



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:07 PM UTC

PDB ID : 7Z6Q / pdb_00007z6q
EMDB ID : EMD-14528
Title : Cryo-EM structure of the whole photosynthetic complex from the green sulfur bacteria
Authors : Xie, H.; Tsiotis, G.
Deposited on : 2022-03-14
Resolution : 2.50 Å (reported)
Based on initial models : 3ENI, 5V8K

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

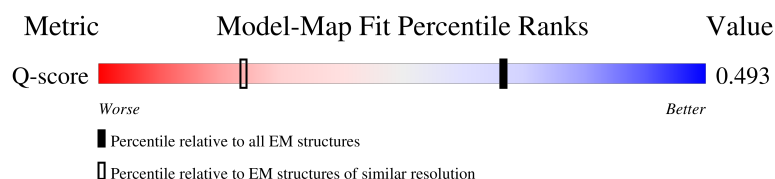
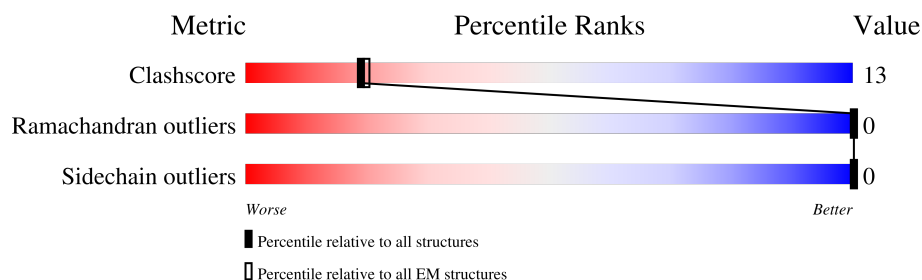
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	731	 78% 13% 9%
1	a	731	 76% 14% 11%
2	B	231	 42% 11% 47%
3	C	206	 50% 9% 41%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	206	
4	D	143	
5	E	366	
5	F	366	
5	G	366	
5	H	366	
5	I	366	
5	J	366	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	F39	A	816	-	X	-	-
9	F39	a	816	-	X	-	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 36557 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 Photosystem P840 reaction center, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	667	Total	C	N	O	S	0	0
			5344	3559	858	900	27		
1	a	654	Total	C	N	O	S	0	0
			5230	3487	834	883	26		

- Molecule 2 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	123	Total	C	N	O	S	0	0
			954	605	165	175	9		

- Molecule 3 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	121	Total	C	N	O	S	0	0
			943	632	148	156	7		
3	c	121	Total	C	N	O	S	0	0
			943	632	148	156	7		

- Molecule 4 is a protein called P840 reaction center 17 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			970	620	168	177	5		

- Molecule 5 is a protein called Bacteriochlorophyll a protein.

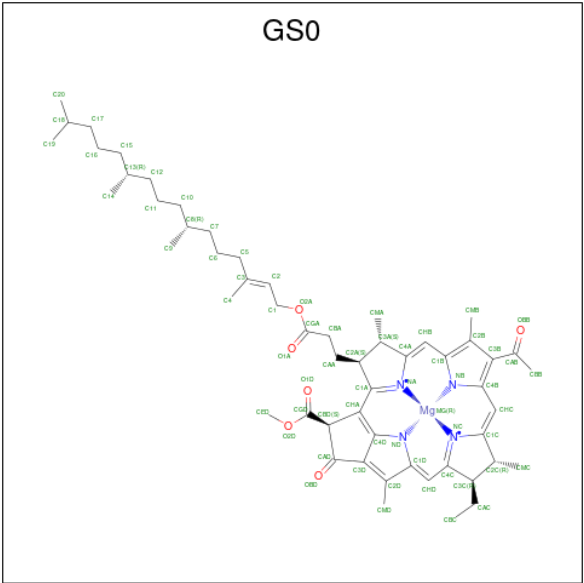
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	359	Total	C	N	O	S	0	0
			2798	1774	497	520	7		
5	F	359	Total	C	N	O	S	0	0
			2798	1774	497	520	7		

Continued on next page...

Continued from previous page...

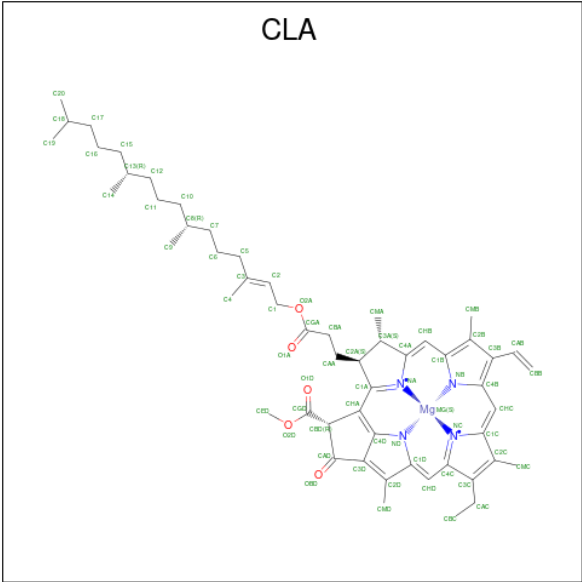
Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	359	Total	C	N	O	S	0	0
			2798	1774	497	520	7		
5	H	358	Total	C	N	O	S	0	0
			2790	1770	496	517	7		
5	I	359	Total	C	N	O	S	0	0
			2798	1774	497	520	7		
5	J	357	Total	C	N	O	S	0	0
			2783	1766	494	516	7		

- Molecule 6 is Bacteriochlorophyll A isomer (CCD ID: GS0) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



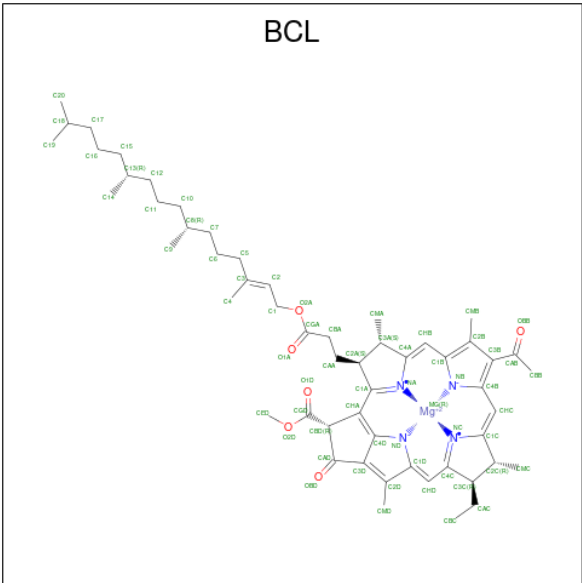
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 7 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
7	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
7	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
7	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	F	1	Total 46	C 35	Mg 1	N 4	O 6	1
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

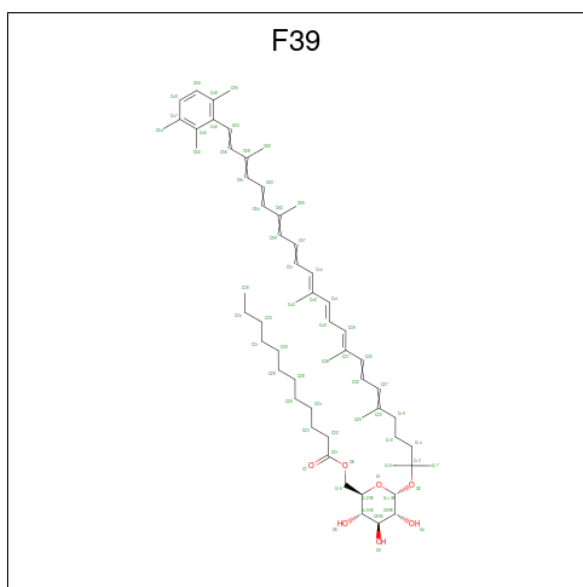
Mol	Chain	Residues	Atoms					AltConf
8	H	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
8	I	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

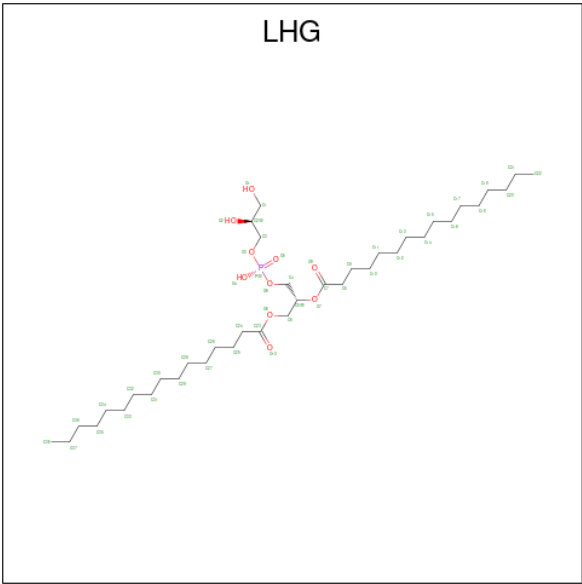
Mol	Chain	Residues	Atoms					AltConf
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55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

- Molecule 9 is [(2R,3S,4S,5R,6R)-6-[(10E,12E,14E)-2,6,10,14,19,23-hexamethyl-25-(2,3,6-trimethylphenyl)pentacos-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl dodecanoate (CCD ID: F39) (formula: C₅₈H₈₆O₇) (labeled as "Ligand of Interest" by depositor).



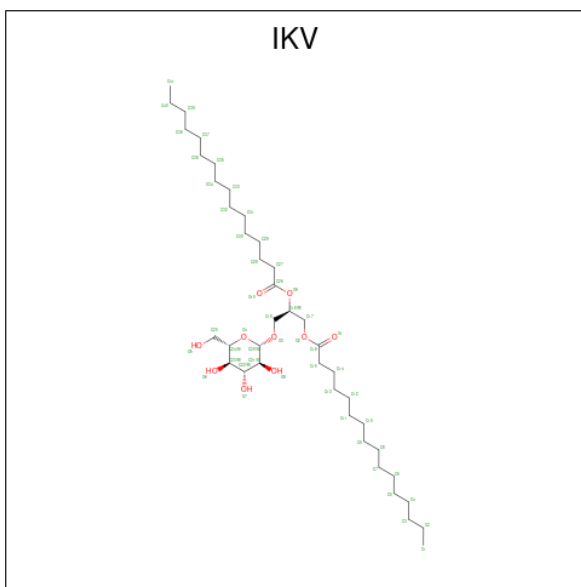
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			65	58	7	
9	a	1	Total	C	O	0
			65	58	7	

- Molecule 10 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	O	P	0
			49	38	10	1	
10	A	1	Total	C	O	P	0
			49	38	10	1	
10	a	1	Total	C	O	P	0
			49	38	10	1	
10	a	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 11 is [(2 {R})-2-hexadecanoyloxy-3-[(2 {S},3 {S},4 {R},5 {R},6 {S})-6-(hydroxy methyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-propyl] hexadecanoate (CCD ID: IKV) (formula: C₄₁H₇₈O₁₀) (labeled as "Ligand of Interest" by depositor).

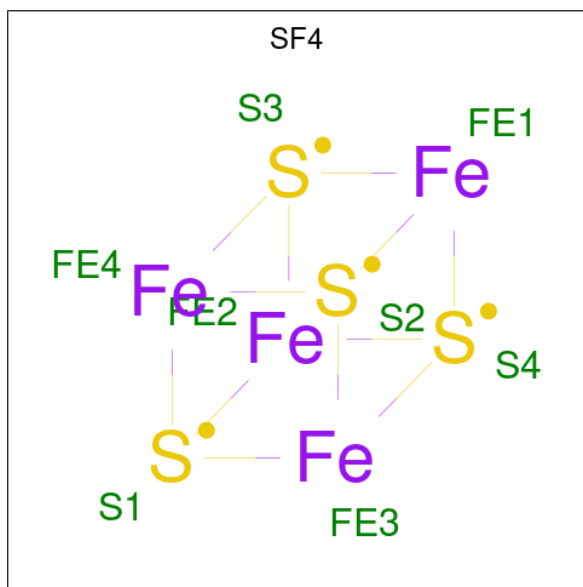


Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	O	0
			51	41	10	
11	a	1	Total	C	O	0
			51	41	10	

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Fe	S	0
			8	4	4	
13	B	1	Total	Fe	S	0
			8	4	4	
13	B	1	Total	Fe	S	0
			8	4	4	

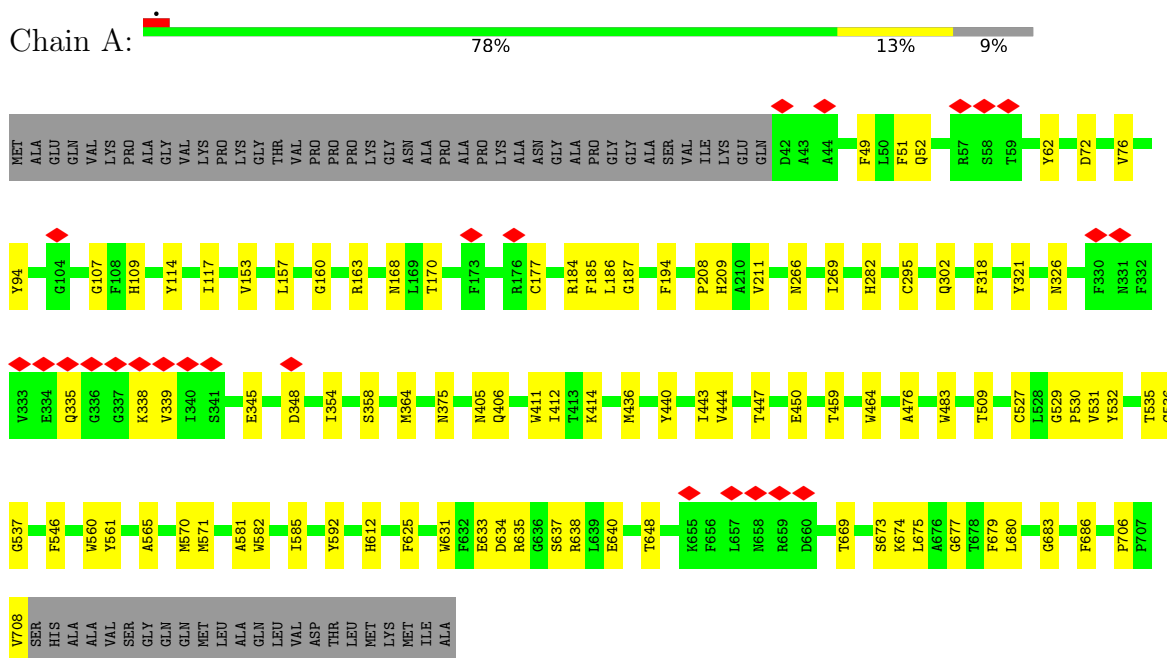
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	A	2	Total	O	0
			2	2	
14	E	2	Total	O	0
			2	2	
14	F	1	Total	O	0
			1	1	
14	H	1	Total	O	0
			1	1	
14	I	1	Total	O	0
			1	1	
14	J	1	Total	O	0
			1	1	
14	a	2	Total	O	0
			2	2	

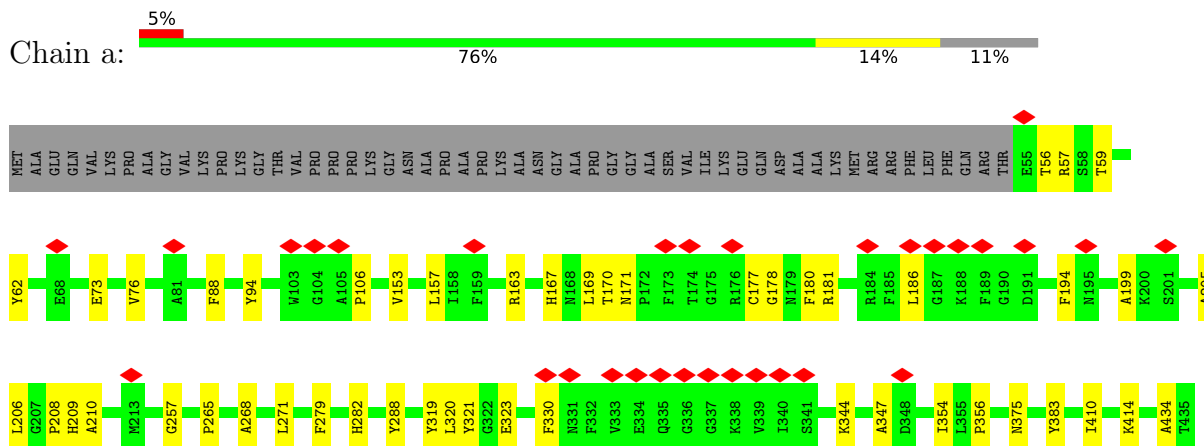
3 Residue-property plots

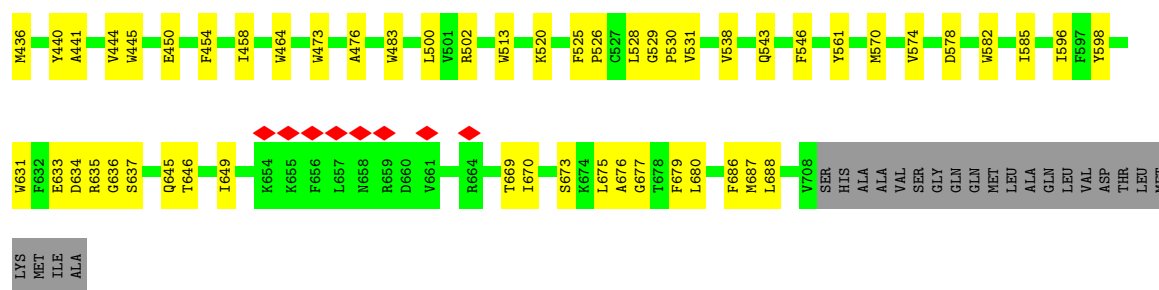
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Photosystem P840 reaction center, large subunit

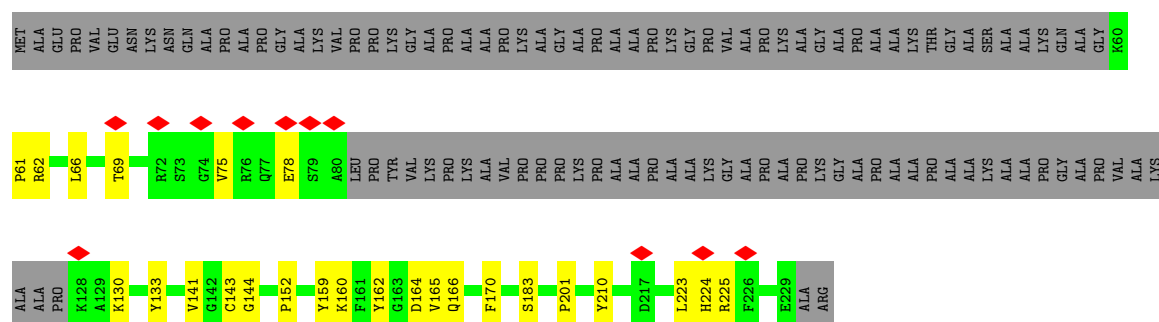


- Molecule 1: Photosystem P840 reaction center, large subunit

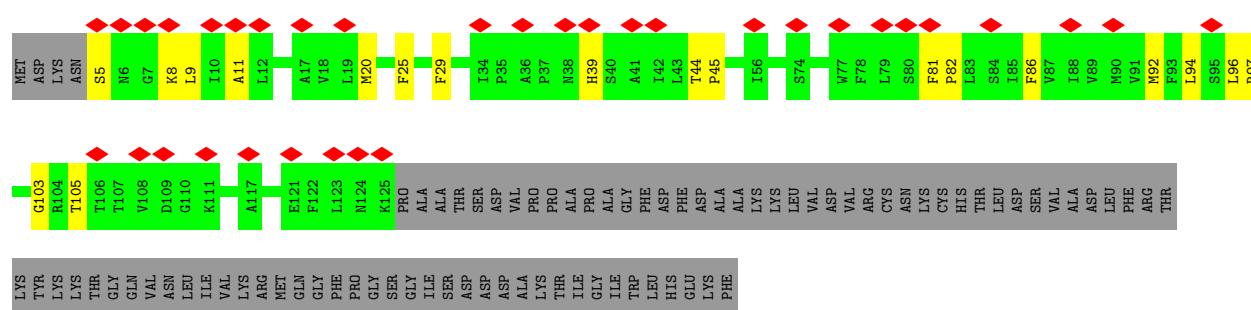




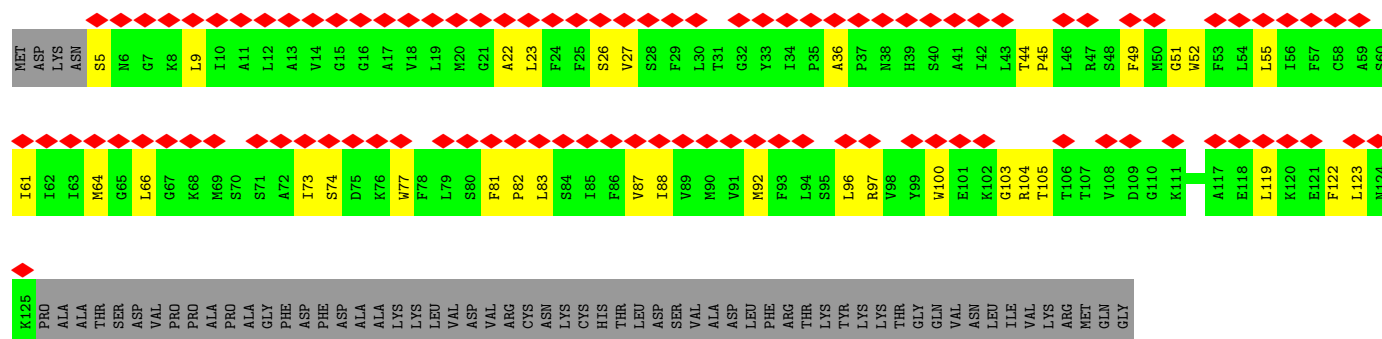
• Molecule 2: Photosystem P840 reaction center iron-sulfur protein



• Molecule 3: Cytochrome c



• Molecule 3: Cytochrome c



PHE
PRO
GLY
SER
GLY
ILE
SER
ASP
ASP
ALA
ALA
LYS
THR
ILE
GLY
ILE
TRP
LEU
HIS
GLU
LYS
PHE

- Molecule 4: P840 reaction center 17 kDa protein

Chain D: 

MET GLN PRO GLN LEU SER ARG PRO GLN THR ASP ALA LYS ASN GLN VAL ARG LYS A18 V19 S20 A27 D42 R43 D44 G45 K46 L47 E85 I86 A87 I88 D89 M90 N91 K92 E93 I94 I95 D96 N97 E98 N99 R100 Y101 VAL ILE ASP PHE ASP LYS ARG G109 V110 R115 E116

H122 C128 V129 H132 N133 K134 T135 Y136 D139 G140 F141 F142 K143

- Molecule 5: Bacteriochlorophyll a protein

Chain E: 

MET ALA LEU PHE GLY SER ASN D8 V9 T11 D15 Y16 E17 K31 P40 P43 D59 P60 A61 K62 G63 F64 E72 L82 A89 R86 V99 V104 G107 D108 F113 E116 V119 Y125 V130 R131 I138 Q141 G142 R143

V152 V167 I180 W184 F185 I186 G187 P188 R199 I203 L208 P214 K215 S221 M232 V254 F258 R259 S260 D261 S262 Q263 I265 E266 V267 F273 V276 S277 G282 G283 L284 R285 L288 P294 N308 Q312 L313 K314 P318

Y321 A326 A327 P328 L335 F360 E361 Q366

- Molecule 5: Bacteriochlorophyll a protein

Chain F: 

MET ALA LEU PHE GLY SER ASN D8 E17 G23 S24 A38 F39 P40 D48 D59 P60 A61 K62 G63 F64 S77 L82 A89 R86 V104 D108 F113 V119 Y125 V130 N133 V134 P137 Q141 V152 T162 I170

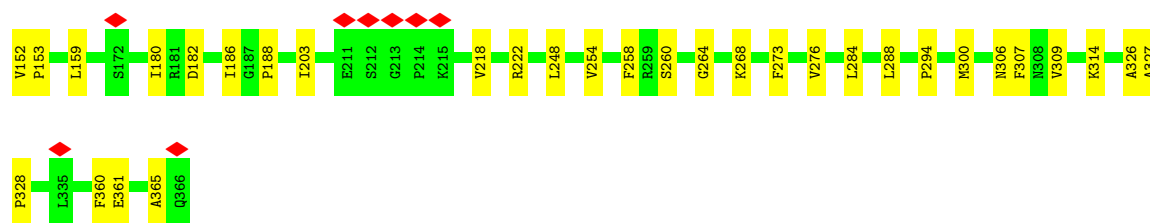
W179 I180 F183 W184 F185 I186 G187 P188 A189 E195 I203 N206 G207 L208 E211 S212 G213 P214 K215 R224 M232 V254 F258 R259 S260 D261 G264 I265 E266 V267 F273 V276 S277 L284 R285 L288 P294 H298 K314 L317 P318

Y321 K322 I323 R324 Y325 A326 A327 P328 R339 R347 Q359 F360 E361 Y364 A365 Q366

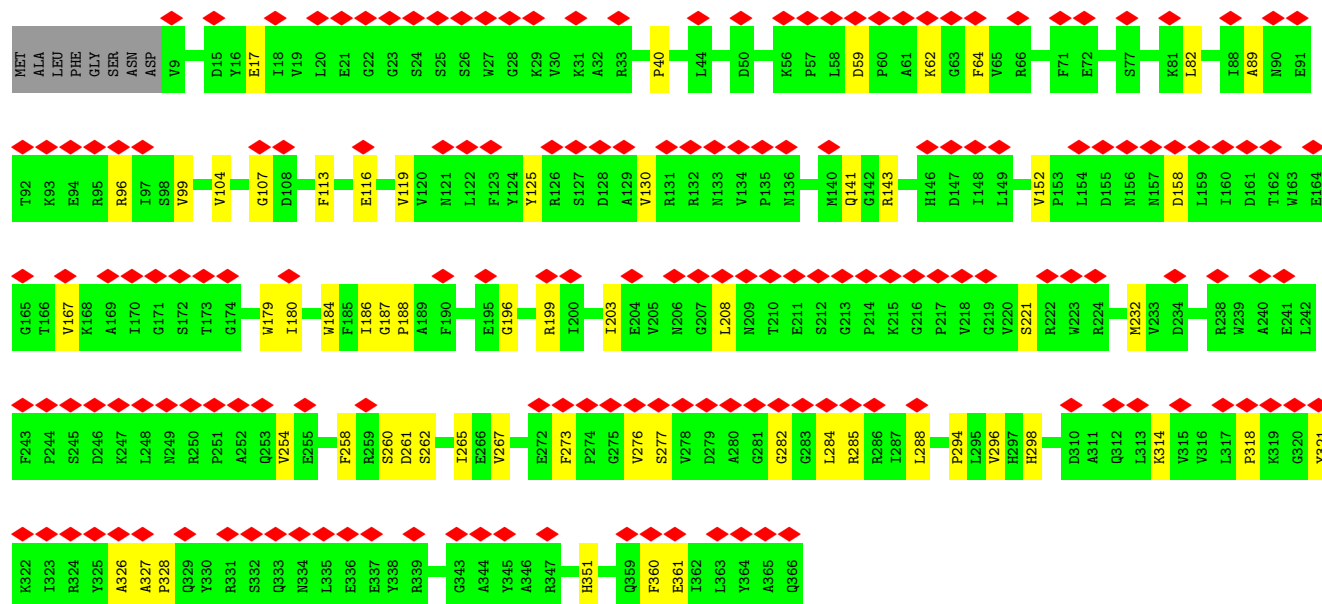
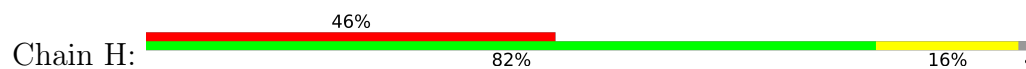
- Molecule 5: Bacteriochlorophyll a protein

Chain G: 

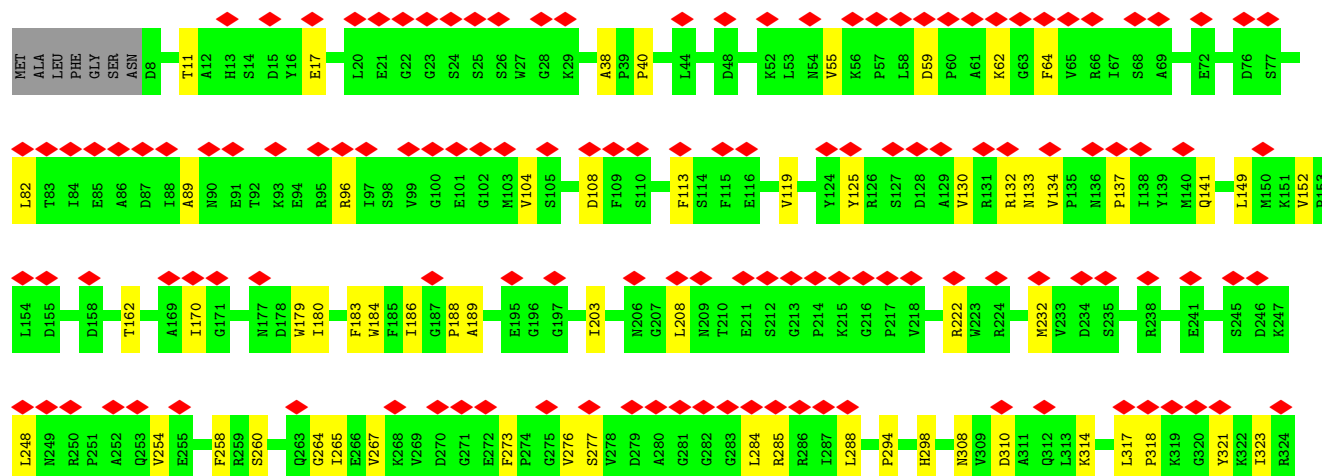
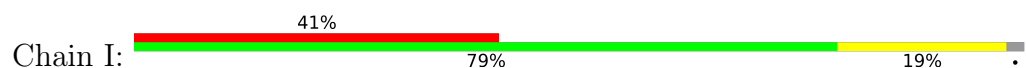
MET ALA LEU PHE GLY SER ASN D8 T10 E17 S24 A38 P39 P40 P43 D46 P57 L58 D59 P60 A61 K62 G63 F64 L82 A89 R96 V104 H111 T112 F113 E116 V119 Y125 R126 S127 R131 V134 Y139 I148

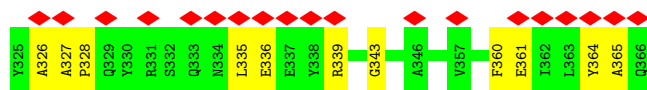


• Molecule 5: Bacteriochlorophyll a protein



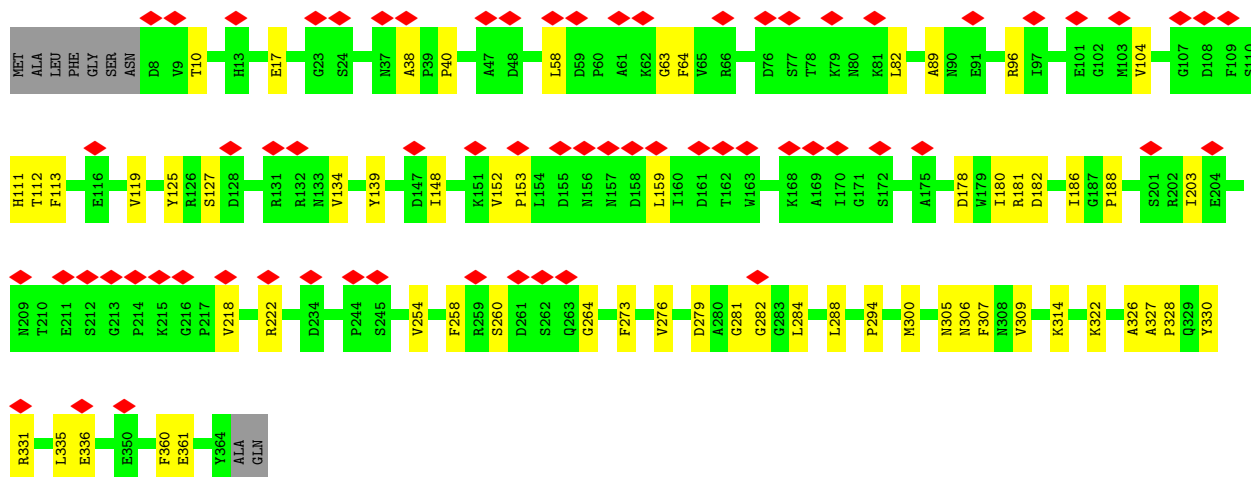
• Molecule 5: Bacteriochlorophyll a protein





• Molecule 5: Bacteriochlorophyll a protein

Chain J: 18% 81% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	481095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.187	Depositor
Minimum map value	-2.014	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.34	Depositor
Map size (Å)	301.32, 301.32, 301.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LHG, BCL, CA, IKV, F39, SF4, GS0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/5528	0.92	1/7527 (0.0%)
1	a	0.73	0/5412	0.98	0/7374
2	B	0.68	0/975	0.89	0/1312
3	C	0.94	0/967	1.23	0/1307
3	c	0.98	0/967	1.31	1/1307 (0.1%)
4	D	0.84	0/990	1.12	1/1331 (0.1%)
5	E	0.85	0/2868	1.09	0/3886
5	F	0.83	0/2868	1.07	0/3886
5	G	0.86	0/2868	1.09	0/3886
5	H	0.85	0/2860	1.08	0/3875
5	I	0.84	0/2868	1.08	0/3886
5	J	0.86	0/2853	1.09	0/3867
All	All	0.81	0/32024	1.05	3/43444 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	104	ARG	N-CA-C	-6.57	99.83	110.20
4	D	86	ILE	N-CA-C	-6.12	106.75	113.43
1	A	592	TYR	CB-CA-C	5.15	118.27	109.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5344	0	5238	128	0
1	a	5230	0	5119	134	0
2	B	954	0	924	39	0
3	C	943	0	989	17	0
3	c	943	0	989	35	0
4	D	970	0	979	29	0
5	E	2798	0	2736	69	0
5	F	2798	0	2736	84	0
5	G	2798	0	2736	54	0
5	H	2790	0	2732	61	0
5	I	2798	0	2736	80	0
5	J	2783	0	2723	72	0
6	A	66	0	0	1	0
6	a	66	0	0	2	0
7	A	130	0	144	17	0
7	a	130	0	144	22	0
8	A	752	0	797	67	0
8	E	574	0	617	65	0
8	F	554	0	579	65	0
8	G	396	0	435	30	0
8	H	508	0	543	51	0
8	I	554	0	579	66	0
8	J	462	0	509	44	0
8	a	752	0	798	68	0
9	A	65	0	0	0	0
9	a	65	0	0	0	0
10	A	98	0	148	11	0
10	a	98	0	148	13	0
11	A	51	0	0	3	0
11	a	51	0	0	2	0
12	A	1	0	0	0	0
12	a	1	0	0	0	0
13	A	8	0	0	1	0
13	B	16	0	0	0	0
14	A	2	0	0	0	0
14	E	2	0	0	0	0
14	F	1	0	0	0	0
14	H	1	0	0	0	0
14	I	1	0	0	0	0
14	J	1	0	0	0	0
14	a	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	36557	0	36078	929	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (929) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLY:HA2	1:a:529:GLY:HA2	1.32	1.05
1:a:178:GLY:HA3	8:a:807:BCL:HMA2	1.49	0.94
1:A:529:GLY:CA	1:a:529:GLY:HA2	1.98	0.93
1:a:634:ASP:HB2	7:a:803:CLA:HMD3	1.53	0.89
4:D:97:MET:HG2	5:J:282:GLY:HA3	1.57	0.86
1:A:163:ARG:HD3	1:A:168:ASN:O	1.75	0.85
1:A:194:PHE:CZ	1:A:208:PRO:HA	2.13	0.83
1:a:450:GLU:OE1	1:a:582:TRP:NE1	2.11	0.83
8:a:806:BCL:H2	8:a:810:BCL:H141	1.61	0.83
1:A:266:ASN:ND2	5:E:11:THR:OG1	2.12	0.82
1:A:581:ALA:HB1	1:a:330:PHE:HZ	1.44	0.82
2:B:160:LYS:HE3	4:D:98:GLU:OE2	1.80	0.82
1:A:358:SER:HB2	3:c:119:LEU:HD23	1.62	0.81
8:A:815:BCL:HAA2	3:c:96:LEU:HD21	1.60	0.81
1:a:635:ARG:HD2	1:a:635:ARG:O	1.81	0.81
1:A:282:HIS:ND1	8:A:804[B]:BCL:OBB	2.14	0.80
5:J:335:LEU:HG	5:J:336:GLU:H	1.46	0.78
1:a:170:THR:O	8:a:807:BCL:HED1	1.84	0.78
1:a:570:MET:HE1	7:a:802:CLA:CMA	2.14	0.78
1:A:326:ASN:OD1	1:A:345:GLU:O	2.02	0.77
1:A:532:TYR:CZ	5:J:322:LYS:NZ	2.52	0.77
8:E:402:BCL:HED2	5:F:134:VAL:HG11	1.67	0.77
8:F:402:BCL:H92	8:F:402:BCL:H52	1.67	0.77
5:E:328:PRO:HD2	5:E:360:PHE:CD1	2.20	0.76
8:E:402:BCL:H92	8:E:402:BCL:H52	1.68	0.76
1:A:530:PRO:HD3	1:a:529:GLY:H	1.50	0.76
8:H:402:BCL:HED2	5:I:134:VAL:HG11	1.67	0.76
1:A:581:ALA:HB1	1:a:330:PHE:CZ	2.20	0.76
5:H:328:PRO:HD2	5:H:360:PHE:CD1	2.20	0.76
1:A:414:LYS:HB3	8:A:805:BCL:H41	1.68	0.76
5:F:328:PRO:HD2	5:F:360:PHE:CD1	2.20	0.76
8:I:402:BCL:H92	8:I:402:BCL:H52	1.67	0.75
1:A:348:ASP:HB3	3:c:122:PHE:HZ	1.52	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:344:LYS:HE3	1:a:347:ALA:HA	1.68	0.75
8:H:402:BCL:H92	8:H:402:BCL:H52	1.67	0.74
5:F:170:ILE:CD1	5:F:208:LEU:HD12	2.17	0.74
8:H:402:BCL:H193	8:H:406:BCL:HMB3	1.69	0.74
8:E:402:BCL:H193	8:E:406:BCL:HMB3	1.69	0.74
8:F:402:BCL:H193	8:F:406:BCL:HMB3	1.69	0.74
8:I:402:BCL:H193	8:I:406:BCL:HMB3	1.69	0.74
3:C:5:SER:HA	3:C:9:LEU:HD23	1.70	0.73
8:A:807:BCL:HBA1	8:A:807:BCL:HBD	1.70	0.73
8:a:807:BCL:HBA1	8:a:807:BCL:HBD	1.70	0.73
1:a:445:TRP:CZ2	3:c:51:GLY:HA3	2.23	0.73
5:I:170:ILE:CD1	5:I:208:LEU:HD12	2.17	0.73
3:c:5:SER:HA	3:c:9:LEU:HD23	1.70	0.73
1:A:683:GLY:HA2	8:A:811:BCL:H102	1.71	0.73
5:J:335:LEU:HG	5:J:336:GLU:N	2.04	0.73
8:A:815:BCL:CAA	3:c:96:LEU:HD21	2.19	0.72
1:A:444:VAL:HG13	7:A:802:CLA:H43	1.72	0.72
8:H:408[B]:BCL:HMD1	5:J:180:ILE:HD13	1.71	0.72
3:C:105:THR:HG21	1:a:354:ILE:O	1.90	0.71
8:E:408[B]:BCL:HMD1	5:G:180:ILE:HD13	1.71	0.71
1:a:634:ASP:CB	7:a:803:CLA:HMD3	2.19	0.71
1:a:634:ASP:HB2	7:a:803:CLA:CMD	2.20	0.71
1:A:535:THR:HA	1:a:636:GLY:HA2	1.72	0.71
1:A:530:PRO:HD3	1:a:529:GLY:N	2.06	0.70
2:B:69:THR:HG21	2:B:75:VAL:HG21	1.71	0.70
1:a:454:PHE:HE2	7:a:802:CLA:C9	2.04	0.70
1:A:706:PRO:HB2	1:A:708:VAL:HG23	1.72	0.70
8:a:807:BCL:HAC2	8:a:807:BCL:H121	1.73	0.70
8:A:806:BCL:HBC2	8:A:810:BCL:H122	1.74	0.69
5:I:179:TRP:HE3	8:I:409[B]:BCL:OBD	1.74	0.69
1:a:680:LEU:HD11	10:a:817:LHG:H101	1.75	0.69
3:C:25:PHE:CE2	3:C:29:PHE:HE2	2.11	0.69
5:F:170:ILE:HD12	5:F:208:LEU:HD12	1.74	0.69
5:F:188:PRO:HG3	8:F:407:BCL:C2	2.23	0.69
2:B:61:PRO:HD2	5:F:77:SER:HB2	1.76	0.68
8:E:408[B]:BCL:CMC	8:G:401:BCL:O2A	2.42	0.68
5:I:170:ILE:HD12	5:I:208:LEU:HD12	1.74	0.68
1:a:199:ALA:HB2	1:a:208:PRO:HG2	1.74	0.68
8:I:408[B]:BCL:HBB3	8:I:408[B]:BCL:HMB1	1.76	0.68
1:a:675:LEU:HD11	8:a:813:BCL:H201	1.75	0.68
5:I:188:PRO:HG3	8:I:407:BCL:C2	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:179:TRP:HE3	8:F:409[B]:BCL:OBD	1.74	0.68
8:H:408[B]:BCL:CMC	8:J:401:BCL:O2A	2.42	0.68
5:I:180:ILE:CD1	8:I:409[B]:BCL:HAC2	2.24	0.68
5:I:183:PHE:CE2	8:I:401:BCL:H191	2.29	0.68
1:a:319:TYR:CE1	1:a:356:PRO:HA	2.28	0.68
1:a:483:TRP:HA	8:a:814:BCL:HED1	1.76	0.68
1:A:675:LEU:HD11	8:A:813:BCL:H201	1.75	0.67
2:B:159:TYR:HE2	1:a:531:VAL:HG21	1.57	0.67
5:E:64:PHE:CG	5:E:89:ALA:HB2	2.30	0.67
5:F:180:ILE:CD1	8:F:409[B]:BCL:HAC2	2.24	0.67
8:H:408[B]:BCL:HMC1	8:J:401:BCL:O2A	1.94	0.67
8:F:408[B]:BCL:HMB1	8:F:408[B]:BCL:HBB3	1.76	0.67
1:a:282:HIS:ND1	8:a:804[B]:BCL:OBB	2.27	0.67
8:a:806:BCL:HBC2	8:a:810:BCL:H122	1.74	0.67
8:A:814:BCL:H151	3:C:20:MET:SD	2.35	0.67
5:H:64:PHE:CG	5:H:89:ALA:HB2	2.29	0.67
5:J:328:PRO:HD2	5:J:360:PHE:CD1	2.29	0.67
5:G:328:PRO:HD2	5:G:360:PHE:CD1	2.29	0.67
1:a:163:ARG:HD3	8:a:807:BCL:HED2	1.75	0.67
5:G:10:THR:HB	5:G:306:ASN:O	1.95	0.67
3:c:81:PHE:HB3	3:c:82:PRO:HD3	1.76	0.67
8:a:814:BCL:HBC3	3:c:27:VAL:HG21	1.77	0.66
2:B:225:ARG:HH11	5:E:312:GLN:HB2	1.59	0.66
4:D:97:MET:HE2	5:J:284:LEU:HB2	1.76	0.66
1:A:109:HIS:HE1	3:c:105:THR:HG23	1.61	0.66
5:F:183:PHE:CE2	8:F:401:BCL:H191	2.29	0.66
5:I:64:PHE:CG	5:I:89:ALA:HB2	2.30	0.66
1:A:269:ILE:HD11	5:F:347:ARG:NH1	2.10	0.66
1:A:476:ALA:N	11:A:819:IKV:O8	2.22	0.66
1:A:483:TRP:HA	8:A:814:BCL:HED1	1.76	0.66
3:C:81:PHE:HB3	3:C:82:PRO:HD3	1.76	0.66
5:F:64:PHE:CG	5:F:89:ALA:HB2	2.30	0.66
8:E:408[B]:BCL:HMC1	8:G:401:BCL:O2A	1.95	0.66
1:A:186:LEU:H	8:A:807:BCL:C6	2.09	0.65
1:A:634:ASP:HB3	1:a:546:PHE:CZ	2.31	0.65
5:J:10:THR:HB	5:J:306:ASN:O	1.95	0.65
5:G:188:PRO:HG3	8:G:406:BCL:H2	1.77	0.65
3:C:86:PHE:CE1	1:a:88:PHE:HB3	2.31	0.65
1:a:436:MET:SD	7:a:802:CLA:HAB	2.37	0.65
5:J:113:PHE:HB3	5:J:152:VAL:HG22	1.79	0.65
1:A:530:PRO:HG2	2:B:170:PHE:CE1	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:17:GLU:HA	5:J:314:LYS:O	1.97	0.65
3:C:8:LYS:HA	3:C:11:ALA:HB3	1.78	0.65
4:D:97:MET:HG2	5:J:281:GLY:O	1.97	0.65
5:H:64:PHE:CD1	5:H:89:ALA:HB2	2.32	0.65
1:a:194:PHE:CZ	1:a:208:PRO:HA	2.32	0.65
5:I:184:TRP:HE1	8:I:406:BCL:HBB1	1.61	0.64
5:G:112:THR:O	5:G:152:VAL:HG13	1.98	0.64
1:a:186:LEU:H	8:a:807:BCL:H72	1.61	0.64
5:G:17:GLU:HA	5:G:314:LYS:O	1.97	0.64
5:I:170:ILE:CD1	5:I:208:LEU:CD1	2.75	0.64
5:J:188:PRO:HG3	8:J:407:BCL:H2	1.77	0.64
1:A:295:CYS:HB3	10:A:818:LHG:HC91	1.78	0.64
5:F:184:TRP:HE1	8:F:406:BCL:HBB1	1.61	0.64
1:a:513:TRP:CZ2	1:a:538:VAL:HG11	2.31	0.64
1:A:443:ILE:HD13	6:A:801:GS0:C14	2.27	0.64
5:G:113:PHE:HB3	5:G:152:VAL:HG22	1.79	0.64
5:J:112:THR:O	5:J:152:VAL:HG13	1.98	0.64
1:a:178:GLY:HA3	8:a:807:BCL:CMA	2.27	0.64
5:F:170:ILE:CD1	5:F:208:LEU:CD1	2.75	0.64
5:I:17:GLU:HA	5:I:314:LYS:O	1.99	0.64
1:A:107:GLY:O	3:c:97:ARG:NE	2.28	0.63
5:E:64:PHE:CD1	5:E:89:ALA:HB2	2.32	0.63
5:H:17:GLU:HA	5:H:314:LYS:O	1.99	0.63
5:I:328:PRO:HD2	5:I:360:PHE:CD1	2.34	0.63
8:H:401:BCL:HAA1	8:H:401:BCL:HBD	1.81	0.63
1:A:633:GLU:HG3	1:a:633:GLU:HG3	1.79	0.63
4:D:97:MET:HE3	5:J:284:LEU:HD22	1.80	0.63
4:D:97:MET:HG2	5:J:282:GLY:CA	2.28	0.63
5:F:17:GLU:HA	5:F:314:LYS:O	1.99	0.63
8:I:401:BCL:HBD	8:I:401:BCL:HAA1	1.81	0.63
1:A:634:ASP:HB2	7:A:803:CLA:HMD3	1.80	0.62
5:E:104:VAL:HG23	5:E:113:PHE:HE2	1.64	0.62
8:E:401:BCL:HAA1	8:E:401:BCL:HBD	1.81	0.62
5:F:104:VAL:HG23	5:F:113:PHE:HE2	1.64	0.62
2:B:164:ASP:HB3	1:a:56:THR:OG1	1.99	0.62
8:F:401:BCL:HAA1	8:F:401:BCL:HBD	1.81	0.62
5:H:104:VAL:HG23	5:H:113:PHE:HE2	1.64	0.62
8:F:401:BCL:HBA1	5:G:127:SER:CB	2.30	0.62
7:A:803:CLA:HHB	7:A:803:CLA:H43	1.82	0.62
8:A:812:BCL:HMB1	8:A:812:BCL:HBB3	1.81	0.62
1:A:535:THR:HA	1:a:636:GLY:CA	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:401:BCL:HAA1	8:G:401:BCL:HBD	1.81	0.62
8:I:401:BCL:HBA1	5:J:127:SER:CB	2.30	0.62
2:B:160:LYS:CE	4:D:98:GLU:OE2	2.47	0.61
5:E:17:GLU:HA	5:E:314:LYS:O	1.99	0.61
5:I:104:VAL:HG23	5:I:113:PHE:HE2	1.64	0.61
8:J:401:BCL:HAA1	8:J:401:BCL:HBD	1.81	0.61
4:D:47:LEU:HD22	4:D:139:ASP:HA	1.83	0.61
4:D:101:TYR:CZ	5:J:284:LEU:HD21	2.36	0.61
5:E:104:VAL:HG21	8:E:401:BCL:HHD	1.83	0.61
5:J:40:PRO:HG2	5:J:260:SER:HB3	1.81	0.61
4:D:97:MET:CG	5:J:282:GLY:HA3	2.30	0.61
5:G:104:VAL:HG21	8:G:401:BCL:HHD	1.83	0.61
1:A:450:GLU:CD	1:A:571:MET:O	2.44	0.61
1:A:459:THR:HG21	3:C:39:HIS:CE1	2.35	0.61
1:a:440:TYR:OH	7:a:802:CLA:O1A	2.19	0.61
1:a:500:LEU:HD12	10:a:818:LHG:H211	1.81	0.61
5:H:261:ASP:CG	5:H:262:SER:H	2.09	0.60
7:a:803:CLA:HBB	7:a:803:CLA:H43	1.82	0.60
8:A:808:BCL:H43	8:A:810:BCL:H8	1.83	0.60
8:E:409:BCL:H203	5:G:113:PHE:CE1	2.37	0.60
1:A:354:ILE:N	3:c:105:THR:HG21	2.16	0.60
5:I:104:VAL:HG21	8:I:401:BCL:HHD	1.83	0.60
4:D:87:ALA:HB2	4:D:143:LYS:N	2.16	0.60
5:H:104:VAL:HG21	8:H:401:BCL:HHD	1.83	0.60
8:a:812:BCL:HBB3	8:a:812:BCL:HHC	1.84	0.60
5:J:104:VAL:HG21	8:J:401:BCL:HHD	1.83	0.59
8:a:808:BCL:H43	8:a:810:BCL:H8	1.84	0.59
5:J:113:PHE:CE1	8:J:402:BCL:H203	2.37	0.59
5:J:186:ILE:CD1	8:J:402:BCL:HAA2	2.32	0.59
1:A:476:ALA:O	11:A:819:IKV:O7	2.19	0.59
8:E:409:BCL:HAA2	5:G:186:ILE:CD1	2.32	0.59
8:F:402:BCL:CED	5:G:139:TYR:O	2.50	0.59
1:a:157:LEU:HD11	8:a:808:BCL:H102	1.84	0.59
2:B:225:ARG:HH11	5:E:312:GLN:CB	2.16	0.59
8:I:402:BCL:CED	5:J:139:TYR:O	2.50	0.59
1:A:339:VAL:HG12	1:A:339:VAL:O	2.01	0.59
4:D:87:ALA:HB2	4:D:143:LYS:CA	2.32	0.59
1:A:440:TYR:O	1:A:444:VAL:HG23	2.02	0.59
5:F:104:VAL:HG21	8:F:401:BCL:HHD	1.83	0.59
5:I:183:PHE:HE2	8:I:401:BCL:H191	1.66	0.59
1:A:535:THR:C	1:a:636:GLY:HA3	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:574:VAL:HG12	1:a:598:TYR:CD1	2.38	0.59
8:A:806:BCL:H2	8:A:810:BCL:H141	1.84	0.59
5:E:186:ILE:HD12	5:F:141:GLN:NE2	2.18	0.59
8:a:814:BCL:CBC	3:c:27:VAL:HG21	2.33	0.59
8:A:805:BCL:HBB1	10:A:818:LHG:H381	1.85	0.58
8:H:408[B]:BCL:HMD1	5:J:180:ILE:CD1	2.32	0.58
1:A:444:VAL:HG13	7:A:802:CLA:C4	2.33	0.58
3:C:25:PHE:CE2	3:C:29:PHE:CE2	2.91	0.58
5:H:186:ILE:HD12	5:I:141:GLN:NE2	2.18	0.58
1:A:157:LEU:HD11	8:A:808:BCL:H102	1.84	0.58
1:A:321:TYR:HB3	8:A:815:BCL:HMA2	1.86	0.58
4:D:87:ALA:HB2	4:D:143:LYS:HA	1.84	0.58
8:E:408[B]:BCL:HMD1	5:G:180:ILE:CD1	2.32	0.58
8:J:403:BCL:H52	8:J:407:BCL:HMA3	1.85	0.58
8:G:402:BCL:H52	8:G:406:BCL:HMA3	1.85	0.58
1:a:669:THR:O	1:a:673:SER:N	2.36	0.58
8:A:810:BCL:H143	8:A:812:BCL:H193	1.86	0.58
5:F:183:PHE:HE2	8:F:401:BCL:H191	1.66	0.58
8:F:406:BCL:HBD	8:F:406:BCL:HAA1	1.86	0.58
1:A:450:GLU:OE1	1:A:571:MET:O	2.22	0.57
1:A:669:THR:O	1:A:673:SER:N	2.37	0.57
2:B:159:TYR:CE2	1:a:531:VAL:HG21	2.38	0.57
5:E:232:MET:SD	5:G:188:PRO:HA	2.44	0.57
8:G:405:BCL:HBD	8:G:405:BCL:HAA1	1.86	0.57
5:I:310:ASP:O	1:a:181:ARG:NH1	2.37	0.57
8:a:810:BCL:H143	8:a:812:BCL:H193	1.86	0.57
5:F:179:TRP:CE3	8:F:409[B]:BCL:OBD	2.57	0.57
8:H:406:BCL:HAA1	8:H:406:BCL:HBD	1.86	0.57
8:I:402:BCL:H193	8:I:406:BCL:CMB	2.34	0.57
8:I:406:BCL:HAA1	8:I:406:BCL:HBD	1.86	0.57
8:J:406:BCL:HAA1	8:J:406:BCL:HBD	1.86	0.57
1:A:674:LYS:HE2	1:a:633:GLU:HB2	1.87	0.57
8:E:402:BCL:H193	8:E:406:BCL:CMB	2.34	0.57
5:I:179:TRP:CE3	8:I:409[B]:BCL:OBD	2.57	0.57
8:H:403:BCL:H52	8:H:407:BCL:HMA3	1.87	0.57
5:E:40:PRO:HD2	5:E:261:ASP:O	2.05	0.57
8:F:402:BCL:H193	8:F:406:BCL:CMB	2.34	0.57
8:H:402:BCL:H193	8:H:406:BCL:CMB	2.34	0.57
3:c:83:LEU:O	3:c:87:VAL:HG23	2.05	0.57
1:A:302:GLN:NE2	10:A:818:LHG:HC12	2.19	0.57
5:I:113:PHE:HB3	5:I:152:VAL:HG22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ARG:HH12	5:F:261:ASP:CG	2.13	0.57
5:G:188:PRO:CG	8:G:406:BCL:H2	2.35	0.57
8:E:403:BCL:H52	8:E:407:BCL:HMA3	1.87	0.56
1:A:185:PHE:CE2	1:A:194:PHE:HE2	2.24	0.56
5:H:265:ILE:HG22	5:H:267:VAL:HG23	1.87	0.56
5:I:265:ILE:HG22	5:I:267:VAL:HG23	1.87	0.56
5:J:188:PRO:CG	8:J:407:BCL:H2	2.35	0.56
1:a:570:MET:HE1	7:a:802:CLA:HMA1	1.87	0.56
1:A:406:GLN:O	5:E:263:GLN:HB2	2.05	0.56
1:A:546:PHE:CZ	1:a:634:ASP:HB3	2.40	0.56
5:H:113:PHE:HB3	5:H:152:VAL:HG22	1.87	0.56
1:A:348:ASP:HB3	3:c:122:PHE:CZ	2.36	0.56
1:A:440:TYR:OH	7:A:802:CLA:O1A	2.19	0.56
5:E:113:PHE:HB3	5:E:152:VAL:HG22	1.87	0.56
5:G:40:PRO:HG2	5:G:260:SER:HB2	1.88	0.56
1:a:62:TYR:HA	8:a:813:BCL:H12	1.87	0.56
3:C:97:ARG:O	3:C:97:ARG:HG3	2.06	0.56
5:F:113:PHE:HB3	5:F:152:VAL:HG22	1.87	0.56
5:H:40:PRO:HG2	5:H:260:SER:HB2	1.88	0.56
1:A:318:PHE:CZ	1:A:364:MET:HG2	2.41	0.56
8:F:402:BCL:O1D	5:G:134:VAL:HG21	2.06	0.56
8:I:403:BCL:H52	8:I:407:BCL:HMA3	1.87	0.56
1:A:49:PHE:O	1:A:52:GLN:HB3	2.07	0.55
1:A:62:TYR:HA	8:A:813:BCL:H12	1.87	0.55
5:E:40:PRO:HG2	5:E:260:SER:HB2	1.88	0.55
1:a:445:TRP:CH2	3:c:51:GLY:HA3	2.41	0.55
5:E:130:VAL:CG1	8:E:409:BCL:CED	2.84	0.55
8:E:406:BCL:HAA1	8:E:406:BCL:HBD	1.86	0.55
5:F:317:LEU:HD11	5:F:323:ILE:HG13	1.88	0.55
1:A:186:LEU:N	8:A:807:BCL:H72	2.21	0.55
1:A:153:VAL:HG13	8:A:808:BCL:H121	1.88	0.55
1:A:536:CYS:O	1:a:636:GLY:N	2.40	0.55
5:F:265:ILE:HG22	5:F:267:VAL:HG23	1.87	0.55
8:I:402:BCL:O1D	5:J:134:VAL:HG21	2.06	0.55
5:F:40:PRO:HG2	5:F:260:SER:HB2	1.88	0.55
8:F:403:BCL:H52	8:F:407:BCL:HMA3	1.87	0.55
5:H:130:VAL:CG1	8:J:402:BCL:CED	2.84	0.55
1:a:153:VAL:HG13	8:a:808:BCL:H121	1.88	0.55
8:A:812:BCL:HMB1	8:A:812:BCL:CBB	2.36	0.55
5:J:330:TYR:CE1	1:a:57:ARG:HD2	2.42	0.55
1:A:631:TRP:CD1	1:A:677:GLY:HA3	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:402:BCL:H141	8:H:402:BCL:H203	1.89	0.54
5:I:40:PRO:HG2	5:I:260:SER:HB2	1.88	0.54
8:a:815:BCL:H121	8:a:815:BCL:C1D	2.38	0.54
1:A:109:HIS:HB2	1:A:321:TYR:CZ	2.41	0.54
5:I:317:LEU:HD11	5:I:323:ILE:HG13	1.88	0.54
1:A:114:TYR:O	1:A:117:ILE:HG12	2.06	0.54
8:E:409:BCL:C5	8:E:409:BCL:C9	2.85	0.54
8:F:402:BCL:H141	8:F:402:BCL:H203	1.89	0.54
1:A:321:TYR:HB2	8:A:815:BCL:O1D	2.08	0.54
5:G:104:VAL:HG23	5:G:113:PHE:HE2	1.72	0.54
5:J:104:VAL:HG23	5:J:113:PHE:HE2	1.72	0.54
1:A:648:THR:HG22	10:A:817:LHG:H381	1.89	0.54
4:D:128:CYS:HA	4:D:136:TYR:O	2.07	0.54
1:A:109:HIS:NE2	3:c:103:GLY:O	2.40	0.54
1:A:170:THR:HB	1:A:177:CYS:SG	2.48	0.54
8:A:815:BCL:C1D	8:A:815:BCL:H121	2.38	0.54
4:D:116:GLU:O	4:D:116:GLU:HG3	2.08	0.54
8:J:402:BCL:C9	8:J:402:BCL:C5	2.85	0.54
1:a:454:PHE:CE2	7:a:802:CLA:C9	2.89	0.54
1:A:321:TYR:HB3	8:A:815:BCL:H2A	1.89	0.54
5:E:152:VAL:HB	8:E:401:BCL:HBB3	1.90	0.54
5:F:152:VAL:HB	8:F:401:BCL:HBB3	1.90	0.54
8:a:806:BCL:H2	8:a:810:BCL:C14	2.36	0.54
2:B:225:ARG:NH1	5:E:312:GLN:HB2	2.23	0.54
1:a:209:HIS:CE1	8:a:808:BCL:C4D	2.91	0.54
8:a:807:BCL:HBD	8:a:807:BCL:CBA	2.38	0.54
2:B:143:CYS:O	1:a:530:PRO:HD2	2.08	0.53
8:E:402:BCL:H141	8:E:402:BCL:H203	1.89	0.53
1:A:570:MET:SD	7:A:802:CLA:H42	2.48	0.53
5:G:254:VAL:HG11	8:G:404:BCL:H41	1.90	0.53
5:J:254:VAL:HG11	8:J:405:BCL:H41	1.91	0.53
8:a:815:BCL:O1A	8:a:815:BCL:H3A	2.08	0.53
5:I:254:VAL:HG11	8:I:405:BCL:H41	1.91	0.53
5:H:119:VAL:HG21	8:H:406:BCL:CHA	2.39	0.53
1:a:676:ALA:HB1	10:a:817:LHG:HC92	1.91	0.53
10:A:818:LHG:H131	10:A:818:LHG:H292	1.90	0.53
1:a:194:PHE:HZ	1:a:208:PRO:HA	1.73	0.53
1:a:288:TYR:CD2	8:a:805:BCL:HMC2	2.44	0.53
1:A:186:LEU:H	8:A:807:BCL:H72	1.72	0.53
8:A:807:BCL:HBD	8:A:807:BCL:CBA	2.38	0.53
2:B:62:ARG:NH1	5:F:261:ASP:HB3	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:119:VAL:HG21	8:E:406:BCL:CHA	2.39	0.53
5:G:119:VAL:HG21	8:G:405:BCL:CHA	2.39	0.53
5:H:254:VAL:HG11	8:H:405:BCL:H41	1.91	0.53
5:J:119:VAL:HG21	8:J:406:BCL:CHA	2.39	0.53
1:A:411:TRP:O	8:A:805:BCL:H11	2.09	0.53
1:A:532:TYR:CE1	5:J:322:LYS:NZ	2.67	0.53
5:I:152:VAL:HB	8:I:401:BCL:HBB3	1.90	0.53
1:A:530:PRO:CG	2:B:165:VAL:HB	2.38	0.53
1:A:266:ASN:HD22	5:E:11:THR:CB	2.22	0.52
5:F:119:VAL:HG21	8:F:406:BCL:CHA	2.39	0.52
8:A:806:BCL:H52	8:A:810:BCL:H141	1.90	0.52
2:B:224:HIS:CG	2:B:224:HIS:O	2.62	0.52
5:I:119:VAL:HG21	8:I:406:BCL:CHA	2.39	0.52
1:a:171:ASN:HB3	8:a:807:BCL:O1A	2.09	0.52
2:B:160:LYS:HZ3	2:B:162:TYR:HB3	1.75	0.52
5:E:254:VAL:HG11	8:E:405:BCL:H41	1.90	0.52
1:A:530:PRO:HG2	2:B:170:PHE:HE1	1.74	0.52
5:H:152:VAL:HB	8:H:401:BCL:HBB3	1.90	0.52
5:I:64:PHE:CD1	5:I:89:ALA:HB2	2.45	0.52
8:A:815:BCL:O1A	8:A:815:BCL:H3A	2.09	0.52
5:H:267:VAL:HG21	8:H:403:BCL:HMA1	1.91	0.52
5:I:186:ILE:HD13	8:I:402:BCL:HAA2	1.92	0.52
1:a:288:TYR:OH	8:a:805:BCL:HBB1	2.10	0.52
1:a:464:TRP:CD1	3:c:44:THR:HG22	2.44	0.52
8:I:402:BCL:H141	8:I:402:BCL:H203	1.89	0.52
1:A:436:MET:HB3	7:a:803:CLA:H51	1.92	0.52
5:F:267:VAL:HG21	8:F:403:BCL:HMA1	1.91	0.52
5:I:188:PRO:CG	8:I:407:BCL:C2	2.88	0.52
3:c:22:ALA:O	3:c:26:SER:N	2.42	0.52
5:E:180:ILE:HG21	5:E:203:ILE:HG12	1.92	0.52
5:F:48:ASP:OD2	5:F:259:ARG:HD2	2.10	0.52
5:F:186:ILE:HD13	8:F:402:BCL:HAA2	1.92	0.52
5:F:254:VAL:HG11	8:F:405:BCL:H41	1.90	0.52
5:F:64:PHE:CD1	5:F:89:ALA:HB2	2.45	0.51
8:H:402:BCL:H91	8:H:407:BCL:H203	1.92	0.51
1:a:169:LEU:HB3	8:a:807:BCL:H2A	1.92	0.51
3:c:119:LEU:O	3:c:123:LEU:HD23	2.10	0.51
2:B:166:GLN:HE21	1:a:526:PRO:HG2	1.73	0.51
5:E:107:GLY:HA3	5:F:133:ASN:OD1	2.11	0.51
5:I:267:VAL:HG21	8:I:403:BCL:HMA1	1.91	0.51
1:a:454:PHE:HA	3:c:100:TRP:HH2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLN:HB3	5:E:261:ASP:OD2	2.10	0.51
8:A:815:BCL:HBC3	8:A:815:BCL:HHD	1.92	0.51
3:C:92:MET:O	3:C:96:LEU:HD23	2.09	0.51
5:I:180:ILE:HG21	5:I:203:ILE:HG12	1.92	0.51
5:J:180:ILE:HG21	5:J:203:ILE:HG12	1.92	0.51
6:a:801:GS0:C14	7:a:802:CLA:HMA1	2.41	0.51
8:a:815:BCL:HBC3	8:a:815:BCL:HHD	1.92	0.51
4:D:97:MET:HG2	5:J:281:GLY:C	2.35	0.51
5:E:267:VAL:HG21	8:E:403:BCL:HMA1	1.91	0.51
5:I:276:VAL:HA	5:I:288:LEU:HD22	1.93	0.51
1:a:585:ILE:HD11	3:c:36:ALA:HB2	1.91	0.51
1:a:646:THR:O	1:a:649:ILE:HG22	2.11	0.51
5:E:276:VAL:HA	5:E:288:LEU:HD22	1.93	0.51
8:F:402:BCL:H91	8:F:407:BCL:H203	1.92	0.51
1:A:411:TRP:O	8:A:805:BCL:C1	2.59	0.51
8:I:402:BCL:H91	8:I:407:BCL:H203	1.92	0.51
1:A:76:VAL:HG13	8:A:808:BCL:HED1	1.92	0.51
5:F:276:VAL:HA	5:F:288:LEU:HD22	1.93	0.51
3:C:44:THR:N	3:C:45:PRO:HD2	2.26	0.51
5:H:180:ILE:HG21	5:H:203:ILE:HG12	1.92	0.51
5:H:276:VAL:HA	5:H:288:LEU:HD22	1.93	0.51
1:a:268:ALA:HB1	1:a:271:LEU:HG	1.92	0.51
8:E:402:BCL:H91	8:E:407:BCL:H203	1.92	0.51
5:H:107:GLY:HA3	5:I:133:ASN:OD1	2.11	0.51
5:H:130:VAL:HG13	8:J:402:BCL:HED3	1.92	0.51
5:J:276:VAL:HA	5:J:288:LEU:HD22	1.93	0.51
3:c:73:ILE:HG23	3:c:73:ILE:O	2.11	0.51
5:H:328:PRO:CD	5:H:360:PHE:CD1	2.93	0.51
5:I:180:ILE:HD11	8:I:409[B]:BCL:HAC2	1.93	0.51
1:a:205:ALA:C	1:a:208:PRO:HD2	2.36	0.51
8:a:815:BCL:HBB2	8:a:815:BCL:HHC	1.92	0.51
8:A:811:BCL:HHC	8:A:811:BCL:HBB3	1.92	0.50
8:I:408[B]:BCL:HMB1	8:I:408[B]:BCL:CBB	2.42	0.50
5:F:180:ILE:HG21	5:F:203:ILE:HG12	1.92	0.50
1:A:464:TRP:CD1	1:A:464:TRP:H	2.28	0.50
8:F:408[B]:BCL:HMB1	8:F:408[B]:BCL:CBB	2.42	0.50
4:D:97:MET:HE2	5:J:281:GLY:O	2.11	0.50
5:F:188:PRO:CG	8:F:407:BCL:C2	2.88	0.50
5:H:125:TYR:HA	8:H:408[B]:BCL:C4B	2.42	0.50
8:a:811:BCL:HHC	8:a:811:BCL:HBB3	1.92	0.50
1:A:527:CYS:HB3	1:A:536:CYS:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:125:TYR:HA	8:E:408[B]:BCL:C4B	2.42	0.50
1:a:206:LEU:HD22	1:a:265:PRO:HG3	1.94	0.50
1:a:570:MET:HE1	7:a:802:CLA:HMA2	1.91	0.50
1:A:612:HIS:CE1	8:A:815:BCL:ND	2.79	0.50
5:H:326:ALA:HA	5:H:361:GLU:O	2.12	0.50
5:I:326:ALA:HA	5:I:361:GLU:O	2.12	0.50
5:F:328:PRO:CD	5:F:360:PHE:CD1	2.93	0.50
5:G:180:ILE:HG21	5:G:203:ILE:HG12	1.92	0.50
1:a:444:VAL:HG22	7:a:802:CLA:H43	1.94	0.50
3:C:92:MET:O	3:C:96:LEU:CD2	2.60	0.50
5:F:326:ALA:HA	5:F:361:GLU:O	2.12	0.50
5:H:261:ASP:CG	5:H:262:SER:N	2.69	0.50
1:a:458:ILE:HB	1:a:578:ASP:HB3	1.93	0.50
8:A:815:BCL:HHC	8:A:815:BCL:HBB2	1.92	0.49
5:G:276:VAL:HA	5:G:288:LEU:HD22	1.93	0.49
5:H:143:ARG:NH2	5:J:182:ASP:OD2	2.41	0.49
5:H:188:PRO:HG3	8:H:407:BCL:C2	2.42	0.49
1:a:500:LEU:CD1	10:a:818:LHG:H211	2.42	0.49
5:E:104:VAL:HG11	8:E:401:BCL:C2D	2.42	0.49
5:F:277:SER:C	5:F:285:ARG:HH21	2.21	0.49
5:I:314:LYS:HD2	5:I:339:ARG:NH1	2.28	0.49
1:a:631:TRP:CD1	1:a:677:GLY:HA3	2.47	0.49
5:E:130:VAL:HG13	8:E:409:BCL:HED3	1.92	0.49
5:E:277:SER:C	5:E:285:ARG:HH21	2.21	0.49
5:G:104:VAL:HG11	8:G:401:BCL:C2D	2.42	0.49
8:H:402:BCL:H93	8:H:403:BCL:H142	1.94	0.49
5:J:111:HIS:HB3	5:J:159:LEU:HD11	1.94	0.49
1:a:635:ARG:HD2	1:a:635:ARG:C	2.36	0.49
3:c:74:SER:H	3:c:77:TRP:HD1	1.60	0.49
5:E:326:ALA:HA	5:E:361:GLU:O	2.12	0.49
5:J:307:PHE:HE2	5:J:309:VAL:HG22	1.77	0.49
1:a:410:ILE:O	1:a:414:LYS:HB2	2.12	0.49
8:F:409[B]:BCL:HMC3	5:G:125:TYR:HB3	1.94	0.49
5:G:10:THR:CB	5:G:306:ASN:O	2.60	0.49
5:H:188:PRO:CG	8:H:407:BCL:C2	2.91	0.49
1:A:582:TRP:HA	1:A:585:ILE:HG22	1.95	0.49
8:E:402:BCL:H93	8:E:403:BCL:H142	1.94	0.49
5:F:180:ILE:HD11	8:F:409[B]:BCL:HAC2	1.93	0.49
5:H:104:VAL:HG11	8:H:401:BCL:C2D	2.42	0.49
5:H:277:SER:C	5:H:285:ARG:HH21	2.21	0.49
5:I:162:THR:HA	8:I:409[B]:BCL:OBB	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:402:BCL:H93	8:I:403:BCL:H142	1.94	0.49
8:a:814:BCL:H122	8:a:814:BCL:OBB	2.12	0.49
1:A:335:GLN:O	1:A:338:LYS:HG3	2.13	0.49
5:E:188:PRO:HG3	8:E:407:BCL:C2	2.42	0.49
5:E:188:PRO:CG	8:E:407:BCL:C2	2.91	0.49
5:E:328:PRO:CD	5:E:360:PHE:CD1	2.93	0.49
3:c:88:ILE:HG22	3:c:92:MET:HE3	1.95	0.49
5:F:104:VAL:HG11	8:F:401:BCL:C2D	2.42	0.49
5:F:318:PRO:HD2	5:F:321:TYR:HB2	1.94	0.49
5:G:326:ALA:HA	5:G:361:GLU:O	2.12	0.49
5:H:187:GLY:HA2	5:I:232:MET:HG3	1.94	0.49
5:I:104:VAL:HG11	8:I:401:BCL:C2D	2.42	0.49
8:I:409[B]:BCL:HMC3	5:J:125:TYR:HB3	1.94	0.49
1:A:633:GLU:HG2	1:a:633:GLU:HG2	1.95	0.49
5:F:314:LYS:HD2	5:F:339:ARG:NH1	2.28	0.49
5:H:152:VAL:HG21	8:H:401:BCL:CHC	2.43	0.49
1:A:209:HIS:CE1	8:A:808:BCL:C4D	2.96	0.49
1:A:186:LEU:H	8:A:807:BCL:H61	1.77	0.48
1:A:375:ASN:HB2	8:A:811:BCL:CHB	2.43	0.48
1:A:570:MET:HE1	7:A:802:CLA:H11	1.95	0.48
1:A:633:GLU:HG3	1:a:633:GLU:CG	2.43	0.48
2:B:223:LEU:HB2	5:E:15:ASP:OD1	2.13	0.48
5:F:284:LEU:HG	5:F:365:ALA:HB2	1.95	0.48
8:F:402:BCL:H93	8:F:403:BCL:H142	1.94	0.48
5:H:130:VAL:HG13	8:J:402:BCL:CED	2.43	0.48
5:H:141:GLN:N	5:H:141:GLN:OE1	2.46	0.48
5:I:284:LEU:HG	5:I:365:ALA:HB2	1.95	0.48
1:a:321:TYR:HB3	8:a:815:BCL:HMA2	1.95	0.48
5:G:111:HIS:HB3	5:G:159:LEU:HD11	1.94	0.48
5:I:152:VAL:HG21	8:I:401:BCL:CHC	2.43	0.48
8:J:402:BCL:H92	8:J:402:BCL:H51	1.95	0.48
1:a:375:ASN:HB2	8:a:811:BCL:CHB	2.43	0.48
5:E:141:GLN:N	5:E:141:GLN:OE1	2.47	0.48
8:E:409:BCL:H51	8:E:409:BCL:H92	1.95	0.48
8:I:401:BCL:HBA1	5:J:127:SER:HB2	1.95	0.48
4:D:129:VAL:HG23	4:D:129:VAL:O	2.13	0.48
5:F:162:THR:HA	8:F:409[B]:BCL:OBB	2.13	0.48
5:J:104:VAL:HG11	8:J:401:BCL:C2D	2.43	0.48
1:a:383:TYR:OH	8:a:812:BCL:HBB1	2.14	0.48
8:E:406:BCL:H72	8:E:406:BCL:H111	1.61	0.48
1:A:354:ILE:H	3:c:105:THR:HG21	1.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:130:VAL:HG13	8:E:409:BCL:CED	2.43	0.48
5:E:187:GLY:HA2	5:F:232:MET:HG3	1.94	0.48
8:H:401:BCL:HBA2	8:H:401:BCL:H3A	1.61	0.48
5:F:125:TYR:HA	8:F:408[B]:BCL:C4B	2.43	0.48
1:a:94:TYR:OH	8:a:806:BCL:O1D	2.32	0.48
4:D:133:ASN:H	5:J:279:ASP:HB3	1.78	0.48
8:E:409:BCL:O2A	8:E:409:BCL:H42	2.14	0.48
5:F:104:VAL:HG21	8:F:401:BCL:CHD	2.44	0.48
5:H:104:VAL:HG21	8:H:401:BCL:CHD	2.44	0.48
5:I:149:LEU:CD1	5:I:222:ARG:HE	2.27	0.48
5:I:277:SER:C	5:I:285:ARG:HH21	2.21	0.48
5:I:318:PRO:HD2	5:I:321:TYR:HB2	1.94	0.48
8:J:402:BCL:O2A	8:J:402:BCL:H42	2.14	0.48
1:a:186:LEU:N	8:a:807:BCL:H72	2.27	0.48
5:E:152:VAL:HG21	8:E:401:BCL:CHC	2.43	0.48
5:G:307:PHE:HE2	5:G:309:VAL:HG22	1.77	0.48
5:I:184:TRP:NE1	8:I:406:BCL:HBB1	2.28	0.48
8:J:402:BCL:HAC2	8:J:407:BCL:H71	1.96	0.48
1:A:680:LEU:HD11	10:A:817:LHG:HC91	1.96	0.47
4:D:98:GLU:HA	4:D:98:GLU:OE1	2.14	0.47
5:F:258:PHE:HB2	5:F:267:VAL:HG22	1.96	0.47
5:I:104:VAL:HG21	8:I:401:BCL:CHD	2.44	0.47
5:J:330:TYR:CE1	1:a:57:ARG:CD	2.96	0.47
4:D:65:GLU:C	4:D:65:GLU:CD	2.82	0.47
4:D:129:VAL:HG21	4:D:141:PHE:CD2	2.49	0.47
5:G:104:VAL:HG21	8:G:401:BCL:CHD	2.44	0.47
8:H:408[B]:BCL:HBB3	8:H:408[B]:BCL:HMB3	1.96	0.47
1:A:483:TRP:HE1	8:A:814:BCL:C1D	2.26	0.47
10:A:817:LHG:H162	10:A:817:LHG:H192	1.66	0.47
5:E:104:VAL:HG21	8:E:401:BCL:CHD	2.44	0.47
5:F:152:VAL:HG21	8:F:401:BCL:CHC	2.43	0.47
8:F:401:BCL:H3A	8:F:401:BCL:HBA2	1.61	0.47
5:G:64:PHE:CG	5:G:89:ALA:HB2	2.49	0.47
8:G:406:BCL:H2	8:G:406:BCL:H61	1.74	0.47
5:I:125:TYR:HA	8:I:408[B]:BCL:C4B	2.43	0.47
5:I:183:PHE:CE2	8:I:409[B]:BCL:HAC1	2.50	0.47
1:A:186:LEU:H	8:A:807:BCL:C7	2.28	0.47
1:a:434:ALA:HB1	8:a:814:BCL:H151	1.97	0.47
1:a:483:TRP:HE1	8:a:814:BCL:C1D	2.26	0.47
3:c:44:THR:N	3:c:45:PRO:HD2	2.29	0.47
5:E:167:VAL:HG22	5:E:208:LEU:HD23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:258:PHE:HB2	5:E:267:VAL:HG22	1.96	0.47
8:F:401:BCL:HBA1	5:G:127:SER:HB2	1.95	0.47
8:F:401:BCL:H8	8:F:401:BCL:H121	1.46	0.47
8:I:401:BCL:OBD	8:I:402:BCL:H3A	2.15	0.47
5:F:183:PHE:CE2	8:F:409[B]:BCL:HAC1	2.50	0.47
5:J:10:THR:CB	5:J:306:ASN:O	2.60	0.47
1:a:679:PHE:HB3	10:a:817:LHG:H141	1.96	0.47
5:I:258:PHE:HB2	5:I:267:VAL:HG22	1.96	0.47
5:E:104:VAL:HG11	8:E:401:BCL:C1D	2.45	0.47
5:F:104:VAL:HG11	8:F:401:BCL:C1D	2.45	0.47
8:F:406:BCL:H111	8:F:406:BCL:H72	1.62	0.47
8:G:401:BCL:HBA2	8:G:401:BCL:H3A	1.61	0.47
5:J:153:PRO:HA	5:J:218:VAL:HG22	1.97	0.47
5:J:188:PRO:HD2	8:J:407:BCL:C9	2.45	0.47
8:F:401:BCL:OBD	8:F:402:BCL:H3A	2.15	0.47
8:F:402:BCL:H141	8:F:402:BCL:H161	1.54	0.47
5:J:104:VAL:HG21	8:J:401:BCL:CHD	2.44	0.47
8:J:401:BCL:H3A	8:J:401:BCL:HBA2	1.61	0.47
8:E:401:BCL:OBD	8:E:402:BCL:H3A	2.15	0.46
5:F:184:TRP:NE1	8:F:406:BCL:HBB1	2.28	0.46
8:H:402:BCL:H203	8:H:402:BCL:H161	1.62	0.46
5:I:104:VAL:HG11	8:I:401:BCL:C1D	2.45	0.46
8:J:402:BCL:H143	8:J:402:BCL:H162	1.74	0.46
1:a:76:VAL:HG13	8:a:808:BCL:HED1	1.96	0.46
3:c:87:VAL:HG12	3:c:87:VAL:O	2.15	0.46
1:A:72:ASP:OD2	8:A:808:BCL:HMD1	2.16	0.46
1:A:447:THR:HA	1:A:450:GLU:OE2	2.14	0.46
2:B:78:GLU:O	2:B:78:GLU:HG2	2.15	0.46
7:A:803:CLA:H41	7:A:803:CLA:H62	1.52	0.46
8:F:409[B]:BCL:HMB3	8:F:409[B]:BCL:HBB3	1.96	0.46
5:G:104:VAL:HG11	8:G:401:BCL:C1D	2.45	0.46
1:a:319:TYR:CE1	1:a:356:PRO:CA	2.97	0.46
7:a:803:CLA:H62	7:a:803:CLA:H41	1.52	0.46
5:H:96:ARG:HG2	8:H:406:BCL:HED2	1.98	0.46
5:J:327:ALA:O	5:J:360:PHE:HD1	1.98	0.46
8:E:409:BCL:HAC2	8:G:406:BCL:H71	1.96	0.46
8:G:405:BCL:H161	8:G:405:BCL:H122	1.49	0.46
1:a:502:ARG:HE	1:a:543:GLN:CD	2.22	0.46
1:A:679:PHE:HB3	10:A:817:LHG:H141	1.96	0.46
8:A:807:BCL:HAC2	8:A:807:BCL:H121	1.98	0.46
2:B:62:ARG:HH12	5:F:261:ASP:HB3	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LEU:HD11	5:F:258:PHE:HA	1.98	0.46
5:F:254:VAL:CG2	5:F:273:PHE:CD2	2.99	0.46
5:G:153:PRO:HA	5:G:218:VAL:HG22	1.97	0.46
5:G:327:ALA:O	5:G:360:PHE:HD1	1.98	0.46
5:I:96:ARG:HG2	8:I:406:BCL:HED2	1.98	0.46
8:I:406:BCL:H72	8:I:406:BCL:H111	1.61	0.46
5:J:104:VAL:HG11	8:J:401:BCL:C1D	2.45	0.46
1:a:645:GLN:O	1:a:649:ILE:HG22	2.16	0.46
8:E:402:BCL:H203	8:E:402:BCL:H161	1.62	0.46
8:E:402:BCL:HED1	5:F:137:PRO:CB	2.46	0.46
5:G:188:PRO:HD2	8:G:406:BCL:C9	2.45	0.46
8:I:405:BCL:HAC2	8:I:406:BCL:H71	1.98	0.46
1:a:520:LYS:HB3	1:a:525:PHE:CE2	2.50	0.46
8:A:811:BCL:H2C	8:A:811:BCL:H93	1.98	0.46
5:E:282:GLY:O	5:E:284:LEU:HD13	2.16	0.46
5:H:167:VAL:HG22	5:H:208:LEU:HD23	1.96	0.46
8:H:402:BCL:HED1	5:I:137:PRO:CB	2.46	0.46
5:J:254:VAL:CG2	5:J:273:PHE:CD2	2.99	0.46
8:E:405:BCL:HAC2	8:E:406:BCL:H71	1.98	0.46
8:E:408[B]:BCL:HBB3	8:E:408[B]:BCL:HMB3	1.96	0.46
5:F:170:ILE:HD11	5:F:208:LEU:HD11	1.97	0.46
1:A:537:GLY:O	1:a:637:SER:HB2	2.16	0.46
5:F:323:ILE:HA	5:F:364:TYR:HA	1.98	0.46
5:H:318:PRO:HD2	5:H:321:TYR:HB2	1.97	0.46
8:H:401:BCL:OBD	8:H:402:BCL:H3A	2.15	0.46
5:I:170:ILE:HD11	5:I:208:LEU:HD11	1.97	0.46
5:I:254:VAL:CG2	5:I:273:PHE:CD2	2.99	0.46
1:a:199:ALA:HB3	8:a:808:BCL:HHC	1.97	0.46
10:a:817:LHG:H242	10:a:817:LHG:H272	1.53	0.46
1:A:184:ARG:HG2	1:A:187:GLY:HA2	1.98	0.45
5:H:104:VAL:HG11	8:H:401:BCL:C1D	2.45	0.45
8:H:405:BCL:HAC2	8:H:406:BCL:H71	1.98	0.45
8:I:409[B]:BCL:HBB3	8:I:409[B]:BCL:HMB3	1.97	0.45
8:J:402:BCL:H143	8:J:403:BCL:H203	1.98	0.45
1:a:528:LEU:O	1:a:531:VAL:HG12	2.16	0.45
1:a:582:TRP:HA	1:a:585:ILE:HG22	1.98	0.45
1:a:686:PHE:HB3	8:a:811:BCL:HBB1	1.99	0.45
8:a:805:BCL:H41	8:a:805:BCL:H61	1.37	0.45
2:B:210:TYR:OH	5:F:325:TYR:CD1	2.67	0.45
3:C:103:GLY:CA	1:a:106:PRO:HB2	2.45	0.45
5:G:254:VAL:CG2	5:G:273:PHE:CD2	2.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:284:LEU:HG	5:G:365:ALA:HB2	1.97	0.45
5:J:58:LEU:HD23	5:J:64:PHE:HB3	1.98	0.45
1:a:441:ALA:CB	3:c:52:TRP:CD1	2.99	0.45
1:A:185:PHE:CE2	1:A:194:PHE:CE2	3.03	0.45
8:A:808:BCL:H62	8:A:808:BCL:H41	1.67	0.45
5:E:143:ARG:NH2	5:G:182:ASP:OD2	2.41	0.45
8:E:402:BCL:HED2	5:F:134:VAL:HG21	1.99	0.45
5:H:258:PHE:HB2	5:H:267:VAL:HG22	1.96	0.45
5:I:323:ILE:HA	5:I:364:TYR:HA	1.98	0.45
10:a:817:LHG:H371	10:a:817:LHG:H332	1.97	0.45
5:E:96:ARG:HG2	8:E:406:BCL:HED2	1.98	0.45
8:G:404:BCL:HAC2	8:G:405:BCL:H71	1.98	0.45
5:H:82:LEU:HB2	8:H:402:BCL:HBB2	1.98	0.45
5:I:343:GLY:N	1:a:177:CYS:SG	2.90	0.45
1:a:279:PHE:HA	8:a:804[B]:BCL:CAB	2.46	0.45
8:a:811:BCL:HED2	8:a:812:BCL:HBA2	1.98	0.45
1:A:530:PRO:HD2	2:B:170:PHE:HZ	1.79	0.45
1:A:686:PHE:HB3	8:A:811:BCL:HBB1	1.99	0.45
5:E:318:PRO:HD2	5:E:321:TYR:HB2	1.97	0.45
8:E:407:BCL:H2	8:E:407:BCL:H61	1.48	0.45
8:E:409:BCL:H143	8:G:402:BCL:H203	1.98	0.45
1:a:320:LEU:HB2	1:a:323:GLU:HG3	1.98	0.45
3:c:23:LEU:O	3:c:27:VAL:HG23	2.17	0.45
5:E:254:VAL:CG2	5:E:273:PHE:CD2	2.99	0.45
5:G:328:PRO:CD	5:G:360:PHE:CD1	2.99	0.45
5:H:254:VAL:CG2	5:H:273:PHE:CD2	2.99	0.45
8:H:402:BCL:HED2	5:I:134:VAL:HG21	1.99	0.45
8:H:404:BCL:HBB2	8:H:405:BCL:H51	1.99	0.45
8:a:806:BCL:H112	8:a:806:BCL:H151	1.45	0.45
8:A:811:BCL:HED2	8:A:812:BCL:HBA2	1.98	0.45
2:B:62:ARG:HH12	5:F:261:ASP:CB	2.29	0.45
5:G:96:ARG:HG2	8:G:405:BCL:HED2	1.98	0.45
8:I:405:BCL:H152	8:I:405:BCL:H112	1.83	0.45
8:I:407:BCL:H2	8:I:407:BCL:H61	1.48	0.45
1:a:319:TYR:CD1	1:a:356:PRO:HA	2.52	0.45
7:A:802:CLA:H152	7:A:802:CLA:H18	1.65	0.45
7:A:803:CLA:H162	7:A:803:CLA:H141	1.67	0.45
5:F:96:ARG:HG2	8:F:406:BCL:HED2	1.98	0.45
5:F:183:PHE:CD2	8:F:401:BCL:H191	2.52	0.45
5:H:282:GLY:O	5:H:284:LEU:HD13	2.16	0.45
5:I:183:PHE:CD2	8:I:401:BCL:H191	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:96:ARG:HG2	8:J:406:BCL:HED2	1.98	0.45
5:J:330:TYR:CD1	1:a:57:ARG:HD2	2.51	0.45
1:A:529:GLY:HA3	1:a:529:GLY:HA2	1.91	0.45
8:I:405:BCL:H41	8:I:405:BCL:H61	1.81	0.45
8:J:406:BCL:H111	8:J:406:BCL:H72	1.61	0.45
1:a:288:TYR:HD2	8:a:805:BCL:HMC2	1.82	0.45
1:A:531:VAL:HG11	2:B:141:VAL:O	2.17	0.45
8:A:807:BCL:H2	8:A:807:BCL:H101	1.98	0.45
3:C:96:LEU:HD11	8:a:815:BCL:CGA	2.46	0.45
8:a:807:BCL:HBB1	8:a:808:BCL:NB	2.32	0.45
10:a:818:LHG:H222	10:a:818:LHG:H191	1.69	0.45
1:A:194:PHE:HZ	1:A:211:VAL:HB	1.83	0.44
8:E:405:BCL:H152	8:E:405:BCL:H112	1.83	0.44
5:F:82:LEU:HB2	8:F:402:BCL:HBB2	1.98	0.44
5:J:331:ARG:HA	1:a:59:THR:HB	1.99	0.44
8:J:401:BCL:H8	8:J:401:BCL:H121	1.46	0.44
8:a:811:BCL:H3A	8:a:811:BCL:HBA2	1.61	0.44
8:A:811:BCL:H13	8:A:811:BCL:H172	1.81	0.44
8:A:812:BCL:CBB	8:A:812:BCL:CMB	2.95	0.44
5:E:108:ASP:OD1	5:E:108:ASP:C	2.60	0.44
8:F:405:BCL:HAC2	8:F:406:BCL:H71	1.98	0.44
5:G:268:LYS:O	5:G:268:LYS:HG3	2.17	0.44
5:G:300:MET:SD	8:G:406:BCL:HBA2	2.57	0.44
5:I:82:LEU:HB2	8:I:402:BCL:HBB2	1.98	0.44
1:A:634:ASP:CB	7:A:803:CLA:HMD3	2.44	0.44
2:B:223:LEU:HD21	5:E:31:LYS:HB3	1.99	0.44
8:E:404:BCL:HBB2	8:E:405:BCL:H51	1.99	0.44
1:a:570:MET:HA	1:a:596:ILE:HB	2.00	0.44
1:A:570:MET:SD	7:A:802:CLA:H11	2.57	0.44
3:C:20:MET:HE3	3:C:20:MET:HA	1.99	0.44
5:J:328:PRO:CD	5:J:360:PHE:CD1	2.99	0.44
1:a:570:MET:SD	7:a:802:CLA:HMA2	2.57	0.44
10:a:818:LHG:H352	10:a:818:LHG:H172	1.99	0.44
4:D:128:CYS:CA	4:D:136:TYR:O	2.66	0.44
5:E:9:VAL:HG11	5:E:308:ASN:CG	2.42	0.44
5:E:82:LEU:HB2	8:E:402:BCL:HBB2	1.98	0.44
5:F:189:ALA:HA	8:F:407:BCL:H3A	1.99	0.44
5:J:300:MET:SD	8:J:407:BCL:HBA2	2.57	0.44
8:a:807:BCL:H2	8:a:807:BCL:H101	1.98	0.44
8:a:808:BCL:HBA2	8:a:808:BCL:HBD	2.00	0.44
1:A:634:ASP:HB2	7:A:803:CLA:CMD	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:809[B]:BCL:HBB2	8:A:809[B]:BCL:HHC	2.00	0.44
13:A:821:SF4:S4	1:a:670:ILE:CD1	3.05	0.44
8:G:403:BCL:HBB2	8:G:404:BCL:H51	1.99	0.44
5:H:125:TYR:CD1	5:H:125:TYR:C	2.96	0.44
8:H:402:BCL:H41	8:H:402:BCL:H61	1.80	0.44
5:I:170:ILE:HD12	5:I:208:LEU:CD1	2.45	0.44
8:I:402:BCL:H41	8:I:402:BCL:H61	1.80	0.44
8:I:404:BCL:HBB2	8:I:405:BCL:H51	1.99	0.44
8:a:812:BCL:HBA2	8:a:812:BCL:H3A	1.56	0.44
8:A:807:BCL:HBB1	8:A:808:BCL:NB	2.32	0.44
5:E:184:TRP:CD1	5:E:184:TRP:C	2.96	0.44
8:E:406:BCL:H161	8:E:406:BCL:H122	1.49	0.44
5:G:148:ILE:O	5:G:222:ARG:HA	2.18	0.44
3:c:66:LEU:HD23	3:c:66:LEU:HA	1.88	0.44
1:A:412:ILE:HD11	8:A:805:BCL:HBD	2.00	0.44
8:A:812:BCL:HBA2	8:A:812:BCL:H3A	1.56	0.44
4:D:132:HIS:CG	4:D:132:HIS:O	2.71	0.44
5:F:108:ASP:OD1	5:F:108:ASP:C	2.60	0.44
8:I:409[B]:BCL:HBC3	8:I:409[B]:BCL:H2C	1.67	0.44
8:J:405:BCL:HAC2	8:J:406:BCL:H71	1.98	0.44
7:a:802:CLA:H152	7:a:802:CLA:H18	1.65	0.44
7:a:803:CLA:H162	7:a:803:CLA:H141	1.67	0.44
8:H:406:BCL:H111	8:H:406:BCL:H72	1.61	0.44
8:a:813:BCL:H51	8:a:813:BCL:H11	1.73	0.44
8:A:805:BCL:CBB	10:A:818:LHG:H381	2.48	0.43
8:G:401:BCL:H8	8:G:401:BCL:H121	1.46	0.43
5:H:158:ASP:OD2	5:I:132:ARG:NH1	2.43	0.43
8:J:405:BCL:H152	8:J:405:BCL:H112	1.83	0.43
8:a:809[B]:BCL:HBB2	8:a:809[B]:BCL:HHC	2.00	0.43
10:a:817:LHG:H341	10:a:817:LHG:H372	1.81	0.43
5:E:99:VAL:HG22	5:E:116:GLU:OE1	2.18	0.43
5:I:258:PHE:C	5:I:258:PHE:CD1	2.96	0.43
8:I:401:BCL:H8	8:I:401:BCL:H121	1.46	0.43
8:a:804[B]:BCL:HBA1	8:a:804[B]:BCL:O1D	2.18	0.43
8:a:810:BCL:H91	8:a:810:BCL:H112	1.59	0.43
5:I:108:ASP:C	5:I:108:ASP:OD1	2.60	0.43
5:I:318:PRO:HD2	5:I:321:TYR:CB	2.49	0.43
1:A:509:THR:HG21	4:D:27:ALA:HB1	2.01	0.43
5:E:125:TYR:CD1	5:E:125:TYR:C	2.96	0.43
5:E:258:PHE:CD1	5:E:258:PHE:C	2.96	0.43
5:H:318:PRO:HD2	5:H:321:TYR:CB	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:188:PRO:CG	8:I:407:BCL:H2	2.48	0.43
5:I:294:PRO:HG3	8:I:407:BCL:HAC1	2.01	0.43
8:J:401:BCL:OBD	8:J:402:BCL:H3A	2.19	0.43
8:J:404:BCL:HBB2	8:J:405:BCL:H51	1.99	0.43
2:B:210:TYR:HB2	5:F:324:ARG:HB3	2.00	0.43
3:C:94:LEU:HD12	3:C:94:LEU:HA	1.80	0.43
5:E:294:PRO:HG3	8:E:407:BCL:HAC1	2.00	0.43
8:E:409:BCL:H3A	8:G:401:BCL:OBD	2.19	0.43
8:F:406:BCL:H61	8:F:406:BCL:H41	1.92	0.43
5:H:99:VAL:HG22	5:H:116:GLU:OE1	2.18	0.43
1:A:321:TYR:CB	8:A:815:BCL:H2A	2.47	0.43
1:A:560:TRP:O	1:A:565:ALA:HB3	2.19	0.43
1:A:625:PHE:HE1	7:A:803:CLA:HAB	1.83	0.43
1:a:450:GLU:HA	1:a:578:ASP:HB2	2.00	0.43
1:A:648:THR:CG2	10:A:817:LHG:H381	2.48	0.43
8:A:805:BCL:H203	8:A:805:BCL:H161	1.66	0.43
5:F:188:PRO:CG	8:F:407:BCL:H2	2.49	0.43
5:H:258:PHE:CD1	5:H:258:PHE:C	2.96	0.43
5:H:294:PRO:HG3	8:H:407:BCL:HAC1	2.00	0.43
1:a:321:TYR:HB2	8:a:815:BCL:H2A	2.00	0.43
1:a:520:LYS:HB3	1:a:525:PHE:HE2	1.84	0.43
7:a:803:CLA:H11	7:a:803:CLA:HBA1	1.75	0.43
5:F:258:PHE:CD1	5:F:258:PHE:C	2.96	0.43
8:F:404:BCL:HBB2	8:F:405:BCL:H51	1.99	0.43
5:J:294:PRO:HG3	8:J:407:BCL:HAC1	2.00	0.43
1:A:405:ASN:O	5:E:259:ARG:NH1	2.52	0.43
1:A:640:GLU:HG3	1:a:502:ARG:HH12	1.84	0.43
8:A:814:BCL:H142	8:A:814:BCL:HHC	2.00	0.43
5:F:318:PRO:HD2	5:F:321:TYR:CB	2.49	0.43
5:H:184:TRP:CD1	5:H:184:TRP:C	2.96	0.43
1:a:441:ALA:HB3	3:c:52:TRP:CD1	2.52	0.43
1:A:530:PRO:HG3	2:B:165:VAL:HB	2.01	0.43
8:A:808:BCL:HBD	8:A:808:BCL:HBA2	1.99	0.43
8:A:811:BCL:HBA2	8:A:811:BCL:H3A	1.61	0.43
4:D:65:GLU:CD	4:D:65:GLU:O	2.62	0.43
5:E:318:PRO:HD2	5:E:321:TYR:CB	2.49	0.43
5:G:258:PHE:CD1	5:G:258:PHE:C	2.96	0.43
5:J:258:PHE:CD1	5:J:258:PHE:C	2.96	0.43
1:A:561:TYR:O	11:A:819:IKV:C25	2.67	0.42
2:B:225:ARG:HD3	2:B:225:ARG:HA	1.66	0.42
5:F:183:PHE:CD2	8:F:409[B]:BCL:HAC1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:409[B]:BCL:HBA1	8:I:409[B]:BCL:H3A	1.69	0.42
1:a:450:GLU:O	1:a:578:ASP:HB2	2.19	0.42
1:a:473:TRP:HH2	10:a:818:LHG:C23	2.32	0.42
1:A:62:TYR:HB2	8:A:813:BCL:H18	2.01	0.42
8:E:401:BCL:HBA2	8:E:401:BCL:H3A	1.61	0.42
5:I:11:THR:HA	5:I:308:ASN:O	2.19	0.42
5:I:189:ALA:HA	8:I:407:BCL:H3A	1.99	0.42
5:J:148:ILE:O	5:J:222:ARG:HA	2.18	0.42
1:a:561:TYR:O	11:a:819:IKV:C25	2.68	0.42
2:B:159:TYR:OH	1:a:531:VAL:HB	2.19	0.42
5:F:294:PRO:HG3	8:F:407:BCL:HAC1	2.00	0.42
8:G:405:BCL:H111	8:G:405:BCL:H72	1.61	0.42
8:J:402:BCL:H193	8:J:406:BCL:CMB	2.49	0.42
7:a:802:CLA:C19	3:c:55:LEU:HG	2.50	0.42
5:E:82:LEU:HD12	5:E:104:VAL:HG22	2.02	0.42
8:E:401:BCL:H8	8:E:401:BCL:H121	1.46	0.42
5:G:294:PRO:HG3	8:G:406:BCL:HAC1	2.00	0.42
8:H:402:BCL:H142	8:H:402:BCL:H111	1.75	0.42
5:I:183:PHE:CD2	8:I:409[B]:BCL:HAC1	2.54	0.42
8:a:813:BCL:H13	8:a:813:BCL:H101	1.89	0.42
3:c:88:ILE:O	3:c:92:MET:HG3	2.20	0.42
1:A:638:ARG:HA	7:A:803:CLA:O2D	2.19	0.42
1:A:680:LEU:HD11	10:A:817:LHG:HC82	2.02	0.42
8:A:810:BCL:H91	8:A:810:BCL:H112	1.60	0.42
8:E:409:BCL:H193	8:G:405:BCL:CMB	2.49	0.42
8:F:401:BCL:HBC2	8:F:401:BCL:H2C	1.85	0.42
1:a:210:ALA:HB3	1:a:257:GLY:HA2	2.01	0.42
8:a:804[B]:BCL:CED	8:a:813:BCL:HBA1	2.50	0.42
5:F:82:LEU:HD12	5:F:104:VAL:HG22	2.02	0.42
5:I:335:LEU:HB3	5:I:336:GLU:H	1.65	0.42
1:A:531:VAL:HG21	2:B:141:VAL:HB	2.01	0.42
8:E:409:BCL:C5	8:E:409:BCL:H92	2.49	0.42
5:F:130:VAL:O	5:F:134:VAL:HG23	2.19	0.42
5:I:38:ALA:O	5:I:264:GLY:HA2	2.20	0.42
5:I:130:VAL:O	5:I:134:VAL:HG23	2.20	0.42
8:J:402:BCL:C5	8:J:402:BCL:H92	2.49	0.42
8:E:405:BCL:H41	8:E:405:BCL:H61	1.81	0.42
5:F:38:ALA:O	5:F:264:GLY:HA2	2.20	0.42
5:G:38:ALA:O	5:G:264:GLY:HA2	2.20	0.42
8:H:406:BCL:H122	8:H:406:BCL:H161	1.49	0.42
5:J:307:PHE:CE2	5:J:309:VAL:HG22	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:62:TYR:HB2	8:a:813:BCL:H18	2.01	0.42
8:a:807:BCL:H2	8:a:807:BCL:C10	2.50	0.42
1:A:635:ARG:HD3	1:A:635:ARG:C	2.45	0.42
8:A:807:BCL:H2	8:A:807:BCL:C10	2.50	0.42
2:B:133:TYR:OH	2:B:183:SER:OG	2.20	0.42
8:E:402:BCL:C4A	8:E:407:BCL:H143	2.50	0.42
8:F:402:BCL:H142	8:F:402:BCL:H111	1.75	0.42
5:J:64:PHE:CG	5:J:89:ALA:HB2	2.55	0.42
8:J:406:BCL:H122	8:J:406:BCL:H161	1.49	0.42
1:a:73:GLU:HA	1:a:180:PHE:CZ	2.55	0.42
1:a:434:ALA:HB1	8:a:814:BCL:H171	2.01	0.42
8:E:408[B]:BCL:HMC1	8:G:401:BCL:C2	2.50	0.42
5:G:64:PHE:CD2	5:G:89:ALA:HB2	2.55	0.42
8:A:814:BCL:H71	8:A:814:BCL:H112	1.37	0.41
5:E:199:ARG:HD3	5:G:182:ASP:OD1	2.20	0.41
5:E:208:LEU:CD1	5:E:221:SER:OG	2.68	0.41
5:E:208:LEU:HD12	5:E:208:LEU:HA	1.89	0.41
5:H:82:LEU:HD12	5:H:104:VAL:HG22	2.02	0.41
5:H:267:VAL:CG2	8:H:403:BCL:HMA1	2.50	0.41
8:H:402:BCL:C4A	8:H:407:BCL:H143	2.50	0.41
5:J:63:GLY:O	5:J:89:ALA:HB1	2.19	0.41
1:A:447:THR:HA	1:A:450:GLU:HG2	2.02	0.41
4:D:97:MET:HE1	4:D:100:ARG:HH21	1.85	0.41
5:I:327:ALA:O	5:I:360:PHE:HD1	2.03	0.41
8:I:402:BCL:H203	8:I:402:BCL:H161	1.62	0.41
8:a:808:BCL:H41	8:a:808:BCL:H62	1.68	0.41
4:D:97:MET:CE	5:J:284:LEU:HD22	2.47	0.41
5:F:188:PRO:HD3	5:G:139:TYR:CZ	2.56	0.41
5:H:208:LEU:CD1	5:H:221:SER:OG	2.68	0.41
8:I:402:BCL:H52	8:I:402:BCL:C9	2.39	0.41
8:I:402:BCL:C4A	8:I:407:BCL:H143	2.50	0.41
8:A:815:BCL:H143	8:A:815:BCL:H111	1.95	0.41
5:H:196:GLY:HA2	5:H:232:MET:SD	2.60	0.41
8:H:402:BCL:H141	8:H:402:BCL:H161	1.55	0.41
8:H:408[B]:BCL:HBA1	8:H:408[B]:BCL:H3A	1.69	0.41
5:I:188:PRO:HD3	5:J:139:TYR:CZ	2.56	0.41
1:a:687:MET:HG3	8:a:815:BCL:HBC2	2.02	0.41
7:a:802:CLA:H2A	7:a:802:CLA:O1D	2.21	0.41
8:a:811:BCL:H61	8:a:811:BCL:H92	1.55	0.41
1:A:51:PHE:CE2	2:B:152:PRO:HB3	2.55	0.41
5:G:57:PRO:HG3	5:G:248:LEU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:82:LEU:HD12	5:G:104:VAL:HG22	2.02	0.41
8:H:402:BCL:H193	8:H:406:BCL:HHB	2.03	0.41
5:I:267:VAL:CG2	8:I:403:BCL:HMA1	2.50	0.41
5:J:326:ALA:HA	5:J:361:GLU:O	2.20	0.41
8:J:406:BCL:H61	8:J:406:BCL:H41	1.91	0.41
8:J:407:BCL:H2	8:J:407:BCL:H61	1.74	0.41
1:a:205:ALA:O	1:a:209:HIS:HB2	2.21	0.41
1:a:476:ALA:N	11:a:819:IKV:O8	2.49	0.41
3:c:49:PHE:HE1	3:c:52:TRP:HZ3	1.69	0.41
1:A:706:PRO:HB3	1:a:330:PHE:CE2	2.56	0.41
2:B:162:TYR:CD1	2:B:162:TYR:C	2.99	0.41
5:E:40:PRO:HG3	5:E:265:ILE:CG1	2.50	0.41
5:E:267:VAL:CG2	8:E:403:BCL:HMA1	2.50	0.41
5:G:59:ASP:CG	5:G:62:LYS:HB2	2.46	0.41
5:G:307:PHE:CE2	5:G:309:VAL:HG22	2.55	0.41
5:H:59:ASP:CG	5:H:62:LYS:HB2	2.46	0.41
5:H:179:TRP:HE3	8:I:408[B]:BCL:OBD	2.04	0.41
8:H:405:BCL:H41	8:H:405:BCL:H61	1.81	0.41
5:J:38:ALA:O	5:J:264:GLY:HA2	2.20	0.41
1:A:640:GLU:HG3	1:a:502:ARG:NH1	2.35	0.41
7:A:802:CLA:H102	7:A:802:CLA:H13	1.65	0.41
2:B:61:PRO:HD2	5:F:77:SER:CB	2.47	0.41
5:E:59:ASP:CG	5:E:62:LYS:HB2	2.46	0.41
5:F:170:ILE:HD11	5:F:208:LEU:CD1	2.51	0.41
5:I:11:THR:HG21	1:a:167:HIS:CD2	2.55	0.41
5:J:178:ASP:OD1	5:J:181:ARG:NH2	2.53	0.41
8:J:402:BCL:H193	8:J:406:BCL:HMB3	2.03	0.41
10:a:817:LHG:H211	10:a:817:LHG:H181	1.80	0.41
8:H:401:BCL:HBC2	8:H:401:BCL:H2C	1.85	0.41
5:E:43:PRO:O	5:F:359:GLN:HB2	2.21	0.41
5:E:138:ILE:HG21	5:G:43:PRO:HB2	2.03	0.41
8:E:402:BCL:H193	8:E:406:BCL:HHB	2.03	0.41
8:E:406:BCL:H161	8:E:406:BCL:H203	1.91	0.41
5:F:298:HIS:HE1	8:F:403:BCL:NC	2.19	0.41
8:F:405:BCL:H152	8:F:405:BCL:H112	1.83	0.41
5:H:199:ARG:HD3	5:J:182:ASP:OD1	2.20	0.41
5:H:327:ALA:O	5:H:360:PHE:HD1	2.04	0.41
5:I:59:ASP:CG	5:I:62:LYS:HB2	2.46	0.41
5:J:314:LYS:O	5:J:314:LYS:HG2	2.21	0.41
1:a:676:ALA:CB	10:a:817:LHG:HC92	2.49	0.41
5:E:141:GLN:NE2	8:E:409:BCL:O1A	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:298:HIS:HE1	8:H:403:BCL:NC	2.19	0.41
5:I:55:VAL:HG13	5:I:248:LEU:HD21	2.03	0.41
5:I:125:TYR:HB3	8:I:408[B]:BCL:C1C	2.51	0.41
5:I:298:HIS:HE1	8:I:403:BCL:NC	2.19	0.41
5:J:82:LEU:HD12	5:J:104:VAL:HG22	2.02	0.41
1:a:646:THR:O	1:a:649:ILE:CG2	2.69	0.41
5:F:206:ASN:HD21	5:F:224:ARG:HH22	1.68	0.40
8:F:407:BCL:H2	8:F:407:BCL:H61	1.48	0.40
5:H:62:LYS:HA	5:H:62:LYS:HD3	1.89	0.40
5:H:232:MET:SD	5:H:296:VAL:HG21	2.61	0.40
8:H:402:BCL:H52	8:H:402:BCL:C9	2.39	0.40
5:I:82:LEU:HD12	5:I:104:VAL:HG22	2.02	0.40
8:a:805:BCL:H93	8:a:805:BCL:H112	1.84	0.40
3:c:61:ILE:HA	3:c:64:MET:HG2	2.03	0.40
1:A:637:SER:OG	7:A:803:CLA:OBD	2.38	0.40
2:B:130:LYS:HB3	2:B:201:PRO:HG3	2.04	0.40
2:B:144:GLY:HA3	1:a:531:VAL:HB	2.04	0.40
4:D:128:CYS:CB	4:D:136:TYR:O	2.70	0.40
5:H:351:HIS:HB2	5:J:305:ASN:HD21	1.86	0.40
8:I:402:BCL:H111	8:I:402:BCL:H142	1.75	0.40
1:a:688:LEU:C	6:a:801:GS0:OBD	2.63	0.40
1:A:160:GLY:HA3	8:A:807:BCL:HHD	2.02	0.40
8:E:405:BCL:CHA	8:E:406:BCL:H143	2.52	0.40
8:F:402:BCL:C4A	8:F:407:BCL:H143	2.50	0.40
8:F:402:BCL:H61	8:F:402:BCL:H41	1.80	0.40
8:H:408[B]:BCL:HMC1	8:J:401:BCL:C2	2.50	0.40
8:J:405:BCL:H193	8:J:407:BCL:H201	2.03	0.40
7:a:802:CLA:H13	7:a:802:CLA:H102	1.65	0.40
1:A:94:TYR:OH	8:A:806:BCL:O1D	2.32	0.40
8:E:402:BCL:HED1	5:F:137:PRO:HB3	2.03	0.40
8:E:409:BCL:H193	8:G:405:BCL:HMB3	2.03	0.40
8:F:402:BCL:H193	8:F:406:BCL:HHB	2.03	0.40
5:F:125:TYR:HB3	8:F:408[B]:BCL:C1C	2.51	0.40
8:F:403:BCL:HBC3	8:F:403:BCL:HHD	2.04	0.40
5:J:188:PRO:HD2	8:J:407:BCL:H93	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	665/731 (91%)	649 (98%)	16 (2%)	0	100	100
1	a	652/731 (89%)	642 (98%)	10 (2%)	0	100	100
2	B	119/231 (52%)	115 (97%)	4 (3%)	0	100	100
3	C	119/206 (58%)	118 (99%)	1 (1%)	0	100	100
3	c	119/206 (58%)	118 (99%)	1 (1%)	0	100	100
4	D	115/143 (80%)	113 (98%)	2 (2%)	0	100	100
5	E	357/366 (98%)	355 (99%)	2 (1%)	0	100	100
5	F	357/366 (98%)	352 (99%)	5 (1%)	0	100	100
5	G	357/366 (98%)	353 (99%)	4 (1%)	0	100	100
5	H	356/366 (97%)	354 (99%)	2 (1%)	0	100	100
5	I	357/366 (98%)	352 (99%)	5 (1%)	0	100	100
5	J	355/366 (97%)	350 (99%)	5 (1%)	0	100	100
All	All	3928/4444 (88%)	3871 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	553/599 (92%)	553 (100%)	0	100	100
1	a	542/599 (90%)	542 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	103/162 (64%)	103 (100%)	0	100	100
3	C	102/173 (59%)	102 (100%)	0	100	100
3	c	102/173 (59%)	102 (100%)	0	100	100
4	D	105/128 (82%)	105 (100%)	0	100	100
5	E	297/302 (98%)	297 (100%)	0	100	100
5	F	297/302 (98%)	297 (100%)	0	100	100
5	G	297/302 (98%)	297 (100%)	0	100	100
5	H	296/302 (98%)	296 (100%)	0	100	100
5	I	297/302 (98%)	297 (100%)	0	100	100
5	J	296/302 (98%)	296 (100%)	0	100	100
All	All	3287/3646 (90%)	3287 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	266	ASN
1	A	645	GLN
2	B	166	GLN
3	C	39	HIS
5	E	37	ASN
5	E	156	ASN
5	E	157	ASN
5	E	198	GLN
5	E	206	ASN
5	E	227	HIS
5	E	263	GLN
5	F	156	ASN
5	F	157	ASN
5	F	198	GLN
5	F	206	ASN
5	F	227	HIS
5	F	305	ASN
5	G	198	GLN
5	G	206	ASN
5	G	227	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	G	305	ASN
5	G	306	ASN
5	H	37	ASN
5	H	156	ASN
5	H	157	ASN
5	H	206	ASN
5	H	227	HIS
5	I	13	HIS
5	I	156	ASN
5	I	157	ASN
5	I	198	GLN
5	I	227	HIS
5	I	305	ASN
5	J	206	ASN
5	J	227	HIS
5	J	305	ASN
5	J	306	ASN
1	a	63	GLN
1	a	74	GLN
1	a	99	GLN
1	a	399	GLN
1	a	521	ASN
1	a	645	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 91 ligands modelled in this entry, 2 are monoatomic - leaving 89 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	BCL	G	405	-	69,74,74	1.03	6 (8%)	79,115,115	1.64	13 (16%)
9	F39	A	816	-	66,66,66	3.84	26 (39%)	83,85,85	4.29	32 (38%)
13	SF4	A	821	1	0,12,12	-	-	-	-	-
8	BCL	G	404	5	69,74,74	1.10	4 (5%)	79,115,115	1.34	8 (10%)
8	BCL	A	809[B]	8,1	49,54,74	1.30	5 (10%)	55,91,115	1.50	6 (10%)
8	BCL	A	811	1	69,74,74	1.10	4 (5%)	79,115,115	1.60	10 (12%)
8	BCL	a	814	-	69,74,74	1.10	6 (8%)	79,115,115	1.39	8 (10%)
8	BCL	H	401	-	69,74,74	1.29	6 (8%)	79,115,115	1.68	13 (16%)
8	BCL	I	402	14	69,74,74	1.34	8 (11%)	79,115,115	1.85	18 (22%)
8	BCL	F	408[B]	5	49,54,74	1.63	10 (20%)	55,91,115	2.07	16 (29%)
8	BCL	E	408[B]	5	49,54,74	1.49	7 (14%)	55,91,115	1.99	14 (25%)
8	BCL	I	406	-	69,74,74	1.05	6 (8%)	79,115,115	1.63	12 (15%)
7	CLA	a	803	14	69,73,73	1.39	8 (11%)	82,113,113	1.49	11 (13%)
8	BCL	F	406	-	69,74,74	1.05	6 (8%)	79,115,115	1.63	12 (15%)
8	BCL	a	812	8,9	69,74,74	1.10	5 (7%)	79,115,115	1.43	8 (10%)
8	BCL	a	813	-	69,74,74	1.13	5 (7%)	79,115,115	1.30	7 (8%)
8	BCL	E	401	-	69,74,74	1.28	6 (8%)	79,115,115	1.68	13 (16%)
10	LHG	A	818	-	48,48,48	0.67	1 (2%)	51,54,54	0.89	3 (5%)
8	BCL	a	810	-	69,74,74	1.19	6 (8%)	79,115,115	1.56	10 (12%)
8	BCL	J	403	-	69,74,74	1.11	4 (5%)	79,115,115	1.38	8 (10%)
7	CLA	a	802	-	69,73,73	1.28	8 (11%)	82,113,113	1.45	9 (10%)
8	BCL	I	407	-	69,74,74	1.33	8 (11%)	79,115,115	1.56	12 (15%)
8	BCL	A	808	-	69,74,74	1.10	5 (7%)	79,115,115	1.40	6 (7%)
8	BCL	F	407	-	69,74,74	1.33	7 (10%)	79,115,115	1.56	12 (15%)
8	BCL	G	403	-	69,74,74	1.10	4 (5%)	79,115,115	1.29	6 (7%)
7	CLA	A	803	14	69,73,73	1.24	9 (13%)	82,113,113	1.87	13 (15%)
8	BCL	A	815	-	69,74,74	1.27	5 (7%)	79,115,115	1.88	13 (16%)
13	SF4	B	302	2	0,12,12	-	-	-	-	-
8	BCL	G	402	-	69,74,74	1.12	4 (5%)	79,115,115	1.38	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	IKV	A	819	-	51,51,51	0.66	1 (1%)	59,59,59	0.67	3 (5%)
8	BCL	J	402	14	69,74,74	1.33	8 (11%)	79,115,115	1.84	17 (21%)
8	BCL	H	406	-	69,74,74	1.05	6 (8%)	79,115,115	1.63	13 (16%)
8	BCL	H	403	-	69,74,74	1.11	4 (5%)	79,115,115	1.37	8 (10%)
8	BCL	G	406	-	69,74,74	1.37	8 (11%)	79,115,115	1.64	17 (21%)
8	BCL	I	401	-	69,74,74	1.28	6 (8%)	79,115,115	1.68	14 (17%)
8	BCL	a	808	-	69,74,74	1.11	5 (7%)	79,115,115	1.41	6 (7%)
6	GS0	A	801	6	69,74,74	2.20	17 (24%)	79,115,115	2.15	26 (32%)
8	BCL	a	807	-	69,74,74	1.31	4 (5%)	79,115,115	1.86	17 (21%)
8	BCL	J	407	-	69,74,74	1.36	8 (11%)	79,115,115	1.64	16 (20%)
10	LHG	A	817	-	48,48,48	0.52	0	51,54,54	0.98	3 (5%)
13	SF4	B	301	2	0,12,12	-	-	-	-	-
8	BCL	I	408[B]	5	49,54,74	1.63	10 (20%)	55,91,115	2.06	17 (30%)
8	BCL	I	405	5	69,74,74	1.10	4 (5%)	79,115,115	1.34	7 (8%)
8	BCL	a	815	-	69,74,74	1.27	5 (7%)	79,115,115	1.88	13 (16%)
8	BCL	A	814	-	69,74,74	1.12	6 (8%)	79,115,115	1.40	8 (10%)
8	BCL	H	404	-	69,74,74	1.10	4 (5%)	79,115,115	1.29	6 (7%)
8	BCL	J	404	-	69,74,74	1.10	4 (5%)	79,115,115	1.29	6 (7%)
8	BCL	a	811	1	69,74,74	1.09	4 (5%)	79,115,115	1.57	10 (12%)
8	BCL	J	401	-	69,74,74	1.29	6 (8%)	79,115,115	1.67	15 (18%)
8	BCL	F	403	-	69,74,74	1.11	4 (5%)	79,115,115	1.38	8 (10%)
8	BCL	a	806	-	69,74,74	1.13	4 (5%)	79,115,115	1.44	10 (12%)
9	F39	a	816	8	66,66,66	3.92	29 (43%)	83,85,85	4.14	33 (39%)
8	BCL	A	813	-	69,74,74	1.13	5 (7%)	79,115,115	1.30	7 (8%)
8	BCL	H	402	14	69,74,74	1.41	7 (10%)	79,115,115	1.73	17 (21%)
8	BCL	E	405	5	69,74,74	1.09	4 (5%)	79,115,115	1.34	8 (10%)
8	BCL	E	406	-	69,74,74	1.05	6 (8%)	79,115,115	1.63	13 (16%)
8	BCL	F	405	5	69,74,74	1.10	4 (5%)	79,115,115	1.34	8 (10%)
8	BCL	a	804[B]	-	49,54,74	1.57	6 (12%)	55,91,115	1.80	13 (23%)
8	BCL	a	805	9,14	69,74,74	1.48	7 (10%)	79,115,115	1.56	13 (16%)
8	BCL	A	810	-	69,74,74	1.19	6 (8%)	79,115,115	1.56	11 (13%)
8	BCL	H	407	-	69,74,74	1.33	7 (10%)	79,115,115	1.56	12 (15%)
8	BCL	F	401	-	69,74,74	1.28	6 (8%)	79,115,115	1.68	14 (17%)
8	BCL	E	404	-	69,74,74	1.10	4 (5%)	79,115,115	1.29	6 (7%)
8	BCL	A	804[B]	-	49,54,74	1.54	5 (10%)	55,91,115	1.74	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	LHG	a	818	-	48,48,48	0.63	1 (2%)	51,54,54	0.83	2 (3%)
8	BCL	E	402	14	69,74,74	1.41	7 (10%)	79,115,115	1.74	17 (21%)
8	BCL	I	403	-	69,74,74	1.11	4 (5%)	79,115,115	1.38	8 (10%)
8	BCL	F	409[B]	5	49,54,74	1.54	8 (16%)	55,91,115	2.01	17 (30%)
8	BCL	E	407	-	69,74,74	1.33	7 (10%)	79,115,115	1.56	12 (15%)
8	BCL	E	409	14	69,74,74	1.33	8 (11%)	79,115,115	1.84	17 (21%)
8	BCL	G	401	-	69,74,74	1.28	6 (8%)	79,115,115	1.67	15 (18%)
8	BCL	J	406	-	69,74,74	1.03	6 (8%)	79,115,115	1.64	13 (16%)
8	BCL	A	812	8	69,74,74	1.23	7 (10%)	79,115,115	1.45	9 (11%)
7	CLA	A	802	-	69,73,73	1.22	8 (11%)	82,113,113	1.40	9 (10%)
8	BCL	H	405	5	69,74,74	1.09	4 (5%)	79,115,115	1.34	8 (10%)
8	BCL	J	405	5	69,74,74	1.10	4 (5%)	79,115,115	1.35	8 (10%)
8	BCL	A	806	-	69,74,74	1.14	4 (5%)	79,115,115	1.38	9 (11%)
8	BCL	E	403	-	69,74,74	1.11	4 (5%)	79,115,115	1.38	8 (10%)
8	BCL	I	404	-	69,74,74	1.09	4 (5%)	79,115,115	1.29	6 (7%)
6	GS0	a	801	6	69,74,74	2.21	17 (24%)	79,115,115	2.21	28 (35%)
8	BCL	H	408[B]	5	49,54,74	1.49	7 (14%)	55,91,115	1.99	15 (27%)
8	BCL	F	404	-	69,74,74	1.09	4 (5%)	79,115,115	1.29	6 (7%)
10	LHG	a	817	-	48,48,48	0.44	0	51,54,54	0.82	3 (5%)
8	BCL	F	402	14	69,74,74	1.34	8 (11%)	79,115,115	1.85	19 (24%)
8	BCL	A	807	-	69,74,74	1.20	3 (4%)	79,115,115	1.88	16 (20%)
8	BCL	I	409[B]	5	49,54,74	1.56	8 (16%)	55,91,115	2.02	17 (30%)
11	IKV	a	819	-	51,51,51	0.73	1 (1%)	59,59,59	0.71	3 (5%)
8	BCL	A	805	14	69,74,74	1.48	11 (15%)	79,115,115	1.98	14 (17%)
8	BCL	a	809[B]	8,1	49,54,74	1.30	5 (10%)	55,91,115	1.49	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	G	405	-	-	4/41/137/137	-
9	F39	A	816	-	-	36/58/78/78	0/2/2/2
13	SF4	A	821	1	-	-	0/6/5/5
8	BCL	G	404	5	-	11/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	A	809[B]	8,1	-	4/17/113/137	-
8	BCL	A	811	1	-	13/41/137/137	-
8	BCL	a	814	-	-	16/41/137/137	-
8	BCL	H	401	-	-	11/41/137/137	-
8	BCL	I	402	14	-	22/41/137/137	-
8	BCL	F	408[B]	5	-	7/17/113/137	-
8	BCL	E	408[B]	5	-	7/17/113/137	-
8	BCL	I	406	-	-	4/41/137/137	-
7	CLA	a	803	14	-	13/39/115/115	-
8	BCL	F	406	-	-	4/41/137/137	-
8	BCL	a	812	8,9	-	8/41/137/137	-
8	BCL	a	813	-	-	5/41/137/137	-
8	BCL	E	401	-	-	11/41/137/137	-
10	LHG	A	818	-	-	32/53/53/53	-
8	BCL	a	810	-	-	10/41/137/137	-
8	BCL	J	403	-	-	11/41/137/137	-
7	CLA	a	802	-	-	23/39/115/115	-
8	BCL	I	407	-	-	10/41/137/137	-
8	BCL	A	808	-	-	6/41/137/137	-
8	BCL	F	407	-	-	10/41/137/137	-
8	BCL	G	403	-	-	3/41/137/137	-
7	CLA	A	803	14	-	13/39/115/115	-
8	BCL	A	815	-	-	19/41/137/137	-
13	SF4	B	302	2	-	-	0/6/5/5
8	BCL	G	402	-	-	11/41/137/137	-
11	IKV	A	819	-	-	26/46/66/66	0/1/1/1
8	BCL	J	402	14	-	17/41/137/137	-
8	BCL	H	406	-	-	4/41/137/137	-
8	BCL	H	403	-	-	11/41/137/137	-
8	BCL	G	406	-	-	12/41/137/137	-
8	BCL	I	401	-	-	11/41/137/137	-
8	BCL	a	808	-	-	6/41/137/137	-
6	GS0	A	801	6	-	7/41/137/137	-
8	BCL	a	807	-	-	10/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	J	407	-	-	12/41/137/137	-
10	LHG	A	817	-	-	24/53/53/53	-
13	SF4	B	301	2	-	-	0/6/5/5
8	BCL	I	408[B]	5	-	7/17/113/137	-
8	BCL	I	405	5	-	11/41/137/137	-
8	BCL	a	815	-	-	19/41/137/137	-
8	BCL	A	814	-	-	18/41/137/137	-
8	BCL	H	404	-	-	3/41/137/137	-
8	BCL	J	404	-	-	3/41/137/137	-
8	BCL	a	811	1	-	14/41/137/137	-
8	BCL	J	401	-	-	11/41/137/137	-
8	BCL	F	403	-	-	11/41/137/137	-
8	BCL	a	806	-	-	9/41/137/137	-
9	F39	a	816	8	-	41/58/78/78	0/2/2/2
8	BCL	A	813	-	-	5/41/137/137	-
8	BCL	H	402	14	-	19/41/137/137	-
8	BCL	E	405	5	-	11/41/137/137	-
8	BCL	E	406	-	-	4/41/137/137	-
8	BCL	F	405	5	-	11/41/137/137	-
8	BCL	a	804[B]	-	-	5/17/113/137	-
8	BCL	a	805	9,14	-	22/41/137/137	-
8	BCL	A	810	-	-	9/41/137/137	-
8	BCL	H	407	-	-	10/41/137/137	-
8	BCL	F	401	-	-	11/41/137/137	-
8	BCL	E	404	-	-	3/41/137/137	-
8	BCL	A	804[B]	-	-	3/17/113/137	-
10	LHG	a	818	-	-	32/53/53/53	-
8	BCL	E	402	14	-	19/41/137/137	-
8	BCL	I	403	-	-	10/41/137/137	-
8	BCL	F	409[B]	5	-	9/17/113/137	-
8	BCL	E	407	-	-	10/41/137/137	-
8	BCL	E	409	14	-	17/41/137/137	-
8	BCL	G	401	-	-	11/41/137/137	-
8	BCL	J	406	-	-	4/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	A	812	8	-	6/41/137/137	-
7	CLA	A	802	-	-	23/39/115/115	-
8	BCL	H	405	5	-	11/41/137/137	-
8	BCL	J	405	5	-	11/41/137/137	-
8	BCL	A	806	-	-	5/41/137/137	-
8	BCL	E	403	-	-	11/41/137/137	-
8	BCL	I	404	-	-	3/41/137/137	-
6	GS0	a	801	6	-	7/41/137/137	-
8	BCL	H	408[B]	5	-	7/17/113/137	-
8	BCL	F	404	-	-	3/41/137/137	-
10	LHG	a	817	-	-	30/53/53/53	-
8	BCL	F	402	14	-	22/41/137/137	-
8	BCL	A	807	-	-	12/41/137/137	-
8	BCL	I	409[B]	5	-	9/17/113/137	-
11	IKV	a	819	-	-	27/46/66/66	0/1/1/1
8	BCL	A	805	14	-	19/41/137/137	-
8	BCL	a	809[B]	8,1	-	4/17/113/137	-

All (539) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	816	F39	C40-C41	10.57	1.62	1.34
9	A	816	F39	C40-C41	10.38	1.61	1.34
9	a	816	F39	C56-C53	10.23	1.59	1.33
9	A	816	F39	C56-C53	10.11	1.58	1.33
9	a	816	F39	C39-C37	9.99	1.58	1.35
9	A	816	F39	C39-C37	9.88	1.58	1.35
9	a	816	F39	C32-C35	8.75	1.57	1.34
9	A	816	F39	C32-C35	8.58	1.57	1.34
9	a	816	F39	C63-C64	8.54	1.57	1.34
9	A	816	F39	C63-C64	8.32	1.56	1.34
9	a	816	F39	C57-C51	7.97	1.58	1.36
9	A	816	F39	C57-C51	7.87	1.57	1.36
9	a	816	F39	C61-C58	7.69	1.53	1.35
9	A	816	F39	C61-C58	7.53	1.53	1.35
9	a	816	F39	C44-C42	7.02	1.52	1.35
9	A	816	F39	C44-C42	6.85	1.51	1.35
9	A	816	F39	C59-C62	6.56	1.51	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	GS0	O1A-CGA	-6.48	1.03	1.22
6	a	801	GS0	O1A-CGA	-6.46	1.03	1.22
6	a	801	GS0	MG-NA	-6.45	1.90	2.06
6	A	801	GS0	MG-NA	-6.45	1.90	2.06
9	a	816	F39	C27-C20	6.30	1.55	1.35
7	a	803	CLA	C1D-ND	6.27	1.46	1.37
9	A	816	F39	C27-C20	6.26	1.55	1.35
6	a	801	GS0	MG-ND	-6.23	1.93	2.05
6	A	801	GS0	MG-ND	-6.22	1.93	2.05
9	a	816	F39	C59-C62	6.00	1.49	1.35
8	a	805	BCL	OBD-CAD	5.72	1.32	1.22
6	A	801	GS0	MG-NB	-5.70	1.94	2.05
6	a	801	GS0	MG-NB	-5.67	1.94	2.05
8	A	807	BCL	MG-NA	5.53	2.19	2.06
8	a	807	BCL	MG-NA	5.51	2.19	2.06
7	a	802	CLA	C1D-ND	5.51	1.45	1.37
8	H	402	BCL	OBD-CAD	5.44	1.31	1.22
8	E	402	BCL	OBD-CAD	5.43	1.31	1.22
6	a	801	GS0	MG-NC	5.41	2.19	2.06
8	a	815	BCL	CHB-C1B	5.39	1.51	1.39
6	A	801	GS0	MG-NC	5.38	2.19	2.06
8	A	815	BCL	CHB-C1B	5.35	1.51	1.39
8	a	804[B]	BCL	MG-NA	5.18	2.18	2.06
8	H	401	BCL	MG-NA	5.15	2.18	2.06
8	F	401	BCL	MG-NA	5.14	2.18	2.06
8	E	401	BCL	MG-NA	5.14	2.18	2.06
8	a	805	BCL	MG-NA	5.14	2.18	2.06
8	J	401	BCL	MG-NA	5.13	2.18	2.06
8	I	401	BCL	MG-NA	5.13	2.18	2.06
8	G	401	BCL	MG-NA	5.12	2.18	2.06
8	A	805	BCL	MG-NA	5.12	2.18	2.06
8	a	810	BCL	MG-NA	5.11	2.18	2.06
8	A	804[B]	BCL	MG-NA	5.09	2.18	2.06
8	A	810	BCL	MG-NA	5.07	2.18	2.06
8	A	806	BCL	MG-NA	5.03	2.18	2.06
8	a	806	BCL	MG-NA	5.02	2.18	2.06
9	a	816	F39	C14-C13	5.01	1.60	1.53
9	A	816	F39	C14-C13	4.98	1.60	1.53
8	I	403	BCL	MG-NA	4.97	2.18	2.06
8	G	402	BCL	MG-NA	4.96	2.18	2.06
8	H	403	BCL	MG-NA	4.95	2.18	2.06
8	J	403	BCL	MG-NA	4.95	2.18	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	809[B]	BCL	MG-NA	4.94	2.18	2.06
8	F	403	BCL	MG-NA	4.93	2.18	2.06
8	a	809[B]	BCL	MG-NA	4.93	2.18	2.06
8	E	403	BCL	MG-NA	4.93	2.18	2.06
8	a	813	BCL	MG-NA	4.88	2.17	2.06
8	A	813	BCL	MG-NA	4.84	2.17	2.06
9	a	816	F39	C56-C58	4.77	1.56	1.46
8	I	404	BCL	MG-NA	4.76	2.17	2.06
8	E	404	BCL	MG-NA	4.74	2.17	2.06
8	F	404	BCL	MG-NA	4.74	2.17	2.06
9	a	816	F39	C38-C37	4.73	1.60	1.50
8	H	404	BCL	MG-NA	4.73	2.17	2.06
8	J	404	BCL	MG-NA	4.73	2.17	2.06
8	G	403	BCL	MG-NA	4.73	2.17	2.06
8	A	814	BCL	MG-NA	4.71	2.17	2.06
9	A	816	F39	C38-C37	4.70	1.60	1.50
9	a	816	F39	C57-C59	4.67	1.57	1.43
8	E	409	BCL	MG-NA	4.66	2.17	2.06
8	H	402	BCL	MG-NA	4.64	2.17	2.06
8	J	402	BCL	MG-NA	4.63	2.17	2.06
9	A	816	F39	C57-C59	4.63	1.57	1.43
8	E	402	BCL	MG-NA	4.63	2.17	2.06
8	F	402	BCL	MG-NA	4.62	2.17	2.06
8	I	402	BCL	MG-NA	4.61	2.17	2.06
7	A	802	CLA	C1D-ND	4.61	1.43	1.37
8	H	408[B]	BCL	MG-NA	4.57	2.17	2.06
8	I	409[B]	BCL	MG-NA	4.57	2.17	2.06
8	F	409[B]	BCL	MG-NA	4.56	2.17	2.06
8	E	408[B]	BCL	MG-NA	4.56	2.17	2.06
8	F	408[B]	BCL	O2A-CGA	4.56	1.45	1.30
8	H	408[B]	BCL	O2A-CGA	4.55	1.45	1.30
8	I	409[B]	BCL	O2A-CGA	4.55	1.45	1.30
8	E	408[B]	BCL	O2A-CGA	4.55	1.45	1.30
8	I	408[B]	BCL	O2A-CGA	4.55	1.45	1.30
8	G	404	BCL	MG-NA	4.55	2.17	2.06
8	H	407	BCL	MG-NA	4.54	2.17	2.06
8	F	405	BCL	MG-NA	4.54	2.17	2.06
8	E	405	BCL	MG-NA	4.54	2.17	2.06
8	J	405	BCL	MG-NA	4.54	2.17	2.06
8	a	804[B]	BCL	O2A-CGA	4.53	1.45	1.30
8	I	405	BCL	MG-NA	4.53	2.17	2.06
8	G	406	BCL	MG-NA	4.53	2.17	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	407	BCL	MG-NA	4.53	2.17	2.06
8	F	409[B]	BCL	O2A-CGA	4.53	1.45	1.30
6	a	801	GS0	OBD-CAD	4.53	1.30	1.22
8	E	407	BCL	MG-NA	4.52	2.17	2.06
8	A	804[B]	BCL	O2A-CGA	4.52	1.45	1.30
8	H	405	BCL	MG-NA	4.51	2.17	2.06
8	A	811	BCL	MG-NA	4.51	2.17	2.06
8	F	408[B]	BCL	MG-NA	4.51	2.17	2.06
6	A	801	GS0	OBD-CAD	4.50	1.30	1.22
8	J	407	BCL	MG-NA	4.50	2.17	2.06
8	I	408[B]	BCL	MG-NA	4.50	2.17	2.06
8	a	811	BCL	MG-NA	4.49	2.16	2.06
8	a	807	BCL	CHB-C1B	4.49	1.49	1.39
9	a	816	F39	C64-C62	4.49	1.55	1.46
8	I	407	BCL	MG-NA	4.48	2.16	2.06
8	a	812	BCL	MG-NA	4.39	2.16	2.06
8	A	812	BCL	MG-NA	4.38	2.16	2.06
8	A	808	BCL	MG-NA	4.38	2.16	2.06
8	F	401	BCL	O2A-CGA	4.37	1.46	1.33
9	A	816	F39	C56-C58	4.37	1.55	1.46
8	J	401	BCL	O2A-CGA	4.36	1.46	1.33
8	E	401	BCL	O2A-CGA	4.36	1.46	1.33
7	A	803	CLA	C1D-ND	4.36	1.43	1.37
8	a	808	BCL	MG-NA	4.35	2.16	2.06
8	G	401	BCL	O2A-CGA	4.34	1.46	1.33
8	I	401	BCL	O2A-CGA	4.34	1.46	1.33
8	H	401	BCL	O2A-CGA	4.34	1.46	1.33
8	I	402	BCL	O2A-CGA	4.32	1.45	1.33
9	A	816	F39	C64-C62	4.32	1.55	1.46
8	a	814	BCL	MG-NA	4.31	2.16	2.06
8	F	402	BCL	O2A-CGA	4.31	1.45	1.33
8	A	805	BCL	C3D-C4D	-4.29	1.34	1.44
8	E	402	BCL	O2A-CGA	4.29	1.45	1.33
8	H	402	BCL	O2A-CGA	4.28	1.45	1.33
11	a	819	IKV	C35-C34	-4.24	1.30	1.51
11	A	819	IKV	C35-C34	-4.24	1.30	1.51
9	a	816	F39	C41-C42	4.20	1.54	1.46
8	A	812	BCL	C4B-NB	-4.16	1.32	1.37
9	a	816	F39	O1-C11	4.16	1.52	1.41
8	G	406	BCL	CHD-C1D	4.13	1.46	1.38
8	H	407	BCL	O2A-CGA	4.13	1.45	1.33
9	A	816	F39	O1-C11	4.13	1.52	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	407	BCL	O2A-CGA	4.12	1.45	1.33
8	J	407	BCL	CHD-C1D	4.12	1.46	1.38
8	E	407	BCL	CHD-C1D	4.12	1.46	1.38
8	I	407	BCL	CHD-C1D	4.12	1.46	1.38
9	A	816	F39	C41-C42	4.11	1.54	1.46
8	F	407	BCL	CHD-C1D	4.11	1.46	1.38
8	E	407	BCL	O2A-CGA	4.11	1.45	1.33
8	I	407	BCL	O2A-CGA	4.11	1.45	1.33
8	H	407	BCL	CHD-C1D	4.10	1.46	1.38
8	J	401	BCL	OBD-CAD	4.09	1.29	1.22
6	a	801	GS0	O1D-CGD	-4.08	1.11	1.21
8	a	805	BCL	C3D-C4D	-4.08	1.35	1.44
8	a	815	BCL	O2A-CGA	4.08	1.45	1.33
8	A	815	BCL	O2A-CGA	4.07	1.45	1.33
6	A	801	GS0	O1D-CGD	-4.07	1.11	1.21
8	J	407	BCL	O2A-CGA	4.05	1.45	1.33
9	a	816	F39	C63-C61	4.05	1.55	1.43
8	F	401	BCL	OBD-CAD	4.04	1.29	1.22
8	G	401	BCL	OBD-CAD	4.04	1.29	1.22
8	G	406	BCL	O2A-CGA	4.04	1.45	1.33
8	H	401	BCL	OBD-CAD	4.03	1.29	1.22
8	E	401	BCL	OBD-CAD	4.01	1.29	1.22
8	I	401	BCL	OBD-CAD	4.01	1.29	1.22
8	J	402	BCL	C3B-C4B	3.97	1.49	1.41
9	A	816	F39	C63-C61	3.96	1.55	1.43
8	A	807	BCL	MG-NC	3.95	2.15	2.06
8	A	805	BCL	CHD-C1D	3.95	1.46	1.38
8	E	409	BCL	C3B-C4B	3.95	1.48	1.41
8	a	807	BCL	MG-NC	3.95	2.15	2.06
8	A	810	BCL	MG-NC	3.91	2.15	2.06
8	E	409	BCL	O2A-CGA	3.91	1.44	1.33
8	J	402	BCL	O2A-CGA	3.90	1.44	1.33
8	H	402	BCL	C3B-C4B	3.89	1.48	1.41
8	E	402	BCL	C3B-C4B	3.89	1.48	1.41
8	F	402	BCL	C3B-C4B	3.87	1.48	1.41
8	a	810	BCL	MG-NC	3.87	2.15	2.06
8	I	402	BCL	C3B-C4B	3.86	1.48	1.41
7	a	803	CLA	OBD-CAD	3.82	1.29	1.22
8	A	805	BCL	OBD-CAD	3.79	1.29	1.22
8	a	805	BCL	MG-NC	3.78	2.15	2.06
8	F	408[B]	BCL	OBD-CAD	3.76	1.29	1.22
8	F	406	BCL	OBD-CAD	3.74	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	408[B]	BCL	OBD-CAD	3.74	1.28	1.22
8	I	406	BCL	OBD-CAD	3.72	1.28	1.22
8	H	406	BCL	OBD-CAD	3.69	1.28	1.22
8	E	406	BCL	OBD-CAD	3.68	1.28	1.22
8	A	804[B]	BCL	C3B-C4B	3.67	1.48	1.41
8	a	808	BCL	MG-NC	3.67	2.15	2.06
8	A	808	BCL	MG-NC	3.66	2.15	2.06
8	A	813	BCL	MG-NC	3.66	2.15	2.06
8	a	813	BCL	MG-NC	3.65	2.14	2.06
8	A	806	BCL	MG-NC	3.65	2.14	2.06
9	a	816	F39	C46-C53	3.64	1.55	1.47
9	a	816	F39	C35-C37	3.64	1.53	1.46
6	a	801	GS0	O2D-CED	3.63	1.53	1.45
9	a	816	F39	C40-C39	3.63	1.54	1.43
8	a	804[B]	BCL	C3B-C4B	3.62	1.48	1.41
8	A	809[B]	BCL	MG-NC	3.61	2.14	2.06
8	a	806	BCL	MG-NC	3.61	2.14	2.06
6	A	801	GS0	O2D-CED	3.61	1.53	1.45
8	a	809[B]	BCL	MG-NC	3.60	2.14	2.06
8	a	805	BCL	CHD-C1D	3.57	1.45	1.38
8	A	804[B]	BCL	MG-NC	3.55	2.14	2.06
8	a	804[B]	BCL	MG-NC	3.53	2.14	2.06
9	A	816	F39	C40-C39	3.52	1.54	1.43
8	A	815	BCL	MG-NC	3.50	2.14	2.06
8	a	815	BCL	MG-NC	3.49	2.14	2.06
9	a	816	F39	C51-C44	3.49	1.54	1.43
8	G	401	BCL	MG-NC	3.49	2.14	2.06
8	A	805	BCL	O2A-CGA	3.49	1.43	1.33
8	J	401	BCL	MG-NC	3.49	2.14	2.06
8	E	401	BCL	MG-NC	3.49	2.14	2.06
8	F	409[B]	BCL	OBD-CAD	3.49	1.28	1.22
8	F	401	BCL	MG-NC	3.48	2.14	2.06
8	F	402	BCL	OBD-CAD	3.48	1.28	1.22
8	I	409[B]	BCL	OBD-CAD	3.47	1.28	1.22
8	I	401	BCL	MG-NC	3.46	2.14	2.06
8	H	401	BCL	MG-NC	3.46	2.14	2.06
8	I	402	BCL	OBD-CAD	3.46	1.28	1.22
9	A	816	F39	C35-C37	3.44	1.53	1.46
9	A	816	F39	C51-C44	3.41	1.53	1.43
8	E	407	BCL	C1D-ND	-3.39	1.33	1.37
8	I	407	BCL	C1D-ND	-3.38	1.33	1.37
8	G	406	BCL	C1D-ND	-3.38	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	407	BCL	C1D-ND	-3.37	1.33	1.37
8	J	407	BCL	MG-NC	3.36	2.14	2.06
8	a	814	BCL	MG-NC	3.35	2.14	2.06
8	I	407	BCL	MG-NC	3.35	2.14	2.06
8	J	407	BCL	C1D-ND	-3.34	1.33	1.37
8	F	407	BCL	MG-NC	3.33	2.14	2.06
8	H	407	BCL	C1D-ND	-3.33	1.33	1.37
8	A	814	BCL	MG-NC	3.33	2.14	2.06
8	E	403	BCL	MG-NC	3.32	2.14	2.06
8	I	408[B]	BCL	C4B-NB	-3.32	1.33	1.37
8	E	407	BCL	MG-NC	3.32	2.14	2.06
8	F	403	BCL	MG-NC	3.32	2.14	2.06
8	G	402	BCL	MG-NC	3.32	2.14	2.06
8	J	403	BCL	MG-NC	3.32	2.14	2.06
8	G	406	BCL	MG-NC	3.31	2.14	2.06
8	a	811	BCL	MG-NC	3.31	2.14	2.06
8	F	408[B]	BCL	C4B-NB	-3.30	1.33	1.37
8	H	403	BCL	MG-NC	3.30	2.14	2.06
8	A	811	BCL	MG-NC	3.29	2.14	2.06
8	I	403	BCL	MG-NC	3.29	2.14	2.06
8	H	407	BCL	MG-NC	3.28	2.14	2.06
8	E	404	BCL	MG-NC	3.27	2.14	2.06
8	I	404	BCL	MG-NC	3.27	2.14	2.06
8	H	404	BCL	MG-NC	3.27	2.14	2.06
8	G	403	BCL	MG-NC	3.26	2.14	2.06
8	F	404	BCL	MG-NC	3.26	2.14	2.06
8	J	404	BCL	MG-NC	3.24	2.14	2.06
8	J	405	BCL	MG-NC	3.24	2.14	2.06
8	H	405	BCL	MG-NC	3.23	2.13	2.06
8	G	404	BCL	MG-NC	3.22	2.13	2.06
8	J	402	BCL	OBD-CAD	3.22	1.28	1.22
8	E	409	BCL	OBD-CAD	3.21	1.28	1.22
8	F	405	BCL	MG-NC	3.21	2.13	2.06
8	I	405	BCL	MG-NC	3.21	2.13	2.06
8	E	405	BCL	MG-NC	3.20	2.13	2.06
9	A	816	F39	C46-C53	3.20	1.54	1.47
8	F	408[B]	BCL	MG-NC	3.12	2.13	2.06
8	I	409[B]	BCL	MG-NC	3.11	2.13	2.06
8	F	409[B]	BCL	MG-NC	3.11	2.13	2.06
8	I	408[B]	BCL	MG-NC	3.11	2.13	2.06
8	G	405	BCL	OBD-CAD	3.11	1.27	1.22
8	J	406	BCL	OBD-CAD	3.10	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	408[B]	BCL	MG-NC	3.09	2.13	2.06
7	A	802	CLA	C4B-NB	3.09	1.41	1.37
8	H	408[B]	BCL	MG-NC	3.08	2.13	2.06
8	a	815	BCL	C3D-C4D	-3.07	1.37	1.44
7	a	802	CLA	C4B-NB	3.07	1.41	1.37
8	J	402	BCL	MG-NC	3.06	2.13	2.06
8	A	815	BCL	C3D-C4D	-3.06	1.37	1.44
8	H	402	BCL	MG-NC	3.05	2.13	2.06
6	a	801	GS0	O2D-CGD	-3.04	1.25	1.33
8	E	402	BCL	MG-NC	3.04	2.13	2.06
6	a	801	GS0	O2A-CGA	-3.04	1.24	1.33
8	F	402	BCL	MG-NC	3.03	2.13	2.06
8	I	402	BCL	MG-NC	3.03	2.13	2.06
6	A	801	GS0	O2A-CGA	-3.02	1.24	1.33
8	E	409	BCL	MG-NC	3.02	2.13	2.06
6	A	801	GS0	O2D-CGD	-3.01	1.25	1.33
8	a	812	BCL	MG-NC	2.97	2.13	2.06
8	A	812	BCL	MG-NC	2.96	2.13	2.06
8	a	812	BCL	C3B-C4B	2.95	1.46	1.41
9	a	816	F39	O6-C21	2.95	1.41	1.33
8	A	805	BCL	C3D-C2D	2.95	1.47	1.39
7	A	803	CLA	C4B-NB	2.92	1.41	1.37
9	A	816	F39	O6-C21	2.90	1.41	1.33
8	J	406	BCL	MG-NC	2.86	2.13	2.06
8	H	406	BCL	MG-NC	2.85	2.13	2.06
8	E	406	BCL	MG-NC	2.84	2.13	2.06
8	E	409	BCL	O2D-CGD	2.84	1.40	1.33
9	A	816	F39	C52-C45	2.84	1.57	1.51
7	a	803	CLA	C4B-NB	2.84	1.41	1.37
8	G	405	BCL	MG-NC	2.84	2.13	2.06
8	a	804[B]	BCL	C3D-C4D	-2.83	1.37	1.44
8	A	812	BCL	C3B-C4B	2.82	1.46	1.41
8	a	809[B]	BCL	C3B-C4B	2.82	1.46	1.41
8	J	402	BCL	O2D-CGD	2.82	1.40	1.33
8	A	809[B]	BCL	C3B-C4B	2.82	1.46	1.41
8	F	406	BCL	MG-NC	2.81	2.12	2.06
8	I	409[B]	BCL	C1B-C2B	2.79	1.49	1.43
8	I	406	BCL	MG-NC	2.78	2.12	2.06
8	E	408[B]	BCL	C1B-C2B	2.78	1.49	1.43
8	F	409[B]	BCL	C1B-C2B	2.77	1.49	1.43
8	I	408[B]	BCL	C1B-C2B	2.76	1.49	1.43
8	H	408[B]	BCL	C1B-C2B	2.76	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	816	F39	C32-C27	2.75	1.51	1.43
8	F	408[B]	BCL	C1B-C2B	2.74	1.49	1.43
8	E	402	BCL	CHD-C1D	2.72	1.43	1.38
8	I	402	BCL	CHD-C1D	2.72	1.43	1.38
8	A	811	BCL	C3B-C4B	2.72	1.46	1.41
7	A	803	CLA	C1B-C2B	2.71	1.49	1.43
8	F	402	BCL	CHD-C1D	2.70	1.43	1.38
8	I	407	BCL	C3D-C4D	-2.70	1.38	1.44
8	E	407	BCL	C3D-C4D	-2.70	1.38	1.44
8	I	409[B]	BCL	C3B-C4B	2.70	1.46	1.41
8	H	408[B]	BCL	C3B-C4B	2.69	1.46	1.41
10	a	818	LHG	O8-C23	2.69	1.41	1.33
8	a	811	BCL	C3B-C4B	2.69	1.46	1.41
8	F	407	BCL	C3D-C4D	-2.69	1.38	1.44
8	H	402	BCL	CHD-C1D	2.69	1.43	1.38
8	A	805	BCL	C3B-C4B	2.69	1.46	1.41
8	G	406	BCL	C3D-C4D	-2.69	1.38	1.44
8	E	408[B]	BCL	C3B-C4B	2.69	1.46	1.41
8	F	409[B]	BCL	C3B-C4B	2.68	1.46	1.41
8	J	407	BCL	C3D-C4D	-2.68	1.38	1.44
8	H	407	BCL	C3D-C4D	-2.68	1.38	1.44
8	a	805	BCL	C3B-C4B	2.67	1.46	1.41
8	E	409	BCL	CHD-C1D	2.66	1.43	1.38
7	a	803	CLA	C1B-C2B	2.66	1.49	1.43
7	a	802	CLA	C1B-C2B	2.66	1.49	1.43
8	J	402	BCL	CHD-C1D	2.65	1.43	1.38
9	a	816	F39	C52-C45	2.65	1.56	1.51
7	A	802	CLA	C1B-C2B	2.64	1.49	1.43
8	A	812	BCL	CHC-C4B	2.61	1.45	1.39
9	A	816	F39	C32-C27	2.61	1.51	1.43
8	A	805	BCL	MG-NC	2.61	2.12	2.06
9	a	816	F39	C55-C48	2.58	1.55	1.51
6	a	801	GS0	OBB-CAB	-2.57	1.17	1.23
6	A	801	GS0	OBB-CAB	-2.57	1.17	1.23
6	a	801	GS0	C1B-C2B	-2.56	1.37	1.43
6	A	801	GS0	C1B-C2B	-2.56	1.37	1.43
6	A	801	GS0	C3D-C4D	-2.55	1.38	1.44
6	a	801	GS0	C3D-C4D	-2.54	1.38	1.44
9	A	816	F39	C55-C48	2.53	1.55	1.51
8	a	812	BCL	CHD-C1D	2.52	1.43	1.38
8	H	406	BCL	CHD-C1D	2.51	1.43	1.38
8	I	406	BCL	CHD-C1D	2.51	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	403	BCL	C3B-C4B	2.51	1.46	1.41
8	A	812	BCL	CHD-C1D	2.50	1.43	1.38
8	E	406	BCL	CHD-C1D	2.50	1.43	1.38
8	F	406	BCL	CHD-C1D	2.49	1.43	1.38
8	J	403	BCL	C3B-C4B	2.48	1.46	1.41
8	H	403	BCL	C3B-C4B	2.48	1.46	1.41
8	E	403	BCL	C3B-C4B	2.48	1.46	1.41
8	J	406	BCL	CHD-C1D	2.48	1.43	1.38
8	a	811	BCL	CHD-C1D	2.48	1.43	1.38
8	F	403	BCL	C3B-C4B	2.47	1.46	1.41
8	G	402	BCL	C3B-C4B	2.47	1.46	1.41
8	A	811	BCL	CHD-C1D	2.46	1.43	1.38
7	A	803	CLA	CHD-C1D	2.46	1.43	1.38
8	H	404	BCL	C3B-C4B	2.45	1.46	1.41
8	G	405	BCL	CHD-C1D	2.45	1.43	1.38
8	A	814	BCL	C1D-C2D	-2.44	1.40	1.45
8	I	404	BCL	C3B-C4B	2.43	1.45	1.41
6	a	801	GS0	C1D-C2D	-2.42	1.40	1.45
8	G	403	BCL	C3B-C4B	2.42	1.45	1.41
8	E	404	BCL	C3B-C4B	2.41	1.45	1.41
8	F	404	BCL	C3B-C4B	2.41	1.45	1.41
8	F	405	BCL	CHD-C1D	2.41	1.43	1.38
8	I	405	BCL	CHD-C1D	2.40	1.43	1.38
8	H	401	BCL	C3B-C4B	2.39	1.45	1.41
8	a	814	BCL	C3B-C4B	2.39	1.45	1.41
8	a	814	BCL	C1D-C2D	-2.39	1.40	1.45
6	A	801	GS0	C1D-C2D	-2.38	1.40	1.45
8	G	404	BCL	CHD-C1D	2.38	1.43	1.38
8	J	405	BCL	CHD-C1D	2.38	1.43	1.38
8	H	405	BCL	CHD-C1D	2.38	1.43	1.38
8	J	404	BCL	C3B-C4B	2.37	1.45	1.41
8	A	814	BCL	C3B-C4B	2.37	1.45	1.41
8	a	810	BCL	C3B-C4B	2.37	1.45	1.41
8	E	405	BCL	CHD-C1D	2.37	1.43	1.38
8	E	401	BCL	C3B-C4B	2.36	1.45	1.41
8	J	407	BCL	CBD-CGD	-2.36	1.45	1.52
6	a	801	GS0	C3B-CAB	2.36	1.54	1.46
8	I	406	BCL	MG-ND	-2.36	2.01	2.05
8	F	401	BCL	C3B-C4B	2.36	1.45	1.41
10	A	818	LHG	O7-C5	-2.35	1.41	1.46
7	a	802	CLA	C3B-C4B	2.35	1.49	1.42
8	A	808	BCL	CHD-C1D	2.35	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	808	BCL	C3B-C4B	2.35	1.45	1.41
8	F	402	BCL	CBB-CAB	2.35	1.54	1.50
8	F	406	BCL	MG-ND	-2.35	2.01	2.05
8	I	405	BCL	C3B-C4B	2.35	1.45	1.41
8	G	406	BCL	CBD-CGD	-2.34	1.45	1.52
7	A	802	CLA	C3B-C4B	2.34	1.49	1.42
8	F	405	BCL	C3B-C4B	2.34	1.45	1.41
8	J	402	BCL	CBB-CAB	2.34	1.54	1.50
8	I	402	BCL	CBB-CAB	2.34	1.54	1.50
8	a	808	BCL	CHD-C1D	2.34	1.42	1.38
8	a	808	BCL	C3B-C4B	2.33	1.45	1.41
8	A	810	BCL	C3B-C4B	2.33	1.45	1.41
6	A	801	GS0	C3B-CAB	2.33	1.54	1.46
8	E	405	BCL	C3B-C4B	2.33	1.45	1.41
8	H	402	BCL	CBB-CAB	2.33	1.54	1.50
8	G	405	BCL	MG-ND	-2.33	2.01	2.05
8	J	405	BCL	C3B-C4B	2.33	1.45	1.41
9	a	816	F39	C46-C45	2.32	1.44	1.41
8	H	406	BCL	MG-ND	-2.32	2.01	2.05
8	A	809[B]	BCL	CHD-C1D	2.32	1.42	1.38
8	J	406	BCL	MG-ND	-2.32	2.01	2.05
8	G	401	BCL	C3B-C4B	2.32	1.45	1.41
8	E	406	BCL	MG-ND	-2.32	2.01	2.05
8	G	404	BCL	C3B-C4B	2.32	1.45	1.41
8	H	405	BCL	C3B-C4B	2.32	1.45	1.41
8	I	401	BCL	C3B-C4B	2.32	1.45	1.41
8	J	401	BCL	C3B-C4B	2.32	1.45	1.41
8	F	402	BCL	O2D-CGD	2.31	1.38	1.33
8	E	409	BCL	CBB-CAB	2.31	1.54	1.50
8	J	404	BCL	CHD-C1D	2.31	1.42	1.38
8	a	809[B]	BCL	CHD-C1D	2.31	1.42	1.38
8	I	402	BCL	O2D-CGD	2.31	1.38	1.33
8	a	813	BCL	CHD-C1D	2.31	1.42	1.38
8	E	402	BCL	CBB-CAB	2.31	1.54	1.50
8	A	813	BCL	CHD-C1D	2.30	1.42	1.38
7	a	803	CLA	C3B-C4B	2.29	1.49	1.42
8	I	406	BCL	C3D-C4D	-2.28	1.39	1.44
8	G	403	BCL	CHD-C1D	2.27	1.42	1.38
7	A	803	CLA	C3B-C4B	2.27	1.49	1.42
8	F	406	BCL	C3D-C4D	-2.27	1.39	1.44
8	F	408[B]	BCL	CHC-C4B	2.26	1.44	1.39
8	H	404	BCL	CHD-C1D	2.26	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	408[B]	BCL	CHC-C4B	2.26	1.44	1.39
8	H	406	BCL	C3D-C4D	-2.25	1.39	1.44
8	A	806	BCL	CHD-C1D	2.25	1.42	1.38
8	a	813	BCL	C3B-C4B	2.25	1.45	1.41
8	E	404	BCL	CHD-C1D	2.25	1.42	1.38
8	A	806	BCL	C3B-C4B	2.25	1.45	1.41
8	E	406	BCL	C3D-C4D	-2.24	1.39	1.44
8	a	806	BCL	C3B-C4B	2.22	1.45	1.41
8	A	813	BCL	C3B-C4B	2.22	1.45	1.41
7	A	803	CLA	CHC-C1C	2.22	1.42	1.38
8	J	406	BCL	C3D-C4D	-2.21	1.39	1.44
8	F	404	BCL	CHD-C1D	2.21	1.42	1.38
8	a	806	BCL	CHD-C1D	2.21	1.42	1.38
8	I	404	BCL	CHD-C1D	2.21	1.42	1.38
8	G	405	BCL	C3D-C4D	-2.21	1.39	1.44
8	G	402	BCL	CHD-C1D	2.20	1.42	1.38
8	H	403	BCL	CHD-C1D	2.20	1.42	1.38
7	a	802	CLA	CHC-C1C	2.20	1.42	1.38
9	a	816	F39	C54-C47	2.19	1.55	1.51
8	a	810	BCL	CHD-C1D	2.19	1.42	1.38
8	E	403	BCL	CHD-C1D	2.19	1.42	1.38
8	A	810	BCL	CHD-C1D	2.18	1.42	1.38
7	a	803	CLA	CHC-C1C	2.18	1.42	1.38
8	F	403	BCL	CHD-C1D	2.18	1.42	1.38
8	J	403	BCL	CHD-C1D	2.17	1.42	1.38
8	a	805	BCL	C1D-ND	-2.17	1.35	1.37
7	A	803	CLA	CMD-C2D	-2.17	1.46	1.50
7	a	803	CLA	CMD-C2D	-2.17	1.46	1.50
8	I	403	BCL	CHD-C1D	2.16	1.42	1.38
8	I	407	BCL	C3B-C4B	2.16	1.45	1.41
7	a	802	CLA	CMB-C2B	-2.15	1.46	1.50
8	G	406	BCL	C3B-C4B	2.15	1.45	1.41
8	F	407	BCL	C3B-C4B	2.15	1.45	1.41
7	A	803	CLA	C4D-CHA	2.14	1.45	1.38
8	J	407	BCL	C3B-C4B	2.14	1.45	1.41
7	A	802	CLA	CMB-C2B	-2.13	1.46	1.50
7	A	802	CLA	CHC-C1C	2.13	1.42	1.38
8	E	407	BCL	C3B-C4B	2.13	1.45	1.41
7	a	803	CLA	MG-NB	-2.12	2.01	2.05
8	a	809[B]	BCL	C3D-C4D	-2.12	1.39	1.44
6	a	801	GS0	CAA-C2A	-2.11	1.50	1.54
8	G	405	BCL	C1A-CHA	-2.11	1.34	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	406	BCL	C1A-CHA	-2.11	1.34	1.43
8	G	401	BCL	CHD-C1D	2.11	1.42	1.38
7	A	803	CLA	MG-NB	-2.11	2.01	2.05
8	J	401	BCL	CHD-C1D	2.11	1.42	1.38
6	A	801	GS0	CAA-C2A	-2.11	1.50	1.54
8	F	408[B]	BCL	C3B-C4B	2.11	1.45	1.41
8	A	809[B]	BCL	C3D-C4D	-2.11	1.39	1.44
8	A	805	BCL	C1D-ND	-2.10	1.35	1.37
8	I	408[B]	BCL	C3B-C4B	2.10	1.45	1.41
8	J	406	BCL	C1A-CHA	-2.10	1.34	1.43
8	H	407	BCL	C3B-C4B	2.10	1.45	1.41
7	a	802	CLA	MG-NB	-2.10	2.01	2.05
8	E	406	BCL	C1A-CHA	-2.10	1.34	1.43
7	a	802	CLA	CMD-C2D	-2.09	1.46	1.50
8	I	406	BCL	C1A-CHA	-2.09	1.34	1.43
8	F	406	BCL	C1A-CHA	-2.09	1.34	1.43
8	E	401	BCL	CHD-C1D	2.09	1.42	1.38
8	H	401	BCL	CHD-C1D	2.09	1.42	1.38
8	H	408[B]	BCL	C3D-C4D	-2.08	1.39	1.44
8	H	408[B]	BCL	CHD-C1D	2.08	1.42	1.38
8	E	408[B]	BCL	CHD-C1D	2.08	1.42	1.38
8	A	814	BCL	CHD-C1D	2.07	1.42	1.38
8	I	401	BCL	CHD-C1D	2.07	1.42	1.38
8	F	401	BCL	CHD-C1D	2.07	1.42	1.38
8	E	408[B]	BCL	C3D-C4D	-2.07	1.39	1.44
8	F	408[B]	BCL	CHD-C1D	2.06	1.42	1.38
8	a	814	BCL	CHD-C1D	2.06	1.42	1.38
8	I	409[B]	BCL	CHD-C1D	2.06	1.42	1.38
8	a	810	BCL	C3D-C4D	-2.06	1.39	1.44
7	A	802	CLA	CMD-C2D	-2.06	1.46	1.50
8	A	810	BCL	O1A-CGA	-2.05	1.16	1.22
6	A	801	GS0	C3D-C2D	-2.05	1.33	1.39
8	A	805	BCL	O2A-C1	-2.05	1.40	1.46
6	a	801	GS0	C3D-C2D	-2.05	1.33	1.39
8	F	408[B]	BCL	C3D-C4D	-2.04	1.39	1.44
8	A	810	BCL	C3D-C4D	-2.04	1.39	1.44
8	A	805	BCL	C1D-C2D	2.04	1.49	1.45
8	A	815	BCL	MG-ND	-2.04	2.01	2.05
8	a	810	BCL	O1A-CGA	-2.04	1.16	1.22
8	I	408[B]	BCL	CHD-C1D	2.04	1.42	1.38
8	I	408[B]	BCL	C3D-C4D	-2.04	1.39	1.44
7	A	802	CLA	MG-NB	-2.04	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	807	BCL	C3D-C4D	-2.04	1.39	1.44
8	F	409[B]	BCL	CHD-C1D	2.03	1.42	1.38
8	A	814	BCL	C3D-C4D	-2.03	1.39	1.44
8	A	807	BCL	C3D-C4D	-2.03	1.39	1.44
9	a	816	F39	O2-C13	2.03	1.49	1.46
8	a	814	BCL	C3D-C4D	-2.03	1.39	1.44
8	A	804[B]	BCL	OBb-CAB	2.03	1.27	1.23
8	F	409[B]	BCL	C3D-C4D	-2.03	1.39	1.44
8	a	804[B]	BCL	OBb-CAB	2.02	1.27	1.23
8	a	812	BCL	C3D-C4D	-2.02	1.39	1.44
8	a	808	BCL	C3D-C4D	-2.01	1.39	1.44
8	I	409[B]	BCL	C3D-C4D	-2.01	1.39	1.44
8	A	812	BCL	C3D-C4D	-2.01	1.39	1.44
8	a	813	BCL	C3D-C4D	-2.01	1.39	1.44
8	A	808	BCL	C3D-C4D	-2.01	1.39	1.44
8	a	815	BCL	MG-ND	-2.01	2.01	2.05
8	A	813	BCL	C3D-C4D	-2.01	1.39	1.44
8	I	407	BCL	C4D-CHA	2.00	1.45	1.38

All (992) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	816	F39	C51-C44-C42	-11.71	110.85	127.28
9	A	816	F39	C32-C27-C20	-11.41	111.64	127.69
9	A	816	F39	C57-C59-C62	-11.40	111.30	127.28
7	A	803	CLA	C1D-ND-C4D	-11.04	98.56	106.31
9	a	816	F39	C32-C27-C20	-10.97	112.26	127.69
9	A	816	F39	C51-C44-C42	-10.92	111.97	127.28
9	A	816	F39	C63-C61-C58	-10.89	112.01	127.28
9	A	816	F39	C40-C39-C37	-10.86	112.05	127.28
8	A	805	BCL	C1-C2-C3	-10.74	108.60	126.20
9	a	816	F39	C40-C39-C37	-10.41	112.68	127.28
9	a	816	F39	C65-C62-C59	-10.40	105.97	122.82
9	a	816	F39	C63-C61-C58	-9.73	113.63	127.28
9	a	816	F39	C64-C62-C59	-8.92	104.98	119.01
9	a	816	F39	C60-C58-C61	-8.49	109.05	122.82
9	A	816	F39	C65-C62-C59	-8.40	109.20	122.82
9	A	816	F39	C43-C42-C44	-8.37	109.25	122.82
9	a	816	F39	C43-C42-C44	-8.29	109.38	122.82
9	A	816	F39	C46-C53-C56	-8.18	109.96	128.50
9	a	816	F39	C51-C57-C59	-7.84	107.47	123.52
9	A	816	F39	C60-C58-C61	-7.76	110.25	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	815	BCL	C4A-NA-C1A	7.56	110.13	106.68
8	A	815	BCL	C4A-NA-C1A	7.47	110.09	106.68
8	F	406	BCL	C1D-ND-C4D	-7.46	101.08	106.31
8	I	406	BCL	C1D-ND-C4D	-7.45	101.09	106.31
8	E	406	BCL	C1D-ND-C4D	-7.44	101.09	106.31
8	H	406	BCL	C1D-ND-C4D	-7.44	101.09	106.31
8	J	406	BCL	C1D-ND-C4D	-7.43	101.10	106.31
8	G	405	BCL	C1D-ND-C4D	-7.40	101.12	106.31
9	A	816	F39	C56-C58-C61	-7.25	107.60	119.01
6	A	801	GS0	C1-C2-C3	7.25	138.07	126.20
6	a	801	GS0	C1-C2-C3	7.22	138.03	126.20
9	A	816	F39	C38-C37-C39	-7.09	111.32	122.82
9	a	816	F39	C38-C37-C39	-6.92	111.61	122.82
9	A	816	F39	C41-C42-C44	-6.66	108.53	119.01
9	a	816	F39	C57-C59-C62	-6.63	117.98	127.28
9	a	816	F39	C53-C56-C58	-6.49	110.84	126.25
8	A	807	BCL	C1-O2A-CGA	6.46	132.30	116.65
7	a	803	CLA	C1D-ND-C4D	-6.44	101.79	106.31
8	a	807	BCL	C1-O2A-CGA	6.44	132.25	116.65
7	A	803	CLA	C4A-NA-C1A	6.44	109.62	106.68
8	A	811	BCL	C1-C2-C3	-6.38	115.74	126.20
8	a	811	BCL	C1-C2-C3	-6.36	115.78	126.20
7	a	802	CLA	C4A-NA-C1A	6.33	109.57	106.68
7	a	803	CLA	C4A-NA-C1A	6.33	109.57	106.68
9	A	816	F39	C64-C62-C59	-6.20	109.26	119.01
7	A	802	CLA	C4A-NA-C1A	6.20	109.51	106.68
9	A	816	F39	C57-C51-C44	-6.11	111.01	123.52
8	a	804[B]	BCL	C1D-ND-C4D	-6.11	102.02	106.31
9	a	816	F39	C41-C42-C44	-6.05	109.49	119.01
8	A	815	BCL	C1D-ND-C4D	-6.03	102.08	106.31
8	a	815	BCL	C1D-ND-C4D	-6.01	102.09	106.31
9	A	816	F39	C65-C62-C64	-5.91	109.06	118.09
9	A	816	F39	C60-C58-C56	-5.78	109.25	118.09
9	A	816	F39	C51-C57-C59	-5.78	111.70	123.52
9	A	816	F39	C63-C64-C62	-5.72	110.67	126.36
9	a	816	F39	C60-C58-C56	-5.71	109.37	118.09
9	A	816	F39	C35-C37-C39	-5.68	110.07	119.01
9	a	816	F39	C43-C42-C41	-5.49	109.70	118.09
9	a	816	F39	C56-C58-C61	-5.48	110.39	119.01
9	A	816	F39	C43-C42-C41	-5.47	109.73	118.09
9	A	816	F39	C53-C56-C58	-5.45	113.31	126.25
8	A	808	BCL	C1-C2-C3	-5.42	117.31	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	808	BCL	C1-C2-C3	-5.41	117.34	126.20
9	A	816	F39	C32-C35-C37	-5.39	111.59	126.36
6	a	801	GS0	O2D-CGD-CBD	5.38	120.63	111.23
6	A	801	GS0	O2D-CGD-CBD	5.37	120.62	111.23
9	A	816	F39	C40-C41-C42	-5.34	111.72	126.36
8	H	404	BCL	C4D-CHA-C1A	5.33	127.60	121.24
8	F	404	BCL	C4D-CHA-C1A	5.33	127.60	121.24
8	I	404	BCL	C4D-CHA-C1A	5.33	127.60	121.24
8	H	408[B]	BCL	O2D-CGD-CBD	5.32	120.52	111.23
8	G	403	BCL	C4D-CHA-C1A	5.31	127.58	121.24
8	E	404	BCL	C4D-CHA-C1A	5.30	127.57	121.24
8	J	404	BCL	C4D-CHA-C1A	5.30	127.56	121.24
8	a	813	BCL	C4D-CHA-C1A	5.30	127.56	121.24
8	A	813	BCL	C4D-CHA-C1A	5.30	127.56	121.24
8	E	401	BCL	C4A-NA-C1A	5.29	109.09	106.68
8	A	809[B]	BCL	C4D-CHA-C1A	5.29	127.56	121.24
8	E	408[B]	BCL	O2D-CGD-CBD	5.29	120.47	111.23
8	F	409[B]	BCL	O2D-CGD-CBD	5.28	120.46	111.23
8	I	408[B]	BCL	O2D-CGD-CBD	5.28	120.46	111.23
8	I	401	BCL	C4A-NA-C1A	5.28	109.09	106.68
8	F	408[B]	BCL	O2D-CGD-CBD	5.28	120.46	111.23
8	F	401	BCL	C4A-NA-C1A	5.27	109.08	106.68
8	H	401	BCL	C4A-NA-C1A	5.27	109.08	106.68
8	a	809[B]	BCL	C4D-CHA-C1A	5.27	127.53	121.24
8	I	409[B]	BCL	O2D-CGD-CBD	5.25	120.42	111.23
8	A	807	BCL	CBA-CAA-C2A	5.25	129.40	113.79
8	a	807	BCL	CBA-CAA-C2A	5.25	129.40	113.79
8	G	401	BCL	C4A-NA-C1A	5.22	109.06	106.68
8	E	407	BCL	C4D-CHA-C1A	5.21	127.46	121.24
8	I	407	BCL	C4D-CHA-C1A	5.21	127.46	121.24
8	F	407	BCL	C4D-CHA-C1A	5.21	127.45	121.24
8	A	805	BCL	C3D-C2D-C1D	-5.21	98.73	105.83
8	H	407	BCL	C4D-CHA-C1A	5.20	127.44	121.24
8	G	406	BCL	C4D-CHA-C1A	5.19	127.44	121.24
8	J	407	BCL	C4D-CHA-C1A	5.18	127.42	121.24
9	a	816	F39	C35-C37-C39	-5.17	110.87	119.01
9	a	816	F39	C40-C41-C42	-5.16	112.22	126.36
8	a	811	BCL	C4D-CHA-C1A	5.13	127.36	121.24
8	J	401	BCL	C4A-NA-C1A	5.13	109.02	106.68
8	A	811	BCL	C4D-CHA-C1A	5.12	127.36	121.24
8	I	407	BCL	C1D-ND-C4D	-5.08	102.75	106.31
8	a	812	BCL	C4D-CHA-C1A	5.07	127.29	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	402	BCL	O2D-CGD-CBD	5.06	120.07	111.23
8	E	409	BCL	O2D-CGD-CBD	5.05	120.06	111.23
8	H	407	BCL	C1D-ND-C4D	-5.05	102.77	106.31
9	A	816	F39	C38-C37-C35	-5.04	110.39	118.09
8	A	814	BCL	C4D-CHA-C1A	5.04	127.25	121.24
8	A	812	BCL	C4D-CHA-C1A	5.03	127.25	121.24
8	E	407	BCL	C1D-ND-C4D	-5.03	102.78	106.31
8	F	407	BCL	C1D-ND-C4D	-5.03	102.78	106.31
8	a	814	BCL	C4D-CHA-C1A	5.03	127.24	121.24
8	J	407	BCL	C1D-ND-C4D	-5.02	102.79	106.31
8	G	406	BCL	C1D-ND-C4D	-5.01	102.80	106.31
8	H	408[B]	BCL	C4D-CHA-C1A	5.00	127.20	121.24
8	a	805	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
8	I	409[B]	BCL	C4D-CHA-C1A	4.99	127.19	121.24
8	I	402	BCL	C4D-C3D-CAD	-4.99	102.69	108.11
8	I	403	BCL	C4D-CHA-C1A	4.98	127.19	121.24
8	F	402	BCL	C4D-C3D-CAD	-4.98	102.70	108.11
8	F	408[B]	BCL	C4D-CHA-C1A	4.97	127.17	121.24
8	F	403	BCL	C4D-CHA-C1A	4.97	127.17	121.24
8	H	403	BCL	C4D-CHA-C1A	4.97	127.17	121.24
8	I	406	BCL	O2D-CGD-CBD	4.96	119.91	111.23
8	E	403	BCL	C4D-CHA-C1A	4.96	127.16	121.24
8	E	408[B]	BCL	C4D-CHA-C1A	4.96	127.16	121.24
8	F	409[B]	BCL	C4D-CHA-C1A	4.95	127.15	121.24
8	J	403	BCL	C4D-CHA-C1A	4.95	127.15	121.24
8	F	406	BCL	O2D-CGD-CBD	4.95	119.88	111.23
8	G	402	BCL	C4D-CHA-C1A	4.95	127.15	121.24
8	E	406	BCL	O2D-CGD-CBD	4.94	119.87	111.23
8	H	406	BCL	O2D-CGD-CBD	4.94	119.86	111.23
9	a	816	F39	C32-C35-C37	-4.94	112.83	126.36
8	I	408[B]	BCL	C4D-CHA-C1A	4.93	127.13	121.24
8	J	406	BCL	O2D-CGD-CBD	4.93	119.84	111.23
8	G	405	BCL	O2D-CGD-CBD	4.92	119.84	111.23
8	a	806	BCL	C4D-CHA-C1A	4.91	127.11	121.24
9	a	816	F39	C46-C53-C56	-4.91	117.38	128.50
8	A	811	BCL	C11-C10-C8	4.89	132.23	115.97
8	A	806	BCL	C4D-CHA-C1A	4.89	127.07	121.24
8	J	405	BCL	C4D-CHA-C1A	4.87	127.05	121.24
8	a	810	BCL	C4D-CHA-C1A	4.87	127.05	121.24
8	E	409	BCL	C1-C2-C3	-4.87	118.22	126.20
9	a	816	F39	C65-C62-C64	-4.86	110.66	118.09
8	J	402	BCL	C1-C2-C3	-4.86	118.23	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	810	BCL	C4D-CHA-C1A	4.85	127.02	121.24
8	F	405	BCL	C4D-CHA-C1A	4.84	127.02	121.24
8	G	404	BCL	C4D-CHA-C1A	4.84	127.02	121.24
8	I	405	BCL	C4D-CHA-C1A	4.84	127.02	121.24
8	E	405	BCL	C4D-CHA-C1A	4.82	127.00	121.24
8	I	401	BCL	C4D-CHA-C1A	4.82	126.99	121.24
8	H	405	BCL	C4D-CHA-C1A	4.82	126.99	121.24
8	F	401	BCL	C4D-CHA-C1A	4.81	126.98	121.24
8	E	401	BCL	C4D-CHA-C1A	4.77	126.93	121.24
8	a	808	BCL	C4D-CHA-C1A	4.77	126.93	121.24
8	A	815	BCL	C4D-CHA-C1A	4.77	126.93	121.24
8	J	401	BCL	C4D-CHA-C1A	4.76	126.93	121.24
8	G	401	BCL	C4D-CHA-C1A	4.76	126.92	121.24
8	H	401	BCL	C4D-CHA-C1A	4.76	126.92	121.24
8	A	808	BCL	C4D-CHA-C1A	4.76	126.92	121.24
8	a	815	BCL	C4D-CHA-C1A	4.73	126.89	121.24
8	A	804[B]	BCL	CBA-CAA-C2A	-4.72	99.75	113.79
8	J	402	BCL	C4D-C3D-CAD	-4.62	103.09	108.11
7	a	802	CLA	C1D-ND-C4D	-4.62	103.07	106.31
8	a	807	BCL	C2A-C1A-CHA	4.61	131.87	123.87
8	A	807	BCL	C2A-C1A-CHA	4.61	131.86	123.87
8	E	409	BCL	C4D-C3D-CAD	-4.60	103.11	108.11
8	A	807	BCL	C1D-ND-C4D	-4.58	103.10	106.31
8	I	402	BCL	O2D-CGD-CBD	4.58	119.23	111.23
8	F	402	BCL	O2D-CGD-CBD	4.55	119.19	111.23
8	a	807	BCL	C1D-ND-C4D	-4.49	103.16	106.31
8	E	402	BCL	C4D-CHA-C1A	4.48	126.59	121.24
8	H	402	BCL	C4D-CHA-C1A	4.48	126.58	121.24
8	E	409	BCL	C4D-CHA-C1A	4.46	126.56	121.24
8	J	402	BCL	C4D-CHA-C1A	4.45	126.56	121.24
8	F	402	BCL	C4D-CHA-C1A	4.45	126.55	121.24
8	a	815	BCL	CHB-C4A-NA	4.44	130.81	124.40
8	I	402	BCL	C4D-CHA-C1A	4.44	126.54	121.24
8	a	812	BCL	C1-O2A-CGA	4.43	127.38	116.65
8	A	815	BCL	CHB-C4A-NA	4.42	130.78	124.40
8	A	812	BCL	C1-O2A-CGA	4.41	127.33	116.65
8	a	807	BCL	CHD-C1D-ND	-4.37	118.65	124.80
6	A	801	GS0	O2D-CGD-O1D	-4.36	115.35	123.85
6	a	801	GS0	O2D-CGD-O1D	-4.36	115.37	123.85
9	a	816	F39	C63-C64-C62	-4.35	114.45	126.36
8	A	807	BCL	CHD-C1D-ND	-4.34	118.69	124.80
6	a	801	GS0	C1D-ND-C4D	-4.32	103.28	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	816	F39	C38-C37-C35	-4.32	111.49	118.09
6	a	801	GS0	CMB-C2B-C1B	-4.31	118.85	125.42
6	a	801	GS0	C11-C10-C8	-4.31	101.66	115.97
6	A	801	GS0	CMB-C2B-C1B	-4.30	118.88	125.42
6	A	801	GS0	C1D-ND-C4D	-4.29	103.30	106.31
8	F	401	BCL	O2D-CGD-CBD	4.26	118.68	111.23
8	E	401	BCL	O2D-CGD-CBD	4.25	118.67	111.23
8	H	401	BCL	O2D-CGD-CBD	4.25	118.66	111.23
8	I	401	BCL	O2D-CGD-CBD	4.25	118.65	111.23
8	J	401	BCL	O2D-CGD-CBD	4.24	118.65	111.23
8	G	401	BCL	O2D-CGD-CBD	4.24	118.65	111.23
9	a	816	F39	C57-C51-C44	-4.21	114.90	123.52
8	A	814	BCL	C1-O2A-CGA	4.17	126.74	116.65
8	I	402	BCL	C1D-ND-C4D	-4.16	103.39	106.31
8	H	402	BCL	C1D-ND-C4D	-4.16	103.39	106.31
8	I	408[B]	BCL	C3B-C4B-NB	4.16	115.24	109.76
8	A	815	BCL	C1-C2-C3	-4.16	119.39	126.20
8	H	408[B]	BCL	CMC-C2C-C1C	4.15	122.94	111.77
8	a	815	BCL	C1-C2-C3	-4.15	119.39	126.20
8	E	408[B]	BCL	CMC-C2C-C1C	4.15	122.93	111.77
8	E	402	BCL	C1D-ND-C4D	-4.15	103.40	106.31
8	a	814	BCL	C1-O2A-CGA	4.14	126.68	116.65
8	F	408[B]	BCL	C3B-C4B-NB	4.14	115.22	109.76
8	E	409	BCL	C1D-ND-C4D	-4.14	103.41	106.31
8	A	810	BCL	CHD-C1D-ND	-4.14	118.98	124.80
8	a	810	BCL	CHD-C1D-ND	-4.13	119.00	124.80
8	F	402	BCL	C1D-ND-C4D	-4.12	103.42	106.31
8	A	812	BCL	CHD-C1D-ND	-4.12	119.00	124.80
8	A	807	BCL	CHA-C1A-NA	-4.10	117.11	126.39
9	a	816	F39	C61-C63-C64	-4.10	111.33	123.20
8	a	812	BCL	CHD-C1D-ND	-4.09	119.04	124.80
8	a	807	BCL	CHA-C1A-NA	-4.09	117.13	126.39
8	A	810	BCL	C11-C10-C8	-4.09	102.38	115.97
8	J	402	BCL	C1D-ND-C4D	-4.08	103.45	106.31
8	a	810	BCL	C11-C10-C8	-4.08	102.40	115.97
8	A	804[B]	BCL	C1D-ND-C4D	-4.05	103.47	106.31
8	J	405	BCL	C4A-NA-C1A	4.04	108.52	106.68
8	a	811	BCL	CHD-C1D-ND	-4.03	119.13	124.80
8	A	811	BCL	CHD-C1D-ND	-4.03	119.13	124.80
8	A	805	BCL	CHA-C1A-NA	-4.00	117.34	126.39
8	H	408[B]	BCL	C4A-NA-C1A	3.99	108.50	106.68
8	a	805	BCL	CHA-C1A-NA	-3.98	117.37	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	402	BCL	CHD-C1D-ND	-3.98	119.20	124.80
8	I	405	BCL	C4A-NA-C1A	3.97	108.49	106.68
8	E	409	BCL	CHD-C1D-ND	-3.97	119.21	124.80
8	J	403	BCL	C16-C15-C13	3.97	129.17	115.97
8	G	402	BCL	C16-C15-C13	3.97	129.16	115.97
8	H	402	BCL	CHD-C1D-ND	-3.96	119.22	124.80
8	E	403	BCL	C16-C15-C13	3.96	129.14	115.97
8	F	403	BCL	C16-C15-C13	3.96	129.14	115.97
8	I	403	BCL	C16-C15-C13	3.96	129.14	115.97
8	J	402	BCL	CHD-C1D-ND	-3.96	119.23	124.80
8	F	405	BCL	C4A-NA-C1A	3.96	108.48	106.68
8	H	403	BCL	C16-C15-C13	3.96	129.12	115.97
8	G	404	BCL	C4A-NA-C1A	3.95	108.48	106.68
8	F	402	BCL	CHD-C1D-ND	-3.95	119.24	124.80
8	E	405	BCL	C4A-NA-C1A	3.94	108.48	106.68
8	I	409[B]	BCL	C4A-NA-C1A	3.94	108.47	106.68
8	H	405	BCL	C4A-NA-C1A	3.93	108.47	106.68
8	I	402	BCL	CHD-C1D-ND	-3.93	119.27	124.80
8	a	810	BCL	C4A-NA-C1A	3.93	108.47	106.68
10	A	817	LHG	O7-C7-C8	3.93	119.98	111.48
8	I	409[B]	BCL	CHD-C1D-ND	-3.92	119.29	124.80
8	E	408[B]	BCL	CHD-C1D-ND	-3.92	119.29	124.80
8	A	815	BCL	O2A-CGA-O1A	-3.91	113.84	123.63
8	A	806	BCL	CHD-C1D-ND	-3.91	119.30	124.80
8	a	806	BCL	CHD-C1D-ND	-3.91	119.30	124.80
8	F	409[B]	BCL	CHD-C1D-ND	-3.90	119.31	124.80
8	a	815	BCL	O2A-CGA-O1A	-3.90	113.88	123.63
8	F	408[B]	BCL	CHD-C1D-ND	-3.90	119.32	124.80
6	a	801	GS0	C16-C15-C13	-3.90	103.02	115.97
8	F	409[B]	BCL	C4A-NA-C1A	3.90	108.46	106.68
8	H	408[B]	BCL	CHD-C1D-ND	-3.89	119.32	124.80
8	A	810	BCL	C4A-NA-C1A	3.89	108.45	106.68
9	A	816	F39	C27-C32-C35	-3.89	111.92	123.20
9	A	816	F39	C39-C40-C41	-3.89	111.92	123.20
8	I	408[B]	BCL	CHD-C1D-ND	-3.89	119.33	124.80
8	E	408[B]	BCL	C4A-NA-C1A	3.88	108.45	106.68
8	A	810	BCL	C1D-ND-C4D	-3.88	103.59	106.31
8	a	810	BCL	C1D-ND-C4D	-3.88	103.59	106.31
8	F	402	BCL	C1-C2-C3	-3.86	119.87	126.20
8	A	805	BCL	C1D-ND-C4D	-3.86	103.60	106.31
8	I	402	BCL	C1-C2-C3	-3.85	119.88	126.20
8	E	402	BCL	C1-C2-C3	-3.85	119.89	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	402	BCL	C1-C2-C3	-3.85	119.89	126.20
10	A	817	LHG	O4-P-O5	3.85	130.35	112.44
8	a	804[B]	BCL	CHD-C1D-ND	-3.83	119.41	124.80
8	a	813	BCL	CHD-C1D-ND	-3.82	119.42	124.80
8	E	401	BCL	C1-C2-C3	-3.81	119.95	126.20
8	H	401	BCL	C1-C2-C3	-3.81	119.95	126.20
8	H	408[B]	BCL	C1D-ND-C4D	-3.81	103.64	106.31
8	A	804[B]	BCL	CHD-C1D-ND	-3.81	119.44	124.80
8	G	401	BCL	CHD-C1D-ND	-3.81	119.44	124.80
8	H	404	BCL	CHD-C1D-ND	-3.81	119.44	124.80
8	E	404	BCL	CHD-C1D-ND	-3.80	119.45	124.80
8	E	401	BCL	CHD-C1D-ND	-3.80	119.45	124.80
8	J	404	BCL	CHD-C1D-ND	-3.80	119.46	124.80
8	F	401	BCL	C1-C2-C3	-3.80	119.98	126.20
8	J	401	BCL	CHD-C1D-ND	-3.80	119.46	124.80
8	A	813	BCL	CHD-C1D-ND	-3.79	119.47	124.80
8	H	401	BCL	CHD-C1D-ND	-3.79	119.47	124.80
8	G	403	BCL	CHD-C1D-ND	-3.79	119.47	124.80
9	A	816	F39	C61-C63-C64	-3.79	112.23	123.20
6	a	801	GS0	CAA-C2A-C3A	-3.78	102.78	113.00
8	G	401	BCL	C1-C2-C3	-3.78	120.00	126.20
8	F	405	BCL	C1D-ND-C4D	-3.78	103.66	106.31
6	A	801	GS0	CAA-C2A-C3A	-3.78	102.79	113.00
8	F	404	BCL	CHD-C1D-ND	-3.78	119.49	124.80
8	I	404	BCL	CHD-C1D-ND	-3.77	119.50	124.80
8	F	405	BCL	CHD-C1D-ND	-3.77	119.50	124.80
8	I	405	BCL	C1D-ND-C4D	-3.77	103.67	106.31
8	J	405	BCL	C1D-ND-C4D	-3.77	103.67	106.31
8	F	401	BCL	CHD-C1D-ND	-3.77	119.50	124.80
8	I	401	BCL	C1-C2-C3	-3.77	120.03	126.20
8	E	405	BCL	CHD-C1D-ND	-3.76	119.51	124.80
8	E	408[B]	BCL	C1D-ND-C4D	-3.76	103.67	106.31
8	J	401	BCL	C1-C2-C3	-3.76	120.04	126.20
8	F	408[B]	BCL	C4A-NA-C1A	3.75	108.39	106.68
8	I	405	BCL	CHD-C1D-ND	-3.75	119.52	124.80
8	A	805	BCL	CHD-C1D-ND	-3.75	119.52	124.80
8	J	405	BCL	CHD-C1D-ND	-3.75	119.52	124.80
8	G	404	BCL	C1D-ND-C4D	-3.75	103.68	106.31
8	I	409[B]	BCL	C1D-ND-C4D	-3.75	103.68	106.31
8	G	404	BCL	CHD-C1D-ND	-3.75	119.52	124.80
8	E	405	BCL	C1D-ND-C4D	-3.75	103.68	106.31
8	I	401	BCL	CHD-C1D-ND	-3.75	119.53	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	405	BCL	CHD-C1D-ND	-3.75	119.53	124.80
8	a	805	BCL	C1-C2-C3	-3.74	120.07	126.20
8	F	409[B]	BCL	C1D-ND-C4D	-3.74	103.69	106.31
8	I	408[B]	BCL	C4A-NA-C1A	3.74	108.38	106.68
8	A	812	BCL	C1D-ND-C4D	-3.73	103.70	106.31
8	H	405	BCL	C1D-ND-C4D	-3.73	103.70	106.31
8	A	807	BCL	CAA-C2A-C1A	3.72	124.15	111.97
8	a	807	BCL	CAA-C2A-C1A	3.71	124.15	111.97
9	a	816	F39	C27-C32-C35	-3.71	112.44	123.20
8	F	408[B]	BCL	C1D-ND-C4D	-3.71	103.71	106.31
8	A	808	BCL	CHD-C1D-ND	-3.71	119.58	124.80
8	a	808	BCL	CHD-C1D-ND	-3.71	119.58	124.80
8	a	808	BCL	C2A-C1A-CHA	3.70	130.28	123.87
8	I	408[B]	BCL	C1D-ND-C4D	-3.70	103.72	106.31
8	a	812	BCL	C1D-ND-C4D	-3.69	103.72	106.31
8	A	808	BCL	C2A-C1A-CHA	3.67	130.24	123.87
10	a	817	LHG	O7-C7-C8	3.66	119.41	111.48
8	a	806	BCL	C1D-ND-C4D	-3.63	103.77	106.31
9	a	816	F39	C39-C40-C41	-3.62	112.71	123.20
8	a	806	BCL	C1-C2-C3	-3.62	120.27	126.20
8	A	806	BCL	C1D-ND-C4D	-3.61	103.78	106.31
8	H	402	BCL	CED-O2D-CGD	3.60	124.09	115.92
6	A	801	GS0	OBB-CAB-CBB	-3.60	111.71	119.77
6	a	801	GS0	OBB-CAB-CBB	-3.59	111.72	119.77
8	E	402	BCL	CED-O2D-CGD	3.59	124.06	115.92
8	A	804[B]	BCL	C4D-CHA-C1A	3.59	125.53	121.24
8	A	815	BCL	CHD-C1D-ND	-3.59	119.75	124.80
8	a	815	BCL	CHD-C1D-ND	-3.58	119.77	124.80
8	A	809[B]	BCL	CHD-C1D-ND	-3.57	119.78	124.80
8	I	406	BCL	CHD-C1D-ND	-3.56	119.79	124.80
8	G	405	BCL	CHD-C1D-ND	-3.56	119.79	124.80
8	H	406	BCL	CHD-C1D-ND	-3.56	119.80	124.80
8	F	406	BCL	CHD-C1D-ND	-3.55	119.81	124.80
8	E	406	BCL	CHD-C1D-ND	-3.55	119.81	124.80
8	a	809[B]	BCL	CHD-C1D-ND	-3.55	119.81	124.80
8	A	815	BCL	O2A-CGA-CBA	3.54	122.63	111.83
8	J	406	BCL	CHD-C1D-ND	-3.54	119.83	124.80
8	a	815	BCL	O2A-CGA-CBA	3.53	122.61	111.83
7	A	802	CLA	C1D-ND-C4D	-3.52	103.84	106.31
8	a	807	BCL	C4D-CHA-C1A	3.52	125.44	121.24
8	A	814	BCL	CHD-C1D-ND	-3.51	119.86	124.80
8	a	815	BCL	C3D-C4D-ND	3.51	115.69	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	815	BCL	C3D-C4D-ND	3.51	115.69	109.99
8	A	807	BCL	C4D-CHA-C1A	3.50	125.41	121.24
8	a	814	BCL	CHD-C1D-ND	-3.49	119.89	124.80
8	H	407	BCL	C1-C2-C3	-3.48	120.49	126.20
8	a	808	BCL	C1D-ND-C4D	-3.47	103.87	106.31
8	E	407	BCL	C1-C2-C3	-3.47	120.51	126.20
8	A	805	BCL	C2D-C1D-ND	3.47	113.56	110.13
8	A	804[B]	BCL	C2A-C1A-CHA	3.47	129.89	123.87
8	I	407	BCL	C1-C2-C3	-3.46	120.53	126.20
8	F	407	BCL	C1-C2-C3	-3.45	120.54	126.20
8	A	814	BCL	C1-C2-C3	-3.45	120.55	126.20
8	a	814	BCL	C1-C2-C3	-3.45	120.55	126.20
8	A	808	BCL	C1D-ND-C4D	-3.43	103.91	106.31
8	a	804[B]	BCL	OBB-CAB-C3B	3.43	126.50	120.43
8	a	805	BCL	CMD-C2D-C1D	3.43	130.76	124.73
8	a	804[B]	BCL	C2A-C1A-CHA	3.41	129.79	123.87
8	A	804[B]	BCL	OBB-CAB-C3B	3.41	126.46	120.43
10	A	818	LHG	O7-C7-C8	3.40	118.84	111.48
8	a	804[B]	BCL	CMB-C2B-C1B	-3.39	120.26	125.42
8	H	402	BCL	CBA-CAA-C2A	-3.37	103.77	113.79
8	H	403	BCL	CHA-C1A-NA	-3.37	118.77	126.39
8	I	402	BCL	CBA-CAA-C2A	-3.36	103.79	113.79
8	E	402	BCL	CBA-CAA-C2A	-3.36	103.79	113.79
8	F	402	BCL	CBA-CAA-C2A	-3.36	103.80	113.79
8	I	407	BCL	CHA-C1A-NA	-3.35	118.79	126.39
8	J	403	BCL	CHA-C1A-NA	-3.35	118.80	126.39
8	E	403	BCL	CHA-C1A-NA	-3.35	118.80	126.39
8	H	401	BCL	C1D-ND-C4D	-3.35	103.96	106.31
8	F	403	BCL	CHA-C1A-NA	-3.35	118.80	126.39
8	G	402	BCL	CHA-C1A-NA	-3.34	118.82	126.39
8	I	403	BCL	CHA-C1A-NA	-3.34	118.82	126.39
8	F	407	BCL	CHA-C1A-NA	-3.34	118.83	126.39
7	A	802	CLA	C1-C2-C3	-3.34	120.73	126.20
8	G	406	BCL	CHA-C1A-NA	-3.33	118.84	126.39
7	a	802	CLA	C1-C2-C3	-3.33	120.74	126.20
8	E	407	BCL	CHA-C1A-NA	-3.33	118.84	126.39
8	J	407	BCL	CHA-C1A-NA	-3.33	118.84	126.39
8	A	804[B]	BCL	CMB-C2B-C1B	-3.33	120.35	125.42
9	a	816	F39	C25-C20-C19	-3.33	109.45	115.23
8	a	813	BCL	C1D-ND-C4D	-3.32	103.98	106.31
8	E	401	BCL	C1D-ND-C4D	-3.32	103.98	106.31
7	A	803	CLA	C3D-C4D-ND	3.32	115.38	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	805	BCL	CHD-C1D-ND	-3.32	120.14	124.80
8	a	806	BCL	C4-C3-C5	3.31	120.98	115.23
8	H	407	BCL	CHA-C1A-NA	-3.31	118.89	126.39
8	J	401	BCL	C1D-ND-C4D	-3.31	103.99	106.31
8	G	401	BCL	C1D-ND-C4D	-3.31	103.99	106.31
6	A	801	GS0	CBB-CAB-C3B	3.30	127.37	120.40
8	I	409[B]	BCL	CMB-C2B-C3B	3.29	136.04	125.67
6	a	801	GS0	CBB-CAB-C3B	3.29	127.33	120.40
8	F	401	BCL	C1D-ND-C4D	-3.27	104.02	106.31
8	G	402	BCL	CHD-C1D-ND	-3.27	120.20	124.80
8	a	814	BCL	CHA-C1A-NA	-3.26	119.00	126.39
8	E	403	BCL	CHD-C1D-ND	-3.26	120.21	124.80
7	a	803	CLA	CHD-C1D-ND	-3.26	120.22	124.80
8	F	409[B]	BCL	CMB-C2B-C3B	3.26	135.95	125.67
8	G	402	BCL	C2A-C1A-CHA	3.25	129.51	123.87
8	F	403	BCL	CHD-C1D-ND	-3.25	120.23	124.80
8	I	401	BCL	C1D-ND-C4D	-3.25	104.03	106.31
8	I	403	BCL	CHD-C1D-ND	-3.25	120.23	124.80
8	E	403	BCL	C2A-C1A-CHA	3.24	129.50	123.87
8	J	403	BCL	CHD-C1D-ND	-3.24	120.24	124.80
8	J	403	BCL	C2A-C1A-CHA	3.24	129.49	123.87
8	J	401	BCL	CHA-C1A-NA	-3.24	119.06	126.39
8	E	402	BCL	O2A-CGA-CBA	3.24	121.71	111.83
8	F	402	BCL	O2A-CGA-CBA	3.24	121.71	111.83
8	F	403	BCL	C2A-C1A-CHA	3.24	129.48	123.87
8	I	403	BCL	C2A-C1A-CHA	3.24	129.48	123.87
8	H	402	BCL	O2A-CGA-CBA	3.23	121.70	111.83
8	H	403	BCL	C2A-C1A-CHA	3.23	129.48	123.87
6	A	801	GS0	CHA-C1A-NA	-3.23	119.07	126.39
8	F	401	BCL	CHA-C1A-NA	-3.23	119.08	126.39
8	I	401	BCL	CHA-C1A-NA	-3.23	119.08	126.39
8	G	401	BCL	CHA-C1A-NA	-3.23	119.09	126.39
8	A	809[B]	BCL	C1D-ND-C4D	-3.23	104.05	106.31
8	E	401	BCL	CHA-C1A-NA	-3.22	119.09	126.39
8	a	807	BCL	C16-C15-C13	3.22	126.68	115.97
6	a	801	GS0	CHA-C1A-NA	-3.22	119.09	126.39
10	a	818	LHG	O4-P-O5	3.22	127.43	112.44
8	I	402	BCL	O2A-CGA-CBA	3.22	121.66	111.83
8	H	401	BCL	CHA-C1A-NA	-3.22	119.10	126.39
8	F	408[B]	BCL	CHA-C1A-NA	-3.22	119.11	126.39
8	A	807	BCL	C16-C15-C13	3.22	126.66	115.97
8	H	403	BCL	CHD-C1D-ND	-3.22	120.28	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	805	BCL	C2A-C1A-CHA	3.21	129.45	123.87
8	a	805	BCL	C2A-C1A-CHA	3.21	129.44	123.87
8	I	408[B]	BCL	CHA-C1A-NA	-3.21	119.12	126.39
8	G	403	BCL	C1D-ND-C4D	-3.21	104.06	106.31
8	A	809[B]	BCL	CHA-C1A-NA	-3.20	119.13	126.39
11	a	819	IKV	O2-C17-C18	3.20	117.63	108.40
8	A	812	BCL	C1-C2-C3	-3.20	120.95	126.20
8	A	813	BCL	C1D-ND-C4D	-3.20	104.06	106.31
8	I	409[B]	BCL	CHA-C1A-NA	-3.20	119.14	126.39
8	A	804[B]	BCL	CHA-C1A-NA	-3.20	119.14	126.39
8	a	809[B]	BCL	CHA-C1A-NA	-3.20	119.15	126.39
8	a	812	BCL	C1-C2-C3	-3.20	120.96	126.20
8	H	408[B]	BCL	CHA-C1A-NA	-3.20	119.16	126.39
8	E	408[B]	BCL	CHA-C1A-NA	-3.19	119.16	126.39
11	A	819	IKV	O2-C17-C18	3.19	117.60	108.40
8	F	409[B]	BCL	CHA-C1A-NA	-3.19	119.16	126.39
8	J	404	BCL	C1D-ND-C4D	-3.19	104.08	106.31
7	A	803	CLA	C4D-CHA-C1A	3.18	125.04	121.24
8	a	804[B]	BCL	CHA-C1A-NA	-3.18	119.20	126.39
8	a	809[B]	BCL	C1D-ND-C4D	-3.18	104.08	106.31
7	a	802	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
8	A	805	BCL	CGD-CBD-CAD	-3.17	100.57	110.85
8	E	404	BCL	C1D-ND-C4D	-3.17	104.09	106.31
8	I	402	BCL	C4-C3-C5	3.17	120.72	115.23
8	A	814	BCL	C2A-C1A-CHA	3.16	129.35	123.87
8	H	404	BCL	C1D-ND-C4D	-3.16	104.09	106.31
8	H	402	BCL	C4-C3-C5	3.15	120.70	115.23
8	A	811	BCL	C1D-ND-C4D	-3.15	104.10	106.31
8	a	808	BCL	CHA-C1A-NA	-3.15	119.26	126.39
8	F	402	BCL	C4-C3-C5	3.15	120.69	115.23
8	E	402	BCL	C4-C3-C5	3.15	120.69	115.23
7	A	802	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
8	a	804[B]	BCL	OBB-CAB-CBB	-3.14	112.73	119.77
8	A	804[B]	BCL	OBB-CAB-CBB	-3.14	112.74	119.77
8	A	808	BCL	CHA-C1A-NA	-3.13	119.29	126.39
8	a	814	BCL	C1D-ND-C4D	-3.13	104.11	106.31
8	E	403	BCL	C1D-ND-C4D	-3.13	104.12	106.31
8	A	814	BCL	CHA-C1A-NA	-3.13	119.31	126.39
8	a	814	BCL	C2A-C1A-CHA	3.12	129.29	123.87
8	G	402	BCL	C4A-NA-C1A	3.12	108.10	106.68
7	a	802	CLA	CHD-C1D-ND	-3.12	120.41	124.80
10	A	818	LHG	O4-P-O5	3.12	126.95	112.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	402	BCL	C1D-ND-C4D	-3.12	104.12	106.31
8	I	403	BCL	C1D-ND-C4D	-3.11	104.13	106.31
8	A	814	BCL	C1D-ND-C4D	-3.11	104.13	106.31
9	A	816	F39	C25-C20-C27	-3.11	109.06	122.50
8	F	404	BCL	C1D-ND-C4D	-3.10	104.13	106.31
8	F	403	BCL	C1D-ND-C4D	-3.10	104.14	106.31
8	I	403	BCL	C4A-NA-C1A	3.09	108.09	106.68
8	J	403	BCL	C1D-ND-C4D	-3.09	104.14	106.31
8	G	406	BCL	C1-C2-C3	-3.09	121.14	126.20
8	I	404	BCL	C1D-ND-C4D	-3.08	104.15	106.31
9	A	816	F39	C25-C20-C19	-3.08	109.88	115.23
8	H	402	BCL	C2A-C1A-CHA	3.08	129.21	123.87
8	F	402	BCL	C2A-C1A-CHA	3.07	129.20	123.87
8	E	402	BCL	C2A-C1A-CHA	3.07	129.20	123.87
8	J	403	BCL	C4A-NA-C1A	3.07	108.08	106.68
8	a	811	BCL	C1D-ND-C4D	-3.06	104.17	106.31
8	A	809[B]	BCL	C2A-C1A-CHA	3.06	129.17	123.87
8	I	408[B]	BCL	CGD-CBD-CAD	-3.05	100.96	110.85
8	G	406	BCL	C4-C3-C5	3.05	120.52	115.23
8	J	407	BCL	C1-C2-C3	-3.05	121.20	126.20
8	E	402	BCL	CHA-C1A-NA	-3.05	119.49	126.39
8	F	408[B]	BCL	CGD-CBD-CAD	-3.05	100.99	110.85
8	I	402	BCL	C2A-C1A-CHA	3.04	129.15	123.87
8	I	402	BCL	CHA-C1A-NA	-3.04	119.50	126.39
8	H	403	BCL	C1D-ND-C4D	-3.04	104.18	106.31
8	F	402	BCL	CHA-C1A-NA	-3.04	119.51	126.39
8	J	407	BCL	C4-C3-C5	3.04	120.50	115.23
8	H	402	BCL	CHA-C1A-NA	-3.04	119.51	126.39
8	A	806	BCL	C4A-NA-C1A	3.04	108.06	106.68
9	a	816	F39	C25-C20-C27	-3.03	109.39	122.50
8	a	810	BCL	CHA-C1A-NA	-3.03	119.53	126.39
6	A	801	GS0	C11-C10-C8	-3.03	105.89	115.97
7	A	803	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
8	A	810	BCL	CHA-C1A-NA	-3.02	119.54	126.39
7	a	803	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
8	E	409	BCL	C4A-NA-C1A	3.02	108.06	106.68
8	I	408[B]	BCL	CMC-C2C-C1C	3.02	119.88	111.77
8	E	409	BCL	CHA-C1A-NA	-3.01	119.57	126.39
8	F	408[B]	BCL	CMC-C2C-C1C	3.01	119.87	111.77
8	I	409[B]	BCL	CGD-CBD-CAD	-3.01	101.11	110.85
8	a	809[B]	BCL	C2A-C1A-CHA	3.01	129.08	123.87
7	A	802	CLA	C3B-C4B-NB	-3.01	107.85	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	403	BCL	C4A-NA-C1A	3.00	108.05	106.68
8	J	402	BCL	C4A-NA-C1A	3.00	108.05	106.68
8	J	402	BCL	CHA-C1A-NA	-3.00	119.60	126.39
8	F	409[B]	BCL	CGD-CBD-CAD	-3.00	101.14	110.85
8	E	403	BCL	C4A-NA-C1A	3.00	108.05	106.68
6	A	801	GS0	C16-C15-C13	-2.99	106.01	115.97
8	F	404	BCL	CHA-C1A-NA	-2.99	119.61	126.39
8	E	407	BCL	O2A-CGA-CBA	2.99	120.95	111.83
8	a	813	BCL	CHA-C1A-NA	-2.99	119.62	126.39
8	a	806	BCL	CHA-C1A-NA	-2.99	119.63	126.39
8	H	407	BCL	O2A-CGA-CBA	2.98	120.93	111.83
8	F	407	BCL	O2A-CGA-CBA	2.98	120.92	111.83
8	A	813	BCL	CHA-C1A-NA	-2.98	119.65	126.39
8	F	407	BCL	C2A-C1A-CHA	2.98	129.03	123.87
8	I	407	BCL	O2A-CGA-CBA	2.98	120.91	111.83
8	a	805	BCL	C4D-CHA-C1A	2.98	124.79	121.24
8	H	404	BCL	CHA-C1A-NA	-2.98	119.65	126.39
8	J	404	BCL	CHA-C1A-NA	-2.97	119.66	126.39
8	E	407	BCL	C2A-C1A-CHA	2.97	129.03	123.87
8	I	407	BCL	C2A-C1A-CHA	2.97	129.02	123.87
8	G	406	BCL	CAA-C2A-C1A	-2.97	102.24	111.97
8	a	805	BCL	CHC-C1C-NC	-2.97	120.11	124.40
8	I	404	BCL	CHA-C1A-NA	-2.97	119.67	126.39
8	I	404	BCL	C4A-NA-C1A	2.97	108.03	106.68
8	J	407	BCL	CAA-C2A-C1A	-2.97	102.26	111.97
8	E	404	BCL	CHA-C1A-NA	-2.96	119.68	126.39
8	H	404	BCL	C2A-C1A-CHA	2.96	129.01	123.87
8	A	806	BCL	CHA-C1A-NA	-2.96	119.69	126.39
8	H	407	BCL	C2A-C1A-CHA	2.96	129.00	123.87
8	I	407	BCL	C3D-C4D-ND	2.96	114.80	109.99
7	A	802	CLA	CHD-C1D-ND	-2.95	120.64	124.80
8	G	403	BCL	C4A-NA-C1A	2.95	108.03	106.68
8	H	401	BCL	CAA-CBA-CGA	-2.95	104.82	113.21
8	G	403	BCL	CHA-C1A-NA	-2.95	119.70	126.39
8	F	401	BCL	CAA-CBA-CGA	-2.95	104.82	113.21
8	A	805	BCL	C4D-CHA-C1A	2.95	124.77	121.24
8	E	401	BCL	CAA-CBA-CGA	-2.95	104.82	113.21
8	A	805	BCL	C1C-NC-C4C	-2.95	105.33	106.68
8	F	404	BCL	C2A-C1A-CHA	2.95	128.99	123.87
8	I	401	BCL	CAA-CBA-CGA	-2.95	104.83	113.21
8	I	404	BCL	C2A-C1A-CHA	2.95	128.99	123.87
8	G	401	BCL	CAA-CBA-CGA	-2.95	104.83	113.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	402	BCL	C4A-NA-C1A	2.94	108.02	106.68
8	H	402	BCL	C4A-NA-C1A	2.94	108.02	106.68
8	J	401	BCL	CAA-CBA-CGA	-2.94	104.86	113.21
8	E	402	BCL	C4A-NA-C1A	2.94	108.02	106.68
8	H	403	BCL	C4A-NA-C1A	2.93	108.02	106.68
8	a	805	BCL	C1D-ND-C4D	-2.93	104.25	106.31
8	E	404	BCL	C2A-C1A-CHA	2.93	128.96	123.87
8	E	404	BCL	C4A-NA-C1A	2.93	108.02	106.68
7	a	802	CLA	C3B-C4B-NB	-2.93	107.92	110.53
8	J	407	BCL	O2A-CGA-CBA	2.92	120.75	111.83
8	G	405	BCL	C4D-C3D-CAD	-2.92	104.93	108.11
8	F	407	BCL	C3D-C4D-ND	2.92	114.74	109.99
8	G	406	BCL	O2A-CGA-CBA	2.92	120.75	111.83
8	A	805	BCL	CHC-C1C-NC	-2.92	120.18	124.40
8	J	407	BCL	C3D-C4D-ND	2.92	114.73	109.99
8	E	407	BCL	C3D-C4D-ND	2.92	114.73	109.99
8	a	813	BCL	C4A-NA-C1A	2.91	108.01	106.68
8	H	407	BCL	C3D-C4D-ND	2.91	114.72	109.99
8	a	806	BCL	C6-C7-C8	-2.91	106.30	115.97
8	G	403	BCL	C2A-C1A-CHA	2.91	128.91	123.87
8	J	404	BCL	C2A-C1A-CHA	2.91	128.91	123.87
8	H	404	BCL	C4A-NA-C1A	2.90	108.00	106.68
8	J	406	BCL	C4D-C3D-CAD	-2.90	104.96	108.11
8	G	406	BCL	C3D-C4D-ND	2.90	114.70	109.99
8	a	806	BCL	C4A-NA-C1A	2.90	108.00	106.68
8	a	804[B]	BCL	C3D-C4D-ND	2.89	114.69	109.99
8	a	812	BCL	CHA-C1A-NA	-2.89	119.85	126.39
8	J	404	BCL	C4A-NA-C1A	2.88	108.00	106.68
8	A	812	BCL	CHA-C1A-NA	-2.88	119.86	126.39
8	I	406	BCL	CHA-C1A-NA	-2.88	119.87	126.39
8	J	406	BCL	CHA-C1A-NA	-2.88	119.88	126.39
8	E	406	BCL	CHA-C1A-NA	-2.88	119.88	126.39
8	F	406	BCL	CHA-C1A-NA	-2.87	119.89	126.39
8	F	404	BCL	C4A-NA-C1A	2.87	107.99	106.68
8	H	401	BCL	O2A-CGA-CBA	2.87	120.58	111.83
8	a	805	BCL	C2D-C1D-ND	2.87	112.96	110.13
8	G	405	BCL	CHA-C1A-NA	-2.87	119.90	126.39
8	E	401	BCL	O2A-CGA-CBA	2.87	120.57	111.83
8	I	401	BCL	O2A-CGA-CBA	2.87	120.57	111.83
8	G	401	BCL	O2A-CGA-CBA	2.86	120.57	111.83
8	J	401	BCL	O2A-CGA-CBA	2.86	120.56	111.83
8	F	401	BCL	O2A-CGA-CBA	2.86	120.56	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	813	BCL	C4A-NA-C1A	2.86	107.98	106.68
7	A	803	CLA	CHA-C4D-ND	-2.86	126.65	132.55
8	H	406	BCL	CHA-C1A-NA	-2.85	119.93	126.39
6	A	801	GS0	CMC-C2C-C3C	-2.85	102.95	113.98
6	a	801	GS0	CMC-C2C-C3C	-2.85	102.95	113.98
8	I	402	BCL	C4A-NA-C1A	2.85	107.98	106.68
6	a	801	GS0	C12-C11-C10	-2.84	100.57	113.28
6	a	801	GS0	O2A-CGA-O1A	-2.83	116.55	123.63
8	E	409	BCL	O2D-CGD-O1D	-2.83	118.35	123.85
6	A	801	GS0	O2A-CGA-O1A	-2.82	116.57	123.63
8	J	402	BCL	O2D-CGD-O1D	-2.82	118.36	123.85
8	a	807	BCL	O2A-CGA-CBA	-2.82	103.24	111.83
9	A	816	F39	O6-C21-C22	2.82	120.42	111.83
8	I	407	BCL	C4-C3-C5	2.81	120.11	115.23
8	H	406	BCL	C4A-NA-C1A	2.81	107.96	106.68
8	A	807	BCL	O2A-CGA-CBA	-2.81	103.28	111.83
8	a	811	BCL	CHA-C1A-NA	-2.80	120.04	126.39
8	F	407	BCL	C4-C3-C5	2.80	120.09	115.23
8	A	815	BCL	C2B-C1B-NB	-2.80	107.42	110.33
7	A	802	CLA	C7-C6-C5	-2.80	105.80	113.26
8	G	405	BCL	C4A-NA-C1A	2.80	107.96	106.68
6	a	801	GS0	C2D-C1D-ND	2.80	112.89	110.13
7	a	802	CLA	C7-C6-C5	-2.80	105.81	113.26
8	A	811	BCL	CHA-C1A-NA	-2.80	120.06	126.39
8	a	812	BCL	C2A-C1A-CHA	2.79	128.71	123.87
8	A	812	BCL	C2A-C1A-CHA	2.79	128.70	123.87
8	I	408[B]	BCL	CHC-C4B-NB	-2.79	119.87	124.05
8	a	811	BCL	CAA-CBA-CGA	2.78	121.10	113.21
8	E	407	BCL	C4-C3-C5	2.78	120.05	115.23
8	a	806	BCL	C2A-C1A-CHA	2.77	128.68	123.87
8	F	406	BCL	C4A-NA-C1A	2.77	107.94	106.68
8	A	811	BCL	CAA-CBA-CGA	2.77	121.08	113.21
8	a	815	BCL	C2B-C1B-NB	-2.77	107.45	110.33
8	A	812	BCL	C4A-NA-C1A	2.77	107.94	106.68
9	a	816	F39	O6-C21-C22	2.77	120.28	111.83
8	F	408[B]	BCL	CHC-C4B-NB	-2.77	119.90	124.05
8	A	806	BCL	C2A-C1A-CHA	2.77	128.67	123.87
8	H	407	BCL	C4-C3-C5	2.76	120.03	115.23
6	A	801	GS0	C2D-C1D-ND	2.76	112.86	110.13
10	a	818	LHG	O8-C23-C24	2.76	120.26	111.83
8	E	406	BCL	C4A-NA-C1A	2.76	107.94	106.68
8	J	406	BCL	C4A-NA-C1A	2.76	107.94	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	816	F39	O1-C12-C10	2.75	114.66	109.70
8	I	409[B]	BCL	CMB-C2B-C1B	-2.75	121.24	125.42
8	I	406	BCL	CHA-C4D-ND	-2.74	126.89	132.55
8	a	812	BCL	C4A-NA-C1A	2.74	107.93	106.68
8	F	406	BCL	CHA-C4D-ND	-2.74	126.90	132.55
8	E	406	BCL	CHA-C4D-ND	-2.73	126.91	132.55
8	I	406	BCL	C4A-NA-C1A	2.73	107.92	106.68
8	H	406	BCL	CHA-C4D-ND	-2.73	126.92	132.55
8	J	406	BCL	CHA-C4D-ND	-2.73	126.92	132.55
8	G	405	BCL	CHA-C4D-ND	-2.72	126.93	132.55
8	I	401	BCL	C2A-C1A-CHA	2.72	128.59	123.87
8	F	401	BCL	C2A-C1A-CHA	2.72	128.59	123.87
8	E	409	BCL	C4-C3-C5	2.72	119.94	115.23
8	F	402	BCL	CAA-C2A-C1A	2.72	120.88	111.97
8	I	402	BCL	CAA-C2A-C1A	2.71	120.87	111.97
8	E	402	BCL	CAA-C2A-C1A	2.71	120.86	111.97
8	J	402	BCL	C4-C3-C5	2.71	119.93	115.23
8	H	402	BCL	CAA-C2A-C1A	2.71	120.84	111.97
8	F	409[B]	BCL	CMB-C2B-C1B	-2.71	121.30	125.42
8	J	407	BCL	O2D-CGD-O1D	-2.70	118.59	123.85
8	E	401	BCL	C2A-C1A-CHA	2.70	128.56	123.87
8	F	405	BCL	CHA-C1A-NA	-2.70	120.29	126.39
6	a	801	GS0	C3B-C4B-NB	-2.69	106.21	109.76
8	G	404	BCL	CHA-C1A-NA	-2.69	120.30	126.39
8	I	405	BCL	CHA-C1A-NA	-2.69	120.31	126.39
8	E	405	BCL	CHA-C1A-NA	-2.68	120.31	126.39
8	H	401	BCL	C2A-C1A-CHA	2.68	128.52	123.87
8	J	405	BCL	CHA-C1A-NA	-2.68	120.32	126.39
6	A	801	GS0	C3B-C4B-NB	-2.68	106.22	109.76
8	A	806	BCL	C6-C7-C8	-2.68	107.06	115.97
8	F	408[B]	BCL	C2A-C1A-CHA	2.68	128.52	123.87
8	J	401	BCL	C2A-C1A-CHA	2.68	128.51	123.87
8	G	401	BCL	C2A-C1A-CHA	2.68	128.51	123.87
8	A	813	BCL	C1-C2-C3	-2.68	121.81	126.20
8	G	406	BCL	O2D-CGD-O1D	-2.68	118.64	123.85
8	H	405	BCL	CHA-C1A-NA	-2.68	120.33	126.39
6	A	801	GS0	CHB-C1B-NB	2.66	128.05	124.05
8	a	810	BCL	C2A-C1A-CHA	2.66	128.48	123.87
6	a	801	GS0	CHB-C1B-NB	2.66	128.04	124.05
8	a	813	BCL	C1-C2-C3	-2.66	121.84	126.20
8	I	408[B]	BCL	C2A-C1A-CHA	2.65	128.46	123.87
6	A	801	GS0	C3D-C2D-C1D	-2.64	102.23	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	811	BCL	C4A-NA-C1A	2.63	107.88	106.68
8	A	811	BCL	C4A-NA-C1A	2.63	107.88	106.68
6	a	801	GS0	C3D-C2D-C1D	-2.62	102.25	105.83
8	I	409[B]	BCL	CHC-C1C-NC	-2.62	120.61	124.40
8	a	815	BCL	C4-C3-C5	2.62	119.78	115.23
8	A	810	BCL	C2A-C1A-CHA	2.61	128.40	123.87
8	E	408[B]	BCL	CHC-C1C-NC	-2.61	120.64	124.40
8	J	406	BCL	C3D-C4D-ND	2.60	114.21	109.99
8	E	408[B]	BCL	CMB-C2B-C3B	2.60	133.86	125.67
8	F	409[B]	BCL	CHC-C1C-NC	-2.60	120.65	124.40
8	a	810	BCL	C11-C12-C13	-2.60	107.33	115.97
8	A	810	BCL	C11-C12-C13	-2.60	107.34	115.97
8	F	408[B]	BCL	CHC-C1C-NC	-2.59	120.65	124.40
8	I	408[B]	BCL	CHC-C1C-NC	-2.59	120.65	124.40
8	J	402	BCL	C2A-C1A-CHA	2.59	128.36	123.87
7	A	803	CLA	C3B-C4B-NB	-2.59	108.22	110.53
8	A	811	BCL	C2A-C1A-CHA	2.58	128.35	123.87
8	E	409	BCL	C2A-C1A-CHA	2.58	128.35	123.87
8	A	815	BCL	C4-C3-C5	2.58	119.71	115.23
8	H	408[B]	BCL	CHC-C1C-NC	-2.58	120.67	124.40
8	F	402	BCL	CGD-CBD-CAD	2.58	119.21	110.85
8	E	402	BCL	CGD-CBD-CAD	2.58	119.21	110.85
8	a	811	BCL	C2A-C1A-CHA	2.58	128.35	123.87
8	I	402	BCL	CGD-CBD-CAD	2.58	119.20	110.85
8	I	406	BCL	C3D-C4D-ND	2.58	114.18	109.99
8	H	402	BCL	CGD-CBD-CAD	2.58	119.19	110.85
8	G	405	BCL	C3D-C4D-ND	2.57	114.17	109.99
8	J	405	BCL	C11-C10-C8	-2.57	107.42	115.97
8	F	406	BCL	C3D-C4D-ND	2.57	114.16	109.99
8	I	401	BCL	C1-O2A-CGA	2.57	122.87	116.65
8	E	409	BCL	O2A-CGA-CBA	2.57	119.66	111.83
8	G	404	BCL	C11-C10-C8	-2.56	107.44	115.97
8	H	405	BCL	C11-C10-C8	-2.56	107.44	115.97
8	J	402	BCL	O2A-CGA-CBA	2.56	119.65	111.83
8	E	406	BCL	C3D-C4D-ND	2.56	114.15	109.99
8	E	405	BCL	C11-C10-C8	-2.56	107.45	115.97
8	F	405	BCL	C11-C10-C8	-2.56	107.45	115.97
8	H	406	BCL	C3D-C4D-ND	2.56	114.15	109.99
8	I	405	BCL	C11-C10-C8	-2.56	107.47	115.97
8	H	408[B]	BCL	O2D-CGD-O1D	-2.56	118.87	123.85
8	A	814	BCL	CBA-CAA-C2A	2.56	121.40	113.79
8	a	814	BCL	CBA-CAA-C2A	2.56	121.40	113.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	803	CLA	C3B-C4B-NB	-2.56	108.25	110.53
8	F	401	BCL	C1-O2A-CGA	2.55	122.83	116.65
8	A	809[B]	BCL	C4A-NA-C1A	2.55	107.84	106.68
8	G	401	BCL	C1-O2A-CGA	2.55	122.83	116.65
8	J	401	BCL	C1-O2A-CGA	2.55	122.83	116.65
8	E	401	BCL	C1-O2A-CGA	2.55	122.82	116.65
8	E	408[B]	BCL	O2D-CGD-O1D	-2.55	118.89	123.85
8	A	813	BCL	C2A-C1A-CHA	2.54	128.28	123.87
8	H	401	BCL	C1-O2A-CGA	2.54	122.80	116.65
8	H	408[B]	BCL	C2A-C1A-CHA	2.54	128.27	123.87
8	F	409[B]	BCL	O2D-CGD-O1D	-2.54	118.91	123.85
8	I	409[B]	BCL	C2A-C1A-CHA	2.53	128.26	123.87
8	a	813	BCL	C2A-C1A-CHA	2.53	128.26	123.87
8	a	809[B]	BCL	C4A-NA-C1A	2.53	107.83	106.68
8	F	408[B]	BCL	O2D-CGD-O1D	-2.53	118.93	123.85
8	E	408[B]	BCL	C2A-C1A-CHA	2.52	128.24	123.87
8	H	406	BCL	C4D-C3D-CAD	-2.52	105.37	108.11
8	H	408[B]	BCL	CMB-C2B-C3B	2.51	133.60	125.67
8	I	408[B]	BCL	O2D-CGD-O1D	-2.51	118.97	123.85
8	E	406	BCL	C4D-C3D-CAD	-2.51	105.39	108.11
8	I	409[B]	BCL	O2D-CGD-O1D	-2.50	118.98	123.85
8	F	409[B]	BCL	C2A-C1A-CHA	2.50	128.20	123.87
10	a	817	LHG	O4-P-O5	2.49	124.03	112.44
9	A	816	F39	C19-C20-C27	-2.48	108.61	122.53
8	F	406	BCL	C11-C10-C8	-2.48	107.72	115.97
8	J	406	BCL	C11-C10-C8	-2.48	107.73	115.97
8	I	406	BCL	C11-C10-C8	-2.48	107.73	115.97
8	E	406	BCL	C11-C10-C8	-2.47	107.74	115.97
8	G	405	BCL	C11-C10-C8	-2.47	107.75	115.97
8	F	406	BCL	C4D-C3D-CAD	-2.47	105.42	108.11
6	a	801	GS0	CMA-C3A-C4A	-2.47	105.15	111.77
6	A	801	GS0	CMA-C3A-C4A	-2.46	105.15	111.77
8	H	406	BCL	C11-C10-C8	-2.45	107.81	115.97
6	a	801	GS0	C3C-C2C-C1C	2.45	105.82	101.87
6	A	801	GS0	C3C-C2C-C1C	2.44	105.82	101.87
8	I	406	BCL	C4D-C3D-CAD	-2.44	105.45	108.11
8	I	407	BCL	CMB-C2B-C1B	-2.43	121.72	125.42
8	G	406	BCL	CMB-C2B-C1B	-2.43	121.72	125.42
8	F	407	BCL	CMB-C2B-C1B	-2.43	121.72	125.42
8	J	407	BCL	CMB-C2B-C1B	-2.43	121.72	125.42
6	A	801	GS0	C20-C18-C19	-2.43	99.70	110.53
8	E	407	BCL	CMB-C2B-C1B	-2.42	121.73	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	407	BCL	CMB-C2B-C1B	-2.42	121.73	125.42
8	a	807	BCL	C6-C5-C3	2.42	119.35	113.47
8	A	805	BCL	CMD-C2D-C1D	2.42	128.98	124.73
8	a	804[B]	BCL	C4D-CHA-C1A	2.41	124.12	121.24
7	a	802	CLA	CHB-C4A-NA	2.40	127.87	124.40
8	I	409[B]	BCL	C4D-C3D-CAD	-2.39	105.50	108.11
8	a	811	BCL	C1C-NC-C4C	2.39	107.77	106.68
7	A	802	CLA	CHB-C4A-NA	2.39	127.84	124.40
8	a	804[B]	BCL	CBA-CAA-C2A	-2.38	106.70	113.79
8	F	409[B]	BCL	C4D-C3D-CAD	-2.38	105.52	108.11
8	a	807	BCL	C1-C2-C3	-2.37	122.32	126.20
8	A	807	BCL	C1-C2-C3	-2.36	122.33	126.20
8	J	406	BCL	C16-C15-C13	-2.35	108.14	115.97
8	E	406	BCL	C16-C15-C13	-2.35	108.15	115.97
8	A	810	BCL	C1-O2A-CGA	2.35	122.33	116.65
8	G	405	BCL	C16-C15-C13	-2.35	108.17	115.97
8	H	406	BCL	C16-C15-C13	-2.35	108.17	115.97
8	F	406	BCL	C16-C15-C13	-2.34	108.17	115.97
8	a	810	BCL	C1-O2A-CGA	2.34	122.31	116.65
7	A	803	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
8	I	406	BCL	C16-C15-C13	-2.34	108.20	115.97
8	A	806	BCL	C17-C16-C15	2.33	123.74	113.28
8	F	405	BCL	C2A-C1A-CHA	2.33	127.91	123.87
8	H	408[B]	BCL	CED-O2D-CGD	2.32	121.19	115.92
8	H	405	BCL	C2A-C1A-CHA	2.32	127.90	123.87
8	J	405	BCL	C2A-C1A-CHA	2.32	127.90	123.87
8	A	811	BCL	C1C-NC-C4C	2.32	107.74	106.68
8	E	408[B]	BCL	CED-O2D-CGD	2.32	121.18	115.92
8	I	405	BCL	C2A-C1A-CHA	2.32	127.89	123.87
7	a	803	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
9	a	816	F39	C19-C20-C27	-2.32	109.52	122.53
8	G	404	BCL	C2A-C1A-CHA	2.32	127.89	123.87
8	a	805	BCL	C4D-C3D-CAD	2.32	110.63	108.11
8	F	408[B]	BCL	CED-O2D-CGD	2.32	121.17	115.92
8	A	806	BCL	C1-C2-C3	2.32	129.99	126.20
8	A	815	BCL	CHA-C1A-NA	-2.31	121.15	126.39
8	I	402	BCL	O2D-CGD-O1D	-2.31	119.35	123.85
8	E	405	BCL	C2A-C1A-CHA	2.31	127.87	123.87
8	I	408[B]	BCL	CED-O2D-CGD	2.30	121.14	115.92
8	F	409[B]	BCL	CED-O2D-CGD	2.30	121.13	115.92
8	a	815	BCL	CHA-C1A-NA	-2.30	121.19	126.39
7	A	803	CLA	CHB-C4A-NA	2.29	127.71	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	402	BCL	OBB-CAB-CBB	-2.29	114.64	119.77
8	F	402	BCL	O2D-CGD-O1D	-2.29	119.39	123.85
8	H	408[B]	BCL	CHC-C4B-NB	-2.29	120.61	124.05
7	a	803	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
8	a	805	BCL	C4-C3-C5	2.28	119.19	115.23
6	a	801	GS0	CHD-C1D-ND	-2.28	121.60	124.80
8	F	409[B]	BCL	CHC-C4B-NB	-2.28	120.63	124.05
8	I	409[B]	BCL	CHC-C4B-NB	-2.28	120.63	124.05
8	I	402	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
8	I	409[B]	BCL	CED-O2D-CGD	2.27	121.07	115.92
7	A	803	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
6	a	801	GS0	C20-C18-C19	-2.27	100.40	110.53
8	G	406	BCL	C2A-C1A-CHA	2.27	127.80	123.87
8	E	402	BCL	OBB-CAB-CBB	-2.26	114.70	119.77
8	a	811	BCL	CMD-C2D-C1D	2.26	128.72	124.73
8	H	402	BCL	OBB-CAB-CBB	-2.26	114.70	119.77
8	J	402	BCL	OBB-CAB-CBB	-2.26	114.70	119.77
6	a	801	GS0	CAA-C2A-C1A	-2.26	104.57	111.97
8	E	408[B]	BCL	CHC-C4B-NB	-2.26	120.67	124.05
6	A	801	GS0	CHD-C1D-ND	-2.26	121.63	124.80
8	H	406	BCL	O2D-CGD-O1D	-2.25	119.46	123.85
6	A	801	GS0	CAA-C2A-C1A	-2.25	104.59	111.97
8	E	406	BCL	O2D-CGD-O1D	-2.25	119.46	123.85
8	J	407	BCL	C2A-C1A-CHA	2.25	127.78	123.87
8	E	409	BCL	OBB-CAB-CBB	-2.25	114.72	119.77
8	I	406	BCL	O2D-CGD-O1D	-2.25	119.47	123.85
8	A	810	BCL	C4D-C3D-CAD	-2.24	105.67	108.11
8	F	406	BCL	O2D-CGD-O1D	-2.24	119.49	123.85
7	a	803	CLA	CHB-C4A-NA	2.24	127.63	124.40
8	G	405	BCL	O2D-CGD-O1D	-2.23	119.50	123.85
6	a	801	GS0	C4-C3-C5	-2.23	111.36	115.23
6	A	801	GS0	C4-C3-C5	-2.23	111.36	115.23
8	H	402	BCL	C1C-NC-C4C	2.22	107.69	106.68
8	J	406	BCL	O2D-CGD-O1D	-2.22	119.52	123.85
11	A	819	IKV	C36-C35-C34	2.22	125.56	114.37
8	F	401	BCL	CAA-C2A-C3A	2.21	118.98	113.00
11	a	819	IKV	C36-C35-C34	2.21	125.55	114.37
8	I	401	BCL	CAA-C2A-C3A	2.21	118.97	113.00
8	E	402	BCL	C1C-NC-C4C	2.21	107.69	106.68
8	H	401	BCL	CAA-C2A-C3A	2.21	118.96	113.00
8	J	405	BCL	C1C-NC-C4C	2.20	107.68	106.68
8	J	406	BCL	C2A-C1A-CHA	2.20	127.68	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	406	BCL	CMA-C3A-C2A	-2.20	105.49	113.98
8	J	407	BCL	CMA-C3A-C2A	-2.20	105.49	113.98
8	G	401	BCL	CAA-C2A-C3A	2.20	118.93	113.00
8	H	408[B]	BCL	CAC-C3C-C4C	-2.20	107.71	112.58
8	a	810	BCL	C4D-C3D-CAD	-2.20	105.72	108.11
8	G	405	BCL	C2A-C1A-CHA	2.19	127.67	123.87
8	E	401	BCL	CAA-C2A-C3A	2.19	118.92	113.00
8	E	408[B]	BCL	CAC-C3C-C4C	-2.19	107.72	112.58
8	E	406	BCL	C2A-C1A-CHA	2.19	127.67	123.87
8	J	401	BCL	CAA-C2A-C3A	2.18	118.90	113.00
11	A	819	IKV	C35-C34-C33	2.18	125.40	114.37
8	I	406	BCL	C2A-C1A-CHA	2.18	127.65	123.87
8	A	805	BCL	C3D-C4D-ND	2.18	113.53	109.99
8	H	406	BCL	C2A-C1A-CHA	2.18	127.64	123.87
8	a	806	BCL	C6-C5-C3	-2.18	108.17	113.47
8	F	406	BCL	C2A-C1A-CHA	2.18	127.64	123.87
11	a	819	IKV	C35-C34-C33	2.18	125.36	114.37
8	J	402	BCL	C1C-NC-C4C	2.17	107.67	106.68
8	a	804[B]	BCL	CHC-C4B-NB	-2.17	120.79	124.05
8	A	807	BCL	C6-C5-C3	2.17	118.75	113.47
8	E	409	BCL	C1C-NC-C4C	2.16	107.67	106.68
8	H	407	BCL	CHD-C1D-ND	-2.16	121.76	124.80
8	A	807	BCL	CAA-CBA-CGA	-2.16	107.08	113.21
8	J	407	BCL	CHD-C1D-ND	-2.16	121.77	124.80
8	A	807	BCL	O2A-C1-C2	-2.15	99.82	108.11
8	G	406	BCL	CHD-C1D-ND	-2.15	121.77	124.80
6	a	801	GS0	CMD-C2D-C1D	2.15	128.52	124.73
8	a	807	BCL	O2A-C1-C2	-2.15	99.83	108.11
8	E	407	BCL	CHD-C1D-ND	-2.15	121.78	124.80
8	F	407	BCL	CHD-C1D-ND	-2.15	121.78	124.80
8	F	408[B]	BCL	C4D-C3D-CAD	-2.15	105.78	108.11
8	H	405	BCL	C1C-NC-C4C	2.15	107.66	106.68
8	H	402	BCL	C3D-C4D-ND	2.14	113.47	109.99
8	G	406	BCL	C16-C15-C13	-2.14	108.84	115.97
8	a	807	BCL	CAA-CBA-CGA	-2.14	107.12	113.21
8	G	404	BCL	C1C-NC-C4C	2.14	107.66	106.68
8	I	407	BCL	CHD-C1D-ND	-2.14	121.79	124.80
8	J	407	BCL	C16-C15-C13	-2.14	108.84	115.97
6	A	801	GS0	CMD-C2D-C1D	2.14	128.49	124.73
10	A	817	LHG	O8-C23-C24	2.14	118.35	111.83
8	F	408[B]	BCL	CMB-C2B-C1B	2.14	128.67	125.42
8	E	402	BCL	C3D-C4D-ND	2.13	113.46	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	402	BCL	C3D-C4D-ND	2.13	113.45	109.99
8	I	402	BCL	C3D-C4D-ND	2.13	113.45	109.99
8	I	408[B]	BCL	CMB-C2B-C1B	2.13	128.66	125.42
8	E	407	BCL	C3D-C2D-C1D	-2.13	102.93	105.83
8	E	405	BCL	C1C-NC-C4C	2.12	107.65	106.68
8	A	804[B]	BCL	CHC-C4B-NB	-2.12	120.86	124.05
8	H	407	BCL	C3D-C2D-C1D	-2.12	102.94	105.83
8	E	409	BCL	CBA-CAA-C2A	-2.12	107.49	113.79
8	A	807	BCL	CHC-C1C-NC	-2.11	121.35	124.40
8	G	406	BCL	C3D-C2D-C1D	-2.11	102.95	105.83
8	J	407	BCL	C3D-C2D-C1D	-2.11	102.95	105.83
10	A	818	LHG	O8-C23-C24	2.11	118.26	111.83
8	I	408[B]	BCL	C4D-C3D-CAD	-2.11	105.82	108.11
8	G	402	BCL	C17-C16-C15	2.11	122.72	113.28
8	J	402	BCL	CBA-CAA-C2A	-2.11	107.52	113.79
8	a	804[B]	BCL	C4A-NA-C1A	2.11	107.64	106.68
8	E	409	BCL	C3D-C4D-ND	2.10	113.41	109.99
8	E	403	BCL	C17-C16-C15	2.10	122.70	113.28
8	J	403	BCL	C17-C16-C15	2.10	122.70	113.28
8	H	403	BCL	C17-C16-C15	2.10	122.69	113.28
6	a	801	GS0	C16-C17-C18	-2.10	106.57	115.94
8	a	807	BCL	CHC-C1C-NC	-2.09	121.38	124.40
8	F	403	BCL	C17-C16-C15	2.09	122.66	113.28
8	E	402	BCL	CMB-C2B-C1B	-2.09	122.23	125.42
8	I	403	BCL	C17-C16-C15	2.09	122.65	113.28
8	F	407	BCL	C3D-C2D-C1D	-2.09	102.98	105.83
8	I	407	BCL	C3D-C2D-C1D	-2.09	102.98	105.83
6	a	801	GS0	CMB-C2B-C3B	2.09	132.25	125.67
10	a	817	LHG	O8-C23-C24	2.09	118.20	111.83
8	E	409	BCL	CMB-C2B-C1B	-2.08	122.25	125.42
6	A	801	GS0	CMB-C2B-C3B	2.08	132.24	125.67
7	a	802	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
6	a	801	GS0	C2B-C1B-NB	-2.08	108.17	110.33
8	J	402	BCL	C3D-C4D-ND	2.08	113.36	109.99
8	A	815	BCL	C2A-C1A-CHA	2.08	127.47	123.87
8	F	409[B]	BCL	CBB-CAB-C3B	-2.08	116.02	120.40
8	F	402	BCL	CMB-C2B-C1B	-2.08	122.26	125.42
7	A	803	CLA	O2D-CGD-CBD	2.07	114.86	111.23
8	F	402	BCL	C1C-NC-C4C	2.07	107.62	106.68
9	a	816	F39	O1-C11-C9	2.07	114.63	110.37
8	J	407	BCL	O1D-CGD-CBD	2.07	128.60	124.52
8	I	402	BCL	CMB-C2B-C1B	-2.07	122.26	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	802	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
7	a	803	CLA	O2D-CGD-CBD	2.07	114.85	111.23
8	J	402	BCL	CMB-C2B-C1B	-2.07	122.27	125.42
8	I	409[B]	BCL	CBB-CAB-C3B	-2.07	116.05	120.40
8	H	402	BCL	CMB-C2B-C1B	-2.06	122.28	125.42
8	H	407	BCL	C2D-C1D-ND	2.06	112.16	110.13
8	G	406	BCL	O1D-CGD-CBD	2.06	128.57	124.52
8	F	405	BCL	C1C-NC-C4C	2.05	107.61	106.68
8	a	815	BCL	C2A-C1A-CHA	2.05	127.42	123.87
8	A	804[B]	BCL	O2A-CGA-CBA	2.05	120.47	114.00
8	A	807	BCL	C4D-C3D-CAD	-2.05	105.88	108.11
6	A	801	GS0	C2B-C1B-NB	-2.04	108.21	110.33
8	J	401	BCL	C4-C3-C5	2.04	118.78	115.23
8	G	401	BCL	C4-C3-C5	2.04	118.77	115.23
8	a	804[B]	BCL	CAA-C2A-C3A	2.04	118.51	113.00
7	A	803	CLA	CMB-C2B-C3B	2.04	131.34	126.55
8	E	401	BCL	C4-C3-C5	2.04	118.76	115.23
8	F	401	BCL	C4D-C3D-CAD	-2.03	105.90	108.11
8	E	407	BCL	C2D-C1D-ND	2.03	112.14	110.13
8	F	401	BCL	C4-C3-C5	2.03	118.75	115.23
8	H	401	BCL	C4-C3-C5	2.03	118.75	115.23
8	H	408[B]	BCL	C3B-C4B-NB	2.03	112.44	109.76
8	I	409[B]	BCL	C3B-C4B-NB	2.03	112.43	109.76
8	A	805	BCL	CHC-C4B-NB	-2.03	121.01	124.05
8	A	812	BCL	C3B-C4B-NB	2.02	112.43	109.76
7	A	803	CLA	C1-C2-C3	-2.02	122.88	126.20
8	G	405	BCL	C17-C16-C15	2.02	122.33	113.28
8	F	409[B]	BCL	C3B-C4B-NB	2.02	112.42	109.76
7	a	803	CLA	C1-C2-C3	-2.02	122.89	126.20
8	H	406	BCL	C17-C16-C15	2.02	122.32	113.28
8	J	401	BCL	C4-C3-C2	-2.02	118.45	123.63
8	I	401	BCL	C4-C3-C5	2.02	118.73	115.23
8	A	810	BCL	C6-C5-C3	2.02	118.38	113.47
8	J	406	BCL	C17-C16-C15	2.02	122.31	113.28
8	E	406	BCL	C17-C16-C15	2.01	122.31	113.28
8	a	805	BCL	CHC-C4B-NB	-2.01	121.03	124.05
7	a	803	CLA	CMB-C2B-C3B	2.01	131.28	126.55
8	a	807	BCL	C4D-C3D-CAD	-2.01	105.92	108.11
8	G	406	BCL	C2D-C1D-ND	2.01	112.11	110.13
8	I	407	BCL	C2D-C1D-ND	2.01	112.11	110.13
8	G	401	BCL	C4D-C3D-CAD	-2.01	105.93	108.11
8	J	401	BCL	C4D-C3D-CAD	-2.01	105.93	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	407	BCL	C2D-C1D-ND	2.01	112.11	110.13
8	I	408[B]	BCL	O1D-CGD-CBD	-2.01	120.56	124.52
8	G	401	BCL	C4-C3-C2	-2.00	118.48	123.63
9	A	816	F39	C13-O2-C11	-2.00	115.68	119.78
8	I	401	BCL	C4-C3-C2	-2.00	118.48	123.63
8	a	807	BCL	O2A-CGA-O1A	2.00	128.64	123.63

There are no chirality outliers.

All (1046) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	GS0	CHA-CBD-CGD-O2D
6	a	801	GS0	CHA-CBD-CGD-O2D
7	A	802	CLA	CAD-CBD-CGD-O1D
7	A	802	CLA	CAD-CBD-CGD-O2D
7	A	802	CLA	CBD-CGD-O2D-CED
7	A	803	CLA	C1A-C2A-CAA-CBA
7	A	803	CLA	C3A-C2A-CAA-CBA
7	A	803	CLA	CBA-CGA-O2A-C1
7	A	803	CLA	O1A-CGA-O2A-C1
7	a	802	CLA	CAD-CBD-CGD-O1D
7	a	802	CLA	CAD-CBD-CGD-O2D
7	a	802	CLA	CBD-CGD-O2D-CED
7	a	803	CLA	C1A-C2A-CAA-CBA
7	a	803	CLA	C3A-C2A-CAA-CBA
7	a	803	CLA	CBA-CGA-O2A-C1
7	a	803	CLA	O1A-CGA-O2A-C1
8	A	804[B]	BCL	C1A-C2A-CAA-CBA
8	A	804[B]	BCL	C3A-C2A-CAA-CBA
8	A	805	BCL	C2B-C3B-CAB-OB
8	A	805	BCL	C2B-C3B-CAB-CB
8	A	805	BCL	C4B-C3B-CAB-OB
8	A	805	BCL	C4B-C3B-CAB-CB
8	A	805	BCL	C2C-C3C-CAC-CB
8	A	805	BCL	C4C-C3C-CAC-CB
8	A	805	BCL	CHA-CBD-CGD-O1D
8	A	805	BCL	CHA-CBD-CGD-O2D
8	A	808	BCL	C1A-C2A-CAA-CBA
8	A	810	BCL	C2-C3-C5-C6
8	A	810	BCL	C4-C3-C5-C6
8	A	811	BCL	C1A-C2A-CAA-CBA
8	A	811	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	811	BCL	C4B-C3B-CAB-CBB
8	A	812	BCL	C3A-C2A-CAA-CBA
8	A	813	BCL	C2B-C3B-CAB-OB
8	A	813	BCL	C2B-C3B-CAB-CBB
8	A	813	BCL	C4B-C3B-CAB-OB
8	A	813	BCL	C4B-C3B-CAB-CBB
8	A	814	BCL	C4C-C3C-CAC-CBC
8	A	815	BCL	C2B-C3B-CAB-OB
8	A	815	BCL	C2B-C3B-CAB-CBB
8	A	815	BCL	C4B-C3B-CAB-OB
8	A	815	BCL	C4B-C3B-CAB-CBB
8	E	401	BCL	C1A-C2A-CAA-CBA
8	E	401	BCL	C3A-C2A-CAA-CBA
8	E	403	BCL	C4B-C3B-CAB-CBB
8	E	403	BCL	C2C-C3C-CAC-CBC
8	E	403	BCL	C4C-C3C-CAC-CBC
8	E	405	BCL	C2B-C3B-CAB-OB
8	E	405	BCL	C2B-C3B-CAB-CBB
8	E	405	BCL	C4B-C3B-CAB-OB
8	E	405	BCL	C4B-C3B-CAB-CBB
8	E	405	BCL	CHA-CBD-CGD-O1D
8	E	405	BCL	CHA-CBD-CGD-O2D
8	E	407	BCL	CHA-CBD-CGD-O1D
8	E	407	BCL	CHA-CBD-CGD-O2D
8	E	408[B]	BCL	CHA-CBD-CGD-O1D
8	E	408[B]	BCL	CHA-CBD-CGD-O2D
8	F	401	BCL	C1A-C2A-CAA-CBA
8	F	401	BCL	C3A-C2A-CAA-CBA
8	F	402	BCL	CBD-CGD-O2D-CED
8	F	403	BCL	C4B-C3B-CAB-CBB
8	F	403	BCL	C2C-C3C-CAC-CBC
8	F	403	BCL	C4C-C3C-CAC-CBC
8	F	405	BCL	C2B-C3B-CAB-OB
8	F	405	BCL	C2B-C3B-CAB-CBB
8	F	405	BCL	C4B-C3B-CAB-OB
8	F	405	BCL	C4B-C3B-CAB-CBB
8	F	405	BCL	CHA-CBD-CGD-O1D
8	F	405	BCL	CHA-CBD-CGD-O2D
8	F	407	BCL	CHA-CBD-CGD-O1D
8	F	407	BCL	CHA-CBD-CGD-O2D
8	F	408[B]	BCL	CHA-CBD-CGD-O1D
8	F	408[B]	BCL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	F	409[B]	BCL	C2C-C3C-CAC-CBC
8	F	409[B]	BCL	C4C-C3C-CAC-CBC
8	F	409[B]	BCL	CHA-CBD-CGD-O1D
8	F	409[B]	BCL	CHA-CBD-CGD-O2D
8	G	401	BCL	C1A-C2A-CAA-CBA
8	G	401	BCL	C3A-C2A-CAA-CBA
8	G	402	BCL	C4B-C3B-CAB-CBB
8	G	402	BCL	C2C-C3C-CAC-CBC
8	G	402	BCL	C4C-C3C-CAC-CBC
8	G	404	BCL	C2B-C3B-CAB-OB
8	G	404	BCL	C2B-C3B-CAB-CBB
8	G	404	BCL	C4B-C3B-CAB-OB
8	G	404	BCL	C4B-C3B-CAB-CBB
8	G	404	BCL	CHA-CBD-CGD-O1D
8	G	404	BCL	CHA-CBD-CGD-O2D
8	G	406	BCL	CHA-CBD-CGD-O1D
8	G	406	BCL	CHA-CBD-CGD-O2D
8	H	401	BCL	C1A-C2A-CAA-CBA
8	H	401	BCL	C3A-C2A-CAA-CBA
8	H	403	BCL	C4B-C3B-CAB-CBB
8	H	403	BCL	C2C-C3C-CAC-CBC
8	H	403	BCL	C4C-C3C-CAC-CBC
8	H	405	BCL	C2B-C3B-CAB-OB
8	H	405	BCL	C2B-C3B-CAB-CBB
8	H	405	BCL	C4B-C3B-CAB-OB
8	H	405	BCL	C4B-C3B-CAB-CBB
8	H	405	BCL	CHA-CBD-CGD-O1D
8	H	405	BCL	CHA-CBD-CGD-O2D
8	H	407	BCL	CHA-CBD-CGD-O1D
8	H	407	BCL	CHA-CBD-CGD-O2D
8	H	408[B]	BCL	CHA-CBD-CGD-O1D
8	H	408[B]	BCL	CHA-CBD-CGD-O2D
8	I	401	BCL	C1A-C2A-CAA-CBA
8	I	401	BCL	C3A-C2A-CAA-CBA
8	I	402	BCL	CBD-CGD-O2D-CED
8	I	403	BCL	C4B-C3B-CAB-CBB
8	I	403	BCL	C2C-C3C-CAC-CBC
8	I	403	BCL	C4C-C3C-CAC-CBC
8	I	405	BCL	C2B-C3B-CAB-OB
8	I	405	BCL	C2B-C3B-CAB-CBB
8	I	405	BCL	C4B-C3B-CAB-OB
8	I	405	BCL	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	I	405	BCL	CHA-CBD-CGD-O1D
8	I	405	BCL	CHA-CBD-CGD-O2D
8	I	407	BCL	CHA-CBD-CGD-O1D
8	I	407	BCL	CHA-CBD-CGD-O2D
8	I	408[B]	BCL	CHA-CBD-CGD-O1D
8	I	408[B]	BCL	CHA-CBD-CGD-O2D
8	I	409[B]	BCL	C2C-C3C-CAC-CBC
8	I	409[B]	BCL	C4C-C3C-CAC-CBC
8	I	409[B]	BCL	CHA-CBD-CGD-O1D
8	I	409[B]	BCL	CHA-CBD-CGD-O2D
8	J	401	BCL	C1A-C2A-CAA-CBA
8	J	401	BCL	C3A-C2A-CAA-CBA
8	J	403	BCL	C4B-C3B-CAB-CBB
8	J	403	BCL	C2C-C3C-CAC-CBC
8	J	403	BCL	C4C-C3C-CAC-CBC
8	J	405	BCL	C2B-C3B-CAB-OB
8	J	405	BCL	C2B-C3B-CAB-CBB
8	J	405	BCL	C4B-C3B-CAB-OB
8	J	405	BCL	C4B-C3B-CAB-CBB
8	J	405	BCL	CHA-CBD-CGD-O1D
8	J	405	BCL	CHA-CBD-CGD-O2D
8	J	407	BCL	CHA-CBD-CGD-O1D
8	J	407	BCL	CHA-CBD-CGD-O2D
8	a	804[B]	BCL	C4C-C3C-CAC-CBC
8	a	805	BCL	C2B-C3B-CAB-OB
8	a	805	BCL	C2B-C3B-CAB-CBB
8	a	805	BCL	C4B-C3B-CAB-OB
8	a	805	BCL	C4B-C3B-CAB-CBB
8	a	805	BCL	C2C-C3C-CAC-CBC
8	a	805	BCL	C4C-C3C-CAC-CBC
8	a	805	BCL	CHA-CBD-CGD-O1D
8	a	805	BCL	CHA-CBD-CGD-O2D
8	a	808	BCL	C1A-C2A-CAA-CBA
8	a	810	BCL	C2-C3-C5-C6
8	a	810	BCL	C4-C3-C5-C6
8	a	811	BCL	C1A-C2A-CAA-CBA
8	a	811	BCL	C3A-C2A-CAA-CBA
8	a	811	BCL	C4B-C3B-CAB-CBB
8	a	812	BCL	C3A-C2A-CAA-CBA
8	a	813	BCL	C2B-C3B-CAB-OB
8	a	813	BCL	C2B-C3B-CAB-CBB
8	a	813	BCL	C4B-C3B-CAB-OB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	a	813	BCL	C4B-C3B-CAB-CBB
8	a	814	BCL	C4C-C3C-CAC-CBC
8	a	815	BCL	C2B-C3B-CAB-OB
8	a	815	BCL	C2B-C3B-CAB-CBB
8	a	815	BCL	C4B-C3B-CAB-OB
8	a	815	BCL	C4B-C3B-CAB-CBB
9	A	816	F39	C13-C14-C18-C19
9	A	816	F39	C19-C20-C27-C32
9	A	816	F39	C25-C20-C27-C32
9	A	816	F39	C22-C21-O6-C15
9	A	816	F39	O7-C21-O6-C15
9	A	816	F39	C27-C32-C35-C37
9	A	816	F39	C32-C35-C37-C38
9	A	816	F39	C32-C35-C37-C39
9	A	816	F39	C40-C41-C42-C43
9	A	816	F39	C43-C42-C44-C51
9	A	816	F39	C44-C51-C57-C59
9	A	816	F39	C60-C58-C61-C63
9	A	816	F39	C57-C59-C62-C65
9	a	816	F39	C16-C13-C14-C18
9	a	816	F39	C17-C13-C14-C18
9	a	816	F39	C19-C20-C27-C32
9	a	816	F39	C25-C20-C27-C32
9	a	816	F39	C22-C21-O6-C15
9	a	816	F39	O7-C21-O6-C15
9	a	816	F39	C27-C32-C35-C37
9	a	816	F39	C38-C37-C39-C40
9	a	816	F39	C39-C40-C41-C42
9	a	816	F39	C40-C41-C42-C43
9	a	816	F39	C43-C42-C44-C51
9	a	816	F39	C44-C51-C57-C59
9	a	816	F39	C46-C53-C56-C58
9	a	816	F39	C53-C56-C58-C61
9	a	816	F39	C56-C58-C61-C63
9	a	816	F39	C60-C58-C61-C63
9	a	816	F39	C57-C59-C62-C65
9	a	816	F39	C61-C63-C64-C62
10	A	817	LHG	C4-O6-P-O3
10	A	818	LHG	C3-O3-P-O6
10	a	817	LHG	O2-C2-C3-O3
10	a	817	LHG	C3-O3-P-O4
10	a	817	LHG	C3-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	a	817	LHG	C4-O6-P-O3
10	a	817	LHG	C4-O6-P-O4
10	a	817	LHG	C4-O6-P-O5
10	a	818	LHG	C1-C2-C3-O3
10	a	818	LHG	C3-O3-P-O5
10	a	818	LHG	C4-O6-P-O3
10	a	818	LHG	C4-O6-P-O5
10	a	818	LHG	C8-C7-O7-C5
8	F	402	BCL	O1D-CGD-O2D-CED
8	I	402	BCL	O1D-CGD-O2D-CED
7	A	802	CLA	O1D-CGD-O2D-CED
7	a	802	CLA	O1D-CGD-O2D-CED
8	E	401	BCL	C8-C10-C11-C12
8	F	401	BCL	C8-C10-C11-C12
8	G	401	BCL	C8-C10-C11-C12
8	H	401	BCL	C8-C10-C11-C12
8	I	401	BCL	C8-C10-C11-C12
8	J	401	BCL	C8-C10-C11-C12
10	A	818	LHG	O9-C7-O7-C5
10	a	818	LHG	O9-C7-O7-C5
8	A	815	BCL	C3-C5-C6-C7
8	E	409	BCL	C3-C5-C6-C7
8	J	402	BCL	C3-C5-C6-C7
8	a	805	BCL	C3-C5-C6-C7
8	a	811	BCL	C3-C5-C6-C7
8	a	815	BCL	C3-C5-C6-C7
8	E	409	BCL	CBD-CGD-O2D-CED
8	J	402	BCL	CBD-CGD-O2D-CED
10	A	818	LHG	C8-C7-O7-C5
7	A	803	CLA	C4-C3-C5-C6
7	a	803	CLA	C4-C3-C5-C6
8	A	808	BCL	C4-C3-C5-C6
8	E	405	BCL	C4-C3-C5-C6
8	F	405	BCL	C4-C3-C5-C6
8	G	404	BCL	C4-C3-C5-C6
8	H	405	BCL	C4-C3-C5-C6
8	I	405	BCL	C4-C3-C5-C6
8	J	405	BCL	C4-C3-C5-C6
8	a	808	BCL	C4-C3-C5-C6
7	A	803	CLA	C2-C3-C5-C6
7	a	803	CLA	C2-C3-C5-C6
8	A	808	BCL	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	E	405	BCL	C2-C3-C5-C6
8	F	405	BCL	C2-C3-C5-C6
8	G	404	BCL	C2-C3-C5-C6
8	H	405	BCL	C2-C3-C5-C6
8	I	405	BCL	C2-C3-C5-C6
8	J	405	BCL	C2-C3-C5-C6
8	a	808	BCL	C2-C3-C5-C6
8	E	407	BCL	C3-C5-C6-C7
8	F	407	BCL	C3-C5-C6-C7
8	H	407	BCL	C3-C5-C6-C7
8	I	407	BCL	C3-C5-C6-C7
9	A	816	F39	C58-C61-C63-C64
9	a	816	F39	C51-C57-C59-C62
8	E	401	BCL	CBA-CGA-O2A-C1
8	F	401	BCL	CBA-CGA-O2A-C1
8	G	401	BCL	CBA-CGA-O2A-C1
8	H	401	BCL	CBA-CGA-O2A-C1
8	I	401	BCL	CBA-CGA-O2A-C1
8	J	401	BCL	CBA-CGA-O2A-C1
11	A	819	IKV	C23-C24-C25-O5
8	F	401	BCL	O1A-CGA-O2A-C1
8	J	401	BCL	O1A-CGA-O2A-C1
11	a	819	IKV	C23-C24-C25-O5
10	a	817	LHG	C34-C35-C36-C37
8	a	805	BCL	C4-C3-C5-C6
8	a	805	BCL	C2-C3-C5-C6
9	a	816	F39	C18-C19-C20-C27
8	E	401	BCL	O1A-CGA-O2A-C1
8	G	401	BCL	O1A-CGA-O2A-C1
8	H	401	BCL	O1A-CGA-O2A-C1
8	I	401	BCL	O1A-CGA-O2A-C1
11	A	819	IKV	O4-C24-C25-O5
11	a	819	IKV	O4-C24-C25-O5
10	a	817	LHG	C18-C19-C20-C21
7	A	803	CLA	CBD-CGD-O2D-CED
7	a	803	CLA	CBD-CGD-O2D-CED
10	a	818	LHG	C34-C35-C36-C37
10	a	817	LHG	C24-C25-C26-C27
10	A	817	LHG	C32-C33-C34-C35
11	a	819	IKV	C12-C13-C14-C15
7	A	802	CLA	C15-C16-C17-C18
7	a	802	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	816	F39	C14-C18-C19-C20
7	A	802	CLA	C14-C13-C15-C16
7	a	802	CLA	C14-C13-C15-C16
8	A	805	BCL	C14-C13-C15-C16
8	A	807	BCL	C6-C7-C8-C9
8	A	814	BCL	C6-C7-C8-C9
8	A	814	BCL	C14-C13-C15-C16
8	E	407	BCL	C6-C7-C8-C9
8	F	407	BCL	C6-C7-C8-C9
8	H	407	BCL	C6-C7-C8-C9
8	I	407	BCL	C6-C7-C8-C9
8	a	805	BCL	C11-C10-C8-C9
8	a	806	BCL	C14-C13-C15-C16
8	a	807	BCL	C6-C7-C8-C9
10	A	817	LHG	C24-C25-C26-C27
8	E	409	BCL	O1D-CGD-O2D-CED
8	J	402	BCL	O1D-CGD-O2D-CED
10	a	818	LHG	O2-C2-C3-O3
9	A	816	F39	C53-C56-C58-C60
9	A	816	F39	C65-C62-C64-C63
9	a	816	F39	C32-C35-C37-C38
9	a	816	F39	C59-C62-C64-C63
11	A	819	IKV	O2-C17-C18-O9
11	a	819	IKV	O2-C17-C18-O9
8	E	409	BCL	CBA-CGA-O2A-C1
8	J	402	BCL	CBA-CGA-O2A-C1
10	A	818	LHG	C7-C8-C9-C10
10	a	818	LHG	C23-C24-C25-C26
8	A	812	BCL	C2-C1-O2A-CGA
8	A	814	BCL	C2-C1-O2A-CGA
8	a	812	BCL	C2-C1-O2A-CGA
8	a	814	BCL	C2-C1-O2A-CGA
8	A	814	BCL	C11-C10-C8-C7
8	A	815	BCL	C6-C7-C8-C10
8	a	815	BCL	C6-C7-C8-C10
9	A	816	F39	C21-C22-C23-C24
9	a	816	F39	C58-C61-C63-C64
6	A	801	GS0	C10-C11-C12-C13
10	a	818	LHG	C7-C8-C9-C10
8	E	409	BCL	O1A-CGA-O2A-C1
8	J	402	BCL	O1A-CGA-O2A-C1
8	a	806	BCL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	804[B]	BCL	C2A-CAA-CBA-CGA
8	E	408[B]	BCL	C2A-CAA-CBA-CGA
8	F	408[B]	BCL	C2A-CAA-CBA-CGA
8	F	409[B]	BCL	C2A-CAA-CBA-CGA
8	H	408[B]	BCL	C2A-CAA-CBA-CGA
8	I	408[B]	BCL	C2A-CAA-CBA-CGA
8	I	409[B]	BCL	C2A-CAA-CBA-CGA
8	E	409	BCL	C15-C16-C17-C18
8	a	814	BCL	C10-C11-C12-C13
11	A	819	IKV	C13-C14-C15-C16
11	A	819	IKV	C34-C35-C36-C37
11	a	819	IKV	C34-C35-C36-C37
8	J	402	BCL	C15-C16-C17-C18
8	a	814	BCL	C8-C10-C11-C12
8	a	814	BCL	C13-C15-C16-C17
8	E	407	BCL	C13-C15-C16-C17
8	F	407	BCL	C13-C15-C16-C17
8	H	407	BCL	C13-C15-C16-C17
8	I	407	BCL	C13-C15-C16-C17
9	a	816	F39	C42-C44-C51-C57
10	A	818	LHG	C24-C23-O8-C6
8	G	406	BCL	C15-C16-C17-C18
8	J	407	BCL	C15-C16-C17-C18
11	a	819	IKV	C1-C2-C3-C4
7	A	803	CLA	C10-C11-C12-C13
7	a	803	CLA	C10-C11-C12-C13
8	E	403	BCL	C10-C11-C12-C13
8	F	403	BCL	C10-C11-C12-C13
8	G	402	BCL	C10-C11-C12-C13
8	H	403	BCL	C10-C11-C12-C13
8	I	403	BCL	C10-C11-C12-C13
8	J	403	BCL	C10-C11-C12-C13
8	A	805	BCL	C15-C16-C17-C18
8	A	806	BCL	C15-C16-C17-C18
8	E	402	BCL	C13-C15-C16-C17
8	F	402	BCL	C13-C15-C16-C17
8	H	402	BCL	C13-C15-C16-C17
8	I	402	BCL	C13-C15-C16-C17
8	A	807	BCL	C4B-C3B-CAB-OBB
8	A	811	BCL	C4B-C3B-CAB-OBB
8	E	403	BCL	C4B-C3B-CAB-OBB
8	F	403	BCL	C4B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	G	402	BCL	C4B-C3B-CAB-OBB
8	H	403	BCL	C4B-C3B-CAB-OBB
8	I	403	BCL	C4B-C3B-CAB-OBB
8	J	403	BCL	C4B-C3B-CAB-OBB
8	a	807	BCL	C4B-C3B-CAB-OBB
8	a	811	BCL	C4B-C3B-CAB-OBB
8	G	406	BCL	C6-C7-C8-C9
8	J	407	BCL	C6-C7-C8-C9
10	a	817	LHG	C15-C16-C17-C18
9	A	816	F39	C38-C37-C39-C40
9	a	816	F39	C53-C56-C58-C60
7	A	802	CLA	C2A-CAA-CBA-CGA
7	a	802	CLA	C2A-CAA-CBA-CGA
8	E	409	BCL	C2A-CAA-CBA-CGA
8	J	402	BCL	C2A-CAA-CBA-CGA
10	A	817	LHG	O1-C1-C2-C3
8	A	811	BCL	C2B-C3B-CAB-CBB
8	E	403	BCL	C2B-C3B-CAB-OBB
8	E	403	BCL	C2B-C3B-CAB-CBB
8	F	403	BCL	C2B-C3B-CAB-OBB
8	F	403	BCL	C2B-C3B-CAB-CBB
8	G	402	BCL	C2B-C3B-CAB-OBB
8	G	402	BCL	C2B-C3B-CAB-CBB
8	H	403	BCL	C2B-C3B-CAB-OBB
8	H	403	BCL	C2B-C3B-CAB-CBB
8	I	403	BCL	C2B-C3B-CAB-OBB
8	I	403	BCL	C2B-C3B-CAB-CBB
8	J	403	BCL	C2B-C3B-CAB-OBB
8	J	403	BCL	C2B-C3B-CAB-CBB
8	a	811	BCL	C2B-C3B-CAB-CBB
8	E	402	BCL	C15-C16-C17-C18
8	F	402	BCL	C15-C16-C17-C18
8	H	402	BCL	C15-C16-C17-C18
8	I	402	BCL	C15-C16-C17-C18
9	A	816	F39	C35-C37-C39-C40
9	A	816	F39	C57-C59-C62-C64
9	a	816	F39	C57-C59-C62-C64
8	E	406	BCL	C10-C11-C12-C13
8	F	406	BCL	C10-C11-C12-C13
8	G	405	BCL	C10-C11-C12-C13
8	H	406	BCL	C10-C11-C12-C13
8	I	406	BCL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	J	406	BCL	C10-C11-C12-C13
8	A	806	BCL	C16-C17-C18-C19
8	G	406	BCL	C16-C17-C18-C19
8	J	407	BCL	C16-C17-C18-C19
10	A	818	LHG	O10-C23-O8-C6
10	A	818	LHG	C10-C11-C12-C13
10	a	817	LHG	C26-C27-C28-C29
9	a	816	F39	C24-C26-C28-C29
10	a	818	LHG	C28-C29-C30-C31
10	A	817	LHG	C26-C27-C28-C29
10	A	818	LHG	C25-C26-C27-C28
11	a	819	IKV	C4-C5-C6-C7
10	a	817	LHG	C9-C10-C11-C12
10	A	818	LHG	C14-C15-C16-C17
10	a	817	LHG	C10-C11-C12-C13
8	a	814	BCL	C16-C17-C18-C19
8	A	812	BCL	C2A-CAA-CBA-CGA
8	E	401	BCL	C2A-CAA-CBA-CGA
8	E	402	BCL	C2A-CAA-CBA-CGA
8	F	401	BCL	C2A-CAA-CBA-CGA
8	F	402	BCL	C2A-CAA-CBA-CGA
8	G	401	BCL	C2A-CAA-CBA-CGA
8	H	401	BCL	C2A-CAA-CBA-CGA
8	H	402	BCL	C2A-CAA-CBA-CGA
8	I	401	BCL	C2A-CAA-CBA-CGA
8	I	402	BCL	C2A-CAA-CBA-CGA
8	J	401	BCL	C2A-CAA-CBA-CGA
8	a	812	BCL	C2A-CAA-CBA-CGA
8	A	805	BCL	C8-C10-C11-C12
9	a	816	F39	C22-C23-C24-C26
10	a	817	LHG	C13-C14-C15-C16
10	a	817	LHG	C7-C8-C9-C10
8	A	814	BCL	C13-C15-C16-C17
10	A	817	LHG	C16-C17-C18-C19
11	a	819	IKV	C2-C3-C4-C5
8	a	804[B]	BCL	C3A-C2A-CAA-CBA
8	a	811	BCL	C5-C6-C7-C8
10	A	818	LHG	C26-C27-C28-C29
8	a	814	BCL	C16-C17-C18-C20
8	E	402	BCL	C5-C6-C7-C8
8	F	402	BCL	C5-C6-C7-C8
8	H	402	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	I	402	BCL	C5-C6-C7-C8
9	A	816	F39	C22-C23-C24-C26
8	E	402	BCL	CBA-CGA-O2A-C1
8	E	407	BCL	CBA-CGA-O2A-C1
8	F	402	BCL	CBA-CGA-O2A-C1
8	F	407	BCL	CBA-CGA-O2A-C1
8	H	402	BCL	CBA-CGA-O2A-C1
8	H	407	BCL	CBA-CGA-O2A-C1
8	I	402	BCL	CBA-CGA-O2A-C1
8	I	407	BCL	CBA-CGA-O2A-C1
7	A	802	CLA	C3-C5-C6-C7
7	a	802	CLA	C3-C5-C6-C7
11	a	819	IKV	C13-C14-C15-C16
9	A	816	F39	C29-C30-C31-C33
11	A	819	IKV	C32-C33-C34-C35
11	a	819	IKV	C3-C4-C5-C6
11	a	819	IKV	C11-C10-C9-C8
11	a	819	IKV	C10-C11-C12-C13
11	a	819	IKV	C32-C33-C34-C35
6	A	801	GS0	O1A-CGA-O2A-C1
6	a	801	GS0	O1A-CGA-O2A-C1
11	A	819	IKV	C6-C7-C8-C9
11	A	819	IKV	C31-C32-C33-C34
11	a	819	IKV	C31-C32-C33-C34
9	a	816	F39	C28-C29-C30-C31
10	A	817	LHG	C17-C18-C19-C20
10	a	817	LHG	C25-C26-C27-C28
10	a	818	LHG	C14-C15-C16-C17
8	G	406	BCL	C16-C17-C18-C20
8	J	407	BCL	C16-C17-C18-C20
10	a	818	LHG	C18-C19-C20-C21
11	A	819	IKV	C9-C10-C11-C12
11	A	819	IKV	C10-C11-C12-C13
10	a	818	LHG	C19-C20-C21-C22
10	a	818	LHG	C13-C14-C15-C16
8	A	807	BCL	C2A-CAA-CBA-CGA
8	a	807	BCL	C2A-CAA-CBA-CGA
9	A	816	F39	C28-C29-C30-C31
9	A	816	F39	C39-C40-C41-C42
8	A	806	BCL	C16-C17-C18-C20
10	A	817	LHG	C33-C34-C35-C36
10	a	818	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	E	409	BCL	C6-C7-C8-C9
8	J	402	BCL	C6-C7-C8-C9
9	a	816	F39	C26-C28-C29-C30
10	A	817	LHG	C34-C35-C36-C37
10	A	818	LHG	C32-C33-C34-C35
10	A	818	LHG	C5-C6-O8-C23
11	A	819	IKV	C21-C20-O3-C19
10	A	817	LHG	C18-C19-C20-C21
10	a	818	LHG	C24-C25-C26-C27
11	a	819	IKV	C29-C30-C31-C32
9	A	816	F39	C20-C27-C32-C35
8	A	805	BCL	C16-C17-C18-C19
11	A	819	IKV	C29-C30-C31-C32
8	H	407	BCL	O1A-CGA-O2A-C1
9	a	816	F39	C31-C33-C34-C36
10	a	817	LHG	C27-C28-C29-C30
8	E	407	BCL	O1A-CGA-O2A-C1
8	E	402	BCL	O1A-CGA-O2A-C1
8	F	402	BCL	O1A-CGA-O2A-C1
8	F	407	BCL	O1A-CGA-O2A-C1
8	H	402	BCL	O1A-CGA-O2A-C1
8	I	402	BCL	O1A-CGA-O2A-C1
8	I	407	BCL	O1A-CGA-O2A-C1
8	a	806	BCL	C10-C11-C12-C13
10	a	817	LHG	C14-C15-C16-C17
7	A	803	CLA	C3-C5-C6-C7
7	a	803	CLA	C3-C5-C6-C7
11	A	819	IKV	C11-C12-C13-C14
7	A	803	CLA	O1D-CGD-O2D-CED
7	a	803	CLA	O1D-CGD-O2D-CED
8	E	409	BCL	C2-C3-C5-C6
8	J	402	BCL	C2-C3-C5-C6
9	A	816	F39	C31-C33-C34-C36
8	A	811	BCL	C2A-CAA-CBA-CGA
8	a	811	BCL	C2A-CAA-CBA-CGA
10	a	817	LHG	O1-C1-C2-O2
10	a	818	LHG	O10-C23-O8-C6
8	A	812	BCL	C1A-C2A-CAA-CBA
8	a	804[B]	BCL	C1A-C2A-CAA-CBA
8	a	812	BCL	C1A-C2A-CAA-CBA
8	E	402	BCL	C3-C5-C6-C7
8	F	402	BCL	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	H	402	BCL	C3-C5-C6-C7
8	I	402	BCL	C3-C5-C6-C7
7	A	802	CLA	C6-C7-C8-C10
7	a	802	CLA	C6-C7-C8-C10
8	a	805	BCL	C11-C10-C8-C7
8	a	805	BCL	C11-C12-C13-C15
8	a	806	BCL	C11-C12-C13-C15
8	A	807	BCL	C2C-C3C-CAC-CBC
8	A	814	BCL	C2C-C3C-CAC-CBC
8	a	804[B]	BCL	C2C-C3C-CAC-CBC
8	a	814	BCL	C2C-C3C-CAC-CBC
8	A	810	BCL	C10-C11-C12-C13
8	a	810	BCL	C10-C11-C12-C13
10	A	817	LHG	C7-C8-C9-C10
10	A	818	LHG	C23-C24-C25-C26
8	G	406	BCL	C2-C3-C5-C6
8	J	407	BCL	C2-C3-C5-C6
8	A	807	BCL	C4B-C3B-CAB-CBB
8	a	807	BCL	C4B-C3B-CAB-CBB
8	a	804[B]	BCL	C2A-CAA-CBA-CGA
8	E	409	BCL	C11-C12-C13-C14
8	G	406	BCL	C11-C10-C8-C9
8	J	402	BCL	C11-C12-C13-C14
8	J	407	BCL	C11-C10-C8-C9
8	a	811	BCL	C6-C7-C8-C9
11	a	819	IKV	C21-C20-O3-C19
10	a	818	LHG	C12-C13-C14-C15
10	a	818	LHG	C25-C26-C27-C28
8	A	815	BCL	CBA-CGA-O2A-C1
8	a	815	BCL	CBA-CGA-O2A-C1
9	A	816	F39	C24-C26-C28-C29
8	E	409	BCL	C4-C3-C5-C6
8	G	406	BCL	C4-C3-C5-C6
8	J	402	BCL	C4-C3-C5-C6
8	J	407	BCL	C4-C3-C5-C6
8	E	407	BCL	C15-C16-C17-C18
8	F	407	BCL	C15-C16-C17-C18
8	H	407	BCL	C15-C16-C17-C18
8	I	407	BCL	C15-C16-C17-C18
10	A	817	LHG	C27-C28-C29-C30
11	A	819	IKV	C5-C6-C7-C8
8	A	811	BCL	C2B-C3B-CAB-OB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	E	409	BCL	O2A-C1-C2-C3
8	J	402	BCL	O2A-C1-C2-C3
8	a	811	BCL	C2B-C3B-CAB-OB
9	A	816	F39	C61-C63-C64-C62
10	A	817	LHG	C28-C29-C30-C31
10	A	818	LHG	C15-C16-C17-C18
9	A	816	F39	C56-C58-C61-C63
8	E	406	BCL	C4-C3-C5-C6
8	F	406	BCL	C4-C3-C5-C6
8	G	405	BCL	C4-C3-C5-C6
8	H	406	BCL	C4-C3-C5-C6
8	I	406	BCL	C4-C3-C5-C6
8	J	406	BCL	C4-C3-C5-C6
10	A	818	LHG	C30-C31-C32-C33
10	A	818	LHG	O7-C5-C6-O8
10	A	817	LHG	C14-C15-C16-C17
7	A	802	CLA	CBA-CGA-O2A-C1
7	a	802	CLA	CBA-CGA-O2A-C1
11	A	819	IKV	C7-C8-C9-C10
6	a	801	GS0	C11-C10-C8-C9
8	A	814	BCL	C11-C10-C8-C9
8	a	805	BCL	C6-C7-C8-C9
8	a	805	BCL	C11-C12-C13-C14
10	A	818	LHG	C27-C28-C29-C30
10	A	818	LHG	C28-C29-C30-C31
8	E	409	BCL	C11-C12-C13-C15
8	G	406	BCL	C11-C10-C8-C7
8	J	402	BCL	C11-C12-C13-C15
8	J	407	BCL	C11-C10-C8-C7
8	a	805	BCL	C6-C7-C8-C10
8	a	806	BCL	C11-C10-C8-C7
8	a	806	BCL	C12-C13-C15-C16
8	E	403	BCL	C8-C10-C11-C12
8	F	403	BCL	C8-C10-C11-C12
8	G	402	BCL	C8-C10-C11-C12
8	H	403	BCL	C8-C10-C11-C12
8	I	403	BCL	C8-C10-C11-C12
8	J	403	BCL	C8-C10-C11-C12
7	A	802	CLA	C4-C3-C5-C6
7	a	802	CLA	C4-C3-C5-C6
8	E	408[B]	BCL	C3A-C2A-CAA-CBA
8	F	408[B]	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	F	409[B]	BCL	C3A-C2A-CAA-CBA
8	H	408[B]	BCL	C3A-C2A-CAA-CBA
8	I	408[B]	BCL	C3A-C2A-CAA-CBA
8	I	409[B]	BCL	C3A-C2A-CAA-CBA
9	a	816	F39	C32-C35-C37-C39
10	a	817	LHG	C1-C2-C3-O3
11	A	819	IKV	O2-C17-C18-C19
11	a	819	IKV	O2-C17-C18-C19
10	A	817	LHG	C29-C30-C31-C32
10	a	818	LHG	C15-C16-C17-C18
10	A	818	LHG	C24-C25-C26-C27
10	A	817	LHG	C35-C36-C37-C38
8	A	814	BCL	C4-C3-C5-C6
8	a	814	BCL	C4-C3-C5-C6
7	A	802	CLA	C2-C3-C5-C6
7	a	802	CLA	C2-C3-C5-C6
9	a	816	F39	C16-C13-O2-C11
9	a	816	F39	C17-C13-O2-C11
8	A	805	BCL	C16-C17-C18-C20
11	A	819	IKV	C26-C27-C28-C29
11	a	819	IKV	C26-C27-C28-C29
8	E	401	BCL	C11-C10-C8-C9
8	F	401	BCL	C11-C10-C8-C9
8	G	401	BCL	C11-C10-C8-C9
8	H	401	BCL	C11-C10-C8-C9
8	I	401	BCL	C11-C10-C8-C9
8	J	401	BCL	C11-C10-C8-C9
8	a	814	BCL	C6-C7-C8-C9
10	A	818	LHG	C9-C10-C11-C12
11	A	819	IKV	C28-C29-C30-C31
11	a	819	IKV	C9-C10-C11-C12
11	a	819	IKV	C28-C29-C30-C31
8	A	809[B]	BCL	C4C-C3C-CAC-CBC
8	A	815	BCL	C4C-C3C-CAC-CBC
8	a	809[B]	BCL	C4C-C3C-CAC-CBC
8	a	815	BCL	C4C-C3C-CAC-CBC
9	a	816	F39	O2-C13-C14-C18
11	A	819	IKV	C11-C10-C9-C8
10	A	817	LHG	O1-C1-C2-O2
8	A	815	BCL	C4-C3-C5-C6
8	a	815	BCL	C4-C3-C5-C6
9	a	816	F39	C13-C14-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	803	CLA	C13-C15-C16-C17
7	a	803	CLA	C13-C15-C16-C17
8	A	814	BCL	C8-C10-C11-C12
10	A	817	LHG	O6-C4-C5-C6
9	a	816	F39	C65-C62-C64-C63
7	A	802	CLA	C11-C12-C13-C15
7	a	802	CLA	C11-C12-C13-C15
8	A	814	BCL	C6-C7-C8-C10
8	E	402	BCL	C6-C7-C8-C10
9	a	816	F39	C40-C41-C42-C44
10	a	818	LHG	C30-C31-C32-C33
8	a	805	BCL	C16-C17-C18-C20
8	A	815	BCL	O1A-CGA-O2A-C1
8	a	815	BCL	O1A-CGA-O2A-C1
8	A	814	BCL	C2-C3-C5-C6
8	A	815	BCL	C2-C3-C5-C6
8	a	814	BCL	C2-C3-C5-C6
8	a	815	BCL	C2-C3-C5-C6
8	E	409	BCL	C13-C15-C16-C17
8	J	402	BCL	C13-C15-C16-C17
10	A	818	LHG	C12-C13-C14-C15
8	A	807	BCL	C2B-C3B-CAB-OBB
8	a	807	BCL	C2B-C3B-CAB-OBB
7	A	802	CLA	O1A-CGA-O2A-C1
7	a	802	CLA	O1A-CGA-O2A-C1
10	A	817	LHG	O6-C4-C5-O7
11	A	819	IKV	O9-C18-C19-O3
11	a	819	IKV	O9-C18-C19-O3
7	A	802	CLA	C11-C12-C13-C14
7	a	802	CLA	C11-C12-C13-C14
8	A	815	BCL	C14-C13-C15-C16
8	E	409	BCL	C14-C13-C15-C16
8	J	402	BCL	C14-C13-C15-C16
8	a	806	BCL	C11-C10-C8-C9
8	a	815	BCL	C14-C13-C15-C16
10	A	818	LHG	C16-C17-C18-C19
8	A	810	BCL	C3-C5-C6-C7
8	J	407	BCL	C3-C5-C6-C7
8	a	810	BCL	C3-C5-C6-C7
9	A	816	F39	C30-C31-C33-C34
8	a	805	BCL	C16-C17-C18-C19
8	G	406	BCL	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	818	LHG	C34-C35-C36-C37
7	A	802	CLA	C16-C17-C18-C19
8	A	815	BCL	C1A-C2A-CAA-CBA
8	E	402	BCL	C1A-C2A-CAA-CBA
8	F	402	BCL	C1A-C2A-CAA-CBA
8	H	402	BCL	C1A-C2A-CAA-CBA
8	I	402	BCL	C1A-C2A-CAA-CBA
8	a	815	BCL	C1A-C2A-CAA-CBA
6	a	801	GS0	C8-C10-C11-C12
7	a	802	CLA	C16-C17-C18-C19
6	a	801	GS0	C11-C10-C8-C7
8	A	805	BCL	C11-C12-C13-C15
8	A	808	BCL	C11-C10-C8-C7
8	A	810	BCL	C12-C13-C15-C16
8	E	402	BCL	C11-C10-C8-C7
8	F	402	BCL	C6-C7-C8-C10
8	F	402	BCL	C11-C10-C8-C7
8	H	402	BCL	C6-C7-C8-C10
8	H	402	BCL	C11-C10-C8-C7
8	I	402	BCL	C6-C7-C8-C10
8	I	402	BCL	C11-C10-C8-C7
8	a	808	BCL	C11-C10-C8-C7
8	a	810	BCL	C12-C13-C15-C16
8	a	814	BCL	C11-C12-C13-C15
8	E	402	BCL	C16-C17-C18-C20
8	F	402	BCL	C16-C17-C18-C20
8	H	402	BCL	C16-C17-C18-C20
8	I	402	BCL	C16-C17-C18-C20
8	A	809[B]	BCL	C2C-C3C-CAC-CBC
8	a	809[B]	BCL	C2C-C3C-CAC-CBC
10	a	818	LHG	C2-C3-O3-P
10	a	818	LHG	O6-C4-C5-O7
10	a	818	LHG	C9-C10-C11-C12
8	A	814	BCL	C4B-C3B-CAB-OB
7	A	802	CLA	C6-C7-C8-C9
7	a	802	CLA	C6-C7-C8-C9
8	E	402	BCL	C6-C7-C8-C9
8	F	402	BCL	C6-C7-C8-C9
8	H	402	BCL	C6-C7-C8-C9
8	I	402	BCL	C6-C7-C8-C9
9	A	816	F39	C42-C44-C51-C57
8	E	401	BCL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	H	401	BCL	C15-C16-C17-C18
8	J	401	BCL	C15-C16-C17-C18
8	F	401	BCL	C15-C16-C17-C18
8	G	401	BCL	C15-C16-C17-C18
8	I	401	BCL	C15-C16-C17-C18
10	A	817	LHG	O7-C5-C6-O8
11	A	819	IKV	C2-C3-C4-C5
10	A	818	LHG	C4-C5-C6-O8
11	A	819	IKV	C17-C18-C19-O3
11	a	819	IKV	C17-C18-C19-O3
10	A	817	LHG	C19-C20-C21-C22
8	A	815	BCL	CAD-CBD-CGD-O2D
8	a	815	BCL	CAD-CBD-CGD-O2D
8	E	409	BCL	C5-C6-C7-C8
8	J	402	BCL	C5-C6-C7-C8
6	A	801	GS0	CHA-CBD-CGD-O1D
6	a	801	GS0	CHA-CBD-CGD-O1D
8	A	815	BCL	CAD-CBD-CGD-O1D
8	F	402	BCL	CHA-CBD-CGD-O1D
8	I	402	BCL	CHA-CBD-CGD-O1D
8	a	815	BCL	CAD-CBD-CGD-O1D
10	A	817	LHG	C4-O6-P-O5
10	A	818	LHG	C3-O3-P-O5
10	A	818	LHG	C4-O6-P-O3
10	A	818	LHG	C4-O6-P-O4
10	A	818	LHG	C4-O6-P-O5
10	a	817	LHG	C3-O3-P-O6
10	a	818	LHG	C3-O3-P-O4
10	a	818	LHG	C3-O3-P-O6
10	a	818	LHG	C4-O6-P-O4
8	H	406	BCL	C2-C3-C5-C6
8	I	406	BCL	C2-C3-C5-C6
8	E	406	BCL	C2-C3-C5-C6
8	F	406	BCL	C2-C3-C5-C6
8	G	405	BCL	C2-C3-C5-C6
8	J	406	BCL	C2-C3-C5-C6
7	A	802	CLA	C16-C17-C18-C20
7	a	802	CLA	C16-C17-C18-C20
8	a	805	BCL	C10-C11-C12-C13
8	a	811	BCL	C11-C12-C13-C14
8	A	806	BCL	C11-C12-C13-C15
8	E	401	BCL	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	F	401	BCL	C11-C10-C8-C7
8	G	401	BCL	C11-C10-C8-C7
8	H	401	BCL	C11-C10-C8-C7
8	I	401	BCL	C11-C10-C8-C7
8	J	401	BCL	C11-C10-C8-C7
8	E	402	BCL	C4-C3-C5-C6
8	F	402	BCL	C4-C3-C5-C6
8	H	402	BCL	C4-C3-C5-C6
8	I	402	BCL	C4-C3-C5-C6
10	A	817	LHG	C4-C5-C6-O8
8	A	815	BCL	C2A-CAA-CBA-CGA
8	a	815	BCL	C2A-CAA-CBA-CGA
9	A	816	F39	C37-C39-C40-C41
8	a	814	BCL	C4B-C3B-CAB-OBB
8	A	806	BCL	C11-C12-C13-C14
8	A	810	BCL	C14-C13-C15-C16
8	E	402	BCL	C14-C13-C15-C16
8	F	402	BCL	C14-C13-C15-C16
8	H	402	BCL	C14-C13-C15-C16
8	I	402	BCL	C14-C13-C15-C16
8	a	810	BCL	C14-C13-C15-C16
8	a	814	BCL	C11-C12-C13-C14
9	A	816	F39	C26-C28-C29-C30
8	A	807	BCL	C8-C10-C11-C12
8	a	807	BCL	C8-C10-C11-C12
8	A	812	BCL	C10-C11-C12-C13
8	A	814	BCL	C16-C17-C18-C20
8	A	815	BCL	C10-C11-C12-C13
8	a	815	BCL	C10-C11-C12-C13
10	A	817	LHG	C11-C10-C9-C8
8	A	814	BCL	C3A-C2A-CAA-CBA
8	a	814	BCL	C3A-C2A-CAA-CBA
7	A	802	CLA	C10-C11-C12-C13
7	a	802	CLA	C10-C11-C12-C13
11	A	819	IKV	C12-C13-C14-C15
8	E	405	BCL	C2-C1-O2A-CGA
8	F	405	BCL	C2-C1-O2A-CGA
8	G	404	BCL	C2-C1-O2A-CGA
8	H	405	BCL	C2-C1-O2A-CGA
8	I	405	BCL	C2-C1-O2A-CGA
8	J	405	BCL	C2-C1-O2A-CGA
8	E	402	BCL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	816	F39	C30-C31-C33-C34
8	F	402	BCL	C10-C11-C12-C13
8	I	402	BCL	C10-C11-C12-C13
8	H	402	BCL	C10-C11-C12-C13
10	A	818	LHG	C11-C10-C9-C8
8	A	808	BCL	C11-C10-C8-C9
8	E	403	BCL	C11-C12-C13-C14
8	F	403	BCL	C11-C12-C13-C14
8	G	402	BCL	C11-C12-C13-C14
8	H	403	BCL	C11-C12-C13-C14
8	I	403	BCL	C11-C12-C13-C14
8	J	403	BCL	C11-C12-C13-C14
8	a	808	BCL	C11-C10-C8-C9
10	a	817	LHG	O1-C1-C2-C3
10	a	817	LHG	C31-C32-C33-C34
8	a	812	BCL	C2B-C3B-CAB-OB
8	a	812	BCL	C2B-C3B-CAB-CB
8	A	811	BCL	C8-C10-C11-C12
8	A	810	BCL	CAA-CBA-CGA-O2A
8	a	810	BCL	CAA-CBA-CGA-O2A
8	A	809[B]	BCL	C2A-CAA-CBA-CGA
8	a	809[B]	BCL	C2A-CAA-CBA-CGA
10	a	817	LHG	C30-C31-C32-C33
8	E	408[B]	BCL	C1A-C2A-CAA-CBA
8	F	408[B]	BCL	C1A-C2A-CAA-CBA
8	F	409[B]	BCL	C1A-C2A-CAA-CBA
8	H	408[B]	BCL	C1A-C2A-CAA-CBA
8	I	408[B]	BCL	C1A-C2A-CAA-CBA
8	I	409[B]	BCL	C1A-C2A-CAA-CBA
8	a	811	BCL	C11-C12-C13-C15
7	A	803	CLA	C2A-CAA-CBA-CGA
7	a	803	CLA	C2A-CAA-CBA-CGA
8	A	815	BCL	C2C-C3C-CAC-CBC
8	a	815	BCL	C2C-C3C-CAC-CBC
10	A	818	LHG	C11-C12-C13-C14
8	A	814	BCL	C4B-C3B-CAB-CB
8	a	814	BCL	C4B-C3B-CAB-CB
8	A	807	BCL	C4C-C3C-CAC-CBC
8	a	808	BCL	C13-C15-C16-C17
11	a	819	IKV	C7-C8-C9-C10
10	a	817	LHG	O10-C23-O8-C6
8	A	808	BCL	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	a	817	LHG	O6-C4-C5-C6
9	A	816	F39	C18-C19-C20-C25
8	I	402	BCL	C11-C10-C8-C9
7	a	803	CLA	C16-C17-C18-C20
8	A	807	BCL	CAA-CBA-CGA-O2A
7	A	803	CLA	C16-C17-C18-C20
8	E	409	BCL	C16-C17-C18-C19
8	J	402	BCL	C16-C17-C18-C19
8	a	807	BCL	CAA-CBA-CGA-O2A
8	A	807	BCL	C2B-C3B-CAB-CBB
8	a	807	BCL	C2B-C3B-CAB-CBB
10	A	818	LHG	C6-C5-O7-C7
11	a	819	IKV	C6-C7-C8-C9
10	a	817	LHG	C24-C23-O8-C6
8	A	814	BCL	C16-C17-C18-C19
8	A	813	BCL	C8-C10-C11-C12
8	a	813	BCL	C8-C10-C11-C12
8	G	406	BCL	C10-C11-C12-C13
8	E	406	BCL	C4B-C3B-CAB-OBB
8	F	406	BCL	C4B-C3B-CAB-OBB
8	G	405	BCL	C4B-C3B-CAB-OBB
8	H	406	BCL	C4B-C3B-CAB-OBB
8	I	406	BCL	C4B-C3B-CAB-OBB
8	J	406	BCL	C4B-C3B-CAB-OBB
8	a	812	BCL	C4B-C3B-CAB-CBB
8	A	805	BCL	C11-C12-C13-C14
8	J	407	BCL	C10-C11-C12-C13
11	a	819	IKV	C11-C12-C13-C14
6	A	801	GS0	C12-C13-C15-C16
7	A	802	CLA	C11-C10-C8-C7
8	A	807	BCL	C6-C7-C8-C10
8	A	810	BCL	C6-C7-C8-C10
8	a	807	BCL	C6-C7-C8-C10
8	a	810	BCL	C6-C7-C8-C10
9	A	816	F39	C45-C46-C53-C56
9	A	816	F39	C48-C46-C53-C56
11	A	819	IKV	O9-C26-C27-C28
11	a	819	IKV	O9-C26-C27-C28
8	E	404	BCL	CAA-CBA-CGA-O2A
8	E	405	BCL	CAA-CBA-CGA-O2A
8	F	405	BCL	CAA-CBA-CGA-O2A
8	G	403	BCL	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	G	404	BCL	CAA-CBA-CGA-O2A
8	H	404	BCL	CAA-CBA-CGA-O2A
8	H	405	BCL	CAA-CBA-CGA-O2A
8	I	404	BCL	CAA-CBA-CGA-O2A
8	I	405	BCL	CAA-CBA-CGA-O2A
8	J	404	BCL	CAA-CBA-CGA-O2A
8	J	405	BCL	CAA-CBA-CGA-O2A
10	a	817	LHG	C32-C33-C34-C35
8	F	404	BCL	CAA-CBA-CGA-O2A
8	E	401	BCL	CAA-CBA-CGA-O2A
8	F	401	BCL	CAA-CBA-CGA-O2A
8	G	401	BCL	CAA-CBA-CGA-O2A
8	H	401	BCL	CAA-CBA-CGA-O2A
8	I	401	BCL	CAA-CBA-CGA-O2A
8	J	401	BCL	CAA-CBA-CGA-O2A
10	a	818	LHG	O8-C23-C24-C25
8	E	402	BCL	C2-C3-C5-C6
8	F	402	BCL	C2-C3-C5-C6
8	H	402	BCL	C2-C3-C5-C6
8	I	402	BCL	C2-C3-C5-C6
11	A	819	IKV	C1-C2-C3-C4
8	A	811	BCL	C11-C12-C13-C14
8	E	402	BCL	C11-C10-C8-C9
8	F	402	BCL	C11-C10-C8-C9
8	H	402	BCL	C11-C10-C8-C9
8	A	811	BCL	CAA-CBA-CGA-O2A
8	E	403	BCL	CAA-CBA-CGA-O2A
8	H	403	BCL	CAA-CBA-CGA-O2A
8	a	811	BCL	CAA-CBA-CGA-O2A
7	A	802	CLA	C4B-C3B-CAB-CBB
7	a	802	CLA	C4B-C3B-CAB-CBB
8	A	805	BCL	C4-C3-C5-C6
8	F	403	BCL	CAA-CBA-CGA-O2A
8	I	403	BCL	CAA-CBA-CGA-O2A
8	G	402	BCL	CAA-CBA-CGA-O2A
8	J	403	BCL	CAA-CBA-CGA-O2A
10	a	818	LHG	C17-C18-C19-C20
8	a	810	BCL	C13-C15-C16-C17
8	E	407	BCL	C2-C1-O2A-CGA
8	F	407	BCL	C2-C1-O2A-CGA
8	H	407	BCL	C2-C1-O2A-CGA
8	I	407	BCL	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	802	CLA	C12-C13-C15-C16
7	a	802	CLA	C11-C10-C8-C7
7	a	802	CLA	C12-C13-C15-C16
8	A	805	BCL	C12-C13-C15-C16
8	A	811	BCL	C11-C12-C13-C15
8	A	811	BCL	C12-C13-C15-C16
8	A	812	BCL	C6-C7-C8-C10
8	A	814	BCL	C12-C13-C15-C16
8	E	407	BCL	C6-C7-C8-C10
8	F	407	BCL	C6-C7-C8-C10
8	H	407	BCL	C6-C7-C8-C10
8	I	407	BCL	C6-C7-C8-C10
6	A	801	GS0	C13-C15-C16-C17
8	A	810	BCL	C13-C15-C16-C17
8	A	809[B]	BCL	C2B-C3B-CAB-CBB
8	a	809[B]	BCL	C2B-C3B-CAB-CBB
10	a	818	LHG	C27-C28-C29-C30
8	a	806	BCL	C8-C10-C11-C12
8	J	404	BCL	CAA-CBA-CGA-O1A
8	A	805	BCL	C2A-CAA-CBA-CGA
8	a	805	BCL	C2A-CAA-CBA-CGA
10	a	817	LHG	O8-C23-C24-C25
8	E	404	BCL	CAA-CBA-CGA-O1A
8	G	403	BCL	CAA-CBA-CGA-O1A
8	H	404	BCL	CAA-CBA-CGA-O1A
8	E	402	BCL	C3A-C2A-CAA-CBA
8	F	402	BCL	C3A-C2A-CAA-CBA
8	H	402	BCL	C3A-C2A-CAA-CBA
8	I	402	BCL	C3A-C2A-CAA-CBA
9	a	816	F39	C14-C13-O2-C11
8	F	404	BCL	CAA-CBA-CGA-O1A
8	E	408[B]	BCL	CAA-CBA-CGA-O2A
8	F	408[B]	BCL	CAA-CBA-CGA-O2A
8	F	409[B]	BCL	CAA-CBA-CGA-O2A
8	H	408[B]	BCL	CAA-CBA-CGA-O2A
8	I	408[B]	BCL	CAA-CBA-CGA-O2A
8	I	409[B]	BCL	CAA-CBA-CGA-O2A
8	I	404	BCL	CAA-CBA-CGA-O1A
8	A	811	BCL	CAA-CBA-CGA-O1A
8	a	811	BCL	CAA-CBA-CGA-O1A
11	A	819	IKV	O10-C26-C27-C28
11	a	819	IKV	O10-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	a	812	BCL	C4B-C3B-CAB-OBB
7	A	802	CLA	C11-C10-C8-C9
7	a	802	CLA	C11-C10-C8-C9
8	a	806	BCL	C11-C12-C13-C14
8	a	810	BCL	C6-C7-C8-C9
8	G	404	BCL	CAA-CBA-CGA-O1A
8	a	805	BCL	C15-C16-C17-C18
8	E	401	BCL	CAA-CBA-CGA-O1A
8	E	405	BCL	CAA-CBA-CGA-O1A
8	F	401	BCL	CAA-CBA-CGA-O1A
8	F	405	BCL	CAA-CBA-CGA-O1A
8	G	401	BCL	CAA-CBA-CGA-O1A
8	H	401	BCL	CAA-CBA-CGA-O1A
8	H	405	BCL	CAA-CBA-CGA-O1A
8	I	401	BCL	CAA-CBA-CGA-O1A
8	I	405	BCL	CAA-CBA-CGA-O1A
8	J	401	BCL	CAA-CBA-CGA-O1A
8	J	405	BCL	CAA-CBA-CGA-O1A
8	F	402	BCL	CAA-CBA-CGA-O2A
8	I	402	BCL	CAA-CBA-CGA-O2A
8	E	402	BCL	CAA-CBA-CGA-O2A
8	H	402	BCL	CAA-CBA-CGA-O2A
10	a	818	LHG	O10-C23-C24-C25
8	A	807	BCL	CAD-CBD-CGD-O2D
8	a	807	BCL	CAD-CBD-CGD-O2D
8	A	815	BCL	C8-C10-C11-C12
8	a	815	BCL	C8-C10-C11-C12
8	A	805	BCL	C2-C1-O2A-CGA
8	E	404	BCL	C2-C1-O2A-CGA
8	F	404	BCL	C2-C1-O2A-CGA
8	G	403	BCL	C2-C1-O2A-CGA
8	H	404	BCL	C2-C1-O2A-CGA
8	I	404	BCL	C2-C1-O2A-CGA
8	J	404	BCL	C2-C1-O2A-CGA
8	E	408[B]	BCL	CAA-CBA-CGA-O1A
8	F	408[B]	BCL	CAA-CBA-CGA-O1A
8	F	409[B]	BCL	CAA-CBA-CGA-O1A
8	H	408[B]	BCL	CAA-CBA-CGA-O1A
8	I	408[B]	BCL	CAA-CBA-CGA-O1A
8	I	409[B]	BCL	CAA-CBA-CGA-O1A
6	A	801	GS0	CAA-CBA-CGA-O2A
6	a	801	GS0	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	818	LHG	O8-C23-C24-C25
8	E	403	BCL	CAA-CBA-CGA-O1A
8	F	403	BCL	CAA-CBA-CGA-O1A
8	G	402	BCL	CAA-CBA-CGA-O1A
8	H	403	BCL	CAA-CBA-CGA-O1A
8	J	403	BCL	CAA-CBA-CGA-O1A
10	a	817	LHG	O10-C23-C24-C25

There are no ring outliers.

85 monomers are involved in 514 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	405	BCL	8	0
13	A	821	SF4	1	0
8	G	404	BCL	3	0
8	A	809[B]	BCL	1	0
8	A	811	BCL	8	0
8	a	814	BCL	7	0
8	H	401	BCL	10	0
8	I	402	BCL	16	0
8	F	408[B]	BCL	4	0
8	E	408[B]	BCL	7	0
8	I	406	BCL	9	0
7	a	803	CLA	8	0
8	F	406	BCL	11	0
8	a	812	BCL	5	0
8	a	813	BCL	6	0
8	E	401	BCL	10	0
10	A	818	LHG	5	0
8	a	810	BCL	6	0
8	J	403	BCL	2	0
7	a	802	CLA	14	0
8	I	407	BCL	9	0
8	A	808	BCL	9	0
8	F	407	BCL	9	0
8	G	403	BCL	1	0
7	A	803	CLA	9	0
8	A	815	BCL	12	0
8	G	402	BCL	2	0
11	A	819	IKV	3	0
8	J	402	BCL	15	0
8	H	406	BCL	9	0

Continued on next page...

Continued from previous page...

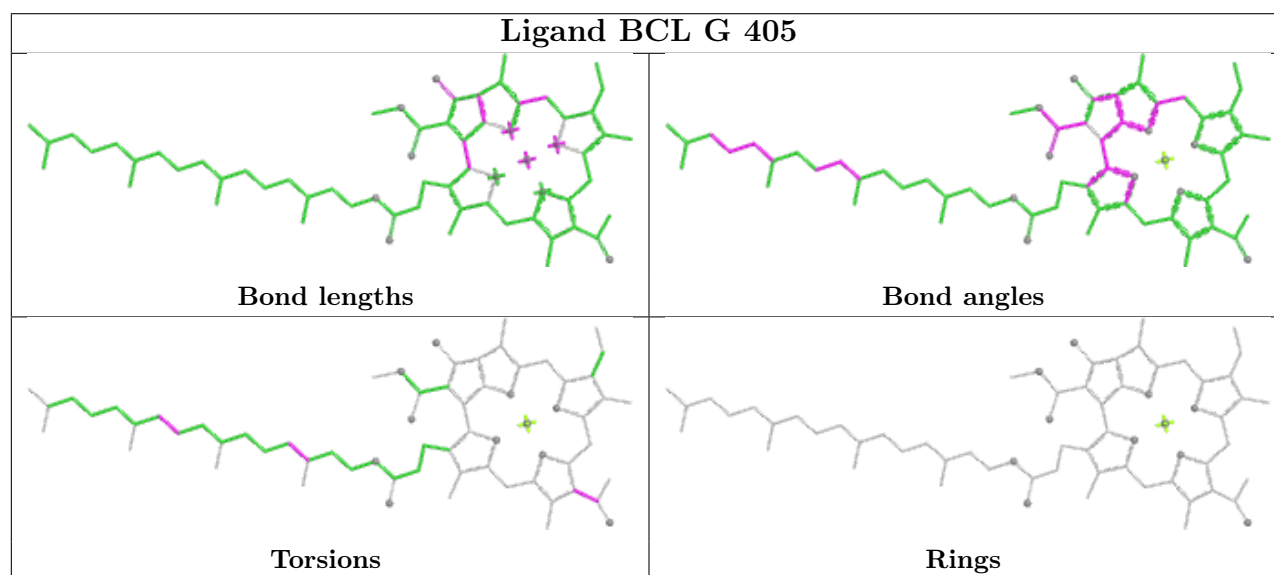
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	403	BCL	5	0
8	G	406	BCL	8	0
8	I	401	BCL	14	0
8	a	808	BCL	9	0
6	A	801	GS0	1	0
8	a	807	BCL	14	0
8	J	407	BCL	10	0
10	A	817	LHG	6	0
8	I	408[B]	BCL	5	0
8	I	405	BCL	5	0
8	a	815	BCL	8	0
8	A	814	BCL	5	0
8	H	404	BCL	1	0
8	J	404	BCL	1	0
8	a	811	BCL	6	0
8	J	401	BCL	11	0
8	F	403	BCL	5	0
8	a	806	BCL	5	0
8	A	813	BCL	3	0
8	H	402	BCL	18	0
8	E	405	BCL	6	0
8	E	406	BCL	11	0
8	F	405	BCL	4	0
8	a	804[B]	BCL	4	0
8	a	805	BCL	5	0
8	A	810	BCL	6	0
8	H	407	BCL	6	0
8	F	401	BCL	16	0
8	E	404	BCL	1	0
8	A	804[B]	BCL	1	0
10	a	818	LHG	5	0
8	E	402	BCL	15	0
8	I	403	BCL	5	0
8	F	409[B]	BCL	9	0
8	E	407	BCL	7	0
8	E	409	BCL	15	0
8	G	401	BCL	11	0
8	J	406	BCL	9	0
8	A	812	BCL	6	0
7	A	802	CLA	8	0
8	H	405	BCL	4	0
8	J	405	BCL	5	0

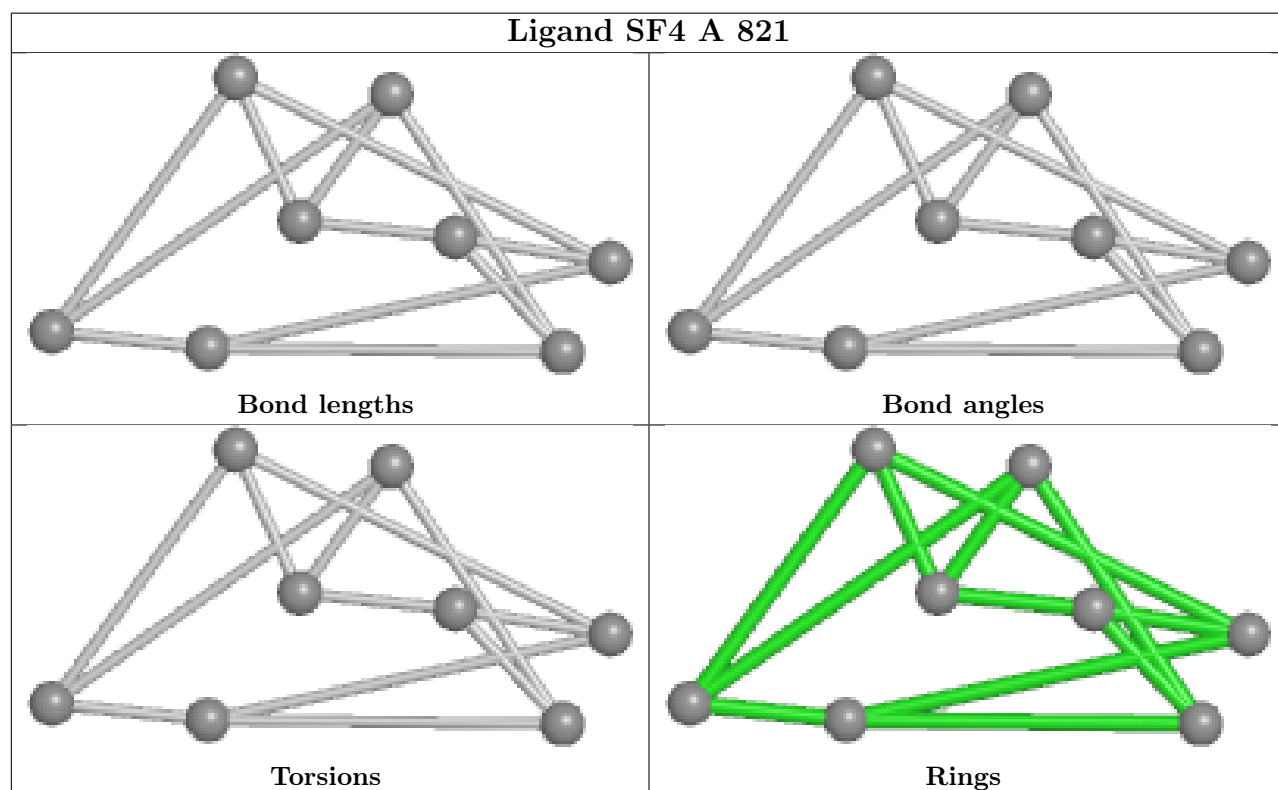
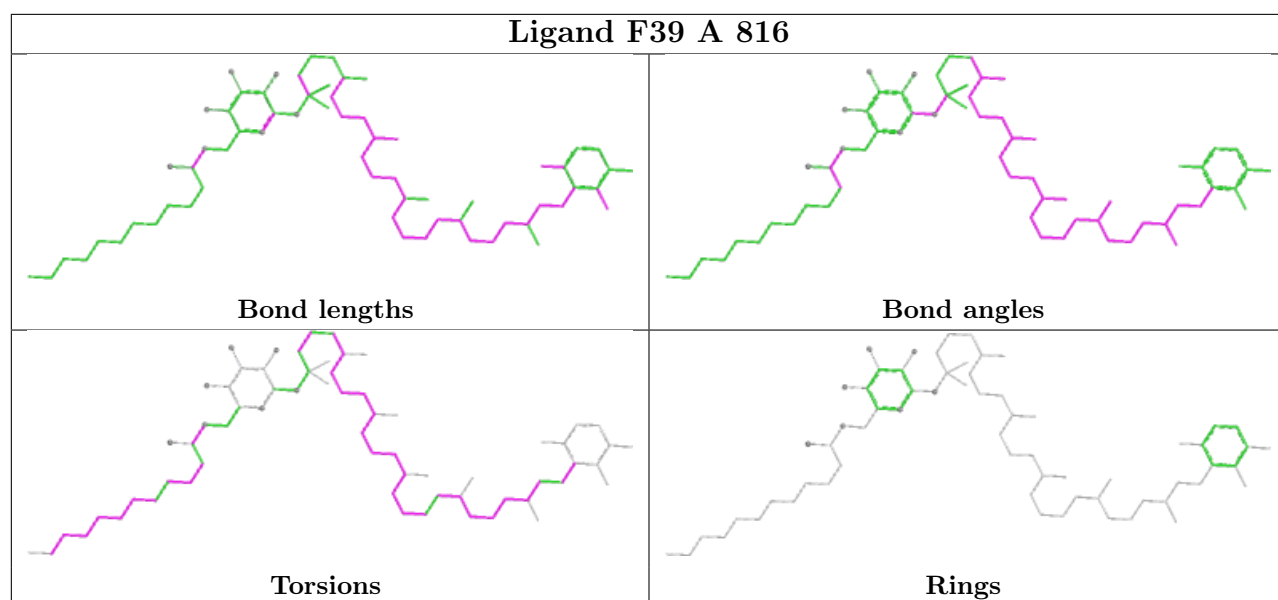
Continued on next page...

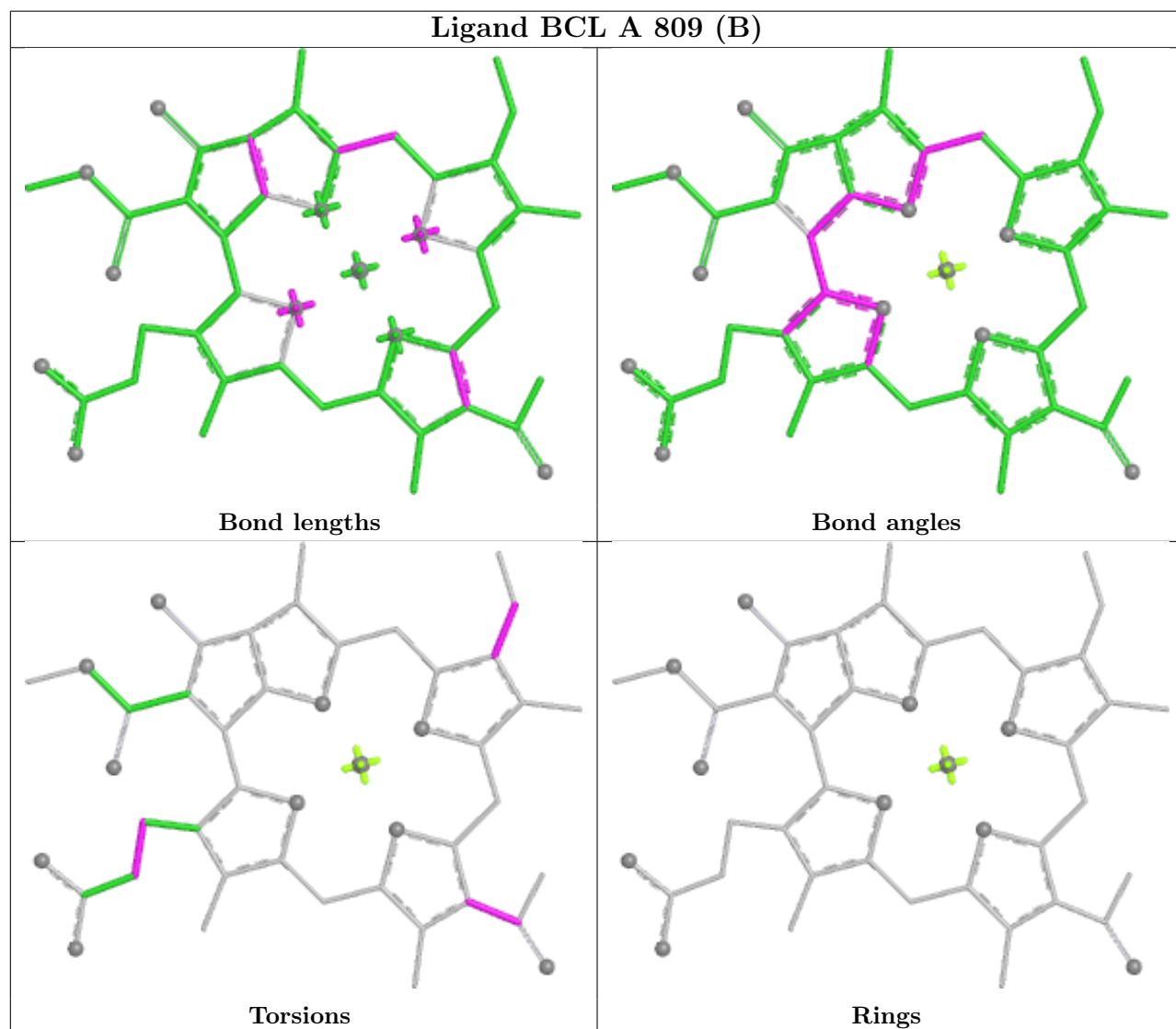
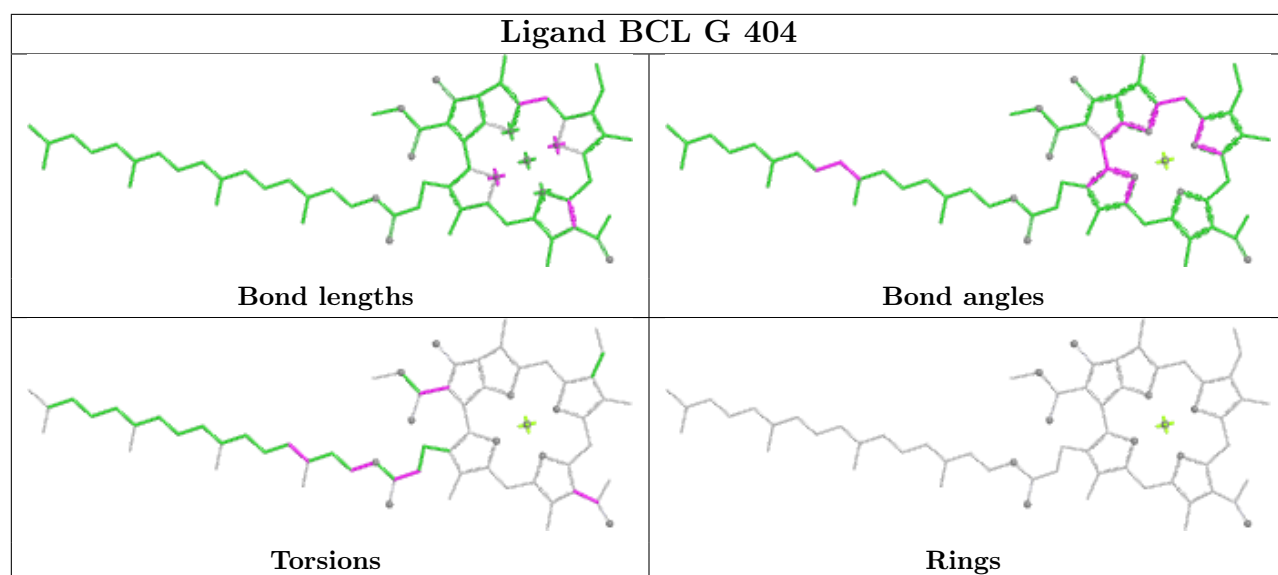
Continued from previous page...

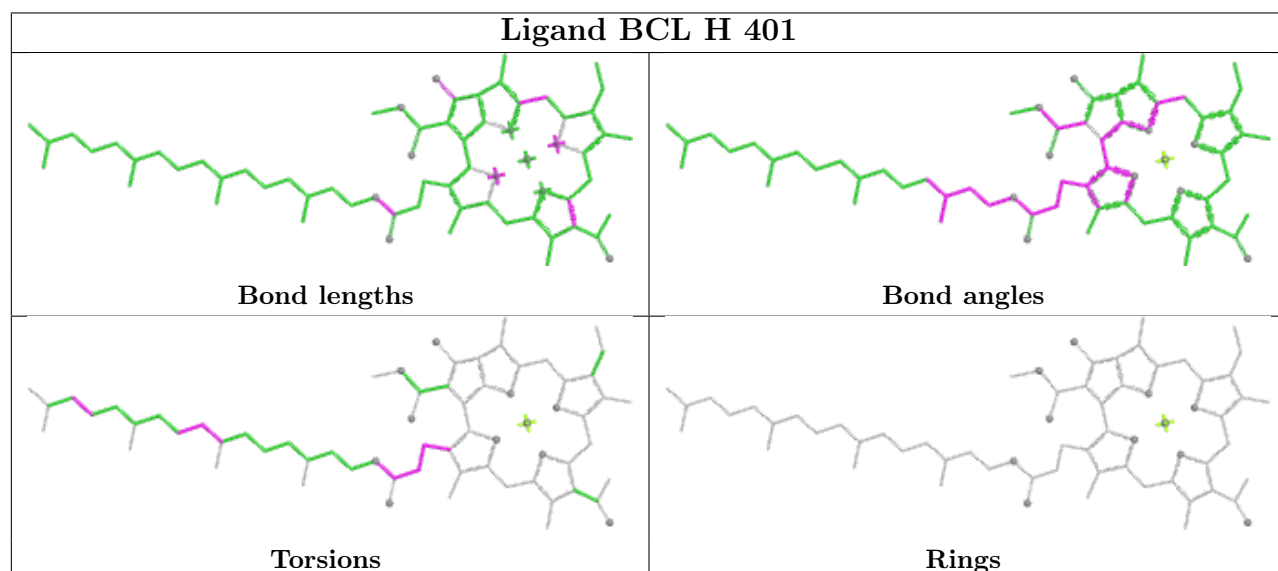
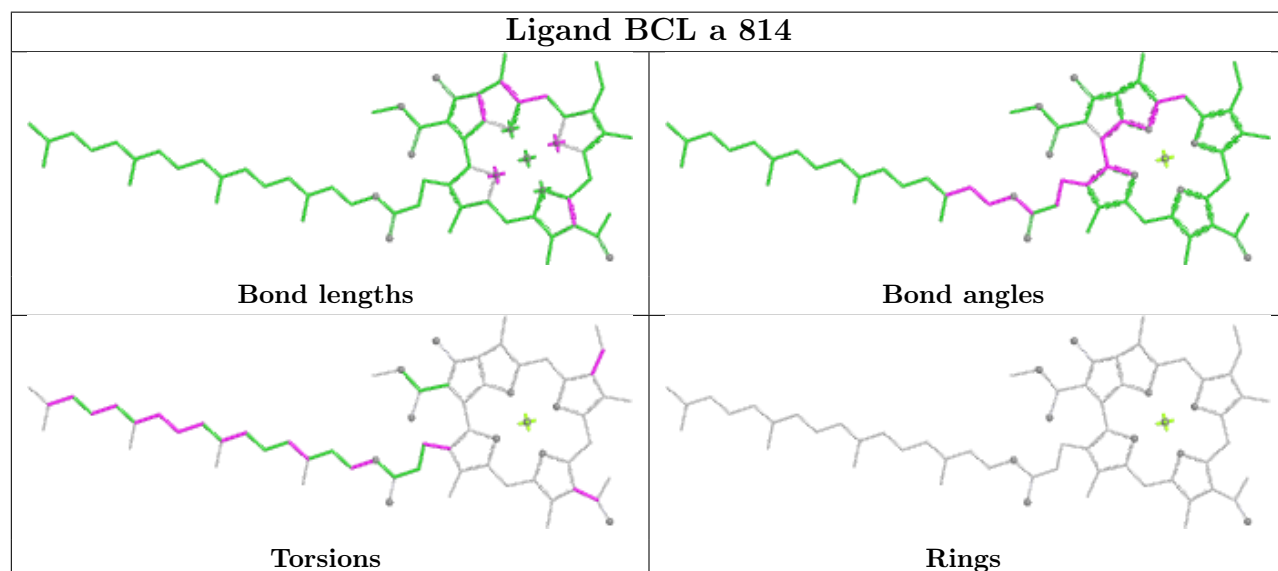
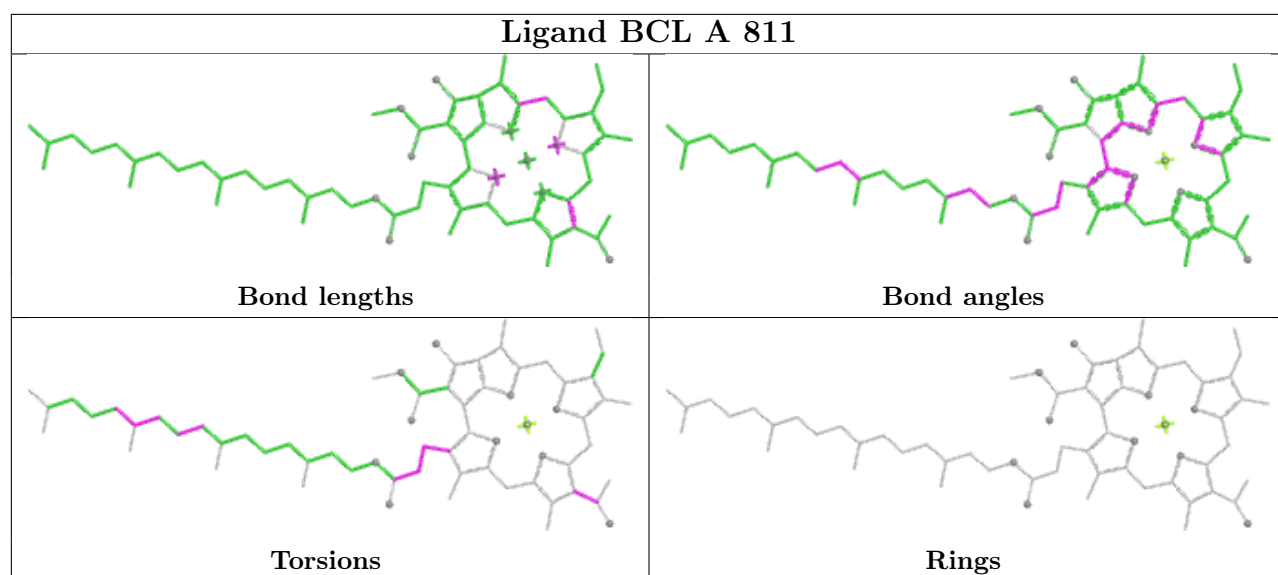
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	806	BCL	4	0
8	E	403	BCL	4	0
8	I	404	BCL	1	0
6	a	801	GS0	2	0
8	H	408[B]	BCL	8	0
8	F	404	BCL	1	0
10	a	817	LHG	8	0
8	F	402	BCL	16	0
8	A	807	BCL	12	0
8	I	409[B]	BCL	11	0
11	a	819	IKV	2	0
8	A	805	BCL	7	0
8	a	809[B]	BCL	1	0

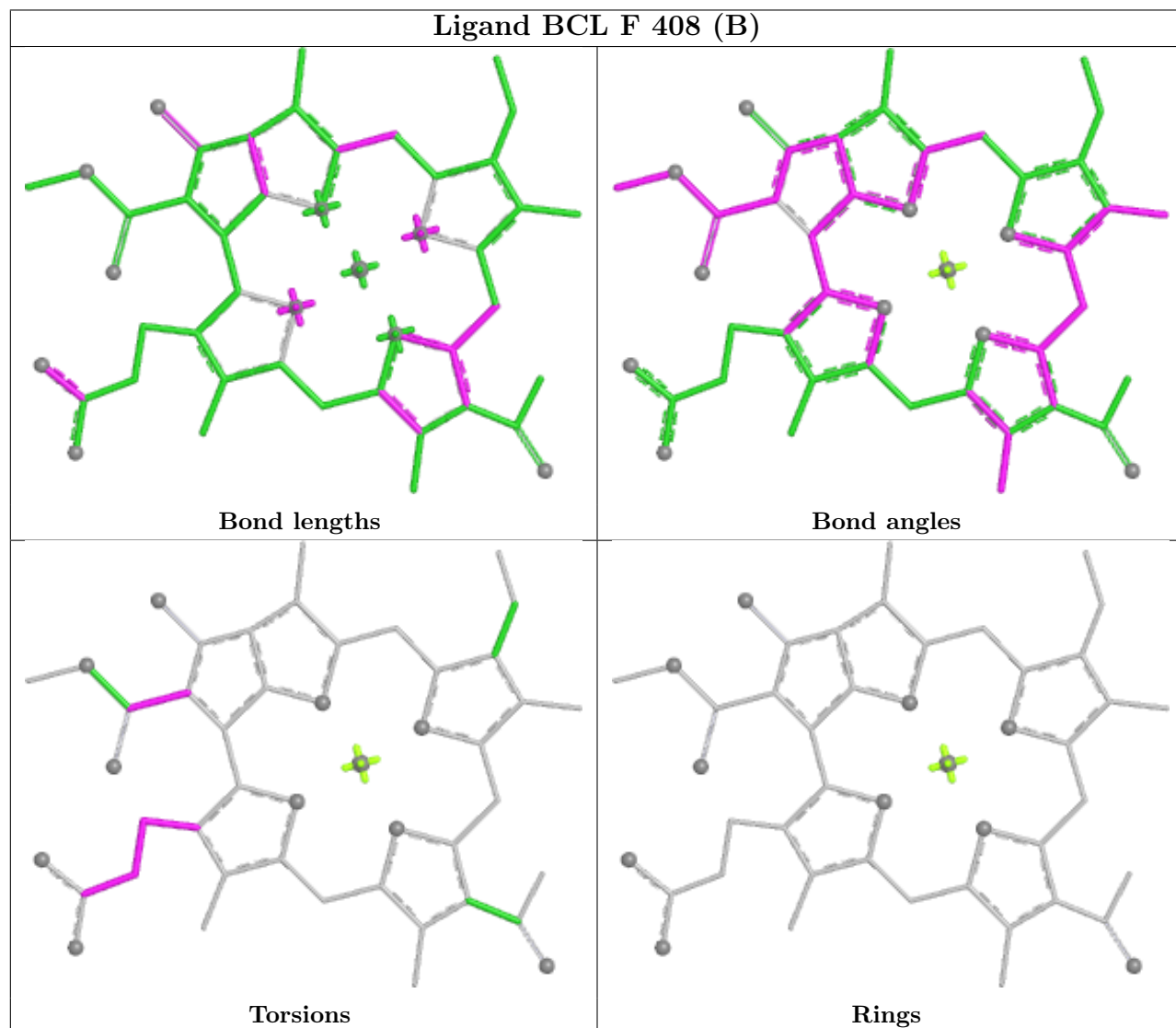
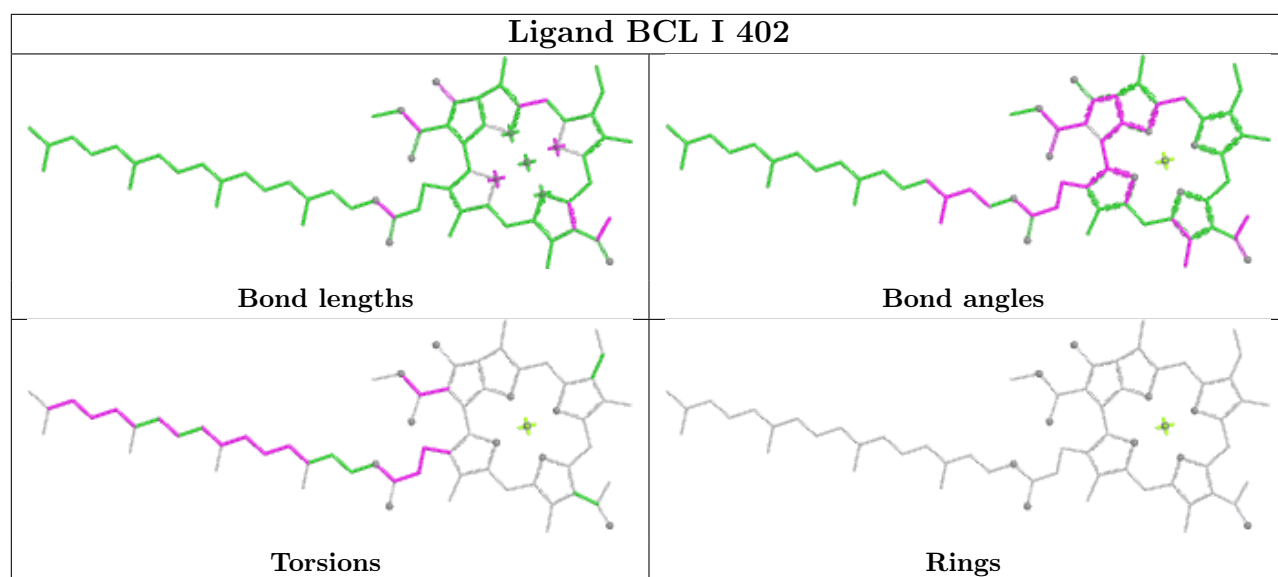
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



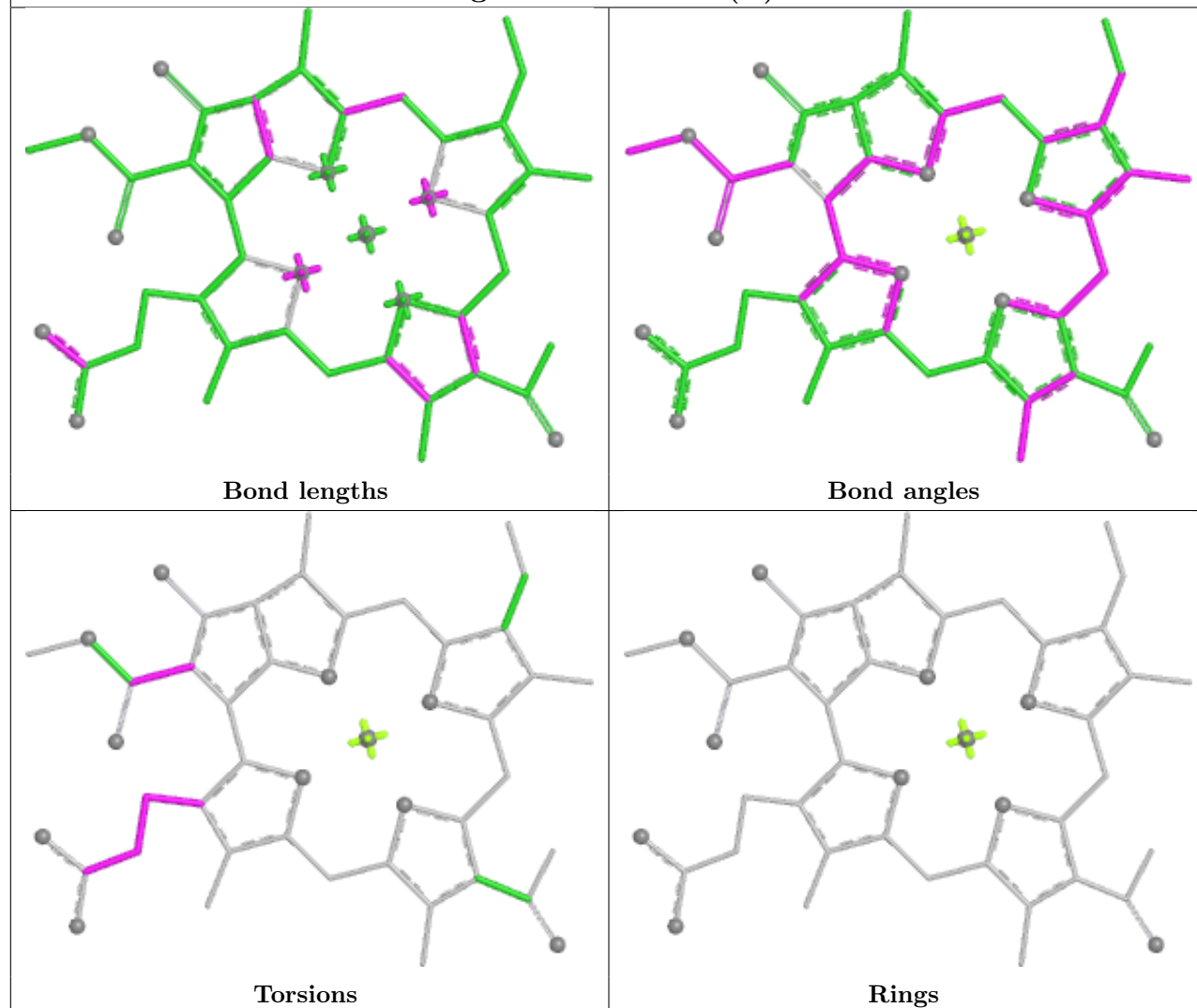




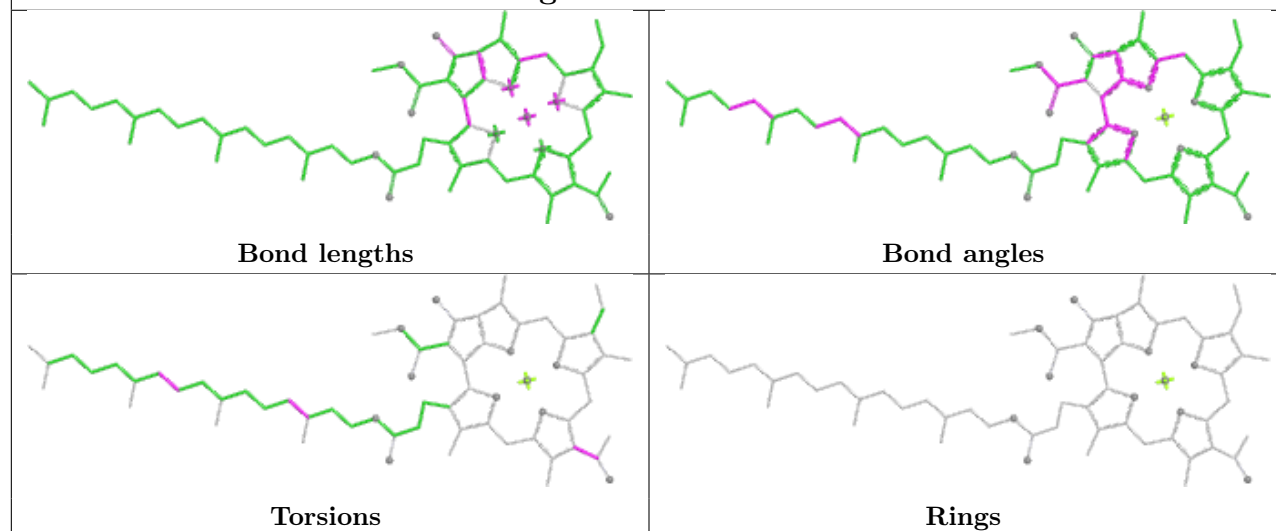


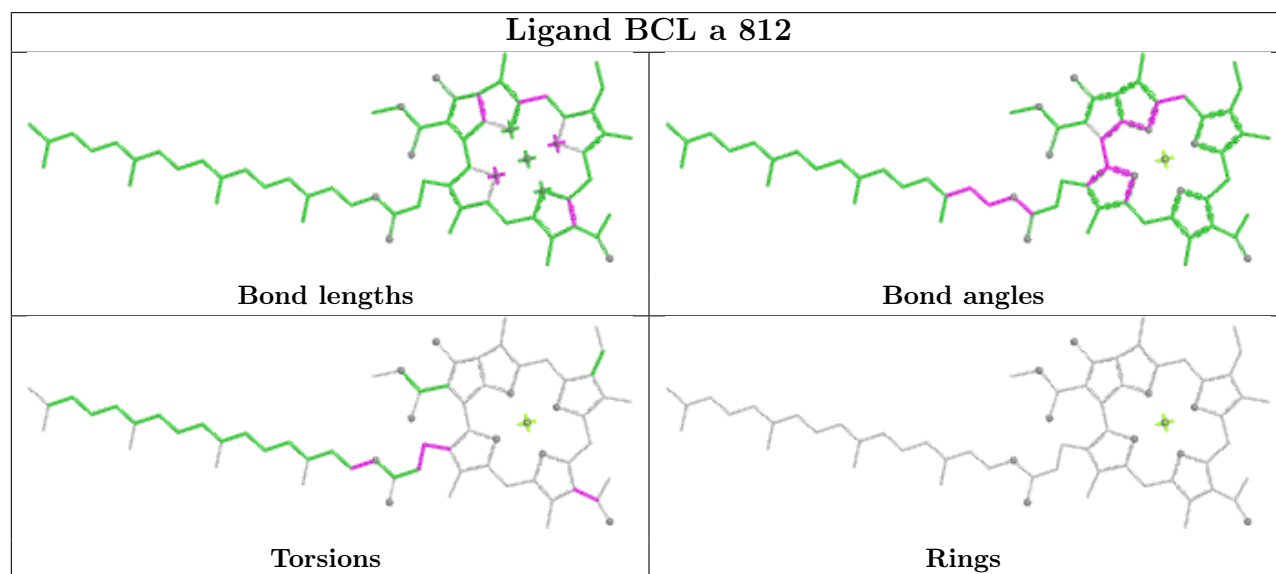
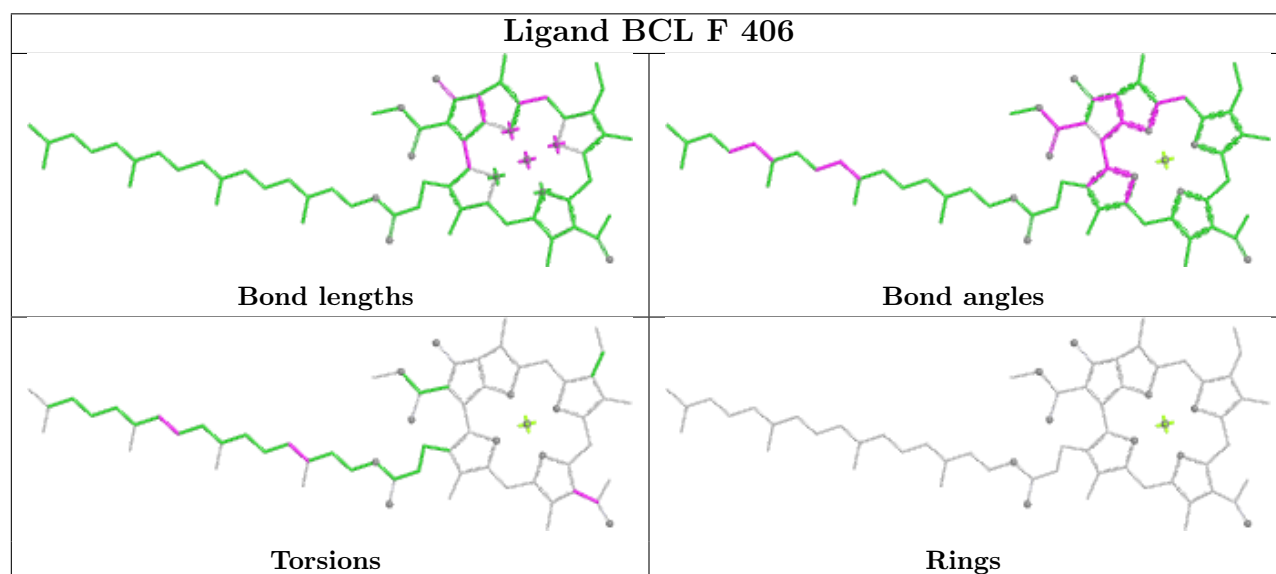
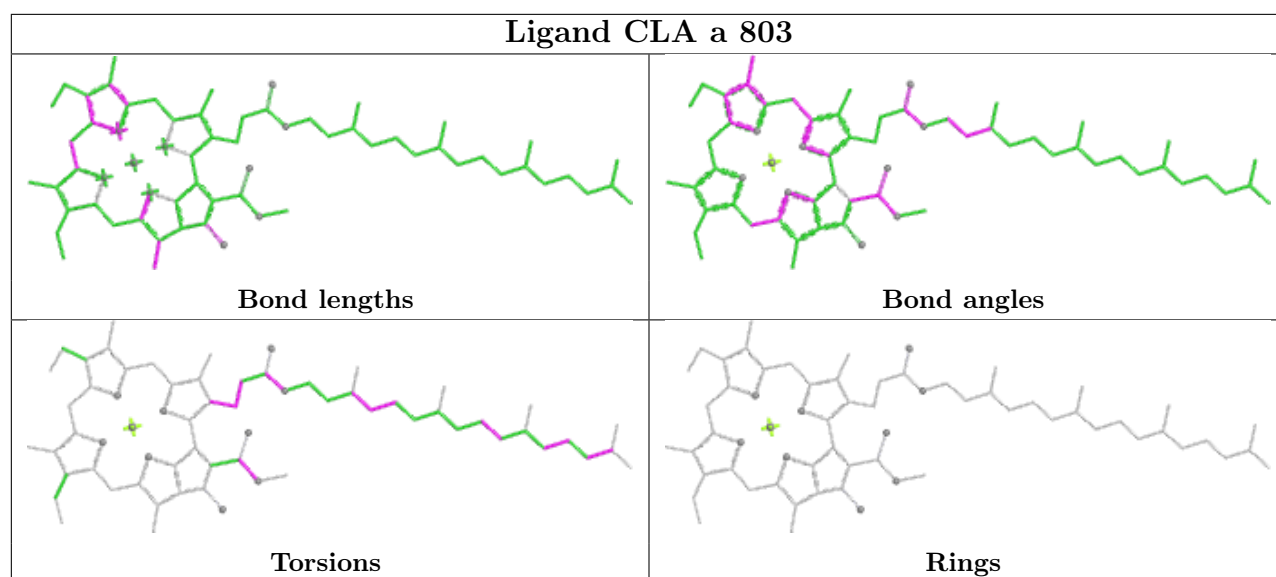


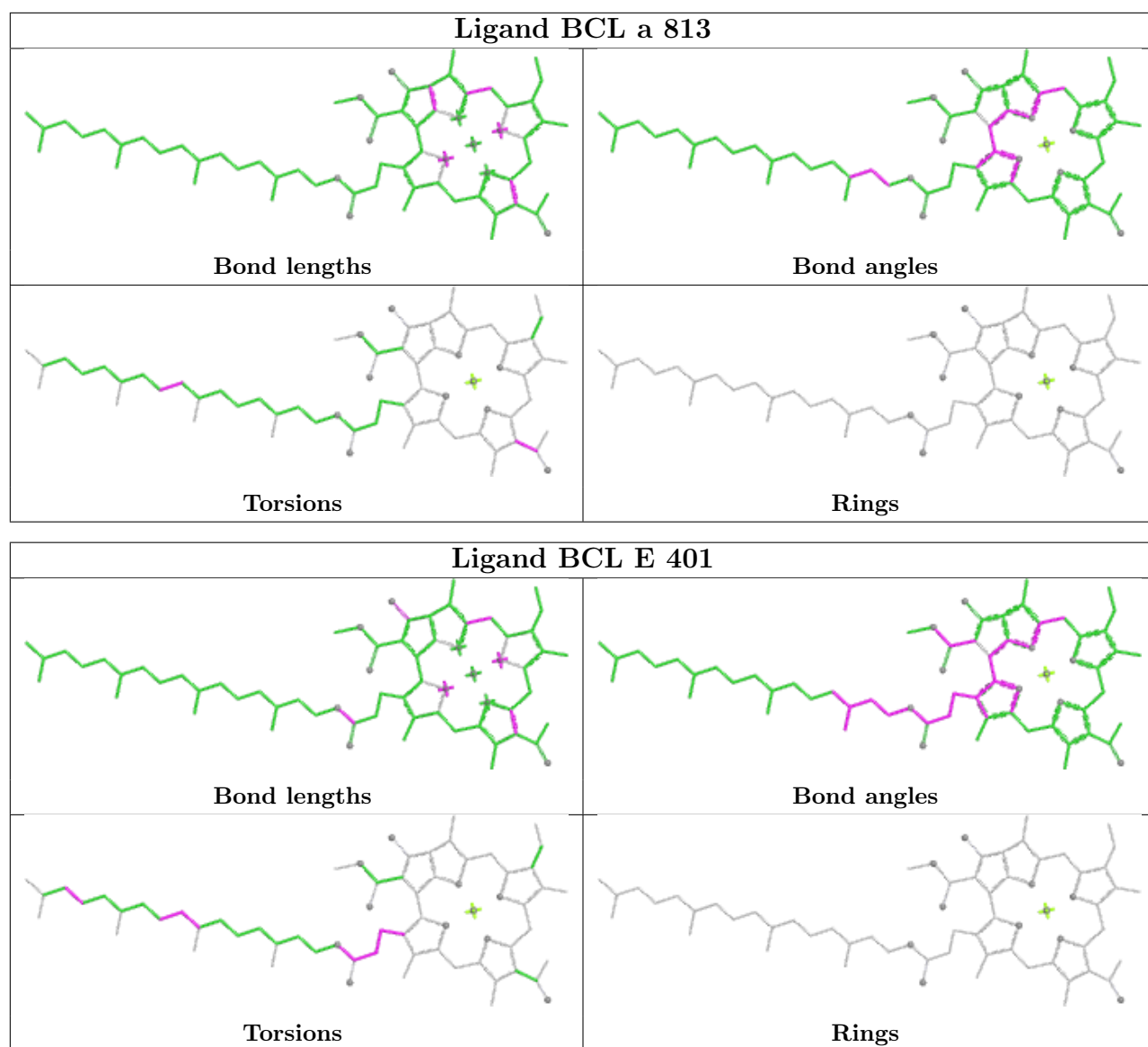
Ligand BCL E 408 (B)

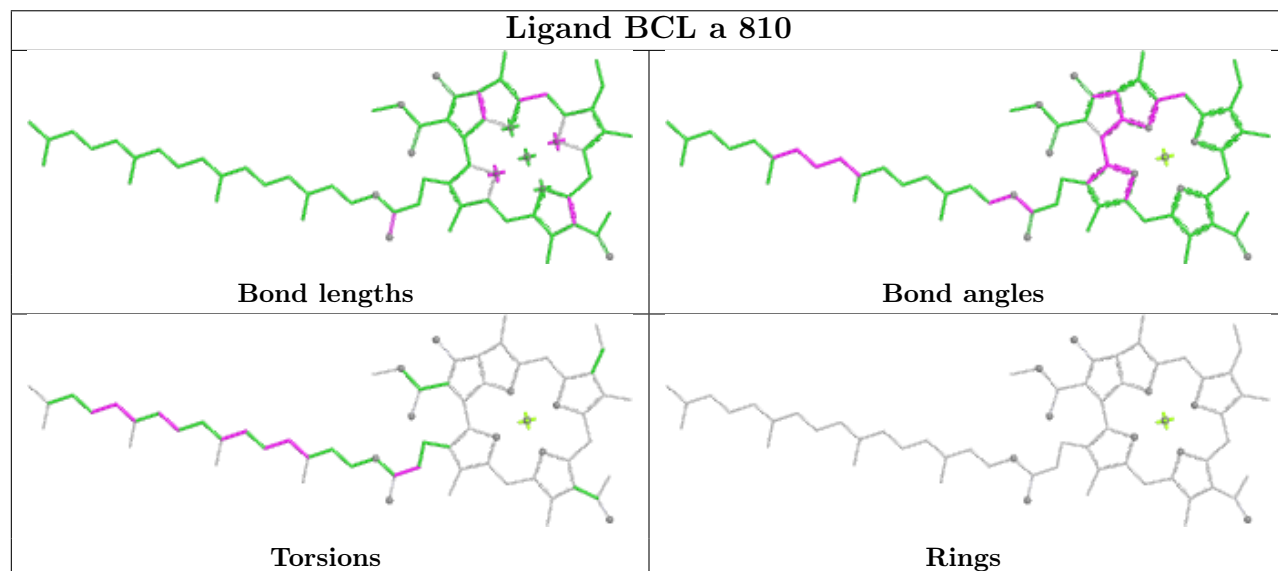
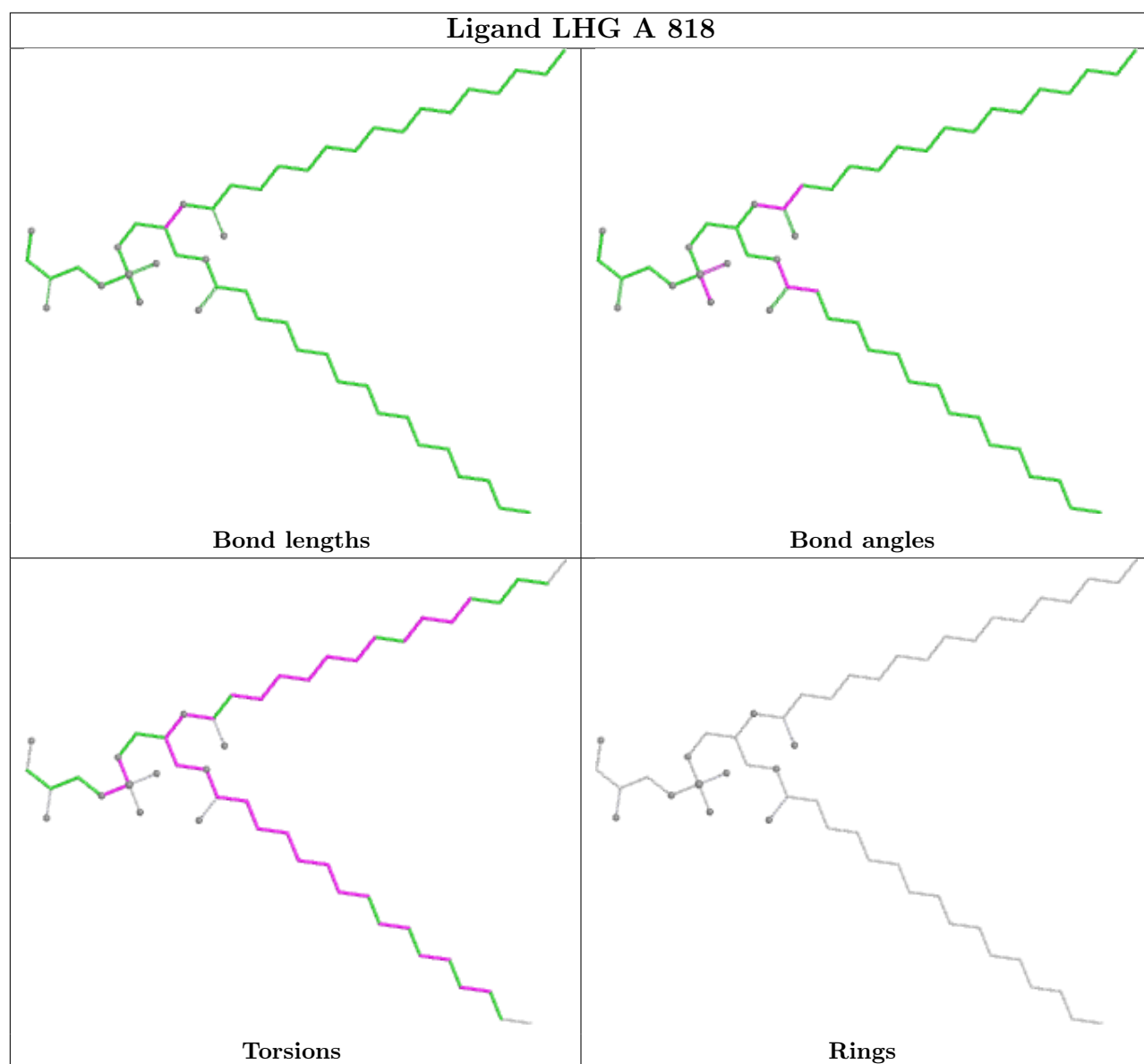


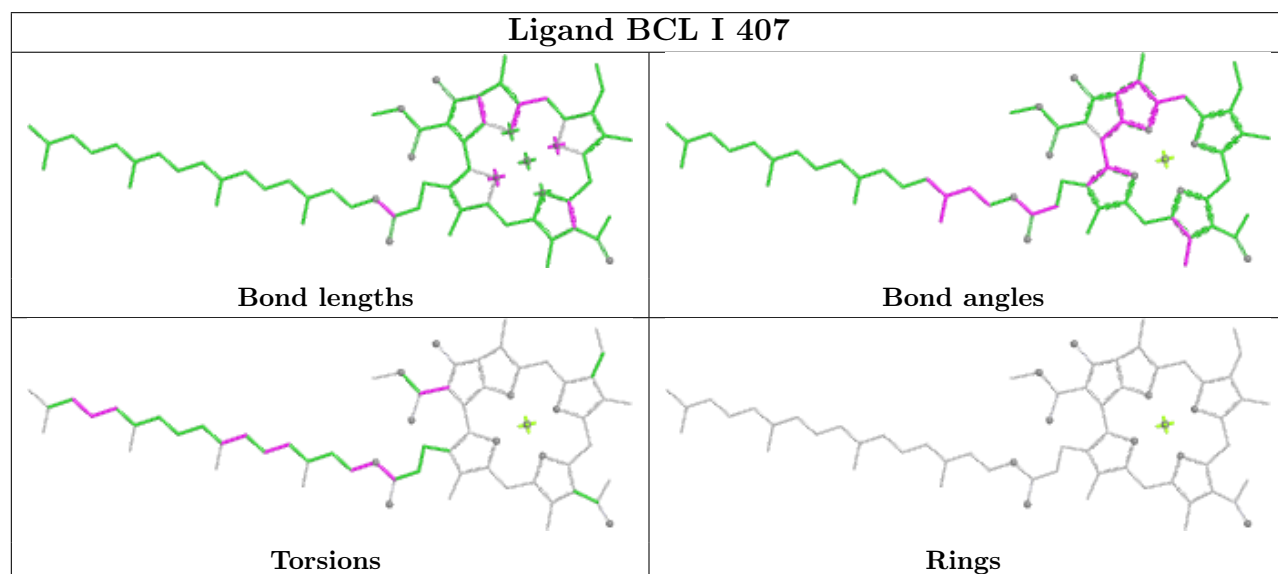
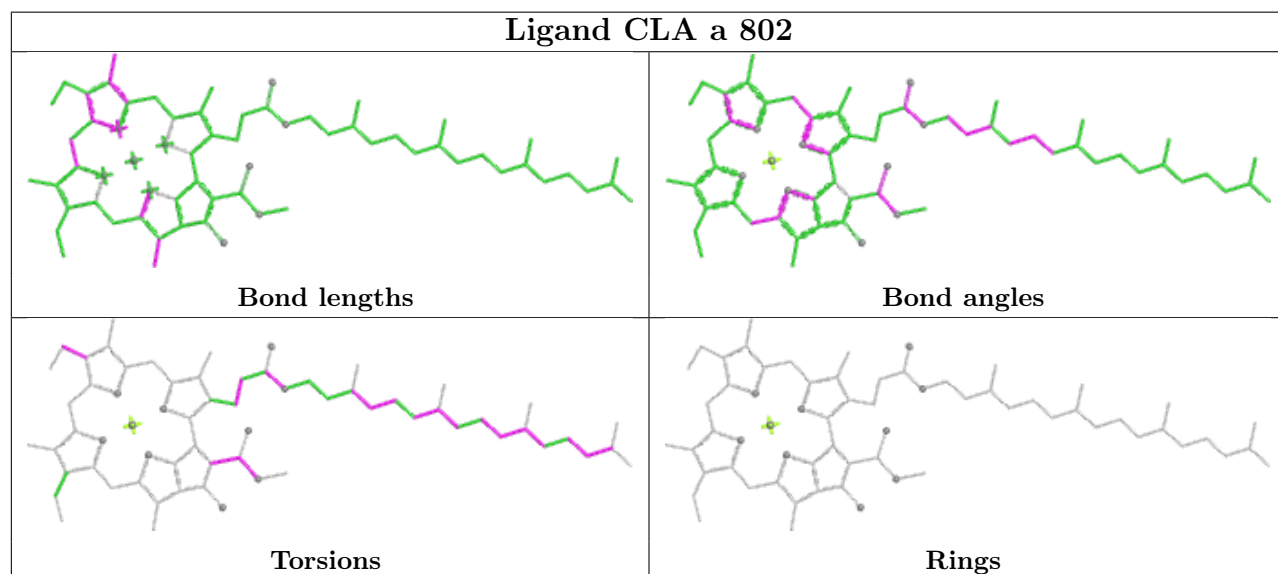
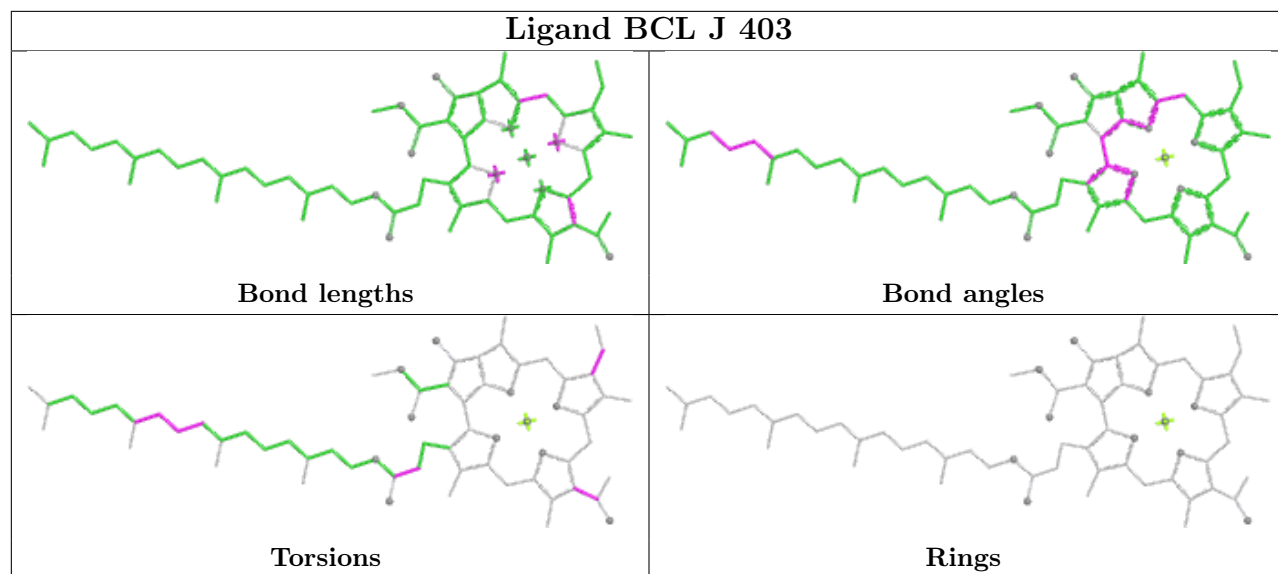
Ligand BCL I 406

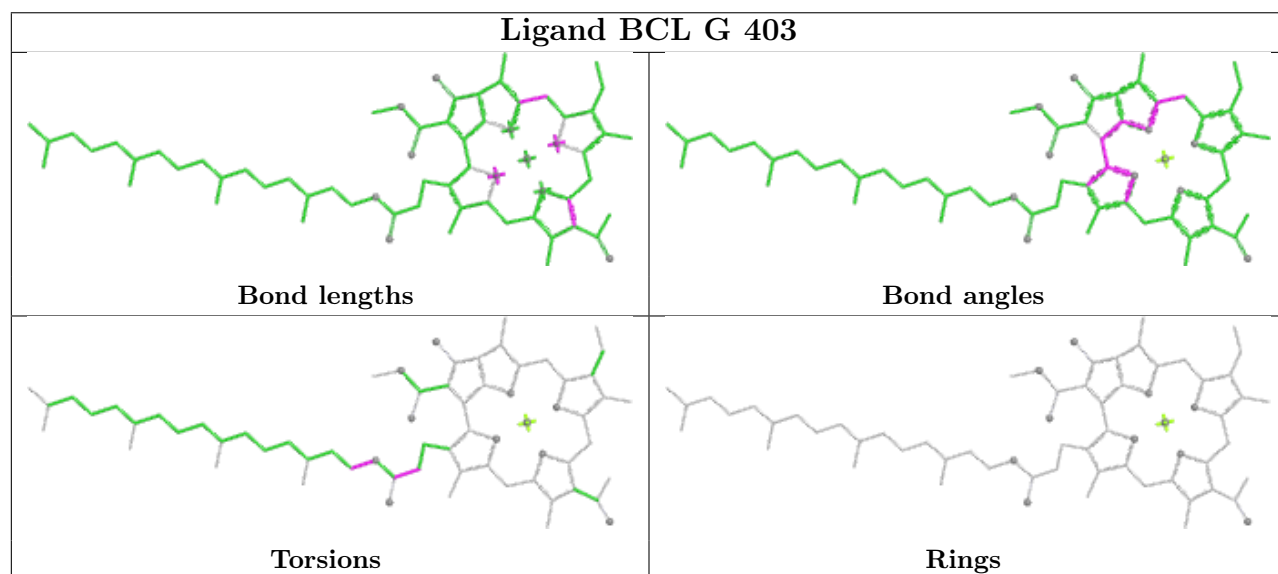
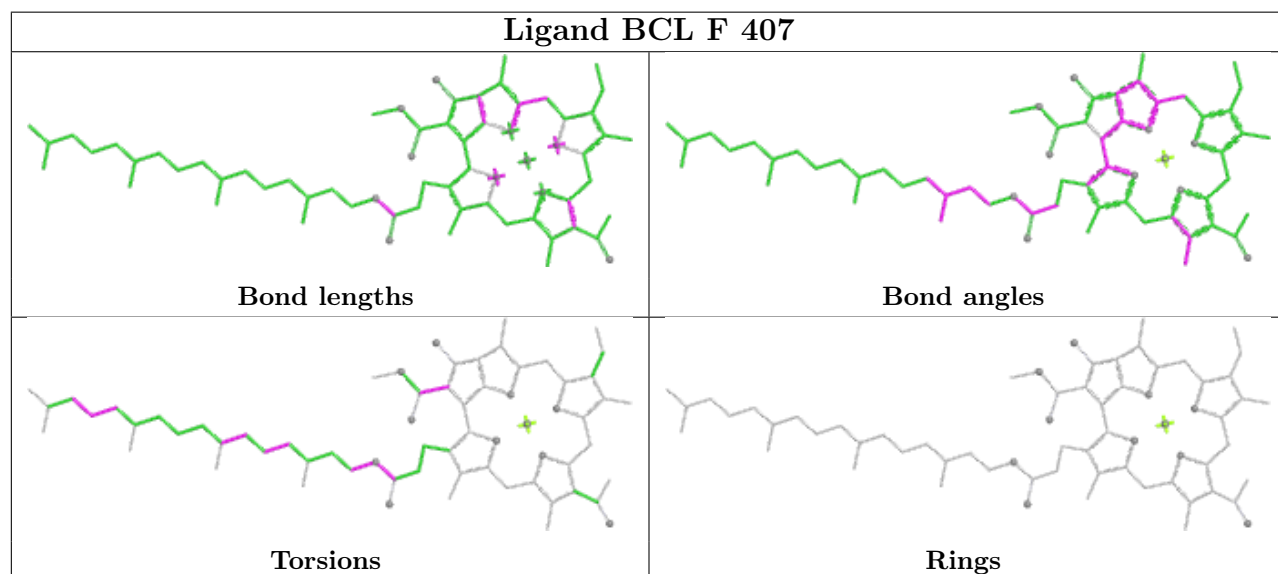
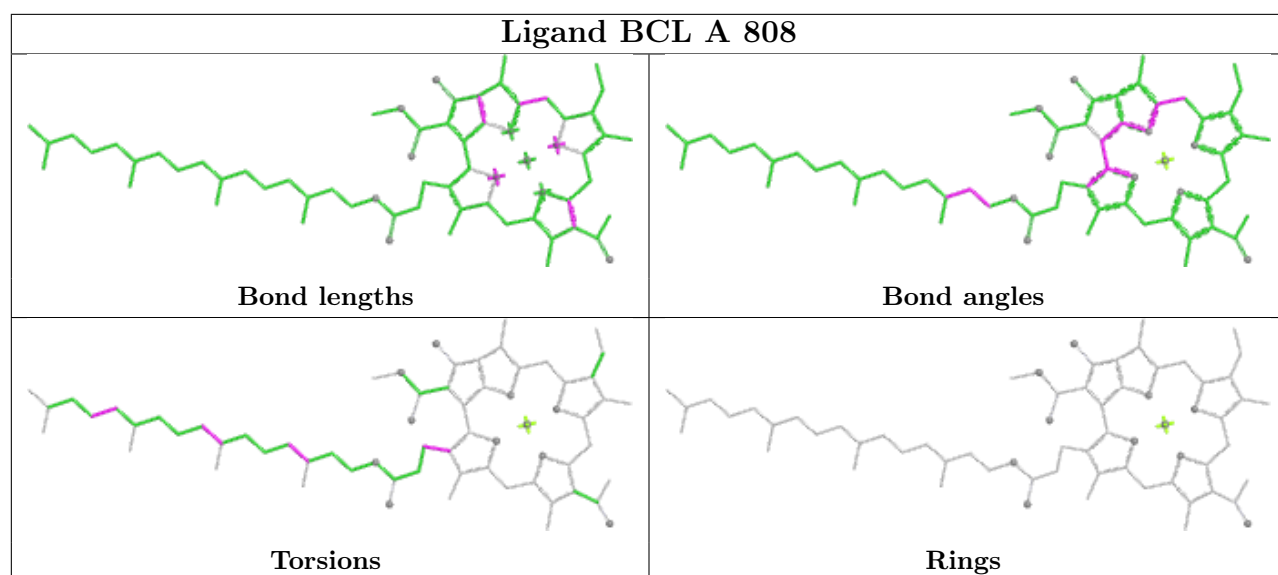


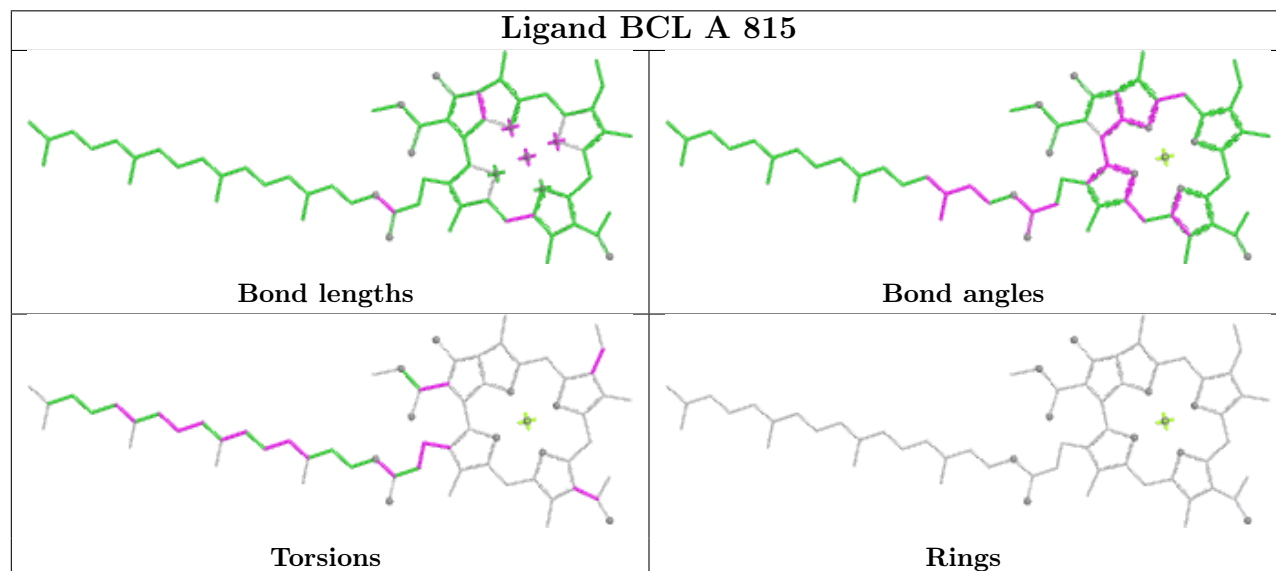
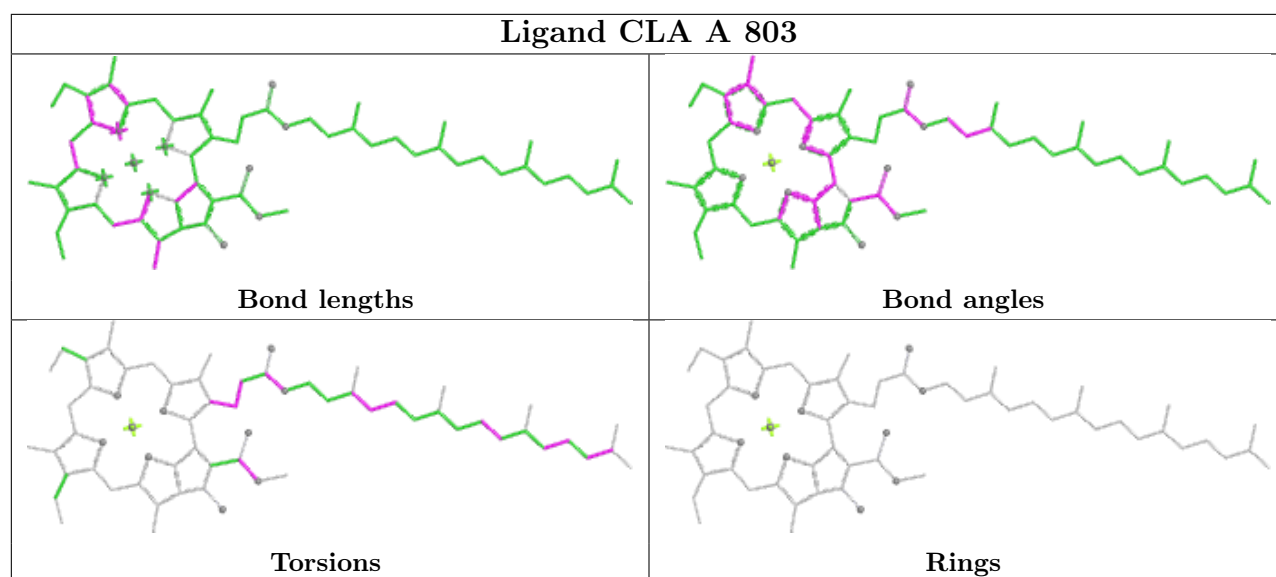


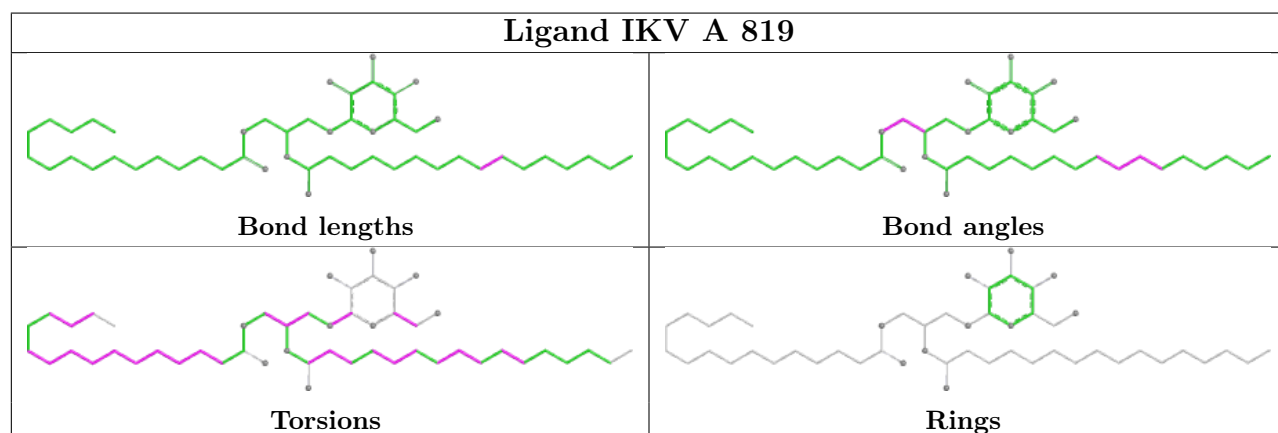
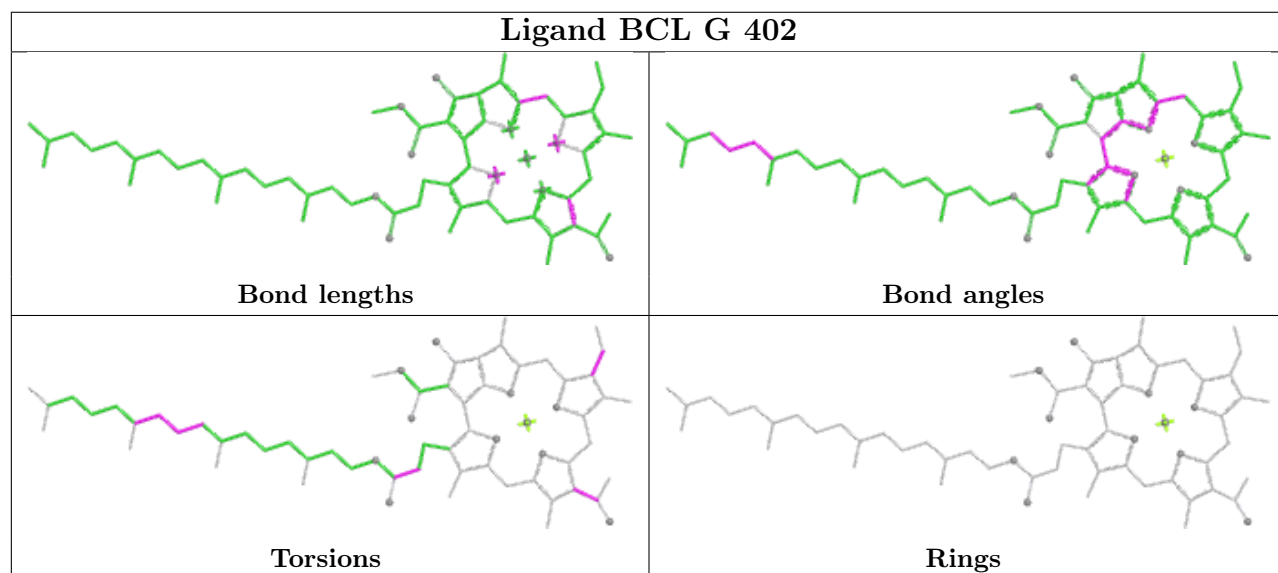
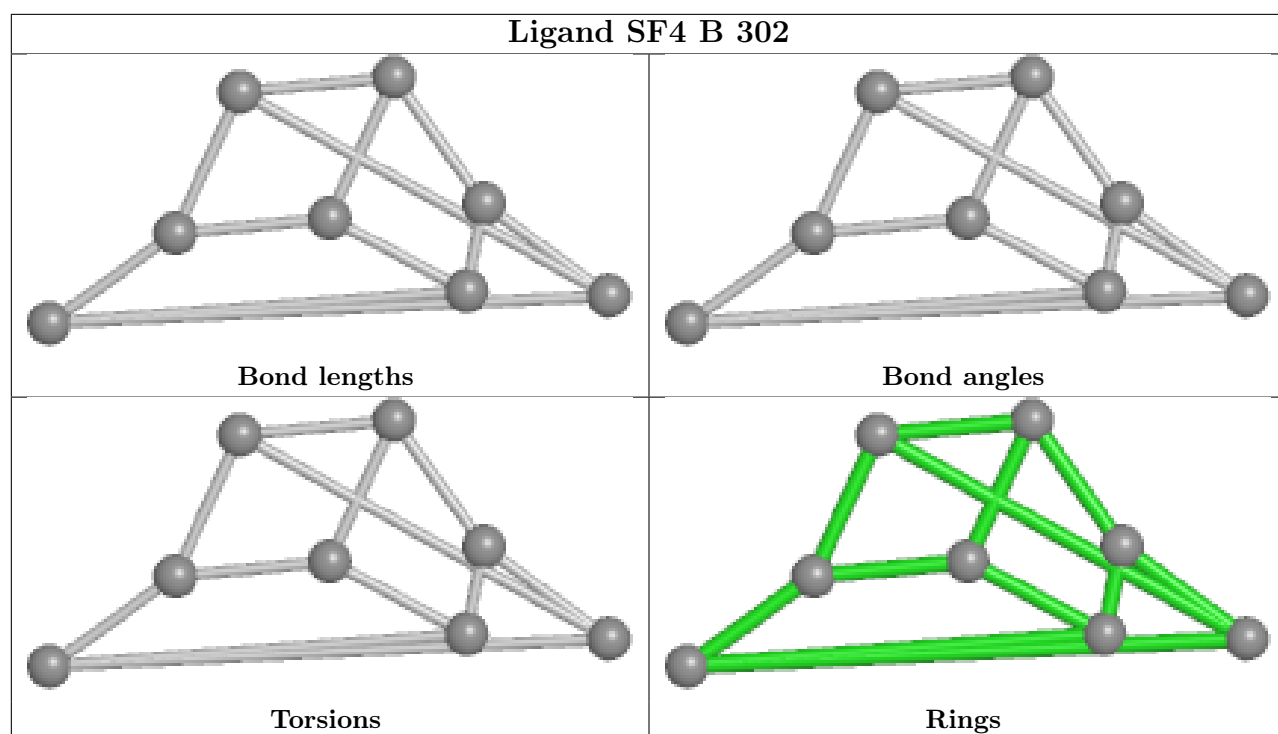


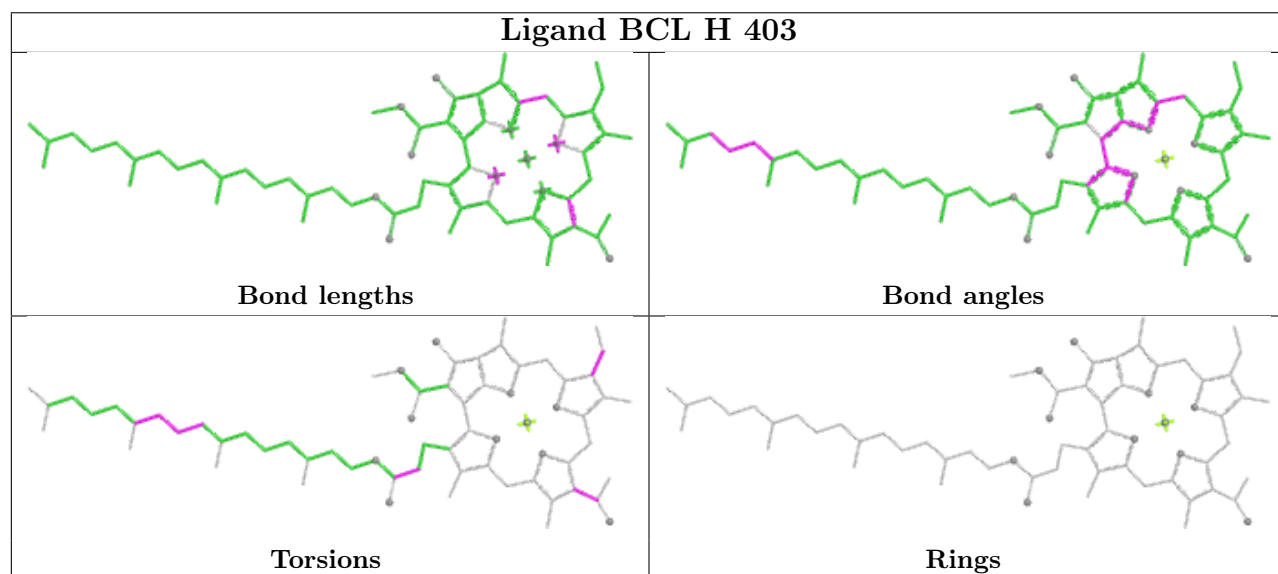
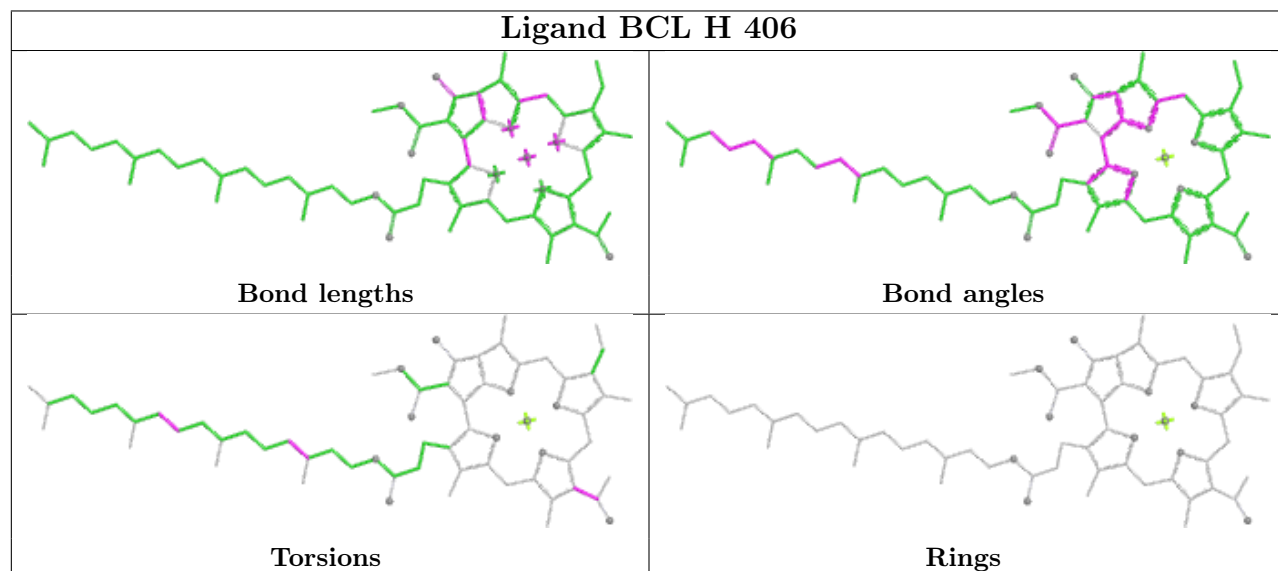
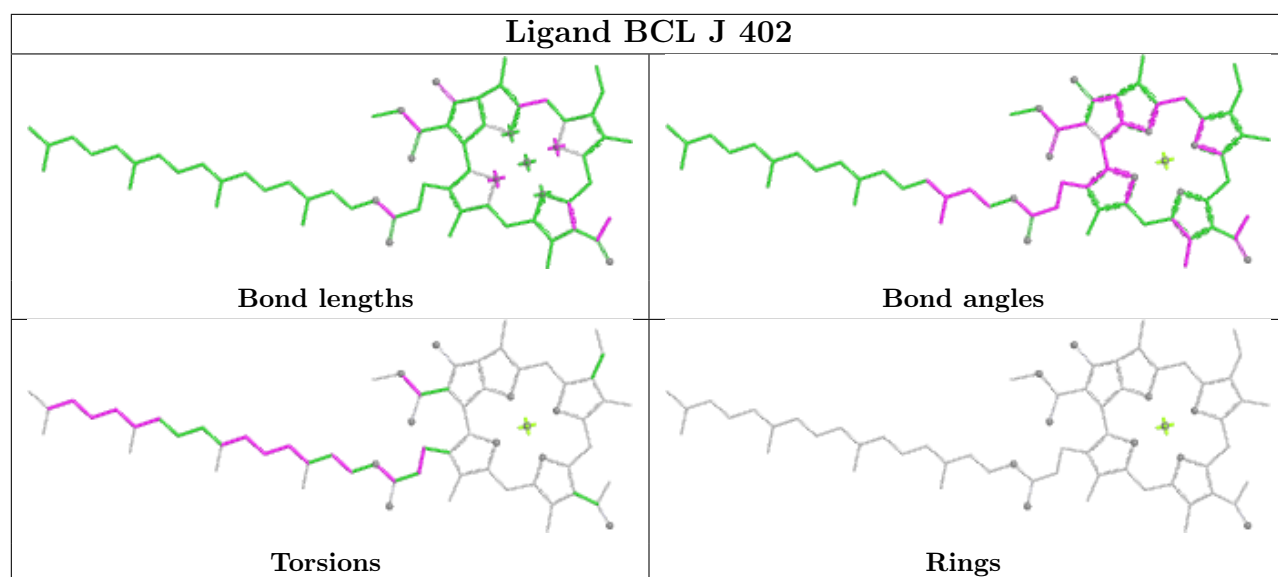


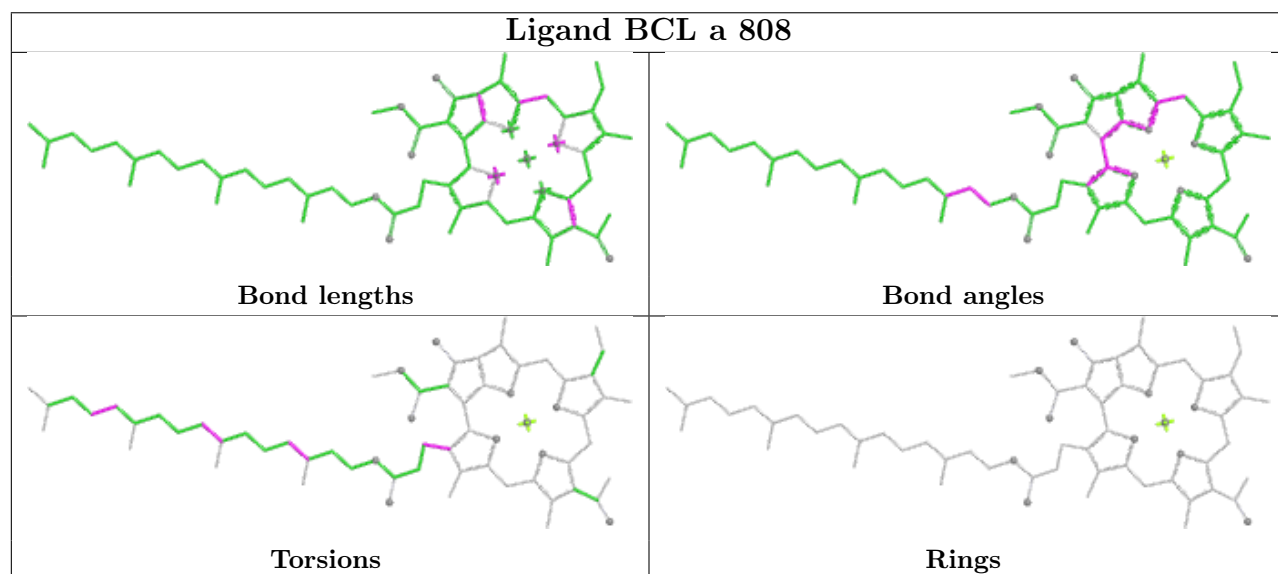
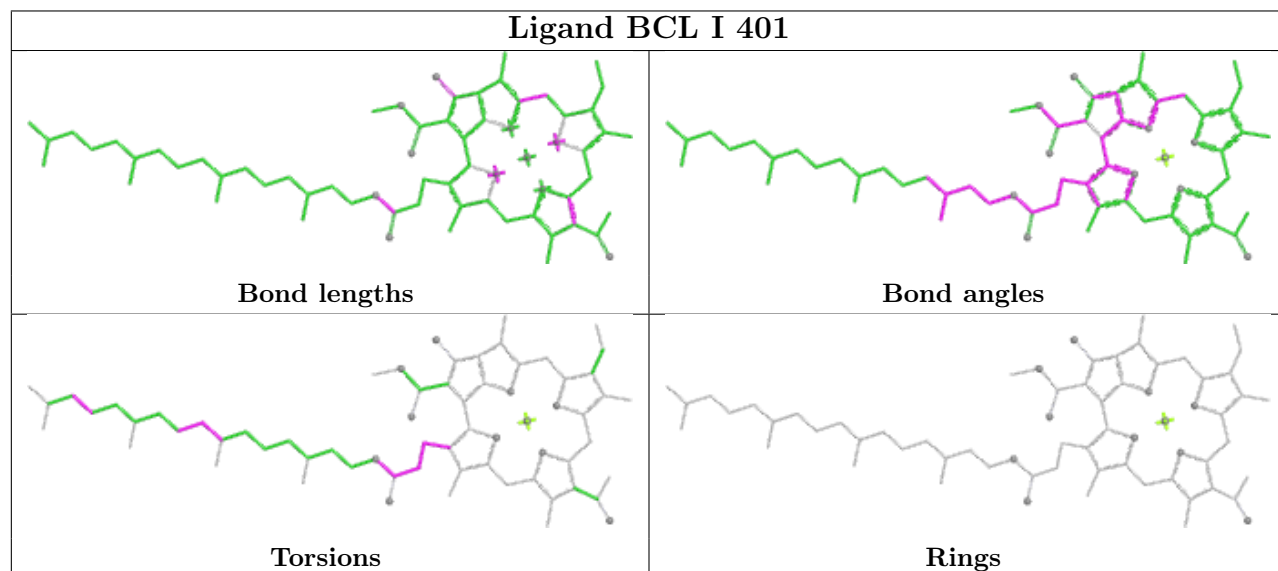
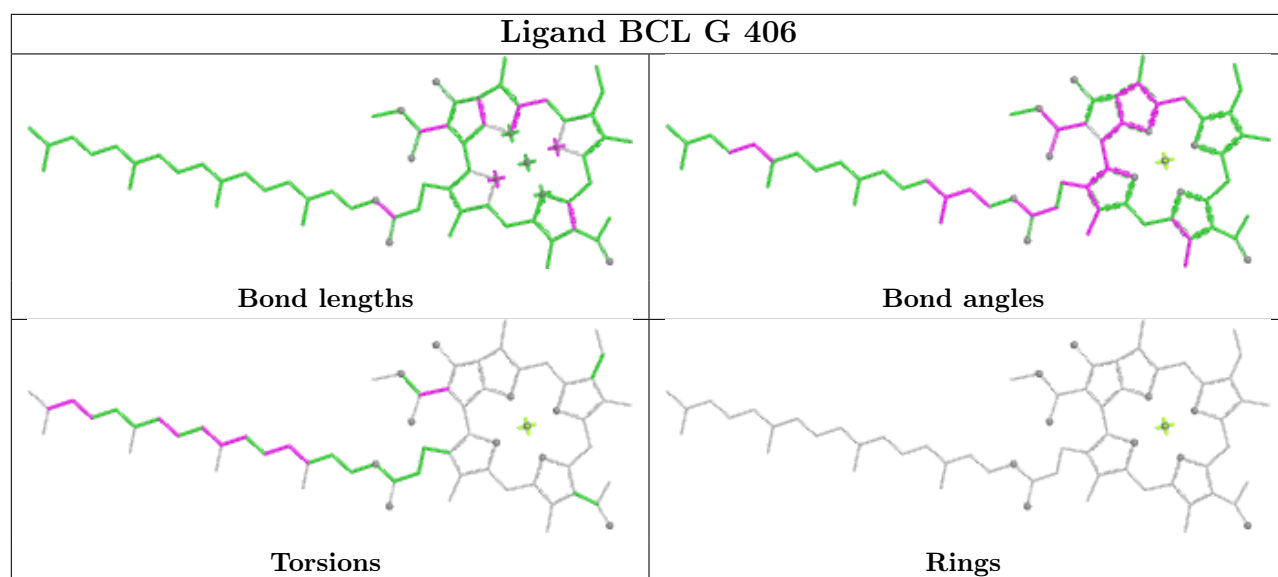


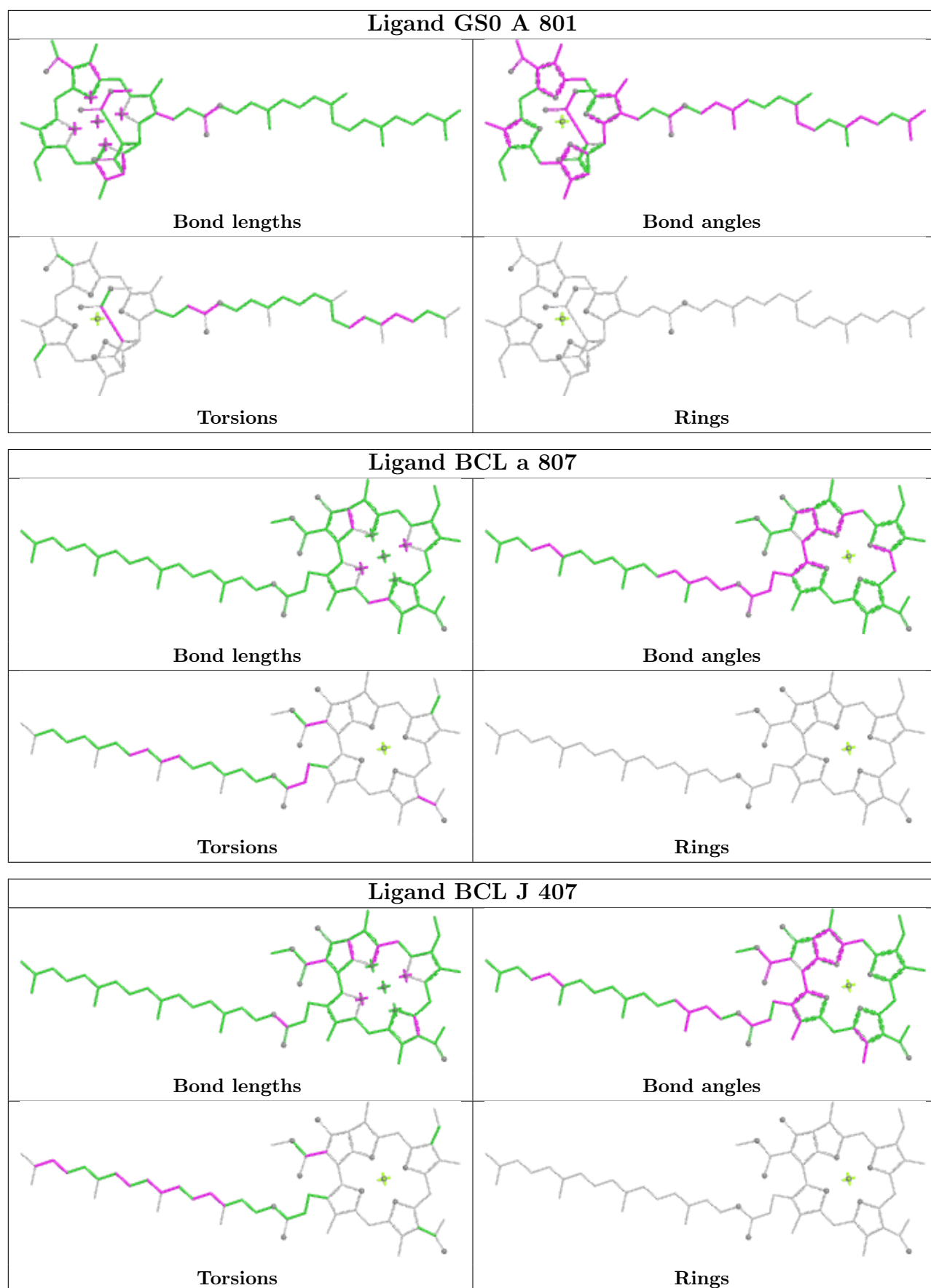


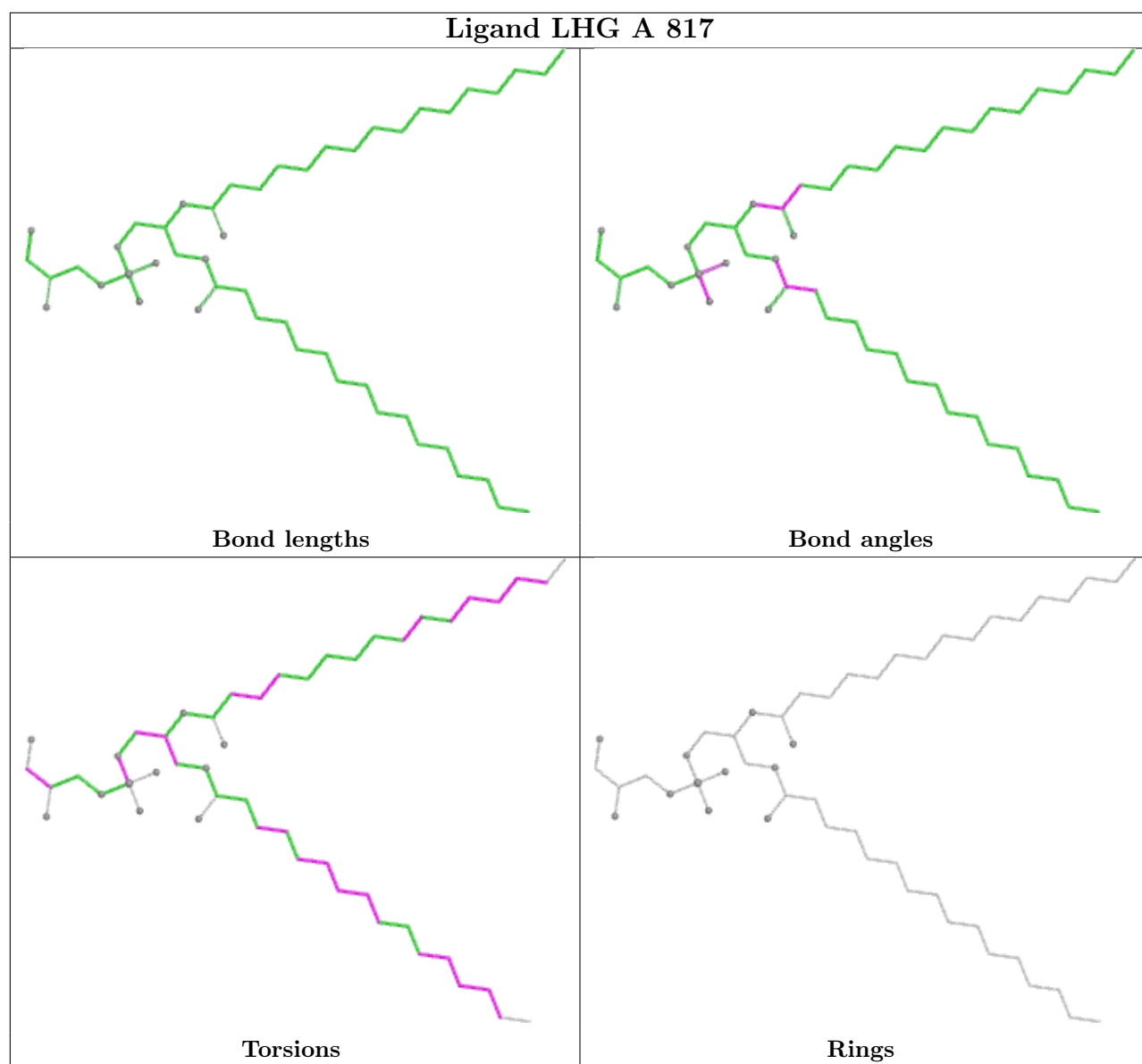


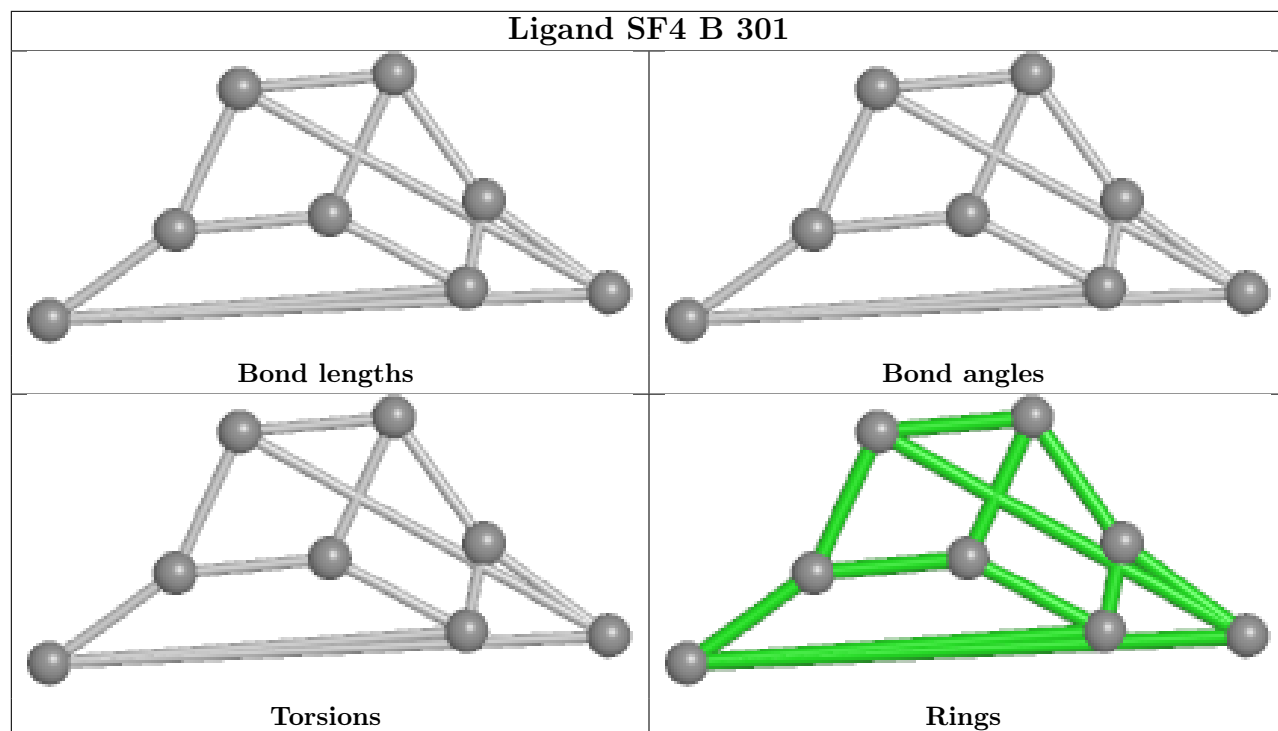




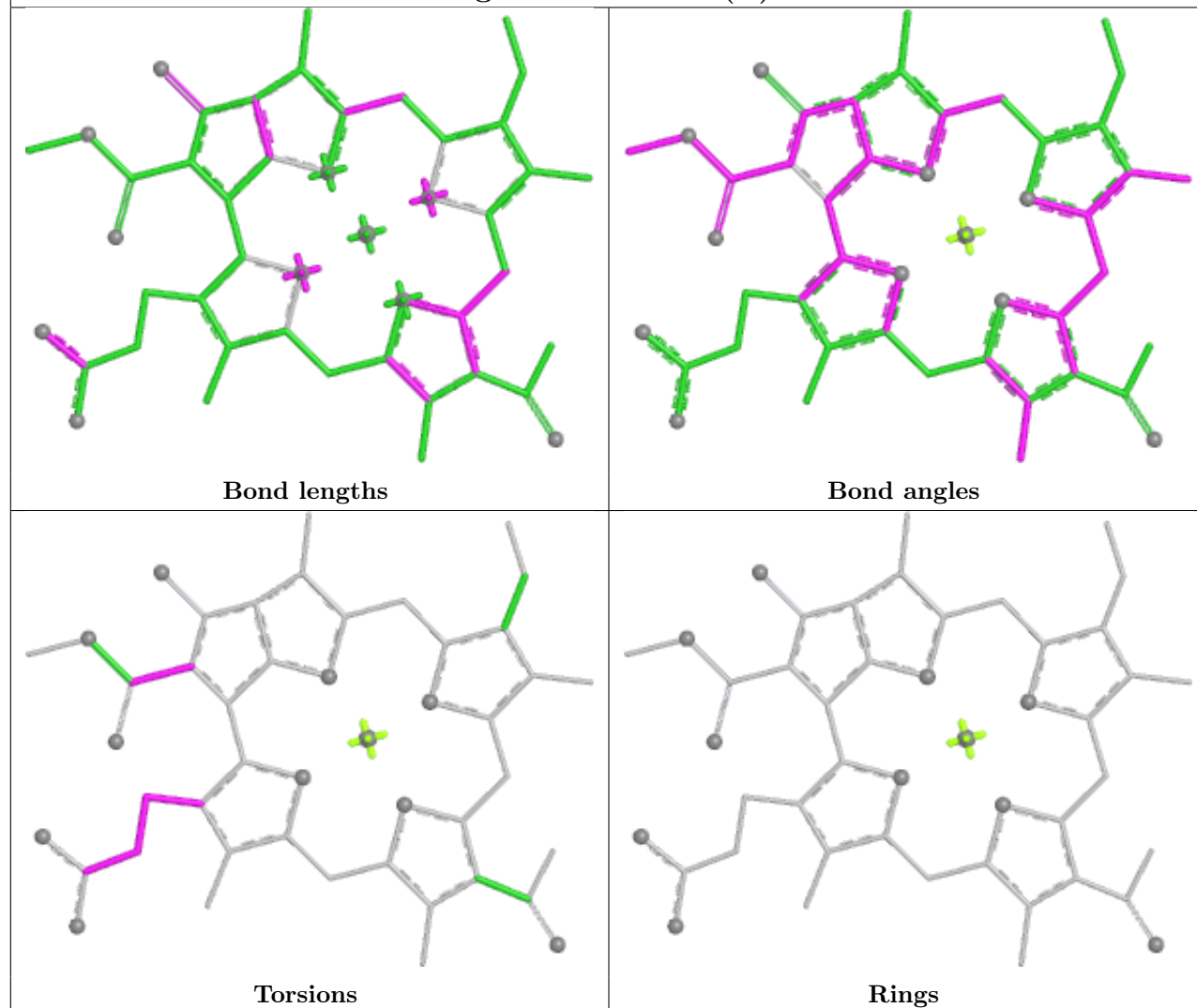




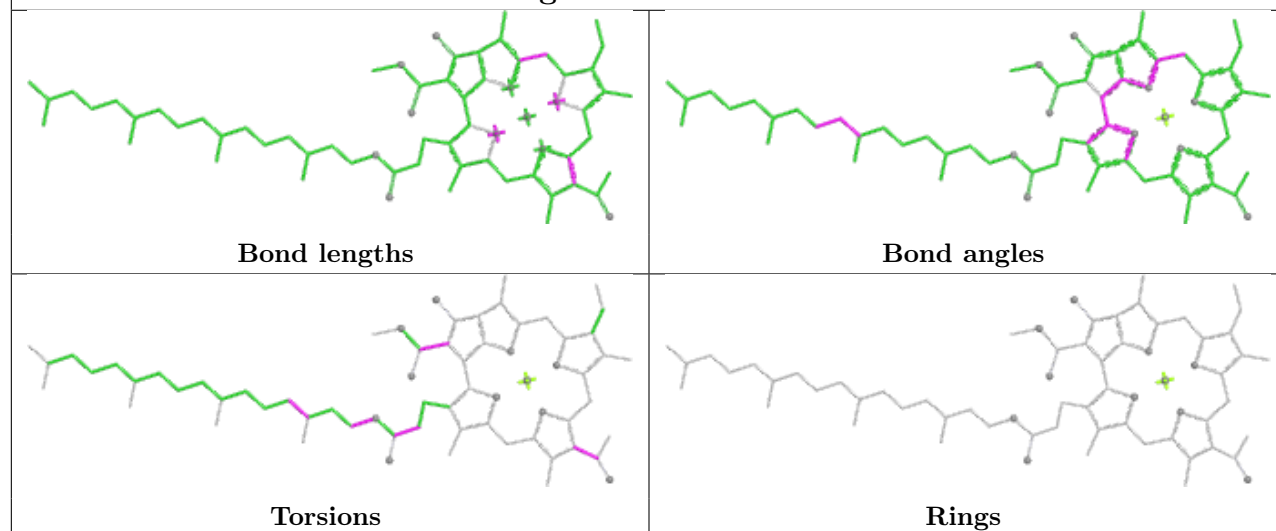


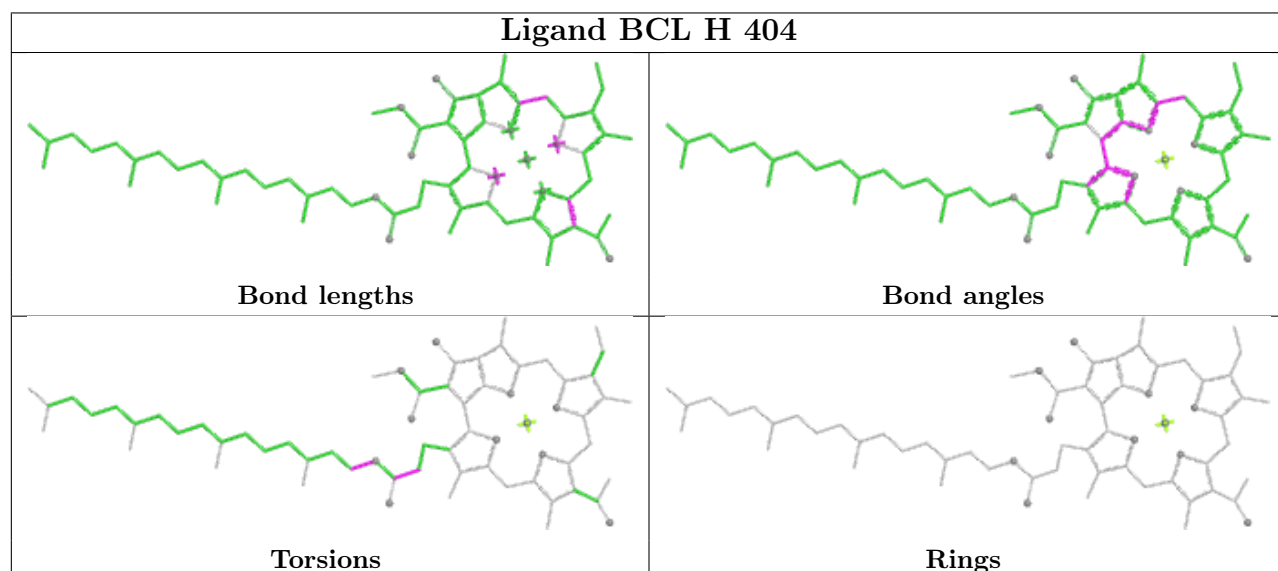
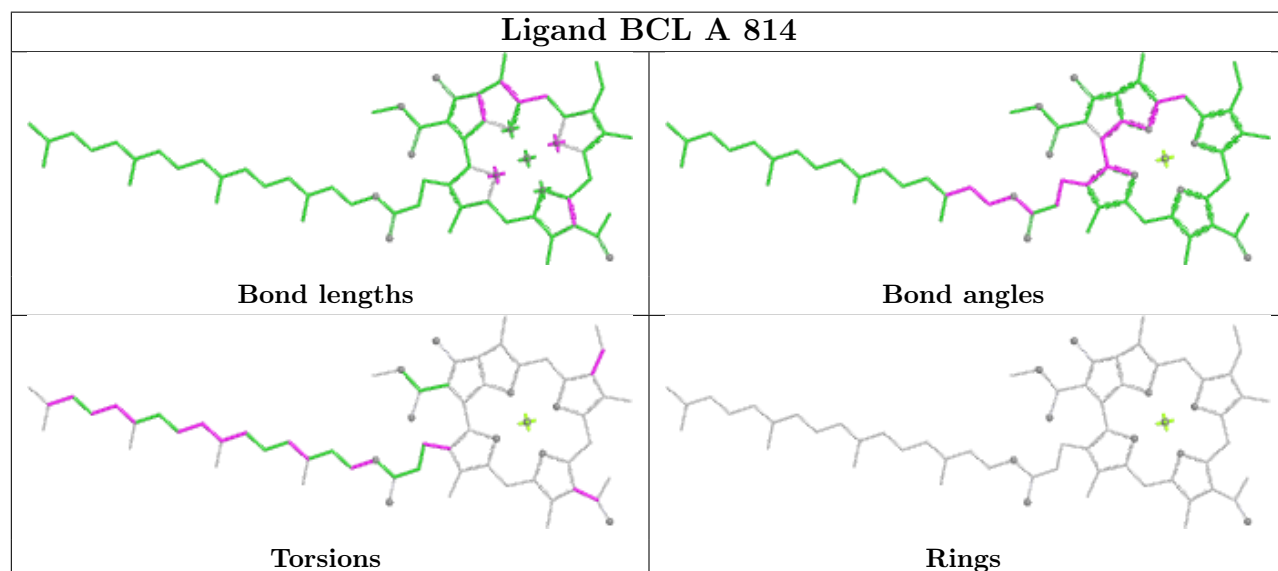
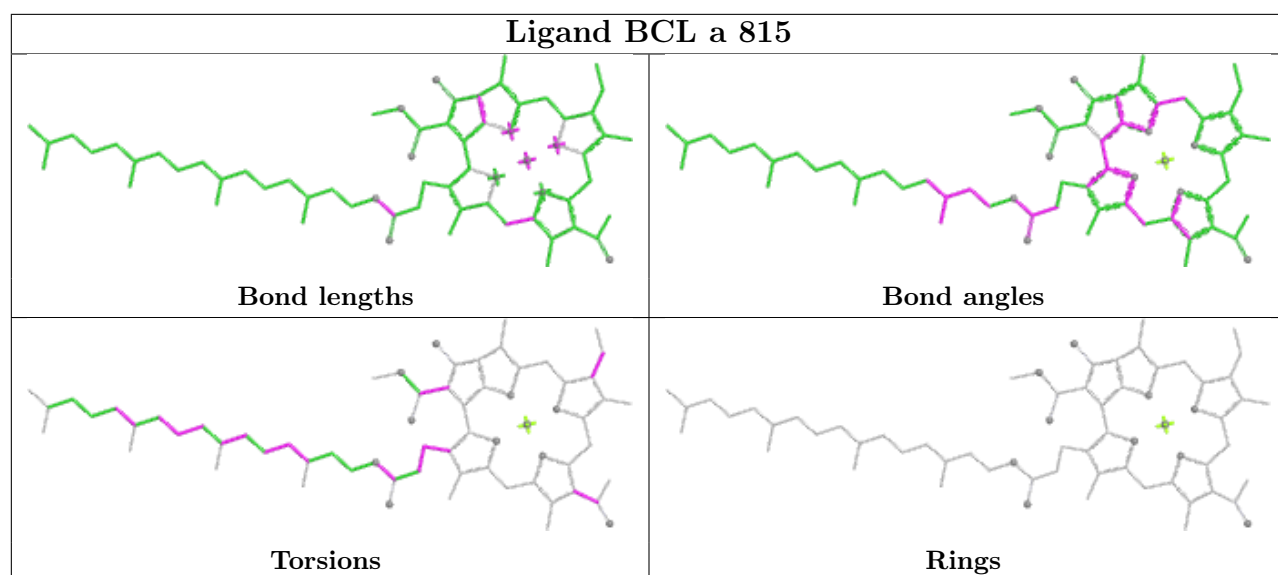


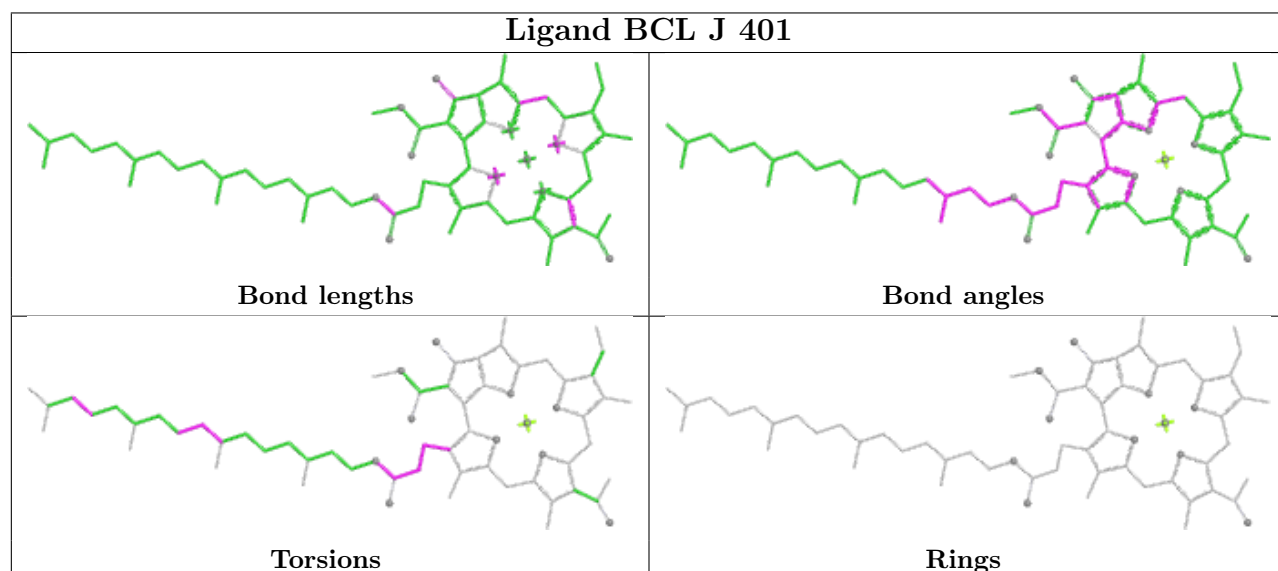
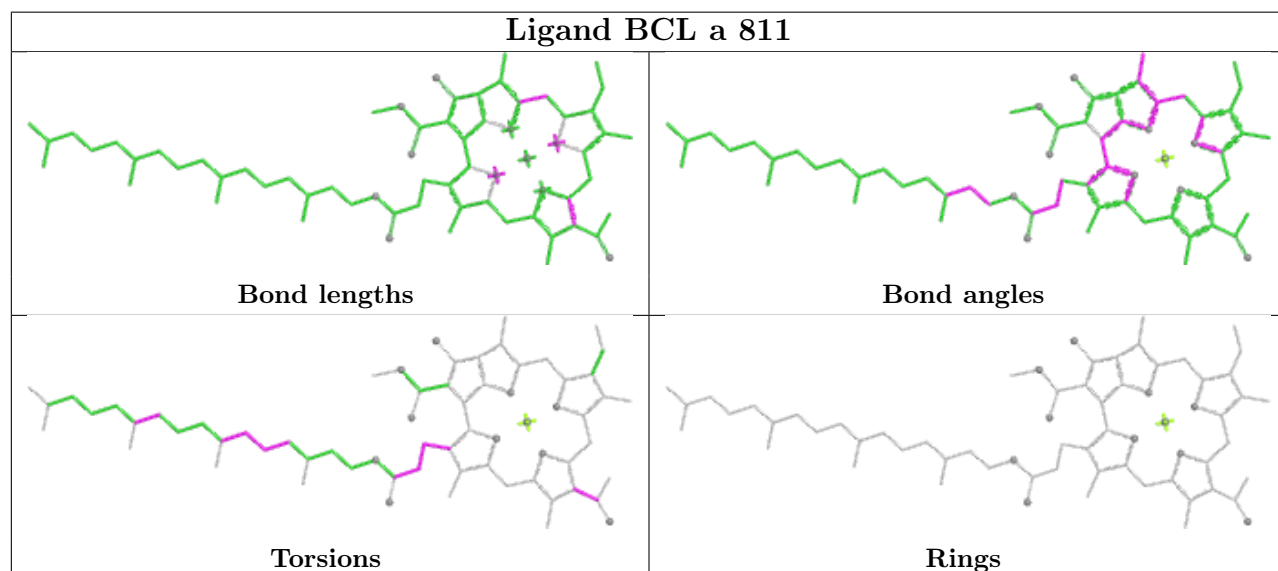
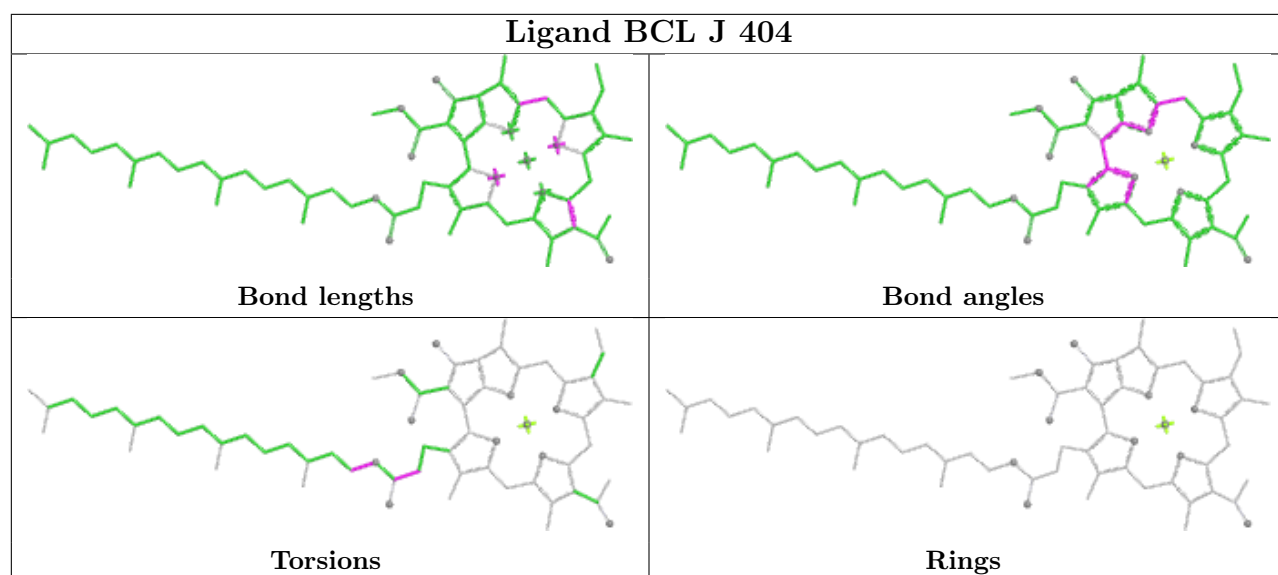
Ligand BCL I 408 (B)

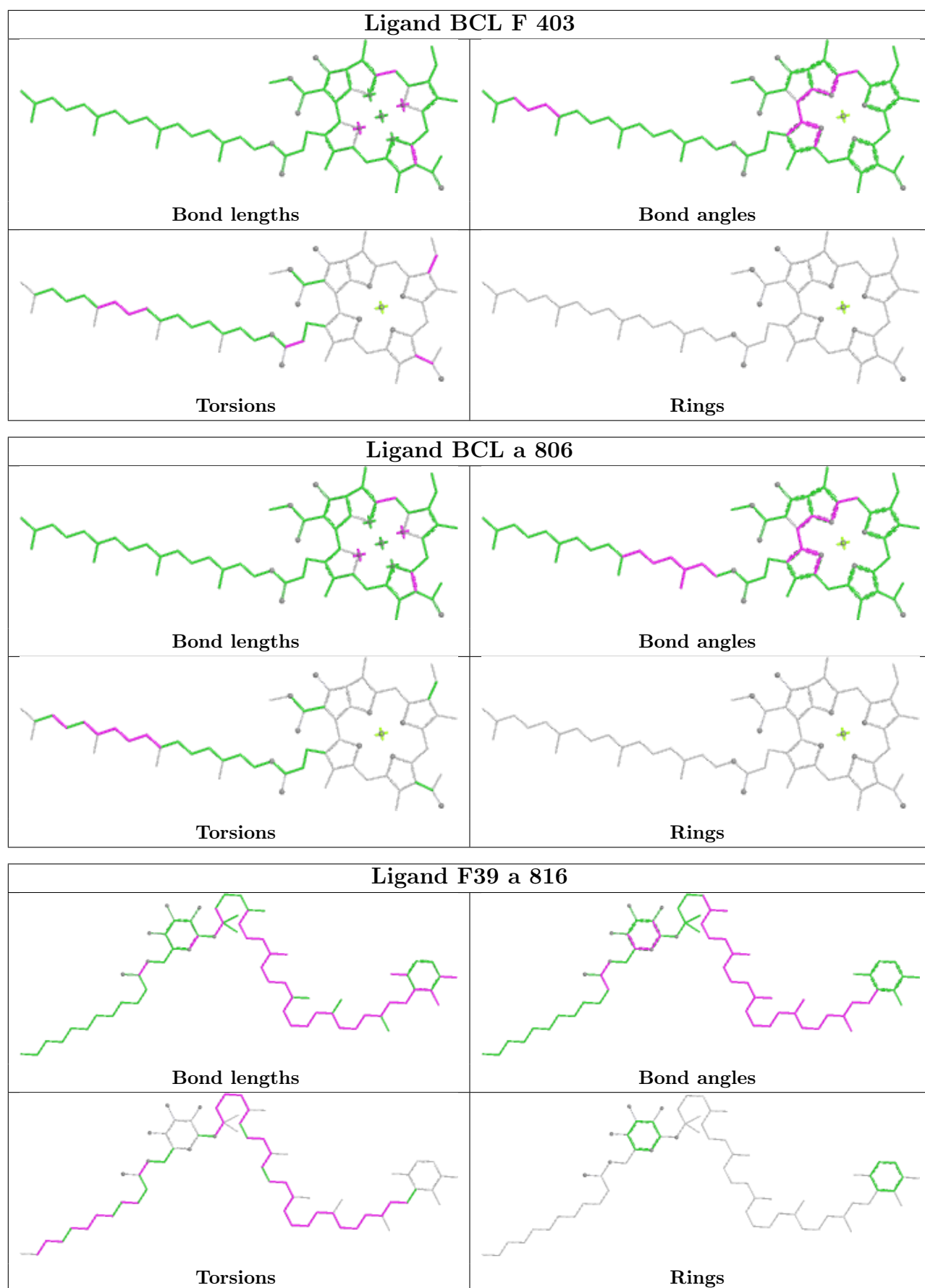


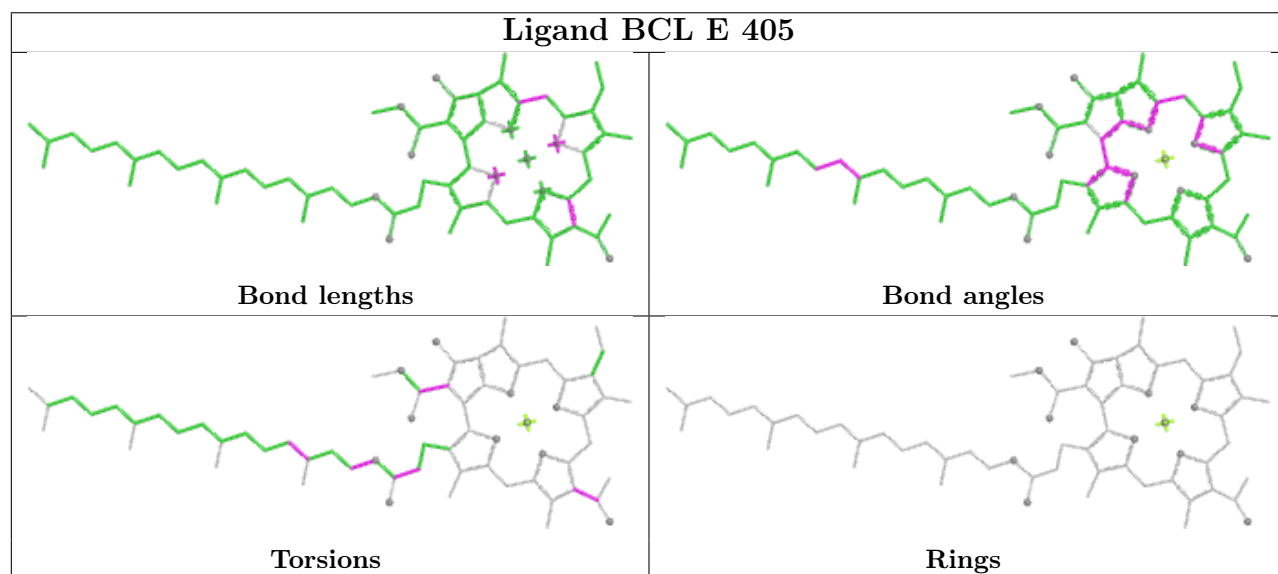
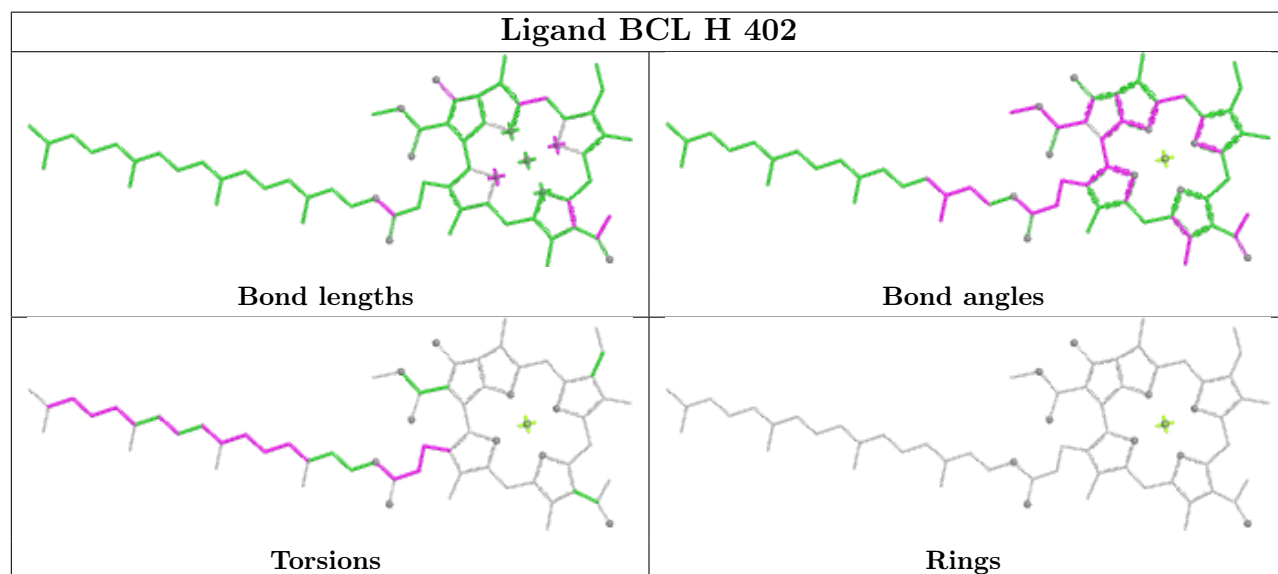
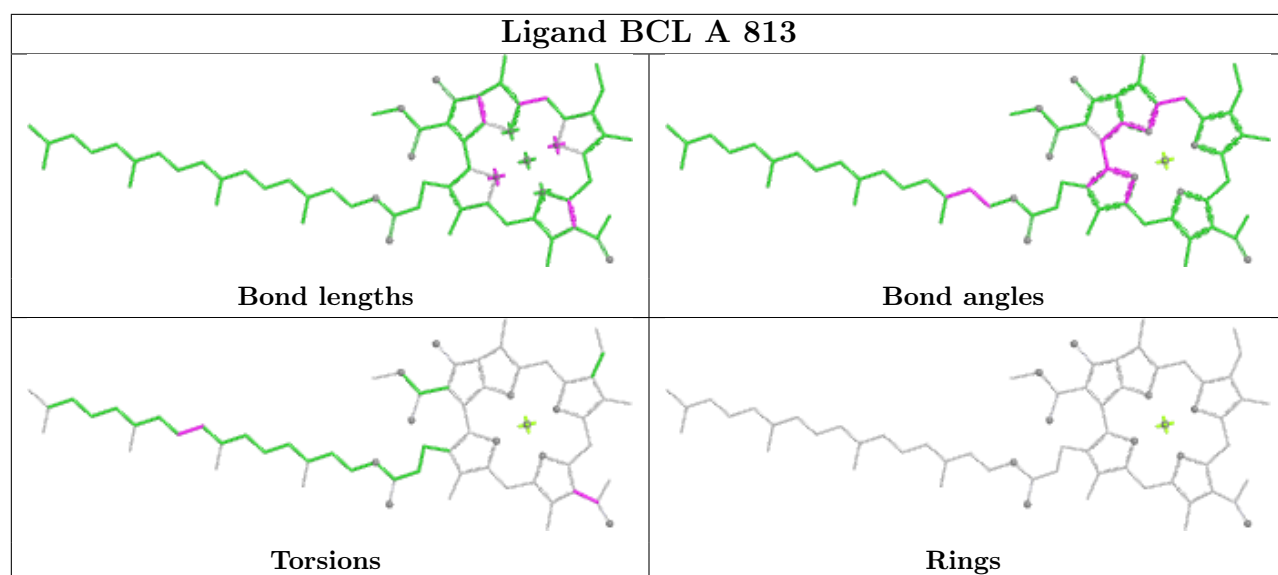
Ligand BCL I 405

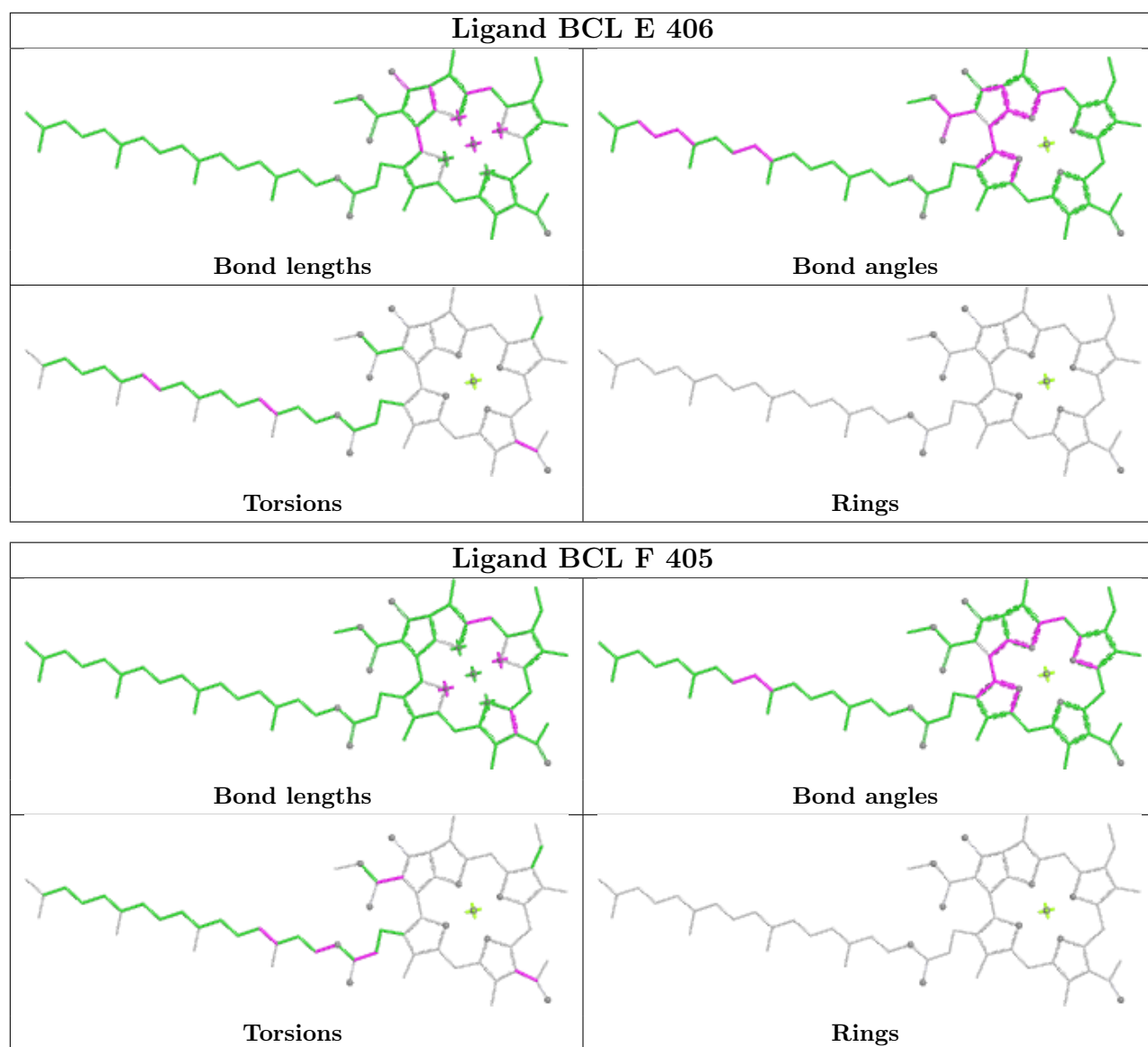




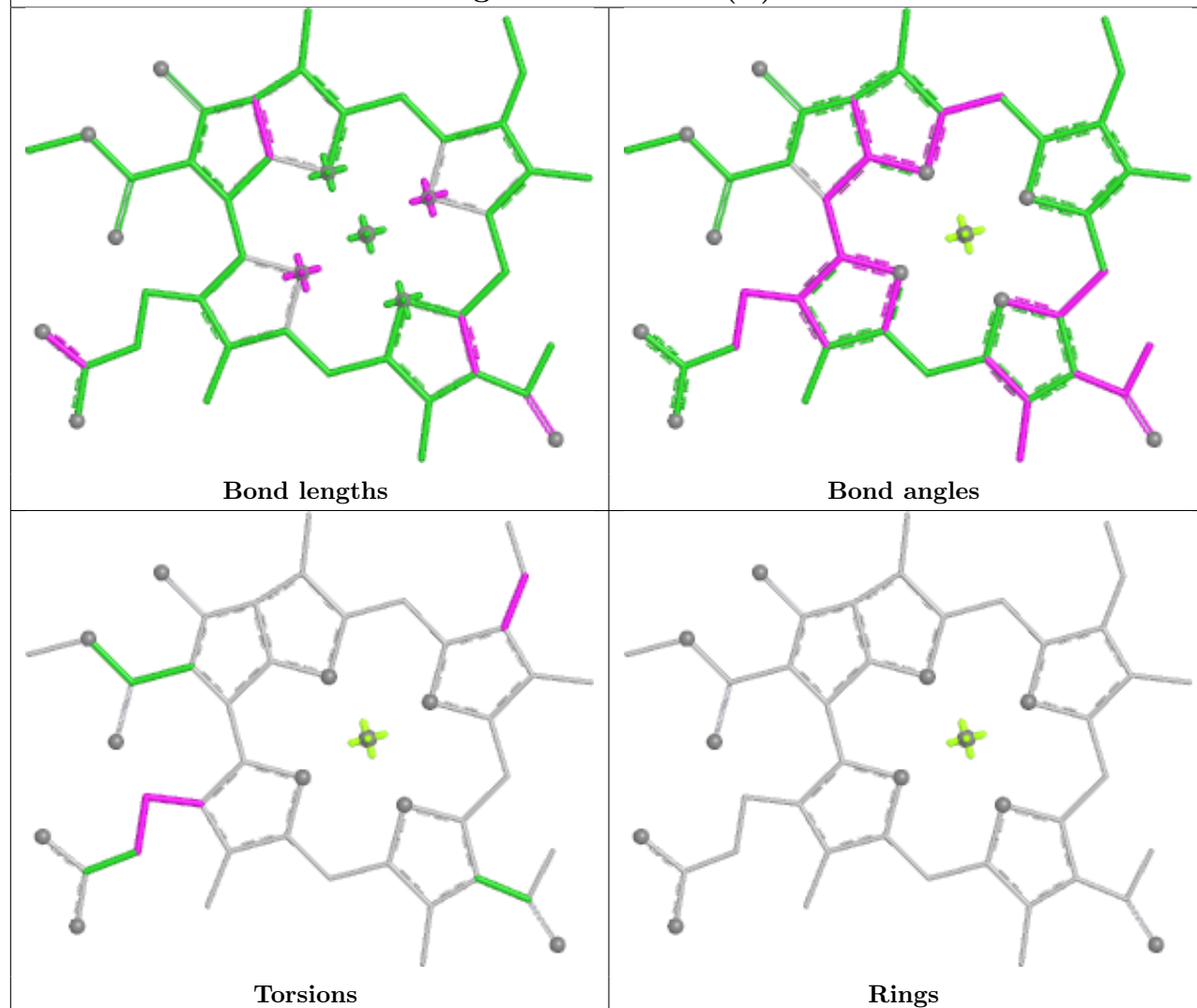




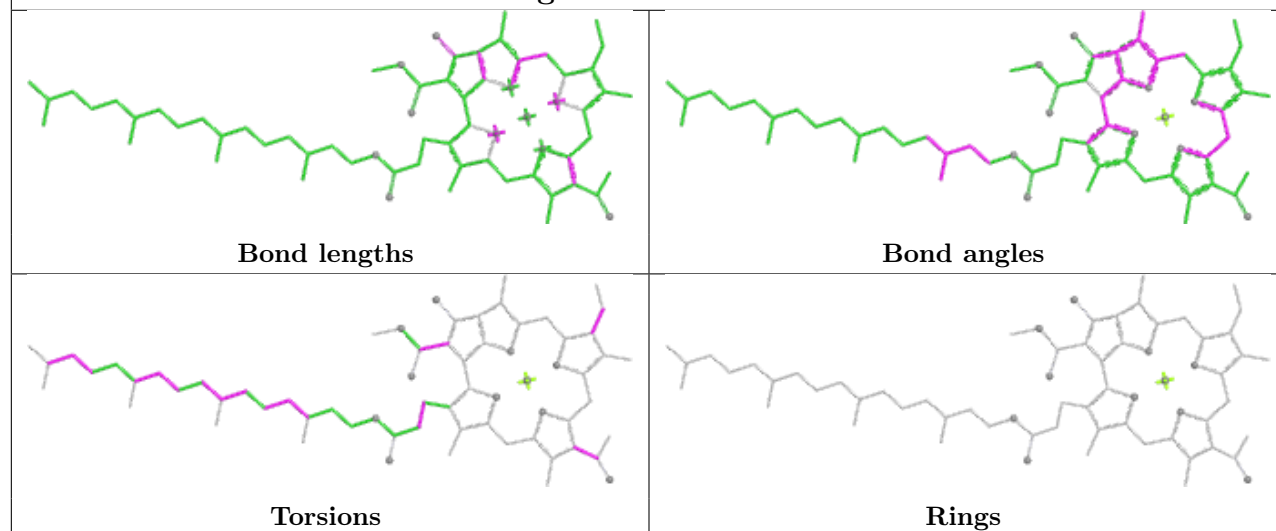


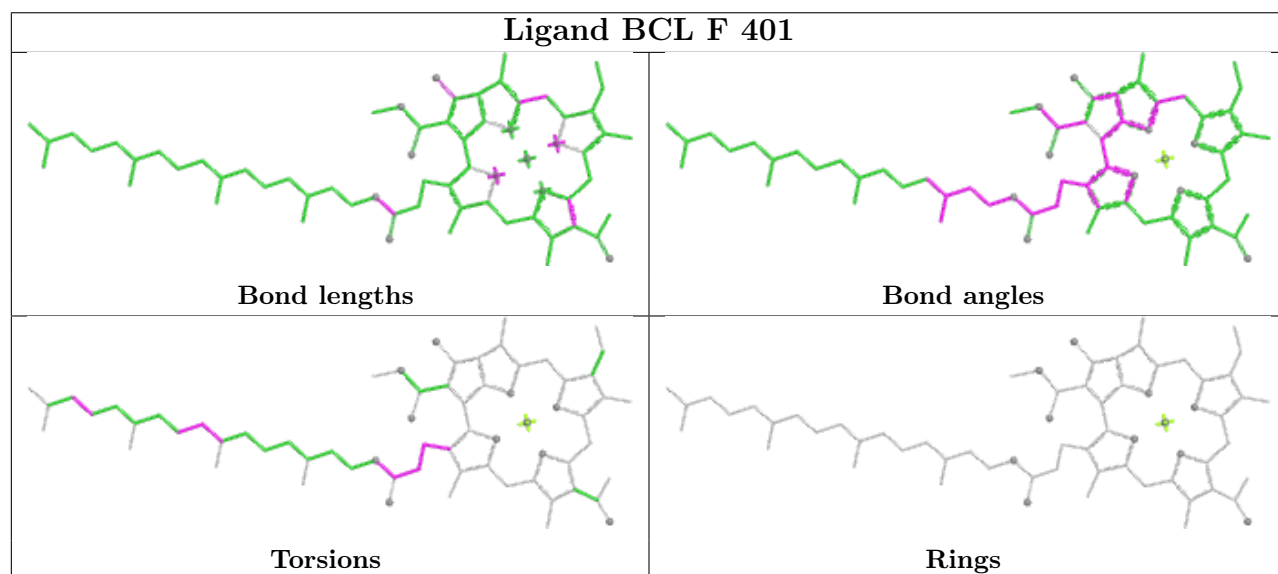
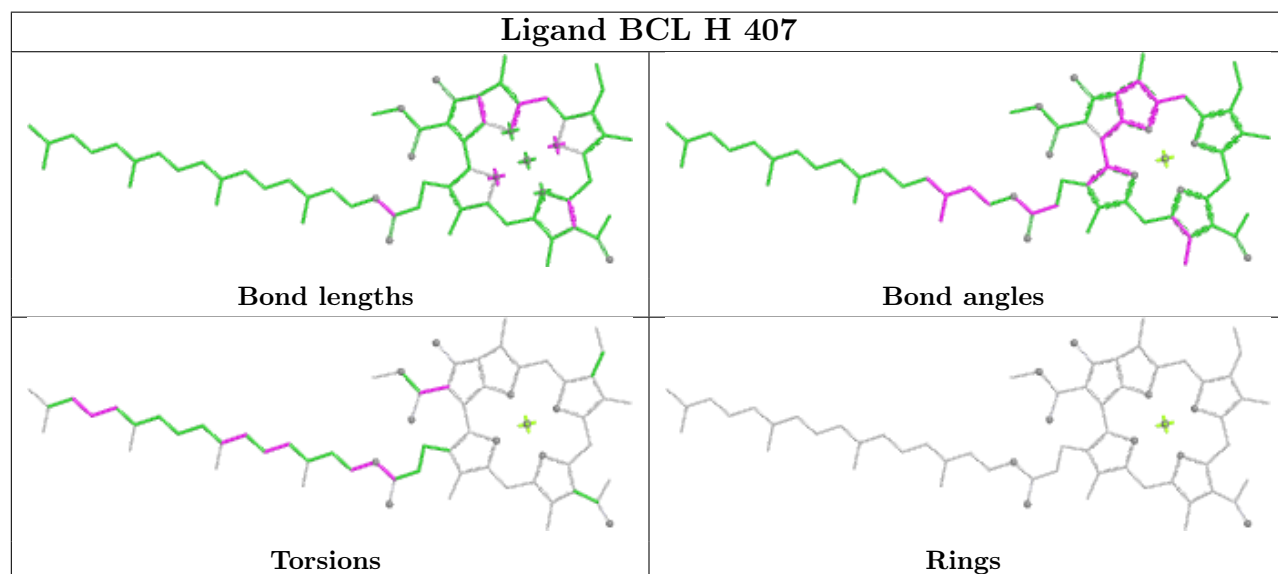
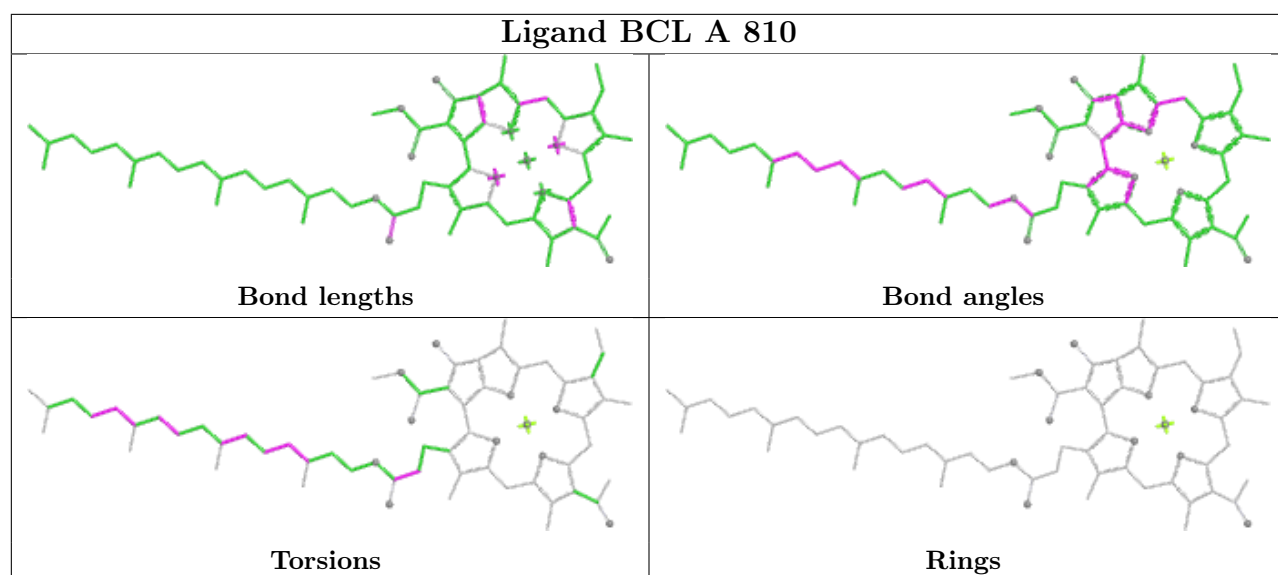


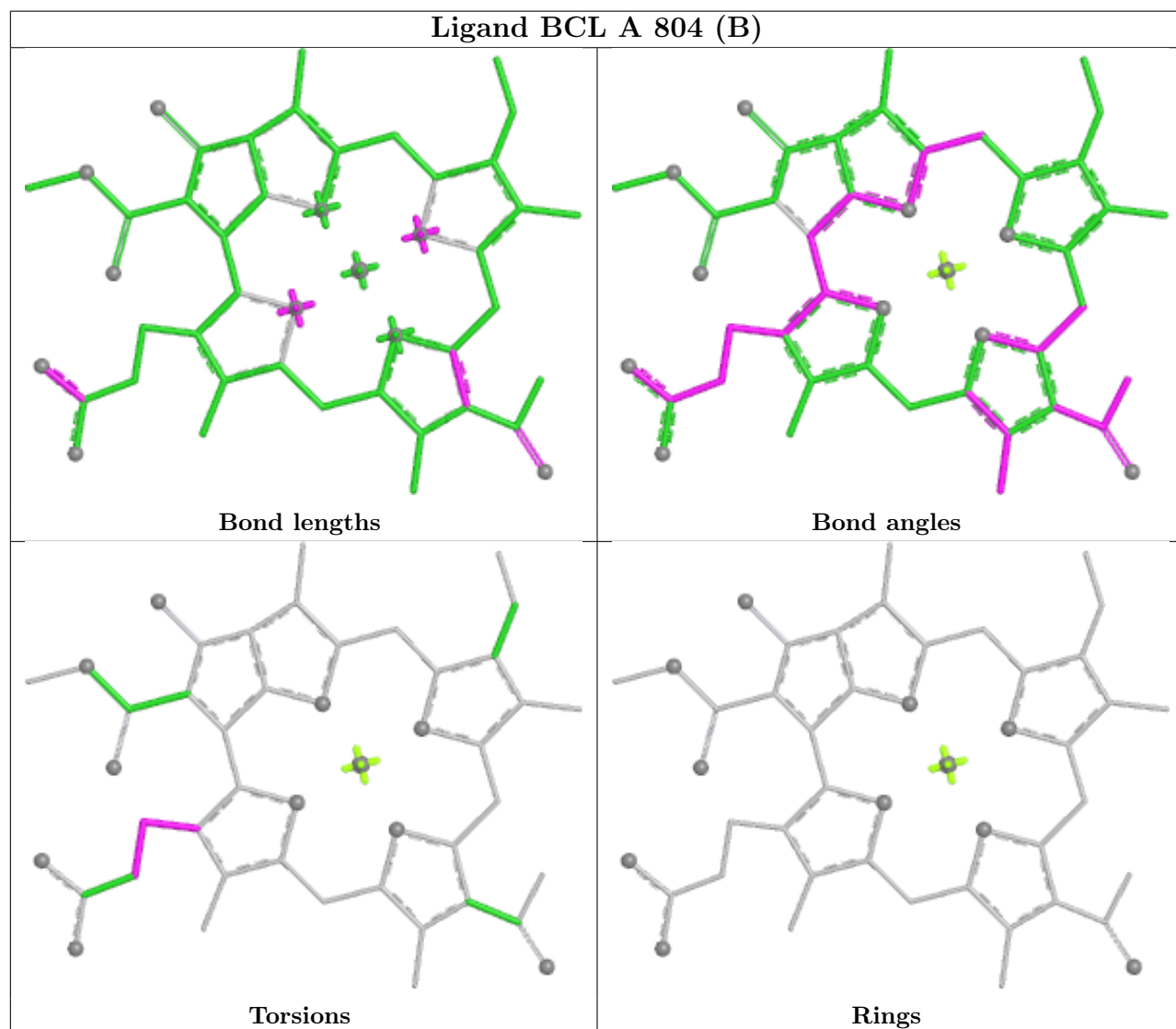
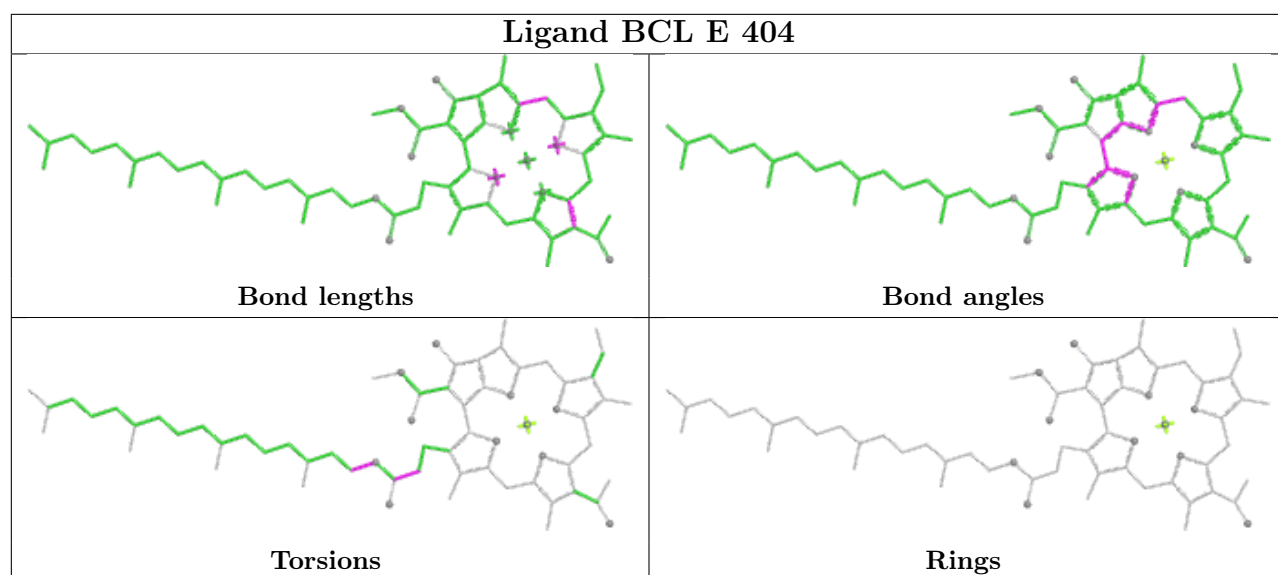
Ligand BCL a 804 (B)

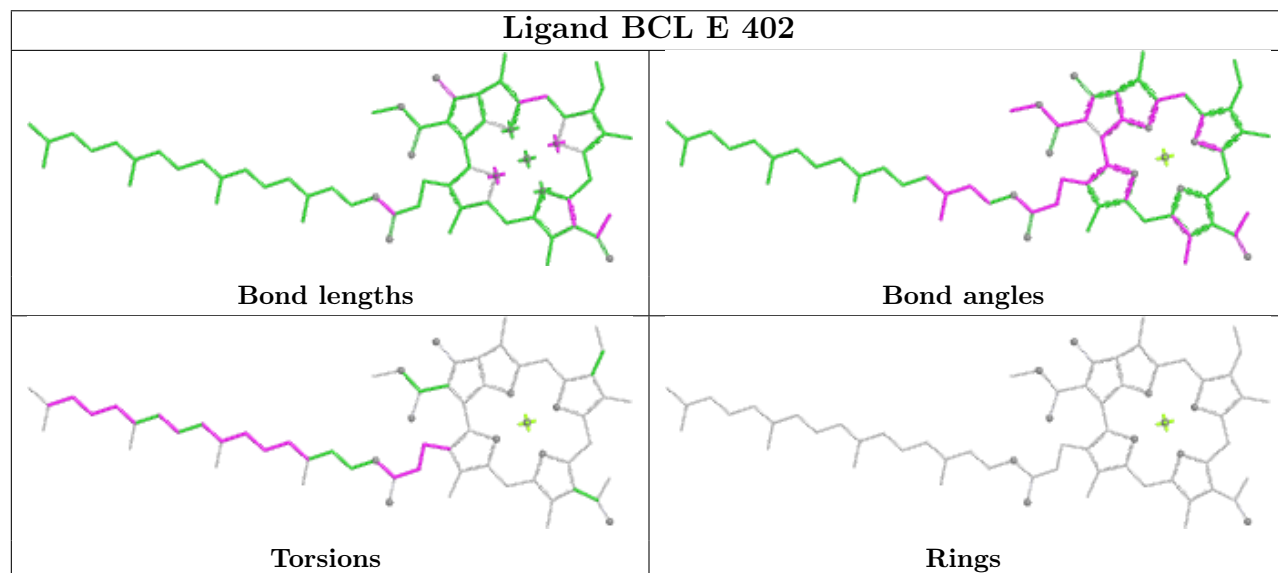
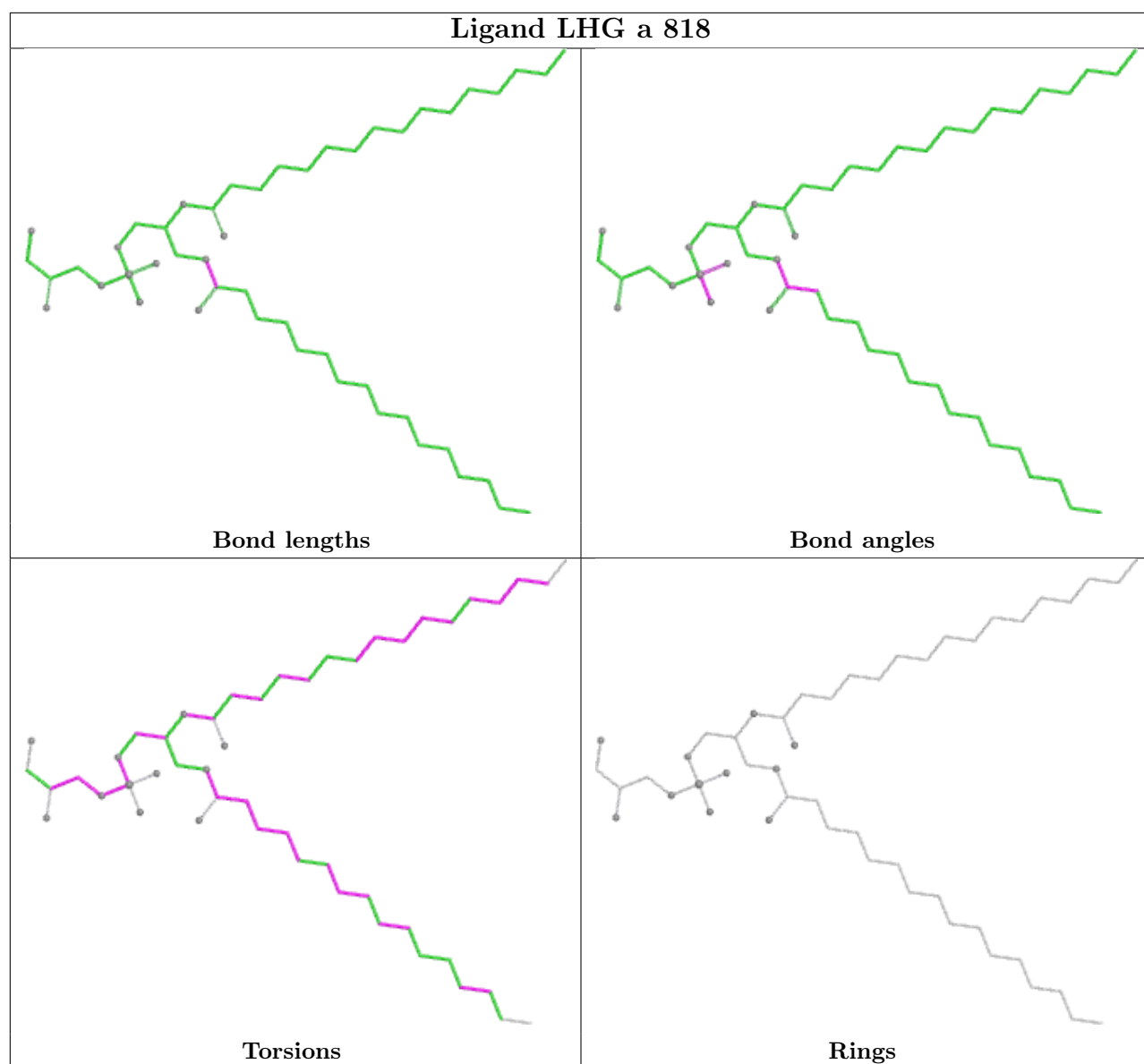


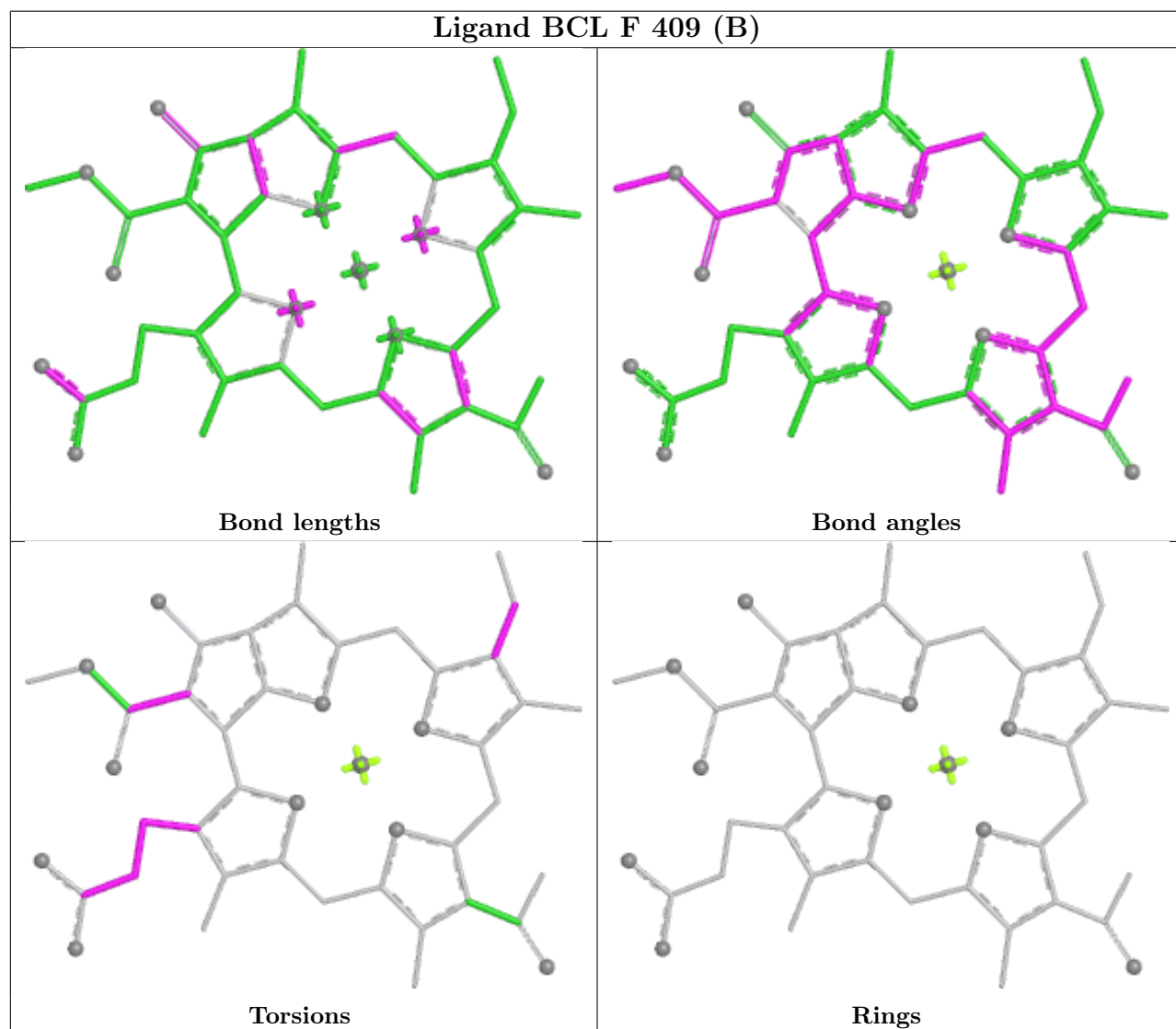
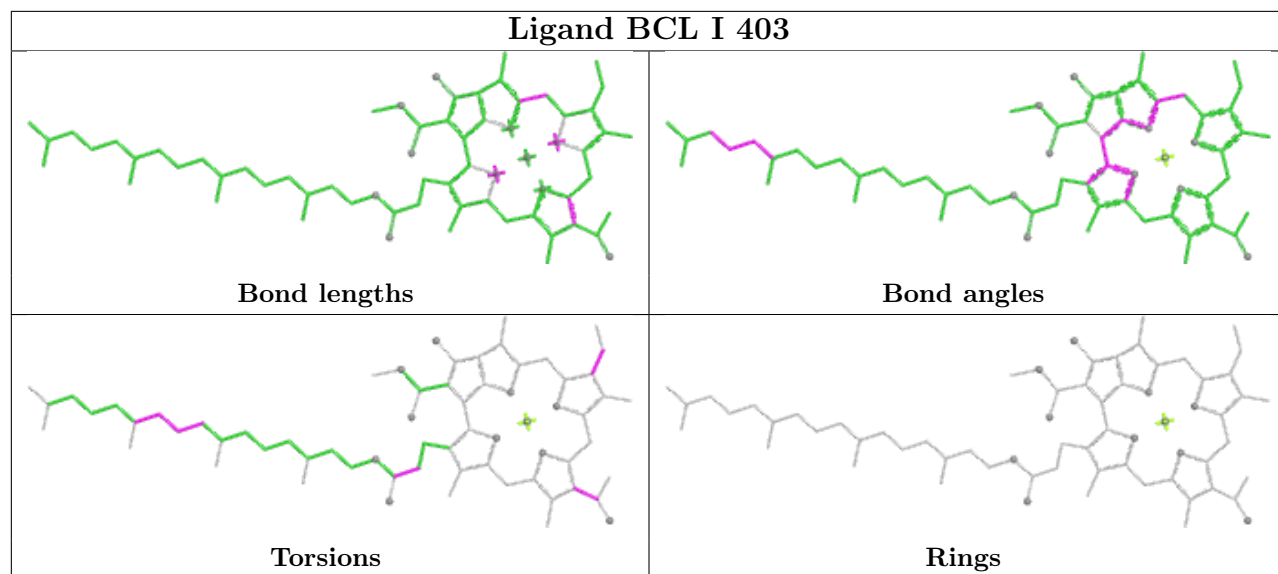
Ligand BCL a 805

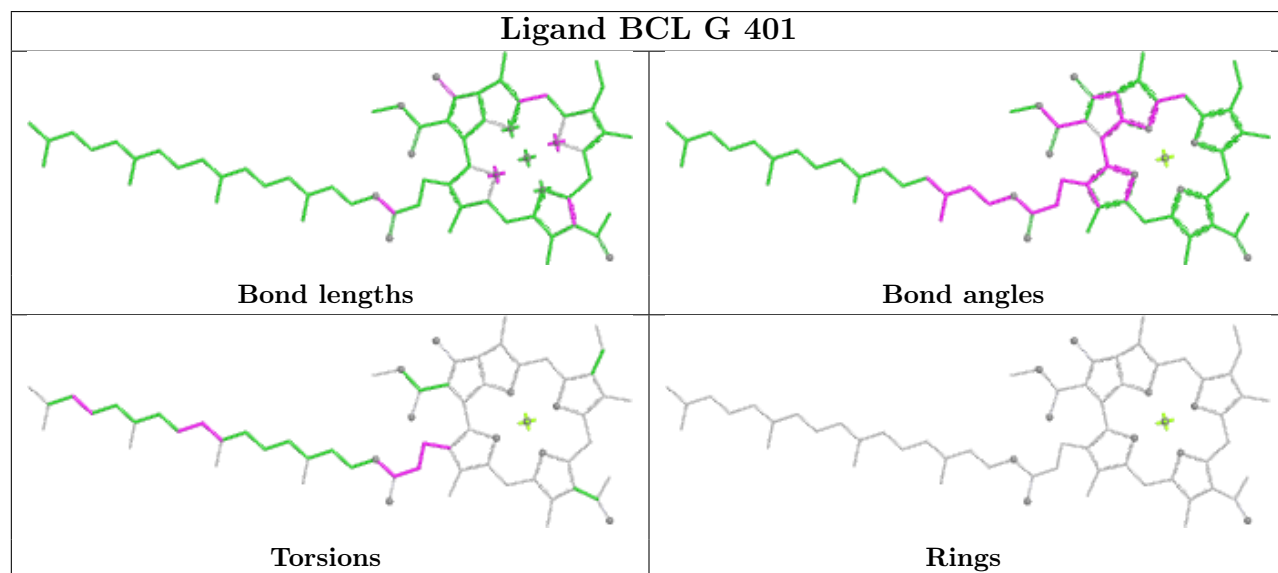
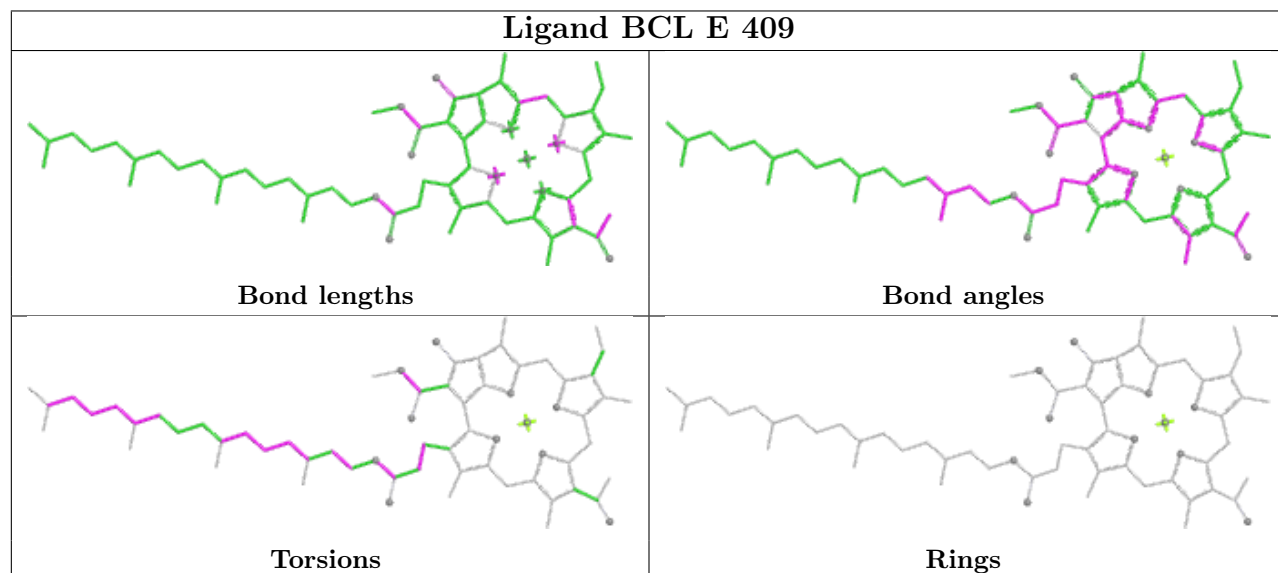
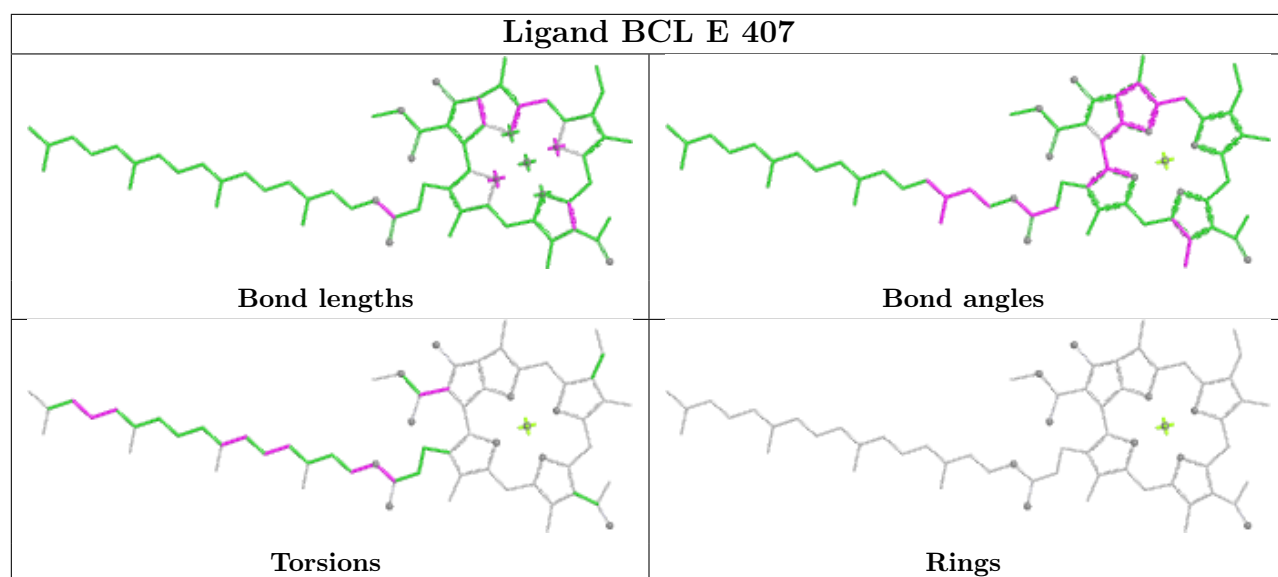


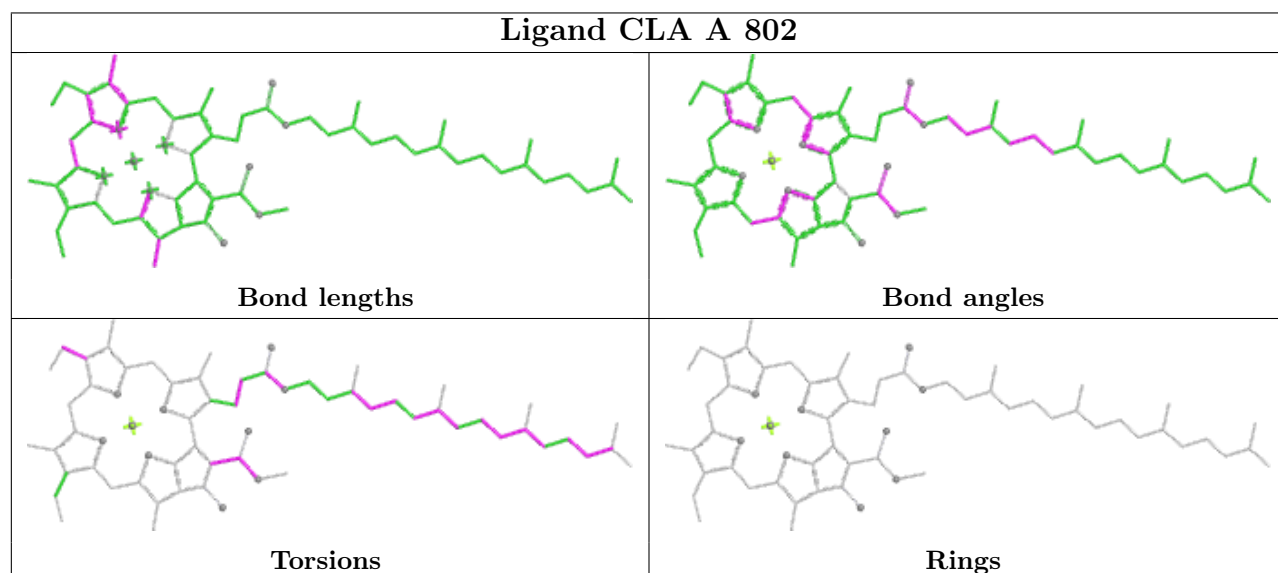
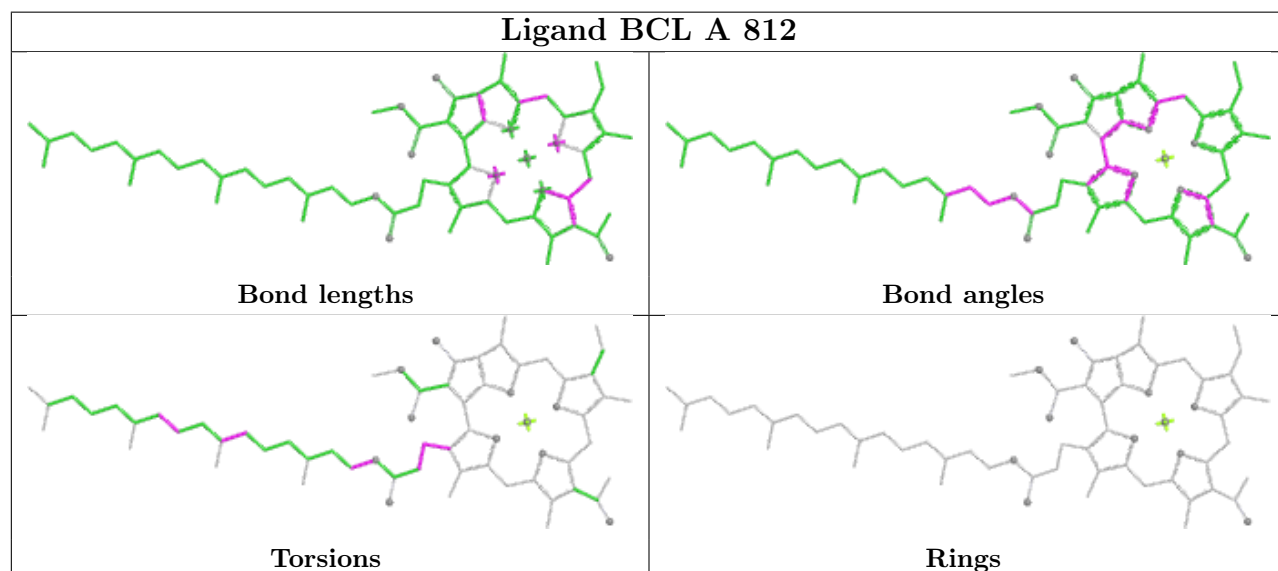
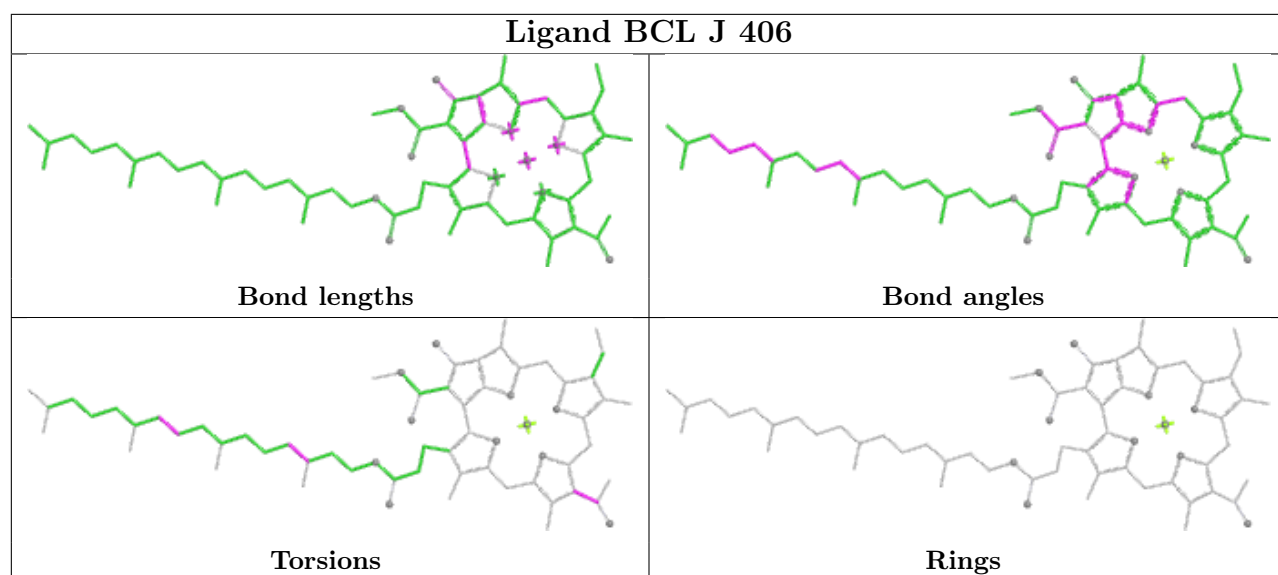


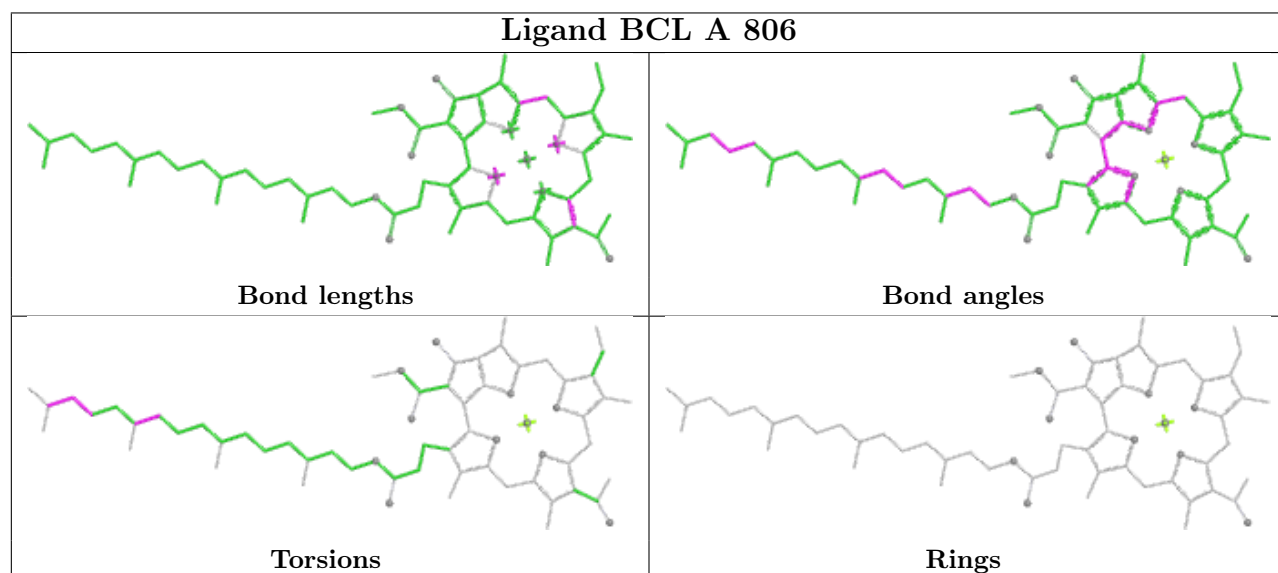
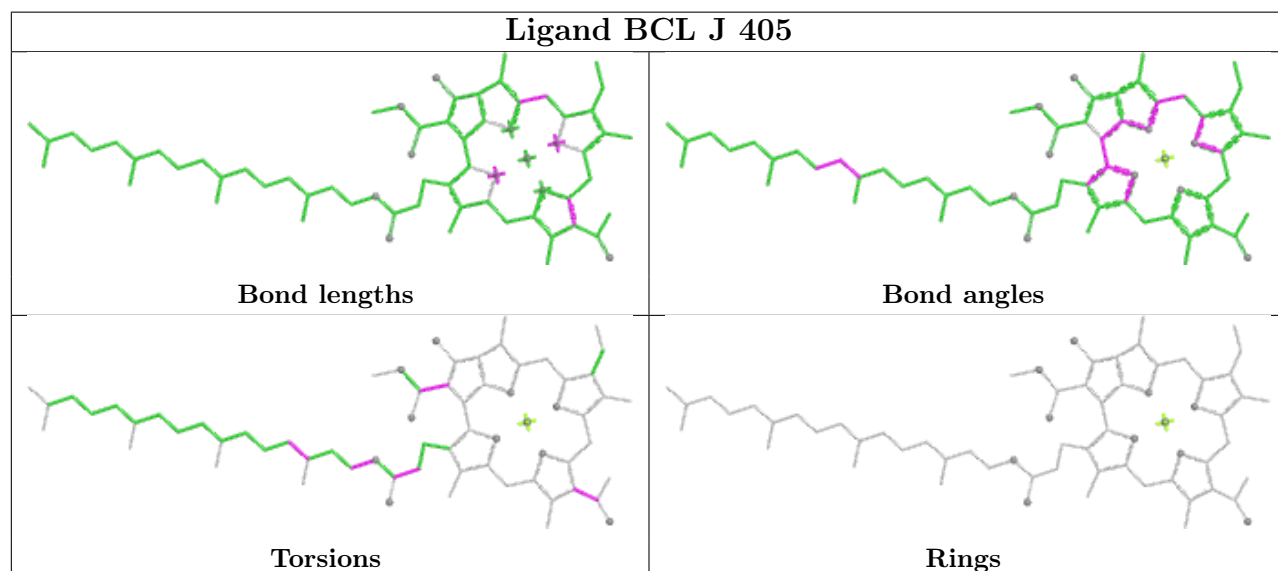
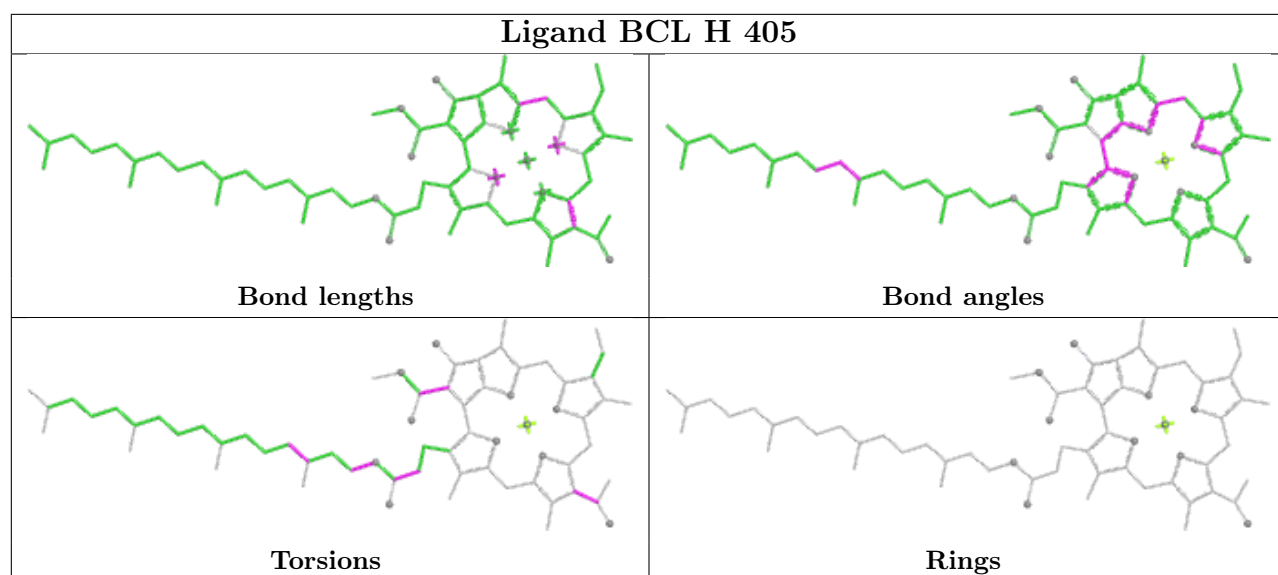


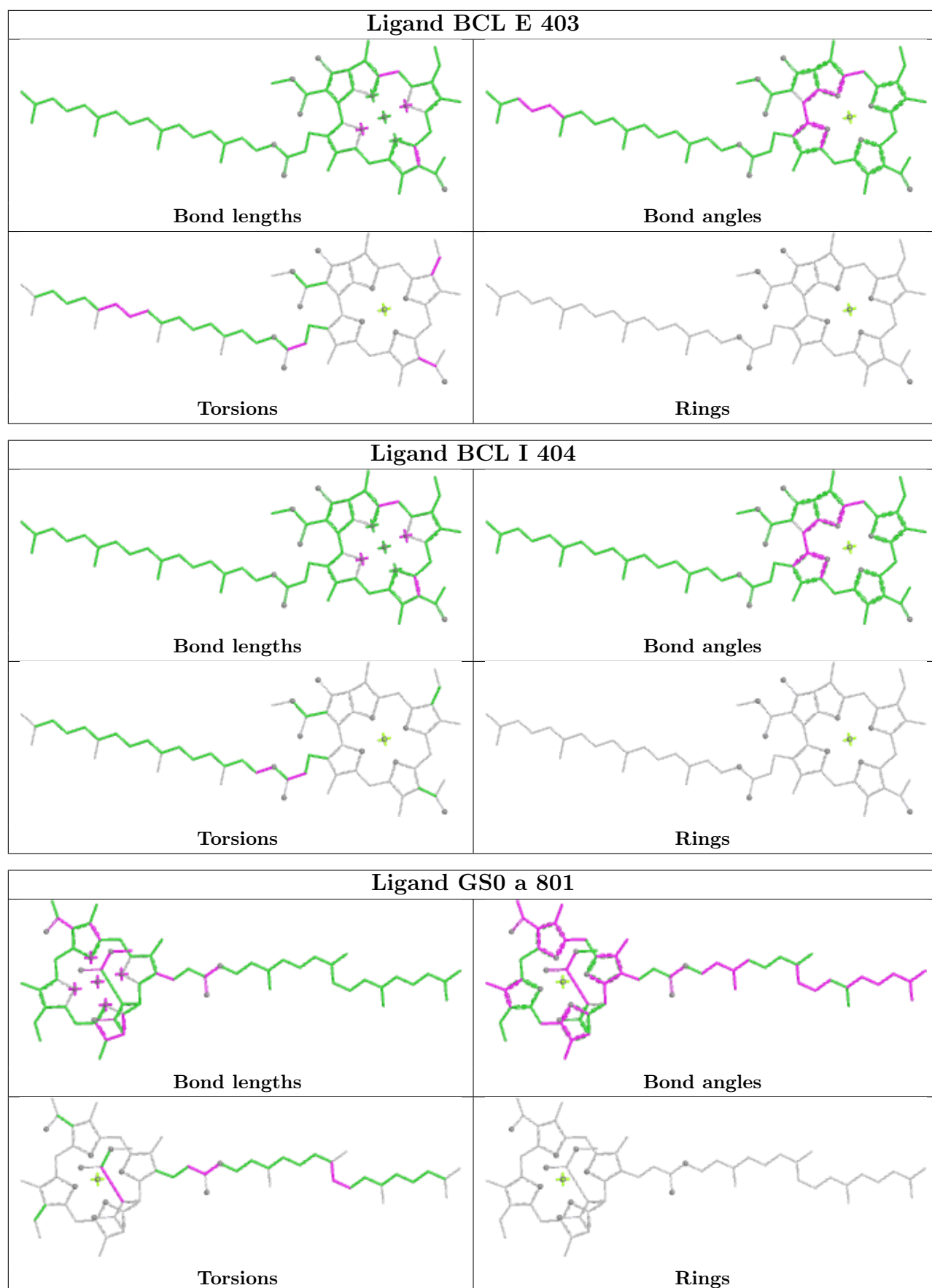




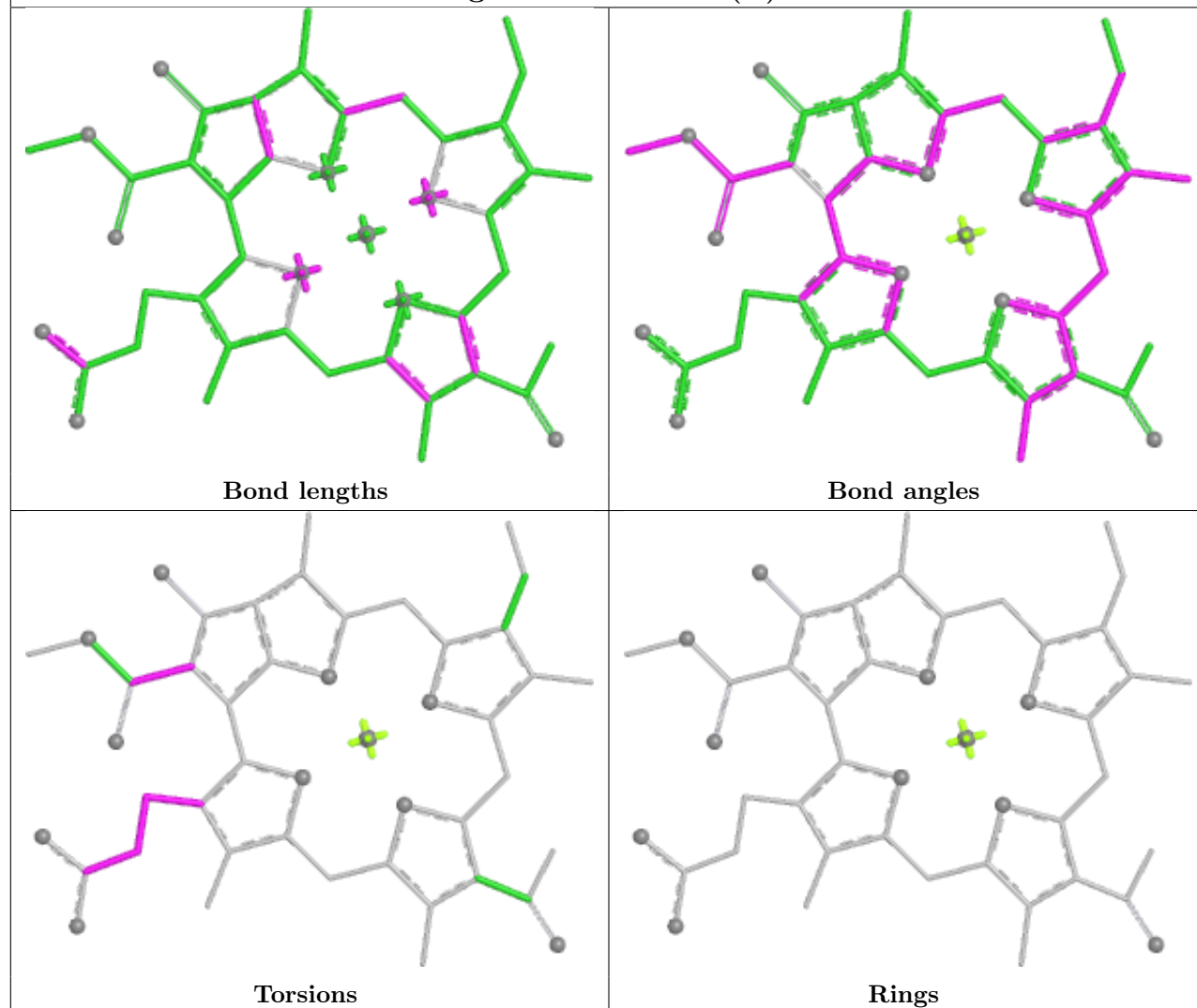




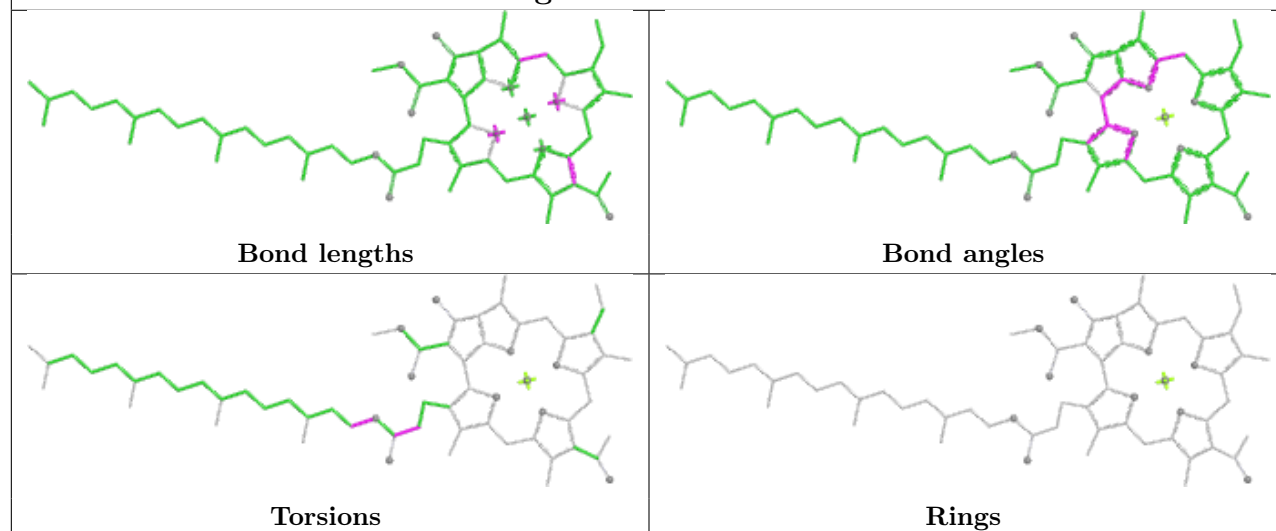


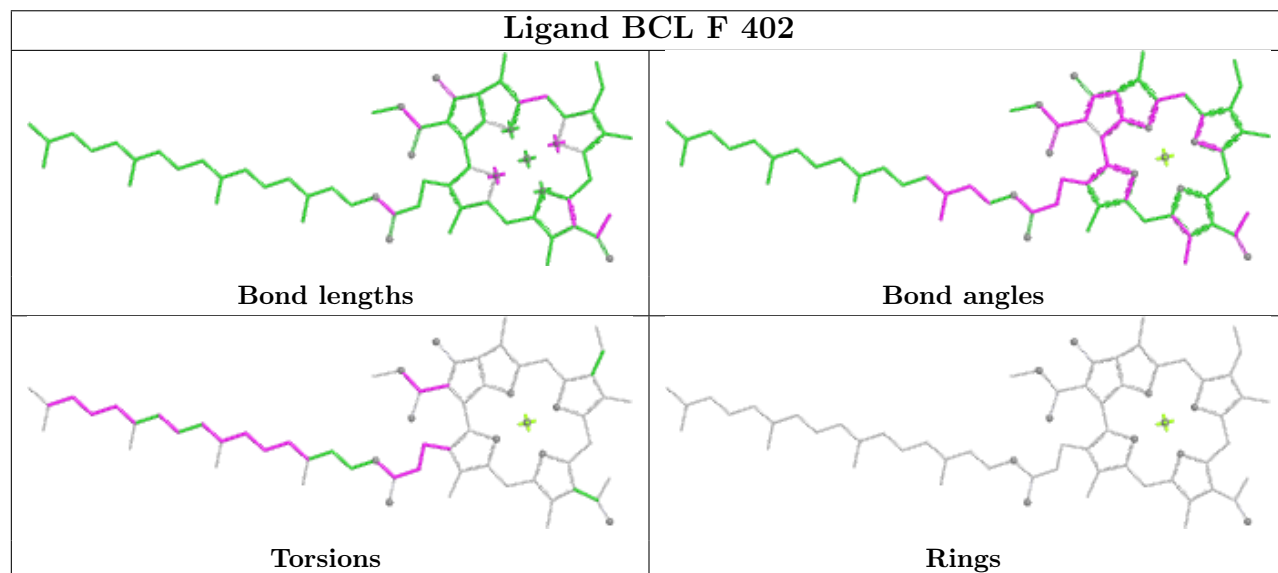
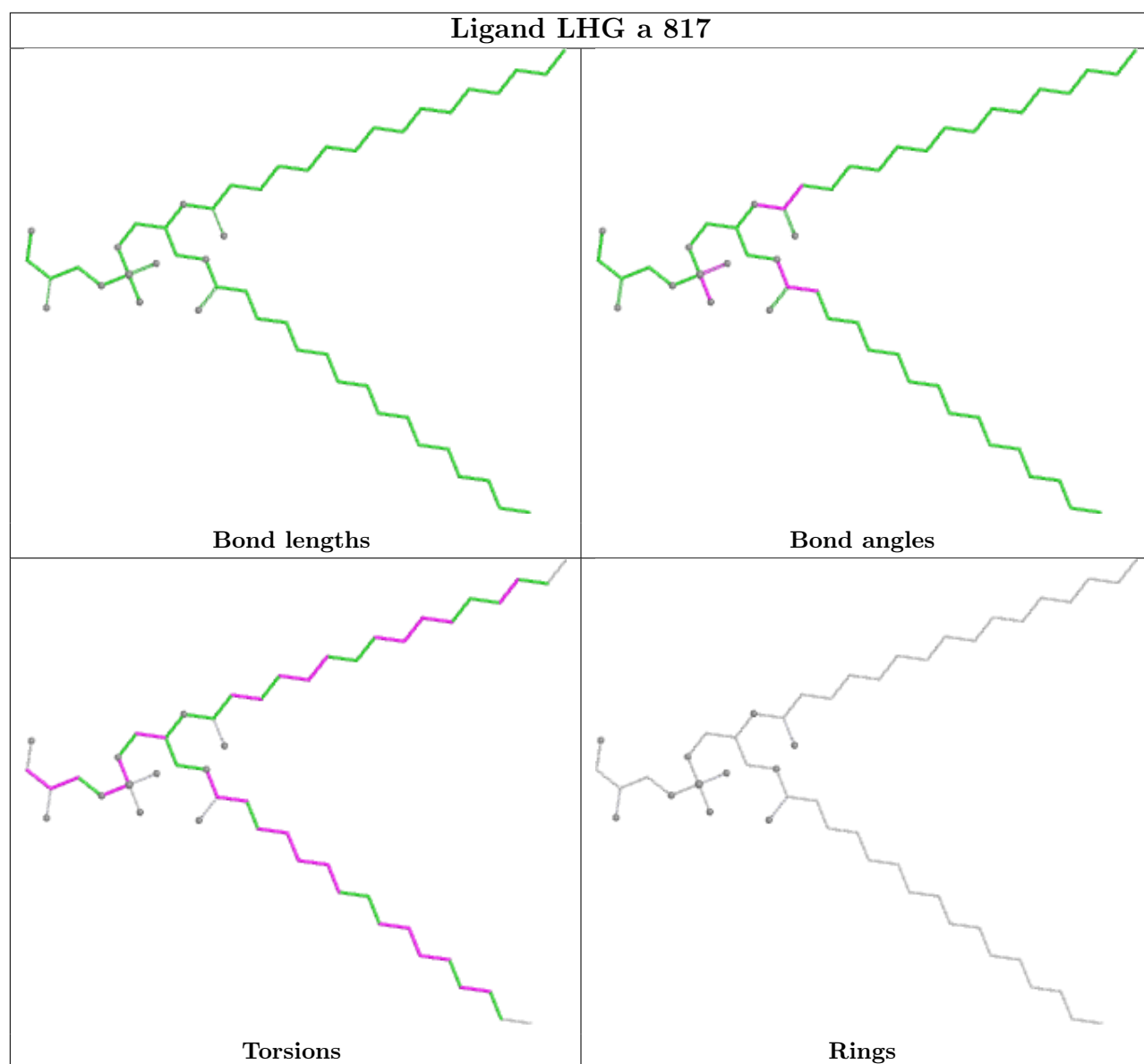


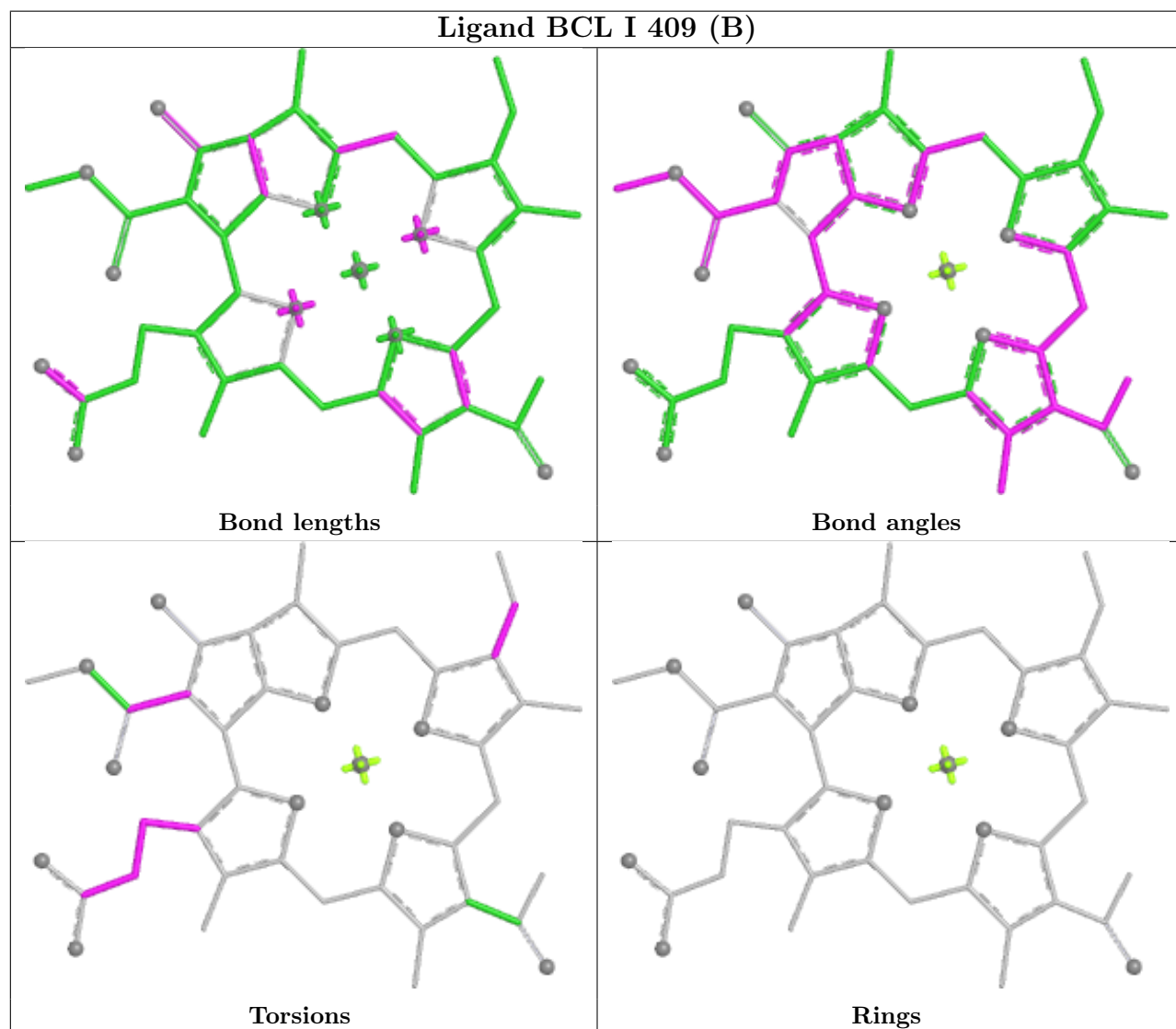
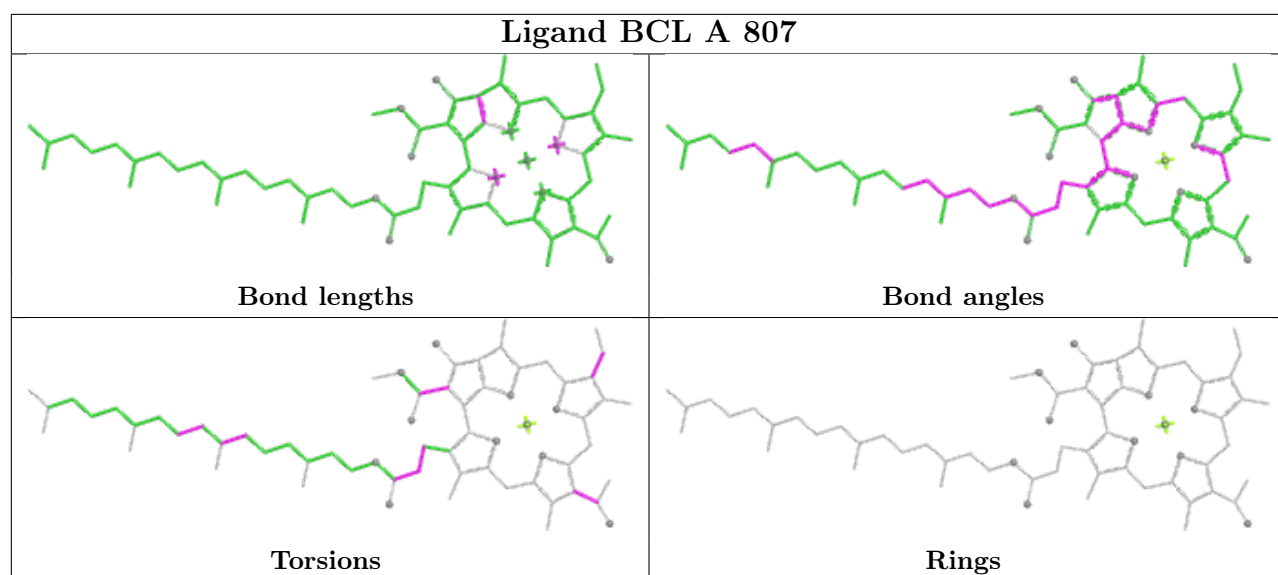
Ligand BCL H 408 (B)

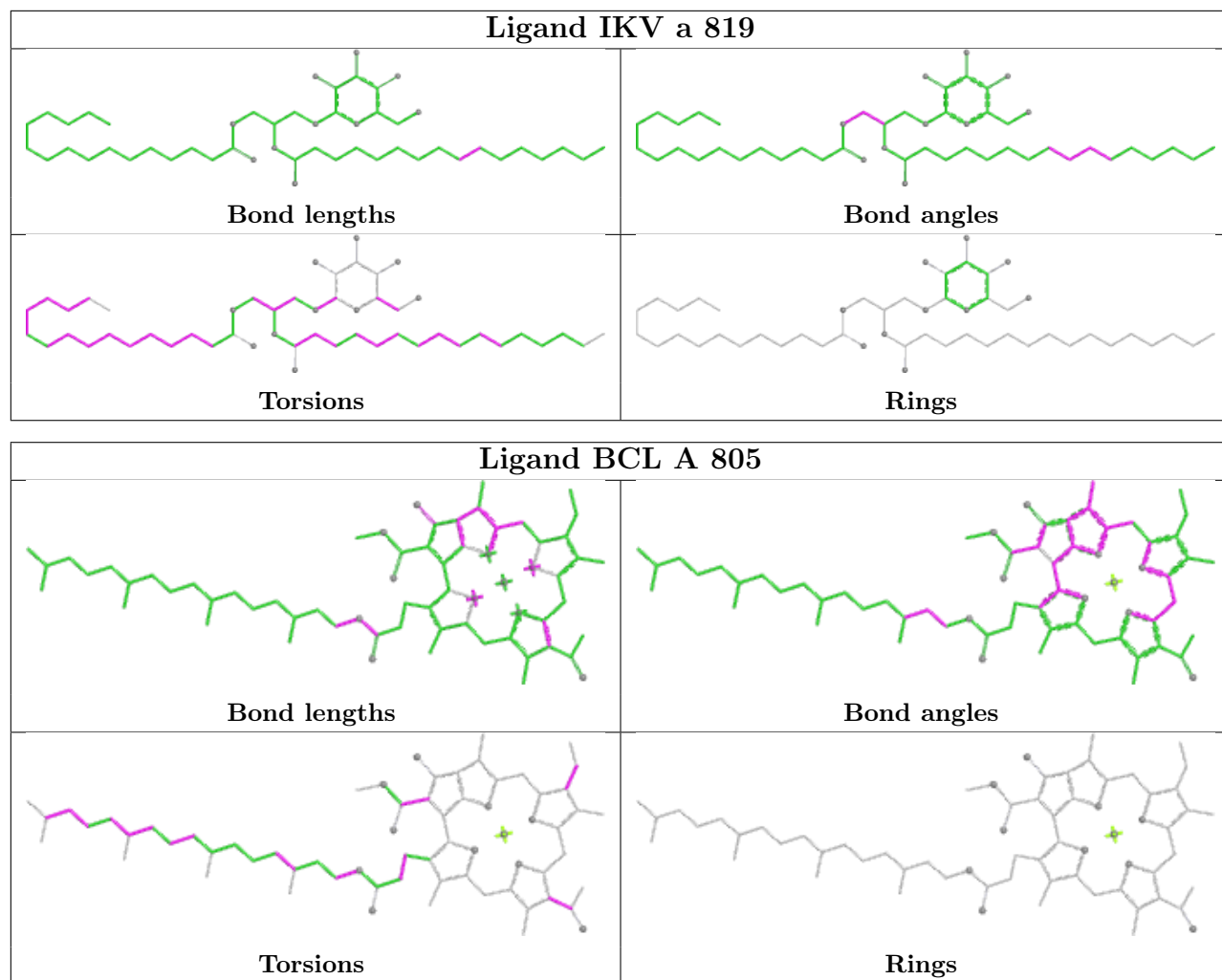


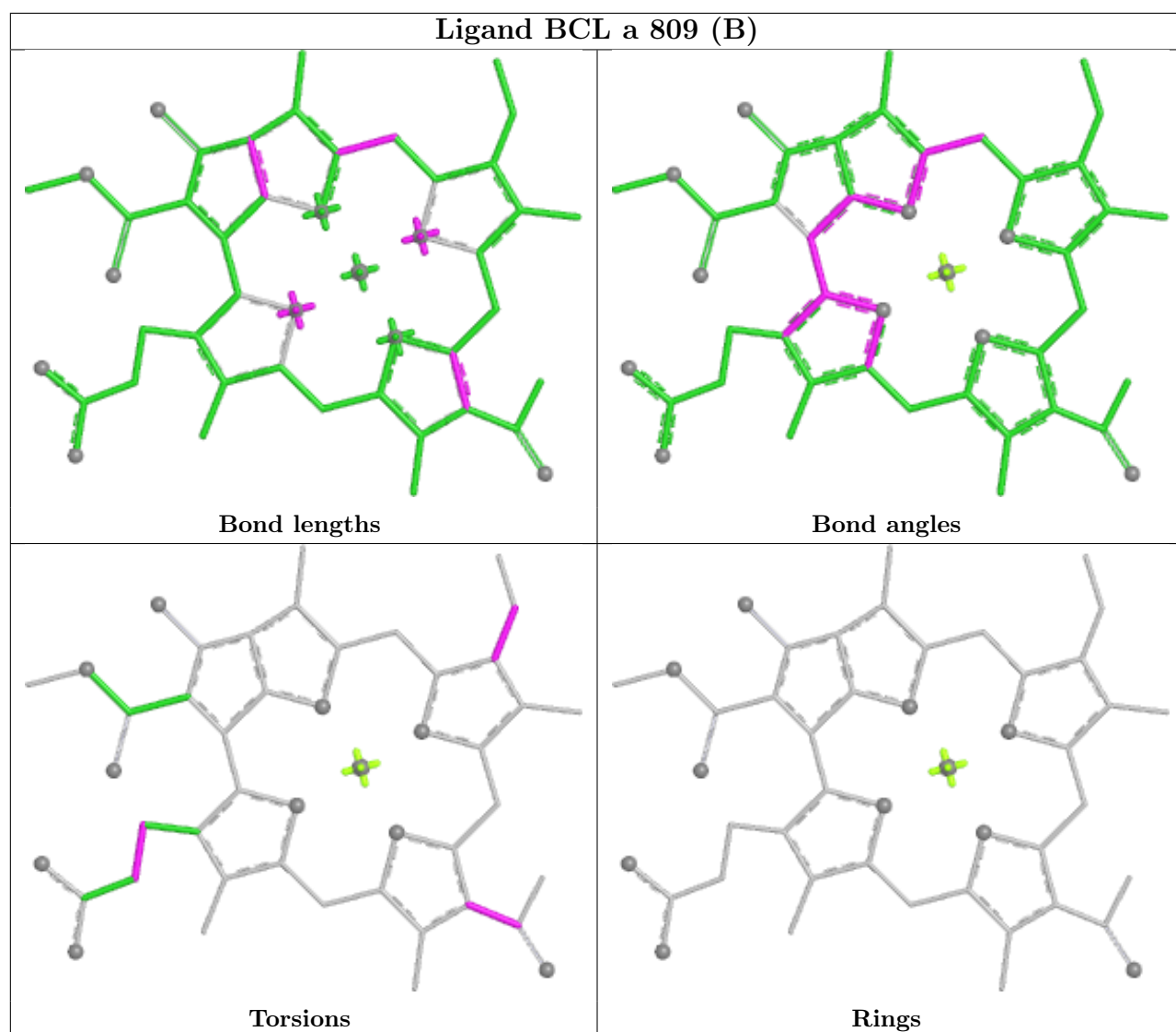
Ligand BCL F 404











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

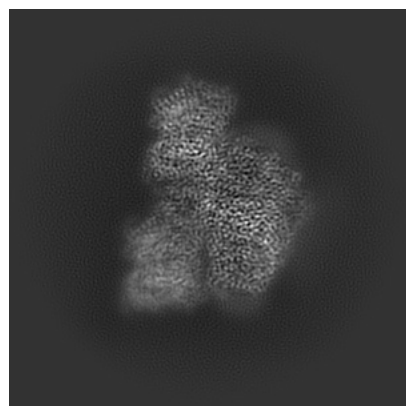
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14528. These allow visual inspection of the internal detail of the map and identification of artifacts.

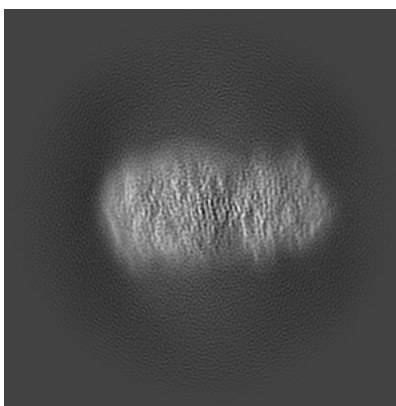
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

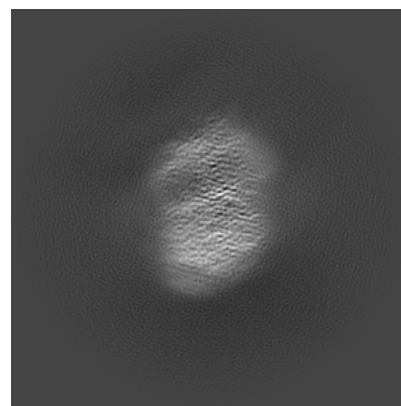
6.1.1 Primary map



X

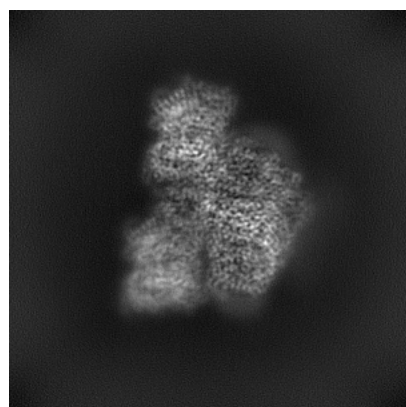


Y

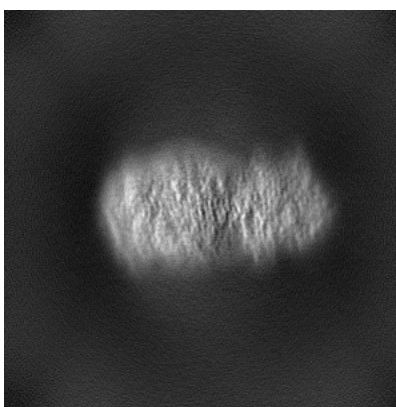


Z

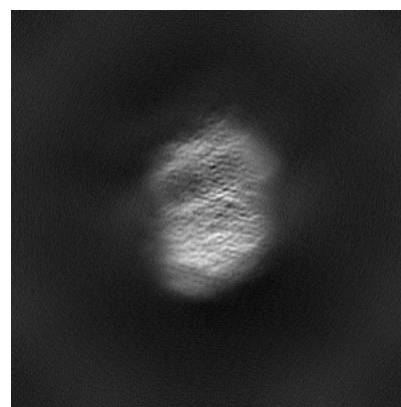
6.1.2 Raw map



X



Y

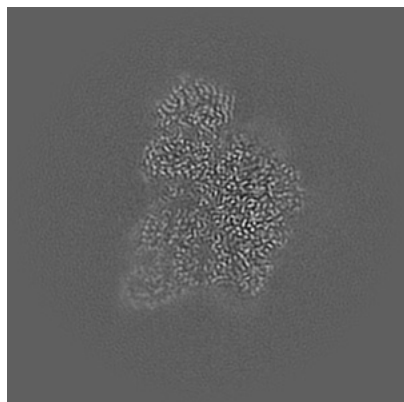


Z

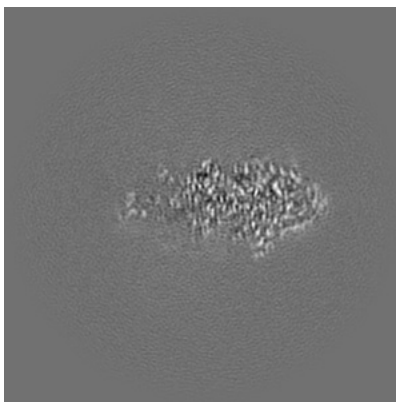
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

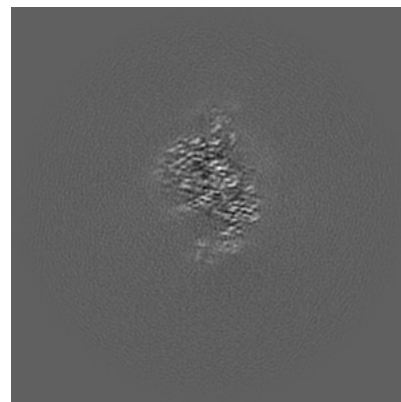
6.2.1 Primary map



X Index: 180

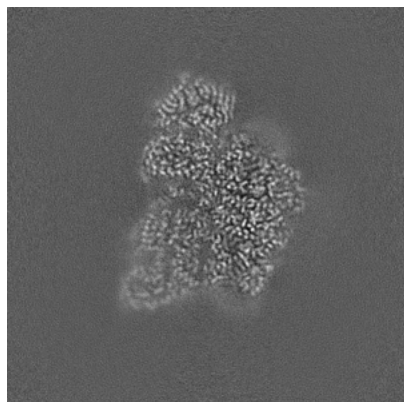


Y Index: 180

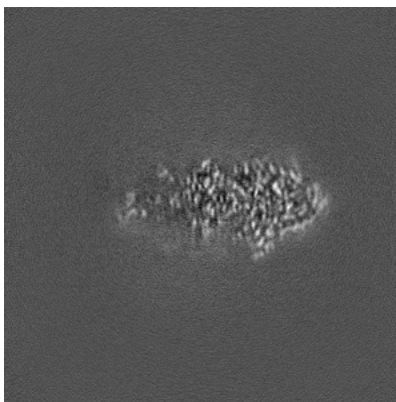


Z Index: 180

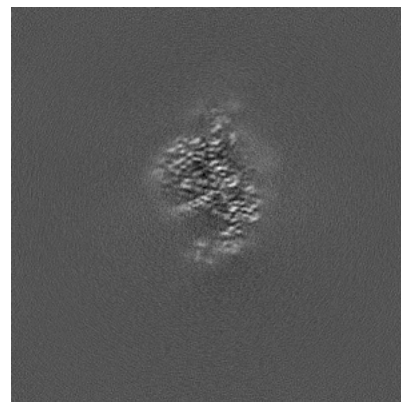
6.2.2 Raw map



X Index: 180



Y Index: 180

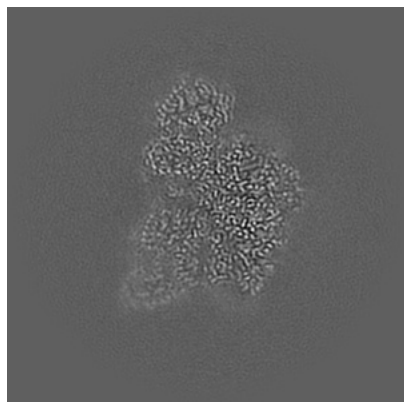


Z Index: 180

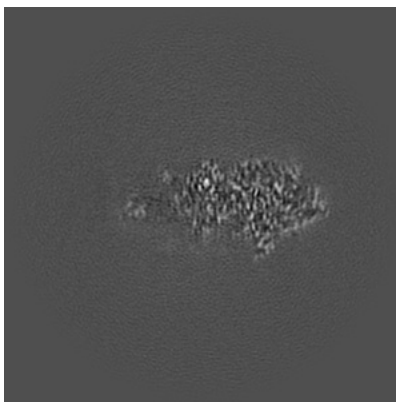
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

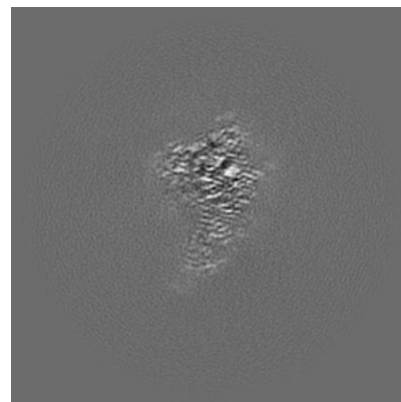
6.3.1 Primary map



X Index: 179

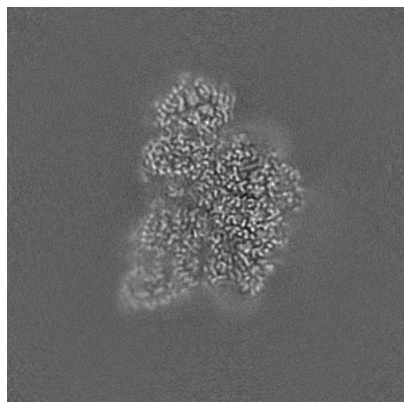


Y Index: 179

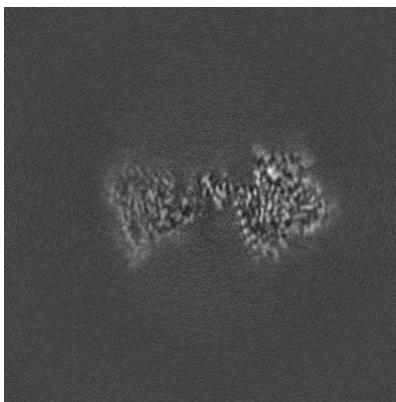


Z Index: 167

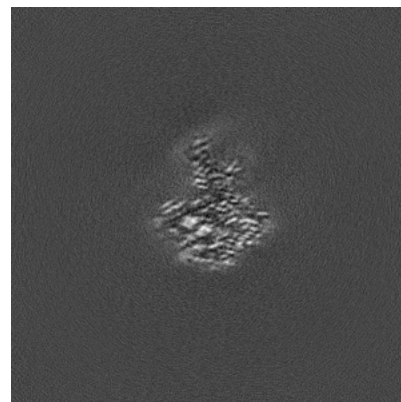
6.3.2 Raw map



X Index: 179



Y Index: 157

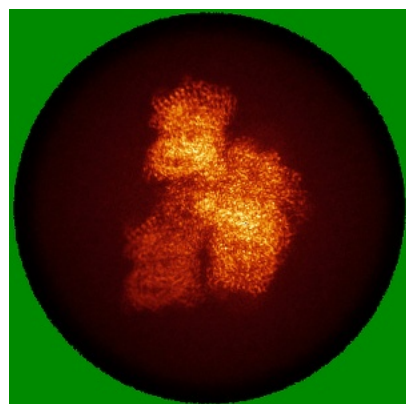


Z Index: 231

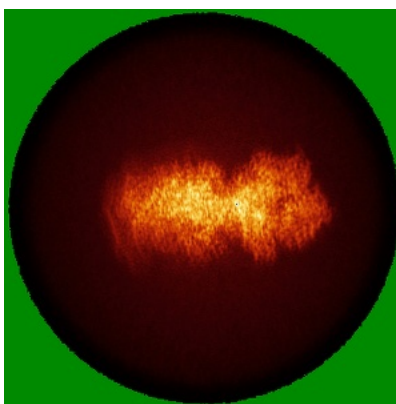
The images above show the largest variance slices of the map in three orthogonal directions.

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

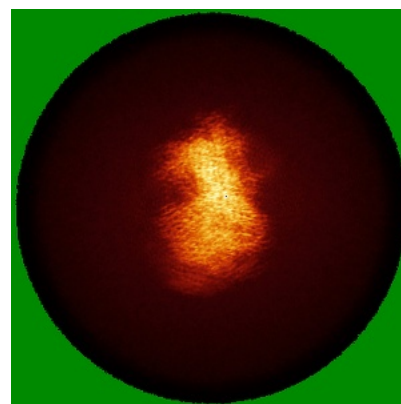
6.4.1 Primary map



X

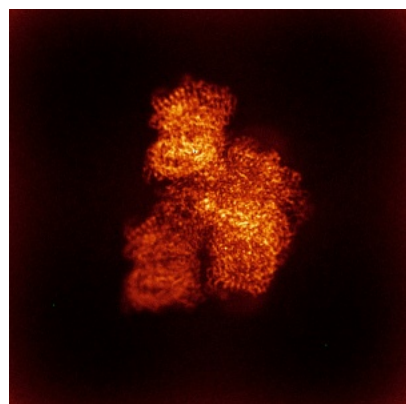


Y

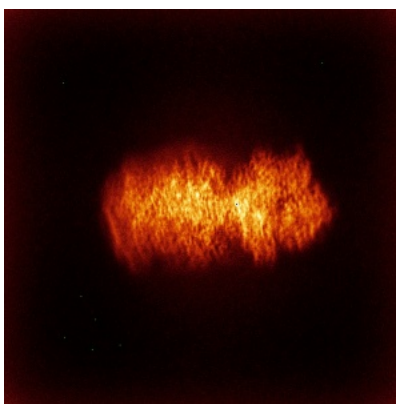


Z

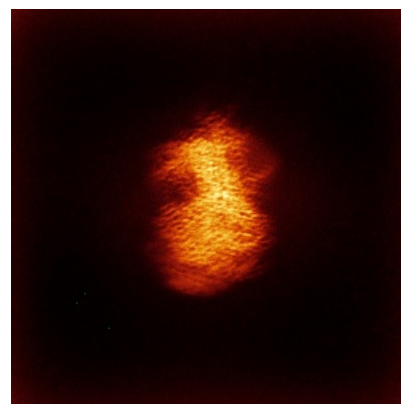
6.4.2 Raw map



X



Y

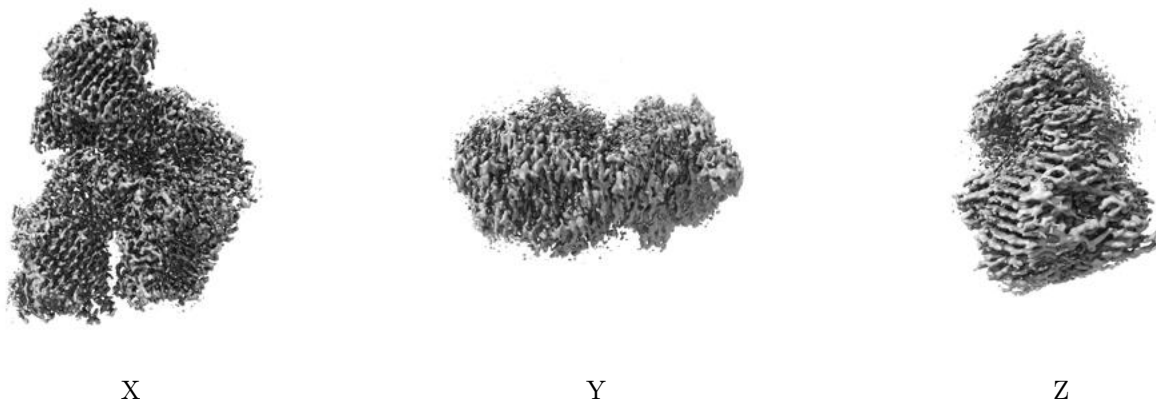


Z

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

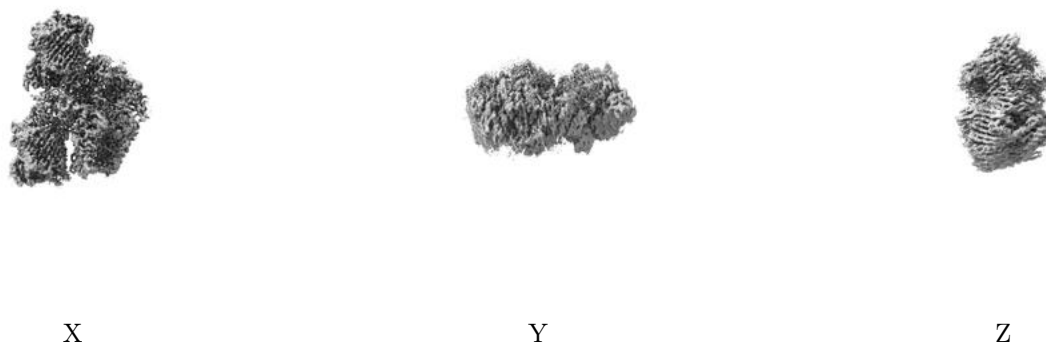
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

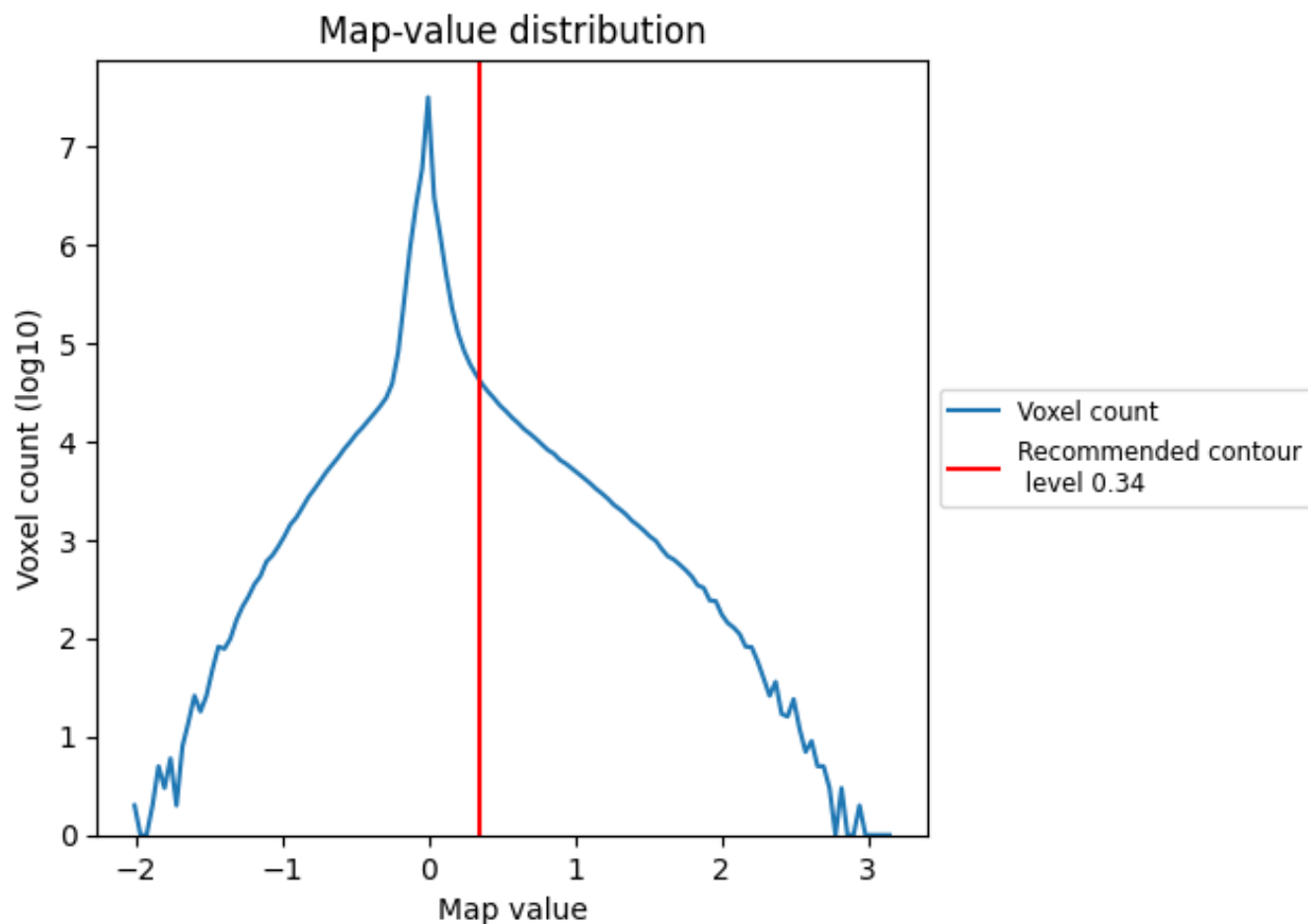
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

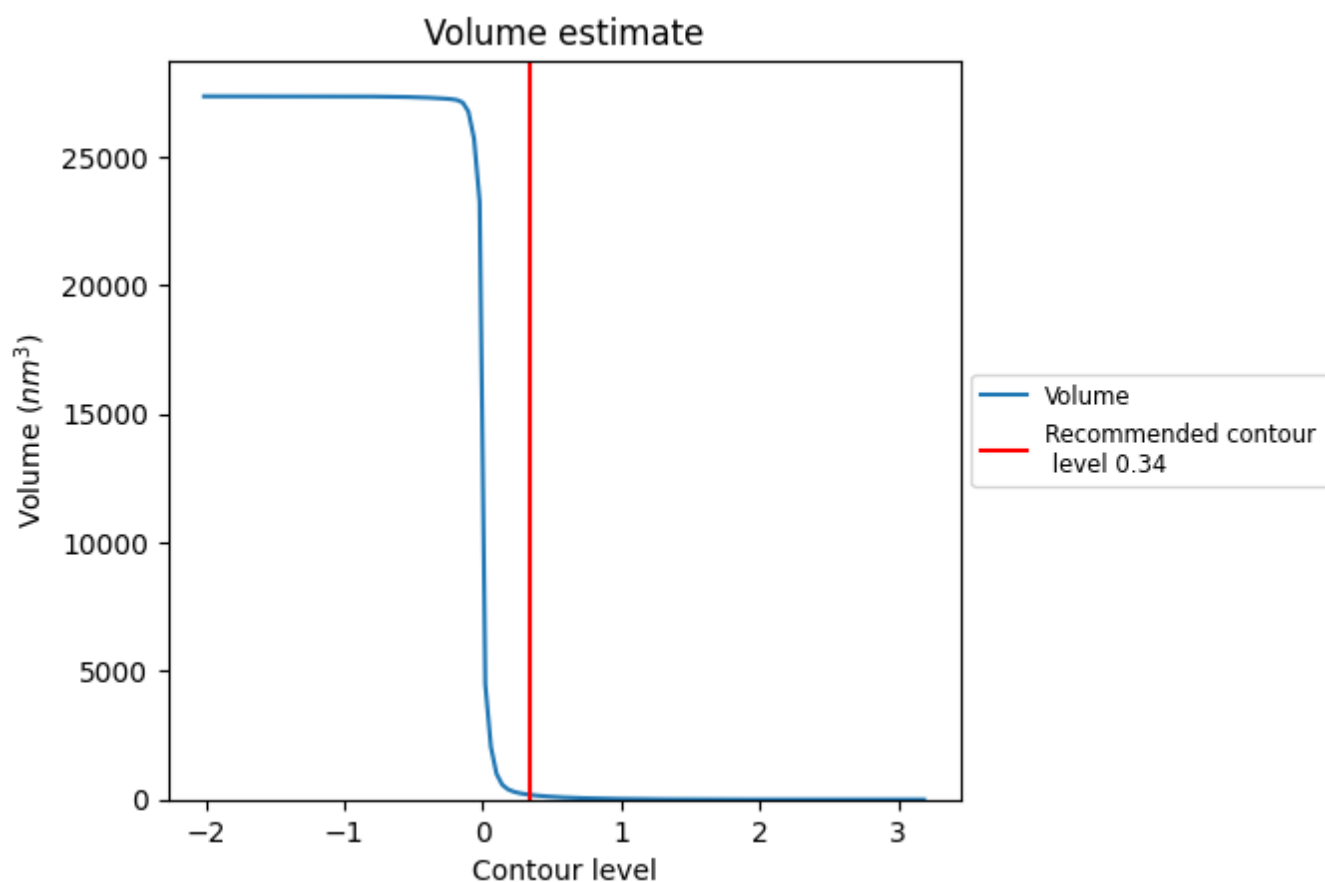
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

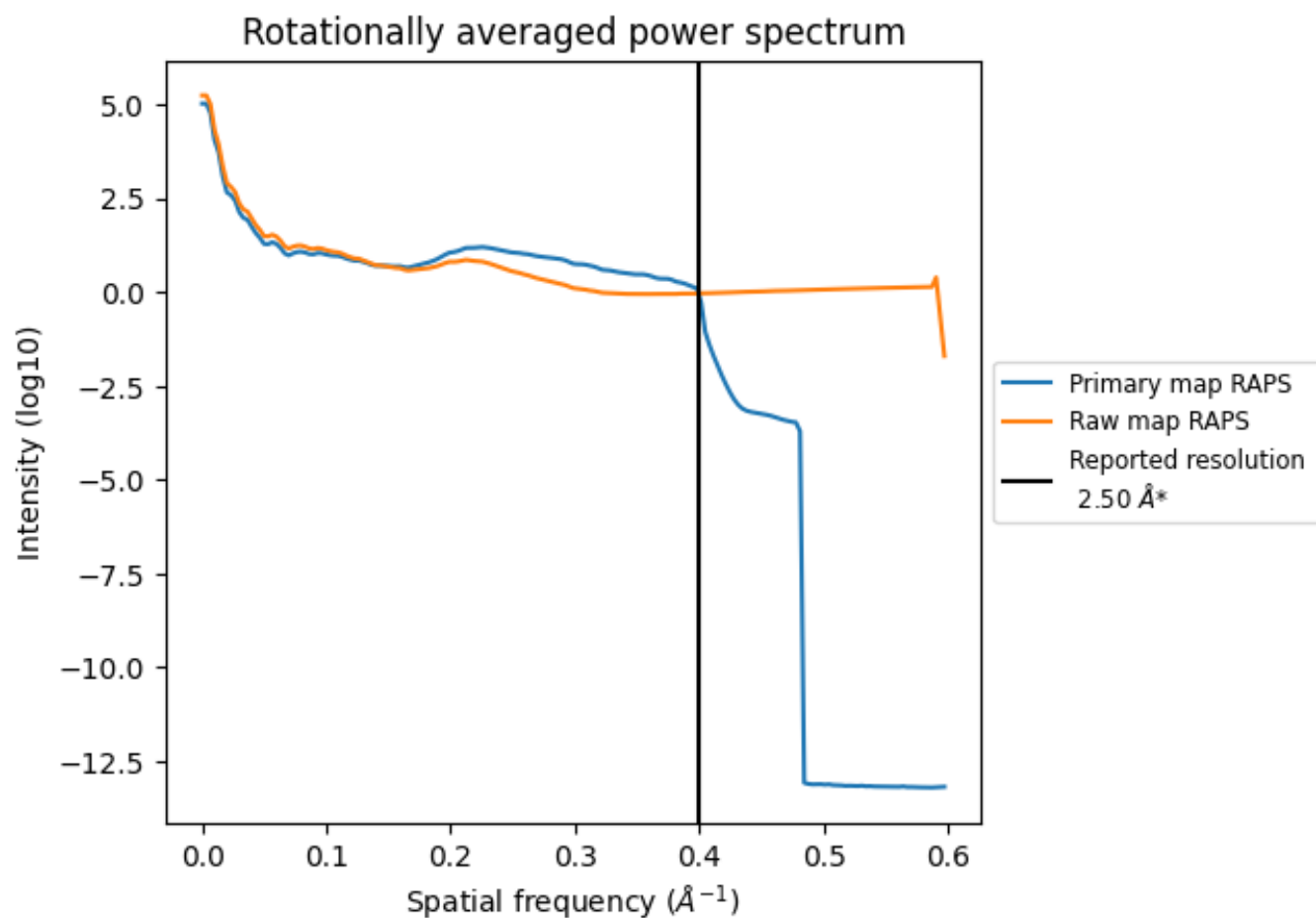
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm³; this corresponds to an approximate mass of 167 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 ⓘ

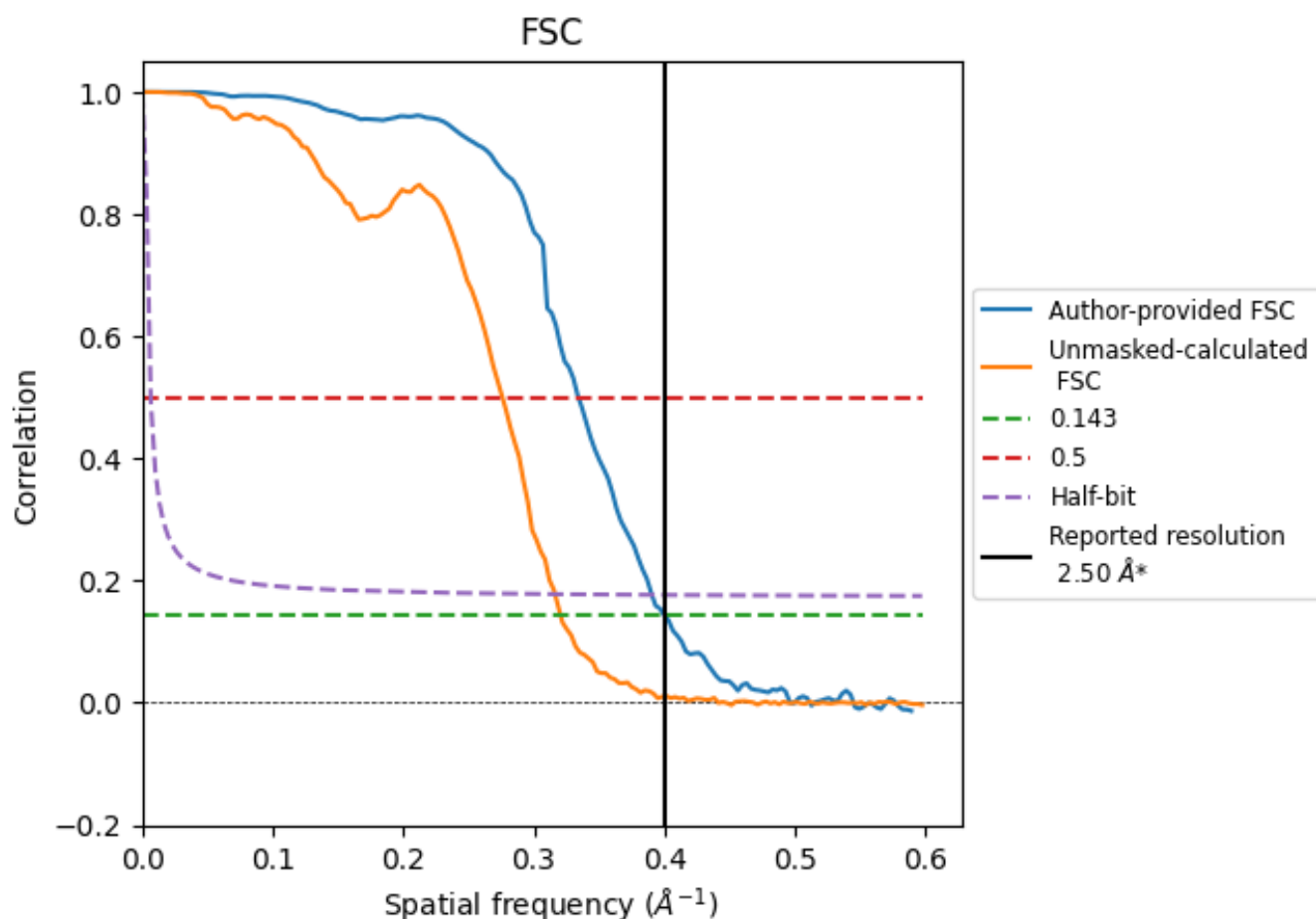


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

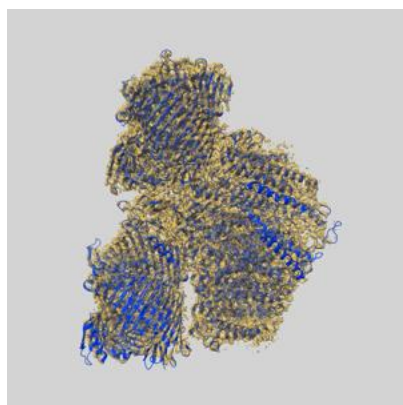
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.99	2.56
Unmasked-calculated*	3.12	3.63	3.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.5 by more than 10 %

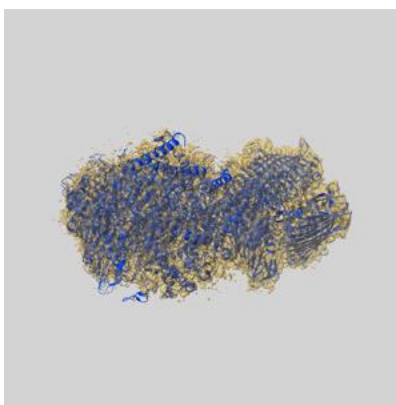
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14528 and PDB model 7Z6Q. Per-residue inclusion information can be found in section [3](#) on page [14](#).

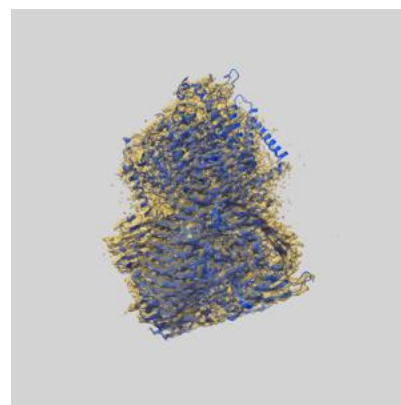
9.1 Map-model overlay [i](#)



X



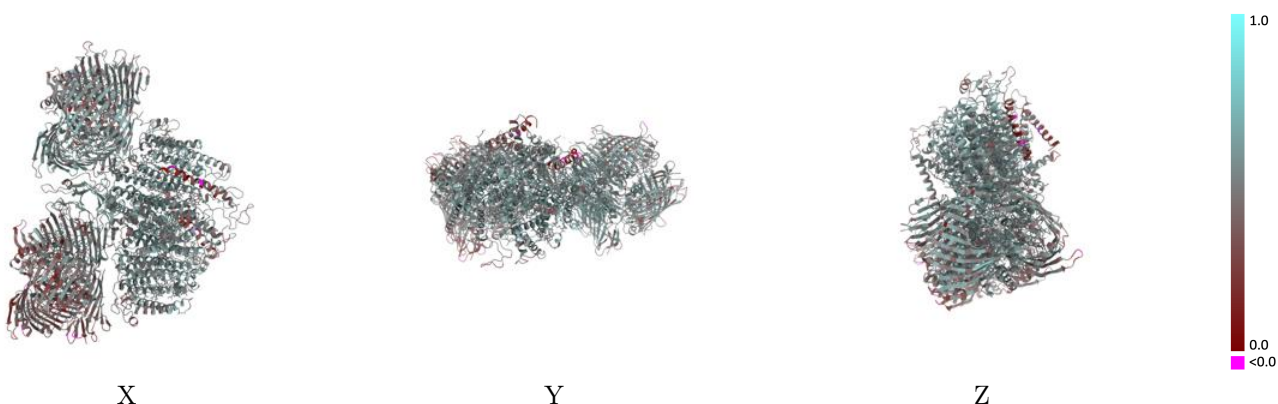
Y



Z

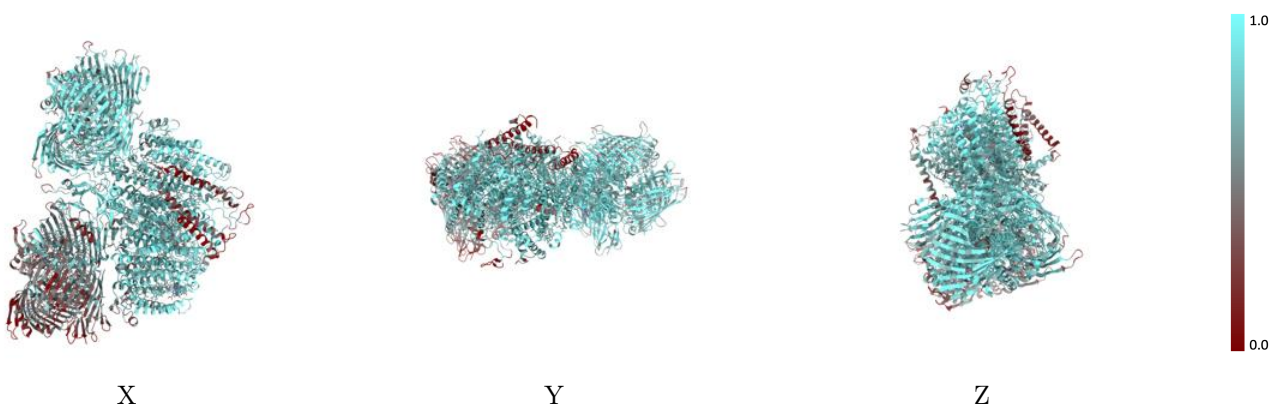
The images above show the 3D surface view of the map at the recommended contour level 0.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



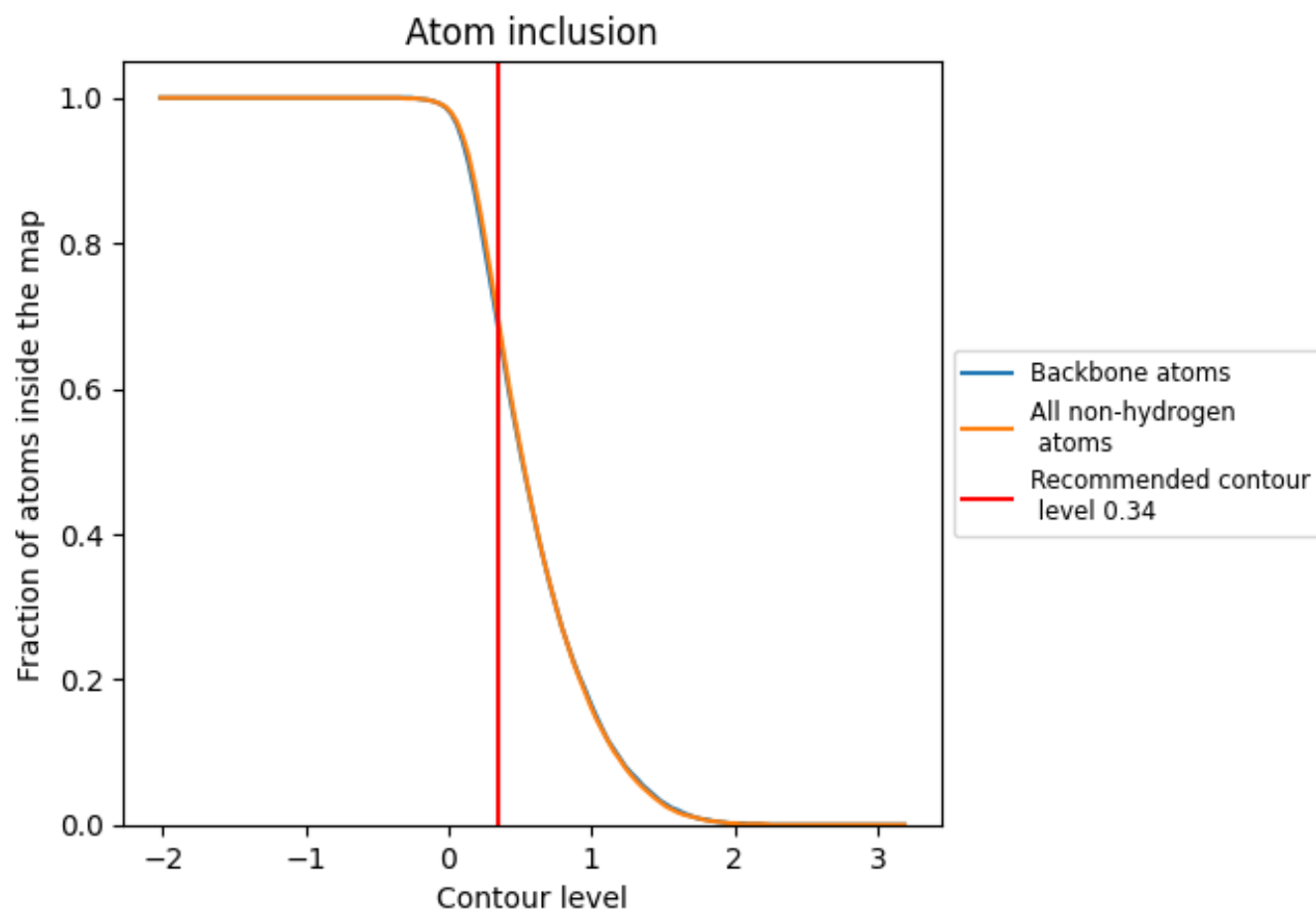
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.34).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 70% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.4930
A	0.8420	0.5570
B	0.7940	0.5370
C	0.5480	0.4780
D	0.6430	0.4970
E	0.8490	0.5410
F	0.8160	0.5030
G	0.7940	0.5010
H	0.4180	0.3670
I	0.4800	0.4080
J	0.6120	0.4590
a	0.8120	0.5370
c	0.2250	0.3330

1.0

0.0

<0.0