



Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 01:10 AM JST

PDB ID : 7VZR
EMDB ID : EMD-32229
Title : Structure of the Acidobacteria homodimeric reaction center bound with cytochrome c (the smaller form)
Authors : Huang, G.Q.; Dong, S.S.; Qin, X.C.; Sui, S.F.
Deposited on : 2021-11-16
Resolution : 2.22 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

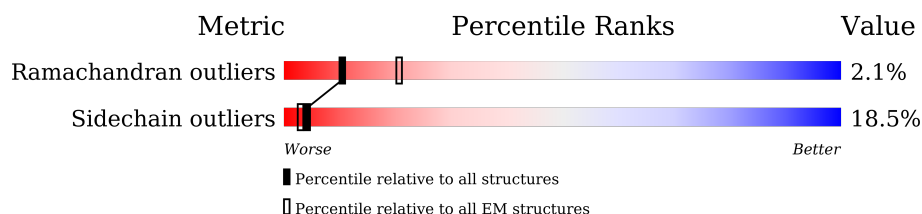
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.22 Å.

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



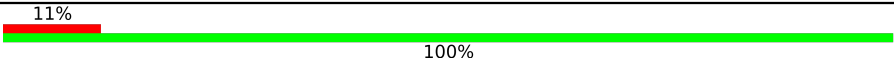
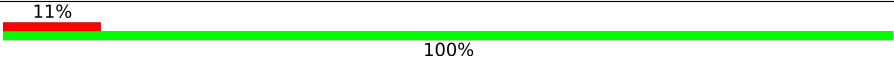

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	865	
1	a	865	
2	C	221	
3	E	35	
3	e	35	
4	F	35	
4	f	35	
5	G	45	
5	g	45	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	19	
6	h	19	
7	c	145	

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
10	CLA	A	910	X	-	-	-
10	CLA	A	911	X	-	-	-
11	LYC	c	201	-	X	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 21354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosynthetic reaction center subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	854	Total	C	N	O	S	0	0
			6960	4602	1155	1170	33		
1	a	858	Total	C	N	O	S	0	0
			6984	4616	1160	1175	33		

- Molecule 2 is a protein called Cytochrome c, mono-and diheme variants.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	193	Total	C	N	O	S	0	0
			1474	900	277	288	9		

- Molecule 3 is a protein called PscE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	35	Total	C	N	O	S	0	0
			258	174	40	42	2		
3	e	35	Total	C	N	O	S	0	0
			258	174	40	42	2		

- Molecule 4 is a protein called PscF.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	35	Total	C	N	O	S	0	0
			273	185	43	43	2		
4	f	35	Total	C	N	O	S	0	0
			273	185	43	43	2		

- Molecule 5 is a protein called PscG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	38	Total	C	N	O	S	0	0
			302	210	45	44	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	38	Total	C	N	O	S	0	0
			302	210	45	44	3		

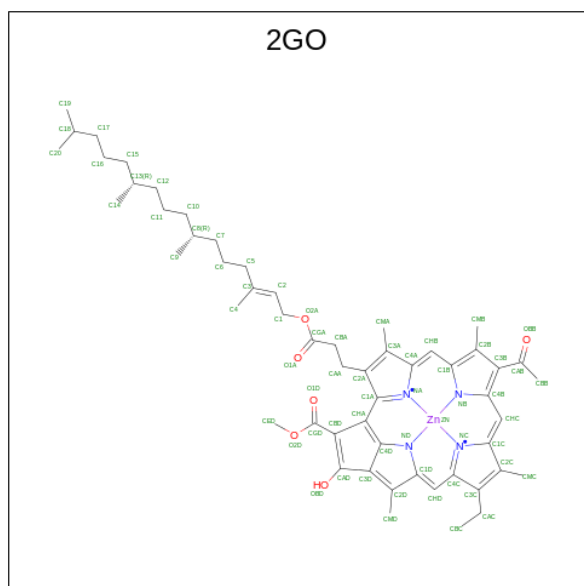
- Molecule 6 is a protein called undefined polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	19	Total	C	N	O	0	0
			95	57	19	19		
6	h	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 7 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	145	Total	C	N	O	S	0	0
			1096	679	200	210	7		

- Molecule 8 is [methyl 9-acetyl-14-ethyl-20-hydroxy-4,8,13,18-tetramethyl-3-{3-oxo-3-[(3,7,11,15-tetramethylhexadec-2-en-1-yl)oxy]propyl}-3,4,20,21-tetradehydrophorbine-21-carboxylato(2-)-kappa 4 N 23 ,N 24 ,N 25 ,N 26]zinc (three-letter code: 2GO) (formula: C₅₅H₇₀N₄O₆Zn) (labeled as "Ligand of Interest" by depositor).



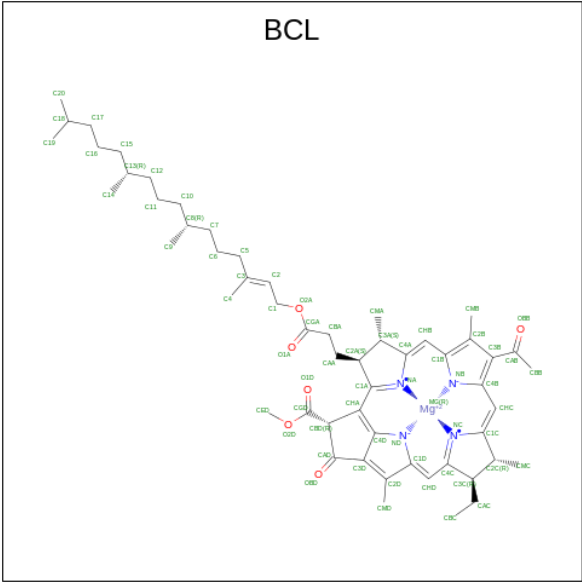
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	Zn	0
			66	55	4	6	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	a	1	Total	C	N	O	Zn	0
			66	55	4	6	1	

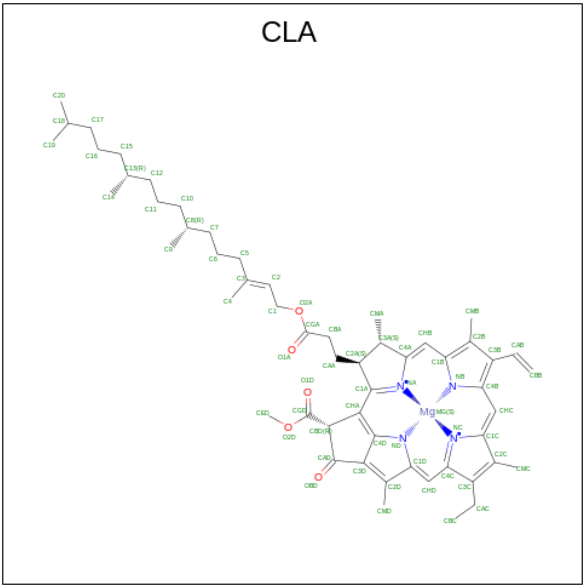
- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



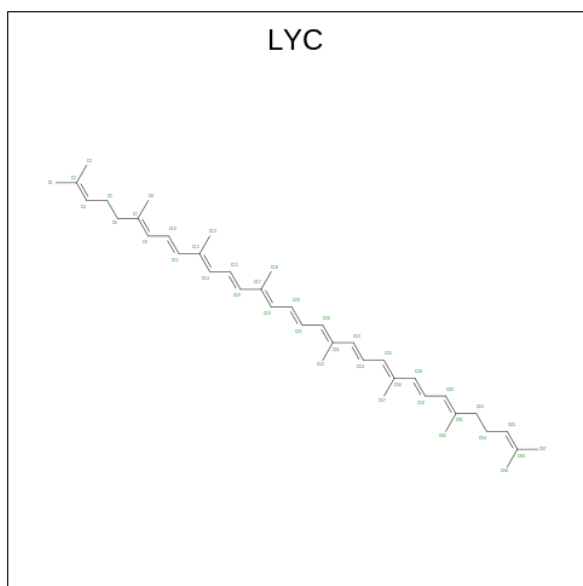
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
10	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

- Molecule 11 is LYCOPENE (three-letter code: LYC) (formula: $C_{40}H_{56}$).

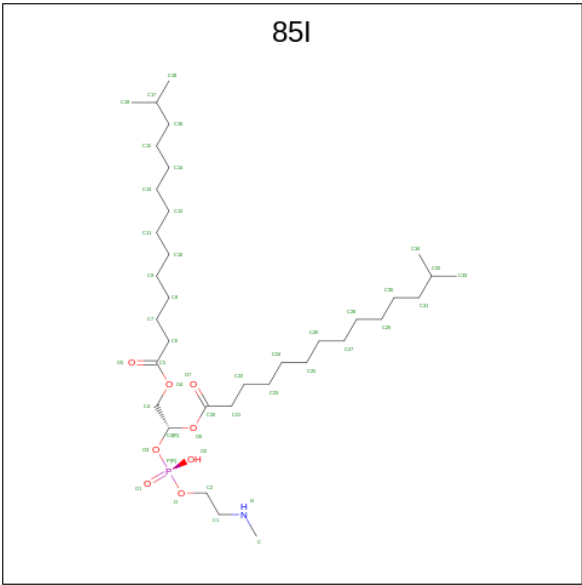


Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	C	0
			40	40	
11	c	1	Total	C	0
			40	40	

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Ca	0
			1	1	
12	a	1	Total	Ca	0
			1	1	

- Molecule 13 is [(2 {R})-2-[2-(methylamino)ethoxy-oxidanyl-phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (three-letter code: 85I) (formula: C₃₅H₇₀NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	a	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 14 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

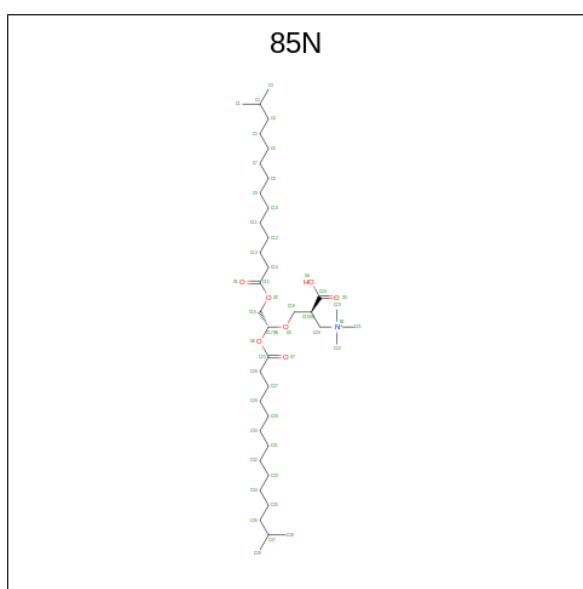
Mol	Chain	Residues	Atoms		AltConf
14	A	13	Total	C	0
			240	240	
14	C	1	Total	C	0
			18	18	
14	E	2	Total	C	0
			26	26	

Continued on next page...

Continued from previous page...

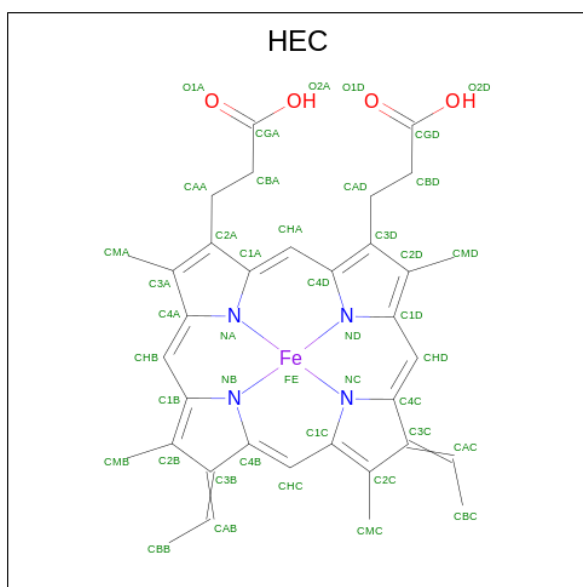
Mol	Chain	Residues	Atoms		AltConf
14	a	13	Total	C	0
			243	243	
14	c	1	Total	C	0
			8	8	
14	e	2	Total	C	0
			26	26	

- Molecule 15 is [(2 {S})-2-[[[(1 {R})-1,2-bis(13-methyltetradecanoyloxy)ethoxy]methyl]-3-oxidanyl-3-oxidanylidene-propyl]-trimethyl-azanium (three-letter code: 85N) (formula: C₃₉H₇₆NO₇) (labeled as "Ligand of Interest" by depositor).



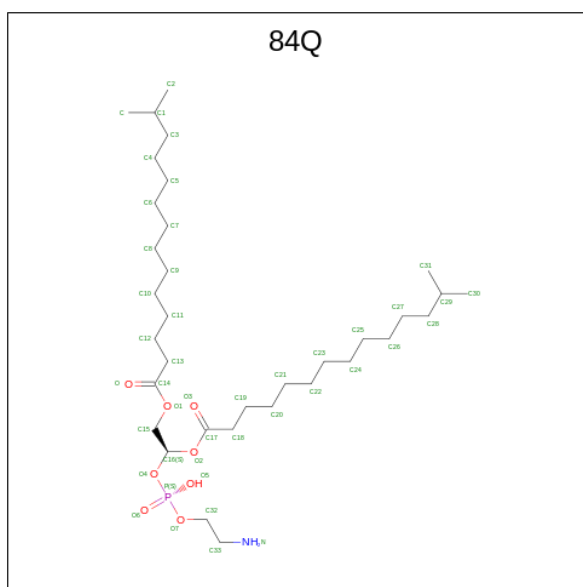
Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	N	O	0
			47	39	1	7	
15	G	1	Total	C	N	O	0
			38	30	1	7	
15	a	1	Total	C	N	O	0
			47	39	1	7	
15	g	1	Total	C	N	O	0
			38	30	1	7	

- Molecule 16 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
16	c	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 17 is [(2S)-2-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (three-letter code: 84Q) (formula: C₃₄H₆₈NO₈P) (labeled as "Ligand of Interest" by depositor).



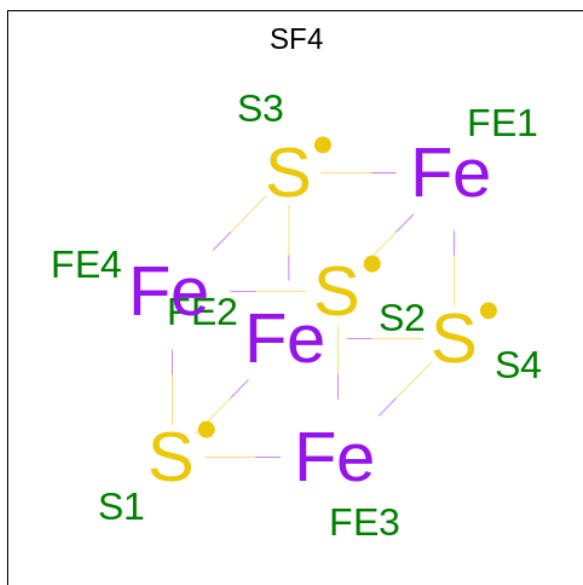
Mol	Chain	Residues	Atoms					AltConf
17	E	1	Total	C	N	O	P	0
			44	34	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	a	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	A	3	Total	O	0
			3	3	
19	a	3	Total	O	0
			3	3	

3 Residue-property plots

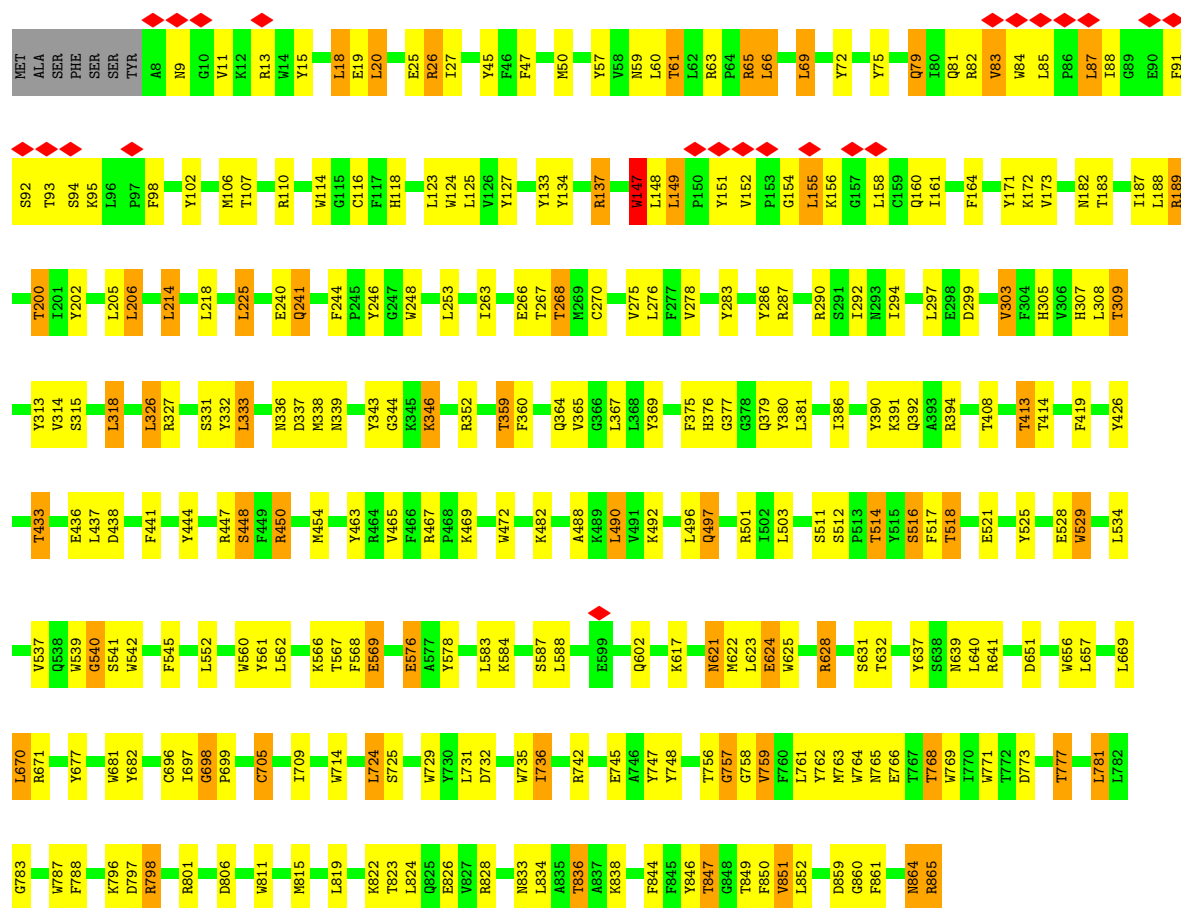
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Photosynthetic reaction center subunit M

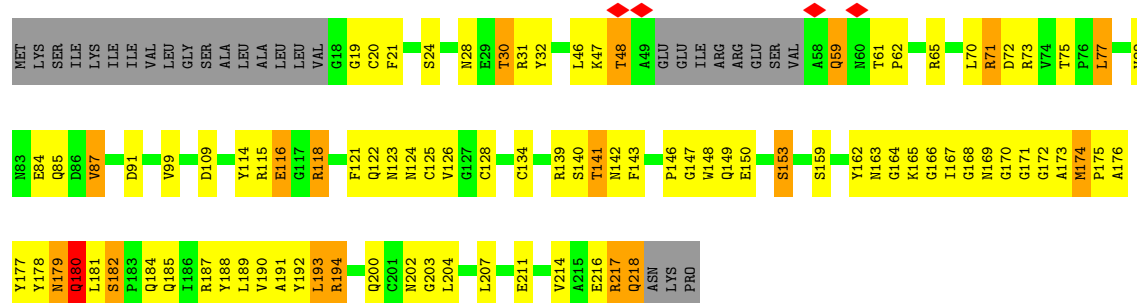


• Molecule 1: Photosynthetic reaction center subunit M





• Molecule 2: Cytochrome c, mono- and di-heme variants

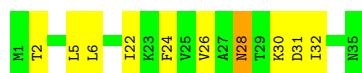


• Molecule 3: PscE

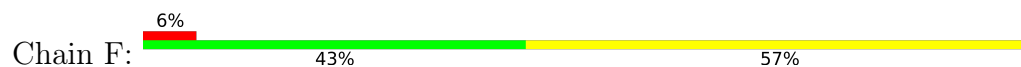


• Molecule 3: PscE

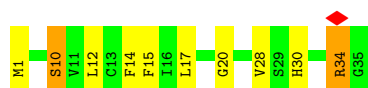




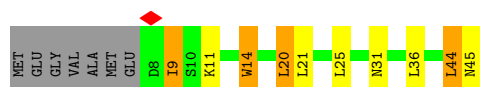
- Molecule 4: PscF



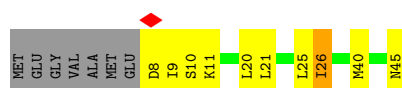
- Molecule 4: PscF



- Molecule 5: PscG



- Molecule 5: PscG



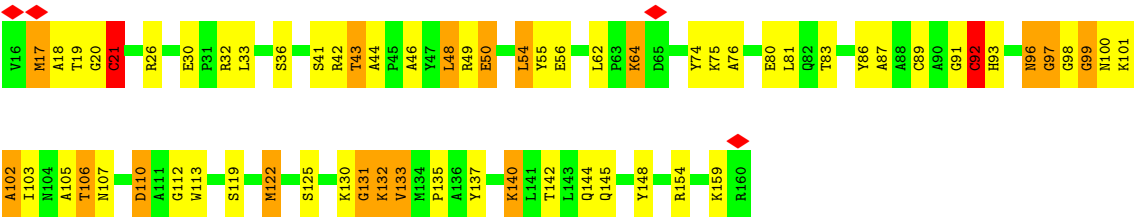
- Molecule 6: undefined polypeptide



- Molecule 6: undefined polypeptide



- Molecule 7: Cytochrome c domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	490075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.661	Depositor
Minimum map value	-2.809	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.48	Depositor
Map size (\AA)	238.15, 238.15, 238.15	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 85N, CA, 84Q, BCL, 85I, SF4, LYC, CLA, 2GO, UNL, HEC

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	1.97	233/7209 (3.2%)	1.33	86/9827 (0.9%)
1	a	1.85	196/7233 (2.7%)	1.28	91/9860 (0.9%)
2	C	2.35	98/1503 (6.5%)	1.67	35/2037 (1.7%)
3	E	2.16	9/262 (3.4%)	1.43	4/356 (1.1%)
3	e	1.50	2/262 (0.8%)	1.14	1/356 (0.3%)
4	F	2.28	15/279 (5.4%)	1.21	0/379
4	f	1.98	6/279 (2.2%)	1.28	1/379 (0.3%)
5	G	1.49	4/311 (1.3%)	1.60	6/421 (1.4%)
5	g	1.25	0/311	1.16	2/421 (0.5%)
7	c	2.54	75/1115 (6.7%)	1.79	36/1506 (2.4%)
All	All	1.98	638/18764 (3.4%)	1.37	262/25542 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	a	0	4
2	C	0	2
7	c	0	1
All	All	0	8

All (638) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	539	TRP	C-O	-15.07	0.94	1.23
7	c	55	TYR	CD1-CE1	-13.98	1.18	1.39
7	c	55	TYR	CD2-CE2	-13.28	1.19	1.39
1	A	309	THR	CB-CG2	-13.10	1.09	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	758	GLY	C-O	-12.33	1.03	1.23
1	a	266	GLU	CD-OE2	-12.24	1.12	1.25
7	c	106	THR	CB-CG2	-12.04	1.12	1.52
1	A	745	GLU	CB-CG	-11.46	1.30	1.52
2	C	141	THR	C-O	-11.41	1.01	1.23
3	E	13	GLY	C-O	-11.34	1.05	1.23
1	a	529	TRP	CB-CG	-11.05	1.30	1.50
1	a	705	CYS	CB-SG	10.68	2.00	1.82
1	a	783	GLY	C-O	-10.64	1.06	1.23
1	A	541	SER	CB-OG	-10.54	1.28	1.42
1	a	860	GLY	C-O	-10.53	1.06	1.23
1	A	266	GLU	CD-OE2	-10.47	1.14	1.25
1	a	758	GLY	C-O	-10.37	1.07	1.23
2	C	179	ASN	C-O	-10.18	1.04	1.23
7	c	20	GLY	C-O	-10.17	1.07	1.23
1	A	766	GLU	CD-OE2	-10.04	1.14	1.25
1	a	852	LEU	C-O	-9.97	1.04	1.23
2	C	140	SER	C-O	-9.89	1.04	1.23
1	a	757	GLY	C-O	-9.89	1.07	1.23
1	a	376	HIS	C-O	-9.83	1.04	1.23
7	c	106	THR	C-O	-9.62	1.05	1.23
1	a	305	HIS	C-O	-9.55	1.05	1.23
7	c	43	THR	CB-CG2	-9.52	1.21	1.52
1	A	638	SER	CB-OG	-9.46	1.29	1.42
7	c	112	GLY	C-O	-9.44	1.08	1.23
1	A	638	SER	C-O	-9.30	1.05	1.23
2	C	147	GLY	C-O	-9.29	1.08	1.23
1	a	541	SER	CB-OG	-9.27	1.30	1.42
1	a	732	ASP	CB-CG	-9.24	1.32	1.51
7	c	98	GLY	CA-C	-9.22	1.37	1.51
2	C	176	ALA	C-O	-9.11	1.06	1.23
1	a	759	VAL	C-O	-9.11	1.06	1.23
4	f	10	SER	CB-OG	-9.09	1.30	1.42
2	C	178	TYR	C-O	-9.05	1.06	1.23
1	a	748	TYR	CD2-CE2	-9.05	1.25	1.39
1	A	306	VAL	C-O	-9.03	1.06	1.23
1	A	313	TYR	CD1-CE1	-9.01	1.25	1.39
1	a	346	LYS	C-O	-9.01	1.06	1.23
1	A	731	LEU	C-O	-9.00	1.06	1.23
1	a	270	CYS	CB-SG	-8.98	1.67	1.82
2	C	182	SER	CB-OG	-8.98	1.30	1.42
2	C	19	GLY	C-O	-8.93	1.09	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	GLU	CD-OE1	-8.89	1.15	1.25
7	c	26	ARG	CZ-NH1	-8.86	1.21	1.33
4	F	4	VAL	C-O	-8.78	1.06	1.23
1	a	380	TYR	CD1-CE1	-8.78	1.26	1.39
1	A	125	LEU	C-O	-8.77	1.06	1.23
7	c	96	ASN	C-O	-8.74	1.06	1.23
1	a	369	TYR	CD1-CE1	-8.74	1.26	1.39
7	c	91	GLY	C-O	-8.72	1.09	1.23
1	a	796	LYS	C-O	-8.68	1.06	1.23
1	A	709	ILE	C-O	-8.66	1.06	1.23
1	a	561	TYR	CD2-CE2	-8.64	1.26	1.39
2	C	179	ASN	CG-OD1	-8.59	1.05	1.24
1	A	733	GLY	C-O	-8.57	1.09	1.23
1	A	61	THR	CB-CG2	-8.54	1.24	1.52
1	a	777	THR	CB-CG2	-8.48	1.24	1.52
7	c	56	GLU	CD-OE1	-8.38	1.16	1.25
1	A	266	GLU	CD-OE1	-8.35	1.16	1.25
2	C	30	THR	C-O	-8.33	1.07	1.23
1	A	541	SER	C-O	-8.27	1.07	1.23
1	A	538	GLN	CD-NE2	-8.24	1.12	1.32
1	A	542	TRP	C-O	-8.22	1.07	1.23
1	A	313	TYR	CD2-CE2	-8.22	1.27	1.39
2	C	142	ASN	CG-ND2	-8.21	1.12	1.32
1	a	426	TYR	CD2-CE2	-8.20	1.27	1.39
1	A	860	GLY	C-O	-8.18	1.10	1.23
4	F	10	SER	CB-OG	-8.16	1.31	1.42
1	a	61	THR	CB-CG2	-8.15	1.25	1.52
1	A	631	SER	CB-OG	-8.13	1.31	1.42
2	C	126	VAL	C-O	-8.06	1.08	1.23
1	A	811	TRP	CE3-CZ3	-8.05	1.24	1.38
1	a	133	TYR	CD1-CE1	-8.02	1.27	1.39
1	A	748	TYR	CD1-CE1	-7.98	1.27	1.39
1	a	332	TYR	CD2-CE2	-7.97	1.27	1.39
2	C	162	TYR	CZ-OH	-7.97	1.24	1.37
1	a	315	SER	CB-OG	-7.95	1.31	1.42
2	C	148	TRP	CG-CD1	-7.94	1.25	1.36
1	a	26	ARG	C-O	-7.93	1.08	1.23
1	A	57	TYR	CD1-CE1	-7.92	1.27	1.39
1	A	849	THR	CB-CG2	-7.90	1.26	1.52
1	A	448	SER	CB-OG	-7.88	1.32	1.42
7	c	86	TYR	CE2-CZ	-7.88	1.28	1.38
1	A	297	LEU	C-O	-7.87	1.08	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	561	TYR	CD1-CE1	-7.86	1.27	1.39
1	A	543	THR	C-O	-7.86	1.08	1.23
1	A	640	LEU	C-O	-7.86	1.08	1.23
7	c	41	SER	CB-OG	-7.84	1.32	1.42
2	C	143	PHE	C-O	-7.83	1.08	1.23
1	A	270	CYS	CB-SG	-7.83	1.69	1.82
2	C	123	ASN	C-O	-7.81	1.08	1.23
2	C	153	SER	CB-OG	-7.80	1.32	1.42
1	A	734	GLY	C-O	-7.80	1.11	1.23
1	a	283	TYR	CD2-CE2	-7.79	1.27	1.39
1	A	682	TYR	CE1-CZ	-7.78	1.28	1.38
4	F	6	GLY	C-O	-7.77	1.11	1.23
1	a	811	TRP	C-O	-7.76	1.08	1.23
7	c	56	GLU	C-O	-7.74	1.08	1.23
2	C	116	GLU	CD-OE2	-7.74	1.17	1.25
2	C	185	GLN	CD-NE2	-7.73	1.13	1.32
7	c	130	LYS	C-O	-7.71	1.08	1.23
1	a	364	GLN	CD-NE2	-7.70	1.13	1.32
1	A	742	ARG	CZ-NH1	-7.70	1.23	1.33
7	c	55	TYR	CZ-OH	-7.68	1.24	1.37
1	A	362	HIS	C-O	-7.66	1.08	1.23
1	A	747	TYR	CD1-CE1	-7.65	1.27	1.39
1	a	521	GLU	CD-OE1	-7.63	1.17	1.25
1	a	639	ASN	CB-CG	-7.63	1.33	1.51
2	C	188	TYR	C-O	-7.62	1.08	1.23
2	C	190	VAL	C-O	-7.62	1.08	1.23
1	A	202	TYR	CE2-CZ	-7.62	1.28	1.38
2	C	178	TYR	CZ-OH	-7.60	1.25	1.37
1	a	764	TRP	CZ3-CH2	-7.60	1.27	1.40
1	A	560	TRP	C-O	-7.59	1.08	1.23
2	C	164	GLY	C-O	-7.59	1.11	1.23
1	a	542	TRP	CE3-CZ3	-7.59	1.25	1.38
7	c	26	ARG	C-O	-7.58	1.08	1.23
2	C	182	SER	C-O	-7.54	1.09	1.23
1	A	764	TRP	C-O	-7.54	1.09	1.23
2	C	166	GLY	C-O	-7.54	1.11	1.23
2	C	188	TYR	CB-CG	-7.51	1.40	1.51
1	A	655	PHE	C-O	-7.50	1.09	1.23
1	A	294	ILE	C-O	-7.49	1.09	1.23
7	c	42	ARG	C-O	-7.47	1.09	1.23
1	A	639	ASN	CG-OD1	-7.46	1.07	1.24
2	C	121	PHE	C-O	-7.43	1.09	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	433	THR	CB-CG2	-7.42	1.27	1.52
2	C	173	ALA	C-O	-7.41	1.09	1.23
1	a	731	LEU	C-O	-7.38	1.09	1.23
1	A	725	SER	CB-OG	-7.38	1.32	1.42
1	A	699	PRO	C-O	-7.38	1.08	1.23
1	a	134	TYR	CB-CG	-7.38	1.40	1.51
1	A	774	ASN	CG-ND2	-7.36	1.14	1.32
1	a	745	GLU	CB-CG	-7.35	1.38	1.52
2	C	142	ASN	N-CA	7.34	1.61	1.46
7	c	93	HIS	C-O	-7.31	1.09	1.23
2	C	180	GLN	C-O	-7.31	1.09	1.23
1	a	57	TYR	CD2-CE2	-7.31	1.28	1.39
2	C	214	VAL	C-O	-7.30	1.09	1.23
1	A	776	LEU	C-O	-7.29	1.09	1.23
1	a	25	GLU	CD-OE1	-7.28	1.17	1.25
2	C	175	PRO	C-O	-7.27	1.08	1.23
1	A	656	TRP	C-O	-7.27	1.09	1.23
2	C	169	ASN	CG-OD1	-7.27	1.07	1.24
2	C	163	ASN	C-O	-7.26	1.09	1.23
7	c	99	GLY	C-O	-7.26	1.12	1.23
1	a	631	SER	C-O	-7.25	1.09	1.23
1	A	124	TRP	C-O	-7.25	1.09	1.23
2	C	128	CYS	C-O	-7.23	1.09	1.23
1	A	766	GLU	CD-OE1	-7.23	1.17	1.25
1	A	810	ARG	CZ-NH1	-7.21	1.23	1.33
1	a	365	VAL	CB-CG2	-7.21	1.37	1.52
1	A	539	TRP	C-O	-7.20	1.09	1.23
1	A	756	THR	C-O	-7.19	1.09	1.23
1	A	248	TRP	C-O	-7.19	1.09	1.23
1	a	414	THR	CB-CG2	-7.19	1.28	1.52
1	A	740	MET	C-O	-7.18	1.09	1.23
1	a	364	GLN	CD-OE1	-7.17	1.08	1.24
1	A	245	PRO	C-O	-7.17	1.08	1.23
2	C	72	ASP	C-O	-7.16	1.09	1.23
2	C	167	ILE	C-O	-7.14	1.09	1.23
4	F	25	ILE	C-O	-7.14	1.09	1.23
1	a	25	GLU	CD-OE2	-7.13	1.17	1.25
2	C	87	VAL	CB-CG2	-7.12	1.37	1.52
2	C	181	LEU	C-O	-7.12	1.09	1.23
1	A	411	VAL	CB-CG2	-7.11	1.38	1.52
1	A	741	ALA	C-O	-7.10	1.09	1.23
1	a	656	TRP	CB-CG	-7.08	1.37	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	788	PHE	CD2-CE2	-7.08	1.25	1.39
4	f	20	GLY	C-O	-7.07	1.12	1.23
4	F	10	SER	C-O	-7.07	1.09	1.23
1	A	628	ARG	CB-CG	-7.06	1.33	1.52
1	A	796	LYS	C-O	-7.05	1.09	1.23
1	a	763	MET	C-O	-7.04	1.09	1.23
1	A	210	TRP	C-O	-7.03	1.10	1.23
1	a	765	ASN	C-O	-7.03	1.10	1.23
1	a	699	PRO	C-O	-7.01	1.09	1.23
1	a	765	ASN	CG-OD1	-7.01	1.08	1.24
7	c	46	ALA	C-O	-7.01	1.10	1.23
2	C	146	PRO	C-O	-7.00	1.09	1.23
1	a	514	THR	CB-CG2	-7.00	1.29	1.52
1	a	748	TYR	CD1-CE1	-7.00	1.28	1.39
1	A	311	ILE	C-O	-7.00	1.10	1.23
1	a	847	THR	CB-CG2	-6.98	1.29	1.52
1	a	202	TYR	CD1-CE1	-6.96	1.28	1.39
1	a	518	THR	CB-CG2	-6.95	1.29	1.52
1	A	762	TYR	CD1-CE1	-6.94	1.28	1.39
1	A	209	ILE	C-O	-6.93	1.10	1.23
1	A	540	GLY	C-O	-6.93	1.12	1.23
1	a	57	TYR	CD1-CE1	-6.92	1.28	1.39
1	A	836	THR	CB-CG2	-6.91	1.29	1.52
1	A	283	TYR	CD2-CE2	-6.91	1.28	1.39
1	a	742	ARG	CZ-NH1	-6.91	1.24	1.33
4	f	17	LEU	C-O	-6.90	1.10	1.23
1	a	528	GLU	CD-OE1	-6.90	1.18	1.25
1	A	252	TYR	CD2-CE2	-6.90	1.29	1.39
1	a	757	GLY	CA-C	-6.89	1.40	1.51
7	c	43	THR	C-O	-6.89	1.10	1.23
1	a	173	VAL	CB-CG1	-6.88	1.38	1.52
2	C	148	TRP	C-O	-6.86	1.10	1.23
1	a	764	TRP	C-O	-6.86	1.10	1.23
2	C	188	TYR	CE2-CZ	-6.85	1.29	1.38
1	A	832	SER	CB-OG	-6.85	1.33	1.42
1	A	203	ILE	C-O	-6.83	1.10	1.23
3	e	28	ASN	C-O	-6.83	1.10	1.23
2	C	170	GLY	C-O	-6.81	1.12	1.23
1	a	413	THR	CB-CG2	-6.80	1.29	1.52
7	c	26	ARG	CZ-NH2	-6.80	1.24	1.33
1	A	861	PHE	C-O	-6.77	1.10	1.23
2	C	189	LEU	C-O	-6.77	1.10	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	102	TYR	CD1-CE1	-6.76	1.29	1.39
2	C	123	ASN	CG-ND2	-6.75	1.16	1.32
1	a	624	GLU	CB-CG	-6.75	1.39	1.52
1	A	480	TRP	C-O	-6.73	1.10	1.23
7	c	99	GLY	CA-C	-6.71	1.41	1.51
1	a	314	VAL	CB-CG2	-6.69	1.38	1.52
1	A	126	VAL	C-O	-6.69	1.10	1.23
1	A	742	ARG	C-O	-6.68	1.10	1.23
2	C	177	TYR	C-O	-6.68	1.10	1.23
1	a	497	GLN	CB-CG	-6.67	1.34	1.52
1	a	569	GLU	CB-CG	-6.66	1.39	1.52
1	A	497	GLN	CB-CG	-6.66	1.34	1.52
1	a	72	TYR	CD2-CE2	-6.64	1.29	1.39
1	A	348	VAL	CB-CG2	-6.63	1.39	1.52
2	C	124	ASN	C-O	-6.62	1.10	1.23
7	c	55	TYR	CE1-CZ	-6.61	1.29	1.38
1	A	75	TYR	CD1-CE1	-6.60	1.29	1.39
7	c	113	TRP	CE3-CZ3	-6.60	1.27	1.38
1	A	283	TYR	CD1-CE1	-6.59	1.29	1.39
1	a	542	TRP	CD1-NE1	-6.59	1.26	1.38
1	A	307	HIS	C-O	-6.59	1.10	1.23
1	a	465	VAL	CB-CG2	-6.59	1.39	1.52
2	C	32	TYR	CD1-CE1	-6.58	1.29	1.39
3	E	2	THR	C-O	-6.58	1.10	1.23
1	a	313	TYR	CD2-CE2	-6.57	1.29	1.39
7	c	125	SER	CB-OG	-6.57	1.33	1.42
1	A	535	TYR	CD1-CE1	-6.57	1.29	1.39
1	a	756	THR	C-O	-6.55	1.10	1.23
1	A	202	TYR	CZ-OH	-6.55	1.26	1.37
1	A	343	TYR	CD2-CE2	-6.51	1.29	1.39
1	a	677	TYR	CD2-CE2	-6.50	1.29	1.39
2	C	31	ARG	C-O	-6.50	1.10	1.23
1	a	448	SER	CB-OG	-6.50	1.33	1.42
1	a	697	ILE	C-O	-6.50	1.11	1.23
2	C	31	ARG	CZ-NH1	-6.48	1.24	1.33
1	a	72	TYR	CD1-CE1	-6.48	1.29	1.39
7	c	105	ALA	C-O	-6.47	1.11	1.23
1	A	268	THR	CB-CG2	-6.47	1.31	1.52
1	A	118	HIS	C-O	-6.46	1.11	1.23
1	A	224	PRO	C-O	-6.46	1.10	1.23
1	A	246	TYR	CE1-CZ	-6.46	1.30	1.38
2	C	192	TYR	CD1-CE1	-6.43	1.29	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	748	TYR	CD2-CE2	-6.43	1.29	1.39
1	a	375	PHE	C-O	-6.43	1.11	1.23
7	c	21	CYS	C-O	-6.43	1.11	1.23
1	a	438	ASP	CB-CG	-6.43	1.38	1.51
2	C	178	TYR	CD1-CE1	-6.42	1.29	1.39
1	a	537	VAL	C-O	-6.42	1.11	1.23
7	c	113	TRP	C-O	-6.42	1.11	1.23
1	A	739	MET	C-O	-6.42	1.11	1.23
1	A	420	VAL	CB-CG1	-6.40	1.39	1.52
2	C	20	CYS	C-O	-6.40	1.11	1.23
1	A	102	TYR	CD2-CE2	-6.40	1.29	1.39
1	a	116	CYS	C-O	-6.40	1.11	1.23
7	c	148	TYR	CD1-CE1	-6.39	1.29	1.39
1	a	541	SER	C-O	-6.39	1.11	1.23
1	a	576	GLU	CB-CG	-6.38	1.40	1.52
2	C	21	PHE	C-O	-6.37	1.11	1.23
1	A	192	TYR	CD1-CE1	-6.37	1.29	1.39
1	A	631	SER	C-O	-6.37	1.11	1.23
1	A	119	ILE	C-O	-6.36	1.11	1.23
7	c	20	GLY	N-CA	-6.34	1.36	1.46
2	C	114	TYR	CE1-CZ	-6.33	1.30	1.38
1	A	677	TYR	CD1-CE1	-6.33	1.29	1.39
1	a	787	TRP	CG-CD1	-6.33	1.27	1.36
1	A	630	ALA	C-O	-6.32	1.11	1.23
1	a	512	SER	CB-OG	-6.32	1.34	1.42
1	A	207	PHE	C-O	-6.30	1.11	1.23
1	A	210	TRP	CG-CD1	-6.30	1.27	1.36
1	A	213	VAL	CB-CG1	-6.29	1.39	1.52
5	G	14	TRP	CB-CG	-6.28	1.39	1.50
1	a	698	GLY	CA-C	-6.28	1.41	1.51
4	F	20	GLY	C-O	-6.27	1.13	1.23
7	c	142	THR	CB-CG2	-6.27	1.31	1.52
1	a	765	ASN	CG-ND2	-6.27	1.17	1.32
1	A	774	ASN	C-O	-6.26	1.11	1.23
1	A	328	ASN	CG-OD1	-6.26	1.10	1.24
1	a	677	TYR	CD1-CE1	-6.26	1.29	1.39
1	A	578	TYR	CD1-CE1	-6.25	1.29	1.39
1	a	529	TRP	CG-CD1	-6.25	1.28	1.36
1	a	332	TYR	CD1-CE1	-6.22	1.30	1.39
1	A	238	PRO	C-O	-6.20	1.10	1.23
1	a	134	TYR	C-O	-6.20	1.11	1.23
2	C	71	ARG	CZ-NH1	-6.20	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	55	TYR	CB-CG	-6.20	1.42	1.51
1	a	725	SER	CB-OG	-6.20	1.34	1.42
1	A	639	ASN	CG-ND2	-6.18	1.17	1.32
1	a	768	THR	CB-CG2	-6.18	1.31	1.52
1	A	308	LEU	C-O	-6.17	1.11	1.23
1	A	656	TRP	CG-CD1	-6.17	1.28	1.36
1	A	625	TRP	CB-CG	-6.17	1.39	1.50
1	A	732	ASP	CG-OD2	-6.16	1.11	1.25
2	C	165	LYS	C-O	-6.16	1.11	1.23
1	a	444	TYR	CD2-CE2	-6.15	1.30	1.39
7	c	154	ARG	CZ-NH1	-6.15	1.25	1.33
1	a	75	TYR	CD1-CE1	-6.15	1.30	1.39
1	a	309	THR	CB-CG2	-6.15	1.32	1.52
1	a	102	TYR	CD2-CE2	-6.14	1.30	1.39
2	C	31	ARG	CZ-NH2	-6.14	1.25	1.33
1	A	639	ASN	CB-CG	-6.13	1.36	1.51
1	A	561	TYR	CD2-CE2	-6.13	1.30	1.39
2	C	134	CYS	CB-SG	-6.13	1.71	1.82
1	a	45	TYR	CD1-CE1	-6.12	1.30	1.39
1	A	273	TRP	CB-CG	-6.11	1.39	1.50
1	a	18	LEU	C-O	-6.11	1.11	1.23
1	A	682	TYR	C-O	-6.11	1.11	1.23
1	A	247	GLY	C-O	-6.10	1.13	1.23
1	A	137	ARG	C-O	-6.10	1.11	1.23
1	a	268	THR	CB-CG2	-6.09	1.32	1.52
1	A	775	HIS	C-O	-6.09	1.11	1.23
1	A	762	TYR	CZ-OH	-6.07	1.27	1.37
2	C	114	TYR	CZ-OH	-6.06	1.27	1.37
7	c	74	TYR	CB-CG	-6.05	1.42	1.51
1	A	246	TYR	CZ-OH	-6.05	1.27	1.37
1	a	377	GLY	C-O	-6.05	1.14	1.23
1	a	202	TYR	CD2-CE2	-6.05	1.30	1.39
7	c	140	LYS	C-O	-6.05	1.11	1.23
1	A	127	TYR	CD2-CE2	-6.04	1.30	1.39
7	c	41	SER	C-O	-6.04	1.11	1.23
1	a	134	TYR	CG-CD1	-6.02	1.31	1.39
1	A	316	PHE	CD2-CE2	-6.02	1.27	1.39
1	A	25	GLU	CD-OE2	-6.02	1.19	1.25
1	a	134	TYR	CE1-CZ	-6.01	1.30	1.38
1	a	246	TYR	CD1-CE1	-6.01	1.30	1.39
1	A	361	ASN	C-O	-6.01	1.11	1.23
1	A	45	TYR	CD1-CE1	-6.00	1.30	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	142	ASN	CG-OD1	-6.00	1.10	1.24
1	a	369	TYR	CD2-CE2	-5.99	1.30	1.39
2	C	177	TYR	CD1-CE1	-5.99	1.30	1.39
1	A	133	TYR	CD1-CE1	-5.98	1.30	1.39
2	C	116	GLU	CG-CD	-5.97	1.43	1.51
7	c	154	ARG	CZ-NH2	-5.96	1.25	1.33
1	A	299	ASP	C-O	-5.96	1.12	1.23
7	c	110	ASP	CG-OD2	-5.96	1.11	1.25
1	A	208	PHE	C-O	-5.95	1.12	1.23
2	C	174	MET	C-O	-5.95	1.12	1.23
7	c	18	ALA	CA-C	-5.94	1.37	1.52
1	a	426	TYR	CD1-CE1	-5.94	1.30	1.39
1	A	677	TYR	CD2-CE2	-5.93	1.30	1.39
1	a	525	TYR	CD2-CE2	-5.93	1.30	1.39
1	A	295	THR	CB-CG2	-5.93	1.32	1.52
2	C	165	LYS	CA-C	-5.93	1.37	1.52
1	A	45	TYR	CD2-CE2	-5.92	1.30	1.39
1	A	117	PHE	C-O	-5.92	1.12	1.23
4	F	24	GLY	C-O	-5.92	1.14	1.23
1	A	134	TYR	CD1-CE1	-5.91	1.30	1.39
7	c	107	ASN	CG-ND2	-5.91	1.18	1.32
2	C	172	GLY	C-O	-5.91	1.14	1.23
2	C	124	ASN	CG-OD1	-5.90	1.10	1.24
1	a	696	CYS	C-O	-5.90	1.12	1.23
1	a	769	TRP	CD1-NE1	-5.89	1.27	1.38
2	C	188	TYR	CZ-OH	-5.89	1.27	1.37
2	C	163	ASN	CG-OD1	-5.89	1.10	1.24
1	a	307	HIS	C-O	-5.88	1.12	1.23
1	a	771	TRP	CE3-CZ3	-5.88	1.28	1.38
3	E	25	VAL	C-O	-5.87	1.12	1.23
1	a	225	LEU	C-O	-5.87	1.12	1.23
1	A	681	TRP	CE3-CZ3	-5.87	1.28	1.38
1	a	512	SER	C-O	-5.86	1.12	1.23
1	a	27	ILE	C-O	-5.86	1.12	1.23
1	A	246	TYR	C-O	-5.86	1.12	1.23
3	E	15	TYR	C-O	-5.85	1.12	1.23
1	A	249	PHE	C-O	-5.85	1.12	1.23
1	A	47	PHE	CD1-CE1	-5.84	1.27	1.39
1	A	183	THR	CB-CG2	-5.84	1.33	1.52
1	a	850	PHE	CD2-CE2	-5.83	1.27	1.39
1	a	742	ARG	C-O	-5.83	1.12	1.23
1	A	108	ASP	C-O	-5.83	1.12	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	578	TYR	CD1-CE1	-5.82	1.30	1.39
1	a	844	PHE	CD1-CE1	-5.82	1.27	1.39
1	A	560	TRP	CB-CG	-5.82	1.39	1.50
1	a	200	THR	CB-CG2	-5.81	1.33	1.52
2	C	177	TYR	CZ-OH	-5.81	1.27	1.37
7	c	55	TYR	CE2-CZ	-5.81	1.30	1.38
7	c	107	ASN	CG-OD1	-5.81	1.11	1.24
7	c	137	TYR	CD2-CE2	-5.80	1.30	1.39
1	a	539	TRP	CB-CG	-5.79	1.39	1.50
2	C	184	GLN	CB-CG	-5.79	1.36	1.52
4	F	15	PHE	C-O	-5.79	1.12	1.23
1	A	15	TYR	CE1-CZ	-5.78	1.31	1.38
1	a	681	TRP	CG-CD1	-5.78	1.28	1.36
1	A	501	ARG	C-O	-5.78	1.12	1.23
1	A	777	THR	CB-CG2	-5.77	1.33	1.52
1	a	283	TYR	CD1-CE1	-5.76	1.30	1.39
1	a	352	ARG	CZ-NH2	-5.76	1.25	1.33
7	c	133	VAL	CB-CG1	-5.76	1.40	1.52
1	a	338	MET	C-O	-5.76	1.12	1.23
1	A	305	HIS	C-O	-5.75	1.12	1.23
3	E	10	PHE	C-O	-5.75	1.12	1.23
1	A	639	ASN	C-O	-5.74	1.12	1.23
1	A	783	GLY	C-O	-5.74	1.14	1.23
1	A	109	PHE	C-O	-5.74	1.12	1.23
1	a	517	PHE	CD1-CE1	-5.74	1.27	1.39
1	a	838	LYS	CB-CG	-5.73	1.37	1.52
1	A	525	TYR	CD1-CE1	-5.73	1.30	1.39
1	A	561	TYR	C-O	-5.72	1.12	1.23
1	A	671	ARG	CZ-NH2	-5.72	1.25	1.33
1	a	516	SER	CB-OG	-5.70	1.34	1.42
1	a	836	THR	CB-CG2	-5.70	1.33	1.52
1	A	414	THR	CB-CG2	-5.69	1.33	1.52
1	a	628	ARG	CB-CG	-5.69	1.37	1.52
1	a	757	GLY	N-CA	-5.69	1.37	1.46
1	a	621	ASN	CB-CG	-5.69	1.38	1.51
1	a	748	TYR	CZ-OH	-5.68	1.28	1.37
1	A	72	TYR	CD1-CE1	-5.68	1.30	1.39
1	A	252	TYR	CD1-CE1	-5.66	1.30	1.39
2	C	185	GLN	C-O	-5.66	1.12	1.23
1	a	15	TYR	CE1-CZ	-5.66	1.31	1.38
1	A	204	GLY	C-O	-5.66	1.14	1.23
1	a	379	GLN	CG-CD	-5.66	1.38	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	MET	C-N	-5.66	1.21	1.34
1	a	540	GLY	N-CA	5.65	1.54	1.46
1	A	107	THR	CB-CG2	-5.65	1.33	1.52
1	A	735	TRP	CD1-NE1	-5.65	1.28	1.38
2	C	114	TYR	C-O	-5.64	1.12	1.23
1	A	424	PHE	CD1-CE1	-5.64	1.27	1.39
1	a	114	TRP	CE3-CZ3	-5.63	1.28	1.38
1	A	231	MET	C-O	-5.62	1.12	1.23
1	A	747	TYR	CD2-CE2	-5.62	1.30	1.39
1	a	560	TRP	C-O	-5.62	1.12	1.23
1	A	310	ALA	C-O	-5.62	1.12	1.23
1	a	747	TYR	CD2-CE2	-5.61	1.30	1.39
1	A	102	TYR	CD1-CE1	-5.61	1.30	1.39
2	C	211	GLU	CB-CG	-5.61	1.41	1.52
1	a	625	TRP	CB-CG	-5.60	1.40	1.50
2	C	32	TYR	CD2-CE2	-5.59	1.30	1.39
7	c	154	ARG	C-O	-5.59	1.12	1.23
1	A	165	THR	C-O	-5.58	1.12	1.23
1	a	20	LEU	C-O	-5.58	1.12	1.23
1	a	241	GLN	CB-CG	-5.58	1.37	1.52
3	e	26	VAL	C-O	-5.57	1.12	1.23
1	A	847	THR	CB-CG2	-5.57	1.33	1.52
4	f	15	PHE	C-O	-5.57	1.12	1.23
7	c	119	SER	CB-OG	-5.57	1.35	1.42
1	a	380	TYR	CD2-CE2	-5.57	1.30	1.39
2	C	114	TYR	CB-CG	-5.56	1.43	1.51
7	c	97	GLY	N-CA	5.56	1.54	1.46
1	a	463	TYR	CD2-CE2	-5.56	1.31	1.39
1	A	57	TYR	CD2-CE2	-5.55	1.31	1.39
2	C	159	SER	CB-OG	-5.55	1.35	1.42
2	C	192	TYR	C-O	-5.53	1.12	1.23
1	A	688	ARG	C-O	-5.53	1.12	1.23
1	a	846	TYR	CD1-CE1	-5.53	1.31	1.39
1	A	463	TYR	CD1-CE1	-5.51	1.31	1.39
1	a	248	TRP	CB-CG	-5.51	1.40	1.50
1	A	729	TRP	CE3-CZ3	-5.51	1.29	1.38
1	A	764	TRP	CD1-NE1	-5.50	1.28	1.38
7	c	21	CYS	CB-SG	-5.50	1.72	1.81
1	A	682	TYR	CG-CD1	-5.49	1.32	1.39
7	c	49	ARG	C-O	-5.49	1.12	1.23
1	a	339	ASN	C-O	-5.49	1.12	1.23
1	a	118	HIS	C-O	-5.48	1.12	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	17	ALA	C-O	-5.47	1.12	1.23
1	A	20	LEU	C-O	-5.47	1.12	1.23
1	A	539	TRP	CG-CD1	-5.47	1.29	1.36
1	A	759	VAL	C-O	-5.47	1.12	1.23
1	a	171	TYR	CD2-CE2	-5.45	1.31	1.39
1	A	542	TRP	CE3-CZ3	-5.45	1.29	1.38
1	A	656	TRP	CD1-NE1	-5.45	1.28	1.38
7	c	74	TYR	CZ-OH	-5.45	1.28	1.37
2	C	148	TRP	CD1-NE1	-5.45	1.28	1.38
1	a	632	THR	C-O	-5.45	1.12	1.23
1	A	521	GLU	CB-CG	-5.45	1.41	1.52
1	a	19	GLU	C-O	-5.44	1.13	1.23
2	C	116	GLU	CB-CG	-5.43	1.41	1.52
1	a	419	PHE	CD1-CE1	-5.43	1.28	1.39
4	F	18	THR	C-O	-5.42	1.13	1.23
1	a	771	TRP	CG-CD1	-5.42	1.29	1.36
1	a	331	SER	CB-OG	-5.41	1.35	1.42
4	F	22	LEU	C-O	-5.41	1.13	1.23
1	a	864	ASN	C-O	-5.39	1.13	1.23
1	A	810	ARG	C-O	-5.39	1.13	1.23
1	A	327	ARG	CZ-NH1	-5.39	1.26	1.33
1	a	79	GLN	C-O	-5.39	1.13	1.23
1	A	123	LEU	C-O	-5.38	1.13	1.23
1	A	418	SER	CB-OG	-5.38	1.35	1.42
2	C	171	GLY	C-O	-5.38	1.15	1.23
2	C	125	CYS	C-O	-5.38	1.13	1.23
1	A	343	TYR	CD1-CE1	-5.38	1.31	1.39
1	a	766	GLU	CD-OE1	-5.37	1.19	1.25
1	A	472	TRP	CB-CG	-5.37	1.40	1.50
2	C	70	LEU	C-O	-5.37	1.13	1.23
2	C	149	GLN	CD-NE2	-5.36	1.19	1.32
1	a	164	PHE	CE1-CZ	-5.36	1.27	1.37
7	c	41	SER	CA-CB	-5.35	1.45	1.52
1	A	828	ARG	C-O	-5.35	1.13	1.23
1	a	359	THR	CB-CG2	-5.35	1.34	1.52
7	c	145	GLN	C-O	-5.35	1.13	1.23
1	a	127	TYR	CD2-CE2	-5.34	1.31	1.39
1	A	47	PHE	CE1-CZ	-5.34	1.27	1.37
1	A	535	TYR	CD2-CE2	-5.33	1.31	1.39
2	C	168	GLY	C-O	-5.33	1.15	1.23
4	F	8	ILE	C-O	-5.33	1.13	1.23
1	a	47	PHE	CE1-CZ	-5.33	1.27	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	131	GLY	C-O	-5.33	1.15	1.23
5	G	31	ASN	CG-OD1	-5.32	1.12	1.24
1	A	560	TRP	CD1-NE1	-5.32	1.28	1.38
1	A	360	PHE	CD1-CE1	-5.31	1.28	1.39
1	A	444	TYR	CD1-CE1	-5.31	1.31	1.39
1	A	611	PHE	C-O	-5.30	1.13	1.23
2	C	148	TRP	CD2-CE2	-5.30	1.34	1.41
1	a	364	GLN	CB-CG	-5.30	1.38	1.52
1	a	286	TYR	CD2-CE2	-5.30	1.31	1.39
1	A	655	PHE	CB-CG	-5.30	1.42	1.51
1	a	764	TRP	CE3-CZ3	-5.30	1.29	1.38
1	A	177	TRP	CB-CG	-5.29	1.40	1.50
1	a	762	TYR	CD2-CE2	-5.28	1.31	1.39
4	F	7	GLN	CD-OE1	-5.27	1.12	1.24
1	A	732	ASP	CG-OD1	-5.27	1.13	1.25
4	F	29	SER	C-O	-5.27	1.13	1.23
7	c	86	TYR	CZ-OH	-5.26	1.28	1.37
1	A	241	GLN	C-O	-5.25	1.13	1.23
1	A	812	VAL	C-O	-5.25	1.13	1.23
1	A	135	GLY	C-O	-5.25	1.15	1.23
5	G	44	LEU	CA-CB	-5.25	1.41	1.53
3	E	12	LEU	C-O	-5.25	1.13	1.23
1	A	498	VAL	CB-CG2	-5.25	1.41	1.52
1	a	568	PHE	CD2-CE2	-5.24	1.28	1.39
2	C	84	GLU	CD-OE2	-5.24	1.19	1.25
2	C	188	TYR	CG-CD1	-5.24	1.32	1.39
7	c	74	TYR	C-O	-5.24	1.13	1.23
1	A	681	TRP	C-O	-5.23	1.13	1.23
1	a	173	VAL	CB-CG2	-5.23	1.41	1.52
1	a	390	TYR	CD1-CE1	-5.23	1.31	1.39
1	a	766	GLU	CD-OE2	-5.22	1.20	1.25
1	A	309	THR	C-O	-5.22	1.13	1.23
1	A	380	TYR	CE1-CZ	-5.22	1.31	1.38
1	A	547	ARG	CZ-NH1	-5.22	1.26	1.33
1	A	242	ALA	C-O	-5.22	1.13	1.23
7	c	36	SER	CB-OG	-5.22	1.35	1.42
1	A	674	PHE	CD1-CE1	-5.22	1.28	1.39
2	C	192	TYR	CE1-CZ	-5.21	1.31	1.38
1	A	110	ARG	C-O	-5.21	1.13	1.23
1	A	449	PHE	CD1-CE1	-5.21	1.28	1.39
7	c	96	ASN	CG-OD1	-5.20	1.12	1.24
1	A	380	TYR	CD2-CE2	-5.20	1.31	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	162	TYR	CE1-CZ	-5.19	1.31	1.38
1	a	764	TRP	CD2-CE2	-5.19	1.35	1.41
1	a	339	ASN	CG-ND2	-5.19	1.19	1.32
1	A	200	THR	CB-CG2	-5.18	1.35	1.52
1	a	133	TYR	CD2-CE2	-5.18	1.31	1.39
2	C	122	GLN	C-O	-5.18	1.13	1.23
2	C	191	ALA	C-O	-5.18	1.13	1.23
1	A	774	ASN	CG-OD1	-5.18	1.12	1.24
7	c	50	GLU	CB-CG	-5.18	1.42	1.52
1	A	472	TRP	CE3-CZ3	-5.17	1.29	1.38
1	a	682	TYR	CD1-CE1	-5.17	1.31	1.39
2	C	116	GLU	CD-OE1	-5.17	1.20	1.25
1	A	851	VAL	CB-CG2	-5.17	1.42	1.52
2	C	115	ARG	CD-NE	-5.16	1.37	1.46
1	a	189	ARG	CG-CD	-5.16	1.39	1.51
1	A	573	LYS	CB-CG	-5.16	1.38	1.52
1	A	730	TYR	CD1-CE1	-5.16	1.31	1.39
1	A	656	TRP	CE3-CZ3	-5.16	1.29	1.38
1	a	732	ASP	CG-OD2	-5.16	1.13	1.25
7	c	148	TYR	CD2-CE2	-5.16	1.31	1.39
1	a	735	TRP	CE3-CZ3	-5.16	1.29	1.38
1	A	578	TYR	CD2-CE2	-5.15	1.31	1.39
2	C	162	TYR	CD1-CE1	-5.15	1.31	1.39
1	a	542	TRP	C-O	-5.15	1.13	1.23
4	f	12	LEU	C-O	-5.15	1.13	1.23
1	A	584	LYS	CB-CG	-5.15	1.38	1.52
1	a	806	ASP	CB-CG	-5.14	1.41	1.51
1	a	864	ASN	CA-C	-5.14	1.39	1.52
4	F	21	THR	C-O	-5.14	1.13	1.23
1	a	275	VAL	CB-CG1	-5.14	1.42	1.52
1	A	45	TYR	CZ-OH	-5.13	1.29	1.37
1	A	690	GLN	C-O	-5.13	1.13	1.23
1	A	171	TYR	CE2-CZ	-5.13	1.31	1.38
1	A	298	GLU	CD-OE2	-5.13	1.20	1.25
1	A	702	GLY	C-O	-5.13	1.15	1.23
1	a	681	TRP	CE3-CZ3	-5.12	1.29	1.38
1	A	426	TYR	CE1-CZ	-5.12	1.31	1.38
1	a	436	GLU	CD-OE2	-5.12	1.20	1.25
1	A	538	GLN	C-O	-5.12	1.13	1.23
7	c	87	ALA	C-O	-5.12	1.13	1.23
1	A	109	PHE	CB-CG	-5.12	1.42	1.51
1	a	511	SER	C-O	-5.11	1.13	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	TRP	CB-CG	-5.10	1.41	1.50
1	a	278	VAL	CB-CG1	-5.10	1.42	1.52
7	c	113	TRP	CD1-NE1	-5.10	1.29	1.38
2	C	114	TYR	CD1-CE1	-5.10	1.31	1.39
1	a	714	TRP	CE3-CZ3	-5.10	1.29	1.38
4	f	14	PHE	C-O	-5.10	1.13	1.23
5	G	20	LEU	C-O	-5.09	1.13	1.23
1	A	680	PRO	C-O	-5.09	1.13	1.23
1	a	528	GLU	C-O	-5.09	1.13	1.23
2	C	216	GLU	CA-CB	-5.08	1.42	1.53
1	A	68	SER	CB-OG	-5.08	1.35	1.42
1	A	720	SER	CB-OG	-5.08	1.35	1.42
7	c	80	GLU	C-O	-5.08	1.13	1.23
1	A	114	TRP	CE3-CZ3	-5.07	1.29	1.38
1	a	545	PHE	CD1-CE1	-5.07	1.29	1.39
7	c	83	THR	C-O	-5.06	1.13	1.23
7	c	89	CYS	C-O	-5.06	1.13	1.23
3	E	18	LEU	C-O	-5.06	1.13	1.23
1	a	346	LYS	N-CA	5.06	1.56	1.46
7	c	76	ALA	C-O	-5.05	1.13	1.23
1	A	735	TRP	C-O	-5.05	1.13	1.23
1	A	732	ASP	CB-CG	-5.05	1.41	1.51
1	a	343	TYR	CD2-CE2	-5.04	1.31	1.39
1	A	202	TYR	C-O	-5.04	1.13	1.23
7	c	44	ALA	C-O	-5.04	1.13	1.23
1	A	75	TYR	CD2-CE2	-5.04	1.31	1.39
1	A	266	GLU	C-O	-5.04	1.13	1.23
1	a	25	GLU	C-O	-5.04	1.13	1.23
7	c	75	LYS	C-O	-5.04	1.13	1.23
1	a	488	ALA	C-O	-5.04	1.13	1.23
7	c	137	TYR	CD1-CE1	-5.04	1.31	1.39
1	a	732	ASP	C-O	-5.03	1.13	1.23
7	c	19	THR	CB-CG2	-5.03	1.35	1.52
1	A	621	ASN	CB-CG	-5.03	1.39	1.51
7	c	135	PRO	C-O	-5.03	1.13	1.23
2	C	187	ARG	CZ-NH2	-5.03	1.26	1.33
3	E	9	LEU	C-O	-5.03	1.13	1.23
7	c	98	GLY	C-O	-5.02	1.15	1.23
1	A	803	GLU	CB-CG	-5.02	1.42	1.52
4	F	27	TYR	CB-CG	-5.02	1.44	1.51
1	A	742	ARG	CZ-NH2	-5.02	1.26	1.33
1	a	441	PHE	CD1-CE1	-5.01	1.29	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	142	THR	C-O	-5.01	1.13	1.23
1	A	40	CYS	CB-SG	-5.01	1.73	1.81
1	a	637	TYR	CD1-CE1	-5.01	1.31	1.39
1	a	116	CYS	CB-SG	-5.01	1.73	1.81

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	A	96	LEU	C-N-CD	-14.30	89.13	120.60
1	A	501	ARG	NE-CZ-NH2	12.88	126.74	120.30
1	a	18	LEU	CA-CB-CG	12.50	144.06	115.30
1	a	18	LEU	CB-CG-CD1	-12.46	89.83	111.00
7	c	26	ARG	NE-CZ-NH1	12.45	126.52	120.30
1	a	801	ARG	NE-CZ-NH1	12.30	126.45	120.30
7	c	26	ARG	NE-CZ-NH2	-12.25	114.18	120.30
1	a	801	ARG	NE-CZ-NH2	-12.21	114.20	120.30
1	A	641	ARG	NE-CZ-NH2	-11.99	114.31	120.30
2	C	194	ARG	NE-CZ-NH2	-11.66	114.47	120.30
2	C	194	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	A	798	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	A	757	GLY	N-CA-C	10.68	139.80	113.10
7	c	110	ASP	CB-CG-OD1	10.28	127.56	118.30
7	c	48	LEU	CB-CG-CD2	-10.13	93.78	111.00
1	A	641	ARG	NE-CZ-NH1	10.02	125.31	120.30
2	C	141	THR	CA-C-N	9.76	138.68	117.20
5	G	44	LEU	CB-CG-CD1	9.76	127.58	111.00
1	A	501	ARG	NE-CZ-NH1	-9.73	115.43	120.30
2	C	179	ASN	O-C-N	-9.63	107.29	122.70
7	c	48	LEU	CA-CB-CG	9.61	137.41	115.30
1	a	539	TRP	CA-C-N	9.59	135.37	116.20
7	c	97	GLY	CA-C-N	-9.54	97.13	116.20
1	a	798	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	a	447	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	A	797	ASP	CB-CG-OD1	9.17	126.55	118.30
2	C	91	ASP	CB-CG-OD1	9.15	126.54	118.30
1	a	346	LYS	N-CA-CB	9.14	127.05	110.60
1	a	65	ARG	NE-CZ-NH1	9.08	124.84	120.30
7	c	48	LEU	CB-CG-CD1	-9.00	95.70	111.00
1	a	859	ASP	CB-CG-OD1	8.98	126.39	118.30
1	A	500	ASP	CB-CG-OD1	8.97	126.37	118.30
1	A	450	ARG	NE-CZ-NH1	8.89	124.74	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	12	LEU	CB-CG-CD2	-8.80	96.05	111.00
1	A	639	ASN	CB-CA-C	-8.74	92.92	110.40
7	c	81	LEU	CA-CB-CG	8.63	135.14	115.30
2	C	71	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	a	450	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	65	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	a	757	GLY	N-CA-C	8.39	134.08	113.10
1	a	188	LEU	CA-CB-CG	8.26	134.29	115.30
2	C	118	ARG	NE-CZ-NH2	-8.16	116.22	120.30
3	E	18	LEU	CB-CG-CD2	8.15	124.85	111.00
1	A	739	MET	CA-CB-CG	8.11	127.08	113.30
1	a	539	TRP	O-C-N	-8.09	109.44	123.20
1	A	724	LEU	CA-CB-CG	7.96	133.60	115.30
7	c	106	THR	O-C-N	-7.92	110.02	122.70
2	C	142	ASN	N-CA-CB	7.91	124.83	110.60
1	a	65	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	135	GLY	N-CA-C	-7.80	93.61	113.10
7	c	21	CYS	N-CA-CB	7.69	124.44	110.60
1	a	333	LEU	CB-CG-CD2	7.69	124.07	111.00
1	a	367	LEU	CA-CB-CG	-7.68	97.63	115.30
1	A	108	ASP	CB-CG-OD1	7.65	125.18	118.30
2	C	202	ASN	CB-CA-C	7.63	125.66	110.40
7	c	26	ARG	CG-CD-NE	-7.62	95.80	111.80
1	A	214	LEU	CA-CB-CG	7.59	132.75	115.30
2	C	174	MET	CG-SD-CE	7.54	112.27	100.20
1	a	326	LEU	CA-CB-CG	7.53	132.61	115.30
3	E	31	ASP	CB-CG-OD1	7.52	125.07	118.30
2	C	193	LEU	CA-CB-CG	7.52	132.59	115.30
1	A	547	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	450	ARG	NE-CZ-NH2	-7.43	116.58	120.30
2	C	141	THR	CA-C-O	-7.40	104.56	120.10
7	c	131	GLY	N-CA-C	7.40	131.60	113.10
1	A	13	ARG	N-CA-C	7.39	130.94	111.00
1	A	700	VAL	CB-CA-C	-7.34	97.45	111.40
1	A	501	ARG	CD-NE-CZ	7.32	133.85	123.60
1	A	266	GLU	OE1-CD-OE2	-7.31	114.52	123.30
7	c	56	GLU	OE1-CD-OE2	-7.31	114.52	123.30
1	a	364	GLN	N-CA-CB	-7.23	97.58	110.60
1	a	333	LEU	CA-CB-CG	7.17	131.80	115.30
1	a	69	LEU	CA-CB-CG	7.17	131.79	115.30
7	c	91	GLY	C-N-CA	7.15	139.58	121.70
1	a	670	LEU	CA-CB-CG	7.14	131.73	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	SER	CB-CA-C	-7.07	96.66	110.10
1	A	761	LEU	CB-CG-CD2	7.05	122.99	111.00
1	A	724	LEU	CB-CG-CD1	7.04	122.97	111.00
5	G	9	ILE	CG1-CB-CG2	-7.02	95.96	111.40
7	c	102	ALA	N-CA-CB	7.01	119.92	110.10
1	a	266	GLU	OE1-CD-OE2	-7.00	114.89	123.30
2	C	179	ASN	CA-C-N	6.97	132.54	117.20
7	c	106	THR	CA-C-O	6.96	134.72	120.10
1	a	450	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	a	724	LEU	CA-CB-CG	6.93	131.25	115.30
1	a	742	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	a	861	PHE	CB-CA-C	6.89	124.19	110.40
1	a	773	ASP	CB-CG-OD1	6.88	124.49	118.30
1	a	865	ARG	NE-CZ-NH1	6.86	123.73	120.30
7	c	98	GLY	C-N-CA	6.84	136.67	122.30
1	a	110	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	475	THR	N-CA-CB	6.82	123.27	110.30
1	a	154	GLY	N-CA-C	-6.82	96.06	113.10
1	A	167	GLU	N-CA-CB	-6.79	98.38	110.60
1	a	26	ARG	NE-CZ-NH1	-6.78	116.91	120.30
2	C	207	LEU	CB-CG-CD1	6.77	122.50	111.00
1	a	824	LEU	CB-CG-CD2	-6.77	99.50	111.00
1	a	851	VAL	CA-CB-CG2	6.77	121.05	110.90
1	A	88	ILE	N-CA-C	6.68	129.04	111.00
1	A	798	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	a	188	LEU	CB-CG-CD2	-6.67	99.66	111.00
1	A	859	ASP	CB-CG-OD2	6.67	124.30	118.30
5	G	25	LEU	CB-CG-CD1	-6.66	99.67	111.00
7	c	26	ARG	CD-NE-CZ	6.64	132.90	123.60
3	E	34	ALA	N-CA-CB	6.63	119.39	110.10
2	C	141	THR	N-CA-C	6.60	128.82	111.00
1	A	367	LEU	CB-CG-CD1	6.59	122.20	111.00
1	A	196	LEU	CB-CG-CD1	6.58	122.19	111.00
2	C	178	TYR	CB-CG-CD1	-6.56	117.07	121.00
7	c	92	CYS	N-CA-C	-6.55	93.31	111.00
2	C	71	ARG	CG-CD-NE	-6.49	98.17	111.80
1	a	528	GLU	OE1-CD-OE2	-6.48	115.52	123.30
1	A	773	ASP	CB-CG-OD1	6.44	124.10	118.30
1	a	318	LEU	CA-CB-CG	6.42	130.06	115.30
1	A	740	MET	CG-SD-CE	6.41	110.45	100.20
7	c	20	GLY	N-CA-C	-6.40	97.10	113.10
2	C	178	TYR	CZ-CE2-CD2	-6.39	114.05	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	437	LEU	CA-CB-CG	6.38	129.97	115.30
1	a	303	VAL	CG1-CB-CG2	6.35	121.06	110.90
1	a	757	GLY	CA-C-N	6.35	128.89	116.20
1	A	333	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	455	ASP	CB-CG-OD1	6.34	124.00	118.30
1	a	732	ASP	CB-CG-OD1	6.33	124.00	118.30
7	c	92	CYS	N-CA-CB	6.32	121.97	110.60
7	c	132	LYS	N-CA-CB	6.30	121.94	110.60
7	c	154	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	696	CYS	CA-CB-SG	6.23	125.22	114.00
1	A	851	VAL	CA-CB-CG1	6.20	120.20	110.90
7	c	54	LEU	CA-CB-CG	6.15	129.44	115.30
1	a	824	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	760	PHE	CB-CG-CD1	6.13	125.09	120.80
5	G	36	LEU	CA-CB-CG	6.12	129.38	115.30
2	C	218	GLN	N-CA-CB	-6.11	99.60	110.60
7	c	106	THR	N-CA-CB	6.11	121.91	110.30
1	a	865	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	206	LEU	CB-CG-CD1	6.10	121.37	111.00
1	A	96	LEU	C-N-CA	6.09	147.59	122.00
2	C	218	GLN	N-CA-C	6.05	127.33	111.00
1	a	834	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	250	ASP	CB-CG-OD1	6.02	123.72	118.30
1	a	182	ASN	C-N-CA	-5.94	106.85	121.70
7	c	98	GLY	O-C-N	5.93	133.28	123.20
1	a	50	MET	CG-SD-CE	-5.93	90.72	100.20
1	A	739	MET	CG-SD-CE	5.91	109.66	100.20
5	g	26	ILE	N-CA-C	-5.91	95.03	111.00
1	A	763	MET	CB-CG-SD	-5.88	94.75	112.40
1	A	706	GLY	N-CA-C	5.88	127.79	113.10
1	a	339	ASN	CB-CA-C	5.87	122.14	110.40
1	A	688	ARG	CB-CG-CD	-5.86	96.35	111.60
2	C	109	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	501	ARG	CG-CD-NE	-5.84	99.53	111.80
1	a	394	ARG	CB-CA-C	-5.83	98.74	110.40
5	G	25	LEU	CA-CB-CG	5.83	128.70	115.30
1	a	299	ASP	CB-CG-OD1	5.79	123.51	118.30
1	a	798	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	a	214	LEU	CA-CB-CG	5.76	128.56	115.30
1	a	137	ARG	CB-CG-CD	-5.76	96.64	111.60
1	A	333	LEU	CB-CG-CD2	5.75	120.78	111.00
1	a	367	LEU	CB-CG-CD2	5.75	120.77	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	21	LEU	CA-CB-CG	-5.74	102.09	115.30
1	a	736	ILE	CG1-CB-CG2	5.73	124.01	111.40
1	A	758	GLY	CA-C-N	5.73	129.80	117.20
1	A	367	LEU	CA-CB-CG	-5.73	102.13	115.30
1	a	326	LEU	CB-CG-CD1	5.72	120.73	111.00
1	A	167	GLU	CB-CA-C	-5.71	98.97	110.40
1	A	813	ARG	NE-CZ-NH1	5.71	123.16	120.30
7	c	110	ASP	OD1-CG-OD2	-5.67	112.52	123.30
1	a	852	LEU	CA-CB-CG	5.67	128.34	115.30
1	a	797	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	196	LEU	C-N-CA	-5.64	107.60	121.70
1	A	447	ARG	NE-CZ-NH1	5.64	123.12	120.30
5	G	44	LEU	N-CA-CB	-5.63	99.14	110.40
1	a	851	VAL	CA-CB-CG1	5.62	119.32	110.90
1	A	66	LEU	CA-CB-CG	5.61	128.19	115.30
2	C	180	GLN	N-CA-C	5.59	126.11	111.00
7	c	122	MET	CG-SD-CE	-5.57	91.28	100.20
1	a	364	GLN	CB-CA-C	5.56	121.52	110.40
1	a	337	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	65	ARG	CG-CD-NE	5.55	123.45	111.80
1	A	729	TRP	CA-CB-CG	5.55	124.24	113.70
1	a	757	GLY	CA-C-O	-5.53	110.64	120.60
1	a	537	VAL	CB-CA-C	-5.53	100.89	111.40
2	C	207	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	214	LEU	CB-CG-CD1	5.52	120.38	111.00
1	A	736	ILE	CA-CB-CG2	5.52	121.94	110.90
7	c	96	ASN	CA-C-N	5.52	127.23	116.20
1	a	206	LEU	CA-CB-CG	5.51	127.97	115.30
7	c	32	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	a	336	ASN	O-C-N	-5.50	113.90	122.70
2	C	87	VAL	CA-CB-CG1	5.49	119.14	110.90
2	C	165	LYS	CB-CA-C	5.49	121.37	110.40
1	A	761	LEU	CB-CG-CD1	5.48	120.31	111.00
1	a	327	ARG	C-N-CA	-5.46	108.06	121.70
1	A	326	LEU	CA-CB-CG	5.43	127.80	115.30
1	a	308	LEU	CB-CG-CD1	5.43	120.23	111.00
1	a	63	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	742	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	a	454	MET	CG-SD-CE	5.42	108.87	100.20
1	a	801	ARG	CD-NE-CZ	5.41	131.18	123.60
1	A	776	LEU	CB-CG-CD2	5.40	120.18	111.00
7	c	133	VAL	CG1-CB-CG2	-5.38	102.28	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	65	ARG	CG-CD-NE	5.38	123.10	111.80
2	C	216	GLU	CB-CA-C	-5.36	99.67	110.40
1	A	73	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	503	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	309	THR	OG1-CB-CG2	-5.35	97.69	110.00
1	A	732	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	687	TRP	N-CA-C	5.34	125.42	111.00
1	A	244	PHE	N-CA-CB	5.32	120.18	110.60
1	a	732	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	a	732	ASP	N-CA-CB	-5.31	101.05	110.60
1	A	108	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	a	671	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	a	781	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	327	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	C	128	CYS	CA-CB-SG	5.29	123.51	114.00
1	A	698	GLY	N-CA-C	5.27	126.27	113.10
1	A	299	ASP	CB-CG-OD1	5.26	123.03	118.30
1	a	266	GLU	CG-CD-OE1	5.26	128.82	118.30
1	A	865	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	147	TRP	N-CA-C	5.26	125.19	111.00
1	A	253	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	447	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	a	798	ARG	CG-CD-NE	-5.24	100.81	111.80
1	a	333	LEU	CB-CG-CD1	-5.23	102.10	111.00
1	a	763	MET	CA-CB-CG	5.23	122.19	113.30
2	C	141	THR	N-CA-CB	5.22	120.22	110.30
7	c	43	THR	OG1-CB-CG2	-5.22	97.99	110.00
2	C	73	ARG	CB-CA-C	-5.22	99.97	110.40
2	C	179	ASN	CB-CA-C	5.22	120.83	110.40
3	E	32	ILE	N-CA-C	-5.21	96.92	111.00
3	e	24	PHE	N-CA-C	-5.20	96.95	111.00
1	A	552	LEU	CA-CB-CG	5.20	127.27	115.30
7	c	19	THR	N-CA-C	-5.19	96.98	111.00
2	C	20	CYS	N-CA-CB	5.19	119.94	110.60
1	a	63	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	a	447	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	a	698	GLY	C-N-CD	-5.16	109.26	120.60
1	a	671	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	a	490	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	713	LEU	CB-CG-CD2	5.11	119.69	111.00
2	C	48	THR	N-CA-C	5.11	124.79	111.00
1	A	638	SER	C-N-CA	5.11	134.46	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	137	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	166	PRO	C-N-CA	5.09	134.43	121.70
7	c	101	LYS	N-CA-C	-5.09	97.25	111.00
1	a	759	VAL	N-CA-C	5.07	124.69	111.00
1	a	344	GLY	C-N-CA	-5.07	109.03	121.70
1	a	66	LEU	CA-CB-CG	5.06	126.95	115.30
1	A	170	TRP	N-CA-C	5.06	124.67	111.00
1	a	731	LEU	CB-CG-CD1	5.06	119.61	111.00
2	C	179	ASN	N-CA-C	-5.06	97.34	111.00
7	c	98	GLY	CA-C-N	-5.06	106.09	116.20
2	C	77	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	90	GLU	O-C-N	-5.04	114.63	122.70
2	C	59	GLN	CB-CA-C	-5.04	100.33	110.40
1	a	147	TRP	N-CA-C	5.03	124.58	111.00
1	a	651	ASP	CB-CG-OD2	5.03	122.82	118.30
7	c	131	GLY	CA-C-O	-5.03	111.55	120.60
1	a	152	VAL	N-CA-C	-5.02	97.44	111.00
1	A	327	ARG	CD-NE-CZ	5.01	130.61	123.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	639	ASN	Mainchain
2	C	141	THR	Mainchain
2	C	179	ASN	Mainchain
1	a	360	PHE	Mainchain
1	a	698	GLY	Peptide
1	a	92	SER	Peptide
1	a	93	THR	Peptide
7	c	97	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles ⓘ

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	852/865 (98%)	793 (93%)	41 (5%)	18 (2%)	7	3
1	a	856/865 (99%)	798 (93%)	46 (5%)	12 (1%)	11	8
2	C	189/221 (86%)	174 (92%)	9 (5%)	6 (3%)	4	1
3	E	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
3	e	33/35 (94%)	32 (97%)	0	1 (3%)	4	2
4	F	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
4	f	33/35 (94%)	30 (91%)	2 (6%)	1 (3%)	4	2
5	G	36/45 (80%)	32 (89%)	3 (8%)	1 (3%)	5	2
5	g	36/45 (80%)	32 (89%)	4 (11%)	0	100	100
7	c	143/145 (99%)	127 (89%)	8 (6%)	8 (6%)	2	0
All	All	2244/2326 (96%)	2080 (93%)	117 (5%)	47 (2%)	10	3

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	97	PRO
1	A	147	TRP
1	A	170	TRP
1	A	346	LYS
2	C	48	THR
2	C	62	PRO
2	C	180	GLN
2	C	203	GLY
1	a	83	VAL
1	a	759	VAL
7	c	99	GLY
7	c	102	ALA
7	c	132	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	LEU
1	A	136	ALA
1	a	137	ARG
1	a	155	LEU
1	a	346	LYS
7	c	17	MET
7	c	21	CYS
7	c	131	GLY
1	A	688	ARG
1	a	9	ASN
1	a	87	LEU
7	c	92	CYS
1	A	94	SER
1	A	155	LEU
1	A	244	PHE
1	A	476	ALA
1	A	542	TRP
5	G	9	ILE
1	a	147	TRP
4	f	34	ARG
1	A	13	ARG
1	A	96	LEU
1	A	757	GLY
2	C	59	GLN
2	C	217	ARG
7	c	64	LYS
1	A	149	LEU
1	A	696	CYS
1	a	529	TRP
1	a	540	GLY
1	a	757	GLY
1	a	149	LEU
3	e	22	ILE

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	718/726 (99%)	589 (82%)	129 (18%)	1	1
1	a	720/726 (99%)	585 (81%)	135 (19%)	1	1
2	C	155/180 (86%)	127 (82%)	28 (18%)	1	1
3	E	25/25 (100%)	23 (92%)	2 (8%)	12	11
3	e	25/25 (100%)	18 (72%)	7 (28%)	0	0
4	F	31/31 (100%)	25 (81%)	6 (19%)	1	1
4	f	31/31 (100%)	26 (84%)	5 (16%)	2	1
5	G	31/36 (86%)	25 (81%)	6 (19%)	1	1
5	g	31/36 (86%)	22 (71%)	9 (29%)	0	0
7	c	112/112 (100%)	91 (81%)	21 (19%)	1	1
All	All	1879/1928 (98%)	1531 (82%)	348 (18%)	4	1

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	13	ARG
1	A	14	TRP
1	A	15	TYR
1	A	17	LYS
1	A	18	LEU
1	A	52	MET
1	A	59	ASN
1	A	60	LEU
1	A	61	THR
1	A	65	ARG
1	A	66	LEU
1	A	69	LEU
1	A	77	THR
1	A	81	GLN
1	A	82	ARG
1	A	84	TRP
1	A	85	LEU
1	A	88	ILE
1	A	90	GLU
1	A	93	THR
1	A	95	LYS
1	A	96	LEU
1	A	101	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	107	THR
1	A	141	THR
1	A	144	GLU
1	A	147	TRP
1	A	148	LEU
1	A	149	LEU
1	A	159	CYS
1	A	161	ILE
1	A	175	LEU
1	A	183	THR
1	A	188	LEU
1	A	200	THR
1	A	203	ILE
1	A	205	LEU
1	A	206	LEU
1	A	214	LEU
1	A	218	LEU
1	A	224	PRO
1	A	240	GLU
1	A	254	ASN
1	A	263	ILE
1	A	267	THR
1	A	268	THR
1	A	276	LEU
1	A	290	ARG
1	A	294	ILE
1	A	301	LYS
1	A	303	VAL
1	A	318	LEU
1	A	326	LEU
1	A	331	SER
1	A	333	LEU
1	A	334	MET
1	A	335	LEU
1	A	339	ASN
1	A	345	LYS
1	A	352	ARG
1	A	359	THR
1	A	381	LEU
1	A	386	ILE
1	A	387	SER
1	A	391	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	408	THR
1	A	413	THR
1	A	414	THR
1	A	433	THR
1	A	450	ARG
1	A	467	ARG
1	A	473	ASP
1	A	475	THR
1	A	479	ASP
1	A	489	LYS
1	A	490	LEU
1	A	494	ARG
1	A	496	LEU
1	A	497	GLN
1	A	501	ARG
1	A	503	LEU
1	A	518	THR
1	A	534	LEU
1	A	552	LEU
1	A	556	ASP
1	A	562	LEU
1	A	567	THR
1	A	572	ARG
1	A	583	LEU
1	A	588	LEU
1	A	601	LYS
1	A	602	GLN
1	A	608	LEU
1	A	612	ARG
1	A	617	LYS
1	A	621	ASN
1	A	624	GLU
1	A	638	SER
1	A	640	LEU
1	A	653	ILE
1	A	657	LEU
1	A	669	LEU
1	A	670	LEU
1	A	684	ASP
1	A	688	ARG
1	A	690	GLN
1	A	700	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	716	CYS
1	A	724	LEU
1	A	736	ILE
1	A	768	THR
1	A	771	TRP
1	A	777	THR
1	A	781	LEU
1	A	790	SER
1	A	798	ARG
1	A	800	SER
1	A	819	LEU
1	A	823	THR
1	A	824	LEU
1	A	826	GLU
1	A	828	ARG
1	A	832	SER
1	A	833	ASN
1	A	836	THR
1	A	847	THR
1	A	849	THR
1	A	851	VAL
2	C	24	SER
2	C	28	ASN
2	C	30	THR
2	C	46	LEU
2	C	47	LYS
2	C	61	THR
2	C	65	ARG
2	C	71	ARG
2	C	75	THR
2	C	77	LEU
2	C	82	VAL
2	C	85	GLN
2	C	87	VAL
2	C	99	VAL
2	C	116	GLU
2	C	118	ARG
2	C	139	ARG
2	C	150	GLU
2	C	153	SER
2	C	174	MET
2	C	180	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	182	SER
2	C	193	LEU
2	C	194	ARG
2	C	200	GLN
2	C	204	LEU
2	C	217	ARG
2	C	218	GLN
3	E	18	LEU
3	E	31	ASP
4	F	1	MET
4	F	2	TRP
4	F	12	LEU
4	F	32	LEU
4	F	33	SER
4	F	34	ARG
5	G	11	LYS
5	G	14	TRP
5	G	20	LEU
5	G	21	LEU
5	G	44	LEU
5	G	45	ASN
1	a	11	VAL
1	a	13	ARG
1	a	18	LEU
1	a	20	LEU
1	a	26	ARG
1	a	59	ASN
1	a	60	LEU
1	a	61	THR
1	a	65	ARG
1	a	66	LEU
1	a	69	LEU
1	a	79	GLN
1	a	81	GLN
1	a	82	ARG
1	a	83	VAL
1	a	84	TRP
1	a	85	LEU
1	a	87	LEU
1	a	88	ILE
1	a	91	PHE
1	a	94	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	95	LYS
1	a	98	PHE
1	a	106	MET
1	a	107	THR
1	a	123	LEU
1	a	124	TRP
1	a	125	LEU
1	a	147	TRP
1	a	148	LEU
1	a	149	LEU
1	a	151	TYR
1	a	155	LEU
1	a	156	LYS
1	a	158	LEU
1	a	160	GLN
1	a	161	ILE
1	a	172	LYS
1	a	183	THR
1	a	187	ILE
1	a	189	ARG
1	a	200	THR
1	a	205	LEU
1	a	206	LEU
1	a	214	LEU
1	a	218	LEU
1	a	225	LEU
1	a	240	GLU
1	a	241	GLN
1	a	244	PHE
1	a	253	LEU
1	a	263	ILE
1	a	267	THR
1	a	268	THR
1	a	276	LEU
1	a	287	ARG
1	a	290	ARG
1	a	292	ILE
1	a	294	ILE
1	a	297	LEU
1	a	303	VAL
1	a	309	THR
1	a	318	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	326	LEU
1	a	333	LEU
1	a	359	THR
1	a	381	LEU
1	a	386	ILE
1	a	391	LYS
1	a	392	GLN
1	a	408	THR
1	a	413	THR
1	a	433	THR
1	a	448	SER
1	a	450	ARG
1	a	467	ARG
1	a	469	LYS
1	a	472	TRP
1	a	482	LYS
1	a	490	LEU
1	a	492	LYS
1	a	496	LEU
1	a	497	GLN
1	a	501	ARG
1	a	503	LEU
1	a	514	THR
1	a	516	SER
1	a	518	THR
1	a	534	LEU
1	a	552	LEU
1	a	562	LEU
1	a	566	LYS
1	a	567	THR
1	a	569	GLU
1	a	576	GLU
1	a	583	LEU
1	a	584	LYS
1	a	587	SER
1	a	588	LEU
1	a	602	GLN
1	a	617	LYS
1	a	621	ASN
1	a	622	MET
1	a	623	LEU
1	a	624	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	628	ARG
1	a	640	LEU
1	a	641	ARG
1	a	657	LEU
1	a	669	LEU
1	a	670	LEU
1	a	705	CYS
1	a	709	ILE
1	a	724	LEU
1	a	729	TRP
1	a	736	ILE
1	a	761	LEU
1	a	768	THR
1	a	777	THR
1	a	781	LEU
1	a	788	PHE
1	a	798	ARG
1	a	815	MET
1	a	819	LEU
1	a	822	LYS
1	a	823	THR
1	a	826	GLU
1	a	828	ARG
1	a	833	ASN
1	a	836	THR
1	a	847	THR
1	a	849	THR
1	a	851	VAL
1	a	864	ASN
1	a	865	ARG
7	c	17	MET
7	c	21	CYS
7	c	30	GLU
7	c	33	LEU
7	c	43	THR
7	c	48	LEU
7	c	50	GLU
7	c	54	LEU
7	c	62	LEU
7	c	64	LYS
7	c	92	CYS
7	c	96	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	c	100	ASN
7	c	103	ILE
7	c	106	THR
7	c	110	ASP
7	c	122	MET
7	c	133	VAL
7	c	140	LYS
7	c	144	GLN
7	c	159	LYS
3	e	2	THR
3	e	5	LEU
3	e	6	LEU
3	e	28	ASN
3	e	30	LYS
3	e	31	ASP
3	e	32	ILE
4	f	1	MET
4	f	10	SER
4	f	28	VAL
4	f	30	HIS
4	f	34	ARG
5	g	8	ASP
5	g	9	ILE
5	g	10	SER
5	g	11	LYS
5	g	20	LEU
5	g	25	LEU
5	g	26	ILE
5	g	40	MET
5	g	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	79	GLN
1	A	81	GLN
1	A	101	GLN
1	A	229	GLN
1	A	241	GLN
1	A	255	GLN
1	A	296	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	339	ASN
1	A	364	GLN
1	A	445	GLN
1	A	470	ASN
1	A	483	ASN
1	A	531	GLN
1	A	538	GLN
1	A	550	ASN
1	A	565	GLN
1	A	602	GLN
1	A	619	HIS
1	A	639	ASN
1	A	643	GLN
1	A	755	HIS
1	A	765	ASN
1	A	808	GLN
1	A	825	GLN
1	A	833	ASN
2	C	40	GLN
2	C	59	GLN
2	C	85	GLN
2	C	136	ASN
2	C	149	GLN
2	C	169	ASN
2	C	185	GLN
2	C	200	GLN
3	E	35	ASN
1	a	16	GLN
1	a	59	ASN
1	a	81	GLN
1	a	382	HIS
1	a	445	GLN
1	a	531	GLN
1	a	538	GLN
1	a	550	ASN
1	a	602	GLN
1	a	619	HIS
1	a	621	ASN
1	a	626	ASN
1	a	643	GLN
1	a	744	ASN
1	a	755	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	765	ASN
1	a	825	GLN
1	a	833	ASN
1	a	864	ASN
7	c	52	GLN
7	c	82	GLN
7	c	96	ASN
7	c	100	ASN
7	c	109	GLN
7	c	144	GLN
7	c	145	GLN
4	f	30	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 79 ligands modelled in this entry, 2 are monoatomic and 32 are unknown - leaving 45 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	$\# Z > 2$
13	85I	A	917	-	43,44,44	1.57	2 (4%)	47,51,51	2.42	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	a	908	1	64,74,74	2.86	24 (37%)	78,115,115	4.42	34 (43%)
9	BCL	A	908	-	64,74,74	2.51	28 (43%)	78,115,115	2.66	27 (34%)
10	CLA	A	911	-	65,73,73	2.62	21 (32%)	76,113,113	3.33	29 (38%)
10	CLA	A	933	-	51,59,73	2.87	18 (35%)	59,96,113	3.90	32 (54%)
15	85N	a	902	-	45,46,46	0.59	0	50,55,55	0.42	0
9	BCL	a	907	-	64,74,74	2.56	23 (35%)	78,115,115	3.69	27 (34%)
9	BCL	A	905	-	64,74,74	2.66	20 (31%)	78,115,115	3.85	32 (41%)
13	85I	A	916	-	43,44,44	2.22	3 (6%)	47,51,51	1.93	6 (12%)
17	84Q	a	921	-	42,43,43	1.35	2 (4%)	47,50,50	1.04	2 (4%)
9	BCL	a	909	-	64,74,74	2.48	23 (35%)	78,115,115	3.89	28 (35%)
15	85N	A	932	-	45,46,46	1.04	1 (2%)	50,55,55	1.82	4 (8%)
11	LYC	c	201	-	39,39,39	1.65	9 (23%)	44,46,46	5.75	28 (63%)
15	85N	g	101	-	36,37,46	0.79	1 (2%)	40,45,55	0.58	0
9	BCL	a	911	-	64,74,74	2.79	22 (34%)	78,115,115	3.46	33 (42%)
10	CLA	A	910	-	65,73,73	2.53	19 (29%)	76,113,113	3.59	36 (47%)
10	CLA	a	915	-	51,59,73	2.93	17 (33%)	59,96,113	3.55	34 (57%)
9	BCL	A	909	-	64,74,74	3.24	27 (42%)	78,115,115	4.30	34 (43%)
16	HEC	C	301	2	32,50,50	2.95	17 (53%)	24,82,82	3.50	12 (50%)
10	CLA	a	912	19	65,73,73	2.79	17 (26%)	76,113,113	3.24	38 (50%)
9	BCL	A	906	1	50,60,74	2.79	14 (28%)	61,98,115	4.91	25 (40%)
13	85I	A	915	-	43,44,44	2.29	10 (23%)	47,51,51	2.44	7 (14%)
9	BCL	A	903	-	64,74,74	2.81	21 (32%)	78,115,115	3.83	33 (42%)
9	BCL	A	904	-	44,54,74	2.53	20 (45%)	54,91,115	3.08	24 (44%)
8	2GO	A	901	1	65,74,74	3.56	18 (27%)	76,115,115	3.49	29 (38%)
9	BCL	A	902	-	64,74,74	2.74	22 (34%)	78,115,115	3.23	31 (39%)
13	85I	a	919	-	43,44,44	1.41	2 (4%)	47,51,51	1.66	3 (6%)
18	SF4	a	917	1	0,12,12	-	-	-	-	-
13	85I	a	918	-	43,44,44	1.06	2 (4%)	47,51,51	1.69	4 (8%)
10	CLA	a	914	-	46,54,73	2.87	19 (41%)	53,90,113	3.60	27 (50%)
13	85I	a	920	-	43,44,44	2.21	2 (4%)	47,51,51	2.04	3 (6%)
8	2GO	a	903	1	65,74,74	3.45	20 (30%)	76,115,115	3.40	28 (36%)
9	BCL	A	907	-	59,69,74	3.30	26 (44%)	72,109,115	4.67	38 (52%)
9	BCL	a	906	-	44,54,74	2.85	19 (43%)	54,91,115	3.11	24 (44%)
10	CLA	A	912	-	46,54,73	2.75	15 (32%)	53,90,113	4.13	29 (54%)
11	LYC	A	913	-	39,39,39	2.05	11 (28%)	44,46,46	2.49	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	84Q	E	101	-	42,43,43	2.09	10 (23%)	47,50,50	1.90	8 (17%)
9	BCL	a	904	-	64,74,74	2.65	17 (26%)	78,115,115	3.42	26 (33%)
10	CLA	A	931	-	65,73,73	3.13	25 (38%)	76,113,113	4.31	38 (50%)
9	BCL	a	905	-	64,74,74	2.75	17 (26%)	78,115,115	3.68	31 (39%)
9	BCL	a	910	-	64,74,74	3.33	19 (29%)	78,115,115	4.08	38 (48%)
10	CLA	a	913	-	65,73,73	2.61	20 (30%)	76,113,113	4.02	34 (44%)
15	85N	G	101	-	36,37,46	0.72	0	40,45,55	0.77	2 (5%)
16	HEC	c	202	7	32,50,50	2.84	14 (43%)	24,82,82	3.87	11 (45%)
10	CLA	a	901	19	65,73,73	2.67	21 (32%)	76,113,113	3.57	32 (42%)

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
13	85I	A	917	-	-	29/47/48/48	-
9	BCL	a	908	1	-	20/37/137/137	-
9	BCL	A	908	-	-	14/37/137/137	-
10	CLA	A	911	-	1/1/15/20	11/37/115/115	-
10	CLA	A	933	-	-	4/21/99/115	-
15	85N	a	902	-	-	25/51/51/51	-
9	BCL	a	907	-	-	12/37/137/137	-
9	BCL	A	905	-	-	16/37/137/137	-
13	85I	A	916	-	-	27/47/48/48	-
17	84Q	a	921	-	-	32/46/47/47	-
9	BCL	a	909	-	-	13/37/137/137	-
15	85N	A	932	-	-	18/51/51/51	-
11	LYC	c	201	-	-	16/43/43/43	-
15	85N	g	101	-	-	19/42/42/51	-
9	BCL	a	911	-	-	5/37/137/137	-
10	CLA	A	910	-	1/1/15/20	9/37/115/115	-
10	CLA	a	915	-	-	7/21/99/115	-
9	BCL	A	909	-	-	12/37/137/137	-
16	HEC	C	301	2	-	3/10/54/54	-
10	CLA	a	912	19	-	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	A	906	1	-	6/21/121/137	-
13	85I	A	915	-	-	19/47/48/48	-
9	BCL	A	903	-	-	21/37/137/137	-
9	BCL	A	904	-	-	6/13/113/137	-
8	2GO	A	901	1	-	4/37/97/97	-
9	BCL	A	902	-	-	16/37/137/137	-
13	85I	a	919	-	-	36/47/48/48	-
18	SF4	a	917	1	-	-	0/6/5/5
13	85I	a	918	-	-	21/47/48/48	-
10	CLA	a	914	-	-	4/15/93/115	-
13	85I	a	920	-	-	30/47/48/48	-
8	2GO	a	903	1	-	9/37/97/97	-
9	BCL	A	907	-	-	16/31/131/137	-
9	BCL	a	906	-	-	6/13/113/137	-
10	CLA	A	912	-	-	2/15/93/115	-
11	LYC	A	913	-	-	1/43/43/43	-
17	84Q	E	101	-	-	27/46/47/47	-
9	BCL	a	904	-	-	12/37/137/137	-
10	CLA	A	931	-	-	18/37/115/115	-
9	BCL	a	905	-	-	17/37/137/137	-
9	BCL	a	910	-	-	11/37/137/137	-
10	CLA	a	913	-	-	11/37/115/115	-
15	85N	G	101	-	-	18/42/42/51	-
16	HEC	c	202	7	-	3/10/54/54	-
10	CLA	a	901	19	-	24/37/115/115	-

All (658) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	910	BCL	C4B-NB	-15.63	1.21	1.35
8	A	901	2GO	C4D-ND	-14.69	1.18	1.37
8	A	901	2GO	C2A-C3A	14.62	1.67	1.36
13	a	920	85I	O6-C3	-14.01	1.20	1.44
8	a	903	2GO	C3C-C2C	11.91	1.62	1.36
10	A	931	CLA	C4B-NB	-11.70	1.24	1.35
9	A	909	BCL	C4B-NB	-10.85	1.25	1.35
9	A	903	BCL	C4B-NB	-10.35	1.26	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	912	CLA	C3D-C4D	-10.25	1.21	1.44
13	A	915	85I	C4-C3	-9.76	1.29	1.51
9	a	904	BCL	C3D-C4D	-9.67	1.22	1.44
9	a	910	BCL	C3D-C4D	-9.66	1.22	1.44
9	A	907	BCL	C1B-NB	-9.46	1.26	1.35
13	A	916	85I	P-O3	9.38	1.85	1.60
10	A	912	CLA	C4B-NB	-9.38	1.26	1.35
10	A	933	CLA	C4B-NB	-9.35	1.26	1.35
9	a	910	BCL	C1B-NB	-9.31	1.26	1.35
8	a	903	2GO	C1D-ND	-9.20	1.25	1.37
10	a	913	CLA	C4B-NB	-9.19	1.27	1.35
8	a	903	2GO	C4D-ND	-9.11	1.25	1.37
9	a	907	BCL	C1D-ND	-9.03	1.26	1.37
10	a	914	CLA	C3D-C4D	-8.99	1.23	1.44
10	A	931	CLA	C3D-C4D	-8.88	1.24	1.44
10	a	915	CLA	C1B-NB	-8.86	1.27	1.35
8	a	903	2GO	C4B-NB	8.82	1.48	1.35
9	a	905	BCL	C3D-C4D	-8.78	1.24	1.44
10	A	911	CLA	C1D-ND	8.78	1.48	1.37
9	A	907	BCL	O2A-CGA	8.61	1.58	1.33
10	A	910	CLA	C3D-C4D	-8.60	1.24	1.44
10	A	910	CLA	C1B-NB	-8.60	1.27	1.35
17	E	101	84Q	P-O4	8.60	1.83	1.60
8	a	903	2GO	OBD-CAD	-8.51	1.09	1.33
13	A	916	85I	C4-C3	8.49	1.71	1.51
9	a	908	BCL	C3D-C4D	-8.45	1.25	1.44
9	A	903	BCL	C3D-C4D	-8.44	1.25	1.44
8	A	901	2GO	C3C-C2C	8.42	1.54	1.36
9	a	905	BCL	C4B-NB	-8.42	1.27	1.35
10	A	912	CLA	C3D-C4D	-8.42	1.25	1.44
10	A	933	CLA	C3D-C4D	-8.34	1.25	1.44
9	a	907	BCL	C3D-C4D	-8.32	1.25	1.44
9	A	902	BCL	C3D-C4D	-8.27	1.25	1.44
9	A	909	BCL	C3D-C4D	-8.24	1.25	1.44
10	A	933	CLA	C4D-ND	-8.22	1.26	1.37
10	a	901	CLA	C1C-NC	-8.21	1.25	1.37
9	a	911	BCL	C4B-NB	-8.20	1.27	1.35
10	A	931	CLA	O1D-CGD	-8.18	1.00	1.21
8	a	903	2GO	C2A-C3A	8.03	1.53	1.36
9	A	905	BCL	CAA-C2A	-8.02	1.39	1.54
9	a	911	BCL	C1B-NB	-7.99	1.28	1.35
10	A	910	CLA	C4B-NB	-7.98	1.28	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	907	BCL	C4B-NB	-7.93	1.28	1.35
10	a	913	CLA	C1B-NB	-7.91	1.28	1.35
17	a	921	84Q	O2-C16	-7.91	1.31	1.44
9	A	909	BCL	C1B-NB	-7.90	1.28	1.35
9	A	906	BCL	C3D-C4D	-7.87	1.26	1.44
13	a	919	85I	O6-C3	7.86	1.58	1.44
9	A	908	BCL	C4B-NB	-7.84	1.28	1.35
10	a	915	CLA	C3D-C4D	-7.83	1.26	1.44
8	A	901	2GO	OBD-CAD	-7.79	1.11	1.33
10	a	901	CLA	C1B-NB	-7.75	1.28	1.35
9	a	909	BCL	C3D-C4D	-7.70	1.26	1.44
10	a	901	CLA	C3D-C4D	-7.69	1.26	1.44
9	a	906	BCL	C3D-C4D	-7.65	1.26	1.44
8	A	901	2GO	C1A-NA	-7.63	1.22	1.38
9	A	906	BCL	C1D-ND	-7.63	1.28	1.37
9	A	902	BCL	C1D-ND	-7.60	1.28	1.37
10	a	914	CLA	C1B-NB	-7.57	1.28	1.35
10	A	911	CLA	C1C-NC	-7.54	1.26	1.37
10	a	914	CLA	C4B-NB	-7.51	1.28	1.35
9	A	905	BCL	C3D-C4D	-7.48	1.27	1.44
9	A	904	BCL	C3D-C4D	-7.41	1.27	1.44
9	a	904	BCL	C3C-C4C	-7.35	1.42	1.51
10	a	901	CLA	C4B-NB	-7.32	1.28	1.35
9	A	909	BCL	C4D-ND	-7.29	1.27	1.37
8	a	903	2GO	C1A-NA	-7.29	1.23	1.38
9	a	911	BCL	C3D-C4D	-7.28	1.27	1.44
9	a	908	BCL	CAA-C2A	-7.26	1.40	1.54
9	a	908	BCL	C4D-ND	-7.21	1.27	1.37
9	a	908	BCL	C1D-ND	-7.16	1.29	1.37
9	A	902	BCL	C1B-NB	-7.15	1.28	1.35
13	A	917	85I	C4-C3	7.10	1.68	1.51
10	a	915	CLA	CHC-C1C	7.10	1.53	1.35
10	a	912	CLA	C1C-NC	-7.05	1.27	1.37
9	A	902	BCL	C4B-NB	-7.00	1.29	1.35
10	a	912	CLA	C9-C8	-6.98	1.30	1.52
9	A	907	BCL	C4D-ND	-6.96	1.28	1.37
9	A	907	BCL	C3D-C4D	-6.88	1.28	1.44
13	A	917	85I	O6-C3	-6.87	1.32	1.44
9	A	908	BCL	C3D-C4D	-6.83	1.28	1.44
10	A	911	CLA	C3D-C4D	-6.81	1.28	1.44
9	a	911	BCL	C1D-ND	-6.80	1.29	1.37
9	a	905	BCL	C1D-ND	-6.80	1.29	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	c	202	HEC	O2A-CGA	-6.79	1.07	1.30
9	a	910	BCL	C3C-C4C	-6.75	1.43	1.51
11	A	913	LYC	C14-C12	-6.69	1.26	1.35
10	a	913	CLA	C3D-C4D	-6.68	1.29	1.44
10	A	931	CLA	C1D-ND	6.61	1.45	1.37
9	A	909	BCL	O1A-CGA	-6.61	1.02	1.22
9	A	907	BCL	O1D-CGD	-6.50	1.04	1.21
9	A	907	BCL	C1D-ND	-6.49	1.29	1.37
9	a	904	BCL	C1D-ND	-6.38	1.29	1.37
10	a	915	CLA	C4B-NB	-6.33	1.29	1.35
10	a	912	CLA	C4B-NB	-6.31	1.29	1.35
9	a	906	BCL	C4B-NB	-6.31	1.29	1.35
9	a	908	BCL	C2A-C1A	-6.27	1.38	1.52
10	a	913	CLA	C1D-ND	6.23	1.45	1.37
9	a	905	BCL	C4D-ND	-6.19	1.29	1.37
10	A	931	CLA	C4D-ND	-6.17	1.29	1.37
10	A	933	CLA	O1D-CGD	-6.15	1.05	1.21
9	A	909	BCL	OBB-CAB	-6.11	1.03	1.22
10	a	913	CLA	C1C-NC	-6.11	1.28	1.37
9	A	909	BCL	C3C-C4C	-6.10	1.43	1.51
9	a	904	BCL	C1B-NB	-6.10	1.29	1.35
9	A	903	BCL	OBB-CAB	-6.09	1.03	1.22
8	a	903	2GO	OBB-CAB	-6.03	1.04	1.22
9	A	905	BCL	C2A-C1A	-6.01	1.38	1.52
10	A	911	CLA	C4D-ND	-6.00	1.29	1.37
9	A	906	BCL	C4B-NB	-5.99	1.29	1.35
10	a	912	CLA	OBD-CAD	-5.99	1.12	1.22
9	a	908	BCL	C4B-NB	-5.95	1.29	1.35
9	a	910	BCL	OBB-CAB	-5.92	1.04	1.22
9	A	905	BCL	C1D-ND	-5.91	1.30	1.37
9	A	905	BCL	C4B-NB	-5.90	1.29	1.35
9	A	904	BCL	C4B-NB	-5.83	1.30	1.35
13	a	918	85I	O6-C3	-5.82	1.34	1.44
10	a	912	CLA	C1B-NB	-5.78	1.30	1.35
9	a	909	BCL	O1D-CGD	-5.78	1.06	1.21
9	A	906	BCL	O2D-CED	-5.76	1.31	1.45
15	A	932	85N	O3-C17	-5.73	1.21	1.40
9	a	905	BCL	C3C-C4C	-5.70	1.44	1.51
10	A	931	CLA	O2D-CED	-5.64	1.32	1.45
9	a	911	BCL	C3C-C4C	-5.61	1.44	1.51
9	a	909	BCL	C4B-NB	-5.56	1.30	1.35
16	C	301	HEC	O2A-CGA	-5.56	1.12	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	901	2GO	C1D-ND	-5.55	1.30	1.37
10	a	915	CLA	C4D-ND	-5.53	1.30	1.37
9	a	909	BCL	C1D-ND	-5.53	1.31	1.37
9	A	909	BCL	C1D-ND	-5.51	1.31	1.37
9	a	910	BCL	C1D-ND	-5.47	1.31	1.37
10	a	912	CLA	CHC-C1C	5.47	1.49	1.35
9	a	907	BCL	C4D-ND	-5.46	1.30	1.37
9	A	908	BCL	C3C-C4C	-5.42	1.44	1.51
9	A	906	BCL	C1B-NB	-5.39	1.30	1.35
10	A	911	CLA	C4B-NB	-5.39	1.30	1.35
17	E	101	84Q	C15-C16	5.38	1.64	1.51
9	a	906	BCL	C4D-ND	-5.38	1.30	1.37
9	A	903	BCL	C3C-C4C	-5.31	1.44	1.51
9	A	903	BCL	C1B-NB	-5.31	1.30	1.35
10	a	912	CLA	C1D-ND	5.29	1.44	1.37
9	a	909	BCL	C1B-NB	-5.28	1.30	1.35
10	a	914	CLA	C1C-NC	-5.26	1.30	1.37
8	A	901	2GO	C3D-C2D	-5.25	1.30	1.39
9	A	903	BCL	C1D-ND	-5.23	1.31	1.37
9	A	908	BCL	C1D-ND	-5.18	1.31	1.37
9	a	906	BCL	C1D-ND	-5.16	1.31	1.37
9	A	905	BCL	C4D-ND	-5.14	1.30	1.37
9	A	903	BCL	O1A-CGA	-5.13	1.07	1.22
9	a	911	BCL	C4D-ND	-5.11	1.30	1.37
9	A	907	BCL	C5-C3	5.10	1.61	1.51
9	a	909	BCL	O2D-CED	-5.09	1.33	1.45
9	A	902	BCL	C2A-C1A	-5.08	1.40	1.52
9	a	908	BCL	C1B-NB	-5.07	1.30	1.35
9	a	905	BCL	O1D-CGD	-5.05	1.08	1.21
9	A	906	BCL	C4D-ND	-5.05	1.30	1.37
9	A	907	BCL	C2-C3	5.02	1.45	1.33
9	A	902	BCL	C4D-ND	-5.00	1.30	1.37
10	A	911	CLA	MG-NC	5.00	2.18	2.06
8	A	901	2GO	C2D-C1D	-4.99	1.31	1.42
9	A	909	BCL	OBD-CAD	-4.99	1.13	1.22
16	c	202	HEC	CAD-C3D	-4.99	1.44	1.52
10	A	931	CLA	O2D-CGD	4.98	1.45	1.33
9	a	911	BCL	OBB-CAB	-4.96	1.07	1.22
16	c	202	HEC	C4B-C3B	-4.93	1.34	1.43
16	C	301	HEC	CBB-CAB	-4.92	1.31	1.49
9	a	906	BCL	CAA-C2A	-4.92	1.45	1.54
10	A	912	CLA	C1B-NB	-4.89	1.30	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	916	85I	O6-C3	4.86	1.52	1.44
10	A	910	CLA	C4D-ND	-4.84	1.31	1.37
10	A	911	CLA	C1B-NB	-4.81	1.30	1.35
9	a	906	BCL	C1B-NB	-4.79	1.30	1.35
16	C	301	HEC	O2D-CGD	-4.79	1.14	1.30
9	a	904	BCL	C4B-NB	-4.78	1.30	1.35
8	a	903	2GO	C4C-C3C	4.77	1.53	1.45
9	A	906	BCL	O1D-CGD	-4.74	1.09	1.21
9	A	905	BCL	C3C-C4C	-4.74	1.45	1.51
16	C	301	HEC	C1B-NB	-4.74	1.26	1.36
10	a	915	CLA	C1C-NC	-4.71	1.30	1.37
16	C	301	HEC	CBC-CAC	-4.70	1.31	1.49
9	a	904	BCL	C4D-ND	-4.69	1.31	1.37
9	a	904	BCL	O1A-CGA	-4.68	1.08	1.22
9	a	909	BCL	C3C-C4C	-4.67	1.45	1.51
9	a	906	BCL	C3C-C4C	-4.65	1.45	1.51
9	A	902	BCL	C3C-C4C	-4.65	1.45	1.51
9	a	907	BCL	C2A-C1A	-4.64	1.41	1.52
9	A	903	BCL	O1D-CGD	-4.59	1.09	1.21
9	a	905	BCL	O2A-CGA	4.57	1.46	1.33
10	a	912	CLA	O2D-CED	-4.57	1.34	1.45
9	A	904	BCL	O2A-CGA	4.57	1.46	1.30
10	A	931	CLA	O2A-CGA	4.55	1.46	1.33
9	a	908	BCL	CBB-CAB	-4.55	1.36	1.49
9	A	906	BCL	CBB-CAB	-4.55	1.36	1.49
9	a	910	BCL	O1D-CGD	-4.53	1.09	1.21
9	A	906	BCL	O1A-CGA	-4.53	1.09	1.22
16	C	301	HEC	C3A-C4A	4.52	1.52	1.42
9	A	908	BCL	C1B-NB	-4.52	1.31	1.35
10	A	912	CLA	C1C-NC	-4.52	1.31	1.37
13	A	915	85I	P-O3	4.50	1.72	1.60
10	A	931	CLA	O1A-CGA	-4.49	1.09	1.22
9	a	907	BCL	C4B-NB	-4.47	1.31	1.35
10	a	915	CLA	C1D-ND	4.45	1.43	1.37
9	a	905	BCL	OBB-CAB	-4.44	1.09	1.22
9	a	911	BCL	OBD-CAD	-4.40	1.14	1.22
10	A	910	CLA	O2D-CED	-4.40	1.35	1.45
9	A	902	BCL	O2D-CED	-4.40	1.35	1.45
9	A	909	BCL	MG-NA	4.39	2.16	2.06
16	c	202	HEC	O2D-CGD	-4.38	1.16	1.30
9	A	905	BCL	C1B-NB	-4.38	1.31	1.35
16	C	301	HEC	C4B-C3B	-4.37	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	914	CLA	O1D-CGD	-4.37	1.10	1.21
10	A	912	CLA	MG-NC	4.34	2.16	2.06
10	a	913	CLA	CHC-C1C	4.34	1.46	1.35
9	a	911	BCL	O2D-CED	-4.33	1.35	1.45
10	A	912	CLA	O1D-CGD	-4.33	1.10	1.21
9	A	907	BCL	OBD-CAD	-4.32	1.15	1.22
10	a	901	CLA	O2A-CGA	4.30	1.45	1.33
16	c	202	HEC	O1A-CGA	-4.30	1.07	1.22
10	a	901	CLA	CHC-C1C	4.28	1.45	1.35
9	a	904	BCL	O2A-CGA	4.27	1.45	1.33
9	A	903	BCL	C2A-C1A	-4.26	1.42	1.52
9	A	907	BCL	O2D-CED	-4.25	1.35	1.45
10	A	910	CLA	C1C-NC	-4.24	1.31	1.37
10	a	912	CLA	O1D-CGD	-4.21	1.10	1.21
16	c	202	HEC	C4D-ND	-4.16	1.27	1.36
10	A	910	CLA	O1D-CGD	-4.16	1.10	1.21
8	A	901	2GO	OBB-CAB	-4.15	1.09	1.22
10	A	933	CLA	C1C-NC	-4.15	1.31	1.37
9	A	905	BCL	OBB-CAB	-4.13	1.10	1.22
9	a	910	BCL	O1A-CGA	-4.10	1.10	1.22
9	A	905	BCL	O2D-CED	-4.10	1.35	1.45
9	a	906	BCL	C3B-C2B	4.09	1.46	1.39
9	a	904	BCL	O2D-CED	-4.06	1.35	1.45
10	A	911	CLA	CHC-C1C	4.05	1.45	1.35
9	a	904	BCL	O1D-CGD	-4.03	1.11	1.21
9	A	905	BCL	C3A-C2A	-4.01	1.43	1.54
13	a	919	85I	C4-C3	-4.00	1.42	1.51
8	a	903	2GO	C2D-C1D	-4.00	1.33	1.42
9	a	908	BCL	O2D-CED	-3.99	1.35	1.45
8	A	901	2GO	ZN-NC	3.99	2.25	2.01
9	a	911	BCL	O2A-C1	-3.98	1.34	1.46
16	C	301	HEC	C3C-C4C	-3.98	1.35	1.43
13	A	915	85I	O4-C5	-3.97	1.21	1.33
9	a	908	BCL	O1D-CGD	-3.97	1.11	1.21
9	a	909	BCL	O1A-CGA	-3.94	1.10	1.22
16	c	202	HEC	C1B-NB	-3.94	1.28	1.36
9	A	908	BCL	O1D-CGD	-3.94	1.11	1.21
9	A	904	BCL	CAA-C2A	-3.92	1.46	1.54
8	A	901	2GO	ZN-NA	3.92	2.24	2.01
11	A	913	LYC	C55-C56	-3.90	1.30	1.35
9	a	907	BCL	OBB-CAB	-3.90	1.10	1.22
10	a	915	CLA	C3C-C2C	3.89	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	933	CLA	O2A-C1	-3.89	1.35	1.46
10	a	901	CLA	O2D-CED	-3.87	1.36	1.45
9	a	911	BCL	O1A-CGA	-3.86	1.11	1.22
9	A	904	BCL	C2A-C1A	-3.86	1.43	1.52
9	A	902	BCL	CAA-C2A	-3.84	1.47	1.54
9	A	905	BCL	O1D-CGD	-3.83	1.11	1.21
9	a	911	BCL	CHD-C1D	3.83	1.45	1.38
9	A	909	BCL	C4B-CHC	3.83	1.51	1.41
11	c	201	LYC	C14-C12	-3.82	1.30	1.35
10	A	931	CLA	OBD-CAD	-3.82	1.15	1.22
9	A	904	BCL	C4D-ND	-3.81	1.32	1.37
9	a	910	BCL	O2D-CGD	3.80	1.42	1.33
9	a	905	BCL	OBD-CAD	-3.79	1.15	1.22
10	a	913	CLA	C3B-C2B	3.79	1.45	1.40
10	a	914	CLA	O2A-CGA	3.79	1.45	1.33
9	A	902	BCL	O2D-CGD	3.77	1.42	1.33
10	A	912	CLA	CHC-C1C	3.76	1.44	1.35
9	a	905	BCL	O2D-CED	-3.76	1.36	1.45
9	a	910	BCL	O2D-CED	-3.75	1.36	1.45
10	a	912	CLA	MG-NC	3.75	2.15	2.06
9	a	910	BCL	C4D-ND	-3.75	1.32	1.37
10	a	915	CLA	MG-NC	3.74	2.15	2.06
9	A	907	BCL	C6-C5	3.73	1.65	1.52
9	a	909	BCL	C3B-C2B	3.73	1.46	1.39
10	a	901	CLA	O1D-CGD	-3.72	1.11	1.21
11	A	913	LYC	C9-C7	-3.72	1.30	1.34
8	a	903	2GO	C1C-C2C	3.70	1.51	1.44
10	a	913	CLA	C4D-ND	-3.70	1.32	1.37
13	A	915	85I	P-O	-3.70	1.44	1.59
9	A	908	BCL	C3A-C2A	-3.68	1.44	1.54
10	a	901	CLA	MG-NC	3.68	2.15	2.06
10	A	912	CLA	C4D-ND	-3.68	1.32	1.37
10	a	901	CLA	CHD-C4C	3.67	1.47	1.39
16	C	301	HEC	C1D-ND	-3.67	1.28	1.36
9	A	907	BCL	OBB-CAB	-3.67	1.11	1.22
9	a	908	BCL	CAA-CBA	-3.66	1.41	1.52
16	C	301	HEC	C3D-C2D	3.66	1.48	1.37
9	a	906	BCL	C2A-C1A	-3.66	1.44	1.52
9	A	909	BCL	MG-ND	-3.65	1.98	2.05
9	a	909	BCL	C4D-ND	-3.64	1.32	1.37
9	A	909	BCL	C2-C3	3.64	1.41	1.33
9	A	902	BCL	O1A-CGA	-3.63	1.11	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	909	BCL	C3A-C2A	-3.62	1.44	1.54
10	a	913	CLA	CAA-C2A	3.61	1.60	1.54
10	a	914	CLA	MG-NC	3.61	2.14	2.06
9	A	909	BCL	O1D-CGD	-3.61	1.12	1.21
10	A	910	CLA	CHC-C1C	3.60	1.44	1.35
10	a	915	CLA	O1A-CGA	-3.59	1.11	1.22
11	c	201	LYC	C19-C17	-3.59	1.31	1.35
9	a	907	BCL	O2A-CGA	3.58	1.43	1.33
9	A	903	BCL	C3A-C2A	-3.58	1.44	1.54
10	a	912	CLA	O2A-CGA	3.57	1.43	1.33
9	a	906	BCL	O2A-CGA	3.56	1.42	1.30
10	A	911	CLA	C10-C8	-3.56	1.33	1.52
8	a	903	2GO	ZN-NC	3.55	2.22	2.01
13	A	915	85I	P-O1	-3.54	1.38	1.50
9	A	909	BCL	CAA-CBA	-3.54	1.41	1.52
9	A	904	BCL	C3B-C2B	3.51	1.45	1.39
9	a	908	BCL	C3B-C2B	3.51	1.45	1.39
10	A	933	CLA	CAA-C2A	-3.48	1.47	1.54
9	A	904	BCL	C4B-CHC	3.48	1.50	1.41
10	a	915	CLA	O1D-CGD	-3.47	1.12	1.21
16	C	301	HEC	CAD-C3D	-3.46	1.47	1.52
10	A	933	CLA	CHC-C1C	3.45	1.43	1.35
9	A	903	BCL	C4D-ND	-3.45	1.33	1.37
9	a	905	BCL	O1A-CGA	-3.44	1.12	1.22
9	a	905	BCL	CBB-CAB	-3.43	1.39	1.49
10	A	933	CLA	O1A-CGA	-3.42	1.12	1.22
9	A	903	BCL	O2A-CGA	3.42	1.43	1.33
9	A	909	BCL	CBD-CGD	-3.41	1.41	1.52
9	a	907	BCL	O2A-C1	-3.41	1.36	1.46
10	A	911	CLA	O1A-CGA	-3.40	1.12	1.22
10	a	901	CLA	C1D-C2D	3.40	1.52	1.45
9	A	903	BCL	CBB-CAB	-3.40	1.39	1.49
11	A	913	LYC	C13-C12	-3.39	1.43	1.50
10	A	911	CLA	O2D-CED	-3.39	1.37	1.45
11	c	201	LYC	C13-C12	-3.39	1.43	1.50
16	c	202	HEC	C2B-C3B	3.38	1.44	1.40
9	a	907	BCL	CHD-C1D	3.37	1.44	1.38
9	a	904	BCL	C3B-C2B	3.37	1.45	1.39
9	a	907	BCL	CAA-C2A	-3.36	1.47	1.54
8	a	903	2GO	C1B-NB	3.36	1.40	1.35
9	A	903	BCL	O2D-CGD	3.35	1.41	1.33
9	a	906	BCL	OB-OB	-3.34	1.12	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	905	BCL	CBA-CGA	-3.34	1.40	1.50
9	A	908	BCL	C4D-ND	-3.34	1.33	1.37
10	A	912	CLA	O2A-CGA	3.33	1.43	1.33
10	A	931	CLA	C4D-CHA	3.31	1.50	1.38
10	A	931	CLA	CHC-C1C	3.31	1.43	1.35
10	A	911	CLA	O2A-C1	-3.30	1.36	1.46
10	a	901	CLA	C7-C8	-3.30	1.35	1.52
16	c	202	HEC	CBA-CGA	-3.30	1.42	1.50
10	a	914	CLA	C3C-C2C	3.29	1.43	1.36
9	a	908	BCL	CBA-CGA	-3.29	1.41	1.50
9	a	905	BCL	CAC-C3C	-3.29	1.47	1.54
8	a	903	2GO	O1D-CGD	-3.27	1.14	1.21
9	A	902	BCL	C3B-C2B	3.24	1.45	1.39
9	a	908	BCL	C5-C3	-3.23	1.44	1.51
9	A	908	BCL	CAA-C2A	-3.21	1.48	1.54
9	a	907	BCL	O1D-CGD	-3.21	1.13	1.21
10	a	914	CLA	CHC-C1C	3.20	1.43	1.35
9	A	907	BCL	CMD-C2D	-3.20	1.44	1.50
9	a	907	BCL	MG-NA	-3.19	1.98	2.06
10	A	910	CLA	CHD-C1D	3.18	1.44	1.38
16	c	202	HEC	CAA-C2A	-3.18	1.46	1.52
9	a	910	BCL	CMB-C2B	-3.18	1.45	1.51
10	a	913	CLA	O1A-CGA	-3.18	1.13	1.22
9	A	908	BCL	CMA-C3A	-3.18	1.46	1.53
9	A	908	BCL	MG-NC	-3.18	1.98	2.06
11	A	913	LYC	C19-C17	-3.16	1.31	1.35
9	A	908	BCL	O2A-CGA	3.16	1.42	1.33
11	A	913	LYC	C10-C11	-3.15	1.26	1.34
9	A	902	BCL	O2A-CGA	3.15	1.42	1.33
9	A	907	BCL	CBB-CAB	-3.12	1.40	1.49
9	a	910	BCL	O2A-CGA	3.11	1.42	1.33
9	A	908	BCL	C3B-CAB	-3.11	1.40	1.49
9	A	902	BCL	C1B-CHB	3.11	1.49	1.41
16	c	202	HEC	CBC-CAC	-3.10	1.37	1.49
9	A	907	BCL	C2C-C3C	-3.09	1.45	1.54
10	A	910	CLA	CHD-C4C	3.08	1.46	1.39
9	a	911	BCL	C1D-C2D	-3.07	1.39	1.45
10	a	915	CLA	O2D-CED	-3.07	1.38	1.45
10	A	931	CLA	C10-C8	-3.07	1.36	1.52
17	E	101	84Q	C3-C1	-3.07	1.30	1.51
9	a	909	BCL	C3A-C2A	-3.06	1.45	1.54
9	a	910	BCL	MG-NA	3.06	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	910	CLA	MG-NC	3.06	2.13	2.06
10	a	901	CLA	O2D-CGD	3.05	1.40	1.33
9	A	909	BCL	CHD-C1D	3.03	1.44	1.38
9	a	907	BCL	C2C-C3C	-3.03	1.46	1.54
10	A	931	CLA	C1D-C2D	-3.03	1.39	1.45
10	A	931	CLA	C3D-C2D	3.02	1.47	1.39
8	A	901	2GO	CHA-C1A	3.02	1.51	1.41
9	A	902	BCL	CHD-C1D	3.01	1.44	1.38
9	a	904	BCL	OBB-CAB	-3.01	1.13	1.22
10	A	911	CLA	C3B-C2B	3.00	1.44	1.40
10	a	914	CLA	C2A-C1A	-3.00	1.45	1.52
16	C	301	HEC	C1C-NC	-2.99	1.30	1.36
10	a	913	CLA	O1D-CGD	-2.99	1.13	1.21
8	a	903	2GO	C3D-C2D	-2.99	1.34	1.39
9	a	911	BCL	C3A-C2A	-2.99	1.46	1.54
9	A	909	BCL	CBB-CAB	-2.99	1.40	1.49
9	a	908	BCL	OBB-CAB	-2.98	1.13	1.22
9	A	902	BCL	CMB-C2B	-2.98	1.45	1.51
16	c	202	HEC	CMD-C2D	-2.97	1.45	1.51
9	A	902	BCL	O1D-CGD	-2.97	1.13	1.21
10	A	911	CLA	O1D-CGD	-2.96	1.13	1.21
9	A	903	BCL	O2D-CED	-2.95	1.38	1.45
9	A	906	BCL	CHD-C1D	2.94	1.44	1.38
9	A	905	BCL	CAA-CBA	-2.94	1.43	1.52
9	a	908	BCL	O2D-CGD	2.93	1.40	1.33
10	a	913	CLA	C10-C8	2.93	1.68	1.52
10	A	931	CLA	CHD-C1D	2.93	1.44	1.38
10	A	931	CLA	CMA-C3A	-2.91	1.46	1.53
9	A	902	BCL	C3A-C2A	-2.90	1.46	1.54
9	A	904	BCL	O2D-CGD	2.90	1.40	1.33
9	a	905	BCL	O2D-CGD	2.90	1.40	1.33
10	A	931	CLA	C1C-C2C	-2.88	1.39	1.44
9	A	903	BCL	C3B-CAB	-2.88	1.41	1.49
10	a	913	CLA	MG-NC	2.87	2.13	2.06
9	A	904	BCL	CMB-C2B	-2.87	1.45	1.51
9	A	908	BCL	O2D-CGD	2.87	1.40	1.33
9	A	908	BCL	C2C-C3C	-2.87	1.46	1.54
9	a	909	BCL	C2C-C3C	-2.87	1.46	1.54
9	a	905	BCL	C2C-C3C	-2.86	1.46	1.54
10	a	914	CLA	C3A-C2A	-2.86	1.46	1.54
10	A	933	CLA	C3A-C2A	-2.85	1.46	1.54
11	A	913	LYC	C59-C58	-2.85	1.27	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	904	BCL	C2C-C3C	-2.85	1.46	1.54
9	A	902	BCL	OBB-CAB	-2.84	1.14	1.22
10	a	901	CLA	CAA-C2A	-2.83	1.48	1.54
9	a	907	BCL	O1A-CGA	-2.83	1.14	1.22
8	A	901	2GO	CBC-CAC	-2.83	1.38	1.51
17	E	101	84Q	C7-C6	-2.80	1.35	1.51
9	A	904	BCL	OBB-CAB	-2.80	1.14	1.22
9	a	910	BCL	C4B-CHC	2.80	1.48	1.41
9	a	908	BCL	O1A-CGA	-2.79	1.14	1.22
10	a	901	CLA	C3C-C2C	2.79	1.42	1.36
9	A	903	BCL	CMD-C2D	-2.78	1.44	1.50
10	A	912	CLA	C1D-C2D	-2.77	1.39	1.45
9	a	907	BCL	C3C-C4C	-2.75	1.48	1.51
8	A	901	2GO	C4B-NB	2.74	1.39	1.35
9	a	911	BCL	C3D-C2D	2.74	1.46	1.39
10	A	912	CLA	C3B-C2B	2.74	1.44	1.40
10	A	910	CLA	C1B-CHB	2.74	1.48	1.41
10	A	933	CLA	O2D-CED	-2.73	1.38	1.45
9	A	908	BCL	MG-NA	-2.73	1.99	2.06
9	a	907	BCL	C1D-C2D	-2.73	1.39	1.45
10	a	915	CLA	O2D-CGD	2.73	1.39	1.33
13	A	915	85I	O5-C5	-2.72	1.14	1.22
9	A	906	BCL	OBB-CAB	-2.72	1.14	1.22
10	A	931	CLA	C1B-NB	2.72	1.37	1.35
13	A	915	85I	O6-C3	-2.71	1.40	1.44
9	A	902	BCL	C2C-C3C	-2.70	1.46	1.54
10	A	911	CLA	CHD-C1D	2.70	1.43	1.38
10	A	912	CLA	C3C-C2C	2.70	1.42	1.36
17	E	101	84Q	C9-C8	-2.69	1.36	1.51
8	a	903	2GO	CHA-C1A	2.69	1.50	1.41
10	A	912	CLA	C2A-C1A	-2.69	1.46	1.52
9	A	907	BCL	C3A-C2A	-2.68	1.47	1.54
10	A	910	CLA	O2A-CGA	2.68	1.41	1.33
16	C	301	HEC	O1A-CGA	-2.68	1.13	1.22
9	A	907	BCL	C1B-CHB	2.68	1.48	1.41
10	A	933	CLA	CBA-CGA	-2.68	1.42	1.50
9	a	906	BCL	O1D-CGD	-2.68	1.14	1.21
9	A	907	BCL	O2A-C1	2.68	1.53	1.46
16	C	301	HEC	CAA-C2A	-2.67	1.47	1.52
13	A	915	85I	P-O2	-2.67	1.42	1.55
9	A	908	BCL	O1A-CGA	-2.67	1.14	1.22
9	a	906	BCL	CHD-C1D	2.65	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	911	CLA	CMC-C2C	-2.65	1.45	1.50
9	a	909	BCL	C5-C3	-2.65	1.45	1.51
16	C	301	HEC	CBA-CGA	-2.64	1.44	1.50
10	A	931	CLA	MG-NC	2.64	2.12	2.06
10	a	901	CLA	O1A-CGA	-2.63	1.14	1.22
9	a	909	BCL	CMD-C2D	-2.63	1.45	1.50
13	A	915	85I	C33-C32	-2.63	1.37	1.51
9	A	907	BCL	C2A-C1A	-2.63	1.46	1.52
17	E	101	84Q	C9-C10	-2.62	1.36	1.51
9	a	909	BCL	O2D-CGD	2.62	1.39	1.33
10	a	914	CLA	O1A-CGA	-2.61	1.14	1.22
9	A	908	BCL	CBD-CGD	-2.60	1.44	1.52
9	A	907	BCL	C3C-C4C	-2.60	1.48	1.51
10	A	931	CLA	MG-NA	2.59	2.12	2.06
9	A	905	BCL	O2A-CGA	2.59	1.40	1.33
10	a	901	CLA	C5-C3	-2.58	1.45	1.51
9	a	909	BCL	CBB-CAB	-2.57	1.42	1.49
10	A	912	CLA	C1B-CHB	2.57	1.48	1.41
9	A	902	BCL	CBB-CAB	-2.57	1.42	1.49
10	A	910	CLA	C1D-C2D	-2.56	1.40	1.45
10	A	933	CLA	MG-ND	2.56	2.10	2.05
17	a	921	84Q	P-O4	2.56	1.67	1.60
8	A	901	2GO	C4C-C3C	-2.56	1.40	1.45
9	a	907	BCL	O2D-CED	-2.55	1.39	1.45
9	A	905	BCL	O2A-C1	-2.54	1.39	1.46
10	A	931	CLA	C3A-C4A	-2.54	1.43	1.51
10	a	901	CLA	C2-C3	-2.54	1.26	1.33
11	c	201	LYC	C1-C2	-2.53	1.43	1.50
11	A	913	LYC	C11-C12	-2.53	1.40	1.45
16	c	202	HEC	C2A-C3A	2.52	1.45	1.37
10	A	910	CLA	C1D-ND	2.52	1.40	1.37
11	c	201	LYC	C15-C16	-2.52	1.28	1.34
16	C	301	HEC	CMB-C2B	-2.52	1.45	1.51
9	A	906	BCL	C2A-C1A	-2.51	1.46	1.52
9	a	910	BCL	C3A-C2A	-2.51	1.47	1.54
10	a	912	CLA	CHD-C4C	2.51	1.45	1.39
8	a	903	2GO	O1A-CGA	-2.50	1.15	1.22
13	a	920	85I	C4-C3	-2.50	1.46	1.51
9	a	907	BCL	C3B-CAB	-2.50	1.42	1.49
9	a	908	BCL	C3D-C2D	2.49	1.45	1.39
9	a	911	BCL	CBA-CGA	-2.49	1.43	1.50
8	A	901	2GO	C3B-C2B	-2.48	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	905	BCL	C2C-C3C	-2.48	1.47	1.54
9	a	907	BCL	C1B-CHB	2.48	1.47	1.41
17	E	101	84Q	C6-C5	-2.48	1.37	1.51
9	a	909	BCL	C3A-C4A	-2.47	1.43	1.51
9	a	908	BCL	MG-ND	2.46	2.10	2.05
13	a	918	85I	C4-C3	2.46	1.57	1.51
10	A	911	CLA	C3B-CAB	-2.46	1.42	1.47
9	a	910	BCL	CBB-CAB	-2.46	1.42	1.49
17	E	101	84Q	C8-C7	-2.46	1.37	1.51
10	a	913	CLA	C5-C3	-2.45	1.46	1.51
9	A	905	BCL	CMB-C2B	-2.43	1.46	1.51
8	a	903	2GO	C3B-C2B	-2.43	1.35	1.39
9	A	906	BCL	MG-ND	2.42	2.10	2.05
9	A	907	BCL	O1A-CGA	-2.42	1.15	1.22
8	A	901	2GO	O1D-CGD	-2.41	1.16	1.21
10	a	914	CLA	C4D-CHA	2.41	1.47	1.38
9	A	904	BCL	C3A-C2A	-2.41	1.47	1.54
9	a	909	BCL	C2C-C1C	-2.40	1.44	1.51
9	A	903	BCL	C1B-CHB	2.40	1.47	1.41
9	A	908	BCL	C3D-C2D	2.40	1.45	1.39
9	a	911	BCL	MG-NA	2.39	2.12	2.06
17	E	101	84Q	C5-C4	-2.39	1.38	1.51
15	g	101	85N	O4-C24	-2.39	1.22	1.30
9	a	906	BCL	CAA-CBA	-2.39	1.45	1.52
9	a	906	BCL	C3D-C2D	2.38	1.45	1.39
10	a	901	CLA	CMC-C2C	-2.38	1.45	1.50
10	A	933	CLA	C2A-C1A	-2.38	1.46	1.52
10	a	913	CLA	C2A-C1A	-2.37	1.46	1.52
11	c	201	LYC	C62-C61	-2.37	1.44	1.50
9	a	911	BCL	C2C-C3C	-2.37	1.47	1.54
9	A	904	BCL	CMA-C3A	-2.36	1.48	1.53
9	a	906	BCL	C3A-C4A	-2.35	1.44	1.51
9	a	911	BCL	O1D-CGD	-2.35	1.15	1.21
10	A	931	CLA	C4C-C3C	-2.35	1.41	1.45
17	E	101	84Q	O-C14	-2.35	1.15	1.22
9	a	905	BCL	C3D-C2D	2.35	1.45	1.39
9	a	904	BCL	CAA-CBA	-2.35	1.45	1.52
9	A	905	BCL	C4B-CHC	2.35	1.47	1.41
8	a	903	2GO	C1A-C2A	2.34	1.50	1.45
11	A	913	LYC	C52-C51	-2.34	1.46	1.50
9	A	908	BCL	C3A-C4A	-2.34	1.44	1.51
10	a	913	CLA	C3A-C2A	-2.34	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	913	CLA	O2A-CGA	2.33	1.40	1.33
9	A	907	BCL	CHD-C1D	2.32	1.42	1.38
9	A	908	BCL	CAC-C3C	-2.32	1.49	1.54
9	a	904	BCL	C2A-C1A	-2.31	1.47	1.52
10	a	914	CLA	C4C-C3C	-2.31	1.41	1.45
16	C	301	HEC	C4D-ND	-2.31	1.31	1.36
10	A	911	CLA	O2A-CGA	2.30	1.40	1.33
10	a	914	CLA	C3D-C2D	2.30	1.45	1.39
9	A	908	BCL	O2D-CED	-2.30	1.39	1.45
13	A	915	85I	O7-C20	-2.30	1.15	1.22
10	A	931	CLA	CBD-CGD	2.30	1.59	1.52
9	A	903	BCL	C4B-CHC	2.28	1.47	1.41
10	A	931	CLA	O2A-C1	-2.28	1.39	1.46
9	a	908	BCL	C4-C3	-2.28	1.44	1.50
10	a	915	CLA	O2A-CGA	2.28	1.40	1.33
10	a	913	CLA	O2A-C1	-2.27	1.39	1.46
9	a	911	BCL	C2A-C1A	-2.27	1.47	1.52
10	a	914	CLA	C3B-CAB	2.26	1.52	1.47
9	a	909	BCL	C4-C3	-2.26	1.44	1.50
9	A	904	BCL	C1B-CHB	2.26	1.47	1.41
9	a	904	BCL	CMA-C3A	-2.25	1.48	1.53
9	a	906	BCL	CBD-CGD	-2.25	1.45	1.52
9	A	904	BCL	C1D-ND	-2.24	1.35	1.37
9	a	907	BCL	C3A-C4A	-2.24	1.44	1.51
9	a	907	BCL	CBA-CGA	-2.24	1.44	1.50
9	A	908	BCL	OBB-CAB	-2.24	1.15	1.22
9	A	904	BCL	CAA-CBA	-2.23	1.45	1.52
9	A	909	BCL	C2A-C1A	-2.23	1.47	1.52
11	A	913	LYC	C18-C17	-2.23	1.46	1.50
9	A	909	BCL	CMD-C2D	-2.22	1.46	1.50
9	A	909	BCL	C9-C8	-2.22	1.45	1.52
10	a	913	CLA	C3C-C2C	2.21	1.41	1.36
11	c	201	LYC	C21-C20	-2.21	1.30	1.36
9	a	908	BCL	O2A-CGA	2.20	1.39	1.33
9	a	909	BCL	CMA-C3A	-2.19	1.48	1.53
10	A	910	CLA	C1C-C2C	-2.19	1.40	1.44
8	a	903	2GO	ZN-NA	2.19	2.14	2.01
9	A	908	BCL	CHD-C1D	2.19	1.42	1.38
9	A	908	BCL	CHD-C4C	2.18	1.45	1.39
11	c	201	LYC	C18-C17	-2.18	1.46	1.50
9	A	908	BCL	CMC-C2C	-2.17	1.48	1.53
10	a	912	CLA	C2A-C1A	-2.17	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	905	BCL	C3A-C2A	-2.17	1.48	1.54
10	a	915	CLA	C3A-C2A	-2.17	1.48	1.54
10	a	901	CLA	C1D-ND	2.17	1.40	1.37
10	A	910	CLA	C3D-C2D	2.17	1.45	1.39
8	A	901	2GO	C1C-NC	-2.17	1.34	1.38
10	a	914	CLA	CBD-CGD	-2.16	1.45	1.52
9	a	909	BCL	CHD-C1D	2.16	1.42	1.38
9	a	906	BCL	C3A-C2A	-2.16	1.48	1.54
10	a	913	CLA	C4B-CHC	2.16	1.47	1.41
9	A	909	BCL	O2D-CED	2.16	1.50	1.45
10	a	915	CLA	C4B-CHC	2.16	1.47	1.41
10	a	912	CLA	C3D-C2D	2.16	1.45	1.39
10	A	910	CLA	C3B-C2B	2.16	1.43	1.40
9	A	908	BCL	CMB-C2B	-2.15	1.47	1.51
9	a	908	BCL	C4B-CHC	2.15	1.47	1.41
9	A	904	BCL	CHD-C1D	2.15	1.42	1.38
9	A	909	BCL	CBA-CGA	-2.14	1.44	1.50
9	A	904	BCL	C4D-CHA	2.14	1.46	1.38
10	A	933	CLA	C1B-NB	-2.14	1.33	1.35
10	a	912	CLA	C4C-C3C	-2.13	1.41	1.45
9	a	907	BCL	CAA-CBA	-2.13	1.46	1.52
10	A	933	CLA	MG-NC	2.13	2.11	2.06
9	A	903	BCL	C2C-C3C	-2.13	1.48	1.54
10	A	912	CLA	CHD-C1D	2.13	1.42	1.38
9	A	906	BCL	O2A-C1	-2.11	1.40	1.46
9	A	905	BCL	C3B-CAB	-2.11	1.43	1.49
10	A	933	CLA	C3D-C2D	2.11	1.44	1.39
9	a	906	BCL	C4B-CHC	2.11	1.46	1.41
10	A	910	CLA	O2D-CGD	2.10	1.38	1.33
11	A	913	LYC	C5-C4	-2.10	1.43	1.50
10	A	911	CLA	C9-C8	2.10	1.59	1.52
9	A	902	BCL	OBD-CAD	-2.10	1.18	1.22
9	a	909	BCL	C2-C3	-2.09	1.28	1.33
10	a	912	CLA	O1A-CGA	-2.09	1.16	1.22
9	A	909	BCL	O2A-CGA	2.09	1.39	1.33
9	A	903	BCL	CAA-CBA	-2.09	1.46	1.52
9	A	909	BCL	CMB-C2B	-2.08	1.47	1.51
9	A	908	BCL	C5-C3	-2.08	1.47	1.51
10	a	914	CLA	CHD-C1D	2.08	1.42	1.38
10	A	911	CLA	CHD-C4C	2.07	1.44	1.39
10	A	933	CLA	C2-C3	-2.07	1.28	1.33
10	a	915	CLA	CHD-C1D	2.07	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	907	BCL	C1-C2	2.06	1.55	1.49
16	c	202	HEC	CAA-CBA	-2.06	1.42	1.52
9	A	909	BCL	C2C-C3C	-2.06	1.48	1.54
9	a	904	BCL	C1B-CHB	2.05	1.46	1.41
9	a	910	BCL	CHD-C4C	2.05	1.45	1.39
9	A	904	BCL	CBA-CGA	-2.05	1.45	1.50
9	a	911	BCL	CAC-C3C	-2.05	1.49	1.54
11	c	201	LYC	C63-C64	-2.05	1.46	1.53
10	A	911	CLA	C2A-C1A	-2.04	1.47	1.52
9	a	911	BCL	CHD-C4C	2.04	1.45	1.39
9	a	908	BCL	C3C-C4C	-2.04	1.49	1.51
9	A	904	BCL	C3D-C2D	2.04	1.44	1.39
10	a	914	CLA	O2D-CED	-2.04	1.40	1.45
10	a	901	CLA	O2A-C1	-2.03	1.40	1.46
9	a	909	BCL	C2A-C1A	-2.03	1.47	1.52
9	A	907	BCL	C6-C7	2.02	1.60	1.52
9	A	907	BCL	C3A-C4A	-2.02	1.45	1.51
9	a	910	BCL	C4D-CHA	2.01	1.45	1.38
9	a	908	BCL	CMC-C2C	-2.01	1.48	1.53
9	a	907	BCL	CMD-C2D	-2.01	1.46	1.50

All (982) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	909	BCL	O2D-CGD-CBD	20.86	148.33	111.27
9	a	908	BCL	C4A-NA-C1A	18.67	115.10	106.71
9	A	906	BCL	O2D-CGD-CBD	18.23	143.67	111.27
10	A	931	CLA	O2D-CGD-CBD	18.08	143.39	111.27
9	a	907	BCL	C4A-NA-C1A	16.53	114.14	106.71
10	a	913	CLA	C1D-ND-C4D	-15.69	95.19	106.33
9	A	906	BCL	O2D-CGD-O1D	-15.51	93.51	123.84
9	a	909	BCL	O2D-CGD-CBD	15.31	138.47	111.27
10	A	912	CLA	C2C-C1C-NC	15.09	124.11	109.97
9	A	905	BCL	O2D-CGD-CBD	14.78	137.52	111.27
11	c	201	LYC	C21-C50-C51	14.71	148.31	127.31
9	A	907	BCL	C4A-NA-C1A	14.57	113.26	106.71
9	A	907	BCL	O2D-CGD-CBD	14.50	137.03	111.27
9	A	903	BCL	O2D-CGD-CBD	14.33	136.73	111.27
10	a	913	CLA	O2D-CGD-CBD	14.11	136.34	111.27
9	a	910	BCL	O2D-CGD-CBD	13.95	136.06	111.27
9	a	904	BCL	O2D-CGD-CBD	13.80	135.79	111.27
9	a	905	BCL	O2D-CGD-CBD	13.71	135.63	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	c	201	LYC	C53-C51-C50	13.56	139.75	118.94
9	A	906	BCL	CHD-C1D-ND	-13.50	112.05	124.45
9	a	910	BCL	C1C-NC-C4C	13.25	112.67	106.71
9	A	906	BCL	C2D-C1D-ND	13.25	119.87	110.10
10	a	913	CLA	O2D-CGD-O1D	-13.14	98.15	123.84
9	a	908	BCL	O2D-CGD-CBD	12.95	134.28	111.27
10	A	910	CLA	O2D-CGD-O1D	-12.76	98.89	123.84
13	A	917	85I	O4-C4-C3	12.74	142.25	109.54
8	A	901	2GO	CMA-C3A-C4A	-12.62	105.83	125.04
9	A	902	BCL	O2D-CGD-CBD	12.47	133.43	111.27
8	a	903	2GO	CMA-C3A-C4A	-12.44	106.09	125.04
9	A	903	BCL	O2D-CGD-O1D	-12.40	99.59	123.84
10	A	910	CLA	O2D-CGD-CBD	11.97	132.54	111.27
10	A	931	CLA	O2D-CGD-O1D	-11.90	100.56	123.84
9	a	911	BCL	C2D-C1D-ND	11.85	118.84	110.10
11	c	201	LYC	C15-C14-C12	11.82	144.19	127.31
9	a	907	BCL	O2D-CGD-CBD	11.81	132.26	111.27
10	A	911	CLA	C1D-ND-C4D	-11.56	98.12	106.33
9	A	909	BCL	O2A-C1-C2	11.47	138.78	108.64
9	a	908	BCL	CBA-CAA-C2A	-11.23	80.73	113.86
8	A	901	2GO	C4A-C3A-C2A	-10.95	95.45	106.96
9	a	907	BCL	C1C-NC-C4C	-10.88	101.81	106.71
9	a	909	BCL	O2D-CGD-O1D	-10.83	102.67	123.84
9	A	909	BCL	O2A-CGA-CBA	10.82	145.86	111.91
8	a	903	2GO	CAD-C3D-C4D	-10.76	102.47	108.47
10	A	933	CLA	O2D-CGD-CBD	10.70	130.28	111.27
10	A	931	CLA	C2D-C1D-ND	-10.69	102.22	110.10
9	a	910	BCL	O2A-CGA-CBA	10.58	145.11	111.91
10	A	933	CLA	O2D-CGD-O1D	-10.54	103.23	123.84
9	a	905	BCL	O2D-CGD-O1D	-10.51	103.29	123.84
11	c	201	LYC	C21-C20-C19	10.48	144.93	123.47
10	a	901	CLA	O2D-CGD-CBD	10.45	129.83	111.27
10	a	915	CLA	O2D-CGD-CBD	10.31	129.58	111.27
11	c	201	LYC	C20-C19-C17	10.30	142.00	127.31
9	A	907	BCL	O2D-CGD-O1D	-10.19	103.91	123.84
13	a	920	85I	O4-C4-C3	10.17	135.66	109.54
15	A	932	85N	C18-O3-C17	10.17	133.50	113.80
9	A	909	BCL	O1D-CGD-CBD	-10.14	103.74	124.48
13	A	917	85I	P-O3-C3	10.14	161.99	120.90
10	A	910	CLA	CED-O2D-CGD	10.13	138.85	115.94
9	A	908	BCL	O2D-CGD-CBD	10.08	129.19	111.27
10	a	914	CLA	O2D-CGD-CBD	10.06	129.14	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	909	BCL	C4A-NA-C1A	9.83	111.12	106.71
9	a	908	BCL	O2D-CGD-O1D	-9.73	104.82	123.84
9	a	910	BCL	O2A-CGA-O1A	-9.72	99.07	123.59
10	A	931	CLA	CED-O2D-CGD	9.66	137.79	115.94
9	A	906	BCL	C4A-NA-C1A	9.66	111.05	106.71
10	A	912	CLA	C3C-C4C-NC	9.59	121.32	110.57
9	A	907	BCL	C6-C5-C3	9.59	138.59	113.45
13	A	916	85I	O4-C4-C3	9.56	134.07	109.54
13	a	918	85I	O4-C4-C3	9.53	134.00	109.54
16	C	301	HEC	C1D-C2D-C3D	-9.51	100.38	107.00
9	a	904	BCL	C4A-NA-C1A	9.50	110.98	106.71
9	a	906	BCL	CMD-C2D-C1D	9.36	141.21	124.71
9	A	905	BCL	O2D-CGD-O1D	-9.34	105.57	123.84
10	A	931	CLA	C1D-ND-C4D	9.32	112.95	106.33
9	A	907	BCL	O2A-CGA-CBA	9.32	141.15	111.91
9	a	905	BCL	CHD-C1D-ND	-9.28	115.93	124.45
9	a	904	BCL	O2D-CGD-O1D	-9.27	105.71	123.84
10	a	914	CLA	C3B-C4B-NB	9.21	121.11	109.21
9	a	909	BCL	CHD-C1D-ND	-9.14	116.05	124.45
9	a	910	BCL	O2A-C1-C2	9.13	132.64	108.64
8	A	901	2GO	CAC-C3C-C2C	-9.13	111.91	127.53
9	A	905	BCL	CHD-C1D-ND	-9.08	116.11	124.45
10	A	911	CLA	C3C-C4C-NC	9.06	120.74	110.57
9	A	906	BCL	C3D-C2D-C1D	-9.03	93.51	105.83
11	c	201	LYC	C13-C12-C14	-9.03	110.27	122.92
9	a	908	BCL	C1-C2-C3	9.02	141.64	126.04
10	A	933	CLA	C4-C3-C5	9.02	126.29	115.98
10	a	912	CLA	O2D-CGD-O1D	-9.00	106.25	123.84
9	a	911	BCL	C3D-C2D-C1D	-8.94	93.63	105.83
9	a	909	BCL	C1-C2-C3	8.90	141.43	126.04
10	a	901	CLA	C3C-C4C-NC	8.89	120.54	110.57
8	A	901	2GO	C1A-NA-C4A	8.84	120.03	106.80
9	A	907	BCL	C3D-C2D-C1D	-8.78	93.85	105.83
9	a	904	BCL	CHD-C1D-ND	-8.75	116.41	124.45
9	A	903	BCL	O2A-CGA-CBA	8.74	139.34	111.91
10	A	911	CLA	C2C-C1C-NC	8.69	118.11	109.97
9	A	906	BCL	C1D-ND-C4D	-8.63	100.20	106.33
9	A	905	BCL	C2D-C1D-ND	8.61	116.45	110.10
9	A	903	BCL	CMD-C2D-C1D	8.56	139.79	124.71
9	a	910	BCL	C1-O2A-CGA	8.53	138.83	116.44
9	A	902	BCL	C1-O2A-CGA	8.50	138.74	116.44
10	a	901	CLA	C1D-ND-C4D	-8.45	100.33	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	915	85I	O6-C3-C4	-8.41	75.45	107.08
16	c	202	HEC	CMC-C2C-C3C	8.40	135.69	125.82
9	A	907	BCL	C1C-NC-C4C	-8.34	102.96	106.71
9	A	907	BCL	C7-C6-C5	8.33	135.99	113.36
9	A	907	BCL	C2D-C1D-ND	8.30	116.22	110.10
9	A	904	BCL	C1C-NC-C4C	-8.28	102.98	106.71
9	A	909	BCL	O2D-CGD-O1D	-8.27	107.67	123.84
9	A	905	BCL	CMD-C2D-C1D	8.24	139.23	124.71
10	A	933	CLA	CED-O2D-CGD	8.23	134.56	115.94
10	a	901	CLA	O2A-CGA-CBA	8.20	137.65	111.91
9	a	905	BCL	O2A-CGA-CBA	8.19	137.62	111.91
9	a	910	BCL	O2D-CGD-O1D	-8.19	107.83	123.84
13	A	915	85I	P-O3-C3	8.16	153.97	120.90
9	A	905	BCL	C3D-C2D-C1D	-8.15	94.71	105.83
9	A	903	BCL	O2A-C1-C2	8.13	130.00	108.64
13	A	915	85I	O4-C4-C3	8.12	130.39	109.54
9	a	909	BCL	O2A-C1-C2	-8.11	87.32	108.64
13	a	919	85I	O3-C3-C4	8.08	137.46	107.08
8	a	903	2GO	C4C-C3C-C2C	-8.08	95.13	106.90
10	A	931	CLA	CMC-C2C-C1C	8.00	137.22	125.04
9	A	907	BCL	CMD-C2D-C1D	7.97	138.76	124.71
9	a	908	BCL	OBB-CAB-CBB	-7.97	102.23	120.17
9	a	911	BCL	O2A-C1-C2	7.96	129.56	108.64
10	a	901	CLA	C6-C7-C8	7.96	141.65	115.92
9	a	909	BCL	CMD-C2D-C1D	7.96	138.74	124.71
9	a	911	BCL	C1-C2-C3	7.94	139.77	126.04
9	A	903	BCL	CHD-C1D-ND	-7.91	117.19	124.45
10	a	913	CLA	CMD-C2D-C1D	7.87	138.59	124.71
10	a	915	CLA	O2D-CGD-O1D	-7.83	108.53	123.84
10	A	931	CLA	C4A-NA-C1A	7.83	110.22	106.71
11	c	201	LYC	C16-C17-C19	7.82	130.94	118.94
9	A	904	BCL	CMD-C2D-C1D	7.82	138.49	124.71
10	a	914	CLA	O2D-CGD-O1D	-7.81	108.56	123.84
16	c	202	HEC	C1D-C2D-C3D	-7.80	101.57	107.00
9	a	909	BCL	O2A-CGA-O1A	-7.74	104.05	123.59
11	c	201	LYC	C52-C51-C50	-7.74	112.08	122.92
9	a	910	BCL	C4A-NA-C1A	-7.72	103.24	106.71
9	a	908	BCL	CHD-C1D-ND	-7.70	117.38	124.45
10	A	910	CLA	C2C-C1C-NC	7.67	117.16	109.97
9	a	911	BCL	C1-O2A-CGA	7.67	136.56	116.44
9	a	905	BCL	CMD-C2D-C1D	7.64	138.18	124.71
13	a	920	85I	O6-C3-C4	7.61	135.72	107.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	911	CLA	C4A-NA-C1A	7.59	110.12	106.71
10	A	933	CLA	C4A-NA-C1A	7.59	110.12	106.71
9	a	906	BCL	CHD-C1D-ND	-7.56	117.50	124.45
9	A	909	BCL	C4A-NA-C1A	-7.51	103.33	106.71
9	a	908	BCL	C3A-C2A-C1A	7.50	112.57	101.34
9	A	907	BCL	C1-O2A-CGA	7.42	135.92	116.44
16	C	301	HEC	C4C-C3C-C2C	7.42	114.36	106.35
8	A	901	2GO	C2A-C1A-NA	-7.42	105.20	109.01
10	a	912	CLA	C1D-ND-C4D	-7.38	101.09	106.33
10	a	901	CLA	C2C-C1C-NC	7.36	116.87	109.97
9	A	905	BCL	C4A-NA-C1A	7.36	110.02	106.71
9	a	905	BCL	C3D-C2D-C1D	-7.36	95.79	105.83
11	c	201	LYC	C15-C16-C17	7.29	146.91	126.42
10	a	901	CLA	C11-C10-C8	-7.27	92.43	115.92
9	A	905	BCL	CBA-CAA-C2A	-7.26	92.43	113.86
8	a	903	2GO	C4C-CHD-C1D	7.22	132.09	122.56
9	A	907	BCL	CED-O2D-CGD	7.21	132.24	115.94
10	A	912	CLA	C1C-C2C-C3C	-7.17	99.42	106.96
9	a	910	BCL	C1-C2-C3	-7.17	113.65	126.04
10	a	913	CLA	C11-C10-C8	-7.16	92.78	115.92
10	a	912	CLA	O2D-CGD-CBD	7.15	123.97	111.27
16	c	202	HEC	O2A-CGA-O1A	-7.15	105.48	123.30
9	a	911	BCL	O2A-CGA-CBA	7.15	134.34	111.91
9	a	908	BCL	C3D-C2D-C1D	-7.14	96.09	105.83
13	a	919	85I	P-O3-C3	7.13	149.82	120.90
10	A	912	CLA	O2D-CGD-O1D	-7.12	109.92	123.84
9	a	907	BCL	C1-C2-C3	-7.12	113.74	126.04
9	A	907	BCL	C1-C2-C3	7.08	138.29	126.04
10	a	912	CLA	CMD-C2D-C1D	7.07	137.18	124.71
10	A	912	CLA	C1D-ND-C4D	-7.04	101.33	106.33
9	a	906	BCL	C3D-C2D-C1D	-7.01	96.27	105.83
9	A	909	BCL	C3D-C2D-C1D	-7.00	96.28	105.83
10	A	911	CLA	CMD-C2D-C1D	6.99	137.03	124.71
9	A	908	BCL	CHD-C1D-ND	-6.99	118.03	124.45
10	A	931	CLA	C1-O2A-CGA	6.97	134.72	116.44
17	E	101	84Q	O1-C15-C16	6.93	127.33	109.54
10	a	914	CLA	C3C-C4C-NC	6.89	118.30	110.57
9	A	903	BCL	C1-O2A-CGA	6.87	134.47	116.44
10	a	913	CLA	C3D-C2D-C1D	-6.86	96.47	105.83
8	A	901	2GO	C1C-NC-C4C	6.85	115.77	106.49
10	A	911	CLA	CHD-C4C-C3C	-6.84	114.78	124.84
10	a	901	CLA	CMD-C2D-C1D	6.84	136.77	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	903	BCL	O1A-CGA-CBA	-6.84	97.06	123.73
9	A	905	BCL	C3A-C2A-C1A	6.77	111.48	101.34
9	A	902	BCL	O2D-CGD-O1D	-6.77	110.61	123.84
10	A	931	CLA	CHD-C4C-C3C	-6.76	114.90	124.84
9	a	908	BCL	OBb-CAB-C3B	6.75	131.98	119.99
11	c	201	LYC	C18-C17-C16	-6.75	107.44	118.08
9	a	911	BCL	CED-O2D-CGD	6.74	131.18	115.94
9	a	904	BCL	O2A-CGA-CBA	6.73	133.03	111.91
9	a	911	BCL	CHD-C1D-ND	-6.73	118.27	124.45
10	a	915	CLA	C4-C3-C5	6.68	123.62	115.98
9	a	908	BCL	CMD-C2D-C1D	6.64	136.41	124.71
9	A	904	BCL	C3D-C2D-C1D	-6.64	96.77	105.83
10	A	912	CLA	O2D-CGD-CBD	6.54	122.90	111.27
8	a	903	2GO	CHA-CBD-CAD	-6.54	100.69	107.17
10	A	911	CLA	C3D-C2D-C1D	-6.54	96.90	105.83
8	a	903	2GO	CAC-C3C-C4C	-6.51	116.37	124.81
8	a	903	2GO	C1A-NA-C4A	6.49	116.52	106.80
10	A	912	CLA	CAC-C3C-C4C	6.47	133.21	124.81
9	a	907	BCL	O2D-CGD-O1D	-6.47	111.19	123.84
10	a	914	CLA	CHD-C4C-C3C	-6.46	115.34	124.84
9	a	911	BCL	CMD-C2D-C1D	6.46	136.09	124.71
9	a	907	BCL	CBA-CAA-C2A	-6.45	94.82	113.86
9	A	907	BCL	CHD-C1D-ND	-6.44	118.54	124.45
9	a	904	BCL	CED-O2D-CGD	6.43	130.48	115.94
9	A	905	BCL	C1D-ND-C4D	-6.43	101.77	106.33
9	A	909	BCL	C4-C3-C5	-6.42	104.46	115.27
10	A	910	CLA	CMD-C2D-C1D	6.42	136.03	124.71
10	a	912	CLA	C2C-C1C-NC	6.42	115.98	109.97
9	A	902	BCL	C4A-NA-C1A	6.41	109.59	106.71
11	A	913	LYC	C18-C17-C19	-6.41	113.95	122.92
9	A	903	BCL	C4A-NA-C1A	6.40	109.58	106.71
8	a	903	2GO	C1A-C2A-C3A	-6.39	98.18	106.61
9	a	905	BCL	C4A-NA-C1A	6.39	109.58	106.71
9	A	906	BCL	OBb-CAB-C3B	6.37	131.29	119.99
11	c	201	LYC	C11-C12-C14	6.36	128.71	118.94
9	a	905	BCL	CHD-C4C-NC	6.33	132.11	125.08
10	a	915	CLA	C4A-NA-C1A	-6.32	103.87	106.71
10	A	912	CLA	CMA-C3A-C4A	6.31	128.73	111.77
8	A	901	2GO	CMC-C2C-C1C	-6.30	115.45	125.04
11	c	201	LYC	C52-C51-C53	-6.29	108.16	118.08
11	c	201	LYC	C20-C21-C50	-6.29	110.60	123.47
10	A	931	CLA	C2C-C1C-NC	6.29	115.86	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	912	CLA	O2A-CGA-CBA	6.26	131.54	111.91
9	A	902	BCL	CHD-C1D-ND	-6.25	118.71	124.45
10	A	910	CLA	C1D-ND-C4D	-6.25	101.90	106.33
9	a	905	BCL	C4-C3-C2	-6.25	107.66	123.68
10	A	933	CLA	C3D-C2D-C1D	-6.24	97.32	105.83
10	a	915	CLA	CMD-C2D-C1D	6.23	135.70	124.71
9	A	905	BCL	CAA-C2A-C3A	-6.23	95.72	112.78
9	A	907	BCL	O1A-CGA-CBA	-6.22	99.46	123.73
10	a	913	CLA	CAC-C3C-C4C	6.22	132.88	124.81
9	a	911	BCL	O2D-CGD-CBD	6.17	122.24	111.27
9	a	911	BCL	C1C-NC-C4C	6.17	109.48	106.71
10	a	915	CLA	C3C-C4C-NC	6.15	117.47	110.57
9	a	904	BCL	CHD-C4C-NC	6.15	131.90	125.08
16	c	202	HEC	C4C-C3C-C2C	6.14	112.98	106.35
9	a	907	BCL	C16-C15-C13	-6.13	96.12	115.92
10	a	901	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
10	A	911	CLA	C4C-C3C-C2C	-6.10	98.01	106.90
9	a	910	BCL	CMD-C2D-C1D	6.09	135.45	124.71
8	a	903	2GO	CMC-C2C-C1C	-6.05	115.82	125.04
10	A	910	CLA	C3C-C4C-NC	6.05	117.35	110.57
9	a	904	BCL	CMD-C2D-C1D	6.03	135.34	124.71
8	a	903	2GO	C16-C15-C13	6.03	135.41	115.92
9	A	902	BCL	CMD-C2D-C1D	5.97	135.23	124.71
9	a	907	BCL	CMD-C2D-C1D	5.96	135.22	124.71
10	a	901	CLA	O2D-CGD-O1D	-5.96	112.19	123.84
16	c	202	HEC	CMB-C2B-C3B	5.92	132.78	125.82
10	A	933	CLA	CMB-C2B-C1B	5.90	137.53	128.46
9	a	909	BCL	C4-C3-C2	-5.89	108.56	123.68
9	A	907	BCL	C4-C3-C2	-5.89	108.57	123.68
8	A	901	2GO	CAC-C3C-C4C	-5.89	117.17	124.81
10	a	901	CLA	CHD-C1D-ND	-5.89	119.04	124.45
9	a	908	BCL	C2A-C3A-C4A	-5.88	92.37	101.87
9	A	909	BCL	C1C-NC-C4C	5.86	109.34	106.71
9	A	909	BCL	CMD-C2D-C1D	5.85	135.02	124.71
9	A	906	BCL	CED-O2D-CGD	5.85	129.16	115.94
9	A	906	BCL	O2A-CGA-O1A	-5.84	108.85	123.59
10	A	933	CLA	O2A-C1-C2	-5.82	93.34	108.64
9	a	909	BCL	C1-O2A-CGA	5.81	131.68	116.44
11	A	913	LYC	C57-C56-C55	5.79	131.03	122.92
10	a	915	CLA	O2A-CGA-O1A	-5.78	109.00	123.59
9	a	910	BCL	CED-O2D-CGD	5.78	129.01	115.94
9	a	906	BCL	CAC-C3C-C4C	-5.78	99.76	112.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	931	CLA	O2A-CGA-CBA	5.78	130.03	111.91
9	a	904	BCL	C3C-C4C-CHD	-5.77	111.06	123.39
9	a	908	BCL	C5-C3-C2	5.76	132.77	121.12
9	A	909	BCL	O2A-CGA-O1A	-5.72	109.16	123.59
10	a	912	CLA	CED-O2D-CGD	5.72	128.87	115.94
10	a	912	CLA	C3B-C4B-NB	5.71	116.60	109.21
9	a	905	BCL	CED-O2D-CGD	5.70	128.82	115.94
9	A	904	BCL	CHD-C1D-ND	-5.68	119.23	124.45
10	a	912	CLA	C3C-C4C-NC	5.67	116.93	110.57
10	A	933	CLA	C3B-C4B-NB	5.67	116.53	109.21
10	a	915	CLA	C3D-C2D-C1D	-5.66	98.10	105.83
10	A	933	CLA	C2C-C1C-NC	5.65	115.27	109.97
16	C	301	HEC	CMC-C2C-C3C	5.61	132.41	125.82
9	a	909	BCL	C3D-C2D-C1D	-5.59	98.20	105.83
9	a	908	BCL	C2D-C1D-ND	5.58	114.21	110.10
11	c	201	LYC	C1-C2-C4	-5.58	106.53	122.65
9	A	902	BCL	C3C-C4C-CHD	-5.56	111.51	123.39
10	a	901	CLA	C4C-C3C-C2C	-5.55	98.81	106.90
10	a	914	CLA	C2C-C1C-NC	5.55	115.17	109.97
9	A	902	BCL	CHD-C4C-NC	5.53	131.22	125.08
10	A	912	CLA	C4A-NA-C1A	5.53	109.19	106.71
9	A	904	BCL	C4A-NA-C1A	5.52	109.19	106.71
10	a	914	CLA	CED-O2D-CGD	5.52	128.42	115.94
9	a	906	BCL	C1C-NC-C4C	-5.51	104.23	106.71
10	a	915	CLA	CMC-C2C-C1C	5.51	133.43	125.04
10	a	914	CLA	CHD-C1D-ND	-5.50	119.40	124.45
9	A	909	BCL	C9-C8-C10	-5.49	91.41	111.29
9	A	905	BCL	CAA-C2A-C1A	-5.46	94.08	111.97
9	A	905	BCL	C1C-NC-C4C	5.45	109.15	106.71
9	a	905	BCL	C1-C2-C3	5.44	135.46	126.04
10	A	910	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
9	a	904	BCL	C1-C2-C3	-5.41	116.68	126.04
13	a	920	85I	P-O3-C3	-5.41	98.98	120.90
10	a	913	CLA	C2D-C1D-ND	5.39	114.08	110.10
10	A	911	CLA	O2D-CGD-O1D	-5.37	113.34	123.84
17	E	101	84Q	P-O4-C16	5.35	142.59	120.90
9	a	908	BCL	CAA-C2A-C1A	-5.33	94.50	111.97
11	c	201	LYC	C3-C2-C4	5.32	138.03	122.65
10	a	914	CLA	CBA-CAA-C2A	-5.31	98.19	113.86
9	a	909	BCL	CED-O2D-CGD	5.30	127.92	115.94
9	a	906	BCL	C3C-C4C-CHD	-5.28	112.12	123.39
16	c	202	HEC	O2A-CGA-CBA	5.26	130.95	114.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	908	BCL	CED-O2D-CGD	5.25	127.82	115.94
13	A	916	85I	P-O3-C3	5.24	142.14	120.90
9	a	904	BCL	C3D-C2D-C1D	-5.23	98.69	105.83
9	A	904	BCL	C3C-C4C-CHD	-5.23	112.23	123.39
9	a	910	BCL	C5-C3-C2	5.22	131.68	121.12
10	a	913	CLA	C3C-C4C-NC	5.21	116.42	110.57
9	A	906	BCL	C1-O2A-CGA	5.21	130.12	116.44
11	c	201	LYC	C8-C7-C9	-5.19	109.19	122.59
9	A	903	BCL	CBA-CAA-C2A	5.19	129.19	113.86
10	A	911	CLA	O2A-CGA-CBA	5.19	128.19	111.91
9	a	905	BCL	C5-C3-C2	5.19	131.61	121.12
10	a	915	CLA	O2A-CGA-CBA	5.17	128.14	111.91
9	A	908	BCL	C3D-C2D-C1D	-5.17	98.77	105.83
9	a	909	BCL	C5-C3-C2	5.14	131.52	121.12
9	A	905	BCL	CMA-C3A-C4A	5.14	125.59	111.77
10	a	901	CLA	C3D-C4D-ND	5.13	118.53	110.24
9	A	903	BCL	C3C-C4C-CHD	-5.12	112.45	123.39
9	a	907	BCL	CHD-C1D-ND	-5.11	119.76	124.45
9	a	909	BCL	O2A-CGA-CBA	5.11	127.93	111.91
9	a	906	BCL	O2D-CGD-O1D	-5.11	113.86	123.84
8	A	901	2GO	C1-O2A-CGA	5.09	129.81	116.44
9	A	908	BCL	CAA-C2A-C3A	-5.08	98.86	112.78
9	A	906	BCL	CMD-C2D-C1D	5.07	133.65	124.71
9	A	902	BCL	O2A-CGA-CBA	5.05	127.75	111.91
9	a	905	BCL	C3C-C4C-CHD	-5.05	112.61	123.39
9	a	906	BCL	C4A-NA-C1A	5.04	108.97	106.71
9	a	907	BCL	C1D-ND-C4D	5.02	109.90	106.33
10	A	911	CLA	CAC-C3C-C4C	5.00	131.30	124.81
11	A	913	LYC	C13-C12-C11	4.99	125.94	118.08
11	c	201	LYC	C14-C15-C16	-4.99	107.65	123.22
10	A	931	CLA	CHD-C4C-NC	4.97	132.04	124.20
8	a	903	2GO	CAA-C2A-C3A	-4.97	118.62	127.88
9	A	903	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
10	A	910	CLA	CHD-C1D-ND	-4.96	119.90	124.45
9	a	911	BCL	C4A-NA-C1A	4.91	108.91	106.71
9	A	902	BCL	CED-O2D-CGD	4.89	127.00	115.94
10	A	931	CLA	C1C-C2C-C3C	-4.89	101.82	106.96
8	A	901	2GO	CHC-C1C-NC	4.88	130.87	124.68
17	a	921	84Q	O1-C15-C16	4.87	122.05	109.54
10	a	913	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
11	c	201	LYC	C5-C4-C2	4.85	144.34	127.75
10	a	913	CLA	O2A-CGA-CBA	4.85	127.14	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	915	CLA	CAC-C3C-C4C	4.85	131.10	124.81
8	A	901	2GO	C4C-CHD-C1D	4.84	128.95	122.56
9	a	908	BCL	CAA-C2A-C3A	-4.83	99.54	112.78
10	A	933	CLA	CAC-C3C-C4C	4.83	131.08	124.81
9	A	904	BCL	O2D-CGD-CBD	4.83	119.85	111.27
10	a	915	CLA	C3B-C4B-NB	4.82	115.45	109.21
9	A	909	BCL	O1A-CGA-CBA	-4.82	104.94	123.73
9	A	904	BCL	CED-O2D-CGD	4.81	126.81	115.94
9	a	904	BCL	C1-O2A-CGA	4.81	129.06	116.44
9	A	903	BCL	OBB-CAB-CBB	-4.81	109.36	120.17
10	A	933	CLA	CMC-C2C-C1C	4.80	132.36	125.04
10	a	914	CLA	C4C-C3C-C2C	-4.80	99.90	106.90
10	a	901	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
11	c	201	LYC	C57-C56-C55	-4.77	116.25	122.92
16	c	202	HEC	O2D-CGD-O1D	-4.75	111.45	123.30
9	a	907	BCL	O2A-CGA-CBA	4.75	126.82	111.91
10	A	912	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
15	A	932	85N	O3-C17-O6	4.75	124.05	110.72
17	E	101	84Q	O4-C16-C15	4.75	124.94	107.08
16	C	301	HEC	C3C-C4C-NC	-4.75	101.98	110.94
11	c	201	LYC	C10-C11-C12	4.74	139.73	126.42
9	a	905	BCL	OBB-CAB-CBB	-4.73	109.52	120.17
9	A	908	BCL	C2D-C1D-ND	4.73	113.59	110.10
10	a	913	CLA	C3D-C4D-ND	4.73	117.89	110.24
9	A	905	BCL	C3C-C4C-CHD	-4.73	113.29	123.39
9	a	911	BCL	OBB-CAB-C3B	-4.72	111.61	119.99
10	a	913	CLA	CHD-C1D-ND	-4.72	120.11	124.45
10	A	910	CLA	C9-C8-C7	4.72	128.37	111.29
9	A	908	BCL	CMD-C2D-C1D	4.70	133.00	124.71
9	A	909	BCL	CHD-C1D-ND	-4.70	120.13	124.45
10	A	910	CLA	C1-O2A-CGA	4.69	128.75	116.44
10	A	933	CLA	C1-O2A-CGA	4.69	128.75	116.44
9	A	904	BCL	CBC-CAC-C3C	4.69	123.90	113.47
8	a	903	2GO	C3A-C4A-NA	-4.68	102.97	109.07
10	a	913	CLA	C1-O2A-CGA	4.67	128.71	116.44
9	A	902	BCL	CBC-CAC-C3C	4.66	123.84	113.47
10	A	912	CLA	CMD-C2D-C1D	4.64	132.89	124.71
9	a	904	BCL	C1D-ND-C4D	-4.64	103.04	106.33
9	a	907	BCL	CED-O2D-CGD	4.63	126.41	115.94
9	a	908	BCL	CHD-C4C-NC	4.63	130.22	125.08
9	A	908	BCL	C1-C2-C3	-4.62	118.06	126.04
17	a	921	84Q	O4-C16-C15	4.61	124.44	107.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	301	HEC	O2A-CGA-O1A	-4.60	111.84	123.30
10	A	912	CLA	CED-O2D-CGD	4.60	126.33	115.94
9	A	907	BCL	C4-C3-C5	4.58	122.97	115.27
9	A	908	BCL	O2A-CGA-CBA	4.58	126.27	111.91
10	a	912	CLA	C1C-C2C-C3C	-4.57	102.16	106.96
9	A	909	BCL	C1-O2A-CGA	4.55	128.39	116.44
9	A	908	BCL	CMB-C2B-C3B	4.55	133.19	124.68
10	a	912	CLA	O2A-CGA-O1A	-4.55	112.11	123.59
11	A	913	LYC	C8-C7-C6	4.55	122.92	115.27
9	A	909	BCL	OBb-CAB-C3B	-4.53	111.95	119.99
9	A	905	BCL	CED-O2D-CGD	4.53	126.19	115.94
10	A	931	CLA	O1D-CGD-CBD	-4.53	115.21	124.48
9	a	905	BCL	O1A-CGA-CBA	-4.53	106.06	123.73
10	A	933	CLA	O2A-CGA-O1A	-4.52	112.19	123.59
9	A	902	BCL	CAA-CBA-CGA	-4.51	100.07	113.25
9	A	908	BCL	O1D-CGD-CBD	-4.50	115.28	124.48
10	A	911	CLA	O2A-CGA-O1A	-4.49	112.25	123.59
13	a	918	85I	P-O3-C3	4.49	139.10	120.90
8	a	903	2GO	C4A-C3A-C2A	-4.48	102.24	106.96
8	a	903	2GO	CHB-C4A-NA	4.48	130.36	124.68
9	A	904	BCL	CAC-C3C-C2C	4.46	125.40	114.26
10	A	931	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
10	A	931	CLA	C3D-C4D-ND	-4.44	103.06	110.24
10	a	915	CLA	CED-O2D-CGD	4.43	125.97	115.94
9	A	903	BCL	C1-C2-C3	4.43	133.70	126.04
8	A	901	2GO	CHB-C4A-NA	4.43	130.29	124.68
9	a	906	BCL	CAA-C2A-C1A	-4.41	97.51	111.97
10	A	910	CLA	CMC-C2C-C1C	4.41	131.76	125.04
9	a	909	BCL	C2D-C1D-ND	4.41	113.36	110.10
10	A	933	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
11	A	913	LYC	C13-C12-C14	-4.40	116.76	122.92
10	a	913	CLA	C2A-C1A-CHA	-4.39	116.19	123.86
9	a	906	BCL	OBb-CAB-CBB	-4.39	110.30	120.17
10	A	912	CLA	C3D-C4D-ND	4.37	117.31	110.24
8	A	901	2GO	C1A-C2A-C3A	-4.37	100.85	106.61
10	a	913	CLA	C4C-C3C-C2C	-4.36	100.54	106.90
10	a	912	CLA	C3D-C4D-ND	4.36	117.30	110.24
9	A	909	BCL	CAA-C2A-C1A	4.36	126.27	111.97
9	a	911	BCL	CMB-C2B-C3B	4.36	132.84	124.68
10	a	914	CLA	O2A-CGA-CBA	4.36	129.47	112.23
8	A	901	2GO	CMC-C2C-C3C	-4.35	114.30	126.12
10	A	931	CLA	C4D-C3D-CAD	-4.35	102.97	108.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	908	BCL	CMB-C2B-C3B	4.34	132.79	124.68
9	A	903	BCL	CBB-CAB-C3B	4.30	133.12	120.34
9	a	910	BCL	OBb-CAB-CBB	-4.30	110.49	120.17
9	A	908	BCL	O2D-CGD-O1D	-4.29	115.46	123.84
10	A	910	CLA	O2A-CGA-O1A	-4.28	112.80	123.59
9	a	904	BCL	O1A-CGA-CBA	-4.28	107.05	123.73
9	A	907	BCL	O2A-C1-C2	4.27	119.85	108.64
10	a	915	CLA	C4C-C3C-C2C	-4.26	100.68	106.90
10	A	931	CLA	C4D-CHA-C1A	-4.25	116.08	121.25
10	A	912	CLA	C4C-C3C-C2C	-4.25	100.70	106.90
10	A	911	CLA	O2D-CGD-CBD	4.24	118.80	111.27
9	A	902	BCL	O1D-CGD-CBD	-4.22	115.85	124.48
9	a	910	BCL	C2A-C1A-CHA	-4.22	116.49	123.86
10	a	914	CLA	CMC-C2C-C1C	4.21	131.45	125.04
10	A	910	CLA	CBA-CAA-C2A	4.21	126.29	113.86
10	a	915	CLA	CMB-C2B-C1B	4.20	134.91	128.46
9	a	910	BCL	CHD-C4C-NC	4.20	129.74	125.08
10	A	933	CLA	CHD-C1D-ND	-4.19	120.61	124.45
10	A	911	CLA	CHC-C1C-NC	-4.16	117.89	124.20
9	A	907	BCL	OBb-CAB-C3B	4.16	127.37	119.99
9	A	903	BCL	CED-O2D-CGD	4.14	125.31	115.94
10	A	910	CLA	C4A-NA-C1A	4.14	108.57	106.71
10	a	901	CLA	C9-C8-C7	4.13	126.26	111.29
10	a	913	CLA	C4-C3-C5	4.13	122.22	115.27
10	A	931	CLA	C4-C3-C5	4.13	122.22	115.27
9	A	908	BCL	C3C-C4C-CHD	-4.13	114.57	123.39
10	a	912	CLA	C6-C7-C8	-4.13	102.58	115.92
10	A	912	CLA	CMC-C2C-C1C	4.12	131.31	125.04
10	A	910	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
11	c	201	LYC	C9-C10-C11	4.11	136.06	123.22
10	a	914	CLA	CMB-C2B-C3B	4.10	132.36	124.68
10	a	915	CLA	CHB-C4A-NA	4.10	130.18	124.51
10	a	901	CLA	O2A-CGA-O1A	-4.10	113.25	123.59
8	A	901	2GO	CAA-C2A-C3A	-4.09	120.25	127.88
9	a	905	BCL	CMB-C2B-C1B	4.09	134.76	128.46
9	a	910	BCL	O1D-CGD-CBD	-4.09	116.11	124.48
10	a	913	CLA	CMC-C2C-C1C	4.09	131.26	125.04
10	a	913	CLA	CED-O2D-CGD	4.08	125.17	115.94
10	a	912	CLA	C4-C3-C2	-4.08	113.22	123.68
9	A	903	BCL	CHD-C4C-NC	4.06	129.59	125.08
9	a	907	BCL	CMC-C2C-C1C	4.06	122.67	111.77
9	a	904	BCL	CMC-C2C-C1C	4.05	122.66	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	911	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
13	A	915	85I	O3-P-O1	4.04	124.61	109.47
9	a	907	BCL	C3C-C4C-CHD	-4.03	114.79	123.39
11	c	201	LYC	C57-C56-C58	4.03	124.42	118.08
10	A	912	CLA	CHC-C1C-C2C	-4.03	115.58	126.72
9	A	905	BCL	CHD-C4C-NC	4.02	129.54	125.08
9	A	906	BCL	O2A-CGA-CBA	4.01	124.48	111.91
9	a	907	BCL	O1D-CGD-CBD	-4.01	116.29	124.48
16	c	202	HEC	CBA-CAA-C2A	-4.00	105.86	112.60
9	a	906	BCL	CED-O2D-CGD	4.00	124.99	115.94
13	A	916	85I	O2-P-O	-4.00	89.18	107.75
10	a	912	CLA	CMB-C2B-C1B	3.99	134.60	128.46
9	A	905	BCL	C1-O2A-CGA	3.98	126.89	116.44
9	A	905	BCL	O2A-C1-C2	3.98	119.09	108.64
9	a	907	BCL	C4-C3-C5	3.98	121.97	115.27
10	a	912	CLA	CAC-C3C-C4C	3.96	129.95	124.81
9	A	902	BCL	C9-C8-C10	-3.96	96.96	111.29
9	A	902	BCL	O2A-C1-C2	3.96	119.03	108.64
10	a	914	CLA	CAC-C3C-C4C	3.95	129.94	124.81
9	a	911	BCL	C1D-ND-C4D	-3.95	103.53	106.33
10	A	911	CLA	CHD-C1D-ND	-3.95	120.83	124.45
9	A	906	BCL	C1-C2-C3	-3.94	119.23	126.04
9	A	904	BCL	CMB-C2B-C1B	3.93	134.50	128.46
9	a	909	BCL	C6-C5-C3	-3.93	103.16	113.45
17	E	101	84Q	O2-C16-C15	-3.92	92.35	107.08
9	a	908	BCL	C3C-C4C-CHD	-3.91	115.03	123.39
15	A	932	85N	O3-C17-C16	3.91	122.01	107.06
10	A	912	CLA	CAA-CBA-CGA	3.90	124.65	113.25
9	A	909	BCL	CMB-C2B-C3B	3.90	131.97	124.68
9	a	909	BCL	CMB-C2B-C3B	3.89	131.96	124.68
9	A	905	BCL	O1D-CGD-CBD	-3.88	116.54	124.48
9	A	908	BCL	CAA-CBA-CGA	-3.87	101.95	113.25
10	a	912	CLA	C12-C11-C10	-3.85	95.53	113.24
10	A	910	CLA	CBC-CAC-C3C	-3.85	101.81	112.43
9	a	910	BCL	C4D-C3D-CAD	3.85	112.63	108.10
10	A	931	CLA	CMB-C2B-C3B	3.84	131.87	124.68
9	A	908	BCL	CHD-C4C-NC	3.84	129.34	125.08
8	A	901	2GO	C3D-C4D-ND	-3.84	104.60	116.21
10	a	912	CLA	C1-C2-C3	-3.83	119.41	126.04
10	a	901	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
9	A	907	BCL	C3C-C4C-CHD	-3.83	115.22	123.39
9	a	907	BCL	C1-O2A-CGA	3.82	126.47	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	915	CLA	C2D-C1D-ND	-3.82	107.29	110.10
10	a	912	CLA	CHD-C1D-ND	-3.82	120.95	124.45
9	a	910	BCL	CAA-C2A-C1A	3.81	124.46	111.97
10	a	913	CLA	C4D-CHA-C1A	-3.81	116.61	121.25
11	c	201	LYC	C6-C7-C9	3.79	133.46	121.98
10	a	901	CLA	O1A-CGA-CBA	-3.79	108.94	123.73
9	a	911	BCL	O1A-CGA-CBA	-3.78	109.00	123.73
9	A	904	BCL	O1A-CGA-CBA	-3.78	110.95	123.08
16	C	301	HEC	O2A-CGA-CBA	3.78	126.16	114.03
10	a	914	CLA	C1D-ND-C4D	-3.77	103.65	106.33
9	A	902	BCL	C11-C12-C13	3.77	128.10	115.92
10	A	933	CLA	C1D-ND-C4D	-3.76	103.66	106.33
9	a	907	BCL	CHB-C4A-NA	3.76	129.71	124.51
9	A	902	BCL	C14-C13-C12	3.75	124.89	111.29
10	a	912	CLA	C3D-C2D-C1D	-3.75	100.72	105.83
9	A	908	BCL	CAC-C3C-C4C	-3.74	104.28	112.58
9	a	904	BCL	C3D-C4D-ND	3.71	116.25	110.24
9	a	906	BCL	CAA-CBA-CGA	-3.71	102.67	112.51
10	a	913	CLA	O2A-CGA-O1A	-3.71	114.24	123.59
10	a	915	CLA	C1-O2A-CGA	3.70	126.16	116.44
9	A	902	BCL	C3D-C2D-C1D	-3.70	100.78	105.83
9	a	904	BCL	C2D-C1D-ND	3.70	112.83	110.10
9	A	904	BCL	O2A-CGA-CBA	3.70	125.92	114.03
9	A	907	BCL	CAA-CBA-CGA	3.70	124.07	113.25
9	a	907	BCL	CMB-C2B-C3B	3.69	131.59	124.68
9	A	907	BCL	C9-C8-C10	-3.69	97.93	111.29
10	A	911	CLA	CED-O2D-CGD	3.69	124.27	115.94
9	a	905	BCL	O2A-C1-C2	3.68	118.31	108.64
10	a	901	CLA	CAC-C3C-C2C	3.67	133.81	127.53
9	A	902	BCL	C2A-C1A-CHA	-3.67	117.44	123.86
9	a	907	BCL	C3D-C2D-C1D	-3.67	100.83	105.83
8	A	901	2GO	C2C-C1C-NC	-3.67	104.30	109.07
13	a	918	85I	O3-C3-C4	3.66	120.84	107.08
9	a	908	BCL	C16-C17-C18	-3.66	98.75	115.98
10	A	911	CLA	C6-C7-C8	3.66	127.74	115.92
9	a	904	BCL	CMB-C2B-C3B	3.65	131.51	124.68
10	a	914	CLA	C3D-C4D-ND	3.64	116.13	110.24
10	a	913	CLA	C9-C8-C7	3.64	124.47	111.29
10	A	911	CLA	C1-O2A-CGA	3.63	125.98	116.44
9	A	903	BCL	C3A-C2A-C1A	3.62	106.77	101.34
10	A	910	CLA	C11-C10-C8	3.61	127.59	115.92
9	A	902	BCL	CMA-C3A-C2A	-3.61	99.27	113.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	903	BCL	C6-C7-C8	3.61	127.58	115.92
10	A	911	CLA	C2A-C1A-CHA	-3.61	117.55	123.86
9	A	907	BCL	C5-C3-C2	3.61	128.41	121.12
8	A	901	2GO	OBb-CAB-CBB	-3.61	112.05	120.17
10	a	912	CLA	CHD-C4C-C3C	-3.61	119.54	124.84
10	A	933	CLA	C1-C2-C3	-3.60	119.81	126.04
9	a	909	BCL	C3C-C4C-CHD	-3.60	115.70	123.39
10	A	933	CLA	C3C-C4C-NC	3.60	114.61	110.57
10	A	933	CLA	CHB-C4A-NA	3.58	129.47	124.51
9	a	906	BCL	C2D-C1D-ND	3.58	112.75	110.10
9	A	902	BCL	C3A-C2A-C1A	3.57	106.68	101.34
9	a	905	BCL	CHB-C4A-NA	3.56	129.43	124.51
10	A	910	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
9	a	905	BCL	CBC-CAC-C3C	-3.55	105.57	113.47
9	a	909	BCL	OBb-CAB-C3B	3.54	126.28	119.99
9	A	903	BCL	C6-C5-C3	3.54	122.75	113.45
9	a	911	BCL	C3C-C4C-CHD	-3.53	115.84	123.39
10	a	901	CLA	CED-O2D-CGD	3.52	123.91	115.94
9	A	907	BCL	C9-C8-C7	3.51	124.02	111.29
8	a	903	2GO	O2D-CGD-CBD	3.50	118.15	111.80
10	A	933	CLA	C6-C5-C3	-3.49	96.56	113.58
10	A	912	CLA	C2A-C1A-CHA	-3.48	117.78	123.86
10	A	933	CLA	CBA-CAA-C2A	-3.47	103.61	113.86
10	a	912	CLA	C4-C3-C5	3.47	121.11	115.27
9	A	903	BCL	C1D-ND-C4D	-3.47	103.87	106.33
9	a	906	BCL	OBd-CAD-C3D	-3.46	120.19	128.52
9	A	909	BCL	C4D-C3D-CAD	3.46	112.17	108.10
10	A	910	CLA	O2A-CGA-CBA	3.46	122.75	111.91
10	a	912	CLA	C9-C8-C10	-3.46	98.78	111.29
9	A	905	BCL	CMB-C2B-C3B	3.44	131.12	124.68
9	A	909	BCL	CED-O2D-CGD	3.44	123.71	115.94
10	a	901	CLA	C4-C3-C5	3.43	121.05	115.27
9	A	903	BCL	C2D-C1D-ND	3.42	112.62	110.10
11	A	913	LYC	C64-C65-C66	-3.41	116.08	127.75
9	A	905	BCL	C2A-C3A-C4A	-3.41	96.36	101.87
10	a	912	CLA	C4A-NA-C1A	-3.41	105.17	106.71
16	C	301	HEC	CMA-C3A-C2A	3.39	131.34	124.94
9	a	905	BCL	OBb-CAB-C3B	3.39	126.02	119.99
9	a	910	BCL	C16-C15-C13	3.39	126.88	115.92
10	A	910	CLA	CAC-C3C-C4C	3.38	129.20	124.81
10	A	931	CLA	CHA-C4D-ND	3.38	139.56	132.50
9	a	909	BCL	C1C-NC-C4C	-3.37	105.19	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	907	BCL	C6-C7-C8	-3.36	105.05	115.92
16	C	301	HEC	CMD-C2D-C3D	3.36	131.28	124.94
11	A	913	LYC	C20-C21-C50	3.36	130.36	123.47
9	A	905	BCL	C3D-C4D-ND	3.36	115.67	110.24
9	A	909	BCL	CMA-C3A-C4A	3.36	120.80	111.77
10	A	931	CLA	O1A-CGA-CBA	-3.35	110.64	123.73
10	a	914	CLA	CHB-C4A-NA	3.35	129.15	124.51
9	A	903	BCL	CAC-C3C-C2C	3.35	122.62	114.26
9	A	902	BCL	CAC-C3C-C4C	-3.35	105.16	112.58
9	a	911	BCL	CHD-C4C-NC	3.34	128.78	125.08
9	a	910	BCL	C4B-CHC-C1C	3.33	136.71	130.12
9	a	906	BCL	O2D-CGD-CBD	3.33	117.19	111.27
16	c	202	HEC	O2D-CGD-CBD	3.33	124.73	114.03
8	a	903	2GO	C3D-C4D-ND	-3.33	106.15	116.21
9	a	908	BCL	C9-C8-C10	-3.32	99.28	111.29
9	A	909	BCL	CHA-C1A-NA	-3.31	118.81	126.40
10	a	912	CLA	C4D-C3D-CAD	-3.31	104.19	108.10
10	A	931	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	A	910	CLA	CHC-C1C-NC	-3.30	119.19	124.20
10	a	912	CLA	CHC-C1C-NC	-3.30	119.19	124.20
9	a	907	BCL	C7-C6-C5	-3.30	104.41	113.36
11	A	913	LYC	C16-C17-C19	3.30	124.00	118.94
10	A	912	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
9	a	904	BCL	O1D-CGD-CBD	-3.29	117.76	124.48
10	a	901	CLA	O1D-CGD-CBD	-3.28	117.78	124.48
10	A	931	CLA	C6-C7-C8	3.28	126.51	115.92
10	A	912	CLA	O2A-CGA-O1A	-3.28	112.87	123.14
10	a	915	CLA	CMA-C3A-C4A	3.28	120.58	111.77
9	A	902	BCL	C4-C3-C2	-3.27	115.29	123.68
9	A	905	BCL	C16-C15-C13	-3.25	105.42	115.92
10	A	910	CLA	C4D-CHA-C1A	-3.25	117.30	121.25
11	A	913	LYC	C58-C56-C55	-3.24	113.96	118.94
10	a	915	CLA	C2A-C1A-CHA	-3.24	118.19	123.86
10	A	911	CLA	C2D-C1D-ND	3.23	112.48	110.10
10	A	912	CLA	C1-O2A-CGA	3.23	126.75	116.11
16	c	202	HEC	CBD-CAD-C3D	-3.22	107.13	112.62
8	a	903	2GO	OBb-CAB-CBB	-3.22	112.93	120.17
9	A	902	BCL	C1-C2-C3	-3.21	120.49	126.04
10	A	910	CLA	CHB-C4A-NA	3.21	128.95	124.51
9	a	905	BCL	C4D-CHA-C1A	3.21	125.15	121.25
9	a	910	BCL	C3D-C2D-C1D	-3.20	101.47	105.83
16	C	301	HEC	O2D-CGD-O1D	-3.19	115.35	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	931	CLA	C11-C10-C8	3.18	126.21	115.92
10	a	912	CLA	CAA-CBA-CGA	-3.18	103.95	113.25
9	A	905	BCL	O2A-CGA-CBA	3.17	121.87	111.91
9	A	909	BCL	C3C-C4C-CHD	-3.17	116.62	123.39
10	a	912	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
9	a	909	BCL	O1D-CGD-CBD	-3.16	118.02	124.48
11	A	913	LYC	C1-C2-C4	-3.16	113.53	122.65
10	A	933	CLA	CMD-C2D-C1D	3.15	130.27	124.71
9	a	905	BCL	C4-C3-C5	3.15	120.57	115.27
10	a	914	CLA	CMD-C2D-C1D	3.15	130.26	124.71
9	A	906	BCL	CMC-C2C-C1C	3.14	120.22	111.77
9	A	909	BCL	C10-C8-C7	3.14	128.65	112.13
9	a	907	BCL	OBB-CAB-C3B	-3.14	114.42	119.99
9	A	903	BCL	CMB-C2B-C3B	3.14	130.55	124.68
10	a	915	CLA	C4D-CHA-C1A	-3.13	117.44	121.25
10	A	931	CLA	C1D-CHD-C4C	-3.12	119.32	126.06
9	a	910	BCL	C11-C12-C13	3.12	126.01	115.92
10	A	931	CLA	CHD-C1D-C2D	3.12	132.02	125.48
10	a	901	CLA	CMB-C2B-C1B	3.11	133.25	128.46
9	A	904	BCL	O2D-CGD-O1D	-3.10	117.77	123.84
10	A	912	CLA	CMB-C2B-C3B	3.09	130.47	124.68
9	a	905	BCL	C2D-C1D-ND	3.08	112.37	110.10
9	a	910	BCL	C4D-CHA-C1A	-3.07	117.52	121.25
9	A	902	BCL	O1A-CGA-CBA	-3.04	111.86	123.73
10	a	901	CLA	C7-C6-C5	-3.03	105.12	113.36
9	a	908	BCL	OBD-CAD-C3D	-3.03	121.23	128.52
10	a	915	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
11	A	913	LYC	C59-C58-C56	-3.03	117.90	126.42
9	a	909	BCL	CHC-C1C-NC	3.02	128.69	124.51
13	A	915	85I	O2-P-O	-3.02	93.70	107.75
9	a	905	BCL	C11-C12-C13	3.02	125.67	115.92
10	a	915	CLA	CHC-C1C-NC	-3.00	119.64	124.20
10	a	912	CLA	C17-C16-C15	-3.00	99.44	113.24
10	a	913	CLA	C4A-NA-C1A	-3.00	105.36	106.71
8	a	903	2GO	CHA-CBD-CGD	-2.98	115.53	125.12
9	A	909	BCL	C5-C3-C2	2.98	127.15	121.12
11	c	201	LYC	C54-C55-C56	2.95	131.53	127.31
9	a	904	BCL	CAC-C3C-C2C	-2.95	106.88	114.26
10	a	914	CLA	C3D-C2D-C1D	-2.95	101.80	105.83
8	A	901	2GO	C4C-C3C-C2C	-2.94	102.61	106.90
9	A	906	BCL	OBB-CAB-CBB	-2.94	113.55	120.17
10	a	913	CLA	CAA-CBA-CGA	2.94	121.83	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	905	BCL	CHD-C1D-C2D	2.94	131.64	125.48
10	A	911	CLA	C10-C8-C7	2.92	127.48	112.13
9	A	907	BCL	O1D-CGD-CBD	-2.92	118.52	124.48
10	A	912	CLA	CAA-C2A-C1A	2.92	121.53	111.97
10	a	901	CLA	C14-C13-C15	-2.91	100.74	111.29
9	A	904	BCL	CHD-C4C-NC	2.91	128.31	125.08
9	a	905	BCL	CMA-C3A-C4A	2.91	119.59	111.77
8	A	901	2GO	O2A-C1-C2	-2.90	101.02	108.64
13	a	919	85I	O4-C4-C3	2.89	116.96	109.54
9	a	911	BCL	C3A-C2A-C1A	2.89	105.67	101.34
8	a	903	2GO	C3C-C4C-NC	2.89	115.93	110.14
9	A	906	BCL	C3D-C4D-ND	2.89	114.91	110.24
9	A	904	BCL	CMA-C3A-C2A	-2.89	102.19	113.83
9	a	905	BCL	O2A-CGA-O1A	-2.88	116.32	123.59
9	A	903	BCL	C3D-C4D-ND	2.88	114.90	110.24
9	A	903	BCL	CMD-C2D-C3D	-2.87	121.00	127.61
9	a	910	BCL	C3D-C4D-ND	2.87	114.88	110.24
10	a	912	CLA	CMC-C2C-C1C	2.87	129.40	125.04
17	E	101	84Q	O7-P-O6	-2.86	97.89	109.07
8	A	901	2GO	CHA-C1A-C2A	2.86	132.92	128.18
10	a	901	CLA	C6-C5-C3	2.85	120.94	113.45
9	a	907	BCL	O1A-CGA-CBA	-2.85	112.60	123.73
10	a	915	CLA	CHD-C4C-C3C	-2.85	120.65	124.84
9	a	907	BCL	CBB-CAB-C3B	2.85	128.79	120.34
9	A	908	BCL	OBB-CAB-C3B	-2.85	114.94	119.99
10	A	910	CLA	CHD-C4C-C3C	-2.83	120.67	124.84
10	A	910	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
9	a	904	BCL	CMC-C2C-C3C	-2.83	102.42	113.83
8	A	901	2GO	CBB-CAB-C3B	2.82	128.72	120.34
9	A	908	BCL	O2A-C1-C2	2.82	116.06	108.64
9	A	903	BCL	CMC-C2C-C1C	2.82	119.36	111.77
9	a	908	BCL	C4-C3-C5	-2.82	110.53	115.27
9	A	907	BCL	C6-C7-C8	2.81	125.01	115.92
8	A	901	2GO	CHA-CBD-CAD	-2.81	104.39	107.17
9	a	911	BCL	CMA-C3A-C4A	2.80	119.29	111.77
9	a	910	BCL	C3A-C2A-C1A	-2.79	97.16	101.34
8	a	903	2GO	CMC-C2C-C3C	-2.78	118.57	126.12
8	a	903	2GO	O1D-CGD-CBD	-2.78	119.49	124.62
10	A	933	CLA	C3D-C4D-ND	2.78	114.73	110.24
10	A	912	CLA	CHC-C1C-NC	-2.78	119.99	124.20
10	a	912	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
9	A	908	BCL	CED-O2D-CGD	2.77	122.19	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	911	BCL	O2A-CGA-O1A	-2.76	116.62	123.59
10	a	915	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
9	a	905	BCL	CMC-C2C-C1C	2.75	119.17	111.77
9	a	908	BCL	C3D-C4D-ND	2.75	114.69	110.24
9	A	903	BCL	CAA-C2A-C3A	2.75	120.30	112.78
9	A	909	BCL	C2D-C1D-ND	2.75	112.13	110.10
9	a	910	BCL	C4-C3-C2	-2.74	116.65	123.68
17	E	101	84Q	O4-P-O6	2.74	119.73	109.47
10	a	912	CLA	C9-C8-C7	2.74	121.20	111.29
10	a	901	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
10	a	913	CLA	C2C-C1C-NC	2.73	112.53	109.97
8	A	901	2GO	CAA-C2A-C1A	-2.73	120.54	128.29
9	a	911	BCL	CAA-C2A-C1A	2.73	120.91	111.97
10	a	913	CLA	CHA-C4D-ND	-2.72	126.80	132.50
9	a	909	BCL	CMA-C3A-C4A	2.72	119.09	111.77
9	a	908	BCL	C4-C3-C2	-2.72	116.70	123.68
9	A	903	BCL	C1C-NC-C4C	-2.71	105.49	106.71
10	a	914	CLA	C1D-CHD-C4C	-2.71	120.21	126.06
10	A	931	CLA	CMD-C2D-C1D	2.71	129.48	124.71
10	A	910	CLA	C6-C7-C8	2.70	124.65	115.92
10	A	910	CLA	CMB-C2B-C3B	2.69	129.72	124.68
10	a	914	CLA	CHD-C1D-C2D	2.69	131.13	125.48
11	A	913	LYC	C5-C4-C2	2.69	136.94	127.75
8	A	901	2GO	C1-C2-C3	2.68	130.67	126.04
8	a	903	2GO	CMB-C2B-C1B	-2.68	124.35	128.46
9	A	902	BCL	C4-C3-C5	2.68	119.77	115.27
9	a	911	BCL	C4D-CHA-C1A	-2.68	117.99	121.25
9	a	911	BCL	C6-C5-C3	2.66	120.44	113.45
8	A	901	2GO	C3A-C4A-NA	-2.66	105.60	109.07
9	A	908	BCL	CHB-C4A-NA	2.66	128.19	124.51
9	A	904	BCL	C4D-CHA-C1A	-2.66	118.02	121.25
9	A	902	BCL	CHD-C1D-C2D	2.65	131.04	125.48
10	a	914	CLA	CMA-C3A-C2A	-2.65	103.13	113.83
10	A	931	CLA	C16-C15-C13	-2.65	107.36	115.92
9	a	910	BCL	CMB-C2B-C1B	2.65	132.53	128.46
10	A	931	CLA	CHB-C4A-NA	2.64	128.16	124.51
10	a	913	CLA	CMB-C2B-C3B	2.64	129.61	124.68
10	A	931	CLA	C11-C12-C13	-2.64	107.39	115.92
10	a	901	CLA	C1-C2-C3	-2.63	121.49	126.04
9	a	905	BCL	OBD-CAD-C3D	-2.63	122.19	128.52
10	A	933	CLA	C4D-C3D-CAD	-2.62	105.01	108.10
9	A	903	BCL	CBC-CAC-C3C	2.62	119.30	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	908	BCL	C4B-C3B-CAB	2.62	132.19	127.13
9	A	905	BCL	C1B-CHB-C4A	-2.62	124.94	130.12
10	A	933	CLA	CHA-C4D-ND	-2.61	127.03	132.50
10	A	910	CLA	CAA-C2A-C3A	2.61	119.93	112.78
9	A	908	BCL	CMA-C3A-C2A	-2.61	103.30	113.83
8	A	901	2GO	CHA-CBD-CGD	-2.60	116.76	125.12
9	A	907	BCL	C2C-C3C-C4C	-2.60	97.45	101.34
9	a	908	BCL	O2A-CGA-O1A	2.60	130.15	123.59
9	A	906	BCL	CBC-CAC-C3C	2.59	119.24	113.47
9	A	904	BCL	C2D-C1D-ND	2.59	112.01	110.10
13	A	915	85I	O-P-O1	-2.59	98.96	109.07
10	a	915	CLA	C2C-C1C-NC	2.59	112.39	109.97
9	A	904	BCL	OBD-CAD-C3D	-2.59	122.30	128.52
9	A	905	BCL	C14-C13-C12	2.58	120.64	111.29
10	a	915	CLA	C4D-C3D-CAD	-2.58	105.05	108.10
9	A	909	BCL	CAC-C3C-C4C	-2.58	106.86	112.58
10	A	911	CLA	CMB-C2B-C3B	2.58	129.50	124.68
9	A	908	BCL	OBB-CAB-CBB	2.58	125.97	120.17
9	A	908	BCL	C7-C6-C5	-2.57	106.37	113.36
11	c	201	LYC	C5-C6-C7	2.57	121.44	112.98
10	a	915	CLA	OBD-CAD-C3D	-2.57	122.33	128.52
9	A	907	BCL	C15-C13-C14	-2.57	98.66	110.51
10	A	911	CLA	C3D-C4D-ND	2.57	114.39	110.24
9	A	909	BCL	C15-C13-C12	2.56	125.60	112.13
10	a	912	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
9	A	903	BCL	C2A-C1A-CHA	-2.56	119.39	123.86
9	A	908	BCL	C3D-C4D-ND	2.56	114.37	110.24
10	A	912	CLA	C3A-C2A-C1A	-2.54	97.53	101.34
9	a	910	BCL	CBA-CAA-C2A	2.54	121.37	113.86
9	A	907	BCL	OBB-CAB-CBB	-2.54	114.45	120.17
10	a	912	CLA	O1D-CGD-CBD	2.54	129.68	124.48
9	A	902	BCL	C9-C8-C7	-2.53	102.12	111.29
9	a	905	BCL	C1D-ND-C4D	2.53	108.13	106.33
10	A	910	CLA	C3A-C2A-C1A	-2.53	97.55	101.34
9	a	904	BCL	O2A-C1-C2	2.52	115.26	108.64
9	A	906	BCL	C4-C3-C5	2.52	118.86	115.98
9	a	909	BCL	C4-C3-C5	2.52	119.51	115.27
9	a	904	BCL	CHD-C1D-C2D	2.51	130.75	125.48
9	a	908	BCL	CAC-C3C-C2C	-2.51	107.98	114.26
11	A	913	LYC	C18-C17-C16	2.51	122.04	118.08
9	A	906	BCL	CBA-CAA-C2A	2.51	121.28	113.86
10	A	910	CLA	C3D-C4D-ND	2.51	114.30	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	904	BCL	CAA-C2A-C1A	-2.51	103.76	111.97
9	a	910	BCL	C3C-C4C-CHD	-2.51	118.04	123.39
10	A	910	CLA	C6-C5-C3	2.50	120.02	113.45
10	A	911	CLA	C1-C2-C3	-2.50	121.72	126.04
10	a	913	CLA	C9-C8-C10	-2.50	102.25	111.29
8	a	903	2GO	C15-C13-C12	-2.49	99.04	112.13
16	c	202	HEC	CMA-C3A-C2A	2.49	129.63	124.94
9	A	906	BCL	CHD-C4C-NC	2.49	127.84	125.08
10	A	911	CLA	C6-C5-C3	2.48	119.97	113.45
9	A	907	BCL	C1D-ND-C4D	-2.48	104.57	106.33
17	E	101	84Q	C19-C18-C17	2.48	122.63	113.62
9	A	907	BCL	C11-C10-C8	2.47	123.91	115.92
10	A	911	CLA	CHB-C4A-NA	2.47	127.93	124.51
10	A	931	CLA	OBD-CAD-C3D	-2.46	122.59	128.52
9	A	906	BCL	C4D-CHA-C1A	2.46	124.25	121.25
9	a	906	BCL	CBC-CAC-C3C	2.46	118.94	113.47
9	a	911	BCL	C4-C3-C2	2.44	129.95	123.68
9	a	909	BCL	CHD-C1D-C2D	2.44	130.59	125.48
8	a	903	2GO	CAC-C3C-C2C	-2.44	123.36	127.53
10	A	912	CLA	CHD-C4C-NC	-2.43	120.37	124.20
9	a	908	BCL	C16-C15-C13	-2.43	108.06	115.92
10	A	910	CLA	C2D-C1D-ND	2.43	111.89	110.10
9	a	910	BCL	C1D-CHD-C4C	-2.43	120.77	126.62
11	A	913	LYC	C20-C19-C17	-2.43	123.85	127.31
9	a	911	BCL	C16-C15-C13	2.42	123.75	115.92
9	a	906	BCL	CMD-C2D-C3D	-2.42	122.04	127.61
9	A	906	BCL	C3C-C4C-CHD	-2.42	118.22	123.39
16	C	301	HEC	CBD-CAD-C3D	-2.42	108.49	112.62
10	a	915	CLA	CAA-CBA-CGA	2.42	120.33	113.25
9	a	909	BCL	C1D-ND-C4D	-2.42	104.62	106.33
10	a	913	CLA	CMA-C3A-C4A	2.42	118.27	111.77
9	A	908	BCL	C1-O2A-CGA	2.41	122.77	116.44
9	A	908	BCL	O1A-CGA-CBA	-2.41	114.35	123.73
13	A	917	85I	O3-C3-C4	2.40	116.12	107.08
9	A	909	BCL	CBA-CAA-C2A	2.40	120.96	113.86
10	A	931	CLA	C9-C8-C10	2.40	119.97	111.29
9	a	904	BCL	C6-C5-C3	2.39	119.73	113.45
9	a	911	BCL	C4-C3-C5	-2.39	111.25	115.27
17	E	101	84Q	O5-P-O4	-2.39	97.34	106.78
11	c	201	LYC	C62-C61-C60	-2.39	116.44	122.59
9	a	910	BCL	CAC-C3C-C2C	2.38	120.20	114.26
10	a	913	CLA	CHC-C1C-NC	-2.37	120.61	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	916	85I	O2-P-O3	2.36	116.09	106.78
9	a	907	BCL	CHD-C1D-C2D	2.35	130.42	125.48
9	A	904	BCL	C2A-C1A-CHA	-2.35	119.74	123.86
10	a	901	CLA	C3B-C4B-NB	2.35	112.25	109.21
10	a	901	CLA	CBA-CAA-C2A	2.35	120.80	113.86
9	A	909	BCL	C4B-C3B-CAB	-2.35	122.59	127.13
13	A	915	85I	O6-C20-C21	2.35	116.56	111.50
9	A	909	BCL	CAC-C3C-C2C	2.35	120.12	114.26
11	c	201	LYC	C59-C58-C56	-2.34	119.83	126.42
15	A	932	85N	O5-C24-C19	-2.34	117.19	122.93
10	A	933	CLA	C5-C3-C2	-2.34	114.71	120.50
10	A	931	CLA	CHD-C1D-ND	-2.34	122.30	124.45
10	a	914	CLA	O1A-CGA-CBA	-2.33	114.63	123.73
11	A	913	LYC	C55-C54-C53	-2.33	115.95	123.22
9	a	910	BCL	CAA-CBA-CGA	2.33	120.06	113.25
9	a	910	BCL	CMC-C2C-C1C	2.33	118.02	111.77
9	A	909	BCL	C11-C12-C13	2.32	123.43	115.92
10	A	931	CLA	CAA-C2A-C3A	2.32	119.13	112.78
10	a	914	CLA	O2A-CGA-O1A	-2.32	115.88	123.14
9	A	902	BCL	C1D-CHD-C4C	-2.32	121.03	126.62
9	a	908	BCL	C11-C10-C8	-2.31	108.44	115.92
10	a	901	CLA	O2A-C1-C2	-2.31	102.56	108.64
10	A	911	CLA	CMA-C3A-C4A	2.31	117.97	111.77
10	a	915	CLA	CHD-C1D-ND	-2.30	122.34	124.45
10	A	910	CLA	CAA-CBA-CGA	2.30	119.98	113.25
8	A	901	2GO	C4B-C3B-CAB	-2.30	122.69	127.13
10	a	915	CLA	CBA-CAA-C2A	-2.29	107.09	113.86
15	G	101	85N	O2-C16-C17	-2.29	103.66	109.54
10	a	913	CLA	C4-C3-C2	-2.29	117.81	123.68
9	a	905	BCL	C6-C5-C3	2.29	119.45	113.45
10	a	912	CLA	C7-C6-C5	2.28	119.56	113.36
9	a	906	BCL	CMC-C2C-C1C	2.28	117.90	111.77
9	A	905	BCL	CHB-C4A-NA	2.28	127.66	124.51
13	A	916	85I	C7-C6-C5	-2.27	105.37	113.62
9	A	907	BCL	C11-C12-C13	2.26	126.64	115.98
9	A	905	BCL	C9-C8-C10	-2.26	103.12	111.29
10	a	915	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
9	A	903	BCL	CHD-C1D-C2D	2.24	130.18	125.48
9	A	902	BCL	C1B-CHB-C4A	2.24	134.55	130.12
9	a	911	BCL	CBB-CAB-C3B	2.24	126.98	120.34
9	A	904	BCL	CAC-C3C-C4C	-2.23	107.63	112.58
10	a	912	CLA	C5-C3-C2	2.23	125.63	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	908	BCL	C1D-ND-C4D	-2.22	104.76	106.33
10	a	913	CLA	CBC-CAC-C3C	2.22	118.54	112.43
10	A	931	CLA	C3C-C4C-NC	2.21	113.05	110.57
10	a	901	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
13	a	918	85I	O6-C3-C4	2.21	115.38	107.08
9	a	906	BCL	O2A-CGA-CBA	2.21	121.11	114.03
9	a	910	BCL	O1A-CGA-CBA	-2.20	115.14	123.73
10	a	915	CLA	C4-C3-C2	-2.20	118.03	123.68
10	a	914	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
9	A	905	BCL	O1A-CGA-CBA	-2.20	115.15	123.73
9	a	906	BCL	OBb-CAB-C3B	2.20	123.89	119.99
10	A	933	CLA	O2A-CGA-CBA	2.19	118.79	111.91
9	A	907	BCL	C4D-C3D-CAD	-2.19	105.51	108.10
9	A	907	BCL	CMA-C3A-C4A	2.19	117.66	111.77
10	A	933	CLA	CHD-C4C-C3C	-2.18	121.63	124.84
9	a	910	BCL	C4-C3-C5	-2.18	111.60	115.27
9	A	907	BCL	C4D-CHA-C1A	2.18	123.90	121.25
9	A	907	BCL	CBA-CAA-C2A	2.17	120.27	113.86
8	a	903	2GO	C1C-C2C-C3C	-2.17	104.68	106.96
9	a	909	BCL	C9-C8-C7	2.17	119.14	111.29
10	A	912	CLA	O2A-CGA-CBA	2.16	120.77	112.23
10	A	912	CLA	CMB-C2B-C1B	2.16	131.78	128.46
15	G	101	85N	O3-C17-O6	2.16	116.77	110.72
11	c	201	LYC	C63-C61-C60	2.15	128.49	121.98
10	A	933	CLA	C4C-C3C-C2C	-2.15	103.76	106.90
10	A	931	CLA	C5-C3-C2	-2.15	116.76	121.12
9	A	904	BCL	C1B-CHB-C4A	-2.15	125.86	130.12
9	a	908	BCL	CHA-C1A-NA	2.15	131.32	126.40
9	a	904	BCL	C4-C3-C2	-2.15	118.16	123.68
10	a	912	CLA	C6-C5-C3	2.15	119.09	113.45
9	a	907	BCL	O2A-C1-C2	-2.14	103.00	108.64
9	a	908	BCL	C1D-CHD-C4C	-2.13	121.49	126.62
9	A	906	BCL	CAC-C3C-C4C	2.12	117.29	112.58
10	a	914	CLA	C4D-CHA-C1A	2.12	123.83	121.25
9	a	904	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
9	a	906	BCL	CMB-C2B-C3B	2.11	128.62	124.68
9	a	910	BCL	C14-C13-C15	2.10	118.91	111.29
10	A	910	CLA	CHD-C4C-NC	-2.10	120.90	124.20
9	a	911	BCL	C15-C13-C12	-2.10	101.10	112.13
9	A	907	BCL	C4B-C3B-CAB	2.09	131.17	127.13
9	a	910	BCL	C20-C18-C17	2.09	124.47	111.54
9	a	910	BCL	CMD-C2D-C3D	-2.09	122.80	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	910	CLA	C4-C3-C5	2.09	118.78	115.27
9	A	909	BCL	CBB-CAB-C3B	2.09	126.53	120.34
8	a	903	2GO	CMD-C2D-C3D	2.09	128.58	124.68
10	a	913	CLA	C2A-C3A-C4A	-2.08	98.50	101.87
10	a	912	CLA	C2D-C1D-ND	-2.08	108.57	110.10
11	A	913	LYC	C15-C14-C12	-2.08	124.34	127.31
9	A	906	BCL	CMD-C2D-C3D	2.08	132.39	127.61
9	a	911	BCL	OBD-CAD-C3D	-2.08	123.52	128.52
9	a	906	BCL	CHD-C4C-NC	2.07	127.38	125.08
8	a	903	2GO	C6-C7-C8	2.07	122.60	115.92
8	A	901	2GO	CAD-C3D-C4D	2.06	109.62	108.47
9	a	906	BCL	CAC-C3C-C2C	2.06	119.41	114.26
10	A	911	CLA	C9-C8-C10	2.06	118.74	111.29
16	C	301	HEC	CAA-C2A-C3A	-2.06	121.34	127.25
10	A	933	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
16	C	301	HEC	CAD-C3D-C2D	-2.05	121.35	127.25
9	a	909	BCL	CMD-C2D-C3D	-2.05	122.91	127.61
9	a	908	BCL	C1-O2A-CGA	-2.04	111.08	116.44
8	a	903	2GO	CAA-C2A-C1A	-2.03	122.53	128.29
9	A	909	BCL	C12-C11-C10	2.03	122.55	113.24
9	a	906	BCL	O1D-CGD-CBD	2.03	128.63	124.48
9	A	908	BCL	C4D-C3D-CAD	-2.02	105.71	108.10
10	a	913	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
10	a	915	CLA	C1-C2-C3	-2.02	122.54	126.04
10	A	931	CLA	CMC-C2C-C3C	-2.02	120.62	126.12
9	A	902	BCL	C6-C5-C3	2.02	118.74	113.45
10	a	914	CLA	CMB-C2B-C1B	-2.02	125.37	128.46
9	A	903	BCL	C12-C11-C10	-2.01	103.99	113.24
9	a	911	BCL	C4B-C3B-CAB	2.01	131.01	127.13
10	A	911	CLA	C15-C13-C12	2.01	122.71	112.13
10	A	912	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
9	A	907	BCL	CAC-C3C-C4C	-2.01	108.12	112.58
13	A	916	85I	O6-C20-C21	2.01	115.83	111.50
9	A	905	BCL	C12-C11-C10	2.01	122.47	113.24
9	a	911	BCL	CAA-C2A-C3A	2.01	118.28	112.78
11	A	913	LYC	C3-C2-C1	2.01	119.04	114.60
10	A	933	CLA	CMD-C2D-C3D	2.01	132.23	127.61
11	A	913	LYC	C57-C56-C58	-2.01	114.92	118.08
9	A	904	BCL	C2C-C3C-C4C	-2.00	98.34	101.34
9	A	905	BCL	CMC-C2C-C3C	-2.00	105.76	113.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	910	CLA	C8
10	A	911	CLA	C8

All (642) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	a	903	2GO	C1A-C2A-CAA-CBA
9	A	902	BCL	C1A-C2A-CAA-CBA
9	A	902	BCL	C3A-C2A-CAA-CBA
9	A	902	BCL	CBD-CGD-O2D-CED
9	A	902	BCL	C11-C12-C13-C14
9	A	903	BCL	C1A-C2A-CAA-CBA
9	A	903	BCL	C2-C3-C5-C6
9	A	903	BCL	C4-C3-C5-C6
9	A	904	BCL	C1A-C2A-CAA-CBA
9	A	904	BCL	CHA-CBD-CGD-O1D
9	A	905	BCL	C1A-C2A-CAA-CBA
9	A	905	BCL	CBA-CGA-O2A-C1
9	A	905	BCL	O1A-CGA-O2A-C1
9	A	905	BCL	CBD-CGD-O2D-CED
9	A	905	BCL	C2-C3-C5-C6
9	A	905	BCL	C4-C3-C5-C6
9	A	906	BCL	CBD-CGD-O2D-CED
9	A	906	BCL	O1D-CGD-O2D-CED
9	A	907	BCL	C2C-C3C-CAC-CBC
9	A	907	BCL	C4C-C3C-CAC-CBC
9	A	907	BCL	CBD-CGD-O2D-CED
9	A	907	BCL	C2-C3-C5-C6
9	A	907	BCL	C4-C3-C5-C6
9	a	904	BCL	C4C-C3C-CAC-CBC
9	a	904	BCL	CBD-CGD-O2D-CED
9	a	905	BCL	C1A-C2A-CAA-CBA
9	a	905	BCL	C3A-C2A-CAA-CBA
9	a	906	BCL	C1A-C2A-CAA-CBA
9	a	907	BCL	C2A-CAA-CBA-CGA
9	a	908	BCL	C1A-C2A-CAA-CBA
9	a	908	BCL	CBD-CGD-O2D-CED
9	a	908	BCL	C2-C3-C5-C6
9	a	908	BCL	C4-C3-C5-C6
9	a	911	BCL	C1A-C2A-CAA-CBA
9	a	911	BCL	C3A-C2A-CAA-CBA
10	A	933	CLA	CHA-CBD-CGD-O2D
10	a	912	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	a	913	CLA	CBD-CGD-O2D-CED
10	a	913	CLA	C6-C7-C8-C9
10	a	915	CLA	C2-C3-C5-C6
10	a	915	CLA	C4-C3-C5-C6
11	c	201	LYC	C4-C5-C6-C7
11	c	201	LYC	C5-C6-C7-C8
11	c	201	LYC	C5-C6-C7-C9
11	c	201	LYC	C57-C56-C58-C59
13	A	915	85I	C4-C3-O3-P
13	A	915	85I	O7-C20-O6-C3
13	A	915	85I	C21-C20-O6-C3
13	A	916	85I	N-C1-C2-O
13	A	916	85I	O3-C3-O6-C20
13	A	916	85I	C3-O3-P-O
13	A	916	85I	O7-C20-O6-C3
13	A	917	85I	C4-C3-O6-C20
13	A	917	85I	C2-O-P-O3
13	A	917	85I	O7-C20-O6-C3
13	a	918	85I	O3-C3-C4-O4
13	a	918	85I	O6-C3-C4-O4
13	a	918	85I	C4-C3-O6-C20
13	a	918	85I	O7-C20-O6-C3
13	a	919	85I	O6-C3-C4-O4
13	a	919	85I	C4-C3-O3-P
13	a	919	85I	O3-C3-O6-C20
13	a	919	85I	C6-C5-O4-C4
13	a	919	85I	C2-O-P-O1
13	a	920	85I	C2-C1-N-C
13	a	920	85I	O3-C3-C4-O4
13	a	920	85I	O6-C3-C4-O4
13	a	920	85I	C4-C3-O6-C20
13	a	920	85I	C2-O-P-O1
13	a	920	85I	C2-O-P-O2
13	a	920	85I	C2-O-P-O3
13	a	920	85I	O7-C20-O6-C3
15	A	932	85N	O3-C17-O6-C25
15	A	932	85N	O2-C16-C17-O6
15	A	932	85N	C16-C17-O3-C18
15	A	932	85N	C20-C19-C24-O4
15	A	932	85N	C20-C19-C24-O5
15	G	101	85N	C19-C20-N1-C21
15	G	101	85N	C19-C20-N1-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	G	101	85N	C19-C20-N1-C23
15	G	101	85N	O3-C18-C19-C20
15	G	101	85N	O3-C18-C19-C24
15	G	101	85N	C20-C19-C24-O4
15	G	101	85N	C20-C19-C24-O5
15	a	902	85N	O7-C25-O6-C17
15	a	902	85N	C26-C25-O6-C17
15	a	902	85N	O2-C16-C17-O3
15	g	101	85N	C16-C17-O6-C25
15	g	101	85N	O7-C25-O6-C17
15	g	101	85N	O2-C16-C17-O6
17	E	101	84Q	O3-C17-O2-C16
17	E	101	84Q	O7-C32-C33-N
17	E	101	84Q	O1-C15-C16-O2
17	E	101	84Q	O1-C15-C16-O4
17	a	921	84Q	O4-C16-O2-C17
17	a	921	84Q	O3-C17-O2-C16
17	a	921	84Q	C32-O7-P-O6
17	a	921	84Q	C32-O7-P-O5
17	a	921	84Q	C32-O7-P-O4
17	a	921	84Q	C16-O4-P-O7
17	a	921	84Q	C15-C16-O4-P
17	a	921	84Q	O1-C15-C16-O4
9	a	904	BCL	O1D-CGD-O2D-CED
9	A	902	BCL	O1D-CGD-O2D-CED
9	A	905	BCL	O1D-CGD-O2D-CED
9	a	909	BCL	O1D-CGD-O2D-CED
9	A	903	BCL	CBD-CGD-O2D-CED
9	a	905	BCL	CBD-CGD-O2D-CED
9	a	909	BCL	CBD-CGD-O2D-CED
9	A	907	BCL	O1A-CGA-O2A-C1
9	a	907	BCL	O1A-CGA-O2A-C1
9	a	911	BCL	O1A-CGA-O2A-C1
13	a	919	85I	O5-C5-O4-C4
9	A	903	BCL	O1D-CGD-O2D-CED
9	A	907	BCL	O1D-CGD-O2D-CED
10	a	913	CLA	O1D-CGD-O2D-CED
10	A	911	CLA	C3-C5-C6-C7
10	a	913	CLA	C3-C5-C6-C7
9	A	907	BCL	CBA-CGA-O2A-C1
9	a	907	BCL	CBA-CGA-O2A-C1
8	a	903	2GO	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	908	BCL	O1A-CGA-O2A-C1
9	a	908	BCL	O1D-CGD-O2D-CED
10	a	901	CLA	CBD-CGD-O2D-CED
9	a	908	BCL	CBA-CGA-O2A-C1
9	a	911	BCL	CBA-CGA-O2A-C1
10	A	911	CLA	CBD-CGD-O2D-CED
9	A	903	BCL	C2A-CAA-CBA-CGA
9	a	910	BCL	C2A-CAA-CBA-CGA
10	a	912	CLA	C2A-CAA-CBA-CGA
9	a	905	BCL	O1D-CGD-O2D-CED
10	a	912	CLA	O1D-CGD-O2D-CED
9	a	909	BCL	C3-C5-C6-C7
15	g	101	85N	C14-C15-O2-C16
8	A	901	2GO	C1A-C2A-CAA-CBA
8	A	901	2GO	C4C-C3C-CAC-CBC
13	A	917	85I	O5-C5-O4-C4
15	G	101	85N	O1-C15-O2-C16
15	a	902	85N	C11-C10-C9-C8
9	A	909	BCL	CBD-CGD-O2D-CED
10	a	914	CLA	CBD-CGD-O2D-CED
10	a	915	CLA	CBD-CGD-O2D-CED
15	G	101	85N	C14-C15-O2-C16
13	a	918	85I	C21-C20-O6-C3
10	a	914	CLA	CBA-CGA-O2A-C1
13	A	915	85I	C12-C13-C14-C15
13	A	917	85I	C7-C8-C9-C10
13	A	917	85I	C25-C26-C27-C28
13	A	917	85I	C10-C11-C12-C13
13	A	917	85I	C6-C5-O4-C4
15	g	101	85N	O1-C15-O2-C16
9	A	902	BCL	C4-C3-C5-C6
9	A	902	BCL	C2-C3-C5-C6
10	a	901	CLA	C2A-CAA-CBA-CGA
9	A	902	BCL	CBA-CGA-O2A-C1
13	A	916	85I	C21-C20-O6-C3
17	E	101	84Q	C13-C14-O1-C15
17	a	921	84Q	C13-C14-O1-C15
10	a	914	CLA	O1A-CGA-O2A-C1
13	A	917	85I	C3-O3-P-O
17	E	101	84Q	C16-O4-P-O7
10	A	910	CLA	C13-C15-C16-C17
17	a	921	84Q	C1-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	a	921	84Q	C11-C12-C13-C14
17	E	101	84Q	O-C14-O1-C15
17	a	921	84Q	O-C14-O1-C15
9	A	903	BCL	C11-C10-C8-C9
9	A	903	BCL	C14-C13-C15-C16
9	A	907	BCL	C11-C10-C8-C9
9	A	908	BCL	C11-C10-C8-C9
9	a	908	BCL	C14-C13-C15-C16
9	a	910	BCL	C14-C13-C15-C16
10	A	910	CLA	C6-C7-C8-C9
10	A	911	CLA	C6-C7-C8-C9
10	A	931	CLA	C6-C7-C8-C9
10	a	901	CLA	C6-C7-C8-C9
11	c	201	LYC	C15-C16-C17-C19
11	c	201	LYC	C55-C56-C58-C59
9	a	908	BCL	C5-C6-C7-C8
10	A	910	CLA	C5-C6-C7-C8
9	a	905	BCL	C15-C16-C17-C18
9	a	909	BCL	C15-C16-C17-C18
10	a	901	CLA	C15-C16-C17-C18
13	a	919	85I	C14-C15-C16-C17
15	A	932	85N	C34-C35-C36-C37
15	a	902	85N	C25-C26-C27-C28
13	a	918	85I	C2-C1-N-C
9	A	909	BCL	C2-C1-O2A-CGA
9	a	907	BCL	C5-C6-C7-C8
9	a	909	BCL	C10-C11-C12-C13
17	E	101	84Q	C18-C17-O2-C16
10	A	911	CLA	C15-C16-C17-C18
9	A	909	BCL	C6-C7-C8-C10
9	a	907	BCL	C11-C12-C13-C15
10	A	910	CLA	C11-C10-C8-C7
10	A	931	CLA	C11-C12-C13-C15
9	A	909	BCL	C3-C5-C6-C7
13	A	915	85I	O5-C5-O4-C4
9	A	905	BCL	C2A-CAA-CBA-CGA
13	A	917	85I	C29-C30-C31-C32
13	a	920	85I	C29-C30-C31-C32
11	A	913	LYC	C4-C5-C6-C7
10	A	931	CLA	O1D-CGD-O2D-CED
9	A	902	BCL	C13-C15-C16-C17
9	a	907	BCL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	909	BCL	C5-C6-C7-C8
10	a	912	CLA	C8-C10-C11-C12
10	a	901	CLA	C5-C6-C7-C8
8	a	903	2GO	C15-C16-C17-C18
10	A	931	CLA	C8-C10-C11-C12
10	A	931	CLA	C13-C15-C16-C17
10	a	901	CLA	C13-C15-C16-C17
13	a	920	85I	C14-C15-C16-C17
13	a	919	85I	C2-O-P-O3
13	A	915	85I	C6-C5-O4-C4
10	A	910	CLA	O1D-CGD-O2D-CED
8	a	903	2GO	C13-C15-C16-C17
9	A	905	BCL	C10-C11-C12-C13
10	A	931	CLA	C15-C16-C17-C18
9	A	908	BCL	C2A-CAA-CBA-CGA
10	A	931	CLA	C2A-CAA-CBA-CGA
13	a	919	85I	C15-C16-C17-C19
9	a	905	BCL	C13-C15-C16-C17
13	A	917	85I	C11-C10-C9-C8
15	A	932	85N	C31-C32-C33-C34
17	E	101	84Q	C7-C8-C9-C10
17	a	921	84Q	C9-C10-C11-C12
10	A	931	CLA	C16-C17-C18-C20
15	a	902	85N	C1-C2-C4-C5
13	a	919	85I	C6-C7-C8-C9
13	a	919	85I	C12-C13-C14-C15
13	a	920	85I	C11-C12-C13-C14
15	A	932	85N	C27-C28-C29-C30
17	a	921	84Q	C4-C5-C6-C7
13	a	919	85I	C21-C22-C23-C24
13	A	916	85I	C25-C26-C27-C28
13	a	920	85I	C9-C10-C11-C12
13	A	915	85I	C22-C23-C24-C25
13	A	916	85I	C22-C23-C24-C25
13	a	920	85I	C20-C21-C22-C23
17	E	101	84Q	C17-C18-C19-C20
9	a	909	BCL	C1-C2-C3-C5
13	a	918	85I	C26-C27-C28-C29
13	a	919	85I	C9-C10-C11-C12
9	A	902	BCL	O1A-CGA-O2A-C1
9	A	903	BCL	C16-C17-C18-C20
10	A	910	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	917	85I	C30-C31-C32-C34
13	A	915	85I	C10-C11-C12-C13
13	a	919	85I	C11-C10-C9-C8
15	G	101	85N	C10-C11-C12-C13
15	a	902	85N	C26-C27-C28-C29
9	A	909	BCL	C11-C10-C8-C9
10	A	911	CLA	O1D-CGD-O2D-CED
13	A	915	85I	C26-C27-C28-C29
13	A	917	85I	C26-C27-C28-C29
15	a	902	85N	C7-C8-C9-C10
15	g	101	85N	C5-C6-C7-C8
17	a	921	84Q	C19-C20-C21-C22
11	c	201	LYC	C15-C16-C17-C18
9	a	908	BCL	C3-C5-C6-C7
13	A	916	85I	C27-C28-C29-C30
13	a	918	85I	C21-C22-C23-C24
13	a	919	85I	C22-C23-C24-C25
15	a	902	85N	C5-C6-C7-C8
13	A	916	85I	C7-C8-C9-C10
13	a	918	85I	C22-C23-C24-C25
13	a	920	85I	C7-C8-C9-C10
15	G	101	85N	C26-C27-C28-C29
15	a	902	85N	C11-C12-C13-C14
17	E	101	84Q	C10-C11-C12-C13
9	a	910	BCL	C16-C17-C18-C19
10	A	931	CLA	C16-C17-C18-C19
17	E	101	84Q	C-C1-C3-C4
10	a	913	CLA	C15-C16-C17-C18
13	A	917	85I	C12-C13-C14-C15
13	a	919	85I	C25-C26-C27-C28
13	a	919	85I	C13-C14-C15-C16
15	g	101	85N	C11-C12-C13-C14
13	A	917	85I	C20-C21-C22-C23
10	A	931	CLA	C5-C6-C7-C8
13	a	920	85I	C25-C26-C27-C28
15	g	101	85N	C27-C28-C29-C30
17	E	101	84Q	C19-C20-C21-C22
9	a	909	BCL	CBA-CGA-O2A-C1
13	a	919	85I	C10-C11-C12-C13
9	A	904	BCL	C3A-C2A-CAA-CBA
9	A	905	BCL	C3A-C2A-CAA-CBA
9	A	909	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	906	BCL	C3A-C2A-CAA-CBA
9	a	908	BCL	C3A-C2A-CAA-CBA
10	a	901	CLA	C3A-C2A-CAA-CBA
9	a	910	BCL	C10-C11-C12-C13
11	c	201	LYC	C17-C19-C20-C21
13	a	919	85I	C7-C8-C9-C10
15	a	902	85N	C10-C11-C12-C13
9	a	910	BCL	C16-C17-C18-C20
13	A	916	85I	C30-C31-C32-C33
13	A	917	85I	C15-C16-C17-C19
17	E	101	84Q	C2-C1-C3-C4
13	A	916	85I	C24-C25-C26-C27
13	A	916	85I	C13-C14-C15-C16
13	a	919	85I	C11-C12-C13-C14
17	E	101	84Q	C20-C21-C22-C23
13	A	916	85I	C20-C21-C22-C23
15	a	902	85N	C12-C13-C14-C15
10	A	931	CLA	C4-C3-C5-C6
15	g	101	85N	C26-C27-C28-C29
10	a	901	CLA	O1D-CGD-O2D-CED
17	a	921	84Q	C3-C4-C5-C6
13	a	919	85I	C30-C31-C32-C34
13	A	916	85I	C11-C10-C9-C8
15	a	902	85N	C28-C29-C30-C31
13	A	917	85I	C22-C23-C24-C25
17	a	921	84Q	C6-C7-C8-C9
17	a	921	84Q	C25-C26-C27-C28
13	A	916	85I	C12-C13-C14-C15
13	A	917	85I	C28-C29-C30-C31
10	a	901	CLA	C8-C10-C11-C12
13	A	916	85I	C5-C6-C7-C8
9	A	909	BCL	C11-C10-C8-C7
10	A	911	CLA	C11-C12-C13-C15
10	A	931	CLA	C11-C10-C8-C7
13	a	920	85I	C26-C27-C28-C29
9	A	903	BCL	C16-C17-C18-C19
13	A	917	85I	C30-C31-C32-C33
13	a	918	85I	C20-C21-C22-C23
9	a	904	BCL	C2A-CAA-CBA-CGA
9	a	908	BCL	C13-C15-C16-C17
13	A	917	85I	C21-C22-C23-C24
15	a	902	85N	C17-C16-O2-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	E	101	84Q	C11-C12-C13-C14
17	a	921	84Q	C5-C6-C7-C8
13	a	920	85I	C21-C20-O6-C3
15	g	101	85N	C26-C25-O6-C17
9	a	904	BCL	CBA-CGA-O2A-C1
13	A	917	85I	C5-C6-C7-C8
13	a	918	85I	C5-C6-C7-C8
13	A	915	85I	C7-C8-C9-C10
13	a	920	85I	C21-C22-C23-C24
15	a	902	85N	C29-C30-C31-C32
17	E	101	84Q	C3-C4-C5-C6
15	G	101	85N	C1-C2-C4-C5
15	a	902	85N	C3-C2-C4-C5
9	A	903	BCL	C10-C11-C12-C13
9	A	908	BCL	C8-C10-C11-C12
9	a	907	BCL	C11-C12-C13-C14
10	A	912	CLA	CBD-CGD-O2D-CED
17	a	921	84Q	C23-C24-C25-C26
15	A	932	85N	C29-C30-C31-C32
8	a	903	2GO	C2C-C3C-CAC-CBC
9	A	908	BCL	C1A-C2A-CAA-CBA
9	A	909	BCL	C1A-C2A-CAA-CBA
9	a	910	BCL	C1A-C2A-CAA-CBA
10	A	910	CLA	C16-C17-C18-C20
13	a	919	85I	C30-C31-C32-C33
13	a	920	85I	C30-C31-C32-C33
15	a	902	85N	C30-C31-C32-C33
10	a	914	CLA	O1D-CGD-O2D-CED
9	A	905	BCL	C5-C6-C7-C8
9	A	909	BCL	C15-C16-C17-C18
17	E	101	84Q	C16-C15-O1-C14
13	A	917	85I	C15-C16-C17-C18
9	A	908	BCL	C3-C5-C6-C7
13	A	917	85I	C6-C7-C8-C9
10	a	901	CLA	CBA-CGA-O2A-C1
9	a	904	BCL	C2C-C3C-CAC-CBC
15	G	101	85N	C7-C8-C9-C10
17	a	921	84Q	C10-C11-C12-C13
10	a	912	CLA	C13-C15-C16-C17
13	a	919	85I	C23-C24-C25-C26
10	a	913	CLA	C16-C17-C18-C19
13	a	918	85I	C30-C31-C32-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	916	85I	C6-C7-C8-C9
10	A	933	CLA	O1D-CGD-O2D-CED
9	A	909	BCL	C8-C10-C11-C12
9	a	909	BCL	O1A-CGA-O2A-C1
17	a	921	84Q	C18-C17-O2-C16
13	a	919	85I	C28-C29-C30-C31
15	G	101	85N	C11-C12-C13-C14
17	E	101	84Q	C22-C23-C24-C25
10	A	912	CLA	O1D-CGD-O2D-CED
9	a	908	BCL	C15-C16-C17-C18
13	A	916	85I	C14-C15-C16-C17
13	A	915	85I	C25-C26-C27-C28
15	a	902	85N	C18-C19-C24-O4
9	a	905	BCL	CBA-CGA-O2A-C1
9	A	908	BCL	C12-C13-C15-C16
9	a	908	BCL	C12-C13-C15-C16
9	a	910	BCL	C11-C12-C13-C15
9	a	910	BCL	C12-C13-C15-C16
10	a	901	CLA	C6-C7-C8-C10
10	a	913	CLA	C11-C10-C8-C7
9	A	903	BCL	C6-C7-C8-C9
9	A	905	BCL	C11-C10-C8-C9
9	a	908	BCL	C6-C7-C8-C9
10	A	931	CLA	C11-C12-C13-C14
10	a	912	CLA	C6-C7-C8-C9
10	a	915	CLA	O1D-CGD-O2D-CED
10	a	912	CLA	CBA-CGA-O2A-C1
17	E	101	84Q	C16-O4-P-O5
9	a	905	BCL	C10-C11-C12-C13
10	a	913	CLA	C16-C17-C18-C20
15	a	902	85N	O2-C16-C17-O6
15	g	101	85N	O2-C16-C17-O3
17	a	921	84Q	O1-C15-C16-O2
15	G	101	85N	C6-C7-C8-C9
9	A	903	BCL	C3A-C2A-CAA-CBA
9	A	908	BCL	C3A-C2A-CAA-CBA
13	a	919	85I	C3-O3-P-O
11	c	201	LYC	C58-C59-C60-C61
15	A	932	85N	C28-C29-C30-C31
13	A	916	85I	C30-C31-C32-C34
9	a	904	BCL	C8-C10-C11-C12
15	G	101	85N	C3-C2-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	E	101	84Q	C6-C7-C8-C9
13	A	915	85I	C2-O-P-O3
9	a	905	BCL	O1A-CGA-O2A-C1
13	A	915	85I	C30-C31-C32-C33
13	a	919	85I	C15-C16-C17-C18
9	a	908	BCL	C10-C11-C12-C13
15	a	902	85N	C2-C4-C5-C6
8	a	903	2GO	C3A-C2A-CAA-CBA
13	a	920	85I	C30-C31-C32-C34
13	a	918	85I	C11-C12-C13-C14
13	a	918	85I	C12-C13-C14-C15
9	A	905	BCL	C2-C1-O2A-CGA
9	a	911	BCL	C2-C1-O2A-CGA
15	A	932	85N	C25-C26-C27-C28
9	a	905	BCL	C11-C12-C13-C14
13	A	917	85I	C21-C20-O6-C3
13	a	918	85I	C30-C31-C32-C33
17	a	921	84Q	C2-C1-C3-C4
17	E	101	84Q	C1-C3-C4-C5
10	A	911	CLA	C10-C11-C12-C13
13	A	915	85I	C24-C25-C26-C27
9	a	905	BCL	C3-C5-C6-C7
8	A	901	2GO	C10-C11-C12-C13
13	a	919	85I	C29-C30-C31-C32
13	A	915	85I	C21-C22-C23-C24
13	a	920	85I	C27-C28-C29-C30
9	A	902	BCL	C11-C12-C13-C15
9	A	902	BCL	C12-C13-C15-C16
9	A	903	BCL	C6-C7-C8-C10
9	A	903	BCL	C11-C10-C8-C7
9	A	905	BCL	C11-C10-C8-C7
9	a	905	BCL	C11-C12-C13-C15
9	a	908	BCL	C6-C7-C8-C10
10	a	901	CLA	C11-C10-C8-C7
9	a	909	BCL	C16-C17-C18-C19
10	A	911	CLA	C16-C17-C18-C19
9	A	902	BCL	C2A-CAA-CBA-CGA
10	a	912	CLA	C3-C5-C6-C7
9	a	909	BCL	CAD-CBD-CGD-O2D
10	A	931	CLA	CAD-CBD-CGD-O2D
10	a	912	CLA	CAD-CBD-CGD-O2D
13	A	916	85I	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	a	920	85I	C13-C14-C15-C16
15	a	902	85N	C33-C34-C35-C36
9	A	903	BCL	C5-C6-C7-C8
17	E	101	84Q	C24-C25-C26-C27
9	A	906	BCL	CHA-CBD-CGD-O2D
9	a	905	BCL	CHA-CBD-CGD-O2D
10	A	933	CLA	CHA-CBD-CGD-O1D
10	a	915	CLA	CHA-CBD-CGD-O1D
10	a	915	CLA	CHA-CBD-CGD-O2D
9	a	904	BCL	O1A-CGA-O2A-C1
10	a	901	CLA	O1A-CGA-O2A-C1
13	a	919	85I	O7-C20-O6-C3
9	A	908	BCL	C14-C13-C15-C16
13	A	916	85I	C10-C11-C12-C13
13	A	917	85I	C3-O3-P-O1
17	a	921	84Q	C16-O4-P-O6
15	A	932	85N	C1-C2-C4-C5
13	a	919	85I	N-C1-C2-O
17	E	101	84Q	C32-O7-P-O4
13	a	918	85I	C27-C28-C29-C30
13	A	915	85I	C2-O-P-O1
13	A	917	85I	C2-O-P-O2
13	a	919	85I	C2-O-P-O2
17	E	101	84Q	C27-C28-C29-C31
9	a	905	BCL	C5-C6-C7-C8
9	a	908	BCL	CAD-CBD-CGD-O1D
13	a	920	85I	C1-C2-O-P
17	a	921	84Q	C33-C32-O7-P
13	a	919	85I	C20-C21-C22-C23
13	a	918	85I	C7-C8-C9-C10
9	A	907	BCL	C8-C10-C11-C12
17	a	921	84Q	C-C1-C3-C4
9	A	905	BCL	C12-C13-C15-C16
9	A	907	BCL	C6-C7-C8-C10
9	A	907	BCL	C11-C10-C8-C7
9	A	908	BCL	C11-C10-C8-C7
9	a	907	BCL	C11-C10-C8-C7
10	A	911	CLA	C11-C10-C8-C7
15	A	932	85N	C19-C18-O3-C17
13	a	918	85I	C23-C24-C25-C26
9	a	909	BCL	CAA-CBA-CGA-O2A
17	a	921	84Q	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	904	BCL	C10-C11-C12-C13
8	a	903	2GO	C14-C13-C15-C16
9	A	902	BCL	C14-C13-C15-C16
9	a	907	BCL	C6-C7-C8-C9
9	a	910	BCL	C11-C12-C13-C14
10	A	911	CLA	C11-C12-C13-C14
10	a	913	CLA	C11-C10-C8-C9
15	G	101	85N	C25-C26-C27-C28
11	c	201	LYC	C9-C10-C11-C12
13	a	920	85I	C6-C7-C8-C9
10	a	912	CLA	O1A-CGA-O2A-C1
9	A	908	BCL	C16-C17-C18-C19
15	g	101	85N	C1-C2-C4-C5
9	A	906	BCL	O1A-CGA-O2A-C1
15	A	932	85N	C3-C2-C4-C5
9	a	904	BCL	C2-C1-O2A-CGA
15	a	902	85N	C18-C19-C24-O5
15	g	101	85N	C7-C8-C9-C10
9	A	902	BCL	CAA-CBA-CGA-O2A
13	a	919	85I	C21-C20-O6-C3
13	a	920	85I	C22-C23-C24-C25
13	a	920	85I	C10-C11-C12-C13
8	a	903	2GO	C11-C12-C13-C15
10	a	901	CLA	C11-C12-C13-C14
11	c	201	LYC	C52-C51-C53-C54
8	a	903	2GO	C8-C10-C11-C12
13	A	916	85I	C26-C27-C28-C29
13	a	919	85I	C24-C25-C26-C27
13	A	915	85I	C6-C7-C8-C9
16	c	202	HEC	CAD-CBD-CGD-O2D
10	a	901	CLA	C16-C17-C18-C20
9	a	906	BCL	CAA-CBA-CGA-O1A
13	A	915	85I	O3-C3-C4-O4
13	a	918	85I	C9-C10-C11-C12
13	a	920	85I	C12-C13-C14-C15
10	a	901	CLA	C14-C13-C15-C16
9	a	908	BCL	C2A-CAA-CBA-CGA
17	E	101	84Q	C23-C24-C25-C26
9	A	904	BCL	CAA-CBA-CGA-O2A
10	a	912	CLA	C4-C3-C5-C6
10	a	901	CLA	C1A-C2A-CAA-CBA
9	A	903	BCL	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	931	CLA	C6-C7-C8-C10
10	a	901	CLA	C12-C13-C15-C16
9	a	909	BCL	C13-C15-C16-C17
16	C	301	HEC	CAD-CBD-CGD-O2D
13	A	916	85I	C15-C16-C17-C19
9	A	904	BCL	CAA-CBA-CGA-O1A
10	A	910	CLA	C10-C11-C12-C13
10	A	911	CLA	C5-C6-C7-C8
9	a	906	BCL	CAA-CBA-CGA-O2A
11	c	201	LYC	C21-C50-C51-C53
10	a	901	CLA	C2-C1-O2A-CGA
13	a	918	85I	C28-C29-C30-C31
9	A	909	BCL	O1D-CGD-O2D-CED
9	a	904	BCL	CAA-CBA-CGA-O2A
16	C	301	HEC	CAD-CBD-CGD-O1D
15	g	101	85N	C3-C2-C4-C5
17	a	921	84Q	C27-C28-C29-C30
13	A	917	85I	C23-C24-C25-C26
10	A	931	CLA	CBD-CGD-O2D-CED
15	g	101	85N	C11-C10-C9-C8
10	a	901	CLA	CAA-CBA-CGA-O2A
8	A	901	2GO	C16-C17-C18-C20
11	c	201	LYC	C13-C12-C14-C15
11	c	201	LYC	C21-C50-C51-C52
13	A	915	85I	C5-C6-C7-C8
9	A	902	BCL	C8-C10-C11-C12
10	A	931	CLA	C2-C3-C5-C6
10	a	912	CLA	C2-C3-C5-C6
9	A	907	BCL	C6-C7-C8-C9
9	A	908	BCL	C6-C7-C8-C9
9	A	909	BCL	C11-C12-C13-C14
9	a	907	BCL	C11-C10-C8-C9
10	A	910	CLA	C11-C10-C8-C9
10	a	901	CLA	C11-C10-C8-C9
9	A	903	BCL	CAA-CBA-CGA-O2A
9	A	903	BCL	CAD-CBD-CGD-O2D
9	A	907	BCL	CAD-CBD-CGD-O2D
10	a	901	CLA	CAD-CBD-CGD-O2D
13	a	918	85I	C24-C25-C26-C27
13	a	920	85I	C11-C10-C9-C8
13	a	919	85I	C26-C27-C28-C29
16	c	202	HEC	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	904	BCL	CHA-CBD-CGD-O2D
9	A	906	BCL	CHA-CBD-CGD-O1D
9	a	904	BCL	CHA-CBD-CGD-O2D
9	a	905	BCL	CHA-CBD-CGD-O1D
9	a	906	BCL	CHA-CBD-CGD-O1D
9	a	908	BCL	CHA-CBD-CGD-O2D
10	a	913	CLA	CHA-CBD-CGD-O2D
11	c	201	LYC	C11-C12-C14-C15
13	a	919	85I	O4-C5-C6-C7
15	a	902	85N	C13-C14-C15-O2
9	a	910	BCL	CAA-CBA-CGA-O2A
9	a	907	BCL	C6-C7-C8-C10
9	A	907	BCL	C11-C12-C13-C14
10	a	901	CLA	C16-C17-C18-C19
13	A	916	85I	O4-C5-C6-C7
16	C	301	HEC	CAA-CBA-CGA-O2A
10	a	901	CLA	CAA-CBA-CGA-O1A
17	a	921	84Q	C22-C23-C24-C25
17	a	921	84Q	C27-C28-C29-C31
13	A	917	85I	N-C1-C2-O
15	g	101	85N	C18-C19-C20-N1
15	A	932	85N	C4-C5-C6-C7
9	a	907	BCL	C13-C15-C16-C17
13	a	919	85I	O5-C5-C6-C7
17	a	921	84Q	C11-C10-C9-C8
15	A	932	85N	C2-C4-C5-C6
9	A	903	BCL	CAA-CBA-CGA-O1A
15	g	101	85N	C13-C14-C15-O2
16	c	202	HEC	CAA-CBA-CGA-O2A
9	a	910	BCL	CAA-CBA-CGA-O1A
15	a	902	85N	C13-C14-C15-O1
9	A	906	BCL	CAD-CBD-CGD-O1D
9	A	908	BCL	CAD-CBD-CGD-O1D
9	a	906	BCL	CAD-CBD-CGD-O1D
10	A	933	CLA	CAD-CBD-CGD-O1D
10	a	915	CLA	CAD-CBD-CGD-O1D
17	E	101	84Q	C33-C32-O7-P
15	g	101	85N	C13-C14-C15-O1
13	a	920	85I	O4-C5-C6-C7
15	g	101	85N	C2-C4-C5-C6
9	A	905	BCL	C14-C13-C15-C16
9	a	905	BCL	C6-C7-C8-C9

Continued on next page...

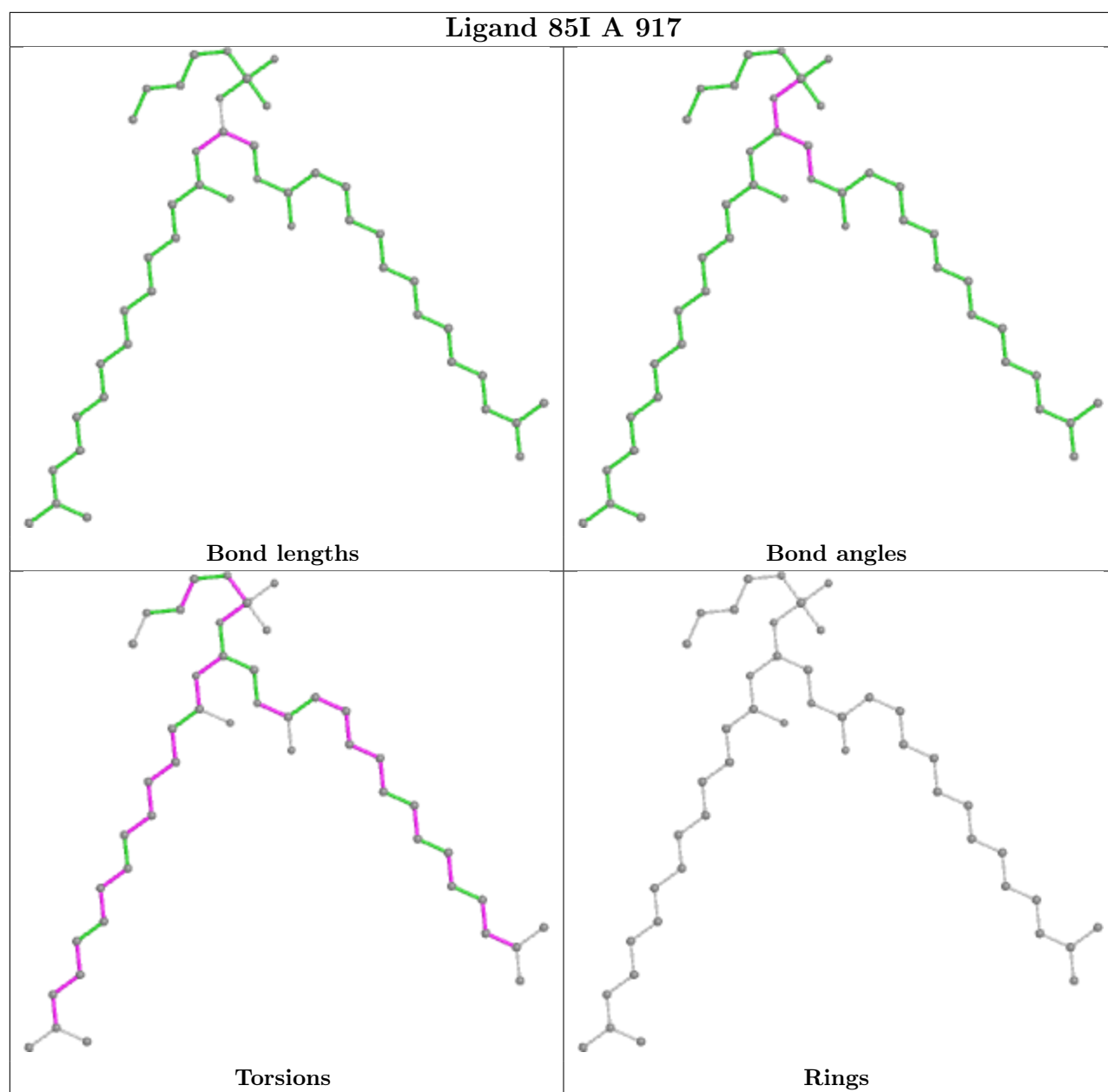
Continued from previous page...

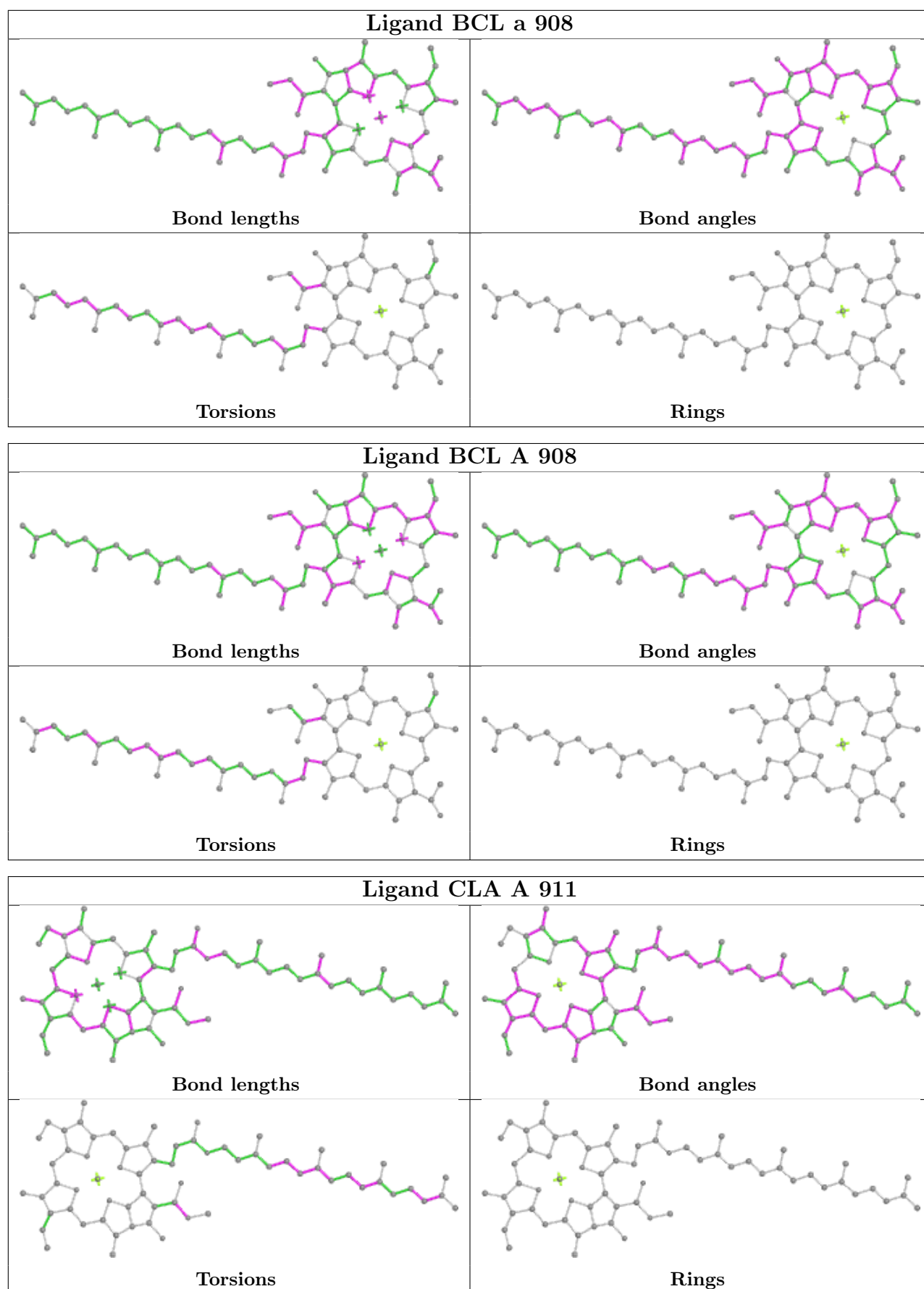
Mol	Chain	Res	Type	Atoms
9	A	908	BCL	CAA-CBA-CGA-O2A
13	A	916	85I	O6-C20-C21-C22
13	A	916	85I	O5-C5-C6-C7
9	A	908	BCL	C6-C7-C8-C10
9	a	905	BCL	C6-C7-C8-C10
10	a	913	CLA	C6-C7-C8-C10
15	A	932	85N	O7-C25-C26-C27
10	A	931	CLA	C3-C5-C6-C7
11	c	201	LYC	C50-C51-C53-C54
9	A	907	BCL	CAA-CBA-CGA-O2A
15	A	932	85N	O6-C25-C26-C27
15	G	101	85N	C13-C14-C15-O2
13	A	917	85I	C14-C15-C16-C17
9	A	903	BCL	O1A-CGA-O2A-C1
13	A	916	85I	O7-C20-C21-C22
13	a	920	85I	O5-C5-C6-C7
15	a	902	85N	C14-C15-O2-C16

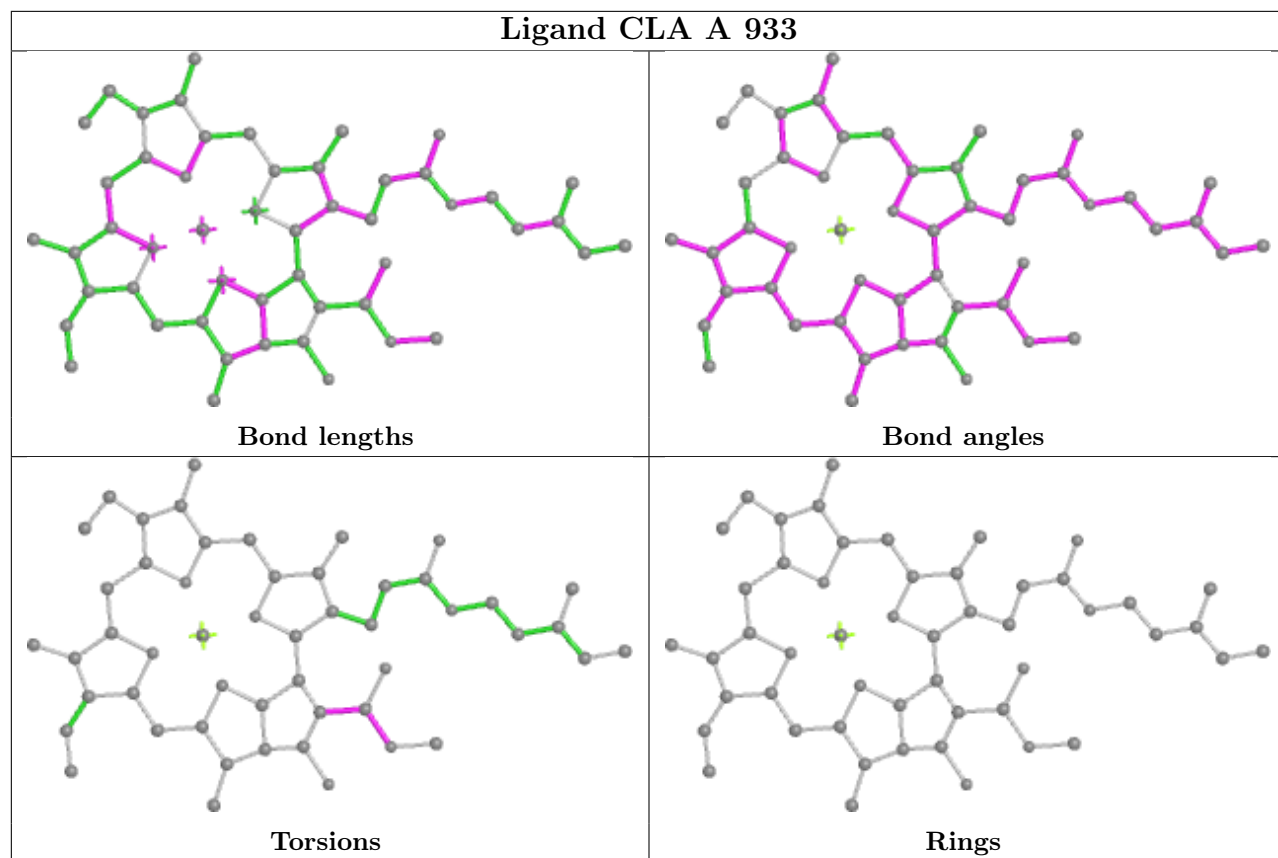
There are no ring outliers.

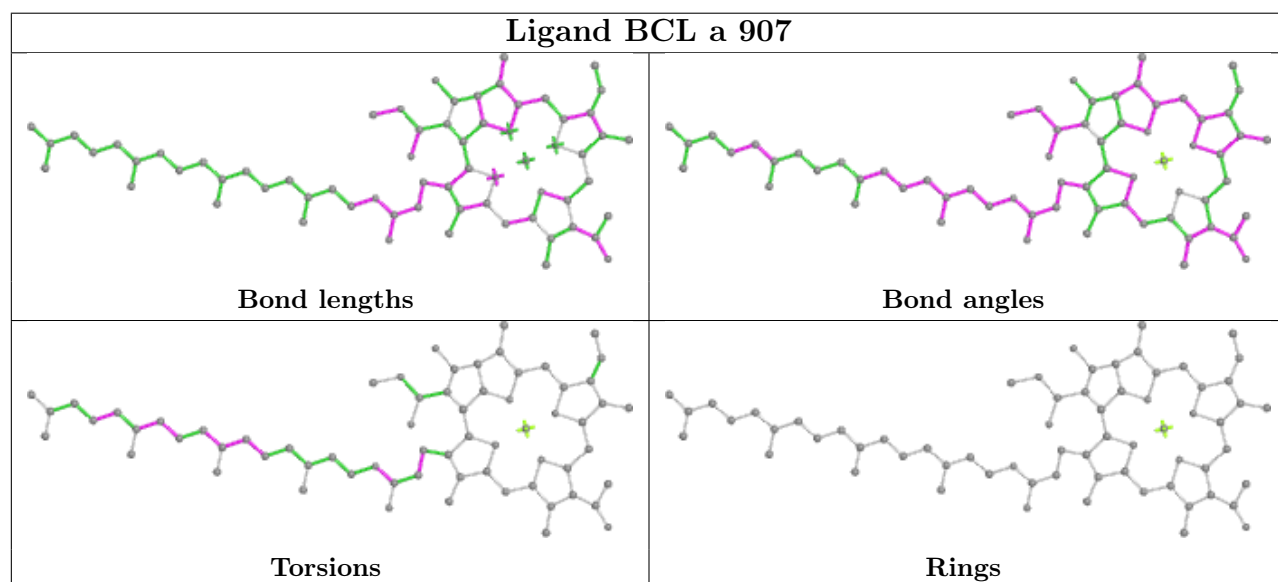
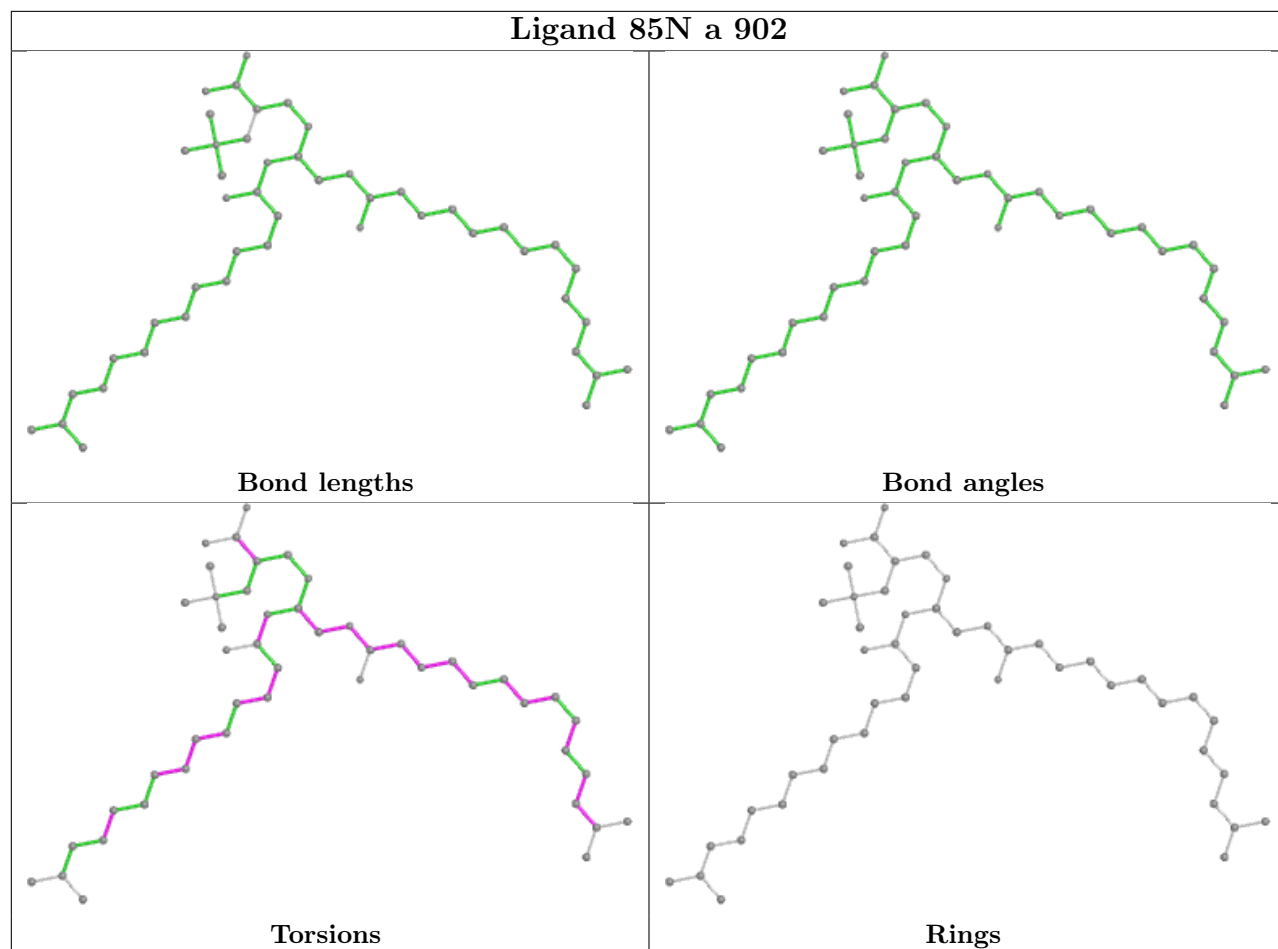
No monomer is involved in short contacts.

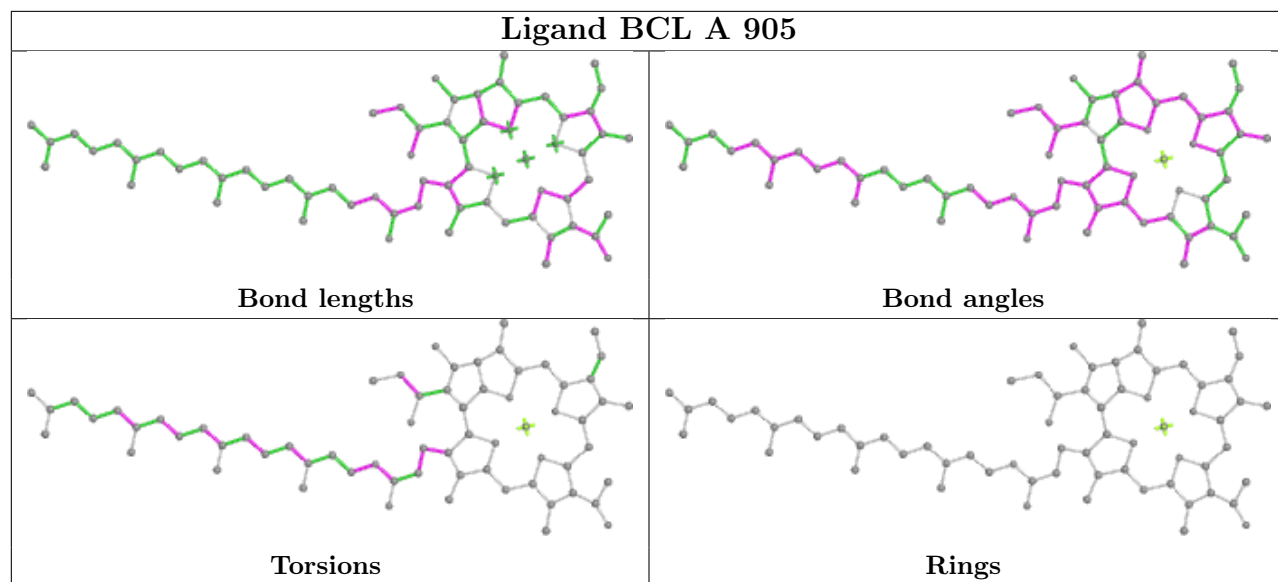
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

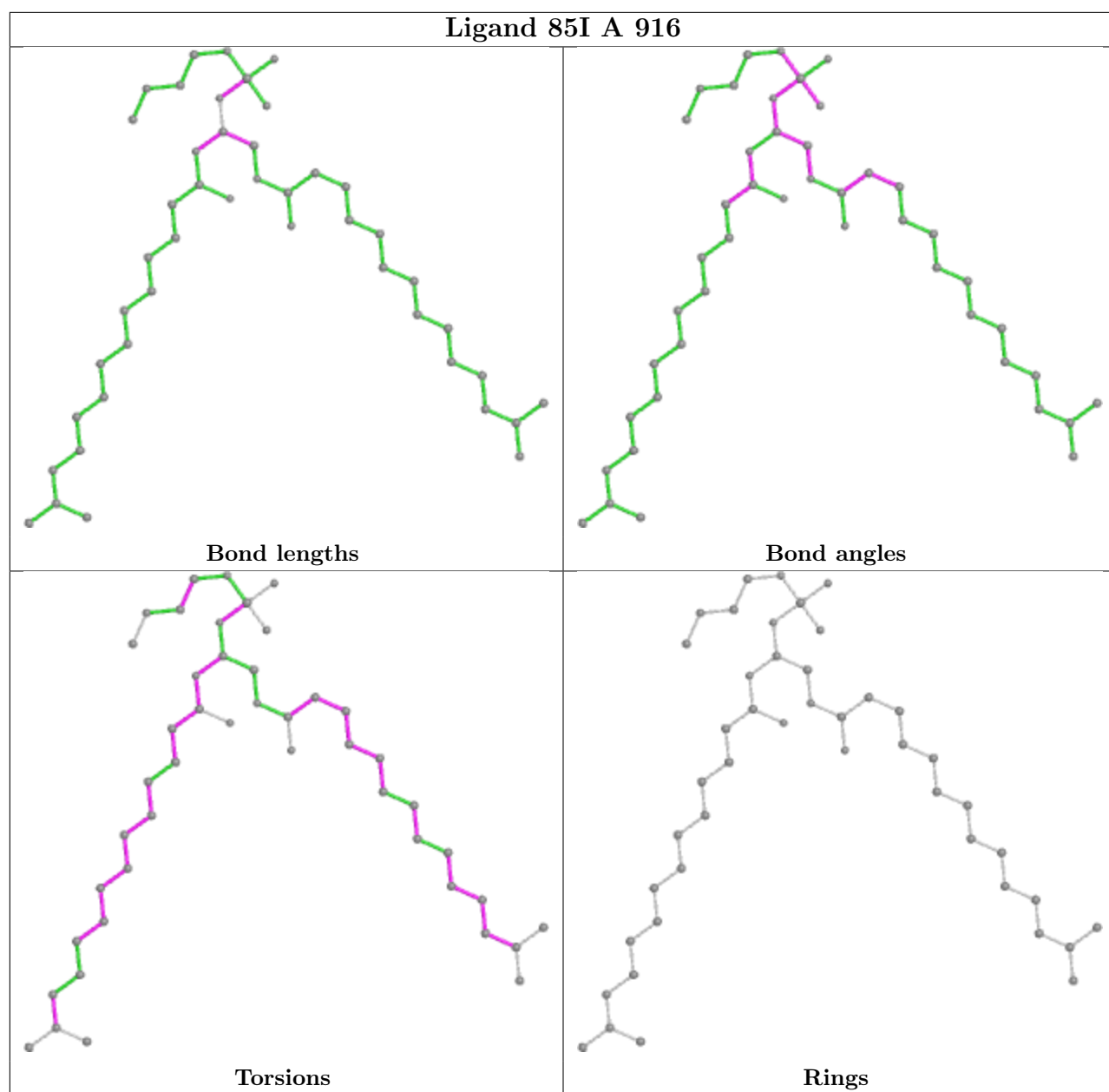


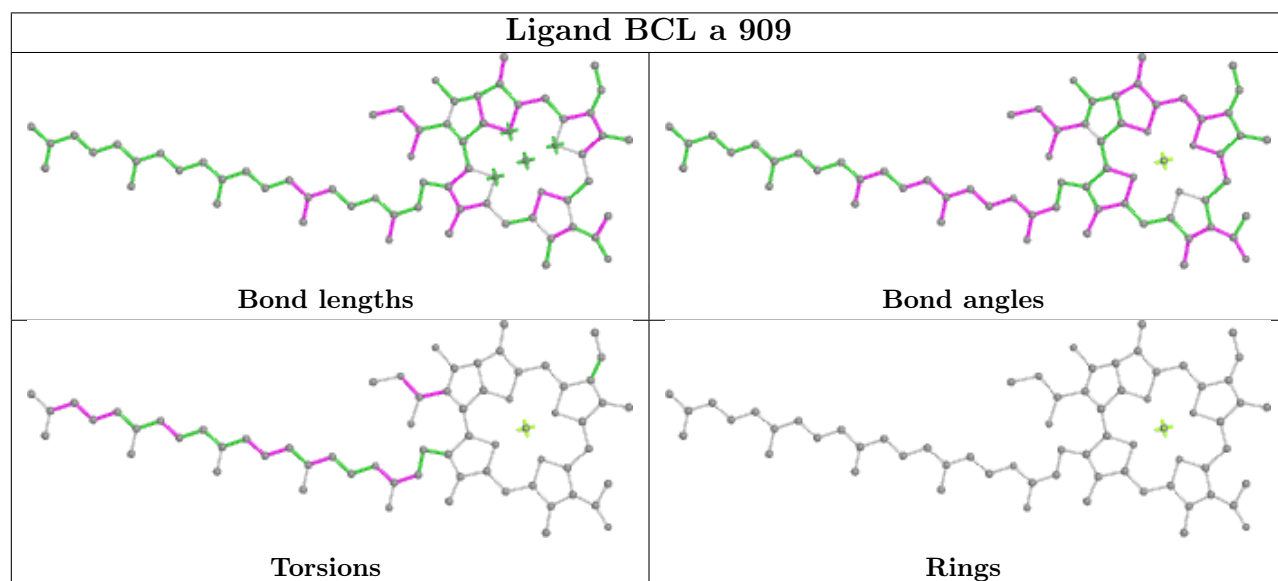
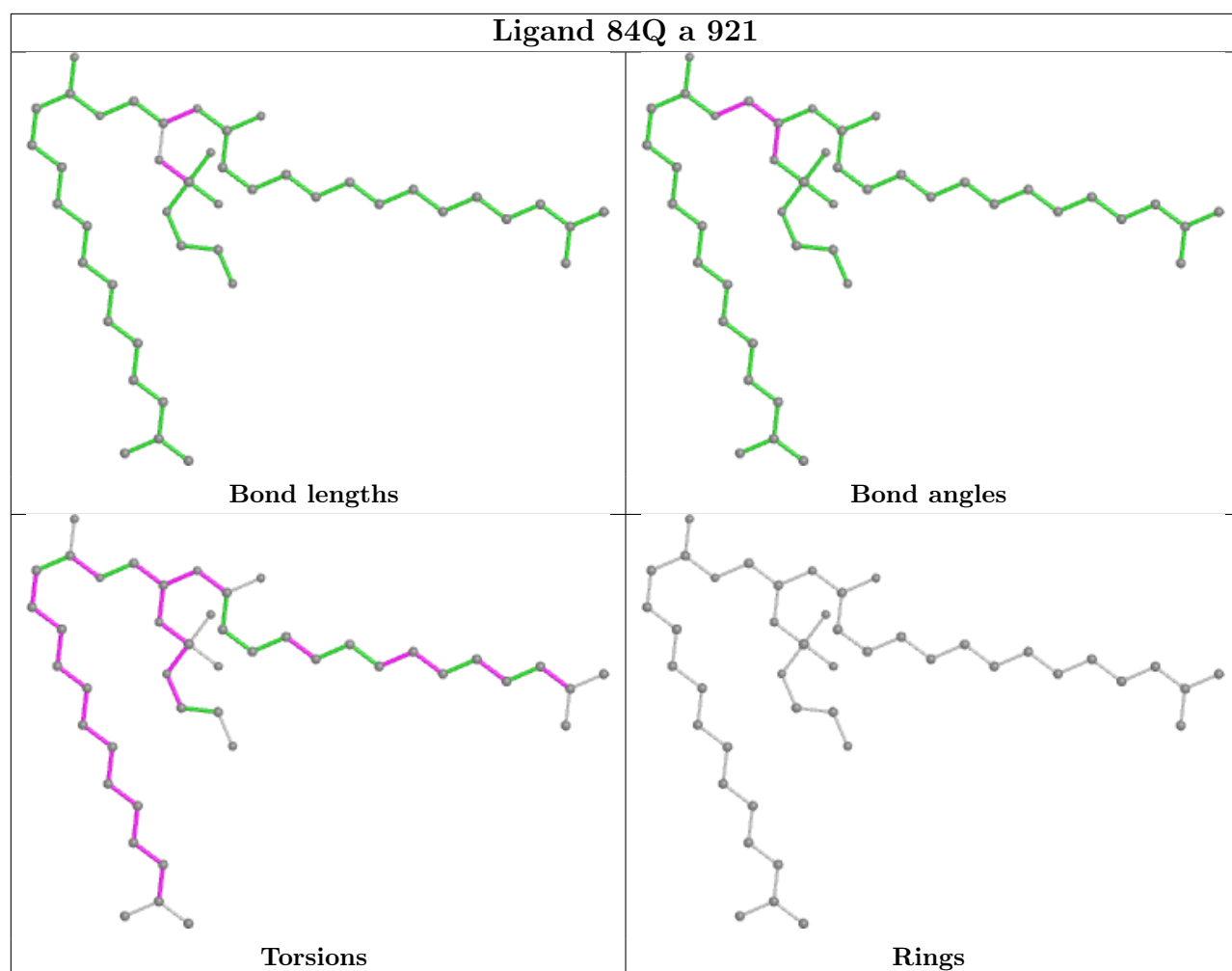


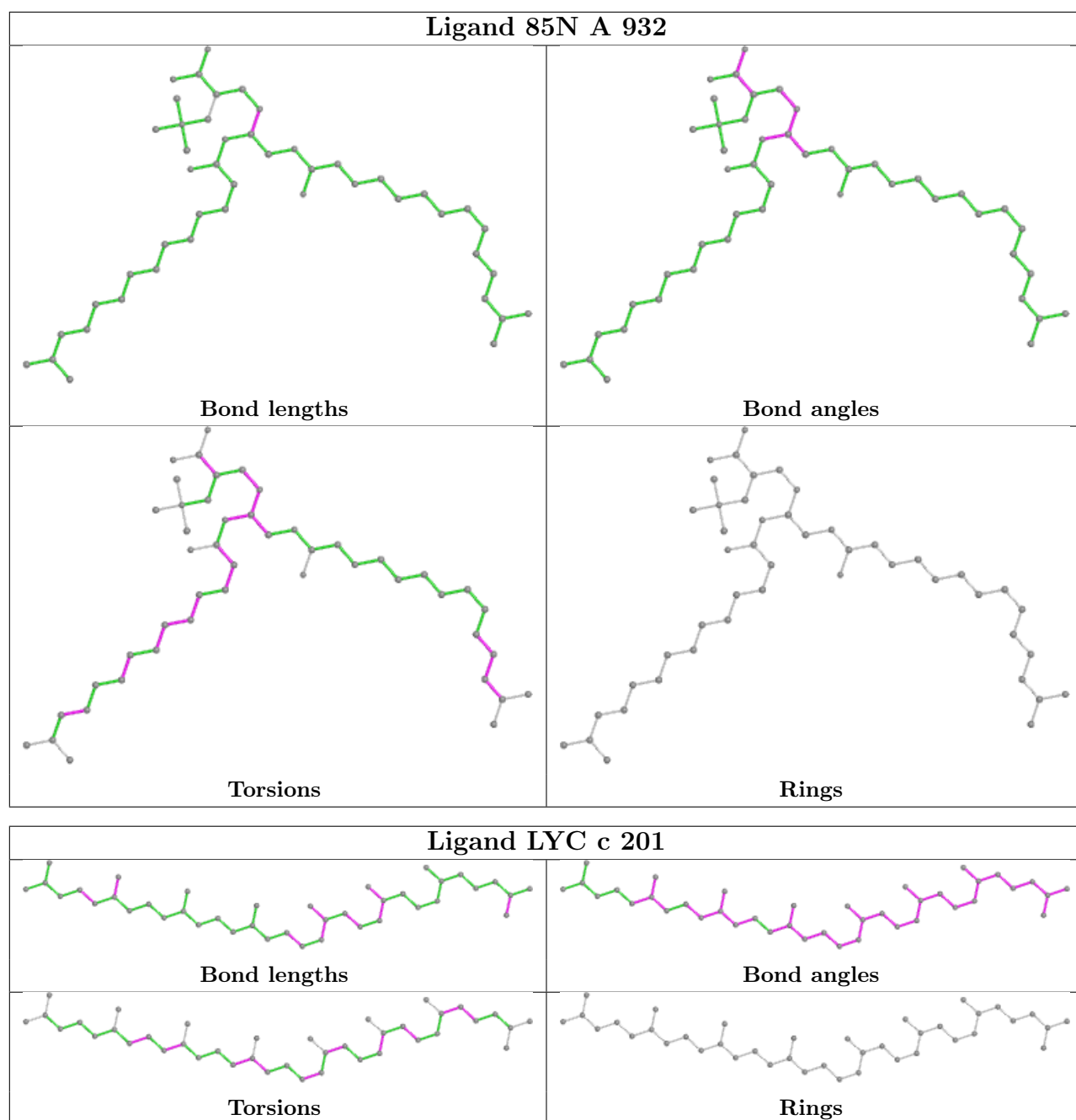


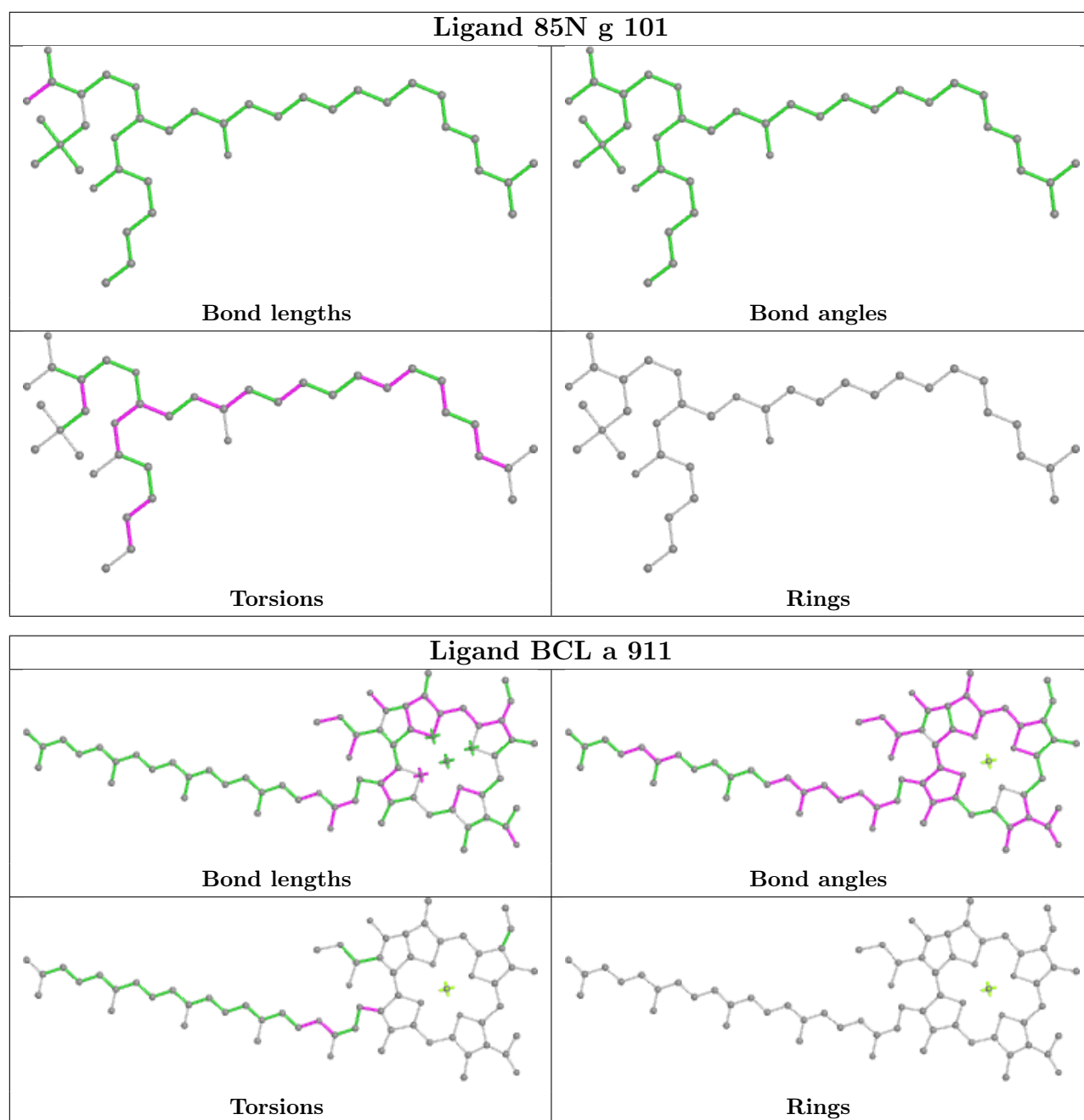




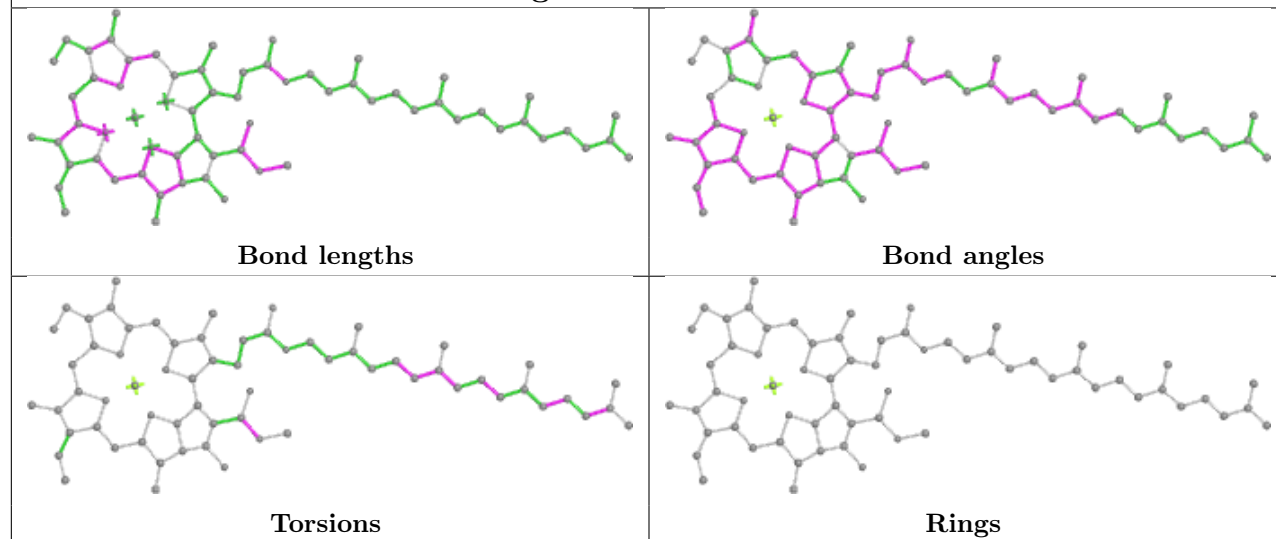




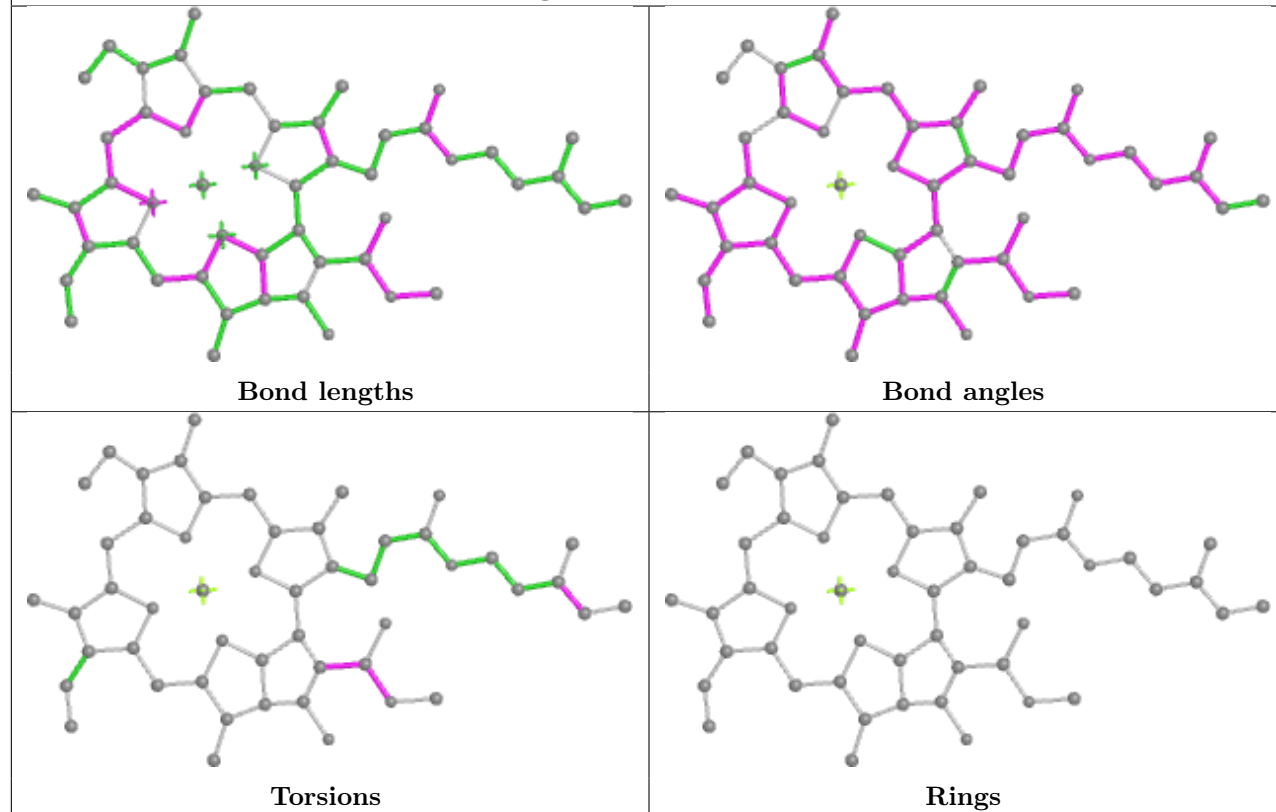


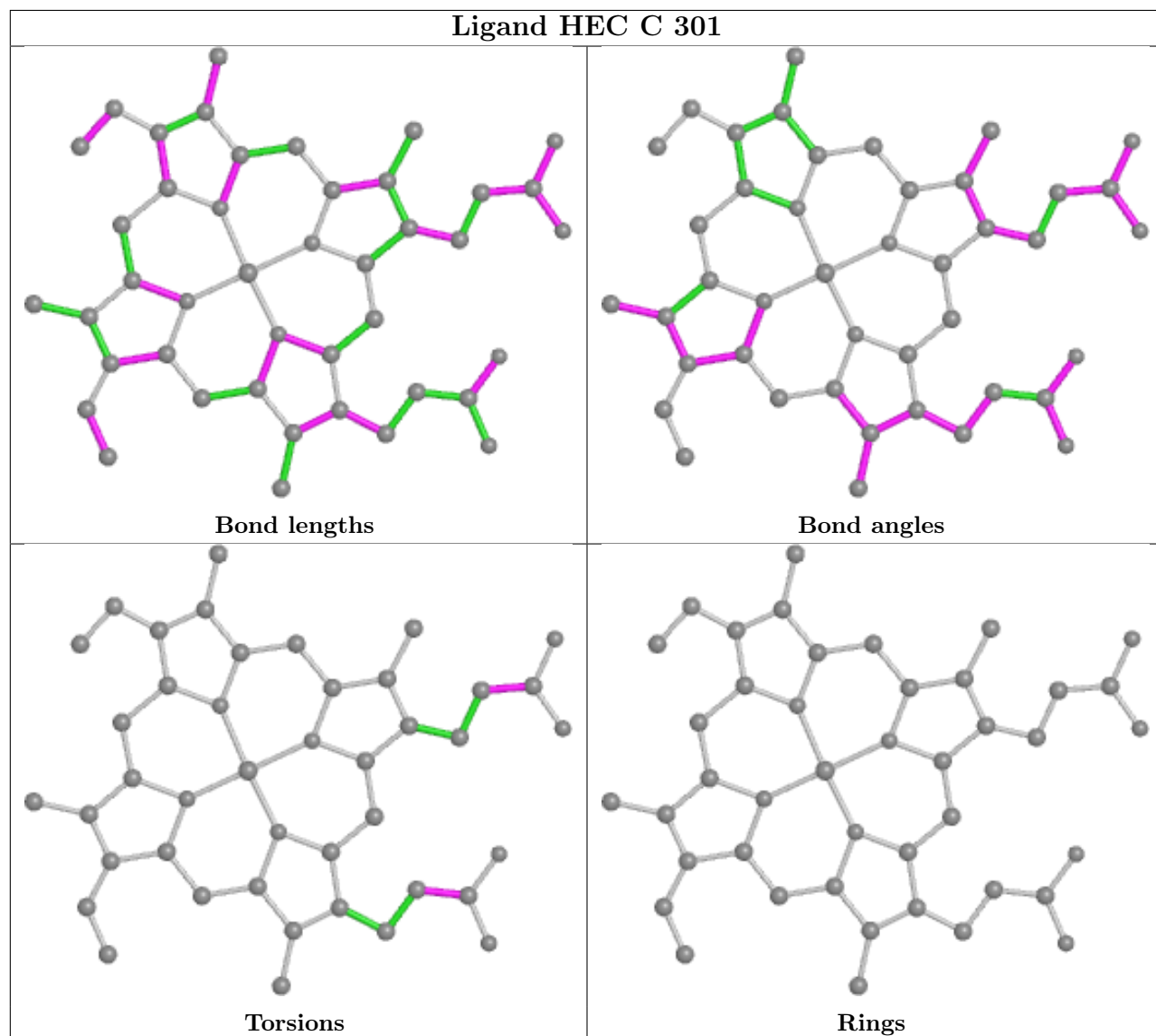
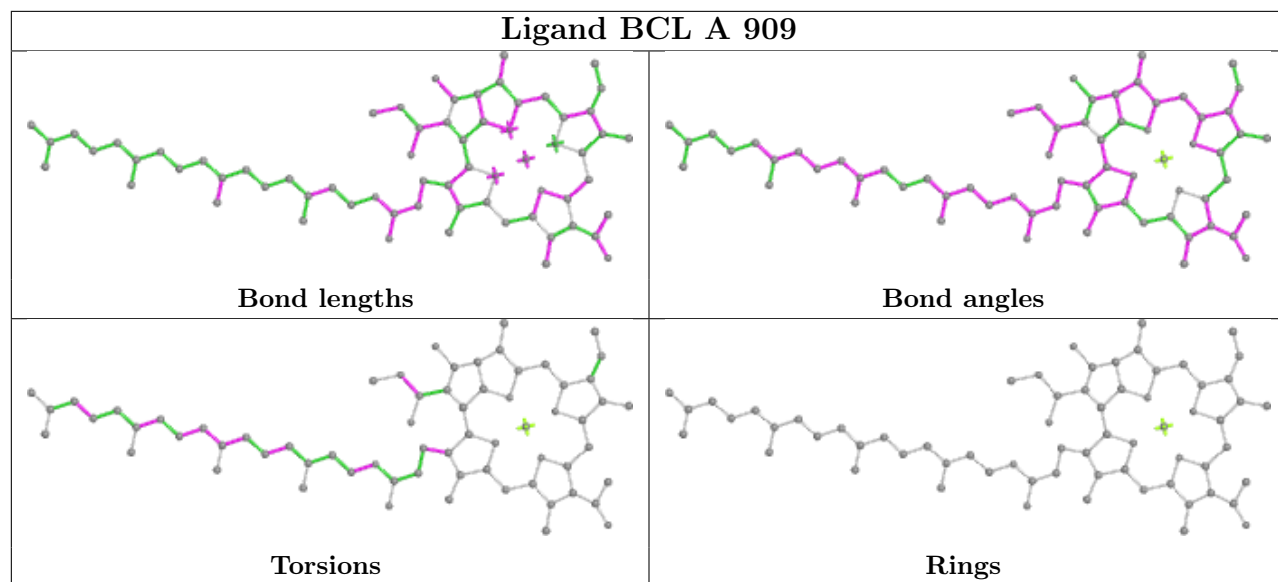


Ligand CLA A 910

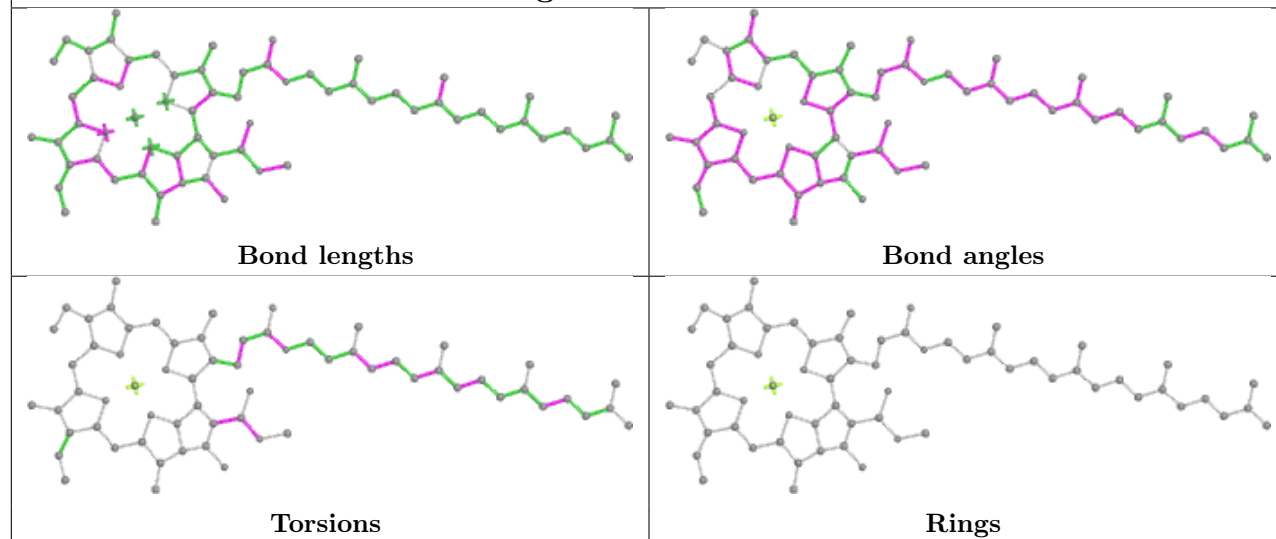


Ligand CLA a 915

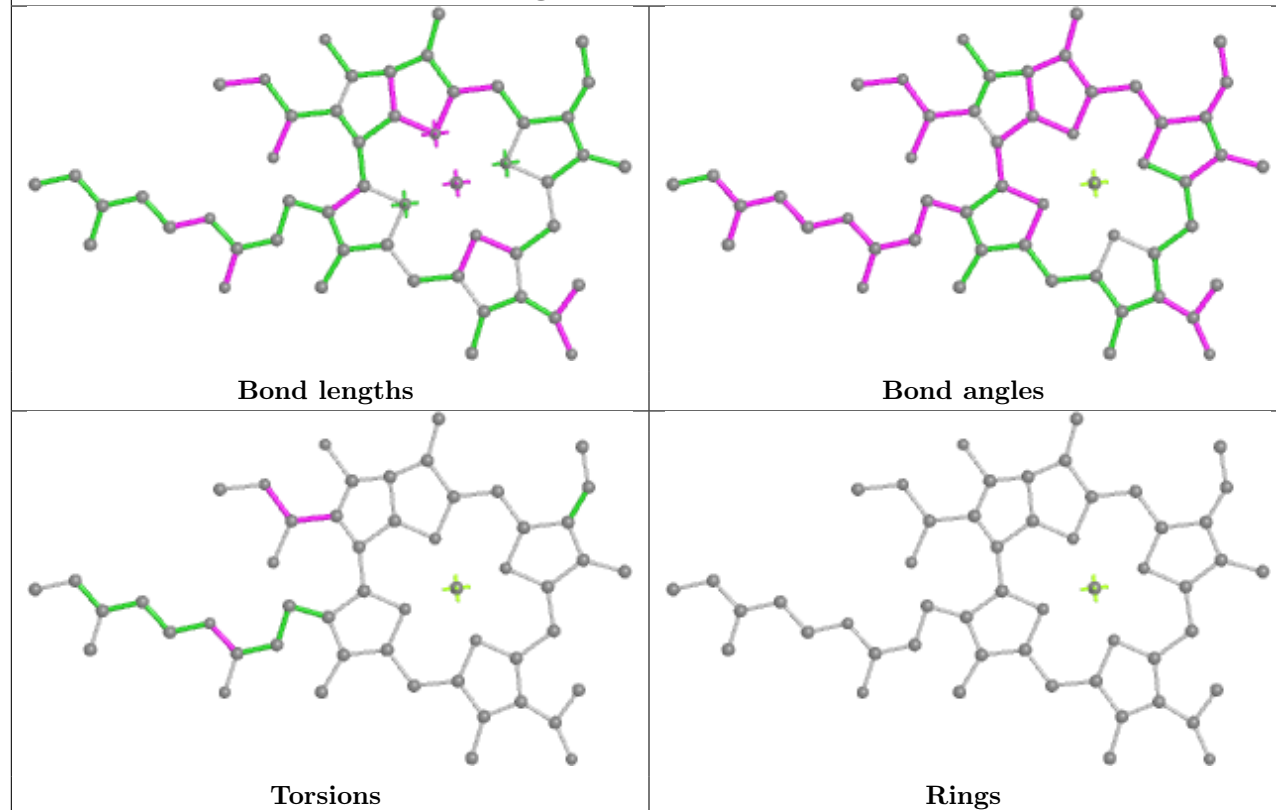




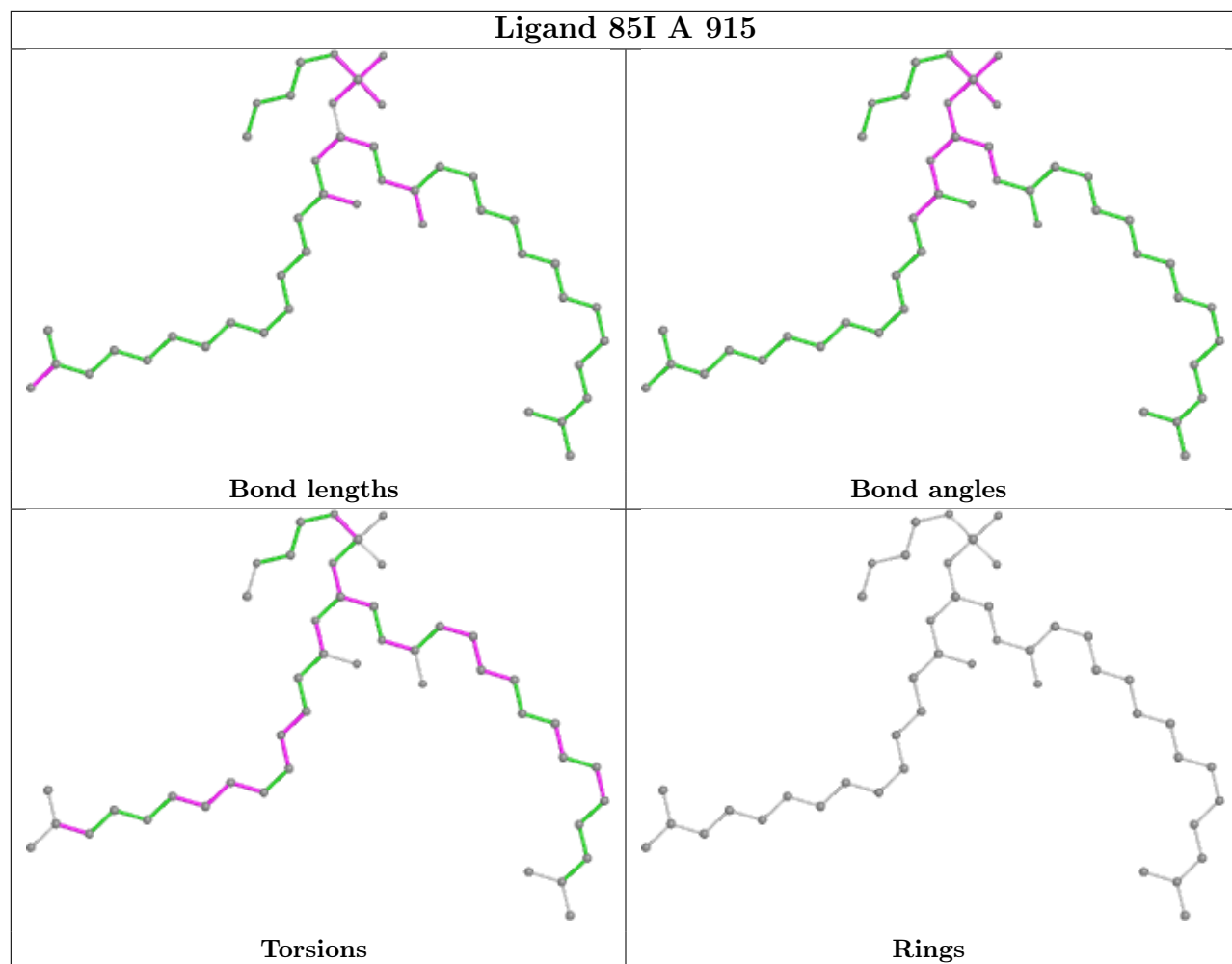
Ligand CLA a 912



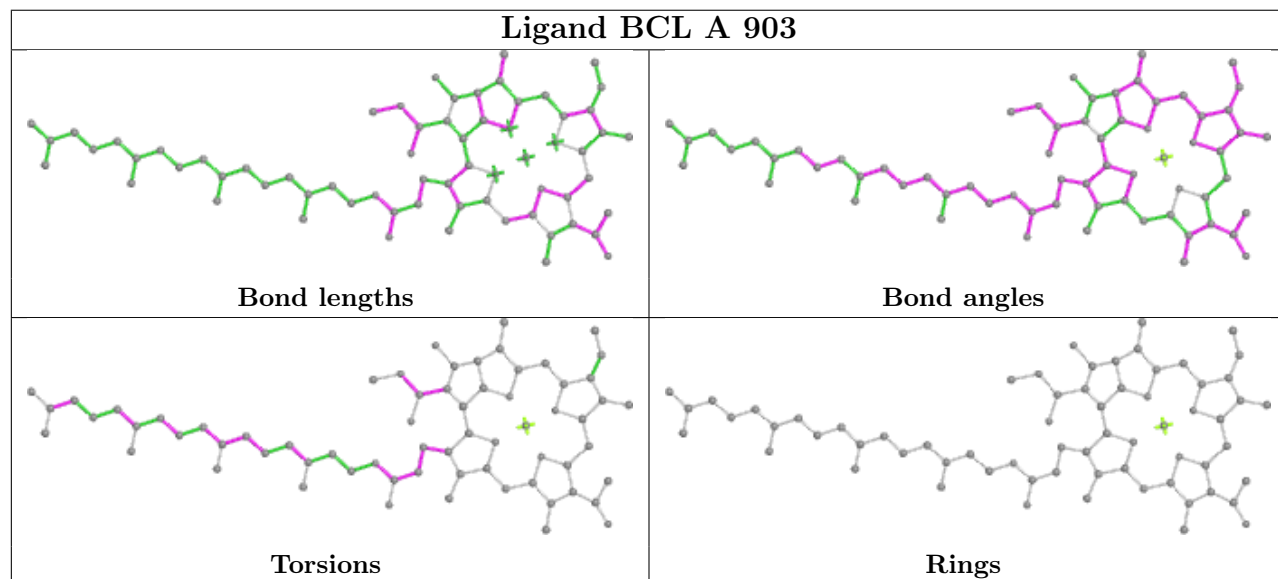
Ligand BCL A 906

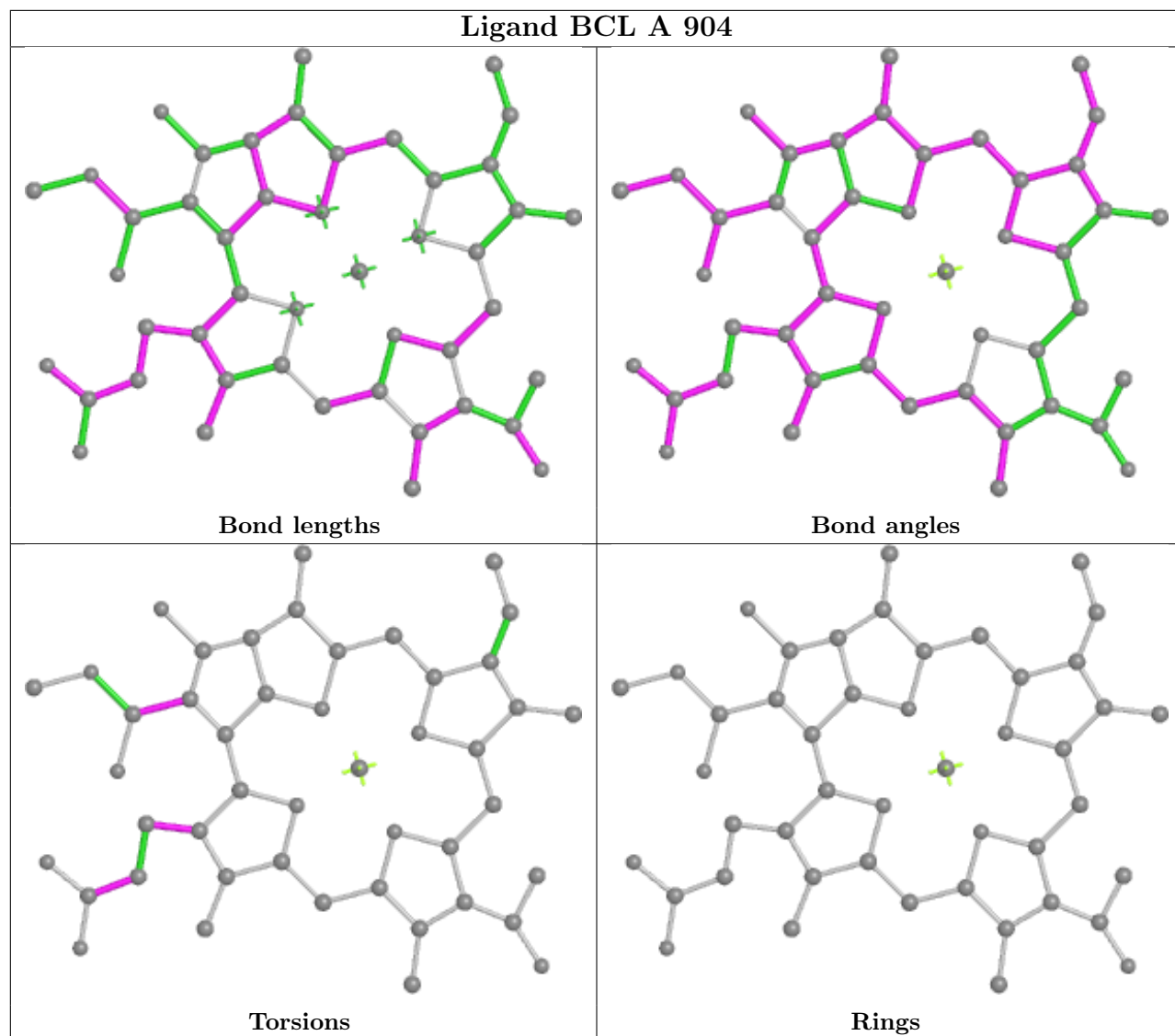


Ligand 85I A 915

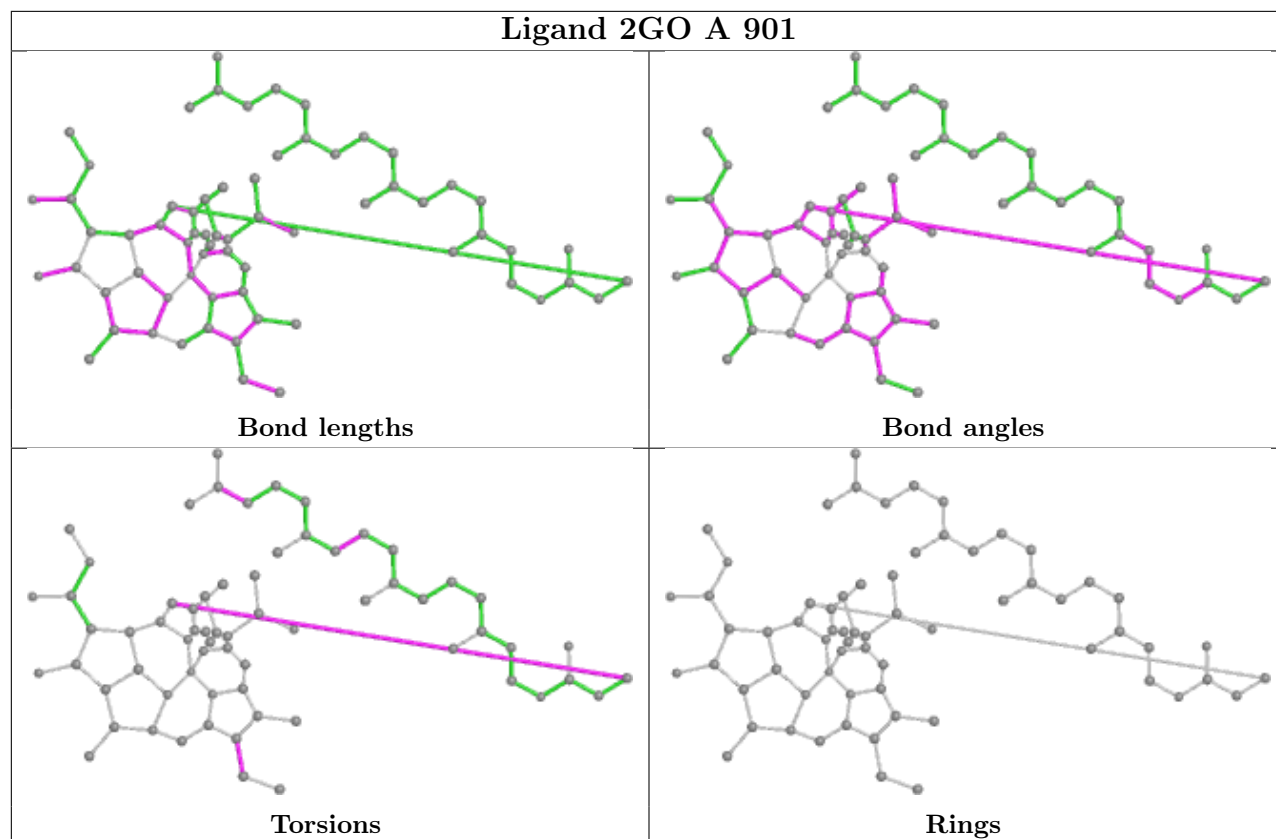


Ligand BCL A 903

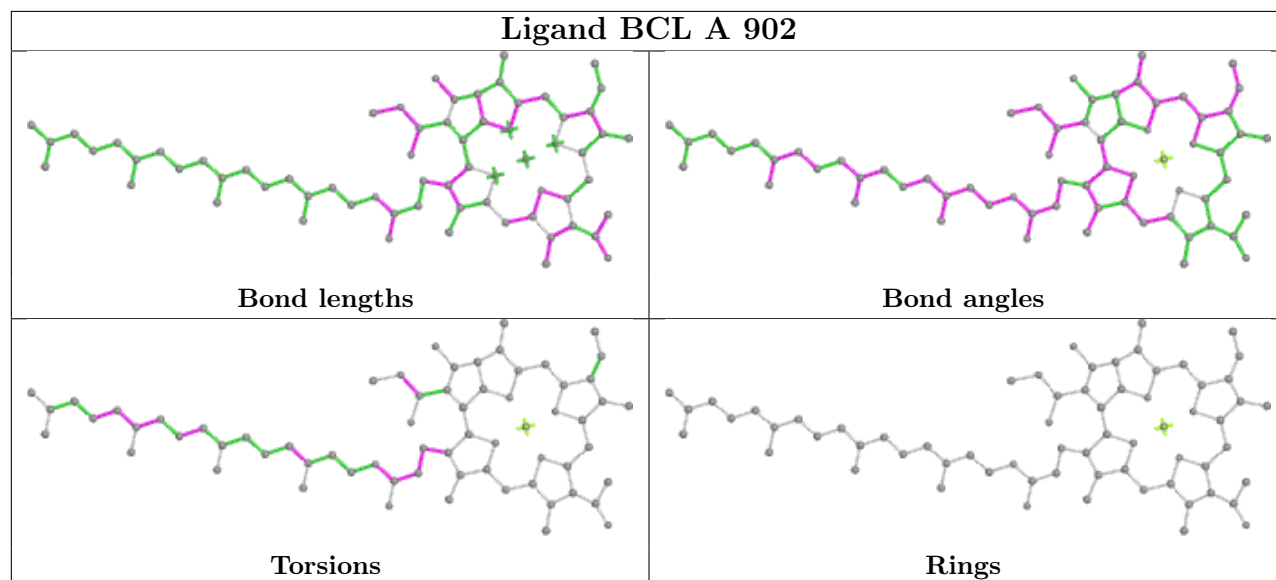


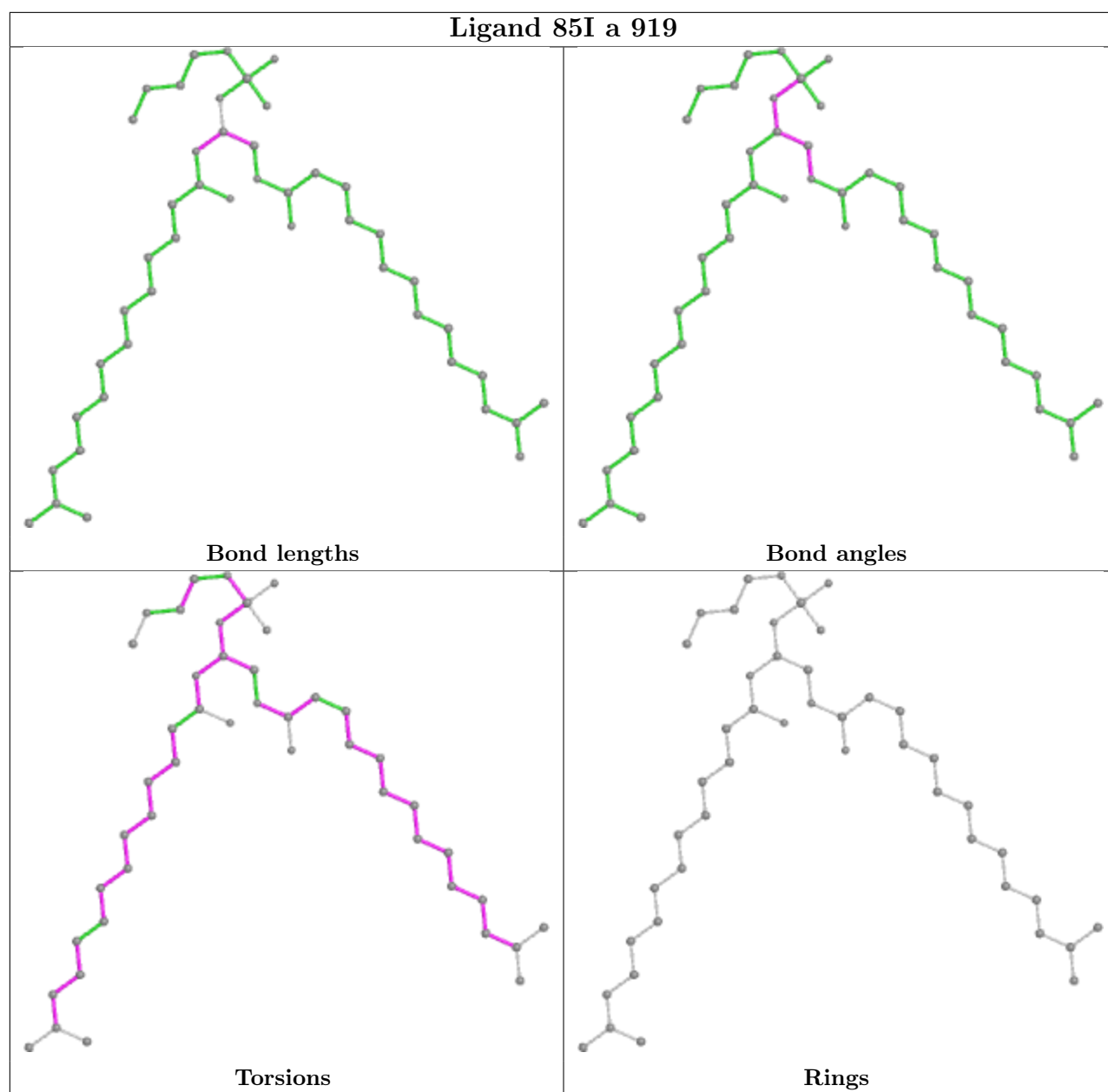


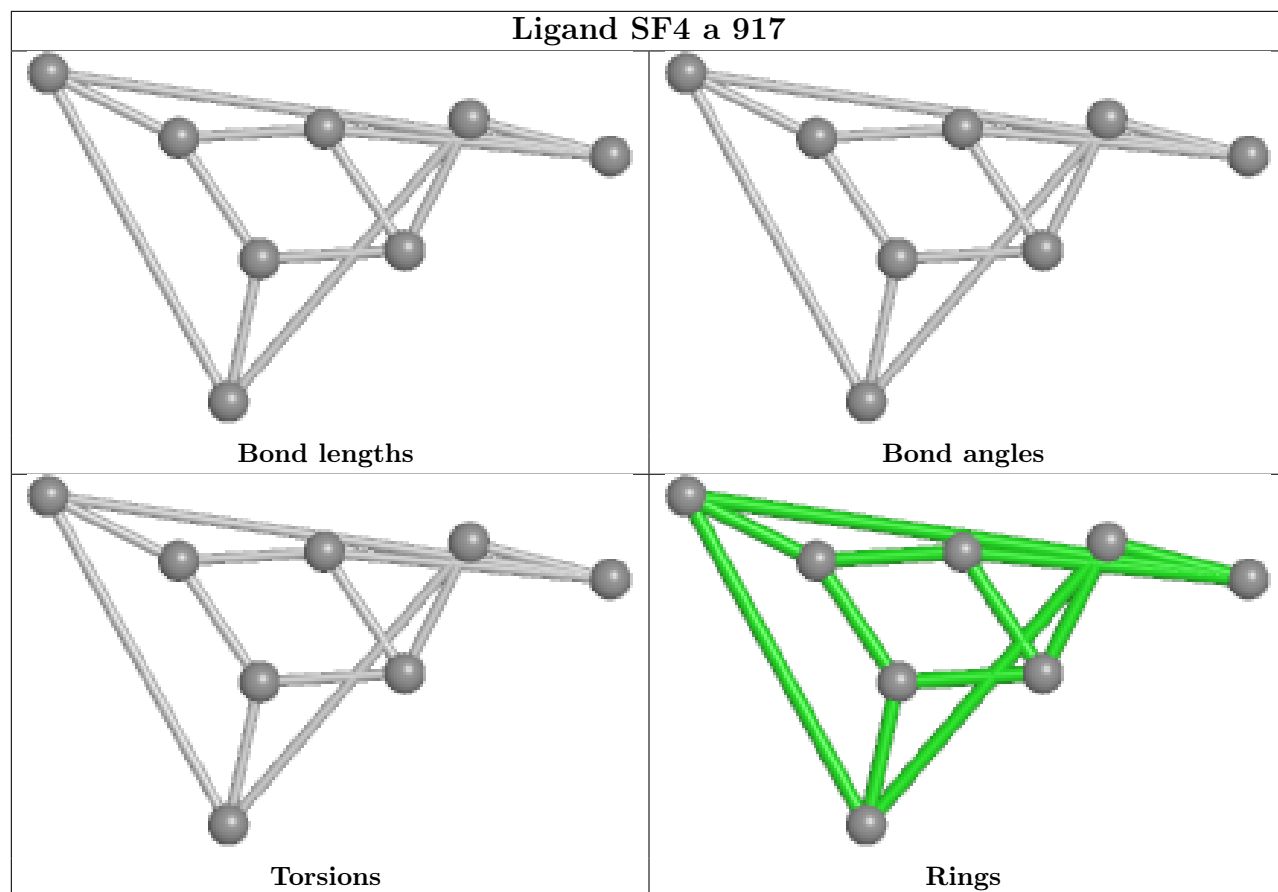
Ligand 2GO A 901

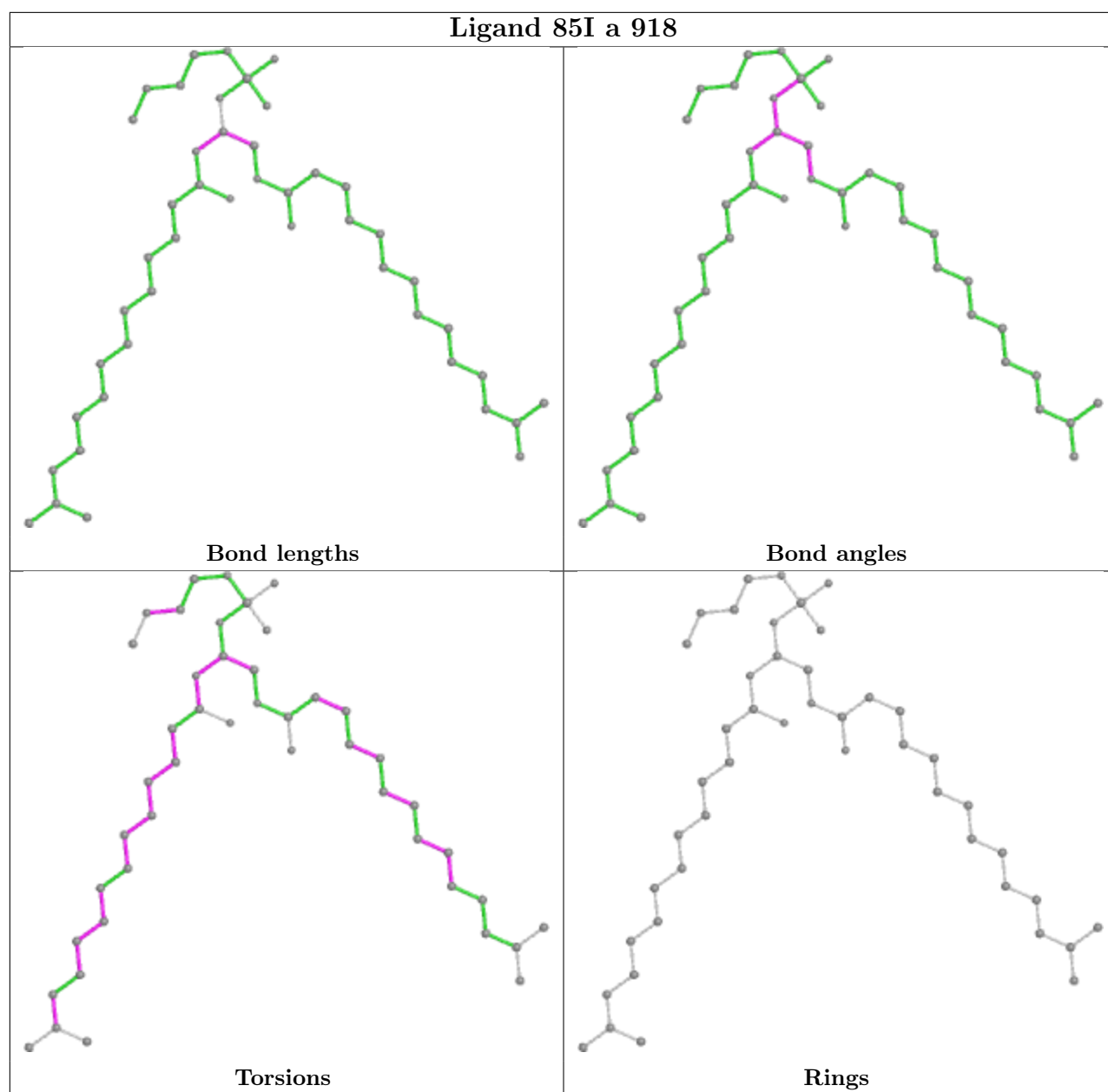


Ligand BCL A 902

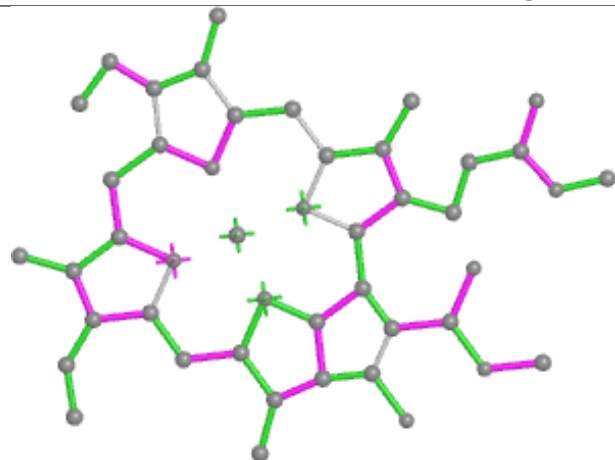




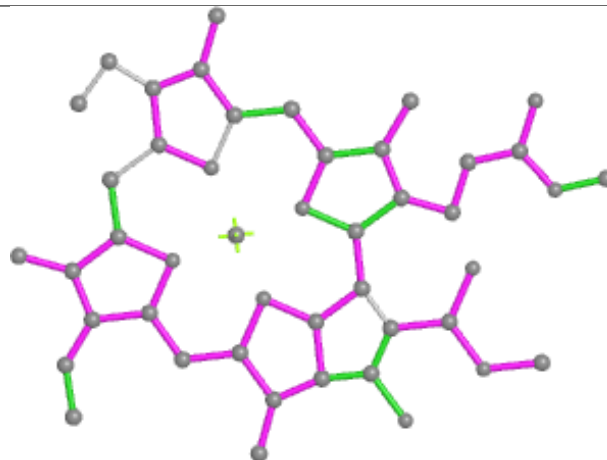




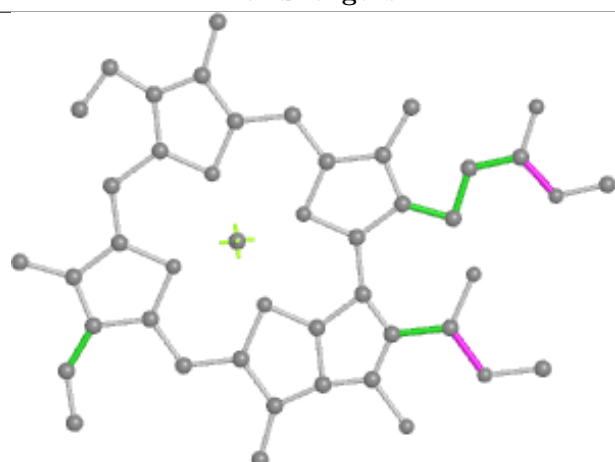
Ligand CLA a 914



Bond lengths



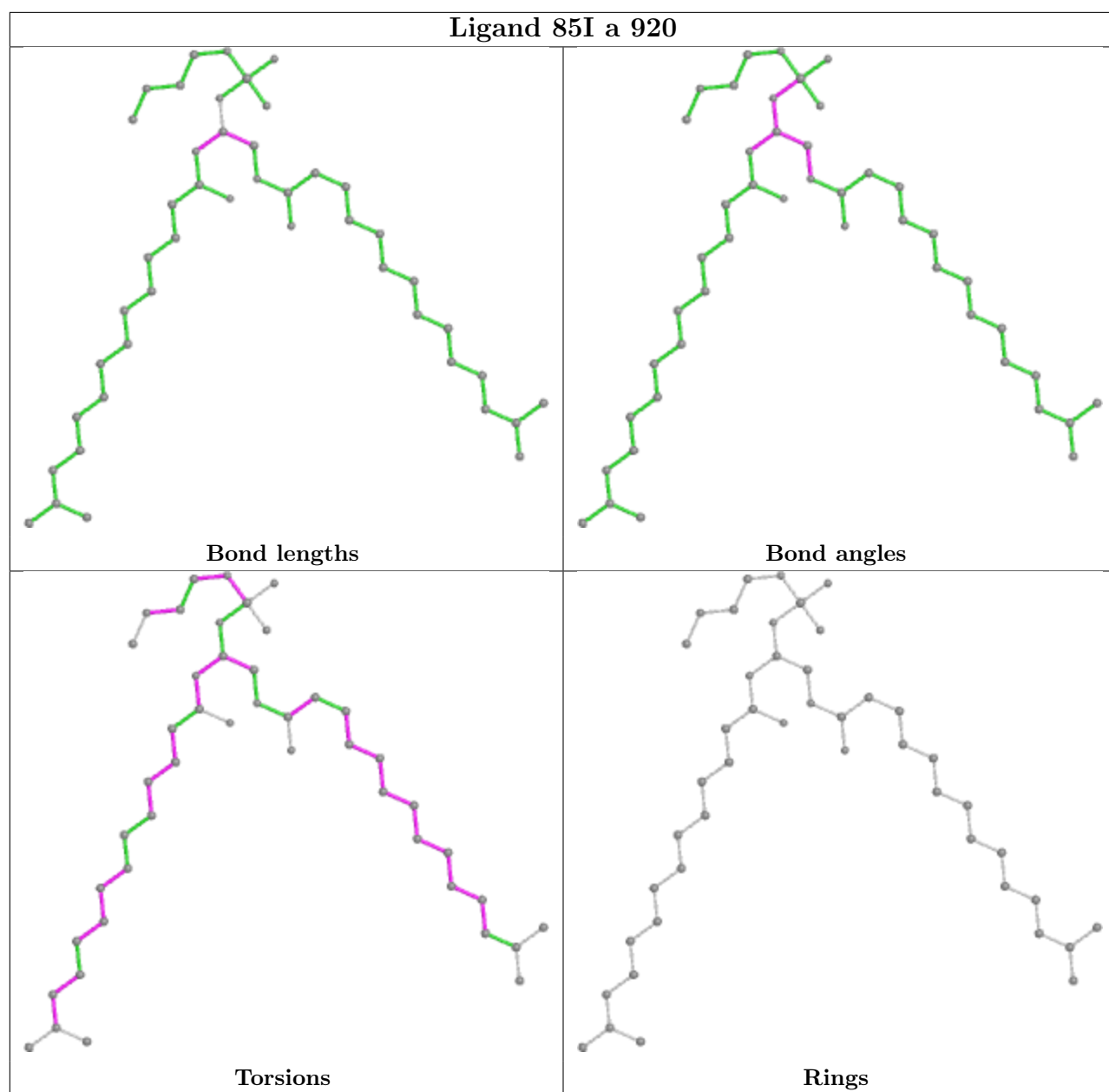
Bond angles



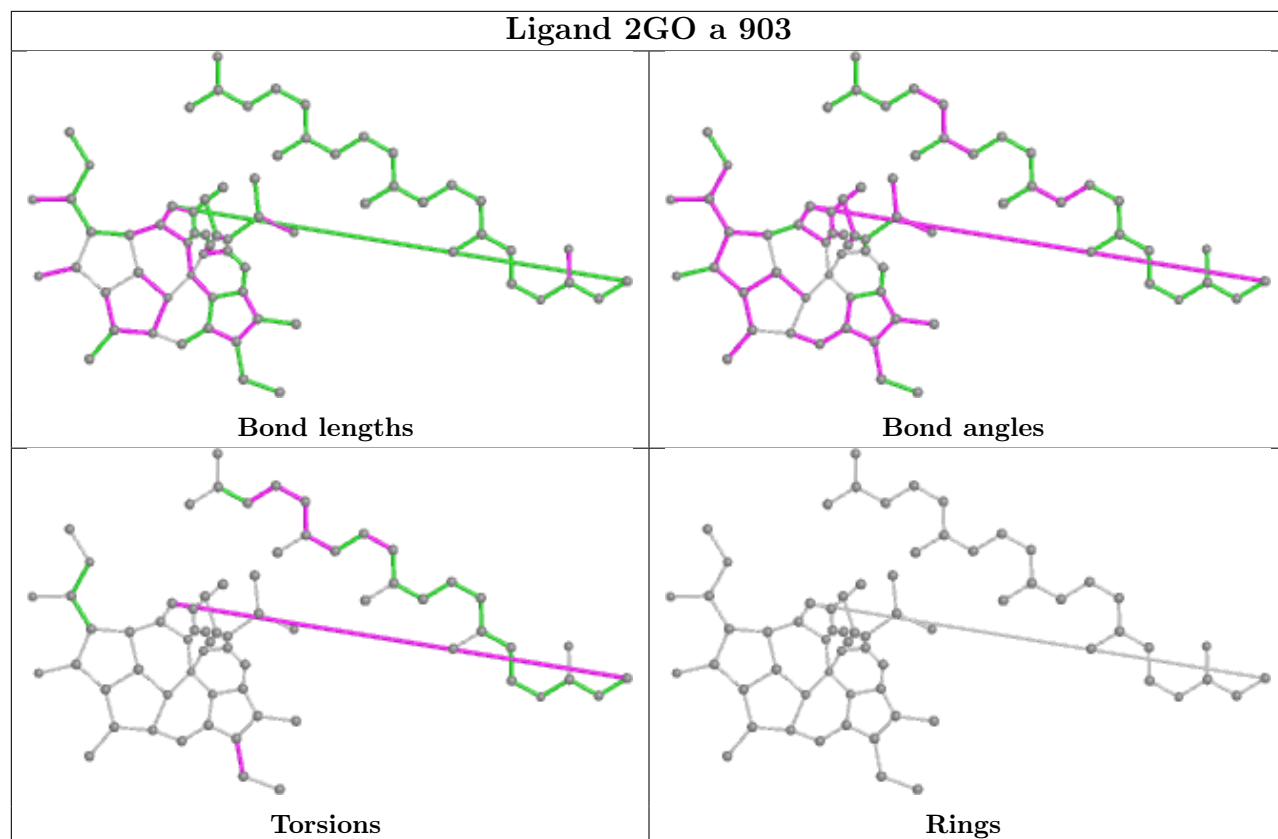
Torsions



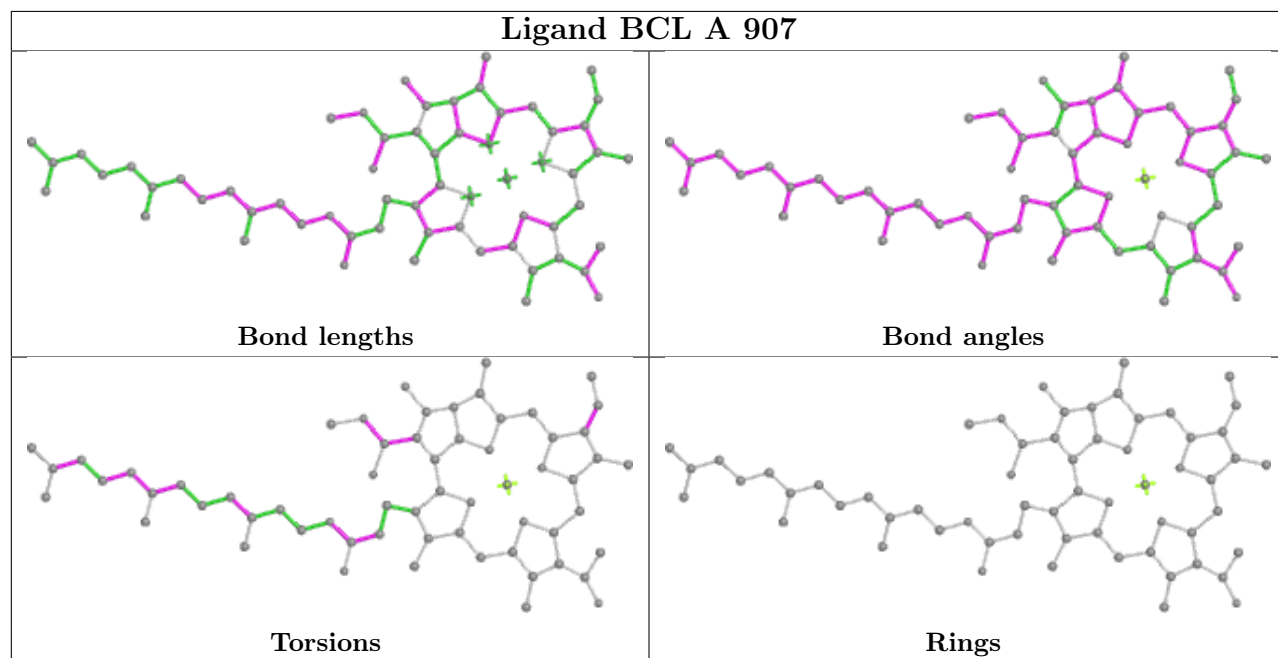
Rings

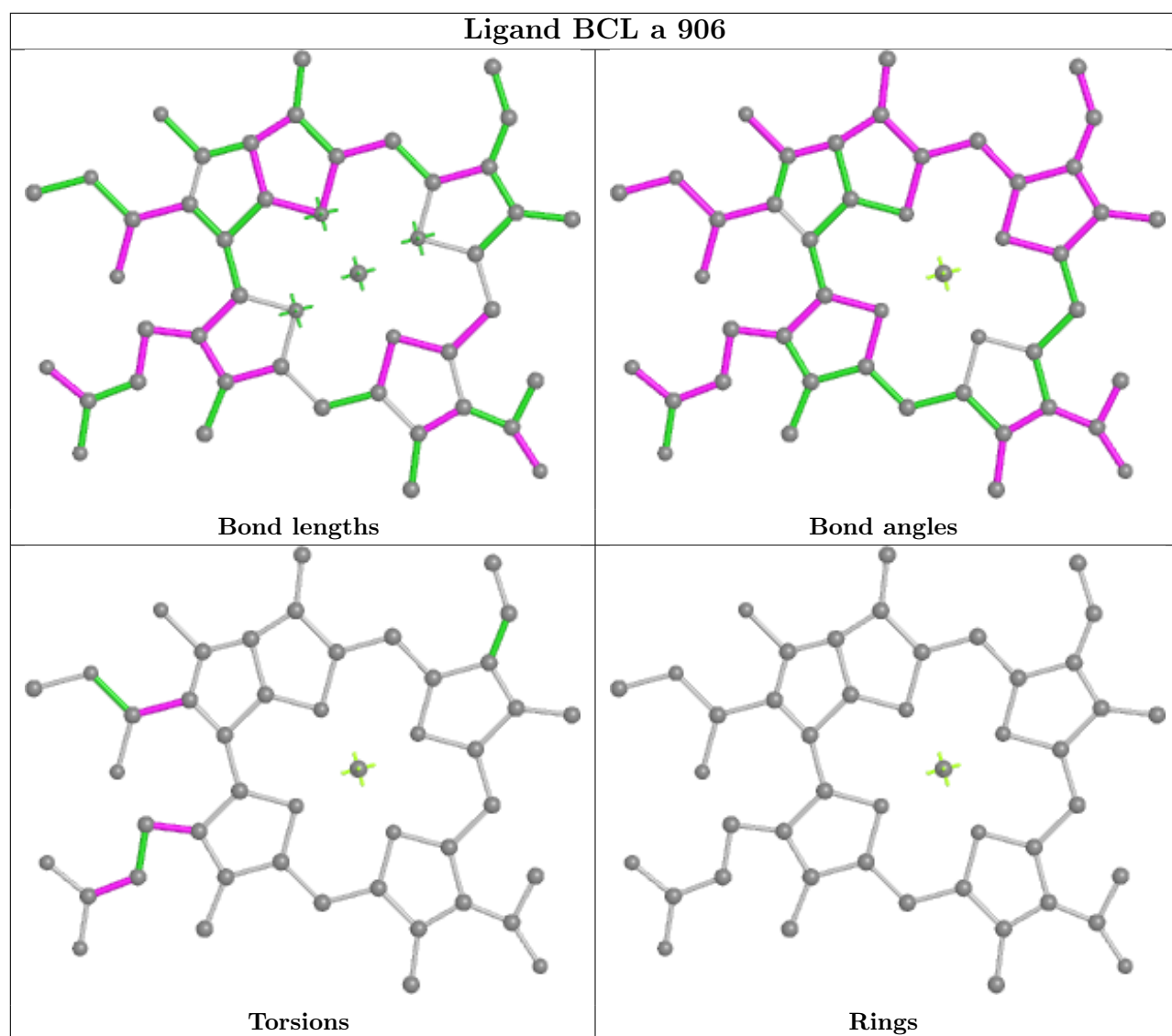


Ligand 2GO a 903

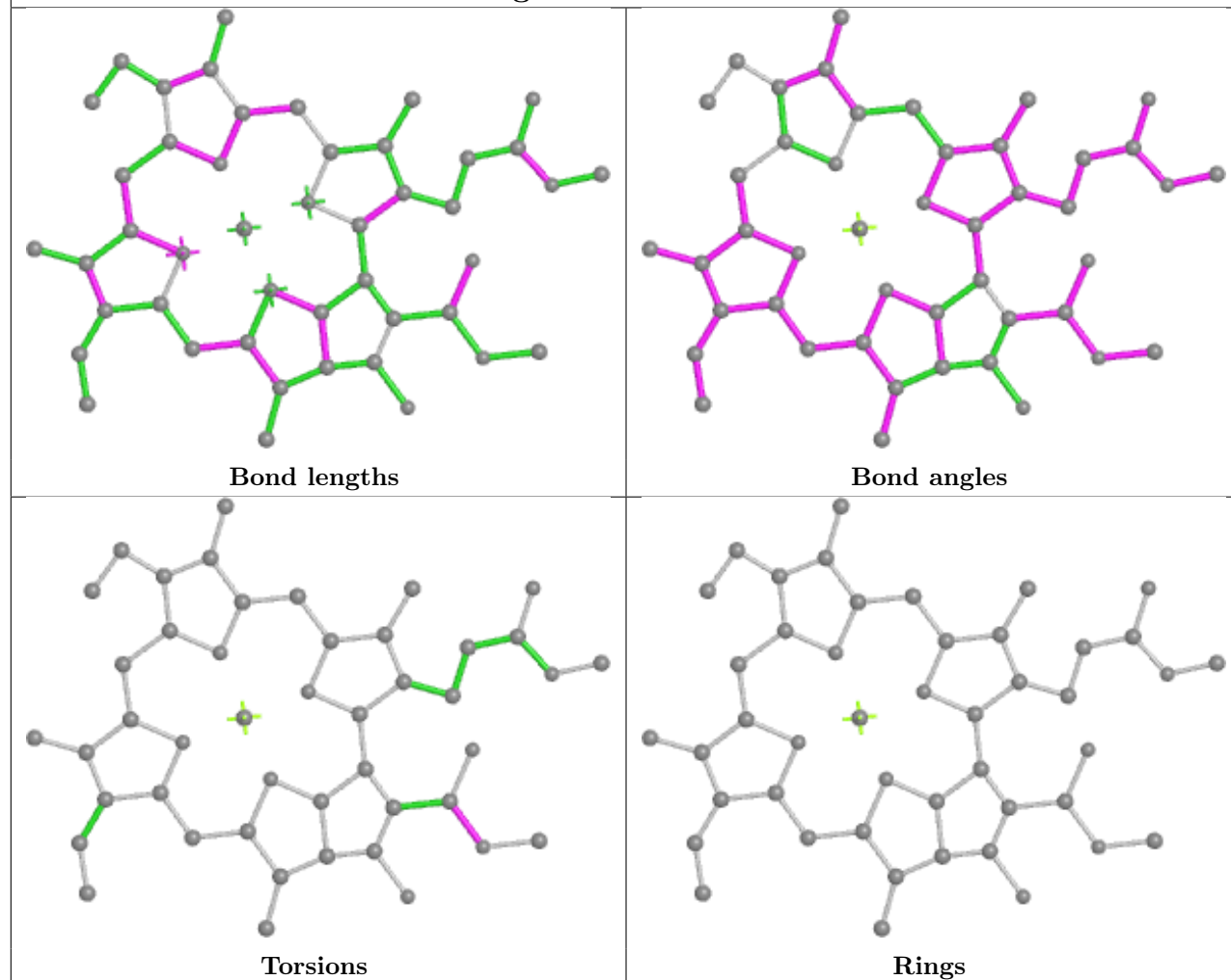


Ligand BCL A 907

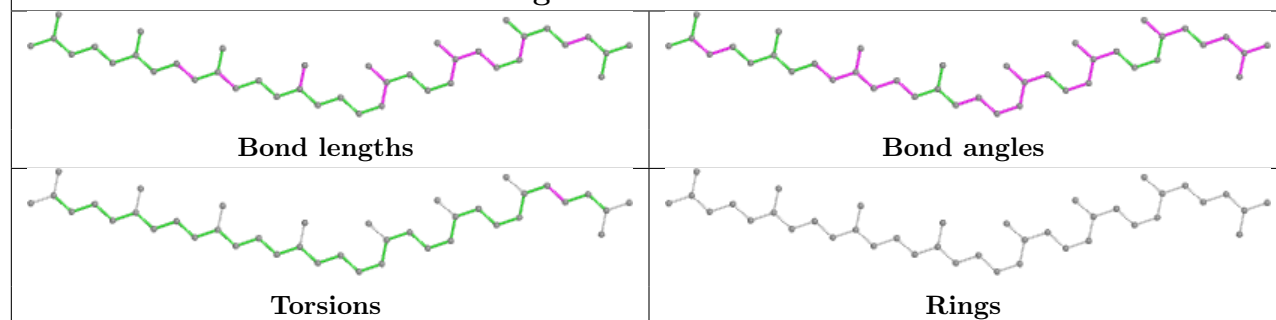


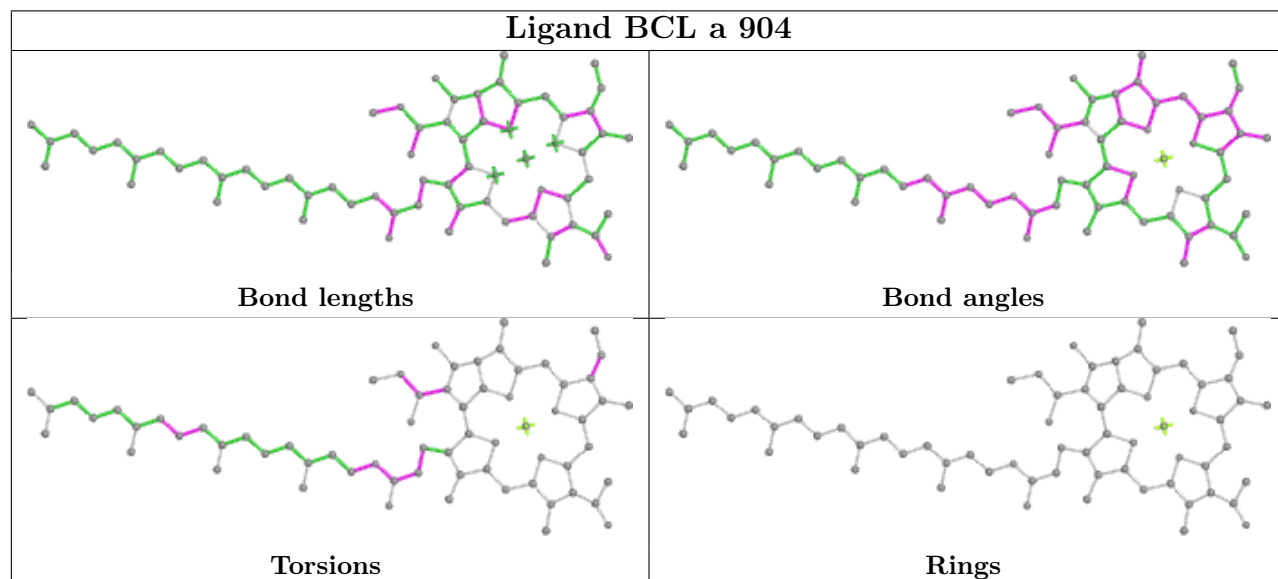
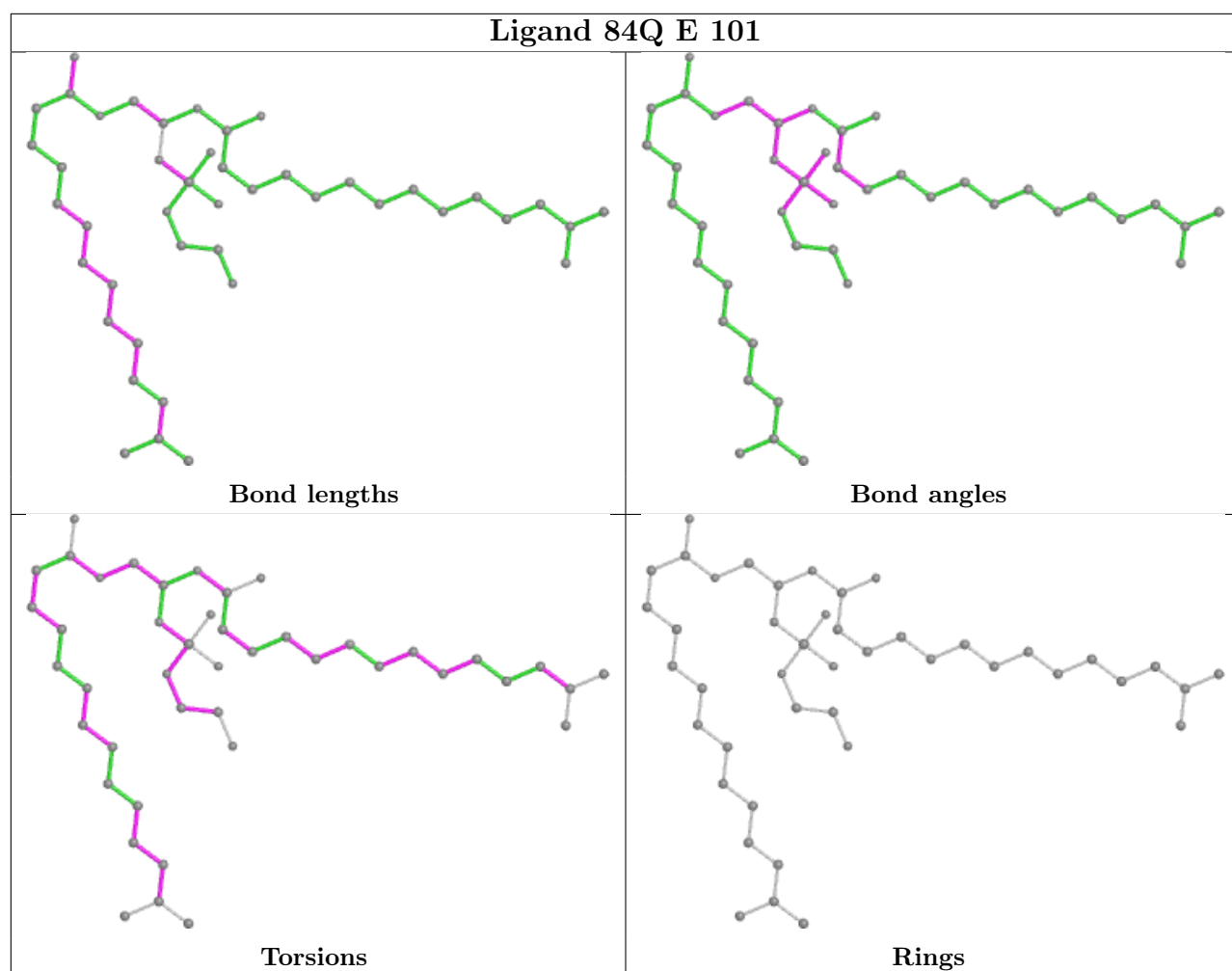


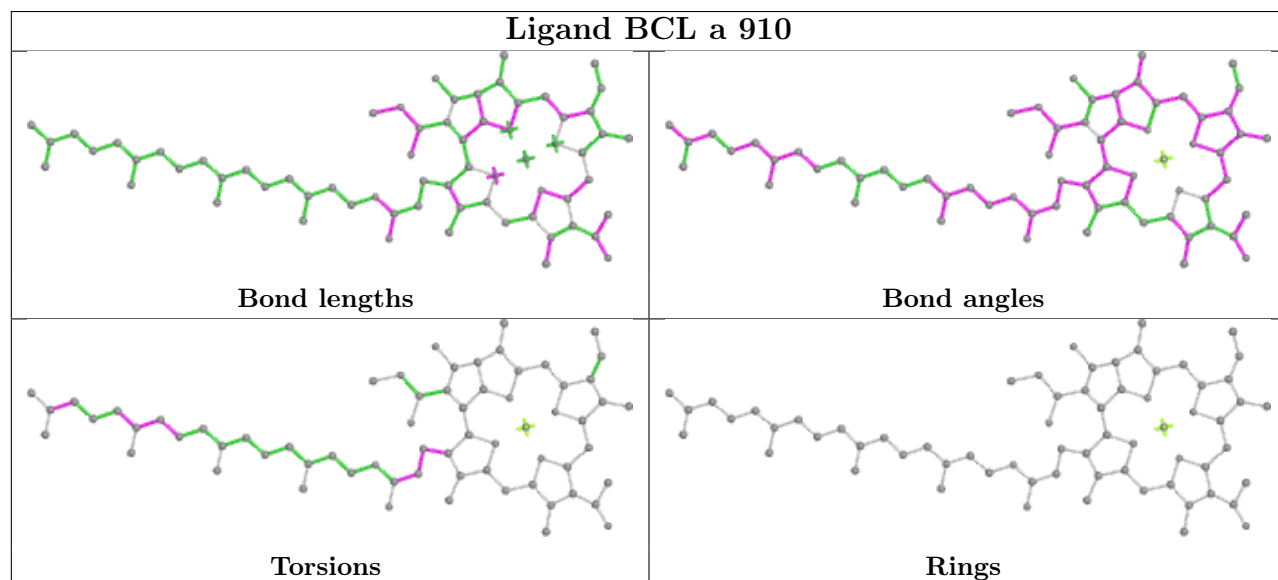
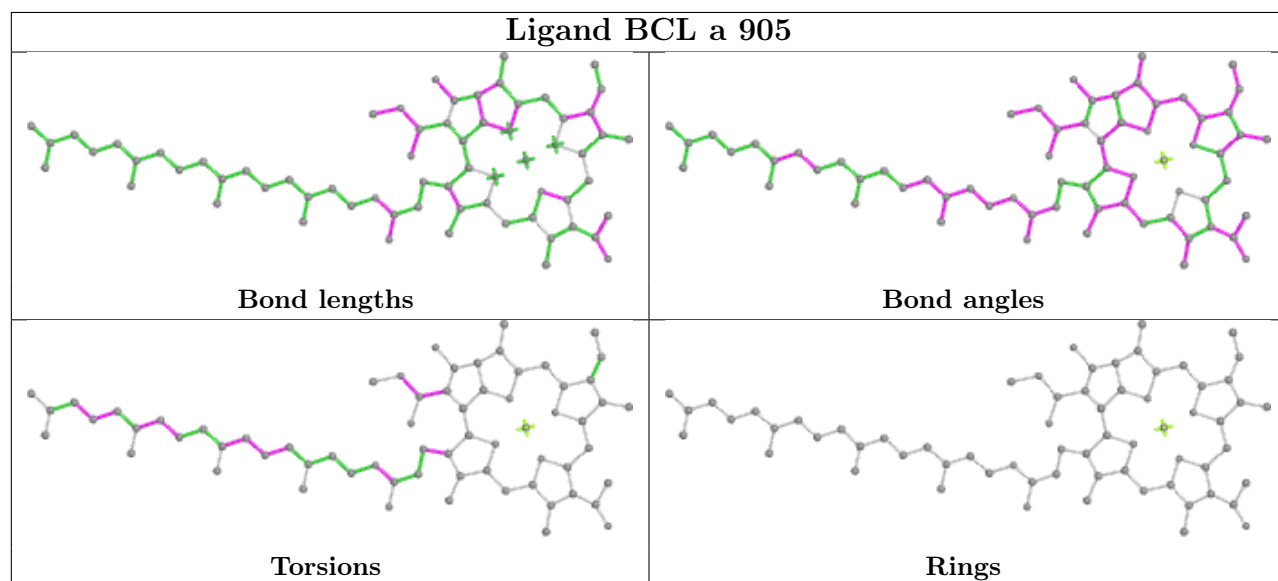
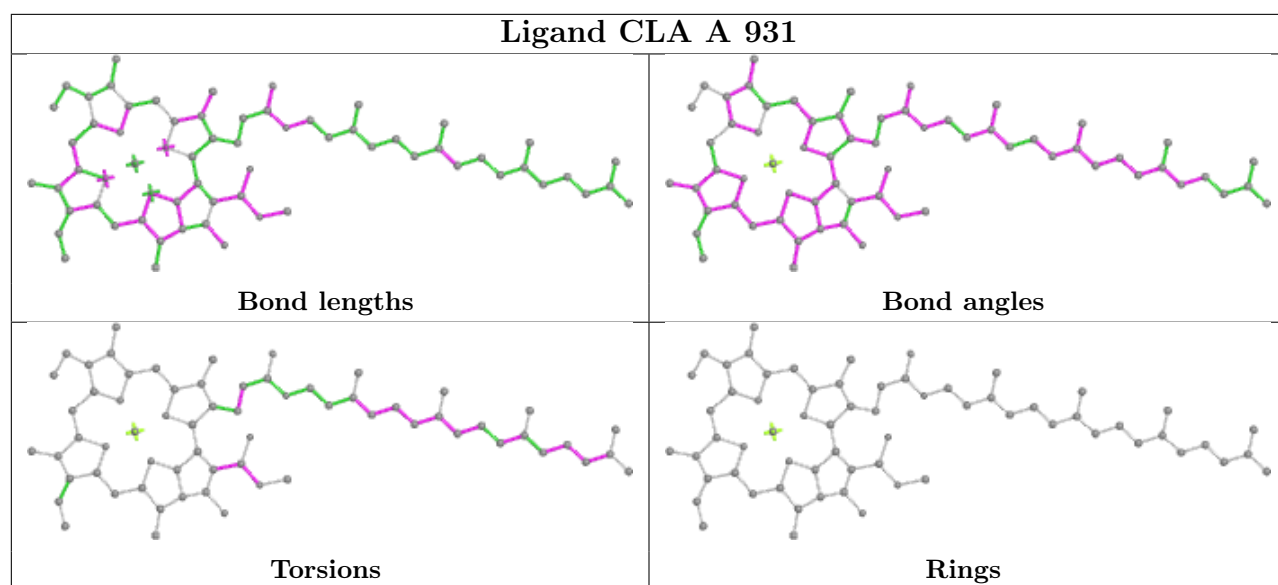
Ligand CLA A 912



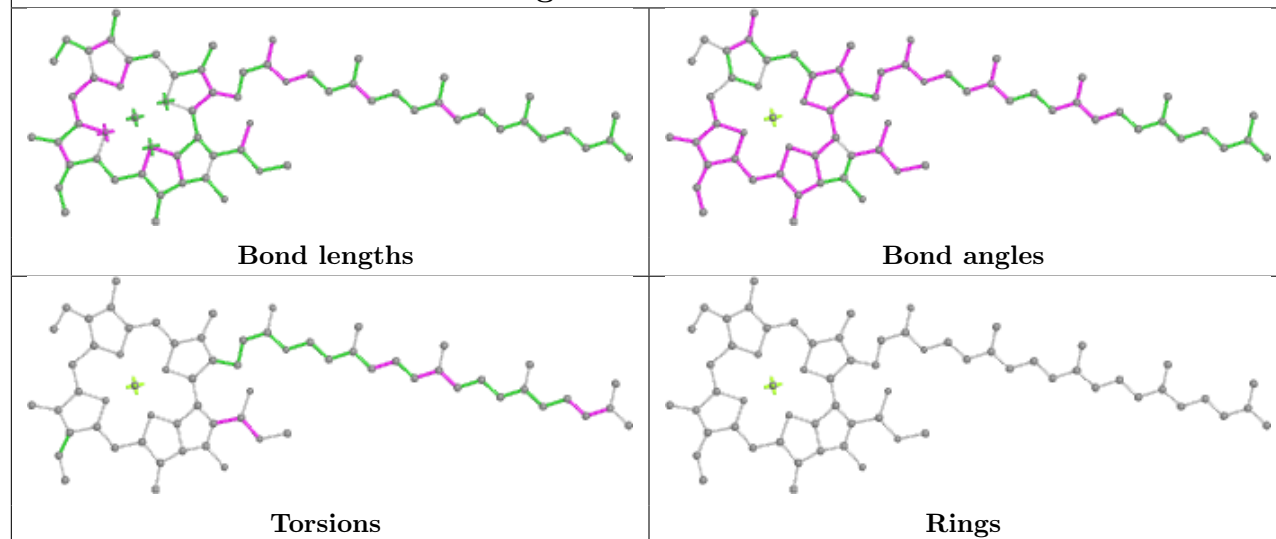
Ligand LYC A 913



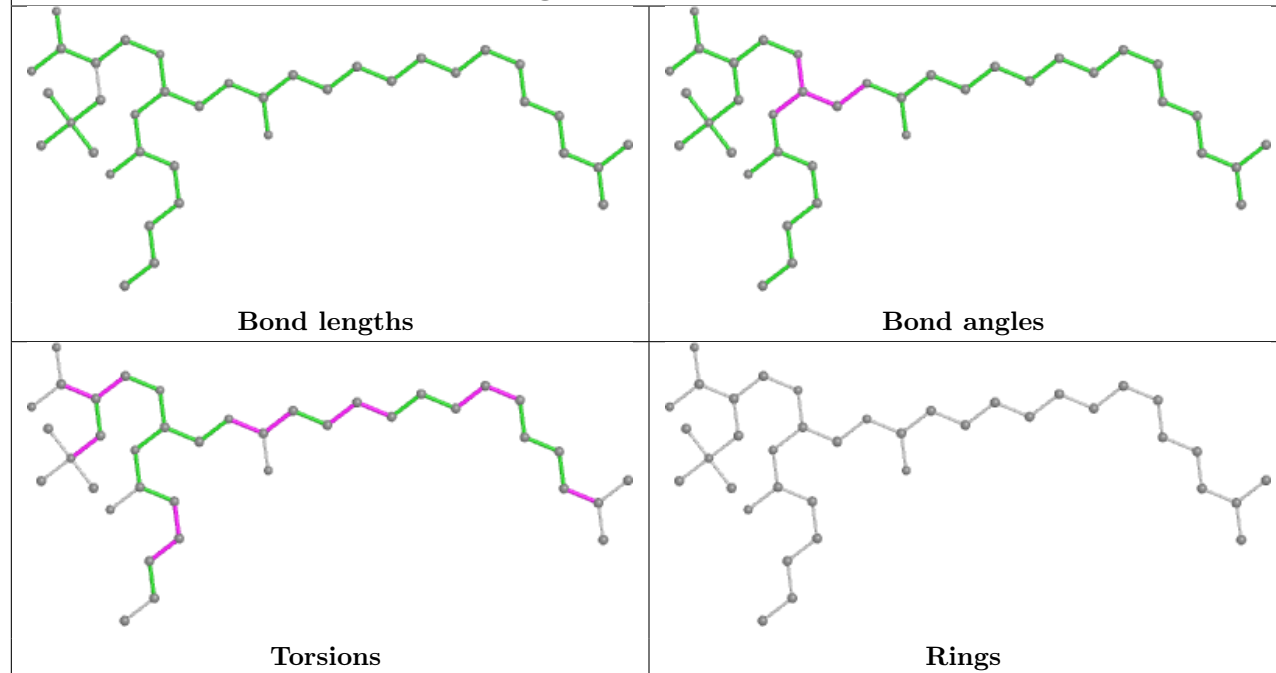




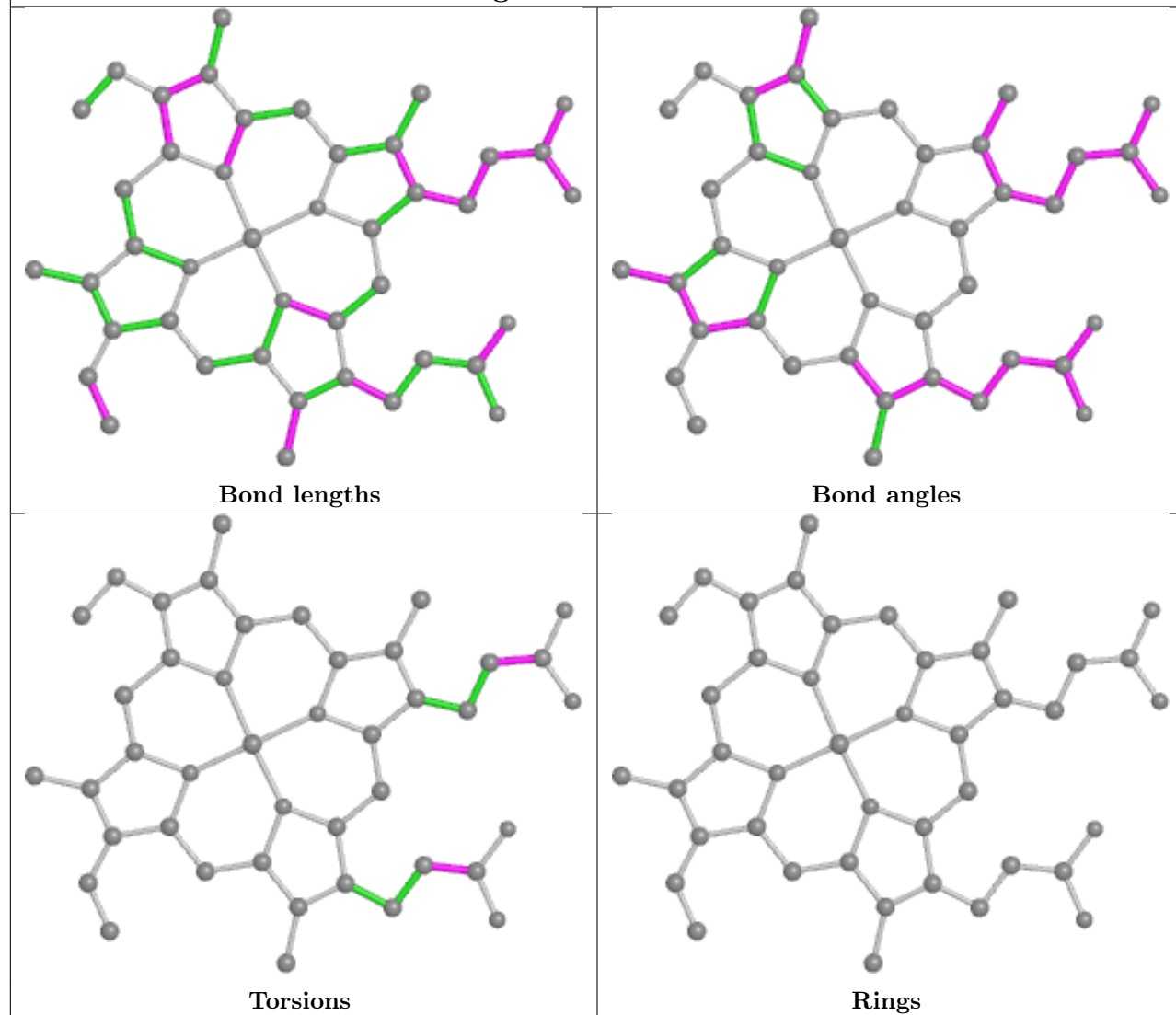
Ligand CLA a 913



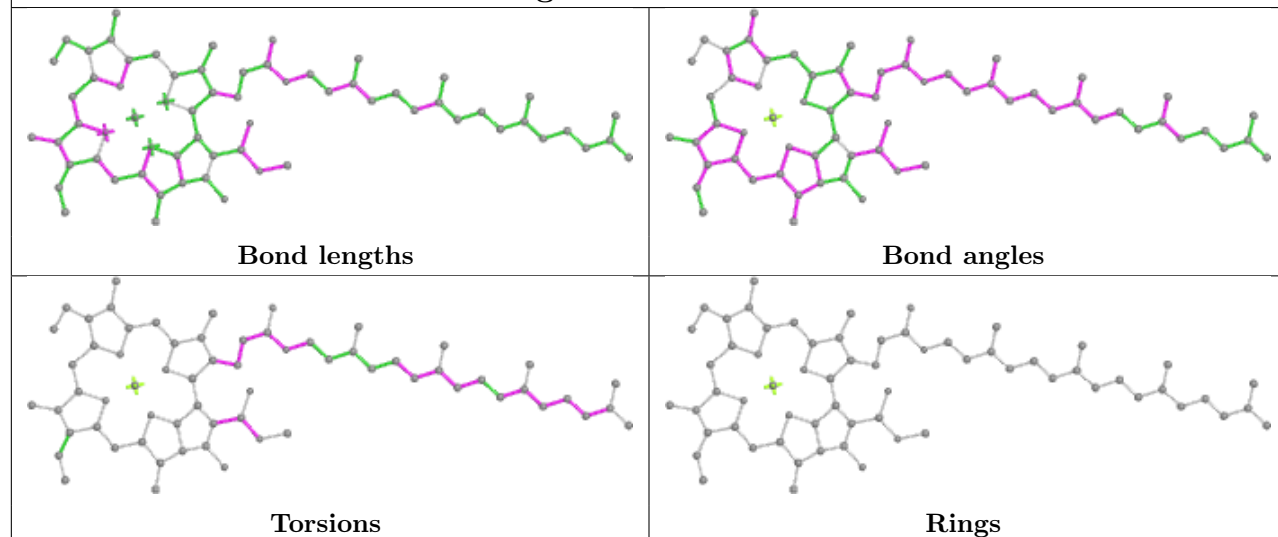
Ligand 85N G 101



Ligand HEC c 202



Ligand CLA a 901



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

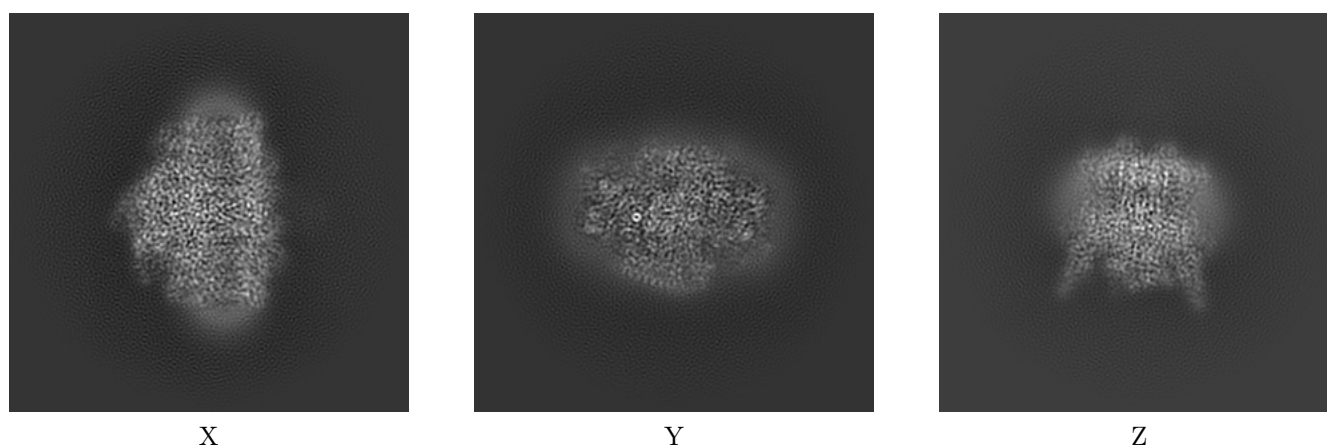
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32229. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

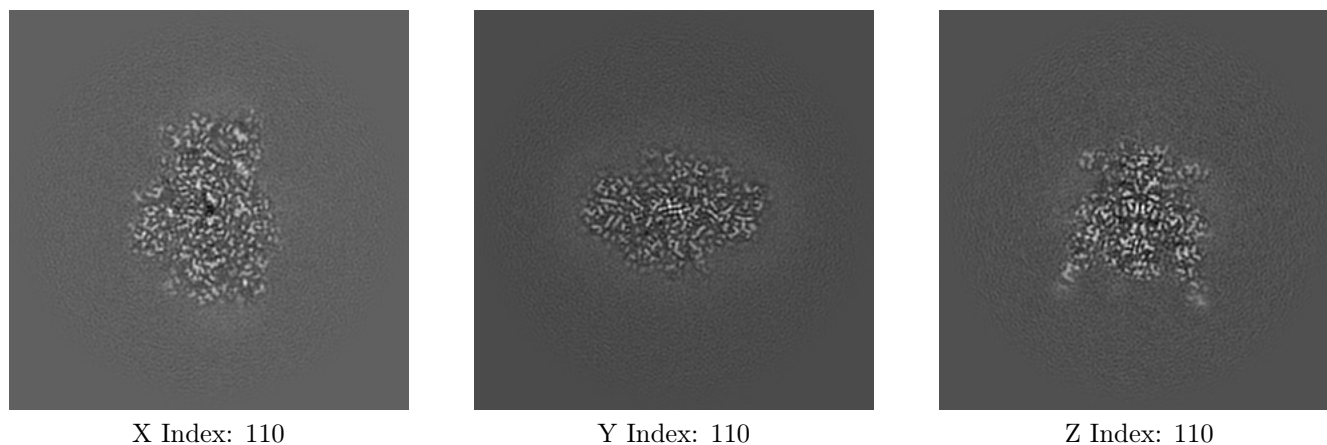
6.1.1 Primary map



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

6.2 Central slices [i](#)

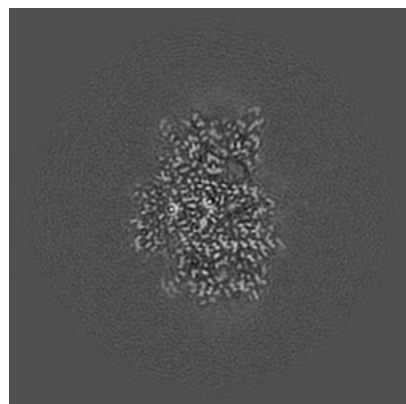
6.2.1 Primary map



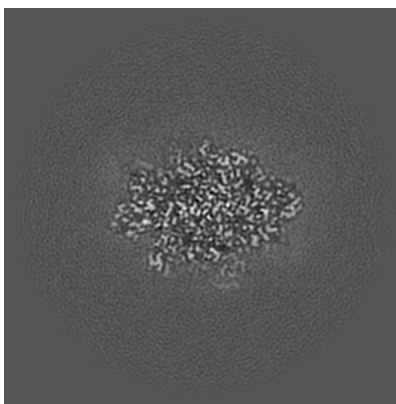
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

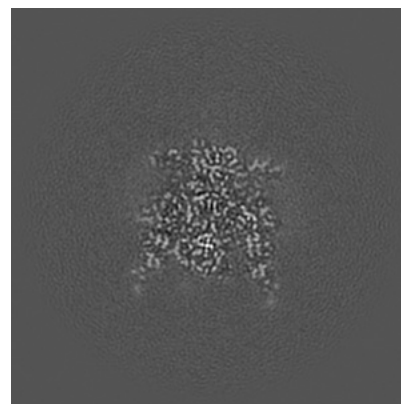
6.3.1 Primary map



X Index: 108



Y Index: 101

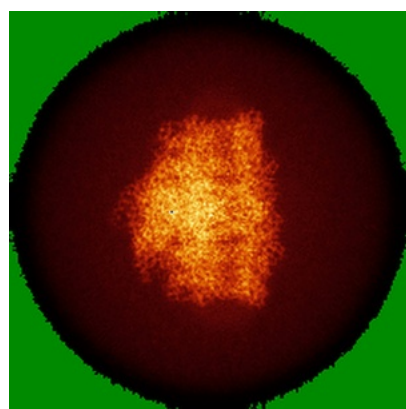


Z Index: 109

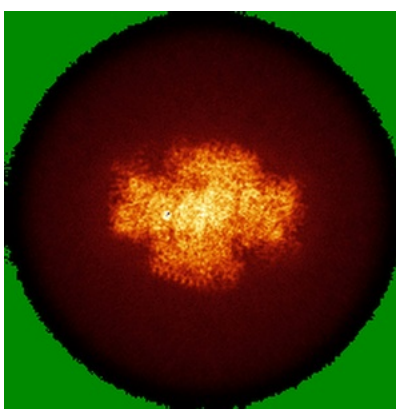
The images above show the largest variance slices of the map in three orthogonal directions.

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

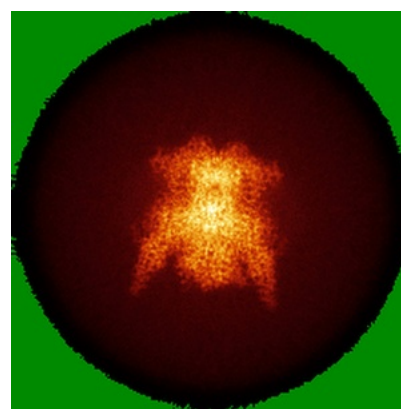
6.4.1 Primary map



X



Y

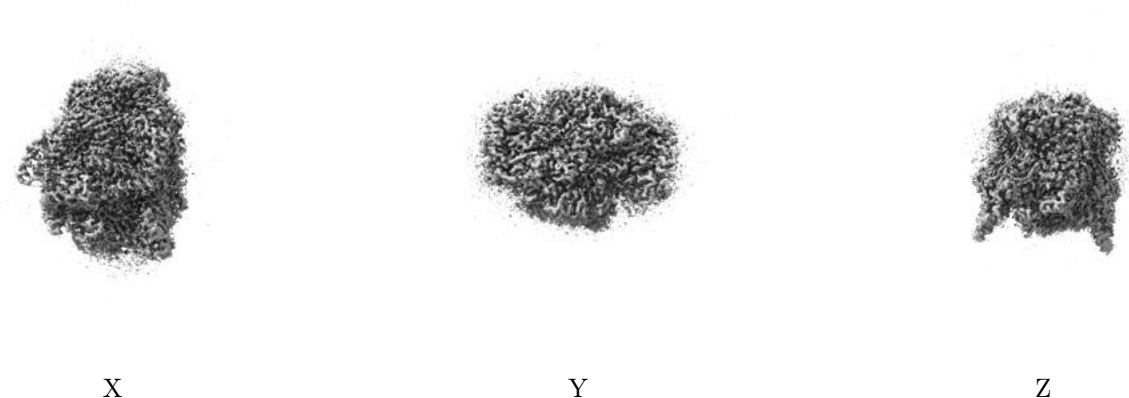


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.48. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

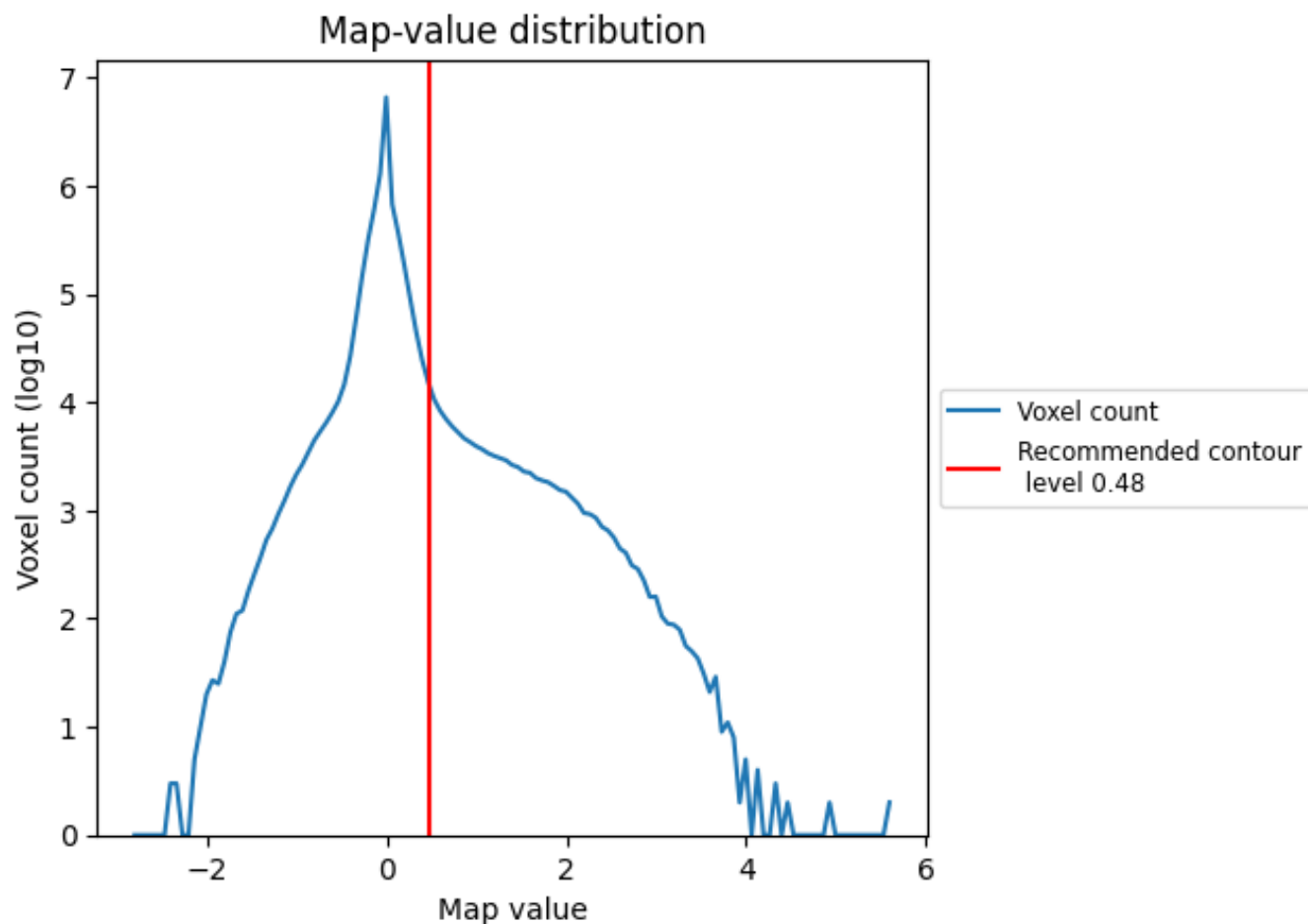
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

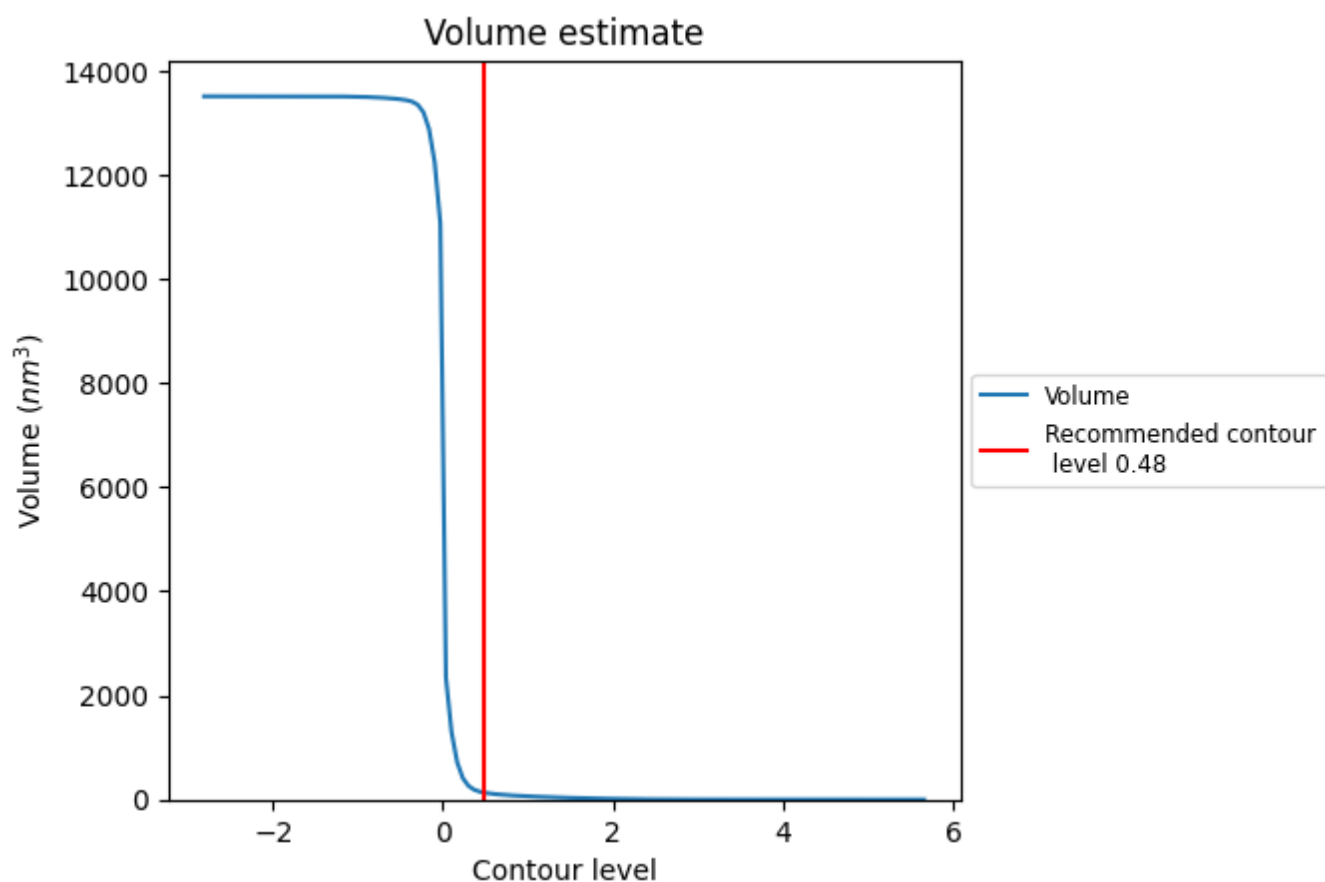
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

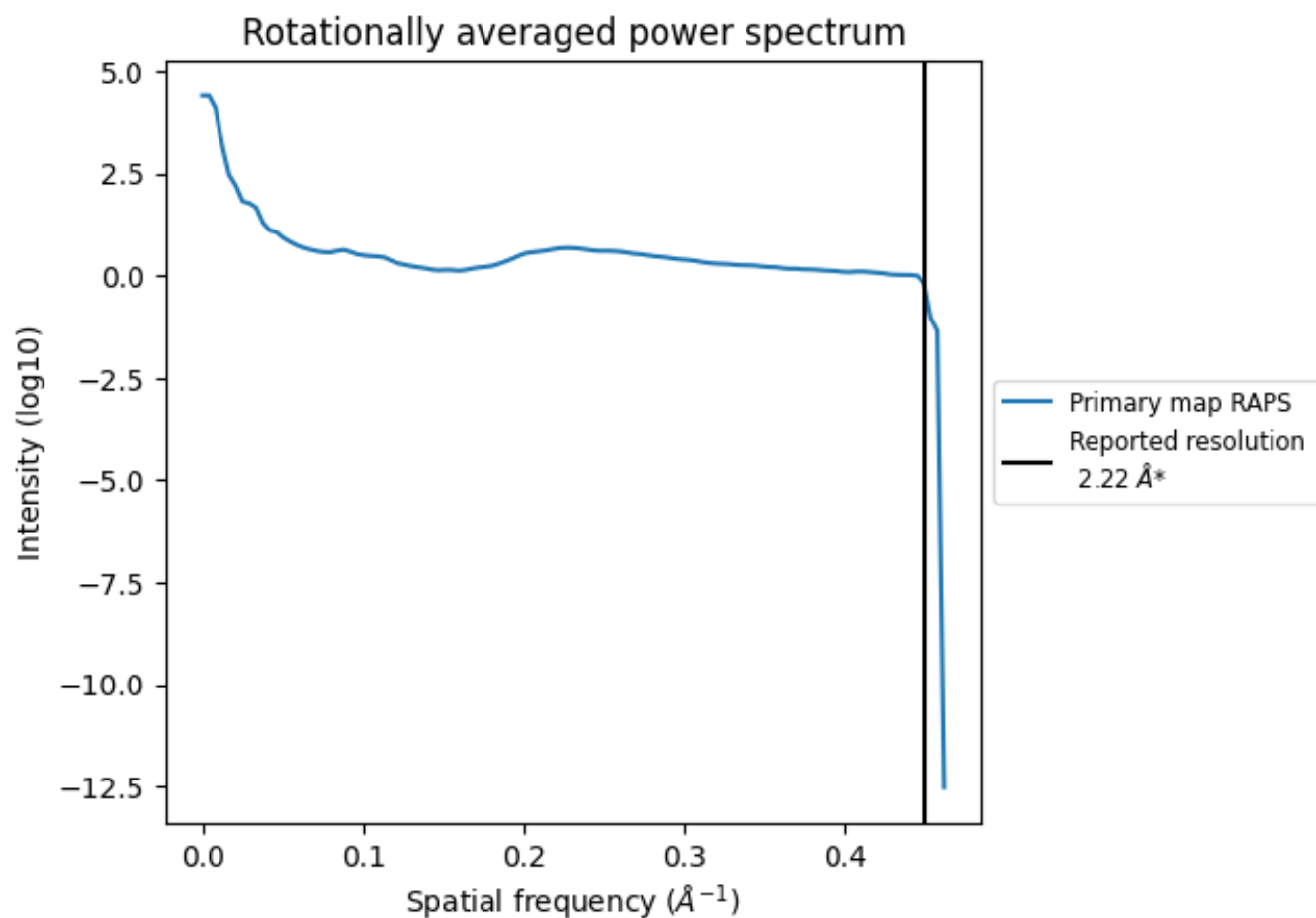
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm³; this corresponds to an approximate mass of 123 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 0.450 Å⁻¹

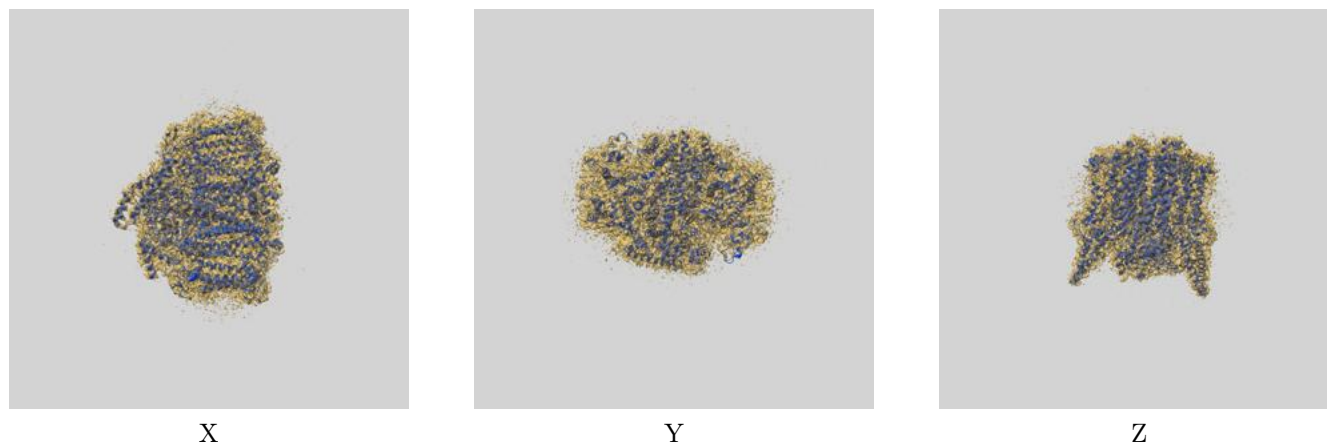
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

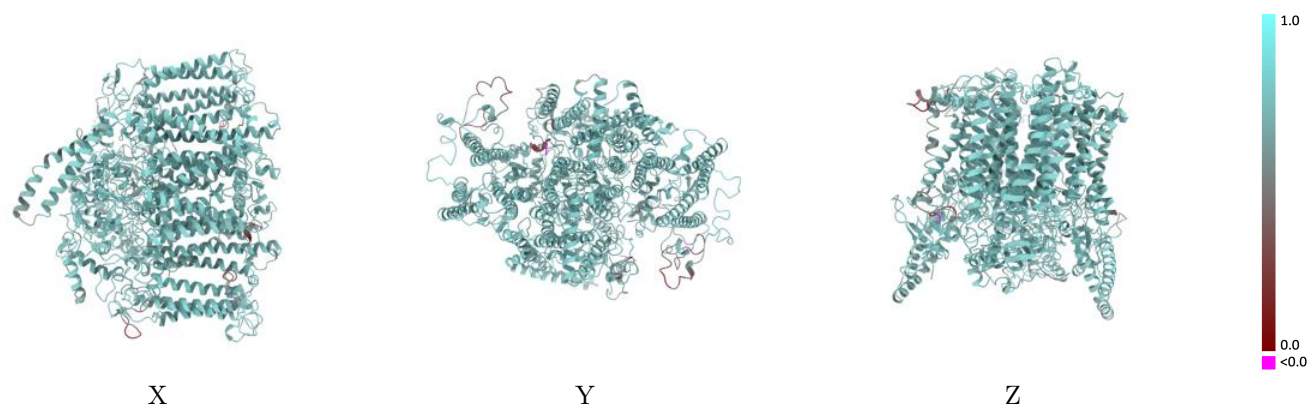
This section contains information regarding the fit between EMDB map EMD-32229 and PDB model 7VZR. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



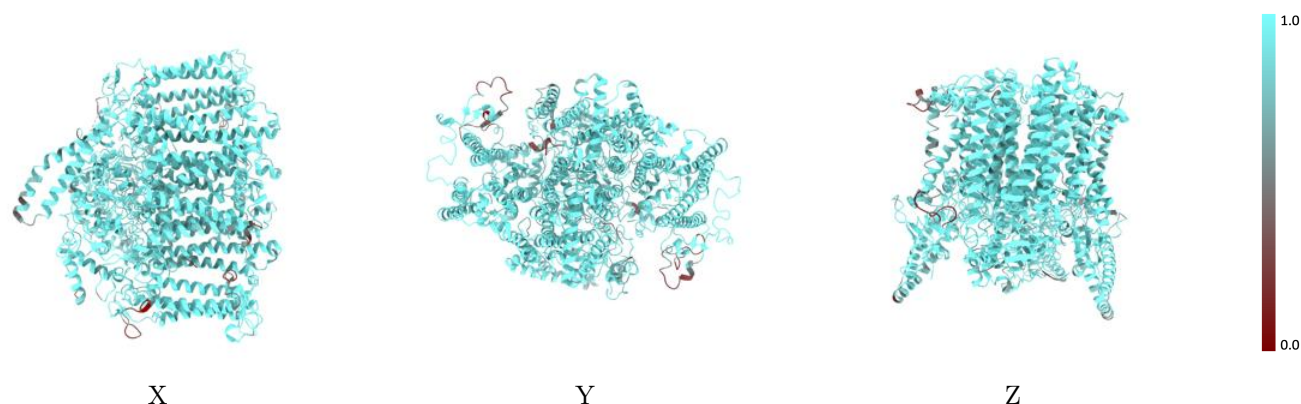
The images above show the 3D surface view of the map at the recommended contour level 0.48 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



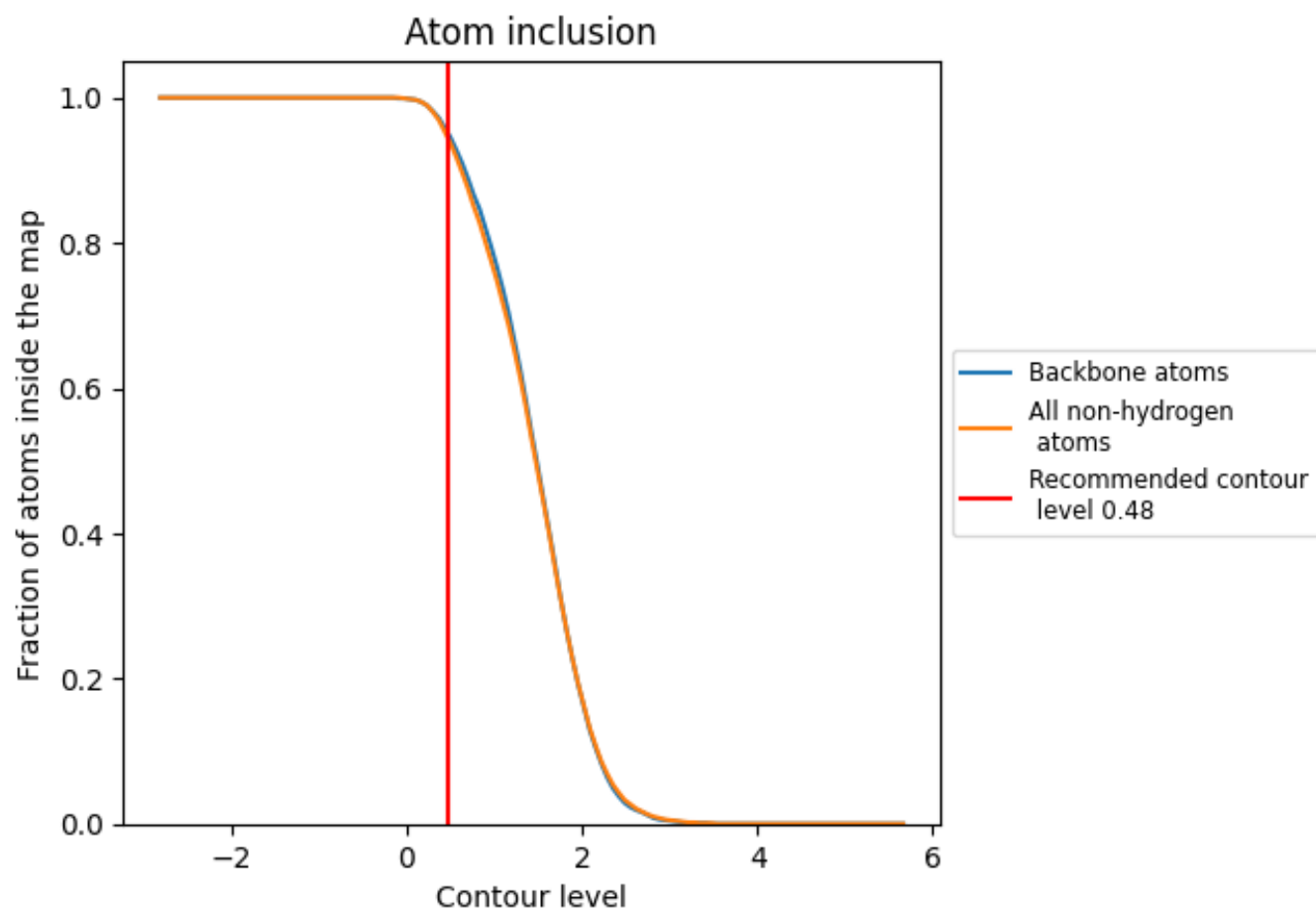
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.48).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9420	<div></div> 0.7050
A	<div></div> 0.9520	<div></div> 0.7100
C	<div></div> 0.9580	<div></div> 0.7210
E	<div></div> 0.9630	<div></div> 0.7140
F	<div></div> 0.9260	<div></div> 0.6700
G	<div></div> 0.7980	<div></div> 0.6490
H	<div></div> 0.8740	<div></div> 0.6670
a	<div></div> 0.9500	<div></div> 0.7060
c	<div></div> 0.9400	<div></div> 0.7060
e	<div></div> 0.9680	<div></div> 0.6970
f	<div></div> 0.9180	<div></div> 0.6770
g	<div></div> 0.7540	<div></div> 0.5870
h	<div></div> 0.8530	<div></div> 0.6610

