



## Full wwPDB EM Validation Report ⓘ

Oct 21, 2023 – 01:54 PM EDT

PDB ID : 8SS7  
EMDB ID : EMD-40746  
Title : Structure of AMPA receptor GluA2 complex with auxiliary subunits TARP gamma-5 and cornichon-2 bound to competitive antagonist ZK, channel blocker spermidine and antiepileptic drug perampanel (closed state)  
Authors : Gangwar, S.P.; Yen, L.Y.; Yelshanskaya, M.V.; Sobolevsky, A.I.  
Deposited on : 2023-05-08  
Resolution : 2.76 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

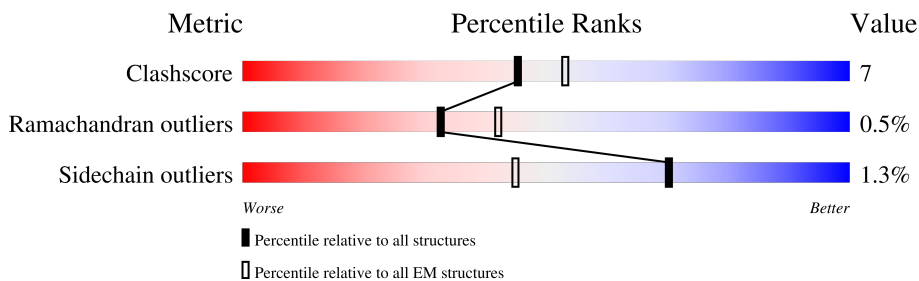
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.76 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1026	
1	B	1026	
1	C	1026	
1	D	1026	
2	E	160	
2	F	160	

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
6	CLR	A	1107	X	-	-	-
6	CLR	A	1108	X	-	-	-
6	CLR	B	1107	X	-	-	-
6	CLR	B	1108	X	-	-	-
6	CLR	C	1107	X	-	-	-
6	CLR	C	1108	X	-	-	-
6	CLR	D	1108	X	-	-	-
6	CLR	D	1109	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19437 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 Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	592	4639	3030	748	830	31	0	0
1	B	401	3134	2036	505	572	21	0	0
1	C	592	4639	3030	748	830	31	0	0
1	D	401	3134	2036	505	572	21	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	754	SER	ASN	conflict	UNP P19491
A	758	VAL	LEU	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	830	SER	-	linker	UNP P19491
A	831	ALA	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	754	SER	ASN	conflict	UNP P19491
B	758	VAL	LEU	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	830	SER	-	linker	UNP P19491
B	831	ALA	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	754	SER	ASN	conflict	UNP P19491
C	758	VAL	LEU	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	830	SER	-	linker	UNP P19491
C	831	ALA	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491

*Continued on next page...*

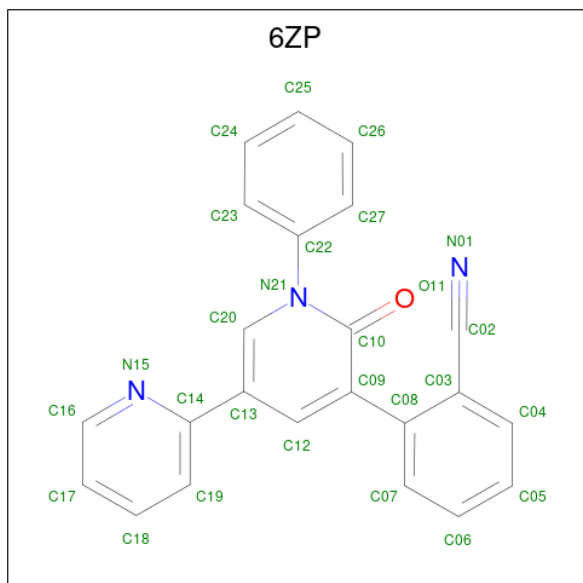
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	754	SER	ASN	conflict	UNP P19491
D	758	VAL	LEU	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	830	SER	-	linker	UNP P19491
D	831	ALA	-	linker	UNP P19491

- Molecule 2 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	140	1166	787	175	191	13	0	0
2	F	140	1166	787	175	191	13	0	0

- Molecule 3 is 2-(6'-oxo-1'-phenyl[1',6'-dihydro[2,3'-bipyridine]]-5'-yl)benzotrile (three-letter code: 6ZP) (formula: C<sub>23</sub>H<sub>15</sub>N<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



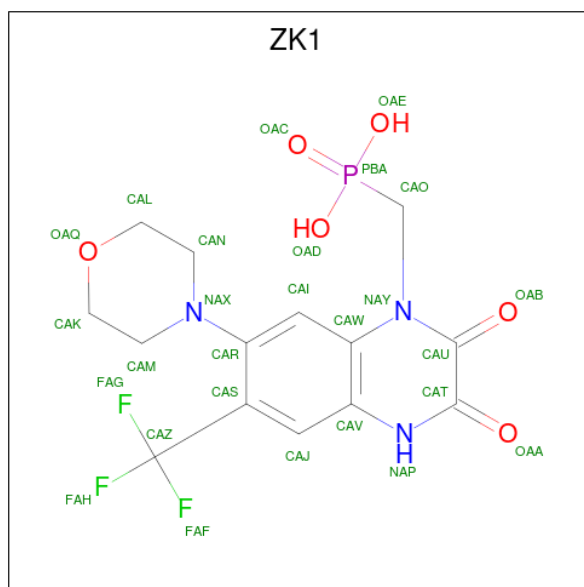
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	27	23	3	1	0
3	B	1	27	23	3	1	0

Continued on next page...

Continued from previous page...

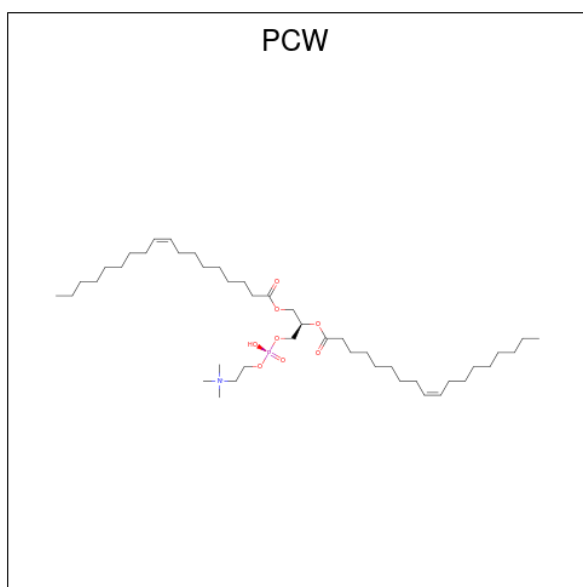
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			27	23	3	1	
3	D	1	Total	C	N	O	0
			27	23	3	1	

- Molecule 4 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
4	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
4	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
4	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
4	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C				0
			11	11				
5	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	B	1	Total	C				0
			11	11				
5	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	C	1	Total	C	N	O	P	0
			51	41	1	8	1	

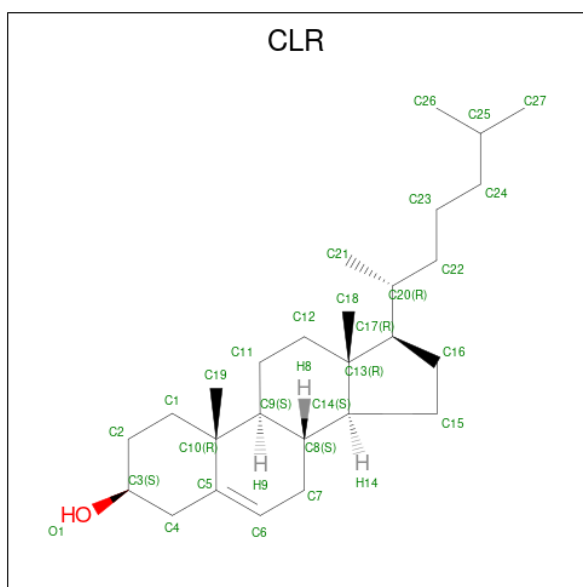
*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	C	1	Total	C				0
			11	11				
5	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	D	1	Total	C				0
			11	11				
5	E	1	Total	C				0
			11	11				
5	E	1	Total	C				0
			11	11				
5	E	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	F	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	F	1	Total	C				0
			11	11				
5	F	1	Total	C				0
			11	11				

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).

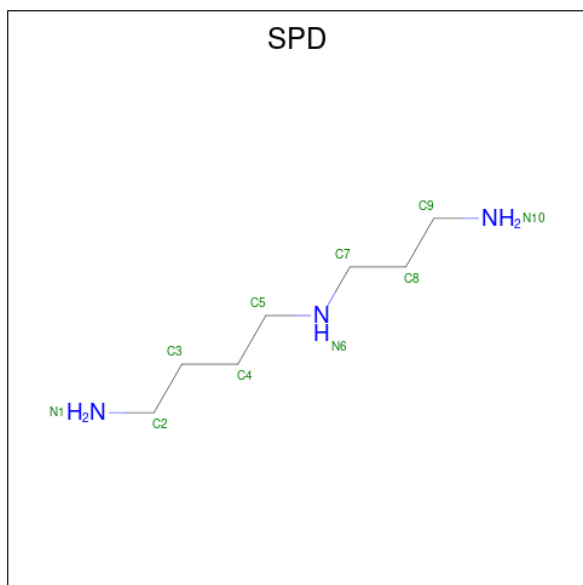


Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Na	0
			1	1	

- Molecule 8 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



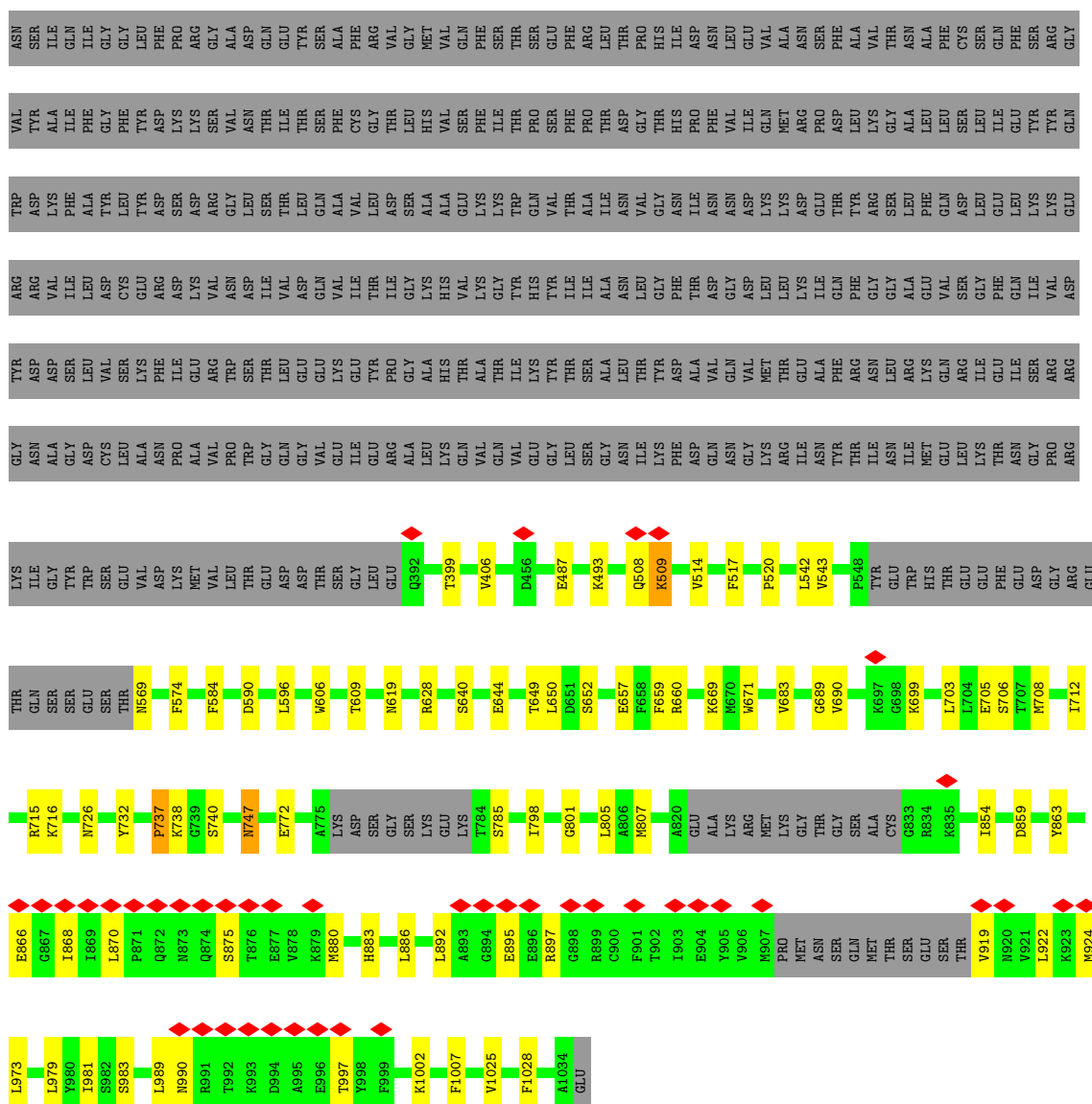
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	N	0
			10	7	3	

### 3 Residue-property plots i

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

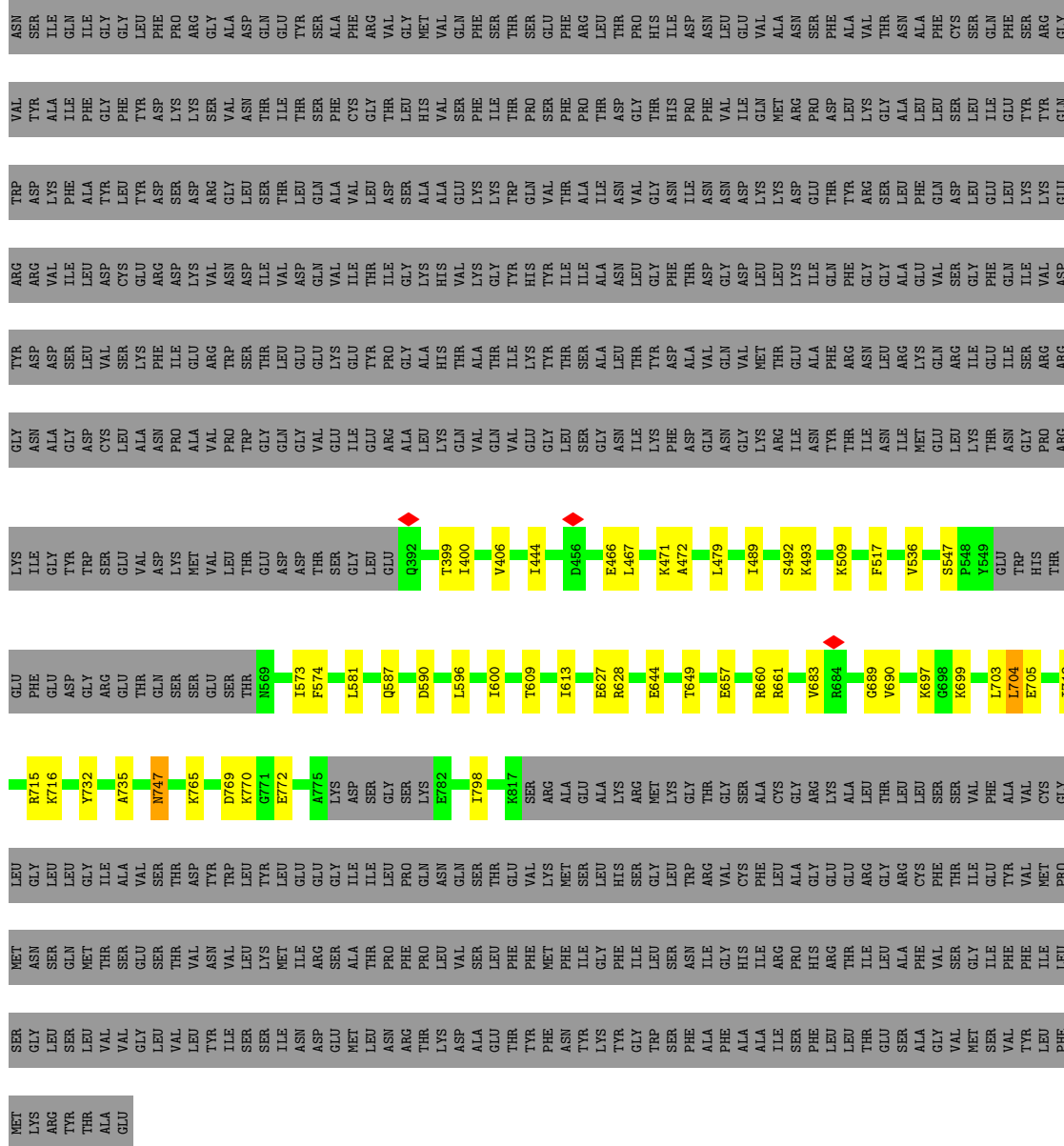
- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

Chain A:



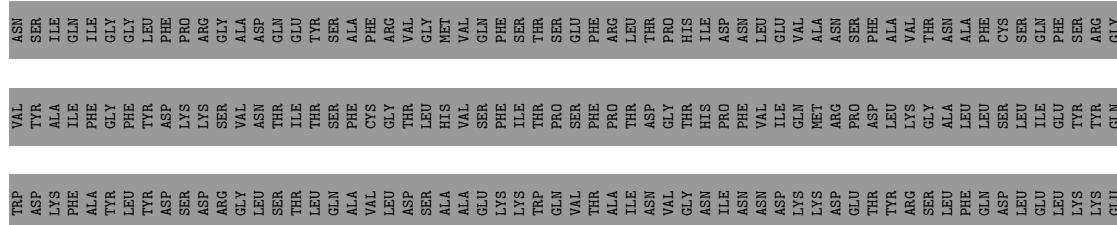
- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

Chain B:  34% 5% 61%



- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

Chain C:  49% 8% 42%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	126263	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	10.298	Depositor
Minimum map value	-6.046	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.172	Depositor
Recommended contour level	1.0	Depositor
Map size ( $\text{\AA}$ )	384.80002, 384.80002, 384.80002	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.9250001, 0.9250001, 0.9250001	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: 6ZP, PCW, SPD, ZK1, NA, CLR

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	0.40	0/4742	0.58	0/6404
1	B	0.42	0/3202	0.58	1/4321 (0.0%)
1	C	0.40	0/4742	0.58	0/6404
1	D	0.42	0/3202	0.58	1/4321 (0.0%)
2	E	0.37	0/1203	0.66	0/1636
2	F	0.37	0/1203	0.66	0/1636
All	All	0.40	0/18294	0.59	2/24722 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
2	E	0	4
2	F	0	4
All	All	0	12

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	704	LEU	CA-CB-CG	7.21	131.88	115.30
1	B	704	LEU	CA-CB-CG	7.20	131.86	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	508	GLN	Peptide
1	A	509	LYS	Peptide
1	C	508	GLN	Peptide
1	C	509	LYS	Peptide
2	E	110	ALA	Peptide
2	E	115	VAL	Peptide
2	E	123	MET	Peptide
2	E	124	ASN	Peptide
2	F	110	ALA	Peptide
2	F	115	VAL	Peptide
2	F	123	MET	Peptide
2	F	124	ASN	Peptide

## 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	4639	0	4714	50	0
1	B	3134	0	3177	33	0
1	C	4639	0	4714	51	0
1	D	3134	0	3177	26	0
2	E	1166	0	1152	13	0
2	F	1166	0	1152	11	0
3	A	27	0	0	1	0
3	B	27	0	0	1	0
3	C	27	0	0	2	0
3	D	27	0	0	1	0
4	A	27	0	13	1	0
4	B	27	0	13	0	0
4	C	27	0	13	1	0
4	D	27	0	13	0	0
5	A	266	0	391	19	0
5	B	215	0	316	26	0
5	C	266	0	391	20	0
5	D	215	0	316	26	0
5	E	73	0	107	9	0
5	F	73	0	107	7	0
6	A	56	0	76	8	0
6	B	56	0	75	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	56	0	76	11	0
6	D	56	0	75	13	0
7	A	1	0	0	0	0
8	A	10	0	19	0	0
All	All	19437	0	20087	266	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 7.

All (266) 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)
6:D:1109:CLR:C14	6:D:1109:CLR:C8	1.85	1.54
6:A:1108:CLR:C14	6:A:1108:CLR:C8	1.85	1.54
6:B:1108:CLR:C14	6:B:1108:CLR:C8	1.85	1.53
6:D:1108:CLR:C14	6:D:1108:CLR:C8	1.87	1.52
6:B:1107:CLR:C14	6:B:1107:CLR:C8	1.87	1.52
6:C:1107:CLR:C14	6:C:1107:CLR:C8	1.85	1.52
6:A:1107:CLR:C14	6:A:1107:CLR:C8	1.85	1.51
6:C:1108:CLR:C14	6:C:1108:CLR:C8	1.85	1.50
6:C:1108:CLR:C14	6:C:1108:CLR:C7	2.60	0.79
6:A:1107:CLR:C14	6:A:1107:CLR:C7	2.60	0.79
6:A:1108:CLR:C14	6:A:1108:CLR:C7	2.60	0.79
6:B:1107:CLR:C8	6:B:1107:CLR:H14	2.10	0.79
6:B:1107:CLR:C14	6:B:1107:CLR:C7	2.60	0.78
6:D:1108:CLR:C14	6:D:1108:CLR:C7	2.60	0.78
6:C:1107:CLR:C14	6:C:1107:CLR:C7	2.61	0.77
1:A:493:LYS:HG2	1:A:747:ASN:HD21	1.52	0.74
1:C:493:LYS:HG2	1:C:747:ASN:HD21	1.52	0.72
6:D:1108:CLR:C8	6:D:1108:CLR:H14	2.11	0.71
6:D:1109:CLR:C14	6:D:1109:CLR:C7	2.65	0.70
6:B:1108:CLR:C14	6:B:1108:CLR:C7	2.66	0.69
6:B:1108:CLR:C14	6:B:1108:CLR:C9	2.64	0.68
6:D:1109:CLR:C14	6:D:1109:CLR:C9	2.64	0.66
1:D:517:PHE:HA	3:D:1102:6ZP:C07	2.26	0.65
5:D:1106:PCW:H11	5:E:203:PCW:H122	1.81	0.63
5:B:1109:PCW:H40	5:C:1105:PCW:H161	1.81	0.62
5:B:1109:PCW:H281	1:C:798:ILE:HD13	1.82	0.62
1:B:547:SER:HB2	1:C:814:PHE:HB2	1.80	0.61
1:C:924:MET:HB3	1:C:983:SER:HB2	1.82	0.61
5:A:1103:PCW:H172	6:A:1107:CLR:H181	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:MET:HB3	1:A:983:SER:HB2	1.82	0.61
2:F:80:LEU:HD22	5:F:201:PCW:H40	1.81	0.60
5:B:1105:PCW:H52	5:F:201:PCW:H31	1.84	0.60
5:D:1106:PCW:H32	5:E:203:PCW:H142	1.83	0.60
5:B:1105:PCW:H11	5:F:201:PCW:H122	1.84	0.60
2:E:57:ILE:HG23	2:E:122:ILE:HD12	1.83	0.59
1:A:708:MET:HG3	4:A:1102:ZK1:HAK	1.84	0.59
1:B:628:ARG:NH1	1:C:785:SER:OG	2.35	0.59
1:A:798:ILE:HD13	5:D:1101:PCW:H281	1.85	0.59
2:F:57:ILE:HG23	2:F:122:ILE:HD12	1.83	0.59
1:B:517:PHE:HA	3:B:1101:6ZP:C07	2.33	0.58
1:A:706:SER:OG	1:A:726:ASN:ND2	2.36	0.58
5:D:1104:PCW:H171	6:D:1108:CLR:H152	1.85	0.58
6:D:1109:CLR:C8	6:D:1109:CLR:H14	2.21	0.58
1:C:706:SER:OG	1:C:726:ASN:ND2	2.37	0.58
1:A:866:GLU:HB3	1:A:880:MET:HB3	1.86	0.58
1:B:493:LYS:HG2	1:B:747:ASN:HD21	1.69	0.57
1:D:493:LYS:HG2	1:D:747:ASN:HD21	1.69	0.57
1:C:866:GLU:HB3	1:C:880:MET:HB3	1.86	0.57
1:A:863:TYR:HB2	1:A:1002:LYS:HB2	1.87	0.57
5:B:1105:PCW:H32	5:F:201:PCW:H142	1.85	0.57
5:C:1103:PCW:H172	6:C:1107:CLR:H181	1.86	0.56
5:D:1106:PCW:H52	5:E:203:PCW:H31	1.88	0.56
1:D:542:LEU:HD21	2:E:74:ILE:HD11	1.88	0.56
1:C:863:TYR:HB2	1:C:1002:LYS:HB2	1.87	0.56
1:A:596:LEU:HB2	5:A:1109:PCW:H31	1.87	0.56
1:B:657:GLU:OE1	1:B:660:ARG:NH2	2.39	0.56
1:C:487:GLU:O	1:C:738:LYS:NZ	2.39	0.55
6:C:1107:CLR:H193	2:F:157:LEU:HD13	1.89	0.55
1:A:487:GLU:O	1:A:738:LYS:NZ	2.39	0.55
1:D:657:GLU:OE1	1:D:660:ARG:NH2	2.40	0.55
1:A:964:ILE:HD13	5:B:1106:PCW:H182	1.89	0.54
1:C:708:MET:HG3	4:C:1102:ZK1:HAK	1.88	0.54
1:C:964:ILE:HD13	5:D:1107:PCW:H182	1.88	0.54
5:D:1104:PCW:H361	5:D:1104:PCW:H142	1.88	0.54
2:E:2:ALA:N	2:E:157:LEU:O	2.40	0.54
2:F:2:ALA:N	2:F:157:LEU:O	2.40	0.54
6:B:1107:CLR:H14	6:B:1107:CLR:C7	2.36	0.54
5:C:1109:PCW:H381	6:D:1109:CLR:H151	1.89	0.54
1:A:868:ILE:HG22	1:A:997:THR:HG22	1.91	0.53
1:C:690:VAL:HG21	1:C:712:ILE:HD13	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:GLU:HG2	1:A:897:ARG:HH21	1.73	0.53
1:C:886:LEU:HD23	1:C:929:THR:HG23	1.91	0.53
1:A:690:VAL:HG21	1:A:712:ILE:HD13	1.91	0.53
1:A:886:LEU:HD23	1:A:929:THR:HG23	1.91	0.53
1:B:406:VAL:HG11	1:B:444:ILE:HD11	1.91	0.53
1:C:868:ILE:HG22	1:C:997:THR:HG22	1.91	0.53
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.90	0.53
5:A:1109:PCW:H361	6:B:1108:CLR:H72	1.91	0.52
6:B:1108:CLR:C8	6:B:1108:CLR:H14	2.22	0.52
1:A:399:THR:HB	1:A:406:VAL:HG21	1.91	0.52
1:A:883:HIS:HD2	1:A:892:LEU:HD23	1.74	0.52
1:C:883:HIS:HD2	1:C:892:LEU:HD23	1.74	0.52
6:C:1107:CLR:C8	6:C:1107:CLR:H14	2.21	0.52
1:A:644:GLU:OE1	1:A:699:LYS:NZ	2.40	0.52
1:C:705:GLU:OE1	1:C:732:TYR:OH	2.28	0.52
5:D:1106:PCW:H262	5:D:1106:PCW:H351	1.91	0.52
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.91	0.52
2:F:37:ASP:O	2:F:56:ASN:ND2	2.43	0.52
1:A:650:LEU:HD23	1:A:652:SER:H	1.74	0.51
1:C:399:THR:HB	1:C:406:VAL:HG21	1.91	0.51
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.91	0.51
1:C:895:GLU:HG2	1:C:897:ARG:HH21	1.73	0.51
2:E:92:GLY:HA2	2:E:95:ILE:HD12	1.92	0.51
1:D:406:VAL:HG11	1:D:444:ILE:HD11	1.91	0.51
2:E:37:ASP:O	2:E:56:ASN:ND2	2.43	0.51
2:F:112:GLY:HA3	2:F:116:MET:HG2	1.93	0.51
1:A:514:VAL:HG21	5:A:1103:PCW:H122	1.92	0.51
1:C:650:LEU:HD23	1:C:652:SER:H	1.74	0.51
1:A:705:GLU:OE1	1:A:732:TYR:OH	2.28	0.51
2:F:92:GLY:HA2	2:F:95:ILE:HD12	1.92	0.51
6:A:1107:CLR:C7	6:A:1107:CLR:H14	2.41	0.51
6:A:1107:CLR:H193	2:E:157:LEU:HD13	1.93	0.51
5:B:1109:PCW:H412	5:C:1105:PCW:H231	1.92	0.51
1:A:785:SER:OG	1:D:628:ARG:NH1	2.45	0.50
5:A:1105:PCW:H161	5:D:1101:PCW:H40	1.93	0.50
1:A:807:MET:HE3	5:E:201:PCW:H20	1.93	0.50
5:B:1105:PCW:H351	5:B:1105:PCW:H241	1.94	0.50
1:C:640:SER:HB2	1:C:669:LYS:HD2	1.94	0.50
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.94	0.50
5:B:1103:PCW:H171	6:B:1107:CLR:H152	1.94	0.50
1:D:715:ARG:NH2	1:D:770:LYS:O	2.44	0.50

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:GLY:HA3	2:E:116:MET:HG2	1.93	0.50
1:A:606:TRP:CG	1:B:587:GLN:HG3	2.47	0.49
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.94	0.49
1:B:715:ARG:NH2	1:B:770:LYS:O	2.44	0.49
1:A:640:SER:HB2	1:A:669:LYS:HD2	1.94	0.48
1:A:574:PHE:HE2	5:A:1105:PCW:H2	1.78	0.48
5:D:1105:PCW:H352	5:D:1105:PCW:H321	1.69	0.48
1:C:517:PHE:HA	3:C:1101:6ZP:C07	2.43	0.48
6:D:1108:CLR:C7	6:D:1108:CLR:H14	2.40	0.48
5:A:1109:PCW:H172	1:B:581:LEU:HD22	1.95	0.48
6:C:1107:CLR:C7	6:C:1107:CLR:H14	2.43	0.48
1:D:466:GLU:HG2	1:D:471:LYS:HE2	1.96	0.48
5:C:1110:PCW:H162	5:D:1107:PCW:H172	1.95	0.47
1:A:584:PHE:HA	1:A:609:THR:HG21	1.96	0.47
5:D:1104:PCW:H151	5:D:1104:PCW:H181	1.63	0.47
1:C:644:GLU:OE1	1:C:699:LYS:NZ	2.40	0.47
2:F:72:TYR:O	2:F:76:GLY:N	2.44	0.47
5:B:1106:PCW:H19	5:B:1106:PCW:H162	1.69	0.47
1:A:716:LYS:HG3	1:A:772:GLU:HB3	1.96	0.47
1:B:466:GLU:HG2	1:B:471:LYS:HE2	1.96	0.47
5:B:1105:PCW:H132	5:B:1105:PCW:H2	1.95	0.47
1:C:584:PHE:HA	1:C:609:THR:HG21	1.96	0.47
1:A:807:MET:HB3	5:E:201:PCW:H182	1.95	0.47
1:C:574:PHE:HE2	5:C:1105:PCW:H2	1.79	0.47
5:D:1106:PCW:H121	5:D:1106:PCW:H151	1.55	0.47
1:A:657:GLU:OE2	1:A:660:ARG:NH1	2.49	0.46
1:C:716:LYS:HG3	1:C:772:GLU:HB3	1.96	0.46
5:A:1105:PCW:H231	5:D:1101:PCW:H412	1.97	0.46
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.97	0.46
1:C:514:VAL:HG21	5:C:1103:PCW:H122	1.96	0.46
1:D:765:LYS:HA	1:D:769:ASP:HB2	1.97	0.46
5:B:1105:PCW:H151	5:B:1105:PCW:H121	1.68	0.46
1:D:609:THR:HG23	1:D:613:ILE:HD13	1.98	0.46
1:A:628:ARG:HH12	1:A:785:SER:HB3	1.81	0.46
1:A:979:LEU:HD21	6:B:1107:CLR:H3	1.98	0.46
1:A:989:LEU:HD11	1:B:509:LYS:HG2	1.96	0.46
1:C:526:TRP:HB3	5:C:1106:PCW:H362	1.98	0.46
5:E:203:PCW:H132	5:E:203:PCW:H321	1.97	0.46
1:D:644:GLU:OE2	1:D:699:LYS:NZ	2.48	0.46
1:C:657:GLU:OE2	1:C:660:ARG:NH1	2.49	0.46
5:F:201:PCW:H321	5:F:201:PCW:H351	1.76	0.46

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:LYS:NZ	1:B:627:GLU:OE1	2.38	0.45
1:D:716:LYS:HG3	1:D:772:GLU:HB3	1.97	0.45
2:E:123:MET:HA	2:E:125:ALA:H	1.82	0.45
1:B:644:GLU:OE2	1:B:699:LYS:NZ	2.48	0.45
2:F:123:MET:HA	2:F:125:ALA:H	1.81	0.45
1:A:517:PHE:HA	3:A:1101:6ZP:C07	2.46	0.45
1:B:573:ILE:HG21	5:B:1104:PCW:H322	1.99	0.45
1:B:716:LYS:HG3	1:B:772:GLU:HB3	1.97	0.45
1:B:705:GLU:OE1	1:B:732:TYR:OH	2.35	0.45
1:C:628:ARG:HH12	1:C:785:SER:HB3	1.81	0.45
1:D:573:ILE:HG21	5:D:1105:PCW:H322	1.98	0.45
1:A:606:TRP:CD2	1:B:587:GLN:HG3	2.52	0.45
1:B:590:ASP:OD1	1:B:590:ASP:N	2.47	0.45
1:D:705:GLU:OE1	1:D:732:TYR:OH	2.35	0.45
5:A:1103:PCW:H232	5:A:1103:PCW:H20	1.66	0.45
5:B:1104:PCW:H281	5:F:201:PCW:H20	1.97	0.45
5:E:203:PCW:H321	5:E:203:PCW:H351	1.67	0.45
1:D:690:VAL:HG21	1:D:712:ILE:HD13	1.98	0.45
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.98	0.45
1:B:609:THR:HG23	1:B:613:ILE:HD13	1.98	0.44
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.98	0.44
1:A:870:LEU:HB2	1:A:875:SER:HB2	1.99	0.44
5:D:1105:PCW:H142	5:D:1105:PCW:H172	1.91	0.44
1:C:599:ARG:HD2	5:C:1109:PCW:H131	1.99	0.44
2:E:72:TYR:O	2:E:76:GLY:N	2.44	0.44
1:C:517:PHE:HA	3:C:1101:6ZP:C06	2.48	0.44
1:D:600:ILE:HA	5:D:1101:PCW:H19	1.98	0.44
6:D:1108:CLR:H25	6:D:1108:CLR:H222	1.55	0.44
5:B:1103:PCW:H182	5:B:1103:PCW:H211	1.73	0.44
1:A:520:PRO:O	1:A:619:ASN:ND2	2.48	0.43
1:A:805:LEU:HD23	5:A:1103:PCW:H261	1.99	0.43
5:A:1106:PCW:H62	5:A:1106:PCW:H41	1.84	0.43
1:B:536:VAL:HG12	1:C:803:LEU:HD11	2.00	0.43
5:C:1109:PCW:H212	5:D:1104:PCW:H262	1.98	0.43
1:B:536:VAL:HG12	1:C:803:LEU:HD21	1.99	0.43
1:B:690:VAL:HG21	1:B:712:ILE:HD13	1.98	0.43
2:F:73:SER:O	2:F:77:LEU:N	2.50	0.43
5:C:1109:PCW:H172	1:D:581:LEU:HD22	1.99	0.43
5:A:1105:PCW:H251	5:D:1101:PCW:H441	1.99	0.43
5:D:1106:PCW:H351	5:D:1106:PCW:H241	1.99	0.43
1:A:542:LEU:HD12	1:A:1025:VAL:HG21	2.00	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1105:PCW:H351	5:B:1105:PCW:H262	2.01	0.43
1:D:683:VAL:HG11	1:D:689:GLY:HA2	2.01	0.43
5:A:1109:PCW:H141	1:B:574:PHE:HD1	1.83	0.43
1:C:870:LEU:HB2	1:C:875:SER:HB2	1.99	0.43
1:A:859:ASP:OD1	1:A:859:ASP:N	2.50	0.43
5:A:1109:PCW:H262	5:A:1109:PCW:H232	1.64	0.43
5:C:1106:PCW:H331	5:C:1106:PCW:H361	1.77	0.43
1:A:683:VAL:HG11	1:A:689:GLY:HA2	2.01	0.43
6:D:1109:CLR:H122	6:D:1109:CLR:H20	1.87	0.43
1:B:596:LEU:HD22	5:B:1109:PCW:H342	2.01	0.43
1:B:683:VAL:HG11	1:B:689:GLY:HA2	2.01	0.43
5:B:1103:PCW:H151	5:B:1103:PCW:H181	1.61	0.43
1:C:1012:ILE:HD11	5:C:1104:PCW:H382	2.00	0.43
5:B:1104:PCW:H322	5:B:1104:PCW:H2	1.92	0.42
1:A:493:LYS:NZ	1:D:492:SER:O	2.51	0.42
1:C:683:VAL:HG11	1:C:689:GLY:HA2	2.01	0.42
5:C:1109:PCW:H41	5:C:1109:PCW:H83	1.82	0.42
1:D:399:THR:HG22	1:D:400:ILE:H	1.84	0.42
1:B:798:ILE:HA	5:B:1103:PCW:H212	2.01	0.42
1:D:467:LEU:HD12	1:D:472:ALA:HB3	2.02	0.42
1:B:600:ILE:HG12	5:B:1109:PCW:H19	2.01	0.42
1:C:520:PRO:O	1:C:619:ASN:ND2	2.48	0.42
1:C:715:ARG:HA	1:C:715:ARG:HD3	1.88	0.42
2:E:73:SER:O	2:E:77:LEU:N	2.50	0.42
1:B:399:THR:HG22	1:B:400:ILE:H	1.84	0.42
1:B:492:SER:O	1:C:493:LYS:NZ	2.52	0.42
2:E:18:ALA:HB1	5:E:201:PCW:H162	2.00	0.42
1:C:859:ASP:OD1	1:C:859:ASP:N	2.50	0.42
5:C:1103:PCW:H19	5:C:1103:PCW:H162	1.79	0.42
1:D:511:LYS:HA	1:D:512:PRO:HD3	1.87	0.42
1:C:737:PRO:HD2	1:C:740:SER:HB2	2.01	0.42
1:A:801:GLY:HA3	5:A:1103:PCW:H212	2.02	0.42
6:C:1108:CLR:H211	6:C:1108:CLR:H232	1.82	0.42
1:D:489:ILE:HD12	1:D:735:ALA:HB1	2.01	0.41
1:B:467:LEU:HD12	1:B:472:ALA:HB3	2.02	0.41
1:C:542:LEU:HD12	1:C:1025:VAL:HG21	2.00	0.41
1:B:489:ILE:HD12	1:B:735:ALA:HB1	2.01	0.41
5:C:1106:PCW:H282	5:C:1106:PCW:H251	1.88	0.41
1:A:596:LEU:HD21	6:B:1108:CLR:H152	2.03	0.41
1:A:715:ARG:HA	1:A:715:ARG:HD3	1.88	0.41
6:C:1108:CLR:C8	6:C:1108:CLR:C15	2.89	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1104:PCW:H412	5:D:1104:PCW:H382	1.85	0.41
5:D:1104:PCW:H421	5:D:1104:PCW:H221	2.02	0.41
5:A:1110:PCW:H162	5:B:1106:PCW:H172	2.03	0.41
1:C:517:PHE:O	1:C:616:TYR:OH	2.28	0.41
6:C:1107:CLR:H25	6:C:1107:CLR:H221	1.71	0.41
5:C:1109:PCW:H372	5:D:1105:PCW:H342	2.01	0.41
2:F:4:THR:HG23	2:F:7:ALA:H	1.85	0.41
5:B:1105:PCW:H62	5:B:1105:PCW:H41	1.83	0.41
1:C:489:ILE:HD12	1:C:735:ALA:HB1	2.03	0.41
5:B:1109:PCW:H252	5:B:1109:PCW:H283	1.80	0.41
1:C:919:VAL:HB	1:C:922:LEU:HD13	2.03	0.41
5:C:1109:PCW:H282	5:D:1106:PCW:H39	2.03	0.41
1:D:590:ASP:OD1	1:D:590:ASP:N	2.47	0.41
6:D:1108:CLR:H162	6:D:1108:CLR:H231	2.03	0.41
1:A:737:PRO:HD2	1:A:740:SER:HB2	2.01	0.41
5:A:1109:PCW:H381	6:B:1108:CLR:H151	2.02	0.40
1:C:596:LEU:HB2	5:C:1109:PCW:H31	2.03	0.40
5:D:1105:PCW:H281	5:E:203:PCW:H20	2.03	0.40
2:E:37:ASP:HB3	2:E:56:ASN:HD22	1.86	0.40
5:A:1109:PCW:H282	5:B:1105:PCW:H39	2.03	0.40
5:B:1103:PCW:H361	5:B:1103:PCW:H142	2.02	0.40
1:C:960:PHE:HB2	1:C:1028:PHE:CG	2.56	0.40
1:A:981:ILE:HD11	1:A:1007:PHE:HZ	1.87	0.40
6:A:1107:CLR:H221	6:A:1107:CLR:H25	1.91	0.40
6:B:1107:CLR:H222	6:B:1107:CLR:H25	1.61	0.40
2:E:4:THR:HG23	2:E:7:ALA:H	1.85	0.40
1:A:919:VAL:HB	1:A:922:LEU:HD13	2.03	0.40
1:A:960:PHE:HB2	1:A:1028:PHE:CG	2.56	0.40
5:A:1106:PCW:H331	5:A:1106:PCW:H361	1.78	0.40
1:C:893:ALA:H	1:C:896:GLU:HG3	1.87	0.40
5:C:1109:PCW:H281	5:D:1106:PCW:H271	2.03	0.40
5:F:201:PCW:H351	5:F:201:PCW:H132	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	582/1026 (57%)	551 (95%)	29 (5%)	2 (0%)	41	60
1	B	395/1026 (38%)	372 (94%)	23 (6%)	0	100	100
1	C	582/1026 (57%)	551 (95%)	29 (5%)	2 (0%)	41	60
1	D	395/1026 (38%)	372 (94%)	23 (6%)	0	100	100
2	E	136/160 (85%)	121 (89%)	11 (8%)	4 (3%)	4	6
2	F	136/160 (85%)	121 (89%)	11 (8%)	4 (3%)	4	6
All	All	2226/4424 (50%)	2088 (94%)	126 (6%)	12 (0%)	32	47

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	123	MET
2	F	123	MET
2	E	116	MET
2	F	116	MET
1	A	509	LYS
1	C	509	LYS
2	E	117	TYR
2	F	117	TYR
2	E	109	PRO
2	F	109	PRO
1	A	737	PRO
1	C	737	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/877 (57%)	494 (99%)	7 (1%)	67	79
1	B	338/877 (38%)	333 (98%)	5 (2%)	65	78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	501/877 (57%)	494 (99%)	7 (1%)	67	79
1	D	338/877 (38%)	333 (98%)	5 (2%)	65	78
2	E	126/143 (88%)	125 (99%)	1 (1%)	81	88
2	F	126/143 (88%)	125 (99%)	1 (1%)	81	88
All	All	1930/3794 (51%)	1904 (99%)	26 (1%)	70	81

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	543	VAL
1	A	569	ASN
1	A	590	ASP
1	A	747	ASN
1	A	854	ILE
1	A	973	LEU
1	A	990	ASN
1	B	479	LEU
1	B	661	ARG
1	B	697	LYS
1	B	704	LEU
1	B	747	ASN
1	C	543	VAL
1	C	569	ASN
1	C	590	ASP
1	C	747	ASN
1	C	854	ILE
1	C	973	LEU
1	C	990	ASN
1	D	479	LEU
1	D	661	ARG
1	D	697	LYS
1	D	704	LEU
1	D	747	ASN
2	E	25	ILE
2	F	25	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	569	ASN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	A	726	ASN
1	A	747	ASN
1	A	990	ASN
1	B	747	ASN
1	C	569	ASN
1	C	726	ASN
1	C	747	ASN
1	C	990	ASN
1	D	747	ASN
2	E	56	ASN
2	F	56	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 1 is monoatomic - leaving 45 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	6ZP	B	1101	-	30,30,30	0.92	1 (3%)	35,41,41	0.99	1 (2%)
4	ZK1	D	1103	-	28,29,29	2.71	8 (28%)	42,45,45	1.81	8 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PCW	D	1107	-	10,10,53	0.75	0	9,9,61	0.38	0
6	CLR	C	1107	-	31,31,31	8.12	17 (54%)	48,48,48	3.05	21 (43%)
5	PCW	B	1104	-	50,50,53	1.11	3 (6%)	56,58,61	0.99	3 (5%)
8	SPD	A	1112	-	9,9,9	0.36	0	8,8,8	0.74	0
5	PCW	C	1104	-	50,50,53	1.13	3 (6%)	56,58,61	1.07	4 (7%)
3	6ZP	A	1101	-	30,30,30	1.04	1 (3%)	35,41,41	1.04	1 (2%)
5	PCW	B	1109	-	50,50,53	1.06	4 (8%)	56,58,61	0.94	4 (7%)
3	6ZP	C	1101	-	30,30,30	1.04	1 (3%)	35,41,41	1.05	1 (2%)
3	6ZP	D	1102	-	30,30,30	0.91	1 (3%)	35,41,41	0.98	1 (2%)
5	PCW	A	1110	-	10,10,53	0.78	0	9,9,61	0.37	0
5	PCW	C	1105	-	50,50,53	1.14	3 (6%)	56,58,61	0.97	3 (5%)
6	CLR	B	1107	-	31,31,31	8.20	19 (61%)	48,48,48	4.94	25 (52%)
5	PCW	D	1105	-	50,50,53	1.10	3 (6%)	56,58,61	0.98	3 (5%)
5	PCW	A	1103	-	50,50,53	1.13	5 (10%)	56,58,61	0.91	3 (5%)
4	ZK1	B	1102	-	28,29,29	2.71	8 (28%)	42,45,45	1.79	8 (19%)
4	ZK1	A	1102	-	28,29,29	2.75	7 (25%)	42,45,45	1.71	7 (16%)
6	CLR	A	1108	-	31,31,31	8.10	17 (54%)	48,48,48	3.44	25 (52%)
5	PCW	A	1106	-	50,50,53	1.11	3 (6%)	56,58,61	0.97	3 (5%)
5	PCW	A	1109	-	50,50,53	1.11	3 (6%)	56,58,61	0.93	3 (5%)
5	PCW	A	1105	-	50,50,53	1.14	3 (6%)	56,58,61	0.99	3 (5%)
5	PCW	C	1110	-	10,10,53	0.79	0	9,9,61	0.37	0
5	PCW	B	1106	-	10,10,53	0.77	0	9,9,61	0.36	0
5	PCW	B	1105	-	50,50,53	1.11	4 (8%)	56,58,61	0.85	3 (5%)
6	CLR	B	1108	-	31,31,31	8.15	17 (54%)	48,48,48	2.99	24 (50%)
5	PCW	F	203	-	10,10,53	0.80	0	9,9,61	0.25	0
5	PCW	E	203	-	50,50,53	1.13	4 (8%)	56,58,61	0.93	3 (5%)
5	PCW	F	201	-	50,50,53	1.13	4 (8%)	56,58,61	0.93	3 (5%)
6	CLR	D	1109	-	31,31,31	8.15	17 (54%)	48,48,48	3.00	24 (50%)
5	PCW	F	202	-	10,10,53	0.80	0	9,9,61	0.35	0
6	CLR	C	1108	-	31,31,31	8.09	17 (54%)	48,48,48	3.34	25 (52%)
6	CLR	D	1108	-	31,31,31	8.19	19 (61%)	48,48,48	4.98	25 (52%)
5	PCW	A	1104	-	50,50,53	1.13	3 (6%)	56,58,61	1.06	4 (7%)
5	PCW	B	1103	-	50,50,53	1.12	3 (6%)	56,58,61	0.94	3 (5%)
4	ZK1	C	1102	-	28,29,29	2.73	7 (25%)	42,45,45	1.69	7 (16%)
5	PCW	D	1106	-	50,50,53	1.11	4 (8%)	56,58,61	0.86	3 (5%)
5	PCW	C	1109	-	50,50,53	1.11	3 (6%)	56,58,61	0.97	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PCW	D	1101	-	50,50,53	1.08	4 (8%)	56,58,61	0.93	4 (7%)
5	PCW	D	1104	-	50,50,53	1.13	4 (8%)	56,58,61	0.93	3 (5%)
6	CLR	A	1107	-	31,31,31	8.13	17 (54%)	48,48,48	3.09	20 (41%)
5	PCW	E	201	-	10,10,53	0.78	0	9,9,61	0.29	0
5	PCW	E	202	-	10,10,53	0.80	0	9,9,61	0.24	0
5	PCW	C	1106	-	50,50,53	1.11	4 (8%)	56,58,61	0.98	3 (5%)
5	PCW	C	1103	-	50,50,53	1.14	5 (10%)	56,58,61	0.92	3 (5%)

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
3	6ZP	B	1101	-	-	0/13/14/14	0/4/4/4
4	ZK1	D	1103	-	-	5/13/23/23	0/3/3/3
5	PCW	D	1107	-	-	3/8/8/57	-
6	CLR	C	1107	-	2/2/10/11	8/10/68/68	0/4/4/4
5	PCW	B	1104	-	-	27/54/54/57	-
8	SPD	A	1112	-	-	0/7/7/7	-
5	PCW	C	1104	-	-	26/54/54/57	-
3	6ZP	A	1101	-	-	0/13/14/14	0/4/4/4
5	PCW	B	1109	-	-	24/54/54/57	-
3	6ZP	C	1101	-	-	0/13/14/14	0/4/4/4
3	6ZP	D	1102	-	-	0/13/14/14	0/4/4/4
5	PCW	A	1110	-	-	2/8/8/57	-
6	CLR	B	1107	-	2/2/10/11	9/10/68/68	0/4/4/4
5	PCW	C	1105	-	-	34/54/54/57	-
5	PCW	D	1105	-	-	27/54/54/57	-
5	PCW	A	1103	-	-	26/54/54/57	-
4	ZK1	B	1102	-	-	5/13/23/23	0/3/3/3
4	ZK1	A	1102	-	-	5/13/23/23	0/3/3/3
6	CLR	A	1108	-	2/2/10/11	8/10/68/68	0/4/4/4
5	PCW	A	1106	-	-	25/54/54/57	-
5	PCW	A	1109	-	-	21/54/54/57	-
5	PCW	A	1105	-	-	33/54/54/57	-
6	CLR	B	1108	-	2/2/10/11	9/10/68/68	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PCW	B	1106	-	-	3/8/8/57	-
5	PCW	B	1105	-	-	34/54/54/57	-
5	PCW	C	1110	-	-	2/8/8/57	-
5	PCW	F	203	-	-	3/8/8/57	-
5	PCW	E	203	-	-	28/54/54/57	-
5	PCW	F	201	-	-	26/54/54/57	-
6	CLR	D	1109	-	2/2/10/11	9/10/68/68	0/4/4/4
5	PCW	F	202	-	-	6/8/8/57	-
6	CLR	C	1108	-	2/2/10/11	8/10/68/68	0/4/4/4
6	CLR	D	1108	-	2/2/10/11	9/10/68/68	0/4/4/4
5	PCW	A	1104	-	-	27/54/54/57	-
5	PCW	B	1103	-	-	21/54/54/57	-
4	ZK1	C	1102	-	-	5/13/23/23	0/3/3/3
5	PCW	D	1106	-	-	32/54/54/57	-
5	PCW	C	1109	-	-	24/54/54/57	-
5	PCW	D	1101	-	-	24/54/54/57	-
5	PCW	D	1104	-	-	25/54/54/57	-
6	CLR	A	1107	-	2/2/10/11	8/10/68/68	0/4/4/4
5	PCW	E	201	-	-	4/8/8/57	-
5	PCW	E	202	-	-	4/8/8/57	-
5	PCW	C	1106	-	-	27/54/54/57	-
5	PCW	C	1103	-	-	27/54/54/57	-

All (246) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1109	CLR	C4-C5	-23.29	1.01	1.51
6	D	1108	CLR	C4-C5	-23.23	1.01	1.51
6	A	1107	CLR	C4-C5	-23.23	1.01	1.51
6	C	1107	CLR	C4-C5	-23.21	1.01	1.51
6	B	1108	CLR	C4-C5	-23.20	1.01	1.51
6	A	1108	CLR	C4-C5	-23.19	1.01	1.51
6	B	1107	CLR	C4-C5	-23.17	1.01	1.51
6	C	1108	CLR	C4-C5	-23.11	1.01	1.51
6	A	1108	CLR	C1-C2	-19.79	1.11	1.53
6	C	1108	CLR	C1-C2	-19.77	1.11	1.53
6	A	1107	CLR	C1-C2	-19.76	1.11	1.53

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1107	CLR	C1-C2	-19.76	1.11	1.53
6	D	1108	CLR	C1-C2	-19.67	1.11	1.53
6	B	1107	CLR	C1-C2	-19.66	1.11	1.53
6	B	1108	CLR	C1-C2	-19.63	1.11	1.53
6	D	1109	CLR	C1-C2	-19.61	1.11	1.53
6	B	1107	CLR	C8-C14	17.59	1.87	1.53
6	D	1108	CLR	C8-C14	17.55	1.87	1.53
6	A	1107	CLR	C8-C14	16.94	1.85	1.53
6	C	1107	CLR	C8-C14	16.92	1.85	1.53
6	C	1108	CLR	C8-C14	16.78	1.85	1.53
6	A	1108	CLR	C8-C14	16.69	1.85	1.53
6	B	1108	CLR	C8-C14	16.65	1.85	1.53
6	D	1109	CLR	C8-C14	16.63	1.85	1.53
6	B	1108	CLR	C8-C9	-14.23	1.26	1.53
6	D	1109	CLR	C8-C9	-14.19	1.26	1.53
6	C	1107	CLR	C8-C9	-13.55	1.27	1.53
6	A	1108	CLR	C8-C9	-13.53	1.27	1.53
6	A	1107	CLR	C8-C9	-13.50	1.27	1.53
6	C	1108	CLR	C8-C9	-13.50	1.27	1.53
6	B	1107	CLR	C8-C9	-12.99	1.28	1.53
6	D	1108	CLR	C8-C9	-12.82	1.29	1.53
6	B	1108	CLR	C7-C6	10.34	1.72	1.50
6	D	1109	CLR	C7-C6	10.27	1.72	1.50
6	D	1108	CLR	C7-C6	10.13	1.72	1.50
6	B	1107	CLR	C7-C6	10.13	1.72	1.50
6	C	1107	CLR	C7-C6	10.11	1.72	1.50
6	C	1108	CLR	C7-C6	10.09	1.71	1.50
6	A	1108	CLR	C7-C6	10.08	1.71	1.50
6	A	1107	CLR	C7-C6	10.00	1.71	1.50
6	D	1109	CLR	C7-C8	-9.61	1.36	1.53
6	B	1108	CLR	C7-C8	-9.60	1.36	1.53
6	B	1107	CLR	C7-C8	-9.41	1.37	1.53
6	B	1107	CLR	C4-C3	9.37	1.68	1.52
6	B	1108	CLR	C4-C3	9.36	1.68	1.52
6	D	1108	CLR	C4-C3	9.34	1.68	1.52
6	C	1108	CLR	C4-C3	9.31	1.68	1.52
6	D	1108	CLR	C7-C8	-9.30	1.37	1.53
6	A	1108	CLR	C4-C3	9.28	1.68	1.52
6	D	1109	CLR	C4-C3	9.24	1.68	1.52
6	A	1107	CLR	C4-C3	9.19	1.68	1.52
6	C	1107	CLR	C4-C3	9.19	1.68	1.52
6	A	1107	CLR	C7-C8	-9.16	1.37	1.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1108	CLR	C6-C5	-9.15	1.12	1.33
6	C	1107	CLR	C7-C8	-9.15	1.37	1.53
6	A	1108	CLR	C6-C5	-9.04	1.13	1.33
6	A	1107	CLR	C6-C5	-9.00	1.13	1.33
6	C	1107	CLR	C6-C5	-8.96	1.13	1.33
6	C	1108	CLR	C7-C8	-8.90	1.38	1.53
6	A	1108	CLR	C7-C8	-8.89	1.38	1.53
6	D	1108	CLR	C6-C5	-8.84	1.13	1.33
6	B	1107	CLR	C6-C5	-8.81	1.13	1.33
6	B	1108	CLR	C6-C5	-8.69	1.13	1.33
6	D	1109	CLR	C6-C5	-8.67	1.13	1.33
4	A	1102	ZK1	OAA-CAT	8.36	1.39	1.23
4	D	1103	ZK1	OAA-CAT	8.36	1.39	1.23
4	B	1102	ZK1	OAA-CAT	8.33	1.39	1.23
4	C	1102	ZK1	OAA-CAT	8.32	1.39	1.23
4	D	1103	ZK1	OAB-CAU	8.11	1.40	1.23
4	B	1102	ZK1	OAB-CAU	8.11	1.40	1.23
4	A	1102	ZK1	OAB-CAU	8.06	1.40	1.23
4	C	1102	ZK1	OAB-CAU	8.01	1.40	1.23
6	D	1108	CLR	C13-C14	-7.90	1.39	1.55
6	B	1107	CLR	C13-C14	-7.86	1.40	1.55
6	B	1108	CLR	C13-C14	-7.41	1.40	1.55
6	D	1109	CLR	C13-C14	-7.28	1.41	1.55
6	A	1107	CLR	C13-C14	-7.24	1.41	1.55
6	D	1108	CLR	C11-C9	7.18	1.65	1.53
6	C	1107	CLR	C13-C14	-7.17	1.41	1.55
6	B	1107	CLR	C11-C9	7.15	1.65	1.53
6	A	1108	CLR	C13-C14	-7.10	1.41	1.55
6	C	1108	CLR	C13-C14	-7.03	1.41	1.55
6	A	1108	CLR	C11-C9	6.55	1.64	1.53
6	C	1108	CLR	C11-C9	6.51	1.64	1.53
6	D	1108	CLR	C12-C13	-6.33	1.42	1.54
6	B	1107	CLR	C12-C13	-6.30	1.42	1.54
6	A	1107	CLR	C11-C9	6.23	1.64	1.53
6	C	1107	CLR	C11-C9	6.23	1.64	1.53
6	D	1109	CLR	C10-C9	6.20	1.66	1.56
6	B	1108	CLR	C10-C9	6.15	1.66	1.56
6	A	1107	CLR	C10-C9	6.14	1.66	1.56
6	A	1107	CLR	C12-C13	-6.14	1.43	1.54
6	C	1107	CLR	C10-C9	6.08	1.66	1.56
6	C	1107	CLR	C12-C13	-6.07	1.43	1.54
6	B	1108	CLR	C11-C9	5.96	1.63	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1109	CLR	C11-C9	5.91	1.63	1.53
6	B	1107	CLR	C13-C17	5.87	1.66	1.55
6	A	1108	CLR	C12-C13	-5.87	1.43	1.54
6	A	1107	CLR	C13-C17	5.86	1.66	1.55
6	C	1108	CLR	C12-C13	-5.85	1.43	1.54
6	A	1108	CLR	C16-C17	-5.83	1.42	1.54
6	B	1108	CLR	C12-C13	-5.82	1.43	1.54
6	D	1109	CLR	C12-C13	-5.81	1.43	1.54
6	D	1108	CLR	C13-C17	5.77	1.66	1.55
6	C	1108	CLR	C10-C9	5.74	1.65	1.56
6	C	1107	CLR	C13-C17	5.73	1.65	1.55
6	C	1108	CLR	C16-C17	-5.68	1.42	1.54
6	A	1108	CLR	C10-C9	5.66	1.65	1.56
6	D	1109	CLR	C13-C17	5.64	1.65	1.55
6	B	1108	CLR	C13-C17	5.59	1.65	1.55
6	D	1109	CLR	C16-C17	-5.56	1.42	1.54
6	C	1108	CLR	C13-C17	5.55	1.65	1.55
6	B	1108	CLR	C16-C17	-5.53	1.42	1.54
6	C	1107	CLR	C16-C17	-5.52	1.42	1.54
6	A	1108	CLR	C13-C17	5.45	1.65	1.55
6	A	1108	CLR	C2-C3	-5.44	1.38	1.51
6	A	1107	CLR	C16-C17	-5.44	1.43	1.54
6	C	1108	CLR	C2-C3	-5.43	1.38	1.51
6	A	1107	CLR	C2-C3	-5.31	1.39	1.51
6	B	1107	CLR	C10-C9	5.28	1.64	1.56
6	C	1107	CLR	C2-C3	-5.27	1.39	1.51
6	D	1109	CLR	C2-C3	-5.27	1.39	1.51
6	B	1108	CLR	C2-C3	-5.27	1.39	1.51
6	D	1108	CLR	C2-C3	-5.26	1.39	1.51
6	D	1108	CLR	C10-C9	5.21	1.64	1.56
6	B	1107	CLR	C2-C3	-5.14	1.39	1.51
3	C	1101	6ZP	C09-C10	-4.82	1.38	1.46
3	A	1101	6ZP	C09-C10	-4.82	1.38	1.46
3	B	1101	6ZP	C09-C10	-4.33	1.39	1.46
3	D	1102	6ZP	C09-C10	-4.31	1.39	1.46
6	D	1109	CLR	C1-C10	4.19	1.62	1.54
6	D	1108	CLR	C16-C17	-4.18	1.45	1.54
6	B	1107	CLR	C16-C17	-4.16	1.45	1.54
6	B	1108	CLR	C1-C10	4.15	1.62	1.54
6	D	1108	CLR	C15-C14	4.13	1.63	1.54
6	A	1107	CLR	C1-C10	4.11	1.62	1.54
6	B	1107	CLR	C15-C14	4.10	1.62	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1107	CLR	C1-C10	4.08	1.62	1.54
6	A	1108	CLR	C1-C10	3.97	1.61	1.54
6	C	1108	CLR	C1-C10	3.96	1.61	1.54
6	D	1108	CLR	C1-C10	3.94	1.61	1.54
6	B	1107	CLR	C1-C10	3.92	1.61	1.54
4	B	1102	ZK1	CAW-NAY	-3.63	1.34	1.41
4	A	1102	ZK1	CAW-NAY	-3.59	1.34	1.41
4	C	1102	ZK1	CAW-NAY	-3.59	1.34	1.41
4	D	1103	ZK1	CAW-NAY	-3.57	1.34	1.41
6	A	1107	CLR	C15-C14	3.37	1.61	1.54
4	A	1102	ZK1	CAV-NAP	-3.36	1.34	1.39
4	C	1102	ZK1	CAV-NAP	-3.36	1.34	1.39
4	A	1102	ZK1	CAV-CAW	-3.35	1.36	1.40
6	C	1107	CLR	C15-C14	3.34	1.61	1.54
6	B	1108	CLR	C15-C14	3.31	1.61	1.54
4	A	1102	ZK1	CAU-NAY	-3.26	1.32	1.38
4	C	1102	ZK1	CAV-CAW	-3.25	1.36	1.40
4	C	1102	ZK1	CAU-NAY	-3.23	1.32	1.38
6	B	1107	CLR	C18-C13	3.20	1.59	1.54
6	D	1109	CLR	C15-C14	3.19	1.61	1.54
4	D	1103	ZK1	CAU-NAY	-3.18	1.32	1.38
4	B	1102	ZK1	CAU-NAY	-3.16	1.32	1.38
6	D	1108	CLR	C18-C13	3.14	1.59	1.54
5	A	1106	PCW	O3-C11	3.11	1.42	1.33
6	C	1108	CLR	C15-C14	3.11	1.60	1.54
4	B	1102	ZK1	CAV-NAP	-3.11	1.34	1.39
5	A	1105	PCW	O2-C31	3.11	1.43	1.34
4	D	1103	ZK1	CAV-NAP	-3.10	1.34	1.39
5	C	1106	PCW	O3-C11	3.09	1.42	1.33
5	C	1105	PCW	O3-C11	3.05	1.42	1.33
6	A	1108	CLR	C15-C14	3.04	1.60	1.54
5	C	1104	PCW	O2-C31	3.04	1.42	1.34
5	C	1105	PCW	O2-C31	3.04	1.42	1.34
5	B	1105	PCW	O3-C11	3.03	1.42	1.33
5	C	1109	PCW	O2-C31	3.03	1.42	1.34
5	D	1106	PCW	O2-C31	3.03	1.42	1.34
5	D	1104	PCW	O3-C11	3.00	1.42	1.33
5	F	201	PCW	O3-C11	3.00	1.42	1.33
5	A	1105	PCW	O3-C11	2.99	1.42	1.33
5	A	1109	PCW	O2-C31	2.99	1.42	1.34
5	D	1106	PCW	O3-C11	2.98	1.42	1.33
5	E	203	PCW	O3-C11	2.98	1.42	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1104	PCW	O2-C31	2.97	1.42	1.34
5	C	1103	PCW	O2-C31	2.96	1.42	1.34
5	A	1103	PCW	O2-C31	2.96	1.42	1.34
5	B	1105	PCW	O2-C31	2.93	1.42	1.34
5	B	1103	PCW	O3-C11	2.91	1.41	1.33
5	C	1104	PCW	O3-C11	2.89	1.41	1.33
5	C	1103	PCW	O3-C11	2.88	1.41	1.33
5	B	1104	PCW	O2-C31	2.88	1.42	1.34
5	D	1104	PCW	O2-C31	2.88	1.42	1.34
5	D	1105	PCW	O2-C31	2.88	1.42	1.34
5	D	1101	PCW	O2-C31	2.87	1.42	1.34
5	A	1103	PCW	O3-C11	2.87	1.41	1.33
5	A	1104	PCW	O3-C11	2.87	1.41	1.33
5	B	1103	PCW	O2-C31	2.84	1.42	1.34
4	A	1102	ZK1	CAT-NAP	-2.84	1.31	1.35
5	B	1109	PCW	O2-C31	2.83	1.42	1.34
4	B	1102	ZK1	CAV-CAW	-2.81	1.37	1.40
5	C	1109	PCW	O3-C11	2.81	1.41	1.33
4	D	1103	ZK1	CAV-CAW	-2.79	1.37	1.40
5	B	1104	PCW	O3-C11	2.79	1.41	1.33
5	C	1106	PCW	O2-C31	2.79	1.42	1.34
5	A	1109	PCW	O3-C11	2.78	1.41	1.33
5	A	1106	PCW	O2-C31	2.78	1.42	1.34
6	D	1108	CLR	C16-C15	2.76	1.61	1.54
5	D	1105	PCW	O3-C11	2.76	1.41	1.33
5	E	203	PCW	O2-C31	2.76	1.42	1.34
6	B	1107	CLR	C16-C15	2.73	1.61	1.54
5	F	201	PCW	O2-C31	2.72	1.42	1.34
4	C	1102	ZK1	CAT-NAP	-2.72	1.32	1.35
4	D	1103	ZK1	CAT-NAP	-2.60	1.32	1.35
5	B	1109	PCW	O2-C2	-2.55	1.40	1.46
5	D	1105	PCW	O2-C2	-2.55	1.40	1.46
5	B	1104	PCW	O2-C2	-2.55	1.40	1.46
5	F	201	PCW	O2-C2	-2.54	1.40	1.46
4	B	1102	ZK1	CAT-NAP	-2.53	1.32	1.35
5	E	203	PCW	O2-C2	-2.52	1.40	1.46
5	D	1101	PCW	O2-C2	-2.52	1.40	1.46
5	D	1101	PCW	O3-C11	2.51	1.40	1.33
5	A	1106	PCW	O2-C2	-2.50	1.40	1.46
5	C	1106	PCW	O2-C2	-2.49	1.40	1.46
5	B	1109	PCW	O3-C11	2.44	1.40	1.33
5	A	1103	PCW	O2-C2	-2.34	1.40	1.46

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1105	PCW	O2-C2	-2.33	1.40	1.46
5	B	1103	PCW	O2-C2	-2.33	1.40	1.46
5	C	1103	PCW	O2-C2	-2.32	1.40	1.46
5	D	1104	PCW	O2-C2	-2.31	1.40	1.46
5	A	1104	PCW	O2-C2	-2.29	1.40	1.46
5	A	1109	PCW	O2-C2	-2.28	1.40	1.46
5	A	1105	PCW	O2-C2	-2.24	1.41	1.46
5	C	1109	PCW	O2-C2	-2.20	1.41	1.46
5	C	1104	PCW	O2-C2	-2.18	1.41	1.46
5	B	1105	PCW	O2-C2	-2.16	1.41	1.46
5	D	1106	PCW	O2-C2	-2.12	1.41	1.46
5	D	1101	PCW	P-O4P	2.10	1.67	1.59
4	B	1102	ZK1	PBA-CAO	2.08	1.86	1.81
5	C	1103	PCW	P-O4P	2.06	1.67	1.59
5	B	1109	PCW	P-O4P	2.05	1.67	1.59
5	A	1103	PCW	P-O4P	2.05	1.67	1.59
5	F	201	PCW	P-O4P	2.04	1.67	1.59
5	C	1103	PCW	P-O3P	2.03	1.67	1.59
5	E	203	PCW	P-O4P	2.03	1.67	1.59
5	B	1105	PCW	P-O4P	2.02	1.67	1.59
5	D	1106	PCW	P-O4P	2.02	1.67	1.59
4	D	1103	ZK1	PBA-CAO	2.02	1.86	1.81
5	A	1103	PCW	P-O3P	2.01	1.67	1.59
5	C	1106	PCW	P-O4P	2.01	1.67	1.59
5	D	1104	PCW	P-O4P	2.00	1.67	1.59

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1108	CLR	C18-C13-C12	-17.66	82.70	110.59
6	B	1107	CLR	C18-C13-C12	-17.59	82.82	110.59
6	D	1108	CLR	C18-C13-C17	-10.11	92.85	111.71
6	B	1107	CLR	C18-C13-C17	-10.08	92.91	111.71
6	D	1108	CLR	C12-C13-C14	9.99	122.78	107.27
6	B	1107	CLR	C12-C13-C14	9.94	122.70	107.27
6	D	1108	CLR	C22-C20-C17	9.43	129.76	110.28
6	B	1107	CLR	C22-C20-C17	9.24	129.37	110.28
6	B	1107	CLR	C12-C13-C17	8.71	129.61	116.57
6	B	1107	CLR	C19-C10-C9	-8.55	101.49	111.68
6	D	1108	CLR	C12-C13-C17	8.54	129.35	116.57
6	A	1107	CLR	C4-C5-C6	-8.40	108.50	120.61
6	C	1107	CLR	C4-C5-C6	-8.31	108.64	120.61

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1108	CLR	C19-C10-C9	-8.21	101.89	111.68
6	D	1108	CLR	C19-C10-C9	-8.08	102.04	111.68
6	D	1109	CLR	C4-C5-C6	-8.07	108.98	120.61
6	C	1108	CLR	C4-C5-C6	-8.07	108.98	120.61
6	B	1107	CLR	C4-C5-C6	-8.03	109.04	120.61
6	D	1108	CLR	C4-C5-C6	-7.97	109.12	120.61
6	A	1108	CLR	C4-C5-C6	-7.87	109.27	120.61
6	B	1108	CLR	C4-C5-C6	-7.85	109.29	120.61
6	D	1109	CLR	C12-C13-C17	-7.80	104.90	116.57
6	A	1108	CLR	C7-C8-C9	7.67	119.01	109.71
6	B	1108	CLR	C12-C13-C17	-7.67	105.09	116.57
6	C	1108	CLR	C7-C8-C9	7.59	118.91	109.71
6	D	1109	CLR	C19-C10-C9	-7.54	102.69	111.68
6	A	1108	CLR	C21-C20-C17	-7.47	101.48	112.92
6	A	1108	CLR	C19-C10-C9	-7.19	103.11	111.68
6	A	1108	CLR	C1-C2-C3	7.11	119.59	110.47
6	A	1107	CLR	C12-C13-C17	-7.04	106.04	116.57
6	C	1108	CLR	C19-C10-C9	-6.89	103.47	111.68
6	B	1108	CLR	C1-C2-C3	6.88	119.30	110.47
6	D	1109	CLR	C1-C2-C3	6.87	119.28	110.47
6	C	1107	CLR	C12-C13-C17	-6.81	106.38	116.57
6	C	1108	CLR	C12-C13-C17	-6.80	106.39	116.57
6	D	1108	CLR	C1-C2-C3	6.62	118.96	110.47
6	C	1107	CLR	C19-C10-C9	-6.60	103.81	111.68
6	A	1108	CLR	C12-C13-C17	-6.56	106.76	116.57
6	B	1107	CLR	C1-C2-C3	6.54	118.87	110.47
6	A	1107	CLR	C19-C10-C9	-6.47	103.96	111.68
6	C	1108	CLR	C1-C2-C3	6.46	118.75	110.47
6	D	1108	CLR	C16-C17-C20	6.38	122.03	112.15
6	D	1108	CLR	C17-C13-C14	6.31	107.55	100.07
6	C	1108	CLR	C21-C20-C17	-6.24	103.36	112.92
6	B	1107	CLR	C16-C17-C20	6.22	121.77	112.15
6	C	1107	CLR	C1-C2-C3	6.21	118.44	110.47
6	A	1107	CLR	C7-C8-C9	6.15	117.17	109.71
6	A	1107	CLR	C1-C2-C3	6.14	118.34	110.47
6	B	1107	CLR	C17-C13-C14	6.11	107.31	100.07
6	C	1107	CLR	C7-C8-C9	5.95	116.92	109.71
6	D	1108	CLR	C21-C20-C17	-5.71	104.18	112.92
6	A	1107	CLR	C14-C8-C9	5.59	116.57	109.09
6	C	1107	CLR	C14-C8-C9	5.52	116.49	109.09
6	B	1107	CLR	C21-C20-C17	-5.40	104.65	112.92
6	A	1108	CLR	C15-C16-C17	-5.31	94.61	105.13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1108	CLR	C7-C8-C9	5.26	116.08	109.71
6	D	1108	CLR	C18-C13-C14	-5.16	102.09	111.71
4	D	1103	ZK1	CAN-NAX-CAM	5.00	122.54	111.52
6	B	1107	CLR	C18-C13-C14	-4.98	102.42	111.71
4	B	1102	ZK1	CAN-NAX-CAM	4.98	122.51	111.52
5	A	1104	PCW	O2-C31-C32	4.95	122.18	111.50
5	C	1104	PCW	O2-C31-C32	4.95	122.17	111.50
6	B	1107	CLR	C14-C8-C9	4.93	115.69	109.09
5	B	1104	PCW	O2-C31-C32	4.90	122.06	111.50
4	A	1102	ZK1	CAI-CAR-NAX	-4.89	115.28	122.52
5	D	1105	PCW	O2-C31-C32	4.85	121.96	111.50
6	A	1108	CLR	C14-C8-C9	4.83	115.56	109.09
6	A	1108	CLR	C12-C13-C14	4.70	114.57	107.27
6	C	1108	CLR	C14-C8-C9	4.70	115.38	109.09
6	D	1108	CLR	C14-C8-C9	4.68	115.36	109.09
4	C	1102	ZK1	CAI-CAR-NAX	-4.68	115.60	122.52
6	C	1108	CLR	C12-C13-C14	4.67	114.52	107.27
4	D	1103	ZK1	CAV-NAP-CAT	-4.59	118.96	124.80
4	B	1102	ZK1	CAV-NAP-CAT	-4.54	119.02	124.80
6	C	1108	CLR	C7-C6-C5	-4.52	116.73	125.06
6	B	1107	CLR	C7-C8-C9	4.49	115.16	109.71
4	A	1102	ZK1	CAN-NAX-CAM	4.48	121.40	111.52
4	D	1103	ZK1	CAI-CAR-NAX	-4.43	115.97	122.52
4	B	1102	ZK1	CAI-CAR-NAX	-4.42	115.99	122.52
6	A	1108	CLR	C7-C6-C5	-4.41	116.92	125.06
4	C	1102	ZK1	CAN-NAX-CAM	4.40	121.23	111.52
6	C	1108	CLR	C15-C16-C17	-4.36	96.48	105.13
6	D	1108	CLR	C10-C9-C8	4.36	119.27	112.73
6	D	1109	CLR	C14-C8-C9	4.34	114.90	109.09
5	C	1109	PCW	O2-C31-C32	4.29	120.75	111.50
6	B	1107	CLR	C10-C9-C8	4.27	119.14	112.73
5	A	1105	PCW	O2-C31-C32	4.26	120.68	111.50
6	A	1107	CLR	C7-C6-C5	-4.25	117.21	125.06
4	A	1102	ZK1	CAS-CAR-NAX	4.24	124.78	119.92
6	C	1107	CLR	C7-C6-C5	-4.21	117.30	125.06
6	D	1109	CLR	C12-C13-C14	4.18	113.76	107.27
5	C	1105	PCW	O2-C31-C32	4.17	120.49	111.50
6	A	1107	CLR	C17-C13-C14	4.14	104.97	100.07
5	A	1109	PCW	O2-C31-C32	4.12	120.39	111.50
6	B	1108	CLR	C14-C8-C9	4.12	114.61	109.09
4	C	1102	ZK1	CAS-CAR-NAX	4.05	124.56	119.92
5	D	1104	PCW	O2-C31-C32	4.04	120.22	111.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1103	PCW	O2-C31-C32	4.04	120.21	111.50
5	B	1103	PCW	O2-C31-C32	4.02	120.17	111.50
6	C	1108	CLR	C3-C4-C5	3.98	118.78	112.03
5	C	1106	PCW	O2-C31-C32	3.96	120.05	111.50
5	E	203	PCW	O2-C31-C32	3.96	120.04	111.50
4	C	1102	ZK1	CAV-NAP-CAT	-3.96	119.76	124.80
6	A	1108	CLR	C15-C14-C8	-3.93	112.60	119.08
6	C	1107	CLR	C17-C13-C14	3.90	104.70	100.07
6	D	1109	CLR	C7-C6-C5	-3.90	117.87	125.06
6	A	1107	CLR	C21-C20-C22	-3.90	104.25	110.36
5	A	1103	PCW	O2-C31-C32	3.90	119.90	111.50
6	B	1108	CLR	C12-C13-C14	3.90	113.32	107.27
5	A	1106	PCW	O2-C31-C32	3.89	119.89	111.50
6	A	1108	CLR	C3-C4-C5	3.85	118.56	112.03
5	F	201	PCW	O2-C31-C32	3.84	119.78	111.50
6	A	1108	CLR	C11-C9-C8	3.82	117.26	111.75
6	D	1108	CLR	C21-C20-C22	-3.82	104.37	110.36
6	C	1108	CLR	C11-C9-C8	3.81	117.25	111.75
6	D	1108	CLR	C23-C22-C20	3.81	125.99	115.03
4	D	1103	ZK1	CAS-CAR-NAX	3.77	124.25	119.92
4	A	1102	ZK1	CAV-NAP-CAT	-3.74	120.05	124.80
6	D	1108	CLR	C7-C6-C5	-3.73	118.17	125.06
4	B	1102	ZK1	CAS-CAR-NAX	3.73	124.19	119.92
5	B	1109	PCW	O2-C31-C32	3.70	119.47	111.50
6	C	1107	CLR	C12-C13-C14	3.68	112.98	107.27
6	B	1107	CLR	C7-C6-C5	-3.67	118.29	125.06
5	D	1101	PCW	O2-C31-C32	3.67	119.40	111.50
6	B	1108	CLR	C3-C4-C5	3.65	118.21	112.03
6	C	1107	CLR	C21-C20-C22	-3.64	104.66	110.36
6	B	1107	CLR	C15-C14-C8	3.64	125.07	119.08
6	B	1108	CLR	C7-C6-C5	-3.63	118.36	125.06
6	A	1107	CLR	C12-C13-C14	3.63	112.90	107.27
6	D	1108	CLR	C15-C14-C8	3.62	125.03	119.08
6	A	1107	CLR	C3-C4-C5	3.52	118.00	112.03
6	B	1107	CLR	C23-C22-C20	3.50	125.10	115.03
6	A	1107	CLR	C9-C10-C5	3.50	115.14	109.65
6	C	1108	CLR	C15-C14-C8	-3.49	113.33	119.08
6	B	1107	CLR	C3-C4-C5	3.45	117.88	112.03
6	C	1107	CLR	C9-C10-C5	3.45	115.06	109.65
6	B	1107	CLR	C7-C8-C14	-3.43	105.93	110.91
6	A	1107	CLR	C11-C9-C8	3.42	116.68	111.75
5	D	1106	PCW	O2-C31-C32	3.41	118.85	111.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1108	CLR	C9-C10-C5	3.40	114.99	109.65
6	B	1108	CLR	C2-C1-C10	3.40	120.11	112.74
6	C	1107	CLR	C3-C4-C5	3.40	117.79	112.03
6	D	1109	CLR	C3-C4-C5	3.39	117.78	112.03
6	D	1109	CLR	C2-C1-C10	3.38	120.07	112.74
6	D	1108	CLR	C3-C4-C5	3.37	117.75	112.03
6	D	1109	CLR	C17-C13-C14	3.32	104.01	100.07
6	B	1108	CLR	C7-C8-C9	3.32	113.74	109.71
3	C	1101	6ZP	C20-C13-C12	3.30	120.34	117.38
6	A	1108	CLR	C9-C10-C5	3.30	114.83	109.65
3	A	1101	6ZP	C20-C13-C12	3.29	120.33	117.38
6	B	1107	CLR	C21-C20-C22	-3.28	105.22	110.36
6	D	1109	CLR	C9-C10-C5	3.28	114.80	109.65
6	D	1108	CLR	C7-C8-C14	-3.28	106.15	110.91
6	C	1107	CLR	C11-C9-C8	3.26	116.45	111.75
5	B	1105	PCW	O2-C31-C32	3.26	118.52	111.50
6	C	1108	CLR	C9-C10-C5	3.25	114.74	109.65
6	A	1107	CLR	C7-C8-C14	-3.24	106.22	110.91
6	B	1108	CLR	C17-C13-C14	3.22	103.89	100.07
4	D	1103	ZK1	CAU-CAT-NAP	3.20	120.78	117.49
6	C	1108	CLR	C7-C8-C14	-3.16	106.33	110.91
6	A	1108	CLR	C7-C8-C14	-3.16	106.33	110.91
6	D	1109	CLR	C21-C20-C17	-3.15	108.09	112.92
6	A	1107	CLR	C15-C14-C13	3.11	107.59	103.84
6	C	1108	CLR	C10-C9-C8	3.10	117.38	112.73
4	B	1102	ZK1	CAU-CAT-NAP	3.09	120.67	117.49
6	C	1108	CLR	C17-C13-C14	3.08	103.72	100.07
6	B	1107	CLR	C9-C10-C5	3.04	114.42	109.65
5	C	1106	PCW	O3-C11-C12	3.02	121.37	111.91
6	D	1109	CLR	C7-C8-C9	3.01	113.36	109.71
5	A	1106	PCW	O3-C11-C12	2.99	121.31	111.91
6	A	1108	CLR	C16-C17-C20	2.99	116.77	112.15
6	B	1108	CLR	C21-C20-C17	-2.97	108.37	112.92
6	D	1108	CLR	C9-C10-C5	2.97	114.31	109.65
6	A	1108	CLR	C10-C9-C8	2.97	117.19	112.73
3	B	1101	6ZP	C20-C13-C12	2.97	120.04	117.38
3	D	1102	6ZP	C20-C13-C12	2.94	120.02	117.38
6	C	1107	CLR	C15-C14-C13	2.92	107.36	103.84
5	C	1105	PCW	O3-C11-C12	2.92	121.07	111.91
6	D	1108	CLR	C11-C9-C8	2.90	115.93	111.75
6	A	1107	CLR	C2-C1-C10	2.85	118.90	112.74
6	C	1107	CLR	C2-C1-C10	2.83	118.87	112.74

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1109	CLR	C8-C7-C6	-2.83	108.67	112.73
5	A	1105	PCW	O3-C11-C12	2.82	120.76	111.91
6	C	1107	CLR	C10-C9-C8	2.80	116.94	112.73
6	A	1107	CLR	C10-C9-C8	2.80	116.93	112.73
6	B	1108	CLR	C8-C7-C6	-2.78	108.74	112.73
6	D	1109	CLR	C15-C16-C17	-2.76	99.66	105.13
6	A	1108	CLR	C22-C20-C17	2.75	115.96	110.28
6	C	1108	CLR	C4-C5-C10	2.74	120.06	116.42
6	D	1108	CLR	C2-C1-C10	2.73	118.65	112.74
4	C	1102	ZK1	CAU-CAT-NAP	2.73	120.30	117.49
6	B	1108	CLR	C13-C17-C20	-2.71	115.23	119.49
6	C	1108	CLR	C16-C17-C20	2.71	116.35	112.15
6	B	1107	CLR	C2-C1-C10	2.70	118.59	112.74
6	A	1108	CLR	C2-C1-C10	2.70	118.58	112.74
6	C	1107	CLR	C7-C8-C14	-2.67	107.04	110.91
6	B	1107	CLR	C11-C9-C8	2.66	115.59	111.75
5	F	201	PCW	C7-N-C5	2.64	120.72	109.92
6	A	1107	CLR	C4-C5-C10	2.63	119.92	116.42
6	C	1108	CLR	C1-C10-C5	2.63	113.57	108.75
4	A	1102	ZK1	CAU-CAT-NAP	2.62	120.19	117.49
5	F	201	PCW	O3-C11-C12	2.62	120.12	111.91
5	C	1104	PCW	O3-C11-C12	2.61	120.11	111.91
6	A	1108	CLR	C1-C10-C5	2.61	113.53	108.75
6	D	1109	CLR	C13-C17-C20	-2.61	115.40	119.49
5	E	203	PCW	C7-N-C5	2.61	120.58	109.92
5	B	1105	PCW	O3-C11-C12	2.60	120.08	111.91
5	A	1103	PCW	O3-C11-C12	2.58	120.02	111.91
5	A	1104	PCW	O3-C11-C12	2.58	120.00	111.91
6	D	1108	CLR	C1-C10-C5	2.57	113.45	108.75
5	C	1103	PCW	O3-C11-C12	2.53	119.86	111.91
6	C	1108	CLR	C2-C1-C10	2.53	118.23	112.74
6	A	1108	CLR	C4-C5-C10	2.52	119.77	116.42
6	B	1108	CLR	C22-C20-C17	2.52	115.49	110.28
5	E	203	PCW	O3-C11-C12	2.52	119.82	111.91
6	D	1109	CLR	C12-C11-C9	-2.50	108.78	113.11
6	A	1107	CLR	C18-C13-C14	-2.48	107.08	111.71
6	C	1107	CLR	C4-C5-C10	2.48	119.71	116.42
6	D	1109	CLR	C22-C20-C17	2.44	115.33	110.28
5	D	1106	PCW	O3-C11-C12	2.44	119.56	111.91
6	D	1109	CLR	C16-C17-C20	2.44	115.92	112.15
6	C	1108	CLR	C22-C20-C17	2.43	115.30	110.28
4	D	1103	ZK1	CAO-NAY-CAU	2.43	118.88	116.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1107	CLR	C1-C10-C5	2.43	113.19	108.75
5	C	1103	PCW	C7-N-C5	2.39	119.70	109.92
5	D	1104	PCW	O3-C11-C12	2.37	119.35	111.91
5	B	1109	PCW	C3-C2-C1	-2.37	106.18	111.79
6	C	1107	CLR	C21-C20-C17	-2.37	109.30	112.92
5	B	1103	PCW	C7-N-C5	2.36	119.59	109.92
6	B	1108	CLR	C15-C16-C17	-2.36	100.45	105.13
5	A	1103	PCW	C7-N-C5	2.36	119.58	109.92
5	D	1104	PCW	C7-N-C5	2.36	119.58	109.92
6	A	1107	CLR	C1-C10-C5	2.36	113.07	108.75
6	C	1107	CLR	C1-C10-C5	2.36	113.07	108.75
4	B	1102	ZK1	CAO-NAY-CAU	2.36	118.81	116.51
6	D	1109	CLR	C15-C14-C13	2.35	106.68	103.84
5	B	1104	PCW	O3-C11-C12	2.35	119.28	111.91
5	D	1101	PCW	C3-C2-C1	-2.35	106.23	111.79
6	B	1108	CLR	C15-C14-C13	2.34	106.67	103.84
4	A	1102	ZK1	CAO-NAY-CAU	2.34	118.79	116.51
6	B	1108	CLR	C2-C3-C4	2.33	113.50	110.31
6	B	1108	CLR	C16-C17-C20	2.33	115.75	112.15
6	B	1108	CLR	C12-C11-C9	-2.32	109.09	113.11
5	B	1103	PCW	O3-C11-C12	2.29	119.09	111.91
5	A	1105	PCW	C7-N-C5	2.28	119.24	109.92
6	D	1109	CLR	C15-C14-C8	-2.28	115.33	119.08
5	D	1106	PCW	C7-N-C5	2.27	119.22	109.92
5	C	1106	PCW	C7-N-C5	2.26	119.16	109.92
5	D	1105	PCW	C7-N-C5	2.26	119.16	109.92
5	A	1106	PCW	C7-N-C5	2.26	119.16	109.92
4	C	1102	ZK1	CAO-NAY-CAU	2.26	118.71	116.51
6	A	1108	CLR	C13-C14-C8	2.25	117.72	114.38
5	A	1109	PCW	C7-N-C5	2.24	119.08	109.92
5	A	1104	PCW	C7-N-C5	2.24	119.08	109.92
5	B	1109	PCW	C7-N-C5	2.24	119.07	109.92
6	C	1108	CLR	C16-C15-C14	-2.23	100.71	105.13
5	B	1105	PCW	C7-N-C5	2.23	119.05	109.92
5	D	1101	PCW	C7-N-C5	2.23	119.03	109.92
5	B	1104	PCW	C7-N-C5	2.22	119.02	109.92
5	C	1104	PCW	C7-N-C5	2.21	118.96	109.92
6	A	1108	CLR	C16-C15-C14	-2.19	100.79	105.13
5	C	1109	PCW	C7-N-C5	2.17	118.81	109.92
5	C	1105	PCW	C7-N-C5	2.17	118.80	109.92
5	D	1101	PCW	O3-C11-C12	2.15	118.66	111.91
5	D	1105	PCW	O3-C11-C12	2.13	118.60	111.91

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1109	PCW	O3-C11-C12	2.13	118.59	111.91
4	A	1102	ZK1	FAG-CAZ-CAS	-2.12	109.00	112.70
4	B	1102	ZK1	CAT-CAU-NAY	2.12	119.75	117.32
6	B	1108	CLR	C10-C5-C6	-2.12	119.67	122.90
6	D	1109	CLR	C1-C10-C5	2.11	112.62	108.75
5	C	1104	PCW	O2-C31-O31	-2.11	118.60	123.70
5	C	1109	PCW	O3-C11-C12	2.11	118.53	111.91
6	D	1109	CLR	C2-C3-C4	2.11	113.20	110.31
4	D	1103	ZK1	CAT-CAU-NAY	2.09	119.72	117.32
6	A	1108	CLR	C17-C13-C14	2.09	102.55	100.07
6	C	1107	CLR	C15-C14-C8	-2.08	115.65	119.08
6	A	1108	CLR	C21-C20-C22	-2.07	107.11	110.36
5	A	1104	PCW	O2-C31-O31	-2.07	118.70	123.70
5	A	1109	PCW	O3-C11-C12	2.07	118.39	111.91
6	C	1108	CLR	C13-C14-C8	2.07	117.44	114.38
4	C	1102	ZK1	FAG-CAZ-CAS	-2.06	109.11	112.70
6	B	1108	CLR	C15-C14-C8	-2.06	115.69	119.08
6	C	1108	CLR	C11-C9-C10	-2.04	110.39	113.08
4	B	1102	ZK1	OAD-PBA-CAO	2.04	111.03	106.66
6	B	1108	CLR	C4-C5-C10	2.02	119.11	116.42
6	D	1109	CLR	C4-C5-C10	2.02	119.11	116.42
4	D	1103	ZK1	FAG-CAZ-CAS	-2.00	109.21	112.70

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1107	CLR	C13
6	A	1107	CLR	C9
6	A	1108	CLR	C13
6	A	1108	CLR	C9
6	B	1107	CLR	C13
6	B	1107	CLR	C9
6	B	1108	CLR	C13
6	B	1108	CLR	C9
6	C	1107	CLR	C13
6	C	1107	CLR	C9
6	C	1108	CLR	C13
6	C	1108	CLR	C9
6	D	1108	CLR	C13
6	D	1108	CLR	C9
6	D	1109	CLR	C13
6	D	1109	CLR	C9

All (653) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1103	PCW	O4P-C4-C5-N
5	A	1103	PCW	C32-C31-O2-C2
5	A	1103	PCW	C1-O3P-P-O1P
5	A	1103	PCW	C1-O3P-P-O2P
5	A	1104	PCW	O4P-C4-C5-N
5	A	1104	PCW	O11-C11-O3-C3
5	A	1104	PCW	O31-C31-O2-C2
5	A	1104	PCW	C1-O3P-P-O2P
5	A	1104	PCW	C1-O3P-P-O4P
5	A	1105	PCW	O4P-C4-C5-N
5	A	1105	PCW	C1-O3P-P-O1P
5	A	1105	PCW	C4-O4P-P-O3P
5	A	1106	PCW	O4P-C4-C5-N
5	A	1106	PCW	O31-C31-O2-C2
5	A	1106	PCW	C1-O3P-P-O1P
5	A	1106	PCW	C1-O3P-P-O2P
5	A	1109	PCW	C32-C31-O2-C2
5	A	1109	PCW	C1-O3P-P-O2P
5	A	1109	PCW	C4-O4P-P-O2P
5	B	1103	PCW	O4P-C4-C5-N
5	B	1103	PCW	C32-C31-O2-C2
5	B	1103	PCW	C4-O4P-P-O1P
5	B	1104	PCW	O4P-C4-C5-N
5	B	1104	PCW	C32-C31-O2-C2
5	B	1104	PCW	O31-C31-O2-C2
5	B	1104	PCW	C4-O4P-P-O2P
5	B	1105	PCW	O4P-C4-C5-N
5	B	1105	PCW	C1-O3P-P-O1P
5	B	1105	PCW	C1-O3P-P-O2P
5	B	1105	PCW	C1-O3P-P-O4P
5	B	1105	PCW	C4-O4P-P-O2P
5	B	1109	PCW	O4P-C4-C5-N
5	B	1109	PCW	C5-C4-O4P-P
5	B	1109	PCW	C1-O3P-P-O2P
5	C	1103	PCW	C32-C31-O2-C2
5	C	1103	PCW	C1-O3P-P-O1P
5	C	1103	PCW	C1-O3P-P-O2P
5	C	1103	PCW	C4-O4P-P-O1P
5	C	1104	PCW	O4P-C4-C5-N
5	C	1104	PCW	C32-C31-O2-C2
5	C	1104	PCW	O31-C31-O2-C2
5	C	1104	PCW	C1-O3P-P-O2P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	1105	PCW	O4P-C4-C5-N
5	C	1105	PCW	C12-C11-O3-C3
5	C	1105	PCW	O11-C11-O3-C3
5	C	1105	PCW	C1-O3P-P-O1P
5	C	1105	PCW	C4-O4P-P-O3P
5	C	1106	PCW	O4P-C4-C5-N
5	C	1106	PCW	O31-C31-O2-C2
5	C	1106	PCW	C1-O3P-P-O1P
5	C	1106	PCW	C1-O3P-P-O2P
5	C	1109	PCW	C32-C31-O2-C2
5	C	1109	PCW	O31-C31-O2-C2
5	C	1109	PCW	C1-O3P-P-O2P
5	D	1101	PCW	O4P-C4-C5-N
5	D	1101	PCW	C5-C4-O4P-P
5	D	1104	PCW	C32-C31-O2-C2
5	D	1104	PCW	C4-O4P-P-O1P
5	D	1105	PCW	O4P-C4-C5-N
5	D	1105	PCW	C32-C31-O2-C2
5	D	1105	PCW	O31-C31-O2-C2
5	D	1105	PCW	C1-O3P-P-O1P
5	D	1105	PCW	C4-O4P-P-O2P
5	D	1106	PCW	C1-O3P-P-O1P
5	D	1106	PCW	C1-O3P-P-O2P
5	D	1106	PCW	C1-O3P-P-O4P
5	D	1106	PCW	C4-O4P-P-O2P
5	E	203	PCW	O4P-C4-C5-N
5	E	203	PCW	O31-C31-O2-C2
5	E	203	PCW	C4-O4P-P-O1P
5	E	203	PCW	C4-O4P-P-O2P
5	F	201	PCW	O3P-C1-C2-O2
5	F	201	PCW	O4P-C4-C5-N
5	F	201	PCW	O31-C31-O2-C2
5	F	201	PCW	C4-O4P-P-O1P
5	F	201	PCW	C4-O4P-P-O2P
5	F	201	PCW	C4-O4P-P-O3P
5	F	202	PCW	C20-C21-C22-C23
6	A	1108	CLR	C13-C17-C20-C21
6	A	1108	CLR	C16-C17-C20-C21
6	A	1108	CLR	C16-C17-C20-C22
6	B	1107	CLR	C17-C20-C22-C23
6	B	1108	CLR	C13-C17-C20-C21
6	C	1108	CLR	C13-C17-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	C	1108	CLR	C16-C17-C20-C22
6	D	1108	CLR	C17-C20-C22-C23
6	D	1109	CLR	C13-C17-C20-C21
5	A	1105	PCW	O11-C11-O3-C3
5	A	1109	PCW	O11-C11-O3-C3
5	C	1109	PCW	O11-C11-O3-C3
5	A	1105	PCW	C12-C11-O3-C3
5	A	1109	PCW	C12-C11-O3-C3
5	C	1109	PCW	C12-C11-O3-C3
5	C	1104	PCW	O11-C11-O3-C3
5	E	203	PCW	O11-C11-O3-C3
5	F	201	PCW	O11-C11-O3-C3
6	C	1108	CLR	C16-C17-C20-C21
6	D	1109	CLR	C16-C17-C20-C21
6	C	1107	CLR	C13-C17-C20-C21
6	A	1108	CLR	C13-C17-C20-C22
5	A	1103	PCW	O31-C31-O2-C2
5	A	1109	PCW	O31-C31-O2-C2
5	B	1103	PCW	O31-C31-O2-C2
5	C	1103	PCW	O31-C31-O2-C2
5	D	1104	PCW	O31-C31-O2-C2
5	A	1104	PCW	C12-C11-O3-C3
5	C	1104	PCW	C12-C11-O3-C3
5	E	203	PCW	C12-C11-O3-C3
5	A	1104	PCW	C32-C31-O2-C2
5	A	1106	PCW	C32-C31-O2-C2
5	C	1106	PCW	C32-C31-O2-C2
5	E	203	PCW	C32-C31-O2-C2
5	F	201	PCW	C32-C31-O2-C2
6	B	1108	CLR	C16-C17-C20-C21
6	C	1107	CLR	C16-C17-C20-C21
6	B	1108	CLR	C16-C17-C20-C22
6	D	1109	CLR	C16-C17-C20-C22
6	B	1108	CLR	C13-C17-C20-C22
6	C	1108	CLR	C13-C17-C20-C22
6	D	1109	CLR	C13-C17-C20-C22
5	F	201	PCW	C12-C11-O3-C3
5	A	1109	PCW	C32-C33-C34-C35
5	B	1105	PCW	O31-C31-O2-C2
5	B	1105	PCW	C32-C31-O2-C2
5	D	1106	PCW	C32-C31-O2-C2
6	D	1108	CLR	C21-C20-C22-C23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	1109	PCW	C32-C33-C34-C35
5	D	1106	PCW	C12-C13-C14-C15
6	C	1107	CLR	C13-C17-C20-C22
5	B	1104	PCW	C32-C33-C34-C35
6	C	1107	CLR	C22-C23-C24-C25
5	C	1103	PCW	C24-C25-C26-C27
6	A	1107	CLR	C22-C23-C24-C25
5	D	1105	PCW	C32-C33-C34-C35
6	D	1109	CLR	C17-C20-C22-C23
5	E	203	PCW	C32-C33-C34-C35
6	D	1108	CLR	C22-C23-C24-C25
5	D	1106	PCW	O31-C31-O2-C2
5	A	1106	PCW	C12-C11-O3-C3
5	C	1106	PCW	C12-C11-O3-C3
5	F	201	PCW	C32-C33-C34-C35
6	B	1107	CLR	C13-C17-C20-C22
6	D	1108	CLR	C13-C17-C20-C22
5	B	1109	PCW	C11-C12-C13-C14
6	B	1108	CLR	C17-C20-C22-C23
5	B	1103	PCW	C15-C16-C17-C18
5	D	1104	PCW	C15-C16-C17-C18
5	A	1106	PCW	O11-C11-O3-C3
5	A	1109	PCW	C31-C32-C33-C34
6	B	1108	CLR	C20-C22-C23-C24
6	D	1109	CLR	C21-C20-C22-C23
5	B	1105	PCW	C11-C12-C13-C14
6	A	1108	CLR	C22-C23-C24-C25
6	D	1109	CLR	C20-C22-C23-C24
6	B	1107	CLR	C16-C17-C20-C21
5	C	1106	PCW	O11-C11-O3-C3
5	C	1109	PCW	C31-C32-C33-C34
5	D	1105	PCW	C31-C32-C33-C34
6	A	1108	CLR	C20-C22-C23-C24
6	C	1107	CLR	C20-C22-C23-C24
6	C	1108	CLR	C22-C23-C24-C25
5	F	201	PCW	C4-C5-N-C7
5	B	1104	PCW	C31-C32-C33-C34
5	C	1106	PCW	C31-C32-C33-C34
5	D	1101	PCW	C11-C12-C13-C14
6	C	1108	CLR	C20-C22-C23-C24
6	D	1108	CLR	C16-C17-C20-C21
6	B	1107	CLR	C13-C17-C20-C21

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	D	1108	CLR	C13-C17-C20-C21
5	C	1103	PCW	C16-C17-C18-C19
5	A	1106	PCW	C31-C32-C33-C34
5	B	1105	PCW	C12-C13-C14-C15
5	E	203	PCW	C15-C16-C17-C18
5	A	1109	PCW	C23-C24-C25-C26
5	A	1103	PCW	C1-O3P-P-O4P
5	A	1105	PCW	C1-O3P-P-O4P
5	A	1106	PCW	C1-O3P-P-O4P
5	A	1106	PCW	C4-O4P-P-O3P
5	A	1109	PCW	C4-O4P-P-O3P
5	B	1103	PCW	C4-O4P-P-O3P
5	B	1104	PCW	C1-O3P-P-O4P
5	B	1109	PCW	C1-O3P-P-O4P
5	B	1109	PCW	C4-O4P-P-O3P
5	C	1103	PCW	C1-O3P-P-O4P
5	C	1105	PCW	C1-O3P-P-O4P
5	C	1106	PCW	C1-O3P-P-O4P
5	C	1106	PCW	C4-O4P-P-O3P
5	C	1109	PCW	C4-O4P-P-O3P
5	D	1101	PCW	C4-O4P-P-O3P
5	D	1104	PCW	C4-O4P-P-O3P
5	D	1105	PCW	C1-O3P-P-O4P
5	E	203	PCW	C4-O4P-P-O3P
5	A	1103	PCW	C11-C12-C13-C14
5	F	201	PCW	C15-C16-C17-C18
6	D	1108	CLR	C20-C22-C23-C24
6	B	1108	CLR	C21-C20-C22-C23
5	F	201	PCW	C4-C5-N-C8
5	F	203	PCW	C15-C16-C17-C18
5	A	1103	PCW	C16-C17-C18-C19
5	C	1105	PCW	C14-C15-C16-C17
5	A	1103	PCW	C22-C23-C24-C25
5	A	1103	PCW	C32-C33-C34-C35
5	B	1109	PCW	C35-C36-C37-C38
5	D	1106	PCW	C14-C15-C16-C17
5	E	203	PCW	C35-C36-C37-C38
6	A	1108	CLR	C23-C24-C25-C26
6	D	1108	CLR	C23-C24-C25-C26
5	A	1106	PCW	C12-C13-C14-C15
5	A	1106	PCW	C32-C33-C34-C35
5	A	1109	PCW	C22-C23-C24-C25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	1109	PCW	C35-C36-C37-C38
5	C	1105	PCW	C22-C23-C24-C25
5	C	1106	PCW	C12-C13-C14-C15
5	D	1101	PCW	C35-C36-C37-C38
5	D	1105	PCW	C15-C16-C17-C18
5	D	1106	PCW	C13-C14-C15-C16
5	A	1109	PCW	C11-C12-C13-C14
5	A	1104	PCW	C33-C34-C35-C36
5	A	1109	PCW	C12-C13-C14-C15
5	B	1104	PCW	C15-C16-C17-C18
5	B	1104	PCW	C21-C22-C23-C24
5	D	1106	PCW	C34-C35-C36-C37
5	B	1109	PCW	C14-C15-C16-C17
5	C	1106	PCW	C32-C33-C34-C35
5	D	1106	PCW	C23-C24-C25-C26
5	A	1105	PCW	C22-C23-C24-C25
5	B	1104	PCW	C24-C25-C26-C27
5	B	1105	PCW	C23-C24-C25-C26
5	C	1103	PCW	C23-C24-C25-C26
5	D	1104	PCW	C32-C33-C34-C35
5	B	1105	PCW	C14-C15-C16-C17
5	C	1103	PCW	C32-C33-C34-C35
5	D	1101	PCW	C14-C15-C16-C17
5	E	203	PCW	C21-C22-C23-C24
5	B	1103	PCW	C32-C33-C34-C35
5	B	1105	PCW	C34-C35-C36-C37
5	B	1109	PCW	C12-C13-C14-C15
5	C	1104	PCW	C24-C25-C26-C27
5	C	1104	PCW	C33-C34-C35-C36
5	D	1101	PCW	C12-C13-C14-C15
5	D	1105	PCW	C21-C22-C23-C24
5	F	201	PCW	C21-C22-C23-C24
5	A	1105	PCW	C14-C15-C16-C17
5	A	1105	PCW	C33-C34-C35-C36
5	B	1104	PCW	C35-C36-C37-C38
5	C	1104	PCW	C13-C14-C15-C16
5	C	1109	PCW	C12-C13-C14-C15
5	C	1109	PCW	C35-C36-C37-C38
5	D	1104	PCW	C21-C22-C23-C24
5	D	1105	PCW	C35-C36-C37-C38
5	F	201	PCW	C35-C36-C37-C38
5	A	1104	PCW	C13-C14-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	1104	PCW	C34-C35-C36-C37
5	A	1105	PCW	C12-C13-C14-C15
5	B	1109	PCW	C40-C41-C42-C43
5	D	1101	PCW	C40-C41-C42-C43
5	D	1106	PCW	C36-C37-C38-C39
5	A	1105	PCW	C31-C32-C33-C34
5	D	1104	PCW	C11-C12-C13-C14
5	A	1109	PCW	C13-C14-C15-C16
5	C	1105	PCW	C33-C34-C35-C36
5	D	1101	PCW	C15-C16-C17-C18
5	D	1105	PCW	C24-C25-C26-C27
5	E	201	PCW	C14-C15-C16-C17
6	A	1107	CLR	C23-C24-C25-C26
5	A	1103	PCW	C33-C34-C35-C36
5	A	1105	PCW	C15-C16-C17-C18
5	D	1105	PCW	C14-C15-C16-C17
5	C	1103	PCW	C33-C34-C35-C36
5	D	1106	PCW	C11-C12-C13-C14
5	D	1106	PCW	C31-C32-C33-C34
5	A	1105	PCW	C32-C33-C34-C35
5	A	1106	PCW	C35-C36-C37-C38
5	C	1106	PCW	C24-C25-C26-C27
5	A	1104	PCW	C21-C22-C23-C24
5	C	1105	PCW	C15-C16-C17-C18
6	A	1107	CLR	C13-C17-C20-C21
5	C	1105	PCW	C12-C13-C14-C15
6	A	1107	CLR	C23-C24-C25-C27
6	C	1107	CLR	C23-C24-C25-C26
6	D	1108	CLR	C23-C24-C25-C27
5	C	1105	PCW	C35-C36-C37-C38
5	C	1109	PCW	C13-C14-C15-C16
5	C	1104	PCW	C21-C22-C23-C24
5	C	1105	PCW	C41-C42-C43-C44
5	C	1106	PCW	C35-C36-C37-C38
5	C	1109	PCW	C23-C24-C25-C26
5	D	1104	PCW	C13-C14-C15-C16
5	D	1104	PCW	C35-C36-C37-C38
5	B	1105	PCW	C12-C11-O3-C3
5	A	1103	PCW	C40-C41-C42-C43
5	A	1105	PCW	C16-C17-C18-C19
5	B	1106	PCW	C16-C17-C18-C19
5	D	1105	PCW	C20-C21-C22-C23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	1106	PCW	C37-C38-C39-C40
5	A	1104	PCW	C12-C13-C14-C15
5	A	1106	PCW	C24-C25-C26-C27
5	D	1101	PCW	C23-C24-C25-C26
5	E	202	PCW	C15-C16-C17-C18
5	B	1109	PCW	C15-C16-C17-C18
5	D	1101	PCW	C24-C25-C26-C27
5	E	203	PCW	C4-C5-N-C7
5	F	201	PCW	C4-C5-N-C6
6	C	1108	CLR	C23-C24-C25-C26
5	B	1103	PCW	C11-C12-C13-C14
5	C	1103	PCW	C11-C12-C13-C14
5	C	1105	PCW	C31-C32-C33-C34
5	A	1105	PCW	C35-C36-C37-C38
5	B	1105	PCW	C31-C32-C33-C34
5	A	1104	PCW	C35-C36-C37-C38
5	B	1105	PCW	O11-C11-O3-C3
5	A	1104	PCW	C16-C17-C18-C19
5	A	1104	PCW	C40-C41-C42-C43
5	A	1109	PCW	C36-C37-C38-C39
5	B	1104	PCW	C20-C21-C22-C23
5	C	1103	PCW	C40-C41-C42-C43
5	C	1104	PCW	C16-C17-C18-C19
5	D	1106	PCW	C16-C17-C18-C19
5	F	201	PCW	C36-C37-C38-C39
5	C	1105	PCW	O31-C31-O2-C2
5	D	1105	PCW	C12-C11-O3-C3
5	B	1103	PCW	C14-C15-C16-C17
5	B	1109	PCW	C21-C22-C23-C24
5	C	1105	PCW	C32-C33-C34-C35
6	A	1107	CLR	C20-C22-C23-C24
5	D	1106	PCW	C24-C25-C26-C27
6	B	1107	CLR	C23-C24-C25-C26
6	C	1107	CLR	C16-C17-C20-C22
5	A	1105	PCW	C32-C31-O2-C2
5	C	1105	PCW	C32-C31-O2-C2
5	B	1109	PCW	C24-C25-C26-C27
5	B	1105	PCW	C24-C25-C26-C27
5	A	1105	PCW	O31-C31-O2-C2
6	B	1107	CLR	C21-C20-C22-C23
5	A	1105	PCW	C41-C42-C43-C44
6	A	1108	CLR	C23-C24-C25-C27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	1103	PCW	C20-C21-C22-C23
5	B	1105	PCW	C36-C37-C38-C39
5	C	1104	PCW	C40-C41-C42-C43
5	D	1101	PCW	C36-C37-C38-C39
5	E	203	PCW	C40-C41-C42-C43
5	F	201	PCW	C40-C41-C42-C43
5	A	1103	PCW	C12-C13-C14-C15
5	C	1106	PCW	C33-C34-C35-C36
5	D	1105	PCW	O11-C11-O3-C3
6	C	1107	CLR	C23-C24-C25-C27
6	C	1108	CLR	C23-C24-C25-C27
6	D	1109	CLR	C23-C24-C25-C27
5	E	203	PCW	C12-C13-C14-C15
5	F	201	PCW	C12-C13-C14-C15
5	B	1105	PCW	C37-C38-C39-C40
5	A	1109	PCW	C1-O3P-P-O4P
5	A	1104	PCW	C24-C25-C26-C27
5	A	1105	PCW	C40-C41-C42-C43
5	B	1109	PCW	C36-C37-C38-C39
5	D	1107	PCW	C16-C17-C18-C19
5	D	1106	PCW	C12-C11-O3-C3
5	B	1103	PCW	C34-C35-C36-C37
5	C	1109	PCW	C34-C35-C36-C37
5	A	1104	PCW	C1-C2-C3-O3
5	A	1106	PCW	C1-C2-C3-O3
5	B	1103	PCW	C1-C2-C3-O3
5	C	1104	PCW	C1-C2-C3-O3
5	C	1106	PCW	C1-C2-C3-O3
5	D	1106	PCW	C1-C2-C3-O3
5	E	203	PCW	C25-C26-C27-C28
5	B	1103	PCW	C35-C36-C37-C38
5	D	1104	PCW	C14-C15-C16-C17
5	F	202	PCW	C13-C14-C15-C16
5	C	1106	PCW	C25-C26-C27-C28
5	B	1105	PCW	C16-C17-C18-C19
5	C	1105	PCW	C16-C17-C18-C19
5	E	203	PCW	C36-C37-C38-C39
5	A	1106	PCW	C41-C42-C43-C44
5	A	1103	PCW	C12-C11-O3-C3
5	C	1103	PCW	C12-C11-O3-C3
5	B	1104	PCW	C25-C26-C27-C28
5	C	1103	PCW	O3-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	F	201	PCW	C25-C26-C27-C28
5	C	1104	PCW	C1-C2-O2-C31
5	B	1103	PCW	C13-C14-C15-C16
5	B	1105	PCW	C41-C42-C43-C44
5	A	1105	PCW	C21-C22-C23-C24
5	E	203	PCW	O3P-C1-C2-O2
5	E	203	PCW	C4-C5-N-C8
6	A	1107	CLR	C16-C17-C20-C21
5	D	1106	PCW	O11-C11-O3-C3
5	D	1105	PCW	C40-C41-C42-C43
5	F	202	PCW	C16-C17-C18-C19
5	C	1105	PCW	C21-C22-C23-C24
6	B	1107	CLR	C22-C23-C24-C25
6	B	1107	CLR	C23-C24-C25-C27
5	C	1103	PCW	C21-C22-C23-C24
5	A	1103	PCW	C34-C35-C36-C37
5	E	203	PCW	C4-C5-N-C6
5	A	1106	PCW	C15-C16-C17-C18
5	C	1109	PCW	C11-C12-C13-C14
5	A	1103	PCW	C24-C25-C26-C27
6	B	1107	CLR	C20-C22-C23-C24
5	E	202	PCW	C20-C21-C22-C23
6	B	1108	CLR	C23-C24-C25-C27
5	B	1106	PCW	C15-C16-C17-C18
5	D	1107	PCW	C15-C16-C17-C18
5	B	1104	PCW	C12-C11-O3-C3
5	C	1109	PCW	C22-C23-C24-C25
5	A	1106	PCW	C25-C26-C27-C28
5	C	1103	PCW	C12-C13-C14-C15
5	C	1109	PCW	C16-C17-C18-C19
5	B	1105	PCW	C1-C2-C3-O3
5	D	1105	PCW	C1-C2-C3-O3
5	B	1105	PCW	C35-C36-C37-C38
5	E	201	PCW	C13-C14-C15-C16
5	C	1103	PCW	O11-C11-O3-C3
5	A	1103	PCW	O3-C11-C12-C13
5	A	1103	PCW	O11-C11-O3-C3
5	D	1106	PCW	C35-C36-C37-C38
5	B	1105	PCW	C4-O4P-P-O3P
5	C	1104	PCW	C1-O3P-P-O4P
5	C	1109	PCW	C1-O3P-P-O4P
5	D	1105	PCW	C4-O4P-P-O3P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	1104	PCW	C14-C15-C16-C17
5	A	1103	PCW	O3P-C1-C2-O2
5	C	1103	PCW	O3P-C1-C2-O2
6	B	1108	CLR	C23-C24-C25-C26
5	A	1106	PCW	O2-C2-C3-O3
5	C	1104	PCW	O2-C2-C3-O3
5	C	1105	PCW	O2-C2-C3-O3
5	C	1106	PCW	O2-C2-C3-O3
5	D	1104	PCW	C42-C43-C44-C45
5	A	1109	PCW	C2-C1-O3P-P
5	F	201	PCW	C41-C42-C43-C44
5	D	1101	PCW	C41-C42-C43-C44
5	C	1110	PCW	C17-C18-C19-C20
5	F	202	PCW	C19-C20-C21-C22
5	A	1106	PCW	C33-C34-C35-C36
5	C	1106	PCW	C14-C15-C16-C17
6	D	1109	CLR	C23-C24-C25-C26
5	D	1106	PCW	C41-C42-C43-C44
5	A	1103	PCW	O3P-C1-C2-C3
5	F	201	PCW	O3P-C1-C2-C3
5	A	1110	PCW	C19-C20-C21-C22
5	B	1109	PCW	C41-C42-C43-C44
5	C	1105	PCW	C13-C14-C15-C16
5	B	1109	PCW	C23-C24-C25-C26
5	C	1110	PCW	C19-C20-C21-C22
5	B	1105	PCW	C1-C2-O2-C31
5	C	1109	PCW	C2-C1-O3P-P
5	D	1104	PCW	C1-C2-C3-O3
4	B	1102	ZK1	CAI-CAR-NAX-CAN
4	D	1103	ZK1	CAI-CAR-NAX-CAN
5	C	1105	PCW	O3P-C1-C2-O2
5	C	1106	PCW	C42-C43-C44-C45
5	A	1104	PCW	O2-C2-C3-O3
5	A	1105	PCW	O2-C2-C3-O3
5	D	1105	PCW	O2-C2-C3-O3
5	B	1104	PCW	O11-C11-O3-C3
4	A	1102	ZK1	NAY-CAO-PBA-OAD
4	A	1102	ZK1	NAY-CAO-PBA-OAE
4	B	1102	ZK1	NAY-CAO-PBA-OAD
4	B	1102	ZK1	NAY-CAO-PBA-OAE
4	C	1102	ZK1	NAY-CAO-PBA-OAD
4	C	1102	ZK1	NAY-CAO-PBA-OAE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	D	1103	ZK1	NAY-CAO-PBA-OAD
4	D	1103	ZK1	NAY-CAO-PBA-OAE
6	A	1107	CLR	C13-C17-C20-C22
5	A	1104	PCW	C23-C24-C25-C26
5	B	1105	PCW	C15-C16-C17-C18
4	A	1102	ZK1	NAY-CAO-PBA-OAC
4	B	1102	ZK1	NAY-CAO-PBA-OAC
4	C	1102	ZK1	NAY-CAO-PBA-OAC
4	D	1103	ZK1	NAY-CAO-PBA-OAC
5	B	1103	PCW	C21-C22-C23-C24
5	B	1103	PCW	C22-C23-C24-C25
5	A	1104	PCW	C4-O4P-P-O3P
5	B	1104	PCW	C4-O4P-P-O3P
5	C	1103	PCW	C4-O4P-P-O3P
5	C	1104	PCW	C4-O4P-P-O3P
5	D	1101	PCW	C1-O3P-P-O4P
5	D	1104	PCW	C1-O3P-P-O4P
5	D	1106	PCW	C4-O4P-P-O3P
5	F	201	PCW	C1-O3P-P-O4P
5	E	203	PCW	C33-C34-C35-C36
5	B	1105	PCW	C2-C1-O3P-P
5	D	1106	PCW	C2-C1-O3P-P
5	A	1103	PCW	C4-O4P-P-O2P
5	A	1104	PCW	C4-O4P-P-O1P
5	A	1104	PCW	C4-O4P-P-O2P
5	A	1105	PCW	C1-O3P-P-O2P
5	A	1105	PCW	C4-O4P-P-O1P
5	A	1106	PCW	C4-O4P-P-O2P
5	B	1103	PCW	C1-O3P-P-O2P
5	B	1103	PCW	C4-O4P-P-O2P
5	B	1104	PCW	C1-O3P-P-O1P
5	B	1109	PCW	C1-O3P-P-O1P
5	B	1109	PCW	C4-O4P-P-O2P
5	C	1103	PCW	C4-O4P-P-O2P
5	C	1104	PCW	C4-O4P-P-O1P
5	C	1104	PCW	C4-O4P-P-O2P
5	C	1105	PCW	C1-O3P-P-O2P
5	C	1106	PCW	C4-O4P-P-O2P
5	C	1109	PCW	C4-O4P-P-O2P
5	D	1101	PCW	C1-O3P-P-O1P
5	D	1101	PCW	C1-O3P-P-O2P
5	D	1101	PCW	C4-O4P-P-O2P

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	1104	PCW	C1-O3P-P-O2P
5	D	1104	PCW	C4-O4P-P-O2P
5	D	1105	PCW	C1-O3P-P-O2P
5	B	1104	PCW	C23-C24-C25-C26
5	C	1103	PCW	O3P-C1-C2-C3
5	E	203	PCW	O3P-C1-C2-C3
5	C	1106	PCW	C21-C22-C23-C24
5	D	1101	PCW	C22-C23-C24-C25
5	A	1109	PCW	C16-C17-C18-C19
5	B	1105	PCW	C13-C14-C15-C16
5	B	1109	PCW	C22-C23-C24-C25
5	A	1105	PCW	O3P-C1-C2-O2
5	B	1104	PCW	C37-C38-C39-C40
5	D	1105	PCW	C25-C26-C27-C28
5	A	1104	PCW	C15-C16-C17-C18
5	C	1103	PCW	O4P-C4-C5-N
5	D	1104	PCW	O4P-C4-C5-N
5	D	1106	PCW	O4P-C4-C5-N
5	B	1103	PCW	O2-C2-C3-O3
5	B	1104	PCW	O2-C2-C3-O3
5	B	1105	PCW	O2-C2-C3-O3
5	D	1106	PCW	O2-C2-C3-O3
5	A	1106	PCW	C14-C15-C16-C17
5	C	1106	PCW	C15-C16-C17-C18
5	B	1104	PCW	C11-C12-C13-C14
5	A	1110	PCW	C17-C18-C19-C20
5	C	1104	PCW	C12-C13-C14-C15
5	B	1104	PCW	C36-C37-C38-C39
5	D	1105	PCW	C36-C37-C38-C39
5	C	1109	PCW	C14-C15-C16-C17
5	F	201	PCW	C23-C24-C25-C26
5	A	1105	PCW	C34-C35-C36-C37
5	A	1109	PCW	C34-C35-C36-C37
5	B	1103	PCW	O3-C11-C12-C13
5	A	1104	PCW	C1-C2-O2-C31
5	D	1106	PCW	C1-C2-O2-C31
5	C	1105	PCW	O3P-C1-C2-C3
5	B	1105	PCW	C42-C43-C44-C45
5	A	1103	PCW	C2-C1-O3P-P
5	D	1104	PCW	O3-C11-C12-C13
4	A	1102	ZK1	CAI-CAR-NAX-CAN
4	C	1102	ZK1	CAI-CAR-NAX-CAN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	1104	PCW	C40-C41-C42-C43
5	C	1106	PCW	C40-C41-C42-C43
5	E	203	PCW	C1-O3P-P-O4P
5	A	1103	PCW	C1-C2-C3-O3
5	C	1103	PCW	C34-C35-C36-C37
5	C	1105	PCW	C34-C35-C36-C37
5	A	1103	PCW	C19-C20-C21-C22
5	B	1103	PCW	C42-C43-C44-C45
5	C	1104	PCW	C15-C16-C17-C18
5	D	1105	PCW	C37-C38-C39-C40
5	E	203	PCW	C23-C24-C25-C26
5	F	202	PCW	C15-C16-C17-C18
5	C	1103	PCW	O11-C11-C12-C13
5	C	1105	PCW	C40-C41-C42-C43
5	D	1101	PCW	C13-C14-C15-C16
5	E	201	PCW	C20-C21-C22-C23
5	D	1101	PCW	C34-C35-C36-C37
5	A	1105	PCW	C11-C12-C13-C14
5	C	1103	PCW	C2-C1-O3P-P
5	B	1105	PCW	C2-C3-O3-C11
5	A	1104	PCW	C20-C21-C22-C23
5	C	1109	PCW	C36-C37-C38-C39
5	C	1104	PCW	C35-C36-C37-C38
6	A	1107	CLR	C16-C17-C20-C22
5	A	1105	PCW	C1-C2-C3-O3
5	C	1103	PCW	C1-C2-C3-O3
5	C	1105	PCW	C1-C2-C3-O3
5	E	202	PCW	C13-C14-C15-C16
5	A	1105	PCW	C19-C20-C21-C22
5	D	1106	PCW	C42-C43-C44-C45
5	D	1104	PCW	C40-C41-C42-C43
5	A	1105	PCW	O3P-C1-C2-C3
5	C	1105	PCW	C19-C20-C21-C22
5	C	1105	PCW	C11-C12-C13-C14
5	D	1104	PCW	O2-C2-C3-O3
5	D	1106	PCW	C21-C22-C23-C24
5	B	1103	PCW	C31-C32-C33-C34
5	B	1105	PCW	C25-C26-C27-C28
5	D	1101	PCW	C16-C17-C18-C19
5	A	1104	PCW	C19-C20-C21-C22
5	C	1106	PCW	C19-C20-C21-C22
5	C	1105	PCW	C25-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	1109	PCW	C25-C26-C27-C28
5	D	1104	PCW	C23-C24-C25-C26
5	F	203	PCW	C13-C14-C15-C16
5	A	1103	PCW	O11-C11-C12-C13
5	A	1109	PCW	C40-C41-C42-C43
5	B	1109	PCW	C13-C14-C15-C16
5	A	1105	PCW	C37-C38-C39-C40
5	B	1105	PCW	C19-C20-C21-C22
5	D	1101	PCW	O3-C11-C12-C13
5	C	1104	PCW	C20-C21-C22-C23
5	A	1106	PCW	C37-C38-C39-C40
5	B	1106	PCW	C19-C20-C21-C22
5	B	1109	PCW	C37-C38-C39-C40
5	C	1105	PCW	C37-C38-C39-C40
5	E	201	PCW	C17-C18-C19-C20
5	F	201	PCW	C37-C38-C39-C40
5	D	1106	PCW	C25-C26-C27-C28
5	B	1109	PCW	O3-C11-C12-C13
5	A	1104	PCW	C37-C38-C39-C40
5	D	1101	PCW	C37-C38-C39-C40
5	D	1106	PCW	C19-C20-C21-C22
5	E	203	PCW	C37-C38-C39-C40
5	F	203	PCW	C19-C20-C21-C22
5	E	203	PCW	C31-C32-C33-C34
5	B	1104	PCW	C1-C2-C3-O3
4	A	1102	ZK1	CAI-CAR-NAX-CAM
4	C	1102	ZK1	CAI-CAR-NAX-CAM
5	A	1104	PCW	C41-C42-C43-C44
5	B	1105	PCW	C22-C23-C24-C25
5	A	1106	PCW	C21-C22-C23-C24
5	C	1106	PCW	C37-C38-C39-C40
5	D	1107	PCW	C19-C20-C21-C22
5	C	1109	PCW	C20-C21-C22-C23
5	D	1104	PCW	C31-C32-C33-C34
5	C	1105	PCW	O2-C31-C32-C33
5	B	1105	PCW	C21-C22-C23-C24
5	B	1104	PCW	C39-C40-C41-C42
5	C	1104	PCW	C19-C20-C21-C22
5	F	202	PCW	C17-C18-C19-C20
5	E	203	PCW	O3-C11-C12-C13
5	C	1104	PCW	C32-C33-C34-C35
5	A	1105	PCW	C25-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	1101	PCW	O11-C11-C12-C13
5	A	1105	PCW	O2-C31-C32-C33
5	C	1109	PCW	C24-C25-C26-C27
5	A	1106	PCW	C11-C12-C13-C14
5	E	203	PCW	O11-C11-C12-C13
5	E	202	PCW	C19-C20-C21-C22
5	B	1109	PCW	O11-C11-C12-C13
5	B	1104	PCW	C1-O3P-P-O2P
5	D	1104	PCW	C1-O3P-P-O1P
5	C	1105	PCW	O31-C31-C32-C33
5	D	1106	PCW	C22-C23-C24-C25
5	D	1104	PCW	C24-C25-C26-C27
5	C	1106	PCW	C11-C12-C13-C14
5	C	1105	PCW	C5-C4-O4P-P
5	D	1105	PCW	C5-C4-O4P-P
5	A	1105	PCW	O31-C31-C32-C33
5	C	1109	PCW	C41-C42-C43-C44
5	D	1105	PCW	C17-C18-C19-C20
5	D	1105	PCW	C39-C40-C41-C42
5	C	1104	PCW	O3-C11-C12-C13
4	B	1102	ZK1	CAS-CAR-NAX-CAN
4	D	1103	ZK1	CAS-CAR-NAX-CAN
5	F	201	PCW	C24-C25-C26-C27

There are no ring outliers.

38 monomers are involved in 133 short contacts:

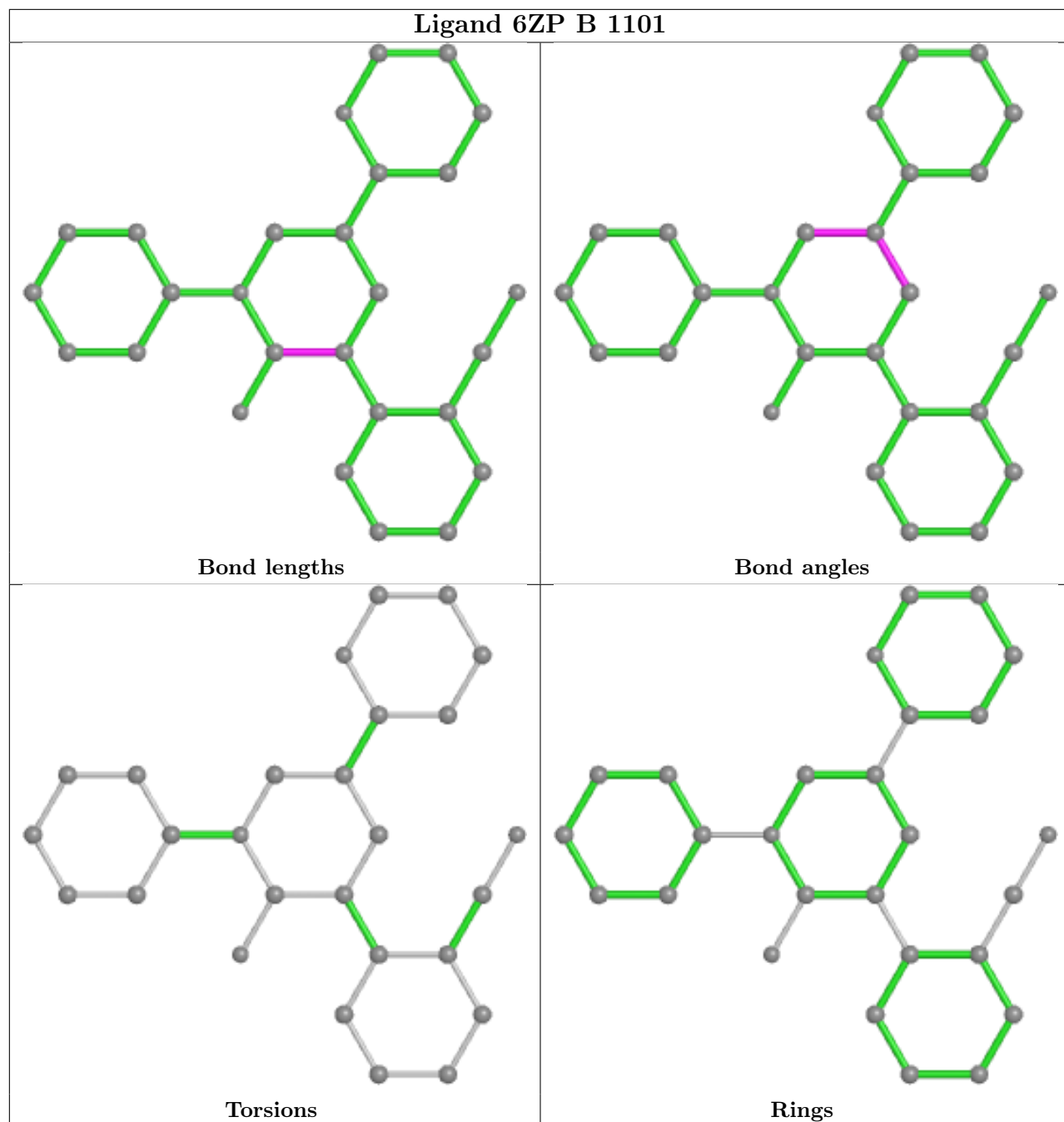
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1101	6ZP	1	0
5	D	1107	PCW	2	0
6	C	1107	CLR	7	0
5	B	1104	PCW	3	0
5	C	1104	PCW	1	0
3	A	1101	6ZP	1	0
5	B	1109	PCW	6	0
3	C	1101	6ZP	2	0
3	D	1102	6ZP	1	0
5	A	1110	PCW	1	0
5	C	1105	PCW	3	0
6	B	1107	CLR	7	0
5	D	1105	PCW	5	0
5	A	1103	PCW	5	0

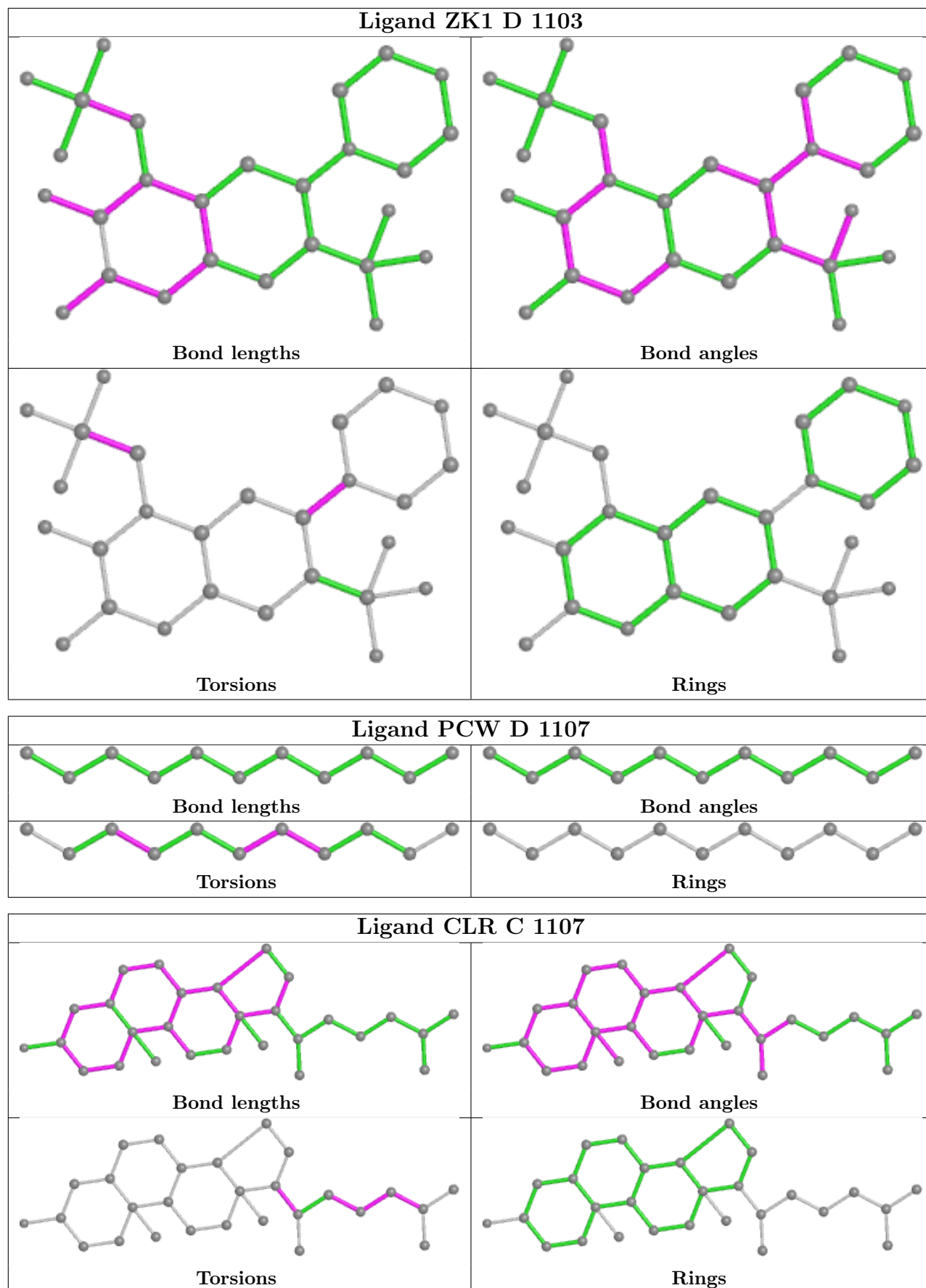
*Continued on next page...*

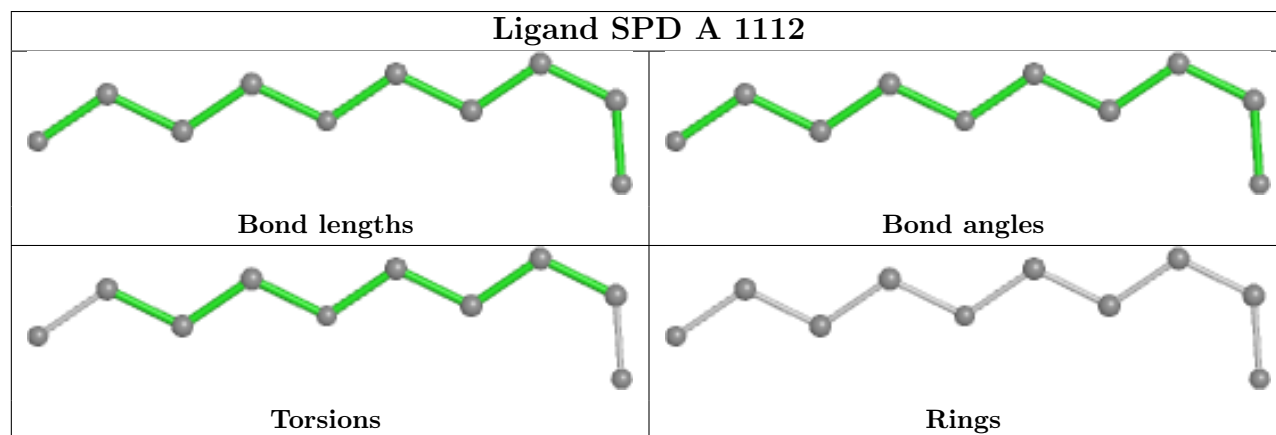
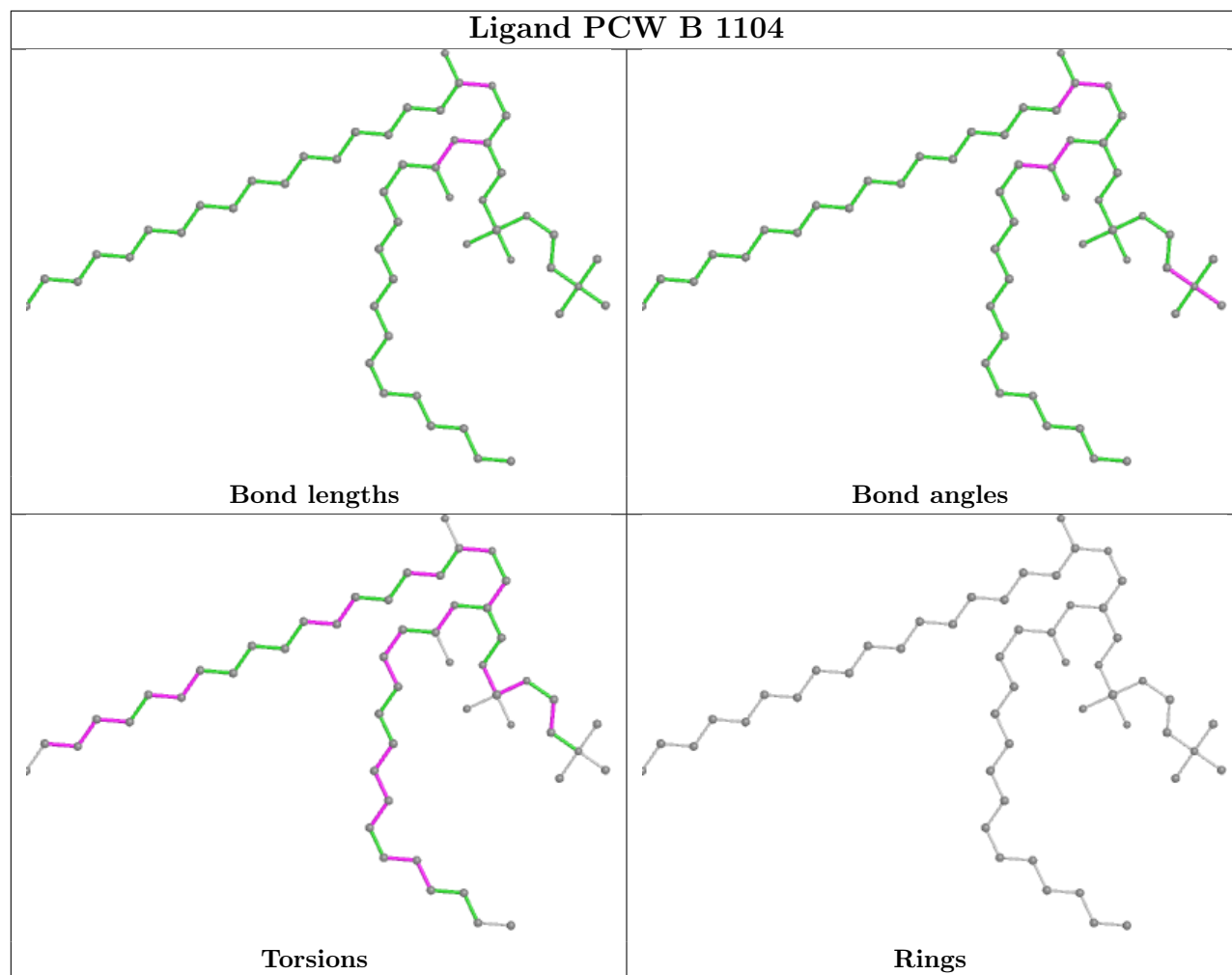
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	ZK1	1	0
6	A	1108	CLR	2	0
5	A	1106	PCW	2	0
5	A	1109	PCW	7	0
5	A	1105	PCW	4	0
5	C	1110	PCW	1	0
5	B	1106	PCW	3	0
5	B	1105	PCW	9	0
6	B	1108	CLR	7	0
5	E	203	PCW	6	0
5	F	201	PCW	7	0
6	D	1109	CLR	6	0
6	C	1108	CLR	4	0
6	D	1108	CLR	7	0
5	B	1103	PCW	5	0
4	C	1102	ZK1	1	0
5	D	1106	PCW	8	0
5	C	1109	PCW	9	0
5	D	1101	PCW	5	0
5	D	1104	PCW	6	0
6	A	1107	CLR	6	0
5	E	201	PCW	3	0
5	C	1106	PCW	3	0
5	C	1103	PCW	3	0

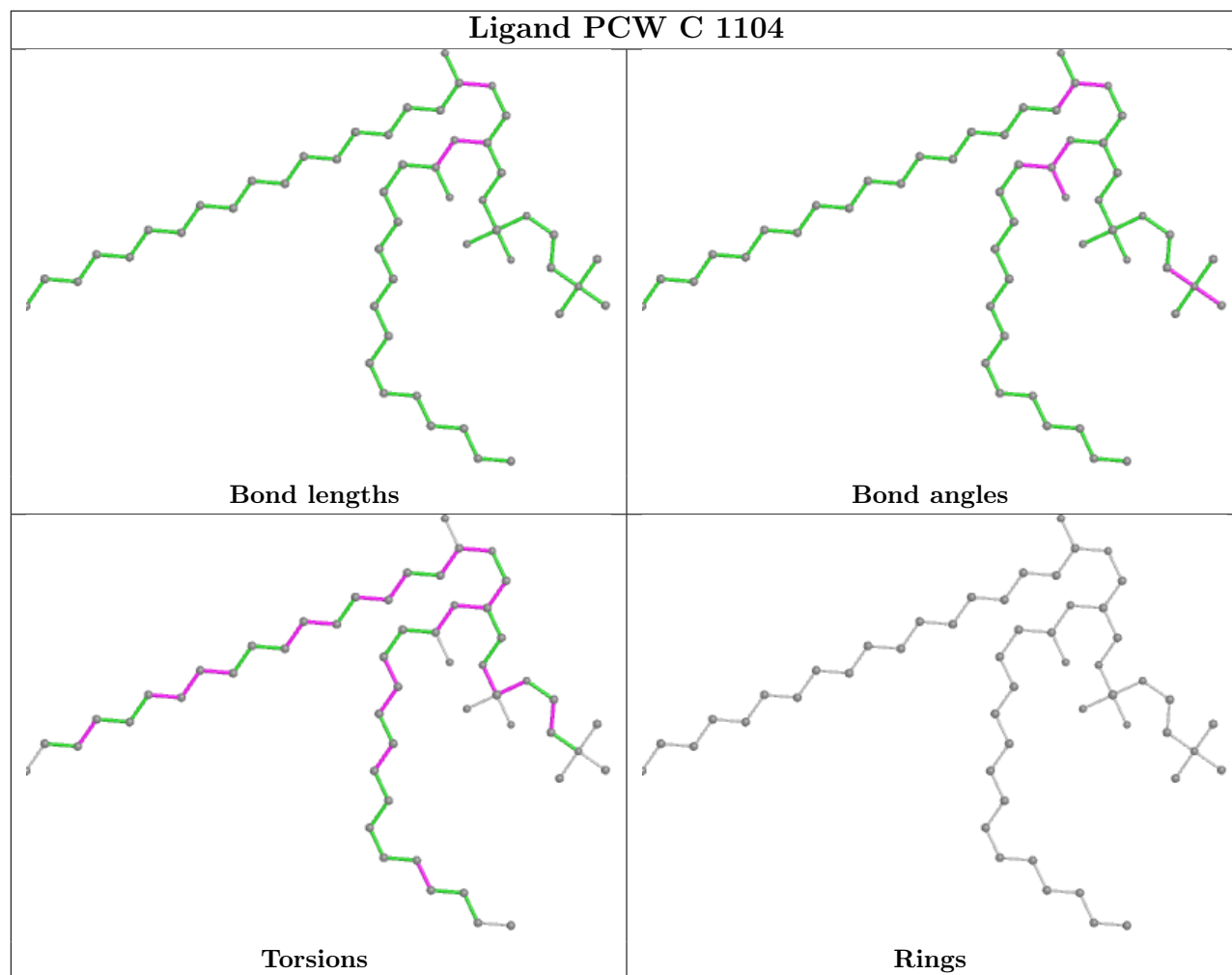
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

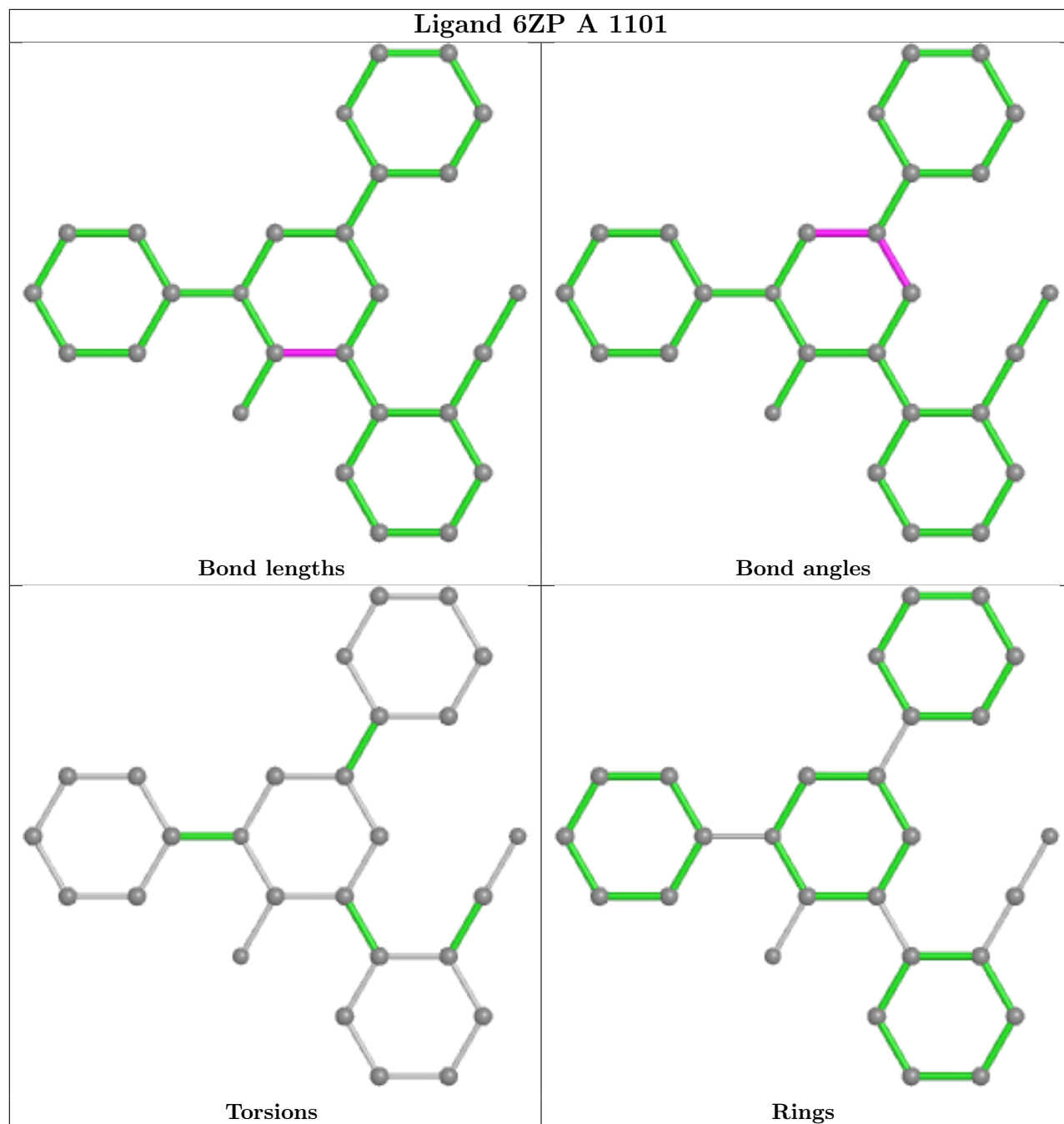


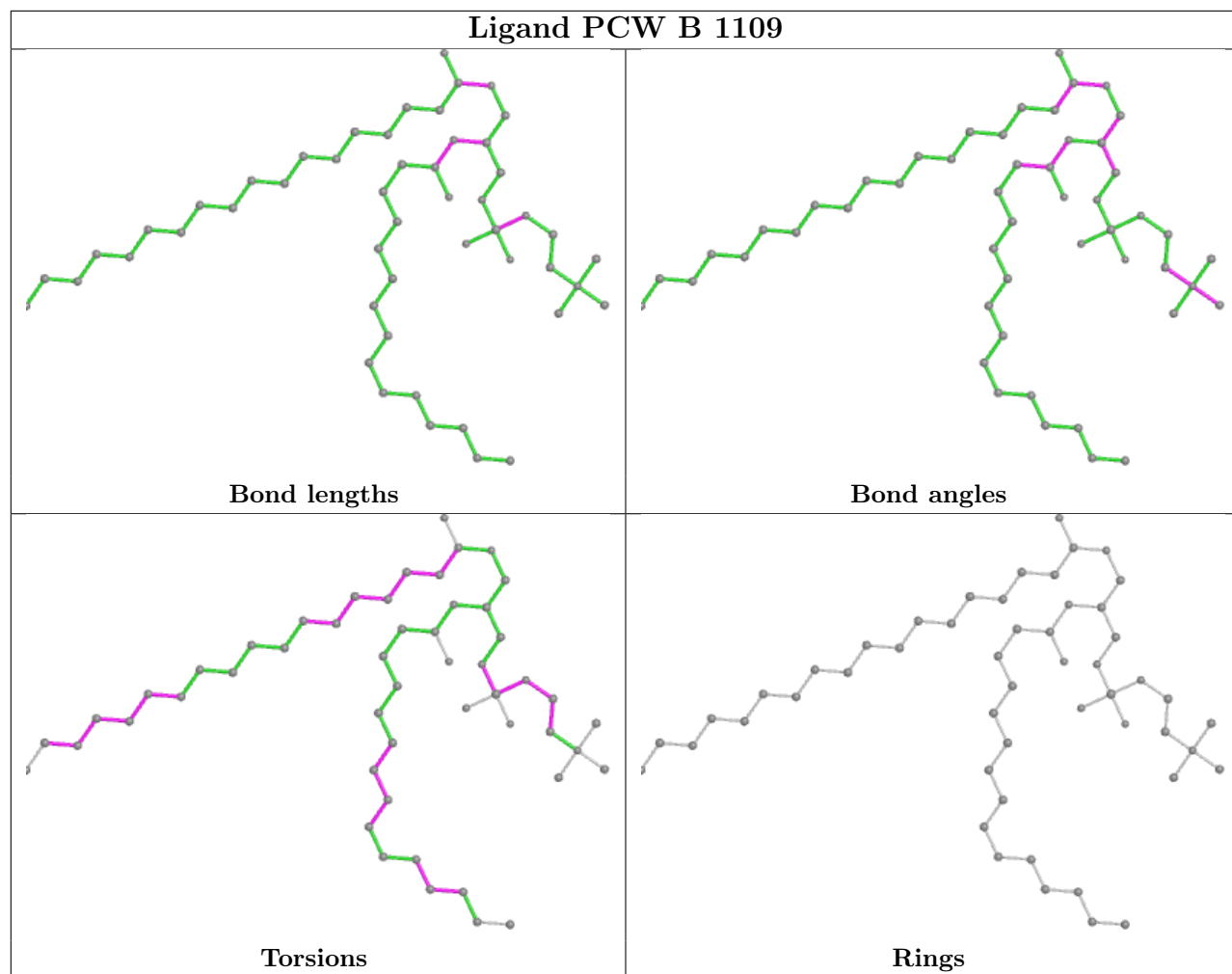


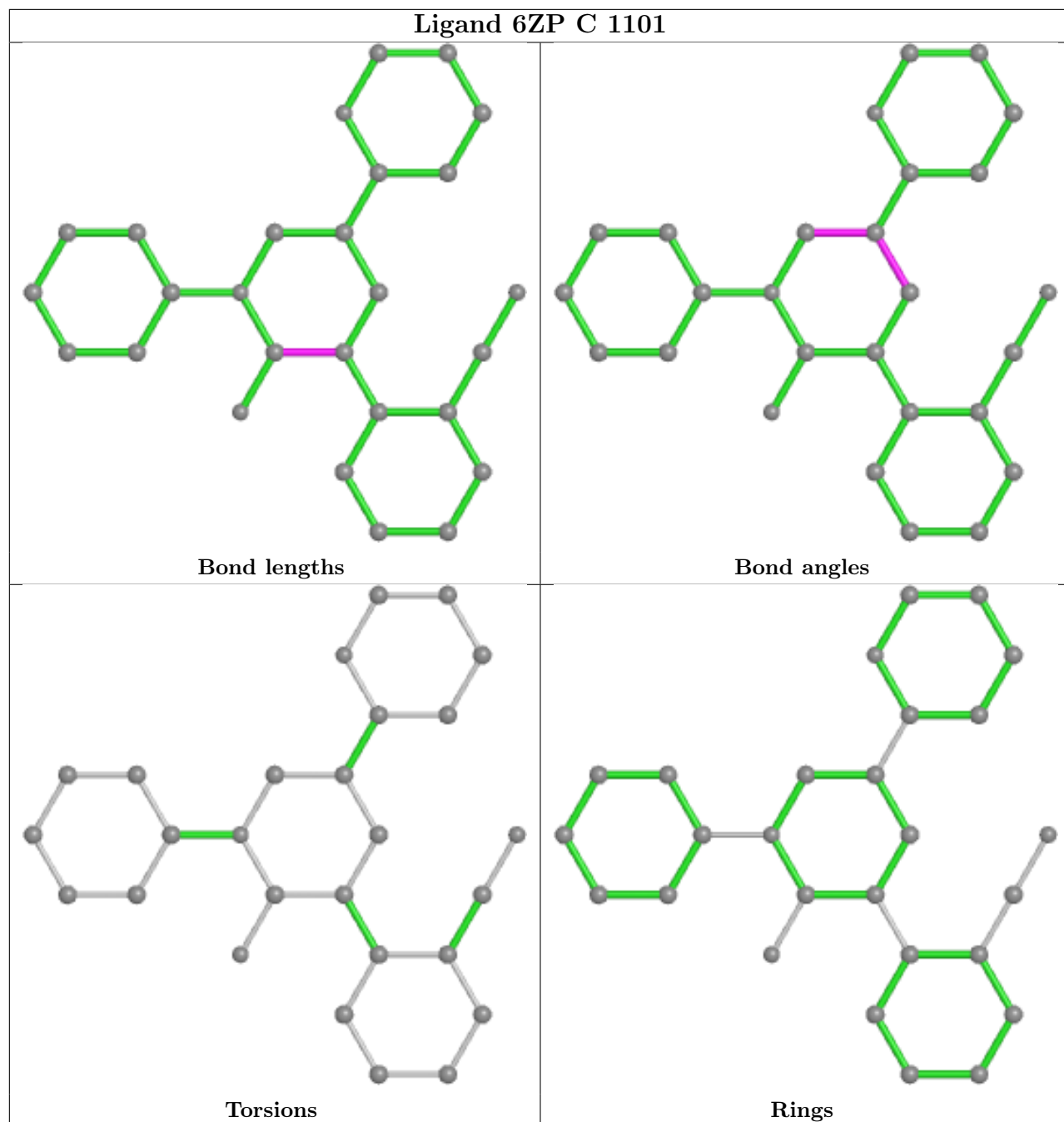


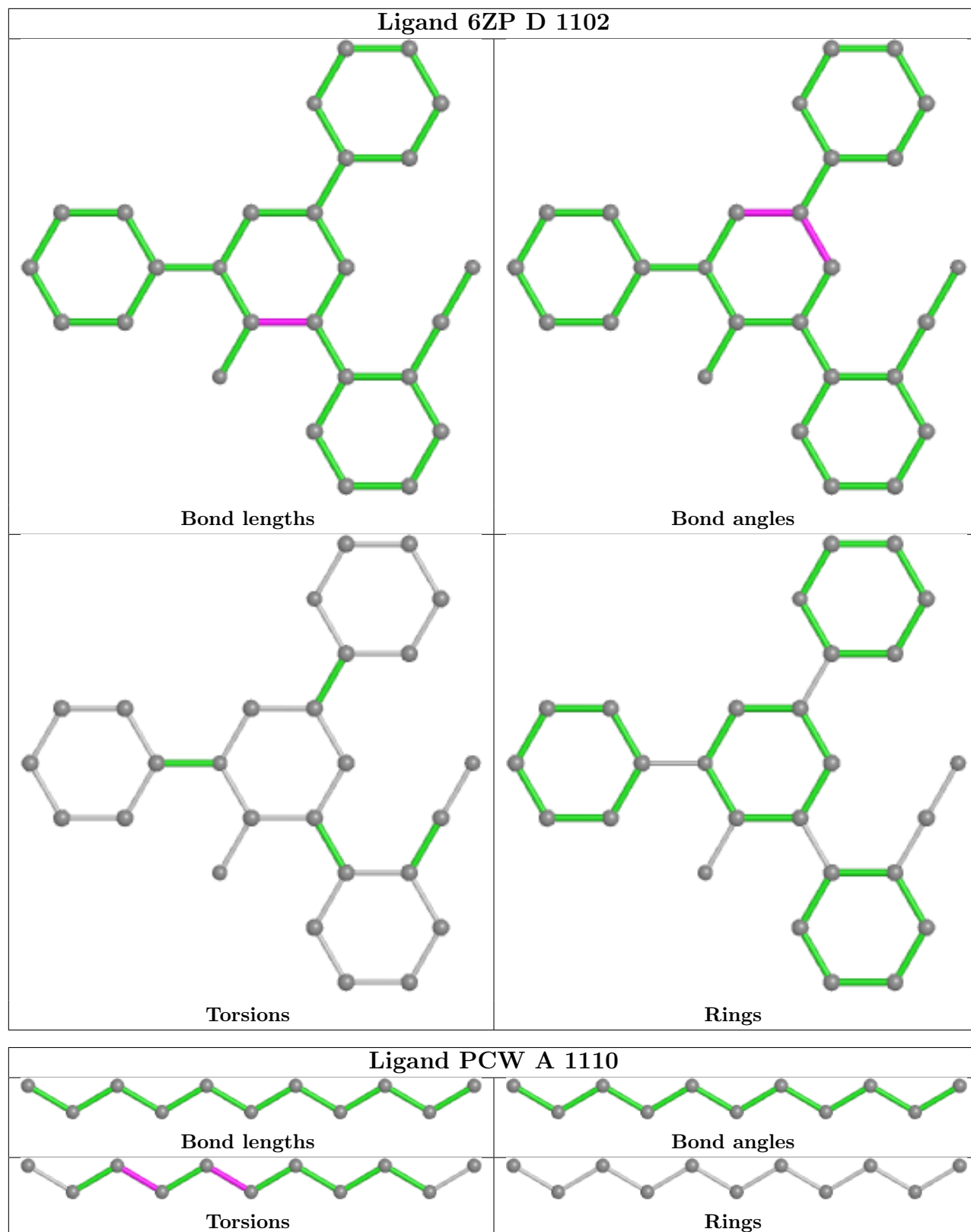


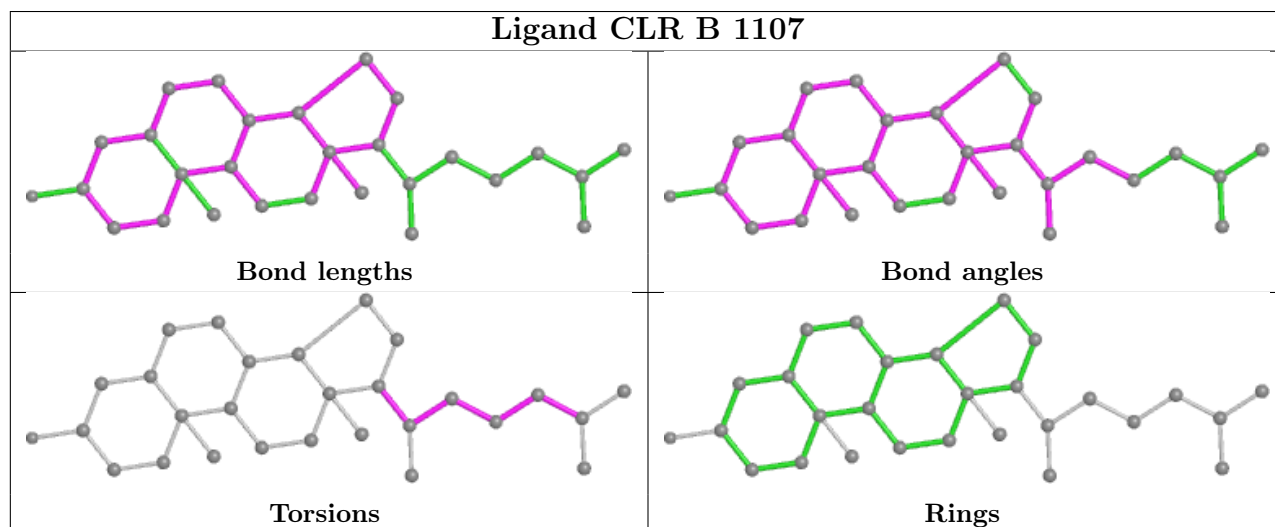
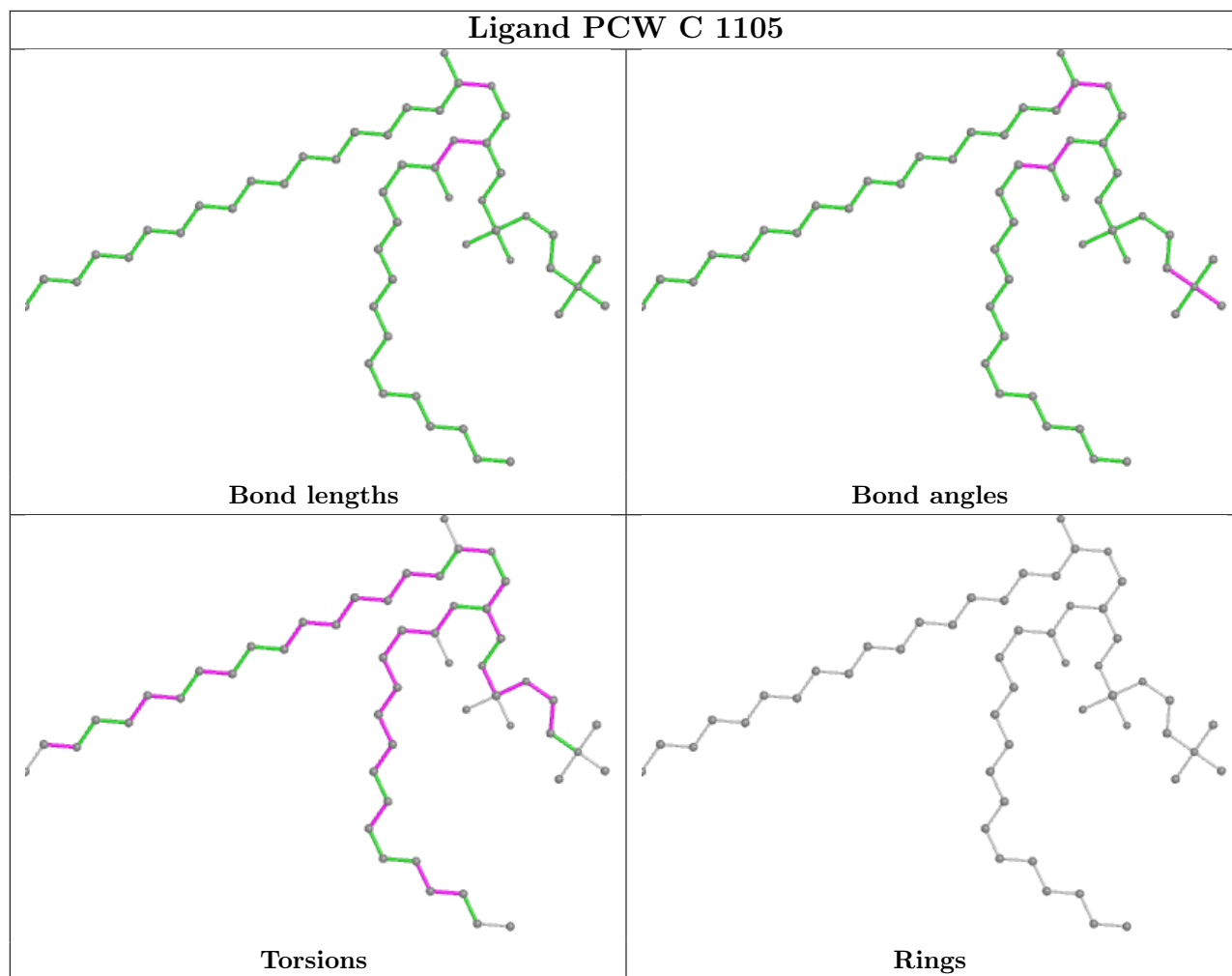


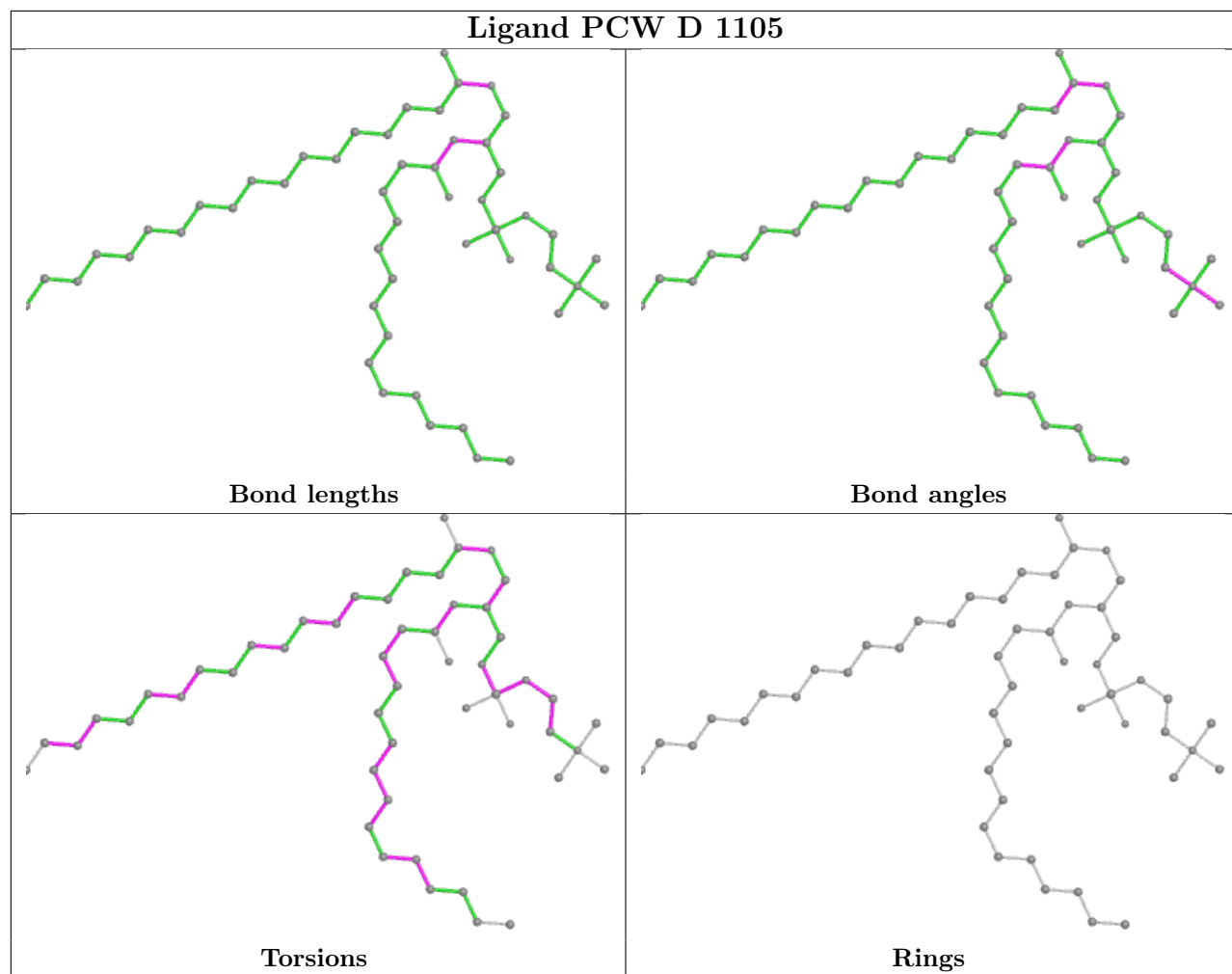


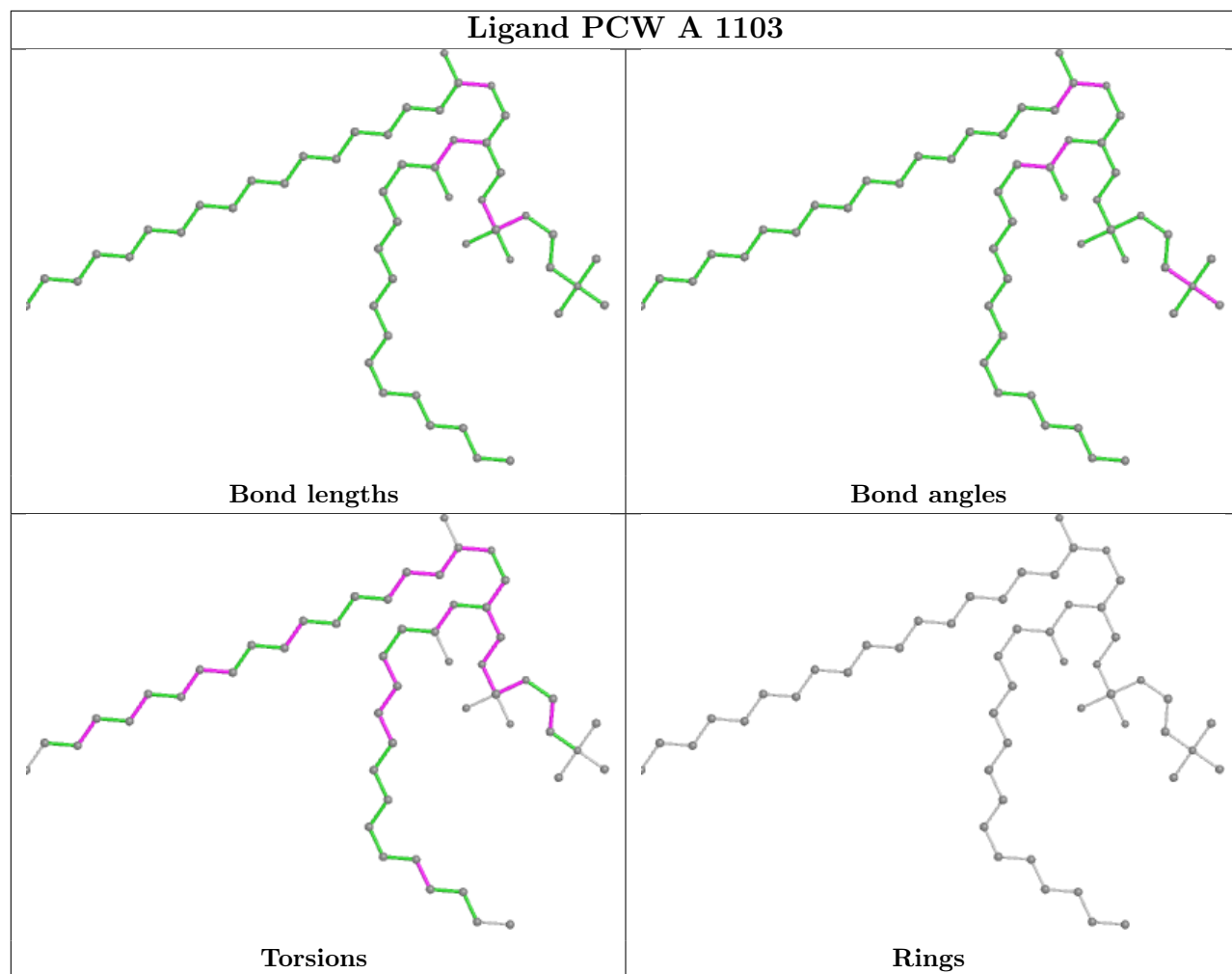




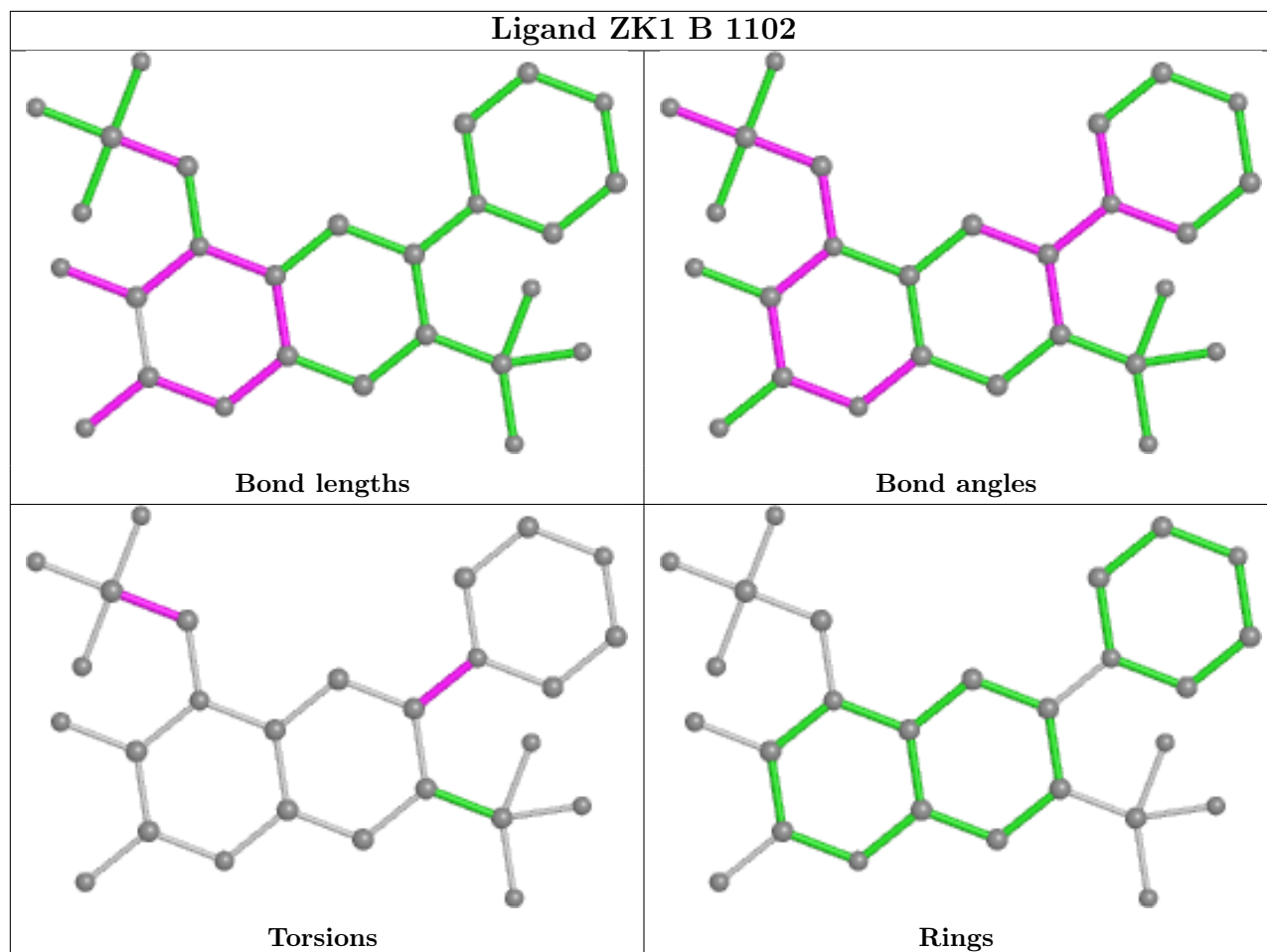


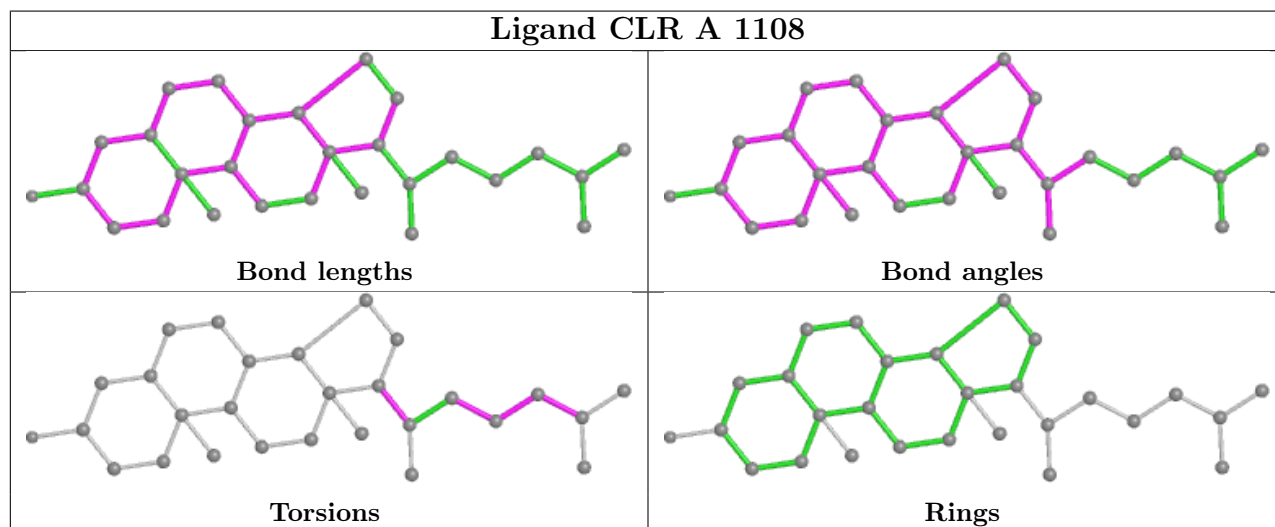
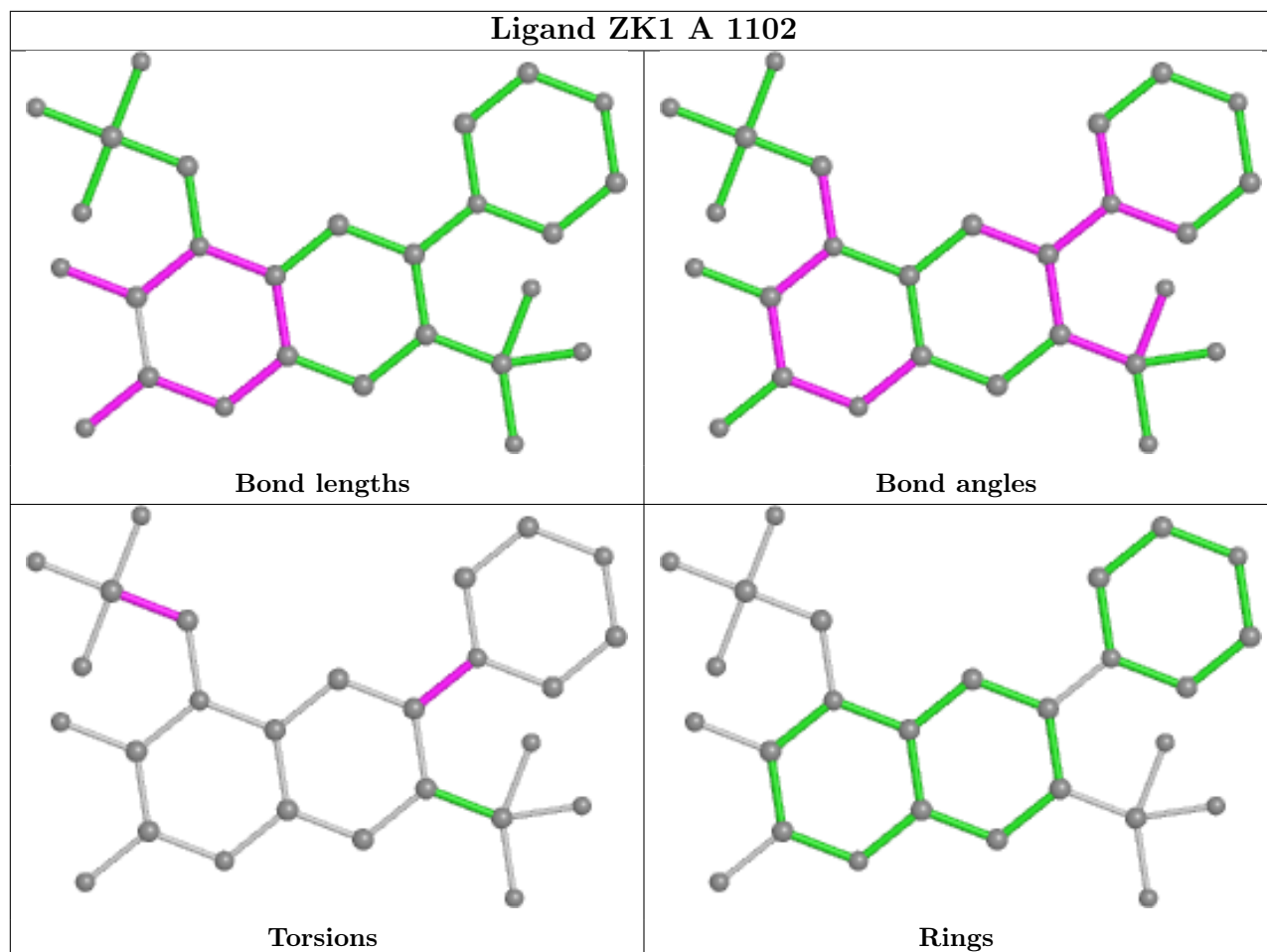


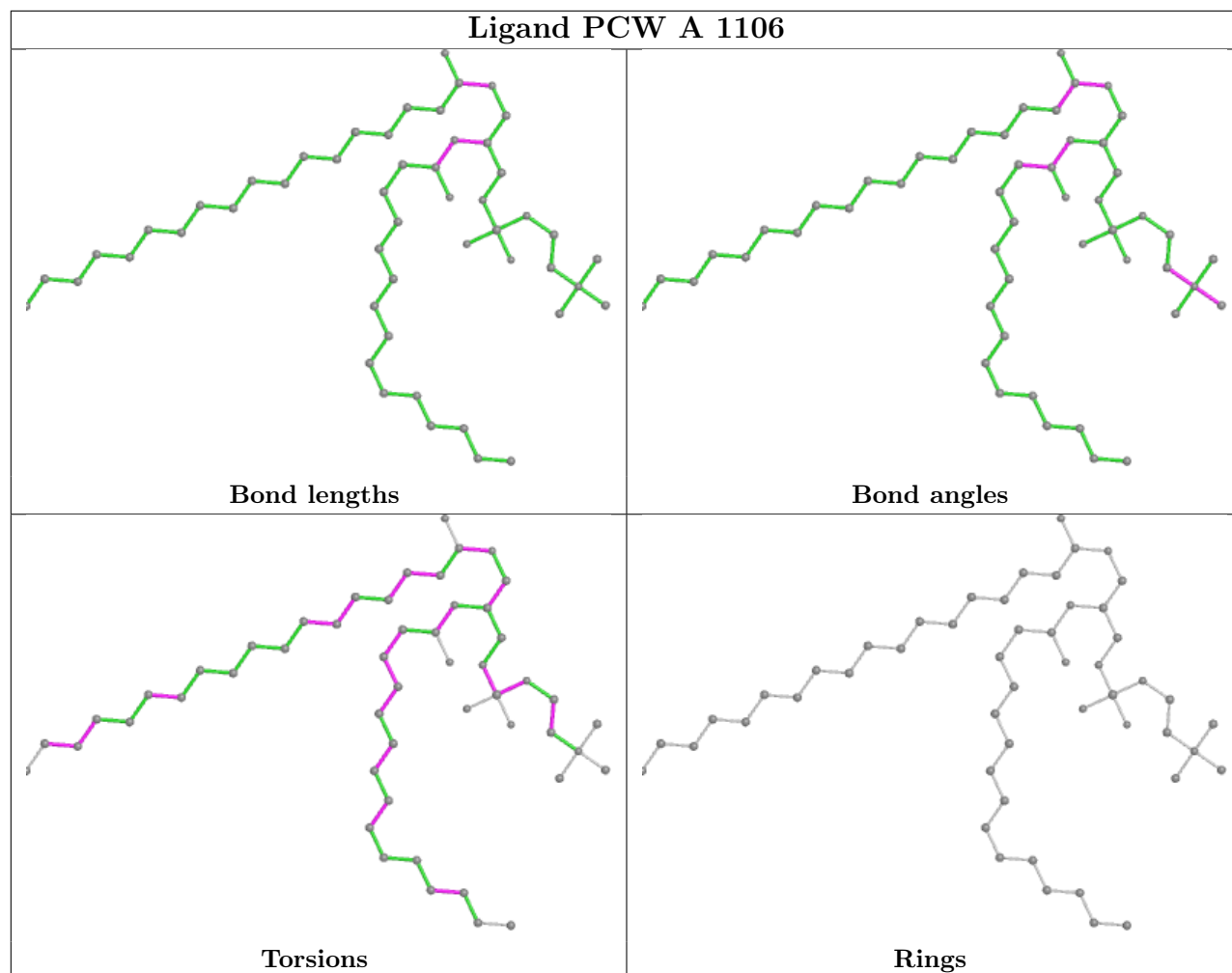


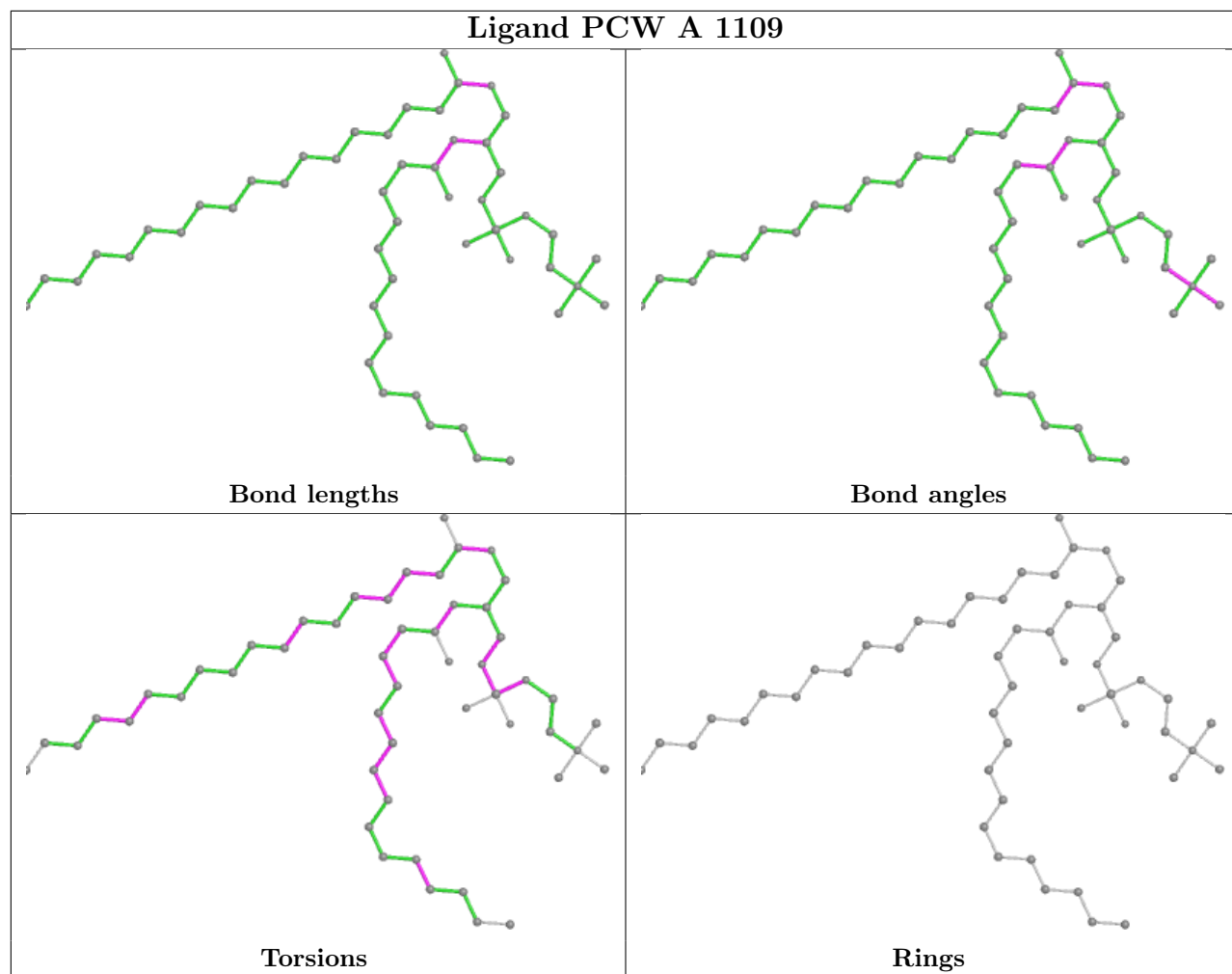


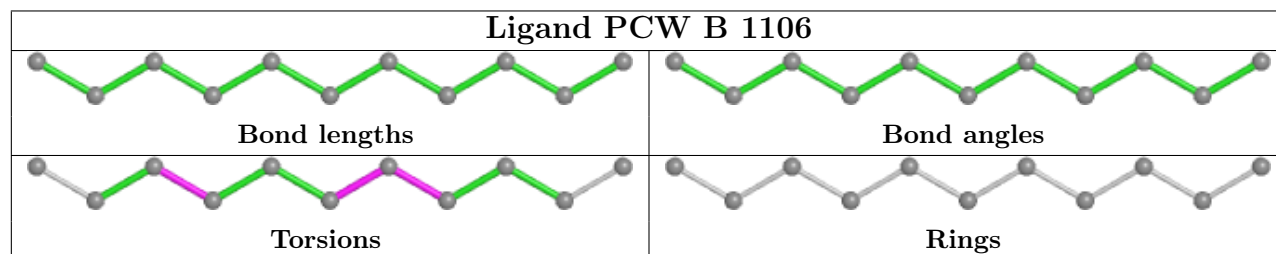
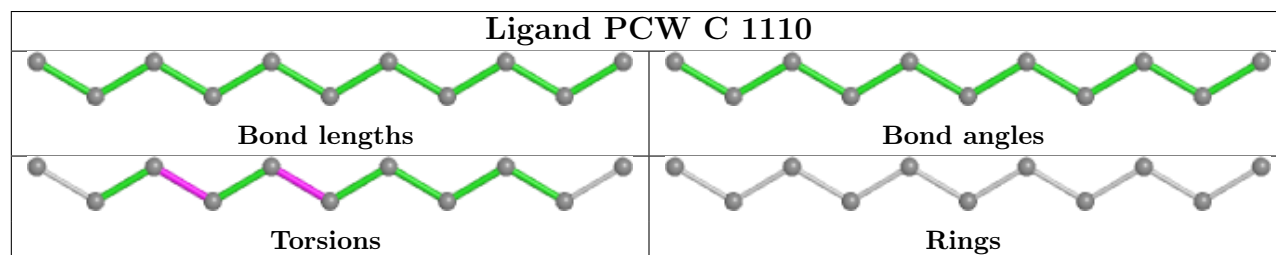
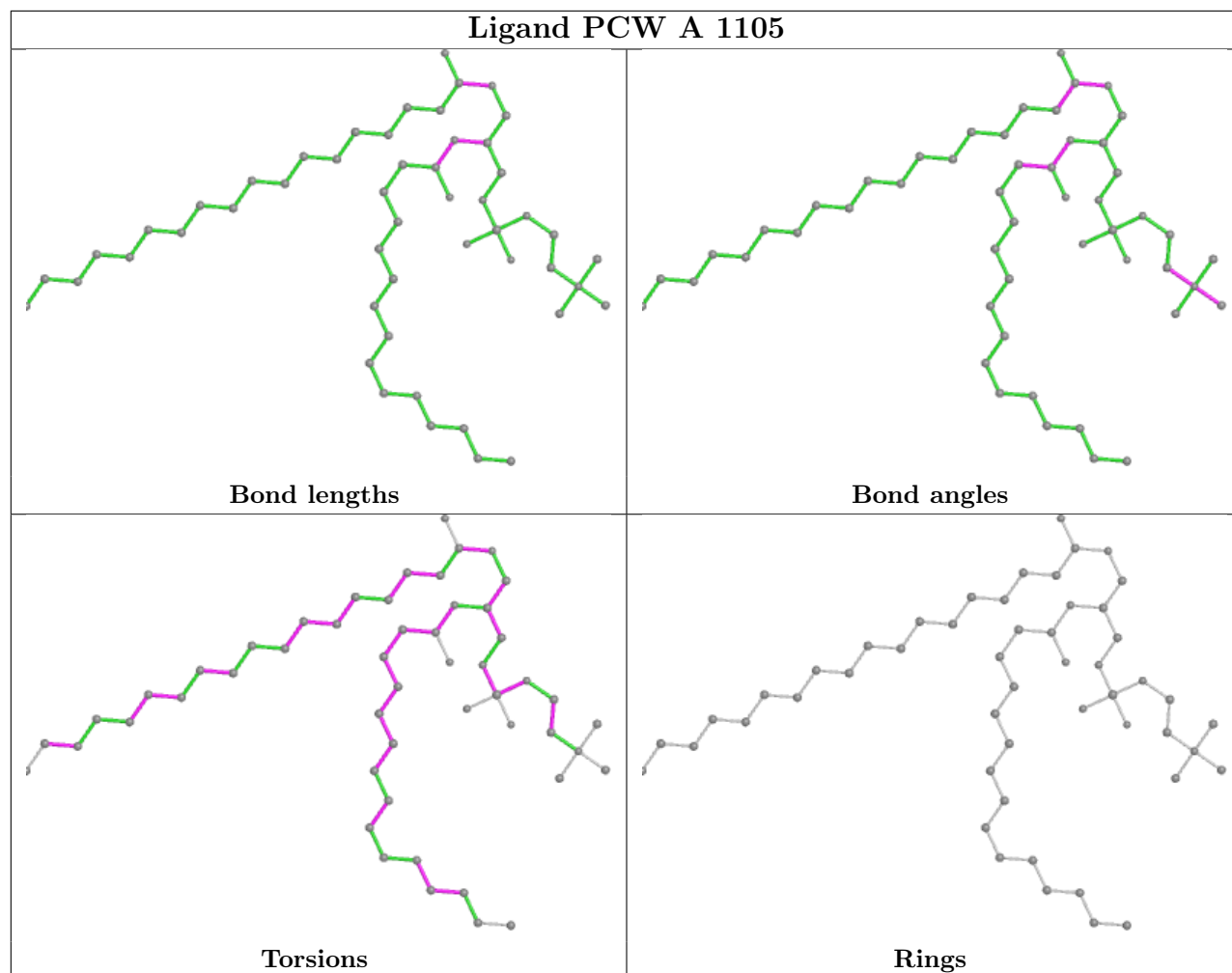


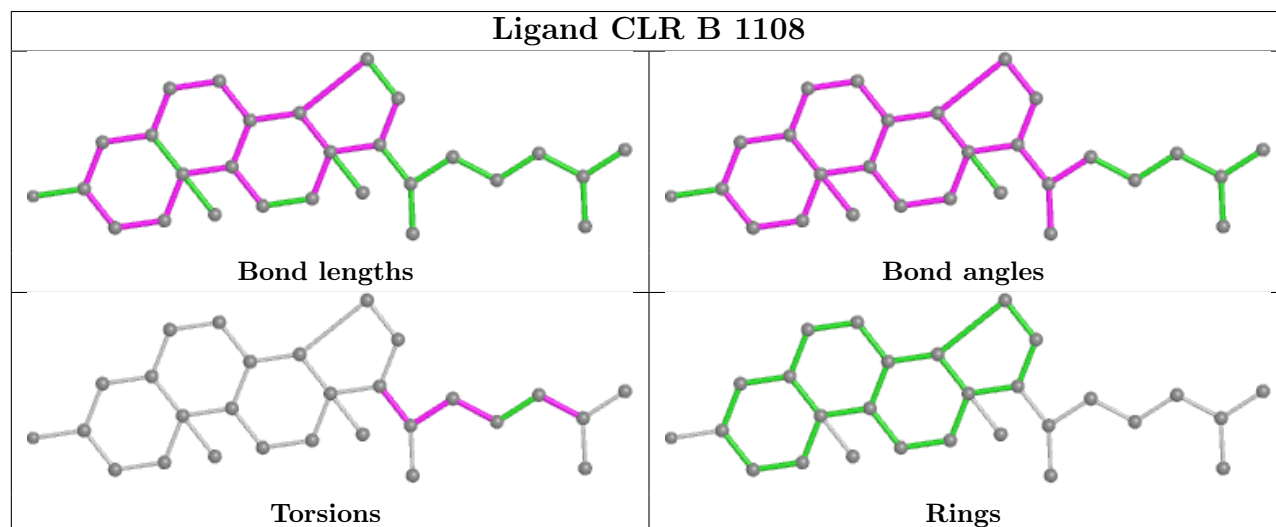
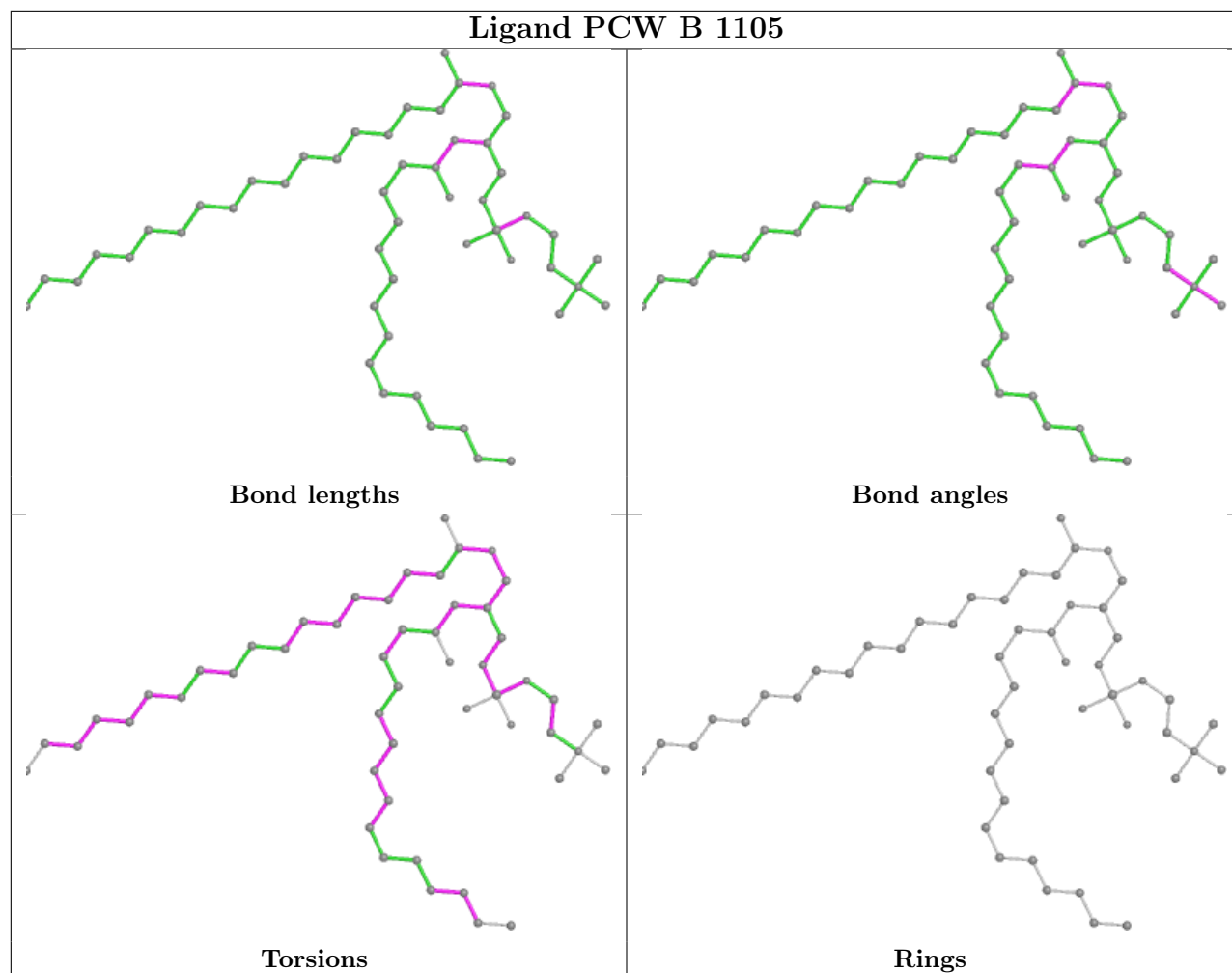


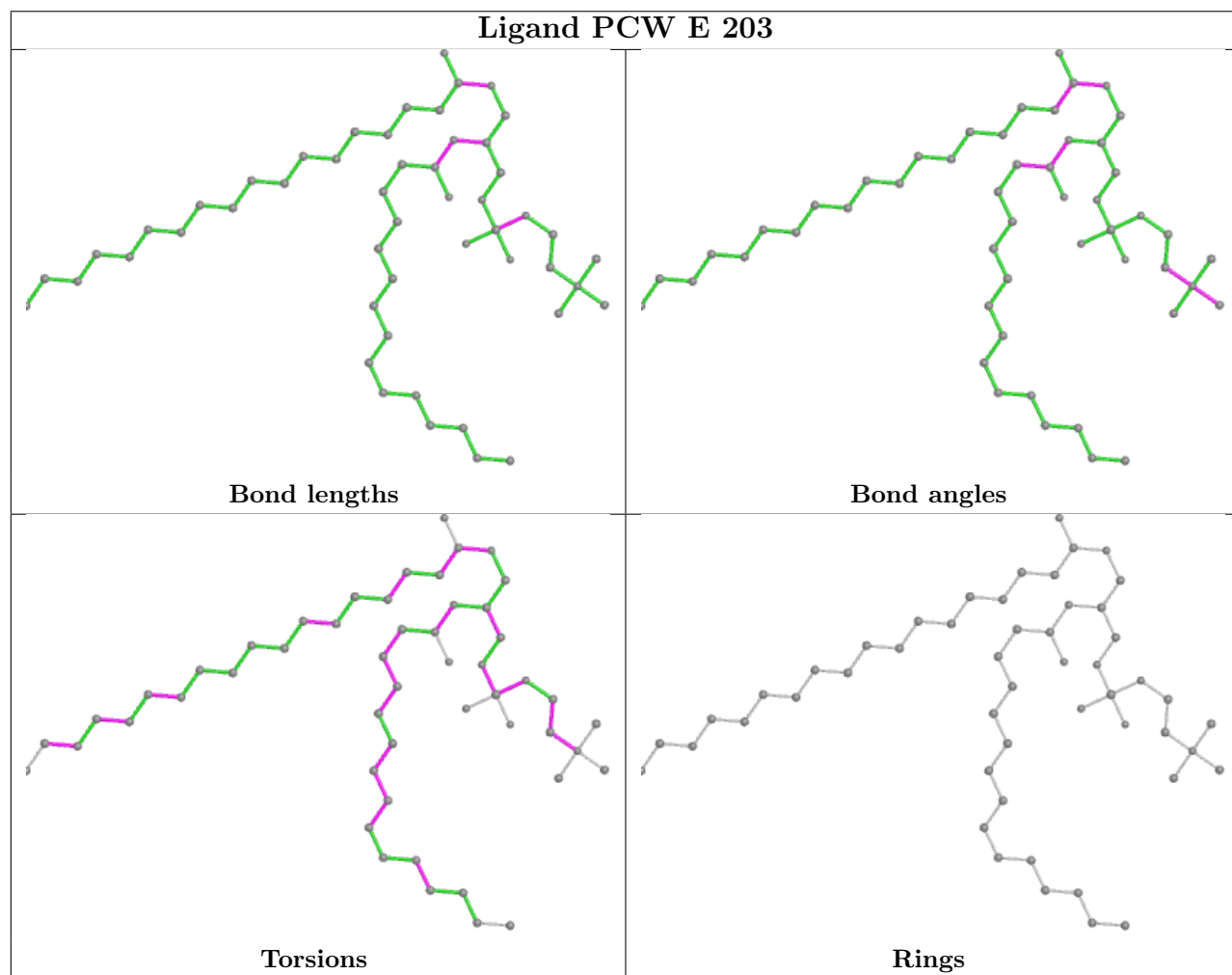
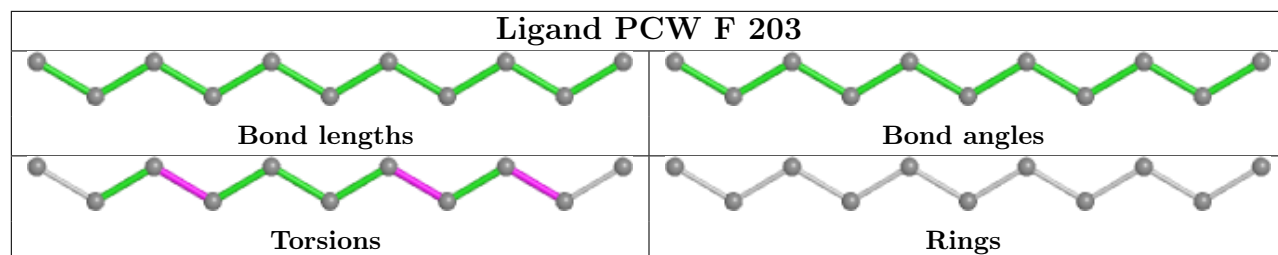


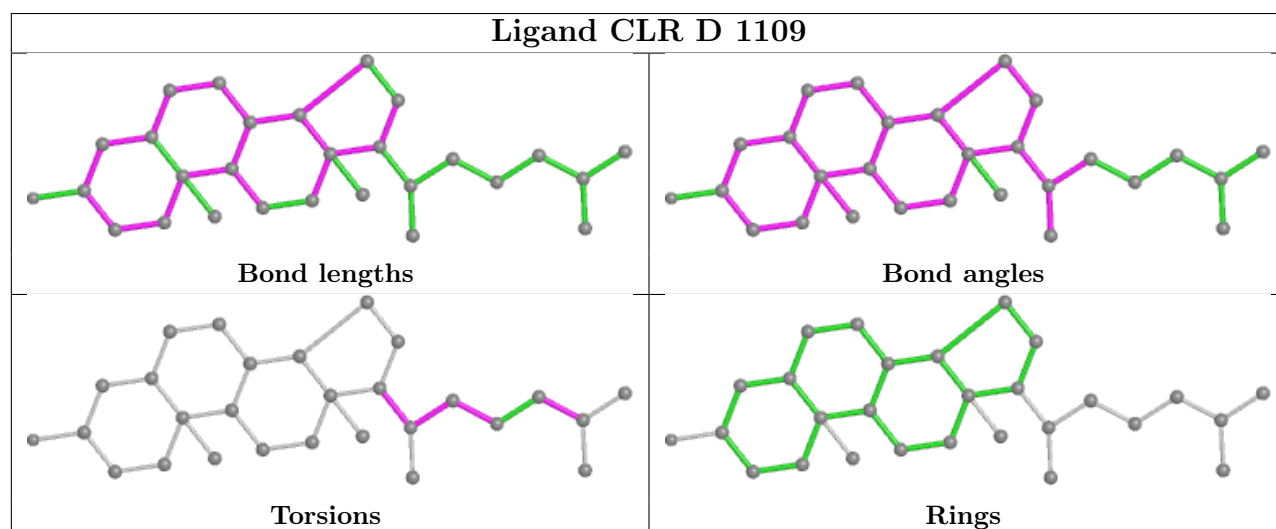
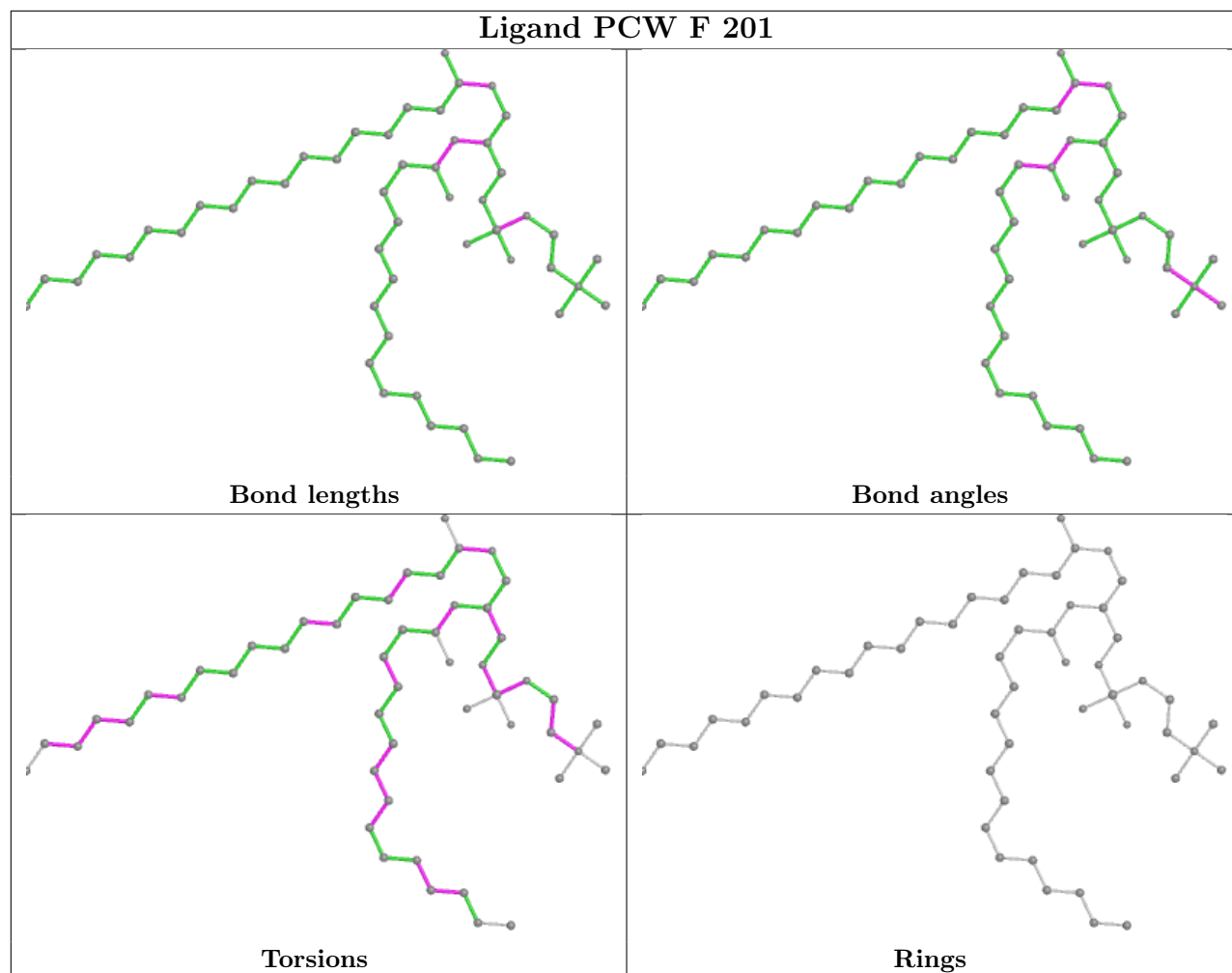




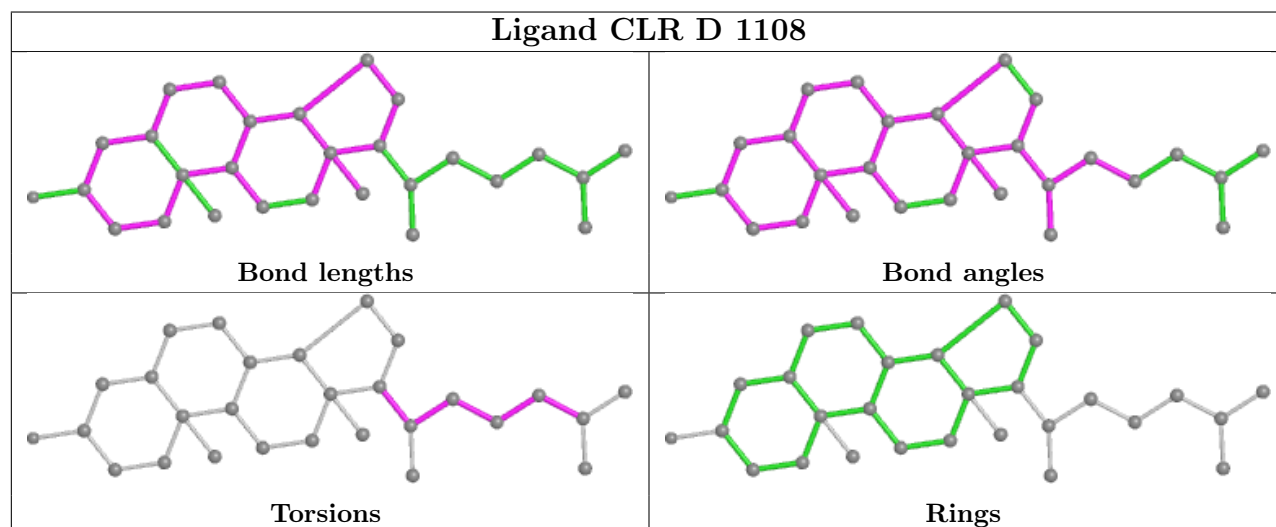
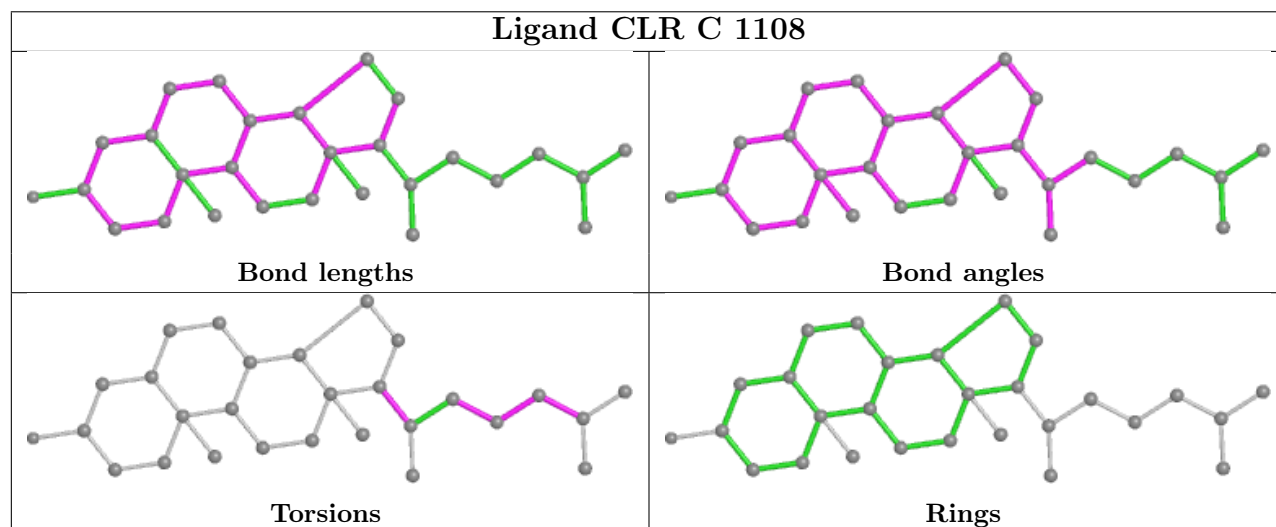
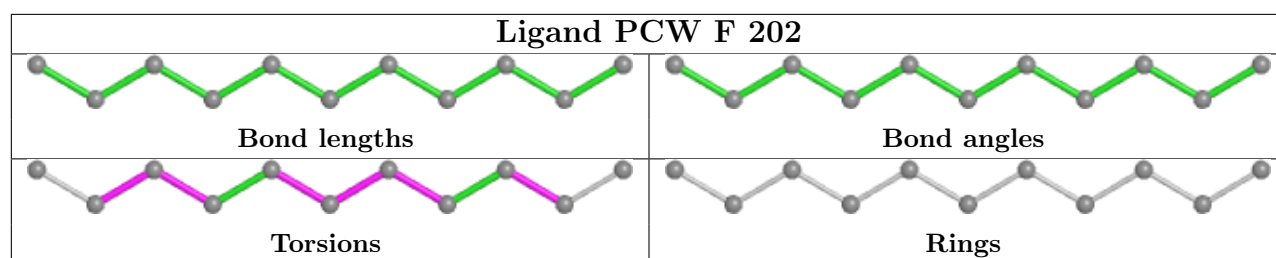


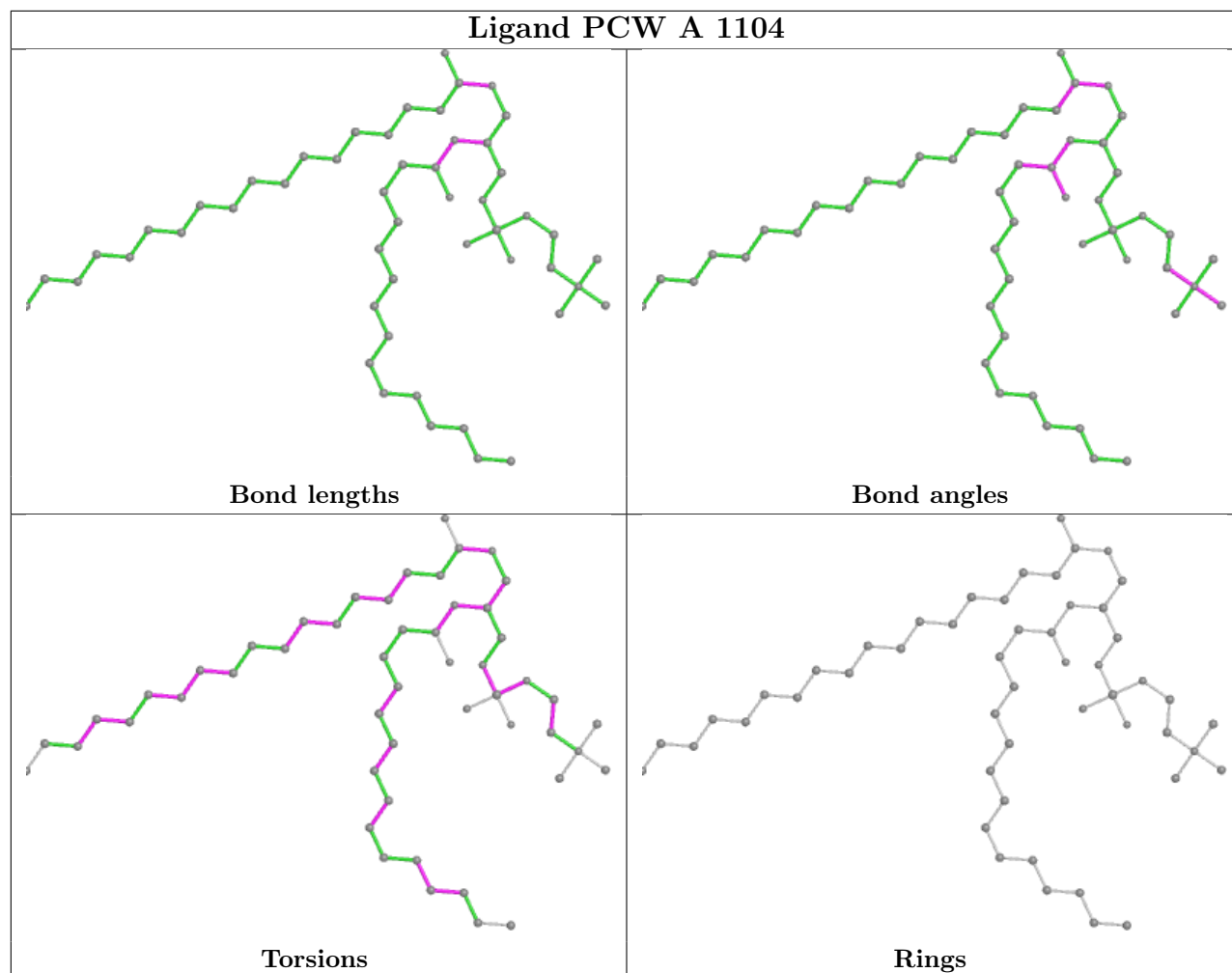


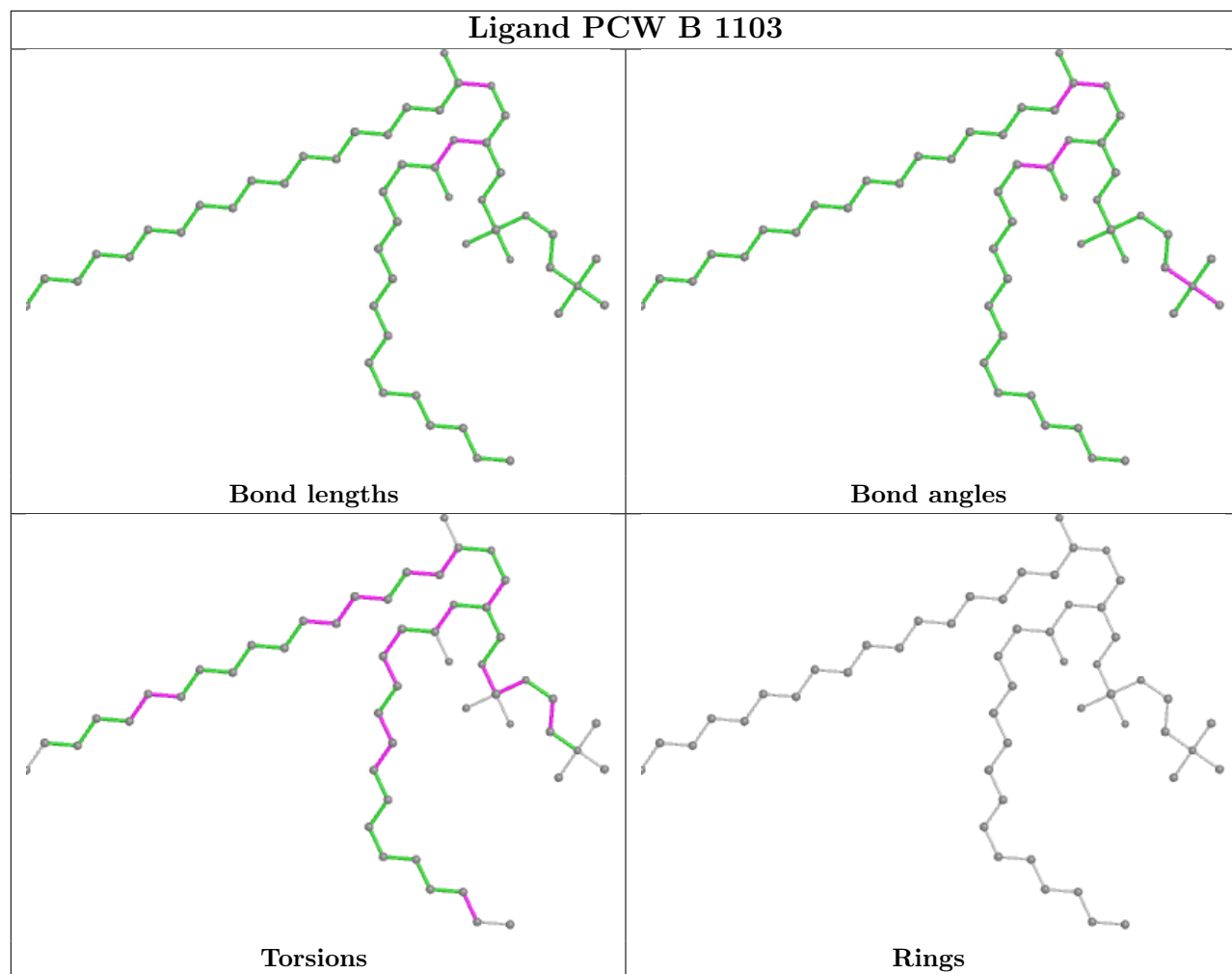


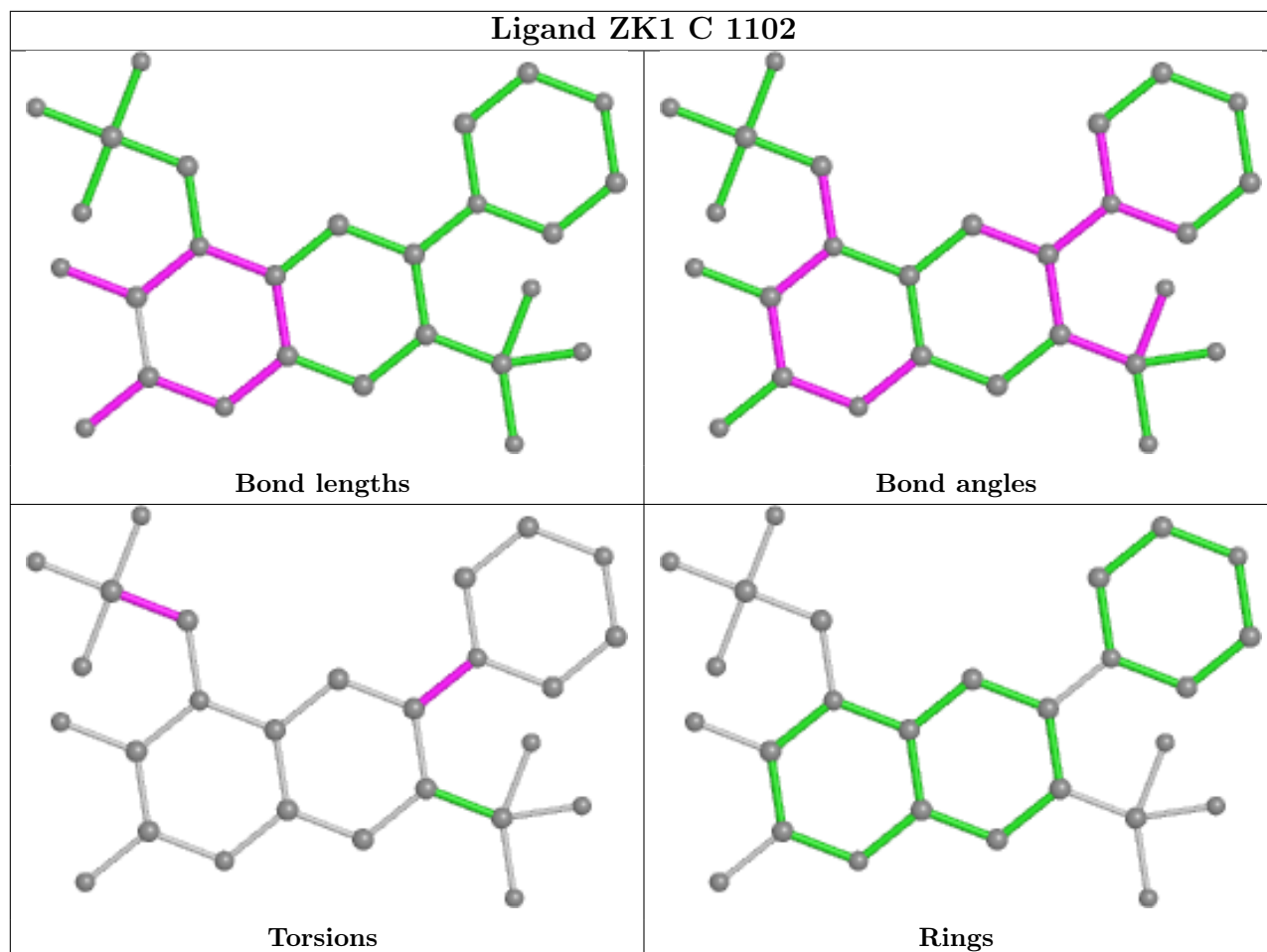


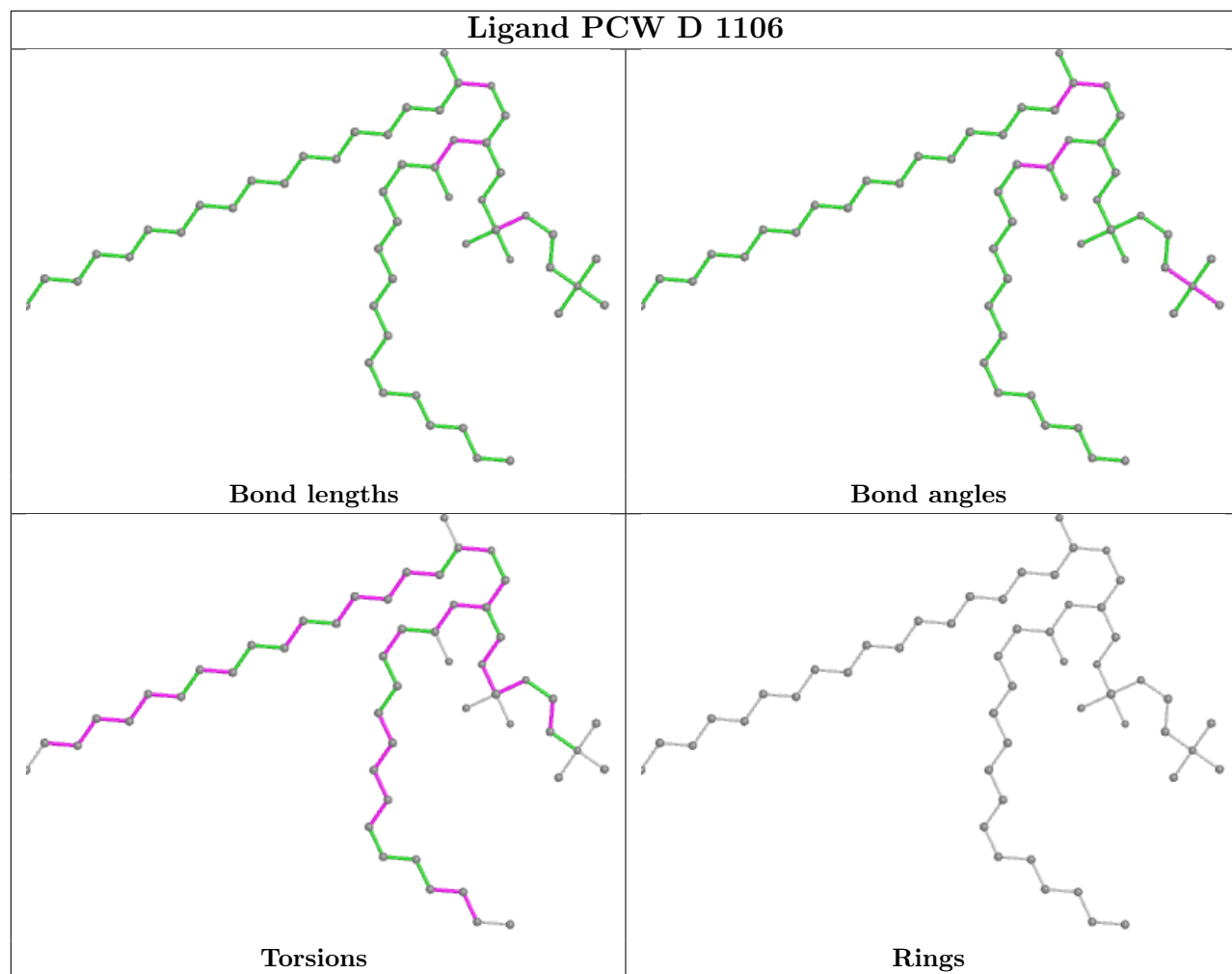


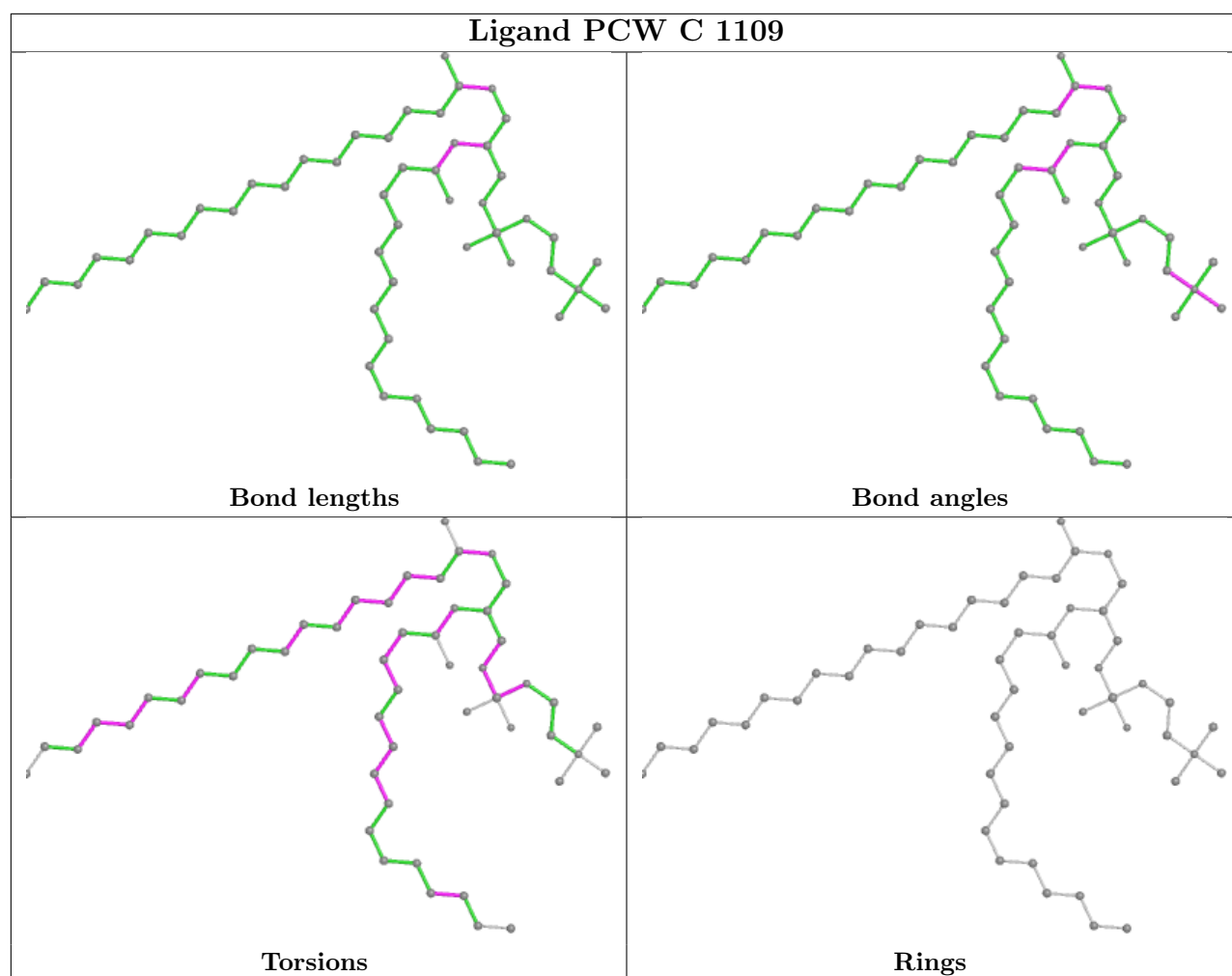


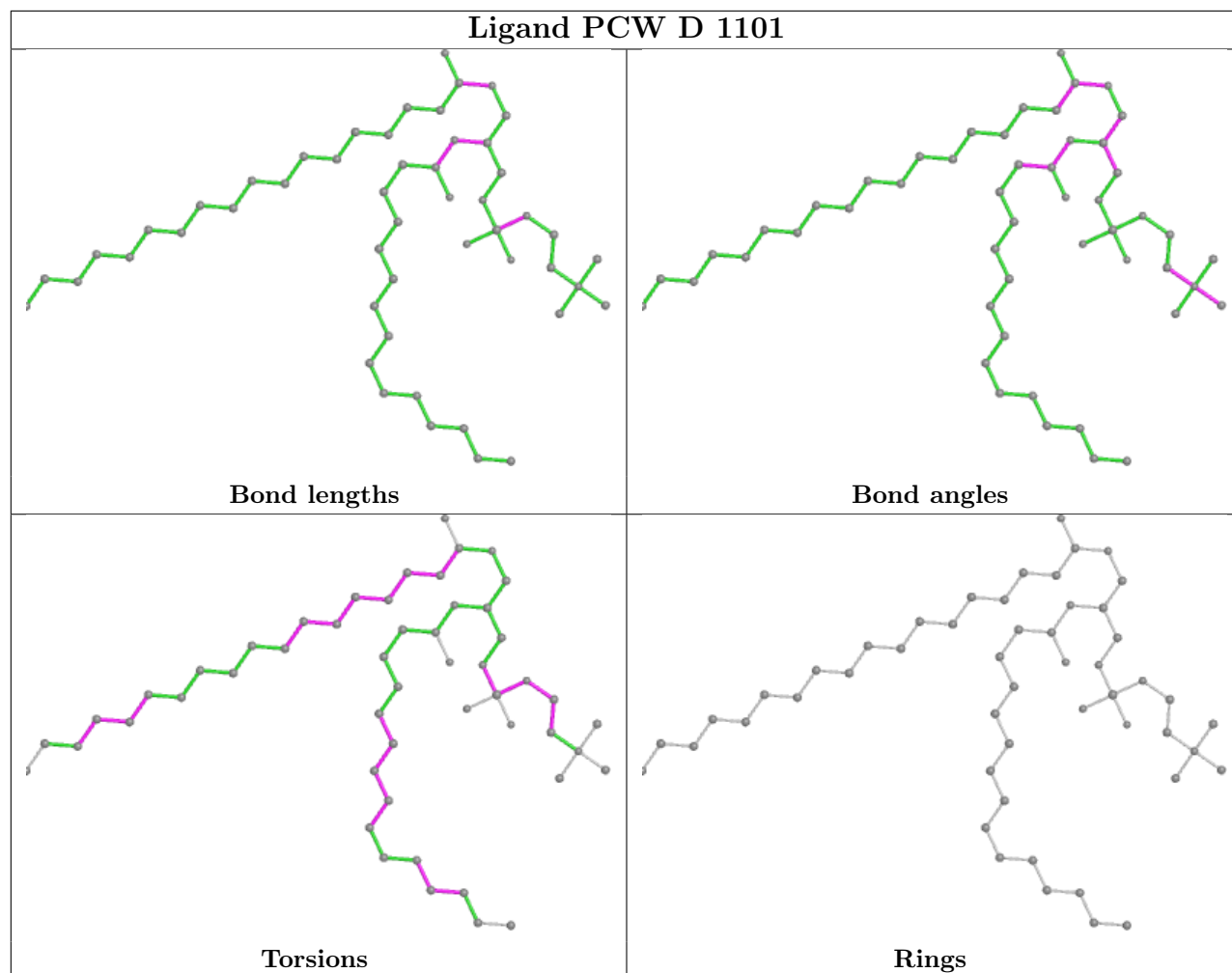


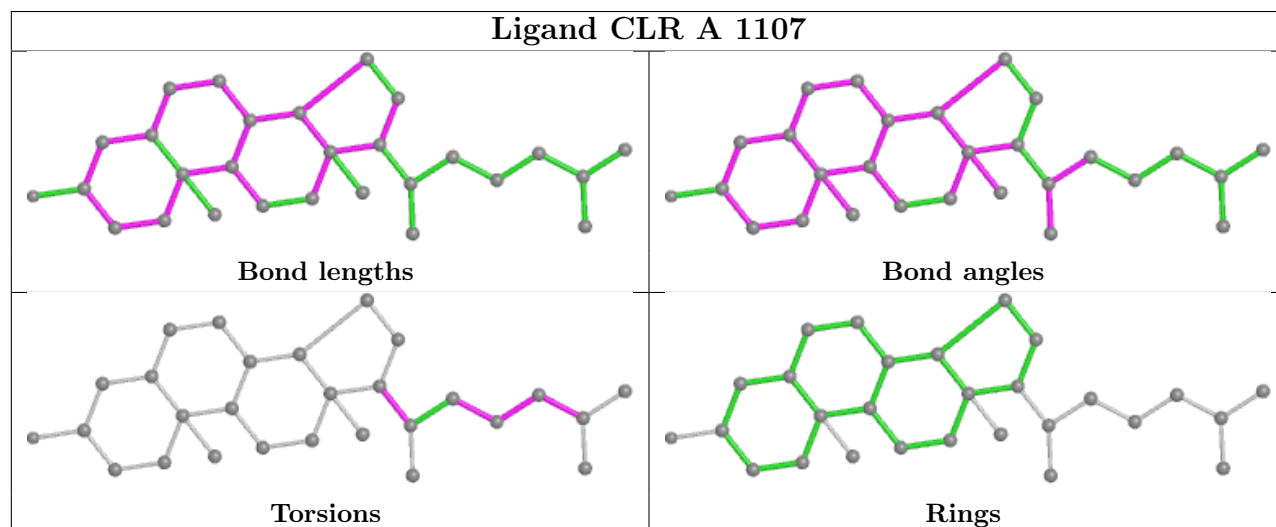
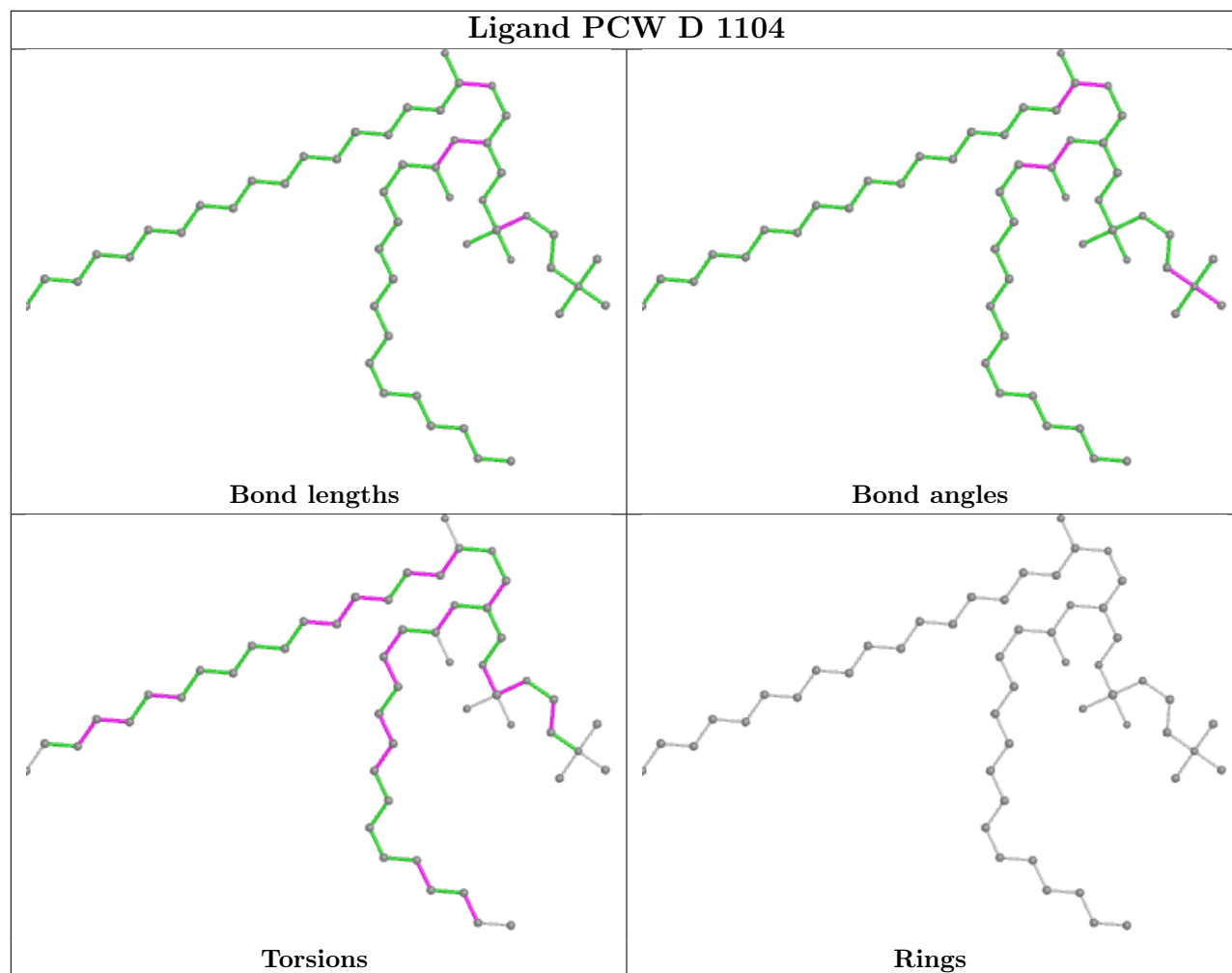




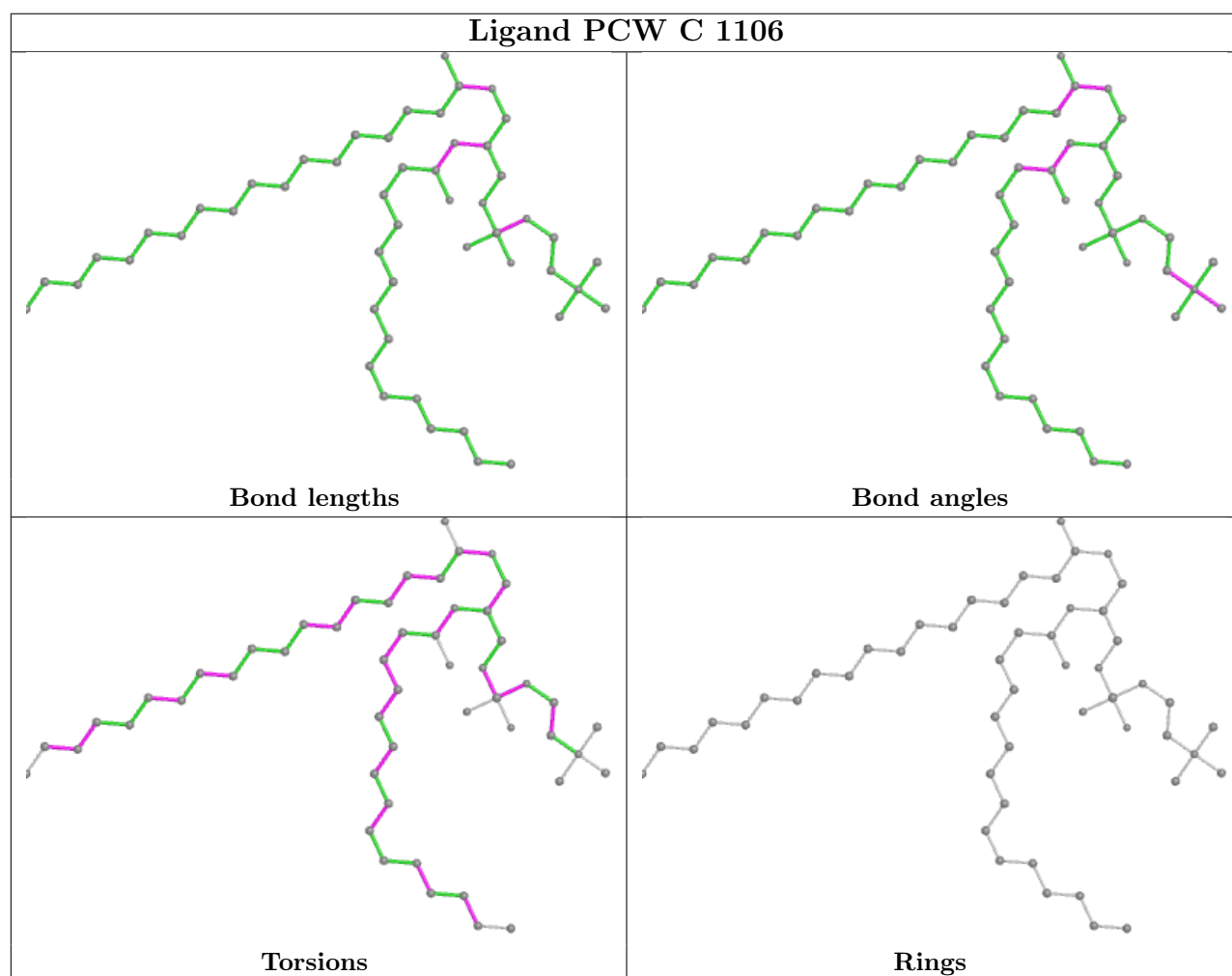
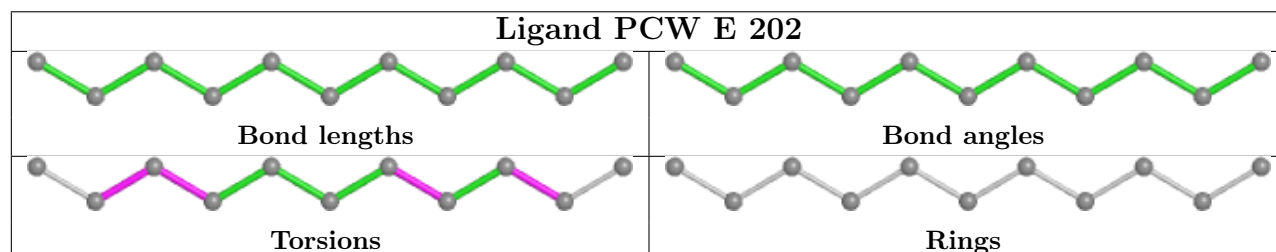
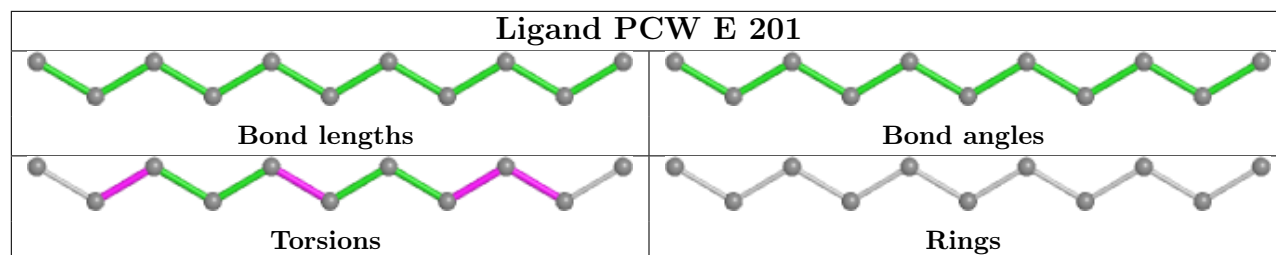


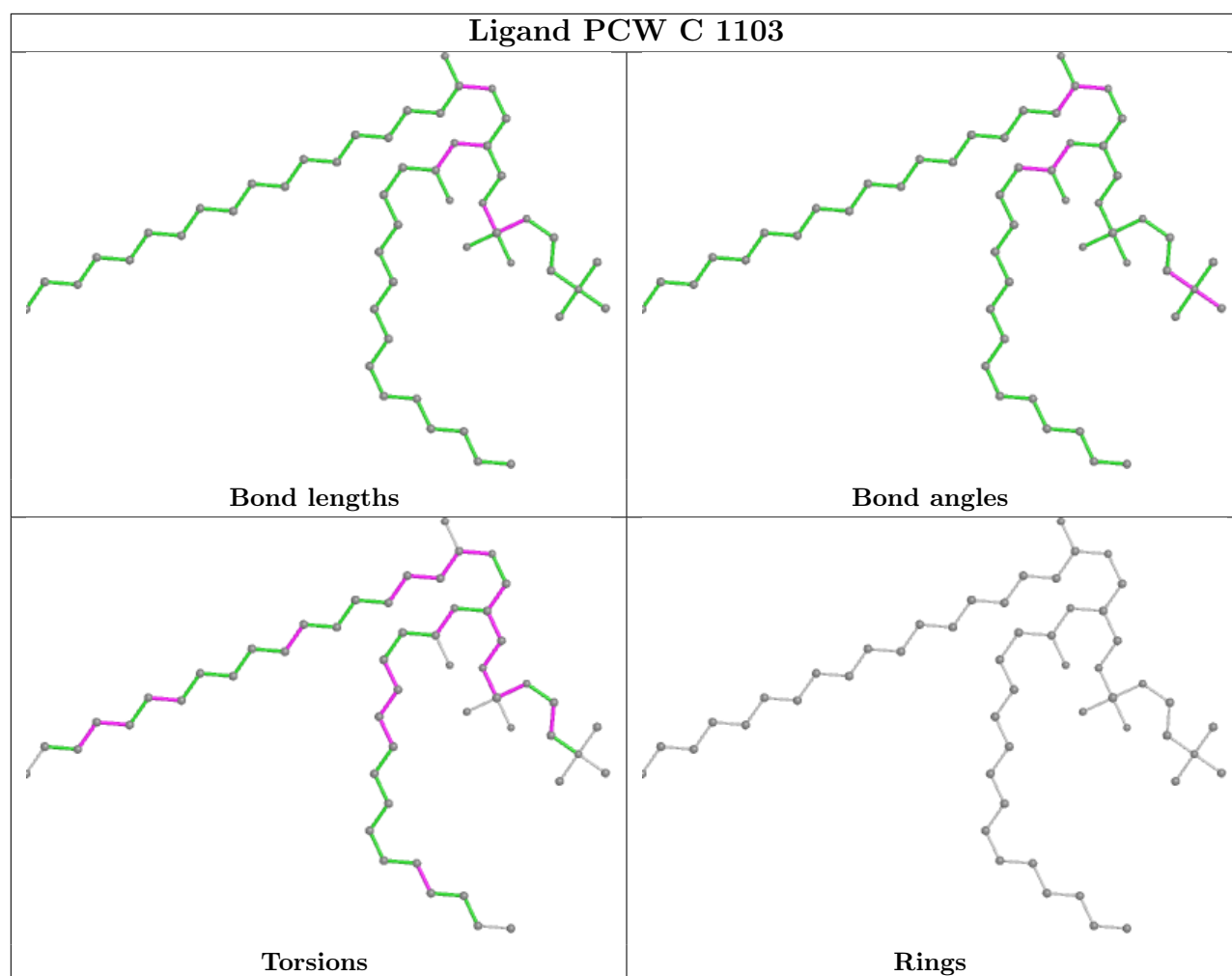












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

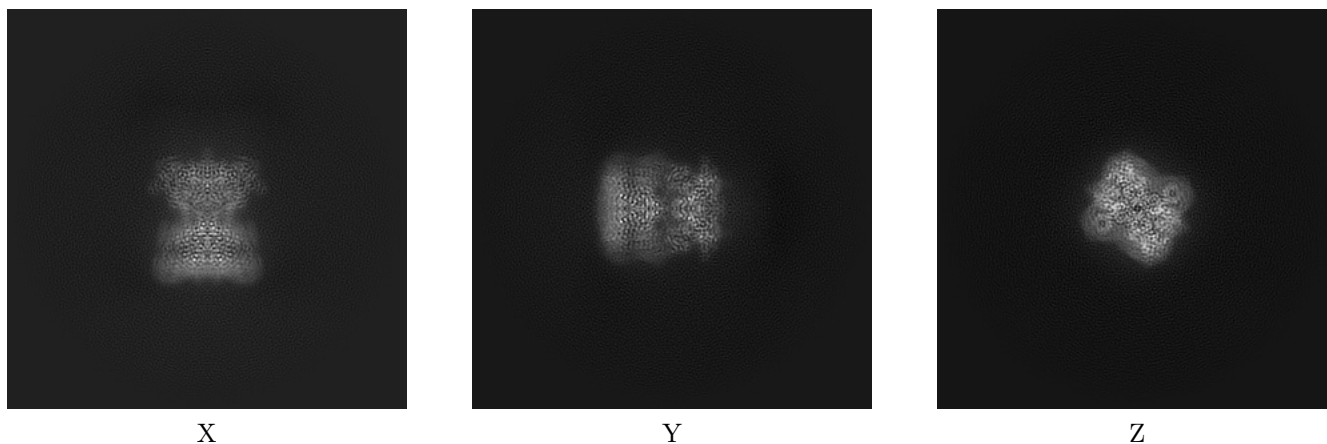
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40746. These allow visual inspection of the internal detail of the map and identification of artifacts.

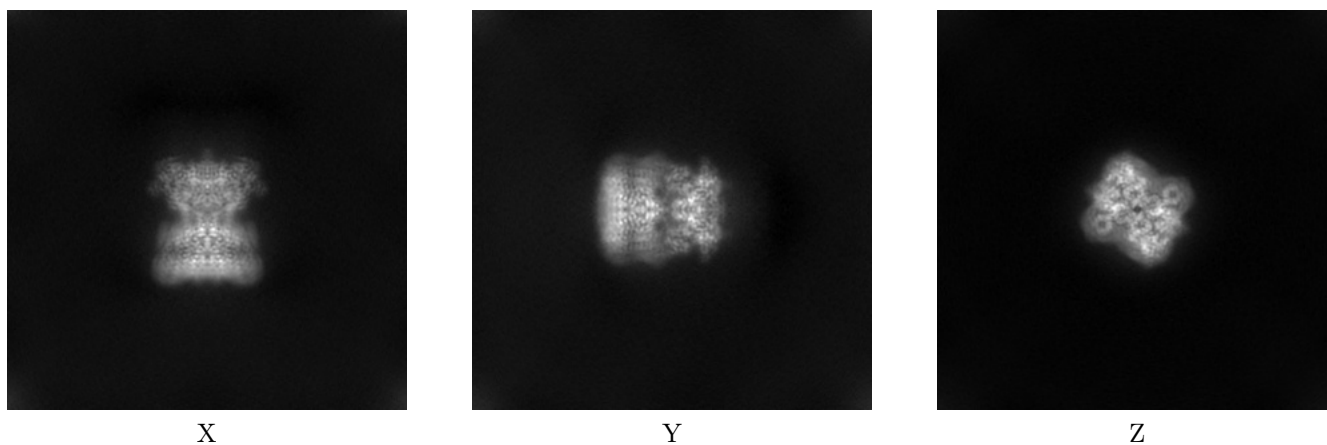
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



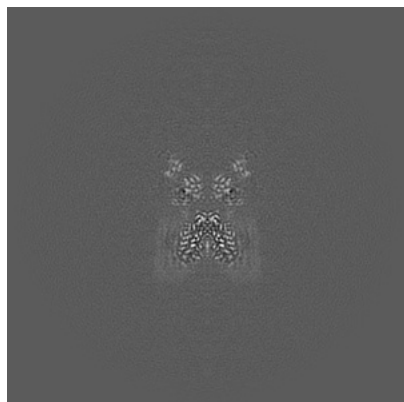
#### 6.1.2 Raw map



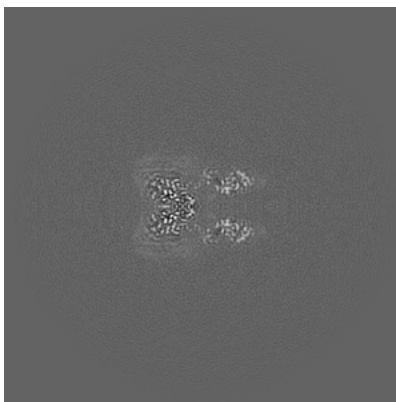
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

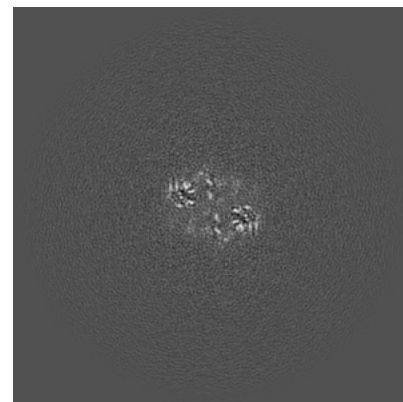
### 6.2.1 Primary map



X Index: 208

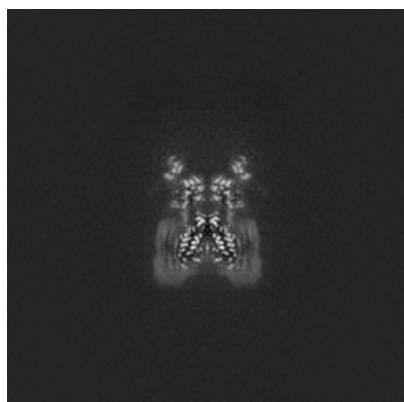


Y Index: 208

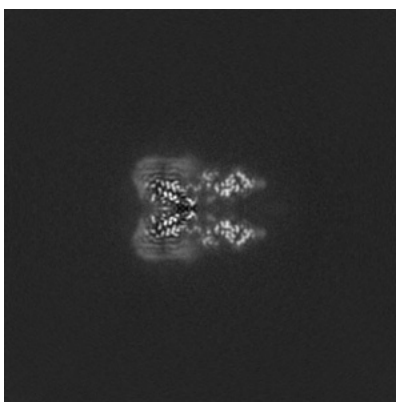


Z Index: 208

### 6.2.2 Raw map



X Index: 208



Y Index: 208

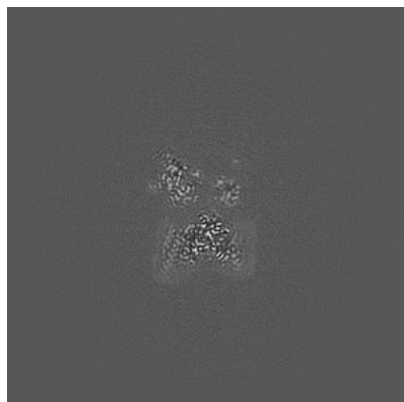


Z Index: 208

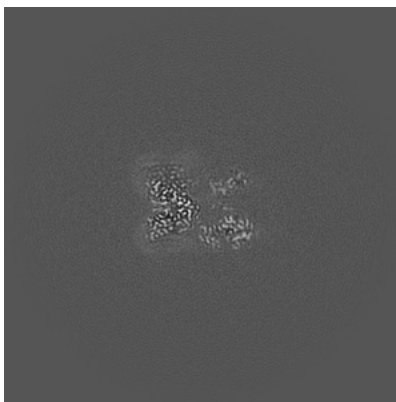
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

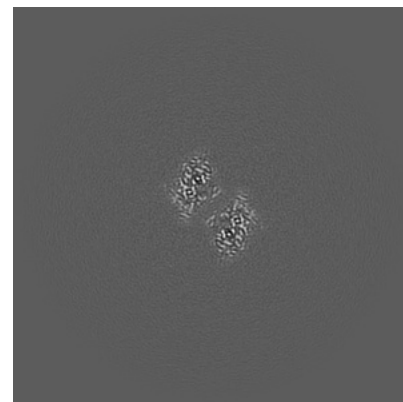
### 6.3.1 Primary map



X Index: 215

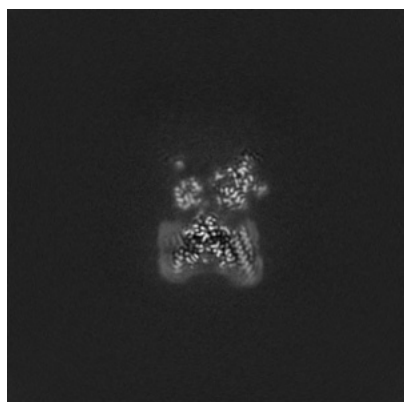


Y Index: 212

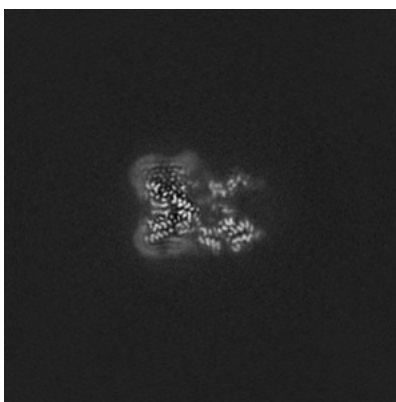


Z Index: 238

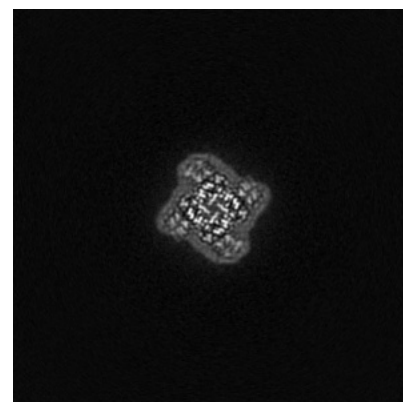
### 6.3.2 Raw map



X Index: 201



Y Index: 212

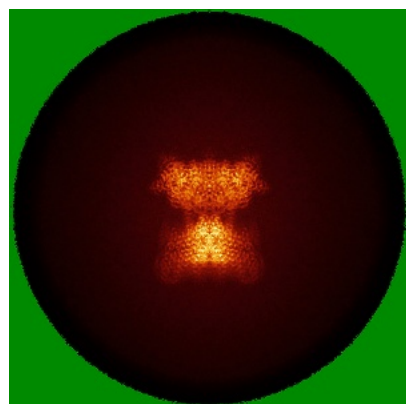


Z Index: 154

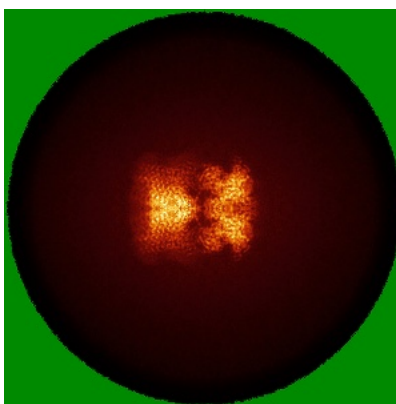
The images above show the largest variance slices of the map in three orthogonal directions.

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

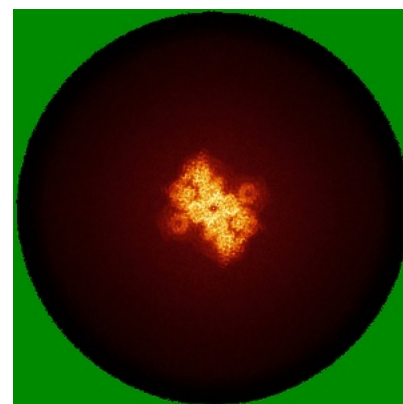
### 6.4.1 Primary map



X

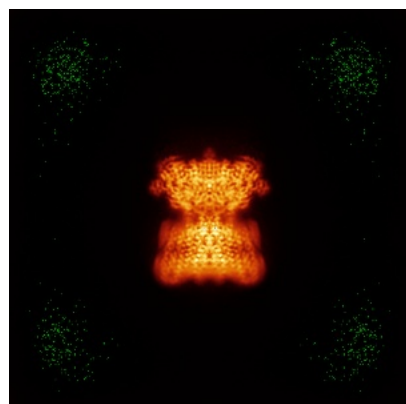


Y

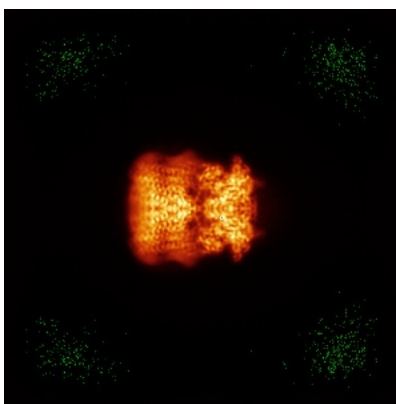


Z

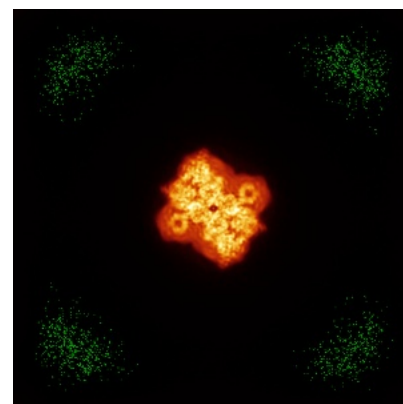
### 6.4.2 Raw map



X



Y

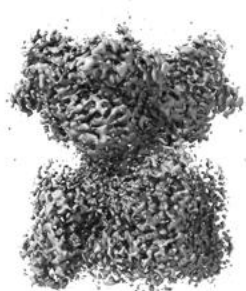


Z

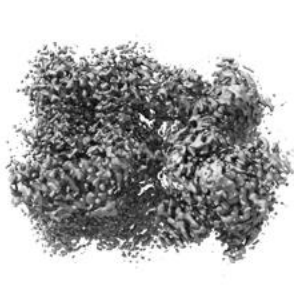
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



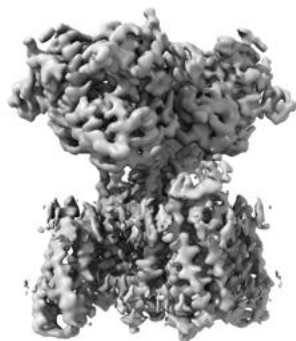
Y



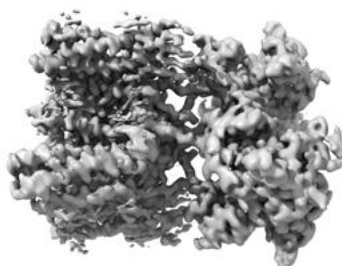
Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

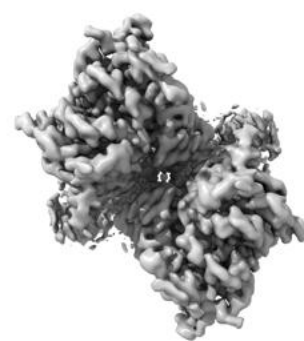
### 6.5.2 Raw map



X



Y



Z

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](#)

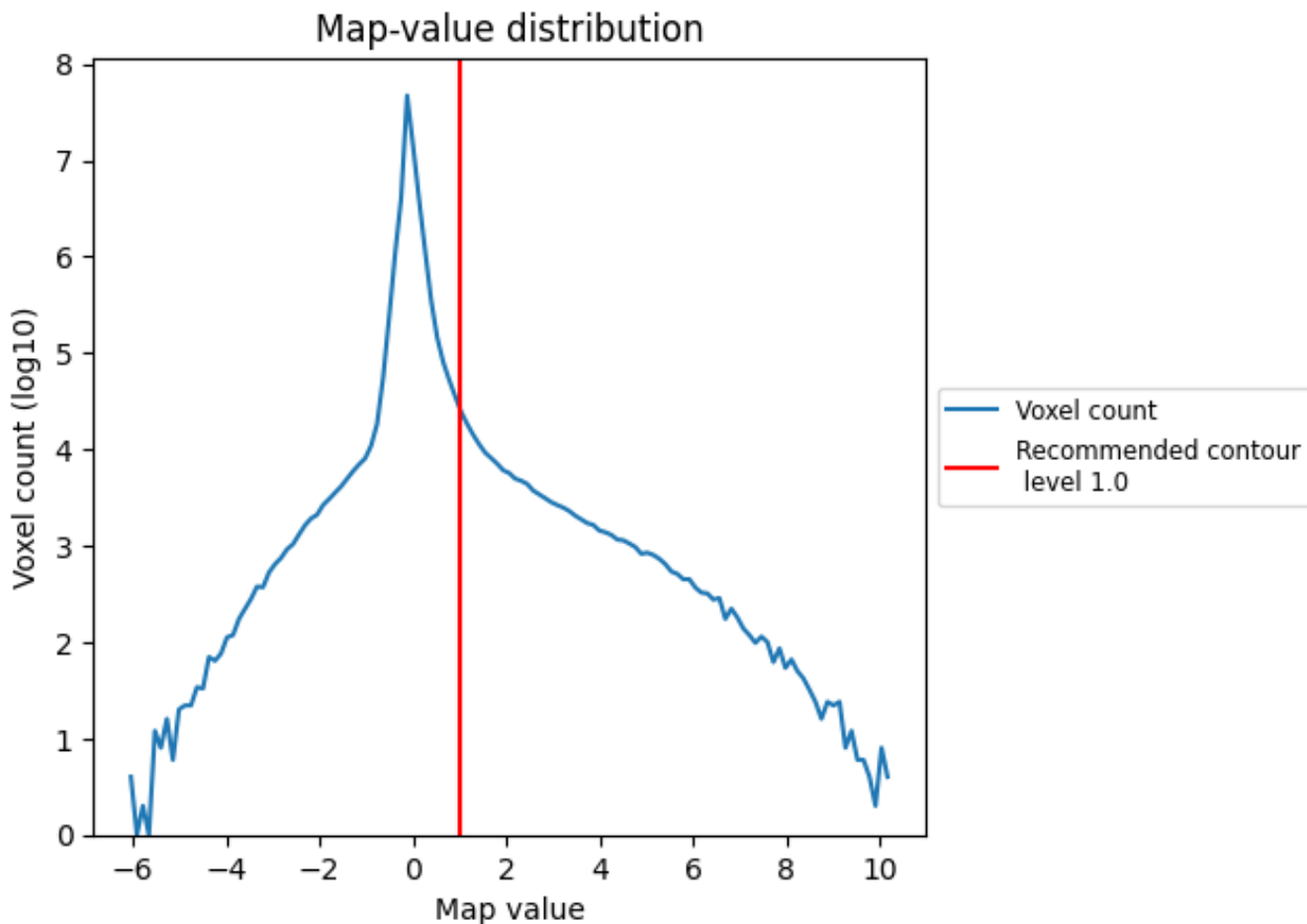
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

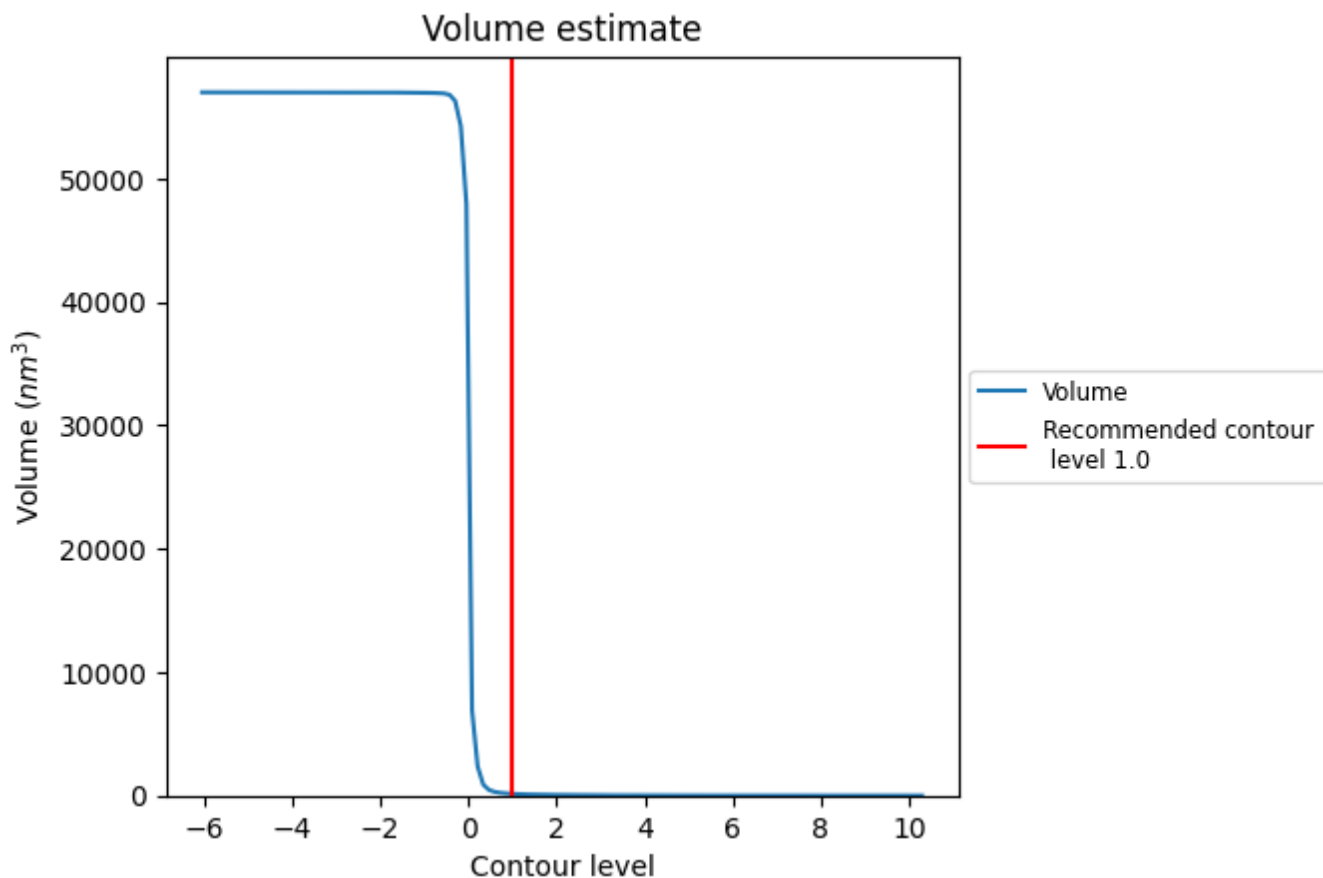
### 7.1 Map-value distribution [i](#)



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.



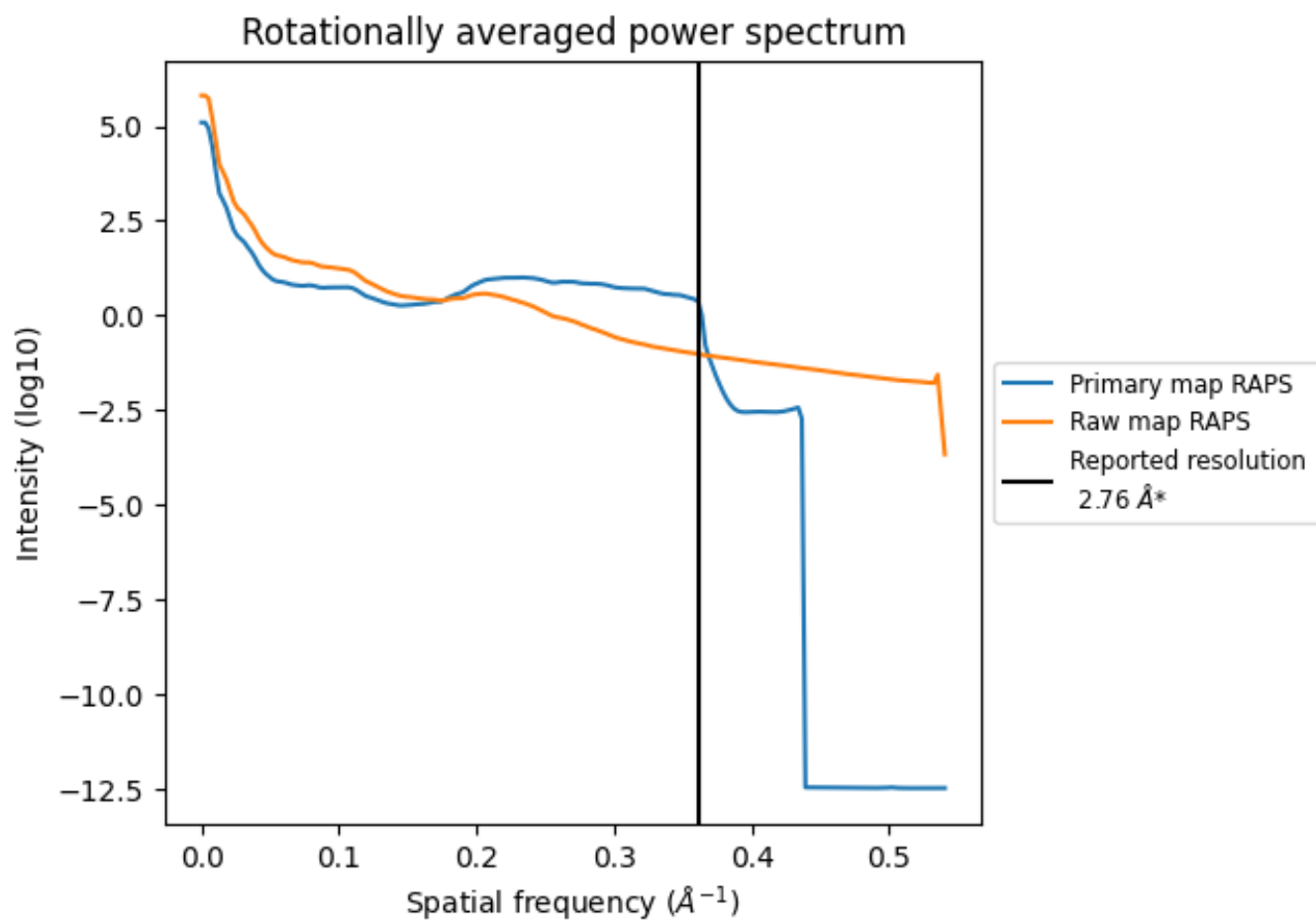
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136  $\text{nm}^3$ ; this corresponds to an approximate mass of 123 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

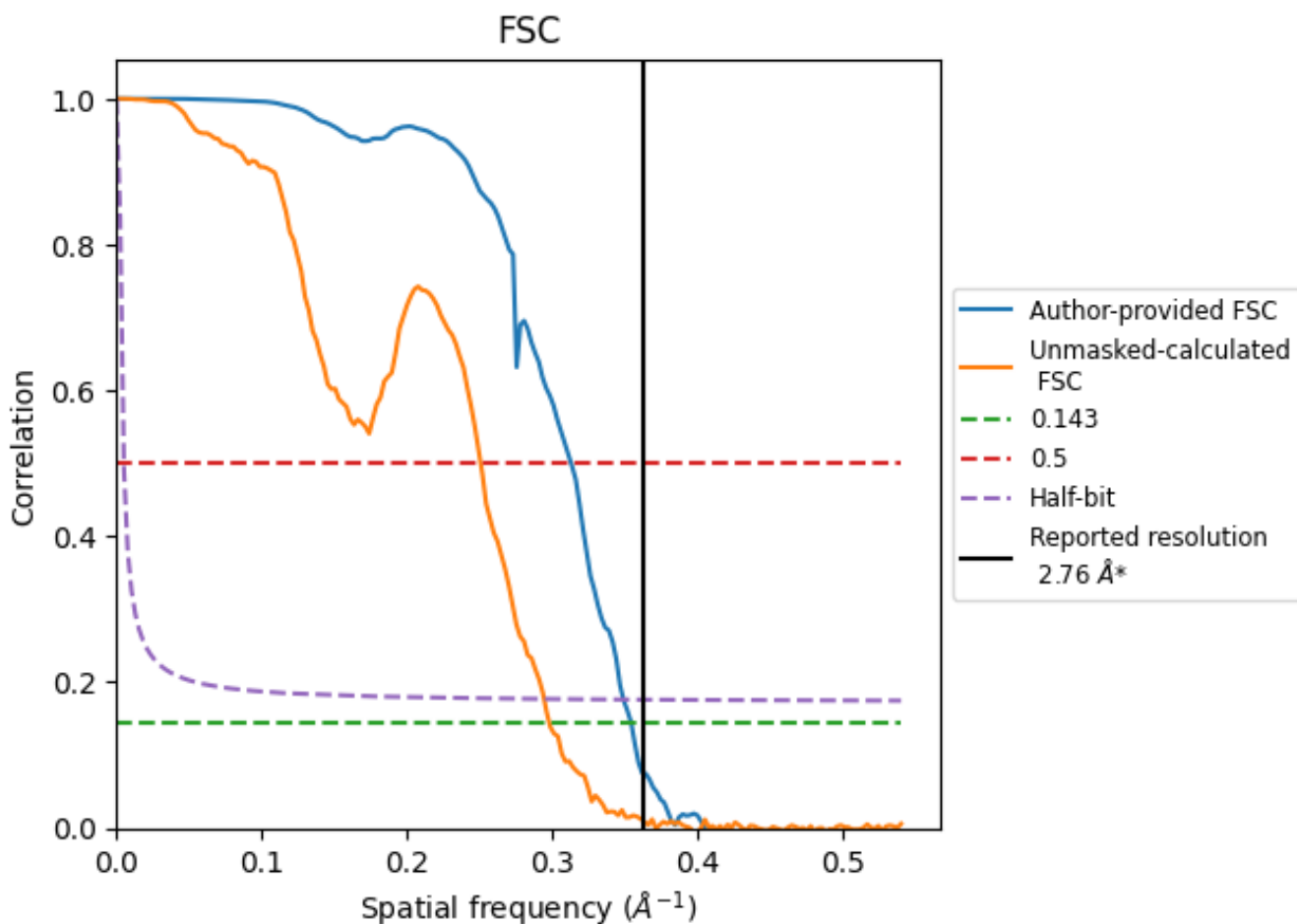


\*Reported resolution corresponds to spatial frequency of 0.362 Å<sup>-1</sup>

## 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  $0.362 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

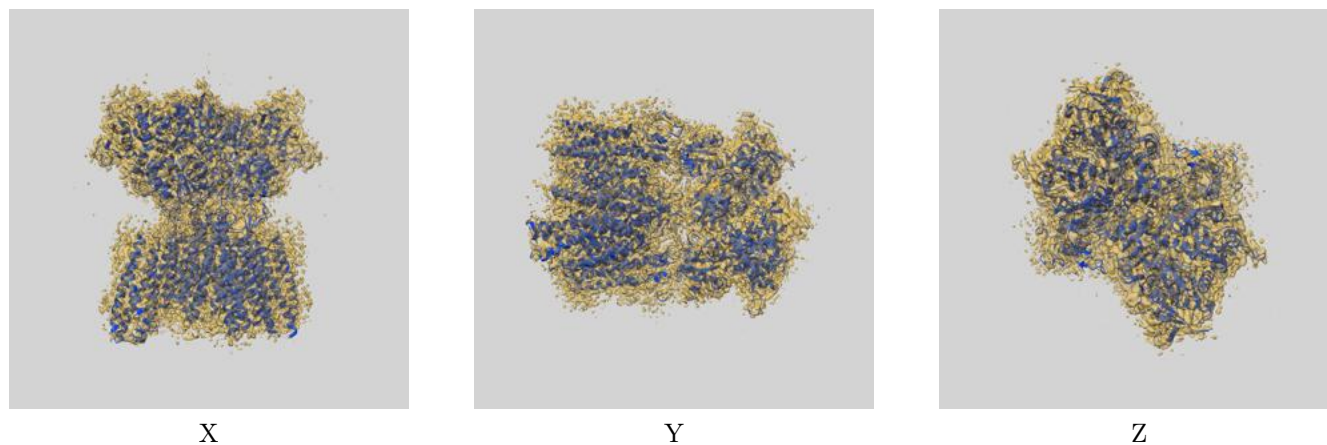
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.82	3.19	2.86
Unmasked-calculated*	3.35	3.99	3.40

\*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 3.35 differs from the reported value 2.76 by more than 10 %

## 9 Map-model fit [i](#)

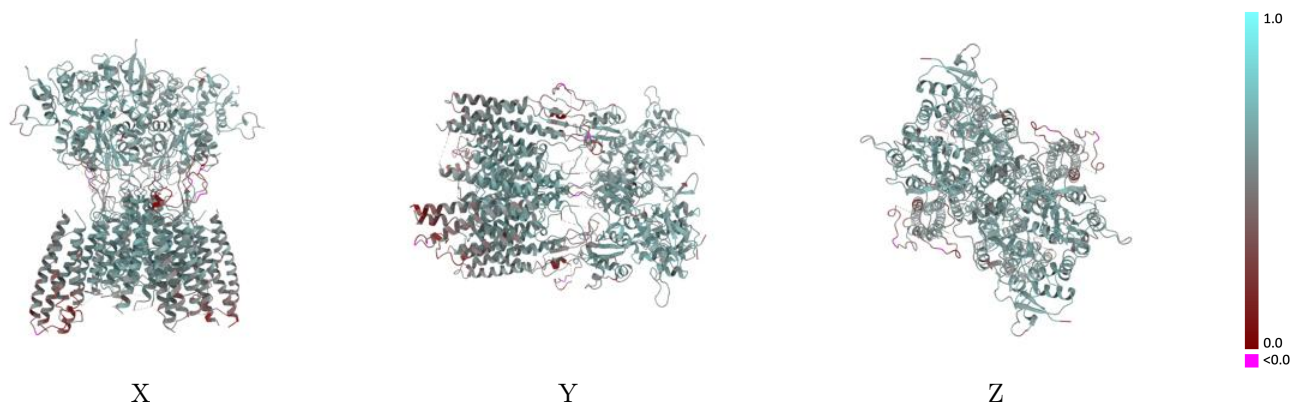
This section contains information regarding the fit between EMDB map EMD-40746 and PDB model 8SS7. Per-residue inclusion information can be found in section 3 on page 12.

### 9.1 Map-model overlay [i](#)



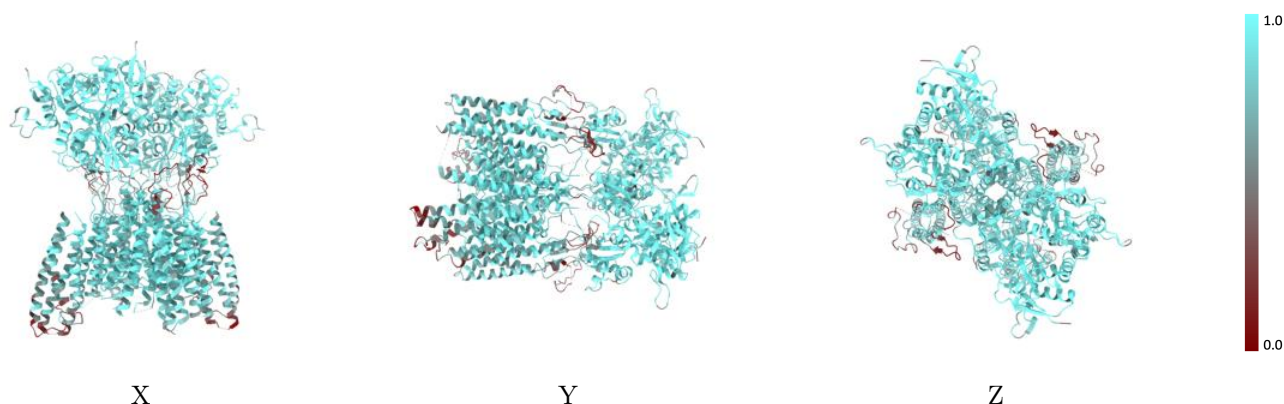
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



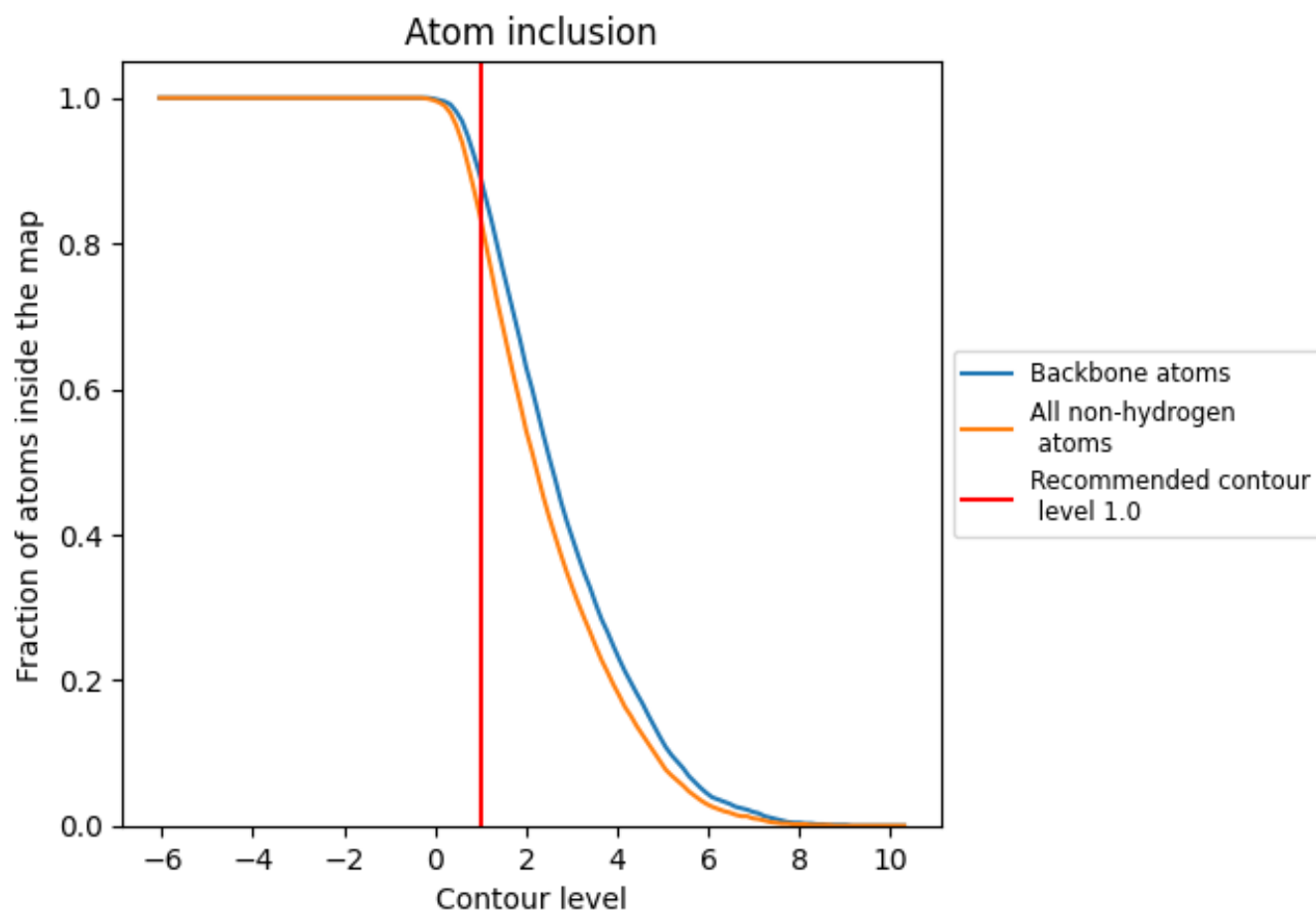
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.0).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8340	 0.5440
A	 0.8300	 0.5450
B	 0.8960	 0.5820
C	 0.8310	 0.5440
D	 0.8960	 0.5790
E	 0.6800	 0.4450
F	 0.6680	 0.4330

