



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 07:09 PM EST

PDB ID : 8SS3  
EMDB ID : EMD-40742  
Title : Structure of LBD-TMD of AMPA receptor GluA2 in complex with auxiliary subunits TARP gamma-5 and cornichon-2 bound to competitive antagonist ZK and channel blocker spermidine (closed state)  
Authors : Gangwar, S.P.; Yen, L.Y.; Yelshanskaya, M.V.; Sobolevsky, A.I.  
Deposited on : 2023-05-08  
Resolution : 3.21 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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

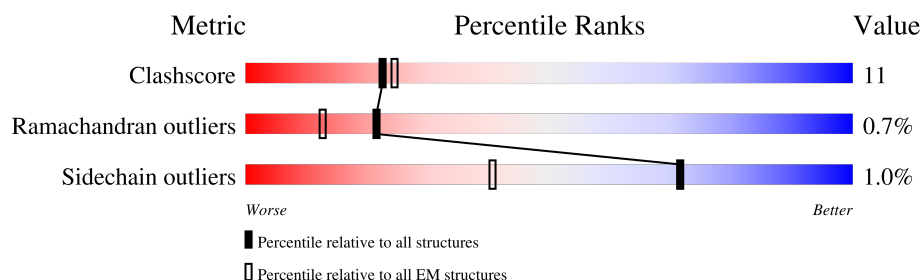
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.21 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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
5	CLR	A	1107	X	-	-	-
5	CLR	A	1112	X	-	-	-
5	CLR	C	1106	X	-	-	-
5	CLR	C	1111	X	-	-	-
6	AJP	A	1110	X	-	X	-
6	AJP	A	1111	X	-	X	-
6	AJP	A	1116	X	-	X	-
6	AJP	C	1109	X	-	X	-
6	AJP	C	1110	X	-	X	-
6	AJP	C	1114	X	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19887 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
1	A	596	Total	C	N	O	S	0	0
			4671	3049	753	838	31		
1	B	404	Total	C	N	O	S	0	0
			3156	2048	511	576	21		
1	C	596	Total	C	N	O	S	0	0
			4671	3049	753	838	31		
1	D	404	Total	C	N	O	S	0	0
			3156	2048	511	576	21		

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

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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

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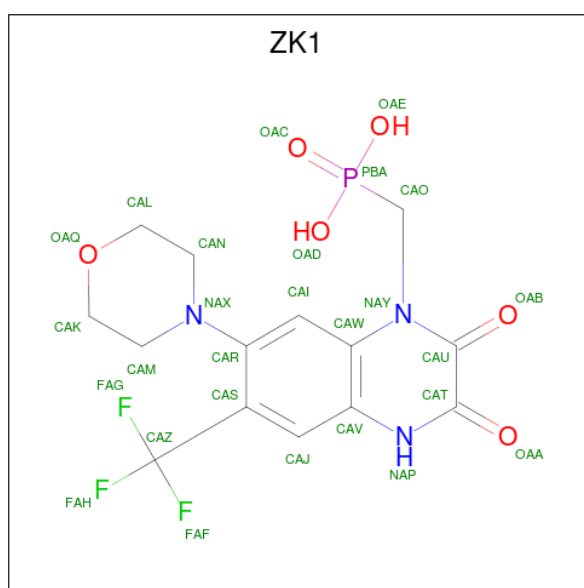
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Chain	Residue	Modelled	Actual	Comment	Reference
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	754	SER	ASN	conflict	UNP P19491
D	758	VAL	LEU	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	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
2	E	140	Total	C	N	O	S	0	0
			1166	787	175	191	13		
2	F	140	Total	C	N	O	S	0	0
			1166	787	175	191	13		

- Molecule 3 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).



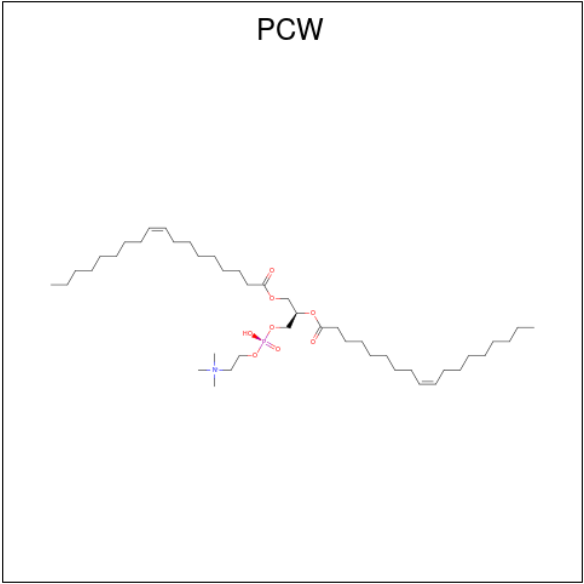
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

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

- Molecule 4 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
4	A	1	Total 51	C 41	N 1	O 8	P 1	0
4	A	1	Total 43	C 33	N 1	O 8	P 1	0
4	A	1	Total 41	C 31	N 1	O 8	P 1	0
4	A	1	Total 51	C 41	N 1	O 8	P 1	0
4	A	1	Total 11		C 11			0
4	A	1	Total 11		C 11			0
4	A	1	Total 11		C 11			0
4	A	1	Total 51	C 41	N 1	O 8	P 1	0
4	A	1	Total 51	C 41	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C				0
			11	11				
4	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	B	1	Total	C				0
			11	11				
4	B	1	Total	C				0
			11	11				
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C				0
			11	11				

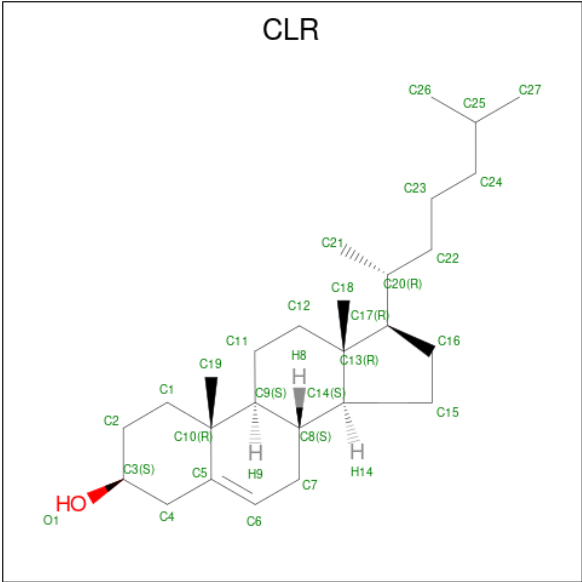
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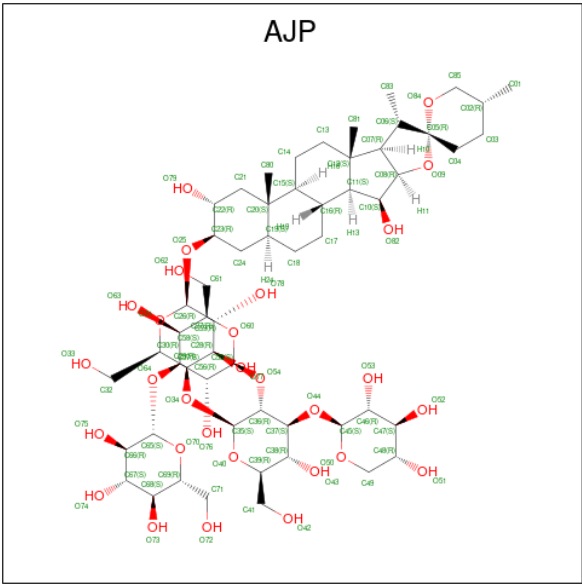
Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C				0
			11	11				
4	D	1	Total	C				0
			11	11				
4	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	D	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	D	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	D	1	Total	C				0
			11	11				
4	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	D	1	Total	C				0
			11	11				
4	E	1	Total	C				0
			11	11				
4	E	1	Total	C				0
			11	11				
4	E	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	E	1	Total	C				0
			11	11				
4	E	1	Total	C				0
			11	11				
4	F	1	Total	C				0
			11	11				
4	F	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	F	1	Total	C				0
			11	11				
4	F	1	Total	C				0
			11	11				
4	F	1	Total	C				0
			11	11				

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



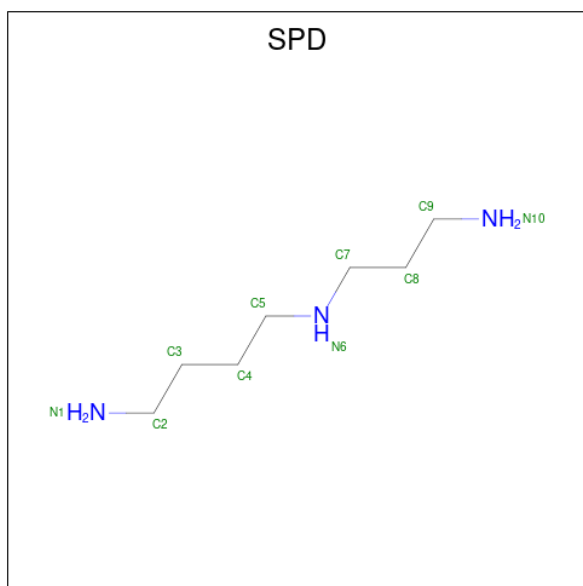
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	C	1	Total	C	O	0
			28	27	1	
5	C	1	Total	C	O	0
			28	27	1	

- Molecule 6 is Digitonin (three-letter code: AJP) (formula:  $C_{56}H_{92}O_{29}$ ).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			42	33	9	
6	A	1	Total	C	O	0
			42	33	9	
6	A	1	Total	C	O	0
			42	33	9	
6	C	1	Total	C	O	0
			41	33	8	
6	C	1	Total	C	O	0
			42	33	9	
6	C	1	Total	C	O	0
			42	33	9	

- Molecule 7 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ) (labeled as "Ligand of Interest" by depositor).

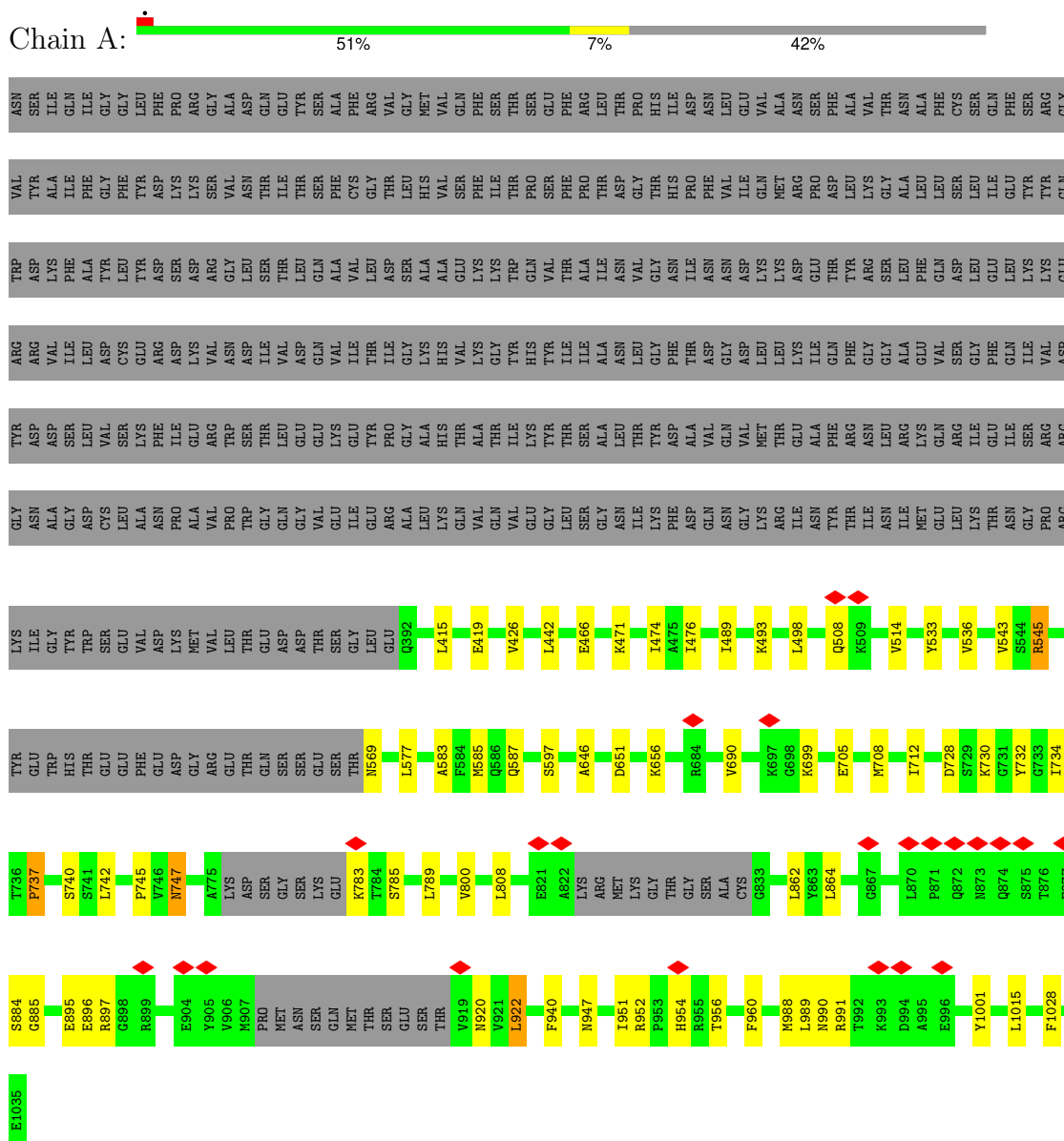


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	N	0
			10	7	3	

### 3 Residue-property plots

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

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



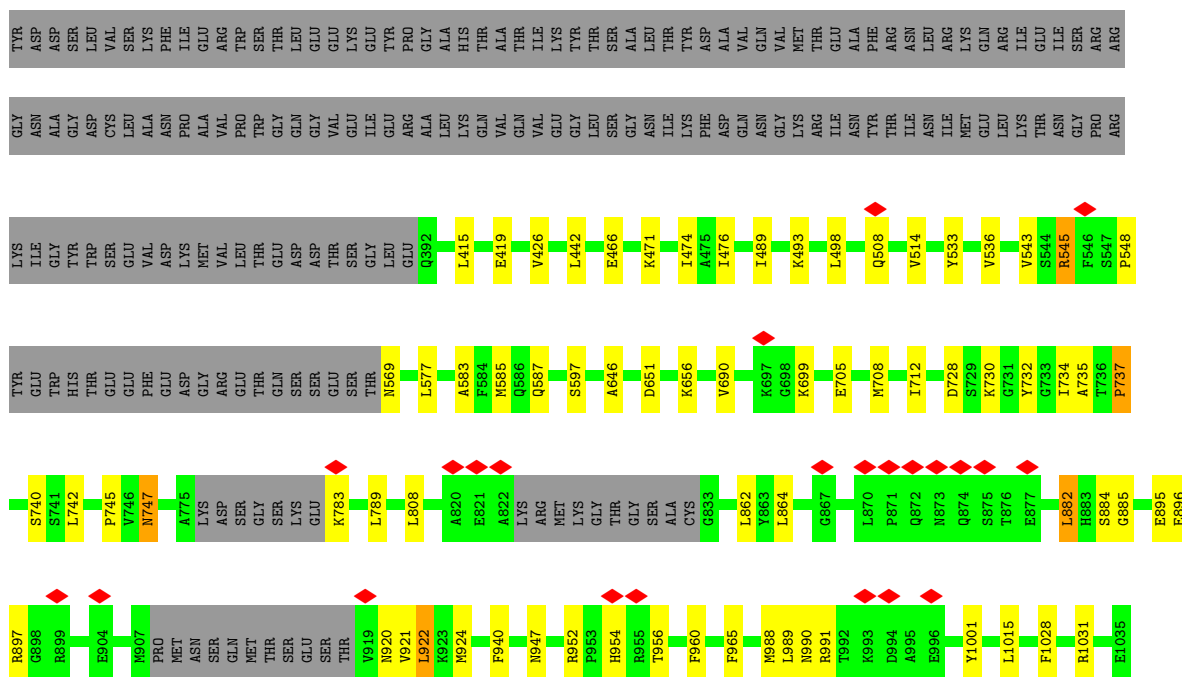
- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

61%

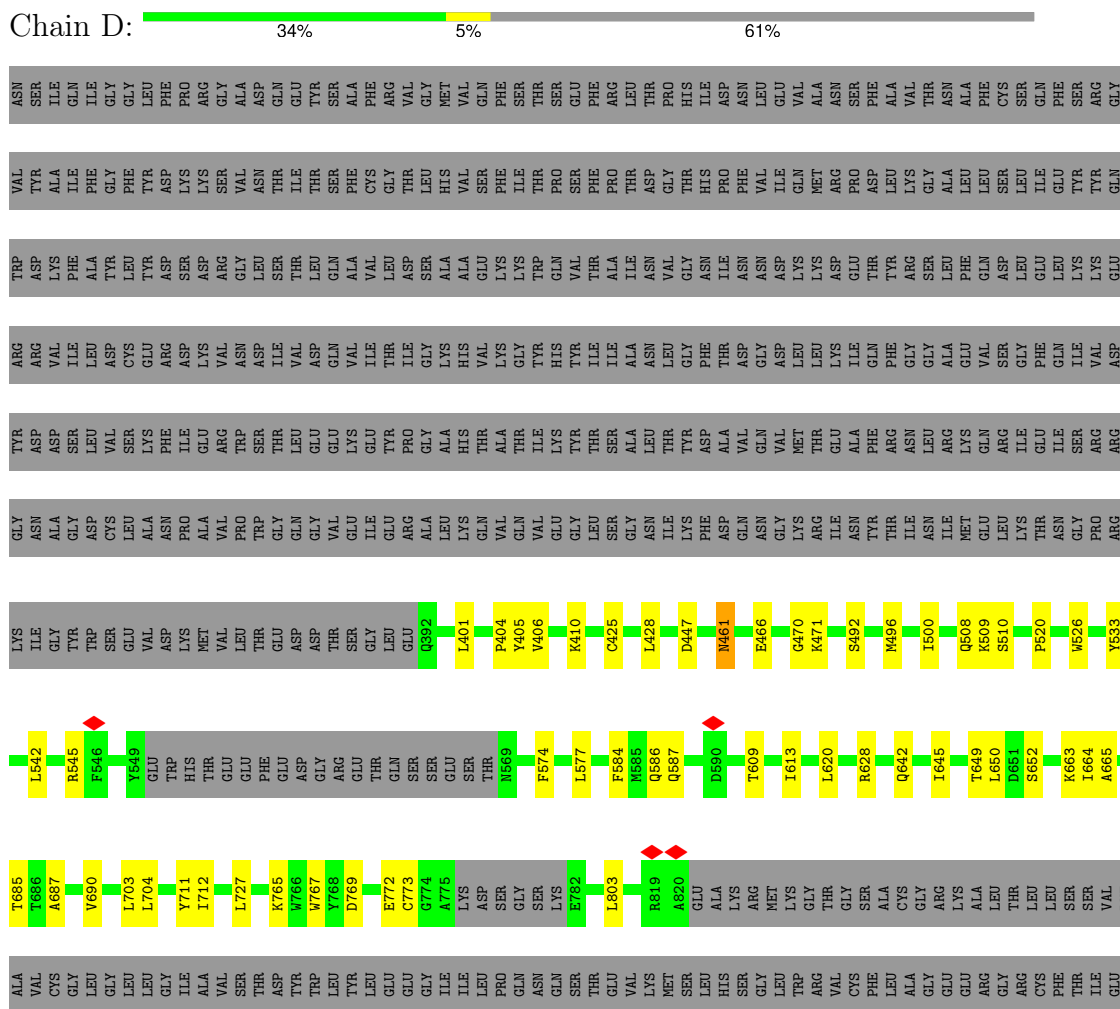
- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

42%

ARG	ARG	ASP	TRP	VAL	ASN
VAL	VAL	ASP	ASP	TYR	SER
ILE	ILE	PHE	LYS	ALA	ILE
LEU	LEU	ALA	PHE	ILE	GLN
ASP	ASP	TYR	GLY	GLY	GLY
CYS	CYS	LEU	LEU	PHE	LEU
GLU	GLU	TYR	TYR	TYR	ASP
ARG	ARG	ASP	ASP	ASP	PHE
ASP	ASP	SER	SER	LYS	PRO
LYS	LYS	ASP	ASP	LYS	ARG
VAL	VAL	ARG	ARG	SER	GLY
ASN	ASN	GLY	GLY	VAL	ALA
ASP	ASP	LEU	LEU	ASN	ASP
ILE	ILE	SER	SER	THR	GLN
VAL	VAL	THR	THR	ILE	GLU
ASP	ASP	LEU	LEU	THR	TYR
GLN	GLN	GLN	GLN	SER	SER
VAL	VAL	ALA	ALA	PHE	ALA
ILE	ILE	VAL	VAL	CYS	PHE
THR	THR	LEU	LEU	GLY	ARG
ILE	ILE	ASP	ASP	THR	VAL
GLY	GLY	SER	SER	LEU	GLY
LYS	LYS	ALA	ALA	HIS	MET
HIS	HIS	ALA	ALA	VAL	VAL
VAL	VAL	GLU	GLU	SER	GLN
LYS	LYS	LYS	LYS	PHE	PHE
GLY	GLY	LYS	LYS	ILE	SER
THR	THR	TRP	TRP	THR	THR
HIS	HIS	GLN	GLN	PRO	SER
TYR	TYR	VAL	VAL	SER	GLU
ILE	ILE	THR	THR	PHE	PHE
ILE	ILE	ALA	ALA	PRO	ARG
ALA	ALA	ILE	ILE	THR	LEU
ASN	ASN	ASN	ASN	ASP	THR
LEU	LEU	VAL	VAL	GLY	PRO
LEU	LEU	GLY	GLY	THR	HIS
PHE	PHE	ASN	ASN	HIS	ILE
THR	THR	ILE	ILE	PRO	ASP
ASP	ASP	ASN	ASN	PHE	ASN
GLY	GLY	ASN	ASN	VAL	LEU
ASP	ASP	ASP	ASP	ILE	GLU
LEU	LEU	LYS	LYS	GLN	VAL
LEU	LEU	LYS	LYS	MET	ALA
LYS	LYS	ASP	ASP	PRO	ASN
GLN	GLN	GLU	GLU	PRO	SER
THR	THR	TYR	TYR	ASP	PHE
GLY	GLY	ARG	ARG	LEU	ALA
ALA	ALA	SER	SER	LYS	VAL
VAL	VAL	LEU	LEU	ALA	ASN
GLU	GLU	PHE	PHE	LEU	ALA
VAL	VAL	GLN	GLN	LEU	PHE
SER	SER	ASP	ASP	SER	CYS
GLY	GLY	LEU	LEU	LEU	SER
ILE	ILE	GLU	GLU	ILE	GLN
VAL	VAL	LEU	LEU	GLU	PHE
ILE	ILE	LYS	LYS	TYR	SER
ASP	ASP	GLU	GLU	GLN	ARG



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	81723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.924	Depositor
Minimum map value	-1.802	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AJP, ZK1, SPD, CLR, PCW

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	0.52	0/4774	0.64	3/6446 (0.0%)
1	B	0.52	0/3224	0.64	1/4350 (0.0%)
1	C	0.52	0/4774	0.64	3/6446 (0.0%)
1	D	0.52	0/3224	0.64	1/4350 (0.0%)
2	E	0.38	0/1203	0.61	0/1636
2	F	0.38	0/1203	0.61	0/1636
All	All	0.51	0/18402	0.64	8/24864 (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	B	0	3
1	C	0	2
1	D	0	3
2	E	0	4
2	F	0	4
All	All	0	18

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	704	LEU	CA-CB-CG	5.93	128.94	115.30
1	D	704	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	1015	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	1015	LEU	CA-CB-CG	5.19	127.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	882	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	A	882	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	C	808	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	808	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	ARG	Peptide
1	A	922	LEU	Peptide
1	B	510	SER	Peptide
1	B	663	LYS	Peptide
1	B	772	GLU	Peptide
1	C	545	ARG	Peptide
1	C	922	LEU	Peptide
1	D	510	SER	Peptide
1	D	663	LYS	Peptide
1	D	772	GLU	Peptide
2	E	109	PRO	Peptide
2	E	115	VAL	Peptide
2	E	116	MET	Peptide
2	E	117	TYR	Peptide
2	F	109	PRO	Peptide
2	F	115	VAL	Peptide
2	F	116	MET	Peptide
2	F	117	TYR	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	4671	0	4745	43	0
1	B	3156	0	3201	28	0
1	C	4671	0	4745	43	0
1	D	3156	0	3201	32	0
2	E	1166	0	1152	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1166	0	1152	14	0
3	A	27	0	13	2	0
3	B	27	0	13	0	0
3	C	27	0	13	1	0
3	D	27	0	13	0	0
4	A	394	0	566	22	0
4	B	331	0	450	18	0
4	C	241	0	341	16	0
4	D	280	0	375	15	0
4	E	87	0	121	4	0
4	F	87	0	121	6	0
5	A	56	0	74	9	0
5	C	56	0	74	9	0
6	A	126	0	0	108	0
6	C	125	0	0	107	0
7	A	10	0	19	0	0
All	All	19887	0	20389	447	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 11.

All (447) 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)
5:A:1107:CLR:C14	5:A:1107:CLR:C15	1.75	1.63
5:A:1107:CLR:C15	5:A:1107:CLR:C16	1.77	1.61
6:C:1109:AJP:C19	6:C:1109:AJP:C24	1.78	1.61
5:C:1106:CLR:C15	5:C:1106:CLR:C16	1.77	1.61
6:C:1114:AJP:C14	6:C:1114:AJP:C15	1.79	1.61
6:A:1111:AJP:C19	6:A:1111:AJP:C24	1.79	1.61
5:A:1112:CLR:C15	5:A:1112:CLR:C16	1.78	1.61
6:A:1110:AJP:C14	6:A:1110:AJP:C15	1.79	1.60
6:C:1109:AJP:C14	6:C:1109:AJP:C15	1.79	1.60
6:C:1114:AJP:C19	6:C:1114:AJP:C24	1.77	1.59
6:A:1111:AJP:C14	6:A:1111:AJP:C15	1.78	1.58
6:A:1116:AJP:C14	6:A:1116:AJP:C15	1.79	1.58
6:C:1110:AJP:C22	6:C:1110:AJP:C21	1.82	1.58
6:A:1110:AJP:C21	6:A:1110:AJP:C22	1.81	1.57
6:A:1110:AJP:C24	6:A:1110:AJP:C19	1.78	1.56
6:C:1109:AJP:C17	6:C:1109:AJP:C18	1.82	1.56
5:C:1111:CLR:C15	5:C:1111:CLR:C16	1.78	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1110:AJP:C15	6:C:1110:AJP:C14	1.78	1.56
6:C:1110:AJP:C18	6:C:1110:AJP:C17	1.82	1.56
5:C:1106:CLR:C15	5:C:1106:CLR:C14	1.75	1.55
6:C:1114:AJP:C10	6:C:1114:AJP:C11	1.84	1.55
6:A:1110:AJP:C17	6:A:1110:AJP:C18	1.82	1.54
6:A:1111:AJP:C21	6:A:1111:AJP:C22	1.82	1.54
6:C:1109:AJP:C21	6:C:1109:AJP:C22	1.81	1.54
6:A:1111:AJP:C17	6:A:1111:AJP:C18	1.82	1.54
6:A:1116:AJP:C10	6:A:1116:AJP:C11	1.84	1.53
6:C:1110:AJP:C10	6:C:1110:AJP:C11	1.86	1.53
6:C:1114:AJP:C17	6:C:1114:AJP:C18	1.81	1.53
6:A:1116:AJP:C21	6:A:1116:AJP:C22	1.81	1.53
6:A:1116:AJP:C19	6:A:1116:AJP:C24	1.78	1.53
6:C:1110:AJP:C24	6:C:1110:AJP:C19	1.79	1.51
6:A:1116:AJP:C17	6:A:1116:AJP:C18	1.82	1.51
6:C:1109:AJP:C10	6:C:1109:AJP:C11	1.86	1.51
6:C:1114:AJP:C21	6:C:1114:AJP:C22	1.81	1.50
6:A:1111:AJP:C27	6:A:1111:AJP:C28	1.89	1.50
6:A:1110:AJP:C10	6:A:1110:AJP:C11	1.85	1.50
6:A:1111:AJP:C11	6:A:1111:AJP:C10	1.86	1.50
6:A:1110:AJP:C28	6:A:1110:AJP:C27	1.88	1.49
6:A:1116:AJP:C27	6:A:1116:AJP:C28	1.89	1.48
6:C:1110:AJP:C27	6:C:1110:AJP:C28	1.91	1.48
6:C:1114:AJP:C27	6:C:1114:AJP:C28	1.92	1.47
6:C:1109:AJP:C27	6:C:1109:AJP:C28	1.94	1.44
6:C:1114:AJP:C11	6:C:1114:AJP:C12	2.08	1.31
6:A:1110:AJP:C11	6:A:1110:AJP:C12	2.09	1.31
6:A:1116:AJP:C11	6:A:1116:AJP:C12	2.08	1.30
6:C:1109:AJP:C11	6:C:1109:AJP:C12	2.09	1.30
6:C:1110:AJP:C11	6:C:1110:AJP:C12	2.09	1.29
6:A:1111:AJP:C11	6:A:1111:AJP:C12	2.09	1.29
6:C:1109:AJP:O31	6:C:1109:AJP:C30	1.81	1.28
6:A:1111:AJP:O31	6:A:1111:AJP:C30	1.82	1.27
6:C:1114:AJP:O31	6:C:1114:AJP:C30	1.82	1.27
6:A:1110:AJP:O31	6:A:1110:AJP:C30	1.82	1.27
6:A:1116:AJP:C30	6:A:1116:AJP:O31	1.82	1.26
6:C:1110:AJP:O31	6:C:1110:AJP:C30	1.83	1.24
6:A:1116:AJP:C08	6:A:1116:AJP:C07	2.21	1.19
6:C:1110:AJP:C07	6:C:1110:AJP:C08	2.22	1.18
6:C:1114:AJP:C07	6:C:1114:AJP:C08	2.21	1.18
6:C:1109:AJP:C07	6:C:1109:AJP:C08	2.22	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1111:AJP:C07	6:A:1111:AJP:C08	2.22	1.17
6:A:1110:AJP:C07	6:A:1110:AJP:C08	2.22	1.17
6:C:1114:AJP:C05	6:C:1114:AJP:O09	2.05	1.04
6:C:1110:AJP:C05	6:C:1110:AJP:O09	2.06	1.04
6:A:1116:AJP:C05	6:A:1116:AJP:O09	2.05	1.03
6:C:1109:AJP:O09	6:C:1109:AJP:C05	2.06	1.03
6:A:1110:AJP:O09	6:A:1110:AJP:C05	2.06	1.03
6:A:1111:AJP:C05	6:A:1111:AJP:O09	2.06	1.03
6:C:1109:AJP:C26	6:C:1109:AJP:C23	2.36	1.02
6:C:1110:AJP:O25	6:C:1110:AJP:C26	2.08	1.02
6:A:1110:AJP:O25	6:A:1110:AJP:C26	2.08	1.02
6:A:1110:AJP:C26	6:A:1110:AJP:C23	2.37	1.02
6:C:1109:AJP:C26	6:C:1109:AJP:O25	2.08	1.01
6:A:1111:AJP:C26	6:A:1111:AJP:O25	2.08	1.01
6:C:1110:AJP:C26	6:C:1110:AJP:C23	2.38	1.01
6:C:1114:AJP:O25	6:C:1114:AJP:C26	2.09	1.01
6:A:1116:AJP:O25	6:A:1116:AJP:C26	2.10	0.99
6:A:1111:AJP:C26	6:A:1111:AJP:C23	2.39	0.99
6:C:1114:AJP:C26	6:C:1114:AJP:C23	2.41	0.98
6:A:1116:AJP:C26	6:A:1116:AJP:C23	2.42	0.97
6:A:1116:AJP:C11	6:A:1116:AJP:C08	2.44	0.95
6:C:1114:AJP:C11	6:C:1114:AJP:C08	2.43	0.95
6:C:1114:AJP:C08	6:C:1114:AJP:C05	2.45	0.95
6:A:1116:AJP:C08	6:A:1116:AJP:C05	2.46	0.94
6:A:1111:AJP:C08	6:A:1111:AJP:C05	2.53	0.86
6:C:1109:AJP:C18	6:C:1109:AJP:C16	2.49	0.86
5:C:1106:CLR:C15	5:C:1106:CLR:C17	2.54	0.86
6:C:1110:AJP:C08	6:C:1110:AJP:C05	2.53	0.85
6:C:1109:AJP:C30	6:C:1109:AJP:C26	2.54	0.85
5:A:1107:CLR:C15	5:A:1107:CLR:C17	2.54	0.84
6:A:1110:AJP:C24	6:A:1110:AJP:C20	2.54	0.84
5:C:1106:CLR:C15	5:C:1106:CLR:C8	2.48	0.83
6:A:1110:AJP:C30	6:A:1110:AJP:C26	2.55	0.83
6:C:1114:AJP:C12	6:C:1114:AJP:C16	2.57	0.83
5:A:1107:CLR:C15	5:A:1107:CLR:C8	2.48	0.82
6:C:1110:AJP:C24	6:C:1110:AJP:C20	2.57	0.82
6:A:1110:AJP:C18	6:A:1110:AJP:C16	2.49	0.82
6:C:1109:AJP:C24	6:C:1109:AJP:C20	2.54	0.81
6:A:1110:AJP:C28	6:A:1110:AJP:C26	2.58	0.81
6:A:1116:AJP:C24	6:A:1116:AJP:C20	2.56	0.81
6:A:1111:AJP:C24	6:A:1111:AJP:C20	2.57	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1116:AJP:C12	6:A:1116:AJP:C16	2.58	0.80
6:C:1109:AJP:C08	6:C:1109:AJP:C05	2.60	0.80
6:A:1111:AJP:C30	6:A:1111:AJP:C26	2.60	0.79
6:C:1109:AJP:C28	6:C:1109:AJP:C26	2.61	0.79
6:C:1114:AJP:C24	6:C:1114:AJP:C20	2.56	0.79
6:A:1110:AJP:C08	6:A:1110:AJP:C05	2.61	0.78
6:A:1110:AJP:C21	6:A:1110:AJP:C23	2.59	0.78
6:A:1116:AJP:C30	6:A:1116:AJP:C26	2.62	0.77
6:C:1110:AJP:C30	6:C:1110:AJP:C26	2.61	0.77
6:C:1114:AJP:C24	6:C:1114:AJP:C18	2.61	0.77
6:C:1109:AJP:C21	6:C:1109:AJP:C23	2.59	0.76
6:A:1116:AJP:C24	6:A:1116:AJP:C18	2.64	0.75
6:C:1109:AJP:C12	6:C:1109:AJP:C16	2.61	0.75
6:C:1114:AJP:C30	6:C:1114:AJP:C26	2.62	0.75
6:A:1110:AJP:C12	6:A:1110:AJP:C16	2.62	0.75
6:C:1109:AJP:C24	6:C:1109:AJP:C18	2.66	0.73
6:C:1110:AJP:C18	6:C:1110:AJP:C24	2.65	0.73
6:A:1111:AJP:C24	6:A:1111:AJP:C18	2.65	0.73
6:C:1110:AJP:C28	6:C:1110:AJP:C26	2.67	0.73
6:A:1110:AJP:C24	6:A:1110:AJP:C18	2.66	0.72
6:A:1111:AJP:C28	6:A:1111:AJP:C26	2.67	0.72
1:A:493:LYS:HG2	1:A:747:ASN:HD21	1.54	0.72
1:C:493:LYS:HG2	1:C:747:ASN:HD21	1.54	0.71
4:A:1102:PCW:H39	4:A:1102:PCW:H331	1.72	0.71
6:A:1116:AJP:C21	6:A:1116:AJP:C23	2.59	0.71
6:C:1110:AJP:C11	6:C:1110:AJP:C08	2.69	0.71
6:A:1111:AJP:C15	6:A:1111:AJP:C13	2.65	0.70
6:C:1114:AJP:C14	6:C:1114:AJP:C16	2.69	0.70
6:A:1111:AJP:C11	6:A:1111:AJP:C08	2.69	0.70
4:C:1102:PCW:H39	4:C:1102:PCW:H331	1.73	0.69
6:C:1110:AJP:C15	6:C:1110:AJP:C13	2.66	0.69
6:A:1111:AJP:C14	6:A:1111:AJP:C16	2.70	0.69
6:A:1111:AJP:C08	6:A:1111:AJP:C06	2.72	0.68
6:C:1110:AJP:C08	6:C:1110:AJP:C06	2.71	0.68
6:C:1114:AJP:C21	6:C:1114:AJP:C23	2.60	0.68
6:A:1116:AJP:C11	6:A:1116:AJP:C07	2.71	0.67
6:A:1116:AJP:C14	6:A:1116:AJP:C16	2.70	0.67
6:C:1114:AJP:C11	6:C:1114:AJP:C07	2.71	0.67
6:A:1111:AJP:C11	6:A:1111:AJP:C07	2.73	0.66
6:C:1114:AJP:C28	6:C:1114:AJP:C26	2.73	0.66
6:C:1110:AJP:C21	6:C:1110:AJP:C23	2.65	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1110:AJP:C19	6:A:1110:AJP:C23	2.73	0.65
6:A:1110:AJP:C27	6:A:1110:AJP:C29	2.63	0.65
1:A:705:GLU:OE2	1:A:732:TYR:OH	2.12	0.65
6:C:1109:AJP:C19	6:C:1109:AJP:C23	2.73	0.65
2:E:28:ILE:HG22	2:E:135:SER:HB2	1.79	0.65
1:C:705:GLU:OE2	1:C:732:TYR:OH	2.12	0.65
6:A:1111:AJP:C21	6:A:1111:AJP:C23	2.64	0.65
6:C:1110:AJP:C27	6:C:1110:AJP:C29	2.63	0.65
1:D:542:LEU:HD11	2:F:74:ILE:HD11	1.78	0.65
6:A:1111:AJP:C12	6:A:1111:AJP:C16	2.69	0.64
6:A:1116:AJP:C18	6:A:1116:AJP:C16	2.53	0.64
2:F:28:ILE:HG22	2:F:135:SER:HB2	1.79	0.64
5:C:1106:CLR:C15	5:C:1106:CLR:C13	2.76	0.64
1:C:548:PRO:HB2	4:D:1107:PCW:H61	1.79	0.64
6:A:1116:AJP:C28	6:A:1116:AJP:C26	2.73	0.63
6:C:1110:AJP:C11	6:C:1110:AJP:C07	2.73	0.63
1:A:737:PRO:HD2	1:A:740:SER:HB2	1.80	0.63
6:A:1111:AJP:C27	6:A:1111:AJP:C29	2.62	0.63
6:C:1109:AJP:C11	6:C:1109:AJP:C08	2.74	0.63
1:D:545:ARG:HH22	2:F:67:LEU:HD23	1.64	0.63
6:C:1110:AJP:C14	6:C:1110:AJP:C16	2.70	0.63
6:C:1109:AJP:C15	6:C:1109:AJP:C13	2.72	0.63
1:C:737:PRO:HD2	1:C:740:SER:HB2	1.80	0.62
5:A:1107:CLR:C15	5:A:1107:CLR:C13	2.75	0.62
6:C:1114:AJP:C15	6:C:1114:AJP:C13	2.72	0.62
6:A:1110:AJP:C11	6:A:1110:AJP:C08	2.74	0.62
6:A:1116:AJP:C27	6:A:1116:AJP:C29	2.63	0.61
6:A:1116:AJP:C19	6:A:1116:AJP:C17	2.68	0.61
2:E:122:ILE:HD12	2:E:123:MET:H	1.65	0.61
6:A:1110:AJP:C15	6:A:1110:AJP:C13	2.72	0.61
6:C:1114:AJP:C18	6:C:1114:AJP:C16	2.52	0.60
2:F:122:ILE:HD12	2:F:123:MET:H	1.65	0.60
5:C:1106:CLR:C15	5:C:1106:CLR:C7	2.80	0.60
1:A:583:ALA:O	1:B:587:GLN:NE2	2.31	0.60
5:A:1107:CLR:C15	5:A:1107:CLR:C7	2.80	0.59
6:C:1109:AJP:C11	6:C:1109:AJP:C07	2.78	0.59
6:C:1114:AJP:C11	6:C:1114:AJP:C13	2.74	0.59
1:C:533:TYR:OH	1:C:577:LEU:O	2.21	0.58
1:C:583:ALA:O	1:D:587:GLN:NE2	2.36	0.58
6:C:1114:AJP:C27	6:C:1114:AJP:C29	2.65	0.58
1:B:492:SER:O	1:C:493:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ASP:HA	1:A:656:LYS:HD2	1.86	0.58
1:A:533:TYR:OH	1:A:577:LEU:O	2.21	0.57
6:C:1110:AJP:C17	6:C:1110:AJP:C19	2.66	0.57
6:C:1110:AJP:C12	6:C:1110:AJP:C16	2.69	0.57
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.84	0.57
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.84	0.57
1:C:862:LEU:HD11	1:C:1001:TYR:HB2	1.86	0.57
1:A:989:LEU:O	1:B:508:GLN:NE2	2.37	0.57
6:A:1110:AJP:C14	6:A:1110:AJP:C16	2.77	0.57
6:A:1110:AJP:C11	6:A:1110:AJP:C07	2.79	0.57
1:C:651:ASP:HA	1:C:656:LYS:HD2	1.86	0.56
6:A:1116:AJP:C15	6:A:1116:AJP:C13	2.71	0.56
6:C:1114:AJP:C24	6:C:1114:AJP:C26	2.84	0.56
6:A:1116:AJP:C10	6:A:1116:AJP:C17	2.83	0.56
1:B:500:ILE:HB	1:B:727:LEU:HB2	1.88	0.56
1:A:545:ARG:NH1	1:A:569:ASN:O	2.39	0.56
1:A:690:VAL:HG21	1:A:712:ILE:HD13	1.87	0.56
1:C:545:ARG:NH1	1:C:569:ASN:O	2.39	0.56
1:A:862:LEU:HD11	1:A:1001:TYR:HB2	1.86	0.56
1:A:940:PHE:HZ	4:A:1108:PCW:H20	1.71	0.56
6:A:1110:AJP:C14	6:A:1110:AJP:C11	2.83	0.56
6:C:1114:AJP:C10	6:C:1114:AJP:C17	2.84	0.56
1:D:500:ILE:HB	1:D:727:LEU:HB2	1.88	0.56
1:C:690:VAL:HG21	1:C:712:ILE:HD13	1.87	0.56
1:C:415:LEU:HD23	1:C:419:GLU:HG3	1.87	0.55
6:C:1109:AJP:C17	6:C:1109:AJP:C10	2.85	0.55
1:D:650:LEU:HD23	1:D:652:SER:H	1.71	0.55
2:F:100:TYR:OH	2:F:134:GLU:OE2	2.21	0.55
6:A:1116:AJP:C11	6:A:1116:AJP:C13	2.74	0.55
1:A:415:LEU:HD23	1:A:419:GLU:HG3	1.87	0.55
1:A:514:VAL:H	4:A:1102:PCW:H63	1.72	0.55
6:C:1109:AJP:C27	6:C:1109:AJP:C29	2.67	0.55
2:F:124:ASN:H	2:F:128:LEU:HD23	1.72	0.55
1:B:650:LEU:HD23	1:B:652:SER:H	1.71	0.55
6:C:1110:AJP:C11	6:C:1110:AJP:C13	2.75	0.55
6:C:1109:AJP:C19	6:C:1109:AJP:C17	2.65	0.54
6:A:1110:AJP:C17	6:A:1110:AJP:C10	2.85	0.54
6:A:1110:AJP:C08	6:A:1110:AJP:C06	2.80	0.54
6:A:1116:AJP:C24	6:A:1116:AJP:C26	2.85	0.54
6:C:1109:AJP:C14	6:C:1109:AJP:C11	2.84	0.54
2:E:124:ASN:H	2:E:128:LEU:HD23	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:990:ASN:HA	1:D:508:GLN:HE22	1.73	0.54
6:C:1114:AJP:C22	6:C:1114:AJP:C20	2.80	0.54
2:E:100:TYR:OH	2:E:134:GLU:OE2	2.21	0.54
1:A:728:ASP:OD2	1:A:730:LYS:NZ	2.38	0.53
1:C:543:VAL:HG22	1:C:597:SER:HB3	1.90	0.53
6:C:1114:AJP:C10	6:C:1114:AJP:C07	2.85	0.53
2:F:22:PHE:HD1	4:F:204:PCW:H19	1.72	0.53
1:A:990:ASN:HA	1:B:508:GLN:HE22	1.74	0.53
1:B:447:ASP:OD2	1:B:461:ASN:ND2	2.42	0.53
6:C:1109:AJP:C08	6:C:1109:AJP:C06	2.81	0.53
1:C:514:VAL:H	4:C:1102:PCW:H63	1.73	0.53
6:A:1111:AJP:C11	6:A:1111:AJP:C13	2.75	0.53
1:A:514:VAL:HB	4:A:1102:PCW:H52	1.91	0.53
6:A:1116:AJP:C10	6:A:1116:AJP:C07	2.86	0.53
6:C:1110:AJP:C12	6:C:1110:AJP:C08	2.83	0.53
1:D:404:PRO:HG2	1:D:767:TRP:CE2	2.44	0.53
1:B:404:PRO:HG2	1:B:767:TRP:CE2	2.44	0.52
1:C:514:VAL:HB	4:C:1102:PCW:H52	1.92	0.52
2:F:71:GLU:OE2	2:F:142:TYR:OH	2.23	0.52
6:C:1114:AJP:C12	6:C:1114:AJP:C08	2.85	0.52
1:D:447:ASP:OD2	1:D:461:ASN:ND2	2.42	0.52
1:A:989:LEU:HD21	1:B:509:LYS:HD3	1.92	0.52
2:E:71:GLU:OE2	2:E:142:TYR:OH	2.23	0.52
4:D:1106:PCW:H381	4:D:1106:PCW:H152	1.92	0.52
1:C:728:ASP:OD2	1:C:730:LYS:NZ	2.38	0.51
1:A:543:VAL:HG22	1:A:597:SER:HB3	1.90	0.51
6:A:1116:AJP:C14	6:A:1116:AJP:C21	2.89	0.51
1:B:574:PHE:HB2	4:B:1107:PCW:H332	1.91	0.51
6:A:1111:AJP:C12	6:A:1111:AJP:C08	2.83	0.51
1:D:690:VAL:HG21	1:D:712:ILE:HD13	1.92	0.51
6:C:1114:AJP:C08	6:C:1114:AJP:C06	2.85	0.51
1:D:404:PRO:HG3	1:D:711:TYR:CD1	2.46	0.51
1:B:690:VAL:HG21	1:B:712:ILE:HD13	1.92	0.50
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.92	0.50
6:A:1116:AJP:C19	6:A:1116:AJP:C23	2.82	0.50
1:A:895:GLU:O	1:A:897:ARG:N	2.44	0.50
4:A:1105:PCW:H19	5:A:1112:CLR:H232	1.92	0.50
4:C:1104:PCW:H351	4:C:1104:PCW:H141	1.92	0.50
1:D:586:GLN:HE21	1:D:613:ILE:HD12	1.76	0.50
1:D:466:GLU:HG2	1:D:471:LYS:HE2	1.94	0.50
1:C:789:LEU:HD22	2:E:3:PHE:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:SER:OG	1:C:885:GLY:N	2.45	0.50
6:C:1114:AJP:C14	6:C:1114:AJP:C21	2.89	0.50
2:E:13:THR:HG21	2:E:82:PHE:HZ	1.77	0.50
2:F:13:THR:HG21	2:F:82:PHE:HZ	1.77	0.50
1:A:884:SER:OG	1:A:885:GLY:N	2.45	0.50
4:B:1106:PCW:H381	4:B:1106:PCW:H152	1.93	0.50
1:C:466:GLU:HG2	1:C:471:LYS:HD2	1.94	0.50
1:C:895:GLU:O	1:C:897:ARG:N	2.44	0.50
1:D:533:TYR:OH	1:D:577:LEU:O	2.26	0.50
1:A:548:PRO:HB2	4:B:1107:PCW:H61	1.94	0.50
6:A:1111:AJP:C24	6:A:1111:AJP:C21	2.85	0.50
6:C:1114:AJP:C07	6:C:1114:AJP:O09	2.55	0.50
1:D:574:PHE:HB2	4:D:1107:PCW:H332	1.94	0.49
1:A:952:ARG:HH21	1:A:954:HIS:HE1	1.59	0.49
6:A:1116:AJP:C12	6:A:1116:AJP:C08	2.85	0.49
1:B:404:PRO:HG3	1:B:711:TYR:CD1	2.46	0.49
1:D:642:GLN:OE1	1:D:645:ILE:N	2.41	0.49
1:C:965:PHE:HZ	5:C:1106:CLR:H152	1.77	0.49
1:C:989:LEU:O	1:D:508:GLN:NE2	2.46	0.49
6:C:1109:AJP:C22	6:C:1109:AJP:C26	2.89	0.49
2:E:22:PHE:HD1	4:E:205:PCW:H19	1.77	0.49
1:B:642:GLN:OE1	1:B:645:ILE:N	2.41	0.49
1:A:466:GLU:HG2	1:A:471:LYS:HD2	1.94	0.49
6:A:1110:AJP:C22	6:A:1110:AJP:C20	2.80	0.49
4:A:1118:PCW:H221	4:B:1101:PCW:H221	1.94	0.49
1:A:489:ILE:HD12	1:A:735:ALA:HB1	1.94	0.49
1:B:466:GLU:HG2	1:B:471:LYS:HE2	1.94	0.49
1:C:952:ARG:HH21	1:C:954:HIS:HE1	1.59	0.49
4:D:1103:PCW:H171	4:D:1104:PCW:H19	1.95	0.49
1:A:493:LYS:NZ	1:D:492:SER:O	2.46	0.48
1:A:708:MET:HG3	3:A:1101:ZK1:HAMA	1.95	0.48
4:E:203:PCW:H132	4:E:203:PCW:H162	1.60	0.48
1:B:586:GLN:HE21	1:B:613:ILE:HD12	1.77	0.48
1:C:956:THR:HG22	1:C:1031:ARG:HG2	1.95	0.48
6:C:1109:AJP:C22	6:C:1109:AJP:C20	2.79	0.48
1:C:864:LEU:HB2	1:C:882:LEU:HB2	1.95	0.48
1:A:864:LEU:HB2	1:A:882:LEU:HB2	1.95	0.48
1:A:956:THR:HG22	1:A:1031:ARG:HG2	1.95	0.48
1:C:489:ILE:HD12	1:C:735:ALA:HB1	1.94	0.48
1:C:989:LEU:HD21	1:D:509:LYS:HD3	1.95	0.48
6:A:1111:AJP:C07	6:A:1111:AJP:O09	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1111:AJP:C22	6:A:1111:AJP:C20	2.82	0.48
6:C:1114:AJP:C14	6:C:1114:AJP:C20	2.87	0.48
6:C:1114:AJP:C19	6:C:1114:AJP:C23	2.82	0.48
4:F:202:PCW:H132	4:F:202:PCW:H162	1.60	0.47
6:C:1114:AJP:C14	6:C:1114:AJP:C11	2.86	0.47
6:A:1111:AJP:C11	6:A:1111:AJP:C81	2.92	0.47
1:C:920:ASN:HA	1:C:991:ARG:HH12	1.80	0.47
2:E:68:VAL:HG21	2:E:117:TYR:HB3	1.95	0.47
1:A:920:ASN:HA	1:A:991:ARG:HH12	1.80	0.47
6:C:1110:AJP:C21	6:C:1110:AJP:C24	2.87	0.47
6:C:1110:AJP:C17	6:C:1110:AJP:C10	2.92	0.47
6:A:1116:AJP:C14	6:A:1116:AJP:C20	2.87	0.47
6:A:1116:AJP:C22	6:A:1116:AJP:C20	2.79	0.47
1:B:533:TYR:OH	1:B:577:LEU:O	2.26	0.47
4:B:1103:PCW:H181	4:B:1103:PCW:H151	1.58	0.47
1:C:708:MET:HG3	3:C:1101:ZK1:HAMA	1.95	0.47
4:B:1110:PCW:C40	4:B:1110:PCW:H20	2.45	0.46
6:C:1110:AJP:C28	6:C:1110:AJP:O31	2.61	0.46
4:A:1103:PCW:H442	4:A:1103:PCW:H412	1.66	0.46
4:A:1114:PCW:H432	4:A:1114:PCW:H40	1.64	0.46
2:F:68:VAL:HG21	2:F:117:TYR:HB3	1.95	0.46
4:A:1104:PCW:H141	4:A:1104:PCW:H172	1.65	0.46
1:C:585:MET:O	1:C:587:GLN:N	2.49	0.46
1:A:988:MET:SD	1:A:988:MET:N	2.88	0.46
1:B:606:TRP:HB3	1:C:585:MET:HB3	1.98	0.46
4:B:1101:PCW:H172	4:B:1101:PCW:H142	1.66	0.46
1:C:988:MET:SD	1:C:988:MET:N	2.88	0.46
6:A:1110:AJP:C26	6:A:1110:AJP:C29	2.93	0.46
1:C:476:ILE:HG13	1:C:734:ILE:HG23	1.98	0.46
4:D:1101:PCW:H221	4:D:1109:PCW:H221	1.97	0.45
1:A:476:ILE:HG13	1:A:734:ILE:HG23	1.98	0.45
5:A:1112:CLR:H211	5:A:1112:CLR:H231	1.71	0.45
6:C:1114:AJP:C11	6:C:1114:AJP:O82	2.44	0.45
4:D:1101:PCW:H212	4:D:1109:PCW:H172	1.98	0.45
4:F:202:PCW:H412	4:F:202:PCW:H381	1.82	0.45
1:A:585:MET:O	1:A:587:GLN:N	2.49	0.45
4:C:1102:PCW:H162	2:E:14:LEU:HD22	1.97	0.45
4:B:1111:PCW:H20	4:B:1111:PCW:H172	1.76	0.45
6:A:1111:AJP:C17	6:A:1111:AJP:C10	2.92	0.45
1:C:940:PHE:HZ	4:C:1107:PCW:H20	1.82	0.45
5:C:1111:CLR:H211	5:C:1111:CLR:H231	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1113:PCW:H181	4:A:1113:PCW:H211	1.74	0.45
6:C:1109:AJP:C12	6:C:1109:AJP:C08	2.89	0.45
1:A:960:PHE:HB2	1:A:1028:PHE:CG	2.53	0.44
6:A:1110:AJP:C19	6:A:1110:AJP:C17	2.66	0.44
4:C:1112:PCW:H342	4:C:1112:PCW:H371	1.78	0.44
6:C:1114:AJP:C08	6:C:1114:AJP:C04	2.95	0.44
1:D:526:TRP:HE3	4:D:1104:PCW:H141	1.82	0.44
4:E:201:PCW:H152	4:E:201:PCW:H181	1.72	0.44
6:A:1116:AJP:C14	6:A:1116:AJP:C11	2.86	0.44
1:C:474:ILE:HD11	1:C:734:ILE:HG22	1.99	0.44
4:D:1103:PCW:H122	4:D:1103:PCW:H152	1.73	0.44
1:B:520:PRO:HG2	1:B:620:LEU:HD12	1.99	0.44
1:B:584:PHE:HA	1:B:609:THR:HG21	2.00	0.44
1:B:685:THR:HG22	1:B:687:ALA:H	1.83	0.44
4:B:1110:PCW:H272	4:B:1111:PCW:H421	2.00	0.44
6:C:1110:AJP:C11	6:C:1110:AJP:C81	2.93	0.44
4:A:1104:PCW:H152	4:A:1104:PCW:H121	1.73	0.44
4:A:1102:PCW:H431	4:A:1114:PCW:H241	2.00	0.44
6:A:1116:AJP:C07	6:A:1116:AJP:O09	2.55	0.44
1:C:960:PHE:HB2	1:C:1028:PHE:CG	2.53	0.44
4:C:1102:PCW:H39	4:C:1102:PCW:H361	1.66	0.44
1:D:685:THR:HG22	1:D:687:ALA:H	1.83	0.44
1:A:951:ILE:HD11	4:A:1108:PCW:H141	1.99	0.43
6:A:1110:AJP:C22	6:A:1110:AJP:C26	2.91	0.43
1:C:864:LEU:HB2	1:C:882:LEU:HD12	2.00	0.43
1:D:584:PHE:HA	1:D:609:THR:HG21	2.00	0.43
1:A:785:SER:OG	1:D:628:ARG:NH1	2.48	0.43
1:C:742:LEU:HA	1:C:745:PRO:HD2	2.00	0.43
6:C:1109:AJP:C14	6:C:1109:AJP:C20	2.89	0.43
6:C:1114:AJP:C19	6:C:1114:AJP:C17	2.68	0.43
4:D:1110:PCW:H181	4:D:1110:PCW:H212	1.86	0.43
4:A:1114:PCW:H172	4:A:1114:PCW:H20	1.74	0.43
4:B:1109:PCW:H181	4:B:1109:PCW:H212	1.84	0.43
4:B:1110:PCW:H441	4:C:1104:PCW:H432	2.01	0.43
4:B:1111:PCW:H241	4:C:1102:PCW:H431	2.00	0.43
1:A:864:LEU:HB2	1:A:882:LEU:HD12	2.00	0.43
4:D:1109:PCW:H382	4:D:1109:PCW:H352	1.81	0.43
4:F:201:PCW:H212	4:F:201:PCW:H181	1.85	0.43
1:D:520:PRO:HG2	1:D:620:LEU:HD12	2.00	0.43
4:A:1105:PCW:C40	4:A:1105:PCW:H20	2.49	0.43
6:A:1111:AJP:C15	6:A:1111:AJP:C12	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:LEU:HA	1:A:745:PRO:HD2	2.00	0.42
4:B:1103:PCW:H122	4:B:1103:PCW:H152	1.75	0.42
1:A:646:ALA:N	1:A:699:LYS:O	2.48	0.42
6:A:1111:AJP:C19	6:A:1111:AJP:C17	2.67	0.42
6:A:1116:AJP:C08	6:A:1116:AJP:C04	2.97	0.42
1:B:401:LEU:HD23	1:B:406:VAL:HG13	2.00	0.42
1:D:405:TYR:OH	1:D:496:MET:SD	2.77	0.42
4:F:202:PCW:H82	4:F:202:PCW:H41	1.85	0.42
1:C:536:VAL:HG22	1:D:803:LEU:HD21	2.01	0.42
4:C:1104:PCW:H141	4:C:1104:PCW:H172	1.65	0.42
1:A:474:ILE:HD11	1:A:734:ILE:HG22	1.99	0.42
4:C:1115:PCW:H182	4:C:1115:PCW:H211	1.82	0.42
4:E:202:PCW:H181	4:E:202:PCW:H212	1.84	0.42
4:A:1104:PCW:H39	4:A:1105:PCW:H40	2.02	0.42
4:D:1103:PCW:H181	4:D:1103:PCW:H151	1.59	0.42
2:F:122:ILE:H	2:F:122:ILE:HG13	1.60	0.42
1:B:664:ILE:HG23	1:B:665:ALA:H	1.85	0.42
4:A:1103:PCW:H332	4:A:1103:PCW:H362	1.75	0.42
1:B:405:TYR:OH	1:B:496:MET:SD	2.77	0.42
1:D:401:LEU:HD23	1:D:406:VAL:HG13	2.00	0.42
1:A:789:LEU:HD22	2:F:3:PHE:HE2	1.85	0.42
6:C:1110:AJP:C14	6:C:1110:AJP:C11	2.92	0.42
4:C:1104:PCW:H121	4:C:1104:PCW:H152	1.75	0.41
1:D:425:CYS:HA	1:D:428:LEU:HB3	2.02	0.41
1:D:508:GLN:HG2	1:D:509:LYS:H	1.85	0.41
4:D:1107:PCW:H83	4:D:1107:PCW:H42	1.90	0.41
2:E:122:ILE:H	2:E:122:ILE:HG13	1.59	0.41
4:A:1102:PCW:H331	4:A:1102:PCW:H361	1.97	0.41
6:A:1111:AJP:C26	6:A:1111:AJP:C29	2.97	0.41
1:B:425:CYS:HA	1:B:428:LEU:HB3	2.02	0.41
2:E:92:GLY:HA2	2:E:95:ILE:HD12	2.02	0.41
2:E:129:ASN:O	2:E:133:LYS:N	2.53	0.41
4:B:1110:PCW:H261	4:B:1111:PCW:H271	2.02	0.41
1:C:426:VAL:HG22	1:C:442:LEU:HD21	2.01	0.41
4:C:1103:PCW:H382	4:C:1103:PCW:H411	1.72	0.41
6:A:1111:AJP:C14	6:A:1111:AJP:C20	2.91	0.41
4:A:1118:PCW:H211	4:A:1118:PCW:H181	1.90	0.41
1:C:921:VAL:HB	1:C:924:MET:HE2	2.03	0.41
4:D:1101:PCW:H172	4:D:1101:PCW:H142	1.69	0.41
1:A:426:VAL:HG22	1:A:442:LEU:HD21	2.01	0.41
6:A:1110:AJP:C12	6:A:1110:AJP:C08	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1113:PCW:H342	4:A:1113:PCW:H371	1.78	0.41
4:B:1110:PCW:H412	4:C:1104:PCW:H181	2.03	0.41
4:B:1111:PCW:H342	4:B:1111:PCW:H371	1.83	0.41
4:C:1103:PCW:H442	4:C:1103:PCW:H412	1.64	0.41
6:C:1110:AJP:C21	6:C:1110:AJP:C14	2.99	0.41
1:D:664:ILE:HG23	1:D:665:ALA:H	1.85	0.41
4:B:1104:PCW:H83	4:B:1104:PCW:H42	1.85	0.41
1:D:577:LEU:HD11	4:D:1103:PCW:H262	2.03	0.41
4:B:1111:PCW:H40	4:B:1111:PCW:H432	1.72	0.40
1:B:409:LYS:HG2	1:B:410:LYS:HD2	2.03	0.40
4:D:1106:PCW:H322	4:D:1106:PCW:H2	1.76	0.40
4:F:204:PCW:H19	4:F:204:PCW:H161	1.78	0.40
3:A:1101:ZK1:HAOA	3:A:1101:ZK1:HAI	1.80	0.40
1:A:800:VAL:HG13	2:F:15:VAL:HG21	2.03	0.40
4:A:1103:PCW:H411	4:A:1103:PCW:H382	1.71	0.40
1:C:646:ALA:N	1:C:699:LYS:O	2.48	0.40
1:D:765:LYS:HA	1:D:769:ASP:HB2	2.03	0.40
2:F:92:GLY:HA2	2:F:95:ILE:HD12	2.02	0.40
4:A:1118:PCW:H382	4:A:1118:PCW:H352	1.89	0.40
1:B:508:GLN:HG2	1:B:509:LYS:H	1.85	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	586/1026 (57%)	538 (92%)	46 (8%)	2 (0%)	37 68
1	B	398/1026 (39%)	369 (93%)	27 (7%)	2 (0%)	25 59
1	C	586/1026 (57%)	538 (92%)	46 (8%)	2 (0%)	37 68
1	D	398/1026 (39%)	369 (93%)	27 (7%)	2 (0%)	25 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	136/160 (85%)	120 (88%)	12 (9%)	4 (3%)	3	23
2	F	136/160 (85%)	120 (88%)	12 (9%)	4 (3%)	3	23
All	All	2240/4424 (51%)	2054 (92%)	170 (8%)	16 (1%)	21	53

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	773	CYS
1	D	773	CYS
2	E	116	MET
2	E	117	TYR
2	F	116	MET
2	F	117	TYR
1	A	737	PRO
1	C	737	PRO
1	A	896	GLU
1	C	896	GLU
2	E	115	VAL
2	E	122	ILE
2	F	115	VAL
2	F	122	ILE
1	B	470	GLY
1	D	470	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	504/877 (58%)	498 (99%)	6 (1%)	67	83
1	B	340/877 (39%)	338 (99%)	2 (1%)	84	91
1	C	504/877 (58%)	498 (99%)	6 (1%)	67	83
1	D	340/877 (39%)	338 (99%)	2 (1%)	84	91
2	E	126/143 (88%)	124 (98%)	2 (2%)	58	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	126/143 (88%)	124 (98%)	2 (2%)	58 78
All	All	1940/3794 (51%)	1920 (99%)	20 (1%)	71 86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	LEU
1	A	508	GLN
1	A	747	ASN
1	A	783	LYS
1	A	922	LEU
1	A	947	ASN
1	B	410	LYS
1	B	461	ASN
1	C	498	LEU
1	C	508	GLN
1	C	747	ASN
1	C	783	LYS
1	C	922	LEU
1	C	947	ASN
1	D	410	LYS
1	D	461	ASN
2	E	122	ILE
2	E	124	ASN
2	F	122	ILE
2	F	124	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	747	ASN
1	A	950	HIS
1	A	954	HIS
1	A	990	ASN
1	B	461	ASN
1	B	508	GLN
1	B	586	GLN
1	C	575	ASN
1	C	747	ASN
1	C	950	HIS
1	C	954	HIS

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Mol	Chain	Res	Type
1	C	990	ASN
1	D	461	ASN
1	D	508	GLN
1	D	586	GLN
2	E	75	HIS
2	E	94	ASN
2	E	124	ASN
2	F	75	HIS
2	F	94	ASN
2	F	124	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

65 ligands are modelled in this entry.

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	$\# Z  > 2$
4	PCW	A	1109	-	10,10,53	0.83	0	9,9,61	0.30	0
4	PCW	B	1104	-	42,42,53	1.20	3 (7%)	48,50,61	1.16	3 (6%)
3	ZK1	A	1101	-	29,29,29	3.40	9 (31%)	45,45,45	1.87	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PCW	A	1117	-	10,10,53	0.84	0	9,9,61	0.29	0
6	AJP	C	1109	-	47,47,95	17.27	38 (80%)	71,76,149	3.32	35 (49%)
4	PCW	F	201	-	10,10,53	0.81	0	9,9,61	0.32	0
6	AJP	C	1110	-	48,48,95	18.95	41 (85%)	72,78,149	3.36	37 (51%)
4	PCW	A	1114	-	50,50,53	1.14	4 (8%)	56,58,61	1.09	4 (7%)
6	AJP	C	1114	-	48,48,95	18.87	40 (83%)	72,78,149	3.47	40 (55%)
4	PCW	A	1104	-	40,40,53	1.25	4 (10%)	46,48,61	1.10	3 (6%)
4	PCW	C	1102	-	50,50,53	1.17	4 (8%)	56,58,61	0.98	3 (5%)
4	PCW	F	204	-	10,10,53	0.84	0	9,9,61	0.30	0
4	PCW	C	1103	-	42,42,53	1.24	4 (9%)	48,50,61	0.98	3 (6%)
4	PCW	A	1105	-	50,50,53	1.17	4 (8%)	56,58,61	1.07	3 (5%)
4	PCW	A	1118	-	50,50,53	1.20	4 (8%)	56,58,61	0.93	3 (5%)
4	PCW	C	1112	-	50,50,53	1.20	5 (10%)	56,58,61	0.99	3 (5%)
4	PCW	D	1101	-	10,10,53	0.76	0	9,9,61	0.44	0
4	PCW	D	1110	-	10,10,53	0.82	0	9,9,61	0.31	0
4	PCW	E	202	-	10,10,53	0.82	0	9,9,61	0.31	0
4	PCW	E	205	-	10,10,53	0.84	0	9,9,61	0.30	0
4	PCW	F	202	-	42,42,53	1.27	5 (11%)	48,50,61	1.06	3 (6%)
7	SPD	A	1119	-	9,9,9	0.31	0	8,8,8	0.50	0
4	PCW	C	1105	-	10,10,53	0.82	0	9,9,61	0.35	0
4	PCW	D	1103	-	40,40,53	1.24	3 (7%)	46,48,61	1.06	3 (6%)
4	PCW	B	1105	-	31,31,53	1.25	2 (6%)	37,39,61	1.35	3 (8%)
4	PCW	C	1108	-	10,10,53	0.83	0	9,9,61	0.29	0
4	PCW	D	1104	-	42,42,53	1.19	3 (7%)	48,50,61	1.19	3 (6%)
4	PCW	A	1113	-	50,50,53	1.20	5 (10%)	56,58,61	1.00	3 (5%)
4	PCW	A	1106	-	10,10,53	0.82	0	9,9,61	0.35	0
4	PCW	B	1110	-	50,50,53	1.16	4 (8%)	56,58,61	1.06	3 (5%)
4	PCW	B	1111	-	50,50,53	1.14	3 (6%)	56,58,61	1.01	4 (7%)
5	CLR	C	1106	-	31,31,31	9.34	22 (70%)	48,48,48	4.38	24 (50%)
3	ZK1	D	1102	-	29,29,29	3.47	9 (31%)	45,45,45	1.77	10 (22%)
5	CLR	A	1107	-	31,31,31	9.34	22 (70%)	48,48,48	4.35	24 (50%)
4	PCW	B	1106	-	40,40,53	1.29	5 (12%)	46,48,61	1.17	3 (6%)
4	PCW	A	1108	-	10,10,53	0.79	0	9,9,61	0.37	0
4	PCW	F	205	-	10,10,53	0.81	0	9,9,61	0.37	0
4	PCW	C	1115	-	10,10,53	0.84	0	9,9,61	0.29	0
4	PCW	B	1107	-	38,38,53	1.29	5 (13%)	44,46,61	1.19	4 (9%)
3	ZK1	C	1101	-	29,29,29	3.39	9 (31%)	45,45,45	1.84	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	AJP	A	1110	-	48,48,95	18.78	39 (81%)	72,78,149	3.67	39 (54%)
4	PCW	A	1115	-	10,10,53	0.81	0	9,9,61	0.35	0
4	PCW	E	203	-	42,42,53	1.27	5 (11%)	48,50,61	1.06	3 (6%)
4	PCW	B	1101	-	10,10,53	0.75	0	9,9,61	0.44	0
4	PCW	D	1109	-	50,50,53	1.21	4 (8%)	56,58,61	0.94	3 (5%)
4	PCW	A	1102	-	50,50,53	1.17	4 (8%)	56,58,61	0.98	3 (5%)
5	CLR	C	1111	-	31,31,31	9.36	22 (70%)	48,48,48	4.12	26 (54%)
4	PCW	C	1107	-	10,10,53	0.80	0	9,9,61	0.37	0
4	PCW	D	1106	-	40,40,53	1.28	5 (12%)	46,48,61	1.18	3 (6%)
4	PCW	B	1108	-	10,10,53	0.82	0	9,9,61	0.31	0
4	PCW	D	1107	-	38,38,53	1.29	5 (13%)	44,46,61	1.23	4 (9%)
4	PCW	C	1104	-	40,40,53	1.25	4 (10%)	46,48,61	1.11	3 (6%)
4	PCW	B	1109	-	10,10,53	0.82	0	9,9,61	0.32	0
4	PCW	C	1113	-	10,10,53	0.81	0	9,9,61	0.35	0
4	PCW	D	1105	-	31,31,53	1.25	2 (6%)	37,39,61	1.40	4 (10%)
4	PCW	E	201	-	10,10,53	0.81	0	9,9,61	0.37	0
4	PCW	D	1108	-	10,10,53	0.80	0	9,9,61	0.37	0
4	PCW	E	204	-	10,10,53	0.81	0	9,9,61	0.39	0
6	AJP	A	1111	-	48,48,95	18.76	41 (85%)	72,78,149	3.37	37 (51%)
4	PCW	F	203	-	10,10,53	0.82	0	9,9,61	0.40	0
3	ZK1	B	1102	-	29,29,29	3.47	9 (31%)	45,45,45	1.77	9 (20%)
4	PCW	A	1103	-	42,42,53	1.24	4 (9%)	48,50,61	0.99	3 (6%)
5	CLR	A	1112	-	31,31,31	9.36	22 (70%)	48,48,48	4.12	25 (52%)
6	AJP	A	1116	-	48,48,95	18.74	40 (83%)	72,78,149	3.44	37 (51%)
4	PCW	B	1103	-	40,40,53	1.24	3 (7%)	46,48,61	1.05	3 (6%)

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
4	PCW	A	1109	-	-	6/8/8/57	-
4	PCW	B	1104	-	-	32/46/46/57	-
3	ZK1	A	1101	-	-	7/13/23/23	0/3/3/3
4	PCW	A	1117	-	-	4/8/8/57	-
6	AJP	C	1109	-	12/12/17/38	2/6/113/220	0/7/7/11
4	PCW	F	201	-	-	4/8/8/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AJP	C	1110	-	9/9/18/38	4/6/117/220	1/7/7/11
4	PCW	A	1114	-	-	22/54/54/57	-
6	AJP	C	1114	-	9/9/18/38	2/6/117/220	0/7/7/11
4	PCW	A	1104	-	-	24/44/44/57	-
4	PCW	C	1102	-	-	25/54/54/57	-
4	PCW	F	204	-	-	4/8/8/57	-
4	PCW	C	1103	-	-	23/46/46/57	-
4	PCW	A	1105	-	-	23/54/54/57	-
4	PCW	A	1118	-	-	21/54/54/57	-
4	PCW	C	1112	-	-	25/54/54/57	-
4	PCW	D	1101	-	-	6/8/8/57	-
4	PCW	D	1110	-	-	5/8/8/57	-
4	PCW	E	202	-	-	4/8/8/57	-
4	PCW	E	205	-	-	4/8/8/57	-
4	PCW	F	202	-	-	22/46/46/57	-
7	SPD	A	1119	-	-	0/7/7/7	-
4	PCW	C	1105	-	-	4/8/8/57	-
4	PCW	D	1103	-	-	24/44/44/57	-
4	PCW	B	1105	-	-	12/34/34/57	-
4	PCW	C	1108	-	-	6/8/8/57	-
4	PCW	D	1104	-	-	31/46/46/57	-
4	PCW	A	1113	-	-	23/54/54/57	-
4	PCW	A	1106	-	-	4/8/8/57	-
4	PCW	B	1110	-	-	29/54/54/57	-
4	PCW	B	1111	-	-	22/54/54/57	-
5	CLR	C	1106	-	2/2/10/11	7/10/68/68	0/4/4/4
3	ZK1	D	1102	-	-	5/13/23/23	0/3/3/3
5	CLR	A	1107	-	2/2/10/11	7/10/68/68	0/4/4/4
4	PCW	B	1106	-	-	23/44/44/57	-
4	PCW	A	1108	-	-	3/8/8/57	-
4	PCW	F	205	-	-	7/8/8/57	-
4	PCW	C	1115	-	-	4/8/8/57	-
4	PCW	B	1107	-	-	24/42/42/57	-
3	ZK1	C	1101	-	-	8/13/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AJP	A	1110	-	13/13/18/38	3/6/117/220	0/7/7/11
4	PCW	A	1115	-	-	2/8/8/57	-
4	PCW	E	203	-	-	23/46/46/57	-
4	PCW	B	1101	-	-	6/8/8/57	-
4	PCW	D	1109	-	-	23/54/54/57	-
4	PCW	A	1102	-	-	26/54/54/57	-
5	CLR	C	1111	-	2/2/10/11	5/10/68/68	0/4/4/4
4	PCW	C	1107	-	-	6/8/8/57	-
4	PCW	D	1106	-	-	22/44/44/57	-
4	PCW	B	1108	-	-	4/8/8/57	-
4	PCW	D	1107	-	-	25/42/42/57	-
4	PCW	C	1104	-	-	23/44/44/57	-
4	PCW	B	1109	-	-	5/8/8/57	-
4	PCW	C	1113	-	-	2/8/8/57	-
4	PCW	D	1105	-	-	12/34/34/57	-
4	PCW	E	201	-	-	7/8/8/57	-
4	PCW	D	1108	-	-	4/8/8/57	-
4	PCW	E	204	-	-	4/8/8/57	-
6	AJP	A	1111	-	9/9/18/38	4/6/117/220	1/7/7/11
4	PCW	F	203	-	-	4/8/8/57	-
5	CLR	A	1112	-	2/2/10/11	4/10/68/68	0/4/4/4
4	PCW	A	1103	-	-	24/46/46/57	-
3	ZK1	B	1102	-	-	5/13/23/23	0/3/3/3
6	AJP	A	1116	-	9/9/18/38	2/6/117/220	0/7/7/11
4	PCW	B	1103	-	-	25/44/44/57	-

All (466) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1110	AJP	O78-C27	-56.92	0.02	1.43
6	A	1111	AJP	O78-C27	-55.60	0.05	1.43
6	C	1114	AJP	O78-C27	-55.22	0.06	1.43
6	A	1110	AJP	O78-C27	-54.71	0.07	1.43
6	A	1116	AJP	O78-C27	-54.01	0.09	1.43
6	C	1109	AJP	O25-C23	-50.72	0.50	1.44
6	C	1110	AJP	O25-C23	-50.61	0.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1111	AJP	O25-C23	-50.33	0.51	1.44
6	A	1110	AJP	O25-C23	-50.32	0.51	1.44
6	C	1114	AJP	O25-C23	-49.54	0.52	1.44
6	A	1116	AJP	O25-C23	-49.49	0.52	1.44
6	C	1110	AJP	C07-C08	41.56	2.22	1.53
6	C	1109	AJP	C07-C08	41.56	2.22	1.53
6	A	1110	AJP	C07-C08	41.55	2.22	1.53
6	A	1111	AJP	C07-C08	41.53	2.22	1.53
6	C	1114	AJP	C07-C08	41.38	2.21	1.53
6	A	1116	AJP	C07-C08	41.29	2.21	1.53
6	C	1114	AJP	C16-C11	-38.04	1.02	1.54
6	A	1116	AJP	C16-C11	-37.91	1.02	1.54
6	C	1109	AJP	C16-C11	-37.31	1.03	1.54
6	A	1110	AJP	C16-C11	-37.24	1.03	1.54
6	C	1110	AJP	C16-C11	-35.51	1.05	1.54
6	A	1111	AJP	C16-C11	-35.46	1.05	1.54
6	A	1110	AJP	O09-C05	30.51	2.06	1.42
6	C	1109	AJP	O09-C05	30.41	2.06	1.42
6	A	1111	AJP	O09-C05	30.21	2.06	1.42
6	C	1110	AJP	O09-C05	30.20	2.06	1.42
6	A	1116	AJP	O09-C05	30.05	2.05	1.42
6	C	1114	AJP	O09-C05	29.97	2.05	1.42
6	A	1110	AJP	C12-C11	29.30	2.09	1.56
6	C	1109	AJP	C12-C11	29.18	2.09	1.56
6	C	1110	AJP	C12-C11	29.16	2.09	1.56
6	A	1111	AJP	C12-C11	29.10	2.09	1.56
5	C	1111	CLR	C8-C14	-28.81	0.99	1.53
5	A	1112	CLR	C8-C14	-28.77	0.99	1.53
6	A	1116	AJP	C12-C11	28.57	2.08	1.56
5	C	1106	CLR	C8-C14	-28.50	1.00	1.53
6	C	1114	AJP	C12-C11	28.44	2.08	1.56
5	A	1107	CLR	C8-C14	-28.43	1.00	1.53
6	C	1114	AJP	C28-C27	25.78	1.92	1.52
6	C	1110	AJP	C28-C27	25.42	1.91	1.52
6	C	1109	AJP	O25-C26	24.67	2.08	1.41
6	C	1110	AJP	O31-C30	24.56	1.83	1.44
6	A	1116	AJP	C28-C27	24.30	1.89	1.52
6	A	1116	AJP	O25-C26	24.24	2.10	1.41
6	C	1109	AJP	C27-C28	24.18	1.94	1.52
6	A	1110	AJP	O31-C30	24.01	1.82	1.44
6	C	1114	AJP	O31-C30	23.99	1.82	1.44
6	C	1114	AJP	O25-C26	23.89	2.09	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1111	AJP	C28-C27	23.86	1.89	1.52
6	A	1111	AJP	O31-C30	23.86	1.82	1.44
6	A	1111	AJP	O25-C26	23.71	2.08	1.41
6	A	1116	AJP	O31-C30	23.69	1.82	1.44
6	C	1110	AJP	O25-C26	23.64	2.08	1.41
6	A	1110	AJP	O25-C26	23.58	2.08	1.41
6	A	1110	AJP	C28-C27	23.47	1.88	1.52
6	C	1109	AJP	O31-C30	23.42	1.81	1.44
6	C	1109	AJP	C29-C28	-22.59	1.12	1.52
6	C	1114	AJP	C13-C12	-22.05	1.15	1.54
6	A	1116	AJP	C13-C12	-22.01	1.15	1.54
6	C	1110	AJP	C13-C12	-21.93	1.15	1.54
6	A	1111	AJP	C13-C12	-21.92	1.16	1.54
6	A	1110	AJP	C13-C12	-21.76	1.16	1.54
6	C	1114	AJP	C17-C16	-21.72	1.15	1.53
6	C	1109	AJP	C13-C12	-21.65	1.16	1.54
6	A	1116	AJP	C29-C28	-21.55	1.11	1.52
5	C	1111	CLR	C12-C11	-21.52	1.10	1.53
6	A	1116	AJP	C17-C16	-21.51	1.15	1.53
5	A	1112	CLR	C12-C11	-21.44	1.10	1.53
6	C	1109	AJP	C17-C16	-21.34	1.15	1.53
6	A	1110	AJP	C17-C16	-21.26	1.16	1.53
6	C	1114	AJP	C29-C28	-21.26	1.12	1.52
6	C	1110	AJP	C29-C28	-21.06	1.12	1.52
5	A	1107	CLR	C12-C11	-21.00	1.11	1.53
6	A	1110	AJP	C29-C28	-21.00	1.12	1.52
6	A	1111	AJP	C17-C16	-20.99	1.16	1.53
6	C	1110	AJP	C17-C16	-20.95	1.16	1.53
5	C	1106	CLR	C12-C11	-20.95	1.11	1.53
6	A	1111	AJP	C29-C28	-20.88	1.13	1.52
6	C	1110	AJP	C21-C22	19.92	1.82	1.53
6	C	1114	AJP	C20-C19	-19.82	1.24	1.55
5	A	1112	CLR	C7-C8	-19.79	1.21	1.53
5	C	1111	CLR	C7-C8	-19.72	1.21	1.53
6	A	1116	AJP	C20-C19	-19.67	1.24	1.55
6	A	1110	AJP	C20-C19	-19.48	1.25	1.55
6	A	1111	AJP	C20-C19	-19.45	1.25	1.55
5	A	1107	CLR	C7-C8	-19.42	1.21	1.53
6	C	1109	AJP	C20-C19	-19.41	1.25	1.55
5	C	1106	CLR	C7-C8	-19.40	1.21	1.53
6	C	1110	AJP	C20-C19	-19.39	1.25	1.55
6	A	1111	AJP	C21-C22	19.38	1.82	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1114	AJP	C21-C22	19.28	1.81	1.53
6	C	1114	AJP	O09-C08	-19.26	1.10	1.43
6	C	1109	AJP	C21-C22	19.21	1.81	1.53
6	A	1116	AJP	O09-C08	-19.20	1.10	1.43
6	A	1116	AJP	C21-C22	19.04	1.81	1.53
6	A	1110	AJP	C21-C22	19.03	1.81	1.53
6	C	1110	AJP	O09-C08	-18.81	1.11	1.43
6	A	1111	AJP	O09-C08	-18.79	1.11	1.43
6	C	1109	AJP	O09-C08	-18.07	1.12	1.43
6	A	1110	AJP	O09-C08	-18.00	1.12	1.43
6	C	1114	AJP	C22-C23	-17.76	1.21	1.52
6	A	1116	AJP	C22-C23	-17.76	1.21	1.52
6	A	1110	AJP	C22-C23	-17.64	1.21	1.52
6	C	1109	AJP	C22-C23	-17.31	1.22	1.52
6	A	1111	AJP	C22-C23	-16.93	1.22	1.52
6	C	1110	AJP	C22-C23	-16.77	1.22	1.52
6	A	1111	AJP	C11-C10	16.58	1.86	1.53
6	C	1110	AJP	C11-C10	16.57	1.86	1.53
6	C	1109	AJP	C11-C10	16.31	1.86	1.53
6	A	1110	AJP	C11-C10	16.29	1.85	1.53
6	C	1110	AJP	C24-C19	15.83	1.79	1.53
6	A	1111	AJP	C24-C19	15.80	1.79	1.53
6	C	1114	AJP	C11-C10	15.63	1.84	1.53
6	A	1116	AJP	C11-C10	15.55	1.84	1.53
6	A	1110	AJP	C14-C15	15.37	1.79	1.53
6	A	1116	AJP	C14-C15	15.36	1.79	1.53
6	C	1109	AJP	C14-C15	15.34	1.79	1.53
6	C	1114	AJP	C14-C15	15.34	1.79	1.53
6	A	1116	AJP	C24-C19	15.29	1.78	1.53
6	A	1110	AJP	C24-C19	15.27	1.78	1.53
6	C	1109	AJP	C24-C19	15.19	1.78	1.53
6	A	1111	AJP	C14-C15	15.14	1.78	1.53
6	C	1110	AJP	C14-C15	15.11	1.78	1.53
6	C	1114	AJP	C24-C19	14.88	1.77	1.53
6	A	1116	AJP	O82-C10	-13.86	1.08	1.43
6	C	1114	AJP	O82-C10	-13.85	1.08	1.43
6	C	1109	AJP	O82-C10	-13.68	1.09	1.43
6	A	1110	AJP	O82-C10	-13.62	1.09	1.43
6	C	1110	AJP	O82-C10	-13.43	1.09	1.43
6	A	1111	AJP	O82-C10	-13.39	1.09	1.43
6	C	1114	AJP	C12-C07	-13.28	1.31	1.56
6	A	1116	AJP	C12-C07	-13.21	1.31	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1110	AJP	C12-C07	-13.01	1.32	1.56
6	A	1111	AJP	C12-C07	-13.00	1.32	1.56
6	C	1109	AJP	C12-C07	-12.96	1.32	1.56
6	A	1110	AJP	C12-C07	-12.88	1.32	1.56
5	A	1107	CLR	C12-C13	-12.30	1.32	1.54
5	C	1106	CLR	C12-C13	-12.23	1.32	1.54
6	A	1111	AJP	C18-C17	12.22	1.82	1.52
6	A	1110	AJP	C18-C17	12.21	1.82	1.52
6	C	1110	AJP	C18-C17	12.13	1.82	1.52
6	C	1109	AJP	C18-C17	12.11	1.82	1.52
5	C	1111	CLR	C12-C13	-12.11	1.33	1.54
5	A	1112	CLR	C12-C13	-12.07	1.33	1.54
6	A	1116	AJP	C18-C17	12.01	1.82	1.52
6	C	1114	AJP	C18-C17	11.96	1.81	1.52
3	B	1102	ZK1	CAU-CAT	-11.23	1.37	1.53
6	C	1114	AJP	O77-C28	-11.18	1.19	1.43
3	D	1102	ZK1	CAU-CAT	-11.17	1.38	1.53
6	A	1116	AJP	O77-C28	-11.04	1.20	1.43
6	A	1110	AJP	O77-C28	-11.03	1.20	1.43
3	A	1101	ZK1	CAU-CAT	-10.92	1.38	1.53
3	C	1101	ZK1	CAU-CAT	-10.87	1.38	1.53
6	C	1110	AJP	O77-C28	-10.76	1.20	1.43
6	C	1114	AJP	C81-C12	10.61	1.71	1.54
6	A	1116	AJP	C81-C12	10.60	1.71	1.54
5	A	1107	CLR	C20-C17	-10.40	1.36	1.54
6	C	1110	AJP	C81-C12	10.37	1.71	1.54
5	C	1106	CLR	C15-C14	10.36	1.75	1.54
5	C	1106	CLR	C20-C17	-10.34	1.36	1.54
5	A	1107	CLR	C15-C14	10.34	1.75	1.54
6	C	1109	AJP	C81-C12	10.23	1.71	1.54
5	A	1112	CLR	C13-C17	10.23	1.73	1.55
6	A	1110	AJP	C81-C12	10.22	1.71	1.54
6	A	1111	AJP	C81-C12	10.18	1.71	1.54
5	C	1111	CLR	C13-C17	10.15	1.73	1.55
6	A	1111	AJP	C20-C15	10.15	1.73	1.56
6	A	1116	AJP	O31-C26	-9.98	1.16	1.41
5	A	1112	CLR	C7-C6	9.97	1.70	1.50
5	A	1107	CLR	C7-C6	9.97	1.70	1.50
5	C	1106	CLR	C7-C6	9.96	1.70	1.50
5	C	1111	CLR	C7-C6	9.95	1.70	1.50
6	A	1110	AJP	O31-C26	-9.94	1.16	1.41
6	C	1110	AJP	C20-C15	9.88	1.73	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1109	AJP	O31-C26	-9.88	1.16	1.42
6	A	1111	AJP	O77-C28	-9.79	1.22	1.43
5	C	1106	CLR	C13-C14	9.74	1.72	1.55
6	C	1114	AJP	O31-C26	-9.73	1.16	1.41
6	A	1110	AJP	C07-C06	-9.69	1.27	1.54
5	A	1107	CLR	C13-C14	9.67	1.72	1.55
6	C	1110	AJP	O31-C26	-9.67	1.17	1.41
6	C	1109	AJP	C07-C06	-9.64	1.27	1.54
6	A	1111	AJP	O31-C26	-9.55	1.17	1.41
6	C	1110	AJP	C80-C20	9.52	1.70	1.54
6	C	1114	AJP	C07-C06	-9.49	1.27	1.54
5	C	1111	CLR	C15-C14	9.48	1.73	1.54
6	A	1111	AJP	C80-C20	9.46	1.70	1.54
6	A	1116	AJP	C07-C06	-9.46	1.27	1.54
5	C	1106	CLR	C13-C17	9.44	1.72	1.55
5	A	1112	CLR	C15-C14	9.43	1.73	1.54
6	C	1114	AJP	C80-C20	9.40	1.69	1.54
6	C	1114	AJP	C20-C15	9.37	1.72	1.56
5	A	1107	CLR	C13-C17	9.37	1.72	1.55
6	A	1116	AJP	C80-C20	9.27	1.69	1.54
5	C	1111	CLR	C4-C5	9.21	1.70	1.51
5	A	1112	CLR	C4-C5	9.18	1.70	1.51
6	A	1116	AJP	C20-C15	9.16	1.72	1.56
5	A	1112	CLR	C10-C5	-9.16	1.35	1.52
5	A	1112	CLR	C20-C17	-9.13	1.38	1.54
6	C	1110	AJP	C07-C06	-9.12	1.28	1.54
5	C	1111	CLR	C20-C17	-9.11	1.38	1.54
6	A	1111	AJP	C07-C06	-9.10	1.28	1.54
5	C	1111	CLR	C10-C5	-9.08	1.35	1.52
5	C	1111	CLR	C13-C14	9.07	1.71	1.55
6	A	1110	AJP	C20-C15	9.07	1.71	1.56
5	C	1106	CLR	C4-C5	9.06	1.69	1.51
5	A	1112	CLR	C13-C14	9.06	1.71	1.55
6	C	1109	AJP	C20-C15	9.04	1.71	1.56
5	A	1107	CLR	C4-C5	9.03	1.69	1.51
6	C	1109	AJP	C80-C20	9.01	1.69	1.54
6	A	1110	AJP	C80-C20	9.00	1.69	1.54
5	A	1107	CLR	C10-C5	-8.97	1.35	1.52
5	C	1106	CLR	C10-C5	-8.97	1.35	1.52
5	C	1111	CLR	C16-C15	8.80	1.78	1.54
5	A	1112	CLR	C16-C15	8.80	1.78	1.54
5	A	1107	CLR	C16-C15	8.72	1.77	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1106	CLR	C16-C15	8.70	1.77	1.54
6	C	1109	AJP	O77-C28	-8.51	1.18	1.43
3	D	1102	ZK1	OAA-CAT	8.45	1.39	1.23
3	A	1101	ZK1	OAA-CAT	8.40	1.39	1.23
3	B	1102	ZK1	OAA-CAT	8.40	1.39	1.23
3	C	1101	ZK1	OAA-CAT	8.35	1.39	1.23
3	B	1102	ZK1	OAB-CAU	8.19	1.39	1.23
3	D	1102	ZK1	OAB-CAU	8.19	1.39	1.23
3	A	1101	ZK1	OAB-CAU	8.13	1.39	1.23
3	C	1101	ZK1	OAB-CAU	8.10	1.39	1.23
6	A	1111	AJP	C32-C30	-7.61	1.32	1.51
6	A	1110	AJP	C32-C30	-7.00	1.34	1.51
6	C	1110	AJP	C32-C30	-6.96	1.34	1.51
6	C	1109	AJP	C32-C30	-6.82	1.34	1.51
5	C	1111	CLR	C16-C17	6.73	1.68	1.54
5	A	1112	CLR	C16-C17	6.72	1.68	1.54
6	A	1116	AJP	C32-C30	-6.70	1.34	1.51
6	C	1114	AJP	C32-C30	-6.68	1.34	1.51
6	A	1116	AJP	C13-C14	-6.37	1.40	1.53
6	C	1114	AJP	C13-C14	-6.31	1.40	1.53
6	A	1110	AJP	C13-C14	-6.29	1.40	1.53
5	A	1107	CLR	C16-C17	6.26	1.67	1.54
5	C	1106	CLR	C16-C17	6.24	1.67	1.54
6	C	1109	AJP	C13-C14	-6.23	1.41	1.53
6	A	1111	AJP	C13-C14	-6.19	1.41	1.53
6	C	1110	AJP	C13-C14	-6.12	1.41	1.53
5	A	1107	CLR	C1-C10	5.60	1.64	1.54
5	C	1106	CLR	C1-C10	5.55	1.64	1.54
6	A	1110	AJP	C26-C27	-5.46	1.36	1.52
6	A	1111	AJP	O84-C85	5.39	1.51	1.43
6	C	1110	AJP	O84-C85	5.30	1.51	1.43
6	C	1110	AJP	C01-C02	5.29	1.69	1.52
6	A	1111	AJP	C01-C02	5.26	1.69	1.52
6	C	1109	AJP	C01-C02	5.22	1.69	1.52
6	A	1110	AJP	C04-C05	-5.21	1.44	1.51
6	A	1110	AJP	C01-C02	5.20	1.69	1.52
5	C	1111	CLR	C1-C10	5.20	1.63	1.54
6	C	1109	AJP	C04-C05	-5.18	1.44	1.51
6	A	1116	AJP	C01-C02	5.16	1.69	1.52
6	C	1114	AJP	C01-C02	5.14	1.68	1.52
5	A	1112	CLR	C1-C10	5.14	1.63	1.54
5	C	1106	CLR	C11-C9	5.03	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1107	CLR	C11-C9	4.95	1.61	1.53
6	C	1109	AJP	O84-C85	4.90	1.50	1.43
6	A	1110	AJP	O84-C85	4.86	1.50	1.43
6	C	1114	AJP	C18-C19	-4.86	1.41	1.53
6	C	1110	AJP	C18-C19	-4.73	1.41	1.53
6	A	1116	AJP	C18-C19	-4.72	1.41	1.53
6	A	1111	AJP	C18-C19	-4.71	1.41	1.53
5	C	1106	CLR	C22-C20	4.61	1.65	1.54
5	A	1107	CLR	C22-C20	4.60	1.65	1.54
6	C	1110	AJP	C83-C06	4.59	1.62	1.53
6	A	1111	AJP	C83-C06	4.57	1.62	1.53
6	A	1116	AJP	O84-C85	4.51	1.50	1.43
6	C	1109	AJP	C18-C19	-4.43	1.42	1.53
6	C	1114	AJP	O84-C85	4.42	1.50	1.43
5	C	1111	CLR	C22-C20	4.41	1.65	1.54
6	A	1110	AJP	C18-C19	-4.38	1.42	1.53
5	A	1112	CLR	C22-C20	4.37	1.65	1.54
5	A	1112	CLR	C11-C9	4.16	1.60	1.53
5	C	1111	CLR	C11-C9	4.14	1.60	1.53
5	A	1107	CLR	C1-C2	4.14	1.61	1.53
5	C	1106	CLR	C1-C2	4.09	1.61	1.53
6	A	1111	AJP	C04-C05	-4.03	1.45	1.51
6	C	1110	AJP	C04-C05	-4.03	1.45	1.51
6	A	1116	AJP	C04-C05	-3.97	1.45	1.51
5	A	1112	CLR	C2-C3	-3.96	1.42	1.51
5	C	1111	CLR	C2-C3	-3.94	1.42	1.51
6	C	1114	AJP	C04-C05	-3.94	1.46	1.51
3	D	1102	ZK1	CAW-NAY	-3.94	1.34	1.41
3	A	1101	ZK1	CAW-NAY	-3.89	1.34	1.41
3	C	1101	ZK1	CAU-NAY	-3.89	1.31	1.38
3	D	1102	ZK1	CAU-NAY	-3.88	1.31	1.38
3	A	1101	ZK1	CAU-NAY	-3.87	1.31	1.38
3	C	1101	ZK1	CAW-NAY	-3.86	1.34	1.41
3	B	1102	ZK1	CAW-NAY	-3.86	1.34	1.41
3	B	1102	ZK1	CAU-NAY	-3.84	1.31	1.38
6	A	1116	AJP	C83-C06	3.84	1.61	1.53
5	C	1111	CLR	C1-C2	3.78	1.60	1.53
5	A	1112	CLR	C1-C2	3.78	1.60	1.53
5	A	1107	CLR	C6-C5	3.76	1.40	1.33
6	C	1114	AJP	C83-C06	3.74	1.60	1.53
6	A	1116	AJP	C26-C27	-3.69	1.41	1.52
5	C	1106	CLR	C6-C5	3.67	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1106	CLR	C2-C3	-3.61	1.43	1.51
5	A	1107	CLR	C2-C3	-3.60	1.43	1.51
3	B	1102	ZK1	CAV-CAW	-3.58	1.36	1.40
3	D	1102	ZK1	CAV-CAW	-3.56	1.36	1.40
5	C	1111	CLR	C18-C13	3.46	1.60	1.54
6	C	1110	AJP	O79-C22	3.44	1.50	1.43
3	B	1102	ZK1	CAV-NAP	-3.44	1.34	1.39
5	A	1112	CLR	C6-C5	3.40	1.40	1.33
5	A	1112	CLR	C18-C13	3.39	1.59	1.54
3	D	1102	ZK1	CAV-NAP	-3.39	1.34	1.39
3	A	1101	ZK1	CAV-CAW	-3.38	1.36	1.40
5	C	1111	CLR	C6-C5	3.37	1.39	1.33
4	D	1105	PCW	O2-C31	3.34	1.43	1.34
6	A	1116	AJP	C24-C23	3.33	1.58	1.52
6	A	1111	AJP	C26-C27	-3.30	1.42	1.52
6	C	1109	AJP	O79-C22	3.30	1.50	1.43
4	B	1105	PCW	O2-C31	3.26	1.43	1.34
6	C	1114	AJP	C26-C27	-3.24	1.43	1.52
6	C	1114	AJP	C24-C23	3.23	1.58	1.52
3	C	1101	ZK1	CAV-CAW	-3.23	1.37	1.40
3	C	1101	ZK1	CAV-NAP	-3.22	1.34	1.39
4	B	1111	PCW	O3-C11	3.18	1.42	1.33
4	A	1114	PCW	O3-C11	3.17	1.42	1.33
6	C	1110	AJP	C24-C23	3.16	1.58	1.52
4	D	1107	PCW	O3-C11	3.16	1.42	1.33
4	C	1104	PCW	O3-C11	3.15	1.42	1.33
4	D	1103	PCW	O2-C31	3.15	1.43	1.34
4	E	203	PCW	O3-C11	3.15	1.42	1.33
4	A	1103	PCW	O3-C11	3.14	1.42	1.33
4	B	1107	PCW	O3-C11	3.14	1.42	1.33
4	F	202	PCW	O3-C11	3.13	1.42	1.33
4	D	1104	PCW	O3-C11	3.13	1.42	1.33
4	A	1104	PCW	O3-C11	3.13	1.42	1.33
4	A	1105	PCW	O3-C11	3.12	1.42	1.33
4	A	1105	PCW	O2-C31	3.12	1.43	1.34
4	A	1113	PCW	O3-C11	3.11	1.42	1.33
4	D	1109	PCW	O3-C11	3.11	1.42	1.33
4	C	1103	PCW	O3-C11	3.11	1.42	1.33
4	B	1110	PCW	O3-C11	3.10	1.42	1.33
4	C	1112	PCW	O3-C11	3.10	1.42	1.33
4	A	1118	PCW	O3-C11	3.10	1.42	1.33
4	B	1110	PCW	O2-C31	3.10	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	ZK1	CAV-NAP	-3.09	1.34	1.39
6	C	1110	AJP	C26-C27	-3.09	1.43	1.52
4	C	1104	PCW	O2-C31	3.08	1.43	1.34
4	B	1104	PCW	O3-C11	3.08	1.42	1.33
4	A	1104	PCW	O2-C31	3.07	1.43	1.34
6	A	1111	AJP	C24-C23	3.06	1.57	1.52
6	C	1109	AJP	C27-C26	-3.06	1.43	1.50
4	B	1106	PCW	O3-C11	3.06	1.42	1.33
4	D	1106	PCW	O3-C11	3.06	1.42	1.33
4	B	1103	PCW	O2-C31	3.06	1.42	1.34
4	E	203	PCW	O2-C31	3.05	1.42	1.34
4	C	1102	PCW	O3-C11	3.05	1.42	1.33
4	F	202	PCW	O2-C31	3.03	1.42	1.34
4	C	1103	PCW	O2-C31	3.03	1.42	1.34
4	A	1102	PCW	O3-C11	3.03	1.42	1.33
6	A	1110	AJP	O79-C22	3.03	1.49	1.43
4	A	1113	PCW	O2-C31	3.02	1.42	1.34
4	A	1103	PCW	O2-C31	3.02	1.42	1.34
4	C	1112	PCW	O2-C31	3.00	1.42	1.34
4	D	1109	PCW	O2-C31	3.00	1.42	1.34
5	C	1106	CLR	C10-C9	2.98	1.60	1.56
4	B	1111	PCW	O2-C2	-2.96	1.39	1.46
5	A	1112	CLR	C10-C9	2.95	1.60	1.56
6	A	1111	AJP	O79-C22	2.94	1.49	1.43
4	A	1118	PCW	O2-C31	2.93	1.42	1.34
4	A	1102	PCW	O2-C31	2.93	1.42	1.34
5	A	1107	CLR	C18-C13	2.92	1.59	1.54
5	C	1106	CLR	C18-C13	2.92	1.59	1.54
5	C	1111	CLR	C10-C9	2.91	1.60	1.56
4	D	1103	PCW	O3-C11	2.91	1.41	1.33
4	B	1103	PCW	O3-C11	2.91	1.41	1.33
4	C	1102	PCW	O2-C31	2.91	1.42	1.34
4	B	1107	PCW	O2-C31	2.90	1.42	1.34
4	B	1106	PCW	O2-C31	2.90	1.42	1.34
4	D	1107	PCW	O2-C31	2.88	1.42	1.34
6	C	1114	AJP	O79-C22	2.88	1.49	1.43
4	D	1106	PCW	O2-C2	-2.86	1.39	1.46
3	B	1102	ZK1	CAT-NAP	-2.86	1.31	1.35
6	A	1116	AJP	O79-C22	2.86	1.49	1.43
4	B	1106	PCW	O2-C2	-2.85	1.39	1.46
5	A	1107	CLR	C10-C9	2.85	1.60	1.56
4	A	1118	PCW	O2-C2	-2.84	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	PCW	O2-C31	2.83	1.42	1.34
4	D	1106	PCW	O2-C31	2.83	1.42	1.34
4	A	1114	PCW	O2-C31	2.79	1.42	1.34
4	D	1104	PCW	O2-C31	2.78	1.42	1.34
4	D	1109	PCW	O2-C2	-2.78	1.40	1.46
6	C	1110	AJP	O84-C05	2.77	1.46	1.42
3	D	1102	ZK1	CAT-NAP	-2.75	1.32	1.35
6	C	1109	AJP	C83-C06	2.74	1.58	1.53
4	A	1114	PCW	O2-C2	-2.73	1.40	1.46
6	A	1111	AJP	O84-C05	2.73	1.46	1.42
3	C	1101	ZK1	CAT-NAP	-2.69	1.32	1.35
4	D	1107	PCW	O2-C2	-2.67	1.40	1.46
4	B	1104	PCW	O2-C2	-2.67	1.40	1.46
6	A	1110	AJP	C24-C23	2.66	1.57	1.52
4	F	202	PCW	O2-C2	-2.66	1.40	1.46
4	B	1107	PCW	O2-C2	-2.66	1.40	1.46
4	C	1102	PCW	O2-C2	-2.65	1.40	1.46
4	D	1104	PCW	O2-C2	-2.64	1.40	1.46
4	A	1102	PCW	O2-C2	-2.62	1.40	1.46
3	A	1101	ZK1	CAT-NAP	-2.60	1.32	1.35
4	A	1113	PCW	O2-C2	-2.60	1.40	1.46
4	B	1111	PCW	O2-C31	2.59	1.41	1.34
4	B	1110	PCW	O2-C2	-2.59	1.40	1.46
4	E	203	PCW	O2-C2	-2.59	1.40	1.46
4	C	1112	PCW	O2-C2	-2.56	1.40	1.46
6	A	1110	AJP	C83-C06	2.56	1.58	1.53
6	A	1110	AJP	C16-C15	-2.54	1.48	1.53
6	C	1110	AJP	C05-C06	2.53	1.58	1.53
6	C	1109	AJP	C16-C15	-2.53	1.48	1.53
4	A	1105	PCW	O2-C2	-2.52	1.40	1.46
5	C	1106	CLR	C4-C3	2.47	1.56	1.52
6	A	1111	AJP	C05-C06	2.47	1.58	1.53
5	C	1111	CLR	C4-C3	2.46	1.56	1.52
5	A	1107	CLR	C4-C3	2.45	1.56	1.52
5	A	1112	CLR	C4-C3	2.44	1.56	1.52
4	B	1103	PCW	O2-C2	-2.43	1.40	1.46
4	C	1103	PCW	O2-C2	-2.43	1.40	1.46
4	C	1104	PCW	O2-C2	-2.41	1.40	1.46
6	A	1116	AJP	C16-C15	-2.40	1.49	1.53
4	A	1103	PCW	O2-C2	-2.39	1.41	1.46
4	A	1104	PCW	O2-C2	-2.39	1.41	1.46
4	D	1103	PCW	O2-C2	-2.36	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1114	AJP	C16-C15	-2.34	1.49	1.53
6	A	1111	AJP	C16-C15	-2.33	1.49	1.53
4	D	1105	PCW	P-O4P	2.29	1.68	1.59
4	B	1105	PCW	P-O4P	2.28	1.68	1.59
3	A	1101	ZK1	CAR-NAX	2.25	1.46	1.41
6	C	1110	AJP	C16-C15	-2.24	1.49	1.53
4	B	1110	PCW	P-O4P	2.17	1.67	1.59
3	C	1101	ZK1	CAR-NAX	2.16	1.46	1.41
4	B	1107	PCW	P-O4P	2.16	1.67	1.59
4	A	1105	PCW	P-O4P	2.16	1.67	1.59
4	D	1106	PCW	P-O4P	2.14	1.67	1.59
4	F	202	PCW	P-O4P	2.13	1.67	1.59
4	A	1113	PCW	P-O4P	2.12	1.67	1.59
4	E	203	PCW	P-O4P	2.12	1.67	1.59
4	B	1106	PCW	P-O4P	2.11	1.67	1.59
4	D	1107	PCW	P-O3P	2.11	1.67	1.59
4	D	1106	PCW	P-O3P	2.11	1.67	1.59
4	B	1107	PCW	P-O3P	2.10	1.67	1.59
6	C	1114	AJP	C05-C06	2.10	1.57	1.53
6	A	1116	AJP	C05-C06	2.09	1.57	1.53
3	B	1102	ZK1	PBA-OAD	-2.08	1.50	1.55
4	D	1107	PCW	P-O4P	2.08	1.67	1.59
4	C	1104	PCW	P-O4P	2.08	1.67	1.59
4	C	1112	PCW	P-O4P	2.07	1.67	1.59
4	B	1106	PCW	P-O3P	2.07	1.67	1.59
4	A	1104	PCW	P-O4P	2.07	1.67	1.59
4	C	1102	PCW	P-O4P	2.06	1.67	1.59
4	A	1103	PCW	P-O4P	2.06	1.67	1.59
4	D	1109	PCW	P-O4P	2.05	1.67	1.59
4	C	1103	PCW	P-O4P	2.05	1.67	1.59
4	A	1118	PCW	P-O4P	2.05	1.67	1.59
6	C	1109	AJP	C24-C23	2.05	1.55	1.52
3	D	1102	ZK1	PBA-OAD	-2.05	1.50	1.55
4	A	1102	PCW	P-O4P	2.04	1.67	1.59
4	C	1112	PCW	P-O3P	2.03	1.67	1.59
4	A	1113	PCW	P-O3P	2.02	1.67	1.59
4	A	1114	PCW	P-O4P	2.01	1.67	1.59
4	F	202	PCW	P-O3P	2.01	1.67	1.59
4	E	203	PCW	P-O3P	2.00	1.67	1.59

All (446) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	CLR	C18-C13-C17	-13.80	86.65	111.68
5	C	1106	CLR	C18-C13-C17	-13.73	86.77	111.68
5	A	1112	CLR	C18-C13-C17	-12.77	88.52	111.68
5	C	1111	CLR	C18-C13-C17	-12.35	89.27	111.68
5	C	1106	CLR	C12-C13-C17	10.83	132.55	116.60
5	A	1107	CLR	C12-C13-C17	10.56	132.16	116.60
6	A	1110	AJP	C04-C05-C06	10.09	133.93	115.66
6	C	1109	AJP	C04-C05-C06	9.98	133.74	115.66
6	C	1110	AJP	C04-C05-C06	9.03	132.02	115.66
6	A	1111	AJP	C04-C05-C06	8.98	131.92	115.66
5	C	1106	CLR	C4-C5-C6	-8.98	108.40	120.57
5	A	1112	CLR	C4-C5-C6	-8.97	108.41	120.57
5	A	1107	CLR	C4-C5-C6	-8.97	108.41	120.57
5	C	1111	CLR	C4-C5-C6	-8.90	108.51	120.57
5	A	1112	CLR	C12-C13-C17	8.73	129.46	116.60
5	C	1111	CLR	C12-C13-C17	8.63	129.31	116.60
6	A	1110	AJP	C83-C06-C05	-8.52	101.21	114.94
6	A	1110	AJP	O78-C27-C28	8.51	127.42	110.05
6	C	1114	AJP	C13-C12-C07	8.31	127.19	115.36
5	C	1106	CLR	C19-C10-C9	-8.28	102.37	111.66
6	A	1116	AJP	C13-C12-C07	8.20	127.04	115.36
5	A	1107	CLR	C19-C10-C9	-8.19	102.47	111.66
6	A	1111	AJP	C13-C12-C07	7.96	126.70	115.36
6	C	1110	AJP	C13-C12-C07	7.82	126.50	115.36
6	A	1116	AJP	C26-O31-C30	7.78	121.75	113.13
6	C	1109	AJP	C83-C06-C05	-7.70	102.53	114.94
5	C	1111	CLR	C7-C6-C5	-7.62	112.15	125.02
6	A	1116	AJP	O78-C27-C28	7.61	125.59	110.05
6	C	1109	AJP	C13-C12-C07	7.59	126.17	115.36
6	A	1110	AJP	C13-C12-C07	7.58	126.15	115.36
5	C	1111	CLR	C10-C5-C6	-7.48	112.00	122.93
6	C	1114	AJP	C26-O31-C30	7.48	121.42	113.13
5	A	1112	CLR	C10-C5-C6	-7.42	112.09	122.93
5	A	1112	CLR	C7-C6-C5	-7.39	112.55	125.02
6	A	1110	AJP	O78-C27-C26	7.34	127.56	110.08
6	C	1114	AJP	O09-C08-C10	7.30	124.99	110.20
6	A	1116	AJP	O09-C08-C10	7.29	124.96	110.20
6	A	1116	AJP	C04-C05-C06	7.16	128.62	115.66
5	C	1106	CLR	C7-C6-C5	-6.98	113.24	125.02
6	C	1114	AJP	C04-C05-C06	6.96	128.26	115.66
5	C	1111	CLR	C19-C10-C9	-6.95	103.86	111.66
5	A	1112	CLR	C13-C14-C8	6.95	124.28	114.41
6	A	1110	AJP	O09-C05-C06	-6.91	95.37	104.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1111	CLR	C11-C12-C13	6.87	124.34	112.74
5	C	1111	CLR	C13-C14-C8	6.86	124.15	114.41
6	A	1111	AJP	C80-C20-C15	-6.85	101.97	111.18
5	A	1107	CLR	C7-C6-C5	-6.84	113.48	125.02
6	C	1114	AJP	O78-C27-C28	-6.83	96.12	110.05
5	A	1112	CLR	C11-C12-C13	6.81	124.23	112.74
5	C	1106	CLR	C10-C5-C6	-6.81	112.99	122.93
6	C	1109	AJP	C03-C02-C85	6.79	116.83	108.59
5	A	1107	CLR	C10-C5-C6	-6.75	113.07	122.93
5	A	1112	CLR	C19-C10-C9	-6.72	104.12	111.66
6	C	1110	AJP	C80-C20-C15	-6.68	102.20	111.18
6	C	1110	AJP	C21-C22-C23	6.65	119.36	110.46
6	A	1110	AJP	C03-C02-C85	6.60	116.60	108.59
6	A	1111	AJP	C21-C22-C23	6.59	119.27	110.46
6	A	1110	AJP	C81-C12-C13	-6.57	100.92	110.61
6	C	1109	AJP	O09-C05-C06	-6.53	95.88	104.56
6	A	1110	AJP	C21-C20-C19	6.52	113.47	107.23
6	A	1110	AJP	C29-C28-C27	6.48	120.00	110.67
6	C	1109	AJP	C81-C12-C13	-6.44	101.11	110.61
6	C	1109	AJP	C21-C20-C19	6.39	113.34	107.23
5	C	1111	CLR	C14-C8-C9	6.27	117.28	109.09
5	A	1112	CLR	C14-C8-C9	6.23	117.23	109.09
6	C	1114	AJP	C24-C23-C22	6.23	117.58	111.07
5	A	1107	CLR	C11-C12-C13	6.15	123.12	112.74
5	C	1106	CLR	C11-C12-C13	6.14	123.10	112.74
6	C	1114	AJP	C29-C28-C27	6.14	119.51	110.67
6	A	1116	AJP	C29-C28-C27	6.09	119.45	110.67
6	A	1110	AJP	O09-C08-C10	6.04	122.43	110.20
6	A	1110	AJP	C81-C12-C07	-5.95	98.64	111.58
5	C	1111	CLR	C8-C7-C6	5.92	120.97	112.76
6	A	1111	AJP	C26-O31-C30	5.89	119.65	113.13
6	C	1109	AJP	O09-C08-C10	5.88	122.10	110.20
5	C	1106	CLR	C13-C14-C8	5.81	122.67	114.41
5	A	1112	CLR	C8-C7-C6	5.79	120.79	112.76
6	C	1109	AJP	C81-C12-C07	-5.79	99.00	111.58
6	A	1116	AJP	C24-C23-C22	5.78	117.11	111.07
5	A	1107	CLR	C13-C14-C8	5.69	122.50	114.41
6	C	1110	AJP	C26-O31-C30	5.60	119.34	113.13
5	C	1106	CLR	C11-C9-C10	5.60	119.99	113.08
6	A	1111	AJP	C29-C28-C27	5.49	118.57	110.67
3	A	1101	ZK1	CAS-CAR-NAX	5.44	126.16	119.92
6	C	1110	AJP	O09-C05-C04	-5.34	97.70	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	CLR	C11-C9-C10	5.32	119.64	113.08
6	A	1111	AJP	O09-C05-C04	-5.30	97.77	108.54
6	C	1114	AJP	C21-C22-C23	5.30	117.55	110.46
6	C	1114	AJP	O25-C23-C24	5.29	119.93	109.64
3	A	1101	ZK1	CAI-CAR-NAX	-5.28	114.90	122.59
6	A	1111	AJP	C81-C12-C11	-5.25	100.17	111.58
5	C	1106	CLR	C8-C7-C6	5.24	120.02	112.76
6	A	1116	AJP	O25-C23-C24	5.22	119.79	109.64
6	A	1111	AJP	C15-C20-C19	5.16	115.69	108.51
6	C	1110	AJP	C29-C28-C27	5.13	118.06	110.67
5	C	1106	CLR	C18-C13-C14	5.12	120.97	111.68
5	C	1106	CLR	C15-C16-C17	-5.12	95.13	105.14
6	C	1114	AJP	O31-C30-C29	-5.11	102.35	110.14
6	A	1111	AJP	O31-C30-C32	5.10	115.01	106.83
3	C	1101	ZK1	CAI-CAR-NAX	-5.09	115.17	122.59
3	C	1101	ZK1	CAS-CAR-NAX	5.08	125.75	119.92
6	A	1111	AJP	O09-C08-C10	5.08	120.47	110.20
6	C	1110	AJP	C81-C12-C11	-5.07	100.55	111.58
6	C	1110	AJP	O09-C08-C10	5.07	120.47	110.20
5	A	1107	CLR	C8-C7-C6	5.06	119.77	112.76
6	C	1110	AJP	O31-C30-C32	5.06	114.94	106.83
6	C	1110	AJP	C15-C20-C19	5.03	115.51	108.51
5	A	1107	CLR	C15-C16-C17	-5.02	95.32	105.14
6	C	1114	AJP	C03-C04-C05	5.01	119.78	111.93
6	A	1116	AJP	O31-C30-C29	-5.00	102.53	110.14
6	C	1110	AJP	C24-C23-C22	4.99	116.29	111.07
5	C	1106	CLR	C14-C8-C9	4.98	115.59	109.09
6	A	1116	AJP	O78-C27-C26	4.92	121.81	110.08
5	A	1107	CLR	C14-C8-C9	4.92	115.52	109.09
5	A	1107	CLR	C18-C13-C14	4.92	120.60	111.68
5	C	1106	CLR	C15-C14-C8	4.85	126.84	119.10
5	A	1107	CLR	C15-C14-C8	4.85	126.83	119.10
6	A	1110	AJP	C11-C12-C07	4.84	107.46	100.16
3	D	1102	ZK1	CAI-CAR-NAX	-4.84	115.54	122.59
5	A	1107	CLR	C1-C10-C9	4.84	115.14	108.74
6	C	1114	AJP	C11-C10-C08	-4.83	92.56	103.05
3	B	1102	ZK1	CAI-CAR-NAX	-4.82	115.57	122.59
6	A	1116	AJP	C80-C20-C15	-4.82	104.70	111.18
6	C	1114	AJP	C26-O25-C23	4.78	123.25	115.27
6	C	1114	AJP	C12-C11-C16	-4.77	107.25	113.90
3	D	1102	ZK1	CAN-NAX-CAM	4.76	122.28	111.57
3	B	1102	ZK1	CAN-NAX-CAM	4.76	122.27	111.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1111	AJP	C03-C02-C85	4.73	114.33	108.59
6	C	1109	AJP	C11-C12-C07	4.69	107.23	100.16
6	C	1110	AJP	C03-C02-C85	4.69	114.28	108.59
6	A	1116	AJP	C11-C10-C08	-4.68	92.88	103.05
6	A	1116	AJP	O31-C30-C32	4.67	114.33	106.83
4	D	1105	PCW	O2-C31-C32	4.65	121.54	111.48
6	C	1110	AJP	O31-C30-C29	-4.65	103.05	110.14
5	C	1106	CLR	C1-C10-C9	4.65	114.89	108.74
6	A	1116	AJP	C28-C29-C30	4.63	119.02	111.19
4	B	1105	PCW	O2-C31-C32	4.62	121.48	111.48
5	C	1111	CLR	C7-C8-C9	4.59	115.03	109.72
4	D	1104	PCW	O2-C31-C32	4.56	121.35	111.48
6	A	1116	AJP	C21-C22-C23	4.54	116.54	110.46
4	B	1104	PCW	O2-C31-C32	4.53	121.28	111.48
6	A	1116	AJP	C26-O25-C23	4.48	122.77	115.27
6	A	1116	AJP	C81-C12-C07	-4.48	101.83	111.58
4	A	1105	PCW	O2-C31-C32	4.47	121.16	111.48
6	A	1111	AJP	O31-C30-C29	-4.47	103.33	110.14
4	D	1107	PCW	O2-C31-C32	4.46	121.13	111.48
6	C	1114	AJP	O31-C30-C32	4.46	113.98	106.83
6	C	1114	AJP	C81-C12-C07	-4.44	101.93	111.58
6	C	1114	AJP	C28-C29-C30	4.43	118.69	111.19
3	D	1102	ZK1	CAS-CAR-NAX	4.41	124.97	119.92
6	A	1110	AJP	C21-C22-C23	4.40	116.34	110.46
4	B	1106	PCW	O2-C31-C32	4.39	120.97	111.48
4	B	1107	PCW	O2-C31-C32	4.38	120.96	111.48
6	A	1110	AJP	O31-C30-C29	-4.37	103.49	110.14
6	C	1109	AJP	C21-C22-C23	4.36	116.29	110.46
3	B	1102	ZK1	CAS-CAR-NAX	4.34	124.89	119.92
6	C	1114	AJP	C81-C12-C13	-4.33	104.22	110.61
6	A	1111	AJP	O25-C26-C27	4.32	118.73	108.09
5	A	1112	CLR	C7-C8-C9	4.32	114.71	109.72
6	A	1110	AJP	C14-C13-C12	4.31	120.01	112.74
3	C	1101	ZK1	CAN-NAX-CAM	4.29	121.22	111.57
6	A	1111	AJP	C24-C23-C22	4.28	115.55	111.07
6	A	1116	AJP	C81-C12-C13	-4.26	104.32	110.61
4	C	1104	PCW	O2-C31-C32	4.25	120.68	111.48
4	D	1106	PCW	O2-C31-C32	4.25	120.67	111.48
6	C	1109	AJP	C14-C13-C12	4.23	119.87	112.74
4	A	1113	PCW	O2-C31-C32	4.21	120.59	111.48
4	C	1112	PCW	O2-C31-C32	4.21	120.59	111.48
6	A	1111	AJP	C17-C16-C15	4.20	115.56	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1104	PCW	O2-C31-C32	4.20	120.57	111.48
5	C	1106	CLR	C16-C15-C14	-4.20	96.92	105.14
6	C	1114	AJP	O78-C27-C26	-4.20	100.07	110.08
6	A	1111	AJP	C26-O25-C23	4.19	122.27	115.27
6	C	1114	AJP	O09-C08-C07	-4.19	94.44	104.08
6	A	1116	AJP	C03-C04-C05	4.18	118.48	111.93
5	A	1107	CLR	C16-C15-C14	-4.18	96.96	105.14
6	C	1114	AJP	C14-C13-C12	4.17	119.78	112.74
6	C	1110	AJP	O78-C27-C26	4.17	120.00	110.08
6	A	1116	AJP	O09-C08-C07	-4.15	94.54	104.08
4	B	1110	PCW	O2-C31-C32	4.14	120.44	111.48
3	A	1101	ZK1	CAN-NAX-CAM	4.13	120.86	111.57
6	C	1109	AJP	O31-C30-C29	-4.13	103.85	110.14
4	C	1102	PCW	O2-C31-C32	4.11	120.38	111.48
5	C	1111	CLR	C16-C15-C14	-4.10	97.13	105.14
4	A	1102	PCW	O2-C31-C32	4.09	120.34	111.48
6	C	1114	AJP	C17-C16-C15	4.09	115.42	110.52
6	A	1116	AJP	C12-C11-C16	-4.07	108.22	113.90
5	C	1106	CLR	C22-C20-C17	-4.07	101.90	110.33
6	A	1116	AJP	C14-C13-C12	4.04	119.56	112.74
5	C	1111	CLR	C12-C11-C9	4.03	119.99	113.14
6	C	1110	AJP	C26-O25-C23	4.03	122.00	115.27
6	A	1110	AJP	C28-C29-C30	4.02	117.99	111.19
5	A	1112	CLR	C12-C11-C9	4.02	119.97	113.14
6	C	1110	AJP	C18-C17-C16	4.01	118.56	112.16
6	A	1111	AJP	C83-C06-C05	-4.01	108.47	114.94
6	C	1110	AJP	O25-C26-C27	4.01	117.95	108.09
6	C	1110	AJP	O09-C08-C07	-4.00	94.87	104.08
6	A	1111	AJP	O09-C08-C07	-4.00	94.87	104.08
5	A	1107	CLR	C22-C20-C17	-3.99	102.06	110.33
6	C	1109	AJP	C28-C29-C30	3.99	118.70	110.63
4	A	1114	PCW	O2-C31-C32	3.98	120.09	111.48
6	C	1114	AJP	C03-C02-C85	3.93	113.36	108.59
6	C	1110	AJP	C17-C16-C15	3.93	115.22	110.52
6	C	1114	AJP	C80-C20-C15	-3.93	105.90	111.18
6	A	1111	AJP	C18-C17-C16	3.92	118.41	112.16
5	A	1112	CLR	C16-C15-C14	-3.92	97.47	105.14
6	C	1110	AJP	C83-C06-C05	-3.90	108.65	114.94
6	A	1110	AJP	O25-C26-C27	3.88	117.64	108.09
4	E	203	PCW	C8-N-C6	3.88	119.17	108.98
4	F	202	PCW	C8-N-C6	3.87	119.14	108.98
4	B	1104	PCW	C8-N-C6	3.87	119.14	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1111	AJP	C81-C12-C07	-3.86	103.18	111.58
6	A	1116	AJP	C15-C20-C19	3.85	113.86	108.51
4	D	1104	PCW	C8-N-C6	3.84	119.07	108.98
6	C	1110	AJP	C06-C07-C08	-3.84	98.11	104.28
6	A	1116	AJP	C17-C16-C15	3.83	115.11	110.52
6	C	1110	AJP	C11-C16-C15	3.81	115.89	109.17
6	C	1110	AJP	O84-C05-O09	-3.81	100.82	109.88
6	C	1109	AJP	C26-C27-C28	-3.80	100.31	111.29
3	A	1101	ZK1	CAV-NAP-CAT	-3.80	119.50	124.82
3	C	1101	ZK1	CAV-NAP-CAT	-3.79	119.52	124.82
6	A	1111	AJP	O84-C05-O09	-3.79	100.87	109.88
4	D	1103	PCW	C8-N-C6	3.78	118.91	108.98
5	A	1112	CLR	C13-C17-C20	3.77	125.32	119.50
4	B	1103	PCW	C8-N-C6	3.77	118.87	108.98
4	D	1109	PCW	C8-N-C6	3.76	118.85	108.98
4	F	202	PCW	O2-C31-C32	3.74	119.56	111.48
5	A	1107	CLR	C12-C11-C9	3.73	119.48	113.14
6	C	1110	AJP	C81-C12-C07	-3.73	103.47	111.58
4	E	203	PCW	O2-C31-C32	3.73	119.55	111.48
4	A	1118	PCW	C8-N-C6	3.71	118.73	108.98
6	C	1109	AJP	C13-C12-C11	3.70	115.34	108.11
6	A	1111	AJP	C11-C16-C15	3.69	115.69	109.17
5	C	1106	CLR	C12-C11-C9	3.69	119.41	113.14
6	C	1109	AJP	O84-C05-O09	-3.68	101.12	109.88
6	A	1111	AJP	C06-C07-C08	-3.67	98.39	104.28
5	A	1107	CLR	C10-C9-C8	3.66	118.06	112.71
6	A	1110	AJP	C13-C12-C11	3.65	115.25	108.11
6	A	1110	AJP	O84-C05-O09	-3.65	101.18	109.88
6	A	1110	AJP	O31-C30-C32	3.65	112.69	106.83
6	C	1109	AJP	C12-C11-C16	-3.65	108.82	113.90
4	A	1104	PCW	C8-N-C6	3.61	118.45	108.98
4	A	1114	PCW	C8-N-C6	3.61	118.45	108.98
4	C	1104	PCW	C8-N-C6	3.60	118.42	108.98
5	C	1111	CLR	C13-C17-C20	3.59	125.05	119.50
6	C	1109	AJP	C29-C28-C27	3.59	119.03	111.10
5	C	1111	CLR	C22-C20-C17	3.58	117.76	110.33
4	B	1111	PCW	C8-N-C6	3.58	118.38	108.98
6	C	1109	AJP	C81-C12-C11	-3.56	103.84	111.58
6	C	1110	AJP	C14-C13-C12	3.56	118.74	112.74
5	C	1106	CLR	C10-C9-C8	3.55	117.91	112.71
4	C	1103	PCW	C8-N-C6	3.54	118.28	108.98
6	C	1114	AJP	C14-C15-C20	-3.54	109.92	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1111	AJP	C14-C13-C12	3.53	118.69	112.74
3	B	1102	ZK1	CAV-NAP-CAT	-3.52	119.89	124.82
6	C	1109	AJP	O31-C30-C32	3.50	112.45	106.83
3	D	1102	ZK1	CAV-NAP-CAT	-3.50	119.92	124.82
6	C	1109	AJP	C12-C07-C06	3.49	130.81	120.50
4	A	1103	PCW	C8-N-C6	3.48	118.12	108.98
6	C	1109	AJP	O25-C26-C27	3.47	114.96	108.28
6	A	1110	AJP	C12-C07-C06	3.46	130.72	120.50
4	B	1110	PCW	C8-N-C6	3.45	118.03	108.98
4	A	1102	PCW	C8-N-C6	3.43	118.00	108.98
4	B	1103	PCW	O2-C31-C32	3.43	118.91	111.48
4	D	1103	PCW	O2-C31-C32	3.42	118.89	111.48
5	C	1111	CLR	C15-C14-C8	3.41	124.55	119.10
5	A	1112	CLR	C17-C13-C14	3.41	104.01	100.10
4	B	1105	PCW	C8-N-C6	3.40	117.92	108.98
6	A	1111	AJP	O84-C05-C04	3.40	113.73	110.76
6	C	1114	AJP	O31-C26-C27	3.39	117.34	110.37
4	D	1105	PCW	C8-N-C6	3.39	117.88	108.98
4	C	1102	PCW	C8-N-C6	3.39	117.88	108.98
6	C	1110	AJP	O84-C05-C04	3.38	113.70	110.76
4	D	1107	PCW	C8-N-C6	3.37	117.83	108.98
5	A	1112	CLR	C15-C14-C8	3.37	124.48	119.10
6	A	1111	AJP	C28-C29-C30	3.37	116.89	111.19
6	A	1110	AJP	C81-C12-C11	-3.36	104.28	111.58
4	A	1105	PCW	C8-N-C6	3.36	117.80	108.98
6	A	1110	AJP	C80-C20-C21	-3.34	104.09	108.99
6	C	1110	AJP	C12-C07-C06	3.33	130.34	120.50
6	A	1116	AJP	C14-C15-C20	-3.33	110.16	113.91
6	A	1110	AJP	C12-C11-C16	-3.32	109.27	113.90
5	C	1111	CLR	C10-C9-C8	3.32	117.56	112.71
6	A	1111	AJP	C85-O84-C05	3.31	119.41	113.69
6	C	1110	AJP	O31-C26-C27	3.31	117.17	110.37
4	D	1109	PCW	O2-C31-C32	3.31	118.64	111.48
4	B	1106	PCW	C8-N-C6	3.31	117.67	108.98
6	A	1111	AJP	C12-C07-C06	3.31	130.28	120.50
4	D	1106	PCW	C8-N-C6	3.31	117.67	108.98
4	A	1118	PCW	O2-C31-C32	3.27	118.55	111.48
6	C	1114	AJP	O84-C05-O09	-3.26	102.12	109.88
6	C	1110	AJP	C85-O84-C05	3.23	119.27	113.69
6	C	1109	AJP	O09-C05-C04	-3.23	101.98	108.54
6	C	1114	AJP	C15-C20-C19	3.22	112.98	108.51
6	A	1116	AJP	C81-C12-C11	-3.22	104.59	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	CLR	C1-C2-C3	3.22	114.74	110.48
6	A	1111	AJP	O25-C26-O31	-3.21	102.23	110.69
6	A	1116	AJP	C03-C02-C85	3.21	112.49	108.59
4	A	1103	PCW	O2-C31-C32	3.21	118.43	111.48
4	C	1112	PCW	C8-N-C6	3.21	117.41	108.98
5	A	1112	CLR	C10-C9-C8	3.20	117.39	112.71
4	A	1113	PCW	C8-N-C6	3.17	117.30	108.98
4	B	1107	PCW	C8-N-C6	3.16	117.28	108.98
6	C	1114	AJP	C81-C12-C11	-3.16	104.72	111.58
6	C	1110	AJP	O25-C26-O31	-3.15	102.40	110.69
6	A	1110	AJP	O09-C05-C04	-3.13	102.18	108.54
5	A	1112	CLR	C11-C9-C10	3.13	116.94	113.08
5	A	1112	CLR	C22-C20-C17	3.13	116.81	110.33
5	C	1111	CLR	C17-C13-C14	3.11	103.67	100.10
5	C	1111	CLR	C9-C10-C5	3.11	114.20	109.65
4	B	1111	PCW	O2-C31-C32	3.09	118.17	111.48
5	A	1112	CLR	C9-C10-C5	3.09	114.18	109.65
6	A	1116	AJP	O84-C05-O09	-3.09	102.53	109.88
5	C	1106	CLR	C1-C2-C3	3.08	114.56	110.48
6	C	1109	AJP	C80-C20-C21	-3.07	104.48	108.99
6	A	1116	AJP	O31-C26-C27	3.05	116.64	110.37
4	D	1105	PCW	C2-O2-C31	3.04	125.08	117.80
5	C	1111	CLR	C11-C9-C10	3.03	116.83	113.08
6	A	1111	AJP	C81-C12-C13	-3.02	106.15	110.61
6	C	1110	AJP	C28-C29-C30	2.99	116.26	111.19
4	D	1106	PCW	O3-C11-C12	2.99	120.95	111.83
6	C	1109	AJP	O31-C26-C27	2.98	115.45	110.84
4	C	1103	PCW	O2-C31-C32	2.97	117.91	111.48
6	C	1114	AJP	O09-C05-C06	-2.95	100.64	104.56
5	C	1106	CLR	C16-C17-C13	2.93	107.28	103.84
5	A	1107	CLR	C16-C17-C13	2.93	107.28	103.84
6	C	1110	AJP	C81-C12-C13	-2.92	106.31	110.61
3	C	1101	ZK1	CAT-CAU-NAY	2.91	120.57	117.41
4	B	1106	PCW	O3-C11-C12	2.87	120.59	111.83
6	A	1116	AJP	C21-C20-C19	2.86	109.96	107.23
6	C	1114	AJP	C21-C20-C19	2.83	109.93	107.23
4	D	1107	PCW	O3-C11-C12	2.82	120.44	111.83
3	A	1101	ZK1	CAT-CAU-NAY	2.80	120.45	117.41
6	A	1110	AJP	O31-C26-C27	2.79	116.10	110.37
6	C	1110	AJP	C83-C06-C07	2.78	120.06	114.50
5	A	1107	CLR	C7-C8-C9	2.78	112.94	109.72
6	A	1111	AJP	C11-C12-C07	2.78	104.35	100.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1107	PCW	O3-C11-C12	2.77	120.29	111.83
6	A	1116	AJP	O09-C05-C06	-2.77	100.88	104.56
6	A	1111	AJP	C83-C06-C07	2.74	119.97	114.50
4	C	1104	PCW	O3-C11-C12	2.71	120.10	111.83
4	A	1113	PCW	O3-C11-C12	2.70	120.06	111.83
3	A	1101	ZK1	CAU-CAT-NAP	2.69	120.21	117.46
4	A	1103	PCW	O3-C11-C12	2.69	120.03	111.83
4	C	1103	PCW	O3-C11-C12	2.69	120.03	111.83
6	A	1110	AJP	C26-O25-C23	2.68	119.75	115.27
3	B	1102	ZK1	FAG-CAZ-CAS	-2.68	107.89	112.65
4	A	1114	PCW	O3-C11-C12	2.67	119.97	111.83
4	A	1104	PCW	O3-C11-C12	2.66	119.95	111.83
3	B	1102	ZK1	CAT-CAU-NAY	2.66	120.30	117.41
4	A	1114	PCW	C2-O2-C31	-2.66	111.44	117.80
4	A	1102	PCW	O3-C11-C12	2.66	119.93	111.83
3	C	1101	ZK1	CAU-CAT-NAP	2.65	120.17	117.46
4	C	1102	PCW	O3-C11-C12	2.65	119.92	111.83
3	B	1102	ZK1	CAU-CAT-NAP	2.65	120.17	117.46
3	A	1101	ZK1	FAG-CAZ-CAS	-2.64	107.97	112.65
6	A	1111	AJP	O31-C26-C27	2.64	115.79	110.37
4	F	202	PCW	O3-C11-C12	2.64	119.87	111.83
4	D	1109	PCW	O3-C11-C12	2.63	119.86	111.83
6	A	1116	AJP	C05-C06-C07	2.63	107.24	103.37
4	A	1118	PCW	O3-C11-C12	2.63	119.85	111.83
3	D	1102	ZK1	CAT-CAU-NAY	2.63	120.26	117.41
4	C	1112	PCW	O3-C11-C12	2.61	119.78	111.83
6	C	1110	AJP	C11-C12-C07	2.60	104.08	100.16
3	C	1101	ZK1	FAG-CAZ-CAS	-2.60	108.04	112.65
4	E	203	PCW	O3-C11-C12	2.60	119.75	111.83
4	B	1111	PCW	O3-C11-C12	2.58	119.71	111.83
3	C	1101	ZK1	CAW-NAY-CAU	-2.57	119.67	122.84
3	D	1102	ZK1	CAU-CAT-NAP	2.57	120.08	117.46
3	D	1102	ZK1	FAG-CAZ-CAS	-2.57	108.09	112.65
4	B	1111	PCW	C2-O2-C31	-2.56	111.66	117.80
5	C	1106	CLR	C7-C8-C9	2.55	112.67	109.72
6	A	1116	AJP	C11-C12-C07	2.54	103.99	100.16
4	B	1105	PCW	C2-O2-C31	2.54	123.86	117.80
6	C	1109	AJP	O77-C28-C29	2.53	114.88	109.84
4	B	1103	PCW	O3-C11-C12	2.51	119.47	111.83
4	D	1103	PCW	O3-C11-C12	2.50	119.46	111.83
5	C	1111	CLR	C12-C13-C14	2.50	110.99	107.25
4	B	1110	PCW	O3-C11-C12	2.49	119.44	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	ZK1	CAW-NAY-CAU	-2.48	119.79	122.84
4	A	1105	PCW	O3-C11-C12	2.44	119.27	111.83
3	B	1102	ZK1	CAW-NAY-CAU	-2.44	119.84	122.84
6	A	1110	AJP	C14-C15-C16	2.44	115.18	111.78
6	A	1110	AJP	C26-O31-C30	2.43	115.82	113.13
5	A	1112	CLR	C23-C22-C20	-2.43	108.29	115.08
6	C	1114	AJP	C05-C06-C07	2.42	106.93	103.37
6	A	1111	AJP	C13-C12-C11	2.42	112.83	108.11
6	A	1110	AJP	C04-C03-C02	2.41	116.48	111.67
6	A	1110	AJP	O09-C08-C07	-2.40	98.55	104.08
5	C	1106	CLR	C3-C4-C5	2.39	115.87	112.05
6	A	1116	AJP	O09-C05-C04	-2.39	103.69	108.54
5	C	1111	CLR	C23-C22-C20	-2.37	108.45	115.08
6	C	1114	AJP	O09-C05-C04	-2.34	103.78	108.54
6	C	1110	AJP	C13-C12-C11	2.34	112.67	108.11
6	C	1114	AJP	C11-C12-C07	2.33	103.68	100.16
5	C	1111	CLR	C16-C17-C13	2.33	106.58	103.84
3	D	1102	ZK1	CAW-NAY-CAU	-2.33	119.98	122.84
6	C	1114	AJP	C13-C12-C11	2.32	112.65	108.11
5	A	1112	CLR	C12-C13-C14	2.32	110.71	107.25
4	D	1107	PCW	C2-O2-C31	-2.30	112.29	117.80
6	C	1109	AJP	C14-C15-C16	2.30	114.99	111.78
6	A	1116	AJP	C13-C12-C11	2.29	112.59	108.11
3	C	1101	ZK1	CAO-NAY-CAU	2.29	118.88	116.55
6	C	1114	AJP	O25-C26-C27	2.28	113.70	108.09
6	C	1114	AJP	C24-C19-C20	2.27	115.08	112.66
4	B	1104	PCW	O3-C11-C12	2.27	118.76	111.83
5	A	1107	CLR	C3-C4-C5	2.26	115.66	112.05
3	A	1101	ZK1	CAO-NAY-CAU	2.26	118.85	116.55
4	D	1104	PCW	O3-C11-C12	2.25	118.69	111.83
5	C	1106	CLR	C18-C13-C12	-2.25	107.29	110.61
6	C	1114	AJP	C04-C03-C02	2.25	116.16	111.67
6	C	1109	AJP	O09-C08-C07	-2.24	98.91	104.08
6	A	1110	AJP	C20-C15-C16	-2.23	110.17	112.43
5	A	1107	CLR	C18-C13-C12	-2.21	107.35	110.61
4	D	1105	PCW	O2-C2-C1	2.20	116.25	108.34
6	C	1114	AJP	O84-C85-C02	-2.18	109.38	112.17
6	A	1111	AJP	C21-C20-C15	2.17	113.01	110.10
6	A	1116	AJP	C18-C17-C16	2.17	115.62	112.16
6	A	1110	AJP	O25-C26-O31	-2.16	105.00	110.69
6	A	1110	AJP	O77-C28-C27	2.16	114.61	110.15
5	A	1112	CLR	C15-C14-C13	-2.15	101.32	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1112	CLR	C16-C17-C13	2.14	106.36	103.84
3	C	1101	ZK1	CAZ-CAS-CAR	2.14	124.80	122.06
5	C	1111	CLR	C1-C10-C9	2.14	111.56	108.74
5	C	1111	CLR	C15-C14-C13	-2.13	101.33	103.84
6	C	1114	AJP	C17-C16-C11	2.13	115.29	112.29
5	C	1111	CLR	C3-C4-C5	2.12	115.44	112.05
6	A	1110	AJP	C17-C16-C11	2.12	115.28	112.29
6	A	1116	AJP	O84-C85-C02	-2.12	109.45	112.17
4	B	1107	PCW	C2-O2-C31	-2.11	112.74	117.80
3	A	1101	ZK1	CAZ-CAS-CAR	2.09	124.73	122.06
3	D	1102	ZK1	CAO-NAY-CAU	2.08	118.67	116.55
3	B	1102	ZK1	CAO-NAY-CAU	2.08	118.67	116.55
6	C	1110	AJP	O79-C22-C21	-2.08	105.13	109.97
3	D	1102	ZK1	CAK-CAM-NAX	2.08	113.86	109.93
6	A	1110	AJP	C13-C14-C15	2.08	116.66	113.14
6	C	1109	AJP	C15-C20-C19	2.07	111.39	108.51
6	A	1110	AJP	C14-C15-C20	-2.06	111.59	113.91
6	C	1109	AJP	C14-C15-C20	-2.06	111.59	113.91
6	C	1109	AJP	C04-C03-C02	2.06	115.78	111.67
6	A	1111	AJP	O78-C27-C28	2.05	114.24	110.05
6	C	1109	AJP	C17-C16-C11	2.03	115.16	112.29
6	C	1109	AJP	C11-C10-C08	2.03	107.45	103.05
6	A	1110	AJP	C11-C10-C08	2.03	107.45	103.05
5	A	1112	CLR	C1-C10-C9	2.00	111.39	108.74
6	C	1109	AJP	C20-C15-C16	-2.00	110.40	112.43

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1107	CLR	C9
5	A	1107	CLR	C17
5	A	1112	CLR	C9
5	A	1112	CLR	C17
5	C	1106	CLR	C9
5	C	1106	CLR	C17
5	C	1111	CLR	C9
5	C	1111	CLR	C17
6	A	1110	AJP	C15
6	A	1110	AJP	C19
6	A	1110	AJP	C02
6	A	1110	AJP	C05
6	A	1110	AJP	C12

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Mol	Chain	Res	Type	Atom
6	A	1110	AJP	C06
6	A	1110	AJP	C20
6	A	1110	AJP	C27
6	A	1110	AJP	C26
6	A	1110	AJP	C28
6	A	1110	AJP	C16
6	A	1110	AJP	C23
6	A	1110	AJP	C11
6	A	1111	AJP	C19
6	A	1111	AJP	C05
6	A	1111	AJP	C06
6	A	1111	AJP	C20
6	A	1111	AJP	C07
6	A	1111	AJP	C27
6	A	1111	AJP	C26
6	A	1111	AJP	C23
6	A	1111	AJP	C11
6	A	1116	AJP	C19
6	A	1116	AJP	C05
6	A	1116	AJP	C22
6	A	1116	AJP	C06
6	A	1116	AJP	C20
6	A	1116	AJP	C07
6	A	1116	AJP	C23
6	A	1116	AJP	C27
6	A	1116	AJP	C28
6	C	1109	AJP	C15
6	C	1109	AJP	C19
6	C	1109	AJP	C02
6	C	1109	AJP	C05
6	C	1109	AJP	C12
6	C	1109	AJP	C06
6	C	1109	AJP	C20
6	C	1109	AJP	C26
6	C	1109	AJP	C28
6	C	1109	AJP	C16
6	C	1109	AJP	C23
6	C	1109	AJP	C11
6	C	1110	AJP	C19
6	C	1110	AJP	C05
6	C	1110	AJP	C06
6	C	1110	AJP	C20

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Mol	Chain	Res	Type	Atom
6	C	1110	AJP	C07
6	C	1110	AJP	C27
6	C	1110	AJP	C26
6	C	1110	AJP	C23
6	C	1110	AJP	C11
6	C	1114	AJP	C19
6	C	1114	AJP	C05
6	C	1114	AJP	C22
6	C	1114	AJP	C06
6	C	1114	AJP	C20
6	C	1114	AJP	C07
6	C	1114	AJP	C23
6	C	1114	AJP	C27
6	C	1114	AJP	C28

All (782) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1102	ZK1	NAY-CAO-PBA-OAC
3	B	1102	ZK1	NAY-CAO-PBA-OAD
3	D	1102	ZK1	NAY-CAO-PBA-OAC
3	D	1102	ZK1	NAY-CAO-PBA-OAD
4	A	1102	PCW	O2-C2-C3-O3
4	A	1102	PCW	C4-O4P-P-O2P
4	A	1102	PCW	C4-O4P-P-O3P
4	A	1103	PCW	O4P-C4-C5-N
4	A	1103	PCW	C1-O3P-P-O4P
4	A	1104	PCW	O4P-C4-C5-N
4	A	1104	PCW	C32-C31-O2-C2
4	A	1104	PCW	O31-C31-O2-C2
4	A	1104	PCW	C1-O3P-P-O1P
4	A	1104	PCW	C1-O3P-P-O2P
4	A	1104	PCW	C1-O3P-P-O4P
4	A	1104	PCW	C4-O4P-P-O3P
4	A	1105	PCW	O3P-C1-C2-O2
4	A	1105	PCW	C1-O3P-P-O1P
4	A	1105	PCW	C1-O3P-P-O4P
4	A	1106	PCW	C20-C21-C22-C23
4	A	1109	PCW	C20-C21-C22-C23
4	A	1113	PCW	O31-C31-O2-C2
4	A	1114	PCW	C1-O3P-P-O2P
4	A	1115	PCW	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
4	A	1117	PCW	C20-C21-C22-C23
4	A	1118	PCW	O2-C2-C3-O3
4	A	1118	PCW	O4P-C4-C5-N
4	A	1118	PCW	C1-O3P-P-O4P
4	A	1118	PCW	C4-O4P-P-O2P
4	B	1103	PCW	C1-O3P-P-O2P
4	B	1104	PCW	O4P-C4-C5-N
4	B	1104	PCW	C32-C31-O2-C2
4	B	1104	PCW	C1-O3P-P-O1P
4	B	1104	PCW	C1-O3P-P-O4P
4	B	1104	PCW	C4-O4P-P-O1P
4	B	1104	PCW	C4-O4P-P-O3P
4	B	1105	PCW	C5-C4-O4P-P
4	B	1105	PCW	C32-C31-O2-C2
4	B	1106	PCW	O4P-C4-C5-N
4	B	1106	PCW	C32-C31-O2-C2
4	B	1106	PCW	O31-C31-O2-C2
4	B	1107	PCW	C4-O4P-P-O2P
4	B	1108	PCW	C16-C17-C18-C19
4	B	1110	PCW	C1-O3P-P-O1P
4	B	1110	PCW	C1-O3P-P-O4P
4	B	1111	PCW	C1-O3P-P-O2P
4	B	1111	PCW	C1-O3P-P-O4P
4	C	1102	PCW	O2-C2-C3-O3
4	C	1102	PCW	C4-O4P-P-O2P
4	C	1102	PCW	C4-O4P-P-O3P
4	C	1103	PCW	C1-O3P-P-O1P
4	C	1103	PCW	C1-O3P-P-O4P
4	C	1104	PCW	O4P-C4-C5-N
4	C	1104	PCW	C32-C31-O2-C2
4	C	1104	PCW	O31-C31-O2-C2
4	C	1104	PCW	C1-O3P-P-O1P
4	C	1104	PCW	C1-O3P-P-O2P
4	C	1104	PCW	C1-O3P-P-O4P
4	C	1104	PCW	C4-O4P-P-O2P
4	C	1104	PCW	C4-O4P-P-O3P
4	C	1105	PCW	C20-C21-C22-C23
4	C	1108	PCW	C20-C21-C22-C23
4	C	1112	PCW	O31-C31-O2-C2
4	C	1112	PCW	C4-O4P-P-O1P
4	C	1112	PCW	C4-O4P-P-O2P
4	C	1112	PCW	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
4	C	1113	PCW	C20-C21-C22-C23
4	C	1115	PCW	C20-C21-C22-C23
4	D	1101	PCW	C20-C21-C22-C23
4	D	1103	PCW	C1-O3P-P-O2P
4	D	1104	PCW	O4P-C4-C5-N
4	D	1104	PCW	C32-C31-O2-C2
4	D	1104	PCW	C1-O3P-P-O1P
4	D	1104	PCW	C1-O3P-P-O4P
4	D	1104	PCW	C4-O4P-P-O1P
4	D	1104	PCW	C4-O4P-P-O3P
4	D	1105	PCW	C5-C4-O4P-P
4	D	1105	PCW	C32-C31-O2-C2
4	D	1106	PCW	O4P-C4-C5-N
4	D	1106	PCW	C32-C31-O2-C2
4	D	1106	PCW	O31-C31-O2-C2
4	D	1107	PCW	O4P-C4-C5-N
4	D	1107	PCW	C1-O3P-P-O2P
4	D	1107	PCW	C4-O4P-P-O2P
4	D	1109	PCW	O2-C2-C3-O3
4	D	1109	PCW	O4P-C4-C5-N
4	D	1109	PCW	C1-O3P-P-O4P
4	D	1109	PCW	C4-O4P-P-O2P
4	E	201	PCW	C20-C21-C22-C23
4	E	203	PCW	O4P-C4-C5-N
4	F	202	PCW	O4P-C4-C5-N
4	F	205	PCW	C20-C21-C22-C23
6	A	1111	AJP	C29-C30-C32-O33
6	A	1111	AJP	O31-C30-C32-O33
6	A	1116	AJP	C29-C30-C32-O33
6	C	1110	AJP	C29-C30-C32-O33
6	C	1110	AJP	O31-C30-C32-O33
6	A	1111	AJP	O31-C26-O25-C23
6	C	1110	AJP	O31-C26-O25-C23
6	A	1111	AJP	C27-C26-O25-C23
6	C	1110	AJP	C27-C26-O25-C23
4	A	1113	PCW	O11-C11-O3-C3
4	B	1104	PCW	O11-C11-O3-C3
4	C	1112	PCW	O11-C11-O3-C3
4	D	1104	PCW	O11-C11-O3-C3
4	B	1104	PCW	C12-C11-O3-C3
4	C	1112	PCW	C12-C11-O3-C3
4	D	1104	PCW	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
4	B	1107	PCW	O11-C11-O3-C3
4	D	1107	PCW	O11-C11-O3-C3
4	A	1103	PCW	O31-C31-O2-C2
4	B	1105	PCW	O31-C31-O2-C2
4	C	1103	PCW	O31-C31-O2-C2
4	D	1105	PCW	O31-C31-O2-C2
4	A	1113	PCW	C12-C11-O3-C3
4	B	1107	PCW	C12-C11-O3-C3
4	D	1107	PCW	C12-C11-O3-C3
4	A	1103	PCW	C32-C31-O2-C2
4	A	1113	PCW	C32-C31-O2-C2
4	C	1112	PCW	C32-C31-O2-C2
4	A	1104	PCW	C12-C11-O3-C3
4	B	1104	PCW	O31-C31-O2-C2
4	D	1104	PCW	O31-C31-O2-C2
4	C	1103	PCW	C33-C34-C35-C36
4	B	1103	PCW	C32-C31-O2-C2
4	C	1103	PCW	C32-C31-O2-C2
4	D	1103	PCW	C32-C31-O2-C2
4	D	1105	PCW	O11-C11-O3-C3
4	A	1104	PCW	O11-C11-O3-C3
4	B	1105	PCW	O11-C11-O3-C3
4	A	1114	PCW	O11-C11-O3-C3
4	A	1114	PCW	C12-C11-O3-C3
4	C	1104	PCW	C12-C11-O3-C3
4	B	1107	PCW	C32-C33-C34-C35
4	C	1104	PCW	C14-C15-C16-C17
4	B	1111	PCW	O11-C11-O3-C3
4	C	1104	PCW	O11-C11-O3-C3
6	C	1109	AJP	O31-C26-O25-C23
4	B	1103	PCW	O31-C31-O2-C2
4	D	1103	PCW	O31-C31-O2-C2
4	A	1103	PCW	C12-C11-O3-C3
4	B	1103	PCW	C12-C11-O3-C3
4	B	1111	PCW	C12-C11-O3-C3
4	C	1103	PCW	C12-C11-O3-C3
4	D	1103	PCW	C12-C11-O3-C3
4	E	203	PCW	C12-C11-O3-C3
4	F	202	PCW	C12-C11-O3-C3
4	A	1103	PCW	C33-C34-C35-C36
4	B	1105	PCW	C4-C5-N-C8
4	C	1112	PCW	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
4	D	1105	PCW	C4-C5-N-C8
4	D	1107	PCW	C4-C5-N-C8
4	A	1113	PCW	C13-C14-C15-C16
4	B	1105	PCW	C12-C11-O3-C3
4	B	1103	PCW	C15-C16-C17-C18
4	C	1103	PCW	O11-C11-O3-C3
4	D	1105	PCW	C12-C11-O3-C3
4	D	1103	PCW	O11-C11-O3-C3
4	B	1106	PCW	O3P-C1-C2-O2
4	B	1110	PCW	O3P-C1-C2-O2
4	F	202	PCW	C13-C14-C15-C16
4	D	1103	PCW	C15-C16-C17-C18
4	F	202	PCW	O11-C11-O3-C3
4	B	1111	PCW	C32-C33-C34-C35
4	E	203	PCW	C13-C14-C15-C16
5	C	1106	CLR	C20-C22-C23-C24
4	A	1104	PCW	C12-C13-C14-C15
4	A	1104	PCW	C14-C15-C16-C17
4	D	1107	PCW	C32-C33-C34-C35
4	B	1105	PCW	C4-C5-N-C7
4	D	1105	PCW	C4-C5-N-C7
4	A	1118	PCW	C31-C32-C33-C34
4	D	1109	PCW	C31-C32-C33-C34
4	B	1103	PCW	O11-C11-O3-C3
4	E	203	PCW	O11-C11-O3-C3
4	E	203	PCW	C32-C31-O2-C2
4	F	202	PCW	C32-C31-O2-C2
5	A	1107	CLR	C20-C22-C23-C24
4	A	1114	PCW	C31-C32-C33-C34
4	A	1114	PCW	C32-C33-C34-C35
5	A	1112	CLR	C20-C22-C23-C24
5	C	1111	CLR	C20-C22-C23-C24
4	A	1103	PCW	O11-C11-O3-C3
4	A	1102	PCW	C36-C37-C38-C39
4	C	1102	PCW	C36-C37-C38-C39
4	B	1106	PCW	C12-C11-O3-C3
6	C	1109	AJP	C27-C26-O25-C23
4	D	1105	PCW	C34-C35-C36-C37
4	E	203	PCW	O31-C31-O2-C2
4	F	202	PCW	O31-C31-O2-C2
4	D	1106	PCW	C12-C11-O3-C3
4	A	1113	PCW	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
4	B	1107	PCW	C4-C5-N-C7
4	B	1107	PCW	C4-C5-N-C8
4	C	1112	PCW	C4-C5-N-C7
5	C	1106	CLR	C23-C24-C25-C27
4	B	1101	PCW	C20-C21-C22-C23
4	D	1110	PCW	C20-C21-C22-C23
5	A	1107	CLR	C23-C24-C25-C27
4	E	202	PCW	C14-C15-C16-C17
4	A	1102	PCW	C12-C11-O3-C3
4	B	1105	PCW	C34-C35-C36-C37
4	B	1107	PCW	C4-C5-N-C6
4	D	1107	PCW	C4-C5-N-C7
4	E	203	PCW	C31-C32-C33-C34
4	A	1103	PCW	C41-C42-C43-C44
4	E	201	PCW	C15-C16-C17-C18
5	C	1111	CLR	C13-C17-C20-C22
4	D	1106	PCW	O11-C11-O3-C3
4	C	1102	PCW	C12-C13-C14-C15
4	F	202	PCW	C35-C36-C37-C38
4	A	1109	PCW	C15-C16-C17-C18
4	C	1108	PCW	C15-C16-C17-C18
4	D	1106	PCW	C14-C15-C16-C17
4	A	1118	PCW	C12-C13-C14-C15
4	B	1106	PCW	O11-C11-O3-C3
4	A	1102	PCW	C13-C14-C15-C16
4	C	1104	PCW	C15-C16-C17-C18
4	D	1109	PCW	C33-C34-C35-C36
4	A	1102	PCW	C12-C13-C14-C15
4	A	1113	PCW	C41-C42-C43-C44
4	C	1112	PCW	C41-C42-C43-C44
4	B	1106	PCW	C14-C15-C16-C17
5	A	1107	CLR	C23-C24-C25-C26
5	C	1106	CLR	C23-C24-C25-C26
5	A	1112	CLR	C13-C17-C20-C22
4	C	1102	PCW	C33-C34-C35-C36
4	F	205	PCW	C15-C16-C17-C18
4	E	201	PCW	C14-C15-C16-C17
4	D	1107	PCW	C31-C32-C33-C34
4	A	1102	PCW	C33-C34-C35-C36
4	A	1103	PCW	C32-C33-C34-C35
4	F	202	PCW	C33-C34-C35-C36
4	A	1118	PCW	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	A	1103	PCW	C35-C36-C37-C38
4	D	1104	PCW	C12-C13-C14-C15
4	A	1102	PCW	C34-C35-C36-C37
4	D	1109	PCW	C12-C13-C14-C15
4	B	1104	PCW	C12-C13-C14-C15
4	C	1102	PCW	C13-C14-C15-C16
4	C	1102	PCW	C34-C35-C36-C37
4	C	1102	PCW	C12-C11-O3-C3
4	D	1109	PCW	C12-C11-O3-C3
4	C	1103	PCW	C1-C2-C3-O3
4	A	1105	PCW	C14-C15-C16-C17
4	A	1118	PCW	C23-C24-C25-C26
4	A	1118	PCW	C33-C34-C35-C36
4	C	1103	PCW	C35-C36-C37-C38
4	C	1103	PCW	C41-C42-C43-C44
4	D	1108	PCW	C14-C15-C16-C17
4	F	205	PCW	C14-C15-C16-C17
4	C	1102	PCW	C23-C24-C25-C26
4	A	1102	PCW	C35-C36-C37-C38
4	F	201	PCW	C14-C15-C16-C17
4	D	1107	PCW	C4-C5-N-C6
4	C	1102	PCW	C35-C36-C37-C38
4	E	203	PCW	C35-C36-C37-C38
4	A	1114	PCW	C21-C22-C23-C24
4	B	1104	PCW	C34-C35-C36-C37
4	D	1109	PCW	C14-C15-C16-C17
4	A	1117	PCW	C16-C17-C18-C19
4	B	1104	PCW	C36-C37-C38-C39
4	C	1115	PCW	C16-C17-C18-C19
4	B	1104	PCW	C32-C33-C34-C35
4	D	1109	PCW	C22-C23-C24-C25
4	A	1102	PCW	O11-C11-O3-C3
4	A	1102	PCW	C23-C24-C25-C26
4	A	1105	PCW	C41-C42-C43-C44
4	C	1104	PCW	C31-C32-C33-C34
4	F	202	PCW	C31-C32-C33-C34
4	A	1118	PCW	C12-C11-O3-C3
4	D	1109	PCW	O11-C11-O3-C3
4	D	1104	PCW	C32-C33-C34-C35
4	A	1113	PCW	C23-C24-C25-C26
4	B	1110	PCW	C14-C15-C16-C17
4	C	1112	PCW	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
4	B	1107	PCW	C32-C31-O2-C2
4	D	1107	PCW	C32-C31-O2-C2
4	D	1106	PCW	C31-C32-C33-C34
4	D	1109	PCW	C23-C24-C25-C26
4	E	203	PCW	C33-C34-C35-C36
4	A	1102	PCW	C16-C17-C18-C19
4	B	1103	PCW	C16-C17-C18-C19
4	D	1103	PCW	C16-C17-C18-C19
4	D	1104	PCW	C36-C37-C38-C39
4	E	203	PCW	C40-C41-C42-C43
4	A	1118	PCW	C14-C15-C16-C17
4	C	1103	PCW	C34-C35-C36-C37
4	A	1105	PCW	C34-C35-C36-C37
4	B	1110	PCW	C24-C25-C26-C27
4	E	203	PCW	C12-C13-C14-C15
6	A	1110	AJP	C27-C26-O25-C23
4	B	1101	PCW	C14-C15-C16-C17
4	F	202	PCW	C12-C13-C14-C15
4	C	1102	PCW	O11-C11-O3-C3
4	B	1106	PCW	C31-C32-C33-C34
4	D	1107	PCW	O31-C31-O2-C2
4	D	1106	PCW	O3P-C1-C2-O2
4	D	1104	PCW	C33-C34-C35-C36
4	F	202	PCW	C15-C16-C17-C18
4	A	1118	PCW	C16-C17-C18-C19
4	C	1102	PCW	C16-C17-C18-C19
4	E	201	PCW	C16-C17-C18-C19
4	E	203	PCW	C16-C17-C18-C19
4	F	202	PCW	C16-C17-C18-C19
4	F	205	PCW	C16-C17-C18-C19
4	B	1110	PCW	C41-C42-C43-C44
4	B	1111	PCW	C21-C22-C23-C24
4	D	1104	PCW	C37-C38-C39-C40
4	E	204	PCW	C14-C15-C16-C17
5	A	1107	CLR	C16-C17-C20-C21
4	D	1103	PCW	C12-C13-C14-C15
4	F	203	PCW	C14-C15-C16-C17
4	C	1104	PCW	C12-C13-C14-C15
4	B	1106	PCW	C34-C35-C36-C37
4	B	1110	PCW	C13-C14-C15-C16
4	A	1103	PCW	C15-C16-C17-C18
4	C	1104	PCW	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	D	1106	PCW	C34-C35-C36-C37
4	A	1109	PCW	C13-C14-C15-C16
4	C	1112	PCW	C15-C16-C17-C18
4	C	1108	PCW	C13-C14-C15-C16
4	C	1103	PCW	C15-C16-C17-C18
4	A	1118	PCW	O11-C11-O3-C3
5	C	1106	CLR	C16-C17-C20-C21
4	D	1101	PCW	C14-C15-C16-C17
4	B	1111	PCW	C22-C23-C24-C25
4	A	1102	PCW	C40-C41-C42-C43
4	A	1109	PCW	C16-C17-C18-C19
4	A	1113	PCW	C16-C17-C18-C19
4	A	1118	PCW	C36-C37-C38-C39
4	B	1106	PCW	C16-C17-C18-C19
4	B	1110	PCW	C40-C41-C42-C43
4	C	1102	PCW	C40-C41-C42-C43
4	C	1108	PCW	C16-C17-C18-C19
4	D	1104	PCW	C40-C41-C42-C43
4	D	1106	PCW	C16-C17-C18-C19
4	E	203	PCW	C36-C37-C38-C39
4	F	202	PCW	C40-C41-C42-C43
4	A	1114	PCW	C22-C23-C24-C25
4	C	1103	PCW	C32-C33-C34-C35
4	B	1110	PCW	O3P-C1-C2-C3
4	C	1102	PCW	O3P-C1-C2-C3
4	D	1106	PCW	O3P-C1-C2-C3
4	D	1109	PCW	O3P-C1-C2-C3
4	B	1107	PCW	O31-C31-O2-C2
4	B	1104	PCW	C33-C34-C35-C36
4	B	1106	PCW	C33-C34-C35-C36
4	A	1105	PCW	C13-C14-C15-C16
4	B	1103	PCW	C12-C13-C14-C15
4	D	1107	PCW	C11-C12-C13-C14
4	D	1106	PCW	C33-C34-C35-C36
4	B	1103	PCW	C17-C18-C19-C20
4	B	1104	PCW	C13-C14-C15-C16
4	A	1102	PCW	C1-C2-C3-O3
4	A	1104	PCW	C1-C2-C3-O3
4	A	1118	PCW	C1-C2-C3-O3
4	B	1106	PCW	C1-C2-C3-O3
4	B	1107	PCW	C1-C2-C3-O3
4	C	1102	PCW	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	1104	PCW	C1-C2-C3-O3
4	D	1103	PCW	C1-C2-C3-O3
4	D	1106	PCW	C1-C2-C3-O3
4	D	1107	PCW	C1-C2-C3-O3
4	D	1109	PCW	C1-C2-C3-O3
4	A	1104	PCW	C40-C41-C42-C43
4	B	1109	PCW	C16-C17-C18-C19
4	C	1107	PCW	C16-C17-C18-C19
4	D	1109	PCW	C36-C37-C38-C39
4	F	202	PCW	C36-C37-C38-C39
4	E	203	PCW	C32-C33-C34-C35
4	E	203	PCW	C15-C16-C17-C18
4	D	1105	PCW	C4-C5-N-C6
4	D	1106	PCW	C12-C13-C14-C15
4	E	204	PCW	C15-C16-C17-C18
4	F	203	PCW	C15-C16-C17-C18
4	B	1107	PCW	C11-C12-C13-C14
4	B	1109	PCW	C20-C21-C22-C23
4	C	1107	PCW	C20-C21-C22-C23
5	A	1107	CLR	C22-C23-C24-C25
4	B	1104	PCW	C15-C16-C17-C18
4	D	1103	PCW	C23-C24-C25-C26
4	D	1104	PCW	C34-C35-C36-C37
4	D	1110	PCW	C13-C14-C15-C16
4	A	1114	PCW	C15-C16-C17-C18
4	B	1109	PCW	C13-C14-C15-C16
4	A	1103	PCW	C1-C2-O2-C31
4	A	1104	PCW	C33-C34-C35-C36
4	D	1104	PCW	C15-C16-C17-C18
4	B	1111	PCW	C36-C37-C38-C39
4	D	1109	PCW	C16-C17-C18-C19
4	D	1110	PCW	C16-C17-C18-C19
4	E	205	PCW	C16-C17-C18-C19
4	B	1107	PCW	C33-C34-C35-C36
4	B	1111	PCW	C15-C16-C17-C18
4	B	1111	PCW	O3P-C1-C2-O2
5	C	1106	CLR	C22-C23-C24-C25
6	A	1116	AJP	O31-C30-C32-O33
4	A	1103	PCW	C42-C43-C44-C45
4	D	1101	PCW	C13-C14-C15-C16
4	A	1104	PCW	C15-C16-C17-C18
4	C	1107	PCW	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	B	1103	PCW	C23-C24-C25-C26
4	B	1109	PCW	C15-C16-C17-C18
5	A	1107	CLR	C13-C17-C20-C21
4	B	1105	PCW	C4-C5-N-C6
4	B	1110	PCW	C34-C35-C36-C37
4	D	1109	PCW	C35-C36-C37-C38
4	F	205	PCW	C13-C14-C15-C16
4	D	1103	PCW	C17-C18-C19-C20
4	E	201	PCW	C19-C20-C21-C22
4	B	1101	PCW	C13-C14-C15-C16
4	C	1112	PCW	C31-C32-C33-C34
4	D	1110	PCW	C15-C16-C17-C18
4	B	1106	PCW	C12-C13-C14-C15
4	A	1114	PCW	C17-C18-C19-C20
4	B	1104	PCW	C37-C38-C39-C40
4	B	1111	PCW	C17-C18-C19-C20
4	F	205	PCW	C19-C20-C21-C22
4	C	1103	PCW	C11-C12-C13-C14
4	A	1105	PCW	C40-C41-C42-C43
4	A	1104	PCW	C31-C32-C33-C34
4	E	201	PCW	C13-C14-C15-C16
4	A	1102	PCW	O3P-C1-C2-C3
4	A	1103	PCW	O3P-C1-C2-C3
4	A	1105	PCW	O3P-C1-C2-C3
4	B	1103	PCW	O3P-C1-C2-C3
4	B	1106	PCW	O3P-C1-C2-C3
4	C	1103	PCW	O3P-C1-C2-C3
4	D	1103	PCW	O3P-C1-C2-C3
5	C	1106	CLR	C13-C17-C20-C21
4	B	1107	PCW	C15-C16-C17-C18
4	F	204	PCW	C13-C14-C15-C16
4	F	204	PCW	C16-C17-C18-C19
4	D	1107	PCW	C33-C34-C35-C36
4	C	1103	PCW	C42-C43-C44-C45
4	B	1104	PCW	C1-C2-C3-O3
4	D	1104	PCW	C1-C2-C3-O3
4	C	1105	PCW	C13-C14-C15-C16
4	A	1102	PCW	O3P-C1-C2-O2
4	A	1113	PCW	O3P-C1-C2-O2
4	A	1114	PCW	O3P-C1-C2-O2
4	A	1118	PCW	O3P-C1-C2-O2
4	C	1102	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	1104	PCW	O3P-C1-C2-O2
4	C	1112	PCW	O3P-C1-C2-O2
4	D	1103	PCW	O3P-C1-C2-O2
4	A	1105	PCW	C21-C22-C23-C24
4	A	1106	PCW	C13-C14-C15-C16
4	B	1109	PCW	C14-C15-C16-C17
4	A	1114	PCW	O2-C2-C3-O3
4	B	1106	PCW	O2-C2-C3-O3
4	C	1104	PCW	O2-C2-C3-O3
4	D	1103	PCW	O2-C2-C3-O3
4	D	1106	PCW	O2-C2-C3-O3
4	D	1107	PCW	C15-C16-C17-C18
4	A	1103	PCW	C11-C12-C13-C14
4	B	1107	PCW	C35-C36-C37-C38
4	D	1110	PCW	C14-C15-C16-C17
4	A	1113	PCW	C31-C32-C33-C34
4	F	201	PCW	C15-C16-C17-C18
4	B	1104	PCW	C16-C17-C18-C19
4	B	1104	PCW	C40-C41-C42-C43
4	D	1104	PCW	C13-C14-C15-C16
3	B	1102	ZK1	CAI-CAR-NAX-CAN
4	C	1104	PCW	C13-C14-C15-C16
4	C	1112	PCW	C13-C14-C15-C16
4	B	1110	PCW	C31-C32-C33-C34
4	B	1106	PCW	C19-C20-C21-C22
4	B	1107	PCW	C39-C40-C41-C42
4	D	1106	PCW	C19-C20-C21-C22
4	D	1107	PCW	C39-C40-C41-C42
3	D	1102	ZK1	CAI-CAR-NAX-CAN
3	A	1101	ZK1	NAY-CAO-PBA-OAD
3	A	1101	ZK1	NAY-CAO-PBA-OAE
3	B	1102	ZK1	NAY-CAO-PBA-OAE
3	C	1101	ZK1	NAY-CAO-PBA-OAD
3	C	1101	ZK1	NAY-CAO-PBA-OAE
3	D	1102	ZK1	NAY-CAO-PBA-OAE
4	D	1108	PCW	C13-C14-C15-C16
4	E	202	PCW	C15-C16-C17-C18
4	C	1112	PCW	C40-C41-C42-C43
4	C	1112	PCW	C21-C22-C23-C24
4	A	1113	PCW	O3P-C1-C2-C3
4	A	1118	PCW	O3P-C1-C2-C3
4	C	1104	PCW	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	1112	PCW	O3P-C1-C2-C3
4	F	202	PCW	C2-C1-O3P-P
4	A	1109	PCW	C14-C15-C16-C17
4	C	1108	PCW	C14-C15-C16-C17
4	C	1115	PCW	C13-C14-C15-C16
4	B	1108	PCW	C20-C21-C22-C23
4	B	1110	PCW	C21-C22-C23-C24
4	A	1117	PCW	C13-C14-C15-C16
4	C	1102	PCW	C11-C12-C13-C14
4	E	202	PCW	C13-C14-C15-C16
4	B	1103	PCW	C14-C15-C16-C17
4	E	205	PCW	C13-C14-C15-C16
4	C	1103	PCW	C1-C2-O2-C31
4	D	1103	PCW	C3-C2-O2-C31
4	A	1113	PCW	C20-C21-C22-C23
4	A	1113	PCW	C40-C41-C42-C43
4	A	1114	PCW	C40-C41-C42-C43
4	D	1106	PCW	C36-C37-C38-C39
4	A	1105	PCW	C24-C25-C26-C27
4	A	1103	PCW	O3P-C1-C2-O2
4	A	1104	PCW	O3P-C1-C2-O2
4	B	1103	PCW	O3P-C1-C2-O2
4	C	1103	PCW	O3P-C1-C2-O2
4	E	203	PCW	C41-C42-C43-C44
4	B	1104	PCW	C35-C36-C37-C38
4	A	1103	PCW	C13-C14-C15-C16
4	A	1105	PCW	C5-C4-O4P-P
4	B	1110	PCW	C5-C4-O4P-P
4	D	1107	PCW	C13-C14-C15-C16
4	A	1104	PCW	O2-C2-C3-O3
4	B	1104	PCW	O2-C2-C3-O3
4	B	1106	PCW	C36-C37-C38-C39
4	B	1111	PCW	O2-C2-C3-O3
4	D	1104	PCW	O2-C2-C3-O3
4	C	1112	PCW	C4-C5-N-C6
4	B	1107	PCW	C12-C13-C14-C15
4	A	1105	PCW	C32-C33-C34-C35
4	B	1107	PCW	C13-C14-C15-C16
4	D	1107	PCW	C12-C13-C14-C15
4	B	1103	PCW	C32-C33-C34-C35
4	A	1102	PCW	O4P-C4-C5-N
4	A	1105	PCW	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
4	A	1114	PCW	O4P-C4-C5-N
4	B	1103	PCW	O4P-C4-C5-N
4	B	1107	PCW	O4P-C4-C5-N
4	B	1110	PCW	O4P-C4-C5-N
4	B	1111	PCW	O4P-C4-C5-N
4	C	1102	PCW	O4P-C4-C5-N
4	C	1103	PCW	O4P-C4-C5-N
4	D	1103	PCW	O4P-C4-C5-N
4	A	1103	PCW	C34-C35-C36-C37
4	B	1110	PCW	C32-C31-O2-C2
4	F	203	PCW	C13-C14-C15-C16
4	D	1103	PCW	C19-C20-C21-C22
4	E	204	PCW	C16-C17-C18-C19
4	F	203	PCW	C16-C17-C18-C19
4	A	1102	PCW	C14-C15-C16-C17
4	A	1104	PCW	O3P-C1-C2-C3
4	B	1107	PCW	O3P-C1-C2-C3
4	E	204	PCW	C13-C14-C15-C16
4	A	1113	PCW	C35-C36-C37-C38
4	C	1112	PCW	C35-C36-C37-C38
4	D	1103	PCW	C14-C15-C16-C17
4	B	1106	PCW	C15-C16-C17-C18
4	D	1107	PCW	C35-C36-C37-C38
4	A	1104	PCW	C37-C38-C39-C40
4	D	1109	PCW	C39-C40-C41-C42
4	D	1106	PCW	C11-C12-C13-C14
4	A	1105	PCW	C2-C1-O3P-P
4	A	1118	PCW	C2-C1-O3P-P
4	B	1103	PCW	C2-C1-O3P-P
4	B	1110	PCW	C2-C1-O3P-P
4	D	1109	PCW	C2-C1-O3P-P
4	C	1102	PCW	C42-C43-C44-C45
4	B	1110	PCW	O31-C31-O2-C2
4	D	1109	PCW	O3P-C1-C2-O2
4	E	202	PCW	C16-C17-C18-C19
4	D	1104	PCW	C17-C18-C19-C20
4	E	205	PCW	C17-C18-C19-C20
4	A	1102	PCW	C11-C12-C13-C14
4	B	1103	PCW	O2-C2-C3-O3
4	C	1103	PCW	O2-C2-C3-O3
4	D	1107	PCW	O2-C2-C3-O3
5	C	1111	CLR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
4	A	1114	PCW	C33-C34-C35-C36
4	D	1106	PCW	C15-C16-C17-C18
4	A	1103	PCW	C1-C2-C3-O3
4	A	1114	PCW	C1-C2-C3-O3
4	B	1103	PCW	C1-C2-C3-O3
4	B	1111	PCW	C1-C2-C3-O3
4	A	1102	PCW	C42-C43-C44-C45
5	C	1111	CLR	C16-C17-C20-C21
4	B	1111	PCW	C42-C43-C44-C45
4	A	1113	PCW	C22-C23-C24-C25
4	D	1104	PCW	C35-C36-C37-C38
4	A	1103	PCW	C4-O4P-P-O3P
4	A	1104	PCW	C4-O4P-P-O2P
4	A	1105	PCW	C4-O4P-P-O2P
4	A	1113	PCW	C4-C5-N-C7
4	A	1113	PCW	C4-O4P-P-O2P
4	A	1114	PCW	C1-O3P-P-O4P
4	A	1118	PCW	C1-O3P-P-O2P
4	B	1103	PCW	C1-O3P-P-O4P
4	B	1104	PCW	C1-O3P-P-O2P
4	B	1107	PCW	C1-O3P-P-O2P
4	B	1107	PCW	C4-O4P-P-O1P
4	B	1107	PCW	C4-O4P-P-O3P
4	B	1110	PCW	C4-O4P-P-O1P
4	B	1110	PCW	C4-O4P-P-O2P
4	B	1110	PCW	C4-O4P-P-O3P
4	B	1111	PCW	C4-O4P-P-O3P
4	C	1112	PCW	C1-O3P-P-O2P
4	D	1104	PCW	C1-O3P-P-O2P
4	D	1107	PCW	C4-O4P-P-O1P
4	D	1107	PCW	C4-O4P-P-O3P
4	D	1109	PCW	C1-O3P-P-O2P
3	C	1101	ZK1	CAI-CAR-NAX-CAN
4	B	1105	PCW	C36-C37-C38-C39
4	B	1106	PCW	C2-C1-O3P-P
4	D	1103	PCW	C2-C1-O3P-P
4	D	1104	PCW	C2-C1-O3P-P
4	D	1106	PCW	C2-C1-O3P-P
4	E	203	PCW	C2-C1-O3P-P
4	C	1107	PCW	C13-C14-C15-C16
4	B	1103	PCW	C19-C20-C21-C22
4	D	1101	PCW	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
4	B	1103	PCW	C3-C2-O2-C31
4	D	1105	PCW	C1-C2-O2-C31
4	C	1103	PCW	C13-C14-C15-C16
4	B	1111	PCW	O3P-C1-C2-C3
4	D	1107	PCW	O3P-C1-C2-C3
4	F	201	PCW	C13-C14-C15-C16
4	F	202	PCW	C32-C33-C34-C35
4	C	1104	PCW	C37-C38-C39-C40
4	D	1104	PCW	C11-C12-C13-C14
4	D	1109	PCW	C11-C12-C13-C14
4	B	1107	PCW	O3P-C1-C2-O2
3	A	1101	ZK1	CAI-CAR-NAX-CAN
4	A	1114	PCW	C36-C37-C38-C39
4	B	1103	PCW	C22-C23-C24-C25
4	C	1112	PCW	C22-C23-C24-C25
4	B	1104	PCW	C2-C1-O3P-P
4	A	1103	PCW	O2-C2-C3-O3
4	B	1107	PCW	O2-C2-C3-O3
4	F	202	PCW	C14-C15-C16-C17
4	D	1103	PCW	C13-C14-C15-C16
4	A	1103	PCW	C12-C13-C14-C15
4	E	203	PCW	C14-C15-C16-C17
4	B	1106	PCW	C32-C33-C34-C35
4	D	1109	PCW	C42-C43-C44-C45
5	C	1111	CLR	C23-C24-C25-C27
4	A	1118	PCW	C39-C40-C41-C42
4	B	1101	PCW	C17-C18-C19-C20
4	F	204	PCW	C17-C18-C19-C20
4	D	1106	PCW	C32-C33-C34-C35
4	A	1104	PCW	C11-C12-C13-C14
4	B	1106	PCW	C11-C12-C13-C14
4	A	1113	PCW	C34-C35-C36-C37
4	C	1112	PCW	C34-C35-C36-C37
4	C	1102	PCW	C14-C15-C16-C17
4	D	1103	PCW	C31-C32-C33-C34
4	A	1102	PCW	C2-C1-O3P-P
5	A	1107	CLR	C13-C17-C20-C22
4	A	1108	PCW	C19-C20-C21-C22
4	B	1104	PCW	C39-C40-C41-C42
4	D	1103	PCW	C22-C23-C24-C25
4	C	1107	PCW	C19-C20-C21-C22
4	B	1101	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	C	1102	PCW	C2-C1-O3P-P
4	B	1103	PCW	C13-C14-C15-C16
4	D	1108	PCW	C20-C21-C22-C23
4	C	1112	PCW	C12-C13-C14-C15
6	A	1110	AJP	O31-C26-O25-C23
4	C	1103	PCW	C12-C13-C14-C15
4	D	1101	PCW	C15-C16-C17-C18
4	A	1108	PCW	C14-C15-C16-C17
4	A	1104	PCW	C32-C33-C34-C35
4	A	1105	PCW	C33-C34-C35-C36
4	B	1105	PCW	C1-C2-O2-C31
4	E	203	PCW	C1-C2-O2-C31
4	E	203	PCW	C3-C2-O2-C31
4	F	202	PCW	C3-C2-O2-C31
4	B	1110	PCW	C16-C17-C18-C19
4	A	1115	PCW	C16-C17-C18-C19
4	C	1113	PCW	C16-C17-C18-C19
4	D	1104	PCW	C16-C17-C18-C19
4	F	202	PCW	C41-C42-C43-C44
4	D	1105	PCW	C32-C33-C34-C35
4	E	203	PCW	C11-C12-C13-C14
4	D	1104	PCW	C39-C40-C41-C42
4	E	203	PCW	O2-C2-C3-O3
4	B	1101	PCW	C16-C17-C18-C19
4	F	201	PCW	C16-C17-C18-C19
4	A	1118	PCW	C11-C12-C13-C14
5	C	1106	CLR	C13-C17-C20-C22
4	A	1114	PCW	C42-C43-C44-C45
4	B	1111	PCW	O31-C31-O2-C2
4	A	1113	PCW	C1-C2-C3-O3
3	A	1101	ZK1	CAI-CAR-NAX-CAM
3	A	1101	ZK1	NAY-CAO-PBA-OAC
3	C	1101	ZK1	NAY-CAO-PBA-OAC
4	F	202	PCW	C11-C12-C13-C14
4	C	1104	PCW	C32-C33-C34-C35
4	A	1114	PCW	O3P-C1-C2-C3
4	F	202	PCW	O2-C2-C3-O3
4	B	1110	PCW	C37-C38-C39-C40
4	B	1110	PCW	C39-C40-C41-C42
4	C	1102	PCW	C19-C20-C21-C22
4	F	204	PCW	C19-C20-C21-C22
4	B	1104	PCW	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
4	A	1104	PCW	C2-C1-O3P-P
4	C	1104	PCW	C2-C1-O3P-P
4	B	1104	PCW	C14-C15-C16-C17
4	C	1105	PCW	C16-C17-C18-C19
4	A	1102	PCW	C19-C20-C21-C22
4	A	1108	PCW	C17-C18-C19-C20
4	A	1114	PCW	C39-C40-C41-C42
4	E	205	PCW	C19-C20-C21-C22
4	F	202	PCW	C1-C2-O2-C31
4	A	1105	PCW	C39-C40-C41-C42
4	C	1103	PCW	C17-C18-C19-C20
4	D	1108	PCW	C17-C18-C19-C20
4	A	1106	PCW	C16-C17-C18-C19
4	A	1113	PCW	C21-C22-C23-C24
4	B	1111	PCW	C39-C40-C41-C42
4	B	1104	PCW	C5-C4-O4P-P
4	D	1104	PCW	C5-C4-O4P-P
4	B	1103	PCW	O3-C11-C12-C13
4	D	1103	PCW	O3-C11-C12-C13
6	A	1110	AJP	O31-C30-C32-O33
6	C	1114	AJP	O31-C30-C32-O33
3	C	1101	ZK1	CAI-CAR-NAX-CAM
4	A	1114	PCW	C16-C17-C18-C19
4	A	1113	PCW	C37-C38-C39-C40
4	B	1106	PCW	C17-C18-C19-C20
4	B	1108	PCW	C17-C18-C19-C20
4	C	1108	PCW	C19-C20-C21-C22
4	C	1112	PCW	C37-C38-C39-C40
4	D	1106	PCW	C17-C18-C19-C20
4	F	205	PCW	C17-C18-C19-C20
4	B	1110	PCW	O2-C31-C32-C33
4	A	1103	PCW	C17-C18-C19-C20
4	A	1113	PCW	C4-C5-N-C6
4	B	1104	PCW	C11-C12-C13-C14
4	A	1109	PCW	C19-C20-C21-C22
4	C	1107	PCW	C17-C18-C19-C20
5	A	1112	CLR	C23-C24-C25-C27
5	A	1112	CLR	C23-C24-C25-C26
4	B	1111	PCW	C32-C31-O2-C2
4	A	1105	PCW	O2-C31-C32-C33
4	B	1110	PCW	O3-C11-C12-C13
4	D	1107	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	1101	ZK1	CAR-CAS-CAZ-FAH
4	C	1105	PCW	C14-C15-C16-C17
4	B	1104	PCW	C31-C32-C33-C34
4	A	1106	PCW	C14-C15-C16-C17
3	B	1102	ZK1	CAS-CAR-NAX-CAN
3	D	1102	ZK1	CAS-CAR-NAX-CAN
3	C	1101	ZK1	CAR-CAS-CAZ-FAF
4	E	201	PCW	C17-C18-C19-C20
4	E	203	PCW	C34-C35-C36-C37
4	B	1104	PCW	O2-C31-C32-C33
4	C	1102	PCW	O3-C11-C12-C13
4	A	1105	PCW	O3-C11-C12-C13
3	A	1101	ZK1	CAR-CAS-CAZ-FAF
4	A	1103	PCW	C40-C41-C42-C43
4	D	1104	PCW	C14-C15-C16-C17
4	D	1104	PCW	O2-C31-C32-C33
6	C	1114	AJP	C29-C30-C32-O33
4	B	1105	PCW	C32-C33-C34-C35
4	C	1115	PCW	C14-C15-C16-C17
3	C	1101	ZK1	CAR-CAS-CAZ-FAG
4	A	1102	PCW	O3-C11-C12-C13
4	B	1103	PCW	O11-C11-C12-C13
4	B	1110	PCW	C33-C34-C35-C36
4	A	1117	PCW	C14-C15-C16-C17
4	B	1110	PCW	O11-C11-O3-C3
4	A	1114	PCW	C12-C13-C14-C15
4	D	1103	PCW	O11-C11-C12-C13
4	D	1105	PCW	C37-C38-C39-C40
4	B	1110	PCW	O11-C11-C12-C13
4	A	1105	PCW	C15-C16-C17-C18
4	A	1105	PCW	O31-C31-C32-C33
4	A	1105	PCW	O11-C11-C12-C13
4	B	1111	PCW	C34-C35-C36-C37
4	B	1104	PCW	O31-C31-C32-C33
4	B	1110	PCW	O31-C31-C32-C33
4	D	1104	PCW	O31-C31-C32-C33
3	A	1101	ZK1	CAR-CAS-CAZ-FAH
4	B	1108	PCW	C13-C14-C15-C16
4	B	1111	PCW	C11-C12-C13-C14
4	C	1102	PCW	O11-C11-C12-C13
4	A	1102	PCW	C31-C32-C33-C34
4	D	1101	PCW	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	B	1106	PCW	C37-C38-C39-C40
4	A	1102	PCW	O11-C11-C12-C13

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1110	AJP	C02-C03-C04-C05-C85-O84
6	A	1111	AJP	C02-C03-C04-C05-C85-O84

48 monomers are involved in 312 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1104	PCW	1	0
3	A	1101	ZK1	2	0
6	C	1109	AJP	33	0
4	F	201	PCW	1	0
6	C	1110	AJP	34	0
4	A	1114	PCW	3	0
6	C	1114	AJP	40	0
4	A	1104	PCW	3	0
4	C	1102	PCW	6	0
4	F	204	PCW	2	0
4	C	1103	PCW	2	0
4	A	1105	PCW	3	0
4	A	1118	PCW	3	0
4	C	1112	PCW	1	0
4	D	1101	PCW	3	0
4	D	1110	PCW	1	0
4	E	202	PCW	1	0
4	E	205	PCW	1	0
4	F	202	PCW	3	0
4	D	1103	PCW	4	0
4	D	1104	PCW	2	0
4	A	1113	PCW	2	0
4	B	1110	PCW	5	0
4	B	1111	PCW	6	0
5	C	1106	CLR	7	0
5	A	1107	CLR	6	0
4	B	1106	PCW	1	0
4	A	1108	PCW	2	0
4	C	1115	PCW	1	0
4	B	1107	PCW	2	0

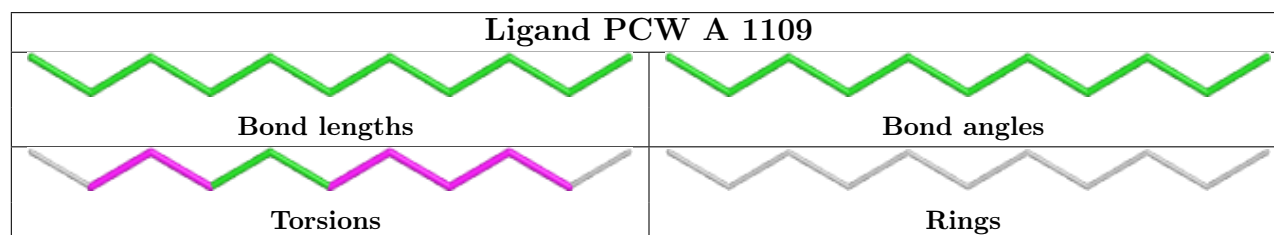
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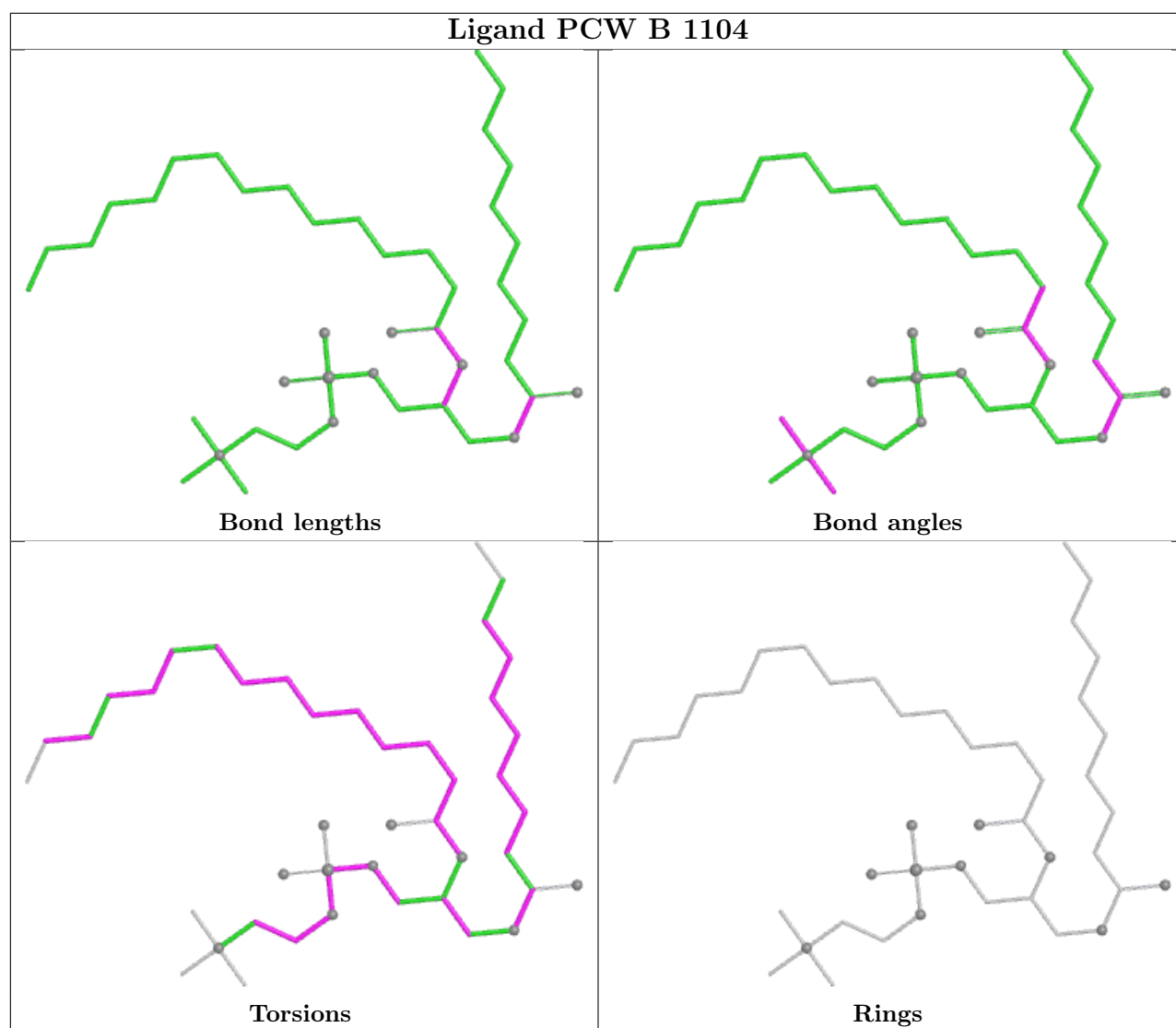


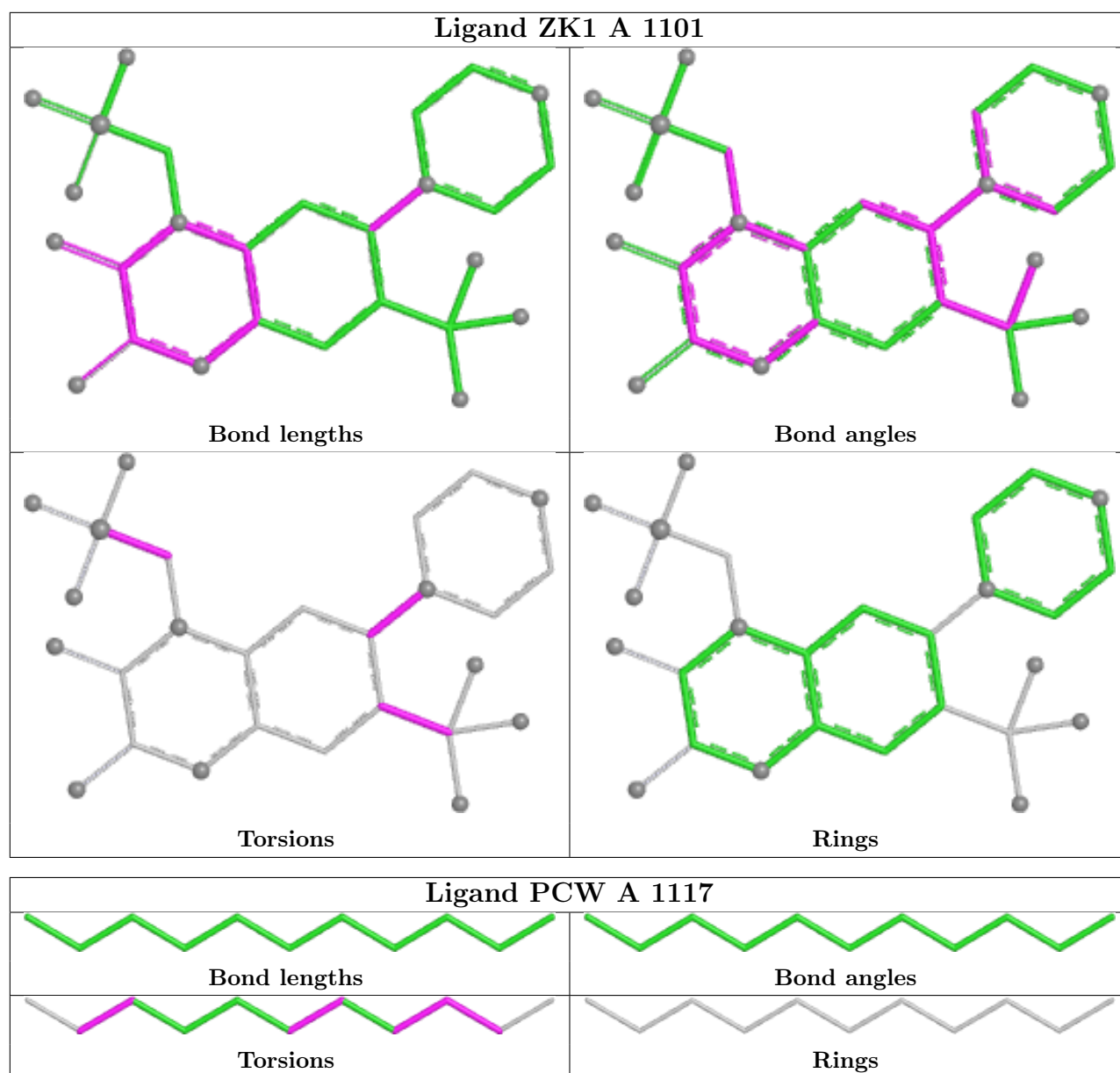
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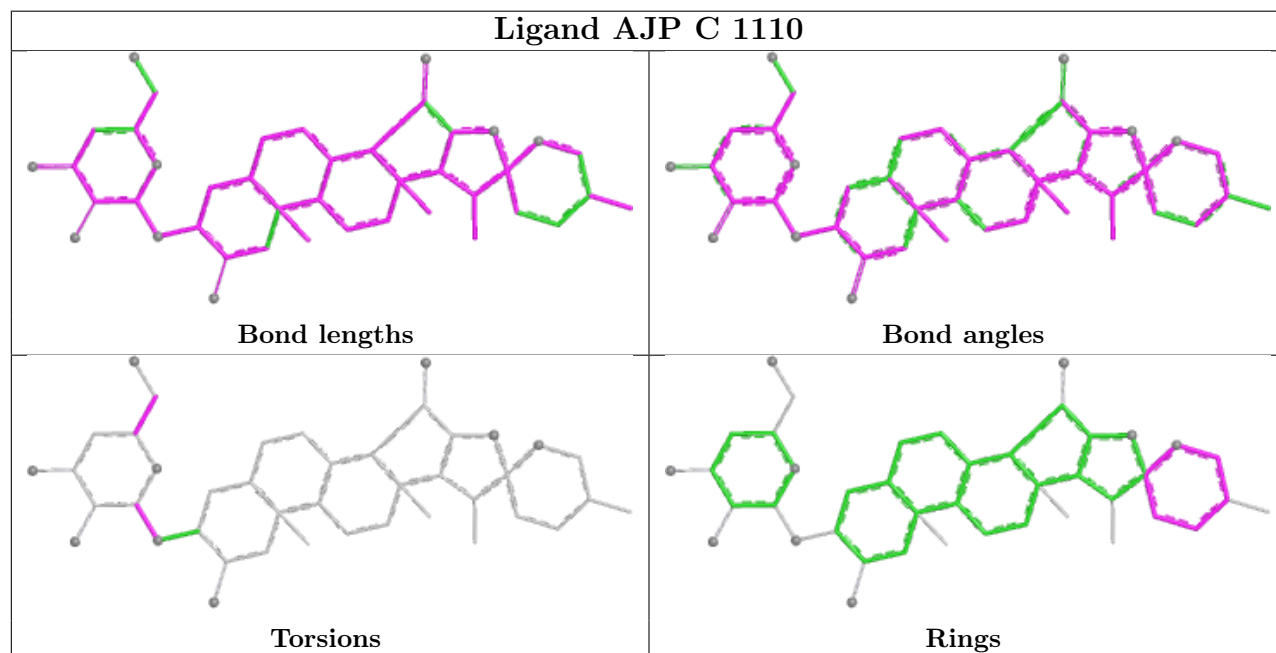
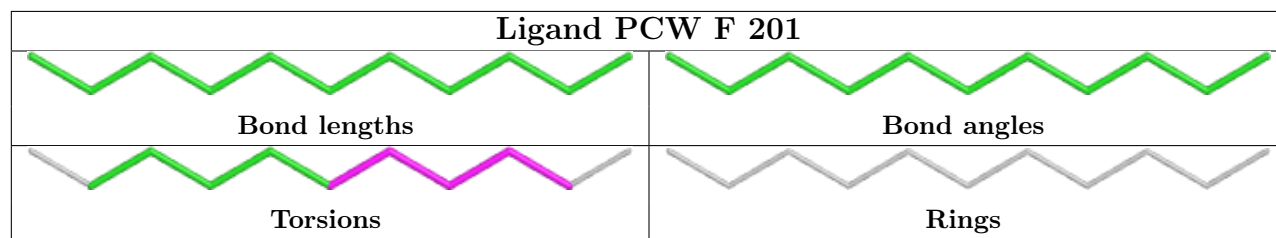
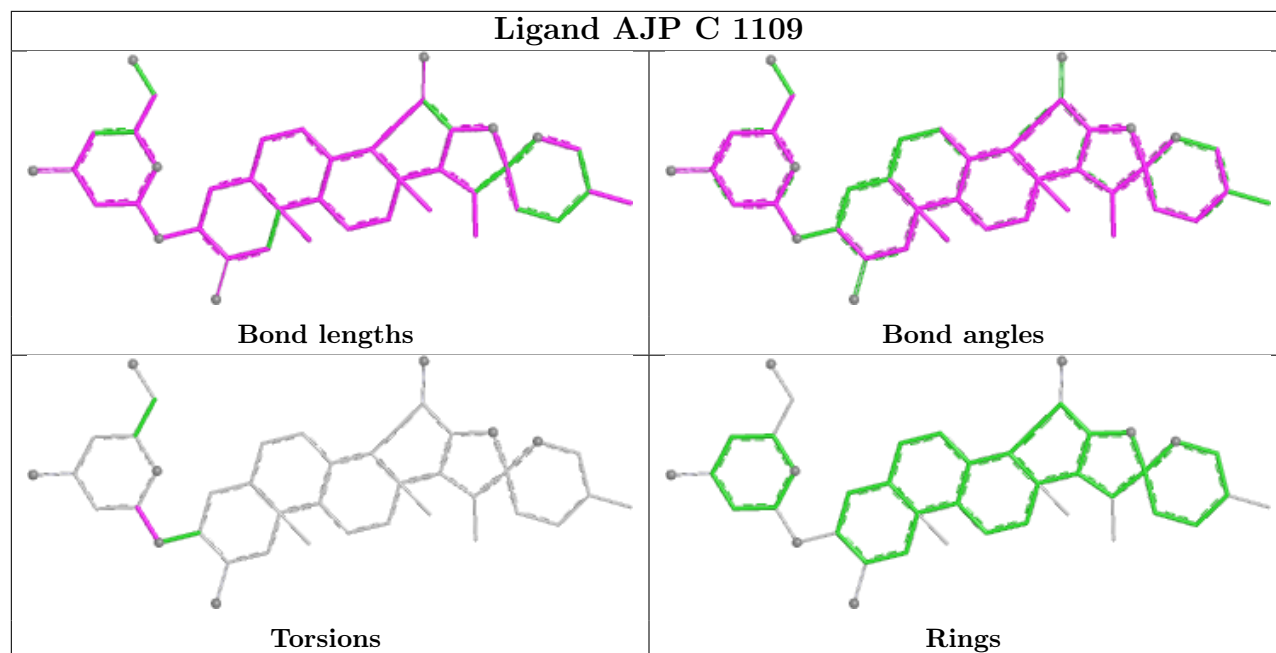
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	ZK1	1	0
6	A	1110	AJP	34	0
4	E	203	PCW	1	0
4	B	1101	PCW	2	0
4	D	1109	PCW	3	0
4	A	1102	PCW	5	0
5	C	1111	CLR	2	0
4	C	1107	PCW	1	0
4	D	1106	PCW	2	0
4	D	1107	PCW	3	0
4	C	1104	PCW	5	0
4	B	1109	PCW	1	0
4	E	201	PCW	1	0
6	A	1111	AJP	36	0
4	A	1103	PCW	3	0
5	A	1112	CLR	3	0
6	A	1116	AJP	38	0
4	B	1103	PCW	2	0

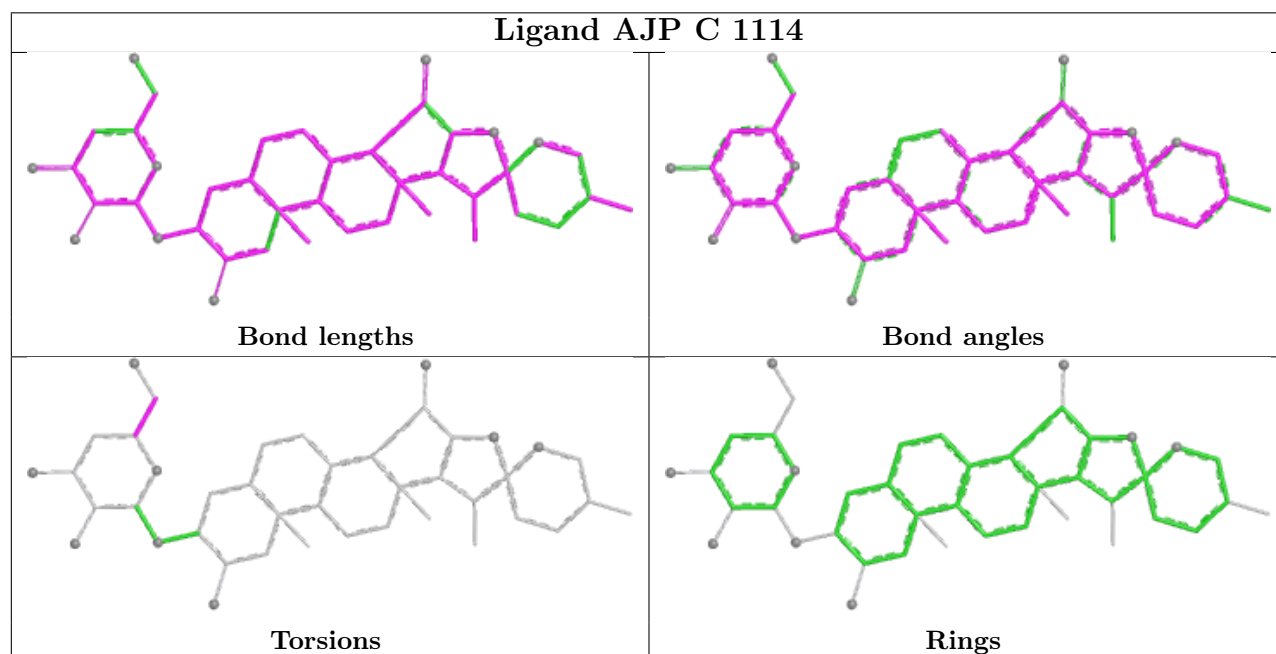
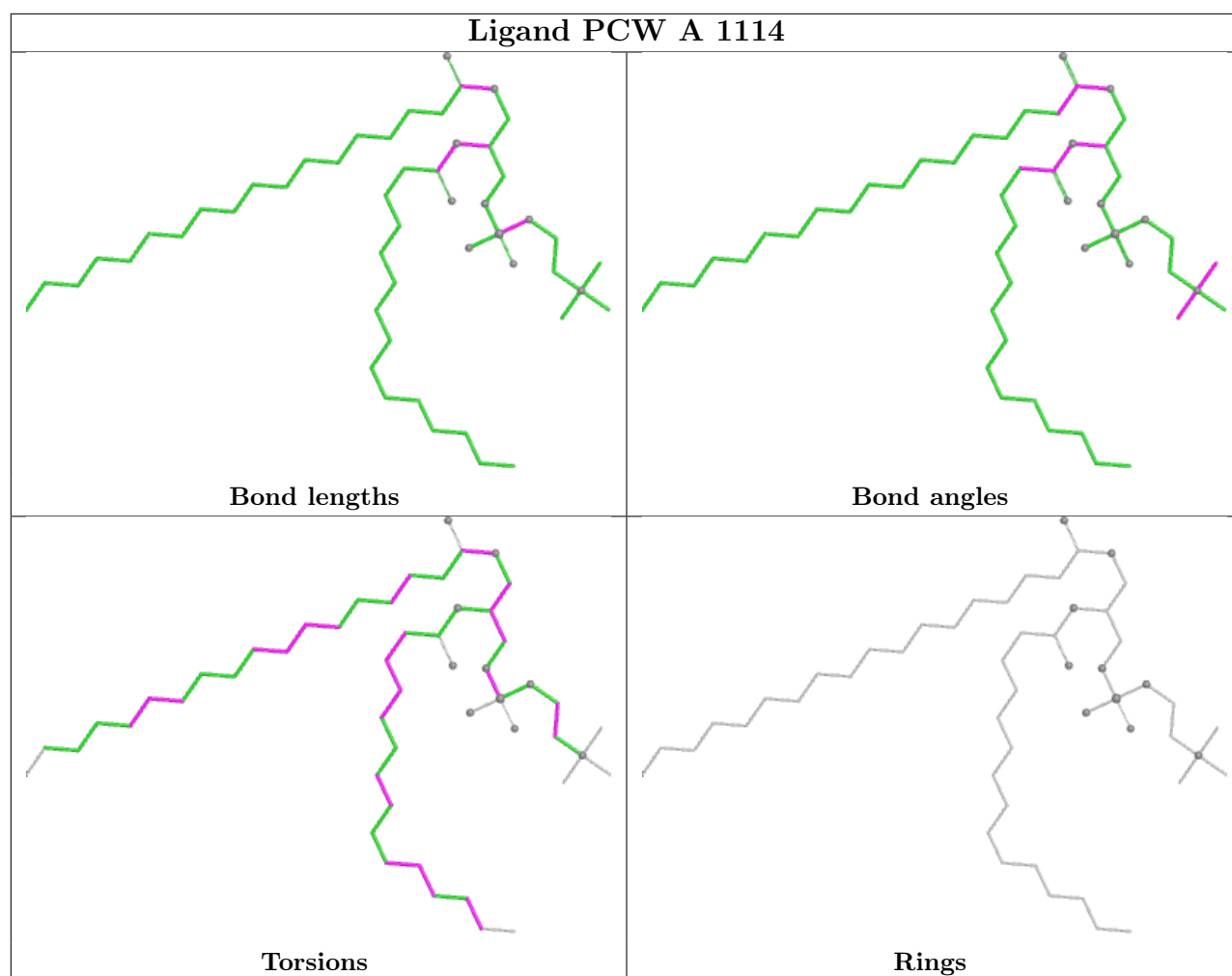
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

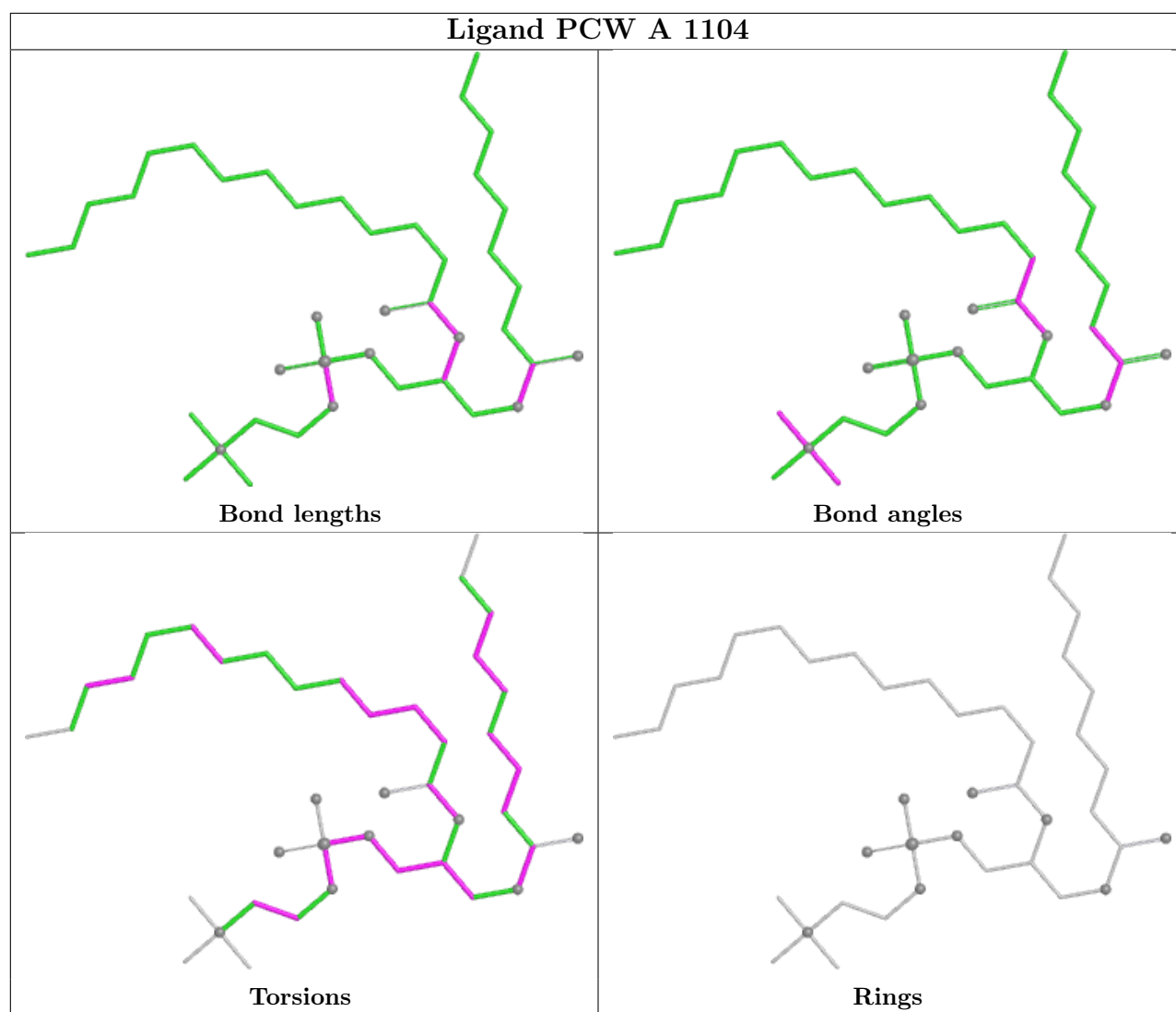


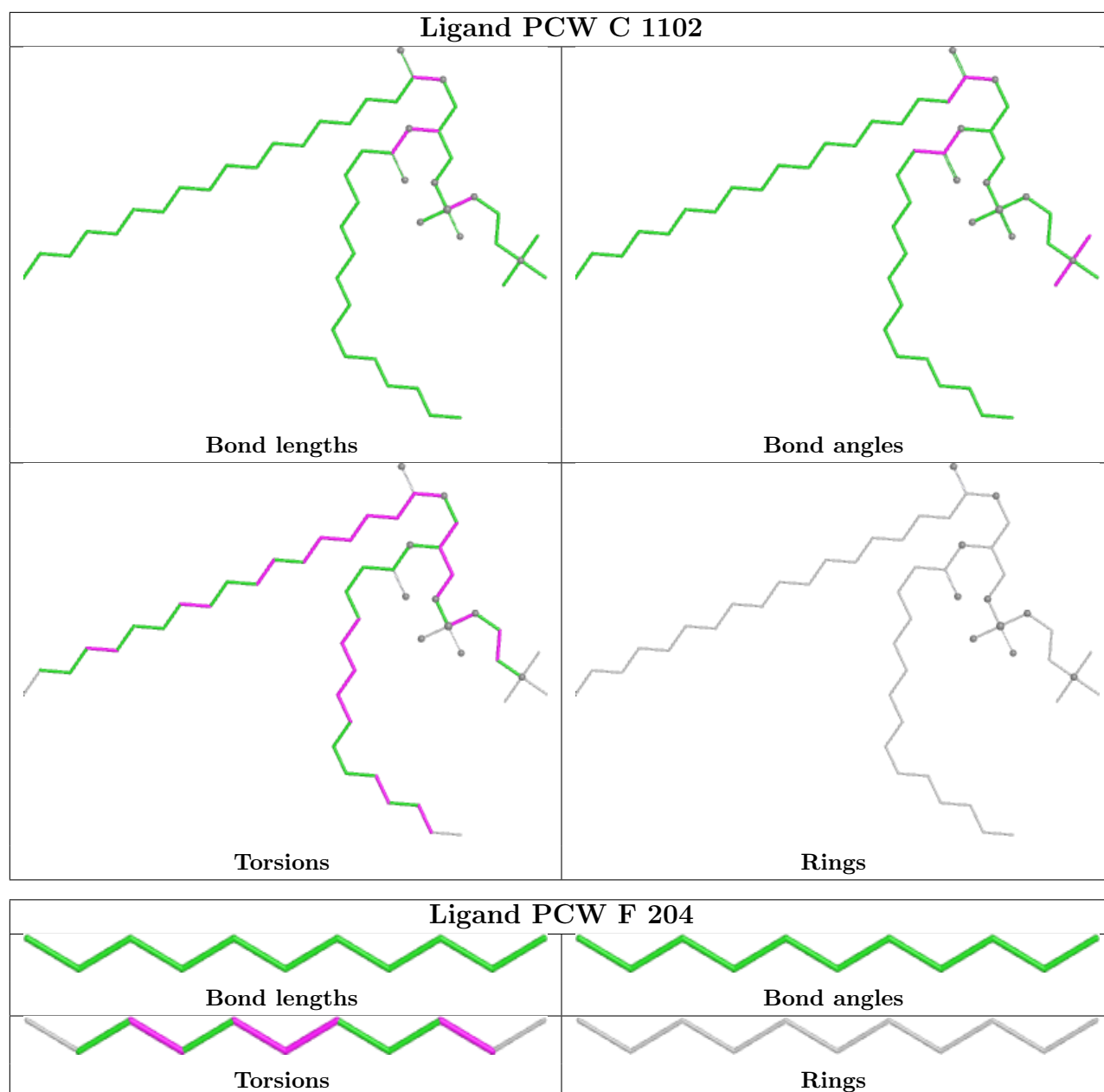


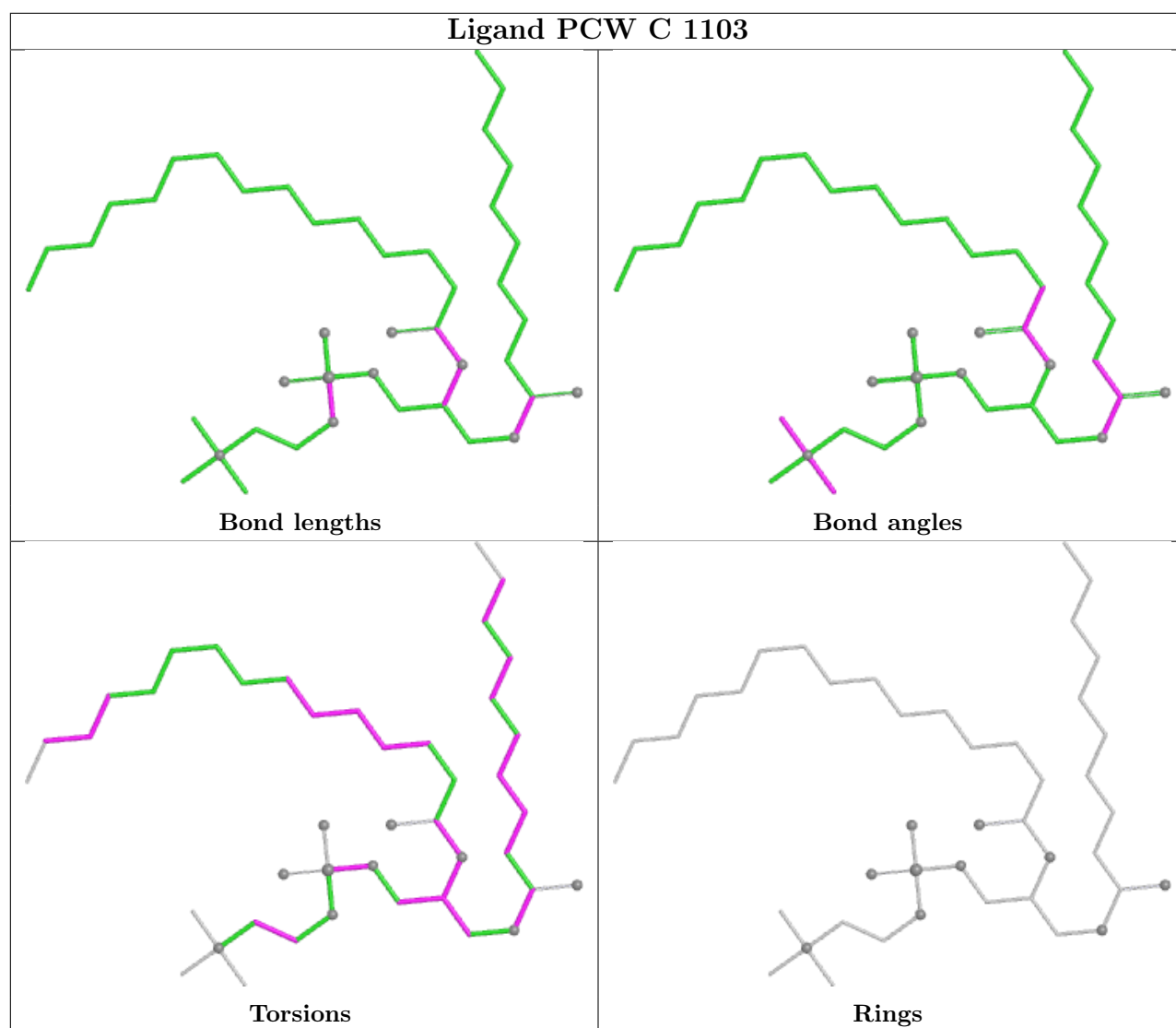




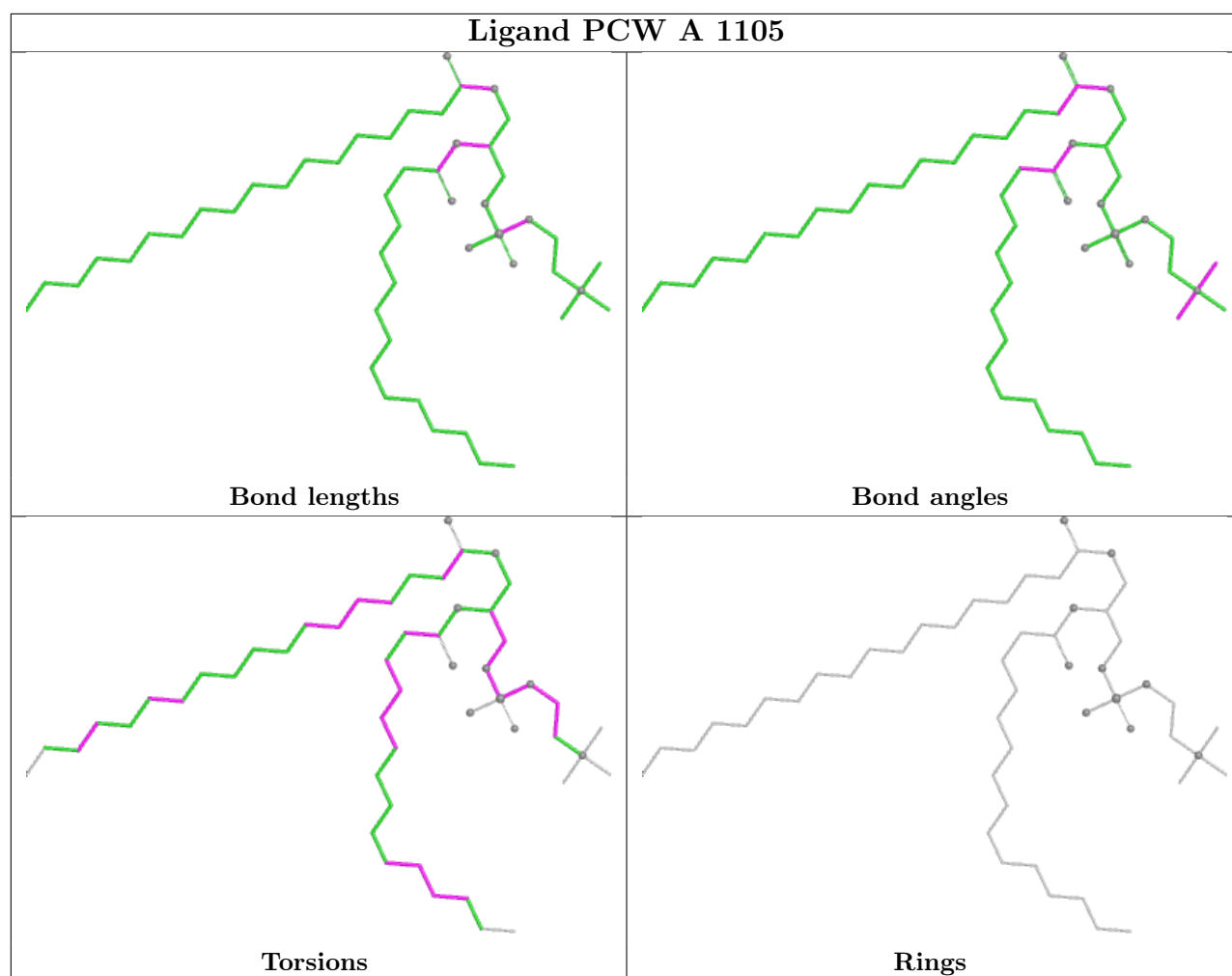


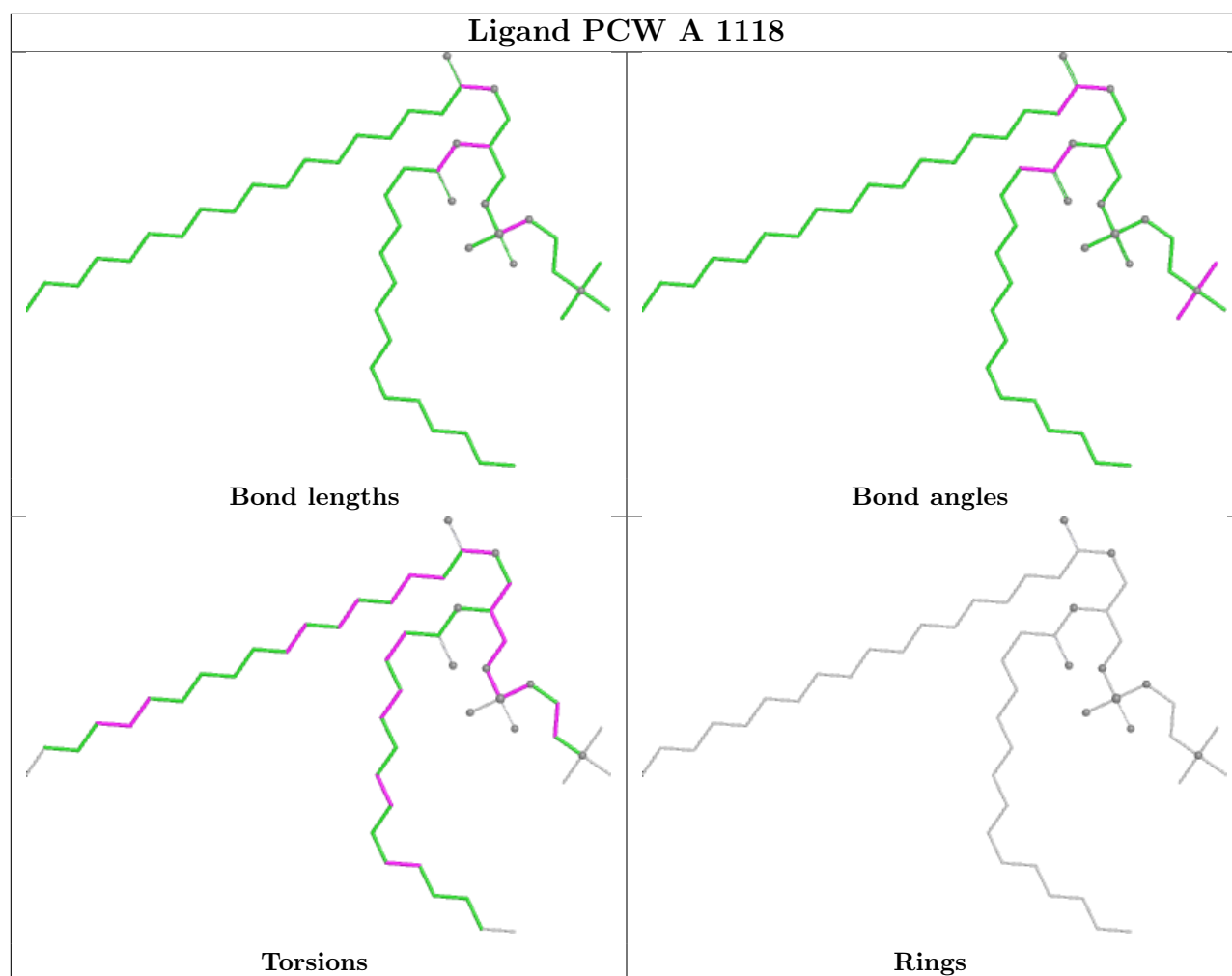


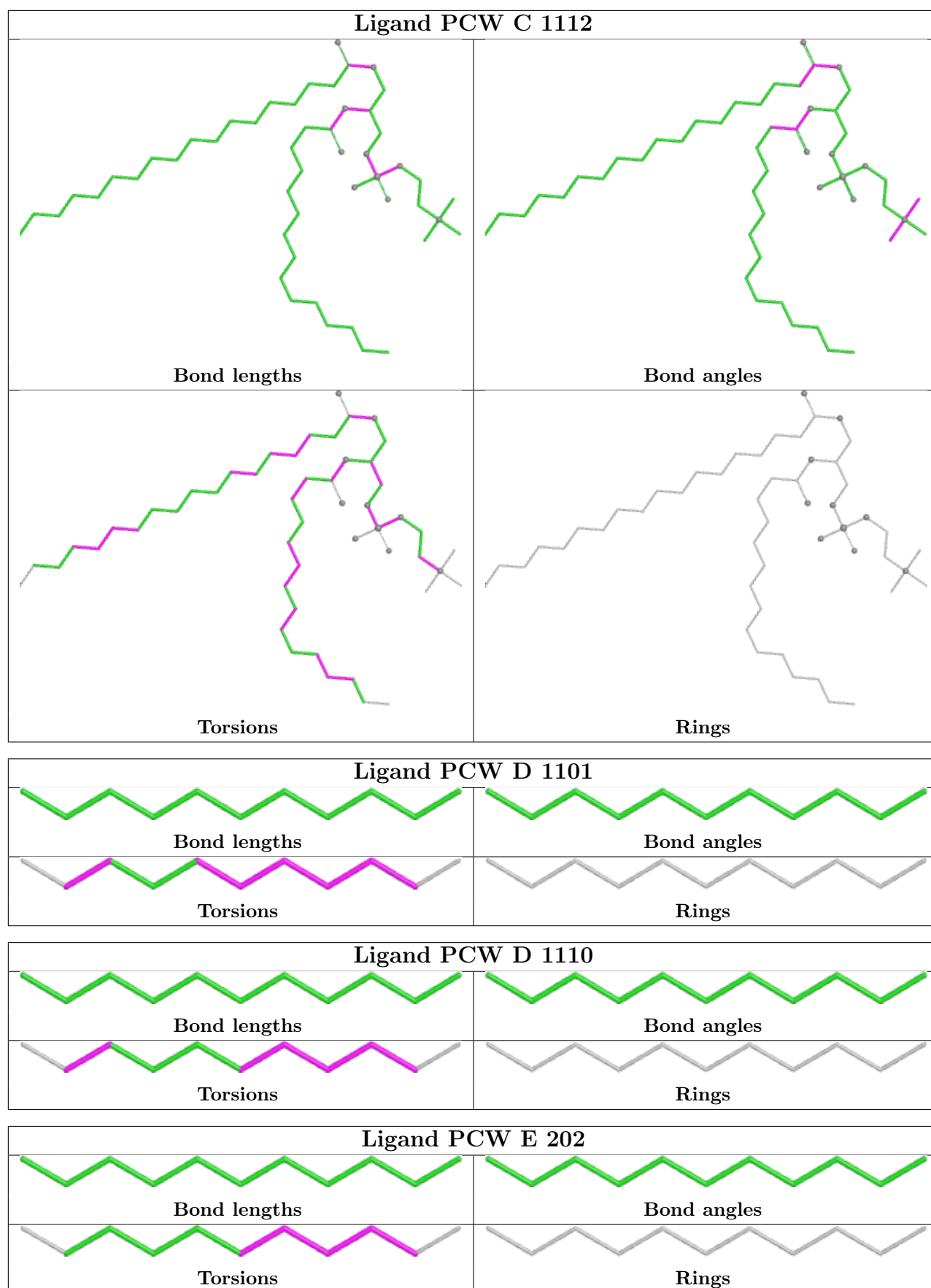


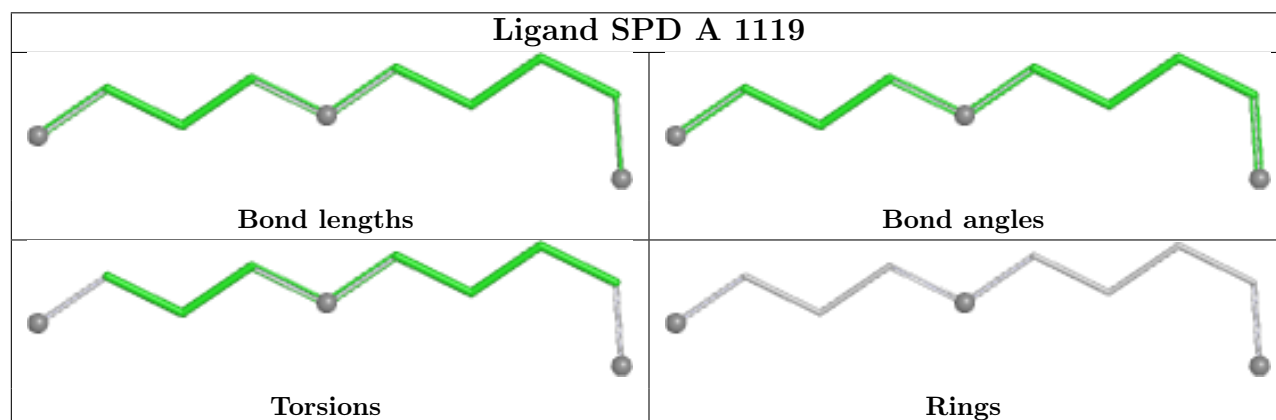
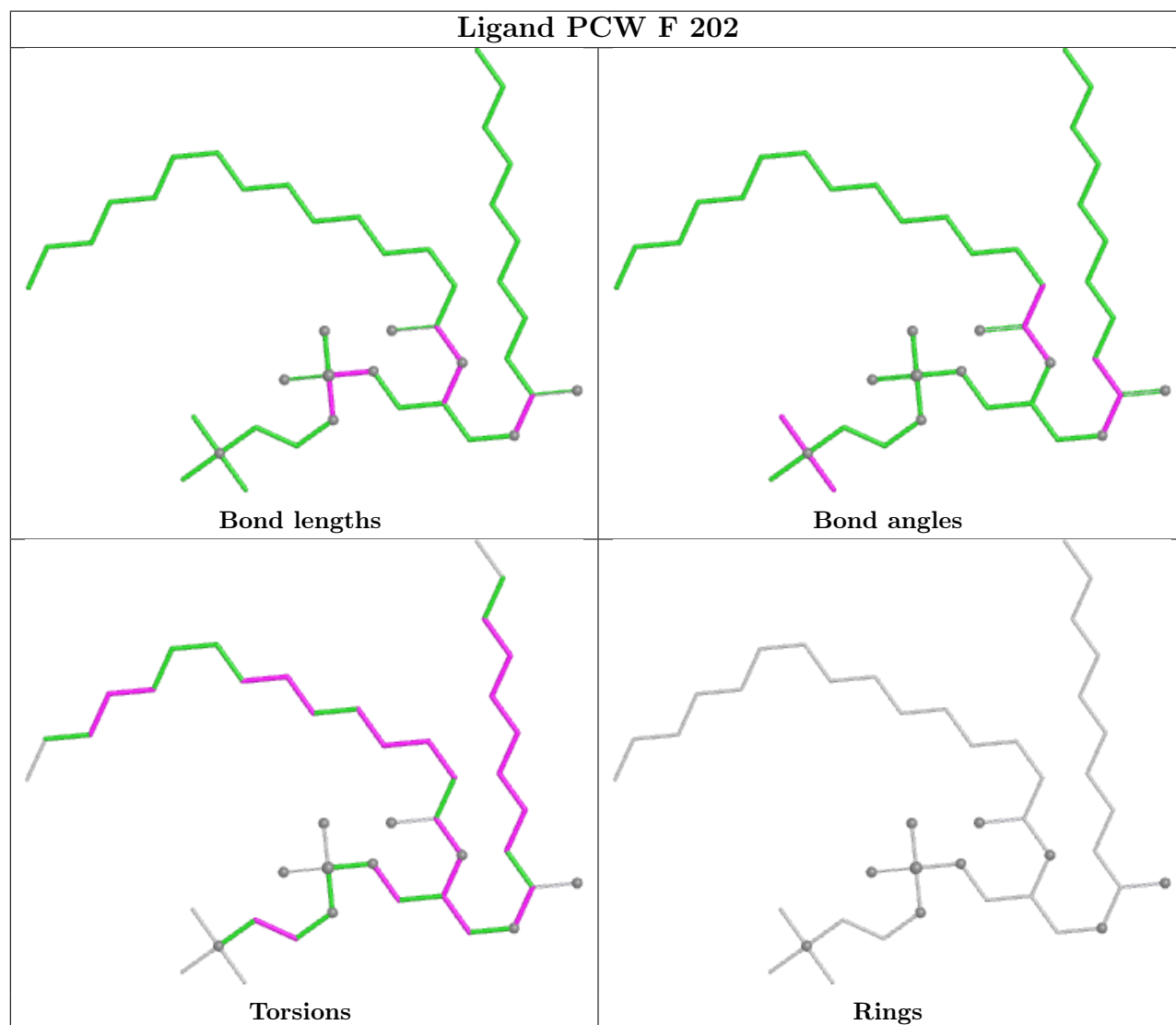
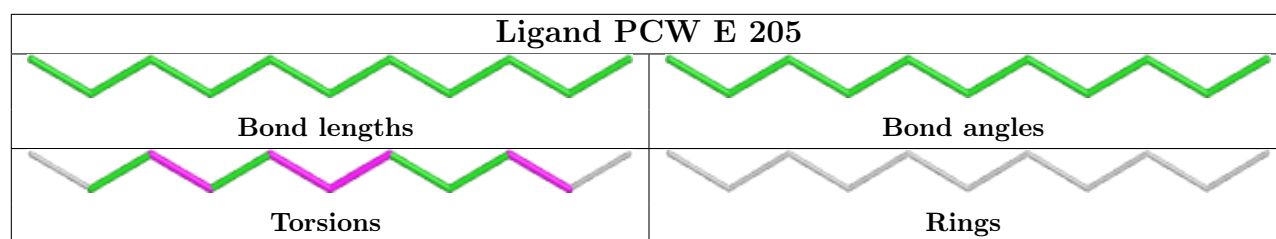


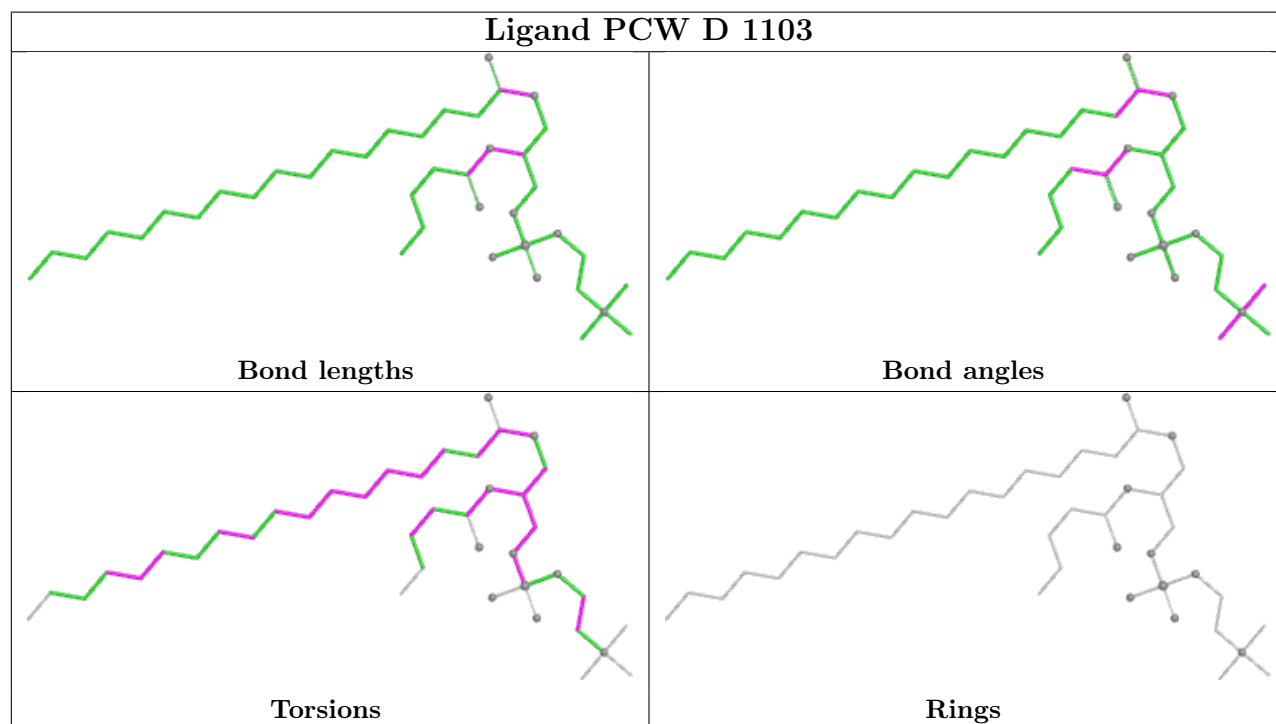
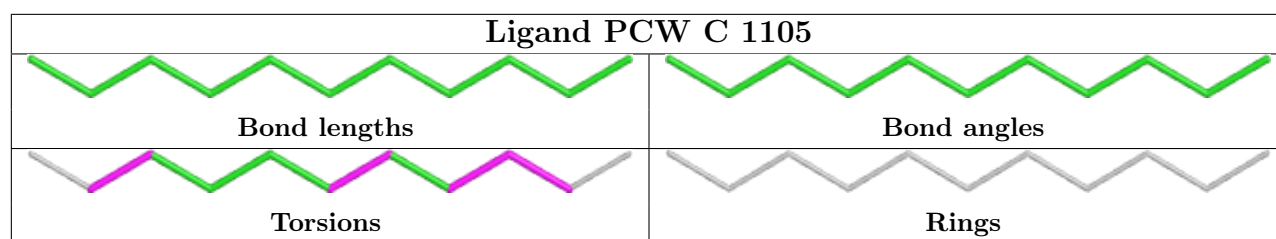


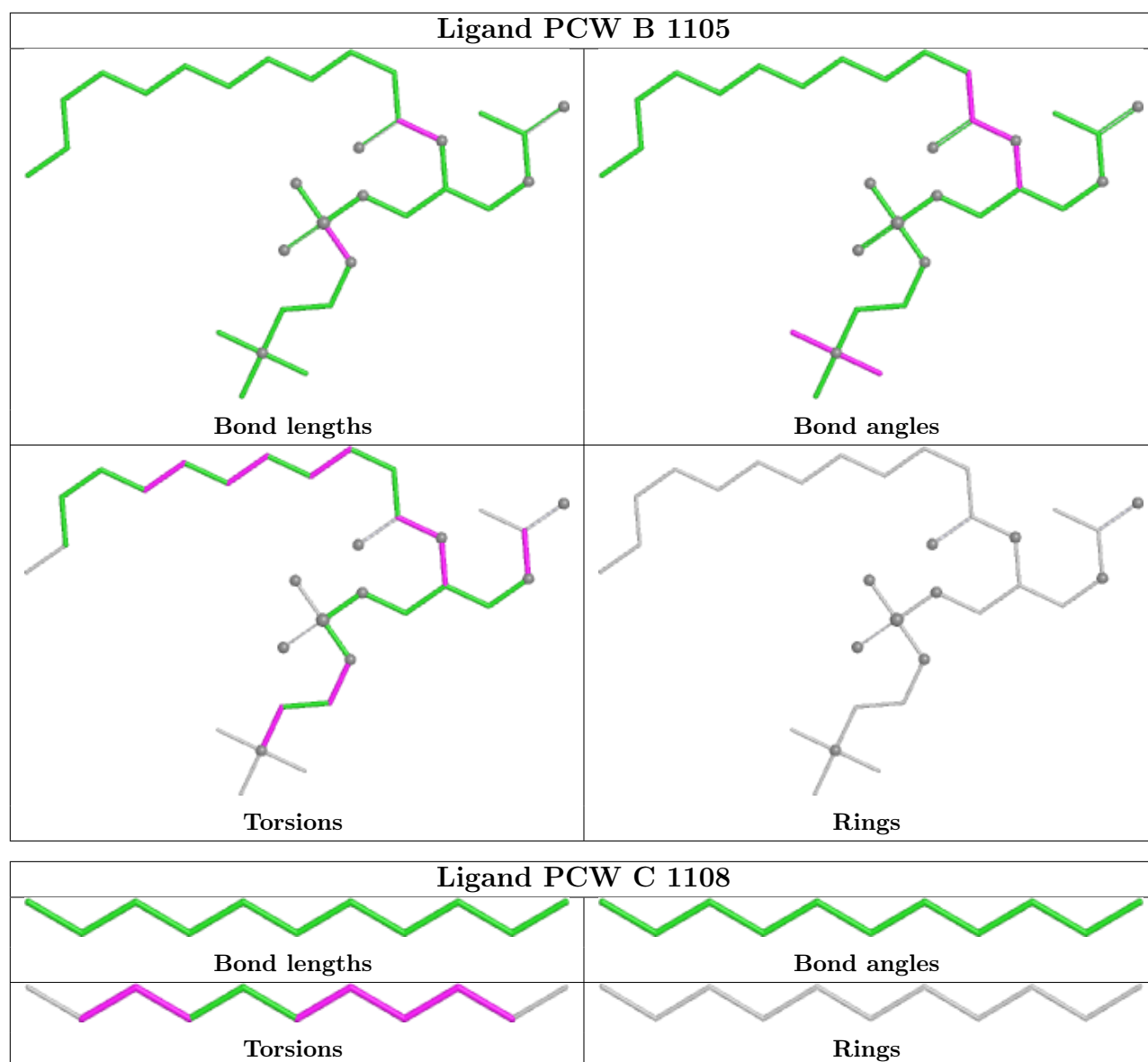


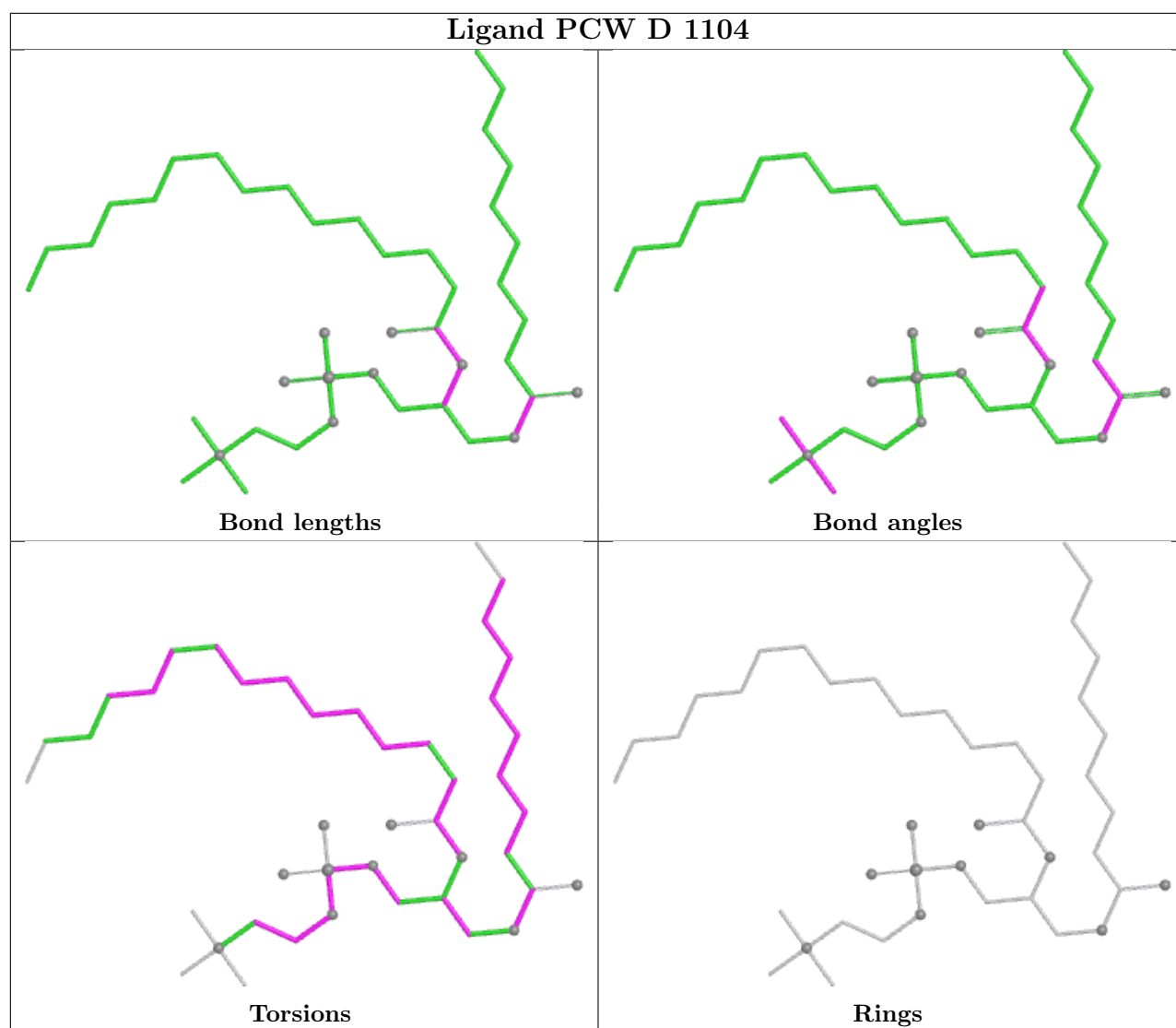


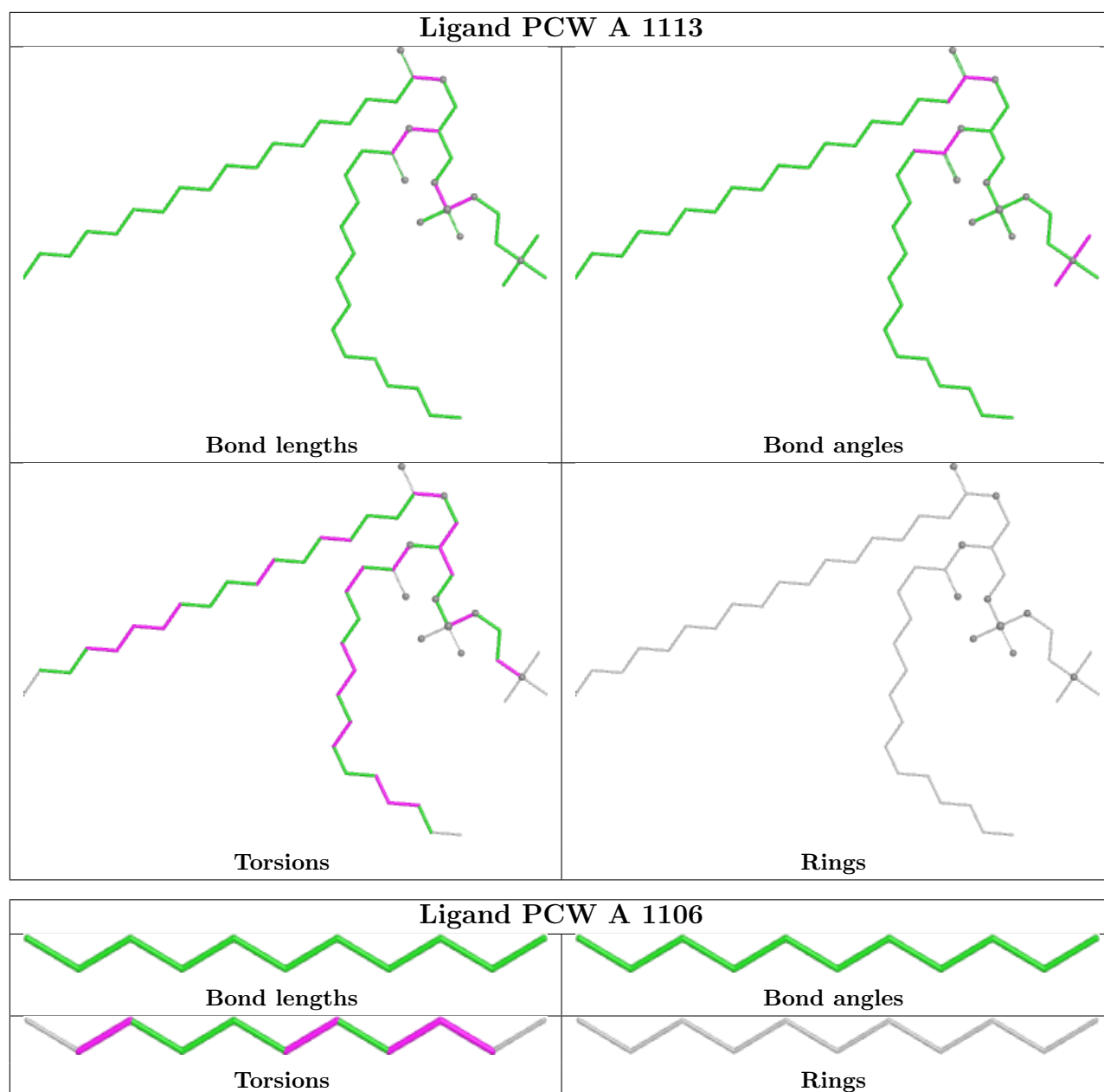




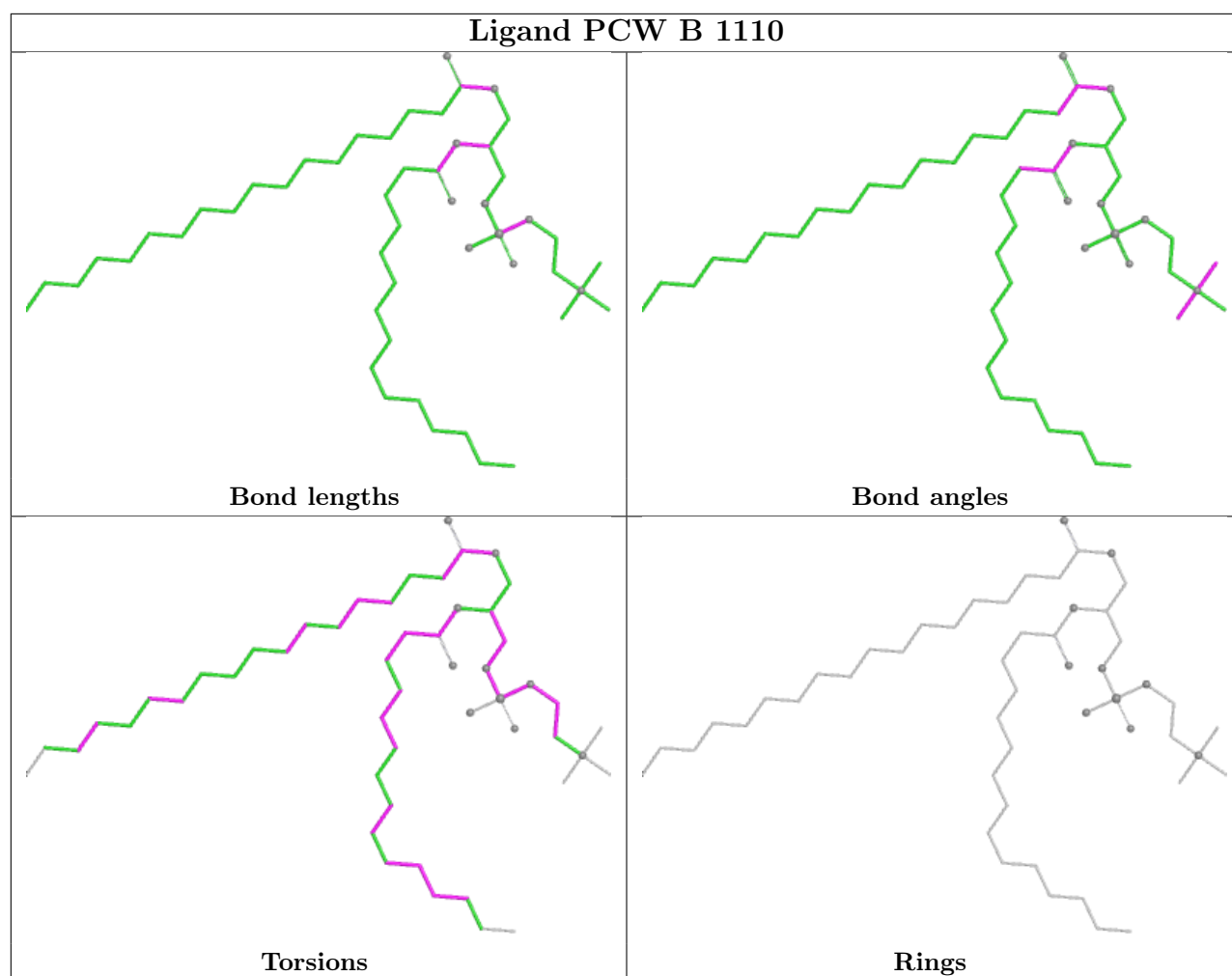


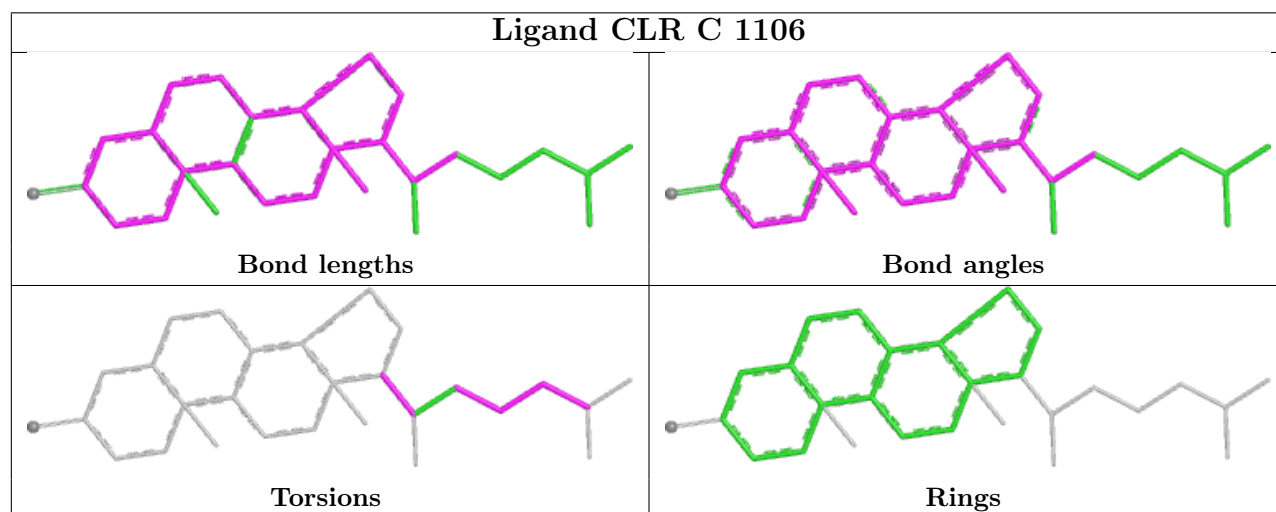
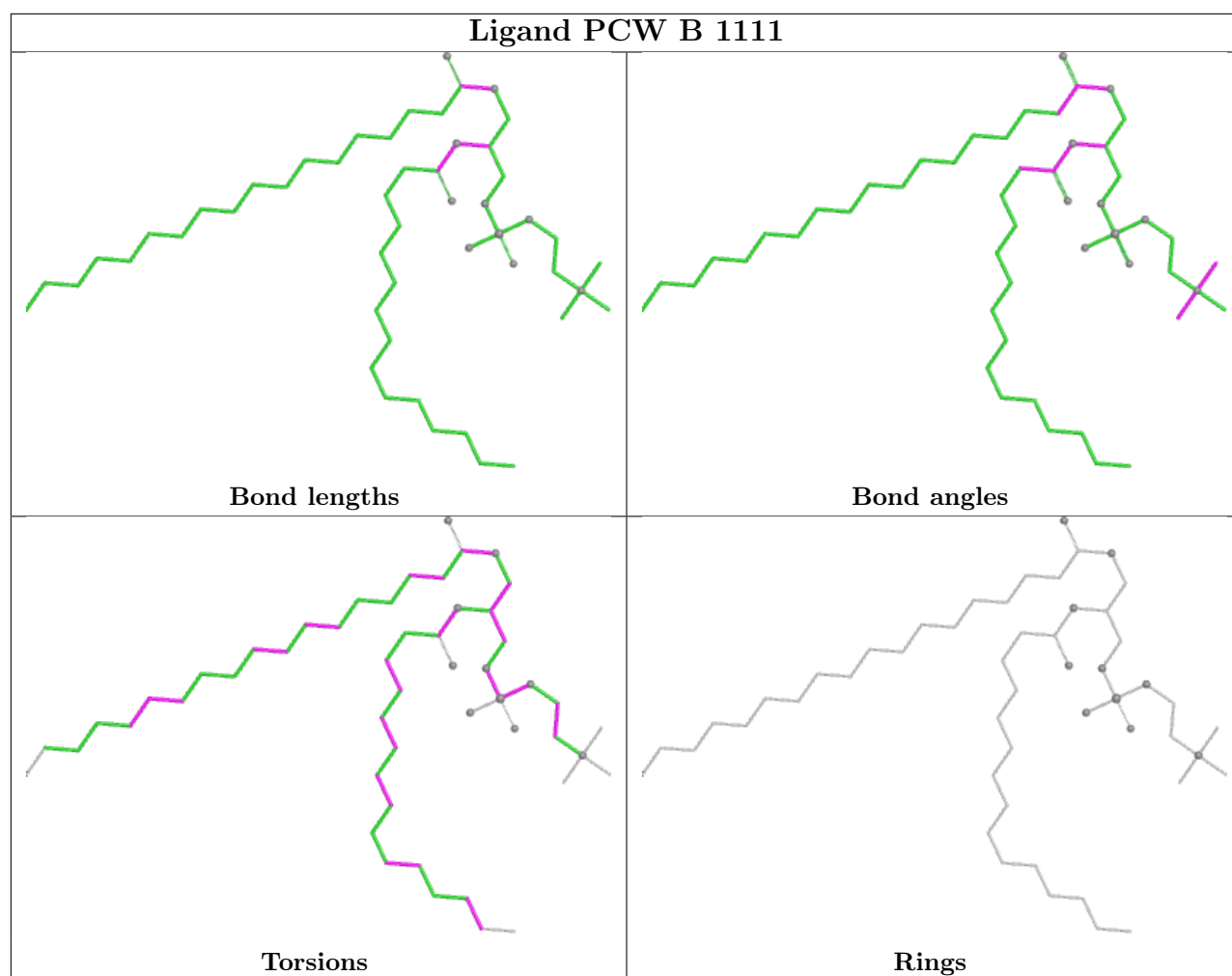


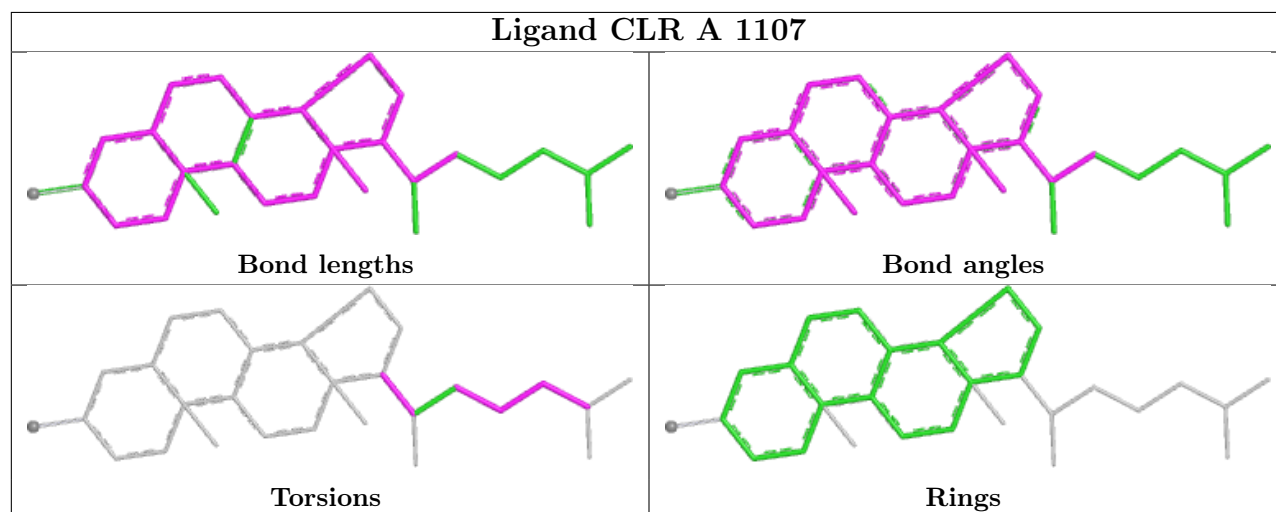
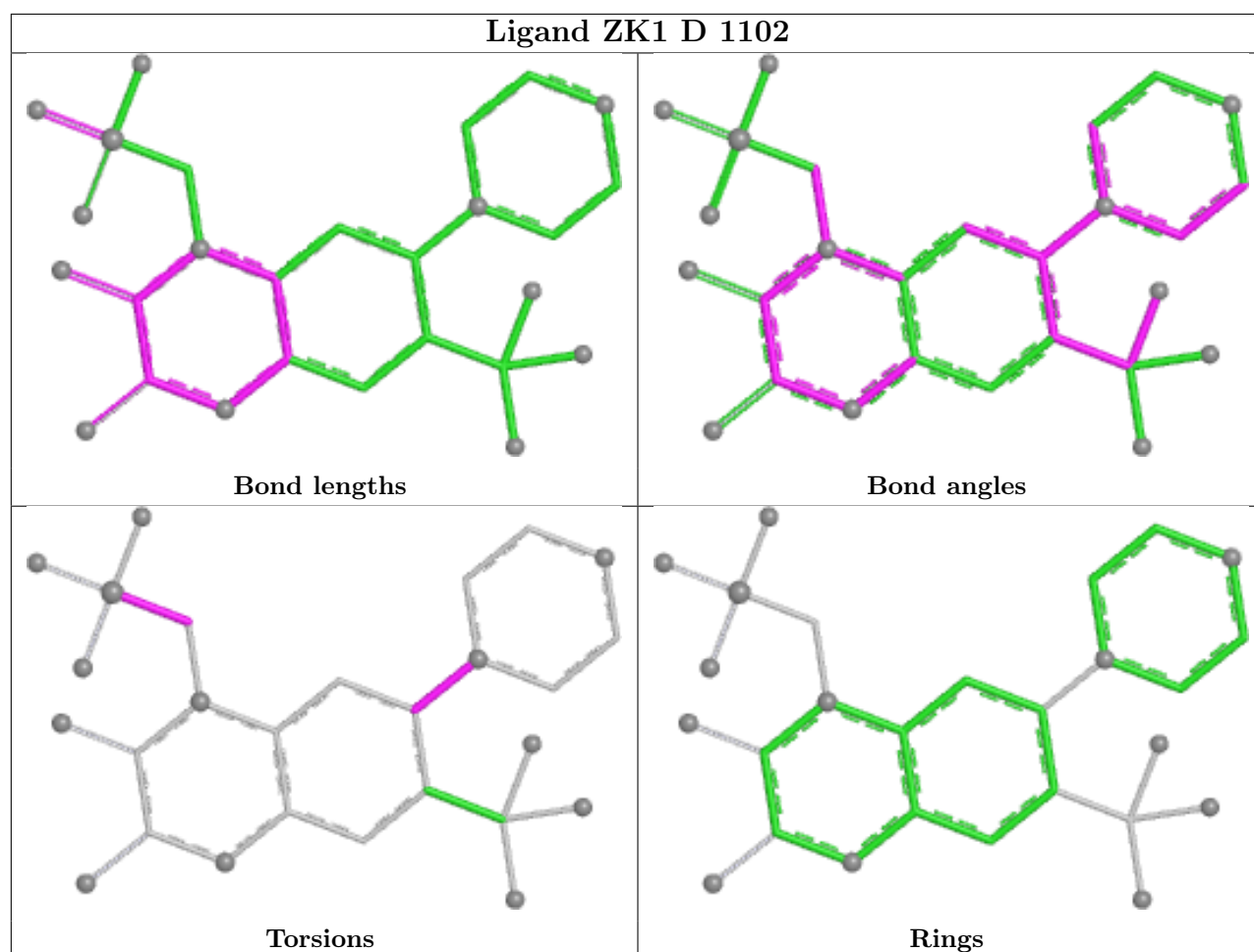


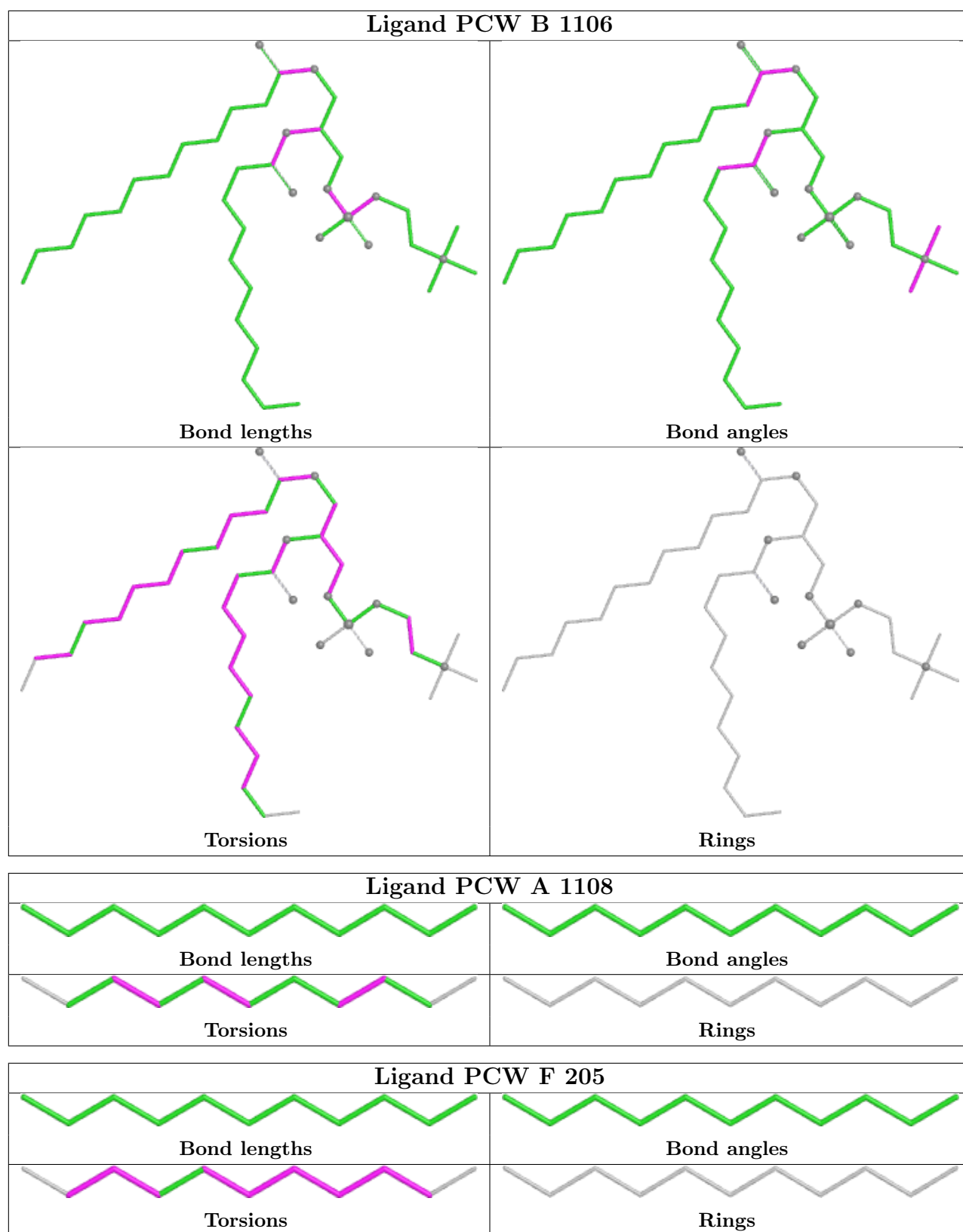


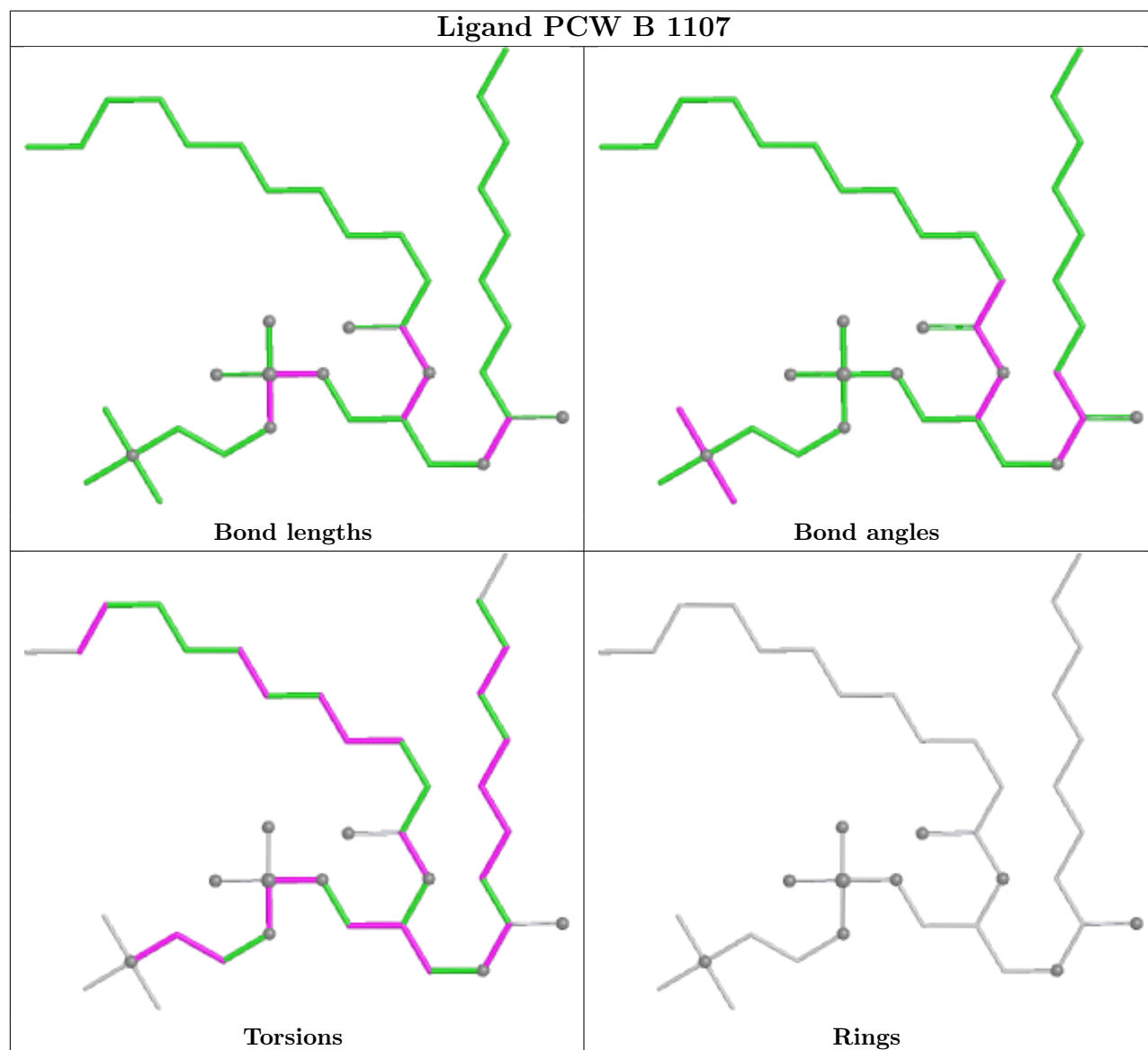
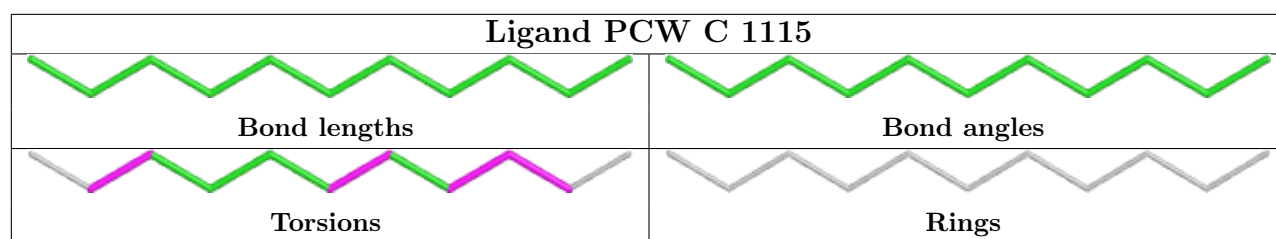


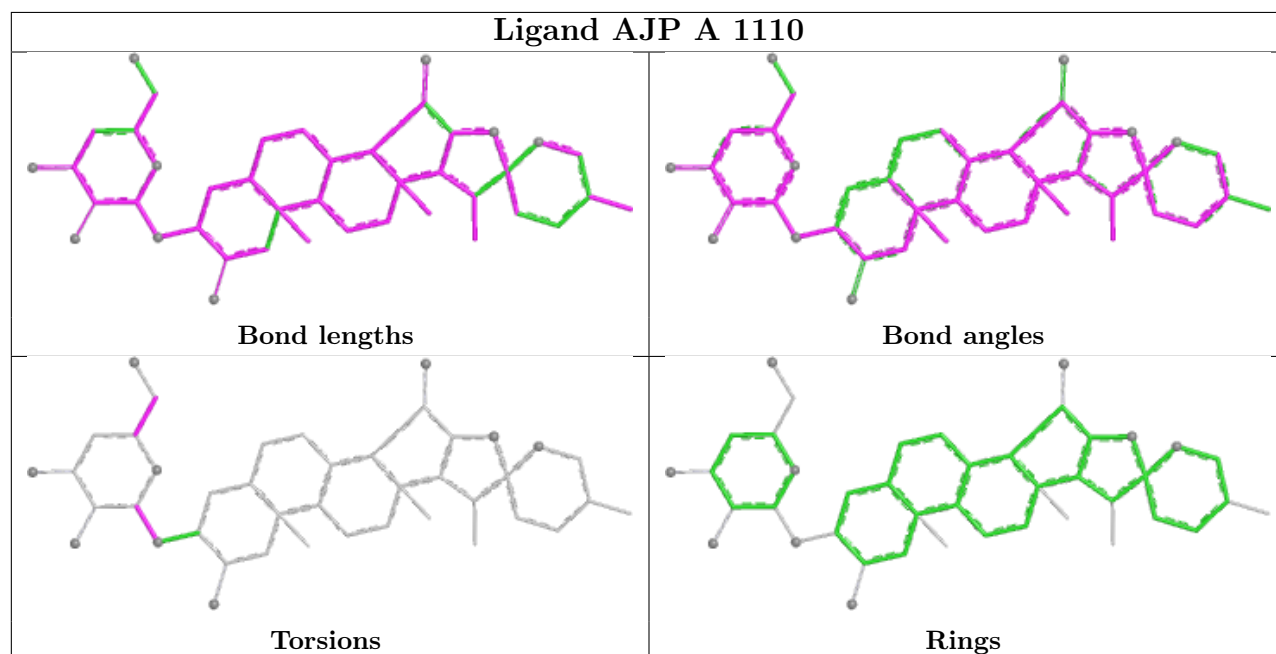
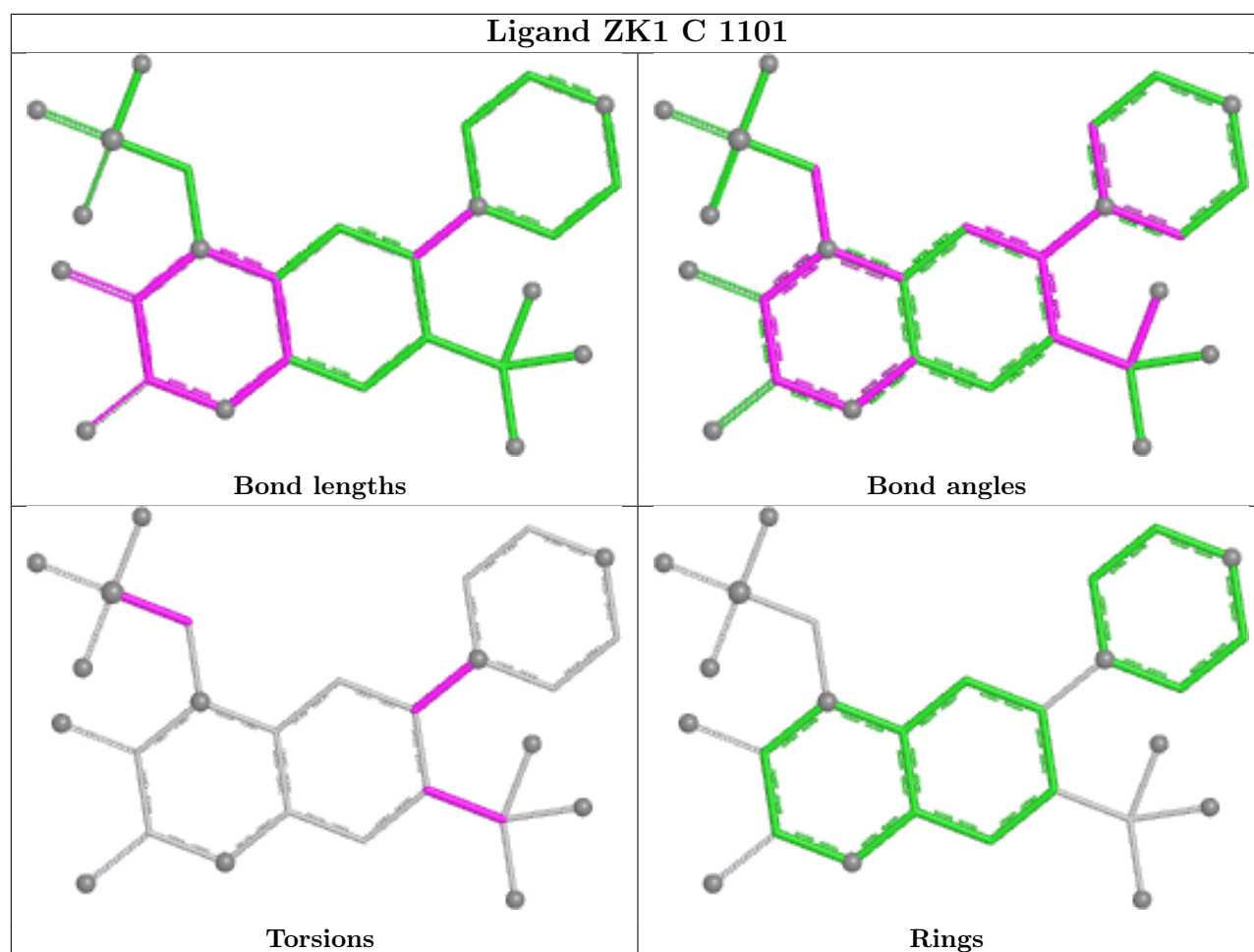


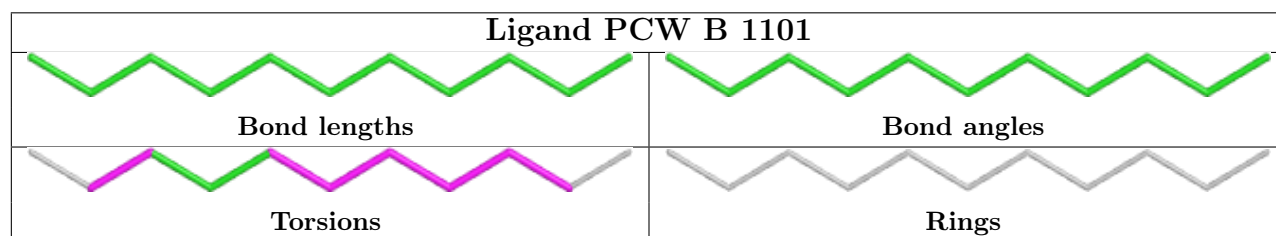
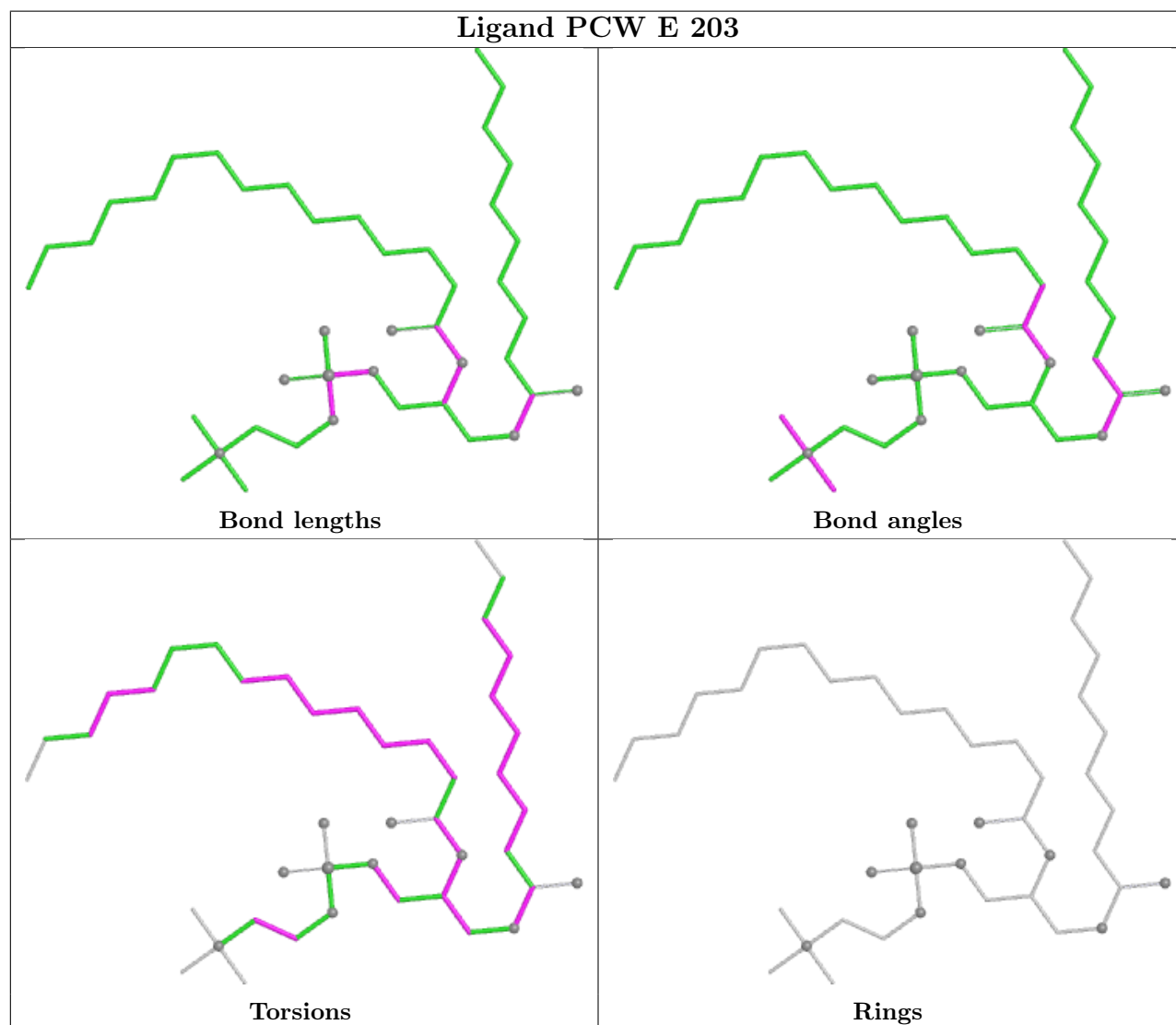
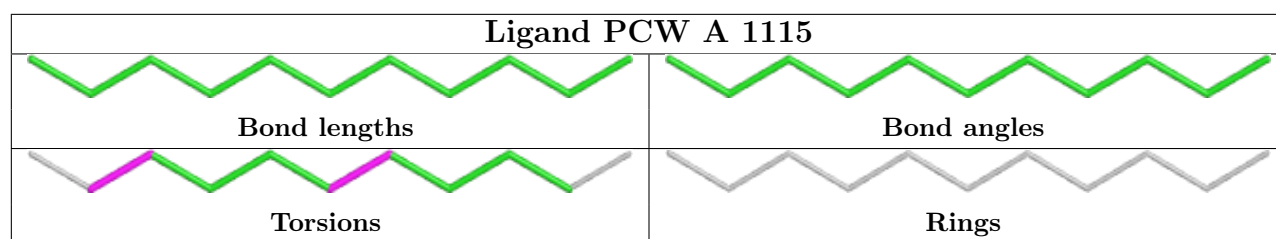


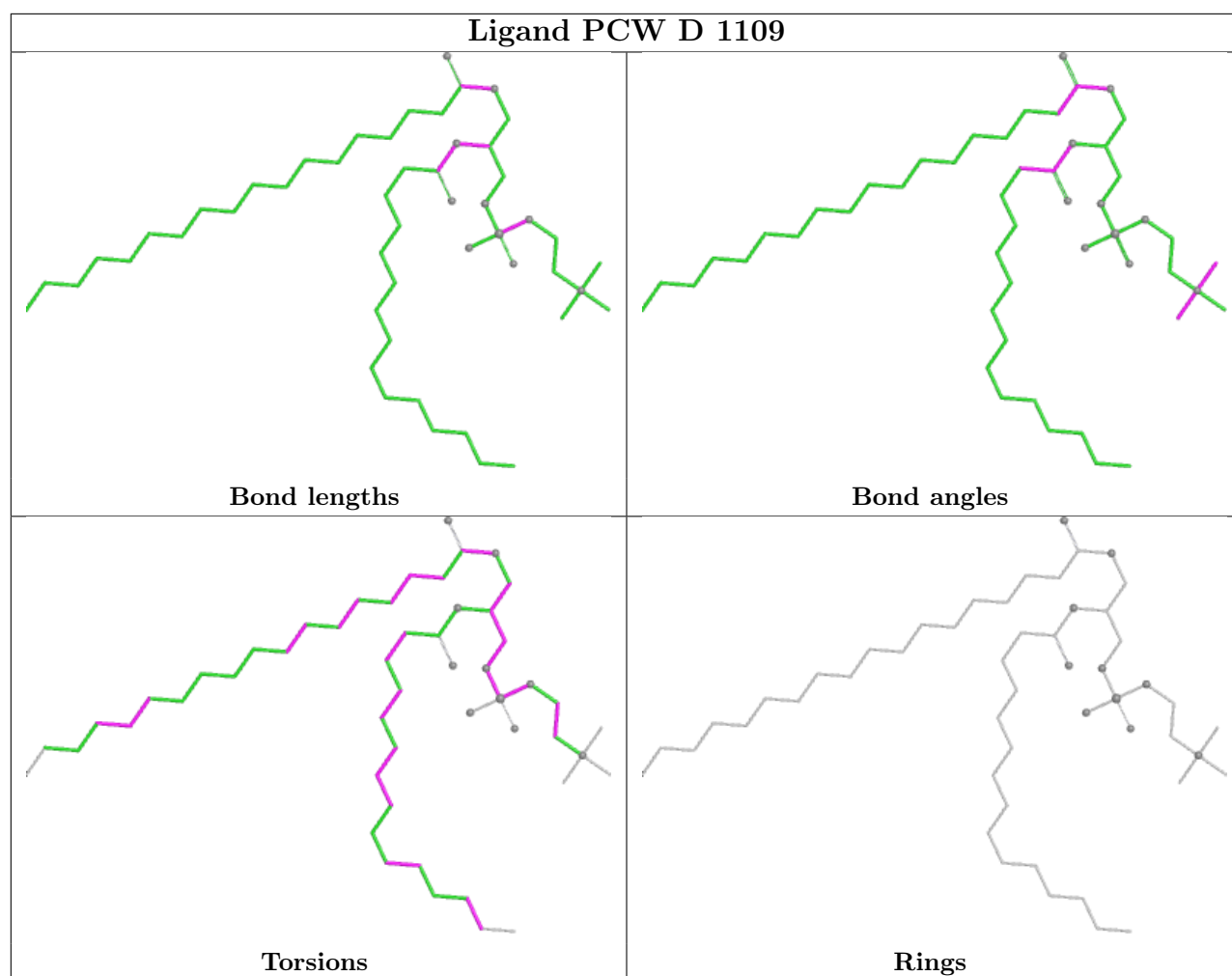




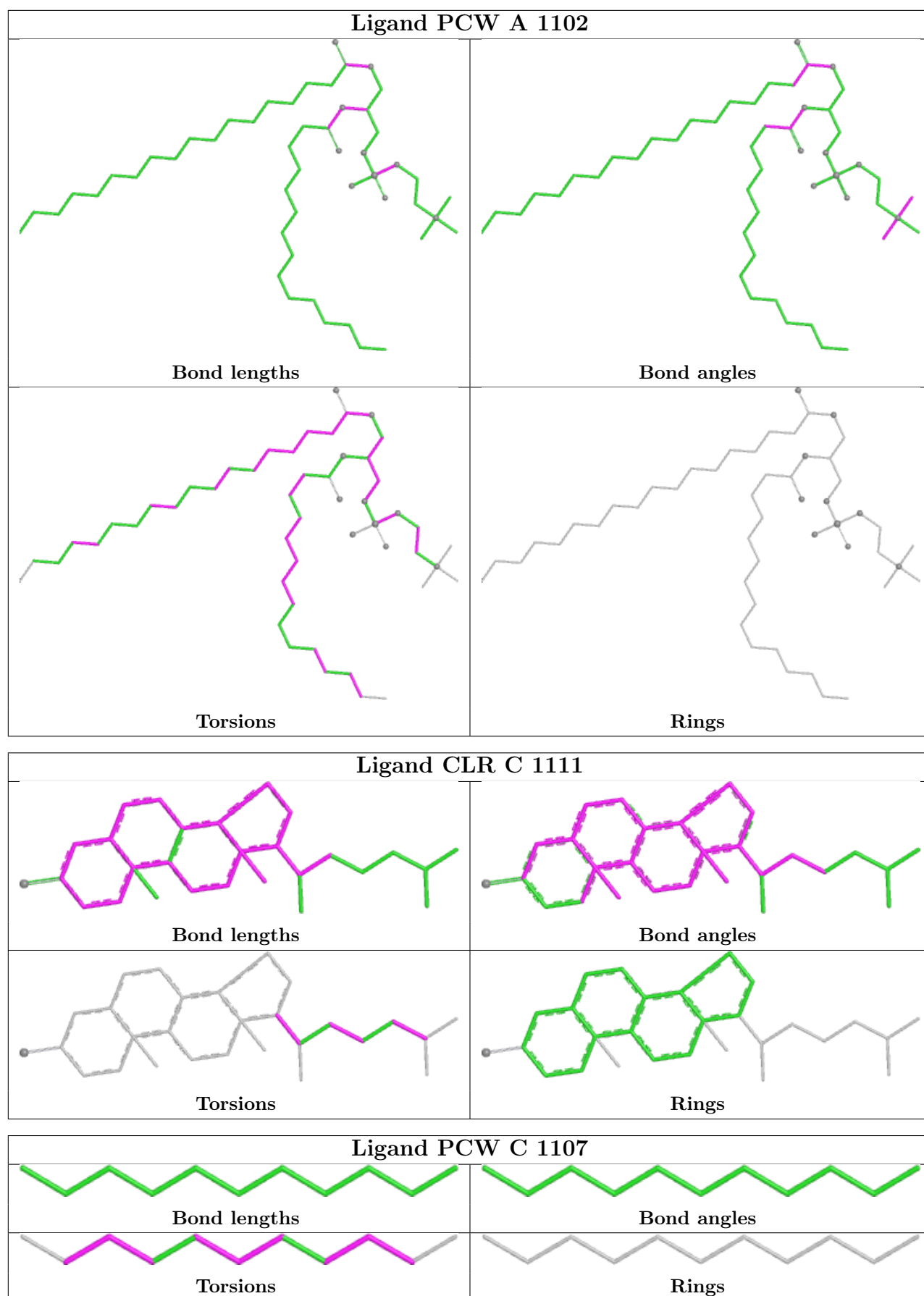


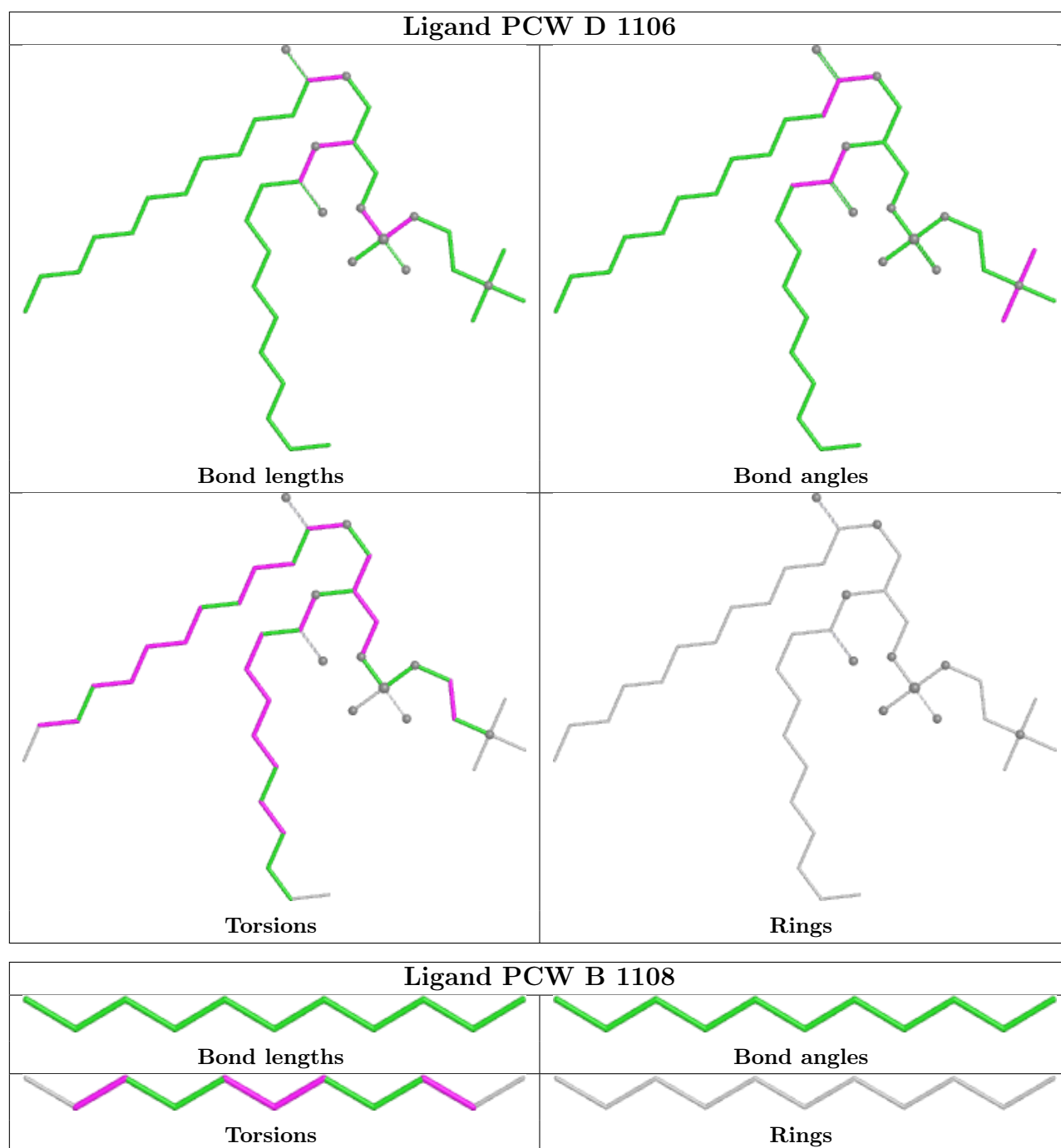


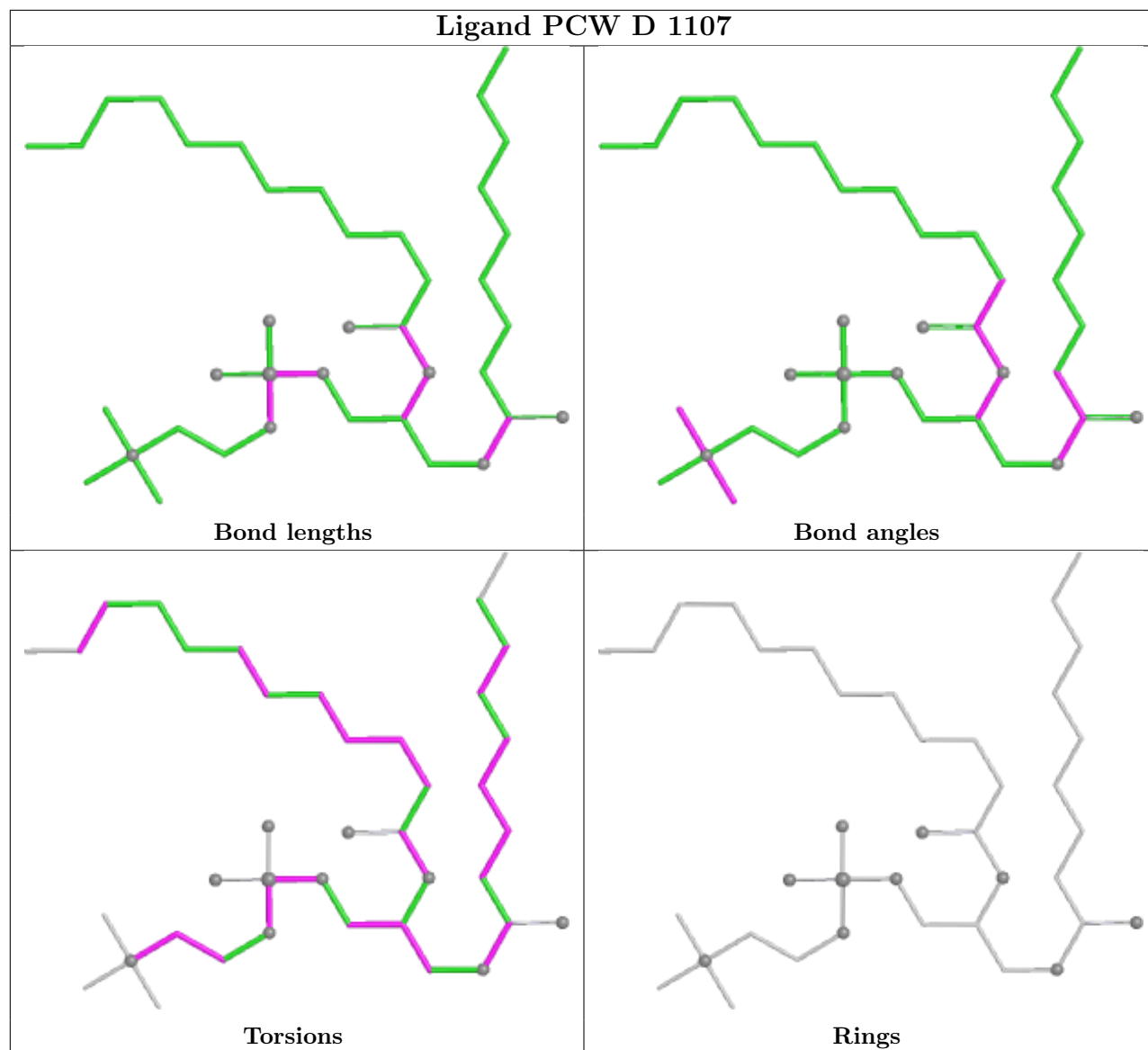


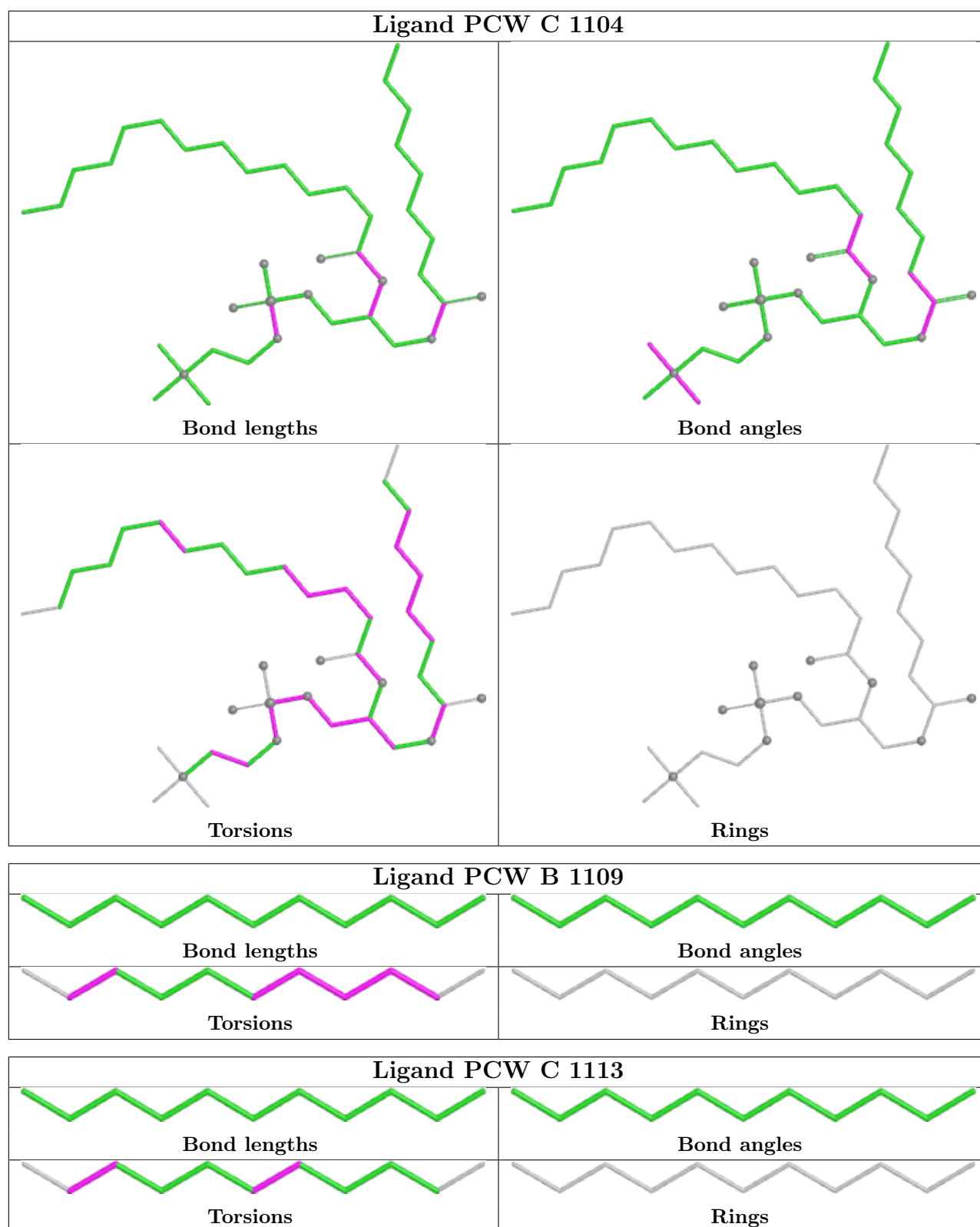


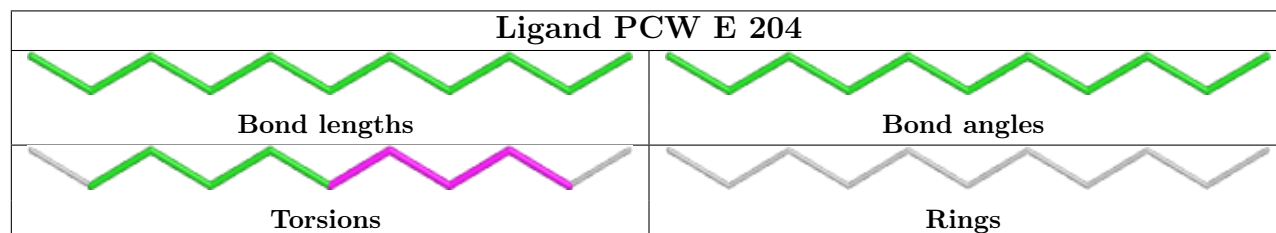
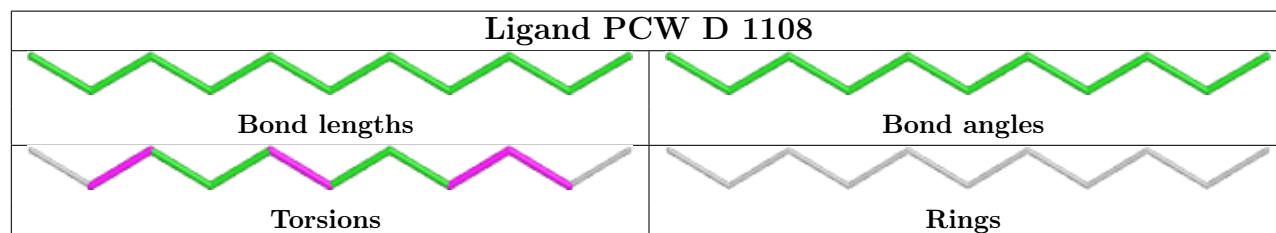
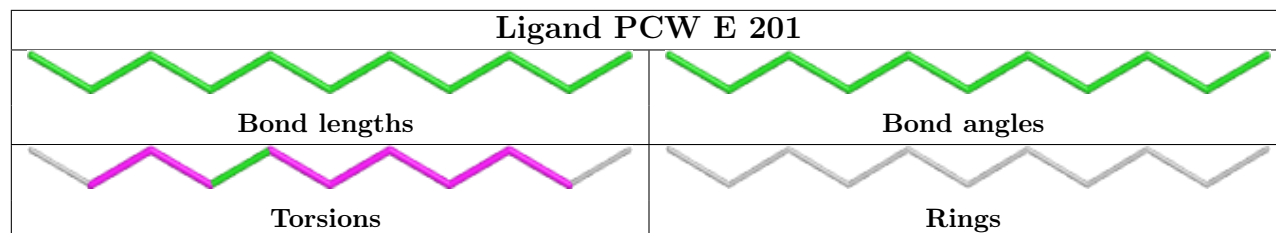
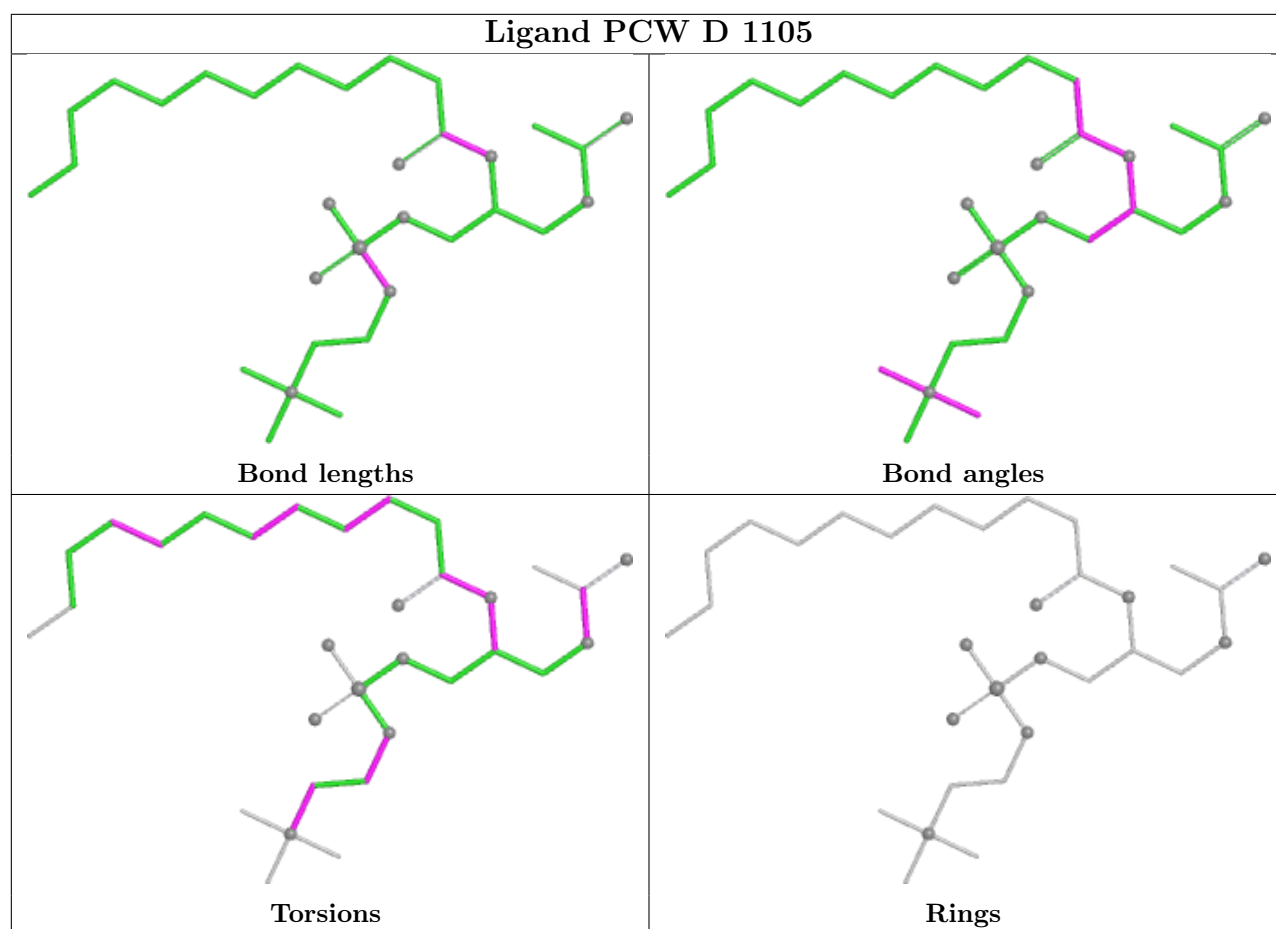


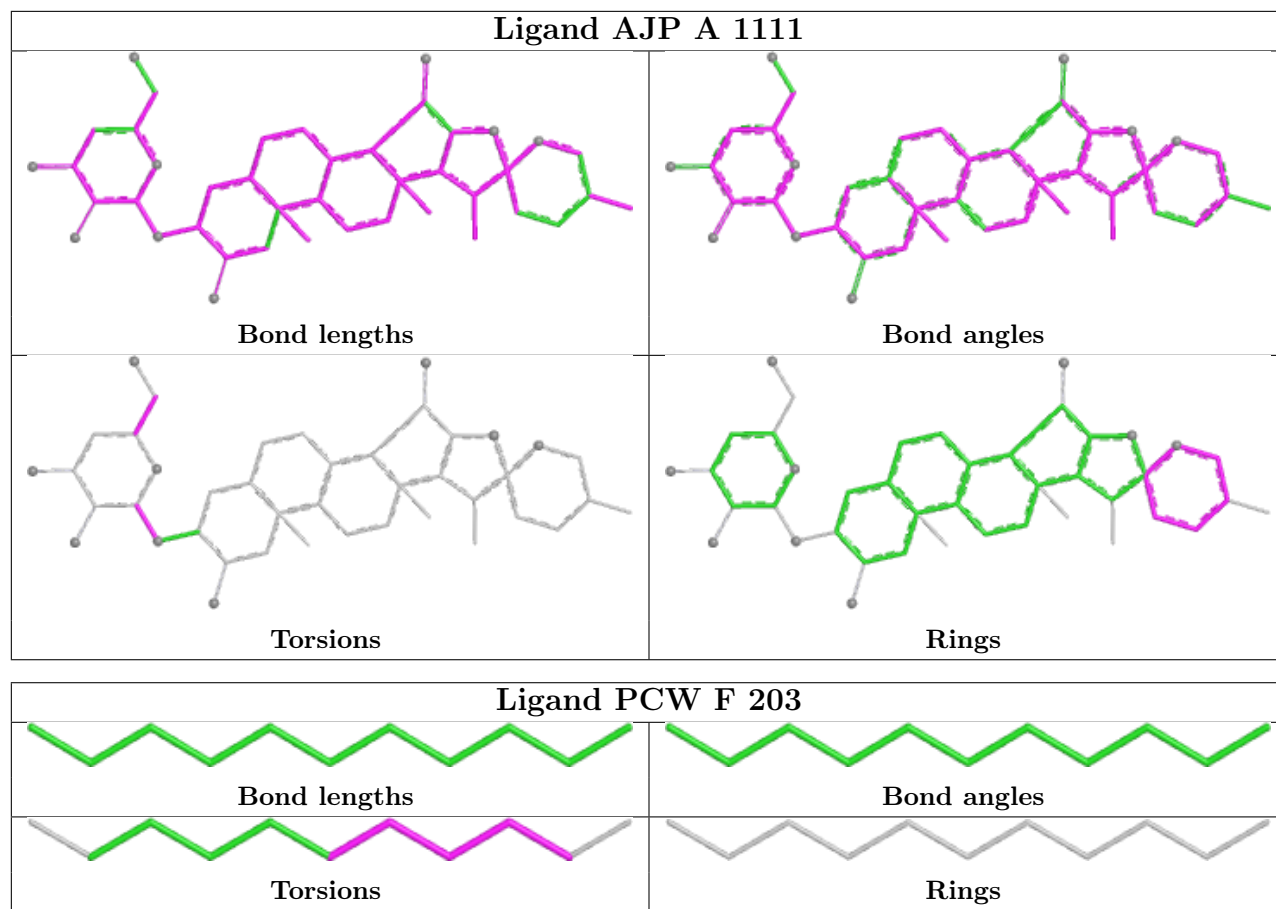


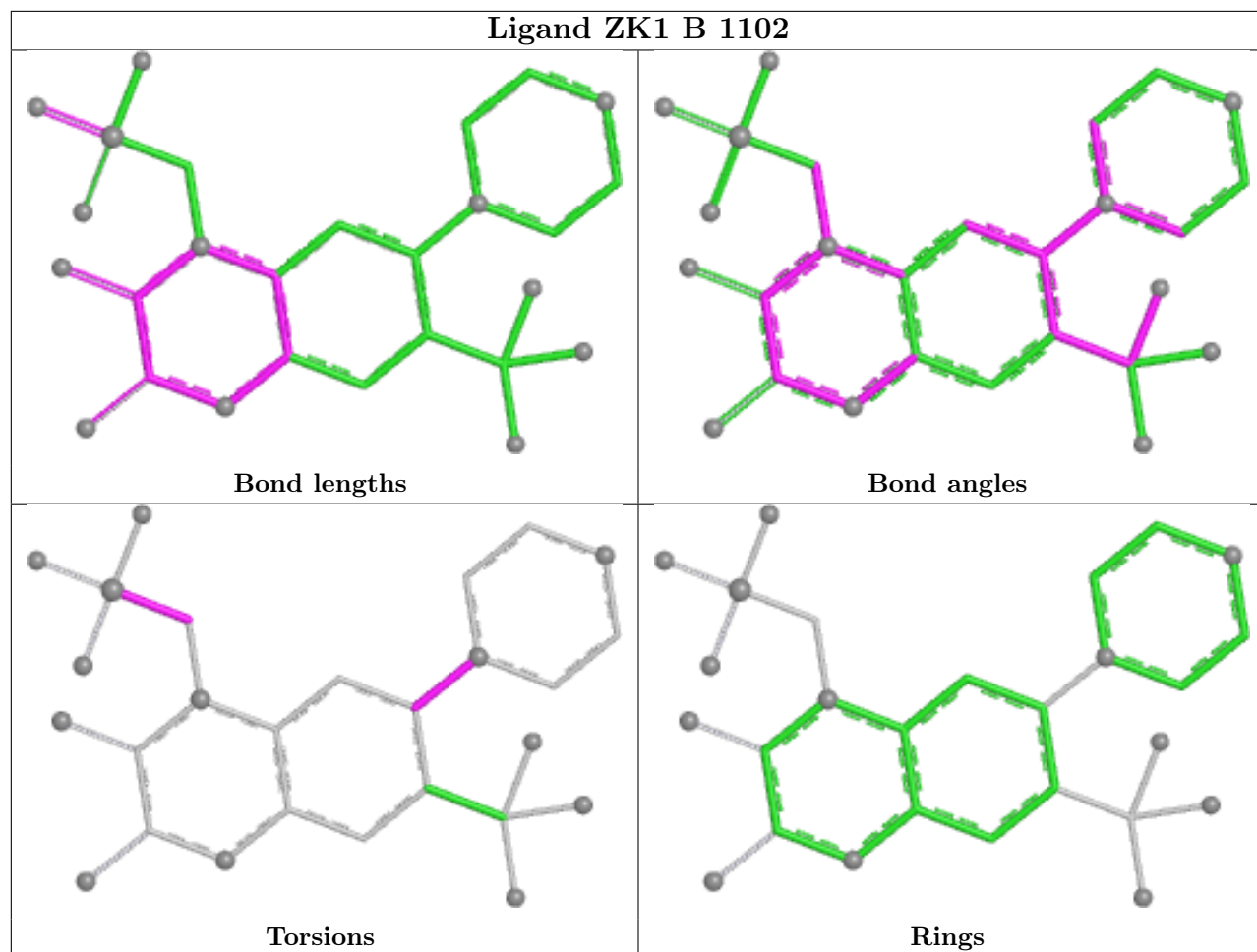




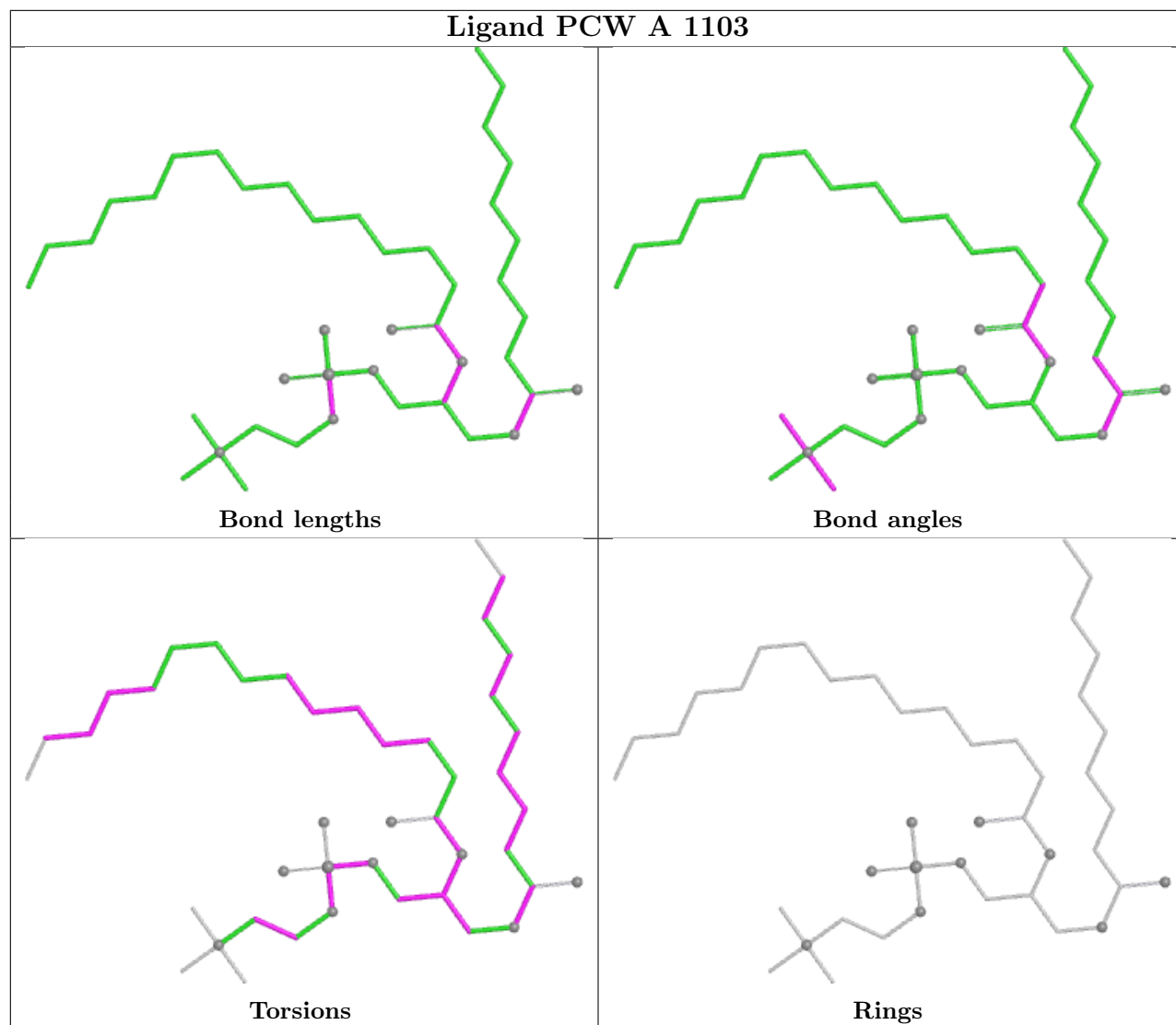




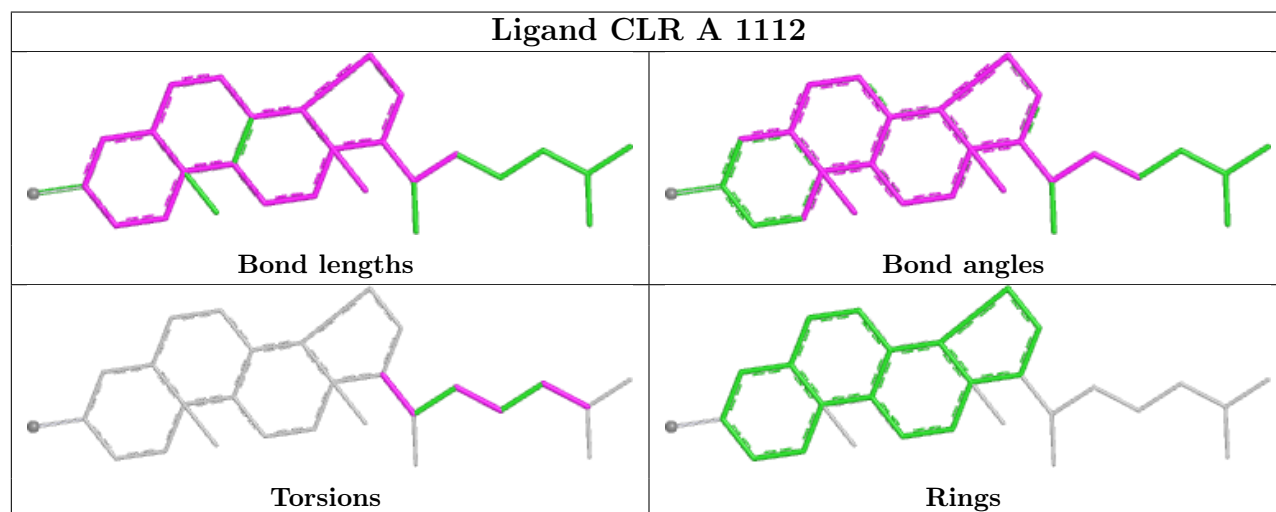




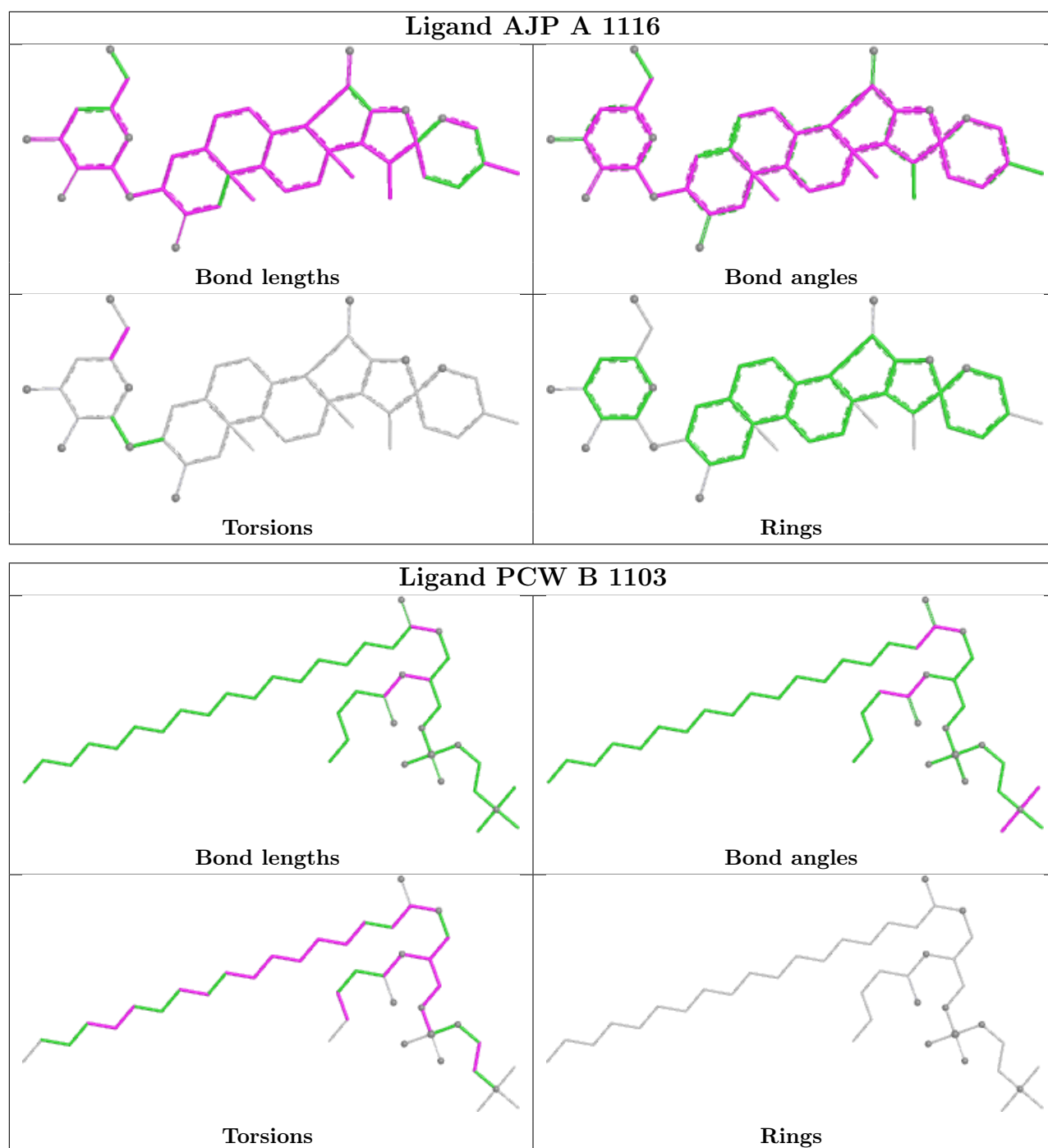
## Ligand PCW A 1103



## Ligand CLR A 1112







## 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.

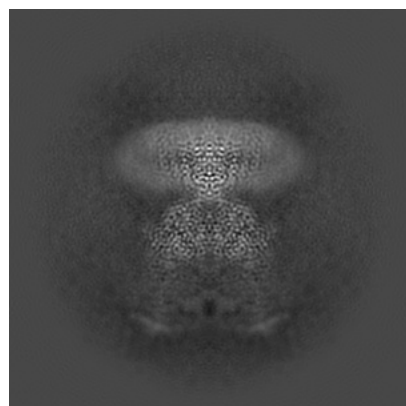
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40742. These allow visual inspection of the internal detail of the map and identification of artifacts.

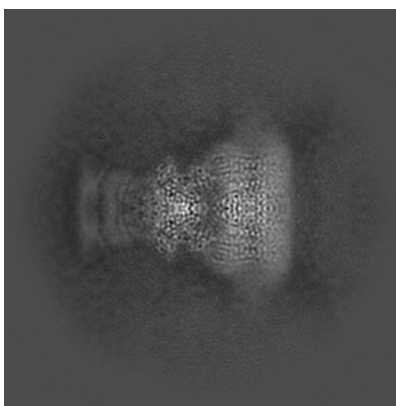
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

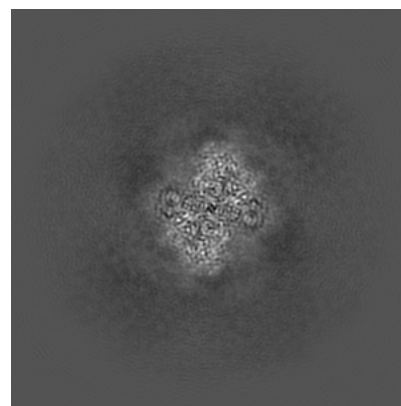
#### 6.1.1 Primary map



X

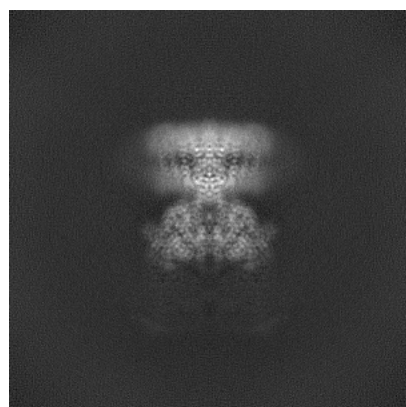


Y

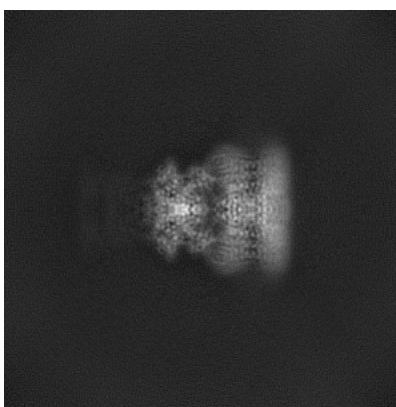


Z

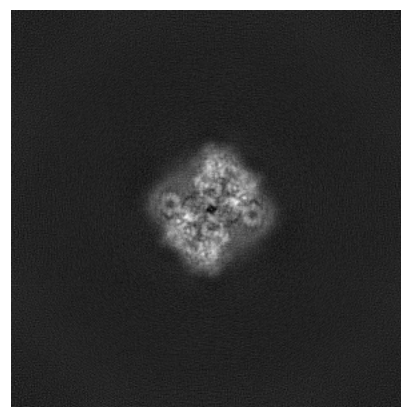
#### 6.1.2 Raw map



X



Y

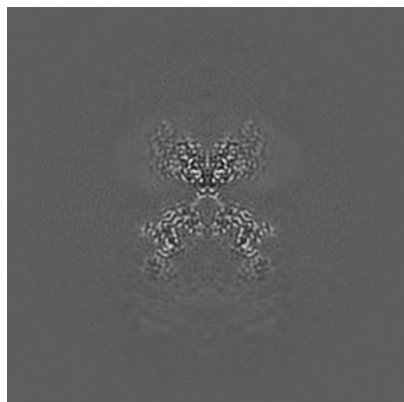


Z

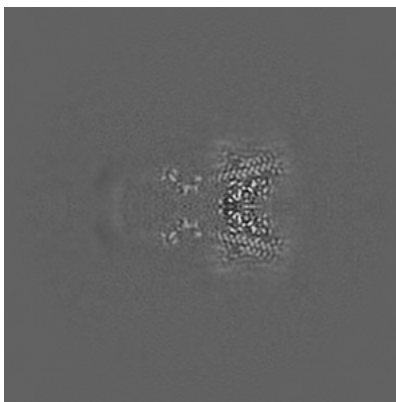
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

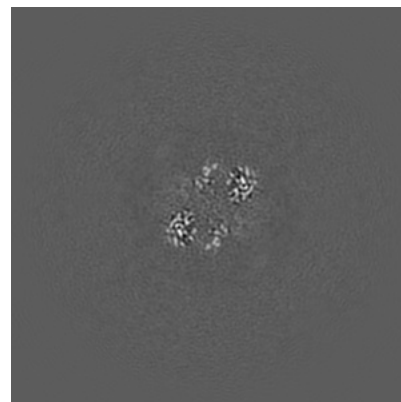
### 6.2.1 Primary map



X Index: 208

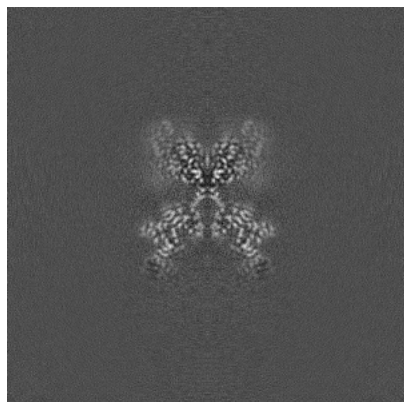


Y Index: 208

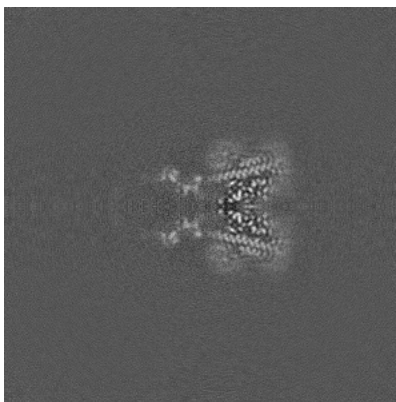


Z Index: 208

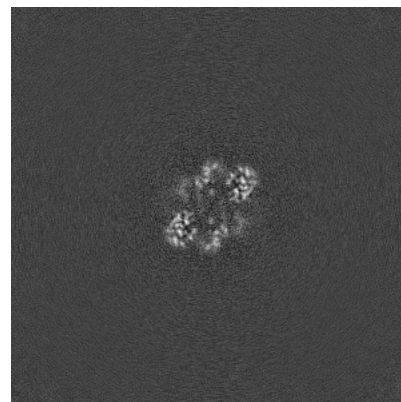
### 6.2.2 Raw map



X Index: 208



Y Index: 208

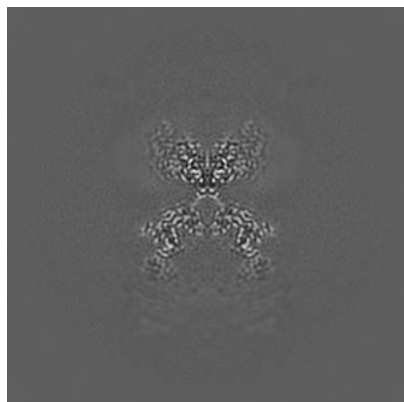


Z Index: 208

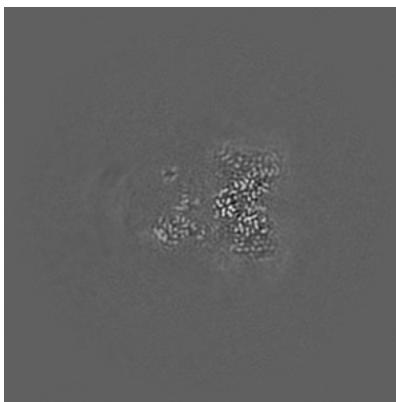
The images above show central slices of the map in three orthogonal directions.

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

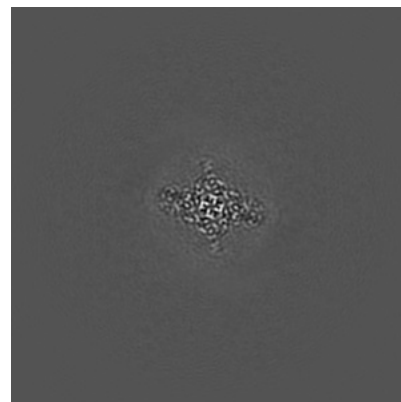
### 6.3.1 Primary map



X Index: 208

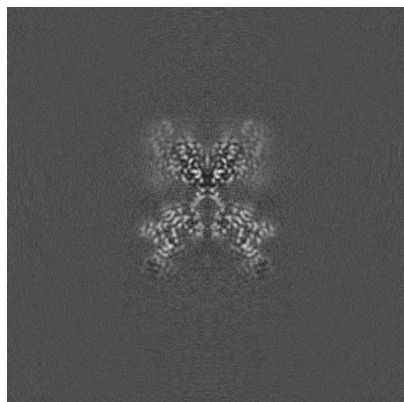


Y Index: 202

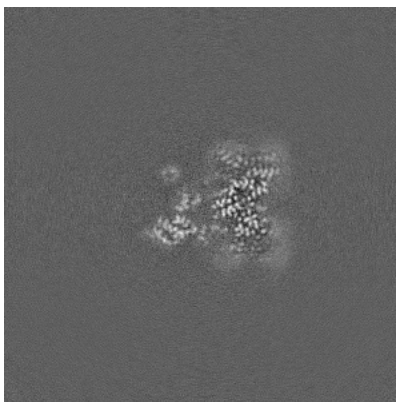


Z Index: 239

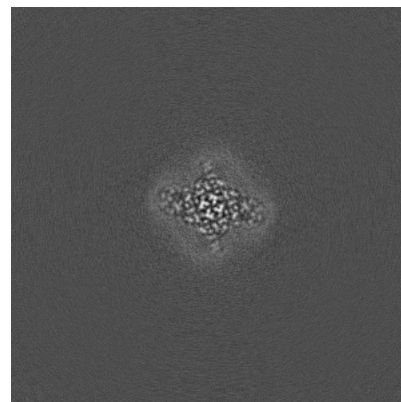
### 6.3.2 Raw map



X Index: 208



Y Index: 201

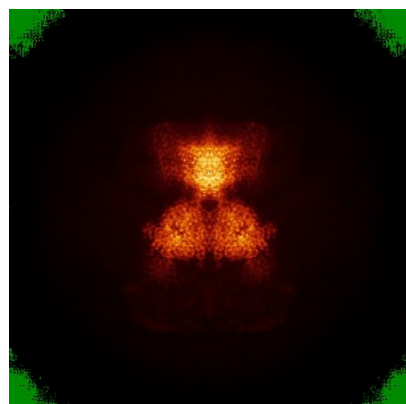


Z Index: 239

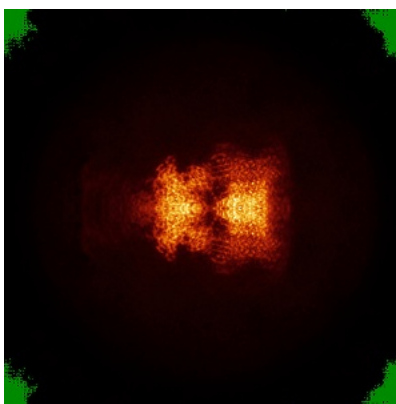
The images above show the largest variance slices of the map in three orthogonal directions.

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

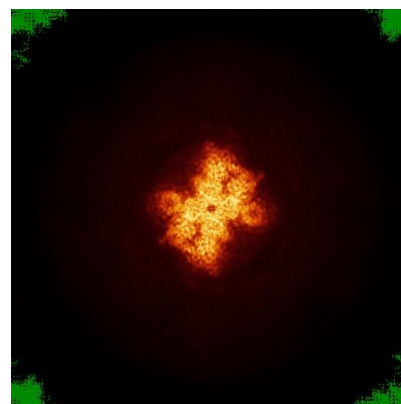
### 6.4.1 Primary map



X

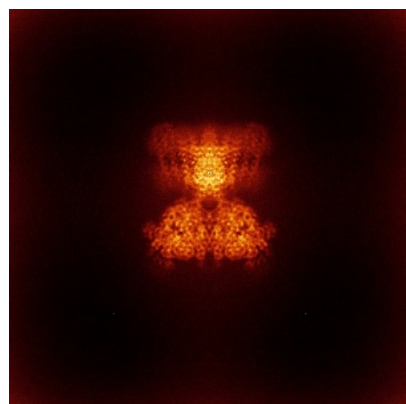


Y

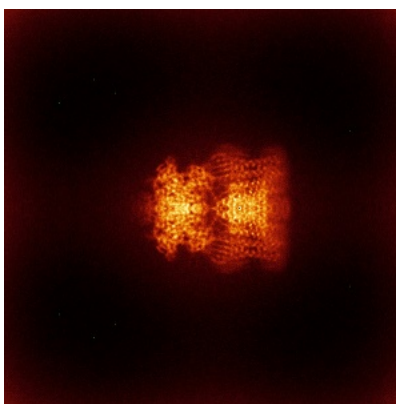


Z

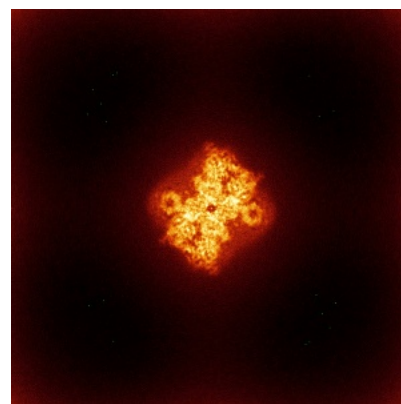
### 6.4.2 Raw map



X



Y



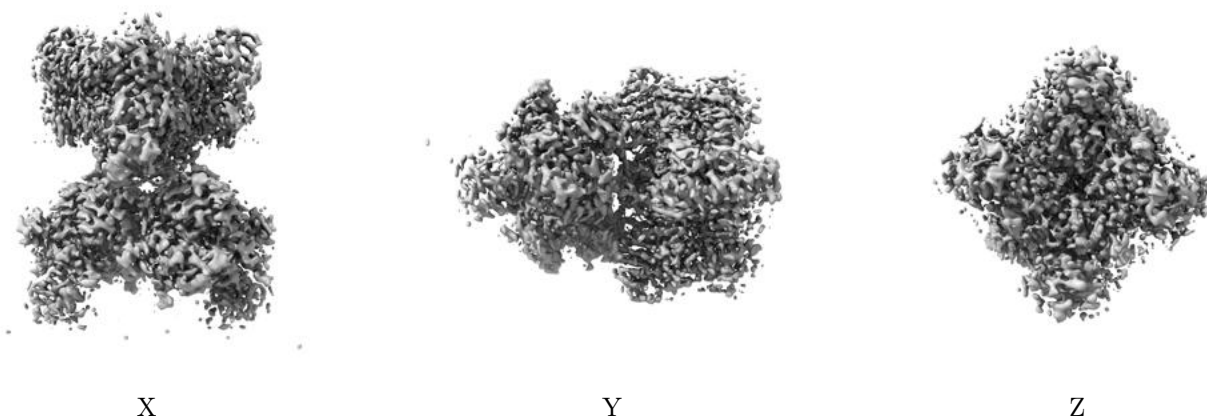
Z

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



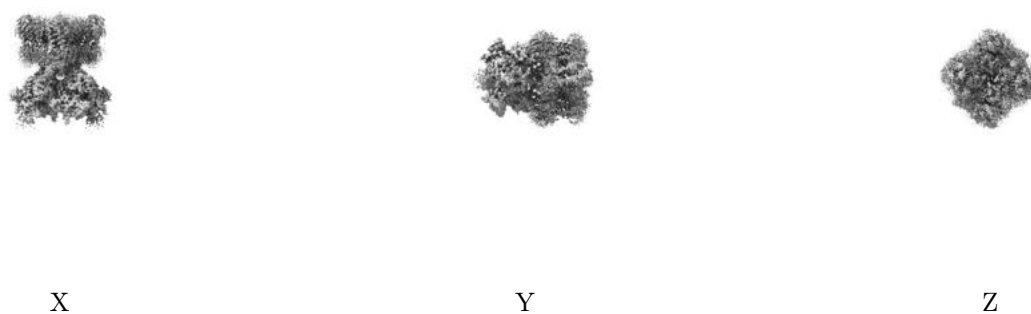
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

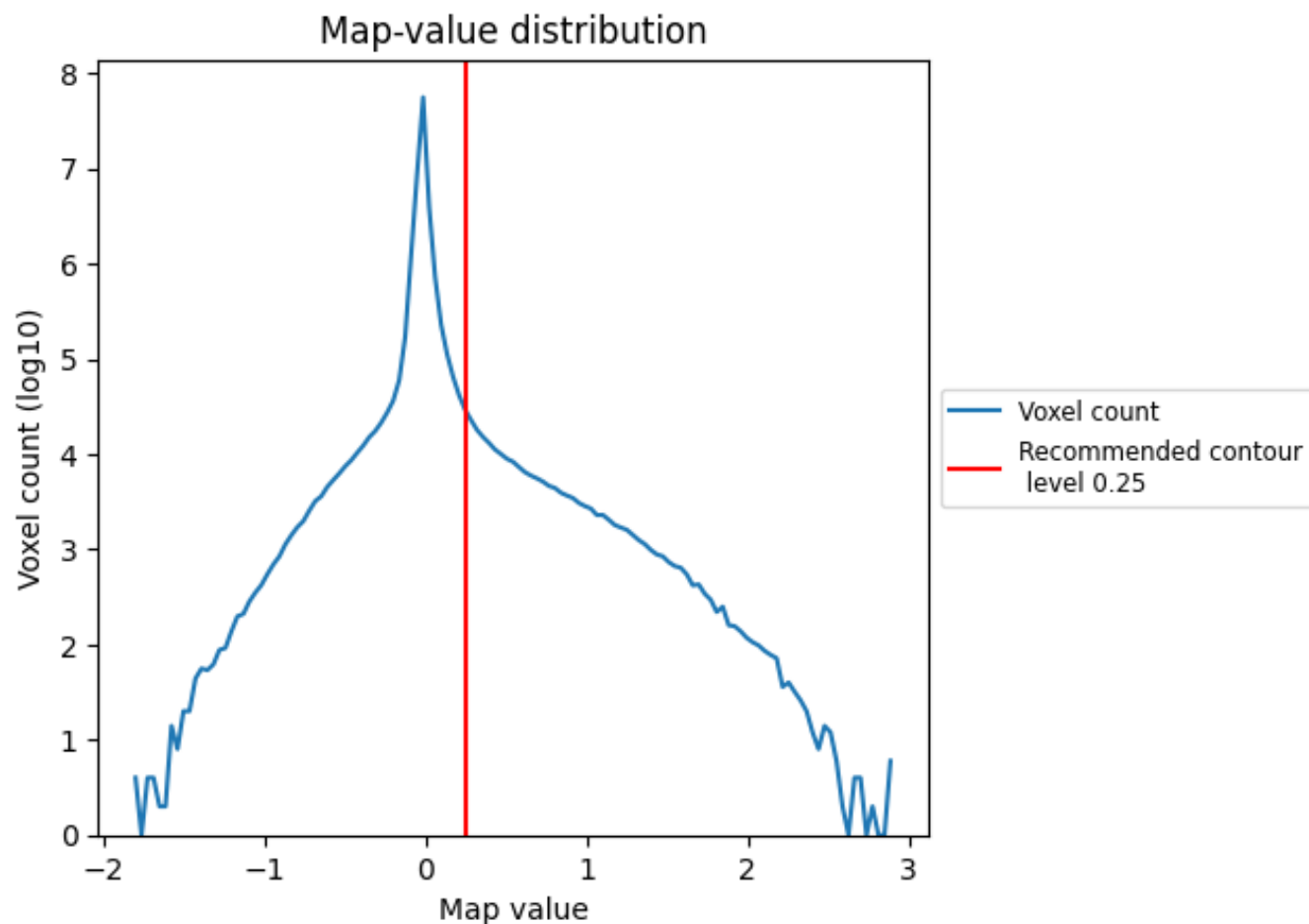
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

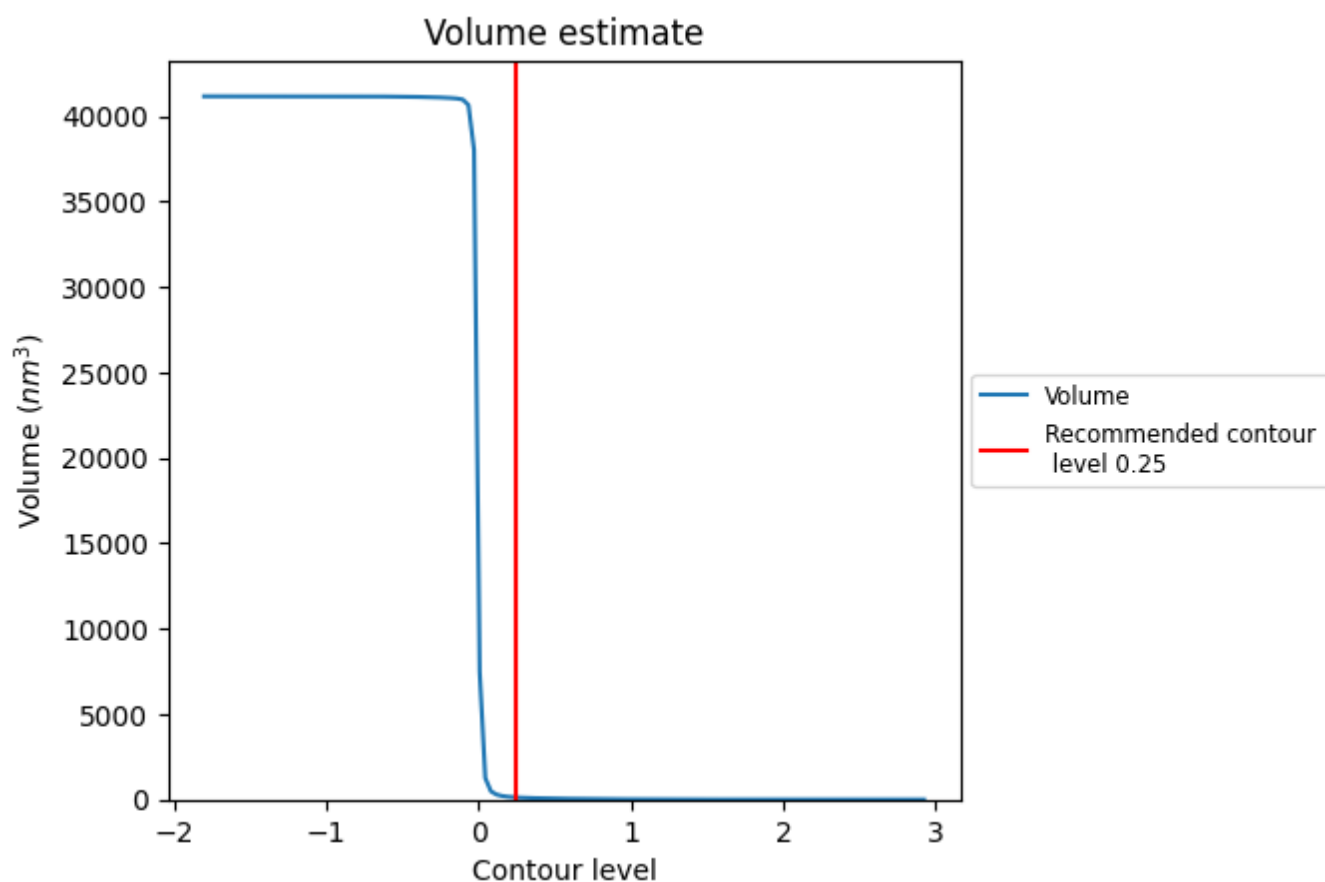
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

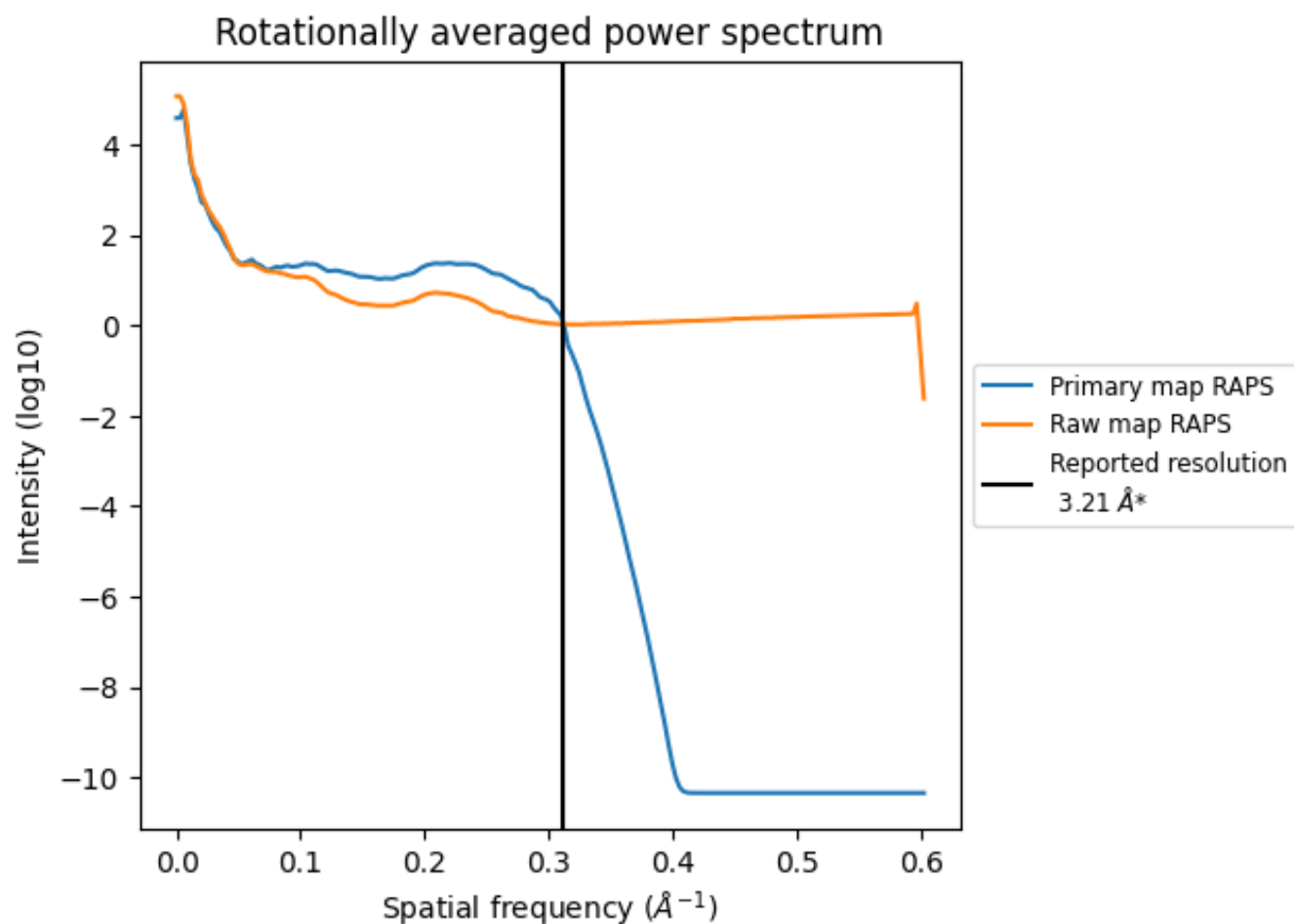


The volume at the recommended contour level is 124  $\text{nm}^3$ ; this corresponds to an approximate mass of 112 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

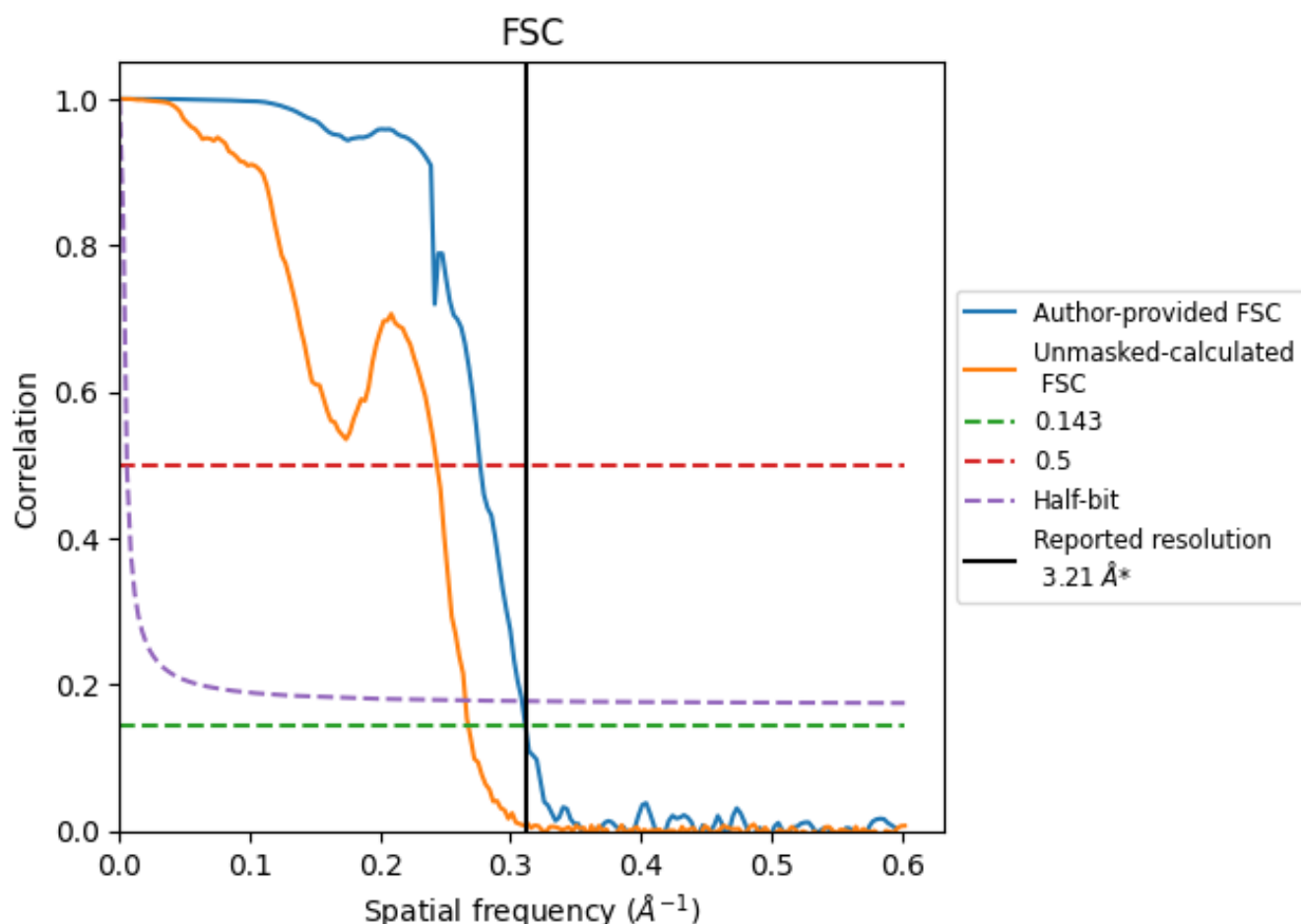


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

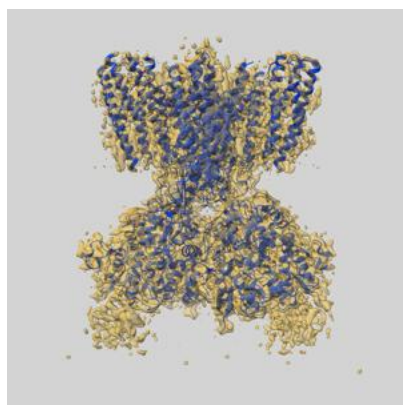
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	3.62	3.24
Unmasked-calculated*	3.74	4.11	3.77

\*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 3.74 differs from the reported value 3.21 by more than 10 %

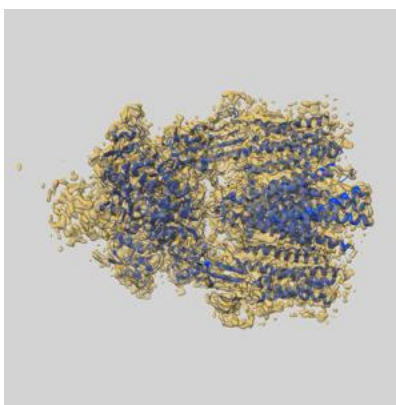
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40742 and PDB model 8SS3. Per-residue inclusion information can be found in section 3 on page 12.

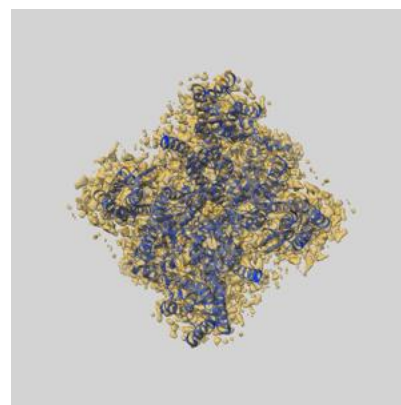
### 9.1 Map-model overlay [i](#)



X



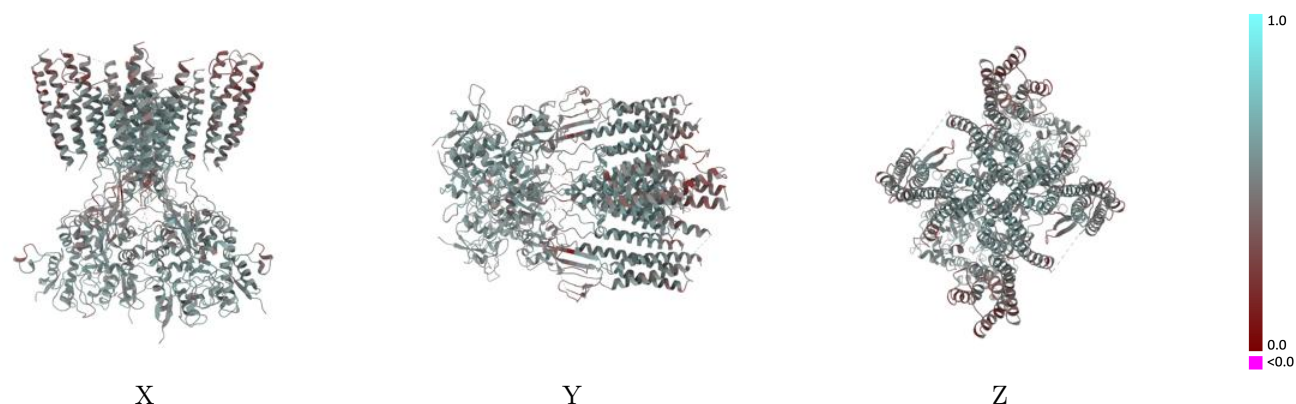
Y



Z

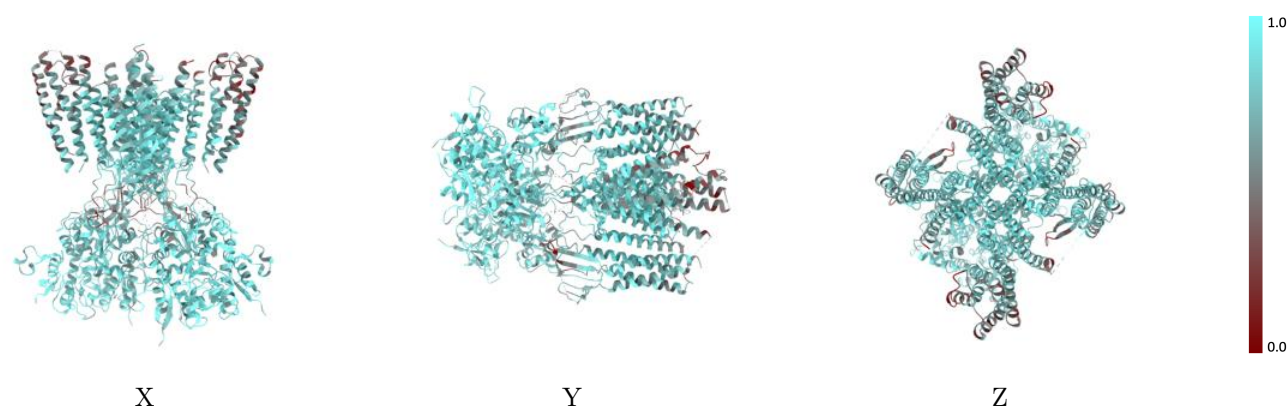
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



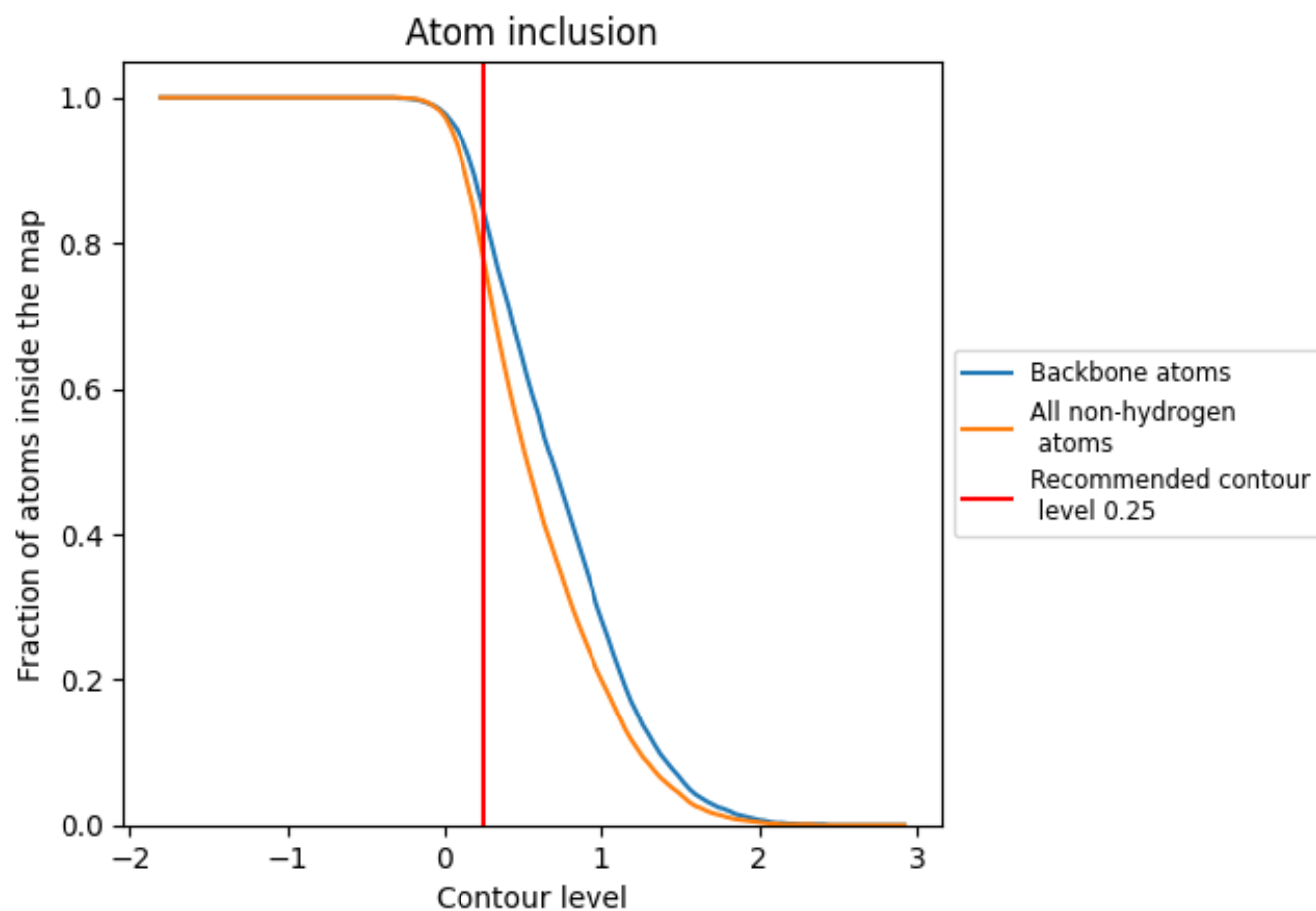
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7790</div>	<div><div></div>0.5070</div>
A	<div><div></div>0.7830</div>	<div><div></div>0.5110</div>
B	<div><div></div>0.8310</div>	<div><div></div>0.5290</div>
C	<div><div></div>0.7870</div>	<div><div></div>0.5090</div>
D	<div><div></div>0.8350</div>	<div><div></div>0.5260</div>
E	<div><div></div>0.6090</div>	<div><div></div>0.4340</div>
F	<div><div></div>0.6030</div>	<div><div></div>0.4360</div>

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