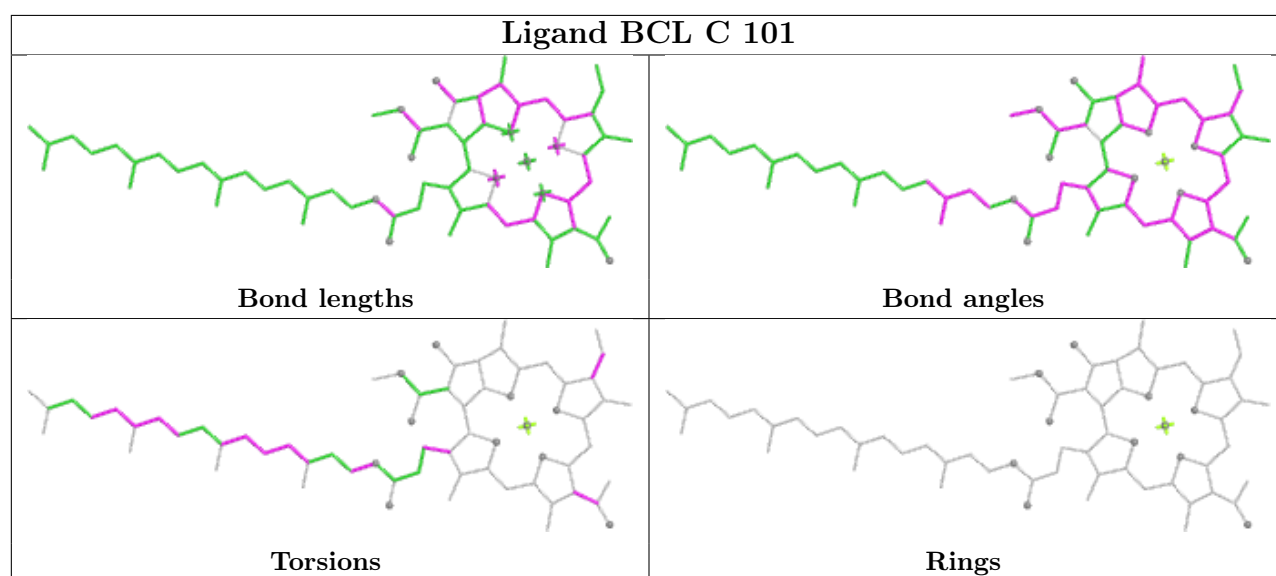
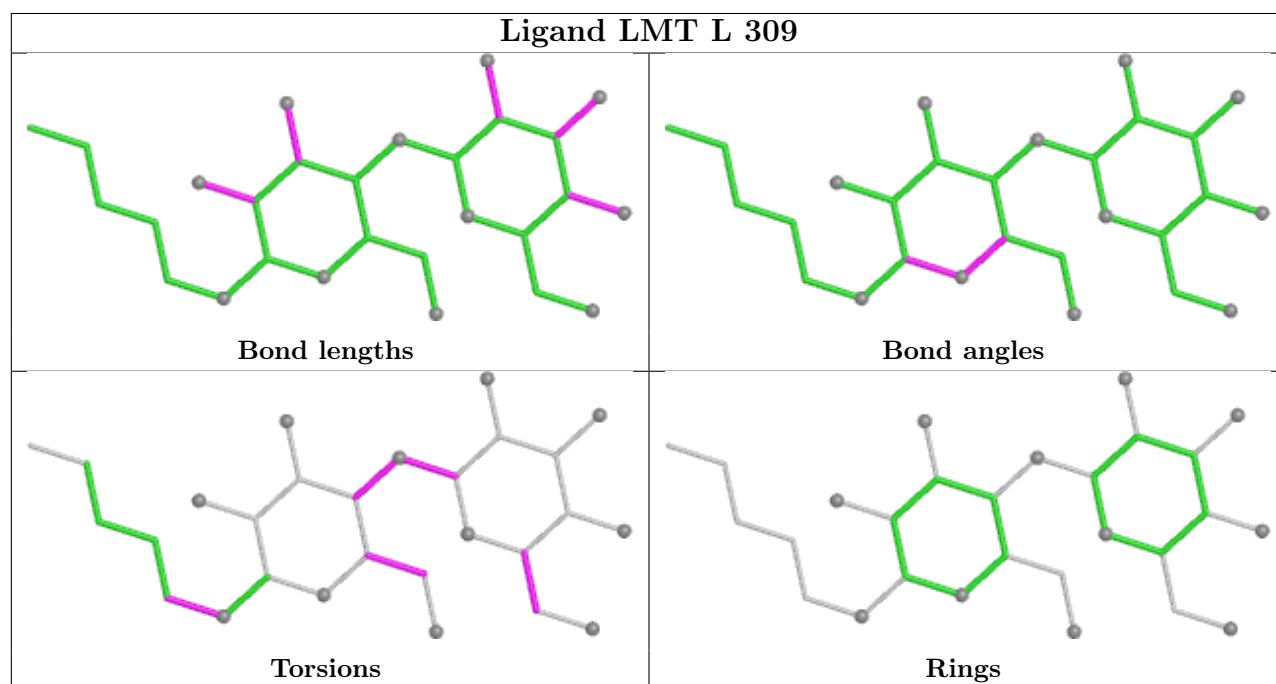
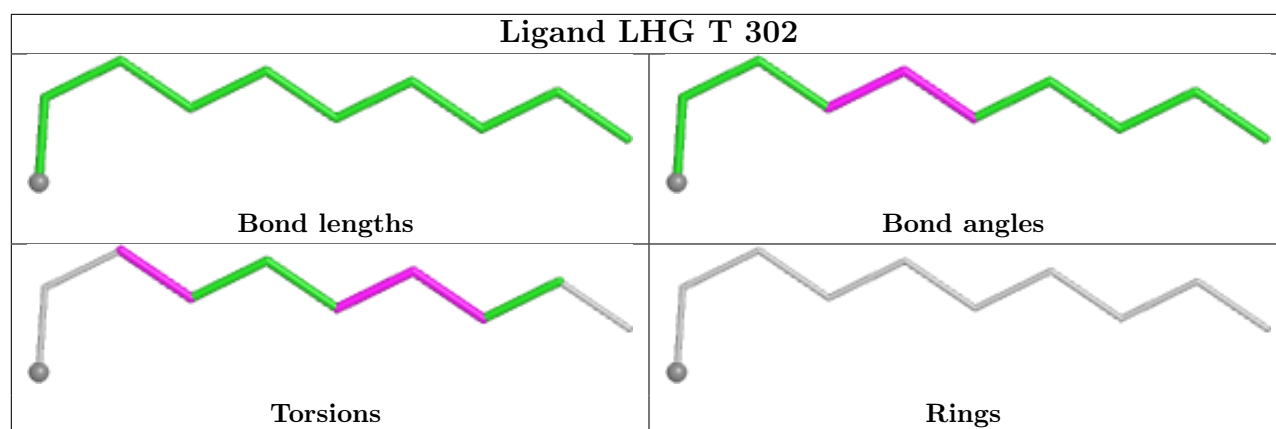


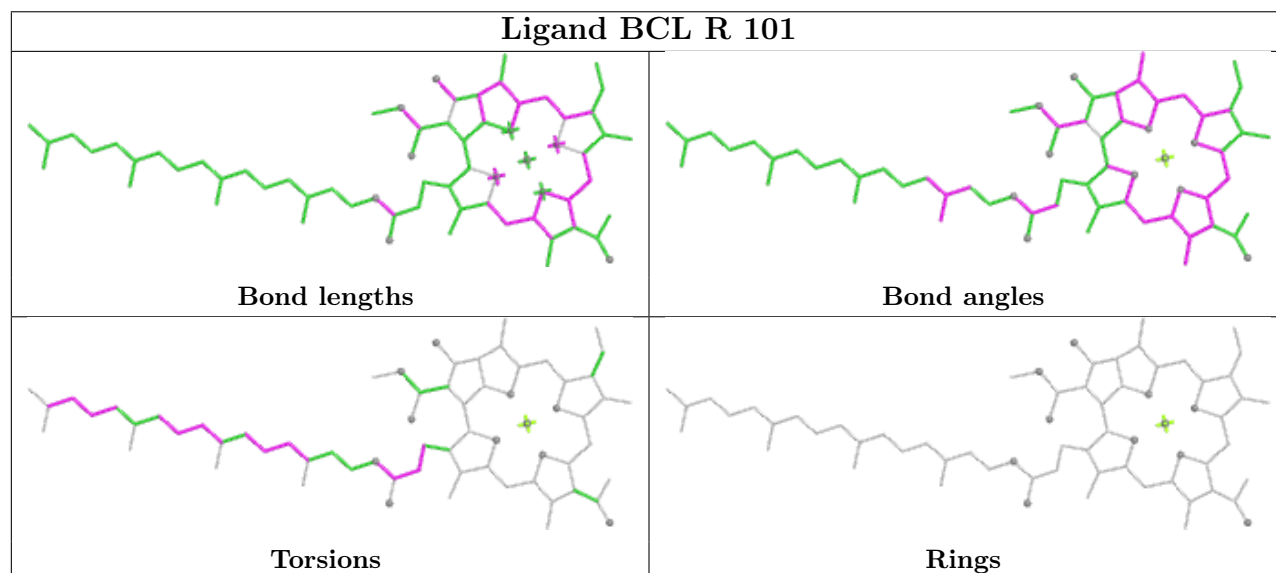
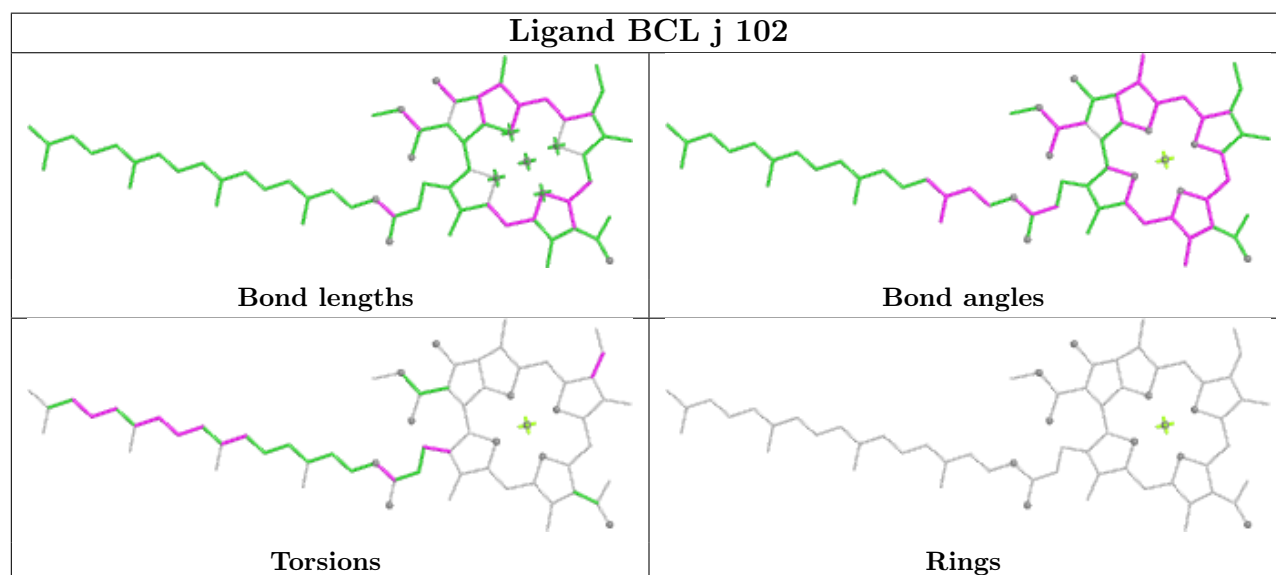
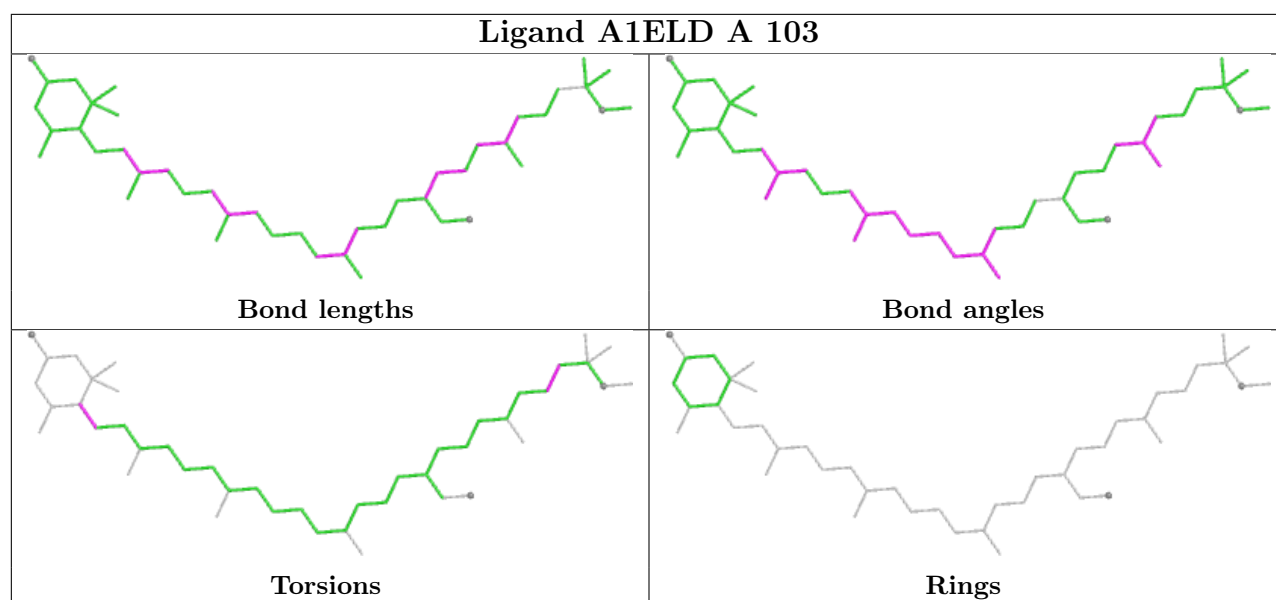


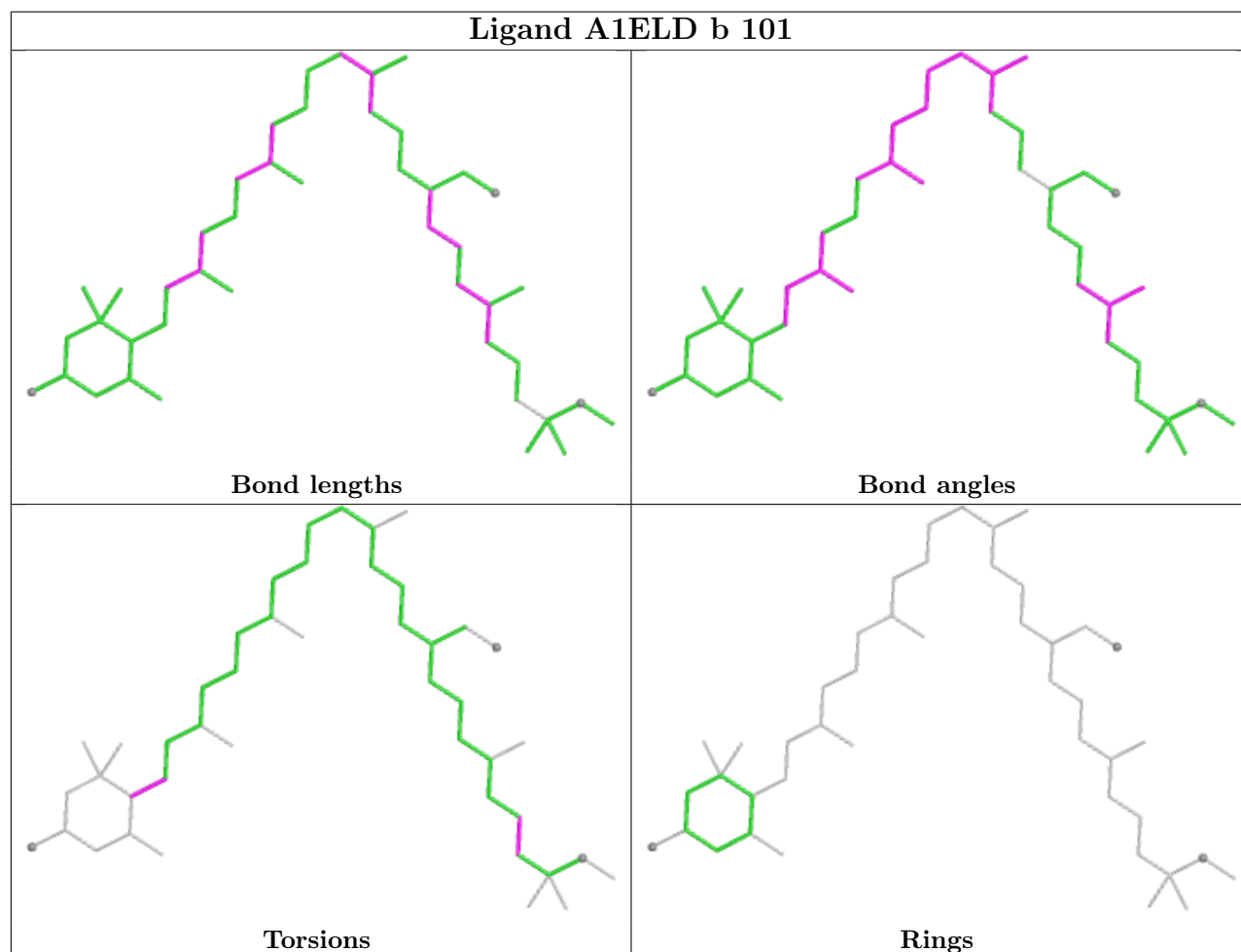
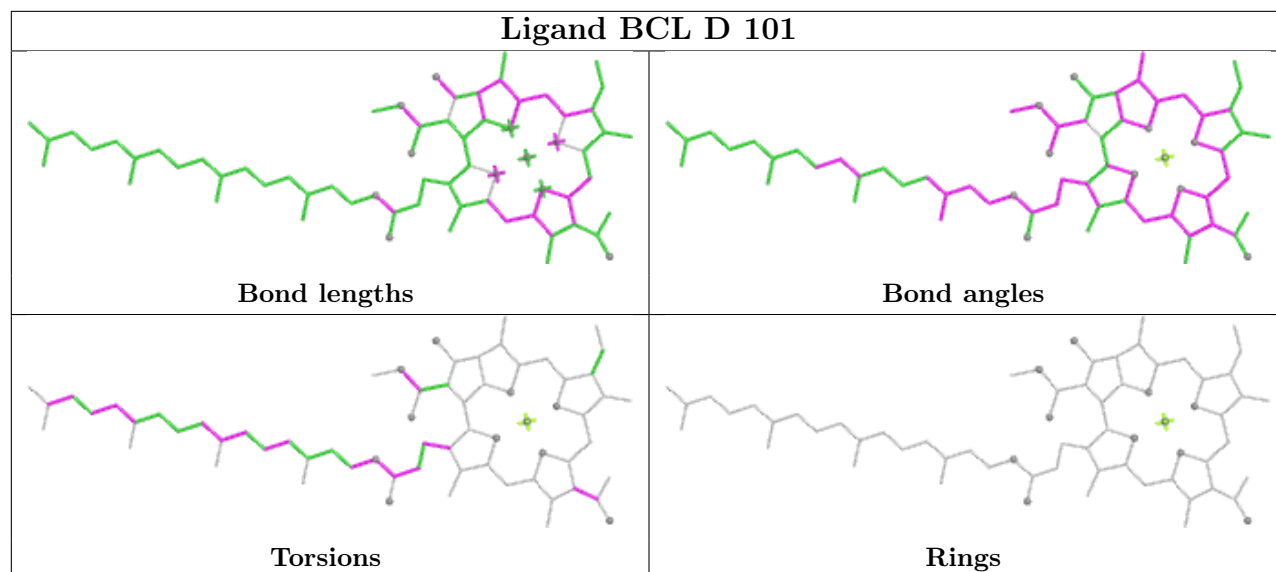


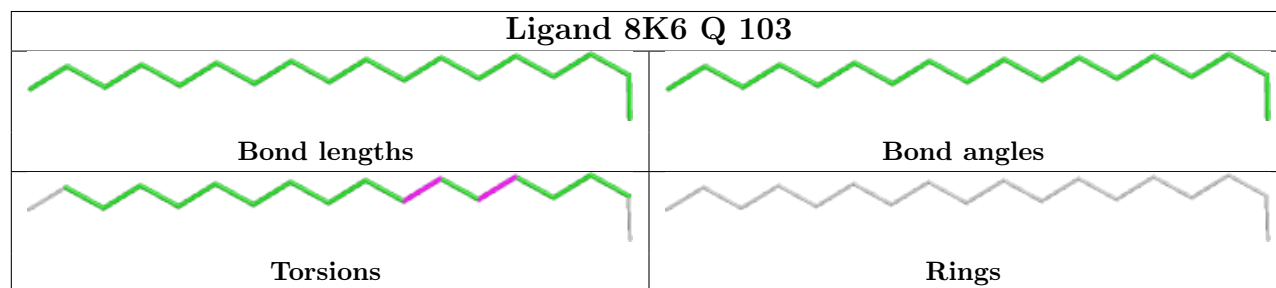
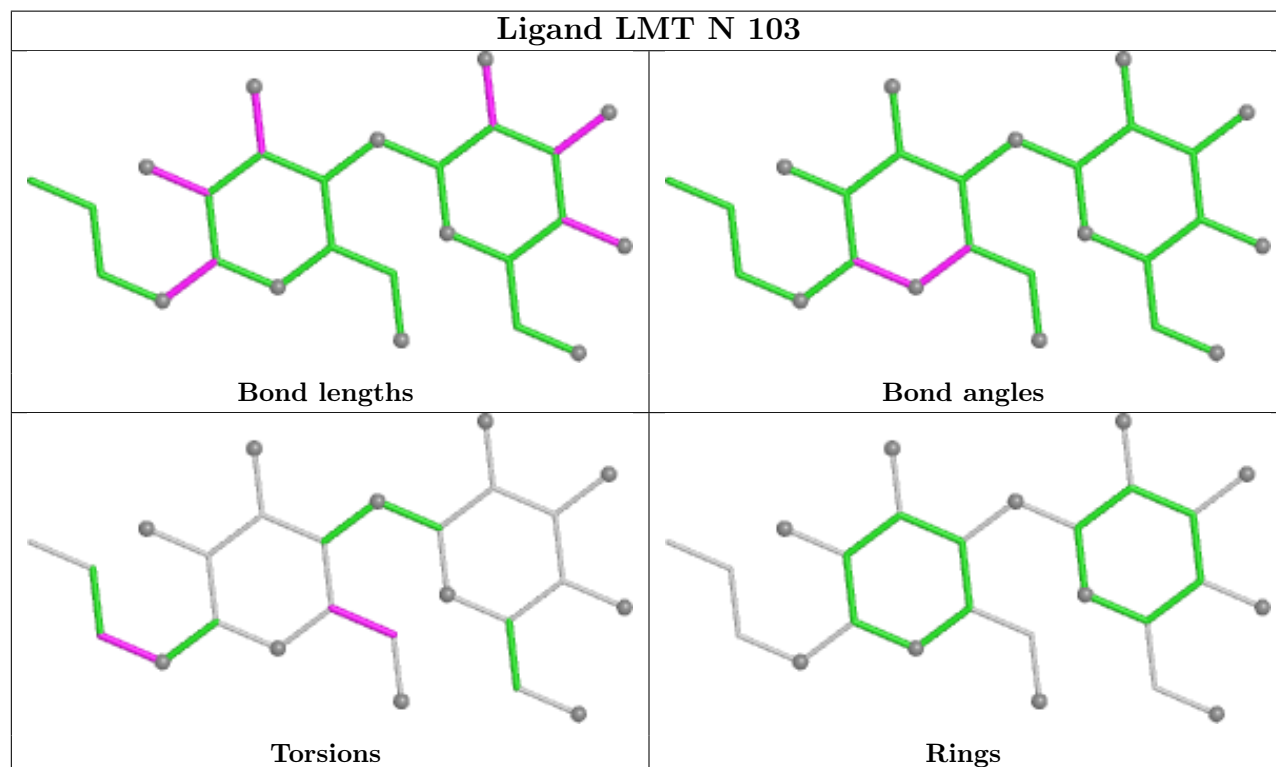
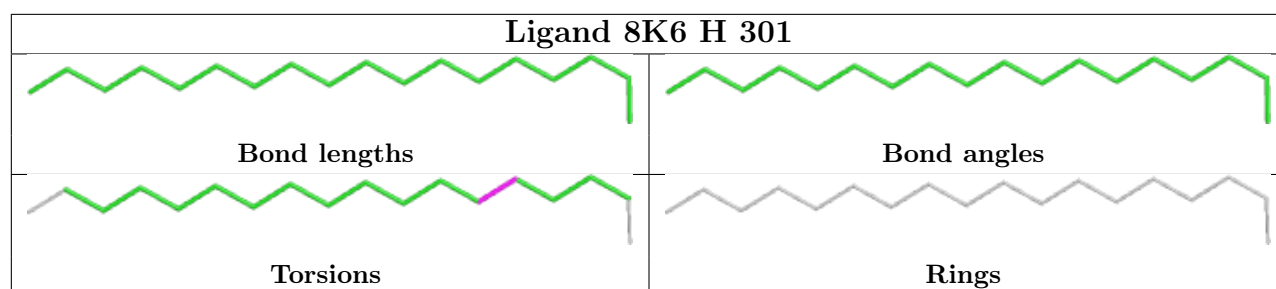


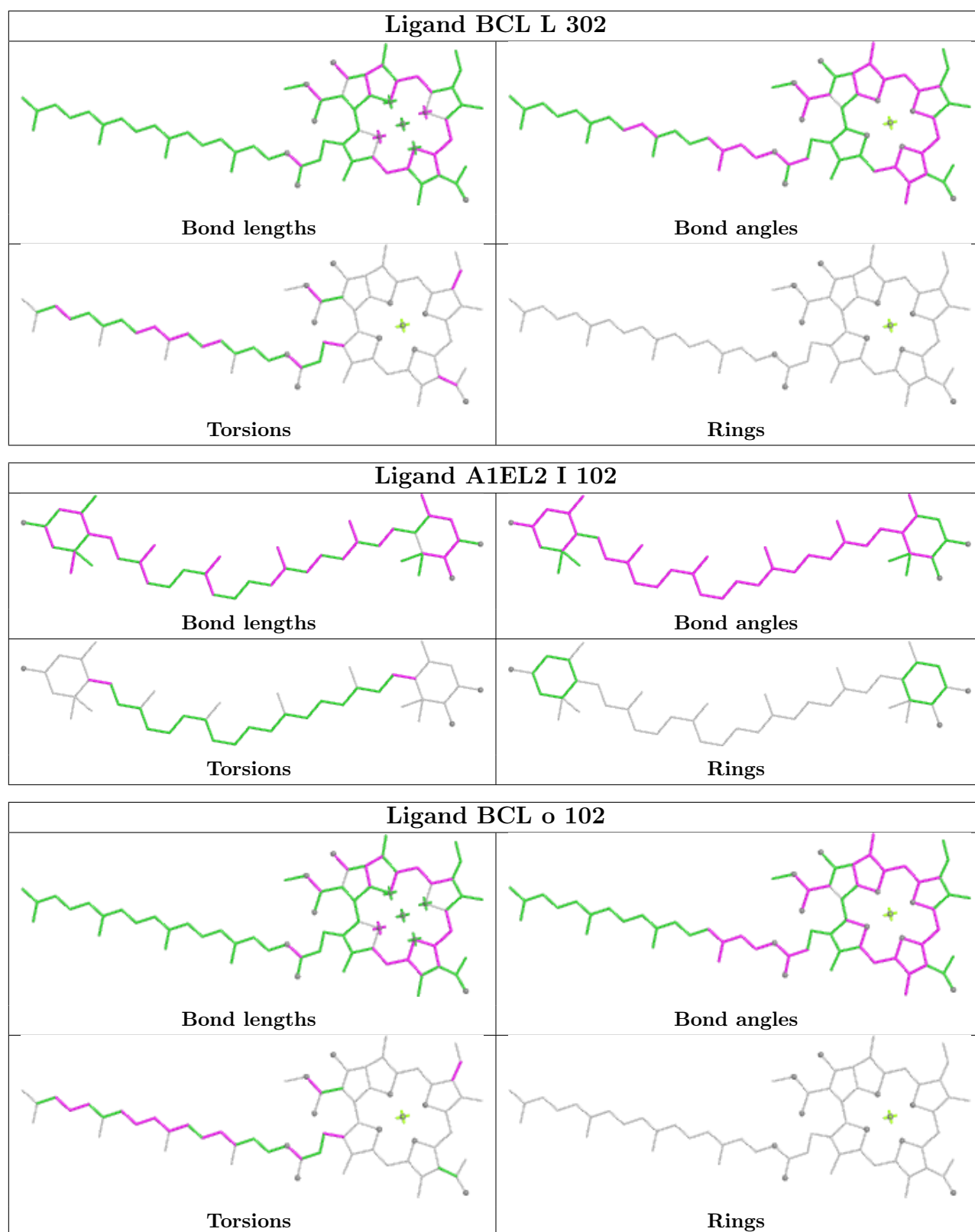


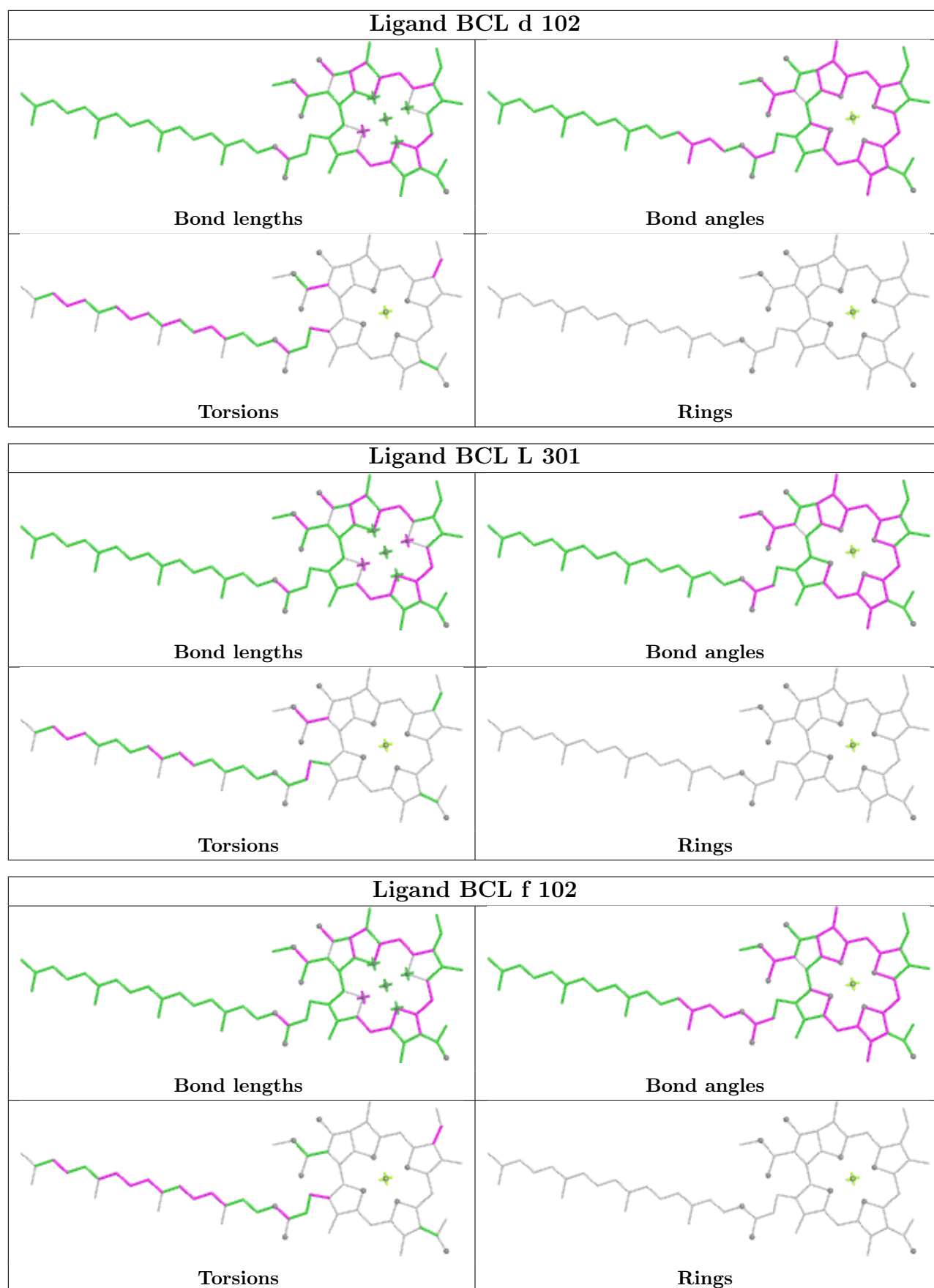


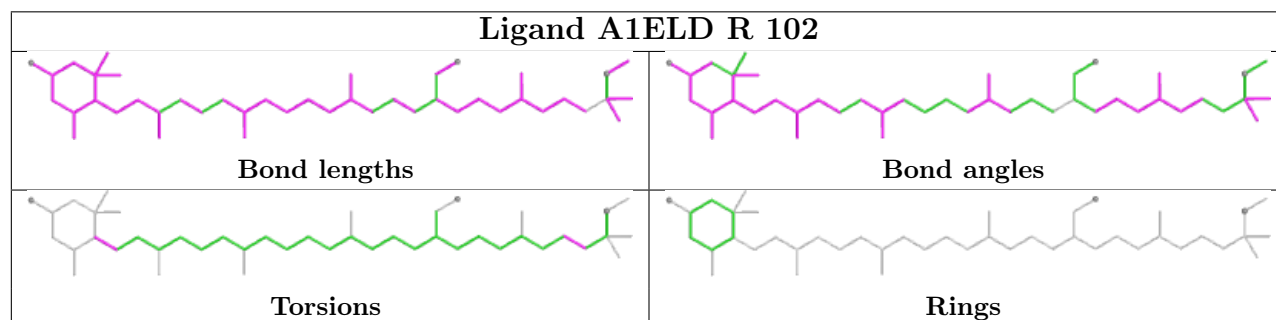
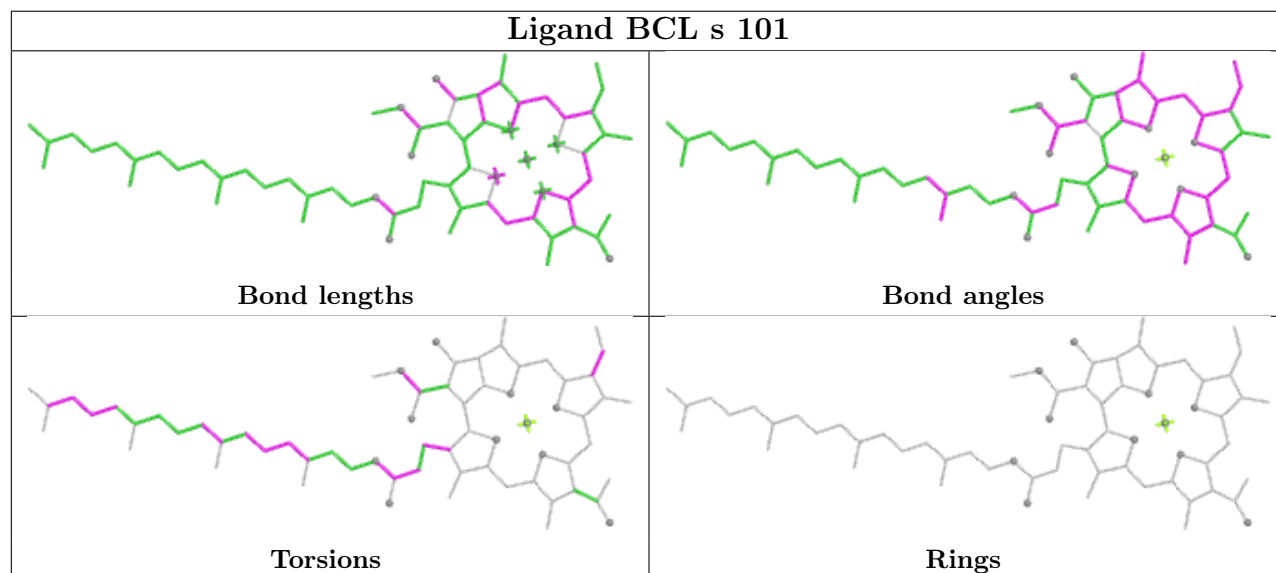
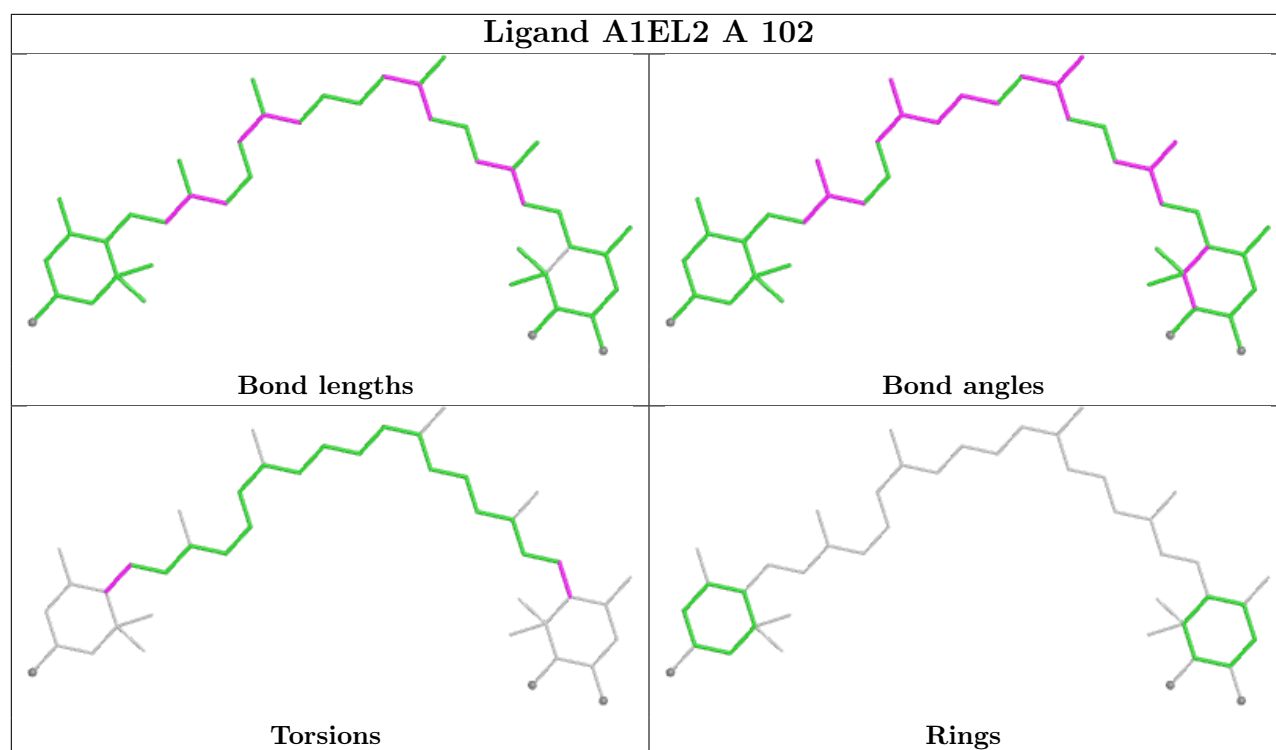


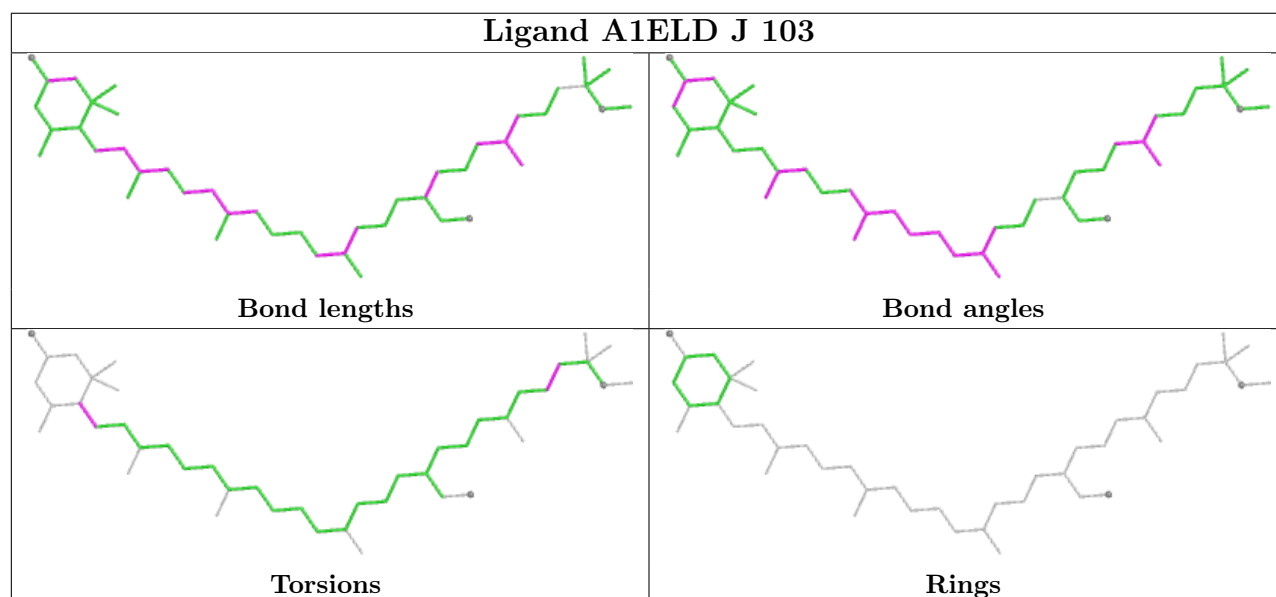
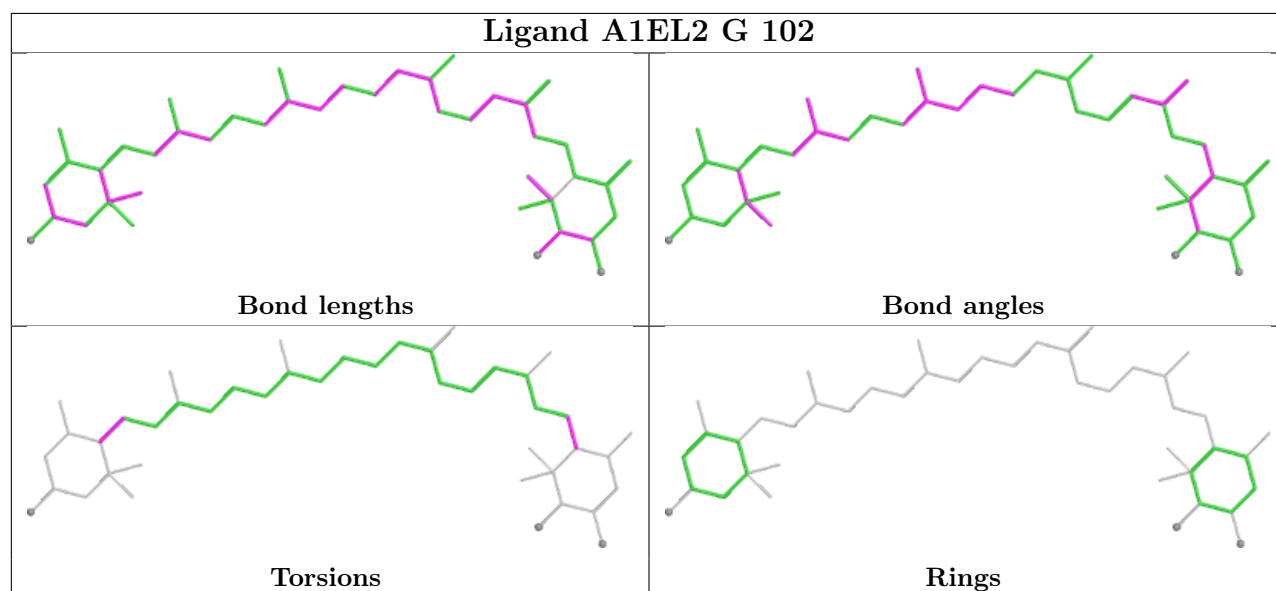
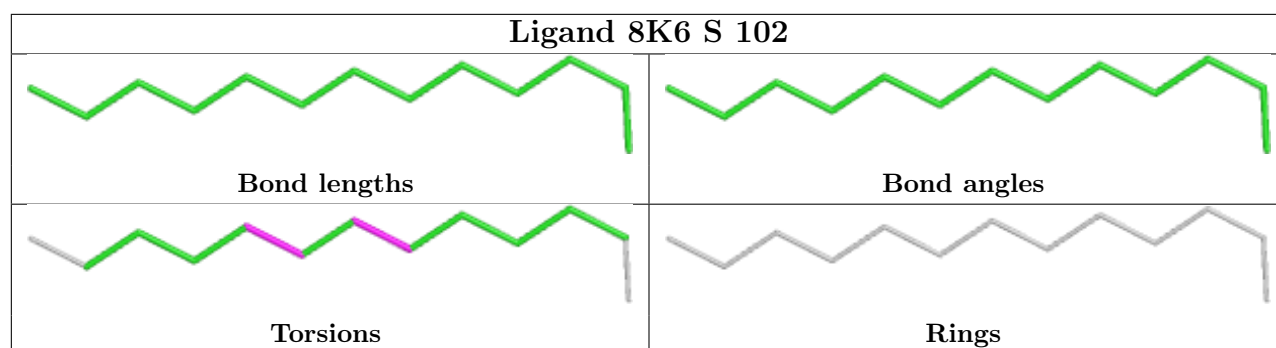


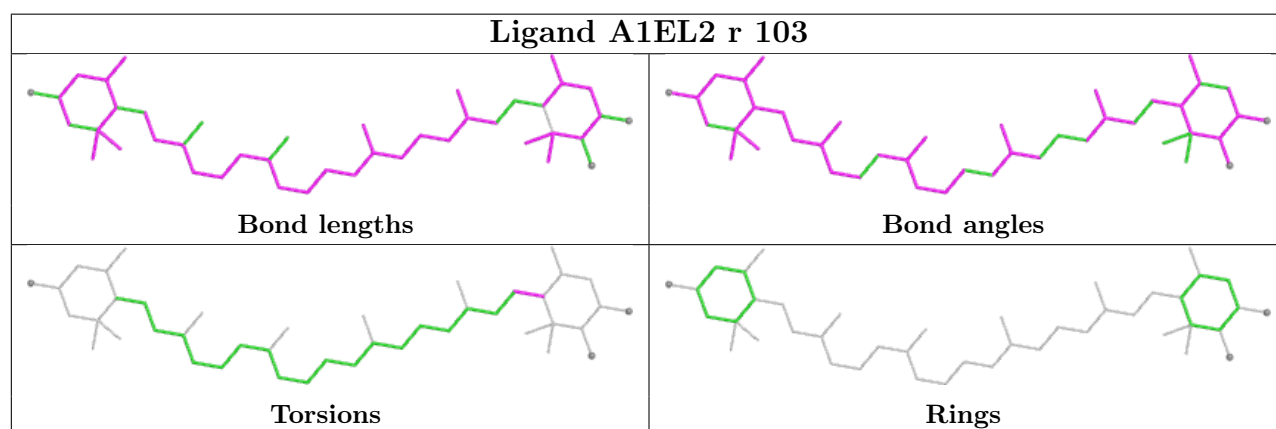
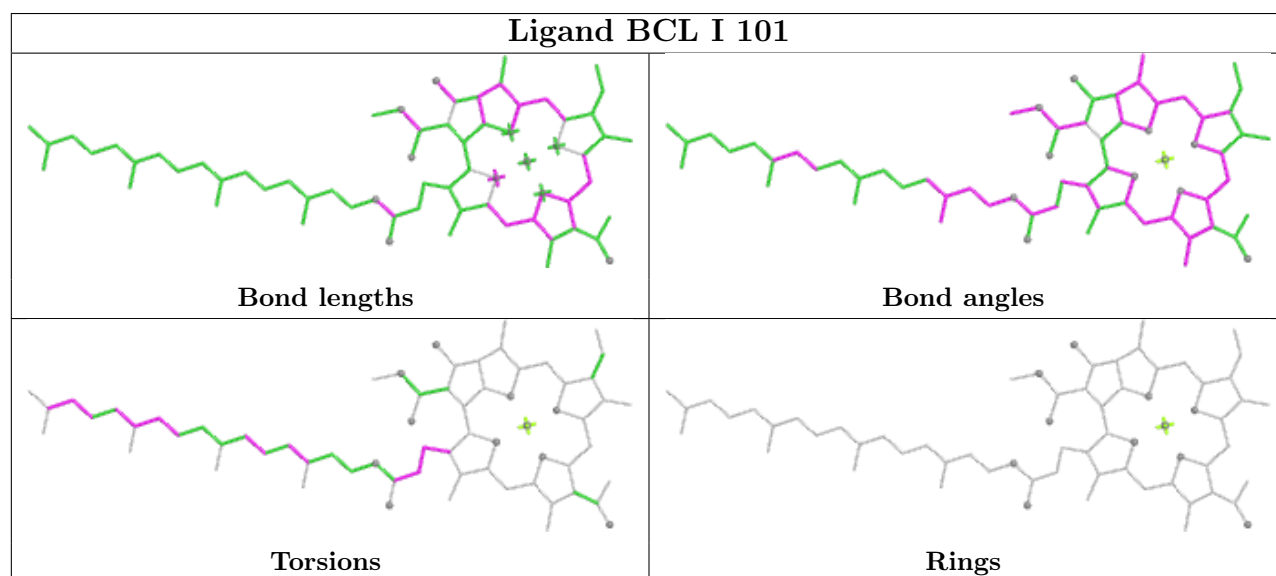
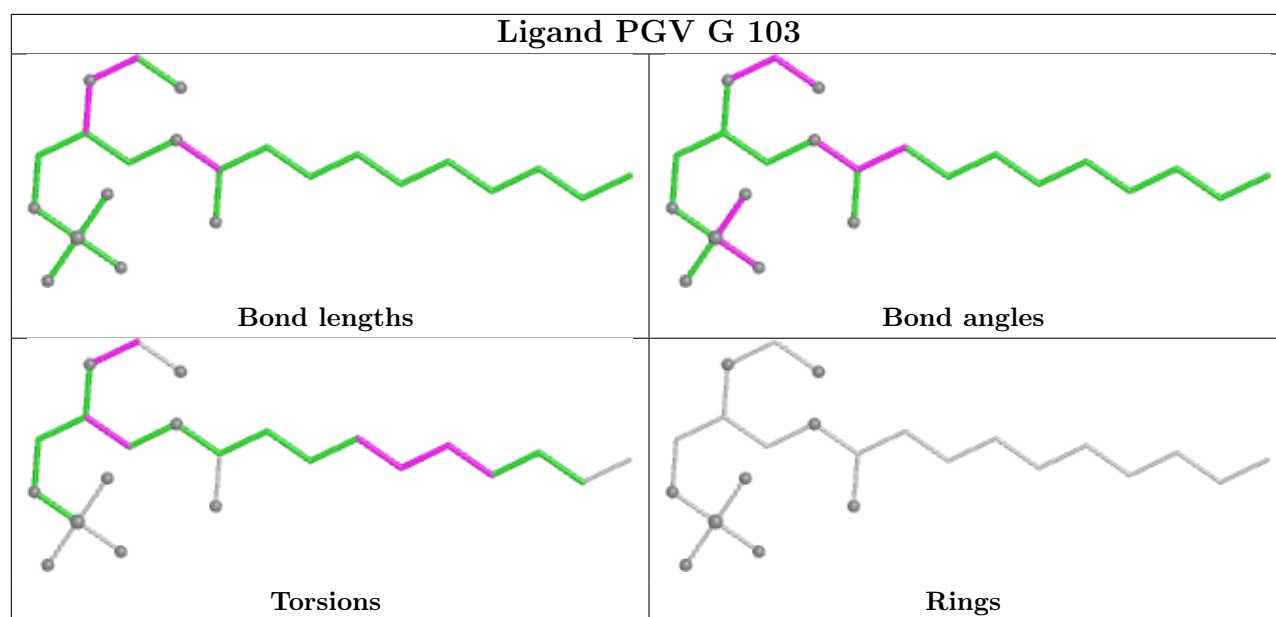


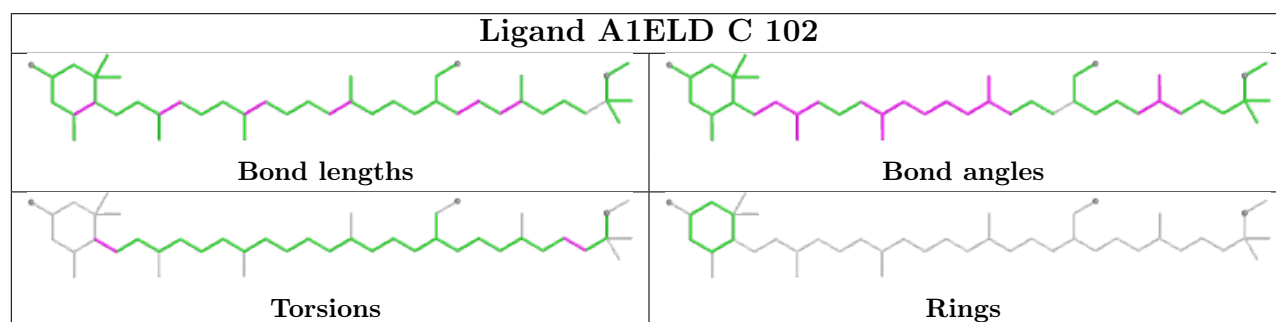
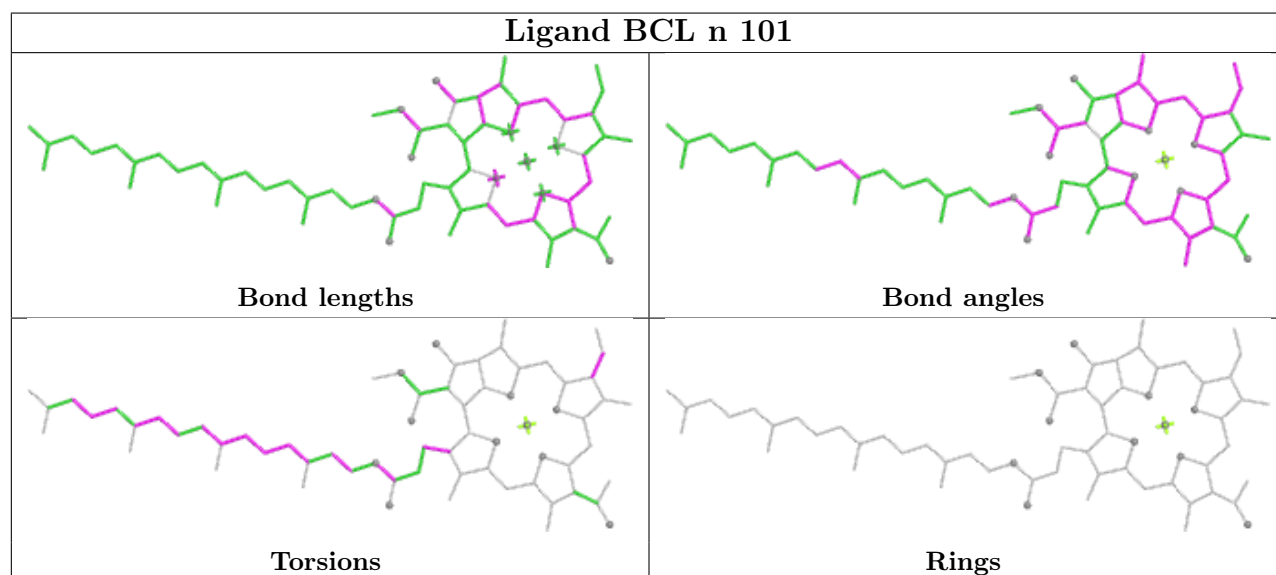
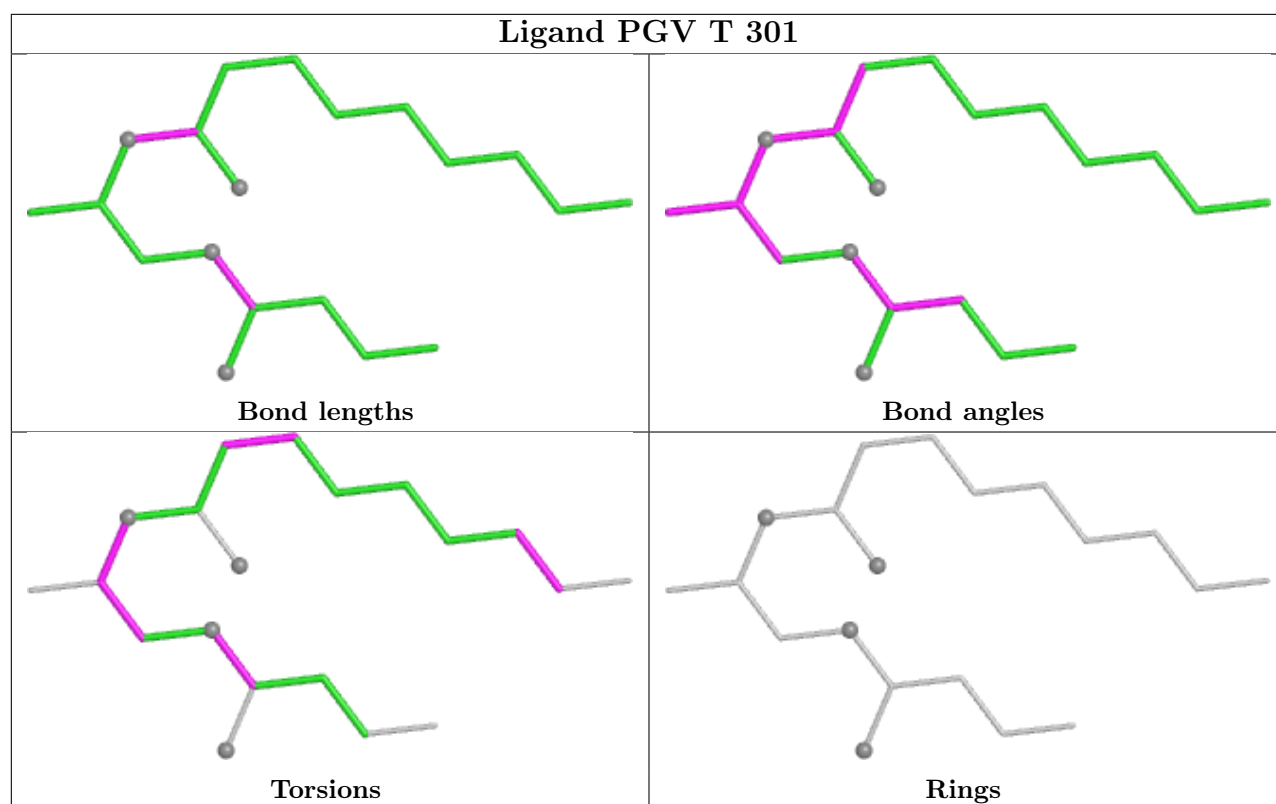


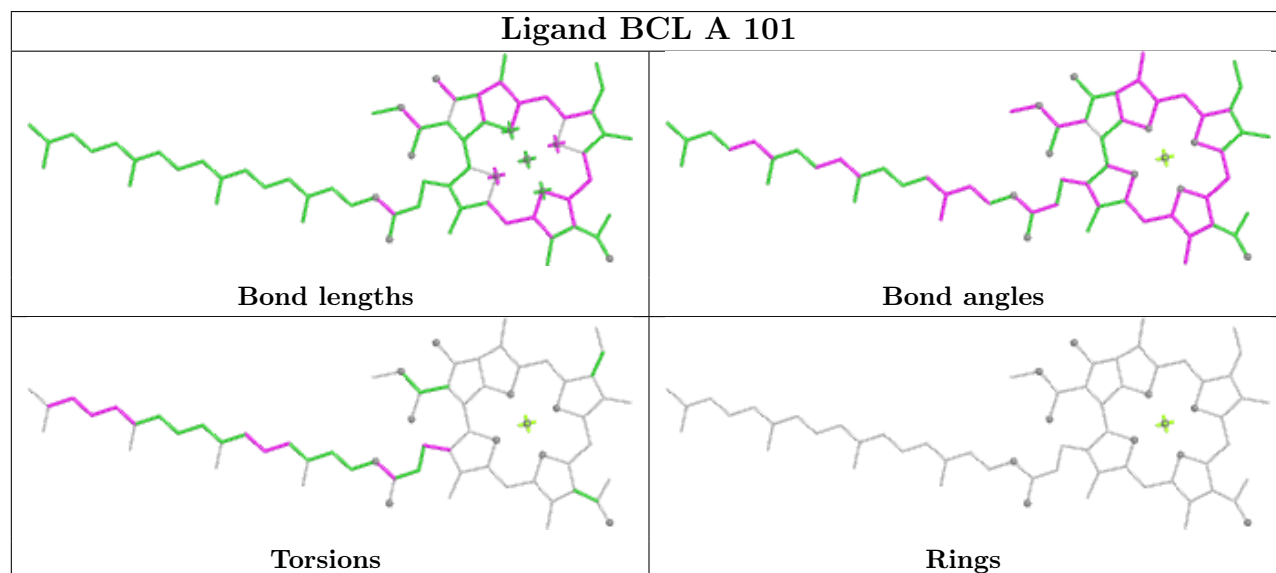
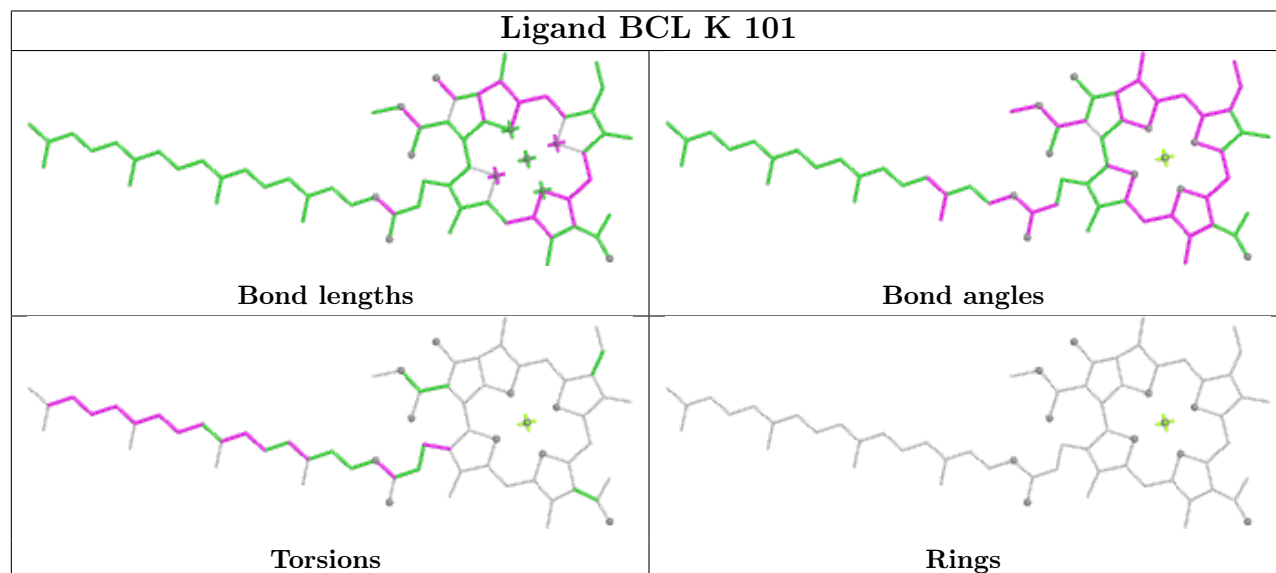
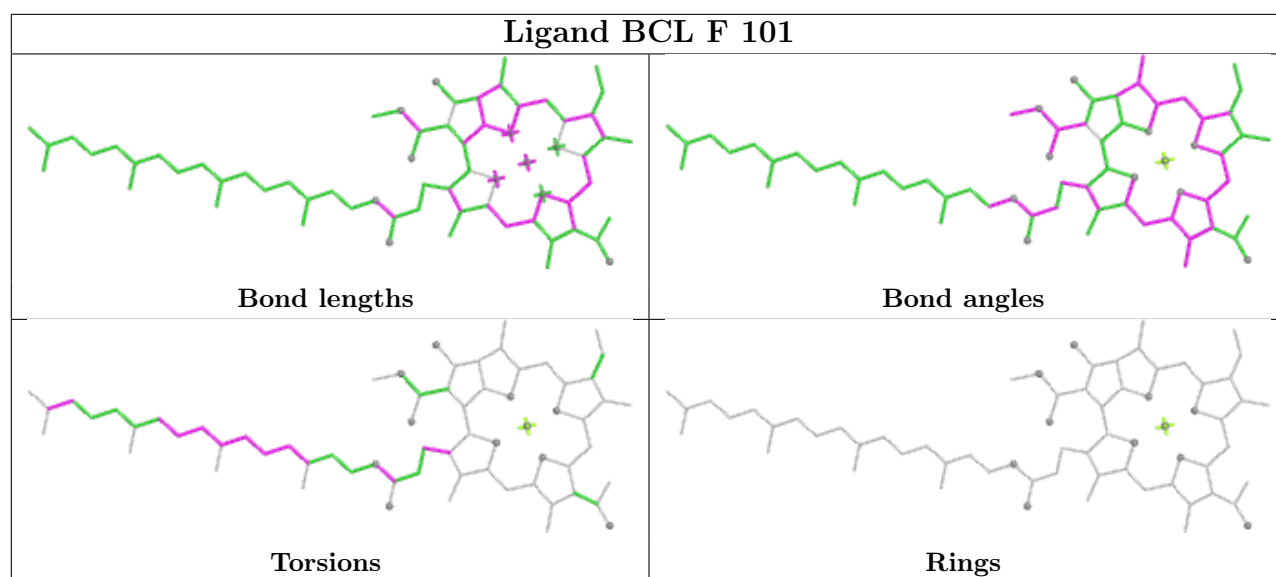


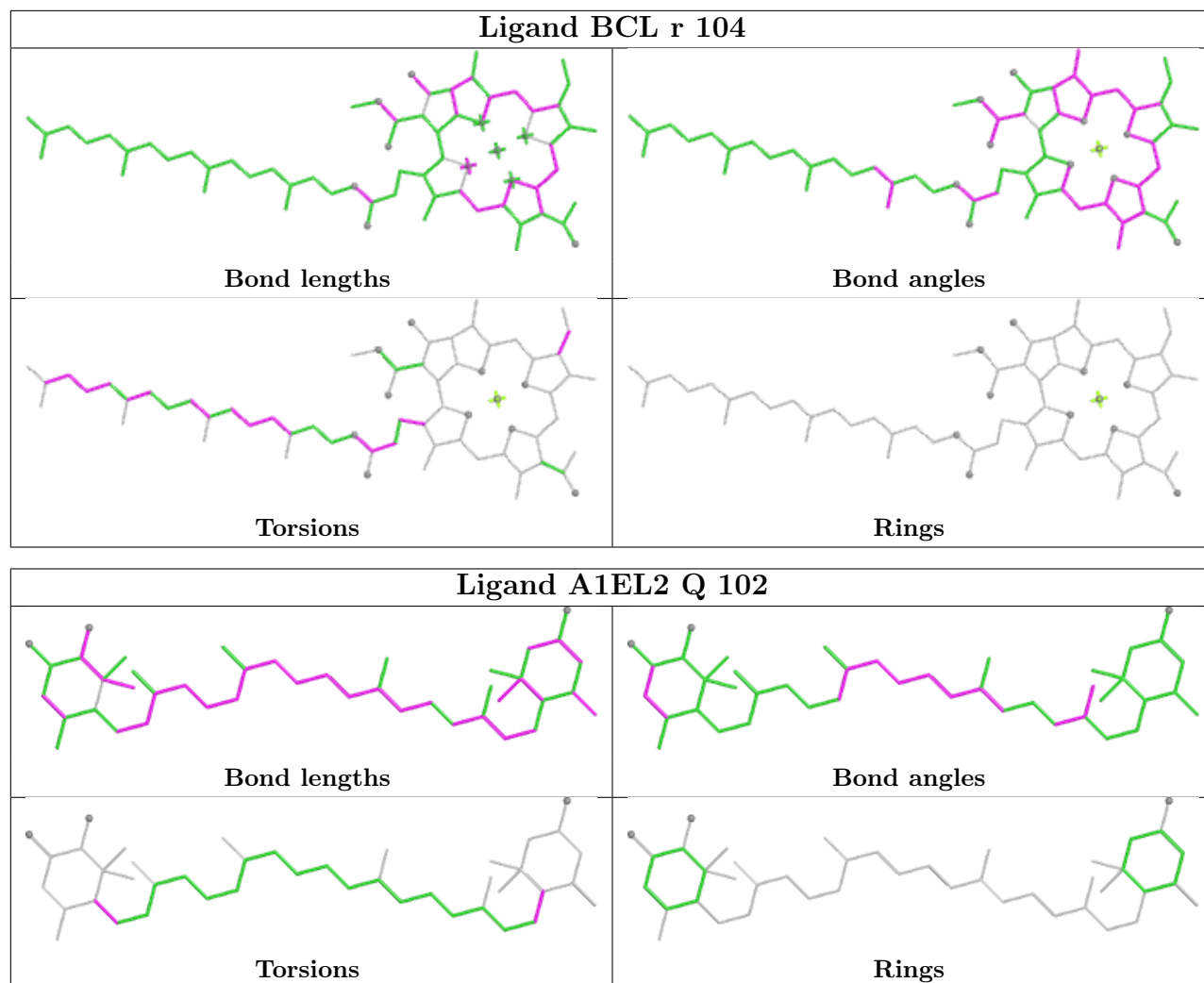


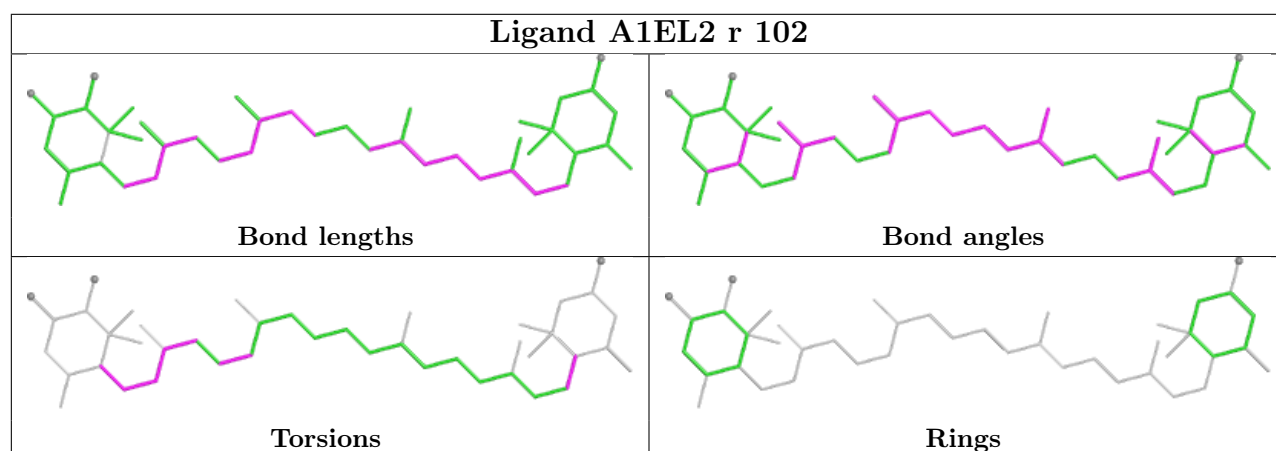
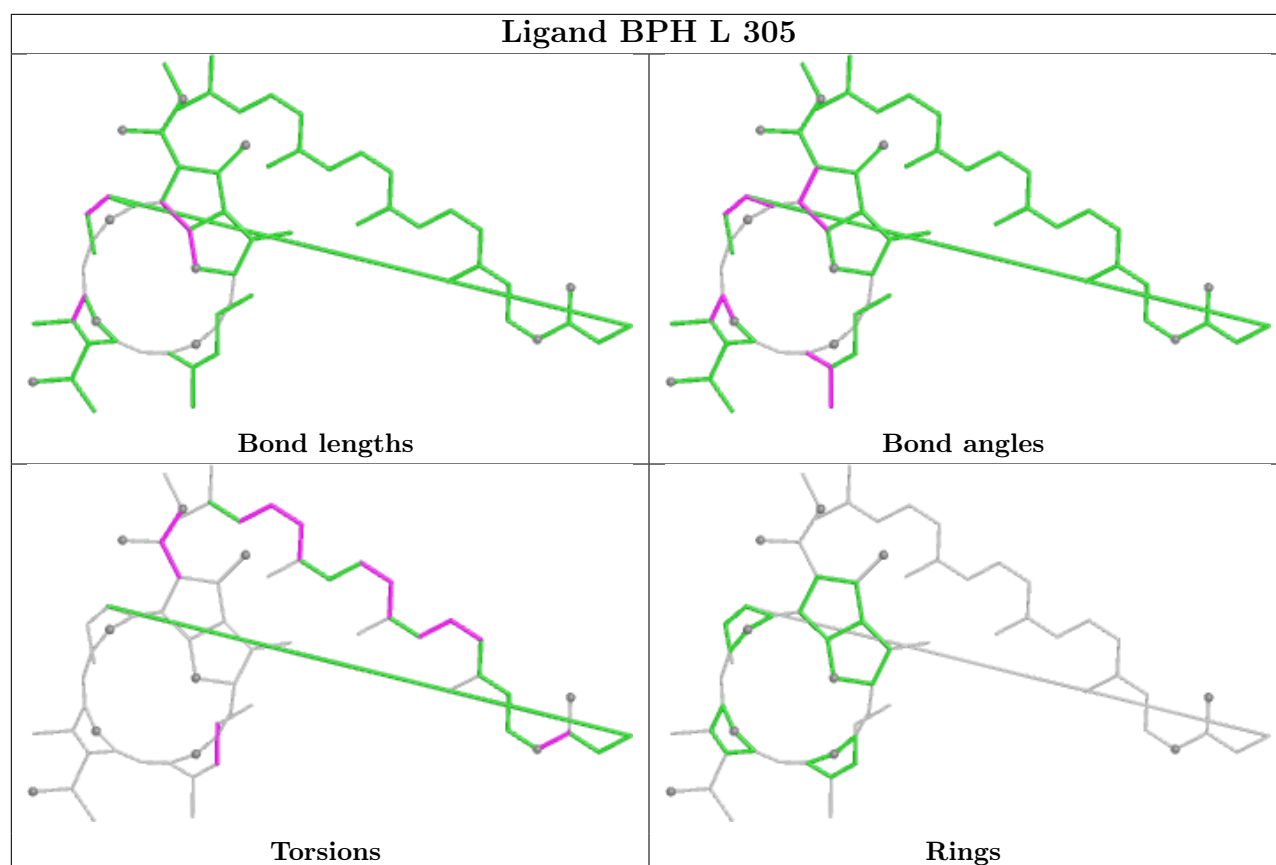


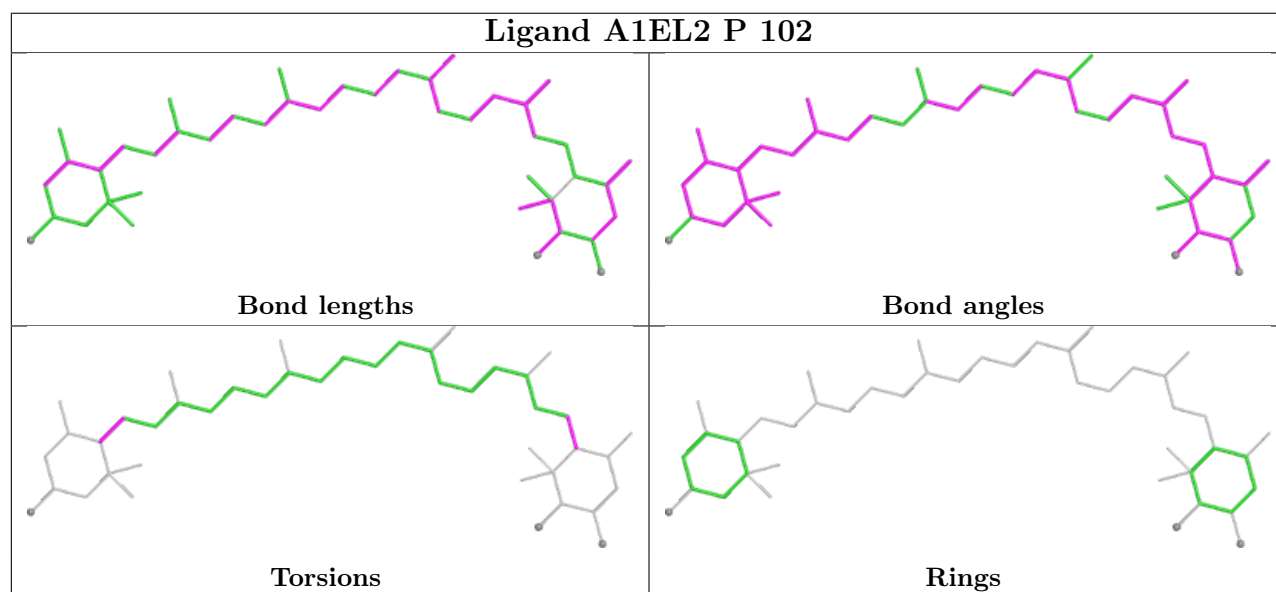
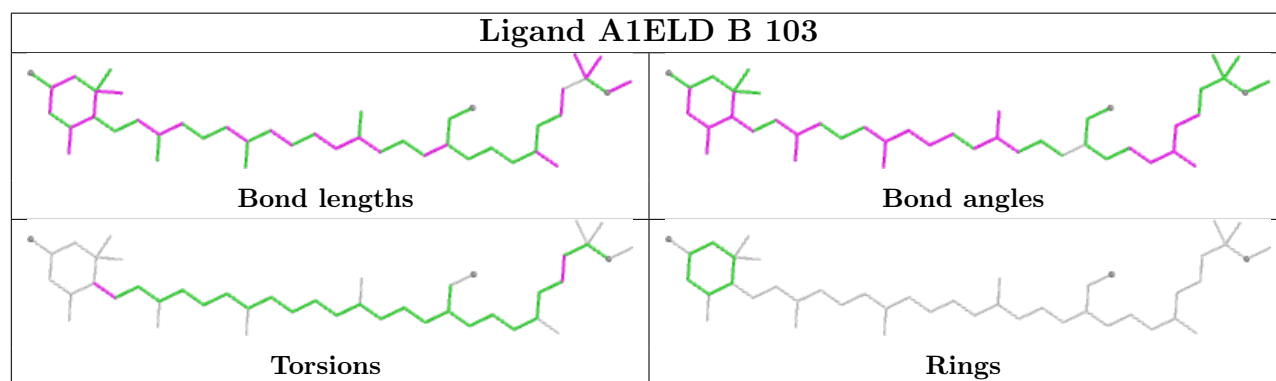
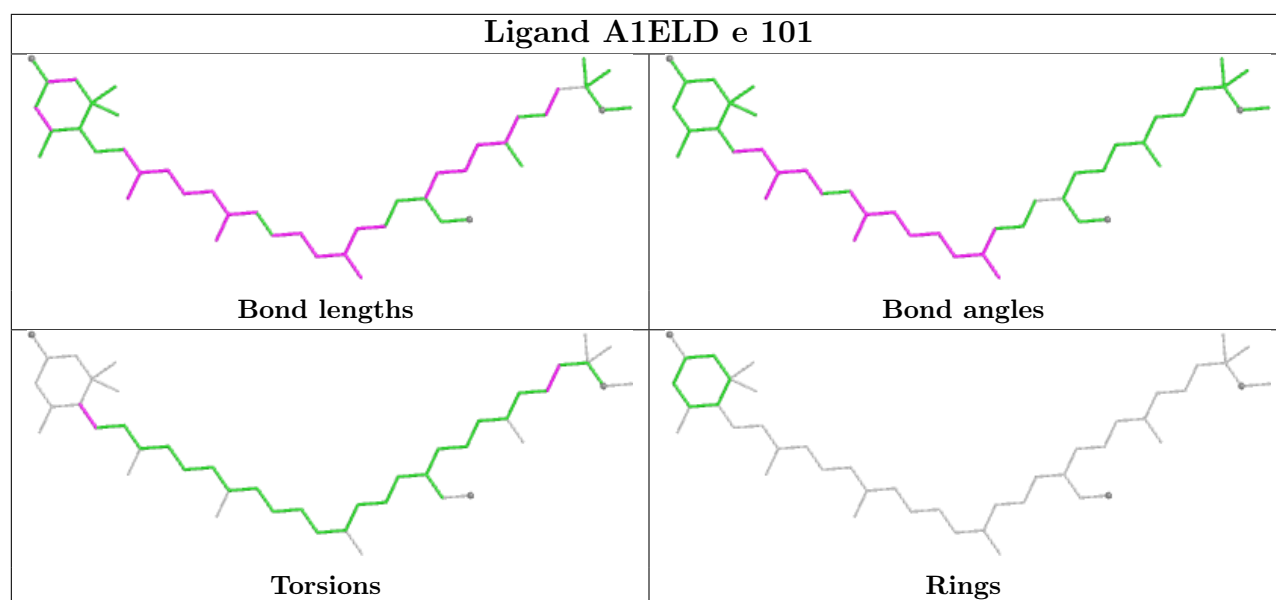


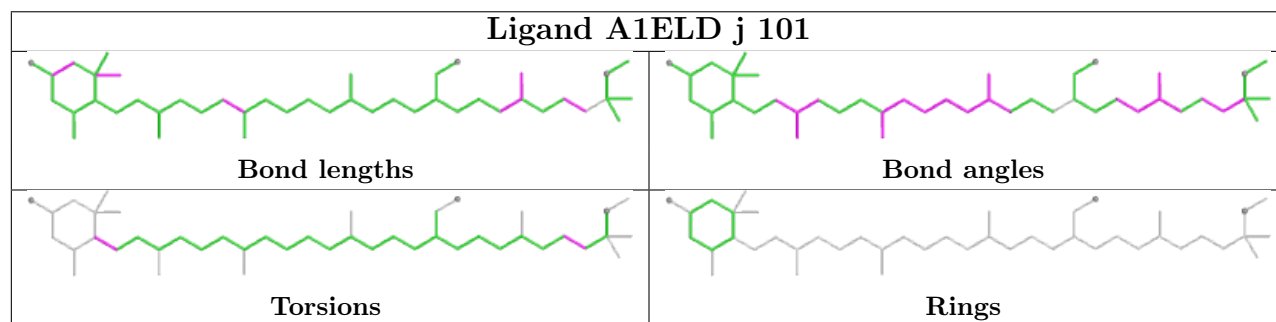
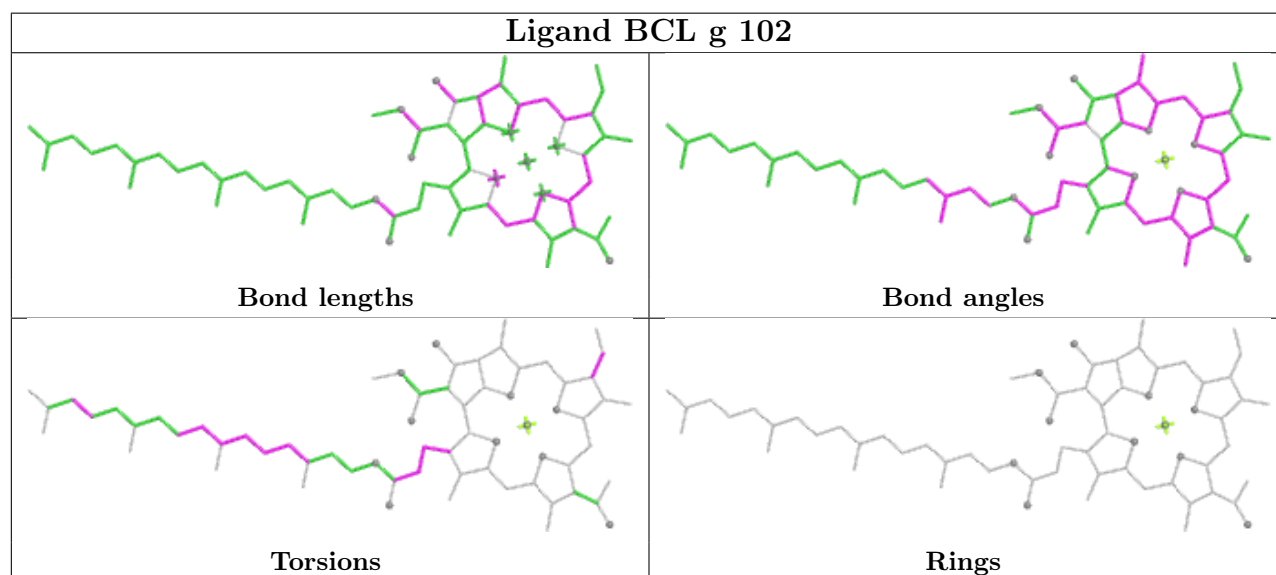
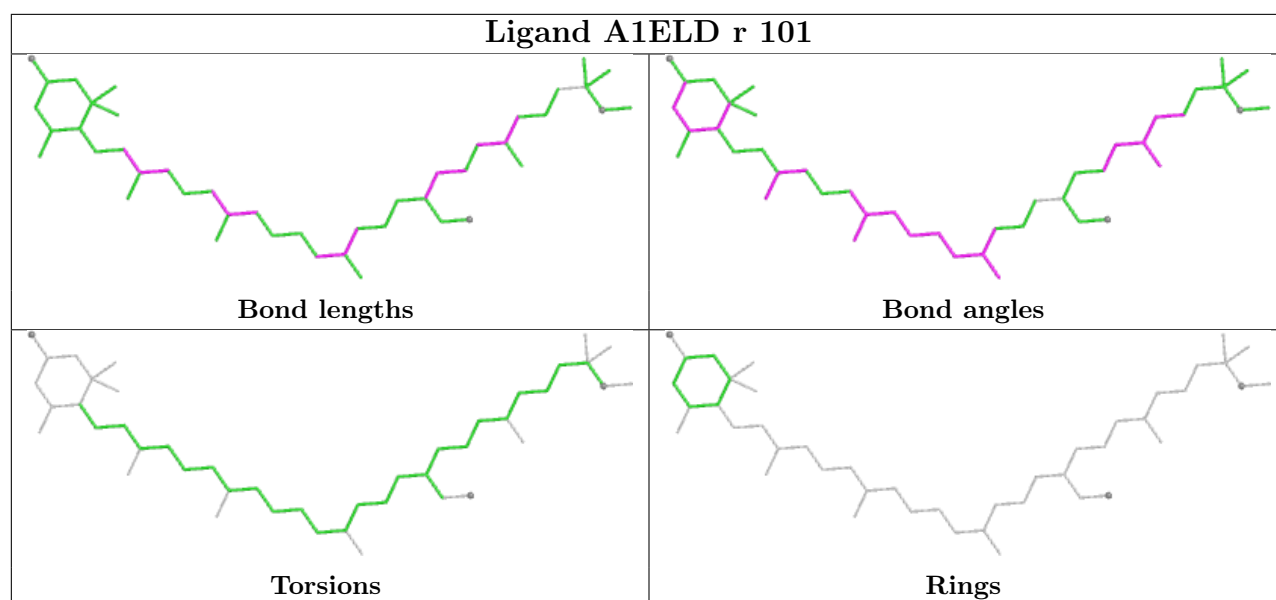


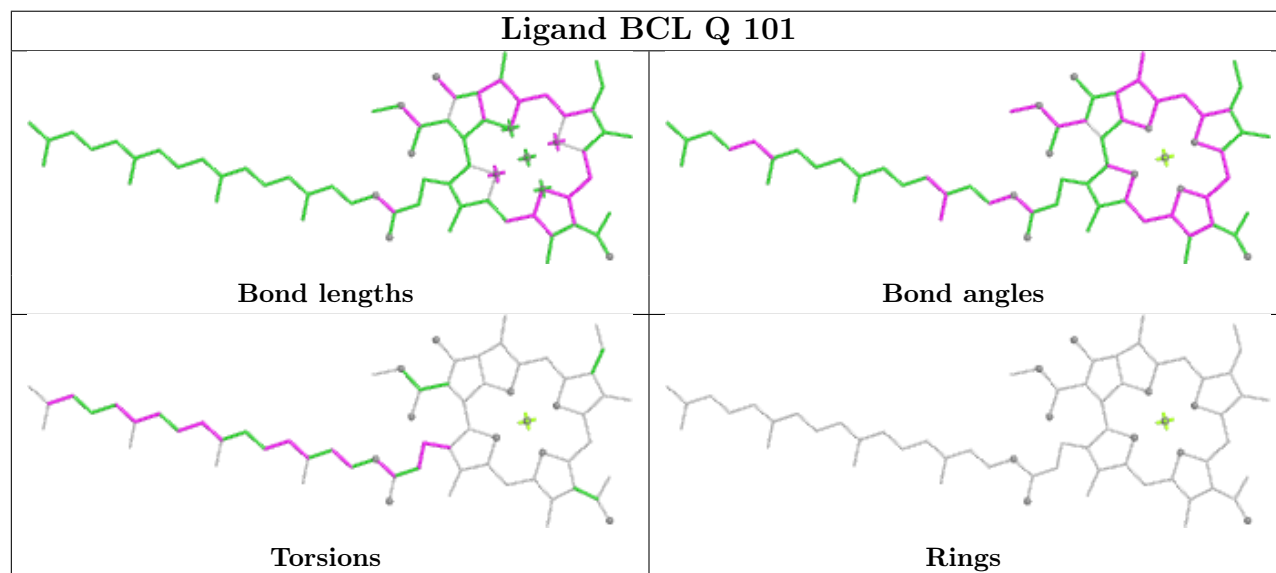
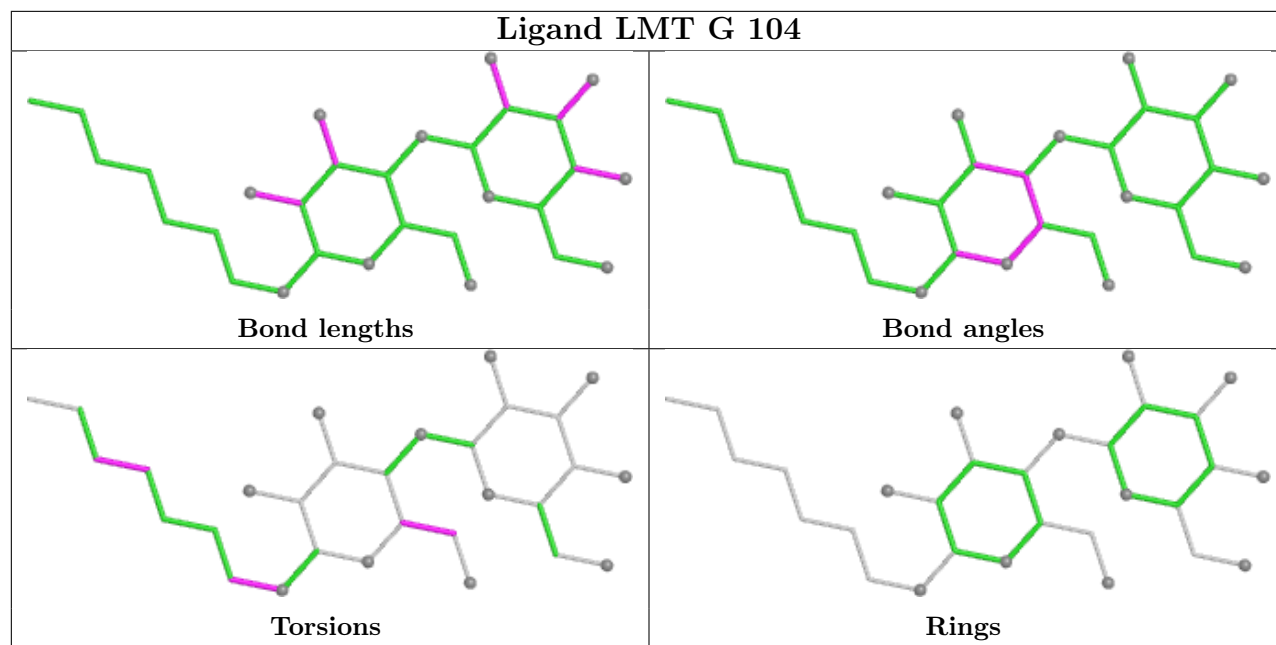


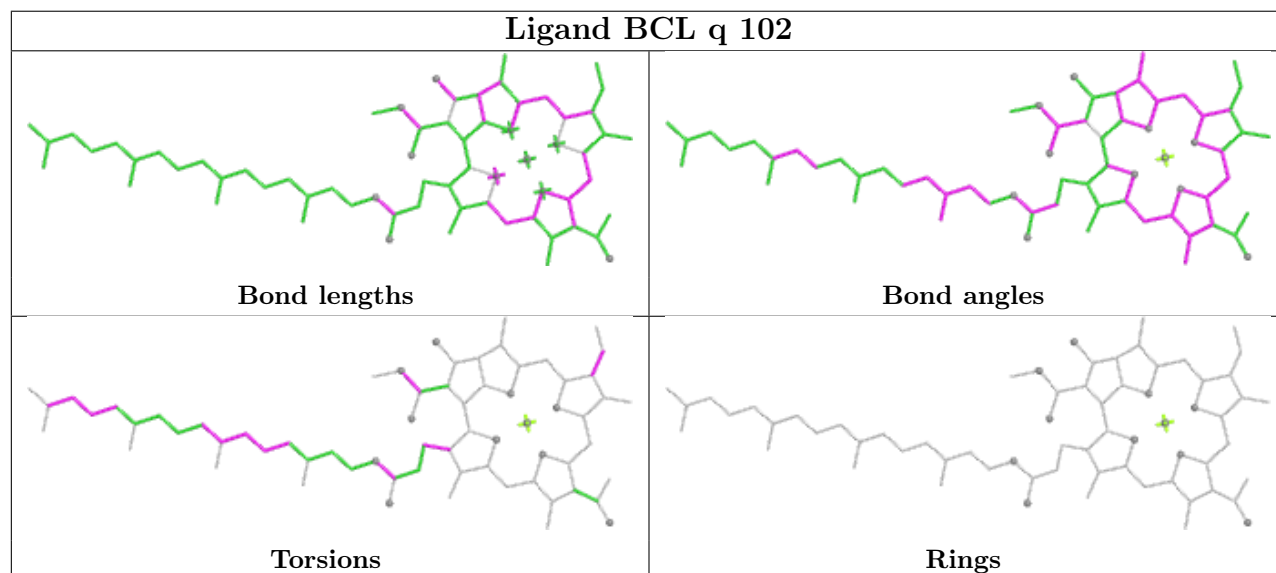
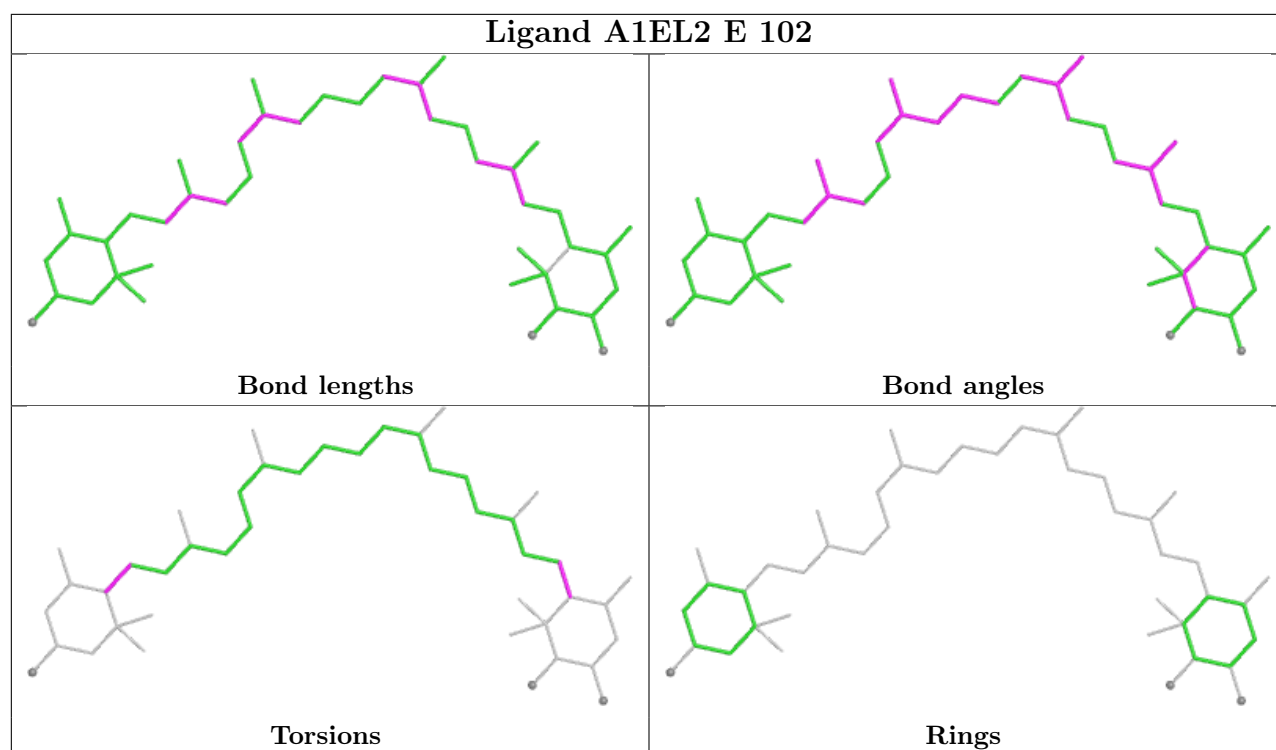


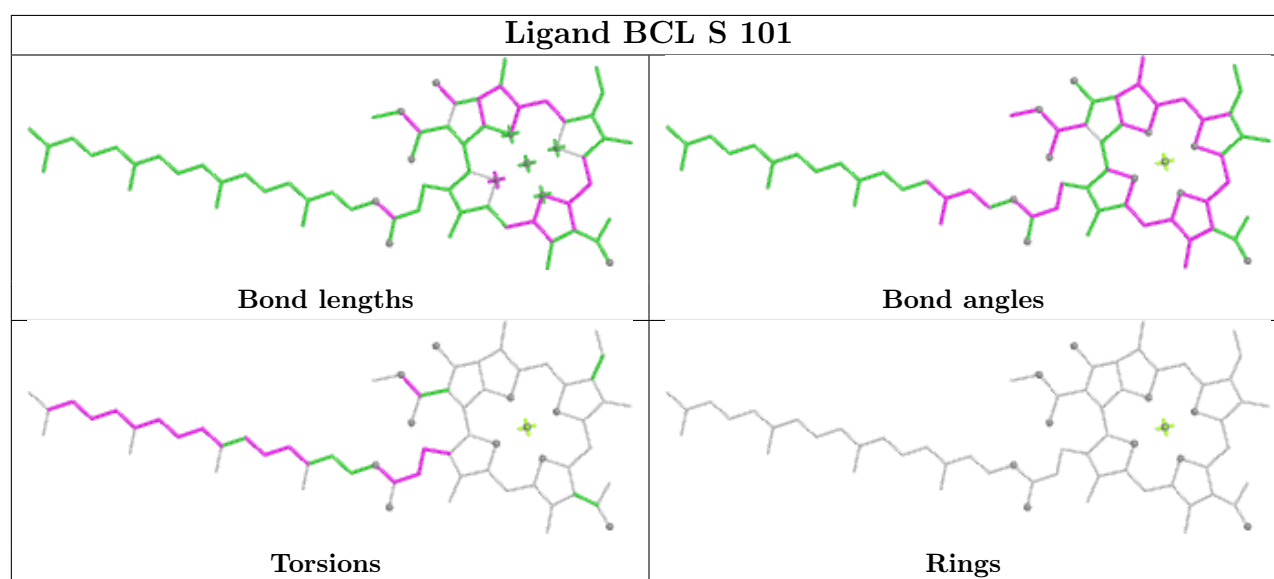
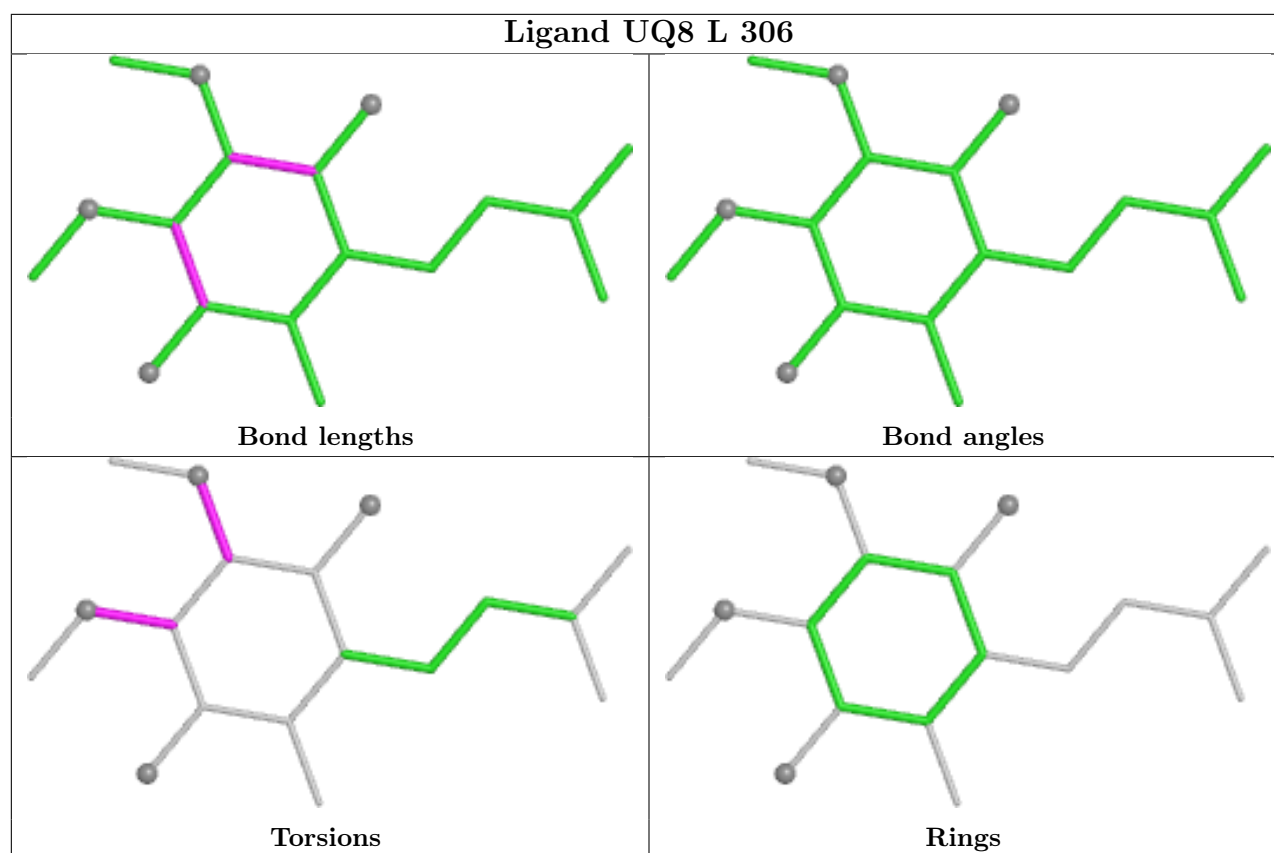


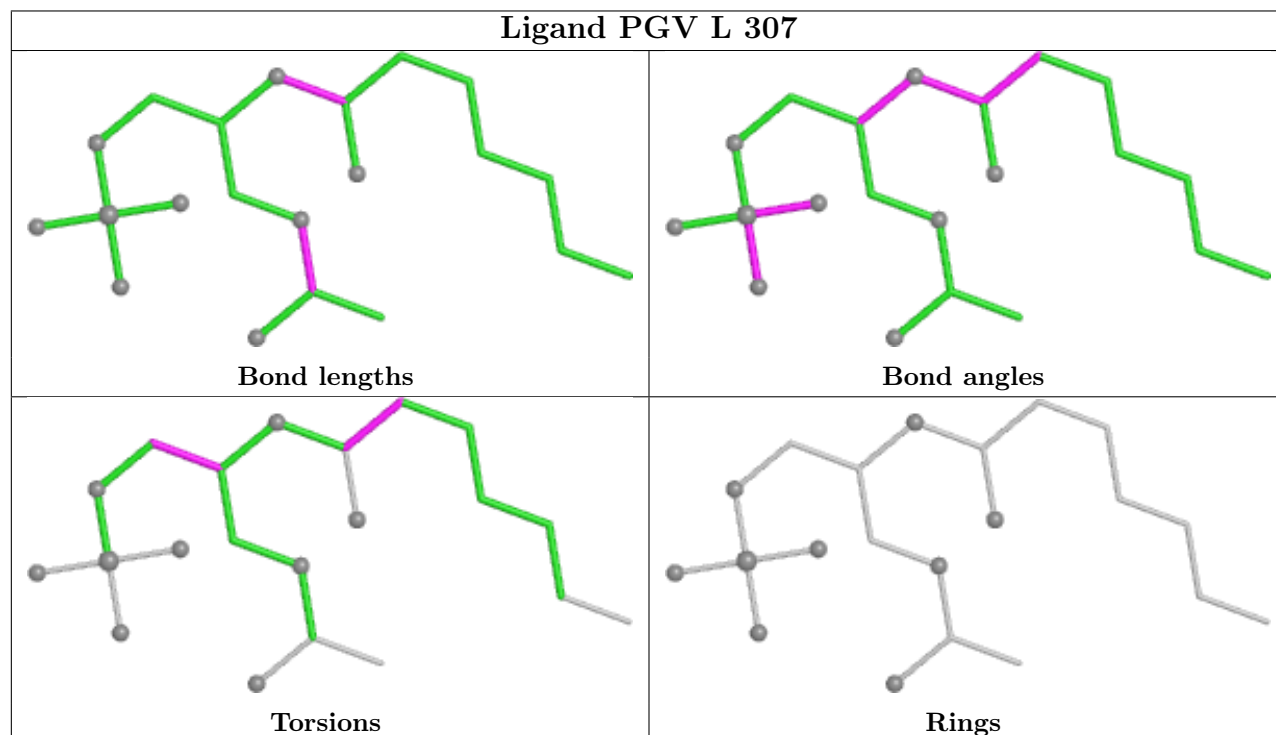
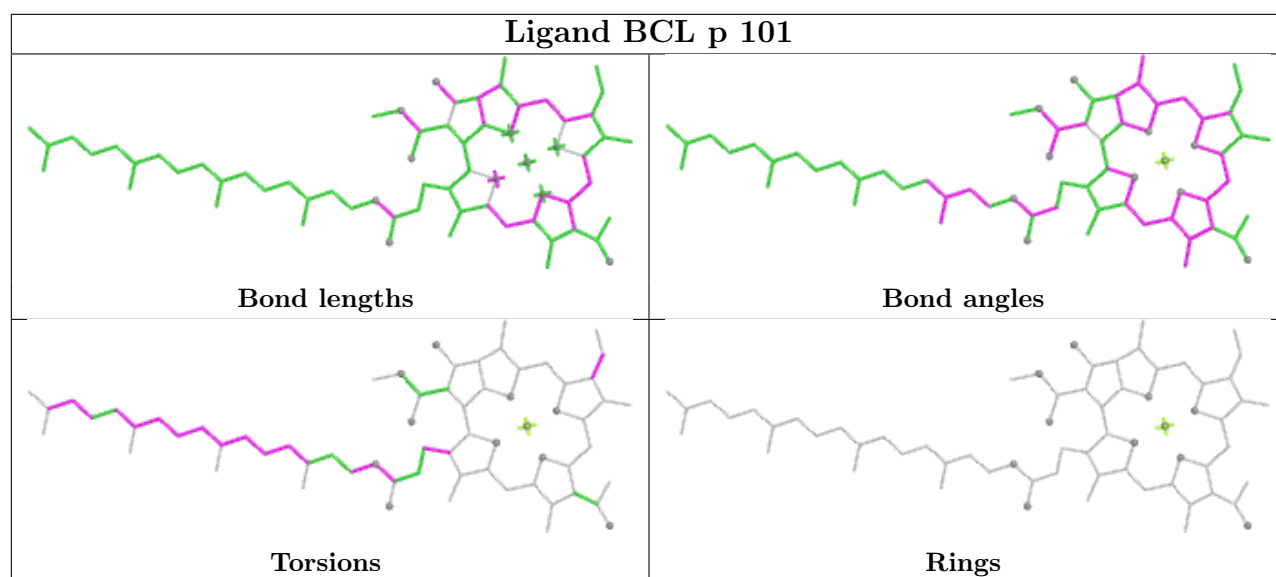


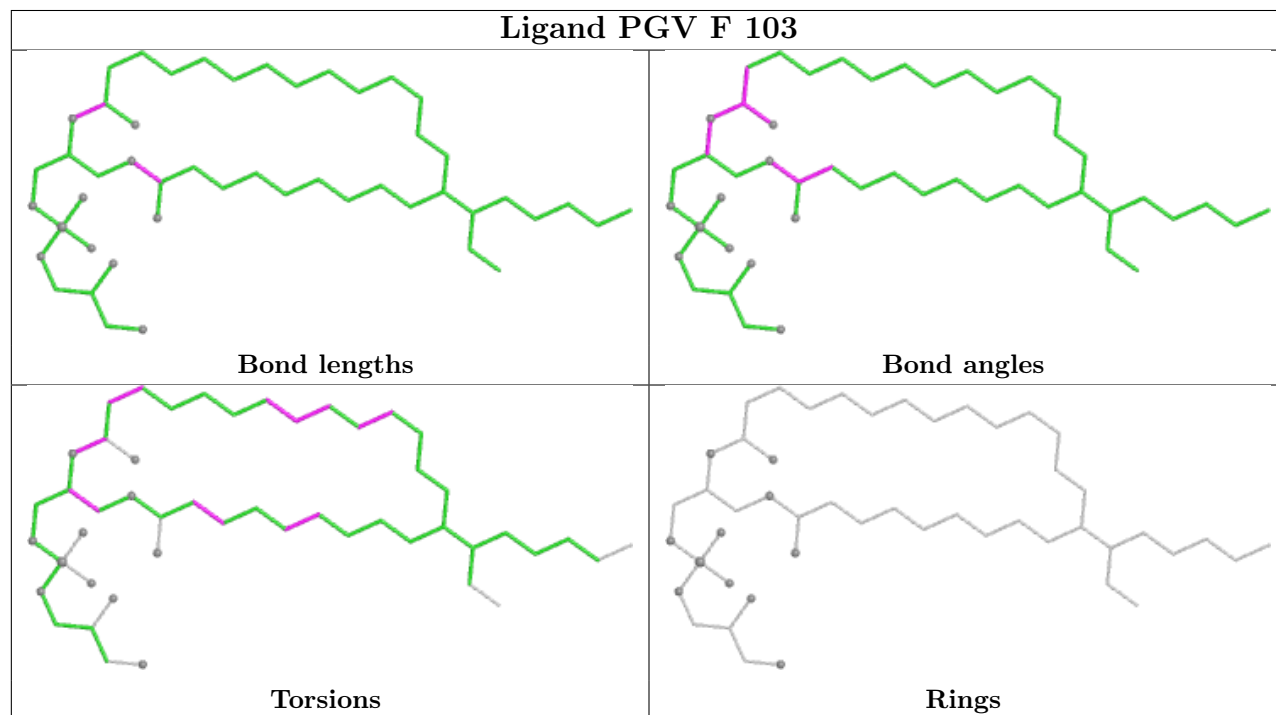
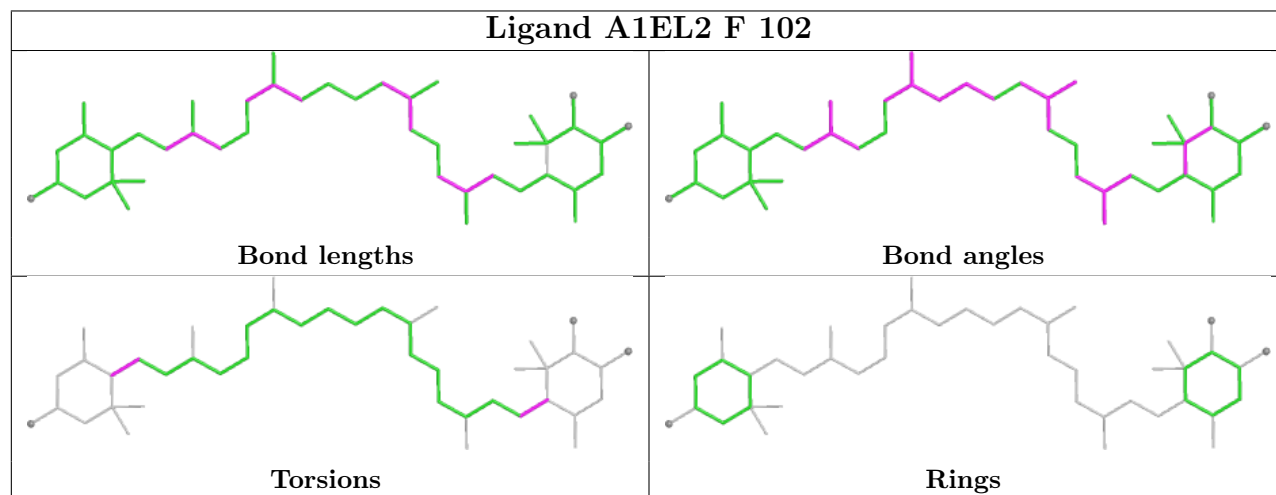
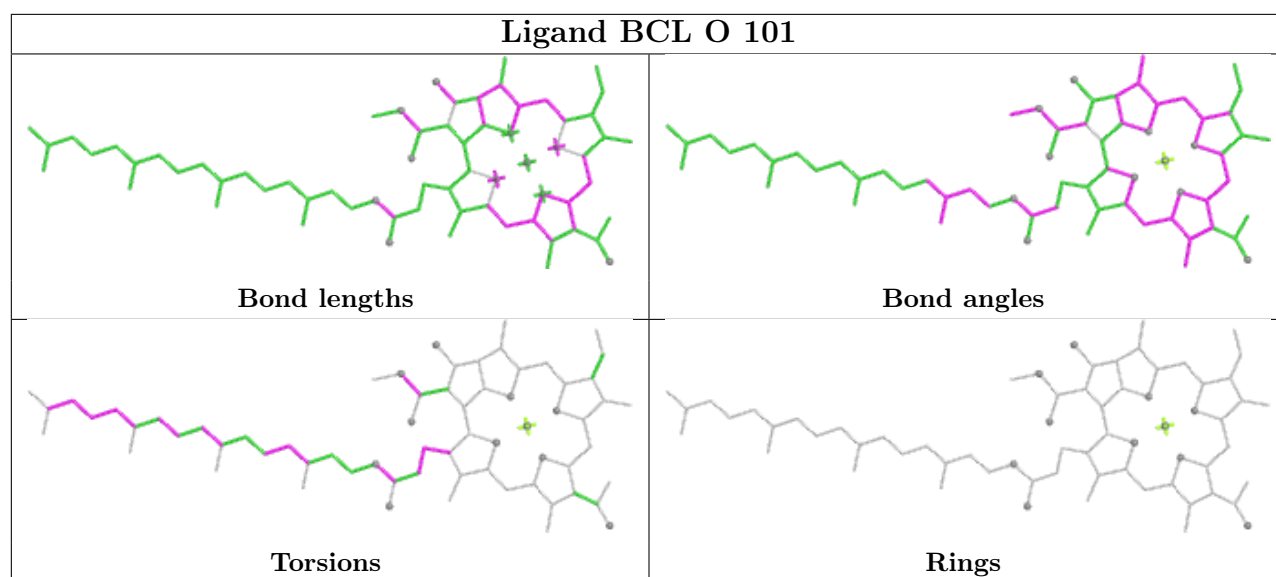


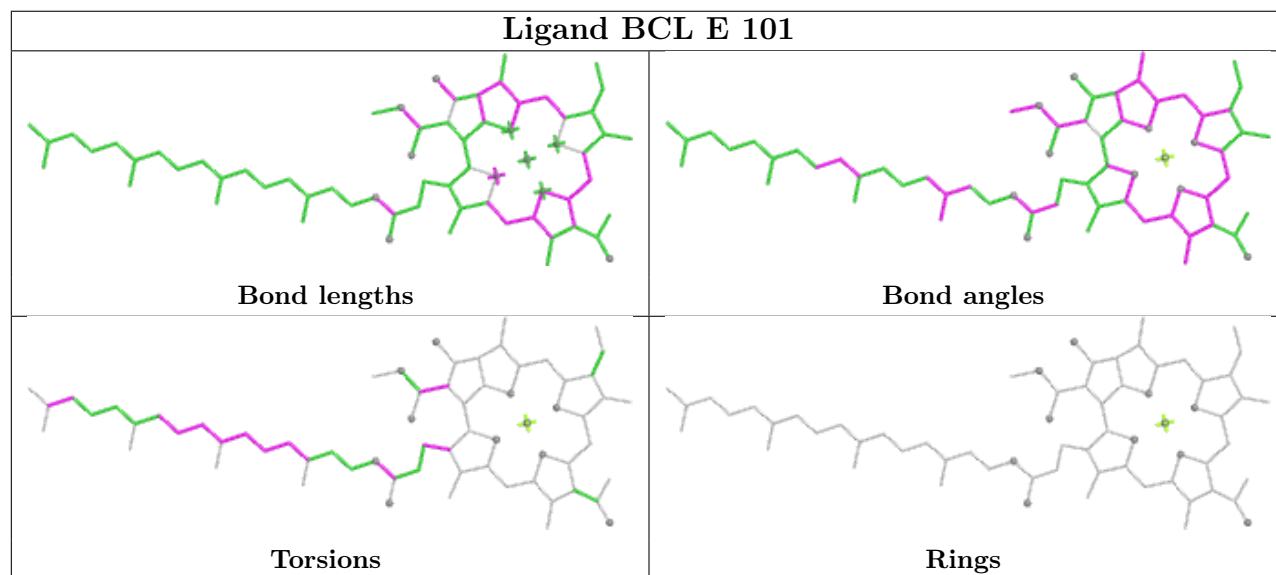
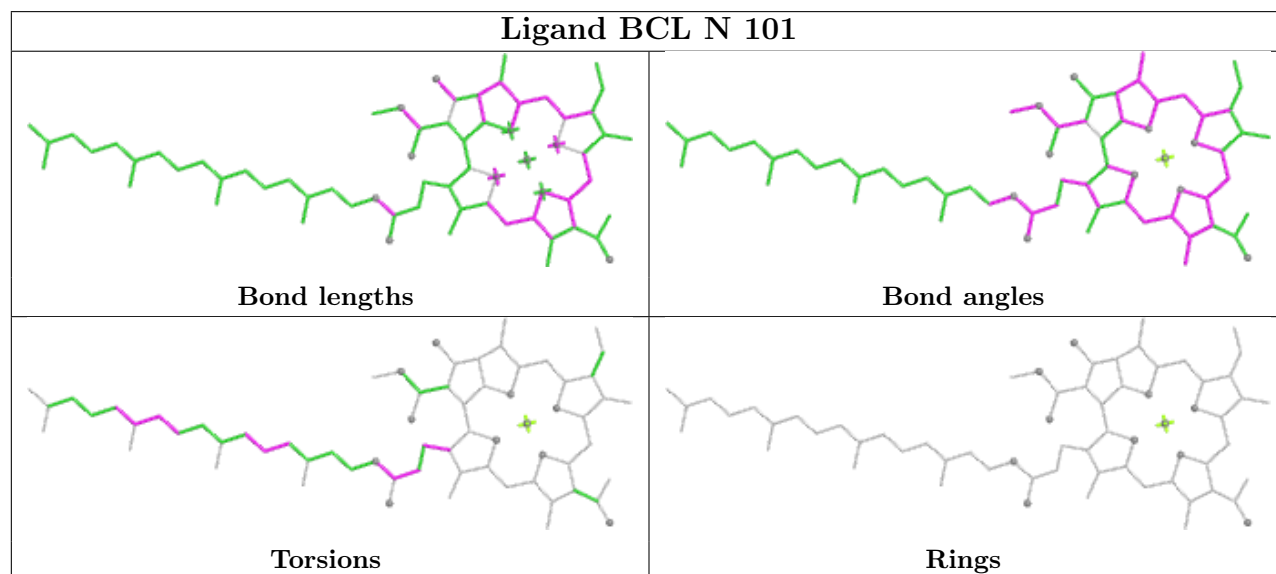
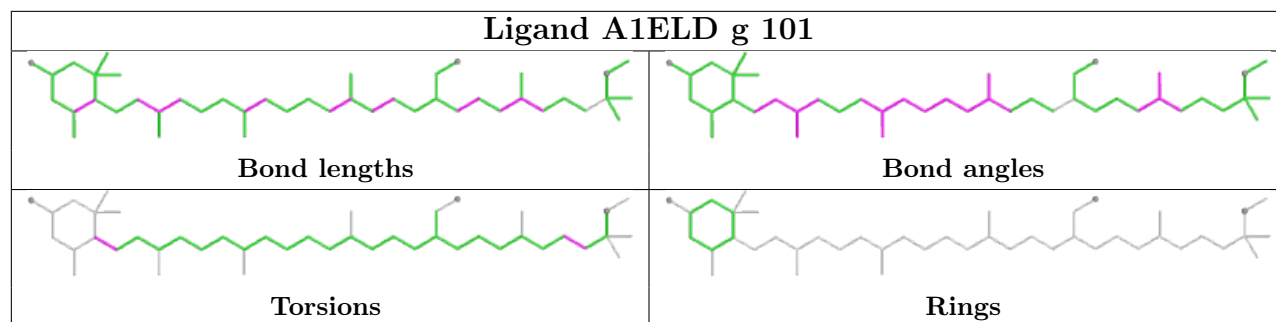


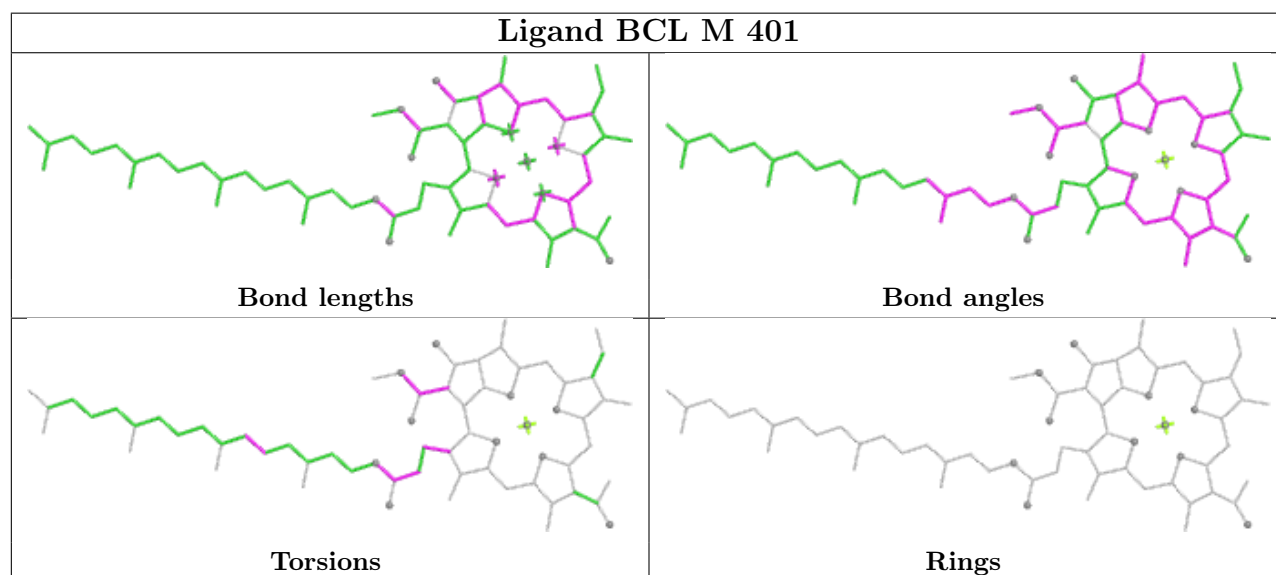
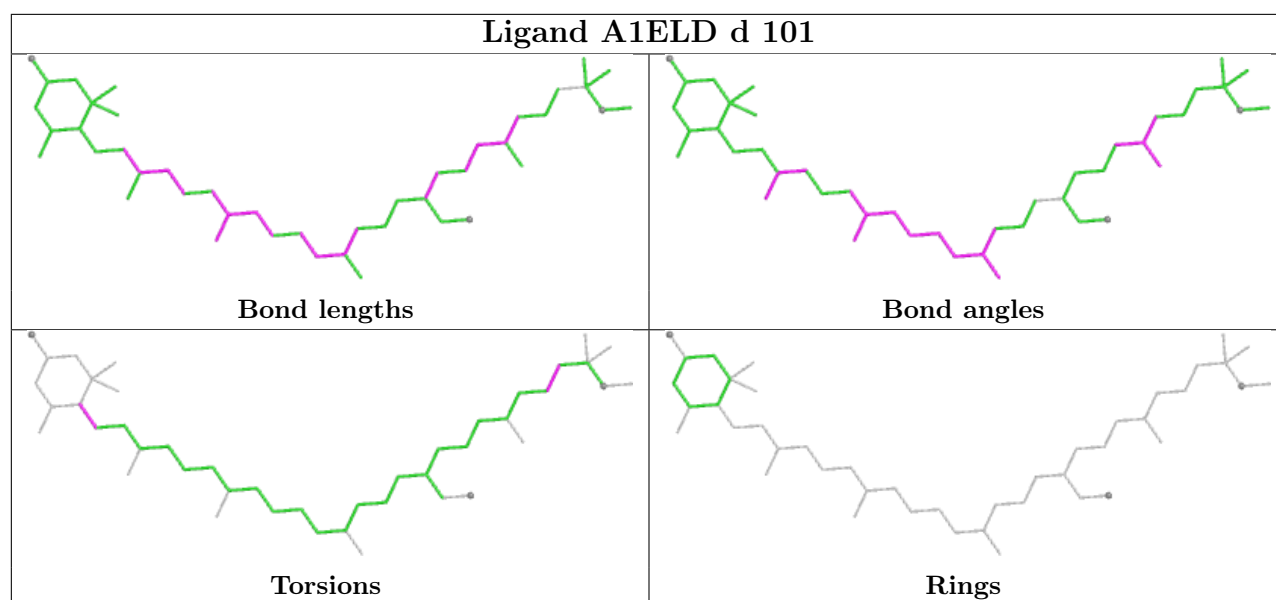


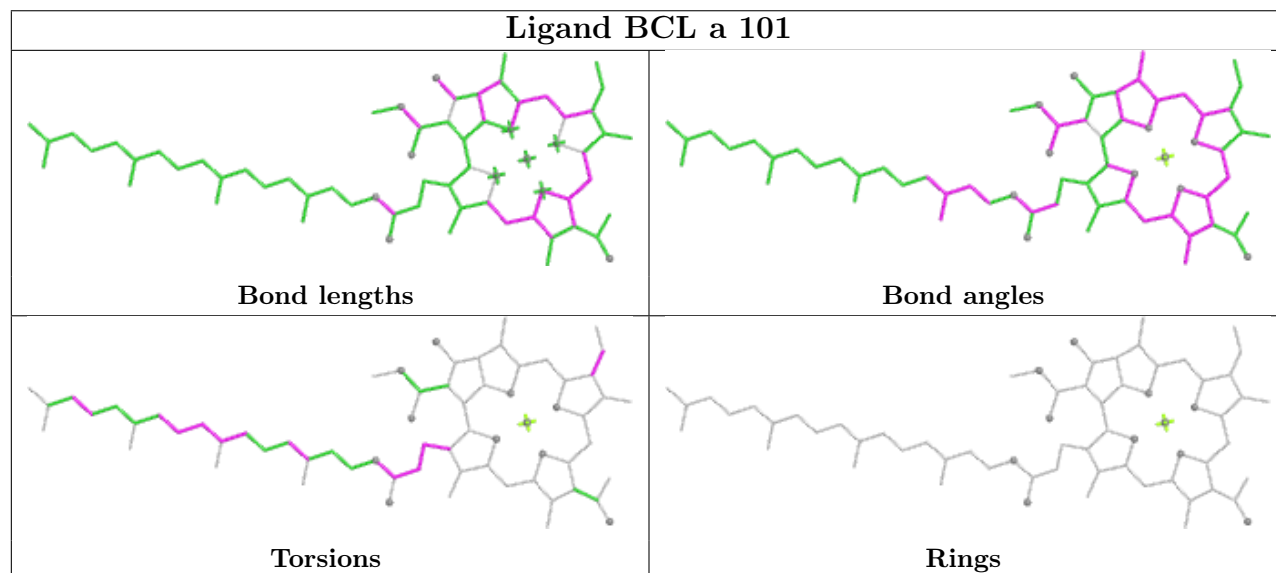
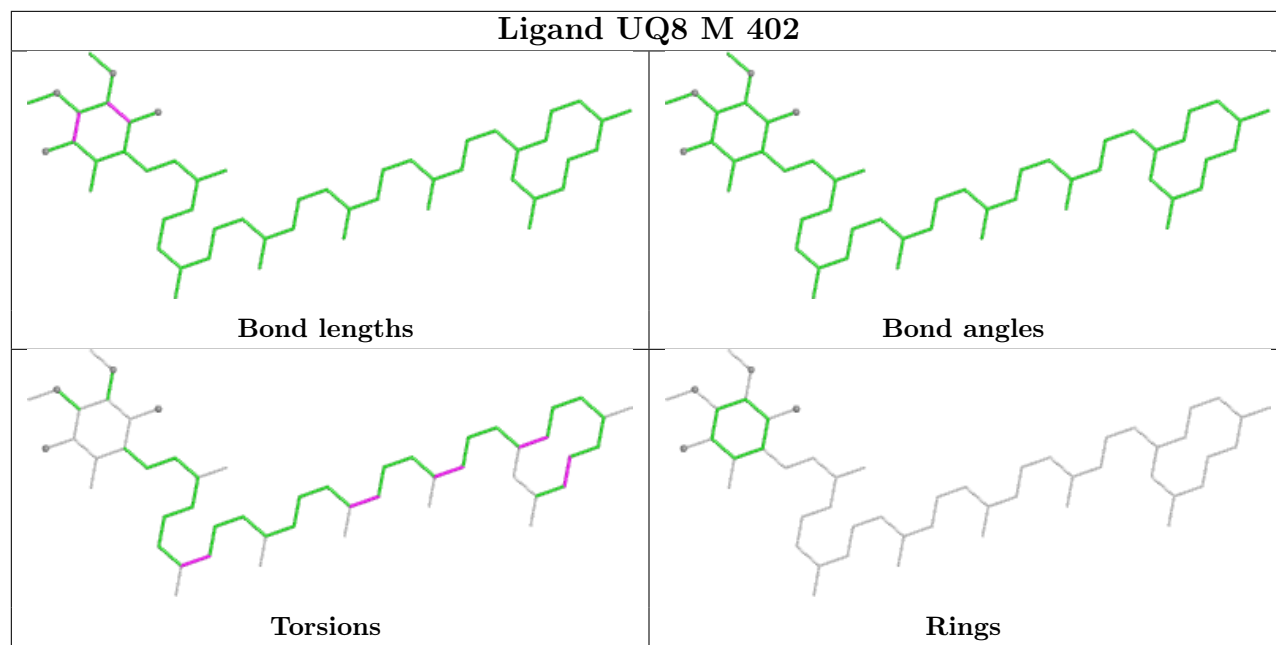


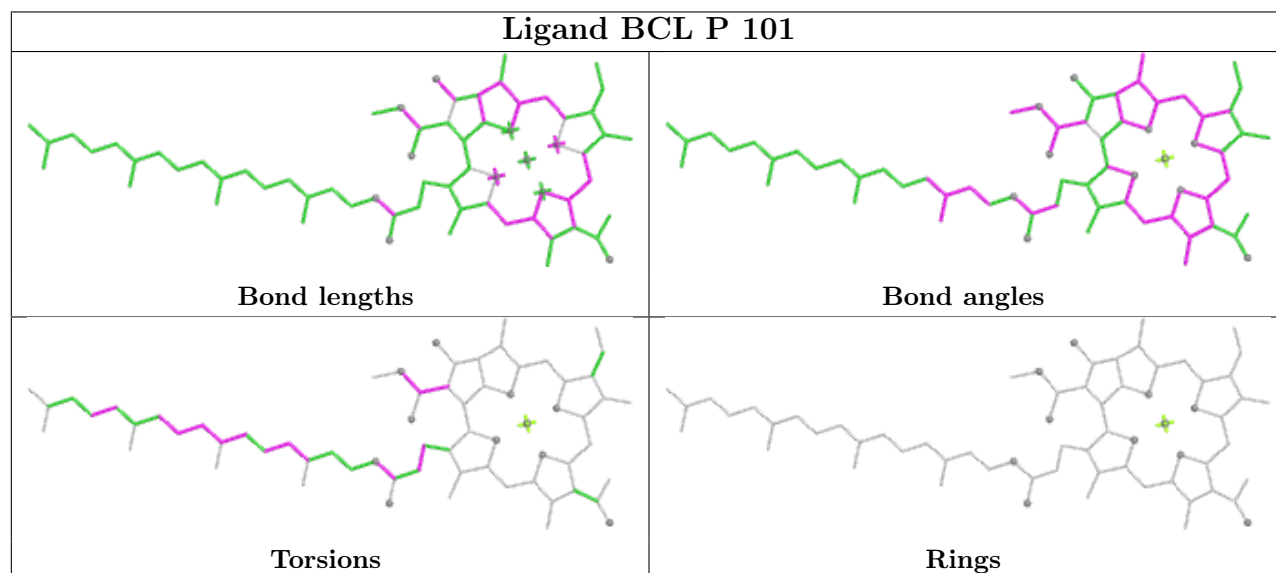
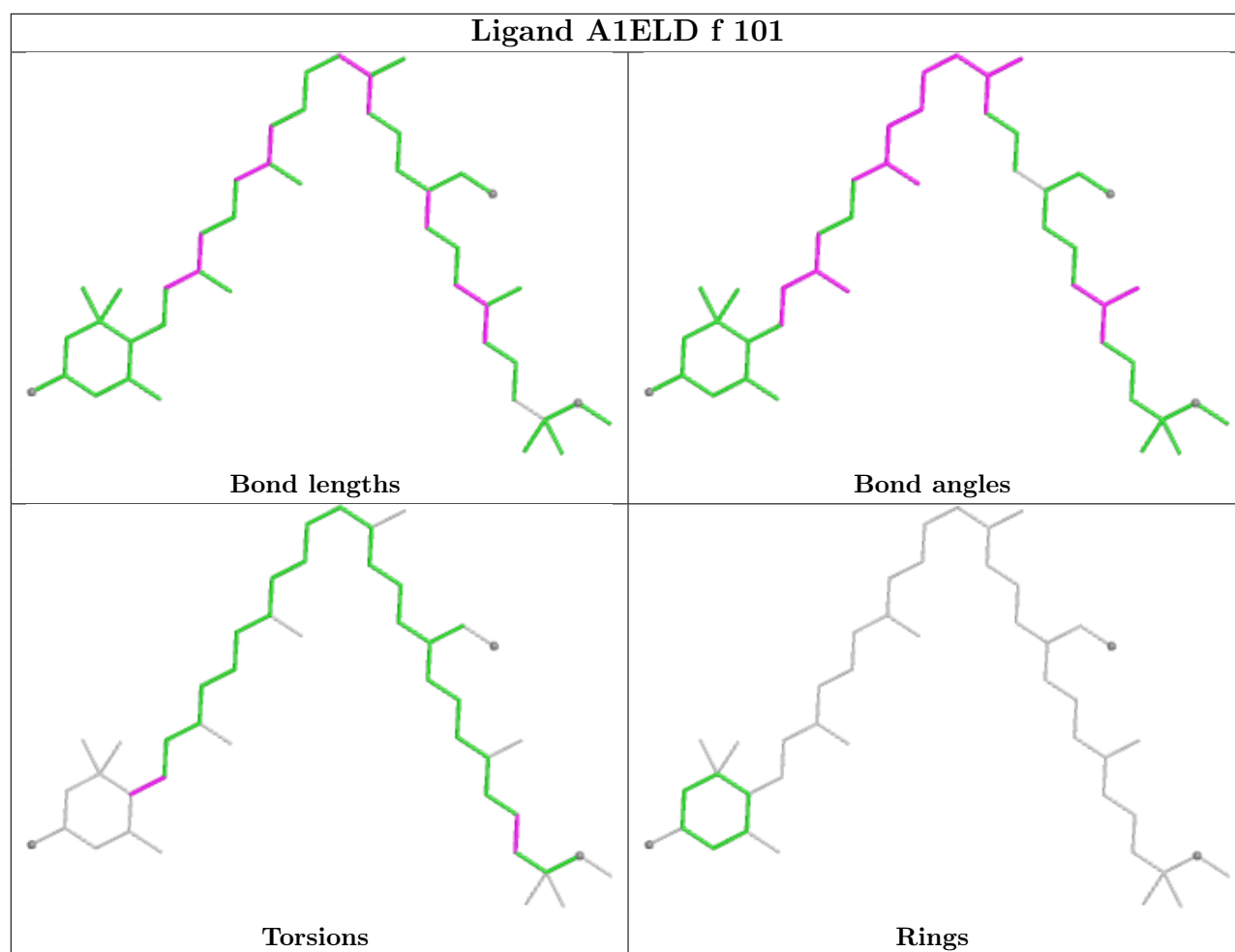


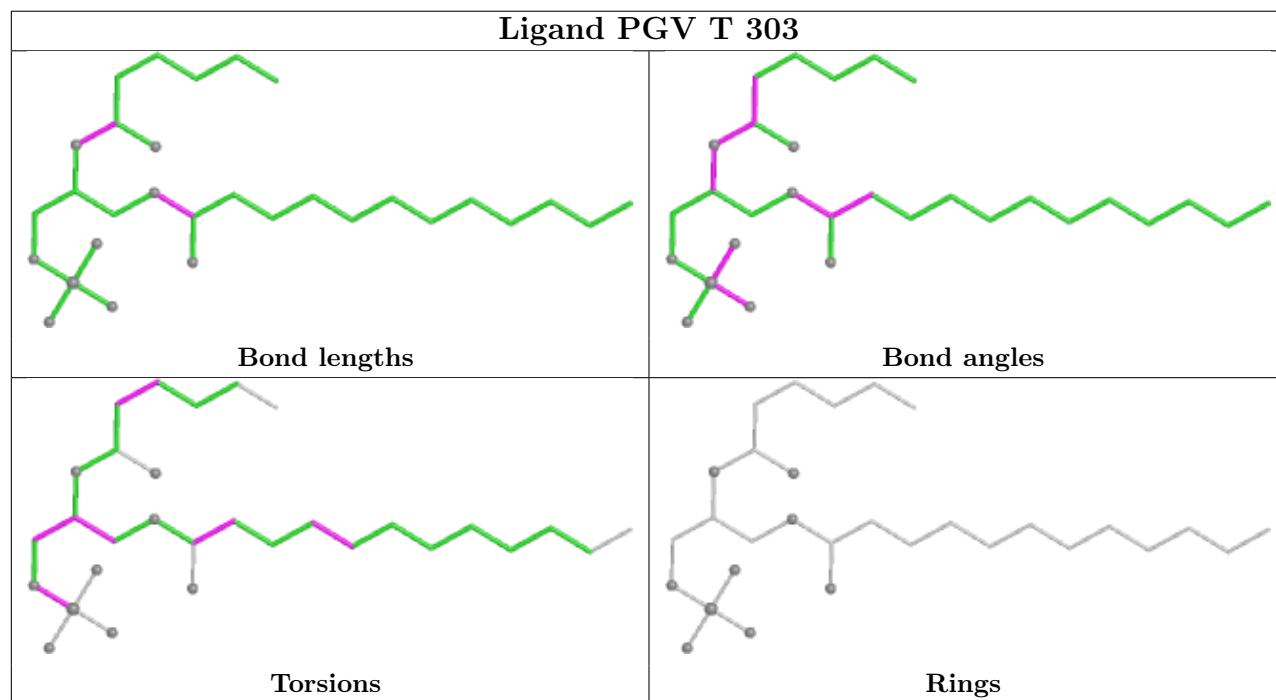
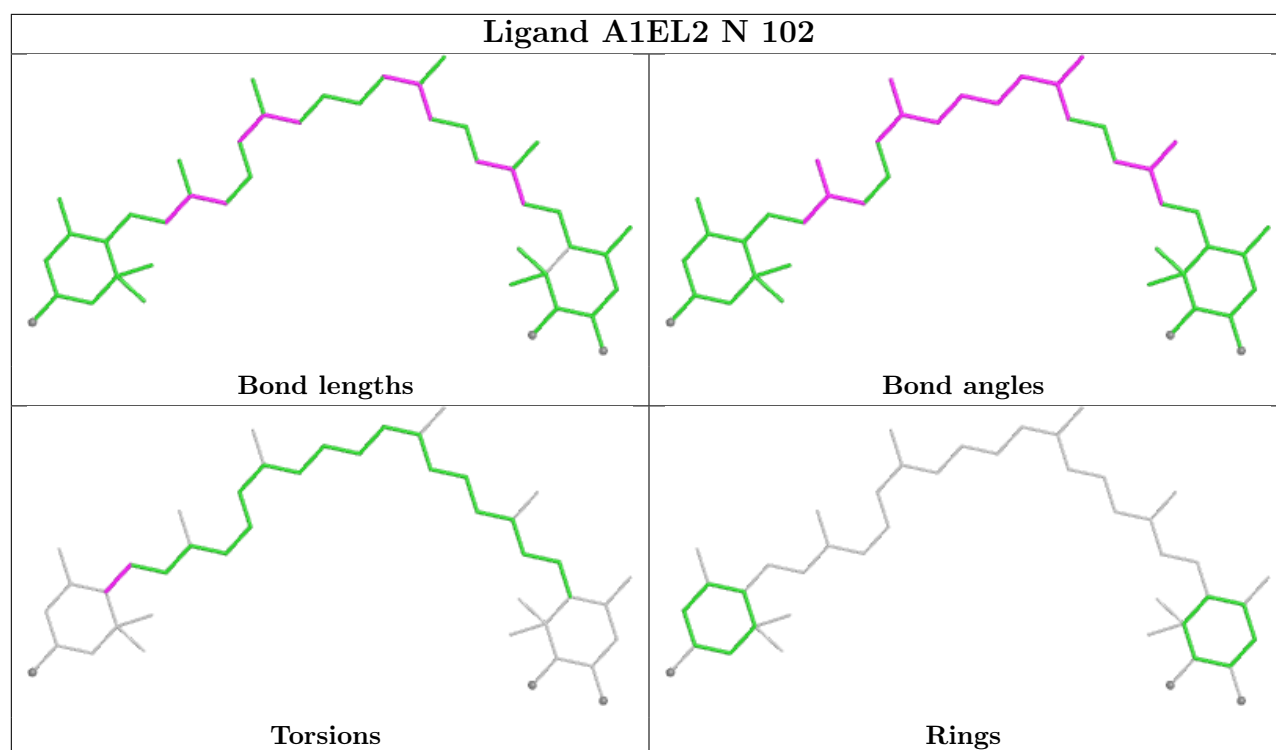


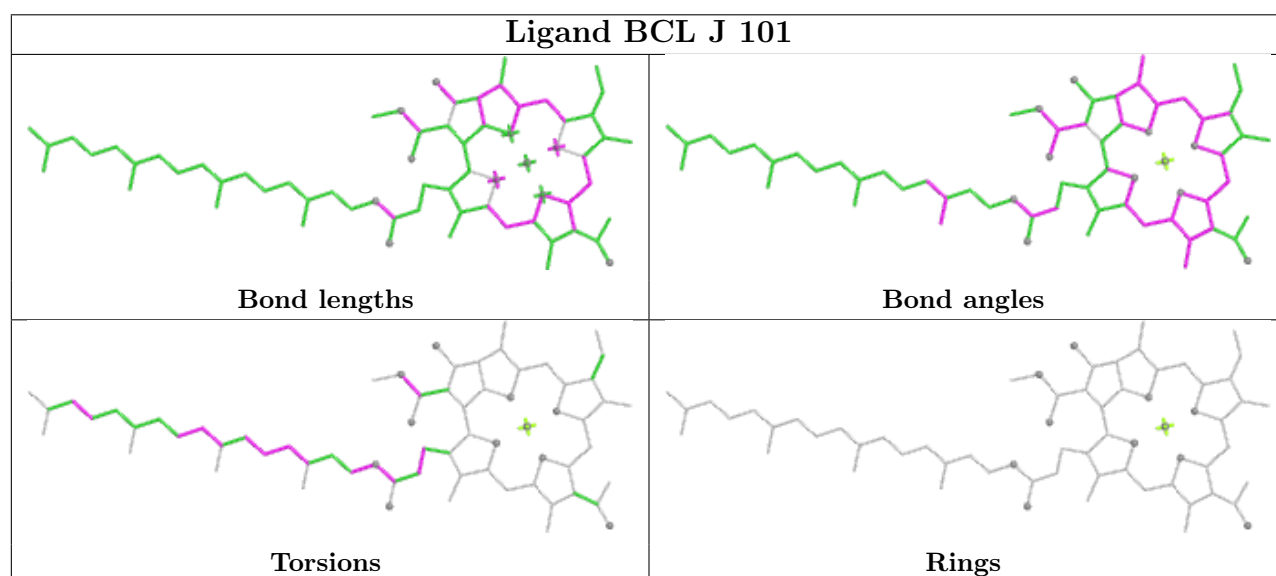
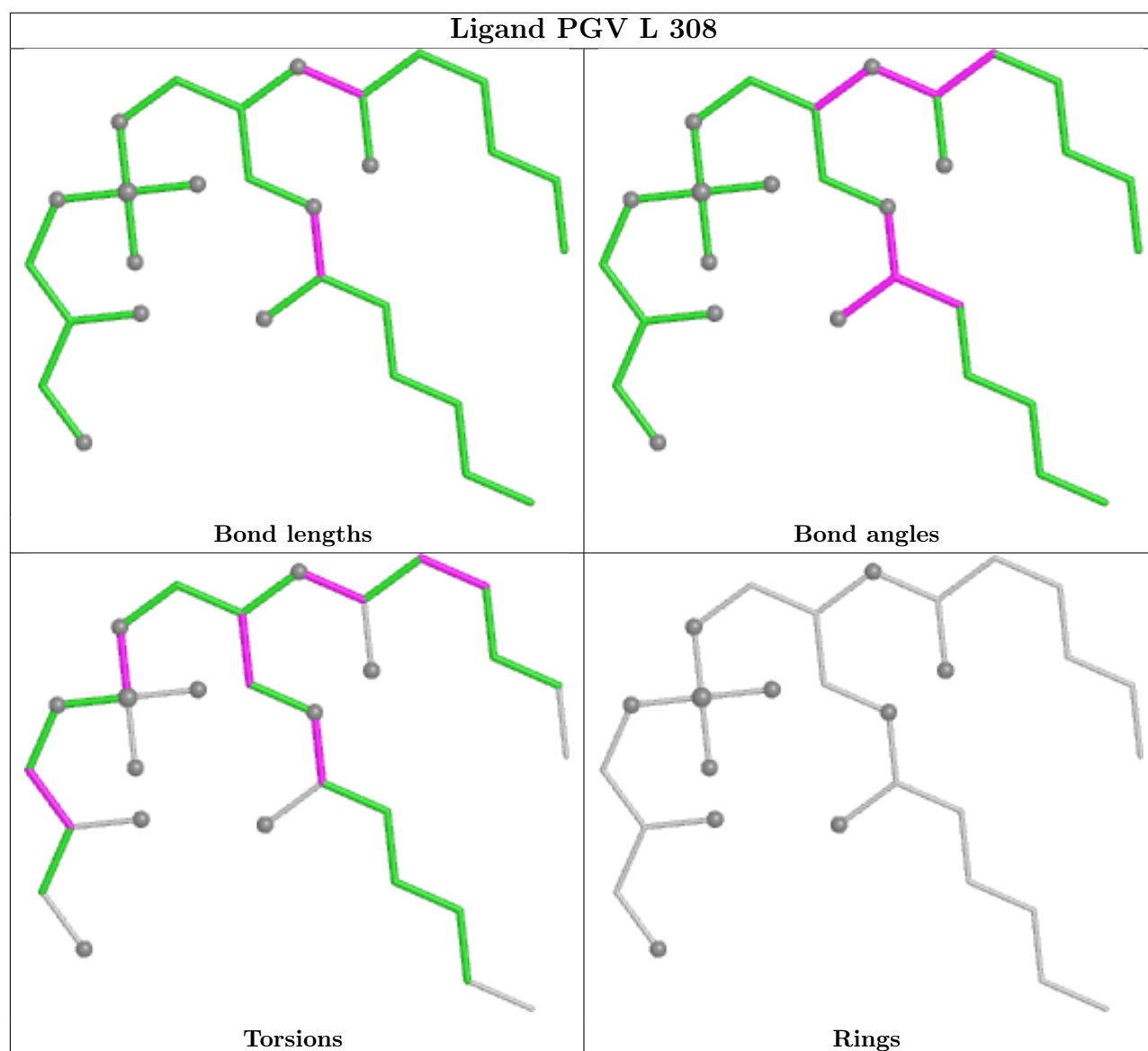


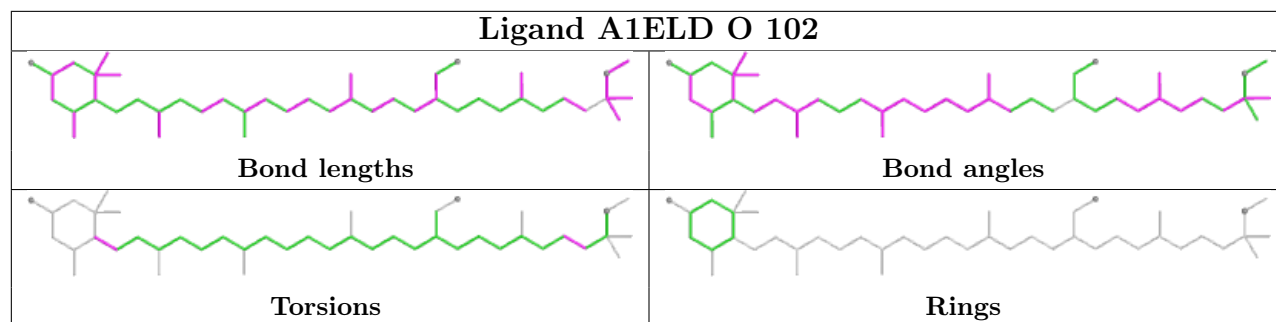












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

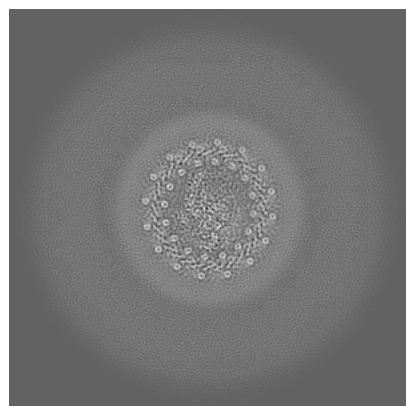
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63370. These allow visual inspection of the internal detail of the map and identification of artifacts.

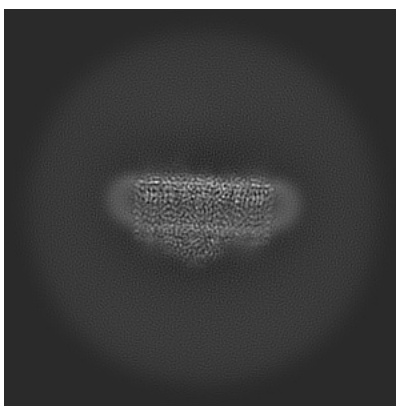
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

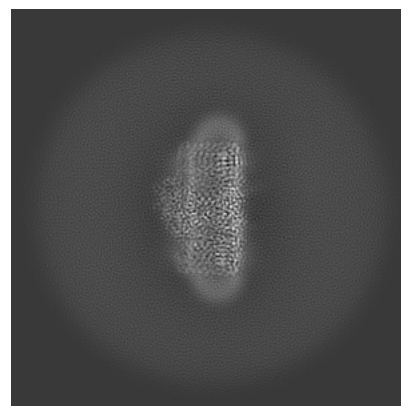
6.1.1 Primary map



X

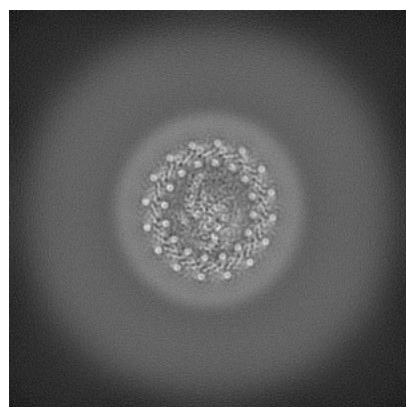


Y

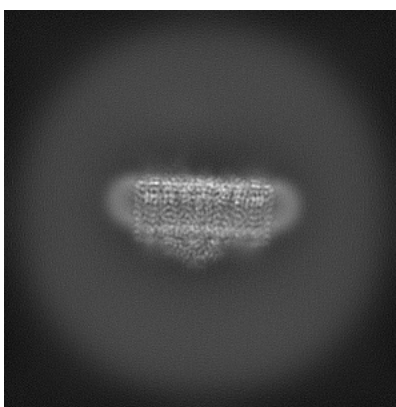


Z

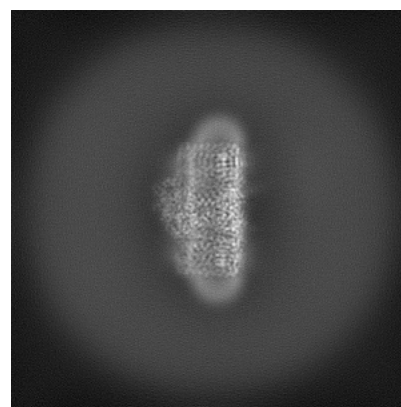
6.1.2 Raw map



X



Y

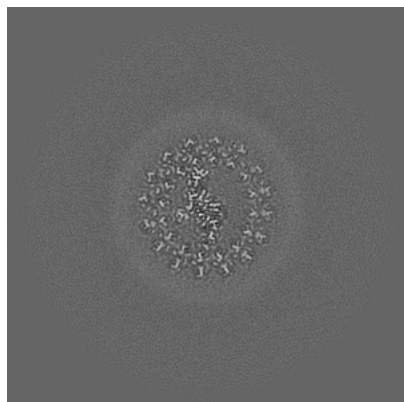


Z

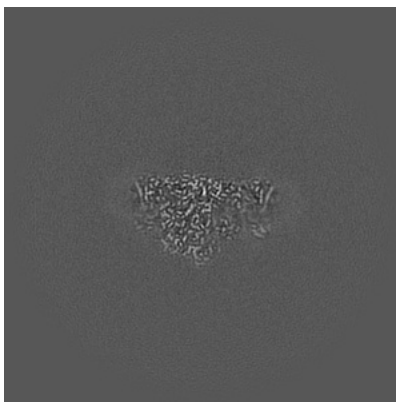
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

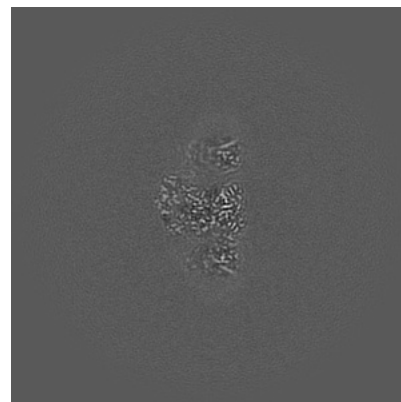
6.2.1 Primary map



X Index: 200

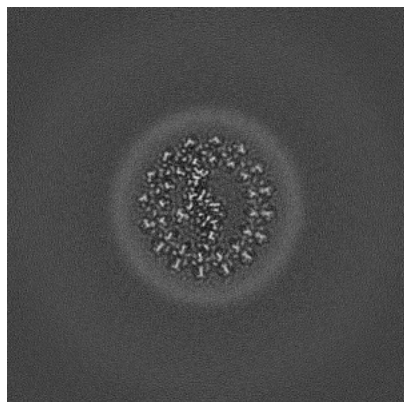


Y Index: 200

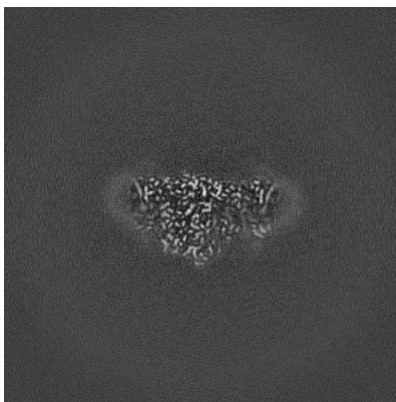


Z Index: 200

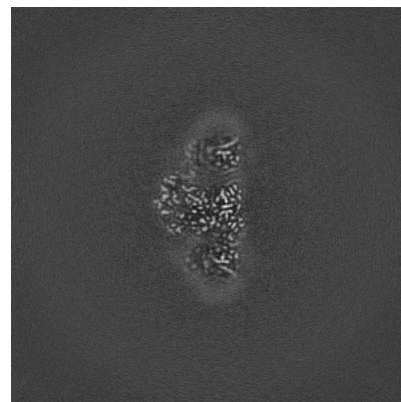
6.2.2 Raw map



X Index: 200



Y Index: 200

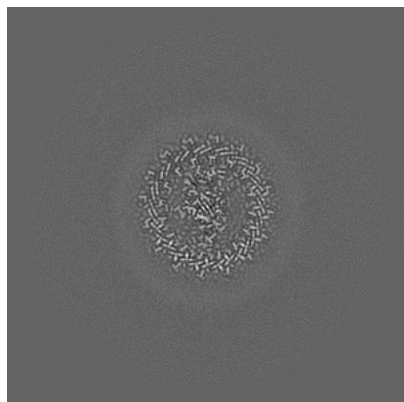


Z Index: 200

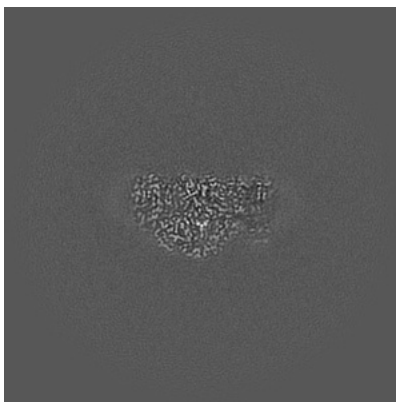
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

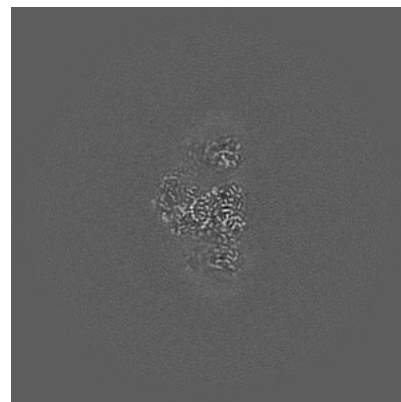
6.3.1 Primary map



X Index: 213

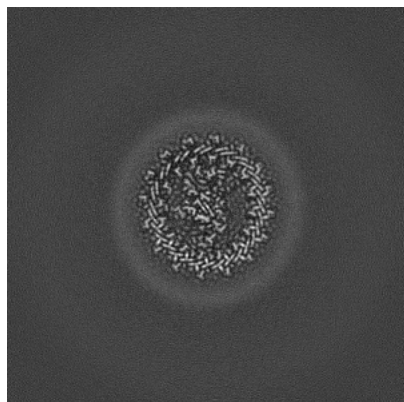


Y Index: 195

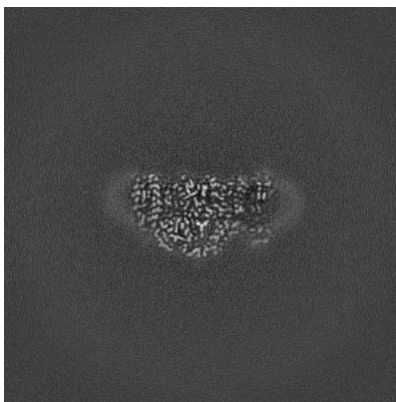


Z Index: 198

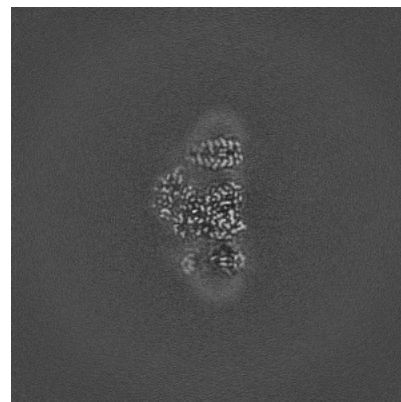
6.3.2 Raw map



X Index: 213



Y Index: 195

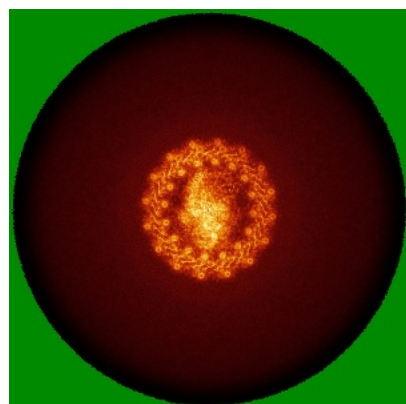


Z Index: 194

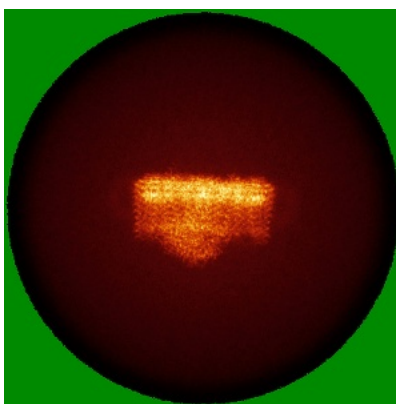
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

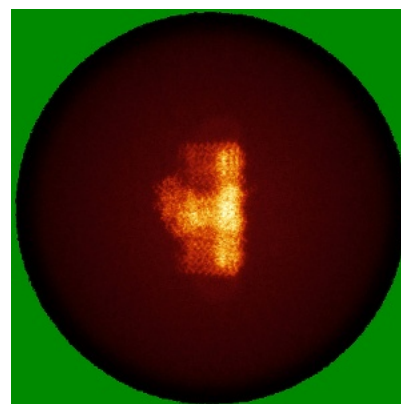
6.4.1 Primary map



X

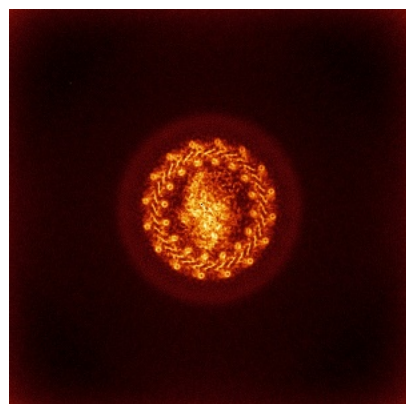


Y

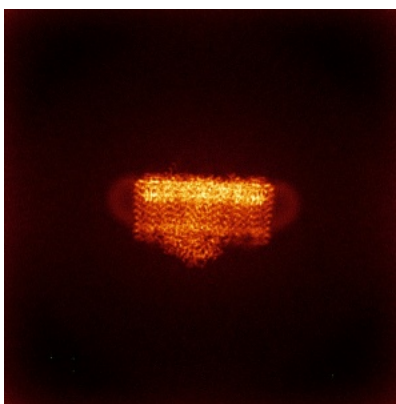


Z

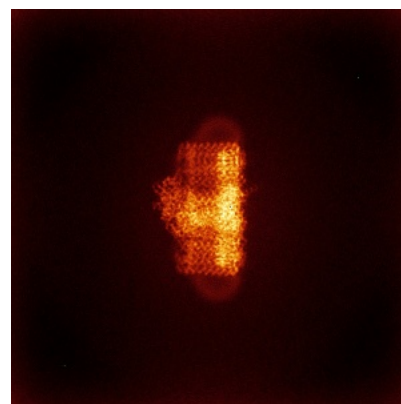
6.4.2 Raw map



X



Y

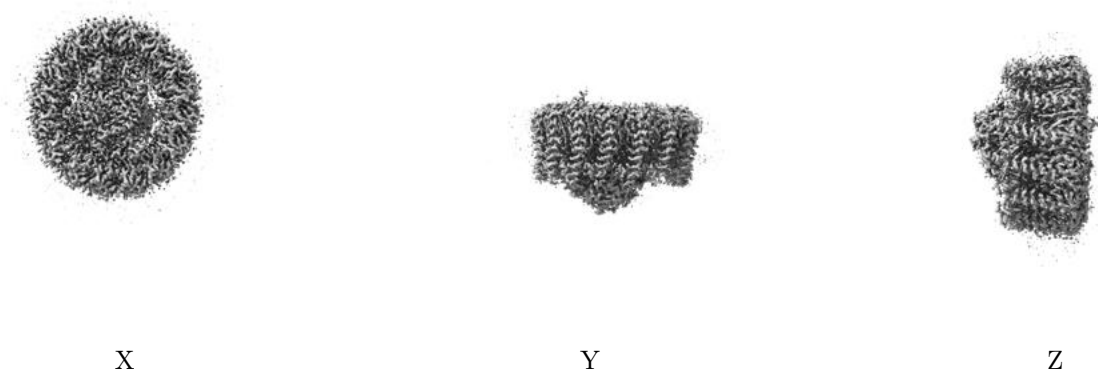


Z

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

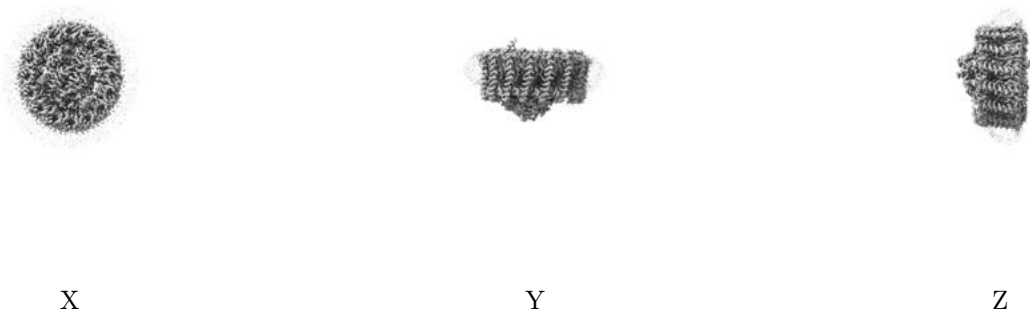
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0961. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

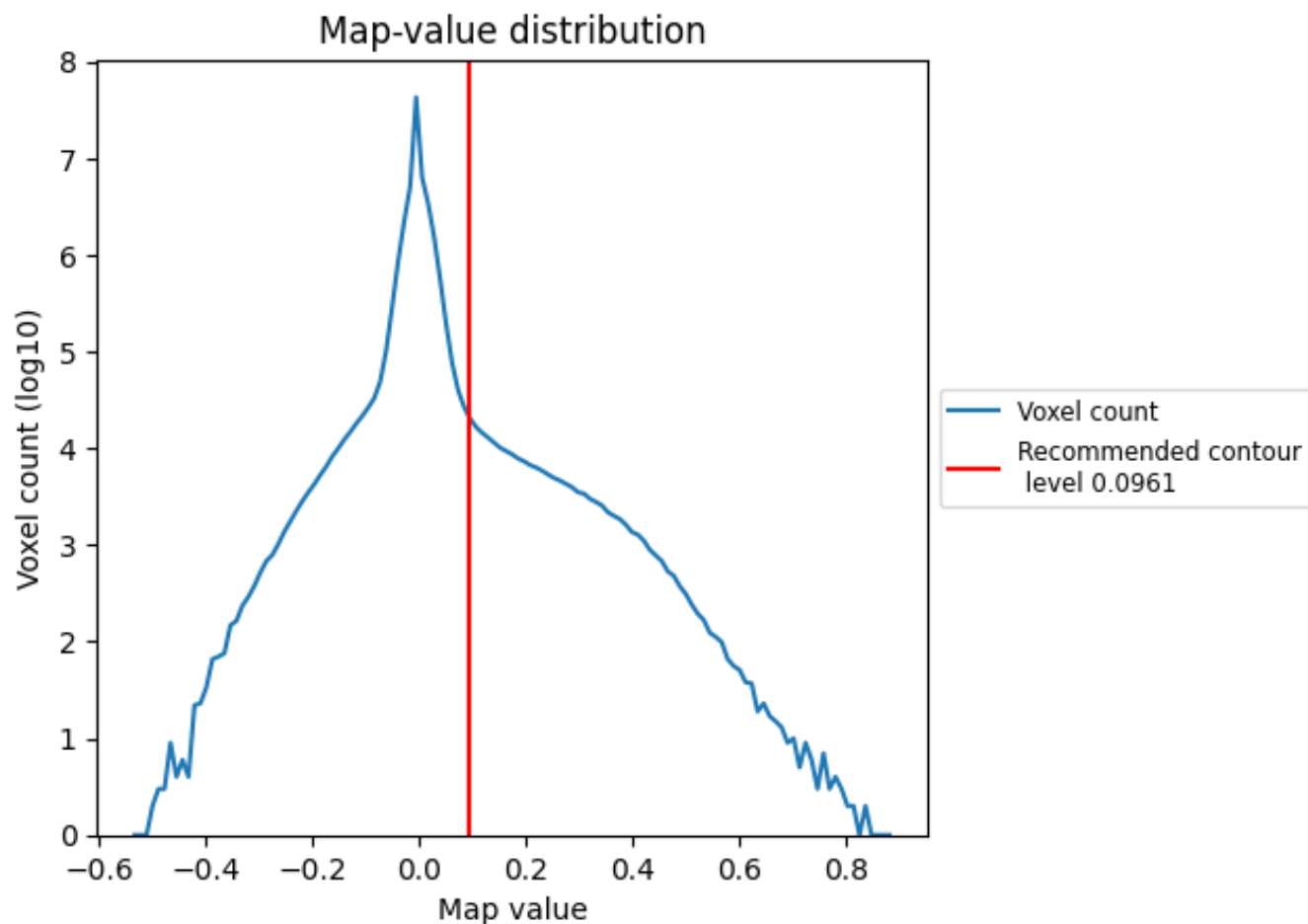
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

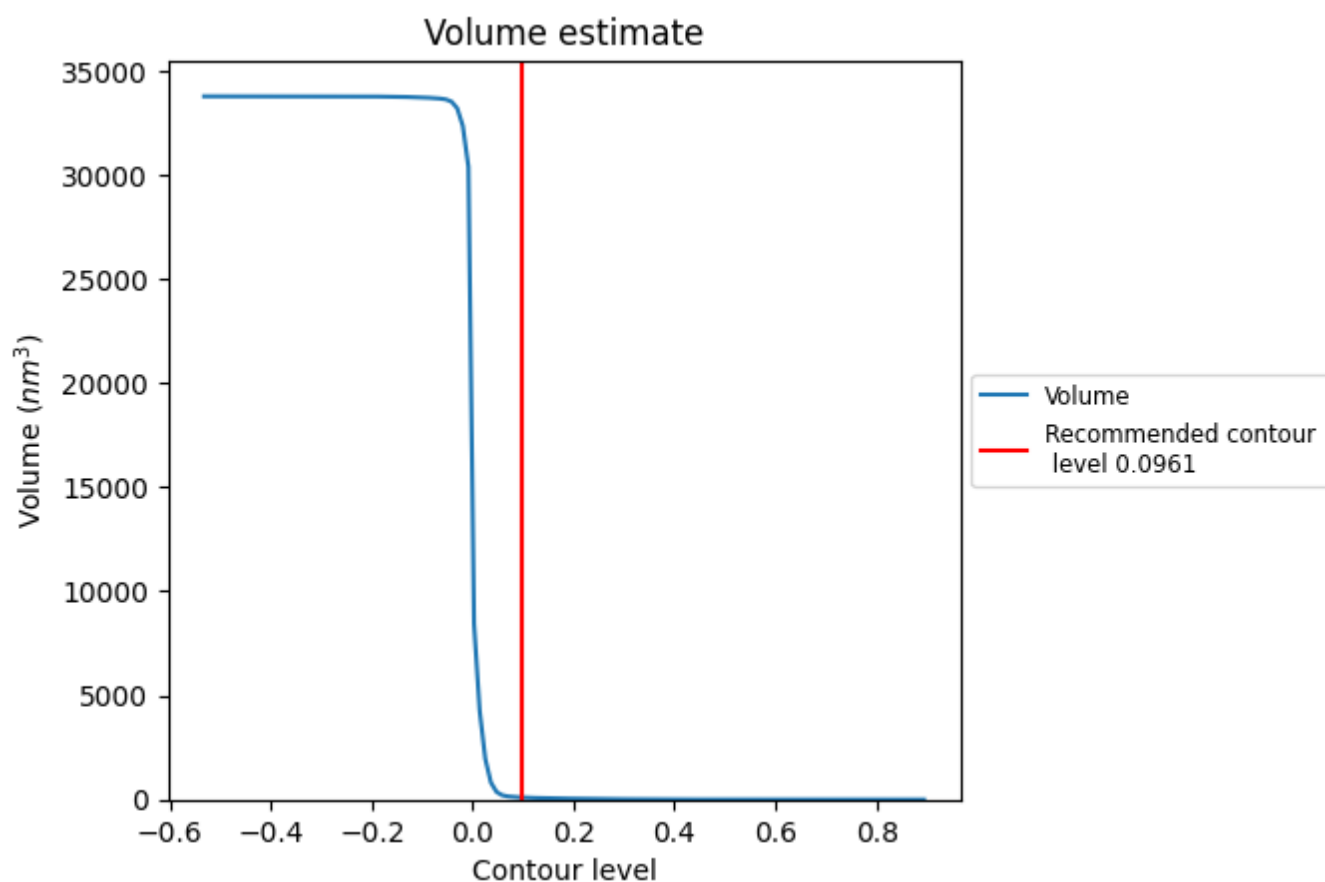
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

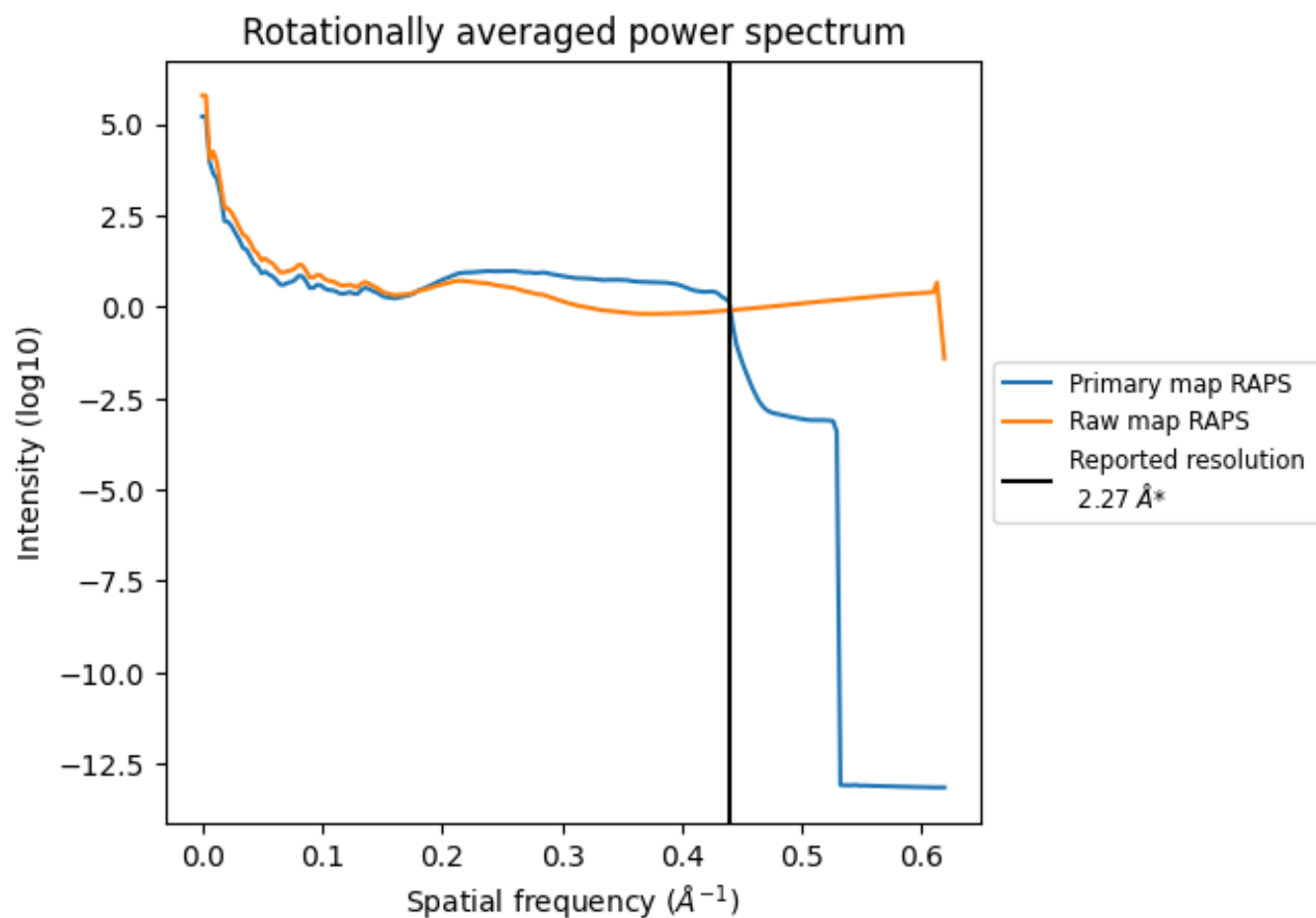
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; 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 ⓘ

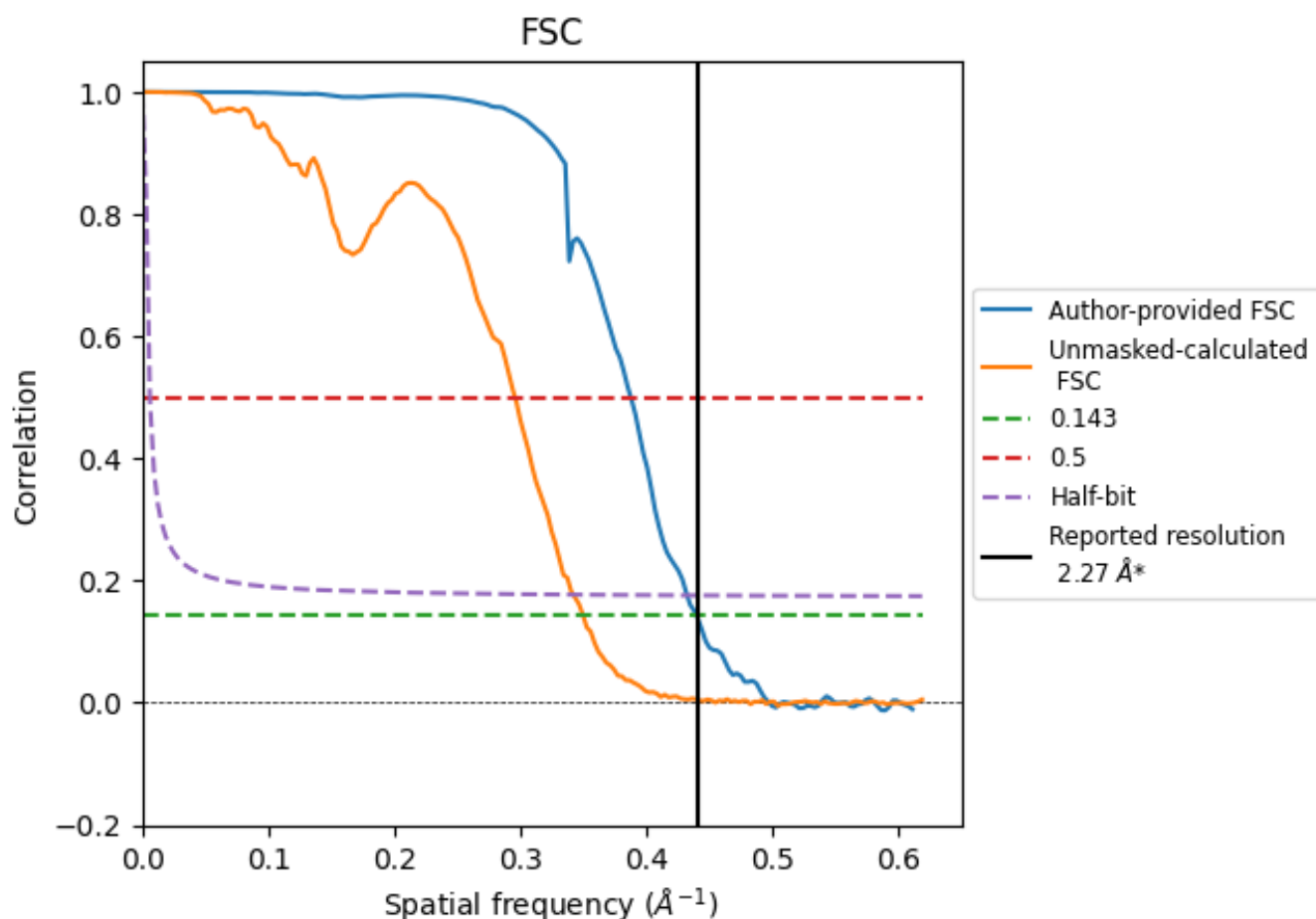


*Reported resolution corresponds to spatial frequency of 0.441 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.441 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

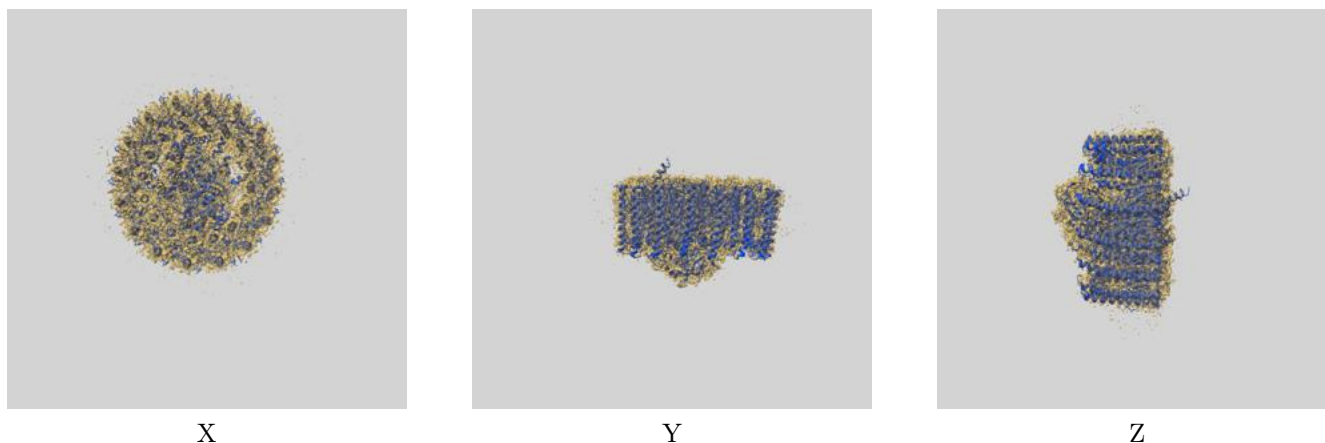
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.27	2.58	2.31
Unmasked-calculated*	2.86	3.38	2.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.86 differs from the reported value 2.27 by more than 10 %

9 Map-model fit [i](#)

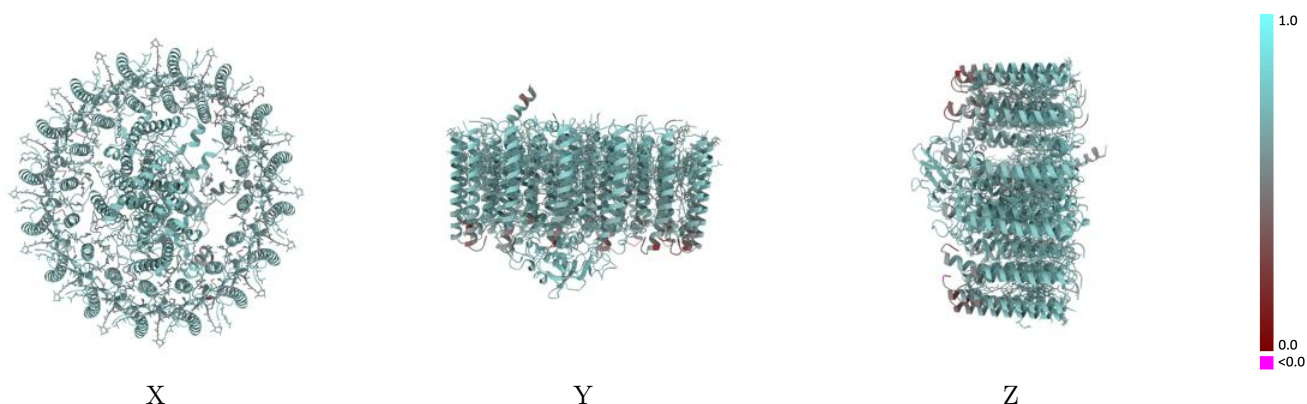
This section contains information regarding the fit between EMDB map EMD-63370 and PDB model 9LTI. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



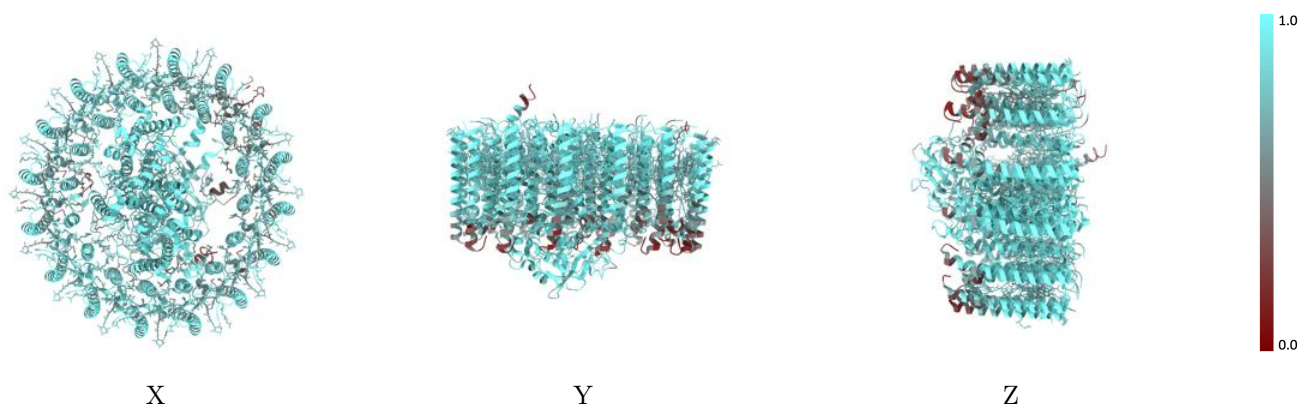
The images above show the 3D surface view of the map at the recommended contour level 0.0961 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



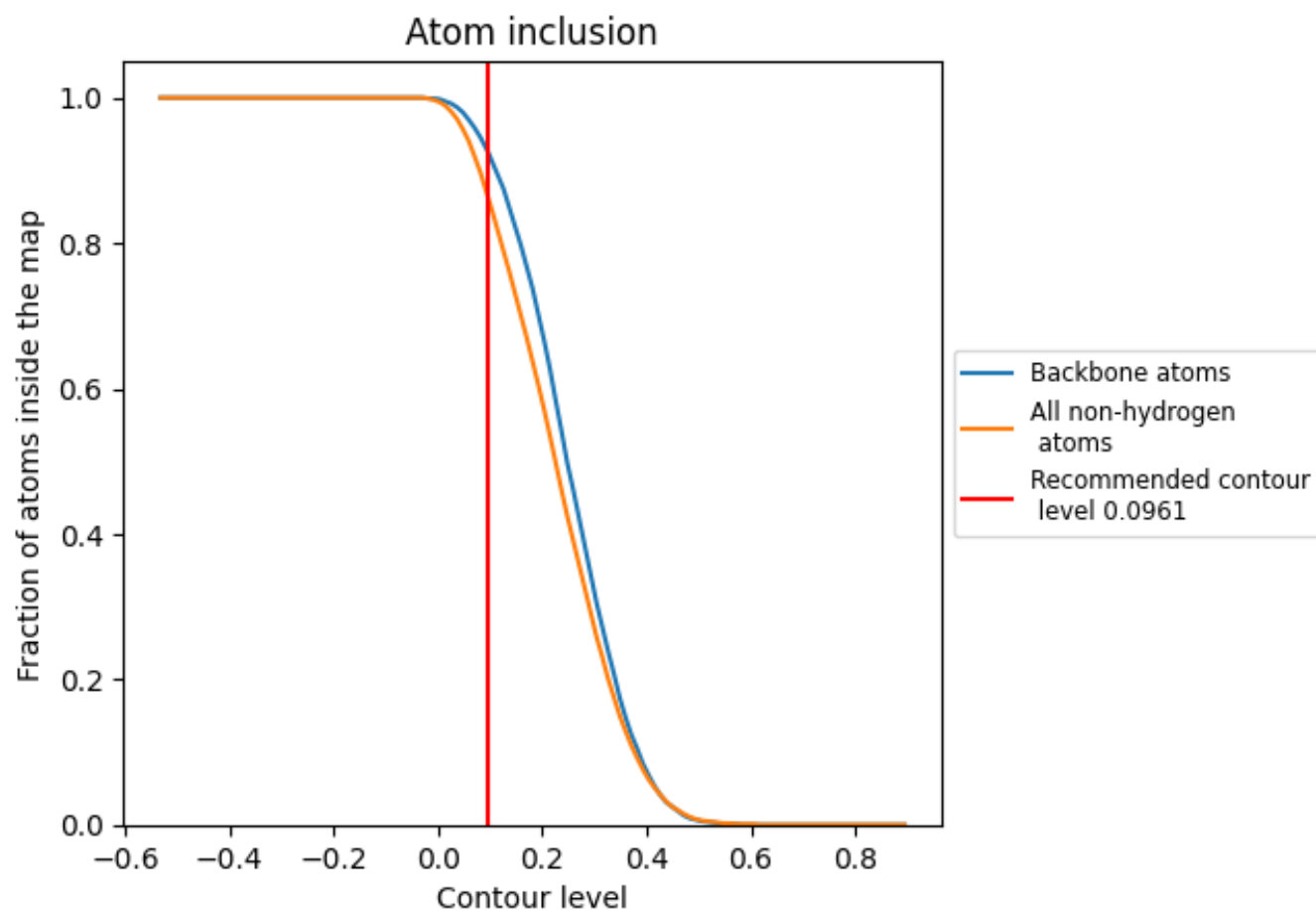
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0961).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.0961) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.6640
A	 0.9270	 0.6780
B	 0.9130	 0.6790
C	 0.9070	 0.6680
D	 0.9100	 0.6810
E	 0.8480	 0.6590
F	 0.7520	 0.6360
G	 0.8710	 0.6620
H	 0.8940	 0.6880
I	 0.9090	 0.6730
J	 0.8420	 0.6580
K	 0.7320	 0.6170
L	 0.9590	 0.7080
M	 0.9540	 0.7100
N	 0.8180	 0.6430
O	 0.7910	 0.6400
P	 0.8230	 0.6310
Q	 0.9040	 0.6670
R	 0.7590	 0.6230
S	 0.8200	 0.6440
T	 0.6500	 0.6150
a	 0.8670	 0.6570
b	 0.8550	 0.6530
c	 0.8720	 0.6620
d	 0.8710	 0.6730
e	 0.7680	 0.6210
f	 0.7730	 0.6240
g	 0.8100	 0.6070
i	 0.8700	 0.6610
j	 0.7680	 0.6350
k	 0.6790	 0.5950
n	 0.7730	 0.6210
o	 0.8080	 0.6320
p	 0.7830	 0.6290
q	 0.8690	 0.6620



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
r	 0.6780	 0.5940
s	 0.8150	 0.6370