



## Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 12:19 PM EDT

PDB ID : 7K4A / pdb\_00007k4a  
EMDB ID : EMD-22662  
Title : Cryo-EM structure of human TRPV6 in the open state  
Authors : Neuberger, A.; Nadezhdin, K.D.; Singh, A.K.; Sobolevsky, A.I.  
Deposited on : 2020-09-15  
Resolution : 3.26 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1

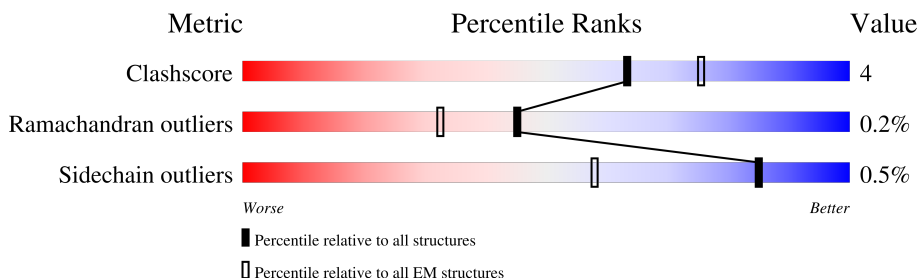
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.26 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	670	<div> <div>14%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>
1	B	670	<div> <div>14%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>
1	C	670	<div> <div>14%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>
1	D	670	<div> <div>14%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20825 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.

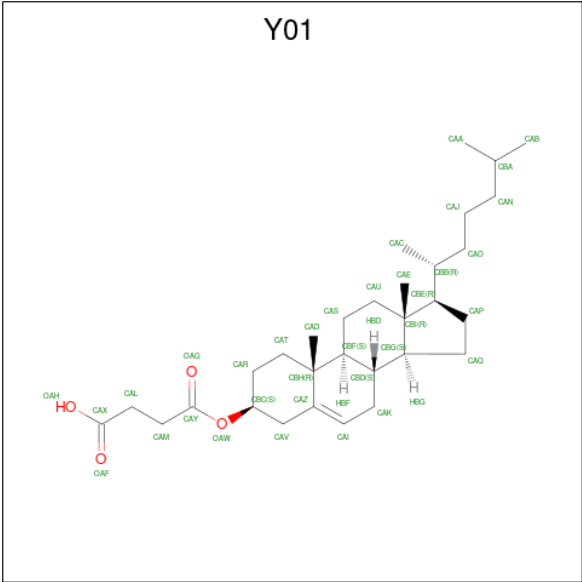
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	605	Total	C	N	O	S	0	0
			4868	3140	829	859	40		
1	B	605	Total	C	N	O	S	0	0
			4868	3140	829	859	40		
1	C	605	Total	C	N	O	S	0	0
			4868	3140	829	859	40		
1	D	605	Total	C	N	O	S	0	0
			4868	3140	829	859	40		

There are 12 discrepancies between the modelled and reference sequences:

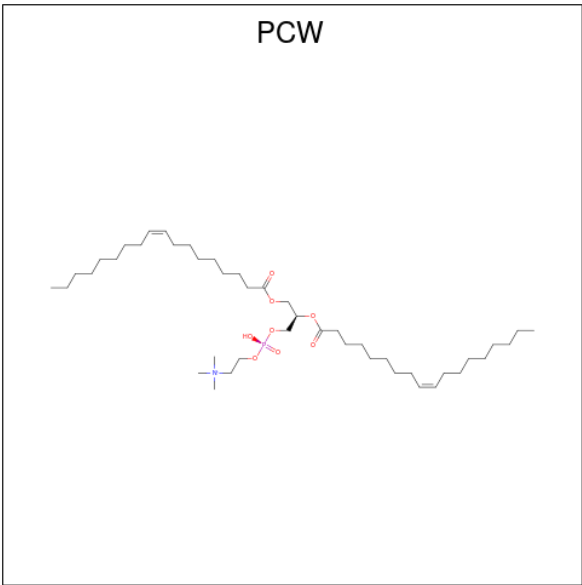
Chain	Residue	Modelled	Actual	Comment	Reference
A	668	VAL	-	expression tag	UNP Q9H1D0
A	669	PRO	-	expression tag	UNP Q9H1D0
A	670	ARG	-	expression tag	UNP Q9H1D0
B	668	VAL	-	expression tag	UNP Q9H1D0
B	669	PRO	-	expression tag	UNP Q9H1D0
B	670	ARG	-	expression tag	UNP Q9H1D0
C	668	VAL	-	expression tag	UNP Q9H1D0
C	669	PRO	-	expression tag	UNP Q9H1D0
C	670	ARG	-	expression tag	UNP Q9H1D0
D	668	VAL	-	expression tag	UNP Q9H1D0
D	669	PRO	-	expression tag	UNP Q9H1D0
D	670	ARG	-	expression tag	UNP Q9H1D0

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C				0
			16	16				
3	A	1	Total	C				0
			13	13				
3	A	1	Total	C				0
			11	11				
3	A	1	Total	C				0
			8	8				
3	A	1	Total	C				0
			8	8				
3	A	1	Total	C				0
			16	16				
3	A	1	Total	C				0
			8	8				
3	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
3	A	1	Total	C				0
			11	11				
3	A	1	Total	C				0
			16	16				
3	A	1	Total	C				0
			16	16				
3	A	1	Total	C				0
			16	16				
3	B	1	Total	C				0
			16	16				

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C 16 16	0
3	B	1	Total C N O P 51 41 1 8 1	0
3	B	1	Total C 16 16	0
3	B	1	Total C 13 13	0
3	B	1	Total C 11 11	0
3	B	1	Total C 8 8	0
3	B	1	Total C 8 8	0
3	B	1	Total C 16 16	0
3	B	1	Total C 8 8	0
3	B	1	Total C N O P 43 33 1 8 1	0
3	B	1	Total C 11 11	0
3	B	1	Total C 16 16	0
3	C	1	Total C 16 16	0
3	C	1	Total C 16 16	0
3	C	1	Total C N O P 51 41 1 8 1	0
3	C	1	Total C 16 16	0
3	C	1	Total C 13 13	0
3	C	1	Total C 11 11	0
3	C	1	Total C 8 8	0
3	C	1	Total C 8 8	0
3	C	1	Total C 16 16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C 8 8	0
3	C	1	Total C N O P 43 33 1 8 1	0
3	C	1	Total C 11 11	0
3	C	1	Total C 16 16	0
3	D	1	Total C N O P 43 33 1 8 1	0
3	D	1	Total C 11 11	0
3	D	1	Total C 16 16	0
3	D	1	Total C 16 16	0
3	D	1	Total C 16 16	0
3	D	1	Total C N O P 51 41 1 8 1	0
3	D	1	Total C 16 16	0
3	D	1	Total C 13 13	0
3	D	1	Total C 11 11	0
3	D	1	Total C 8 8	0
3	D	1	Total C 8 8	0
3	D	1	Total C 16 16	0
3	D	1	Total C 8 8	0

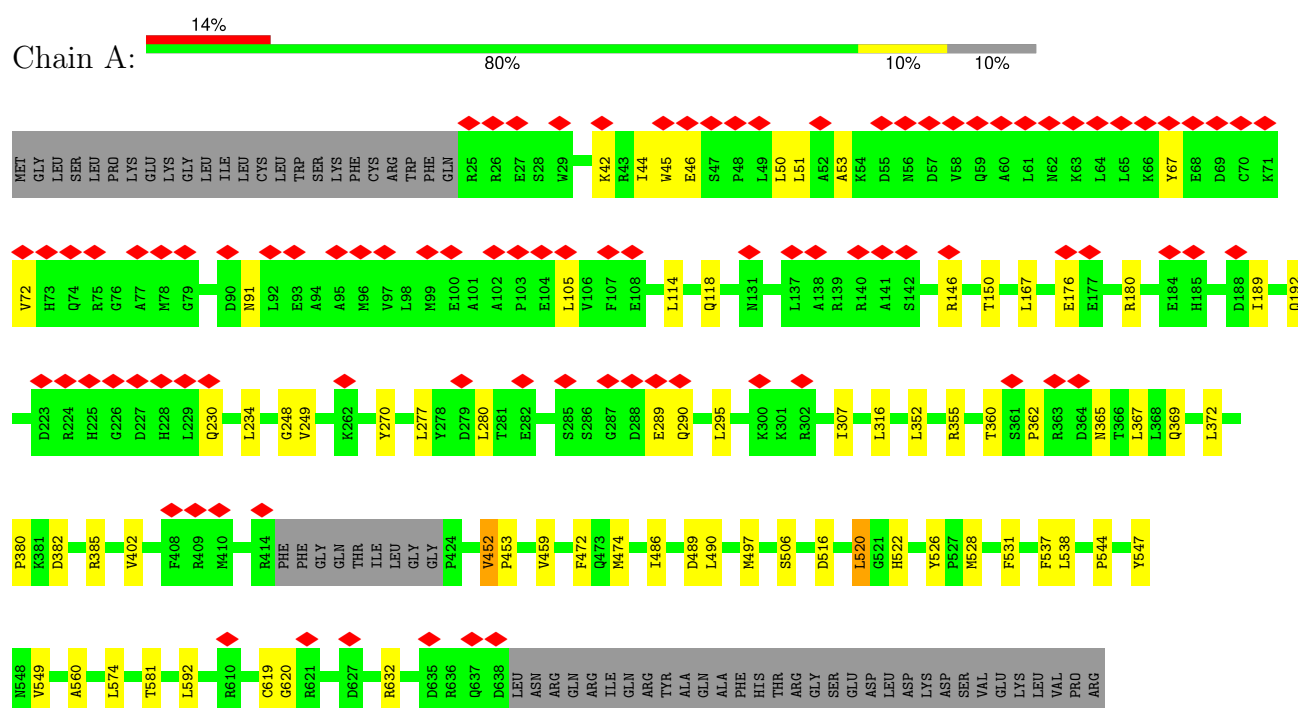
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0

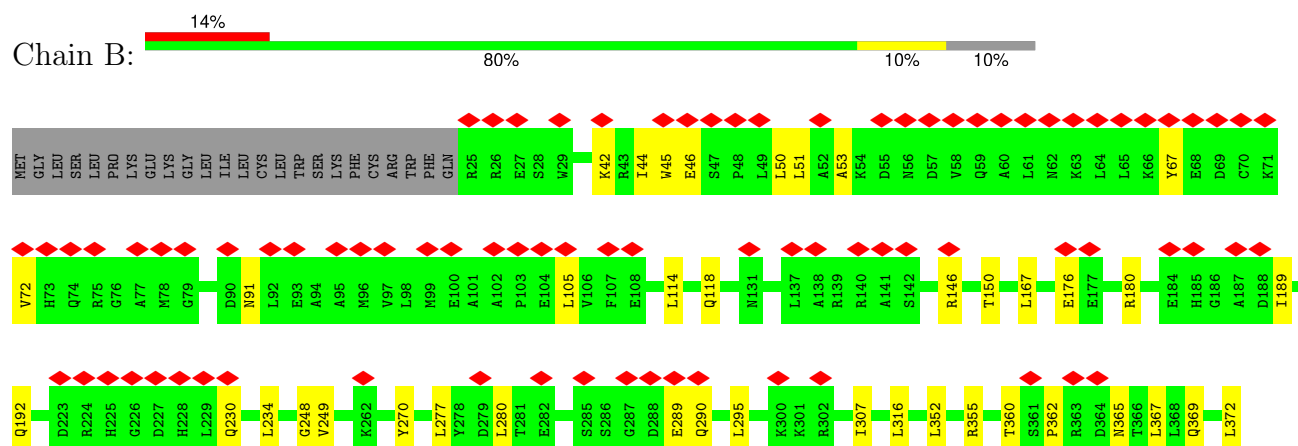
### 3 Residue-property plots

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.

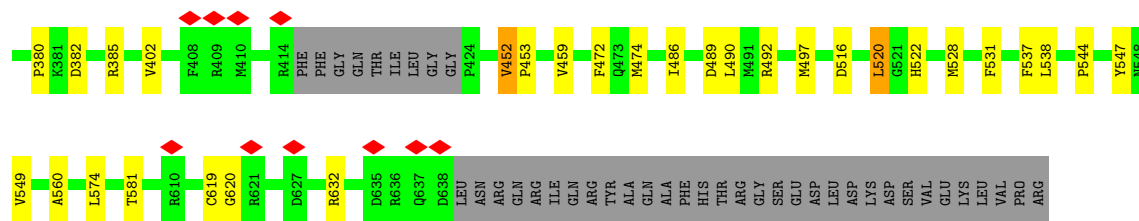
- Molecule 1: Transient receptor potential cation channel subfamily V member 6



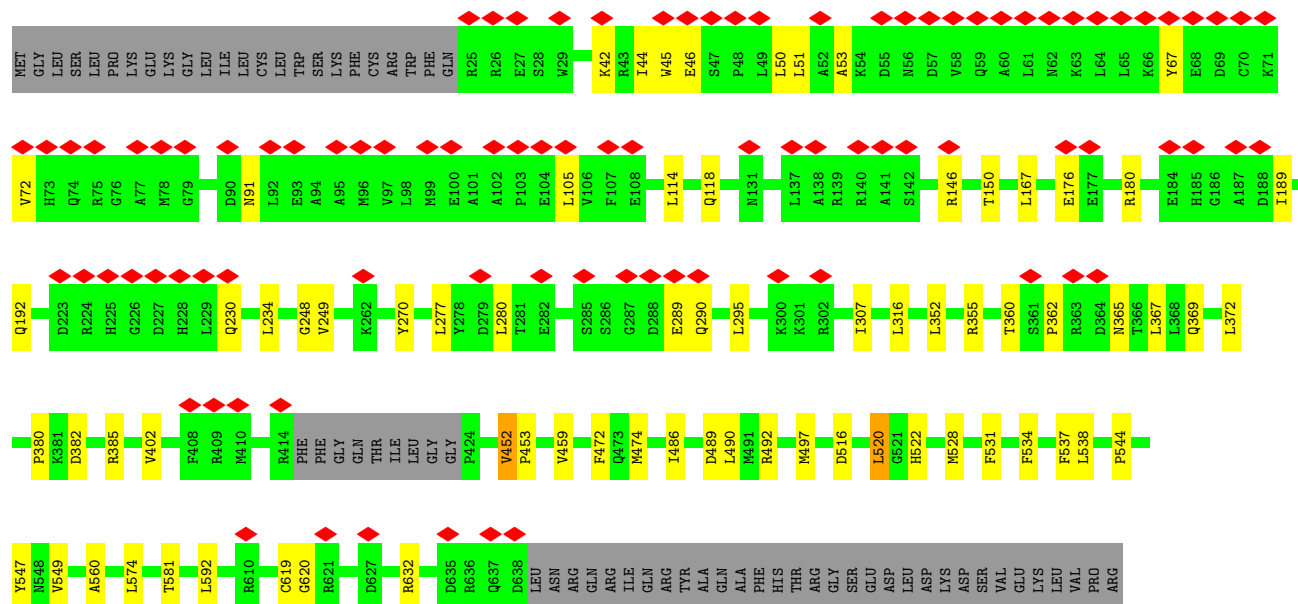
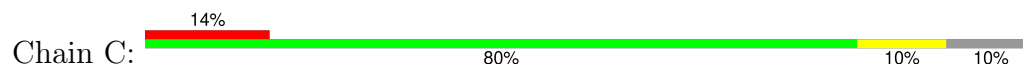
- Molecule 1: Transient receptor potential cation channel subfamily V member 6



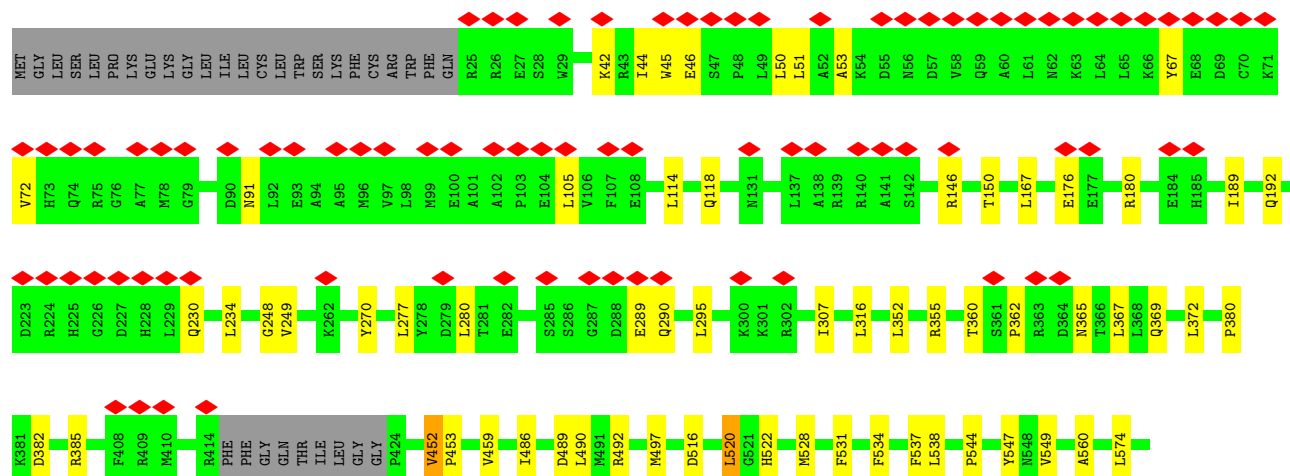
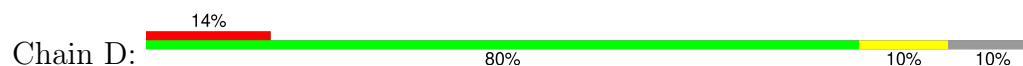


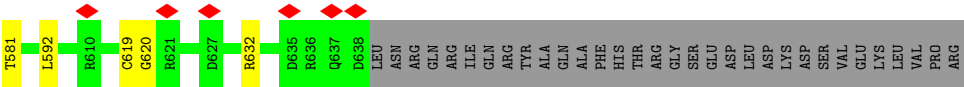


- Molecule 1: Transient receptor potential cation channel subfamily V member 6



- Molecule 1: Transient receptor potential cation channel subfamily V member 6





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	261133	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.405	Depositor
Minimum map value	-0.811	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	216.064, 216.064, 216.064	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.844, 0.844, 0.844	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, Y01, CA

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	0.32	0/4978	0.67	0/6751
1	B	0.32	0/4978	0.67	0/6751
1	C	0.32	0/4978	0.67	0/6751
1	D	0.32	0/4978	0.67	0/6751
All	All	0.32	0/19912	0.67	0/27004

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	TYR	Peptide
1	B	67	TYR	Peptide
1	C	67	TYR	Peptide
1	D	67	TYR	Peptide

## 5.2 Too-close contacts ⓘ

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	4868	0	4926	43	0
1	B	4868	0	4926	43	0
1	C	4868	0	4926	44	0
1	D	4868	0	4926	41	0
2	A	105	0	147	9	0
2	B	140	0	196	11	0
2	C	105	0	147	7	0
2	D	70	0	98	3	0
3	A	233	0	349	3	0
3	B	233	0	349	3	0
3	C	233	0	349	3	0
3	D	233	0	349	2	0
4	A	1	0	0	0	0
All	All	20825	0	21688	169	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 4.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:HG13	1:B:453:PRO:HD3	1.83	0.61
1:C:452:VAL:HG13	1:C:453:PRO:HD3	1.82	0.60
1:A:452:VAL:HG13	1:A:453:PRO:HD3	1.83	0.60
1:D:452:VAL:HG13	1:D:453:PRO:HD3	1.83	0.60
1:A:118:GLN:NE2	1:D:270:TYR:OH	2.36	0.58
1:A:459:VAL:HG11	2:A:802:Y01:HAN2	1.86	0.57
1:C:459:VAL:HG11	2:C:704:Y01:HAN2	1.87	0.57
1:D:459:VAL:HG11	2:D:707:Y01:HAN2	1.87	0.57
1:C:270:TYR:OH	1:D:118:GLN:NE2	2.37	0.56
1:A:270:TYR:OH	1:B:118:GLN:NE2	2.39	0.56
1:B:270:TYR:OH	1:C:118:GLN:NE2	2.38	0.56
1:B:367:LEU:HD12	1:C:516:ASP:HB3	1.88	0.55
1:B:459:VAL:HG11	2:B:705:Y01:HAN2	1.89	0.55
1:B:45:TRP:HA	1:B:51:LEU:HD12	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TRP:HA	1:A:51:LEU:HD12	1.88	0.55
1:A:289:GLU:HG3	1:A:290:GLN:HG2	1.89	0.55
1:D:146:ARG:NH2	1:D:192:GLN:O	2.40	0.55
1:A:146:ARG:NH2	1:A:192:GLN:O	2.40	0.55
1:C:146:ARG:NH2	1:C:192:GLN:O	2.40	0.55
1:B:289:GLU:HG3	1:B:290:GLN:HG2	1.89	0.54
1:D:289:GLU:HG3	1:D:290:GLN:HG2	1.89	0.54
1:C:45:TRP:HA	1:C:51:LEU:HD12	1.88	0.54
1:B:42:LYS:NZ	1:B:46:GLU:OE2	2.40	0.54
1:B:146:ARG:NH2	1:B:192:GLN:O	2.40	0.54
1:D:277:LEU:HD12	1:D:632:ARG:HB3	1.91	0.53
1:C:277:LEU:HD12	1:C:632:ARG:HB3	1.91	0.53
1:C:289:GLU:HG3	1:C:290:GLN:HG2	1.89	0.53
1:C:489:ASP:OD2	1:C:581:THR:OG1	2.26	0.53
1:D:45:TRP:HA	1:D:51:LEU:HD12	1.88	0.53
1:B:382:ASP:OD1	1:B:385:ARG:NH2	2.39	0.53
1:C:382:ASP:OD1	1:C:385:ARG:NH2	2.39	0.53
1:A:42:LYS:NZ	1:A:46:GLU:OE2	2.40	0.53
1:D:42:LYS:NZ	1:D:46:GLU:OE2	2.40	0.52
1:B:486:ILE:HD12	2:B:705:Y01:HAD3	1.92	0.52
1:B:277:LEU:HD12	1:B:632:ARG:HB3	1.90	0.52
1:D:53:ALA:O	1:D:91:ASN:ND2	2.43	0.52
1:C:42:LYS:NZ	1:C:46:GLU:OE2	2.40	0.52
1:C:53:ALA:O	1:C:91:ASN:ND2	2.43	0.52
1:A:367:LEU:HD12	1:B:516:ASP:HB3	1.92	0.52
1:A:516:ASP:HB3	1:D:367:LEU:HD12	1.92	0.52
1:C:230:GLN:HB2	1:C:234:LEU:HB2	1.93	0.51
1:A:277:LEU:HD12	1:A:632:ARG:HB3	1.91	0.51
1:D:230:GLN:HB2	1:D:234:LEU:HB2	1.93	0.51
1:B:230:GLN:HB2	1:B:234:LEU:HB2	1.93	0.51
1:D:352:LEU:HA	1:D:372:LEU:HA	1.93	0.51
1:A:352:LEU:HA	1:A:372:LEU:HA	1.93	0.51
1:C:352:LEU:HA	1:C:372:LEU:HA	1.93	0.51
1:B:53:ALA:O	1:B:91:ASN:ND2	2.43	0.51
1:C:367:LEU:HD12	1:D:516:ASP:HB3	1.93	0.51
1:B:489:ASP:OD2	1:B:581:THR:OG1	2.26	0.51
1:A:53:ALA:O	1:A:91:ASN:ND2	2.43	0.51
1:C:360:THR:HG23	1:C:362:PRO:HD2	1.93	0.51
1:C:486:ILE:HD12	2:C:704:Y01:HAD3	1.93	0.51
1:A:230:GLN:HB2	1:A:234:LEU:HB2	1.93	0.51
1:D:486:ILE:HD12	2:D:707:Y01:HAD3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:THR:HG23	1:B:362:PRO:HD2	1.93	0.50
1:B:352:LEU:HA	1:B:372:LEU:HA	1.93	0.50
1:D:360:THR:HG23	1:D:362:PRO:HD2	1.93	0.50
1:D:176:GLU:O	1:D:180:ARG:NE	2.38	0.50
1:D:382:ASP:OD1	1:D:385:ARG:NH2	2.39	0.49
1:A:382:ASP:OD1	1:A:385:ARG:NH2	2.39	0.49
1:B:176:GLU:O	1:B:180:ARG:NE	2.38	0.49
1:A:360:THR:HG23	1:A:362:PRO:HD2	1.93	0.49
1:B:248:GLY:HA2	1:B:307:ILE:HD13	1.95	0.49
1:A:176:GLU:O	1:A:180:ARG:NE	2.38	0.49
1:A:560:ALA:HB2	1:D:531:PHE:HE1	1.78	0.49
1:A:248:GLY:HA2	1:A:307:ILE:HD13	1.95	0.49
2:B:701:Y01:HAO2	2:B:701:Y01:HAP1	1.55	0.49
1:A:280:LEU:HD11	1:A:316:LEU:HD13	1.95	0.48
1:D:248:GLY:HA2	1:D:307:ILE:HD13	1.95	0.48
1:A:486:ILE:HD12	2:A:802:Y01:HAD3	1.95	0.48
1:D:280:LEU:HD11	1:D:316:LEU:HD13	1.95	0.48
1:C:248:GLY:HA2	1:C:307:ILE:HD13	1.95	0.48
1:C:280:LEU:HD11	1:C:316:LEU:HD13	1.95	0.48
1:D:489:ASP:OD2	1:D:581:THR:OG1	2.26	0.48
1:B:280:LEU:HD11	1:B:316:LEU:HD13	1.95	0.47
2:A:814:Y01:HAP1	2:A:814:Y01:HAO2	1.55	0.47
3:D:701:PCW:H172	3:D:701:PCW:H141	1.71	0.47
1:A:114:LEU:HA	1:A:150:THR:HG22	1.97	0.46
2:B:706:Y01:HAA1	2:B:706:Y01:HAJ1	1.75	0.46
1:C:531:PHE:HE1	1:D:560:ALA:HB2	1.81	0.46
1:D:114:LEU:HA	1:D:150:THR:HG22	1.97	0.46
1:A:549:VAL:HA	1:D:365:ASN:HA	1.97	0.46
1:A:619:CYS:SG	1:A:620:GLY:N	2.89	0.46
1:C:619:CYS:SG	1:C:620:GLY:N	2.89	0.46
1:A:489:ASP:OD2	1:A:581:THR:OG1	2.26	0.46
1:B:114:LEU:HA	1:B:150:THR:HG22	1.97	0.46
1:B:619:CYS:SG	1:B:620:GLY:N	2.89	0.46
1:D:537:PHE:HD2	1:D:538:LEU:HD12	1.81	0.46
1:A:537:PHE:HD2	1:A:538:LEU:HD12	1.81	0.46
3:A:811:PCW:H172	3:A:811:PCW:H141	1.71	0.46
1:D:619:CYS:SG	1:D:620:GLY:N	2.89	0.45
1:A:44:ILE:HD12	1:A:50:LEU:HB3	1.99	0.45
1:A:531:PHE:HE1	1:B:560:ALA:HB2	1.81	0.45
1:B:44:ILE:HD12	1:B:50:LEU:HB3	1.99	0.45
1:C:365:ASN:HA	1:D:549:VAL:HA	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:708:PCW:H182	3:D:708:PCW:H212	1.80	0.45
1:B:531:PHE:HE1	1:C:560:ALA:HB2	1.82	0.45
1:C:114:LEU:HA	1:C:150:THR:HG22	1.97	0.45
3:C:714:PCW:H172	3:C:714:PCW:H141	1.71	0.45
1:B:537:PHE:HD2	1:B:538:LEU:HD12	1.81	0.45
1:B:522:HIS:CD2	1:B:544:PRO:HB3	2.52	0.45
1:D:522:HIS:CD2	1:D:544:PRO:HB3	2.52	0.45
1:A:522:HIS:CD2	1:A:544:PRO:HB3	2.52	0.44
1:C:44:ILE:HD12	1:C:50:LEU:HB3	1.99	0.44
1:C:176:GLU:O	1:C:180:ARG:NE	2.38	0.44
1:C:537:PHE:HD2	1:C:538:LEU:HD12	1.81	0.44
1:D:44:ILE:HD12	1:D:50:LEU:HB3	1.99	0.44
2:B:701:Y01:HAC2	2:B:701:Y01:HAJ1	1.70	0.44
1:C:522:HIS:CD2	1:C:544:PRO:HB3	2.52	0.44
3:C:706:PCW:H182	3:C:706:PCW:H212	1.79	0.44
2:C:705:Y01:HAO2	2:C:705:Y01:HAP1	1.55	0.44
1:C:474:MET:HB3	1:D:492:ARG:HD2	1.99	0.44
2:C:705:Y01:HAA1	2:C:705:Y01:HAJ1	1.75	0.43
2:B:704:Y01:HAE2	2:B:704:Y01:HBB	1.92	0.43
1:A:365:ASN:HA	1:B:549:VAL:HA	1.99	0.43
2:A:814:Y01:HAC2	2:A:814:Y01:HAJ1	1.70	0.43
1:A:474:MET:HB3	1:B:492:ARG:HD2	2.00	0.43
1:D:72:VAL:HG22	1:D:105:LEU:HD11	2.01	0.43
1:A:355:ARG:HD3	1:A:369:GLN:HA	2.01	0.43
1:A:402:VAL:HG21	2:A:801:Y01:HAK1	2.01	0.43
1:A:167:LEU:HD21	1:A:189:ILE:HD12	2.01	0.43
1:B:355:ARG:HD3	1:B:369:GLN:HA	2.01	0.43
1:C:72:VAL:HG22	1:C:105:LEU:HD11	2.01	0.43
1:D:167:LEU:HD21	1:D:189:ILE:HD12	2.00	0.43
1:D:355:ARG:HD3	1:D:369:GLN:HA	2.01	0.43
1:A:72:VAL:HG22	1:A:105:LEU:HD11	2.01	0.43
1:B:474:MET:HB3	1:C:492:ARG:HD2	2.00	0.43
1:B:490:LEU:HD11	2:B:706:Y01:HAB1	2.01	0.42
1:C:355:ARG:HD3	1:C:369:GLN:HA	2.01	0.42
1:B:365:ASN:HA	1:C:549:VAL:HA	1.99	0.42
1:B:528:MET:HE2	1:C:547:TYR:HE1	1.83	0.42
1:A:249:VAL:HG22	1:A:295:LEU:HB3	2.01	0.42
1:B:72:VAL:HG22	1:B:105:LEU:HD11	2.01	0.42
1:B:520:LEU:HD21	1:B:544:PRO:HB2	2.02	0.42
1:A:528:MET:HE2	1:B:547:TYR:HE1	1.84	0.42
2:B:701:Y01:HAJ1	2:B:701:Y01:HAA1	1.75	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:LEU:HD11	2:C:705:Y01:HAB1	2.02	0.42
1:D:520:LEU:HD21	1:D:544:PRO:HB2	2.02	0.42
1:C:249:VAL:HG22	1:C:295:LEU:HB3	2.01	0.42
1:D:249:VAL:HG22	1:D:295:LEU:HB3	2.01	0.42
1:A:520:LEU:HD21	1:A:544:PRO:HB2	2.02	0.42
1:C:520:LEU:HD21	1:C:544:PRO:HB2	2.02	0.42
3:A:803:PCW:H182	3:A:803:PCW:H212	1.79	0.41
1:A:472:PHE:HE1	3:A:811:PCW:H12	1.85	0.41
2:A:814:Y01:HAE2	2:A:814:Y01:HBB	1.90	0.41
1:C:167:LEU:HD21	1:C:189:ILE:HD12	2.01	0.41
1:C:528:MET:HE2	1:D:547:TYR:HE1	1.84	0.41
1:B:167:LEU:HD21	1:B:189:ILE:HD12	2.00	0.41
2:B:706:Y01:HAO2	2:B:706:Y01:HAP1	1.55	0.41
1:A:490:LEU:HD11	2:B:701:Y01:HAB1	2.01	0.41
1:A:506:SER:OG	1:A:526:TYR:OH	2.38	0.41
3:B:707:PCW:H212	3:B:707:PCW:H182	1.80	0.41
3:B:715:PCW:H172	3:B:715:PCW:H141	1.71	0.41
1:C:472:PHE:HE1	3:C:714:PCW:H12	1.86	0.41
1:B:472:PHE:HE1	3:B:715:PCW:H12	1.85	0.41
1:A:547:TYR:HE1	1:D:528:MET:HE2	1.85	0.41
2:A:814:Y01:HAB1	1:D:490:LEU:HD11	2.02	0.41
1:B:249:VAL:HG22	1:B:295:LEU:HB3	2.01	0.41
1:B:402:VAL:HG21	2:B:704:Y01:HAK1	2.03	0.41
1:D:497:MET:HE1	1:D:574:LEU:HD22	2.03	0.41
1:A:497:MET:HE1	1:A:574:LEU:HD22	2.03	0.40
1:B:497:MET:HE1	1:B:574:LEU:HD22	2.03	0.40
2:A:801:Y01:HAE2	2:A:801:Y01:HBB	1.92	0.40
1:C:402:VAL:HG21	2:C:703:Y01:HAK1	2.02	0.40
1:C:497:MET:HE1	1:C:574:LEU:HD22	2.04	0.40
2:A:814:Y01:HAA2	1:D:534:PHE:HE1	1.87	0.40
1:C:534:PHE:HE1	2:C:705:Y01:HAA2	1.86	0.40
2:D:706:Y01:HAE2	2:D:706:Y01:HBB	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	601/670 (90%)	537 (89%)	63 (10%)	1 (0%)	44	71
1	B	601/670 (90%)	537 (89%)	63 (10%)	1 (0%)	44	71
1	C	601/670 (90%)	537 (89%)	63 (10%)	1 (0%)	44	71
1	D	601/670 (90%)	537 (89%)	63 (10%)	1 (0%)	44	71
All	All	2404/2680 (90%)	2148 (89%)	252 (10%)	4 (0%)	45	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	PRO
1	B	380	PRO
1	C	380	PRO
1	D	380	PRO

### 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	527/584 (90%)	524 (99%)	3 (1%)	84	89
1	B	527/584 (90%)	525 (100%)	2 (0%)	89	92
1	C	527/584 (90%)	524 (99%)	3 (1%)	84	89
1	D	527/584 (90%)	524 (99%)	3 (1%)	84	89
All	All	2108/2336 (90%)	2097 (100%)	11 (0%)	85	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	VAL
1	A	520	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	592	LEU
1	B	452	VAL
1	B	520	LEU
1	C	452	VAL
1	C	520	LEU
1	C	592	LEU
1	D	452	VAL
1	D	520	LEU
1	D	592	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	122	HIS
1	A	127	ASN
1	A	128	GLN
1	A	165	HIS
1	A	206	GLN
1	A	208	ASN
1	A	237	ASN
1	A	290	GLN
1	A	426	HIS
1	B	118	GLN
1	B	122	HIS
1	B	127	ASN
1	B	128	GLN
1	B	165	HIS
1	B	197	ASN
1	B	208	ASN
1	B	237	ASN
1	B	290	GLN
1	B	426	HIS
1	C	118	GLN
1	C	122	HIS
1	C	127	ASN
1	C	128	GLN
1	C	165	HIS
1	C	206	GLN
1	C	208	ASN
1	C	237	ASN
1	C	290	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	426	HIS
1	D	118	GLN
1	D	122	HIS
1	D	127	ASN
1	D	128	GLN
1	D	165	HIS
1	D	206	GLN
1	D	208	ASN
1	D	237	ASN
1	D	290	GLN
1	D	426	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 65 ligands modelled in this entry, 1 is monoatomic - leaving 64 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PCW	A	810	-	7,7,53	0.94	0	6,6,61	0.23	0
3	PCW	A	806	-	10,10,53	0.94	0	9,9,61	0.49	0
3	PCW	C	708	-	12,12,53	0.84	0	11,11,61	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PCW	D	710	-	12,12,53	0.83	0	11,11,61	0.46	0
3	PCW	D	704	-	15,15,53	1.56	2 (13%)	14,14,61	0.61	0
2	Y01	D	706	-	38,38,38	0.47	0	57,57,57	0.64	0
3	PCW	B	709	-	12,12,53	0.83	0	11,11,61	0.46	0
3	PCW	A	803	-	50,50,53	1.22	6 (12%)	56,58,61	1.02	4 (7%)
3	PCW	B	716	-	10,10,53	0.98	0	9,9,61	0.49	0
3	PCW	C	707	-	15,15,53	1.54	2 (13%)	14,14,61	0.73	0
3	PCW	C	709	-	10,10,53	0.94	0	9,9,61	0.49	0
3	PCW	D	708	-	50,50,53	1.22	6 (12%)	56,58,61	1.03	4 (7%)
2	Y01	C	703	-	38,38,38	0.47	0	57,57,57	0.64	0
3	PCW	A	813	-	15,15,53	1.54	2 (13%)	14,14,61	0.74	0
3	PCW	C	702	-	15,15,53	1.53	2 (13%)	14,14,61	0.70	0
3	PCW	B	713	-	15,15,53	1.52	2 (13%)	14,14,61	0.73	0
3	PCW	B	710	-	10,10,53	0.94	0	9,9,61	0.49	0
2	Y01	C	704	-	38,38,38	0.45	0	57,57,57	0.45	0
3	PCW	D	709	-	15,15,53	1.54	2 (13%)	14,14,61	0.73	0
3	PCW	C	713	-	7,7,53	0.95	0	6,6,61	0.24	0
2	Y01	B	705	-	38,38,38	0.45	0	57,57,57	0.45	0
3	PCW	B	711	-	7,7,53	0.91	0	6,6,61	0.34	0
3	PCW	A	804	-	15,15,53	1.54	2 (13%)	14,14,61	0.73	0
3	PCW	D	701	-	42,42,53	1.32	6 (14%)	48,50,61	1.03	3 (6%)
3	PCW	B	712	-	7,7,53	0.93	0	6,6,61	0.32	0
3	PCW	A	815	-	15,15,53	1.56	2 (13%)	14,14,61	0.60	0
3	PCW	C	701	-	15,15,53	1.56	2 (13%)	14,14,61	0.60	0
3	PCW	C	711	-	7,7,53	0.93	0	6,6,61	0.31	0
3	PCW	A	811	-	42,42,53	1.31	6 (14%)	48,50,61	1.03	3 (6%)
3	PCW	D	713	-	7,7,53	0.93	0	6,6,61	0.31	0
2	Y01	B	701	-	38,38,38	0.47	0	57,57,57	0.63	0
3	PCW	A	807	-	7,7,53	0.91	0	6,6,61	0.34	0
3	PCW	B	715	-	42,42,53	1.32	6 (14%)	48,50,61	1.03	3 (6%)
3	PCW	D	702	-	10,10,53	0.98	0	9,9,61	0.48	0
3	PCW	D	714	-	15,15,53	1.52	2 (13%)	14,14,61	0.73	0
3	PCW	C	714	-	42,42,53	1.31	6 (14%)	48,50,61	1.03	3 (6%)
3	PCW	D	705	-	15,15,53	1.53	2 (13%)	14,14,61	0.70	0
2	Y01	A	802	-	38,38,38	0.45	0	57,57,57	0.45	0
3	PCW	D	703	-	15,15,53	1.53	2 (13%)	14,14,61	0.74	0
3	PCW	D	715	-	7,7,53	0.94	0	6,6,61	0.23	0
3	PCW	B	717	-	15,15,53	1.53	2 (13%)	14,14,61	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PCW	D	712	-	7,7,53	0.91	0	6,6,61	0.34	0
2	Y01	C	705	-	38,38,38	0.47	0	57,57,57	0.64	0
3	PCW	C	715	-	10,10,53	0.98	0	9,9,61	0.49	0
2	Y01	B	704	-	38,38,38	0.47	0	57,57,57	0.64	0
3	PCW	B	702	-	15,15,53	1.56	2 (13%)	14,14,61	0.60	0
3	PCW	C	716	-	15,15,53	1.53	2 (13%)	14,14,61	0.73	0
3	PCW	C	712	-	15,15,53	1.53	2 (13%)	14,14,61	0.73	0
2	Y01	A	801	-	38,38,38	0.47	0	57,57,57	0.63	0
3	PCW	D	711	-	10,10,53	0.94	0	9,9,61	0.49	0
3	PCW	B	708	-	15,15,53	1.54	2 (13%)	14,14,61	0.73	0
3	PCW	B	703	-	15,15,53	1.53	2 (13%)	14,14,61	0.70	0
3	PCW	A	805	-	12,12,53	0.83	0	11,11,61	0.46	0
3	PCW	C	706	-	50,50,53	1.22	6 (12%)	56,58,61	1.03	4 (7%)
2	Y01	B	706	-	38,38,38	0.47	0	57,57,57	0.64	0
3	PCW	C	710	-	7,7,53	0.91	0	6,6,61	0.34	0
3	PCW	B	707	-	50,50,53	1.22	5 (10%)	56,58,61	1.01	4 (7%)
3	PCW	A	809	-	15,15,53	1.52	2 (13%)	14,14,61	0.73	0
3	PCW	A	816	-	15,15,53	1.53	2 (13%)	14,14,61	0.70	0
3	PCW	A	812	-	10,10,53	0.98	0	9,9,61	0.48	0
2	Y01	A	814	-	38,38,38	0.47	0	57,57,57	0.64	0
3	PCW	B	714	-	7,7,53	0.95	0	6,6,61	0.24	0
3	PCW	A	808	-	7,7,53	0.92	0	6,6,61	0.31	0
2	Y01	D	707	-	38,38,38	0.45	0	57,57,57	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	810	-	-	3/5/5/57	-
3	PCW	A	806	-	-	5/8/8/57	-
3	PCW	C	708	-	-	4/10/10/57	-
3	PCW	D	710	-	-	4/10/10/57	-
3	PCW	D	704	-	-	8/13/13/57	-
2	Y01	D	706	-	-	11/19/77/77	0/4/4/4
3	PCW	B	709	-	-	4/10/10/57	-
3	PCW	A	803	-	-	27/54/54/57	-
3	PCW	B	716	-	-	4/8/8/57	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	C	707	-	-	9/13/13/57	-
3	PCW	C	709	-	-	5/8/8/57	-
3	PCW	D	708	-	-	26/54/54/57	-
2	Y01	C	703	-	-	11/19/77/77	0/4/4/4
3	PCW	A	813	-	-	5/13/13/57	-
3	PCW	C	702	-	-	9/13/13/57	-
3	PCW	B	713	-	-	8/13/13/57	-
3	PCW	B	710	-	-	5/8/8/57	-
2	Y01	C	704	-	-	10/19/77/77	0/4/4/4
3	PCW	D	709	-	-	9/13/13/57	-
3	PCW	C	713	-	-	3/5/5/57	-
2	Y01	B	705	-	-	10/19/77/77	0/4/4/4
3	PCW	B	711	-	-	3/5/5/57	-
3	PCW	A	804	-	-	9/13/13/57	-
3	PCW	D	701	-	-	21/46/46/57	-
3	PCW	B	712	-	-	3/5/5/57	-
3	PCW	A	815	-	-	8/13/13/57	-
3	PCW	C	701	-	-	8/13/13/57	-
3	PCW	C	711	-	-	3/5/5/57	-
3	PCW	A	811	-	-	22/46/46/57	-
3	PCW	D	713	-	-	3/5/5/57	-
2	Y01	B	701	-	-	15/19/77/77	0/4/4/4
3	PCW	A	807	-	-	3/5/5/57	-
3	PCW	B	715	-	-	22/46/46/57	-
3	PCW	D	702	-	-	4/8/8/57	-
3	PCW	D	714	-	-	8/13/13/57	-
3	PCW	C	714	-	-	22/46/46/57	-
3	PCW	D	705	-	-	9/13/13/57	-
2	Y01	A	802	-	-	10/19/77/77	0/4/4/4
3	PCW	D	703	-	-	5/13/13/57	-
3	PCW	D	715	-	-	3/5/5/57	-
3	PCW	B	717	-	-	5/13/13/57	-
3	PCW	D	712	-	-	3/5/5/57	-
2	Y01	C	705	-	-	15/19/77/77	0/4/4/4

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	C	715	-	-	4/8/8/57	-
2	Y01	B	704	-	-	11/19/77/77	0/4/4/4
3	PCW	B	702	-	-	8/13/13/57	-
3	PCW	C	716	-	-	5/13/13/57	-
3	PCW	C	712	-	-	8/13/13/57	-
2	Y01	A	801	-	-	11/19/77/77	0/4/4/4
3	PCW	D	711	-	-	5/8/8/57	-
3	PCW	B	708	-	-	9/13/13/57	-
3	PCW	B	703	-	-	9/13/13/57	-
3	PCW	A	805	-	-	4/10/10/57	-
3	PCW	C	706	-	-	26/54/54/57	-
2	Y01	B	706	-	-	15/19/77/77	0/4/4/4
3	PCW	C	710	-	-	3/5/5/57	-
3	PCW	B	707	-	-	26/54/54/57	-
3	PCW	A	809	-	-	8/13/13/57	-
3	PCW	A	816	-	-	10/13/13/57	-
3	PCW	A	812	-	-	4/8/8/57	-
2	Y01	A	814	-	-	15/19/77/77	0/4/4/4
3	PCW	B	714	-	-	3/5/5/57	-
3	PCW	A	808	-	-	3/5/5/57	-
2	Y01	D	707	-	-	10/19/77/77	0/4/4/4

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	PCW	C20-C19	4.23	1.55	1.31
3	D	704	PCW	C20-C19	4.23	1.55	1.31
3	A	815	PCW	C20-C19	4.23	1.55	1.31
3	B	702	PCW	C20-C19	4.22	1.55	1.31
3	A	813	PCW	C20-C19	4.21	1.55	1.31
3	C	707	PCW	C20-C19	4.21	1.55	1.31
3	A	804	PCW	C20-C19	4.20	1.55	1.31
3	D	709	PCW	C20-C19	4.19	1.55	1.31
3	B	717	PCW	C20-C19	4.19	1.55	1.31
3	B	708	PCW	C20-C19	4.19	1.55	1.31
3	D	703	PCW	C20-C19	4.19	1.55	1.31
3	C	716	PCW	C20-C19	4.19	1.55	1.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	816	PCW	C20-C19	4.18	1.55	1.31
3	C	712	PCW	C20-C19	4.17	1.55	1.31
3	B	703	PCW	C20-C19	4.17	1.55	1.31
3	C	702	PCW	C20-C19	4.17	1.55	1.31
3	D	705	PCW	C20-C19	4.16	1.55	1.31
3	B	713	PCW	C20-C19	4.15	1.55	1.31
3	D	714	PCW	C20-C19	4.15	1.55	1.31
3	A	809	PCW	C20-C19	4.15	1.55	1.31
3	D	701	PCW	O3-C11	3.66	1.44	1.33
3	A	811	PCW	O3-C11	3.62	1.43	1.33
3	B	715	PCW	O3-C11	3.62	1.43	1.33
3	C	714	PCW	O3-C11	3.60	1.43	1.33
3	A	803	PCW	O3-C11	3.56	1.43	1.33
3	D	708	PCW	O3-C11	3.56	1.43	1.33
3	B	707	PCW	O3-C11	3.56	1.43	1.33
3	C	706	PCW	O3-C11	3.55	1.43	1.33
3	D	701	PCW	O2-C2	-2.91	1.39	1.46
3	B	715	PCW	O2-C2	-2.90	1.39	1.46
3	C	706	PCW	O2-C31	2.89	1.42	1.34
3	C	714	PCW	O2-C2	-2.88	1.39	1.46
3	A	803	PCW	O2-C31	2.88	1.42	1.34
3	C	706	PCW	O2-C2	-2.87	1.39	1.46
3	B	707	PCW	O2-C31	2.86	1.42	1.34
3	D	708	PCW	O2-C2	-2.86	1.39	1.46
3	D	708	PCW	O2-C31	2.86	1.42	1.34
3	B	707	PCW	O2-C2	-2.85	1.39	1.46
3	D	701	PCW	O2-C31	2.85	1.42	1.34
3	B	715	PCW	O2-C31	2.84	1.42	1.34
3	A	811	PCW	O2-C2	-2.84	1.39	1.46
3	C	714	PCW	O2-C31	2.84	1.42	1.34
3	A	803	PCW	O2-C2	-2.84	1.39	1.46
3	A	811	PCW	O2-C31	2.82	1.42	1.34
3	C	712	PCW	C18-C19	-2.73	1.35	1.50
3	C	701	PCW	C18-C19	-2.73	1.35	1.50
3	B	713	PCW	C18-C19	-2.73	1.35	1.50
3	D	714	PCW	C18-C19	-2.73	1.35	1.50
3	A	809	PCW	C18-C19	-2.72	1.35	1.50
3	D	705	PCW	C18-C19	-2.72	1.35	1.50
3	D	704	PCW	C18-C19	-2.72	1.35	1.50
3	A	816	PCW	C18-C19	-2.72	1.35	1.50
3	C	702	PCW	C18-C19	-2.71	1.35	1.50
3	B	703	PCW	C18-C19	-2.71	1.35	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	815	PCW	C18-C19	-2.71	1.35	1.50
3	C	707	PCW	C18-C19	-2.71	1.35	1.50
3	D	709	PCW	C18-C19	-2.71	1.35	1.50
3	B	702	PCW	C18-C19	-2.70	1.35	1.50
3	A	804	PCW	C18-C19	-2.69	1.35	1.50
3	B	708	PCW	C18-C19	-2.69	1.35	1.50
3	A	813	PCW	C18-C19	-2.67	1.35	1.50
3	D	703	PCW	C18-C19	-2.67	1.35	1.50
3	C	716	PCW	C18-C19	-2.67	1.35	1.50
3	B	717	PCW	C18-C19	-2.66	1.35	1.50
3	B	715	PCW	P-O3P	2.35	1.68	1.59
3	B	707	PCW	P-O3P	2.34	1.68	1.59
3	D	701	PCW	P-O3P	2.34	1.68	1.59
3	D	708	PCW	P-O3P	2.34	1.68	1.59
3	C	706	PCW	P-O3P	2.33	1.68	1.59
3	C	714	PCW	P-O3P	2.32	1.68	1.59
3	A	803	PCW	P-O3P	2.32	1.68	1.59
3	A	811	PCW	P-O3P	2.31	1.68	1.59
3	C	706	PCW	C12-C11	2.15	1.56	1.50
3	B	707	PCW	C12-C11	2.15	1.56	1.50
3	A	803	PCW	C12-C11	2.14	1.56	1.50
3	B	715	PCW	P-O4P	2.14	1.67	1.59
3	C	714	PCW	P-O4P	2.14	1.67	1.59
3	D	708	PCW	C12-C11	2.13	1.56	1.50
3	A	811	PCW	P-O4P	2.13	1.67	1.59
3	D	701	PCW	P-O4P	2.13	1.67	1.59
3	B	715	PCW	C12-C11	2.05	1.56	1.50
3	D	701	PCW	C12-C11	2.04	1.56	1.50
3	A	811	PCW	C12-C11	2.04	1.56	1.50
3	C	714	PCW	C12-C11	2.03	1.56	1.50
3	A	803	PCW	P-O4P	2.02	1.67	1.59
3	C	706	PCW	P-O4P	2.00	1.67	1.59
3	D	708	PCW	P-O4P	2.00	1.67	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	PCW	O2-C31-C32	4.20	120.57	111.48
3	D	708	PCW	O2-C31-C32	4.18	120.52	111.48
3	B	707	PCW	O2-C31-C32	4.18	120.52	111.48
3	C	706	PCW	O2-C31-C32	4.17	120.50	111.48
3	C	714	PCW	O2-C31-C32	3.57	119.20	111.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	715	PCW	O2-C31-C32	3.56	119.18	111.48
3	D	701	PCW	O2-C31-C32	3.55	119.16	111.48
3	A	811	PCW	O2-C31-C32	3.55	119.16	111.48
3	D	708	PCW	C8-N-C7	3.50	118.16	108.98
3	C	706	PCW	C8-N-C7	3.47	118.09	108.98
3	A	803	PCW	C8-N-C7	3.38	117.85	108.98
3	B	707	PCW	C8-N-C7	3.34	117.76	108.98
3	D	701	PCW	C8-N-C7	3.27	117.56	108.98
3	B	715	PCW	C8-N-C7	3.26	117.53	108.98
3	A	811	PCW	C8-N-C7	3.24	117.49	108.98
3	C	714	PCW	C8-N-C7	3.24	117.48	108.98
3	C	714	PCW	O3-C11-C12	2.99	120.95	111.83
3	A	811	PCW	O3-C11-C12	2.98	120.91	111.83
3	D	701	PCW	O3-C11-C12	2.98	120.91	111.83
3	B	715	PCW	O3-C11-C12	2.96	120.87	111.83
3	C	706	PCW	O3-C11-C12	2.55	119.62	111.83
3	A	803	PCW	O3-C11-C12	2.55	119.62	111.83
3	D	708	PCW	O3-C11-C12	2.53	119.55	111.83
3	B	707	PCW	O3-C11-C12	2.53	119.54	111.83
3	C	706	PCW	C3-C2-C1	-2.09	106.92	111.78
3	D	708	PCW	C3-C2-C1	-2.08	106.93	111.78
3	B	707	PCW	C3-C2-C1	-2.04	107.03	111.78
3	A	803	PCW	C3-C2-C1	-2.01	107.09	111.78

There are no chirality outliers.

All (581) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	814	Y01	CAV-CBC-OAW-CAY
2	A	814	Y01	CAM-CAY-OAW-CBC
2	B	701	Y01	CAV-CBC-OAW-CAY
2	B	701	Y01	CAM-CAY-OAW-CBC
2	B	706	Y01	CAV-CBC-OAW-CAY
2	B	706	Y01	CAM-CAY-OAW-CBC
2	C	705	Y01	CAV-CBC-OAW-CAY
2	C	705	Y01	CAM-CAY-OAW-CBC
3	A	803	PCW	C4-O4P-P-O1P
3	A	803	PCW	C4-O4P-P-O2P
3	A	803	PCW	C4-O4P-P-O3P
3	A	811	PCW	C12-C11-O3-C3
3	A	811	PCW	O11-C11-O3-C3
3	B	707	PCW	C4-O4P-P-O1P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	707	PCW	C4-O4P-P-O2P
3	B	707	PCW	C4-O4P-P-O3P
3	B	715	PCW	C12-C11-O3-C3
3	B	715	PCW	O11-C11-O3-C3
3	C	706	PCW	C4-O4P-P-O1P
3	C	706	PCW	C4-O4P-P-O2P
3	C	706	PCW	C4-O4P-P-O3P
3	C	714	PCW	C12-C11-O3-C3
3	C	714	PCW	O11-C11-O3-C3
3	D	701	PCW	C12-C11-O3-C3
3	D	701	PCW	O11-C11-O3-C3
3	D	708	PCW	C4-O4P-P-O1P
3	D	708	PCW	C4-O4P-P-O2P
3	D	708	PCW	C4-O4P-P-O3P
2	A	801	Y01	CAJ-CAO-CBB-CAC
2	B	704	Y01	CAJ-CAO-CBB-CAC
2	C	703	Y01	CAJ-CAO-CBB-CAC
2	D	706	Y01	CAJ-CAO-CBB-CAC
2	A	801	Y01	CAC-CBB-CBE-CAP
2	B	704	Y01	CAC-CBB-CBE-CAP
2	C	703	Y01	CAC-CBB-CBE-CAP
2	D	706	Y01	CAC-CBB-CBE-CAP
2	A	801	Y01	CAC-CBB-CBE-CBI
2	B	704	Y01	CAC-CBB-CBE-CBI
2	C	703	Y01	CAC-CBB-CBE-CBI
2	D	706	Y01	CAC-CBB-CBE-CBI
2	A	802	Y01	CAO-CBB-CBE-CBI
2	B	705	Y01	CAO-CBB-CBE-CBI
2	C	704	Y01	CAO-CBB-CBE-CBI
2	D	707	Y01	CAO-CBB-CBE-CBI
2	A	814	Y01	OAG-CAY-OAW-CBC
2	B	701	Y01	OAG-CAY-OAW-CBC
2	B	706	Y01	OAG-CAY-OAW-CBC
2	C	705	Y01	OAG-CAY-OAW-CBC
2	A	814	Y01	CAJ-CAO-CBB-CAC
2	B	701	Y01	CAJ-CAO-CBB-CAC
2	B	706	Y01	CAJ-CAO-CBB-CAC
2	C	705	Y01	CAJ-CAO-CBB-CAC
3	A	803	PCW	O11-C11-O3-C3
3	C	706	PCW	O11-C11-O3-C3
3	D	708	PCW	O11-C11-O3-C3
2	A	802	Y01	CAC-CBB-CBE-CAP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	705	Y01	CAC-CBB-CBE-CAP
2	C	704	Y01	CAC-CBB-CBE-CAP
2	D	707	Y01	CAC-CBB-CBE-CAP
2	A	802	Y01	CAC-CBB-CBE-CBI
2	B	705	Y01	CAC-CBB-CBE-CBI
2	C	704	Y01	CAC-CBB-CBE-CBI
2	D	707	Y01	CAC-CBB-CBE-CBI
2	A	801	Y01	CAO-CBB-CBE-CBI
2	B	704	Y01	CAO-CBB-CBE-CBI
2	C	703	Y01	CAO-CBB-CBE-CBI
2	D	706	Y01	CAO-CBB-CBE-CBI
3	B	707	PCW	O11-C11-O3-C3
3	A	803	PCW	C12-C11-O3-C3
3	C	706	PCW	C12-C11-O3-C3
3	D	708	PCW	C12-C11-O3-C3
3	B	707	PCW	C12-C11-O3-C3
2	A	802	Y01	CAJ-CAO-CBB-CAC
2	B	705	Y01	CAJ-CAO-CBB-CAC
2	C	704	Y01	CAJ-CAO-CBB-CAC
2	D	707	Y01	CAJ-CAO-CBB-CAC
3	A	810	PCW	C13-C14-C15-C16
3	B	714	PCW	C13-C14-C15-C16
3	D	715	PCW	C13-C14-C15-C16
3	C	713	PCW	C13-C14-C15-C16
3	A	815	PCW	C18-C19-C20-C21
3	B	702	PCW	C18-C19-C20-C21
3	C	701	PCW	C18-C19-C20-C21
3	D	704	PCW	C18-C19-C20-C21
2	A	814	Y01	CAO-CBB-CBE-CBI
2	B	701	Y01	CAO-CBB-CBE-CBI
2	B	706	Y01	CAO-CBB-CBE-CBI
2	C	705	Y01	CAO-CBB-CBE-CBI
2	A	814	Y01	CAJ-CAO-CBB-CBE
2	B	701	Y01	CAJ-CAO-CBB-CBE
2	B	706	Y01	CAJ-CAO-CBB-CBE
2	C	705	Y01	CAJ-CAO-CBB-CBE
3	B	707	PCW	C11-C12-C13-C14
3	C	706	PCW	C11-C12-C13-C14
2	A	801	Y01	CAO-CBB-CBE-CAP
2	B	704	Y01	CAO-CBB-CBE-CAP
2	C	703	Y01	CAO-CBB-CBE-CAP
2	D	706	Y01	CAO-CBB-CBE-CAP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	803	PCW	C11-C12-C13-C14
3	D	708	PCW	C11-C12-C13-C14
2	A	814	Y01	CAC-CBB-CBE-CAP
2	B	701	Y01	CAC-CBB-CBE-CAP
2	B	706	Y01	CAC-CBB-CBE-CAP
2	C	705	Y01	CAC-CBB-CBE-CAP
2	A	814	Y01	CAC-CBB-CBE-CBI
2	B	701	Y01	CAC-CBB-CBE-CBI
2	B	706	Y01	CAC-CBB-CBE-CBI
2	C	705	Y01	CAC-CBB-CBE-CBI
2	A	802	Y01	CAO-CBB-CBE-CAP
2	B	705	Y01	CAO-CBB-CBE-CAP
2	C	704	Y01	CAO-CBB-CBE-CAP
2	D	707	Y01	CAO-CBB-CBE-CAP
2	A	814	Y01	CAX-CAL-CAM-CAY
2	B	701	Y01	CAX-CAL-CAM-CAY
2	B	706	Y01	CAX-CAL-CAM-CAY
2	C	705	Y01	CAX-CAL-CAM-CAY
2	A	801	Y01	CAJ-CAN-CBA-CAB
2	B	704	Y01	CAJ-CAN-CBA-CAB
2	C	703	Y01	CAJ-CAN-CBA-CAB
2	D	706	Y01	CAJ-CAN-CBA-CAB
3	A	803	PCW	C33-C34-C35-C36
3	B	702	PCW	C14-C15-C16-C17
3	C	707	PCW	C13-C14-C15-C16
3	D	709	PCW	C13-C14-C15-C16
3	A	804	PCW	C13-C14-C15-C16
3	B	708	PCW	C13-C14-C15-C16
3	C	701	PCW	C14-C15-C16-C17
3	C	702	PCW	C15-C16-C17-C18
3	D	704	PCW	C14-C15-C16-C17
3	A	816	PCW	C15-C16-C17-C18
3	D	705	PCW	C15-C16-C17-C18
3	A	815	PCW	C14-C15-C16-C17
3	B	703	PCW	C15-C16-C17-C18
2	A	802	Y01	CAJ-CAN-CBA-CAB
2	B	705	Y01	CAJ-CAN-CBA-CAB
2	C	704	Y01	CAJ-CAN-CBA-CAB
2	D	707	Y01	CAJ-CAN-CBA-CAB
3	B	708	PCW	C14-C15-C16-C17
3	C	707	PCW	C14-C15-C16-C17
3	D	709	PCW	C14-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	706	PCW	C33-C34-C35-C36
3	A	804	PCW	C14-C15-C16-C17
3	A	811	PCW	C15-C16-C17-C18
3	B	707	PCW	C33-C34-C35-C36
3	B	715	PCW	C15-C16-C17-C18
3	C	714	PCW	C15-C16-C17-C18
3	D	708	PCW	C33-C34-C35-C36
3	D	701	PCW	C15-C16-C17-C18
2	A	814	Y01	CAO-CBB-CBE-CAP
2	B	701	Y01	CAO-CBB-CBE-CAP
2	B	706	Y01	CAO-CBB-CBE-CAP
2	C	705	Y01	CAO-CBB-CBE-CAP
3	C	714	PCW	C35-C36-C37-C38
3	D	705	PCW	C14-C15-C16-C17
3	C	702	PCW	C14-C15-C16-C17
3	D	705	PCW	C12-C13-C14-C15
3	A	816	PCW	C14-C15-C16-C17
3	A	803	PCW	C32-C31-O2-C2
3	B	707	PCW	C32-C31-O2-C2
3	A	806	PCW	C16-C17-C18-C19
3	D	704	PCW	C16-C17-C18-C19
3	A	806	PCW	C15-C16-C17-C18
3	B	715	PCW	C35-C36-C37-C38
3	D	701	PCW	C35-C36-C37-C38
3	B	710	PCW	C15-C16-C17-C18
2	A	801	Y01	CAJ-CAN-CBA-CAA
2	B	704	Y01	CAJ-CAN-CBA-CAA
2	C	703	Y01	CAJ-CAN-CBA-CAA
2	D	706	Y01	CAJ-CAN-CBA-CAA
3	A	811	PCW	C35-C36-C37-C38
3	A	816	PCW	C12-C13-C14-C15
3	C	702	PCW	C12-C13-C14-C15
3	B	703	PCW	C12-C13-C14-C15
3	B	703	PCW	C14-C15-C16-C17
2	B	701	Y01	CAN-CAJ-CAO-CBB
3	C	709	PCW	C15-C16-C17-C18
3	B	717	PCW	C12-C13-C14-C15
3	C	716	PCW	C12-C13-C14-C15
2	A	814	Y01	CAN-CAJ-CAO-CBB
2	B	706	Y01	CAN-CAJ-CAO-CBB
2	C	705	Y01	CAN-CAJ-CAO-CBB
3	D	703	PCW	C12-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	711	PCW	C15-C16-C17-C18
3	A	813	PCW	C12-C13-C14-C15
3	A	806	PCW	C19-C20-C21-C22
3	A	812	PCW	C19-C20-C21-C22
3	B	710	PCW	C19-C20-C21-C22
3	B	716	PCW	C19-C20-C21-C22
3	C	709	PCW	C19-C20-C21-C22
3	C	715	PCW	C19-C20-C21-C22
3	D	702	PCW	C19-C20-C21-C22
3	D	711	PCW	C19-C20-C21-C22
3	A	813	PCW	C13-C14-C15-C16
3	C	706	PCW	C32-C31-O2-C2
3	D	708	PCW	C32-C31-O2-C2
3	A	803	PCW	C20-C21-C22-C23
3	A	803	PCW	C36-C37-C38-C39
3	B	707	PCW	C20-C21-C22-C23
3	B	707	PCW	C36-C37-C38-C39
3	B	710	PCW	C16-C17-C18-C19
3	C	701	PCW	C16-C17-C18-C19
3	C	706	PCW	C20-C21-C22-C23
3	C	706	PCW	C36-C37-C38-C39
3	C	709	PCW	C16-C17-C18-C19
3	D	708	PCW	C20-C21-C22-C23
3	D	708	PCW	C36-C37-C38-C39
3	D	711	PCW	C16-C17-C18-C19
3	C	716	PCW	C13-C14-C15-C16
3	D	714	PCW	C18-C19-C20-C21
3	B	717	PCW	C13-C14-C15-C16
3	D	703	PCW	C13-C14-C15-C16
3	A	808	PCW	C13-C14-C15-C16
3	B	712	PCW	C13-C14-C15-C16
3	C	711	PCW	C13-C14-C15-C16
3	D	713	PCW	C13-C14-C15-C16
3	B	702	PCW	C16-C17-C18-C19
3	A	804	PCW	C12-C13-C14-C15
3	B	707	PCW	C24-C25-C26-C27
3	B	708	PCW	C12-C13-C14-C15
3	C	706	PCW	C24-C25-C26-C27
3	D	709	PCW	C12-C13-C14-C15
3	C	707	PCW	C12-C13-C14-C15
3	D	708	PCW	C24-C25-C26-C27
3	C	706	PCW	O31-C31-O2-C2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	708	PCW	O31-C31-O2-C2
2	A	801	Y01	CAX-CAL-CAM-CAY
2	B	704	Y01	CAX-CAL-CAM-CAY
2	C	703	Y01	CAX-CAL-CAM-CAY
2	D	706	Y01	CAX-CAL-CAM-CAY
3	A	803	PCW	C24-C25-C26-C27
3	D	712	PCW	C13-C14-C15-C16
3	A	807	PCW	C13-C14-C15-C16
3	B	711	PCW	C13-C14-C15-C16
3	C	710	PCW	C13-C14-C15-C16
3	A	811	PCW	C36-C37-C38-C39
3	A	815	PCW	C16-C17-C18-C19
3	B	715	PCW	C36-C37-C38-C39
3	C	714	PCW	C36-C37-C38-C39
3	D	701	PCW	C36-C37-C38-C39
3	A	811	PCW	O3P-C1-C2-C3
3	B	715	PCW	O3P-C1-C2-C3
3	C	714	PCW	O3P-C1-C2-C3
3	D	701	PCW	O3P-C1-C2-C3
3	A	803	PCW	O31-C31-O2-C2
3	B	707	PCW	O31-C31-O2-C2
3	D	701	PCW	C14-C15-C16-C17
2	A	802	Y01	CAX-CAL-CAM-CAY
2	B	705	Y01	CAX-CAL-CAM-CAY
2	C	704	Y01	CAX-CAL-CAM-CAY
2	D	707	Y01	CAX-CAL-CAM-CAY
3	A	811	PCW	C14-C15-C16-C17
3	A	809	PCW	C18-C19-C20-C21
3	C	712	PCW	C18-C19-C20-C21
3	B	715	PCW	C14-C15-C16-C17
3	C	714	PCW	C14-C15-C16-C17
3	A	813	PCW	C14-C15-C16-C17
3	A	803	PCW	C12-C13-C14-C15
3	D	703	PCW	C14-C15-C16-C17
3	A	804	PCW	C21-C22-C23-C24
3	B	708	PCW	C21-C22-C23-C24
3	A	804	PCW	C20-C21-C22-C23
3	B	708	PCW	C20-C21-C22-C23
3	C	707	PCW	C20-C21-C22-C23
3	D	709	PCW	C20-C21-C22-C23
3	C	707	PCW	C21-C22-C23-C24
3	D	709	PCW	C21-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	713	PCW	C18-C19-C20-C21
3	C	706	PCW	C12-C13-C14-C15
3	B	717	PCW	C14-C15-C16-C17
3	D	708	PCW	C12-C13-C14-C15
3	C	716	PCW	C14-C15-C16-C17
3	B	703	PCW	C23-C24-C25-C26
3	C	702	PCW	C23-C24-C25-C26
3	B	703	PCW	C13-C14-C15-C16
3	A	816	PCW	C23-C24-C25-C26
3	D	705	PCW	C23-C24-C25-C26
3	C	702	PCW	C13-C14-C15-C16
3	A	816	PCW	C13-C14-C15-C16
3	B	707	PCW	C12-C13-C14-C15
3	C	712	PCW	C11-C12-C13-C14
3	A	809	PCW	C11-C12-C13-C14
3	B	713	PCW	C11-C12-C13-C14
3	D	705	PCW	C13-C14-C15-C16
3	D	714	PCW	C11-C12-C13-C14
3	A	805	PCW	C21-C22-C23-C24
3	A	803	PCW	C1-C2-C3-O3
3	B	707	PCW	C1-C2-C3-O3
3	C	706	PCW	C1-C2-C3-O3
3	D	708	PCW	C1-C2-C3-O3
3	A	804	PCW	C22-C23-C24-C25
3	B	707	PCW	C14-C15-C16-C17
3	B	708	PCW	C22-C23-C24-C25
3	C	706	PCW	C14-C15-C16-C17
3	C	707	PCW	C22-C23-C24-C25
3	C	708	PCW	C21-C22-C23-C24
3	D	704	PCW	C13-C14-C15-C16
3	D	708	PCW	C14-C15-C16-C17
3	D	709	PCW	C22-C23-C24-C25
3	B	702	PCW	C11-C12-C13-C14
3	B	709	PCW	C21-C22-C23-C24
3	C	713	PCW	C15-C16-C17-C18
3	D	715	PCW	C15-C16-C17-C18
3	A	815	PCW	C11-C12-C13-C14
3	A	810	PCW	C15-C16-C17-C18
3	B	714	PCW	C15-C16-C17-C18
3	D	710	PCW	C21-C22-C23-C24
3	A	803	PCW	C14-C15-C16-C17
3	C	701	PCW	C13-C14-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	708	PCW	C13-C14-C15-C16
2	A	802	Y01	CAJ-CAN-CBA-CAA
2	B	705	Y01	CAJ-CAN-CBA-CAA
2	C	704	Y01	CAJ-CAN-CBA-CAA
2	D	707	Y01	CAJ-CAN-CBA-CAA
3	C	701	PCW	C11-C12-C13-C14
3	D	704	PCW	C11-C12-C13-C14
3	C	706	PCW	C13-C14-C15-C16
3	A	803	PCW	C13-C14-C15-C16
3	A	815	PCW	C13-C14-C15-C16
3	D	708	PCW	C35-C36-C37-C38
3	B	707	PCW	C35-C36-C37-C38
3	C	706	PCW	C32-C33-C34-C35
3	C	706	PCW	C35-C36-C37-C38
3	A	803	PCW	C35-C36-C37-C38
3	D	710	PCW	C22-C23-C24-C25
3	B	702	PCW	C13-C14-C15-C16
3	B	707	PCW	C13-C14-C15-C16
3	C	708	PCW	C22-C23-C24-C25
3	D	708	PCW	C32-C33-C34-C35
3	B	709	PCW	C22-C23-C24-C25
3	B	707	PCW	C32-C33-C34-C35
3	C	709	PCW	C13-C14-C15-C16
3	D	711	PCW	C13-C14-C15-C16
3	C	714	PCW	C32-C33-C34-C35
3	A	803	PCW	C32-C33-C34-C35
3	D	702	PCW	C13-C14-C15-C16
3	A	805	PCW	C22-C23-C24-C25
3	B	715	PCW	C32-C33-C34-C35
3	B	710	PCW	C13-C14-C15-C16
3	A	811	PCW	C32-C33-C34-C35
3	A	803	PCW	O4P-C4-C5-N
3	A	811	PCW	O4P-C4-C5-N
3	B	707	PCW	O4P-C4-C5-N
3	B	715	PCW	O4P-C4-C5-N
3	C	706	PCW	O4P-C4-C5-N
3	C	714	PCW	O4P-C4-C5-N
3	D	701	PCW	O4P-C4-C5-N
3	D	708	PCW	O4P-C4-C5-N
3	B	716	PCW	C13-C14-C15-C16
3	C	715	PCW	C13-C14-C15-C16
3	D	708	PCW	C40-C41-C42-C43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	808	PCW	C15-C16-C17-C18
3	A	812	PCW	C13-C14-C15-C16
3	C	711	PCW	C15-C16-C17-C18
3	D	701	PCW	C32-C33-C34-C35
3	D	713	PCW	C15-C16-C17-C18
3	B	712	PCW	C15-C16-C17-C18
3	A	805	PCW	C17-C18-C19-C20
3	B	709	PCW	C17-C18-C19-C20
3	C	708	PCW	C17-C18-C19-C20
3	D	710	PCW	C17-C18-C19-C20
3	C	706	PCW	C40-C41-C42-C43
3	A	804	PCW	C11-C12-C13-C14
3	D	709	PCW	C11-C12-C13-C14
3	C	707	PCW	C11-C12-C13-C14
3	B	708	PCW	C11-C12-C13-C14
3	D	704	PCW	C17-C18-C19-C20
3	A	807	PCW	C15-C16-C17-C18
3	C	716	PCW	C15-C16-C17-C18
3	A	811	PCW	O3P-C1-C2-O2
3	B	715	PCW	O3P-C1-C2-O2
3	C	714	PCW	O3P-C1-C2-O2
3	B	711	PCW	C15-C16-C17-C18
3	C	710	PCW	C15-C16-C17-C18
3	D	712	PCW	C15-C16-C17-C18
3	A	815	PCW	C17-C18-C19-C20
3	B	702	PCW	C17-C18-C19-C20
3	C	701	PCW	C17-C18-C19-C20
3	A	803	PCW	O2-C2-C3-O3
3	B	707	PCW	O2-C2-C3-O3
3	C	706	PCW	O2-C2-C3-O3
3	D	708	PCW	O2-C2-C3-O3
3	B	714	PCW	C16-C17-C18-C19
3	A	810	PCW	C16-C17-C18-C19
3	C	713	PCW	C16-C17-C18-C19
3	B	717	PCW	C15-C16-C17-C18
3	D	715	PCW	C16-C17-C18-C19
3	A	806	PCW	C13-C14-C15-C16
3	A	811	PCW	C1-O3P-P-O1P
3	A	811	PCW	C4-O4P-P-O2P
3	B	715	PCW	C1-O3P-P-O1P
3	B	715	PCW	C4-O4P-P-O2P
3	C	714	PCW	C1-O3P-P-O1P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	714	PCW	C4-O4P-P-O2P
3	D	701	PCW	C1-O3P-P-O1P
3	D	701	PCW	C4-O4P-P-O2P
2	A	801	Y01	CAJ-CAO-CBB-CBE
2	B	704	Y01	CAJ-CAO-CBB-CBE
2	C	703	Y01	CAJ-CAO-CBB-CBE
2	D	706	Y01	CAJ-CAO-CBB-CBE
3	A	807	PCW	C14-C15-C16-C17
3	A	816	PCW	C11-C12-C13-C14
3	C	702	PCW	C11-C12-C13-C14
3	B	711	PCW	C14-C15-C16-C17
3	D	705	PCW	C11-C12-C13-C14
3	D	712	PCW	C14-C15-C16-C17
3	C	710	PCW	C14-C15-C16-C17
3	B	708	PCW	C15-C16-C17-C18
3	B	703	PCW	C11-C12-C13-C14
3	B	713	PCW	C23-C24-C25-C26
3	C	712	PCW	C23-C24-C25-C26
3	B	713	PCW	C22-C23-C24-C25
3	D	701	PCW	O3P-C1-C2-O2
3	C	707	PCW	C15-C16-C17-C18
3	C	712	PCW	C22-C23-C24-C25
3	A	809	PCW	C22-C23-C24-C25
3	A	809	PCW	C23-C24-C25-C26
3	C	715	PCW	C15-C16-C17-C18
3	D	709	PCW	C15-C16-C17-C18
3	B	716	PCW	C15-C16-C17-C18
3	D	702	PCW	C15-C16-C17-C18
3	A	811	PCW	C39-C40-C41-C42
3	B	715	PCW	C39-C40-C41-C42
3	C	714	PCW	C39-C40-C41-C42
3	D	701	PCW	C39-C40-C41-C42
3	A	812	PCW	C15-C16-C17-C18
3	B	703	PCW	C18-C19-C20-C21
3	C	702	PCW	C18-C19-C20-C21
3	D	705	PCW	C18-C19-C20-C21
3	A	808	PCW	C16-C17-C18-C19
3	B	712	PCW	C16-C17-C18-C19
3	C	711	PCW	C16-C17-C18-C19
3	D	713	PCW	C16-C17-C18-C19
3	B	707	PCW	C40-C41-C42-C43
2	A	814	Y01	CAO-CAJ-CAN-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	701	Y01	CAO-CAJ-CAN-CBA
2	B	706	Y01	CAO-CAJ-CAN-CBA
2	C	705	Y01	CAO-CAJ-CAN-CBA
3	A	803	PCW	C40-C41-C42-C43
3	D	708	PCW	C41-C42-C43-C44
3	A	804	PCW	C15-C16-C17-C18
3	A	803	PCW	C25-C26-C27-C28
3	A	812	PCW	C17-C18-C19-C20
3	B	716	PCW	C17-C18-C19-C20
3	C	715	PCW	C17-C18-C19-C20
3	D	702	PCW	C17-C18-C19-C20
3	A	816	PCW	C18-C19-C20-C21
3	D	703	PCW	C15-C16-C17-C18
3	D	714	PCW	C23-C24-C25-C26
3	C	706	PCW	C41-C42-C43-C44
3	D	704	PCW	C19-C20-C21-C22
3	D	701	PCW	C13-C14-C15-C16
3	B	707	PCW	C41-C42-C43-C44
3	A	811	PCW	C13-C14-C15-C16
3	B	707	PCW	C25-C26-C27-C28
3	A	813	PCW	C15-C16-C17-C18
3	A	803	PCW	C41-C42-C43-C44
3	C	701	PCW	C19-C20-C21-C22
2	A	814	Y01	CAM-CAL-CAX-OAH
2	B	701	Y01	CAM-CAL-CAX-OAH
2	B	706	Y01	CAM-CAL-CAX-OAH
2	C	705	Y01	CAM-CAL-CAX-OAH
3	D	708	PCW	C25-C26-C27-C28
3	C	706	PCW	C25-C26-C27-C28
3	A	811	PCW	C16-C17-C18-C19
3	B	715	PCW	C16-C17-C18-C19
3	C	714	PCW	C16-C17-C18-C19
3	D	701	PCW	C16-C17-C18-C19
3	A	815	PCW	C12-C13-C14-C15
3	C	714	PCW	C13-C14-C15-C16
3	B	715	PCW	C13-C14-C15-C16
2	A	814	Y01	CAM-CAL-CAX-OAF
2	B	701	Y01	CAM-CAL-CAX-OAF
2	B	706	Y01	CAM-CAL-CAX-OAF
2	C	705	Y01	CAM-CAL-CAX-OAF
3	D	704	PCW	C12-C13-C14-C15
2	A	802	Y01	CAM-CAL-CAX-OAF

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	705	Y01	CAM-CAL-CAX-OAF
2	C	704	Y01	CAM-CAL-CAX-OAF
2	D	707	Y01	CAM-CAL-CAX-OAF
3	A	815	PCW	C19-C20-C21-C22
3	B	702	PCW	C19-C20-C21-C22
2	A	802	Y01	CAM-CAL-CAX-OAH
2	B	705	Y01	CAM-CAL-CAX-OAH
2	C	704	Y01	CAM-CAL-CAX-OAH
2	D	707	Y01	CAM-CAL-CAX-OAH
3	B	713	PCW	C12-C13-C14-C15
3	D	714	PCW	C12-C13-C14-C15
3	D	708	PCW	C42-C43-C44-C45
3	C	712	PCW	C15-C16-C17-C18
3	C	701	PCW	C12-C13-C14-C15
3	B	713	PCW	C15-C16-C17-C18
3	C	706	PCW	C42-C43-C44-C45
3	C	712	PCW	C12-C13-C14-C15
3	D	714	PCW	C15-C16-C17-C18
2	A	814	Y01	CAJ-CAN-CBA-CAA
2	B	701	Y01	CAJ-CAN-CBA-CAA
2	B	706	Y01	CAJ-CAN-CBA-CAA
2	C	705	Y01	CAJ-CAN-CBA-CAA
3	D	714	PCW	C22-C23-C24-C25
3	A	803	PCW	C39-C40-C41-C42
3	B	707	PCW	C39-C40-C41-C42
3	B	710	PCW	C17-C18-C19-C20
3	C	706	PCW	C39-C40-C41-C42
3	A	816	PCW	C20-C21-C22-C23
3	B	703	PCW	C20-C21-C22-C23
3	D	705	PCW	C20-C21-C22-C23
3	A	809	PCW	C21-C22-C23-C24
3	A	806	PCW	C17-C18-C19-C20
3	B	707	PCW	C42-C43-C44-C45
3	B	713	PCW	C21-C22-C23-C24
3	B	715	PCW	C4-C5-N-C7
3	C	714	PCW	C4-C5-N-C7
3	A	811	PCW	C19-C20-C21-C22
3	B	715	PCW	C19-C20-C21-C22
3	D	708	PCW	C39-C40-C41-C42
3	C	702	PCW	C20-C21-C22-C23
3	A	811	PCW	C17-C18-C19-C20
3	C	714	PCW	C17-C18-C19-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	714	PCW	C19-C20-C21-C22
3	D	701	PCW	C17-C18-C19-C20
3	D	711	PCW	C17-C18-C19-C20
3	C	712	PCW	C21-C22-C23-C24
3	B	715	PCW	C17-C18-C19-C20
3	C	709	PCW	C17-C18-C19-C20
3	D	701	PCW	C19-C20-C21-C22
3	A	811	PCW	C5-C4-O4P-P
3	B	715	PCW	C5-C4-O4P-P
3	C	714	PCW	C5-C4-O4P-P
3	D	701	PCW	C5-C4-O4P-P
3	A	809	PCW	C12-C13-C14-C15
3	C	714	PCW	C12-C13-C14-C15
3	A	803	PCW	C22-C23-C24-C25
3	A	805	PCW	C23-C24-C25-C26
3	B	715	PCW	C12-C13-C14-C15
3	D	701	PCW	C12-C13-C14-C15
3	B	702	PCW	C12-C13-C14-C15
3	A	811	PCW	C12-C13-C14-C15
3	A	811	PCW	C4-C5-N-C7
3	B	709	PCW	C23-C24-C25-C26
2	A	801	Y01	CAM-CAL-CAX-OAH
2	A	801	Y01	CAM-CAL-CAX-OAF
2	B	704	Y01	CAM-CAL-CAX-OAH
2	B	704	Y01	CAM-CAL-CAX-OAF
2	C	703	Y01	CAM-CAL-CAX-OAH
2	C	703	Y01	CAM-CAL-CAX-OAF
2	D	706	Y01	CAM-CAL-CAX-OAH
2	D	706	Y01	CAM-CAL-CAX-OAF
3	B	707	PCW	C22-C23-C24-C25
3	C	708	PCW	C23-C24-C25-C26
3	C	706	PCW	C22-C23-C24-C25
3	D	708	PCW	C22-C23-C24-C25
3	D	710	PCW	C23-C24-C25-C26
3	D	714	PCW	C21-C22-C23-C24
3	A	803	PCW	C42-C43-C44-C45
3	A	809	PCW	C15-C16-C17-C18
3	D	701	PCW	O2-C31-C32-C33
3	A	811	PCW	O2-C31-C32-C33
3	B	715	PCW	O2-C31-C32-C33
3	C	714	PCW	O2-C31-C32-C33
3	A	804	PCW	C17-C18-C19-C20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	809	PCW	C17-C18-C19-C20
3	A	813	PCW	C17-C18-C19-C20
3	A	816	PCW	C17-C18-C19-C20
3	B	703	PCW	C17-C18-C19-C20
3	B	708	PCW	C17-C18-C19-C20
3	B	713	PCW	C17-C18-C19-C20
3	B	717	PCW	C17-C18-C19-C20
3	C	702	PCW	C17-C18-C19-C20
3	C	707	PCW	C17-C18-C19-C20
3	C	712	PCW	C17-C18-C19-C20
3	C	716	PCW	C17-C18-C19-C20
3	D	703	PCW	C17-C18-C19-C20
3	D	705	PCW	C17-C18-C19-C20
3	D	709	PCW	C17-C18-C19-C20
3	D	714	PCW	C17-C18-C19-C20
3	A	803	PCW	C21-C22-C23-C24
3	D	701	PCW	O31-C31-C32-C33
3	A	816	PCW	C21-C22-C23-C24
3	A	811	PCW	O31-C31-C32-C33
3	B	715	PCW	O31-C31-C32-C33
3	C	714	PCW	O31-C31-C32-C33

There are no ring outliers.

20 monomers are involved in 41 short contacts:

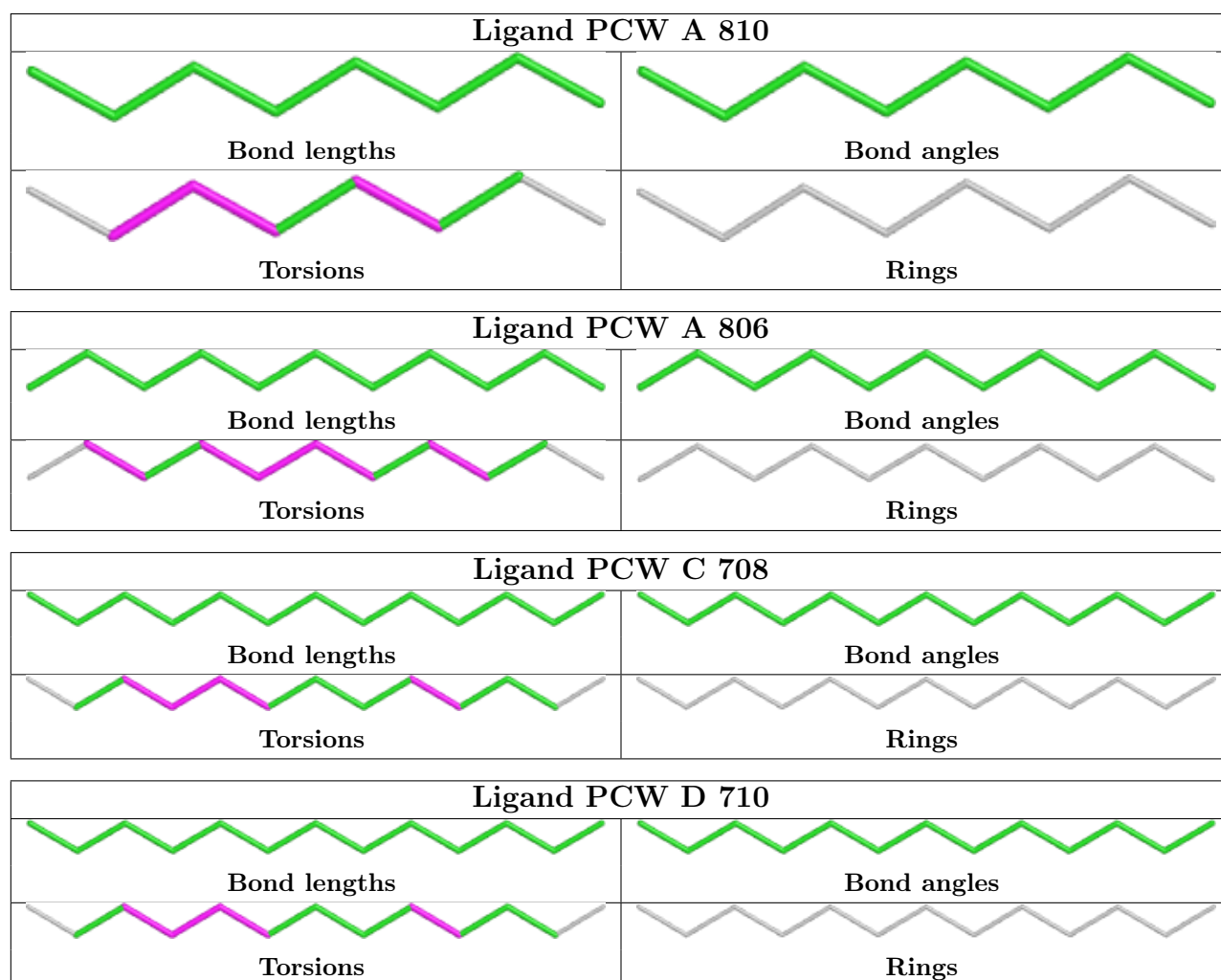
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	706	Y01	1	0
3	A	803	PCW	1	0
3	D	708	PCW	1	0
2	C	703	Y01	1	0
2	C	704	Y01	2	0
2	B	705	Y01	2	0
3	D	701	PCW	1	0
3	A	811	PCW	2	0
2	B	701	Y01	4	0
3	B	715	PCW	2	0
3	C	714	PCW	2	0
2	A	802	Y01	2	0
2	C	705	Y01	4	0
2	B	704	Y01	2	0
2	A	801	Y01	2	0
3	C	706	PCW	1	0

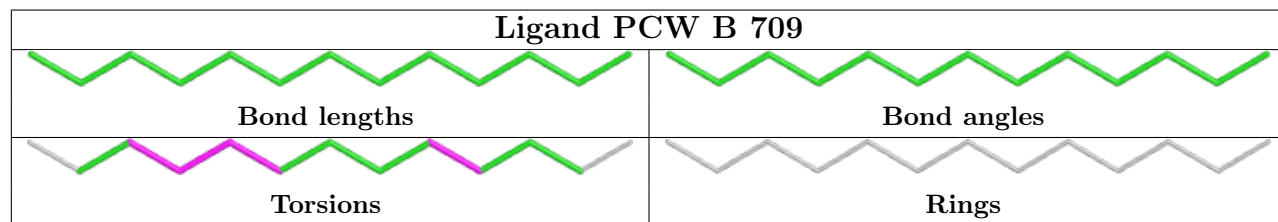
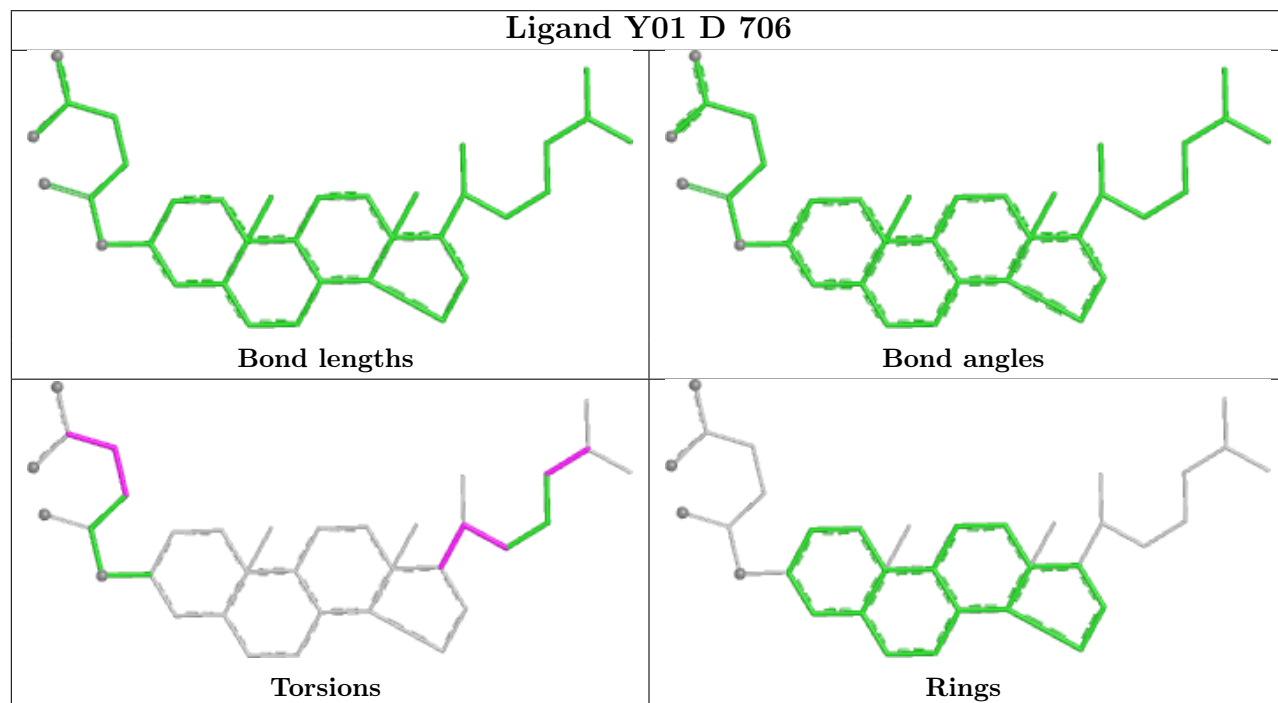
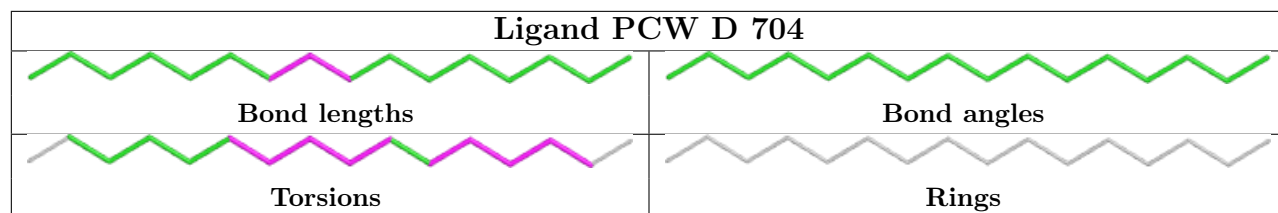
*Continued on next page...*

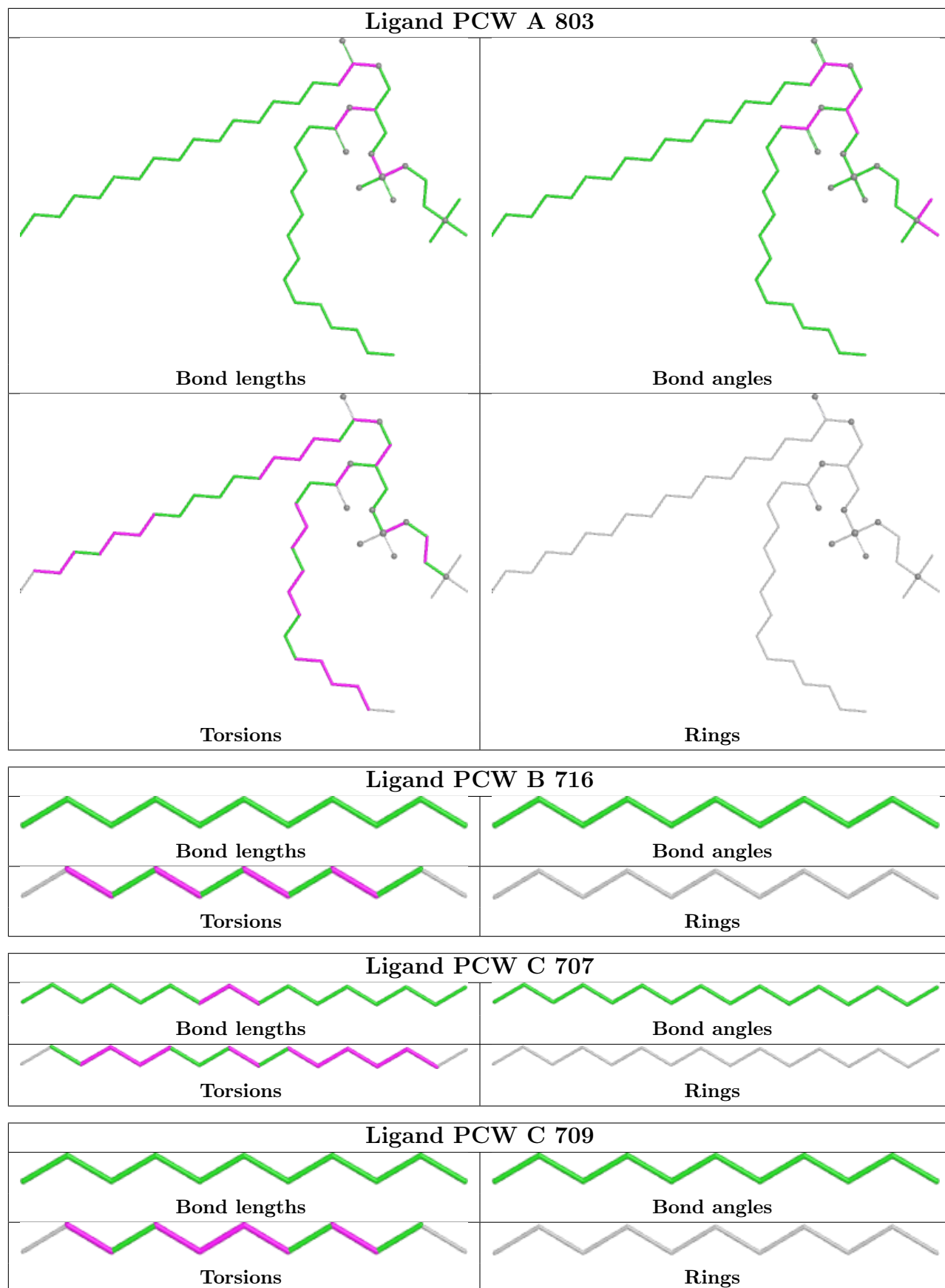
*Continued from previous page...*

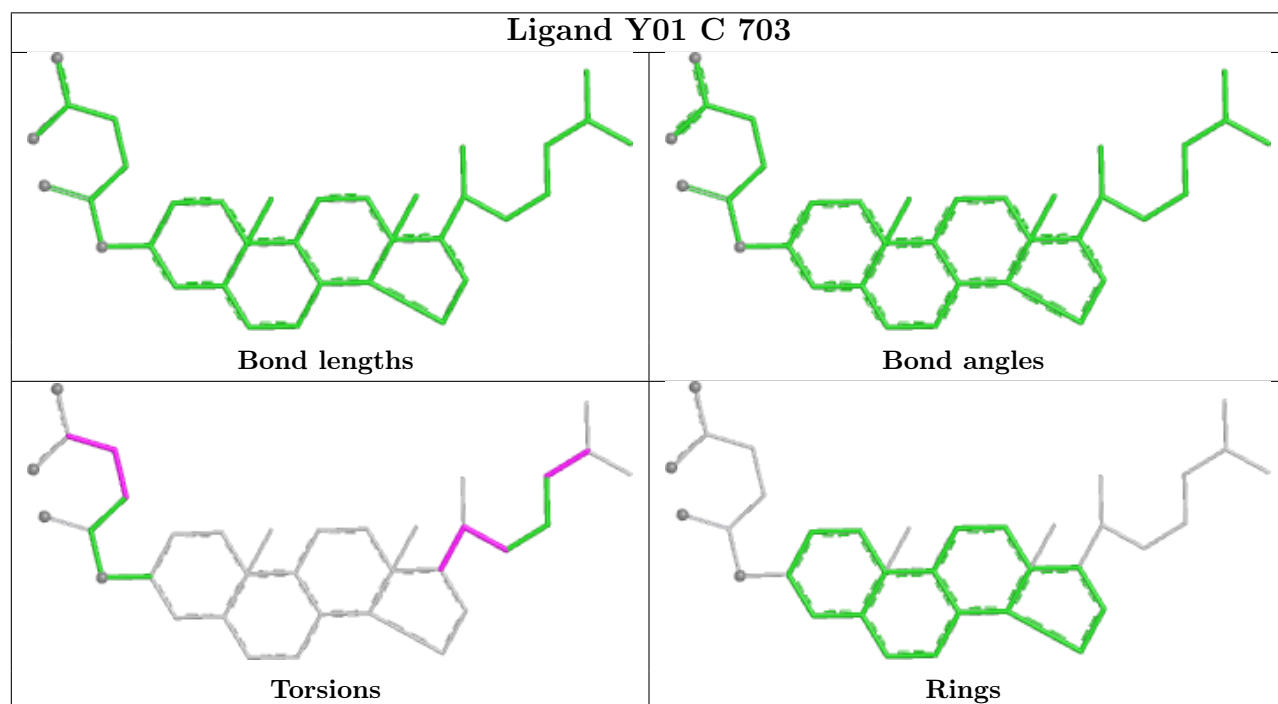
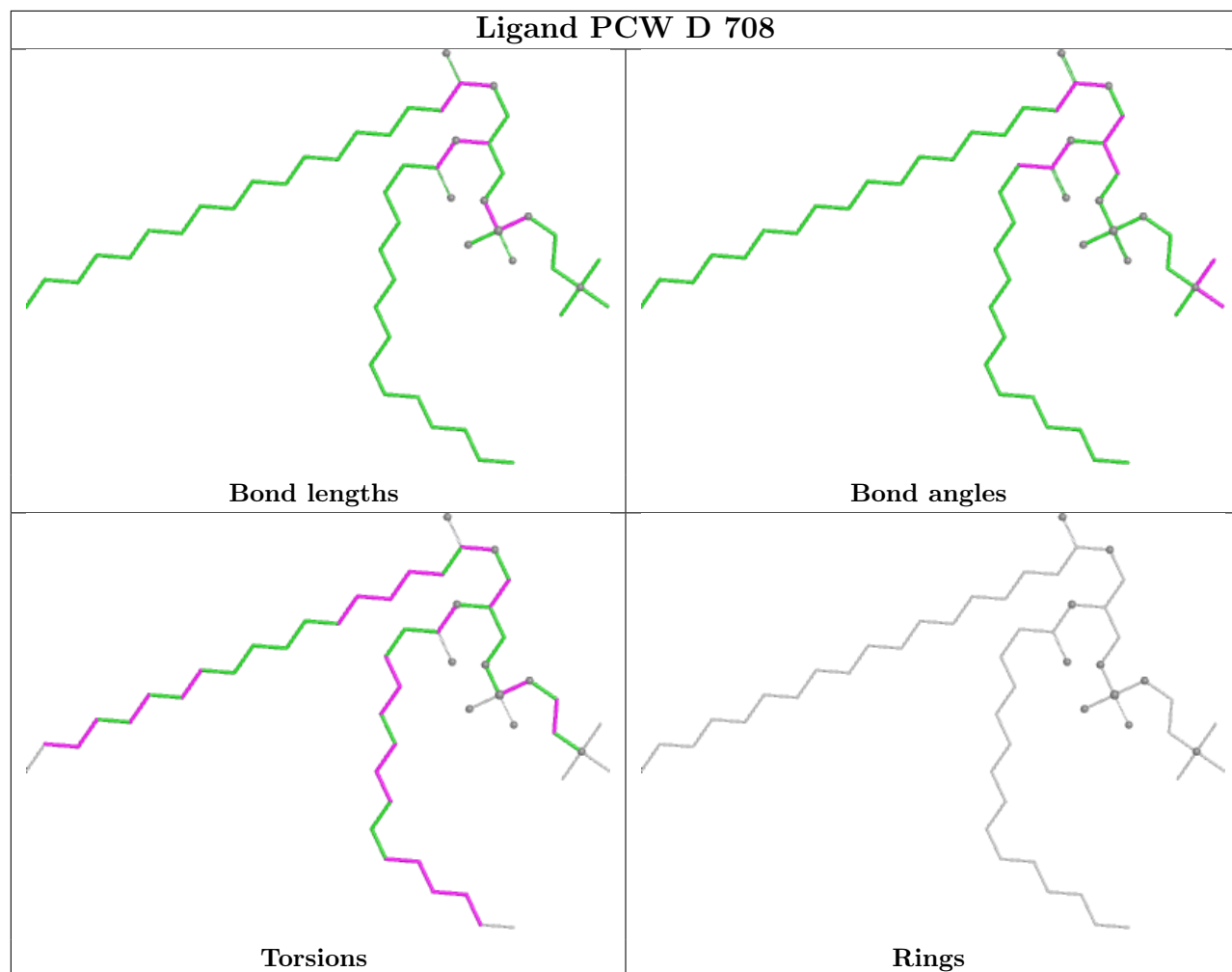
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	706	Y01	3	0
3	B	707	PCW	1	0
2	A	814	Y01	5	0
2	D	707	Y01	2	0





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.








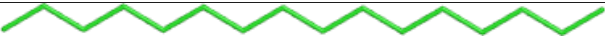




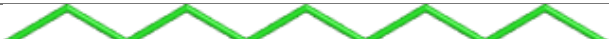
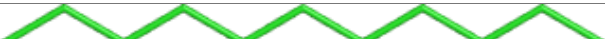

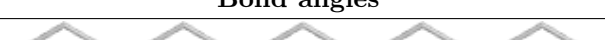


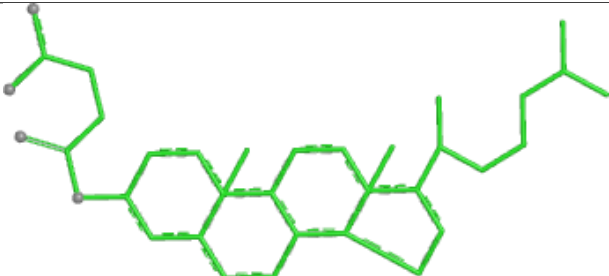
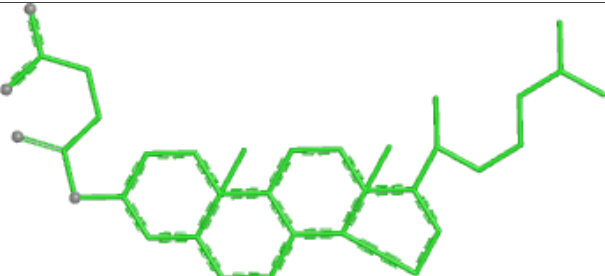
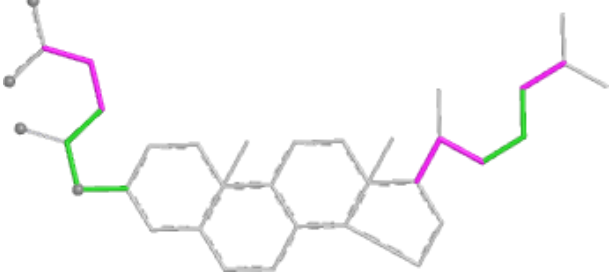
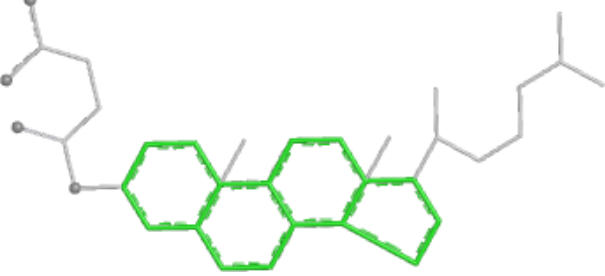


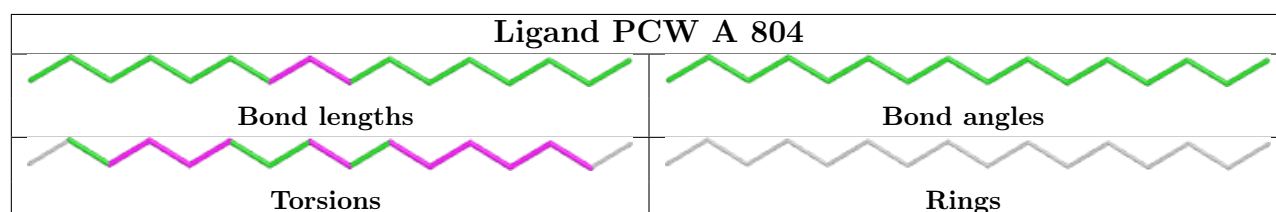
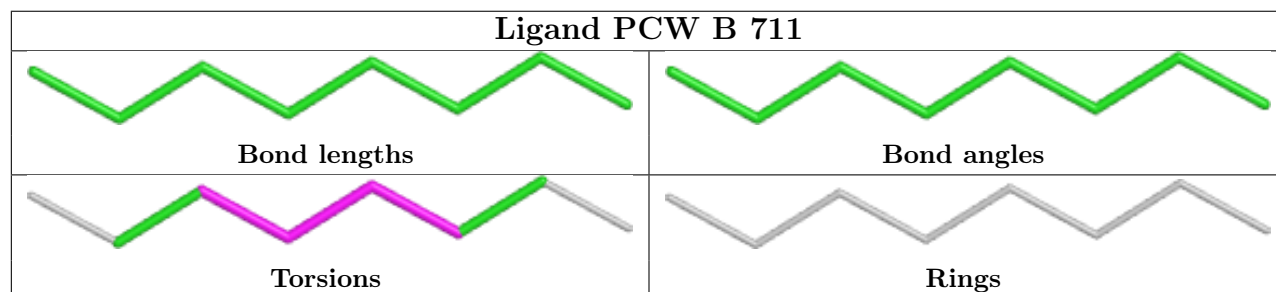
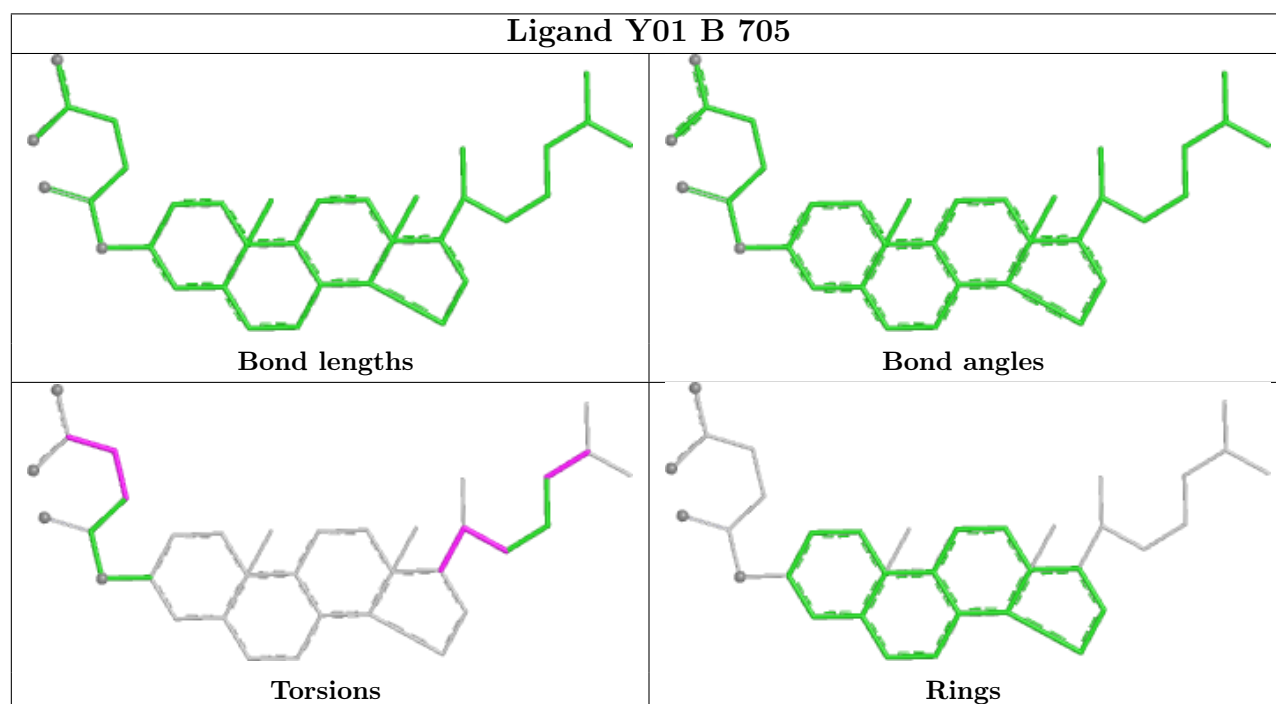
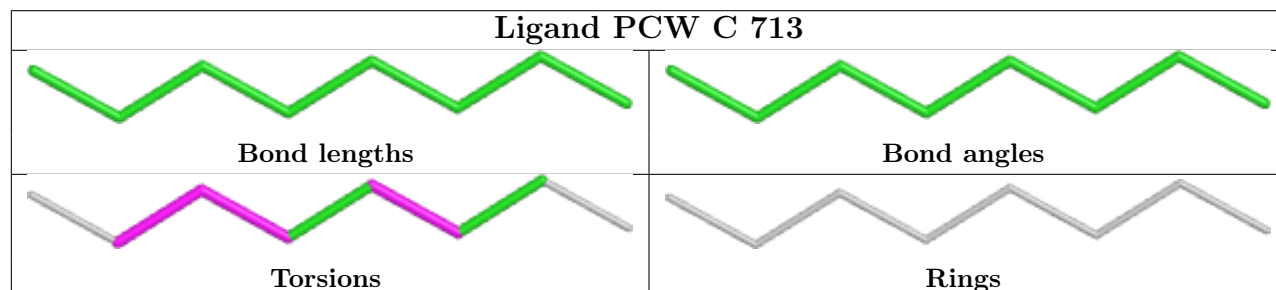
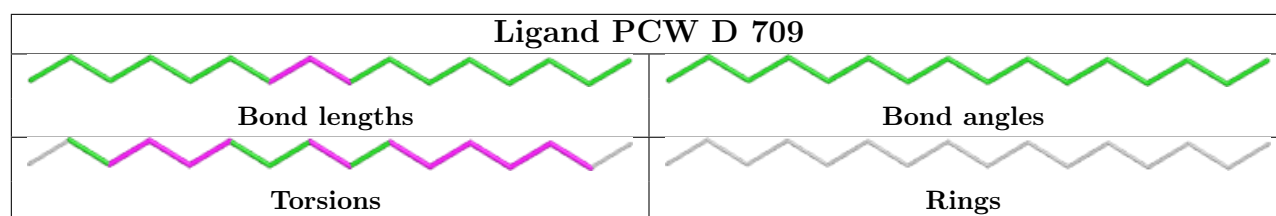
Ligand PCW A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

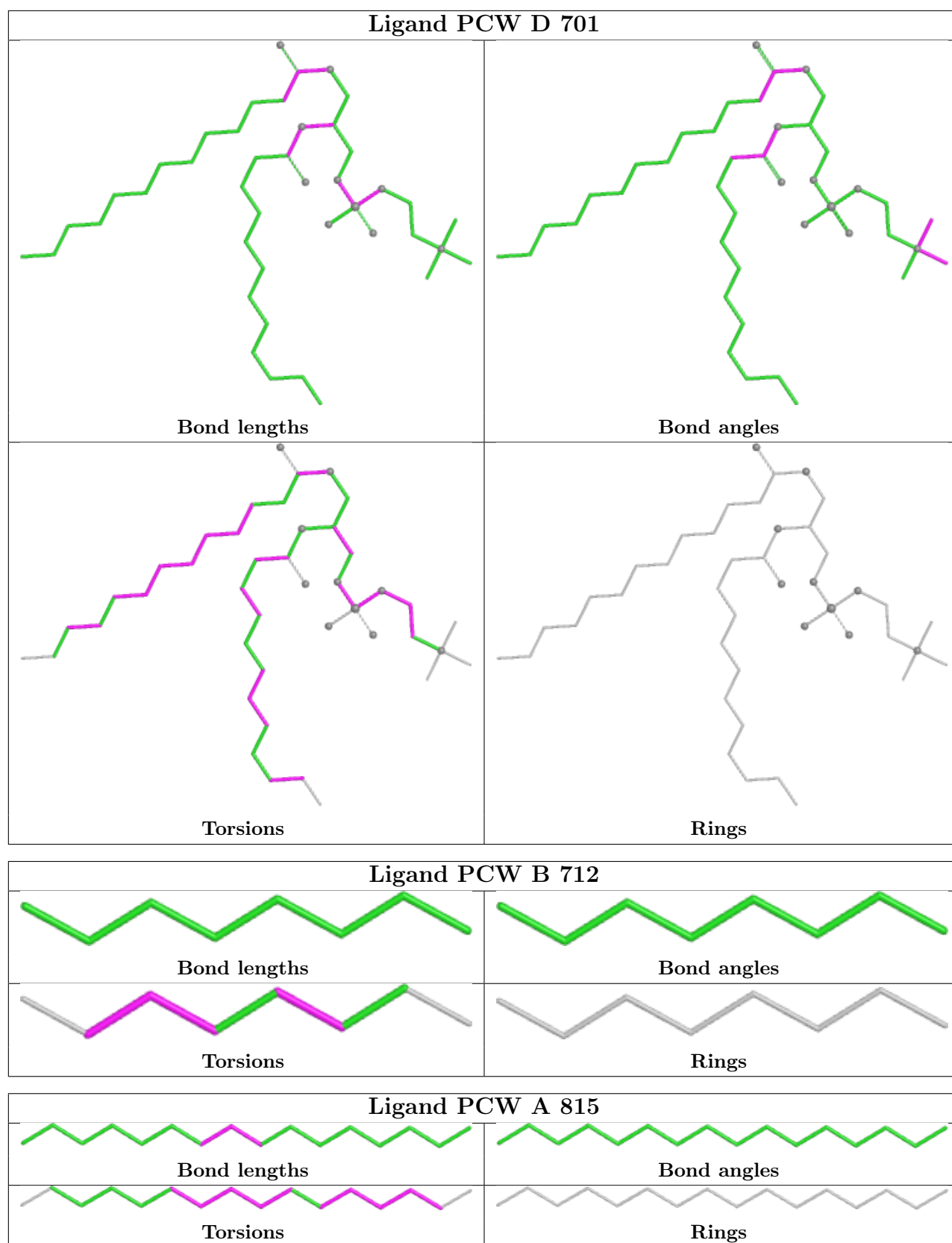
Ligand PCW C 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW B 713	
 Bond lengths	 Bond angles
 Torsions	 Rings

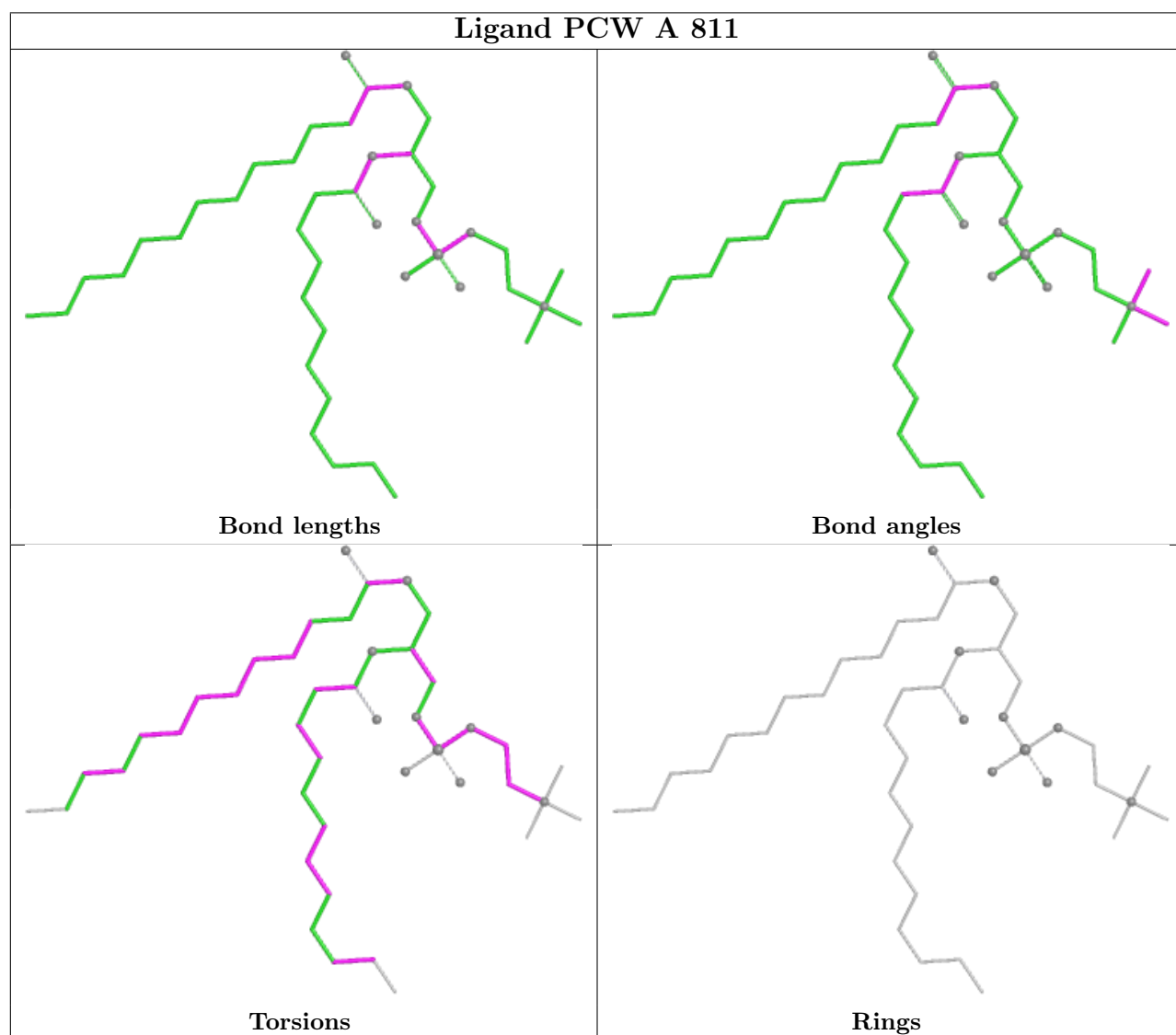
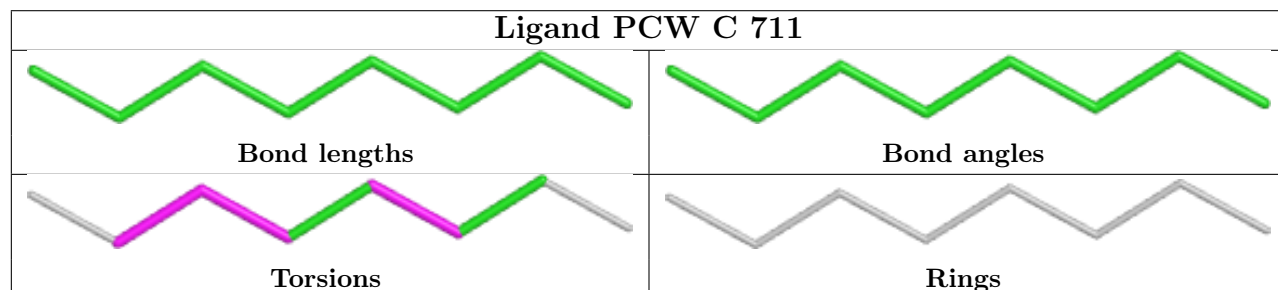
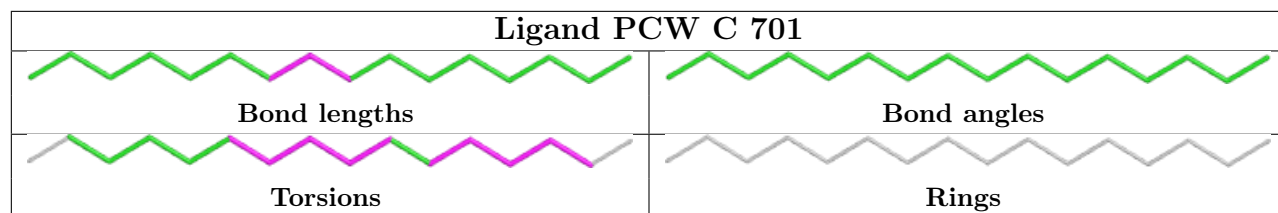
Ligand PCW B 710	
 Bond lengths	 Bond angles
 Torsions	 Rings

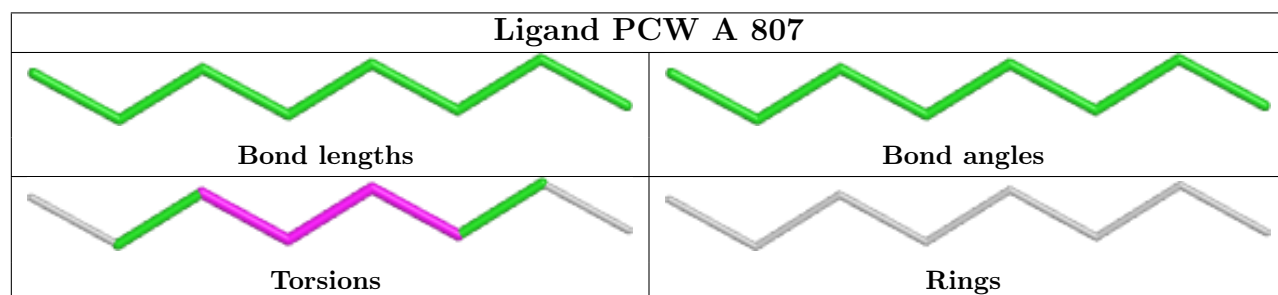
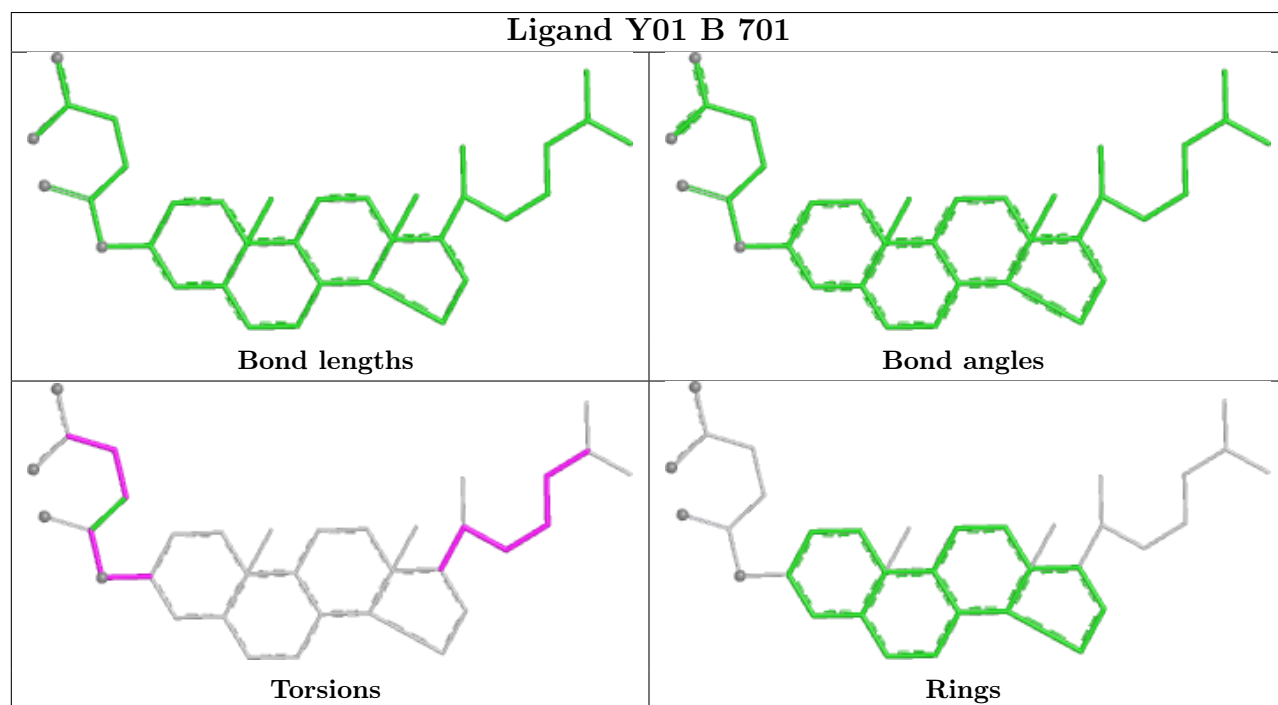
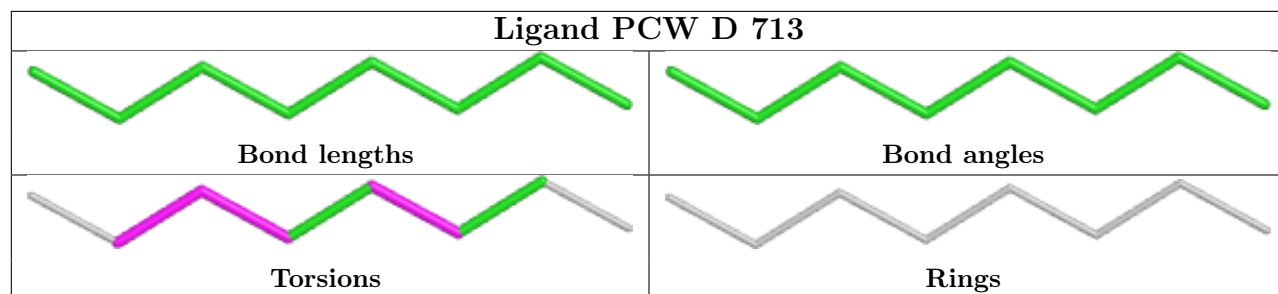
Ligand Y01 C 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

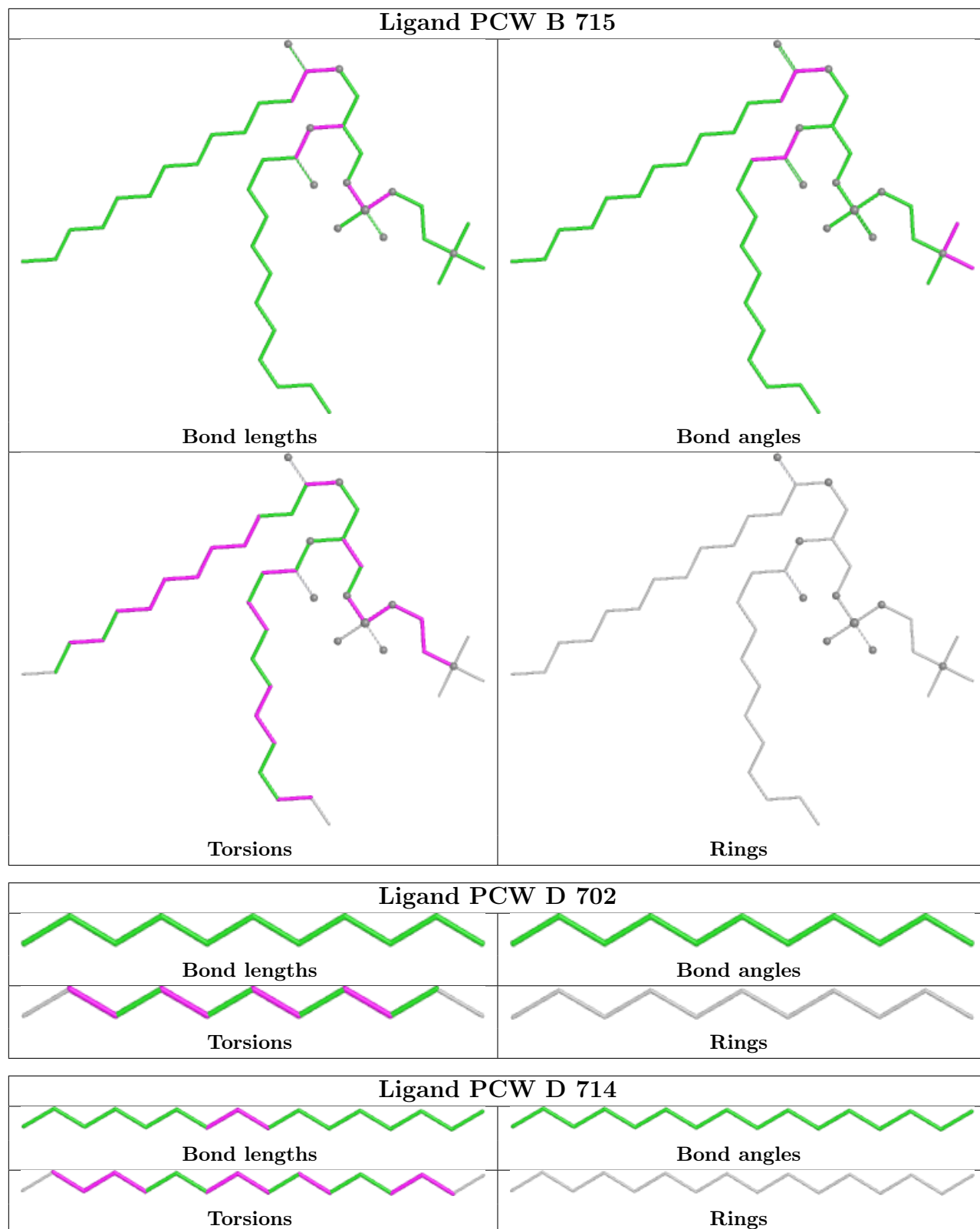


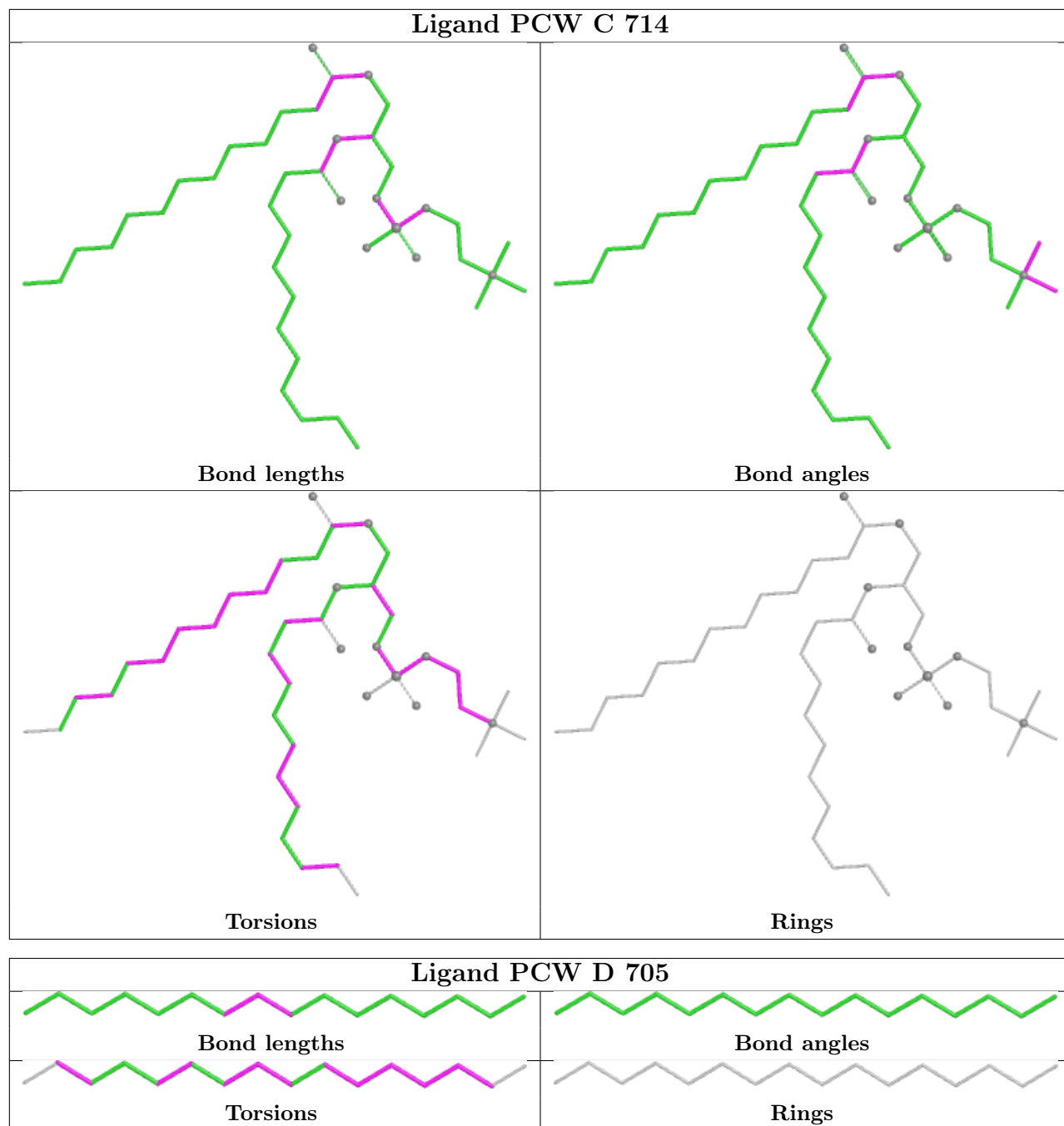


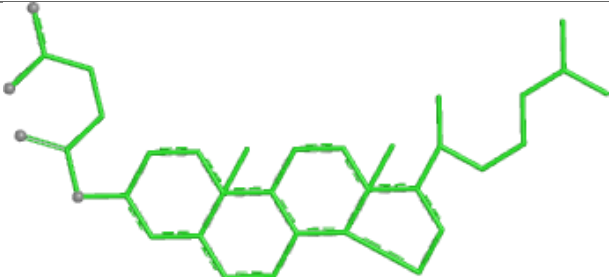
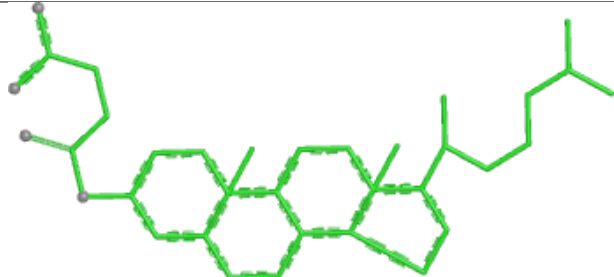
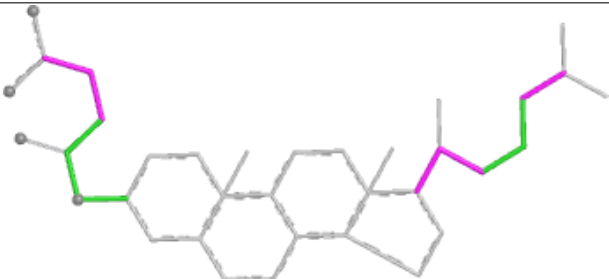
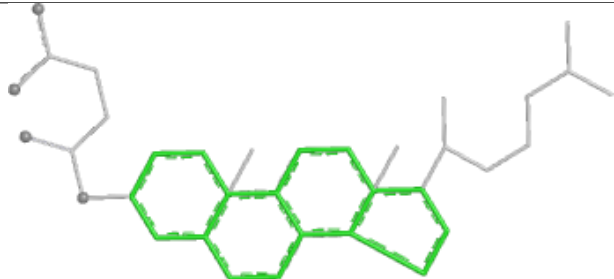




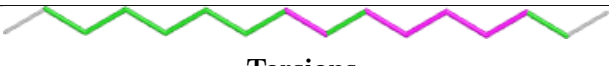
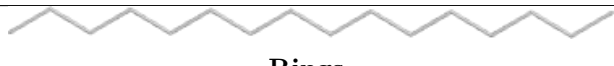









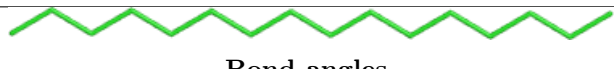
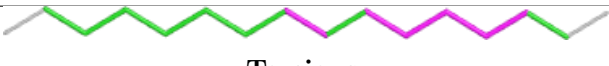
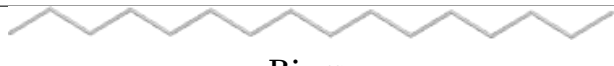








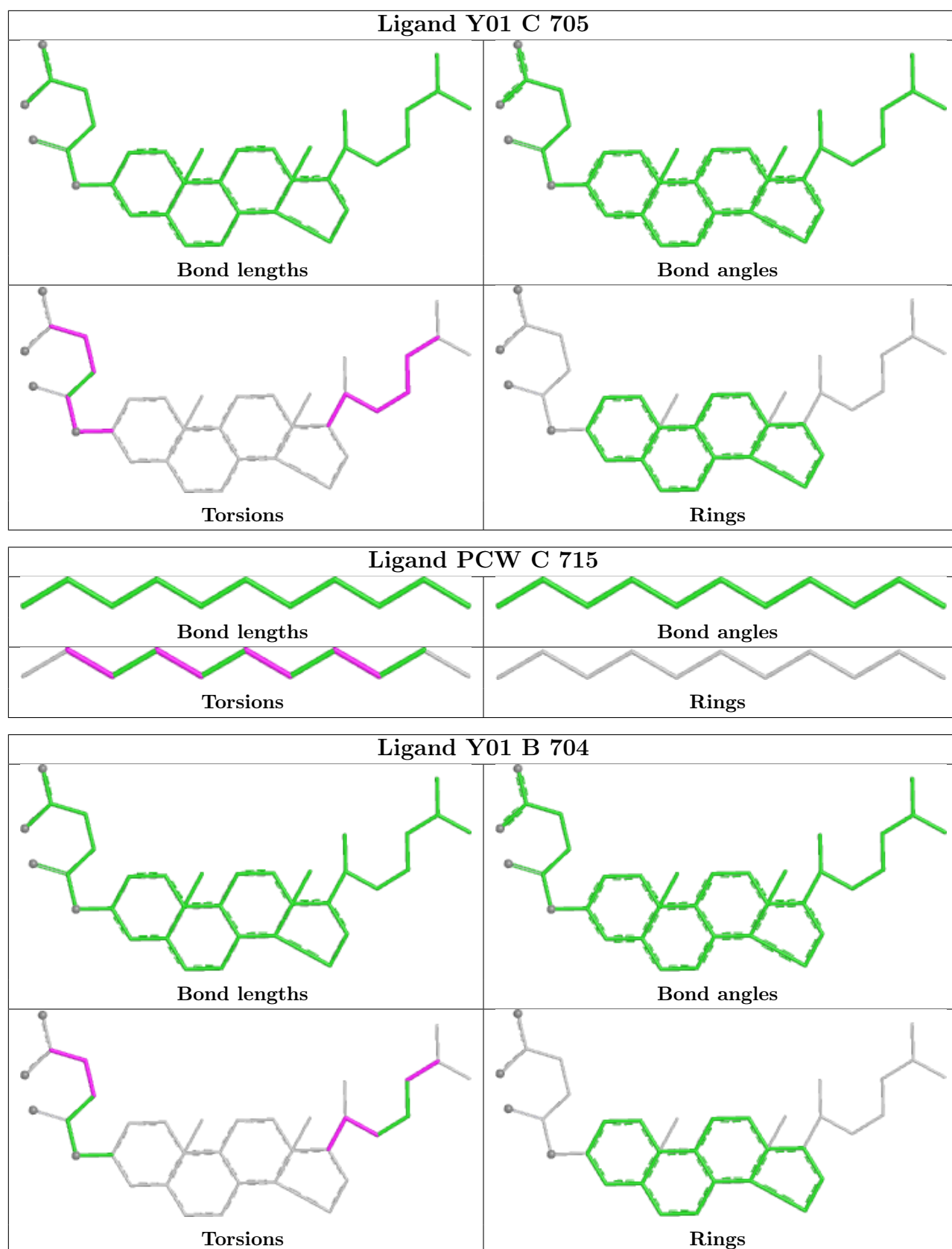
Ligand Y01 A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings


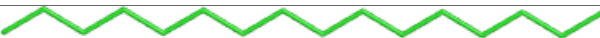


Ligand PCW D 703	
	
Bond lengths	Bond angles
	
Torsions	Rings





Ligand PCW D 715	
	
Bond lengths	Bond angles
	
Torsions	Rings


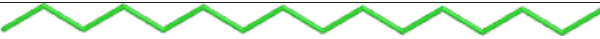


Ligand PCW B 717	
	
Bond lengths	Bond angles
	
Torsions	Rings

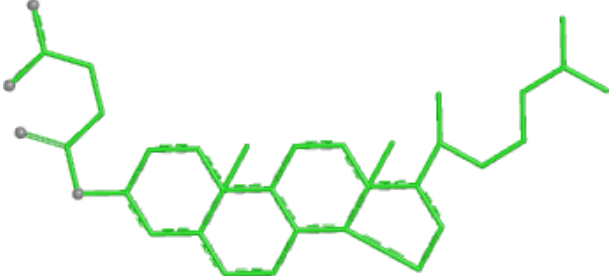
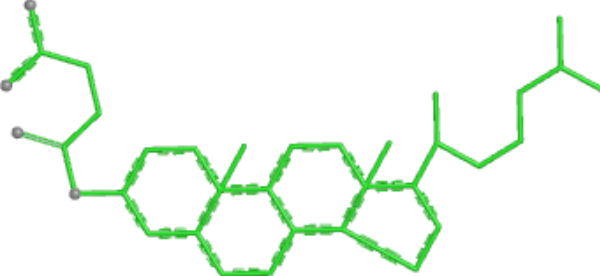

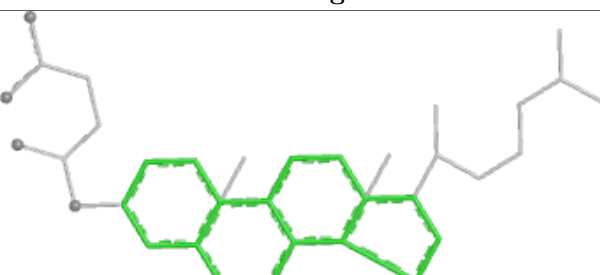
Ligand PCW D 712	
	
Bond lengths	Bond angles
	
Torsions	Rings




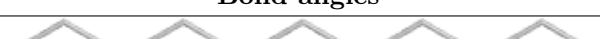


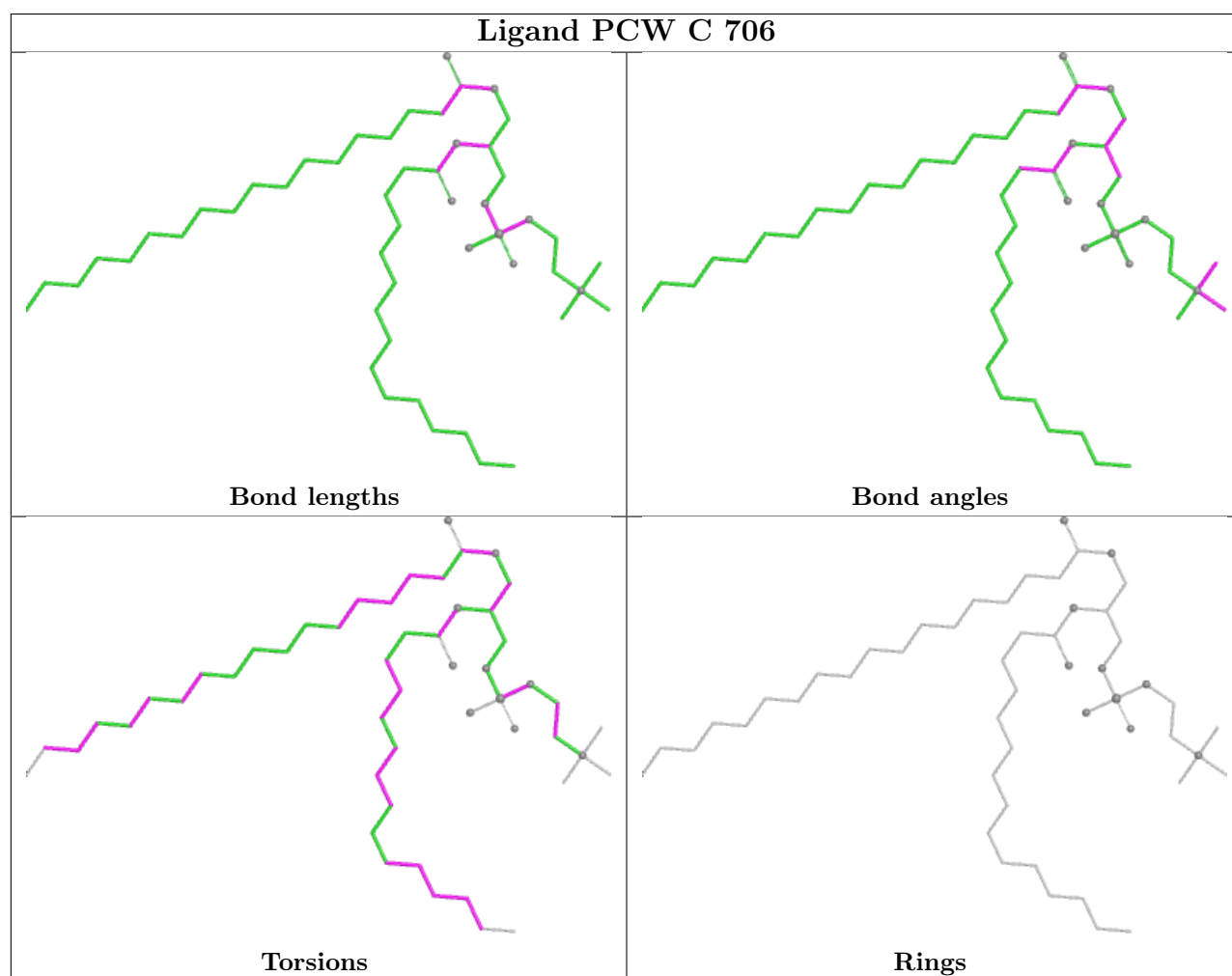
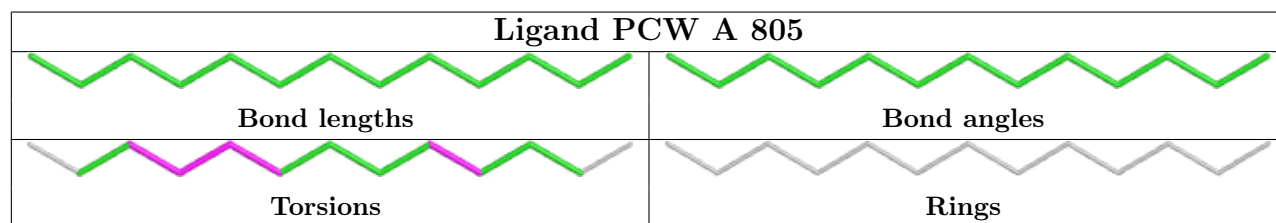
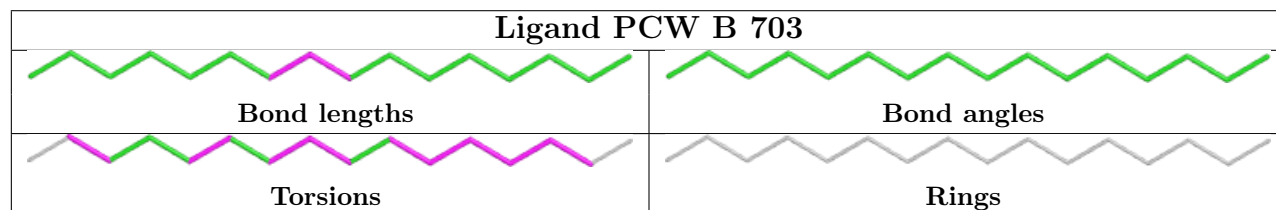
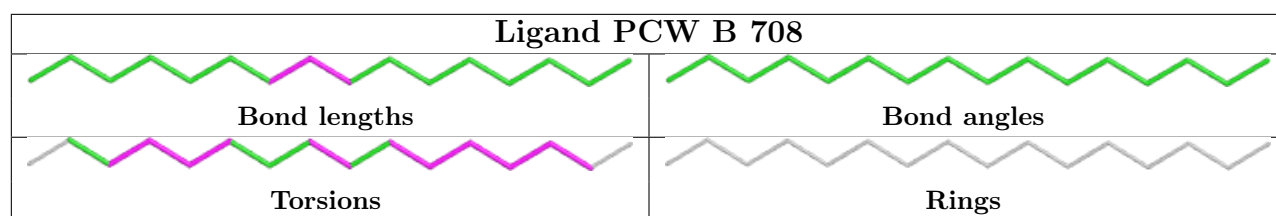
Ligand PCW B 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW C 716	
 Bond lengths	 Bond angles
 Torsions	 Rings

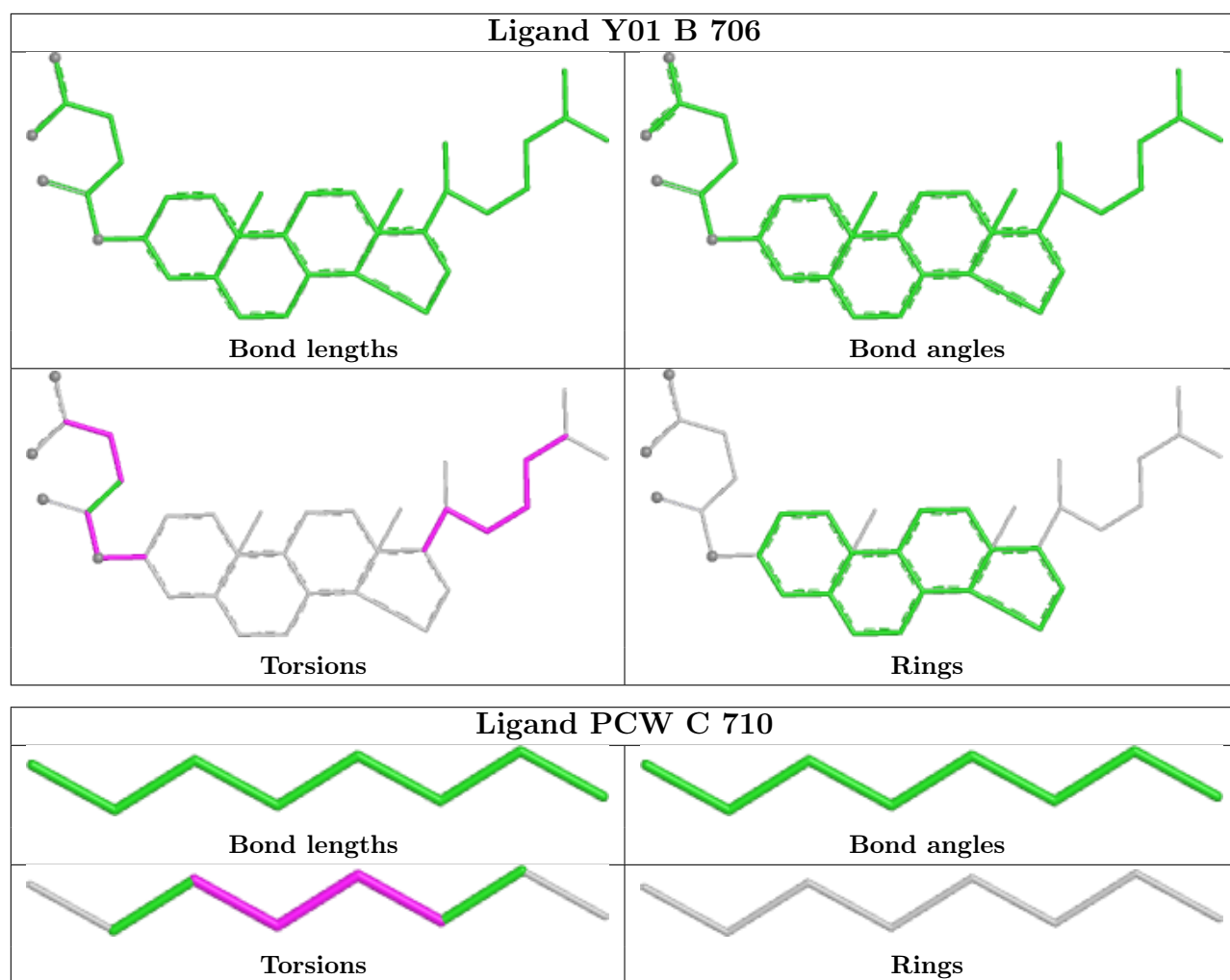
Ligand PCW C 712	
 Bond lengths	 Bond angles
 Torsions	 Rings

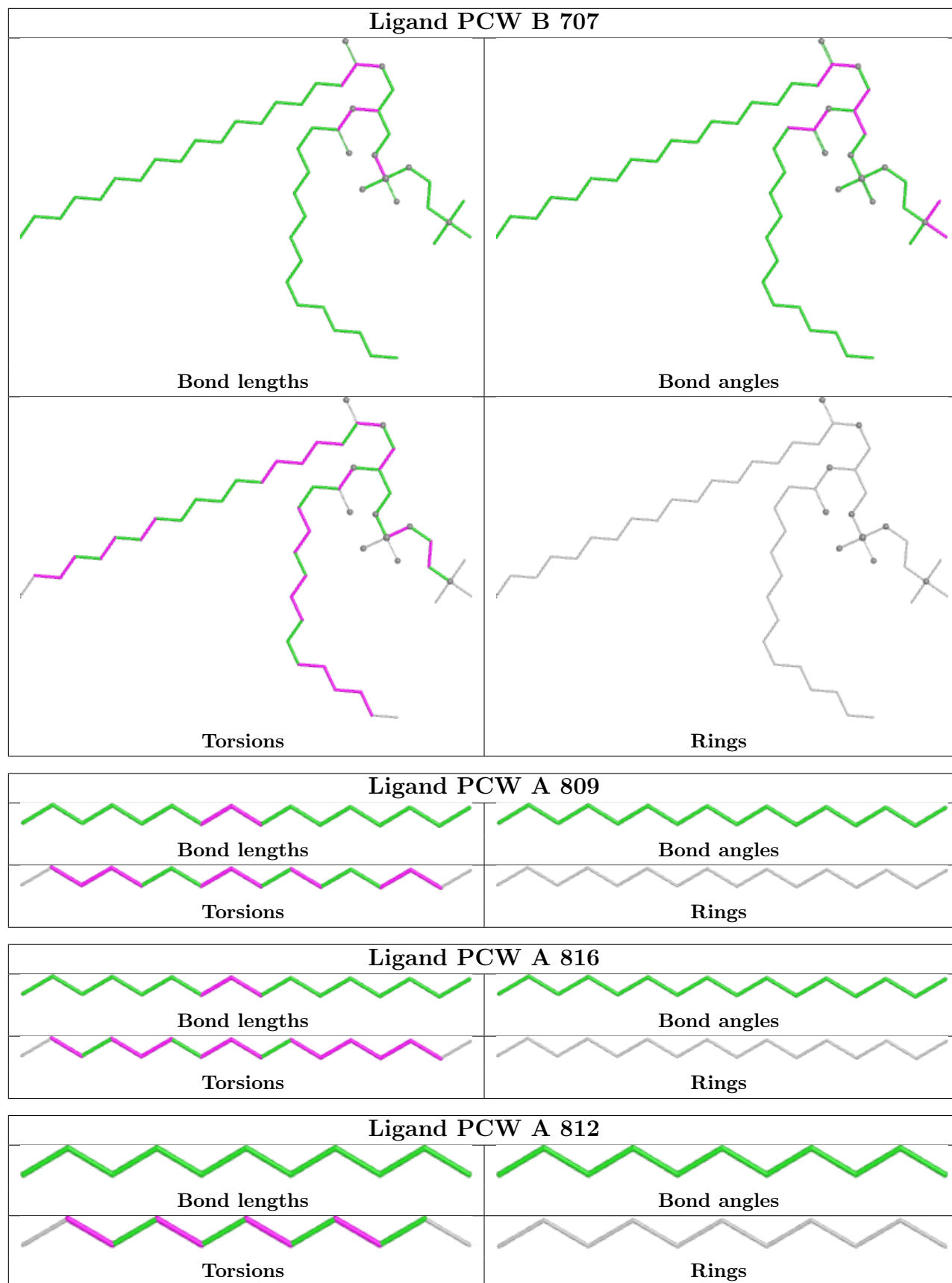
Ligand Y01 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

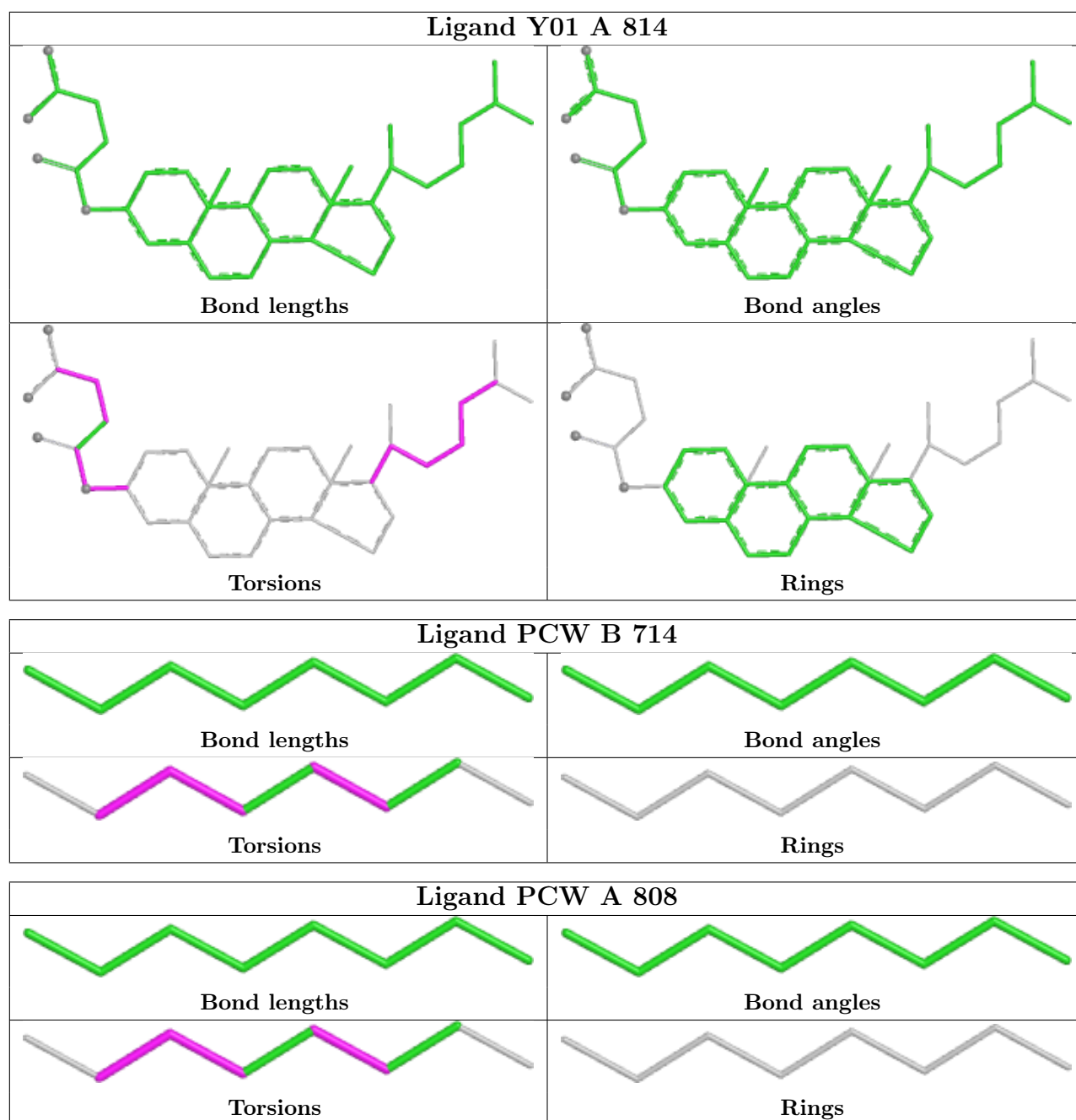
Ligand PCW D 711	
 Bond lengths	 Bond angles
 Torsions	 Rings

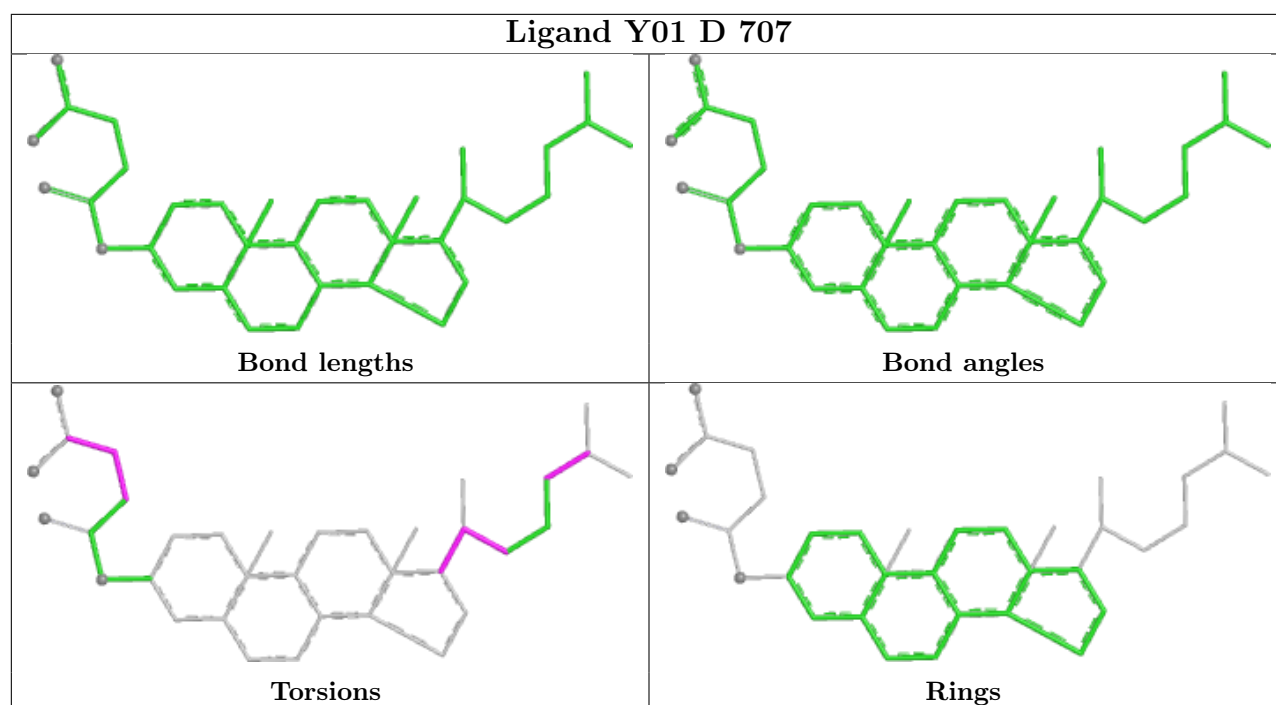












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

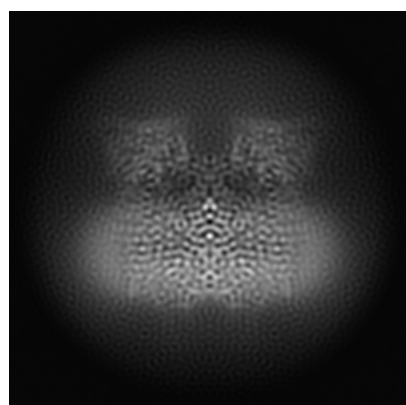
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22662. These allow visual inspection of the internal detail of the map and identification of artifacts.

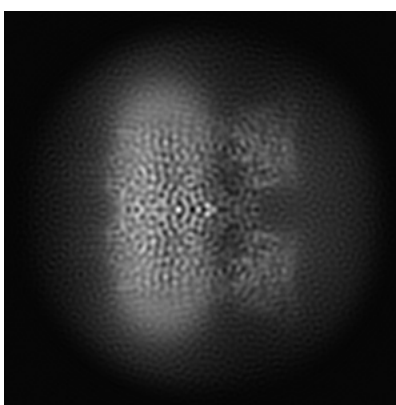
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

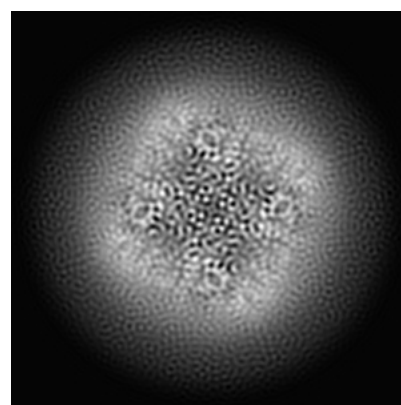
#### 6.1.1 Primary map



X



Y

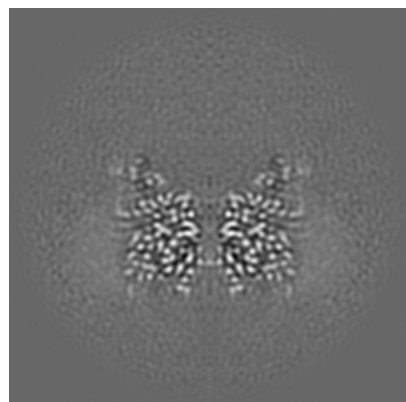


Z

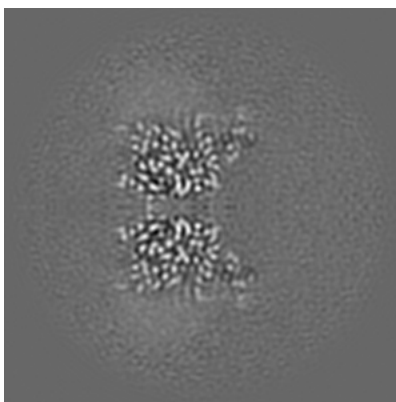
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

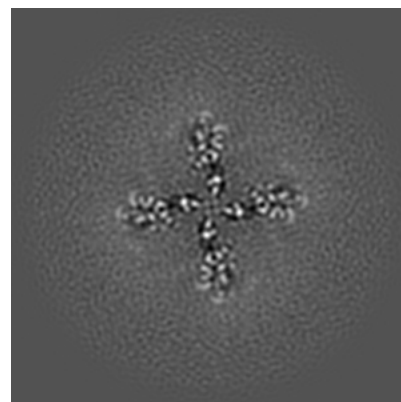
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

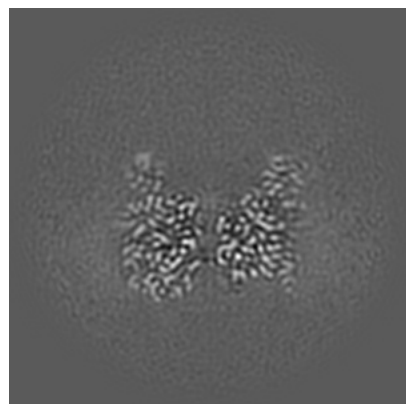


Z Index: 128

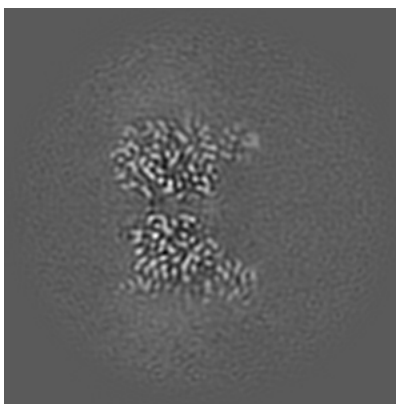
The images above show central slices of the map in three orthogonal directions.

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

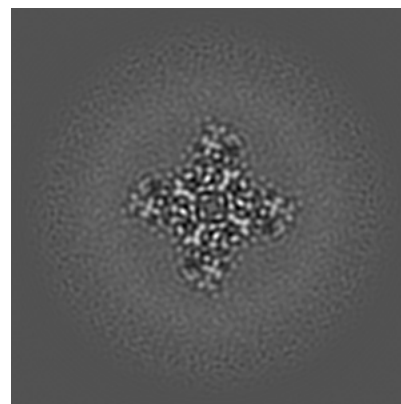
### 6.3.1 Primary map



X Index: 125



Y Index: 125

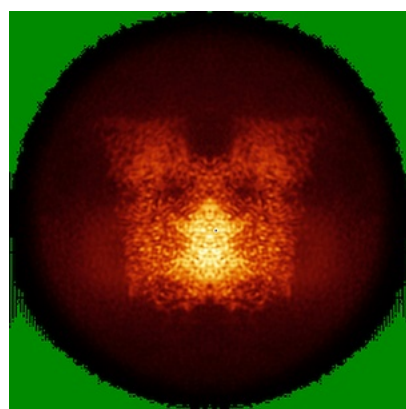


Z Index: 96

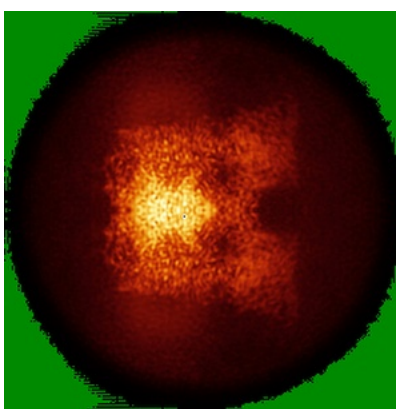
The images above show the largest variance slices of the map in three orthogonal directions.

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

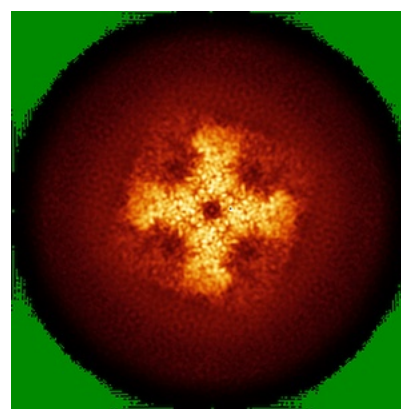
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

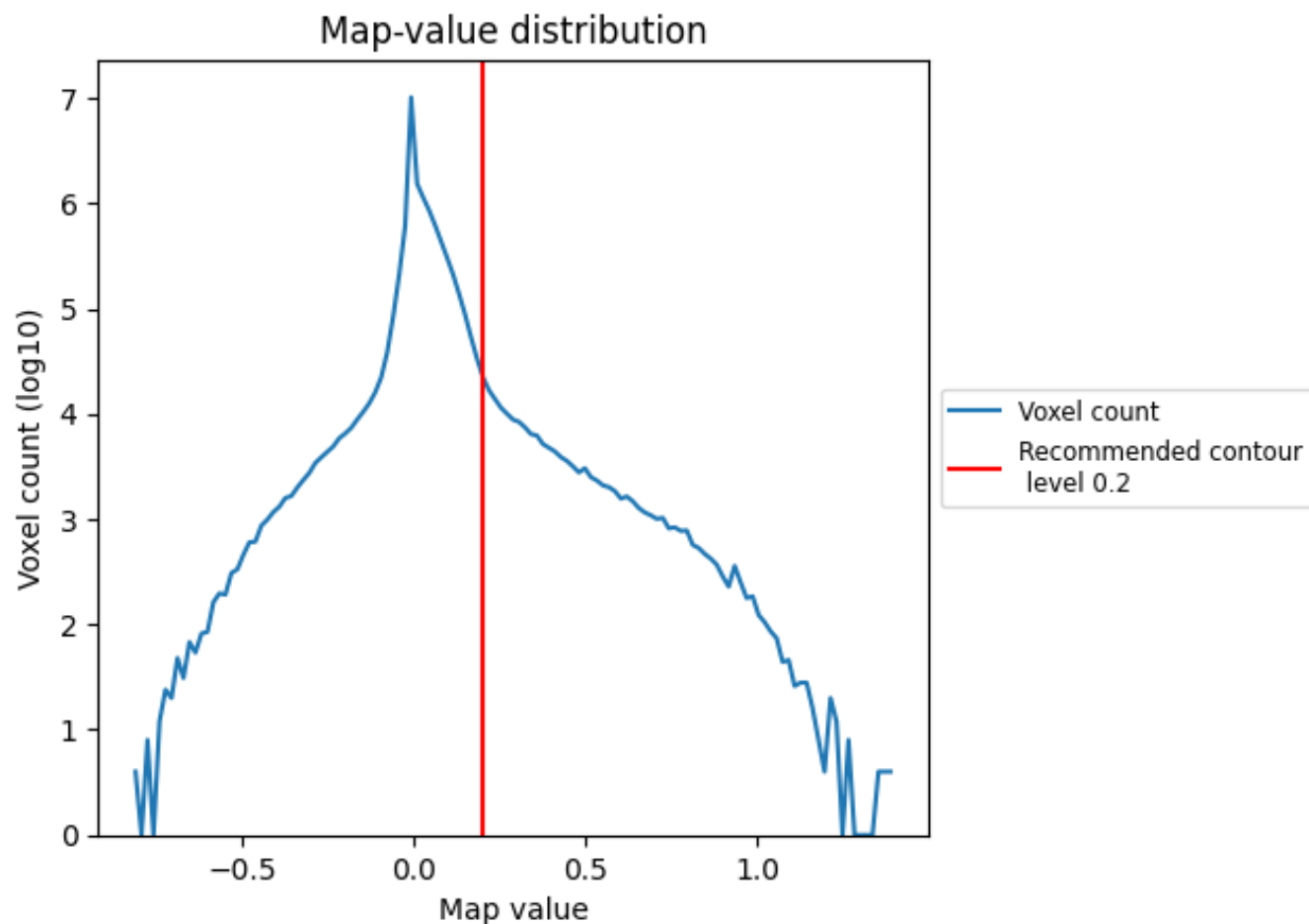
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

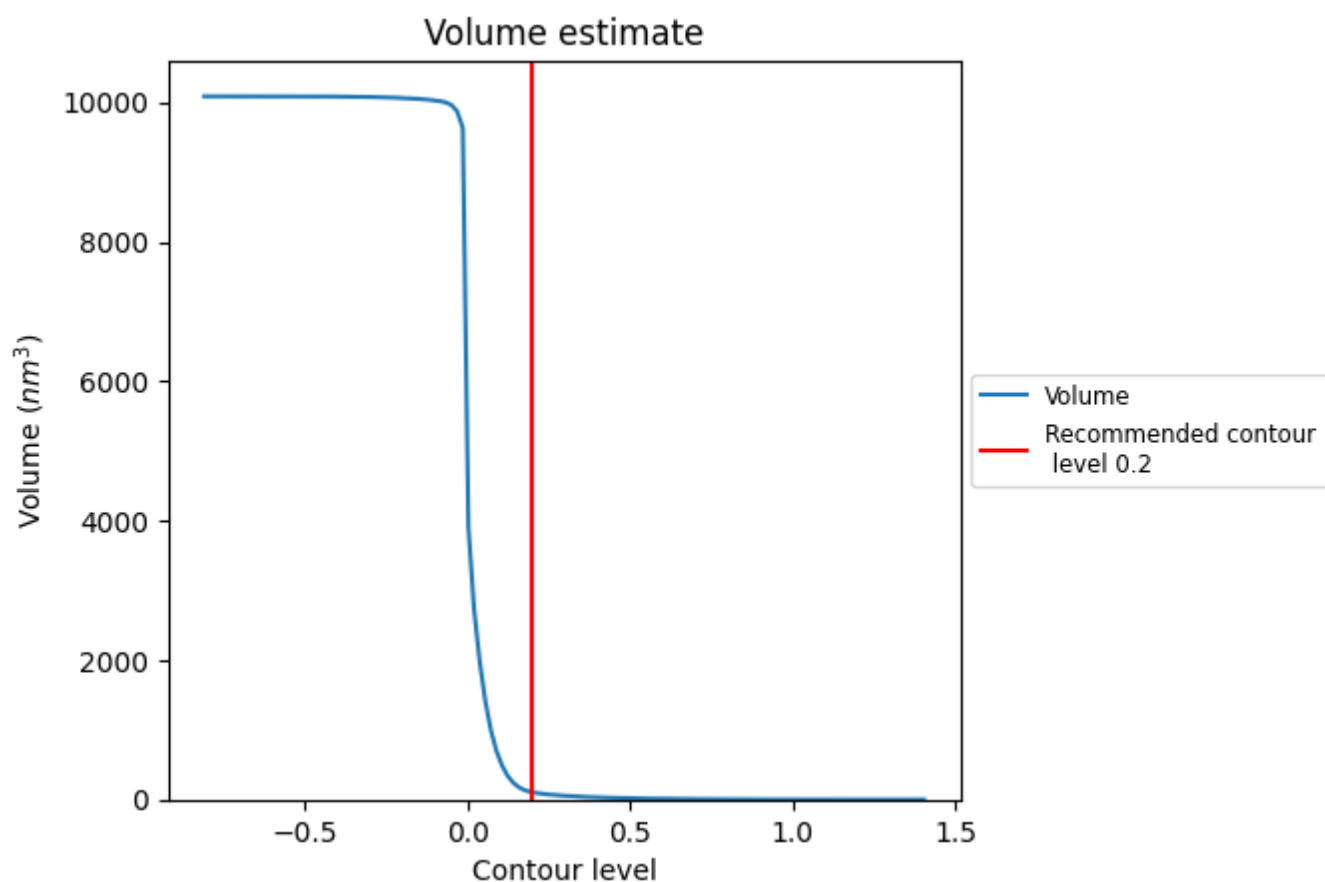
### 7.1 Map-value distribution [i](#)



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.



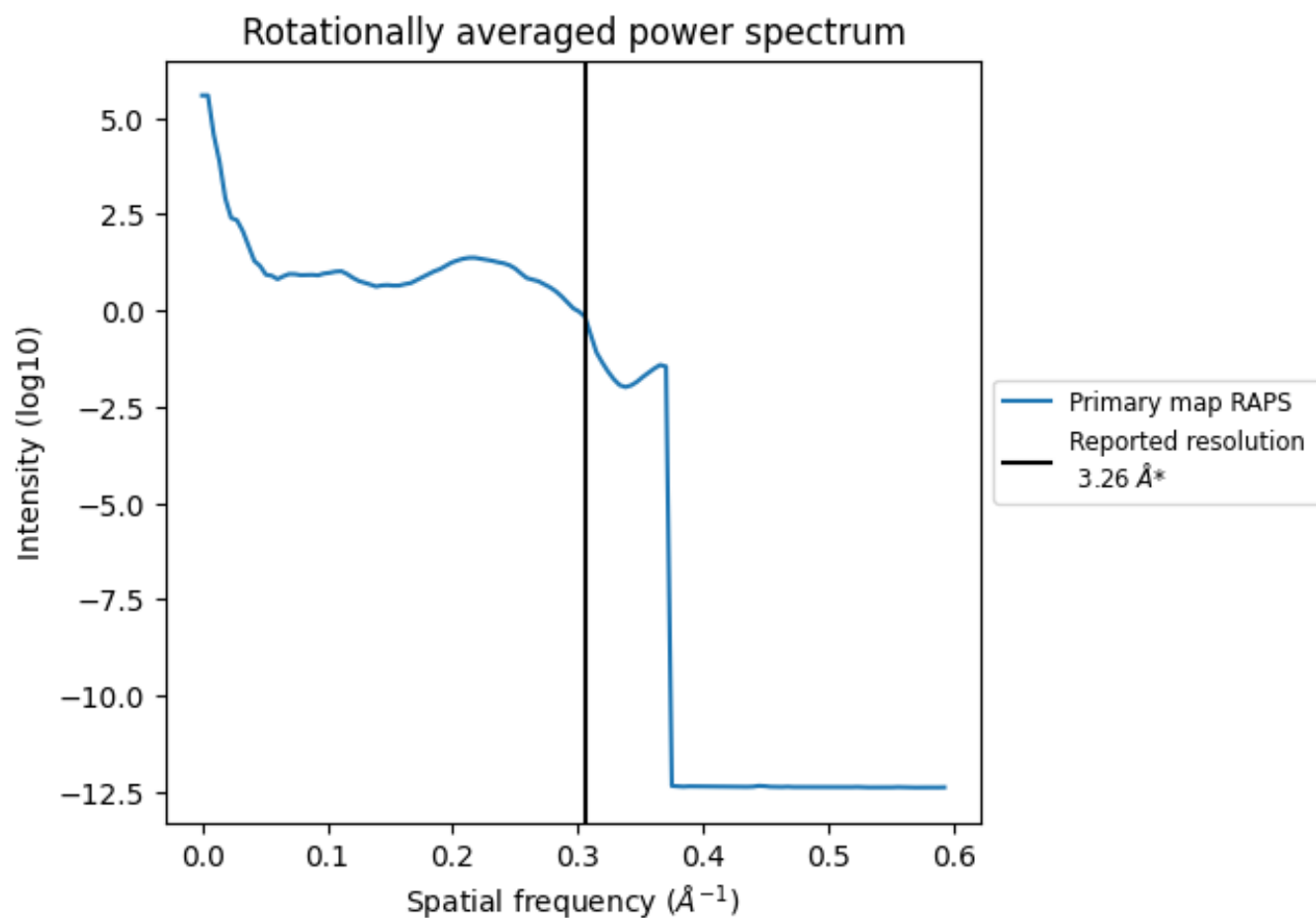
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm<sup>3</sup>; this corresponds to an approximate mass of 95 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 0.307 Å<sup>-1</sup>

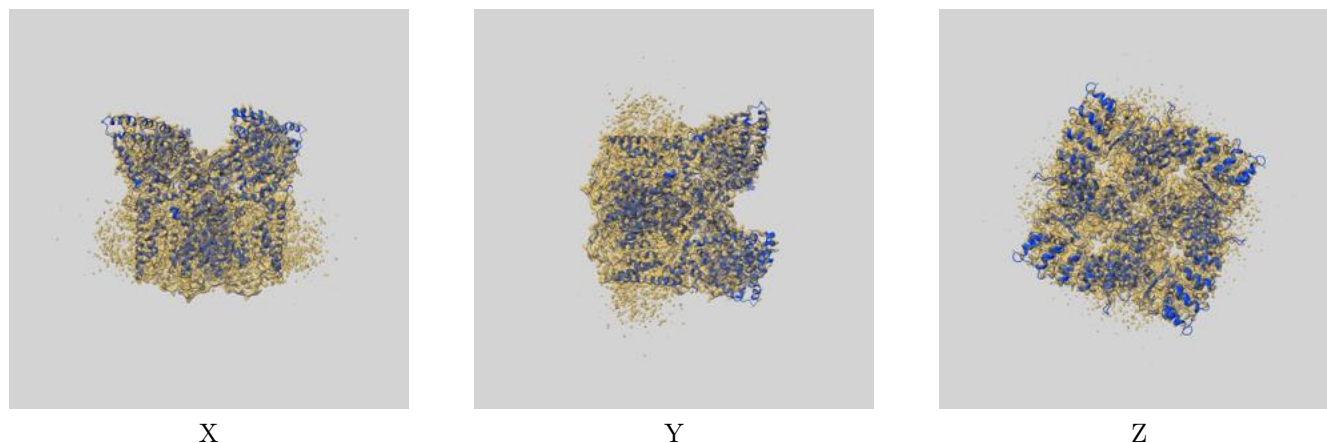
## 8 Fourier-Shell correlation

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

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

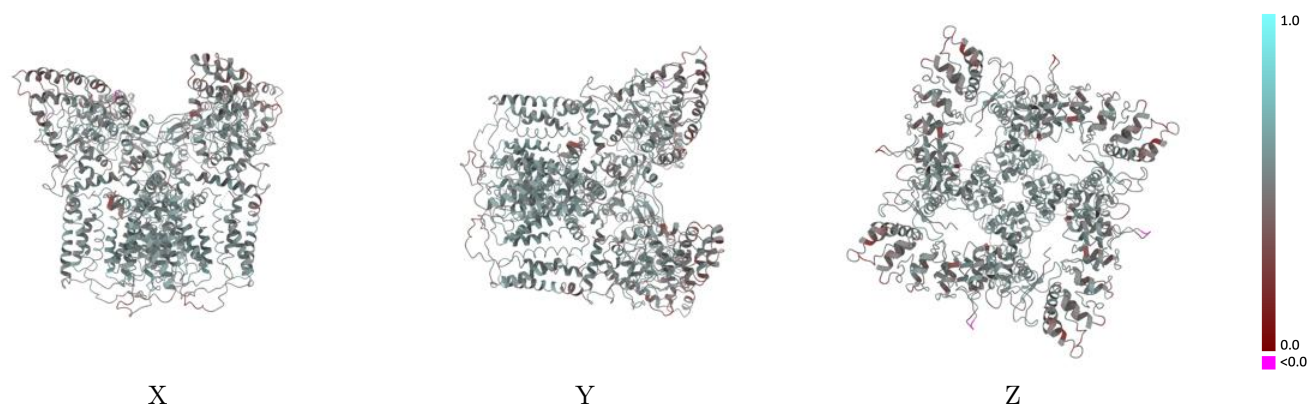
This section contains information regarding the fit between EMDB map EMD-22662 and PDB model 7K4A. Per-residue inclusion information can be found in section 3 on page 8.

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



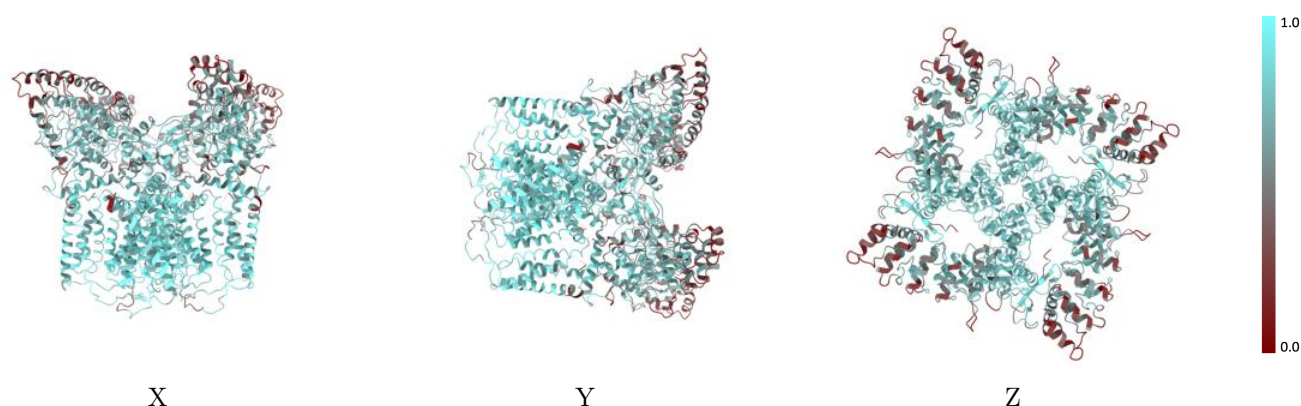
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



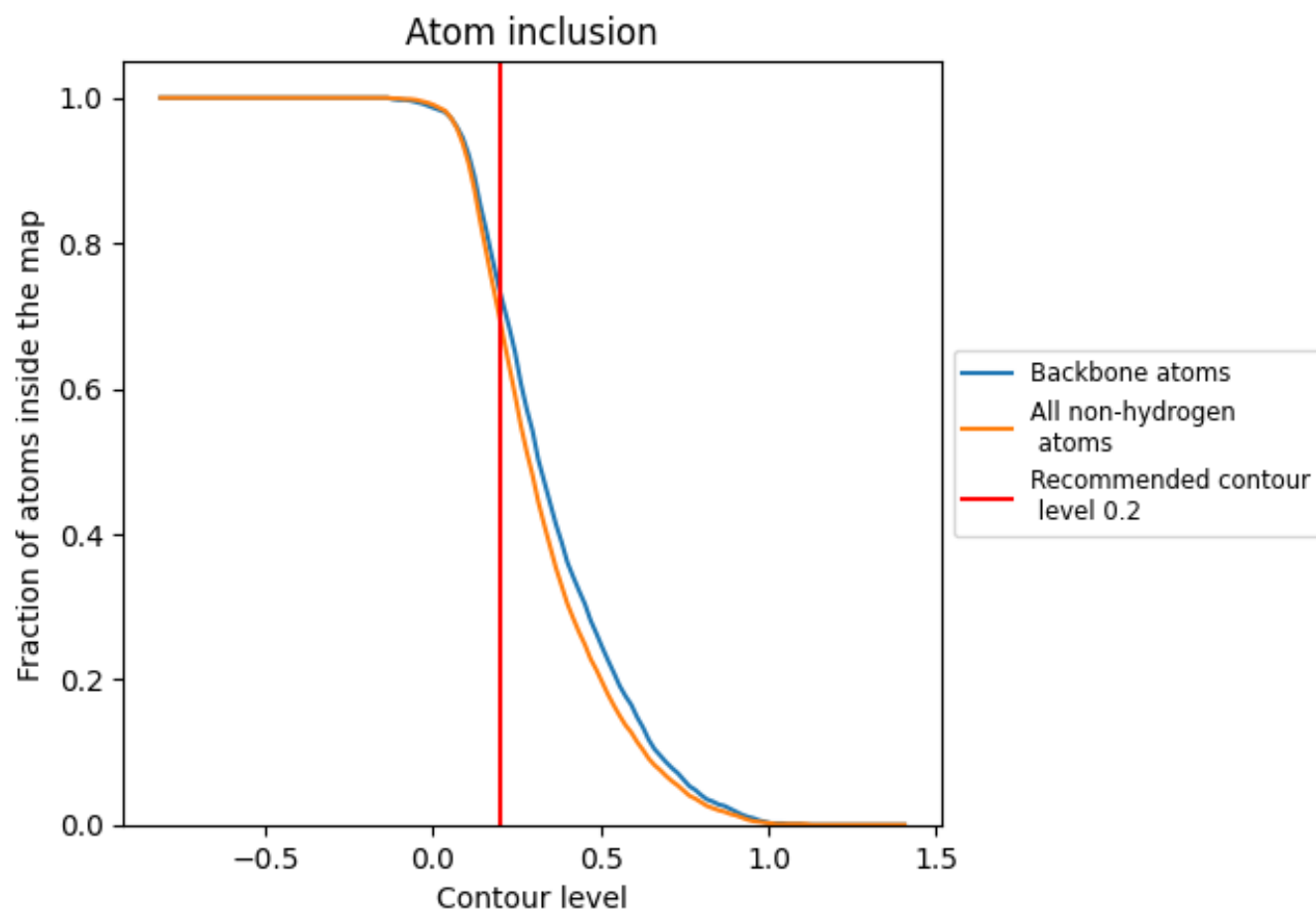
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6960	<div><div></div></div> 0.5120
A	<div><div></div></div> 0.6960	<div><div></div></div> 0.5120
B	<div><div></div></div> 0.6960	<div><div></div></div> 0.5120
C	<div><div></div></div> 0.6960	<div><div></div></div> 0.5120
D	<div><div></div></div> 0.6950	<div><div></div></div> 0.5110

