



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:48 PM UTC

PDB ID : 9ZPW / pdb_00009zpw
EMDB ID : EMD-74535
Title : CNGA1 channel intermediate state in nanodisc cGMP-bound
Authors : Park, T.; Nimigean, C.M.
Deposited on : 2025-12-17
Resolution : 2.47 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

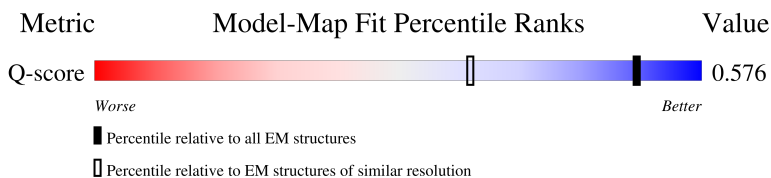
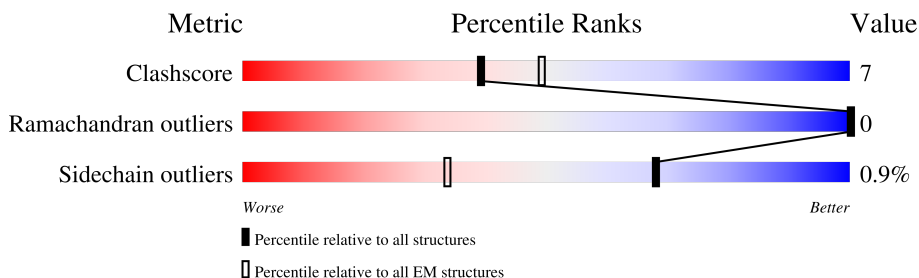
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.47 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6086 (1.98 - 2.97)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	
1	B	559	
1	C	559	
1	D	559	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16007 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 Cyclic nucleotide-gated channel alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3680	2405	593	663	19		
1	B	449	Total	C	N	O	S	0	0
			3680	2405	593	663	19		
1	C	449	Total	C	N	O	S	0	0
			3680	2405	593	663	19		
1	D	449	Total	C	N	O	S	0	0
			3680	2405	593	663	19		

There are 48 discrepancies between the modelled and reference sequences:

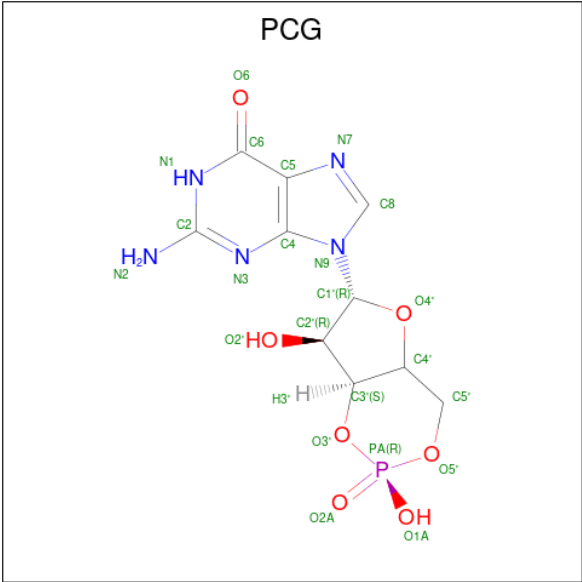
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ASP	-	expression tag	UNP P29973
A	133	TYR	-	expression tag	UNP P29973
A	134	LYS	-	expression tag	UNP P29973
A	135	ASP	-	expression tag	UNP P29973
A	136	ASP	-	expression tag	UNP P29973
A	137	ASP	-	expression tag	UNP P29973
A	138	ASP	-	expression tag	UNP P29973
A	139	LYS	-	expression tag	UNP P29973
A	140	GLY	-	expression tag	UNP P29973
A	141	GLY	-	expression tag	UNP P29973
A	142	SER	-	expression tag	UNP P29973
A	143	ALA	-	expression tag	UNP P29973
B	132	ASP	-	expression tag	UNP P29973
B	133	TYR	-	expression tag	UNP P29973
B	134	LYS	-	expression tag	UNP P29973
B	135	ASP	-	expression tag	UNP P29973
B	136	ASP	-	expression tag	UNP P29973
B	137	ASP	-	expression tag	UNP P29973
B	138	ASP	-	expression tag	UNP P29973
B	139	LYS	-	expression tag	UNP P29973
B	140	GLY	-	expression tag	UNP P29973
B	141	GLY	-	expression tag	UNP P29973

Continued on next page...

Continued from previous page...

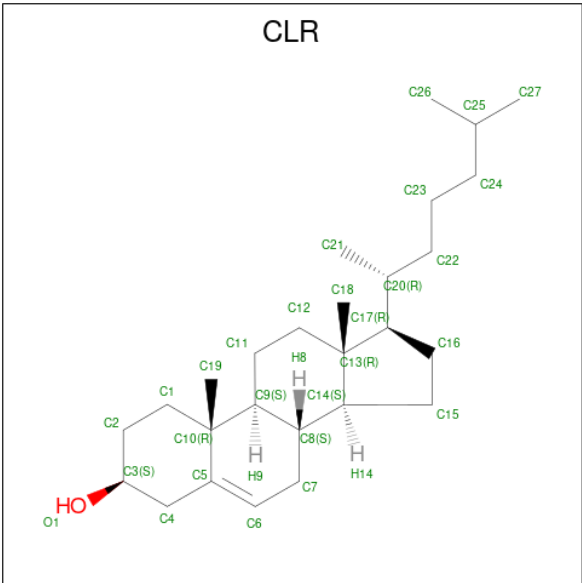
Chain	Residue	Modelled	Actual	Comment	Reference
B	142	SER	-	expression tag	UNP P29973
B	143	ALA	-	expression tag	UNP P29973
C	132	ASP	-	expression tag	UNP P29973
C	133	TYR	-	expression tag	UNP P29973
C	134	LYS	-	expression tag	UNP P29973
C	135	ASP	-	expression tag	UNP P29973
C	136	ASP	-	expression tag	UNP P29973
C	137	ASP	-	expression tag	UNP P29973
C	138	ASP	-	expression tag	UNP P29973
C	139	LYS	-	expression tag	UNP P29973
C	140	GLY	-	expression tag	UNP P29973
C	141	GLY	-	expression tag	UNP P29973
C	142	SER	-	expression tag	UNP P29973
C	143	ALA	-	expression tag	UNP P29973
D	132	ASP	-	expression tag	UNP P29973
D	133	TYR	-	expression tag	UNP P29973
D	134	LYS	-	expression tag	UNP P29973
D	135	ASP	-	expression tag	UNP P29973
D	136	ASP	-	expression tag	UNP P29973
D	137	ASP	-	expression tag	UNP P29973
D	138	ASP	-	expression tag	UNP P29973
D	139	LYS	-	expression tag	UNP P29973
D	140	GLY	-	expression tag	UNP P29973
D	141	GLY	-	expression tag	UNP P29973
D	142	SER	-	expression tag	UNP P29973
D	143	ALA	-	expression tag	UNP P29973

- Molecule 2 is CYCLIC GUANOSINE MONOPHOSPHATE (CCD ID: PCG) (formula: C₁₀H₁₂N₅O₇P) (labeled as "Ligand of Interest" by depositor).



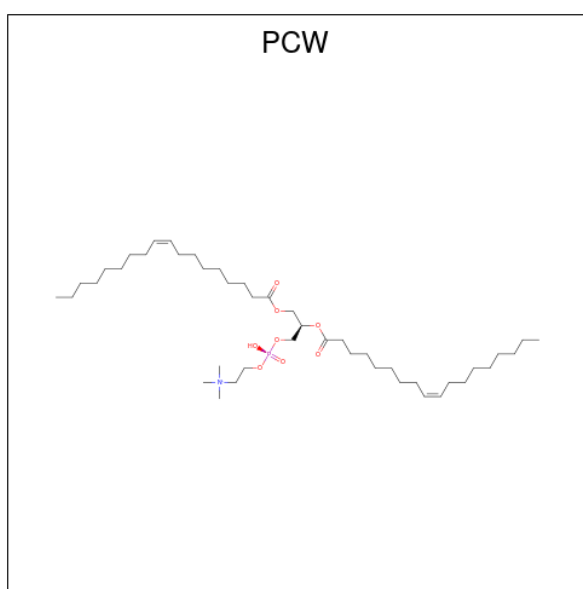
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
4	A	1	Total 48	C 39	O 8	P 1	0	
4	A	1	Total 43	C 33	N 1	O 8	P 1	0
4	A	1	Total 25	C 16	O 8	P 1	0	
4	A	1	Total 38	C 33	O 5		0	
4	A	1	Total 39	C 29	N 1	O 8	P 1	0
4	A	1	Total 34	C 25	O 8	P 1	0	
4	A	1	Total 45	C 36	O 8	P 1	0	

Continued on next page...

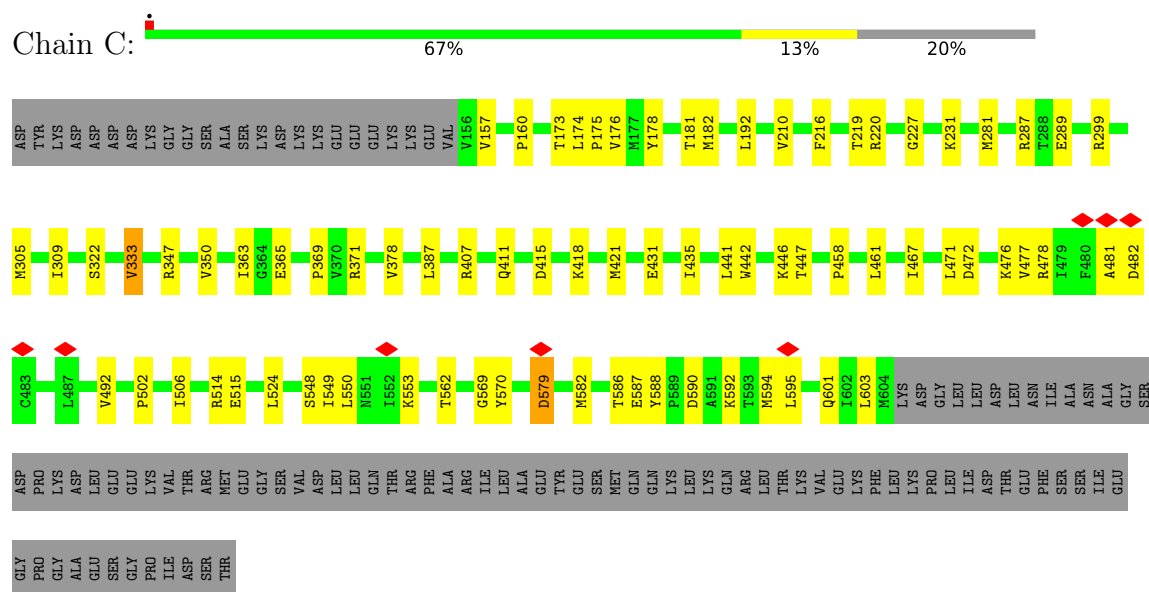
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	O	P	0
			44	35	8	1	
4	B	1	Total	C	N	O	P
			43	33	1	8	1
4	B	1	Total	C	O	P	0
			25	16	8	1	
4	B	1	Total	C	O		0
			38	33	5		
4	B	1	Total	C	N	O	P
			37	27	1	8	1
4	B	1	Total	C	O	P	0
			48	39	8	1	
4	B	1	Total	C	N	O	P
			37	27	1	8	1
4	B	1	Total	C	O	P	0
			34	25	8	1	
4	C	1	Total	C	O	P	0
			44	35	8	1	
4	C	1	Total	C	N	O	P
			42	32	1	8	1
4	C	1	Total	C	O	P	0
			26	17	8	1	
4	C	1	Total	C	O	P	0
			48	39	8	1	
4	C	1	Total	C	O		0
			38	33	5		
4	C	1	Total	C	O	P	0
			34	25	8	1	
4	D	1	Total	C	O	P	0
			34	25	8	1	
4	D	1	Total	C	O	P	0
			43	34	8	1	
4	D	1	Total	C	N	O	P
			44	34	1	8	1
4	D	1	Total	C	O	P	0
			25	16	8	1	
4	D	1	Total	C	N	O	P
			35	25	1	8	1
4	D	1	Total	C	O		0
			38	33	5		
4	D	1	Total	C	O	P	0
			48	39	8	1	

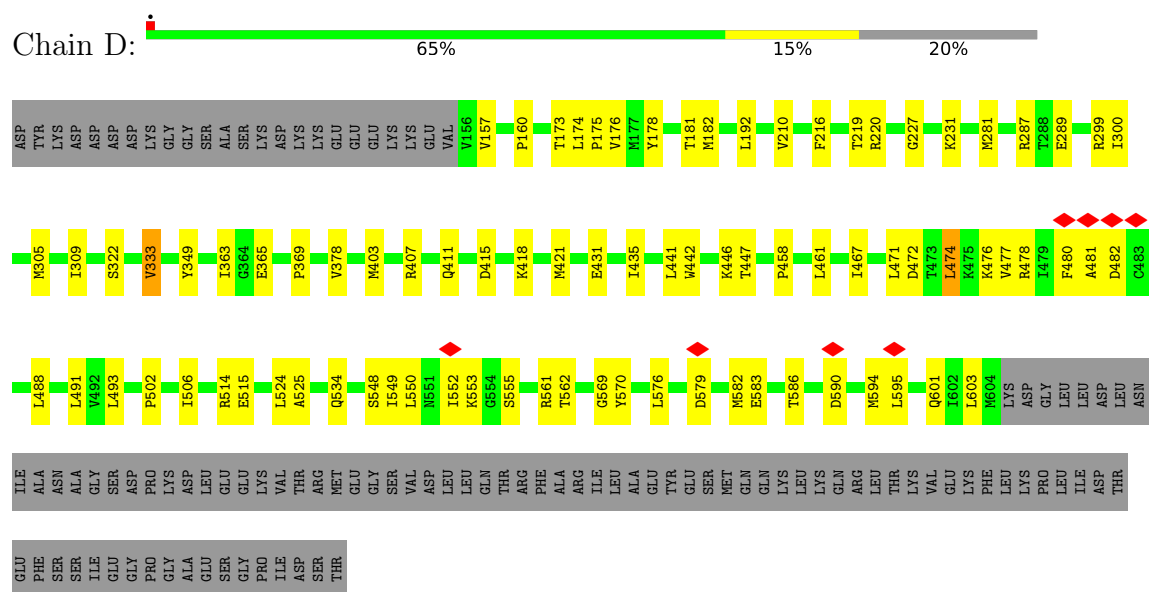
- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	5	Total 5	K 5	0
5	D	1	Total 1	K 1	0

- Molecule 1: Cyclic nucleotide-gated channel alpha-1



- Molecule 1: Cyclic nucleotide-gated channel alpha-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, CLR, PCW, PCG

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	0.10	0/3765	0.27	0/5102
1	B	0.10	0/3765	0.27	0/5102
1	C	0.10	0/3765	0.29	0/5102
1	D	0.10	0/3765	0.27	0/5102
All	All	0.10	0/15060	0.27	0/20408

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3680	0	3725	52	0
1	B	3680	0	3725	49	0
1	C	3680	0	3725	52	0
1	D	3680	0	3725	58	0
2	A	23	0	9	4	0
2	B	23	0	9	4	0
2	C	23	0	9	4	0
2	D	23	0	9	4	0
3	A	28	0	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	46	0	0
3	C	28	0	46	1	0
3	D	28	0	46	0	0
4	A	272	0	356	7	0
4	B	306	0	396	15	0
4	C	232	0	304	8	0
4	D	267	0	347	7	0
5	A	5	0	0	0	0
5	D	1	0	0	0	0
All	All	16007	0	16523	234	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (234) 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)
2:D:703:PCG:C4'	2:D:703:PCG:C3'	1.81	1.52
2:B:702:PCG:C3'	2:B:702:PCG:C4'	1.81	1.50
2:A:701:PCG:C4'	2:A:701:PCG:C3'	1.81	1.43
2:C:702:PCG:C4'	2:C:702:PCG:C3'	1.81	1.39
1:A:407:ARG:HH21	1:A:411:GLN:HG2	1.54	0.72
1:B:407:ARG:HH21	1:B:411:GLN:HG2	1.54	0.71
1:A:474:LEU:HB3	1:A:488:LEU:HD23	1.74	0.70
1:D:525:ALA:HB1	1:D:534:GLN:HG2	1.80	0.64
1:D:407:ARG:NH2	1:D:411:GLN:OE1	2.30	0.64
1:C:458:PRO:HG2	1:C:461:LEU:HB2	1.79	0.64
1:B:458:PRO:HG2	1:B:461:LEU:HB2	1.79	0.64
1:C:407:ARG:NH2	1:C:411:GLN:OE1	2.30	0.64
1:A:458:PRO:HG2	1:A:461:LEU:HB2	1.79	0.63
1:D:458:PRO:HG2	1:D:461:LEU:HB2	1.79	0.63
1:A:594:MET:HE3	1:A:594:MET:H	1.64	0.62
1:C:178:TYR:HB2	4:C:706:PCW:H241	1.80	0.62
1:C:502:PRO:HB3	1:C:569:GLY:HA2	1.83	0.61
1:A:502:PRO:HB3	1:A:569:GLY:HA2	1.82	0.60
1:C:562:THR:OG1	2:C:702:PCG:N2	2.33	0.60
1:D:502:PRO:HB3	1:D:569:GLY:HA2	1.82	0.60
1:B:562:THR:OG1	2:B:702:PCG:N2	2.34	0.60
1:B:160:PRO:O	1:B:287:ARG:NH1	2.34	0.60
1:B:502:PRO:HB3	1:B:569:GLY:HA2	1.82	0.60
1:C:363:ILE:HG22	1:C:365:GLU:HG2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:HG22	1:A:365:GLU:HG2	1.84	0.59
1:B:467:ILE:HG23	1:B:471:LEU:HD22	1.84	0.59
1:D:363:ILE:HG22	1:D:365:GLU:HG2	1.84	0.59
1:D:562:THR:OG1	2:D:703:PCG:N2	2.33	0.59
1:A:562:THR:OG1	2:A:701:PCG:N2	2.33	0.59
1:B:363:ILE:HG22	1:B:365:GLU:HG2	1.84	0.59
1:C:322:SER:HA	1:C:333:VAL:HG22	1.86	0.58
1:C:594:MET:HE3	1:C:594:MET:H	1.66	0.58
1:C:467:ILE:HG23	1:C:471:LEU:HD22	1.86	0.57
1:D:322:SER:HA	1:D:333:VAL:HG22	1.86	0.57
1:A:322:SER:HA	1:A:333:VAL:HG22	1.87	0.57
1:C:160:PRO:O	1:C:287:ARG:NH1	2.33	0.57
1:B:322:SER:HA	1:B:333:VAL:HG22	1.87	0.57
1:D:160:PRO:O	1:D:287:ARG:NH1	2.33	0.56
1:A:553:LYS:HD3	1:A:553:LYS:C	2.31	0.56
1:D:553:LYS:C	1:D:553:LYS:HD3	2.30	0.56
1:A:173:THR:HG23	1:A:281:MET:HG3	1.88	0.56
1:A:467:ILE:HG23	1:A:471:LEU:HD22	1.87	0.56
1:B:553:LYS:HD3	1:B:553:LYS:C	2.30	0.56
1:B:372:ASP:HB2	4:B:707:PCW:H12	1.88	0.55
2:A:701:PCG:C3'	2:A:701:PCG:C5'	2.79	0.55
4:A:704:PCW:H19	4:B:701:PCW:H432	1.88	0.55
1:C:553:LYS:HD3	1:C:553:LYS:C	2.30	0.55
1:A:160:PRO:O	1:A:287:ARG:NH1	2.34	0.55
1:D:514:ARG:HG2	1:D:515:GLU:HG3	1.87	0.55
1:D:467:ILE:HG23	1:D:471:LEU:HD22	1.87	0.55
1:A:514:ARG:HG2	1:A:515:GLU:HG3	1.88	0.55
1:B:300:ILE:HG21	4:B:704:PCW:H362	1.89	0.55
1:C:514:ARG:HG2	1:C:515:GLU:HG3	1.89	0.54
1:A:182:MET:HE1	1:A:192:LEU:HD21	1.89	0.54
2:D:703:PCG:C3'	2:D:703:PCG:C5'	2.80	0.54
1:D:173:THR:HG23	1:D:281:MET:HG3	1.89	0.54
4:B:709:PCW:H41	1:C:371:ARG:HB3	1.90	0.54
1:B:514:ARG:HG2	1:B:515:GLU:HG3	1.88	0.53
4:B:704:PCW:H40	4:C:701:PCW:H221	1.88	0.53
1:C:157:VAL:HG21	1:C:231:LYS:HA	1.90	0.53
1:D:182:MET:HE1	1:D:192:LEU:HD21	1.90	0.53
1:D:594:MET:H	1:D:594:MET:HE3	1.72	0.53
1:B:387:LEU:HD13	4:B:701:PCW:H40	1.91	0.53
1:C:173:THR:HG23	1:C:281:MET:HG3	1.90	0.53
1:C:182:MET:HE1	1:C:192:LEU:HD21	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:HG21	1:B:231:LYS:HA	1.91	0.53
1:B:173:THR:HG23	1:B:281:MET:HG3	1.89	0.53
1:B:582:MET:O	1:B:586:THR:HG23	2.09	0.52
1:B:178:TYR:HB2	4:B:708:PCW:H431	1.92	0.52
2:B:702:PCG:C3'	2:B:702:PCG:C5'	2.80	0.52
1:C:442:TRP:HE3	1:C:447:THR:HG21	1.74	0.52
1:D:178:TYR:HB2	4:D:709:PCW:H241	1.91	0.52
2:C:702:PCG:C3'	2:C:702:PCG:C5'	2.80	0.52
1:D:442:TRP:HE3	1:D:447:THR:HG21	1.74	0.52
1:C:369:PRO:HG3	1:C:378:VAL:HG21	1.92	0.52
1:D:421:MET:HE3	1:D:431:GLU:HG2	1.92	0.52
1:D:474:LEU:HD12	1:D:488:LEU:HD22	1.92	0.52
1:A:594:MET:H	1:A:594:MET:CE	2.23	0.52
1:B:472:ASP:N	1:B:472:ASP:OD1	2.41	0.51
1:D:157:VAL:HG21	1:D:231:LYS:HA	1.91	0.51
1:B:369:PRO:HG3	1:B:378:VAL:HG21	1.91	0.51
1:B:442:TRP:HE3	1:B:447:THR:HG21	1.75	0.51
4:B:705:PCW:H322	4:B:706:PCW:H382	1.93	0.51
1:C:421:MET:HE3	1:C:431:GLU:HG2	1.92	0.51
1:A:157:VAL:HG21	1:A:231:LYS:HA	1.92	0.51
1:A:421:MET:HE3	1:A:431:GLU:HG2	1.93	0.51
1:A:442:TRP:HE3	1:A:447:THR:HG21	1.76	0.51
1:C:582:MET:O	1:C:586:THR:HG23	2.10	0.51
4:B:704:PCW:H332	4:C:701:PCW:H132	1.93	0.51
1:B:421:MET:HE3	1:B:431:GLU:HG2	1.92	0.50
4:B:701:PCW:H411	4:B:701:PCW:H19	1.94	0.50
1:D:369:PRO:HG3	1:D:378:VAL:HG21	1.91	0.50
1:B:289:GLU:OE2	1:B:299:ARG:NH1	2.41	0.50
1:C:549:ILE:HG23	1:C:550:LEU:HG	1.93	0.50
1:A:472:ASP:OD1	1:A:472:ASP:N	2.44	0.50
1:A:582:MET:O	1:A:586:THR:HG23	2.11	0.50
1:C:477:VAL:O	1:C:481:ALA:N	2.45	0.49
1:D:472:ASP:N	1:D:472:ASP:OD1	2.44	0.49
1:B:594:MET:HE3	1:B:594:MET:H	1.74	0.49
1:C:289:GLU:OE2	1:C:299:ARG:NH1	2.40	0.49
1:D:418:LYS:HD3	1:D:435:ILE:HD11	1.95	0.49
1:D:594:MET:H	1:D:594:MET:CE	2.26	0.49
1:D:549:ILE:HG23	1:D:550:LEU:HG	1.94	0.48
4:A:709:PCW:H381	4:D:705:PCW:H342	1.95	0.48
1:D:550:LEU:HD11	1:D:595:LEU:HD12	1.95	0.48
1:C:418:LYS:HD3	1:C:435:ILE:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LEU:HD22	1:C:446:LYS:HB2	1.96	0.48
1:C:579:ASP:OD1	1:C:579:ASP:N	2.47	0.48
1:A:472:ASP:O	1:A:476:LYS:HG2	2.13	0.47
1:B:418:LYS:HD3	1:B:435:ILE:HD11	1.96	0.47
1:A:418:LYS:HD3	1:A:435:ILE:HD11	1.96	0.47
1:C:472:ASP:OD1	1:C:472:ASP:N	2.44	0.47
1:A:289:GLU:OE2	1:A:299:ARG:NH1	2.41	0.47
4:B:708:PCW:H212	4:B:710:PCW:H181	1.96	0.47
1:C:176:VAL:HG12	1:C:281:MET:HE2	1.95	0.47
1:D:441:LEU:HD22	1:D:446:LYS:HB2	1.97	0.47
1:B:441:LEU:HD22	1:B:446:LYS:HB2	1.97	0.47
1:C:472:ASP:O	1:C:476:LYS:HG2	2.15	0.47
1:D:493:LEU:HD12	1:D:493:LEU:H	1.80	0.47
1:B:549:ILE:HG23	1:B:550:LEU:HG	1.96	0.47
1:D:480:PHE:HB3	1:D:488:LEU:HD21	1.97	0.47
1:C:216:PHE:O	1:C:219:THR:OG1	2.27	0.46
1:D:579:ASP:N	1:D:579:ASP:OD1	2.47	0.46
1:A:369:PRO:HG3	1:A:378:VAL:HG21	1.96	0.46
1:A:478:ARG:HA	1:A:481:ALA:HB3	1.97	0.46
1:B:294:TYR:HD1	4:B:704:PCW:H42	1.80	0.46
1:B:478:ARG:HA	1:B:481:ALA:HB3	1.98	0.46
1:B:477:VAL:O	1:B:481:ALA:N	2.48	0.46
4:D:705:PCW:H132	4:D:705:PCW:H332	1.97	0.46
1:A:441:LEU:HD22	1:A:446:LYS:HB2	1.98	0.46
1:A:592:LYS:HE3	1:A:592:LYS:HB3	1.76	0.46
1:A:579:ASP:OD1	1:A:579:ASP:N	2.47	0.46
1:C:471:LEU:HD12	1:C:471:LEU:HA	1.80	0.46
1:D:472:ASP:O	1:D:476:LYS:HG2	2.15	0.46
1:D:289:GLU:OE2	1:D:299:ARG:NH1	2.41	0.46
1:A:216:PHE:O	1:A:219:THR:OG1	2.27	0.46
4:B:708:PCW:H152	4:B:710:PCW:H31	1.98	0.46
1:C:175:PRO:HG2	1:C:210:VAL:HG11	1.98	0.46
1:C:594:MET:H	1:C:594:MET:CE	2.30	0.45
1:C:411:GLN:NE2	1:C:415:ASP:OD1	2.48	0.45
1:D:482:ASP:OD1	1:D:482:ASP:N	2.47	0.45
4:C:701:PCW:H422	4:C:707:PCW:H482	1.98	0.45
3:C:703:CLR:H72	4:C:705:PCW:H332	1.97	0.45
1:A:482:ASP:OD1	1:A:482:ASP:N	2.48	0.45
1:B:594:MET:H	1:B:594:MET:CE	2.29	0.45
1:C:482:ASP:OD1	1:C:482:ASP:N	2.49	0.45
1:B:216:PHE:O	1:B:219:THR:OG1	2.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:PRO:HG2	1:D:210:VAL:HG11	1.99	0.45
1:A:176:VAL:HG12	1:A:281:MET:HE2	1.97	0.45
1:D:411:GLN:NE2	1:D:415:ASP:OD1	2.49	0.45
1:B:175:PRO:HG2	1:B:210:VAL:HG11	1.99	0.45
1:D:548:SER:HB3	2:D:703:PCG:O1A	2.16	0.45
1:B:550:LEU:HD11	1:B:595:LEU:HD12	1.99	0.45
1:C:550:LEU:HD11	1:C:595:LEU:HD12	1.98	0.44
1:D:583:GLU:O	1:D:586:THR:OG1	2.34	0.44
1:A:175:PRO:HG2	1:A:210:VAL:HG11	1.98	0.44
1:D:176:VAL:HG12	1:D:281:MET:HE2	1.97	0.44
1:D:478:ARG:HA	1:D:481:ALA:HB3	1.99	0.44
1:A:549:ILE:HG23	1:A:550:LEU:HG	1.99	0.44
1:B:548:SER:HB3	2:B:702:PCG:O1A	2.18	0.44
1:D:216:PHE:O	1:D:219:THR:OG1	2.27	0.44
1:A:548:SER:HB3	2:A:701:PCG:O1A	2.18	0.44
1:A:491:LEU:HD22	1:A:576:LEU:HD21	1.98	0.44
1:A:493:LEU:H	1:A:493:LEU:HD12	1.82	0.44
1:B:176:VAL:HG12	1:B:281:MET:HE2	2.00	0.44
4:C:707:PCW:H121	4:C:707:PCW:H32	1.75	0.44
1:A:175:PRO:HG3	4:A:703:PCW:H262	1.98	0.44
1:C:548:SER:HB3	2:C:702:PCG:O1A	2.18	0.44
1:B:473:THR:O	1:B:477:VAL:HG13	2.18	0.44
1:B:485:ALA:H	1:B:488:LEU:HD13	1.82	0.44
1:B:570:TYR:O	1:C:227:GLY:HA3	2.18	0.44
4:B:706:PCW:H171	4:B:706:PCW:H20	1.81	0.43
1:A:477:VAL:O	1:A:481:ALA:N	2.51	0.43
1:C:570:TYR:O	1:D:227:GLY:HA3	2.19	0.43
1:D:477:VAL:O	1:D:481:ALA:N	2.51	0.43
1:B:600:LYS:HA	1:B:600:LYS:HD2	1.92	0.43
1:B:305:MET:O	1:B:309:ILE:HG12	2.19	0.43
1:A:570:TYR:O	1:B:227:GLY:HA3	2.19	0.43
1:C:592:LYS:HD2	1:C:592:LYS:O	2.19	0.43
1:A:227:GLY:HA3	1:D:570:TYR:O	2.19	0.42
1:D:300:ILE:HD13	1:D:300:ILE:HA	1.92	0.42
1:D:220:ARG:HA	1:D:220:ARG:HD3	1.82	0.42
1:A:305:MET:O	1:A:309:ILE:HG12	2.19	0.42
1:B:491:LEU:HD22	1:B:576:LEU:HD21	2.01	0.42
1:D:594:MET:SD	1:D:594:MET:N	2.92	0.42
1:D:349:TYR:CZ	4:D:701:PCW:H371	2.54	0.42
1:D:552:ILE:HB	1:D:555:SER:HB3	2.01	0.42
1:A:181:THR:HG22	1:A:309:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ARG:H	1:B:561:ARG:HG2	1.69	0.42
1:C:220:ARG:HD3	1:C:220:ARG:HA	1.82	0.42
1:D:582:MET:HE2	1:D:582:MET:HA	2.02	0.42
1:A:300:ILE:HD13	1:A:300:ILE:HA	1.90	0.42
4:A:707:PCW:H331	4:D:701:PCW:H151	2.00	0.42
1:D:305:MET:O	1:D:309:ILE:HG12	2.19	0.42
1:B:592:LYS:HB3	1:B:592:LYS:HE3	1.78	0.42
4:D:701:PCW:H32	4:D:701:PCW:H122	1.70	0.42
1:A:600:LYS:HA	1:A:600:LYS:HD2	1.93	0.41
1:B:601:GLN:C	1:B:601:GLN:OE1	2.63	0.41
1:C:305:MET:O	1:C:309:ILE:HG12	2.19	0.41
1:A:471:LEU:HD12	1:A:471:LEU:HA	1.81	0.41
1:A:601:GLN:C	1:A:601:GLN:OE1	2.63	0.41
1:D:181:THR:HG22	1:D:309:ILE:HD12	2.01	0.41
1:D:601:GLN:C	1:D:601:GLN:OE1	2.63	0.41
1:D:174:LEU:HB2	1:D:175:PRO:HD3	2.03	0.41
1:D:471:LEU:HD12	1:D:471:LEU:HA	1.81	0.41
1:A:506:ILE:HD13	1:A:524:LEU:HD13	2.03	0.41
4:A:703:PCW:H483	4:A:703:PCW:H20	2.02	0.41
1:B:485:ALA:HA	1:B:488:LEU:HB2	2.01	0.41
1:B:506:ILE:HD13	1:B:524:LEU:HD13	2.02	0.41
1:C:181:THR:HG22	1:C:309:ILE:HD12	2.01	0.41
1:D:491:LEU:HD22	1:D:576:LEU:HD21	2.02	0.41
1:C:601:GLN:OE1	1:C:601:GLN:C	2.63	0.41
1:D:590:ASP:O	1:D:594:MET:HE1	2.21	0.41
1:A:525:ALA:HB1	1:A:534:GLN:HG2	2.03	0.41
1:A:174:LEU:HB2	1:A:175:PRO:HD3	2.03	0.41
1:A:178:TYR:HB2	4:A:703:PCW:H221	2.03	0.41
4:A:709:PCW:H331	1:D:403:MET:HE1	2.01	0.41
1:B:437:TRP:HH2	1:B:499:VAL:HB	1.86	0.41
1:B:488:LEU:O	1:B:492:VAL:HG23	2.21	0.41
1:C:387:LEU:HD12	4:C:701:PCW:H232	2.03	0.41
1:C:467:ILE:HG13	1:C:492:VAL:HG11	2.02	0.41
1:C:590:ASP:O	1:C:594:MET:HE1	2.21	0.41
1:D:561:ARG:H	1:D:561:ARG:HG2	1.69	0.41
1:C:587:GLU:C	1:C:588:TYR:HD1	2.29	0.41
1:A:592:LYS:HA	1:A:595:LEU:HD12	2.02	0.40
1:C:174:LEU:HB2	1:C:175:PRO:HD3	2.03	0.40
4:D:709:PCW:H19	4:D:709:PCW:H40	2.03	0.40
1:A:587:GLU:C	1:A:588:TYR:HD1	2.28	0.40
1:C:347:ARG:HA	1:C:350:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:ARG:HA	1:C:481:ALA:HB3	2.03	0.40
4:C:706:PCW:H441	4:C:706:PCW:H211	2.02	0.40
1:D:506:ILE:HD13	1:D:524:LEU:HD13	2.03	0.40
4:B:708:PCW:H141	4:B:708:PCW:H322	2.04	0.40
1:C:506:ILE:HD13	1:C:524:LEU:HD13	2.02	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	447/559 (80%)	435 (97%)	12 (3%)	0	100	100
1	B	447/559 (80%)	436 (98%)	11 (2%)	0	100	100
1	C	447/559 (80%)	437 (98%)	10 (2%)	0	100	100
1	D	447/559 (80%)	436 (98%)	11 (2%)	0	100	100
All	All	1788/2236 (80%)	1744 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/501 (81%)	400 (99%)	5 (1%)	63	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	405/501 (81%)	401 (99%)	4 (1%)	68	84
1	C	405/501 (81%)	402 (99%)	3 (1%)	76	88
1	D	405/501 (81%)	402 (99%)	3 (1%)	76	88
All	All	1620/2004 (81%)	1605 (99%)	15 (1%)	68	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	VAL
1	A	411	GLN
1	A	417	ILE
1	A	474	LEU
1	A	603	LEU
1	B	234	LEU
1	B	333	VAL
1	B	411	GLN
1	B	603	LEU
1	C	333	VAL
1	C	579	ASP
1	C	603	LEU
1	D	333	VAL
1	D	474	LEU
1	D	603	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	ASN
1	A	534	GLN
1	B	444	ASN
1	C	444	ASN
1	D	444	ASN

5.3.3 RNA ⓘ

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 42 ligands modelled in this entry, 6 are monoatomic - leaving 36 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$
4	PCW	C	704	-	41,41,53	0.54	0	47,49,61	0.50	0
3	CLR	C	703	-	31,31,31	0.37	0	48,48,48	0.57	0
4	PCW	D	707	-	34,34,53	0.60	0	40,42,61	0.53	0
4	PCW	B	704	-	42,42,53	0.54	0	48,50,61	0.51	0
4	PCW	A	709	-	44,44,53	0.55	1 (2%)	47,49,61	0.50	0
4	PCW	C	708	-	33,33,53	0.61	0	36,38,61	0.49	0
4	PCW	B	710	-	33,33,53	0.60	0	36,38,61	0.53	0
4	PCW	B	708	-	47,47,53	0.62	1 (2%)	50,52,61	0.79	2 (4%)
4	PCW	A	707	-	38,38,53	0.56	0	44,46,61	0.52	0
4	PCW	B	709	-	36,36,53	0.58	0	42,44,61	0.55	0
4	PCW	C	707	-	37,37,53	0.41	0	39,39,61	0.42	0
4	PCW	A	706	-	37,37,53	0.41	0	39,39,61	0.42	0
4	PCW	A	705	-	24,24,53	0.66	0	27,29,61	0.79	2 (7%)
4	PCW	B	707	-	36,36,53	0.58	0	42,44,61	0.54	0
4	PCW	A	703	-	47,47,53	0.62	1 (2%)	50,52,61	0.77	2 (4%)
4	PCW	D	708	-	37,37,53	0.41	0	39,39,61	0.43	0
4	PCW	A	708	-	33,33,53	0.61	0	36,38,61	0.54	0
4	PCW	B	705	-	24,24,53	0.66	0	27,29,61	0.79	2 (7%)
3	CLR	D	704	-	31,31,31	0.38	0	48,48,48	0.59	0
4	PCW	C	701	-	43,43,53	0.56	1 (2%)	46,48,61	0.52	0
4	PCW	D	706	-	24,24,53	0.66	0	27,29,61	0.78	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PCW	B	701	-	43,43,53	0.55	1 (2%)	46,48,61	0.53	0
2	PCG	B	702	-	26,26,26	6.31	20 (76%)	39,41,41	2.14	14 (35%)
4	PCW	D	709	-	47,47,53	0.61	1 (2%)	50,52,61	0.81	2 (4%)
2	PCG	A	701	-	26,26,26	6.32	20 (76%)	39,41,41	2.15	14 (35%)
4	PCW	D	702	-	42,42,53	0.57	1 (2%)	45,47,61	0.53	0
4	PCW	D	705	-	43,43,53	0.53	0	49,51,61	0.50	0
4	PCW	C	706	-	47,47,53	0.62	1 (2%)	50,52,61	0.78	2 (4%)
2	PCG	C	702	-	26,26,26	6.32	20 (76%)	39,41,41	2.15	14 (35%)
3	CLR	A	702	-	31,31,31	0.38	0	48,48,48	0.57	0
4	PCW	D	701	-	33,33,53	0.61	0	36,38,61	0.53	0
4	PCW	A	704	-	42,42,53	0.54	0	48,50,61	0.50	0
4	PCW	B	706	-	37,37,53	0.40	0	39,39,61	0.42	0
4	PCW	C	705	-	25,25,53	0.68	0	28,30,61	0.59	0
2	PCG	D	703	-	26,26,26	6.33	20 (76%)	39,41,41	2.15	14 (35%)
3	CLR	B	703	-	31,31,31	0.38	0	48,48,48	0.57	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
4	PCW	C	704	-	-	15/45/45/57	-
3	CLR	C	703	-	-	0/10/68/68	0/4/4/4
4	PCW	D	707	-	-	10/38/38/57	-
4	PCW	B	704	-	-	12/46/46/57	-
4	PCW	A	709	-	-	12/48/48/57	-
4	PCW	C	708	-	-	11/37/37/57	-
4	PCW	B	710	-	-	11/37/37/57	-
4	PCW	B	708	-	-	10/49/49/57	-
4	PCW	A	707	-	-	12/42/42/57	-
4	PCW	B	709	-	-	14/40/40/57	-
4	PCW	C	707	-	-	9/39/39/57	-
4	PCW	A	706	-	-	6/39/39/57	-
4	PCW	A	705	-	-	7/28/28/57	-
4	PCW	B	707	-	-	9/40/40/57	-
4	PCW	A	703	-	-	15/49/49/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	D	708	-	-	8/39/39/57	-
4	PCW	A	708	-	-	15/37/37/57	-
4	PCW	B	705	-	-	7/28/28/57	-
3	CLR	D	704	-	-	0/10/68/68	0/4/4/4
4	PCW	C	701	-	-	18/47/47/57	-
4	PCW	D	706	-	-	7/28/28/57	-
4	PCW	B	701	-	-	11/47/47/57	-
2	PCG	B	702	-	-	0/4/31/31	0/4/4/4
4	PCW	D	709	-	-	17/49/49/57	-
2	PCG	A	701	-	-	0/4/31/31	0/4/4/4
4	PCW	D	702	-	-	8/46/46/57	-
4	PCW	D	705	-	-	10/47/47/57	-
4	PCW	C	706	-	-	14/49/49/57	-
2	PCG	C	702	-	-	0/4/31/31	0/4/4/4
3	CLR	A	702	-	-	0/10/68/68	0/4/4/4
4	PCW	D	701	-	-	13/37/37/57	-
4	PCW	A	704	-	-	16/46/46/57	-
4	PCW	B	706	-	-	12/39/39/57	-
4	PCW	C	705	-	-	6/29/29/57	-
2	PCG	D	703	-	-	0/4/31/31	0/4/4/4
3	CLR	B	703	-	-	0/10/68/68	0/4/4/4

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	PCG	C2'-C3'	-15.12	1.19	1.53
2	C	702	PCG	C2'-C3'	-15.11	1.19	1.53
2	A	701	PCG	C2'-C3'	-15.09	1.20	1.53
2	B	702	PCG	C2'-C3'	-15.07	1.20	1.53
2	A	701	PCG	PA-O5'	14.06	1.73	1.57
2	D	703	PCG	PA-O5'	13.99	1.73	1.57
2	C	702	PCG	PA-O5'	13.96	1.73	1.57
2	B	702	PCG	PA-O5'	13.95	1.73	1.57
2	D	703	PCG	C3'-C4'	11.17	1.81	1.52
2	A	701	PCG	C3'-C4'	11.14	1.81	1.52
2	B	702	PCG	C3'-C4'	11.14	1.81	1.52
2	C	702	PCG	C3'-C4'	11.13	1.81	1.52
2	D	703	PCG	C1'-N9	-8.84	1.22	1.47
2	C	702	PCG	C1'-N9	-8.83	1.22	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PCG	C1'-N9	-8.81	1.22	1.47
2	B	702	PCG	C1'-N9	-8.78	1.22	1.47
2	A	701	PCG	O4'-C4'	-8.41	1.26	1.45
2	C	702	PCG	O4'-C4'	-8.41	1.26	1.45
2	D	703	PCG	O4'-C4'	-8.40	1.26	1.45
2	B	702	PCG	O4'-C4'	-8.39	1.26	1.45
2	D	703	PCG	O4'-C1'	7.63	1.59	1.42
2	C	702	PCG	O4'-C1'	7.61	1.59	1.42
2	A	701	PCG	O4'-C1'	7.60	1.59	1.42
2	B	702	PCG	O4'-C1'	7.59	1.59	1.42
2	C	702	PCG	PA-O3'	7.06	1.69	1.57
2	D	703	PCG	PA-O3'	7.04	1.69	1.57
2	B	702	PCG	PA-O3'	7.01	1.69	1.57
2	A	701	PCG	PA-O3'	6.99	1.69	1.57
2	B	702	PCG	O5'-C5'	6.81	1.56	1.46
2	A	701	PCG	O5'-C5'	6.80	1.56	1.46
2	C	702	PCG	O5'-C5'	6.77	1.55	1.46
2	D	703	PCG	O5'-C5'	6.77	1.55	1.46
2	C	702	PCG	C4-N3	6.72	1.49	1.34
2	A	701	PCG	C4-N3	6.70	1.49	1.34
2	D	703	PCG	C4-N3	6.69	1.49	1.34
2	B	702	PCG	C4-N3	6.68	1.49	1.34
2	D	703	PCG	C2-N3	5.56	1.46	1.33
2	B	702	PCG	C2'-C1'	5.55	1.70	1.53
2	C	702	PCG	C2'-C1'	5.55	1.70	1.53
2	D	703	PCG	C2'-C1'	5.54	1.70	1.53
2	B	702	PCG	C2-N3	5.54	1.46	1.33
2	A	701	PCG	C2'-C1'	5.53	1.70	1.53
2	A	701	PCG	C2-N3	5.53	1.46	1.33
2	C	702	PCG	C2-N3	5.50	1.46	1.33
2	C	702	PCG	C2-N2	4.87	1.45	1.34
2	A	701	PCG	C2-N2	4.86	1.45	1.34
2	B	702	PCG	C2-N2	4.85	1.45	1.34
2	D	703	PCG	C2-N2	4.83	1.45	1.34
4	B	708	PCW	P-O4P	2.92	1.65	1.54
4	C	706	PCW	P-O4P	2.92	1.65	1.54
4	A	703	PCW	P-O4P	2.91	1.65	1.54
4	D	709	PCW	P-O4P	2.90	1.65	1.54
2	A	701	PCG	C5-N7	-2.85	1.33	1.39
2	D	703	PCG	C5-N7	-2.85	1.33	1.39
2	B	702	PCG	C2-N1	2.82	1.44	1.37
2	C	702	PCG	C5-N7	-2.81	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	PCG	C5-N7	-2.81	1.33	1.39
2	C	702	PCG	C2-N1	2.80	1.44	1.37
2	D	703	PCG	C2-N1	2.79	1.44	1.37
2	A	701	PCG	C2-N1	2.76	1.44	1.37
2	B	702	PCG	C5-C6	2.50	1.53	1.44
2	C	702	PCG	C5-C6	2.50	1.53	1.44
2	D	703	PCG	C6-N1	2.50	1.43	1.38
2	D	703	PCG	C5-C6	2.50	1.53	1.44
2	A	701	PCG	C5-C6	2.49	1.53	1.44
2	B	702	PCG	C6-N1	2.47	1.43	1.38
2	B	702	PCG	O6-C6	-2.47	1.18	1.23
2	C	702	PCG	C6-N1	2.46	1.43	1.38
2	A	701	PCG	O2'-C2'	2.46	1.49	1.43
2	A	701	PCG	C6-N1	2.45	1.43	1.38
2	D	703	PCG	O2'-C2'	2.44	1.49	1.43
2	C	702	PCG	O2'-C2'	2.44	1.49	1.43
2	C	702	PCG	O6-C6	-2.44	1.18	1.23
2	D	703	PCG	O6-C6	-2.44	1.18	1.23
2	B	702	PCG	O2'-C2'	2.42	1.49	1.43
2	A	701	PCG	O6-C6	-2.41	1.19	1.23
2	C	702	PCG	C5'-C4'	2.35	1.55	1.51
2	D	703	PCG	C5'-C4'	2.34	1.55	1.51
2	B	702	PCG	C5'-C4'	2.33	1.55	1.51
2	A	701	PCG	C5'-C4'	2.31	1.55	1.51
2	D	703	PCG	PA-O1A	2.10	1.65	1.55
2	A	701	PCG	PA-O1A	2.10	1.65	1.55
2	C	702	PCG	PA-O1A	2.10	1.65	1.55
2	B	702	PCG	PA-O1A	2.09	1.65	1.55
4	C	701	PCW	P-O4P	2.08	1.65	1.58
4	D	702	PCW	P-O4P	2.07	1.65	1.58
4	B	701	PCW	P-O4P	2.07	1.65	1.58
4	A	709	PCW	P-O4P	2.06	1.65	1.58

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	PCG	C5-C4-N3	-5.20	120.11	128.39
2	C	702	PCG	C5-C4-N3	-5.19	120.13	128.39
2	B	702	PCG	C5-C4-N3	-5.18	120.14	128.39
2	A	701	PCG	C5-C4-N3	-5.18	120.14	128.39
2	A	701	PCG	O5'-PA-O3'	5.14	112.58	105.70
2	C	702	PCG	O5'-PA-O3'	5.12	112.56	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	PCG	O5'-PA-O3'	5.08	112.50	105.70
2	D	703	PCG	O5'-PA-O3'	5.03	112.44	105.70
2	D	703	PCG	C2-N3-C4	4.55	120.13	112.30
2	B	702	PCG	C2-N3-C4	4.54	120.12	112.30
2	A	701	PCG	C2-N3-C4	4.53	120.10	112.30
2	C	702	PCG	C2-N3-C4	4.52	120.09	112.30
4	D	709	PCW	O4P-P-O3P	-3.80	96.77	106.67
4	B	708	PCW	O4P-P-O3P	-3.80	96.77	106.67
4	C	706	PCW	O4P-P-O3P	-3.74	96.91	106.67
4	A	703	PCW	O4P-P-O3P	-3.66	97.13	106.67
2	D	703	PCG	C4'-O4'-C1'	-3.28	102.22	109.47
2	A	701	PCG	C4'-O4'-C1'	-3.26	102.28	109.47
2	B	702	PCG	C4'-O4'-C1'	-3.25	102.29	109.47
2	B	702	PCG	N9-C4-N3	3.24	132.44	125.95
2	D	703	PCG	N9-C4-N3	3.24	132.42	125.95
2	C	702	PCG	C4'-O4'-C1'	-3.23	102.33	109.47
2	C	702	PCG	N9-C4-N3	3.22	132.39	125.95
2	A	701	PCG	N9-C4-N3	3.21	132.37	125.95
2	A	701	PCG	N9-C8-N7	-3.11	107.64	113.40
2	C	702	PCG	N9-C8-N7	-3.10	107.65	113.40
2	B	702	PCG	N9-C8-N7	-3.09	107.67	113.40
2	D	703	PCG	N9-C8-N7	-3.07	107.71	113.40
2	C	702	PCG	C2-N1-C6	-3.01	119.65	125.11
2	B	702	PCG	C2-N1-C6	-3.01	119.65	125.11
2	D	703	PCG	C2-N1-C6	-3.00	119.67	125.11
2	A	701	PCG	C2-N1-C6	-2.99	119.69	125.11
2	D	703	PCG	O3'-C3'-C2'	2.76	118.31	115.61
2	A	701	PCG	O3'-C3'-C2'	2.72	118.28	115.61
2	C	702	PCG	O3'-C3'-C2'	2.71	118.26	115.61
2	A	701	PCG	C3'-C2'-C1'	2.66	105.75	99.89
2	B	702	PCG	O3'-C3'-C2'	2.66	118.22	115.61
2	C	702	PCG	C3'-C2'-C1'	2.65	105.71	99.89
2	B	702	PCG	C5-C6-N1	2.65	119.99	113.25
2	A	701	PCG	C5-C6-N1	2.64	119.98	113.25
2	D	703	PCG	C5-C6-N1	2.64	119.98	113.25
2	D	703	PCG	C3'-C2'-C1'	2.64	105.70	99.89
2	C	702	PCG	C5-C6-N1	2.64	119.97	113.25
2	B	702	PCG	C3'-C2'-C1'	2.62	105.65	99.89
2	A	701	PCG	O6-C6-C5	-2.48	119.98	126.53
2	C	702	PCG	O6-C6-C5	-2.46	120.05	126.53
2	D	703	PCG	O6-C6-C5	-2.46	120.05	126.53
2	B	702	PCG	O6-C6-C5	-2.45	120.08	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	709	PCW	O1P-P-O2P	2.42	120.27	110.83
4	B	708	PCW	O1P-P-O2P	2.42	120.26	110.83
2	A	701	PCG	O4'-C4'-C5'	2.36	119.52	112.38
4	C	706	PCW	O1P-P-O2P	2.35	119.99	110.83
4	A	703	PCW	O1P-P-O2P	2.35	119.97	110.83
2	C	702	PCG	O4'-C4'-C5'	2.34	119.47	112.38
2	B	702	PCG	O4'-C4'-C5'	2.34	119.46	112.38
2	D	703	PCG	O4'-C4'-C5'	2.34	119.46	112.38
4	A	705	PCW	C3-C2-C1	2.26	117.06	111.78
4	D	706	PCW	C3-C2-C1	2.23	117.00	111.78
4	B	705	PCW	C3-C2-C1	2.23	116.97	111.78
2	A	701	PCG	C8-N7-C5	2.21	108.19	104.26
2	D	703	PCG	C8-N7-C5	2.18	108.15	104.26
2	C	702	PCG	C8-N7-C5	2.18	108.14	104.26
2	D	703	PCG	O5'-C5'-C4'	2.17	110.76	105.71
2	B	702	PCG	C8-N7-C5	2.17	108.12	104.26
2	C	702	PCG	O5'-C5'-C4'	2.16	110.74	105.71
2	A	701	PCG	O5'-C5'-C4'	2.16	110.74	105.71
2	B	702	PCG	O5'-C5'-C4'	2.16	110.74	105.71
4	A	705	PCW	C2-O2-C31	2.07	122.76	117.80
4	B	705	PCW	C2-O2-C31	2.06	122.72	117.80

There are no chirality outliers.

All (315) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	PCW	C1-O3P-P-O1P
4	A	703	PCW	C1-O3P-P-O4P
4	A	704	PCW	C1-O3P-P-O1P
4	A	704	PCW	C1-O3P-P-O2P
4	A	704	PCW	C1-O3P-P-O4P
4	A	706	PCW	O3P-C1-C2-C3
4	A	706	PCW	O3P-C1-C2-O2
4	A	707	PCW	C1-O3P-P-O1P
4	A	707	PCW	C1-O3P-P-O4P
4	A	708	PCW	C1-O3P-P-O1P
4	A	708	PCW	C4-O4P-P-O3P
4	A	709	PCW	C1-O3P-P-O1P
4	A	709	PCW	C1-O3P-P-O2P
4	A	709	PCW	C1-O3P-P-O4P
4	B	701	PCW	C1-O3P-P-O1P
4	B	701	PCW	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	704	PCW	C1-O3P-P-O1P
4	B	704	PCW	C1-O3P-P-O2P
4	B	704	PCW	C1-O3P-P-O4P
4	B	706	PCW	O3P-C1-C2-C3
4	B	706	PCW	O3P-C1-C2-O2
4	B	706	PCW	C32-C31-O2-C2
4	B	707	PCW	C1-O3P-P-O1P
4	B	707	PCW	C1-O3P-P-O4P
4	B	709	PCW	O4P-C4-C5-N
4	B	709	PCW	C32-C31-O2-C2
4	B	709	PCW	C1-O3P-P-O1P
4	B	709	PCW	C1-O3P-P-O2P
4	B	709	PCW	C1-O3P-P-O4P
4	B	710	PCW	C32-C31-O2-C2
4	B	710	PCW	C1-O3P-P-O1P
4	B	710	PCW	C1-O3P-P-O2P
4	C	701	PCW	C1-O3P-P-O1P
4	C	701	PCW	C1-O3P-P-O4P
4	C	704	PCW	C32-C31-O2-C2
4	C	705	PCW	C1-O3P-P-O1P
4	C	705	PCW	C1-O3P-P-O2P
4	C	705	PCW	C1-O3P-P-O4P
4	C	706	PCW	C2-C1-O3P-P
4	C	706	PCW	C12-C11-O3-C3
4	C	706	PCW	C1-O3P-P-O1P
4	C	706	PCW	C1-O3P-P-O2P
4	C	706	PCW	C1-O3P-P-O4P
4	C	707	PCW	O3P-C1-C2-C3
4	C	707	PCW	O3P-C1-C2-O2
4	C	708	PCW	C1-O3P-P-O1P
4	C	708	PCW	C1-O3P-P-O2P
4	C	708	PCW	C1-O3P-P-O4P
4	D	702	PCW	C1-O3P-P-O1P
4	D	702	PCW	C1-O3P-P-O4P
4	D	705	PCW	C1-O3P-P-O1P
4	D	705	PCW	C1-O3P-P-O2P
4	D	705	PCW	C1-O3P-P-O4P
4	D	705	PCW	C4-O4P-P-O2P
4	D	707	PCW	O4P-C4-C5-N
4	D	708	PCW	O3P-C1-C2-C3
4	D	708	PCW	O3P-C1-C2-O2
4	D	709	PCW	C2-C1-O3P-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	709	PCW	C1-O3P-P-O1P
4	D	709	PCW	C1-O3P-P-O4P
4	A	706	PCW	O11-C11-O3-C3
4	C	704	PCW	O11-C11-O3-C3
4	C	706	PCW	O11-C11-O3-C3
4	C	707	PCW	O11-C11-O3-C3
4	D	701	PCW	O11-C11-O3-C3
4	A	706	PCW	C12-C11-O3-C3
4	C	704	PCW	C12-C11-O3-C3
4	C	707	PCW	C12-C11-O3-C3
4	D	701	PCW	C12-C11-O3-C3
4	B	707	PCW	O11-C11-O3-C3
4	A	708	PCW	O31-C31-O2-C2
4	B	706	PCW	O31-C31-O2-C2
4	B	709	PCW	O31-C31-O2-C2
4	B	710	PCW	O31-C31-O2-C2
4	C	704	PCW	O31-C31-O2-C2
4	B	707	PCW	C12-C11-O3-C3
4	D	709	PCW	C12-C11-O3-C3
4	A	708	PCW	C32-C31-O2-C2
4	D	709	PCW	O11-C11-O3-C3
4	D	709	PCW	C32-C31-O2-C2
4	D	709	PCW	O31-C31-O2-C2
4	B	709	PCW	C12-C11-O3-C3
4	D	708	PCW	C31-C32-C33-C34
4	C	704	PCW	C21-C22-C23-C24
4	A	703	PCW	C11-C12-C13-C14
4	A	708	PCW	C31-C32-C33-C34
4	B	701	PCW	C31-C32-C33-C34
4	C	707	PCW	C31-C32-C33-C34
4	B	701	PCW	C11-C12-C13-C14
4	D	708	PCW	C11-C12-C13-C14
4	D	701	PCW	C11-C12-C13-C14
4	B	709	PCW	O11-C11-O3-C3
4	A	709	PCW	C31-C32-C33-C34
4	D	705	PCW	C4-C5-N-C6
4	A	704	PCW	C32-C31-O2-C2
4	A	704	PCW	O31-C31-O2-C2
4	C	706	PCW	C32-C31-O2-C2
4	A	703	PCW	C32-C33-C34-C35
4	A	707	PCW	C33-C34-C35-C36
4	B	709	PCW	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	705	PCW	C31-C32-C33-C34
4	D	709	PCW	C31-C32-C33-C34
4	B	706	PCW	C15-C16-C17-C18
4	C	704	PCW	C32-C33-C34-C35
4	D	702	PCW	C13-C14-C15-C16
4	B	706	PCW	C1-C2-C3-O3
4	B	710	PCW	C13-C14-C15-C16
4	A	707	PCW	C32-C31-O2-C2
4	A	706	PCW	C16-C17-C18-C19
4	D	707	PCW	C31-C32-C33-C34
4	A	706	PCW	C41-C42-C43-C44
4	B	701	PCW	C14-C15-C16-C17
4	C	706	PCW	O31-C31-O2-C2
4	D	702	PCW	C31-C32-C33-C34
4	D	708	PCW	C32-C33-C34-C35
4	C	701	PCW	C12-C13-C14-C15
4	B	708	PCW	C32-C33-C34-C35
4	C	708	PCW	C34-C35-C36-C37
4	C	701	PCW	C32-C31-O2-C2
4	D	707	PCW	C32-C31-O2-C2
4	D	707	PCW	O31-C31-O2-C2
4	A	704	PCW	C20-C21-C22-C23
4	C	708	PCW	C36-C37-C38-C39
4	D	702	PCW	C40-C41-C42-C43
4	C	704	PCW	C15-C16-C17-C18
4	D	705	PCW	C4-C5-N-C7
4	C	708	PCW	C31-C32-C33-C34
4	B	704	PCW	O3P-C1-C2-O2
4	A	708	PCW	C12-C13-C14-C15
4	A	709	PCW	C13-C14-C15-C16
4	A	703	PCW	C12-C13-C14-C15
4	B	701	PCW	C2-C1-O3P-P
4	A	707	PCW	O31-C31-O2-C2
4	D	709	PCW	C34-C35-C36-C37
4	D	708	PCW	C33-C34-C35-C36
4	B	706	PCW	C20-C21-C22-C23
4	A	705	PCW	O3P-C1-C2-C3
4	B	705	PCW	O3P-C1-C2-C3
4	B	709	PCW	O3P-C1-C2-C3
4	C	704	PCW	O3P-C1-C2-C3
4	D	705	PCW	O3P-C1-C2-C3
4	D	701	PCW	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	705	PCW	C4-C5-N-C8
4	A	703	PCW	C21-C22-C23-C24
4	C	708	PCW	C11-C12-C13-C14
4	D	701	PCW	C31-C32-C33-C34
4	A	703	PCW	C1-O3P-P-O2P
4	C	707	PCW	C16-C17-C18-C19
4	D	702	PCW	C34-C35-C36-C37
4	B	707	PCW	O3P-C1-C2-O2
4	C	701	PCW	O2-C2-C3-O3
4	B	701	PCW	C15-C16-C17-C18
4	B	708	PCW	C22-C23-C24-C25
4	A	704	PCW	C2-C1-O3P-P
4	C	701	PCW	C2-C1-O3P-P
4	B	708	PCW	C40-C41-C42-C43
4	B	704	PCW	O3P-C1-C2-C3
4	B	710	PCW	O3P-C1-C2-C3
4	C	701	PCW	O3P-C1-C2-C3
4	D	706	PCW	O3P-C1-C2-C3
4	B	704	PCW	C41-C42-C43-C44
4	B	707	PCW	C13-C14-C15-C16
4	A	703	PCW	C20-C21-C22-C23
4	C	701	PCW	O31-C31-O2-C2
4	B	710	PCW	O3P-C1-C2-O2
4	D	705	PCW	O3P-C1-C2-O2
4	C	704	PCW	C14-C15-C16-C17
4	C	701	PCW	C34-C35-C36-C37
4	A	707	PCW	C35-C36-C37-C38
4	B	704	PCW	C35-C36-C37-C38
4	D	709	PCW	C32-C33-C34-C35
4	D	707	PCW	C12-C13-C14-C15
4	B	707	PCW	C36-C37-C38-C39
4	A	703	PCW	O3P-C1-C2-C3
4	D	709	PCW	C45-C46-C47-C48
4	B	708	PCW	C1-O3P-P-O1P
4	A	709	PCW	C14-C15-C16-C17
4	D	706	PCW	C32-C31-O2-C2
4	A	708	PCW	O3P-C1-C2-O2
4	A	704	PCW	C1-C2-C3-O3
4	B	709	PCW	C5-C4-O4P-P
4	C	704	PCW	C5-C4-O4P-P
4	D	707	PCW	C5-C4-O4P-P
4	A	704	PCW	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	706	PCW	O2-C2-C3-O3
4	C	701	PCW	C20-C21-C22-C23
4	A	704	PCW	C13-C14-C15-C16
4	A	704	PCW	C31-C32-C33-C34
4	D	706	PCW	O31-C31-O2-C2
4	D	706	PCW	O3-C11-C12-C13
4	C	707	PCW	C32-C33-C34-C35
4	A	708	PCW	O3P-C1-C2-C3
4	D	708	PCW	C34-C35-C36-C37
4	A	705	PCW	O3-C11-C12-C13
4	C	706	PCW	C14-C15-C16-C17
4	A	703	PCW	O3P-C1-C2-O2
4	A	705	PCW	O3P-C1-C2-O2
4	B	705	PCW	O3P-C1-C2-O2
4	C	701	PCW	O3P-C1-C2-O2
4	C	704	PCW	O3P-C1-C2-O2
4	D	706	PCW	O3P-C1-C2-O2
4	D	709	PCW	O3P-C1-C2-O2
4	B	705	PCW	O3-C11-C12-C13
4	C	701	PCW	C1-C2-C3-O3
4	C	705	PCW	C1-C2-C3-O3
4	C	706	PCW	C44-C45-C46-C47
4	A	707	PCW	C1-O3P-P-O2P
4	A	707	PCW	C4-O4P-P-O2P
4	A	708	PCW	C1-O3P-P-O2P
4	A	708	PCW	C1-O3P-P-O4P
4	A	708	PCW	C4-O4P-P-O2P
4	B	710	PCW	C1-O3P-P-O4P
4	C	701	PCW	C1-O3P-P-O2P
4	D	701	PCW	C1-O3P-P-O1P
4	D	701	PCW	C1-O3P-P-O2P
4	D	701	PCW	C1-O3P-P-O4P
4	D	702	PCW	C1-O3P-P-O2P
4	D	707	PCW	C4-O4P-P-O2P
4	A	703	PCW	C2-C1-O3P-P
4	A	709	PCW	C2-C1-O3P-P
4	B	704	PCW	C2-C1-O3P-P
4	A	709	PCW	C44-C45-C46-C47
4	C	706	PCW	C12-C13-C14-C15
4	A	703	PCW	C15-C16-C17-C18
4	C	708	PCW	C35-C36-C37-C38
4	A	705	PCW	C3-C2-O2-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	706	PCW	C3-C2-O2-C31
4	B	707	PCW	O3P-C1-C2-C3
4	A	703	PCW	C37-C38-C39-C40
4	B	710	PCW	O11-C11-O3-C3
4	B	709	PCW	O3P-C1-C2-O2
4	A	705	PCW	C11-C12-C13-C14
4	B	705	PCW	C11-C12-C13-C14
4	D	706	PCW	C11-C12-C13-C14
4	A	704	PCW	C21-C22-C23-C24
4	B	710	PCW	C12-C11-O3-C3
4	B	706	PCW	C16-C17-C18-C19
4	A	704	PCW	C22-C23-C24-C25
4	C	708	PCW	O3-C11-C12-C13
4	B	708	PCW	C43-C44-C45-C46
4	B	710	PCW	C33-C34-C35-C36
4	C	704	PCW	C4-C5-N-C6
4	A	707	PCW	C34-C35-C36-C37
4	C	701	PCW	C36-C37-C38-C39
4	C	707	PCW	C35-C36-C37-C38
4	B	705	PCW	O31-C31-O2-C2
4	B	704	PCW	C37-C38-C39-C40
4	D	709	PCW	C44-C45-C46-C47
4	B	704	PCW	C34-C35-C36-C37
4	A	709	PCW	C4-O4P-P-O2P
4	B	705	PCW	C3-C2-O2-C31
4	D	706	PCW	C3-C2-O2-C31
4	B	708	PCW	O11-C11-O3-C3
4	B	708	PCW	C12-C11-O3-C3
4	A	704	PCW	O3P-C1-C2-O2
4	D	707	PCW	C11-C12-C13-C14
4	B	706	PCW	O3-C11-C12-C13
4	A	707	PCW	O2-C2-C3-O3
4	C	708	PCW	O2-C2-C3-O3
4	C	704	PCW	C4-C5-N-C8
4	A	709	PCW	O31-C31-O2-C2
4	A	708	PCW	C12-C11-O3-C3
4	D	709	PCW	C12-C13-C14-C15
4	A	708	PCW	O11-C11-O3-C3
4	B	708	PCW	C41-C42-C43-C44
4	C	701	PCW	C32-C33-C34-C35
4	D	705	PCW	C40-C41-C42-C43
4	D	707	PCW	O3-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	705	PCW	C32-C31-O2-C2
4	C	704	PCW	C4-C5-N-C7
4	D	709	PCW	O3P-C1-C2-C3
4	B	704	PCW	C32-C33-C34-C35
4	B	701	PCW	O2-C2-C3-O3
4	B	704	PCW	O3-C11-C12-C13
4	C	704	PCW	C11-C12-C13-C14
4	B	708	PCW	C39-C40-C41-C42
4	A	705	PCW	O31-C31-O2-C2
4	A	708	PCW	C15-C16-C17-C18
4	B	701	PCW	C12-C11-O3-C3
4	B	701	PCW	O11-C11-O3-C3
4	C	707	PCW	C43-C44-C45-C46
4	D	702	PCW	C33-C34-C35-C36
4	A	709	PCW	C17-C18-C19-C20
4	A	704	PCW	O3P-C1-C2-C3
4	C	708	PCW	C32-C33-C34-C35
4	D	709	PCW	C23-C24-C25-C26
4	A	704	PCW	C17-C18-C19-C20
4	B	708	PCW	C19-C20-C21-C22
4	A	709	PCW	C32-C31-O2-C2
4	C	701	PCW	C25-C26-C27-C28
4	B	706	PCW	C17-C18-C19-C20
4	C	705	PCW	O3P-C1-C2-O2
4	A	703	PCW	O2-C31-C32-C33
4	C	701	PCW	O3-C11-C12-C13
4	B	701	PCW	C1-C2-C3-O3
4	C	706	PCW	O2-C31-C32-C33
4	D	701	PCW	O2-C2-C3-O3
4	B	709	PCW	O2-C31-C32-C33
4	A	707	PCW	O11-C11-O3-C3
4	A	708	PCW	C19-C20-C21-C22
4	D	701	PCW	C2-C1-O3P-P
4	A	707	PCW	C12-C11-O3-C3
4	A	705	PCW	C32-C31-O2-C2
4	D	701	PCW	O3-C11-C12-C13
4	D	709	PCW	C35-C36-C37-C38
4	D	708	PCW	O3-C11-C12-C13
4	C	701	PCW	O11-C11-C12-C13
4	D	701	PCW	C1-C2-C3-O3
4	A	703	PCW	O31-C31-C32-C33
4	B	706	PCW	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	707	PCW	C32-C33-C34-C35
4	D	701	PCW	O11-C11-C12-C13
4	B	709	PCW	O31-C31-C32-C33
4	C	706	PCW	O31-C31-C32-C33
4	B	707	PCW	C12-C13-C14-C15

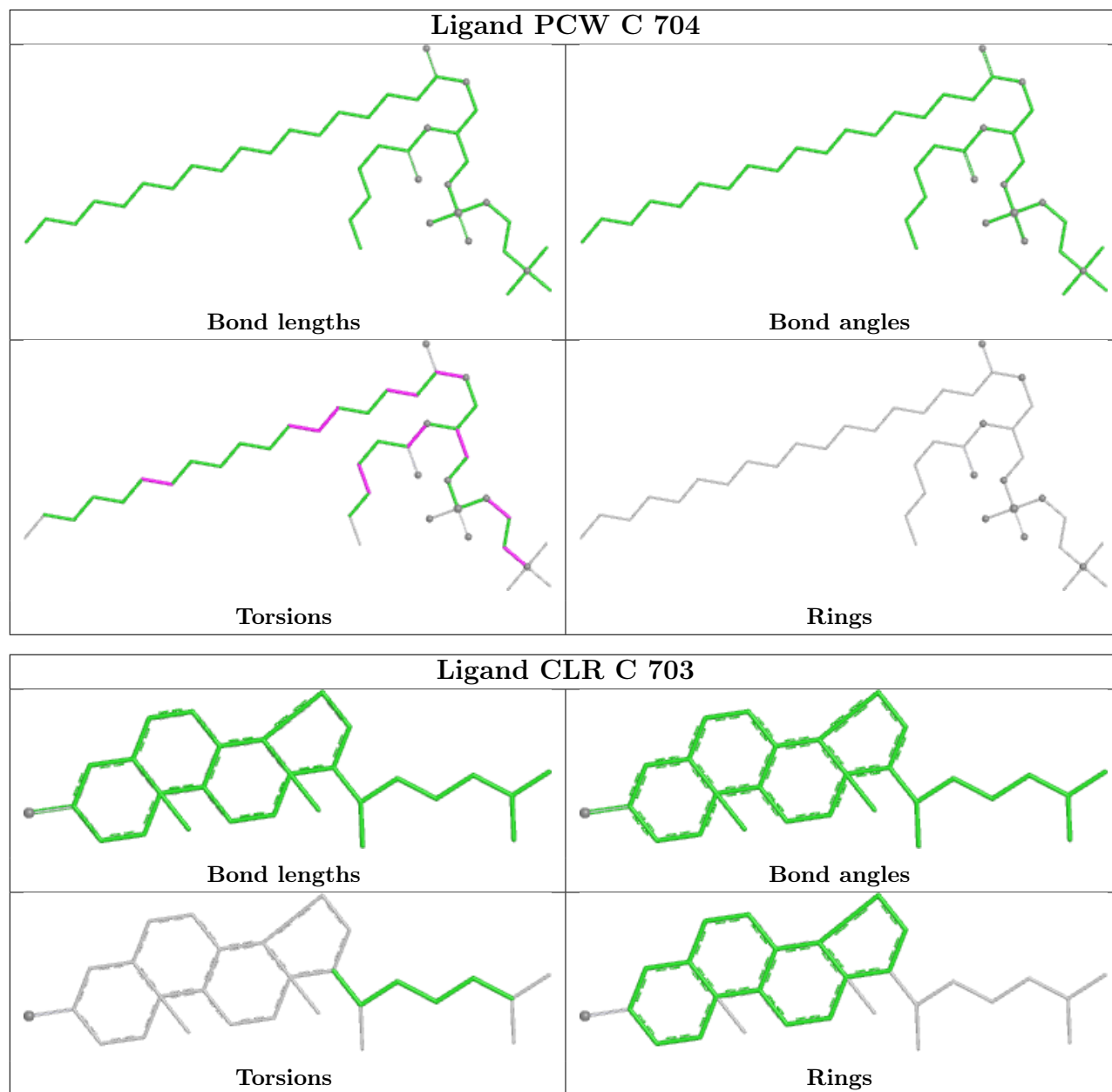
There are no ring outliers.

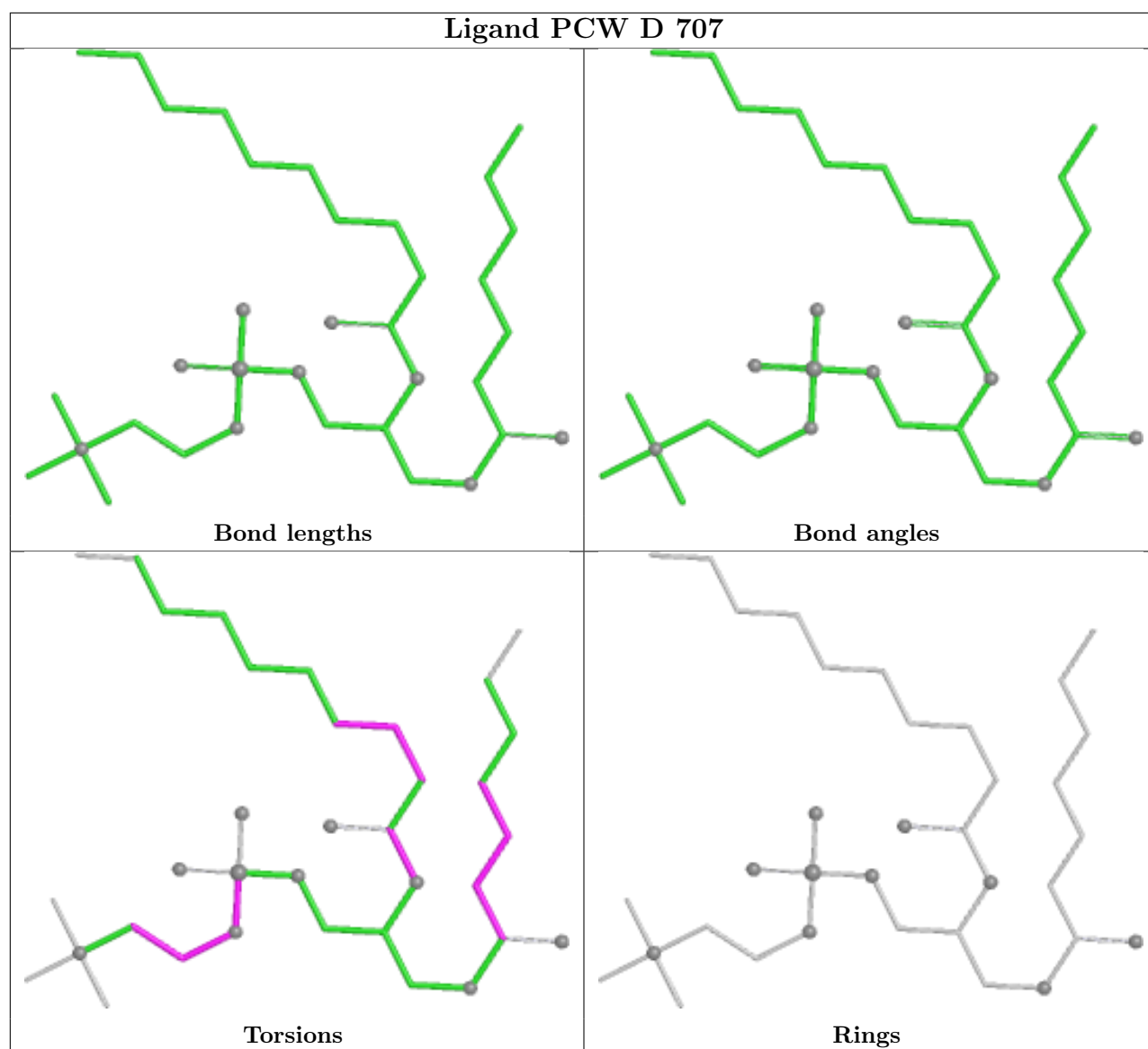
24 monomers are involved in 48 short contacts:

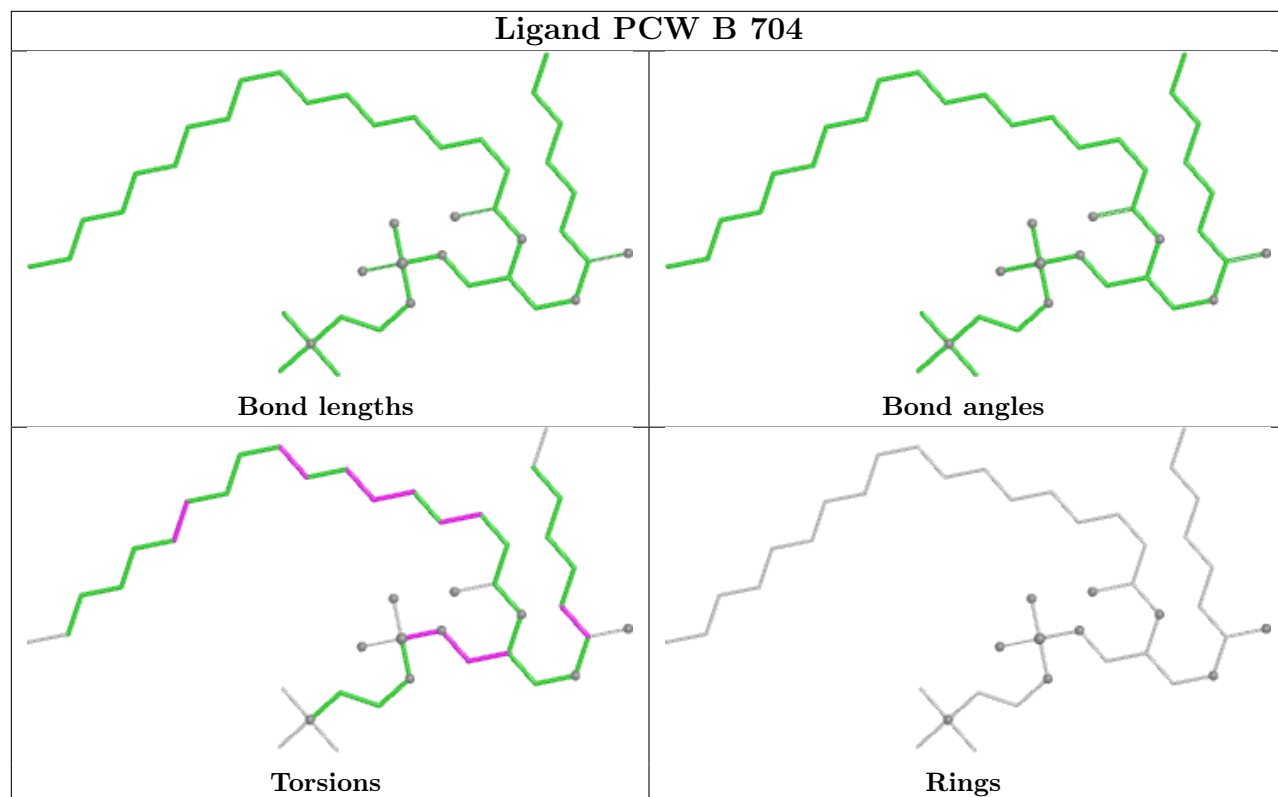
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	CLR	1	0
4	B	704	PCW	4	0
4	A	709	PCW	2	0
4	B	710	PCW	2	0
4	B	708	PCW	4	0
4	A	707	PCW	1	0
4	B	709	PCW	1	0
4	C	707	PCW	2	0
4	B	707	PCW	1	0
4	A	703	PCW	3	0
4	B	705	PCW	1	0
4	C	701	PCW	4	0
4	B	701	PCW	3	0
2	B	702	PCG	4	0
4	D	709	PCW	2	0
2	A	701	PCG	4	0
4	D	705	PCW	2	0
4	C	706	PCW	2	0
2	C	702	PCG	4	0
4	D	701	PCW	3	0
4	A	704	PCW	1	0
4	B	706	PCW	2	0
4	C	705	PCW	1	0
2	D	703	PCG	4	0

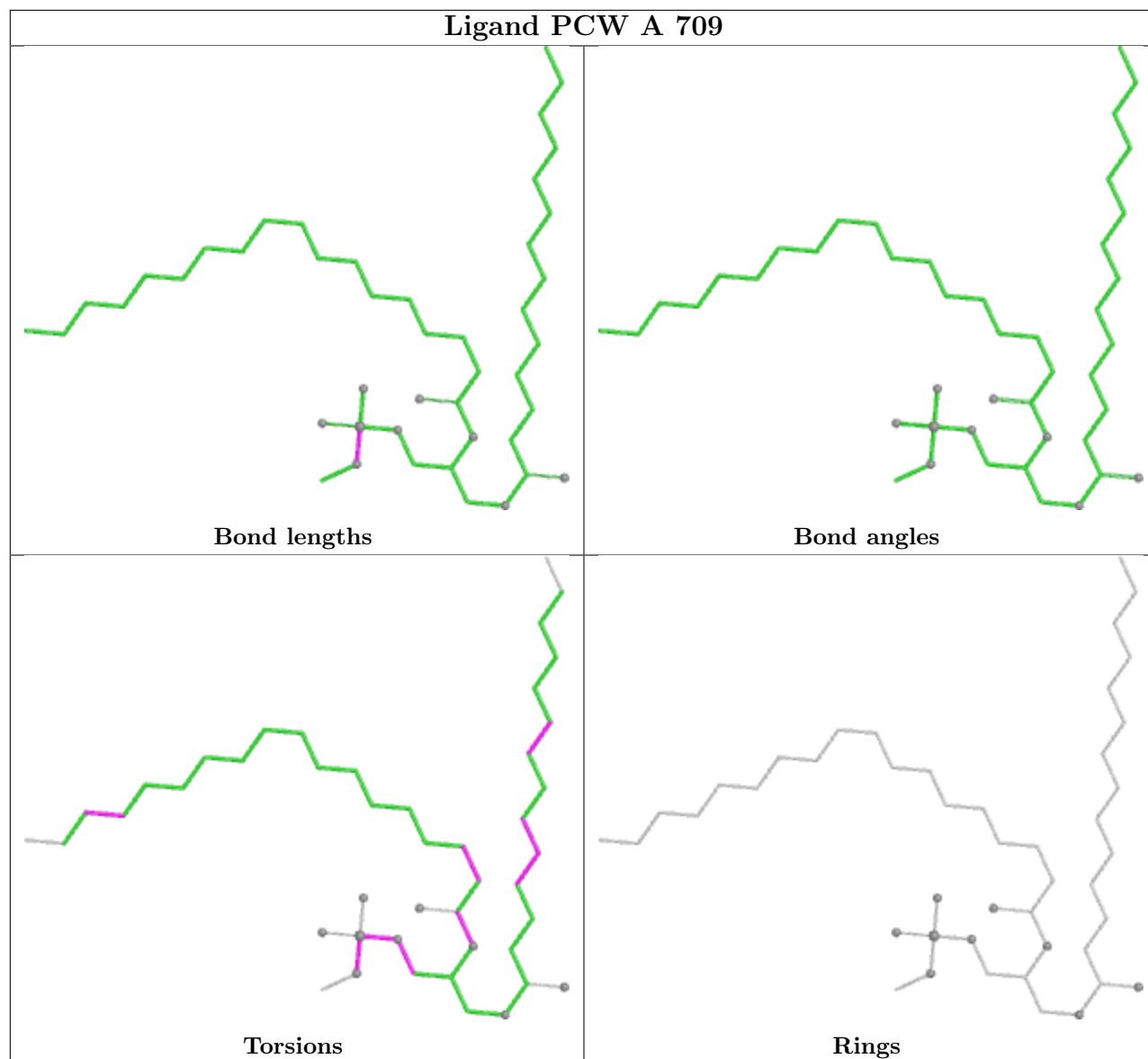
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

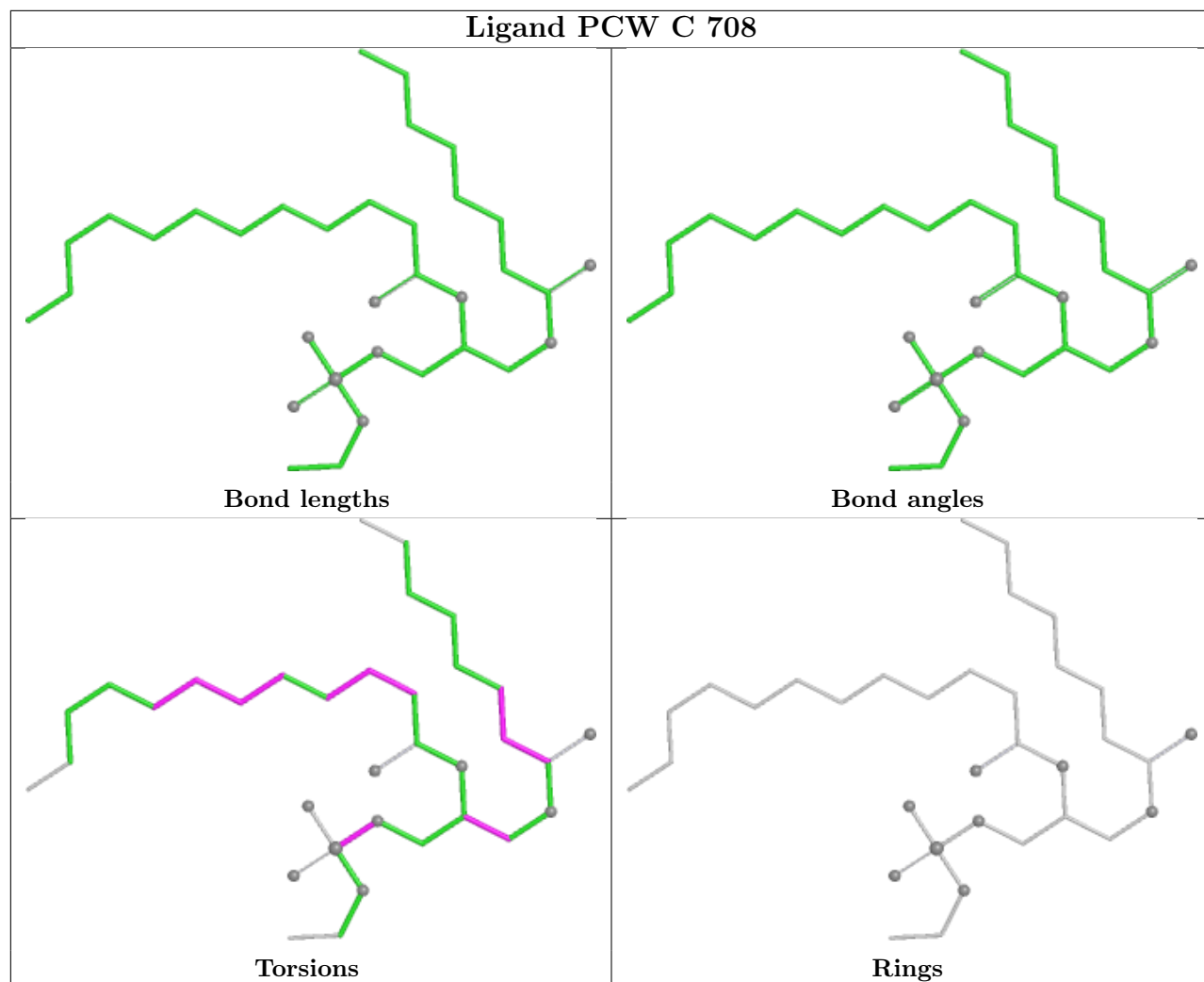
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

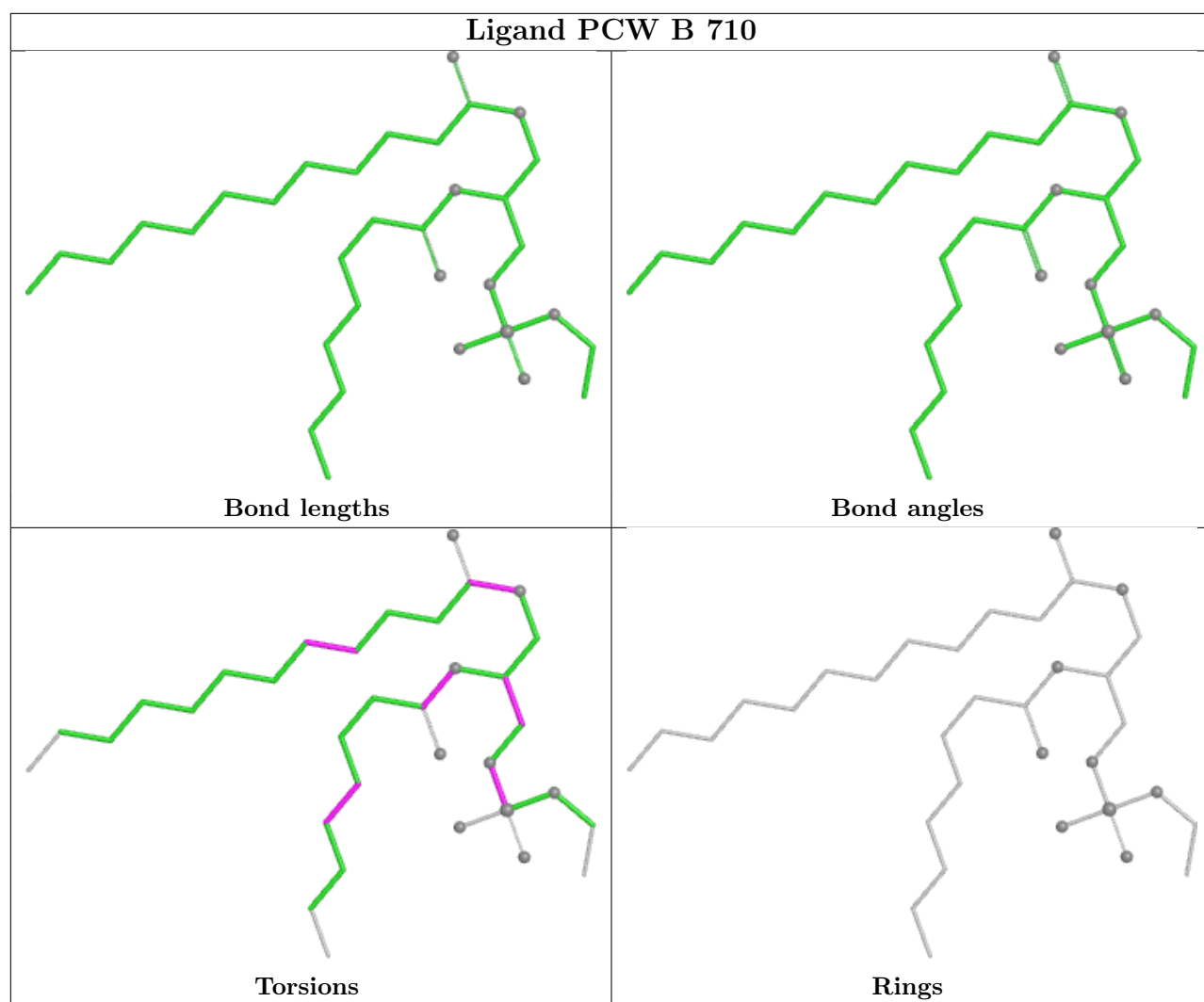


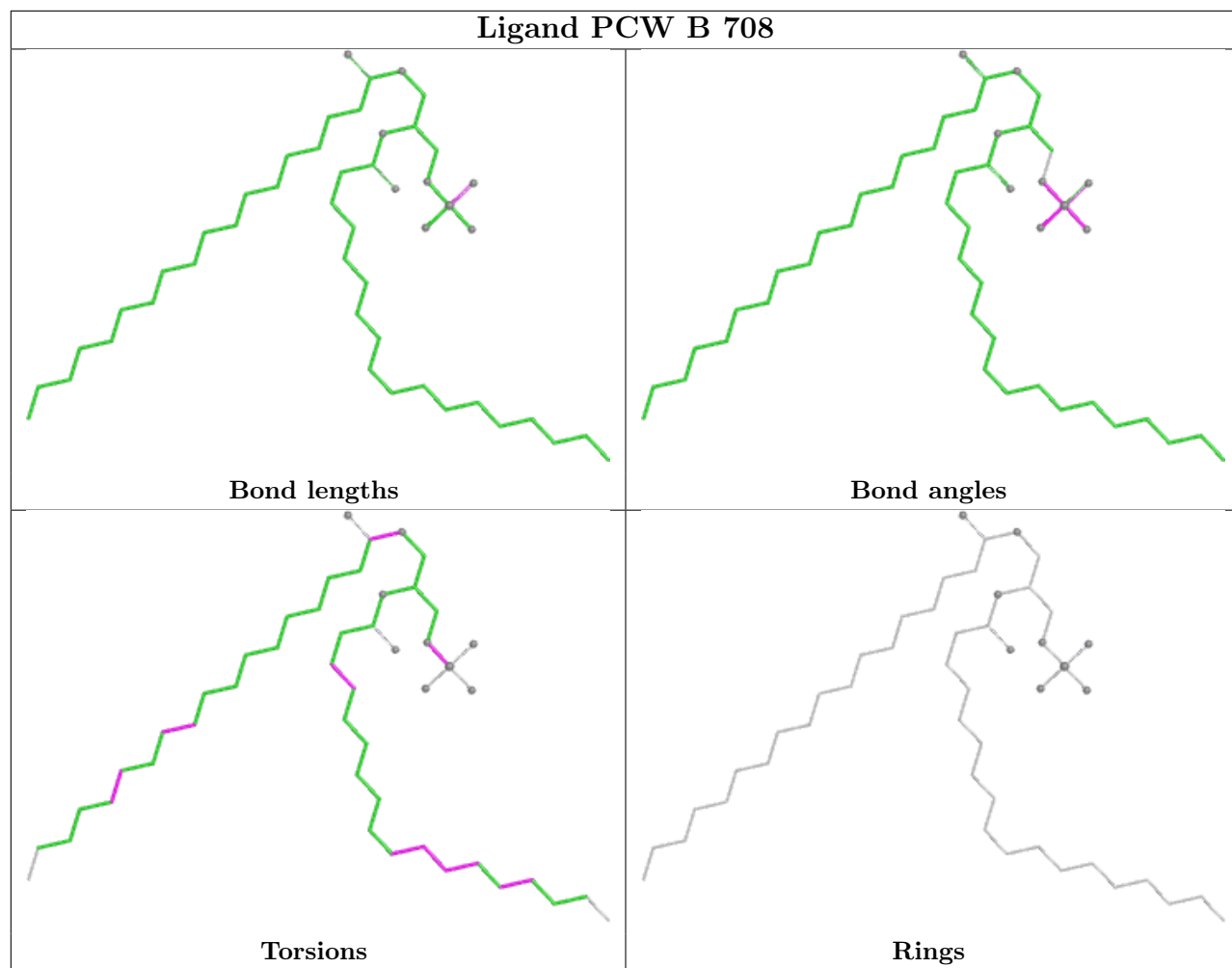


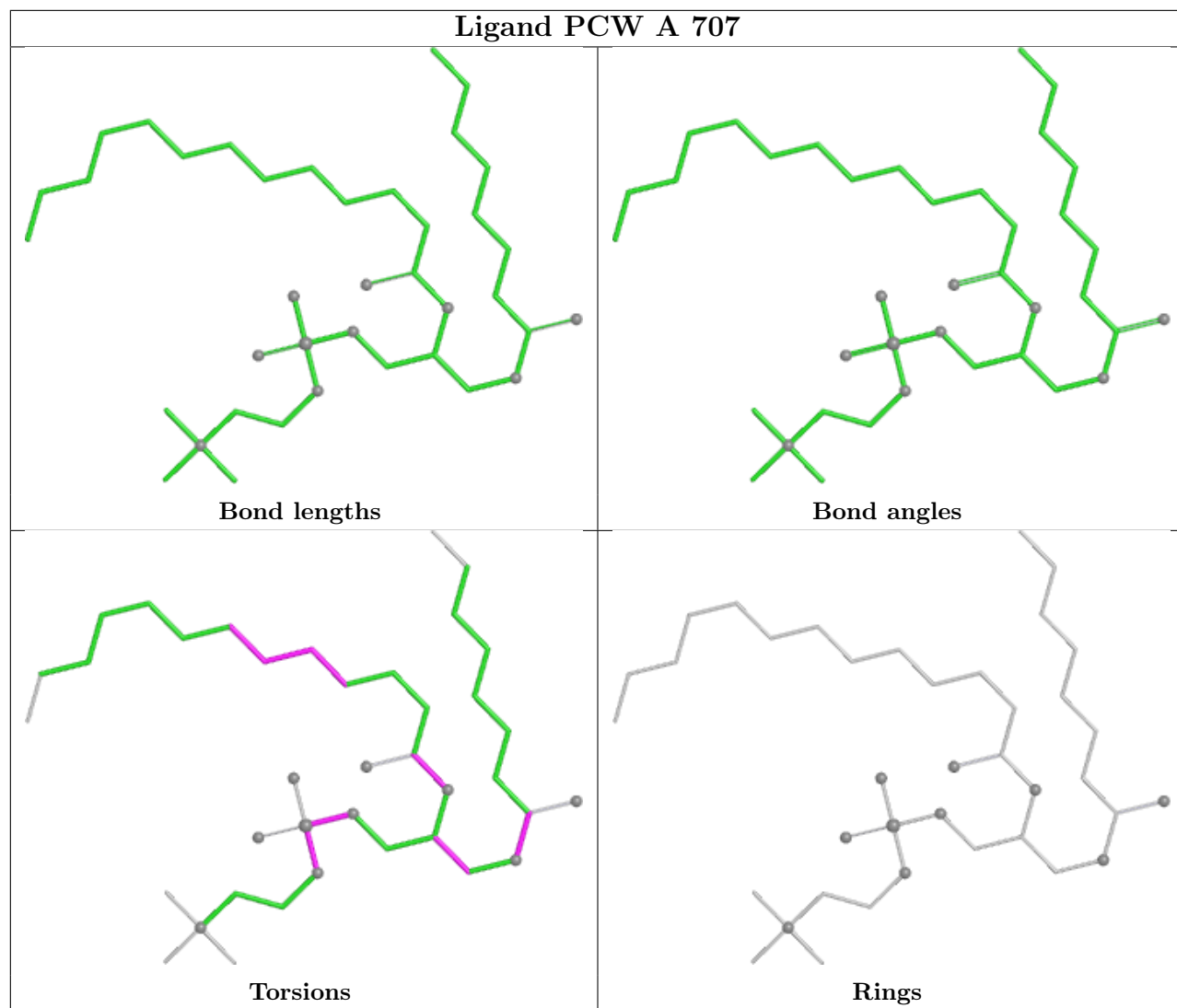


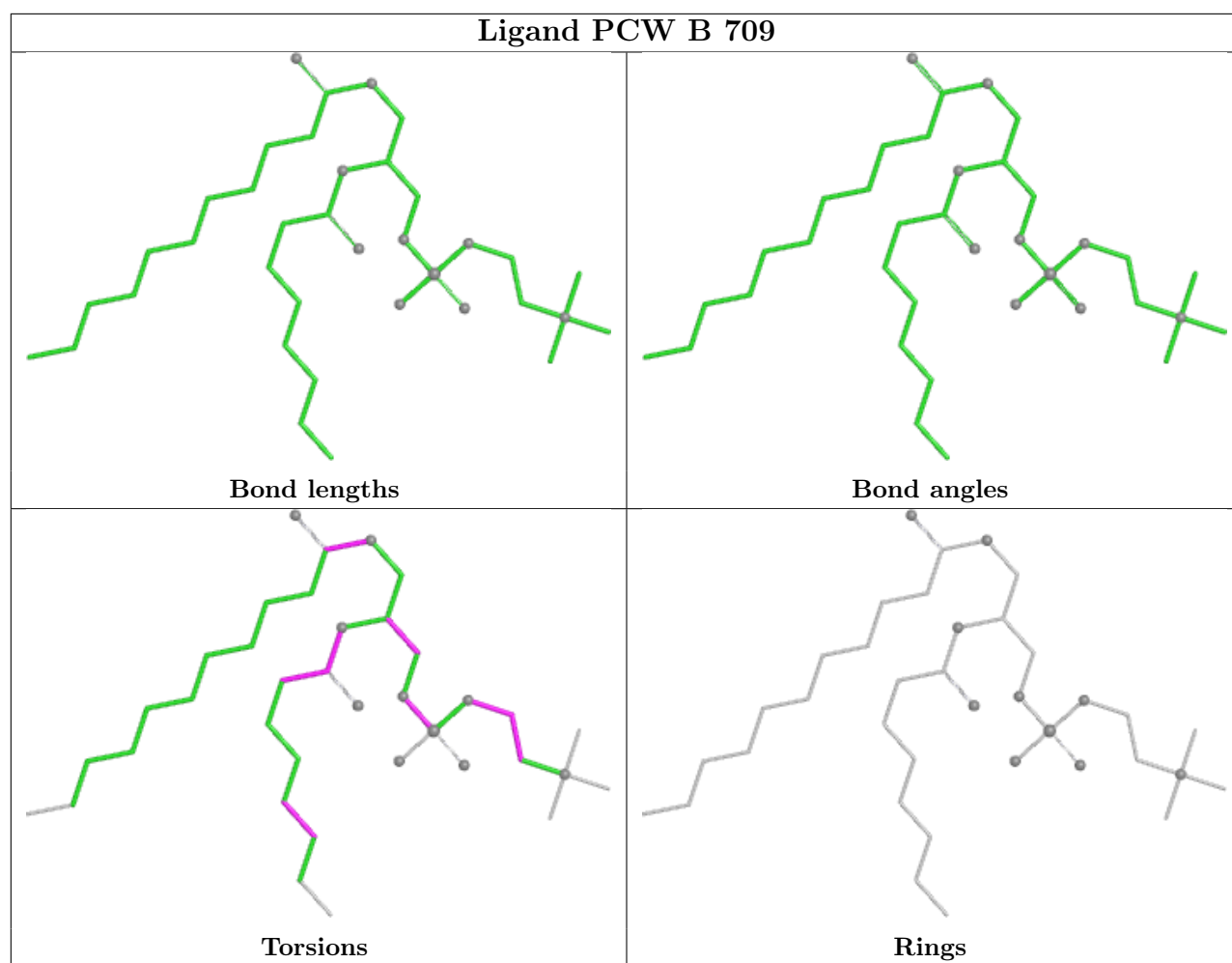


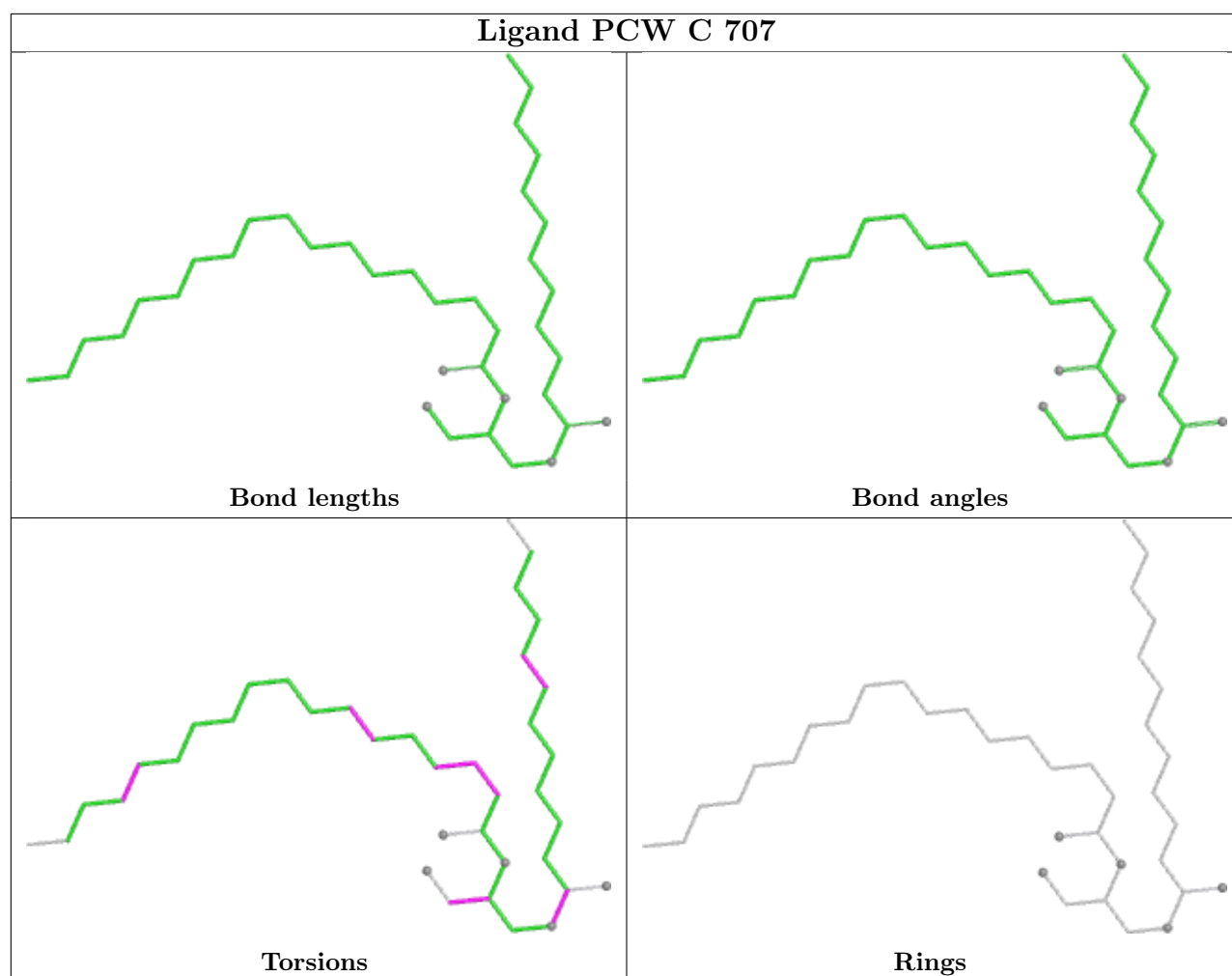


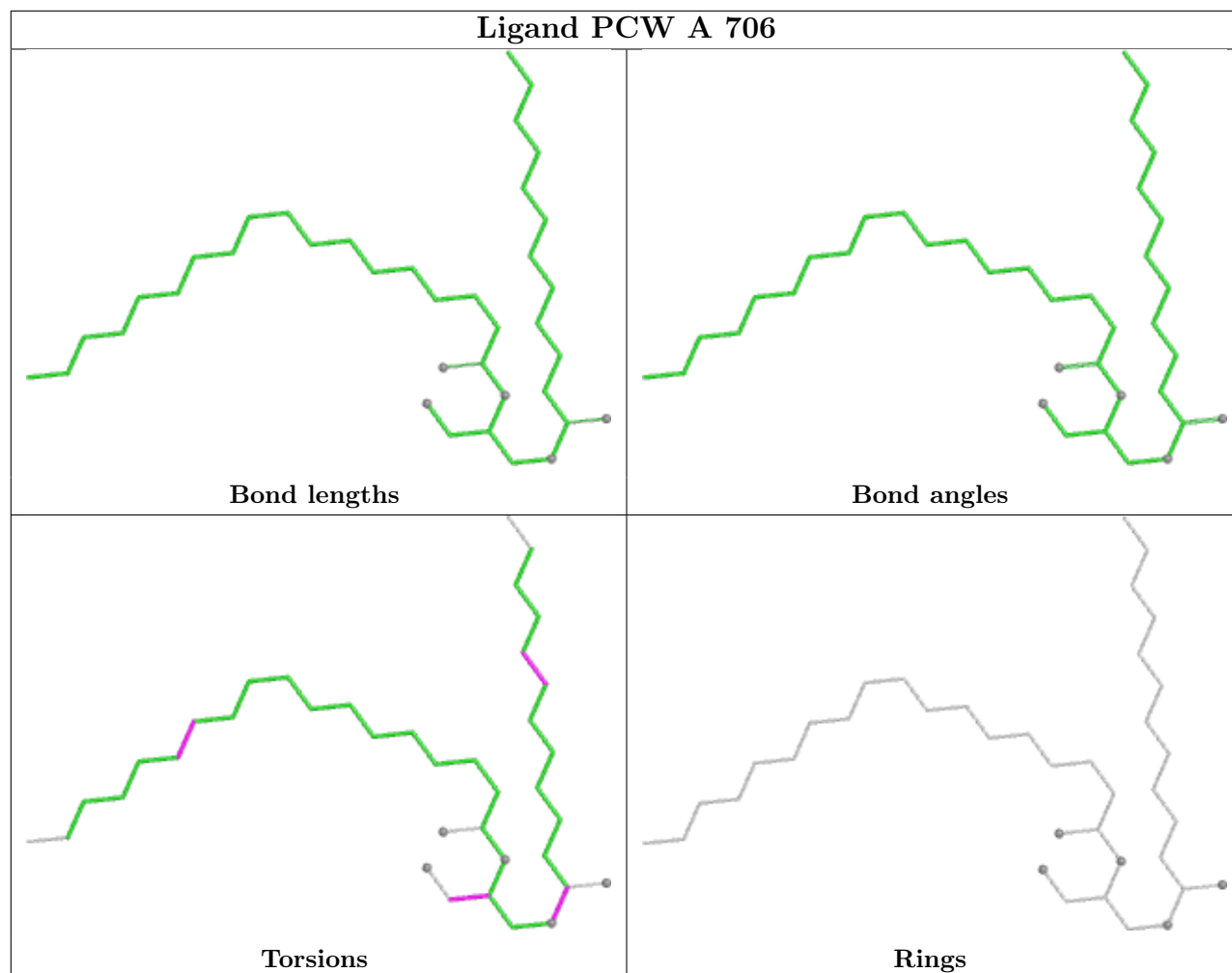


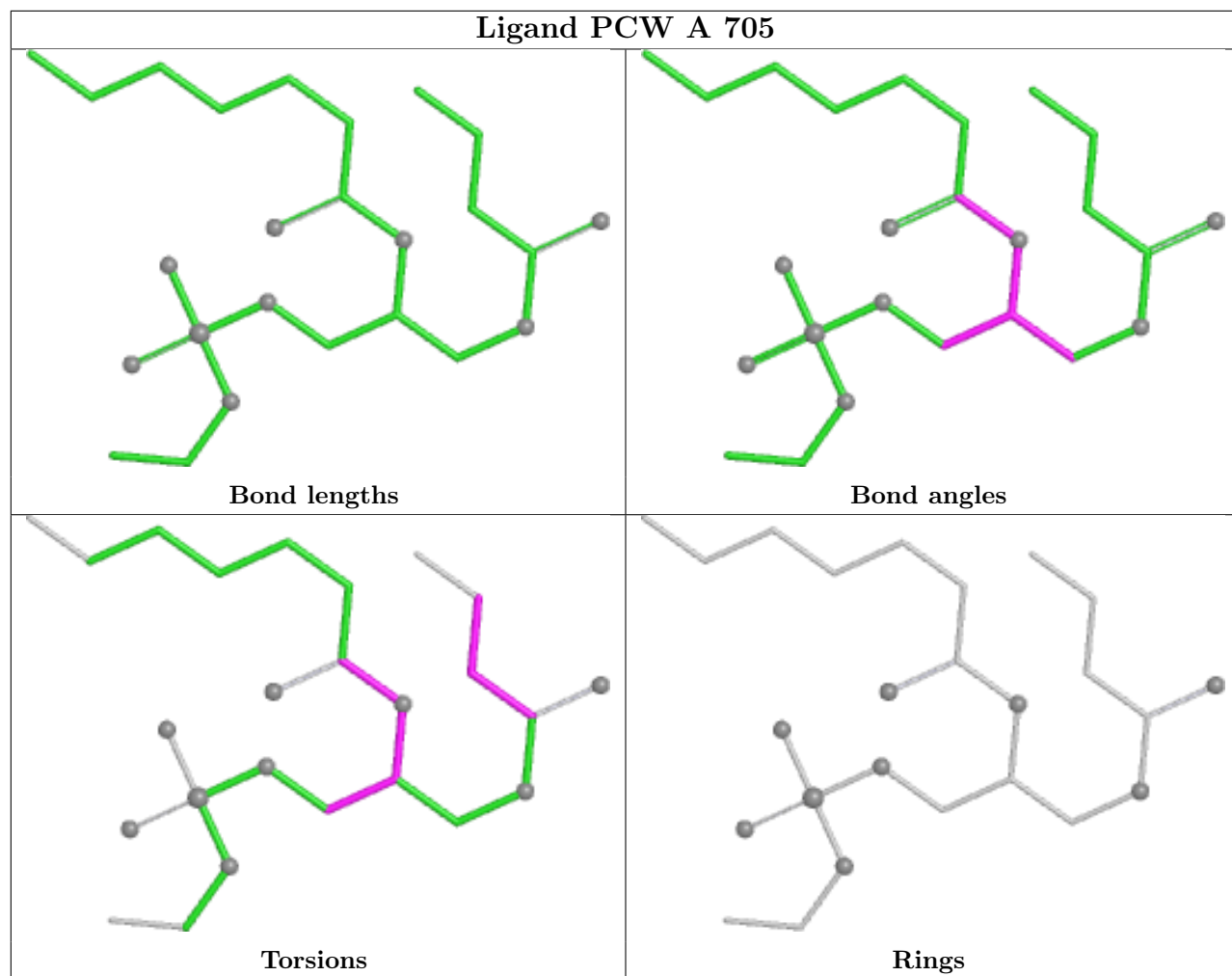


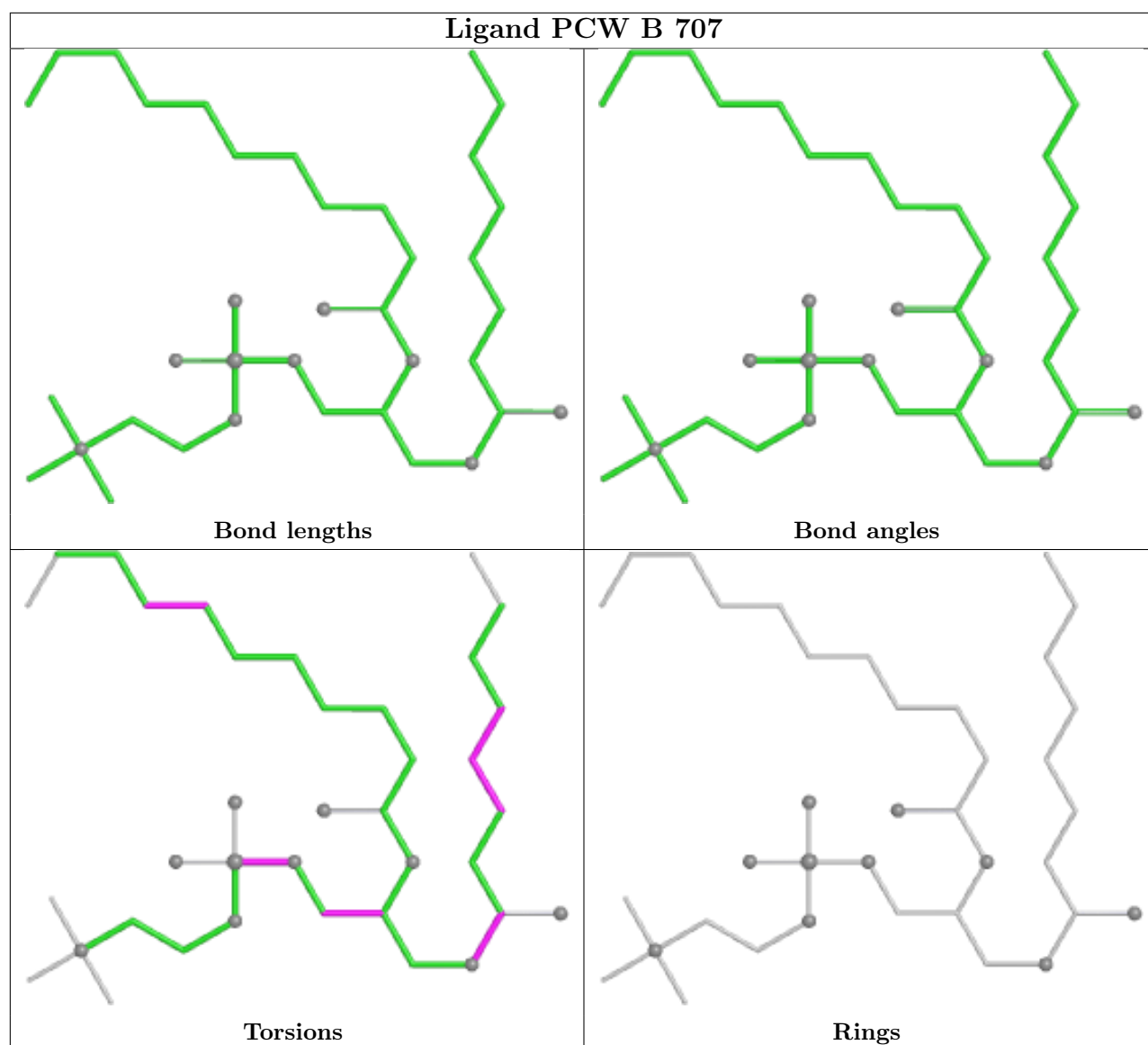


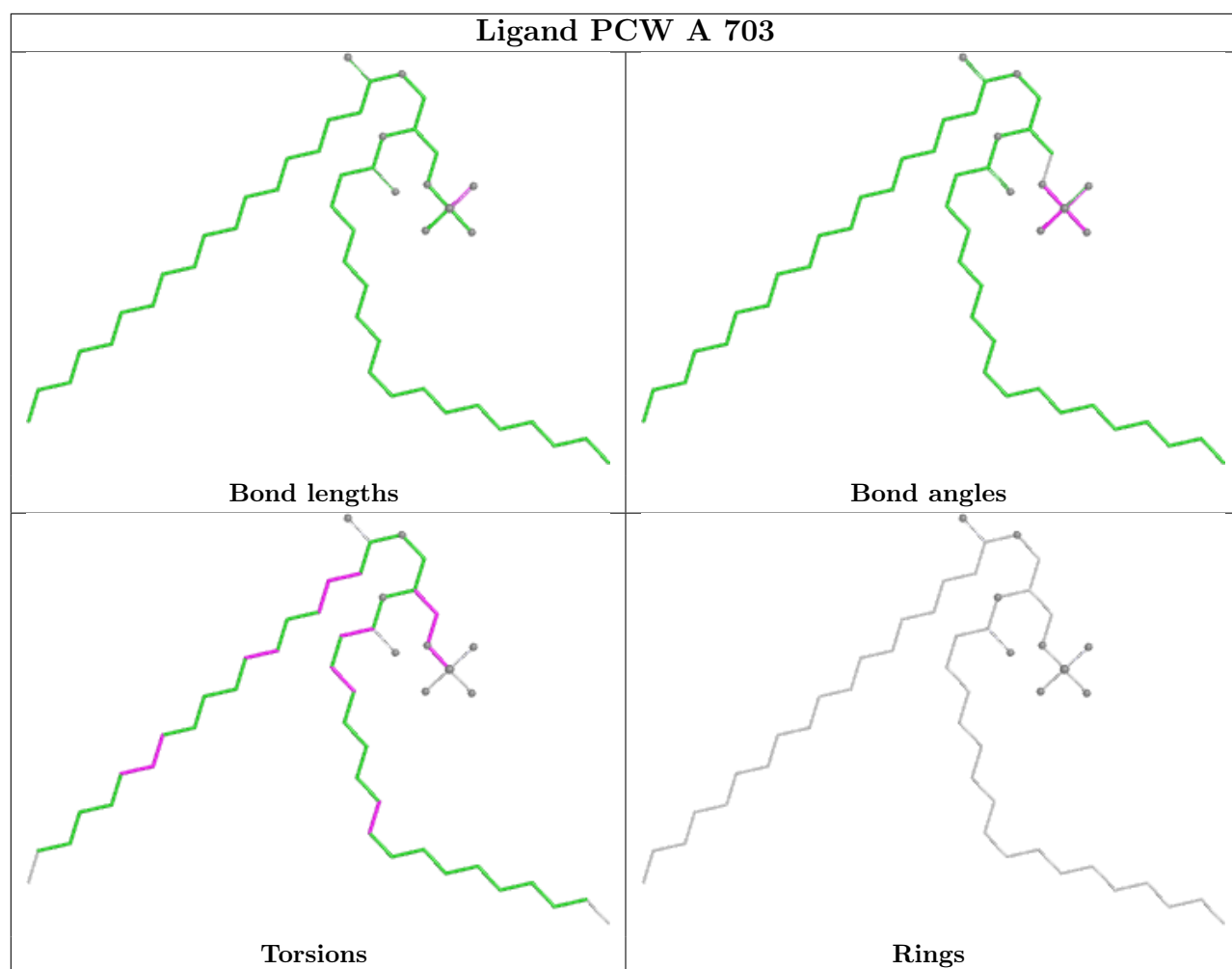


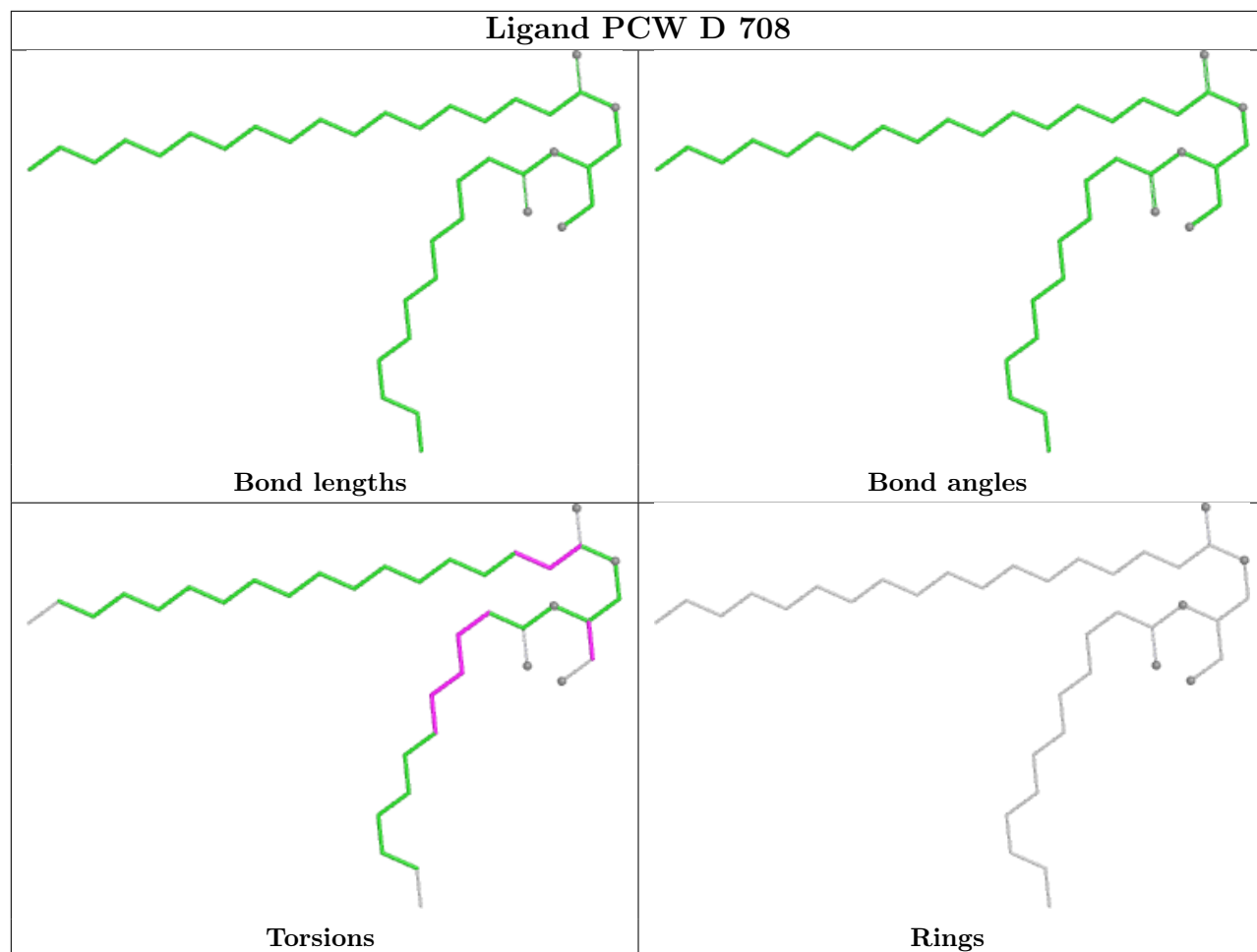


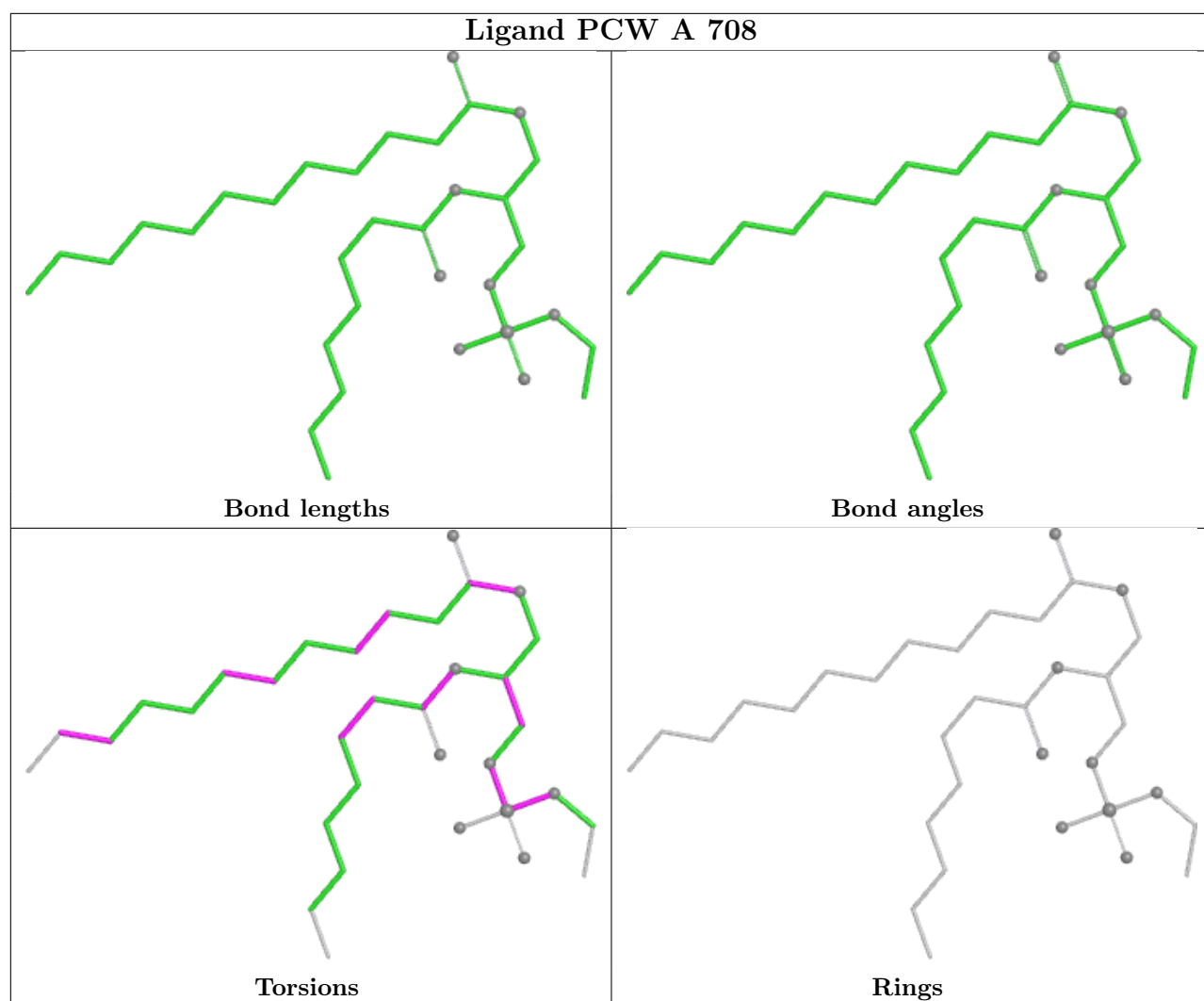


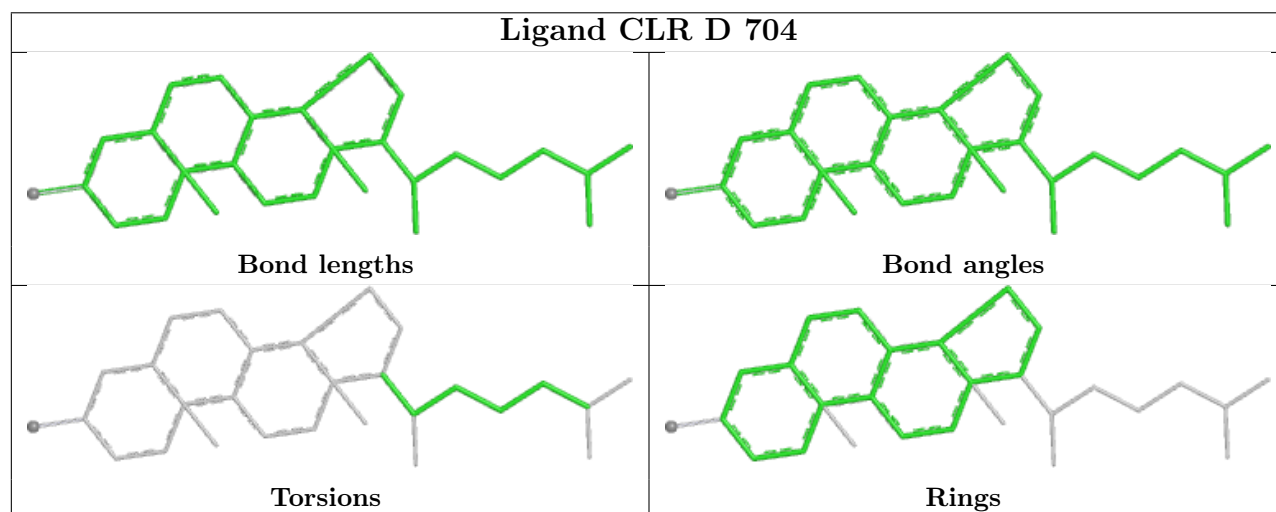
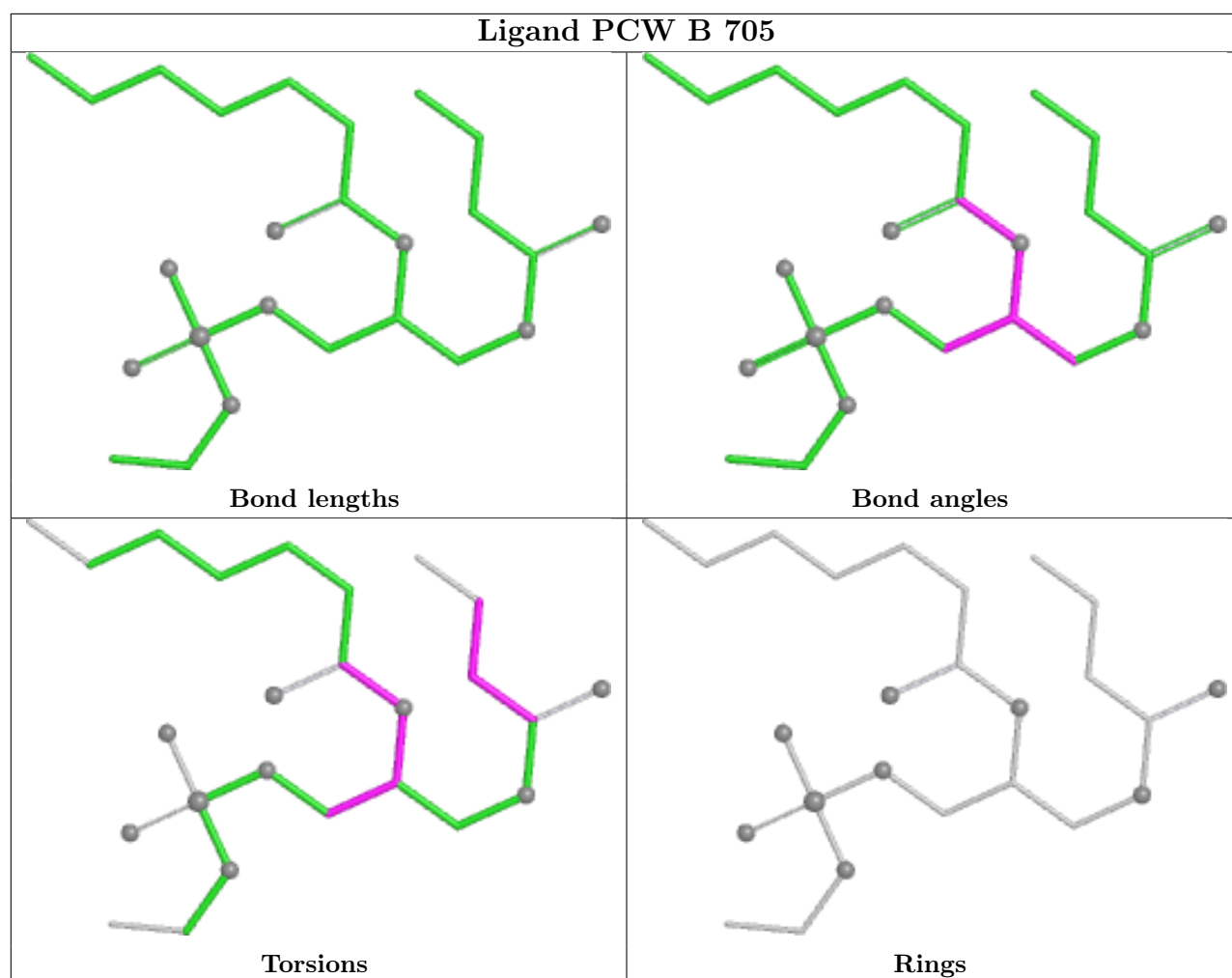


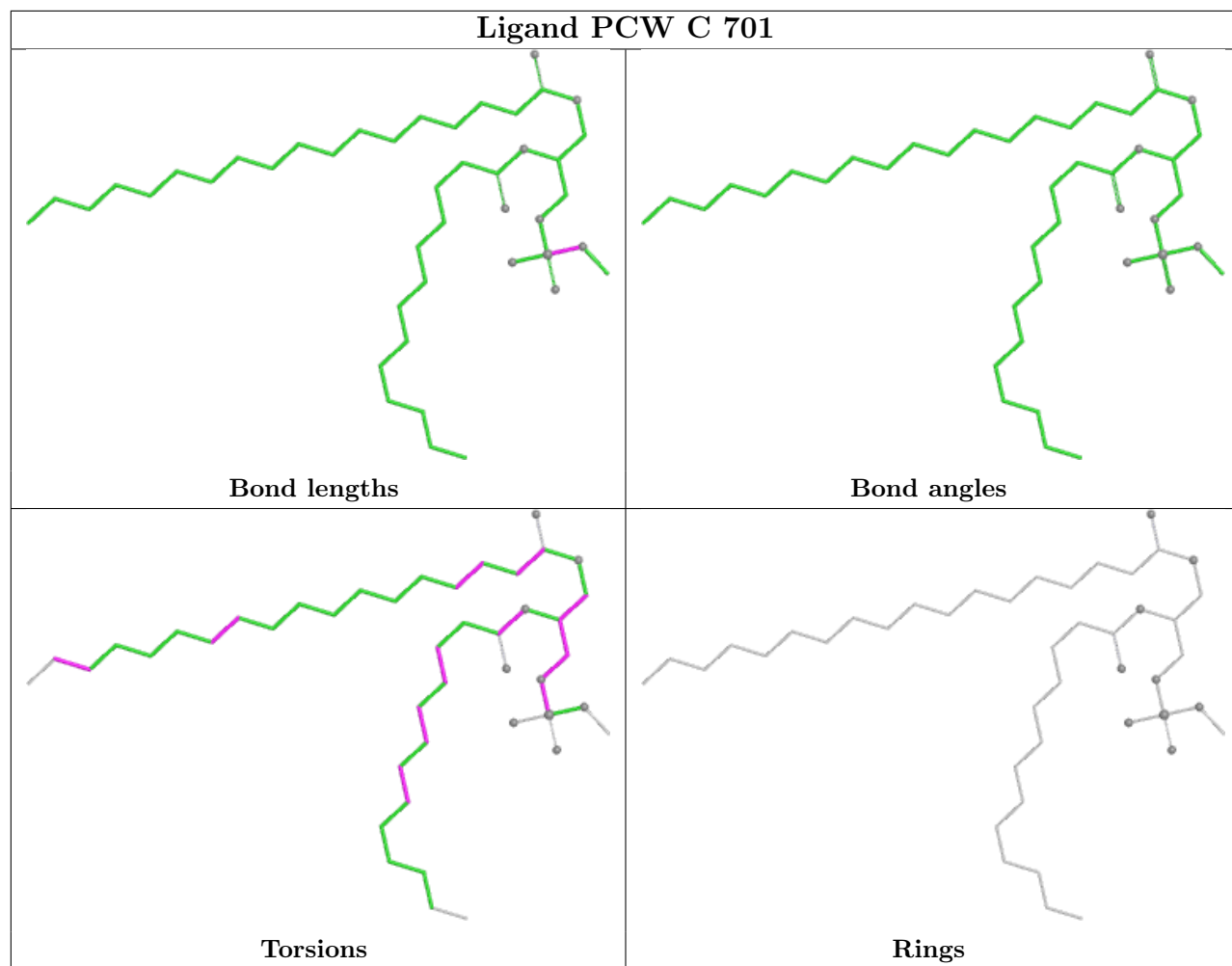


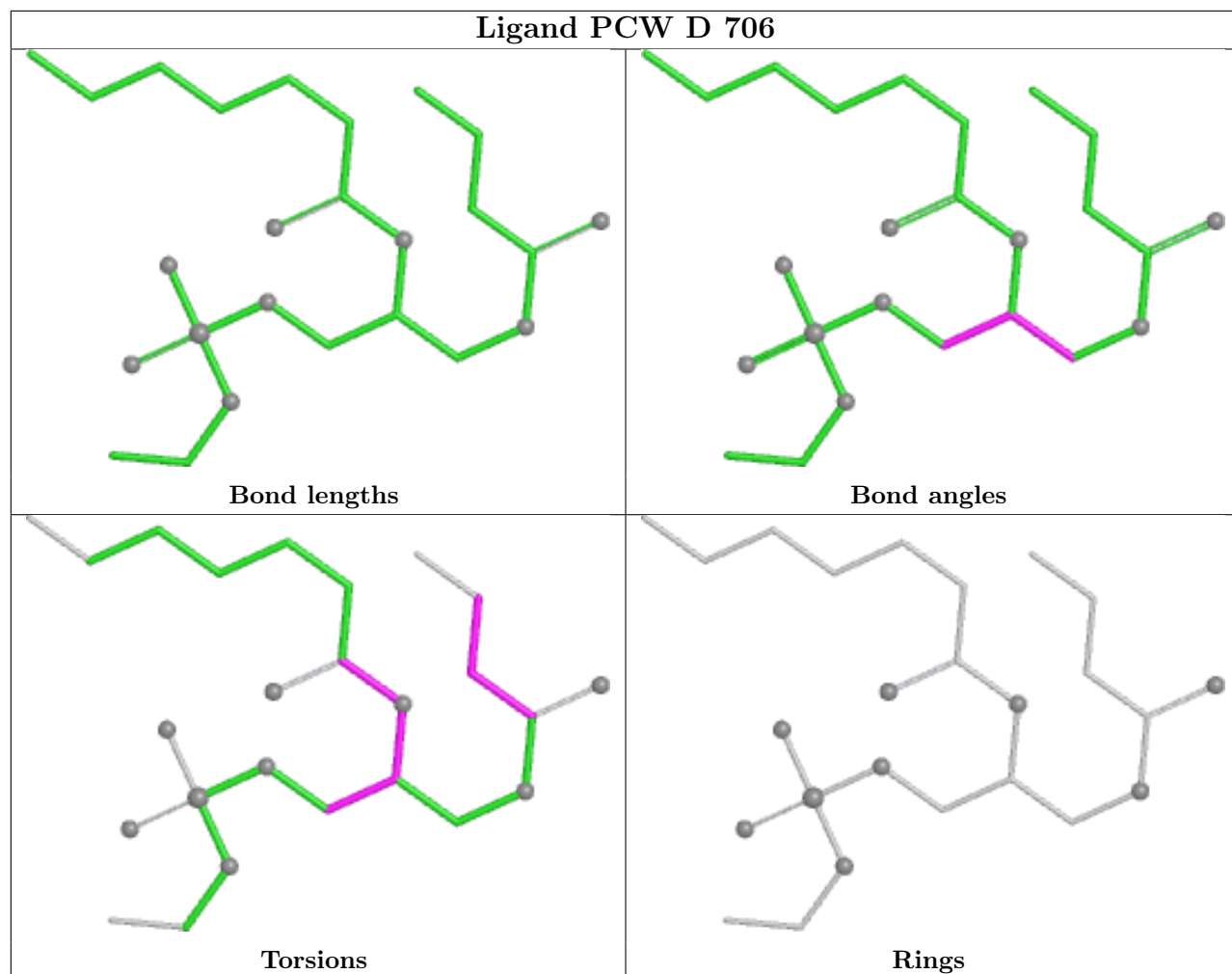


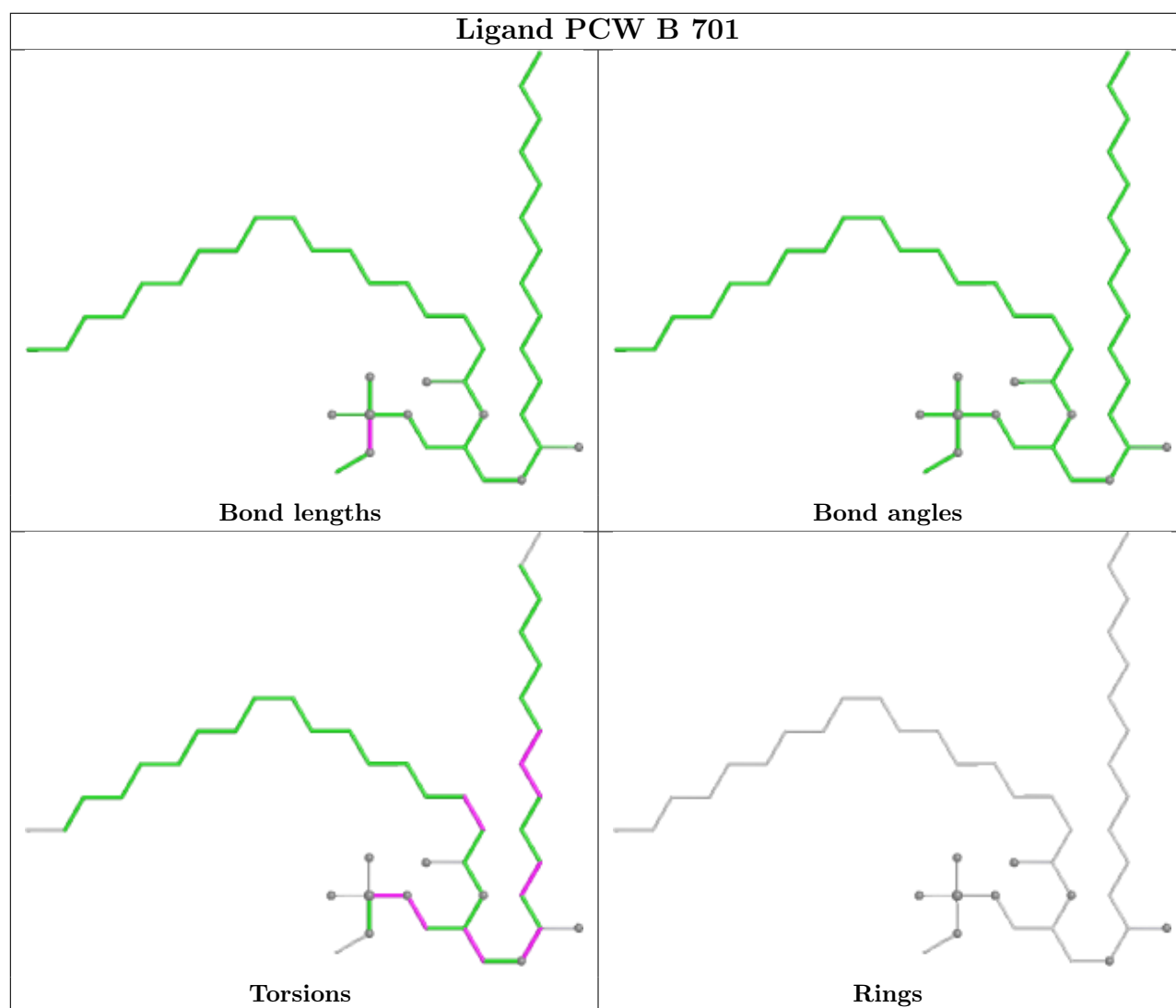


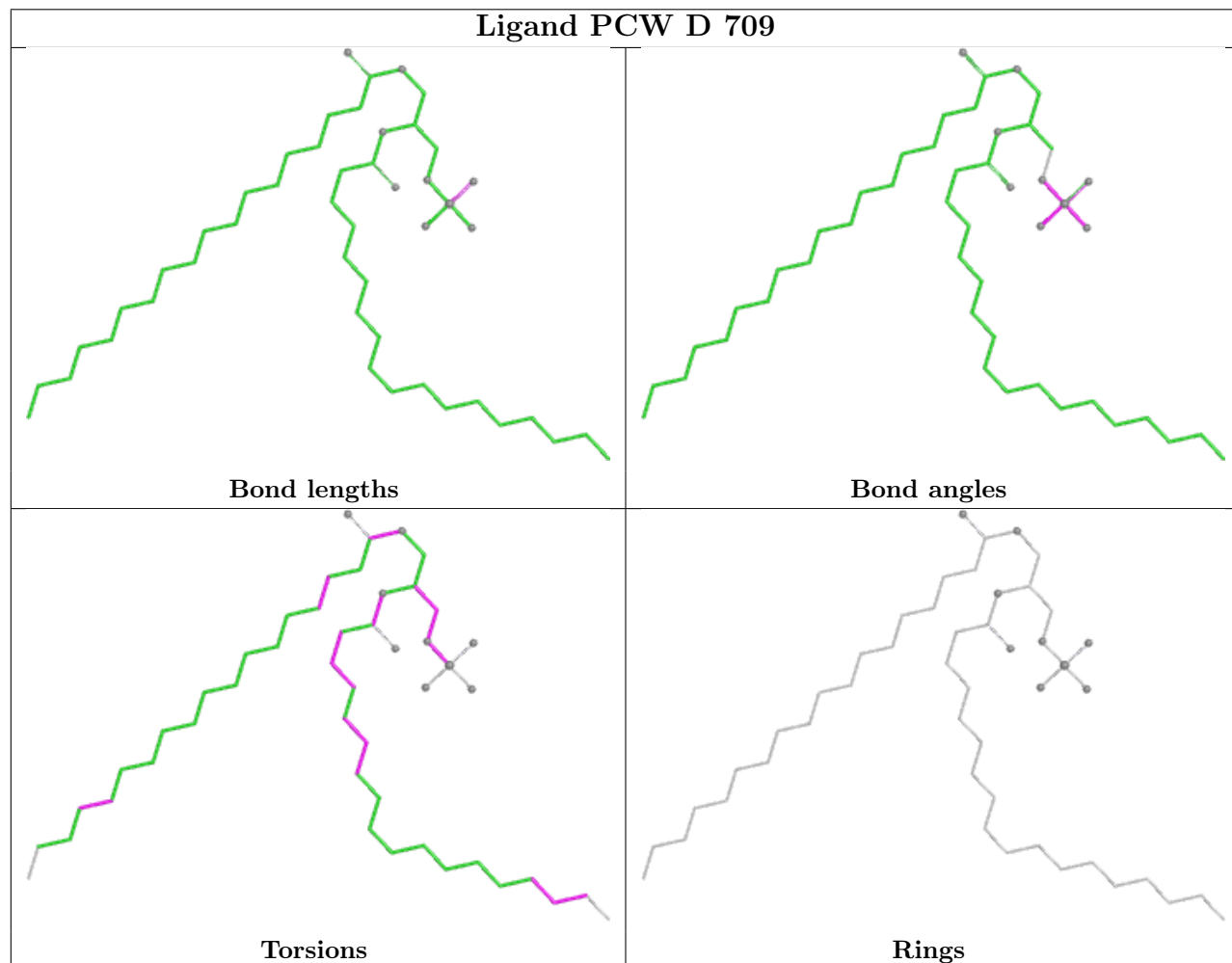
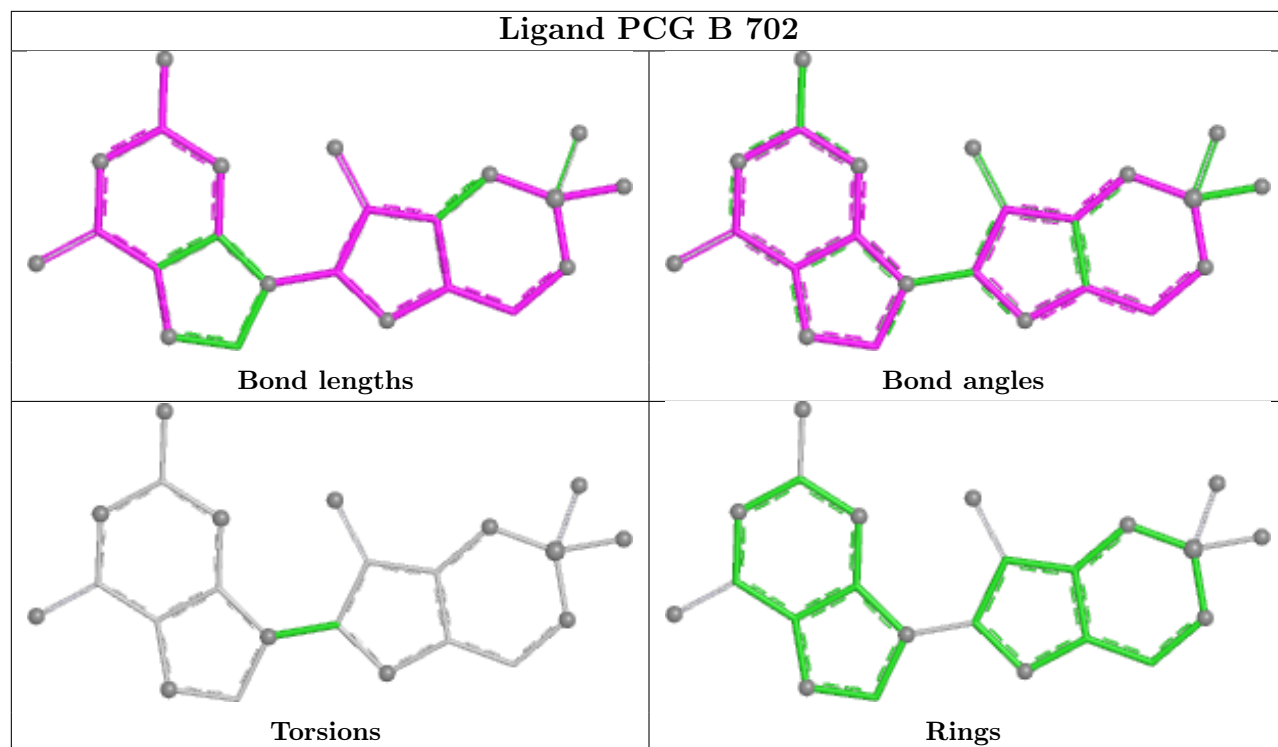


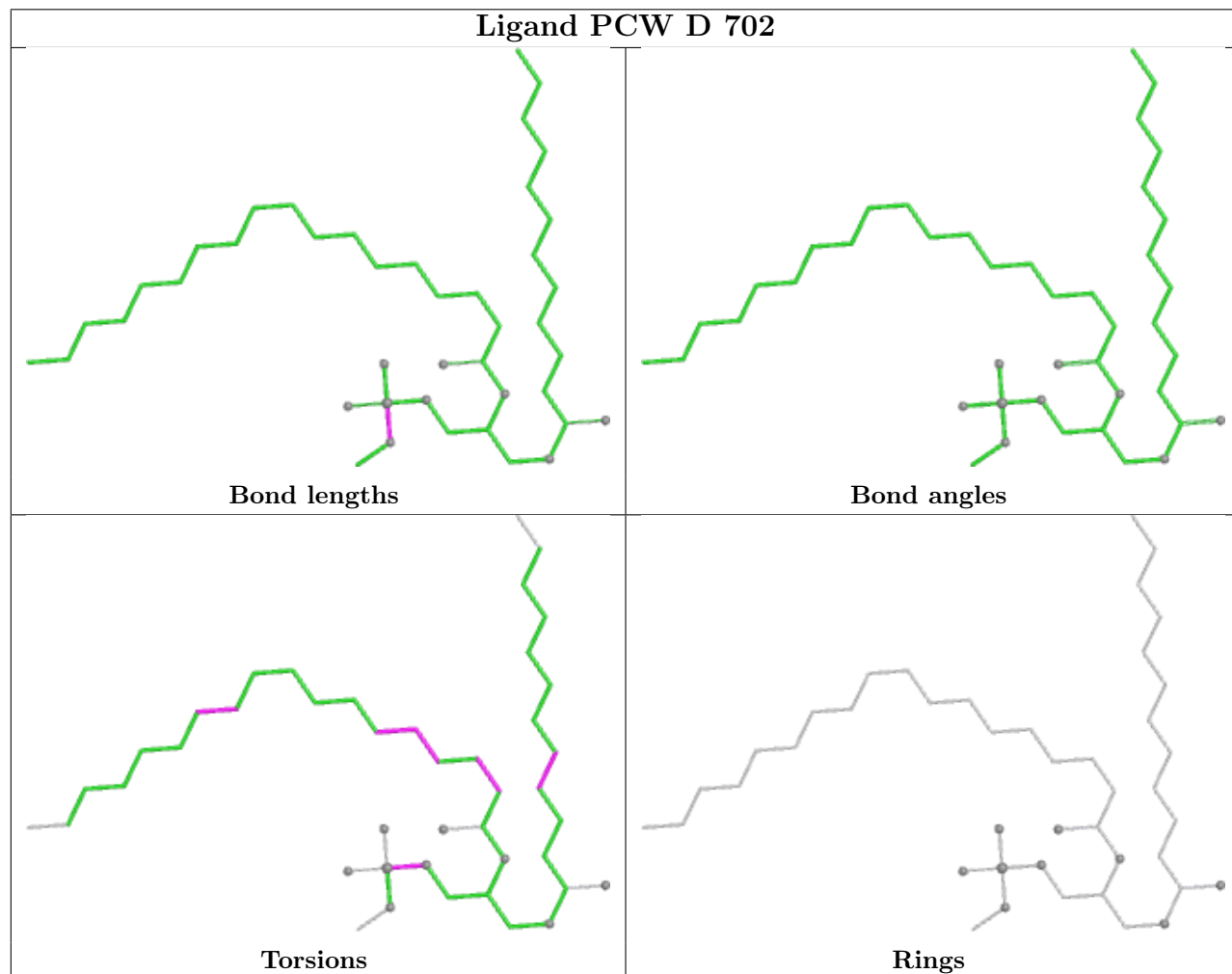
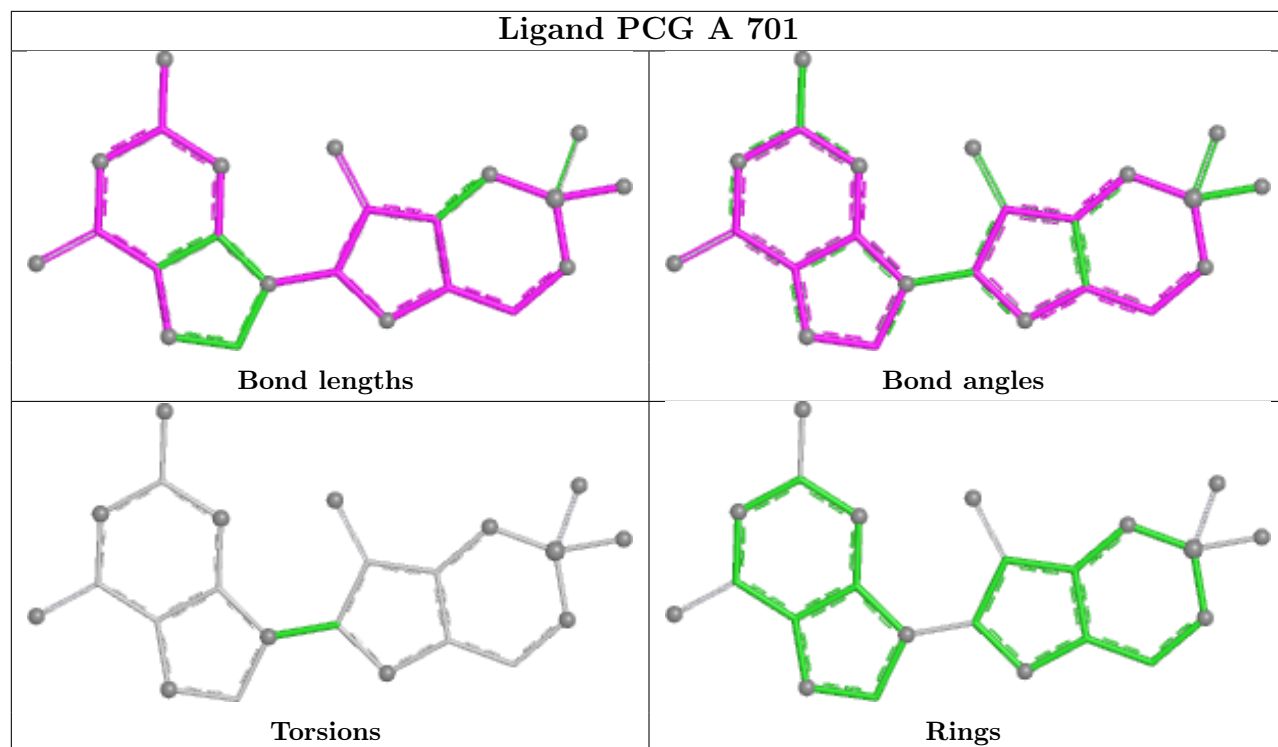


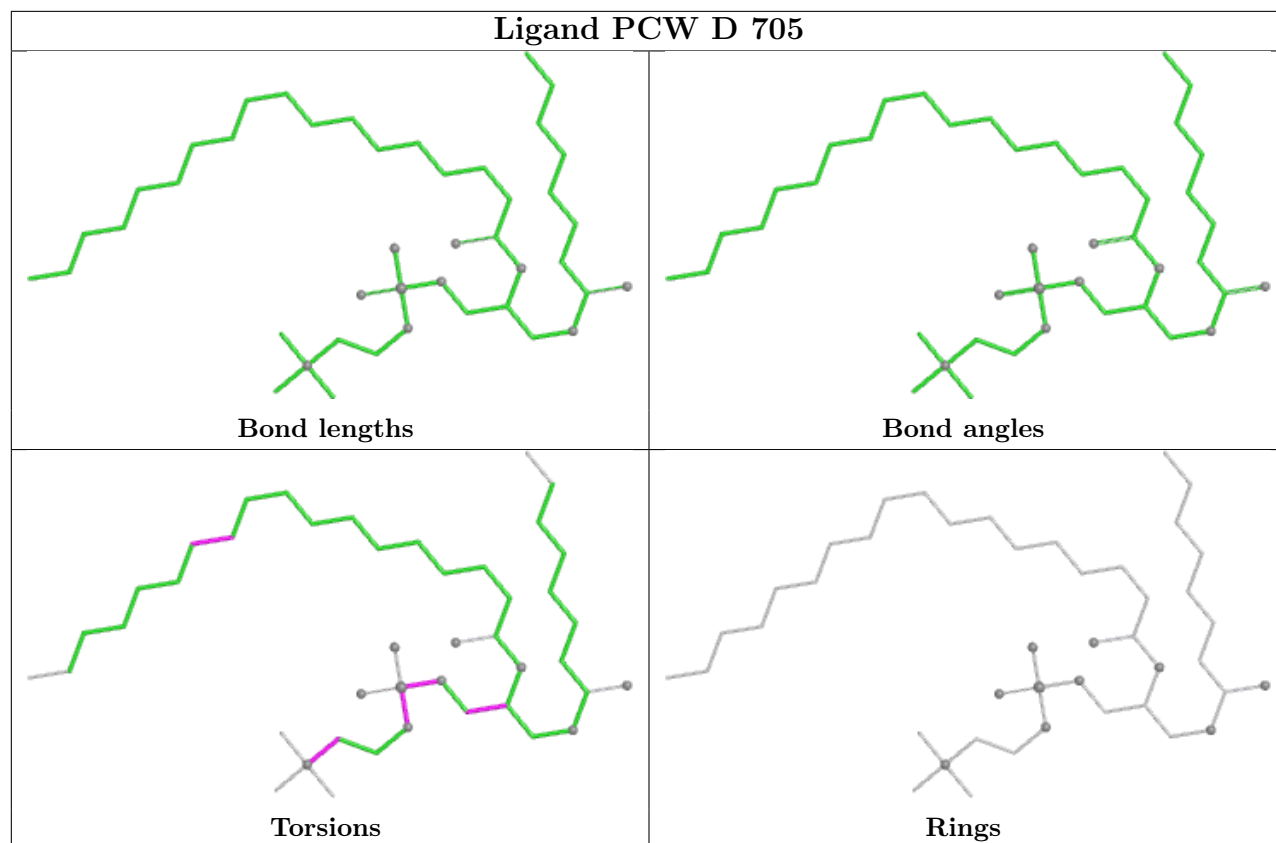


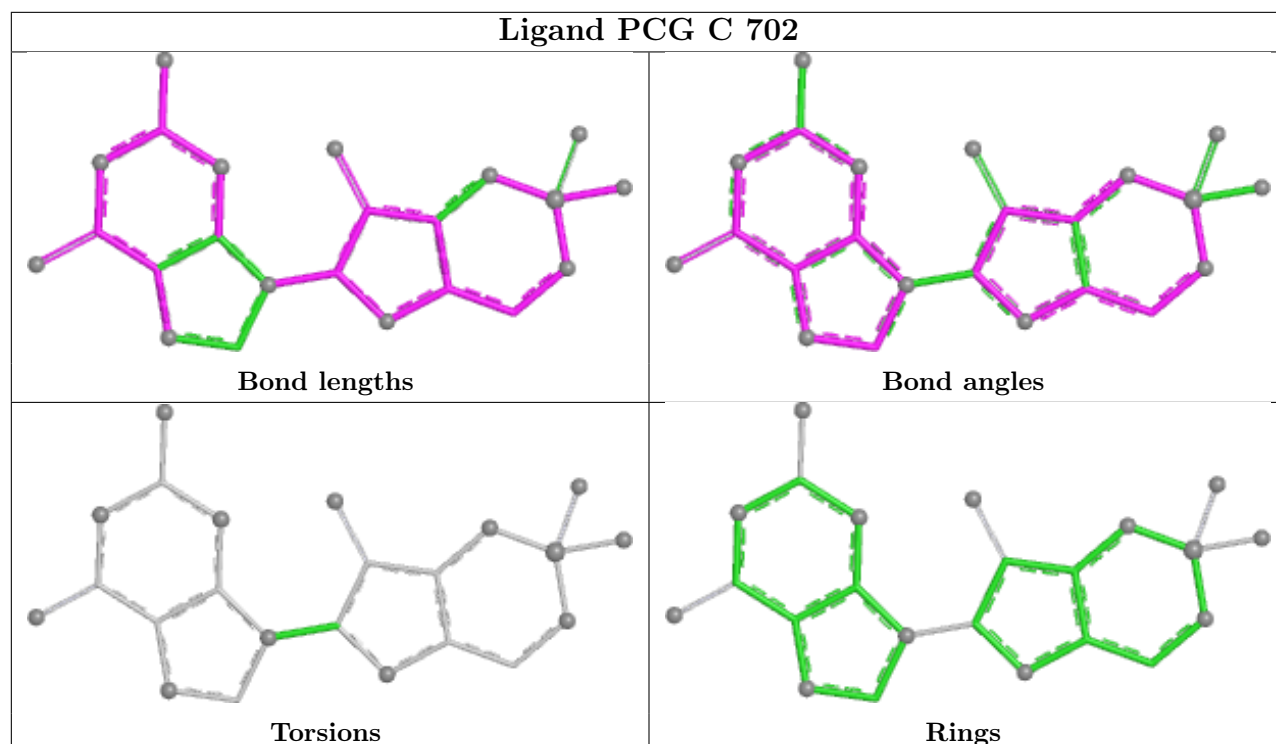
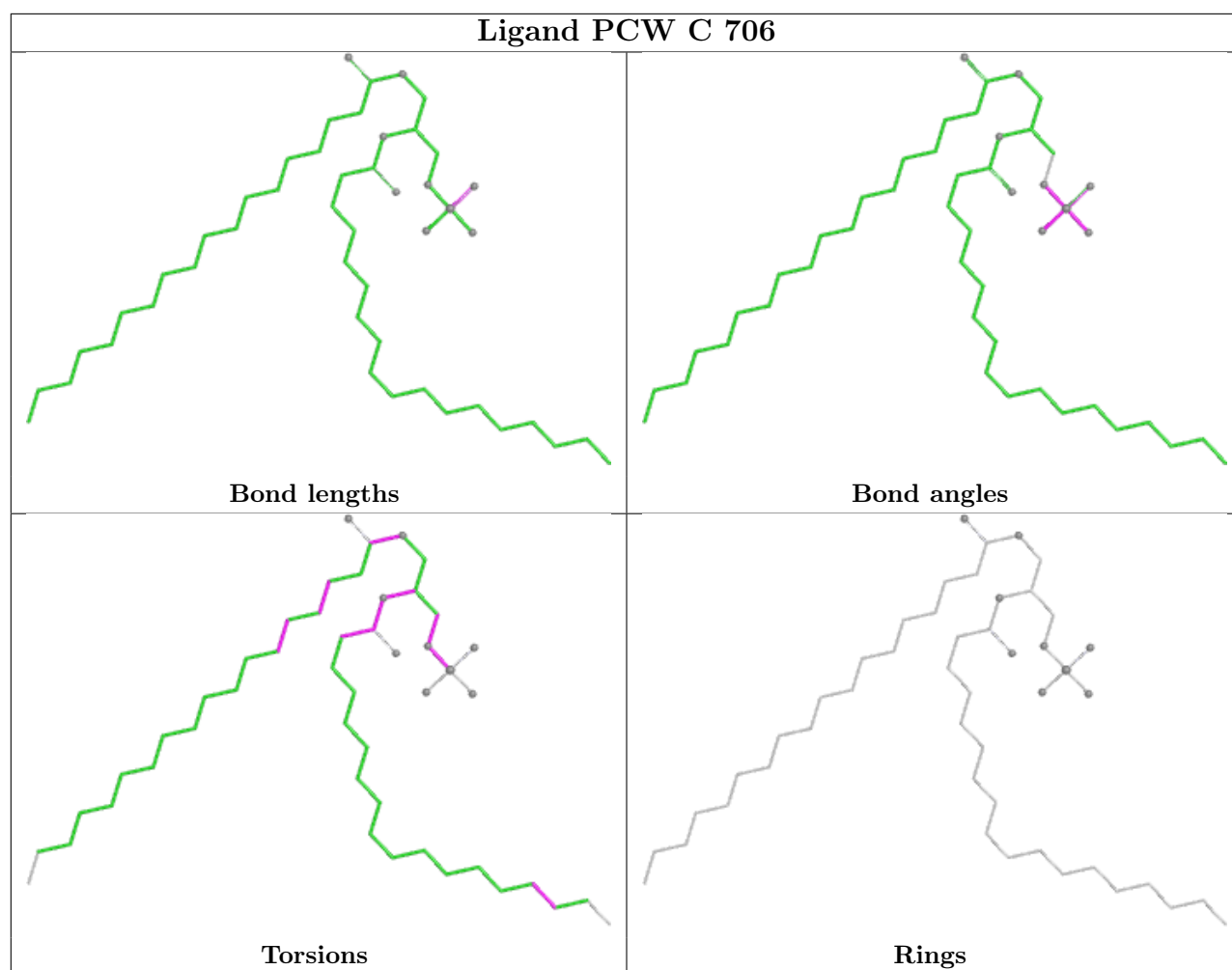


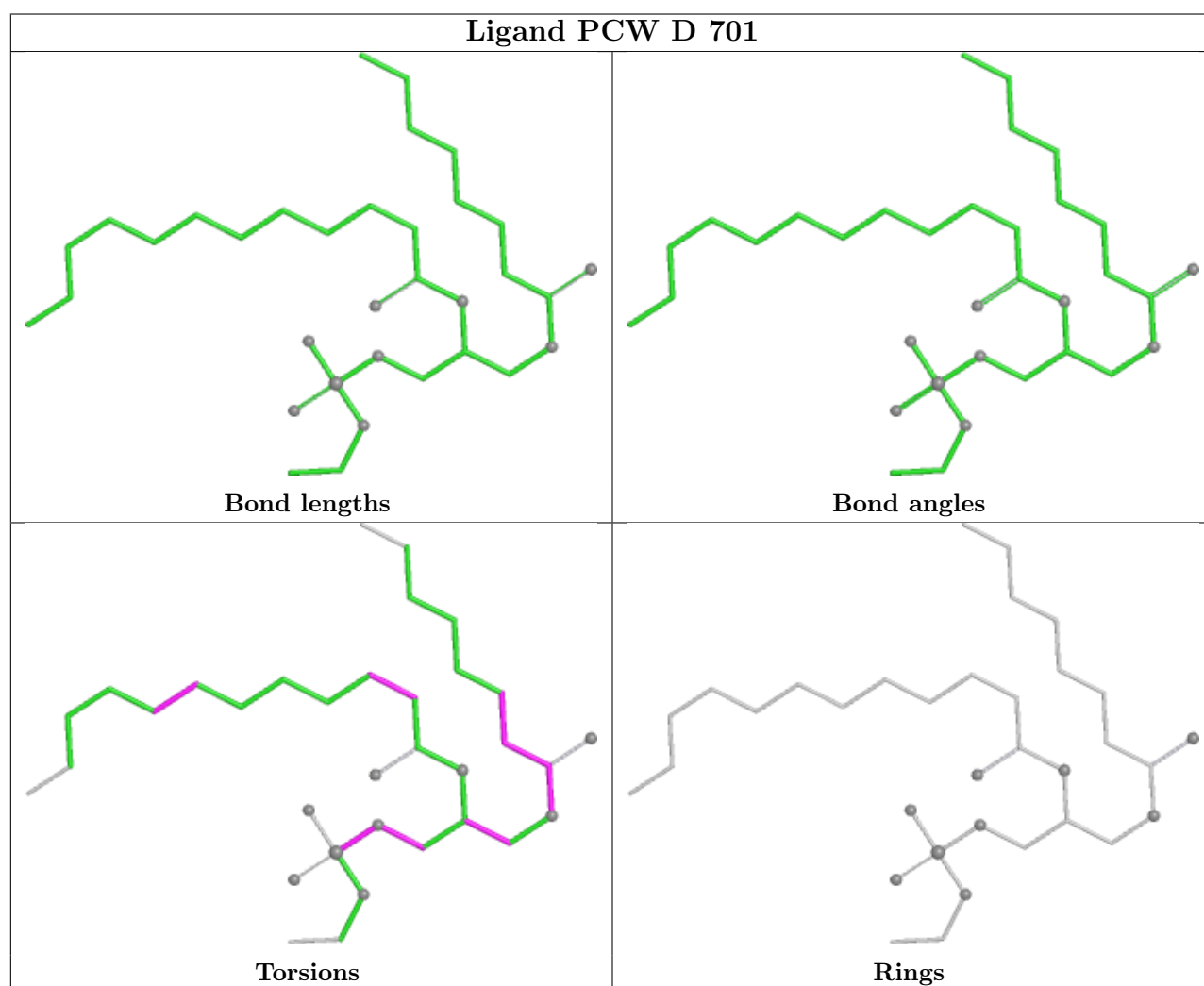
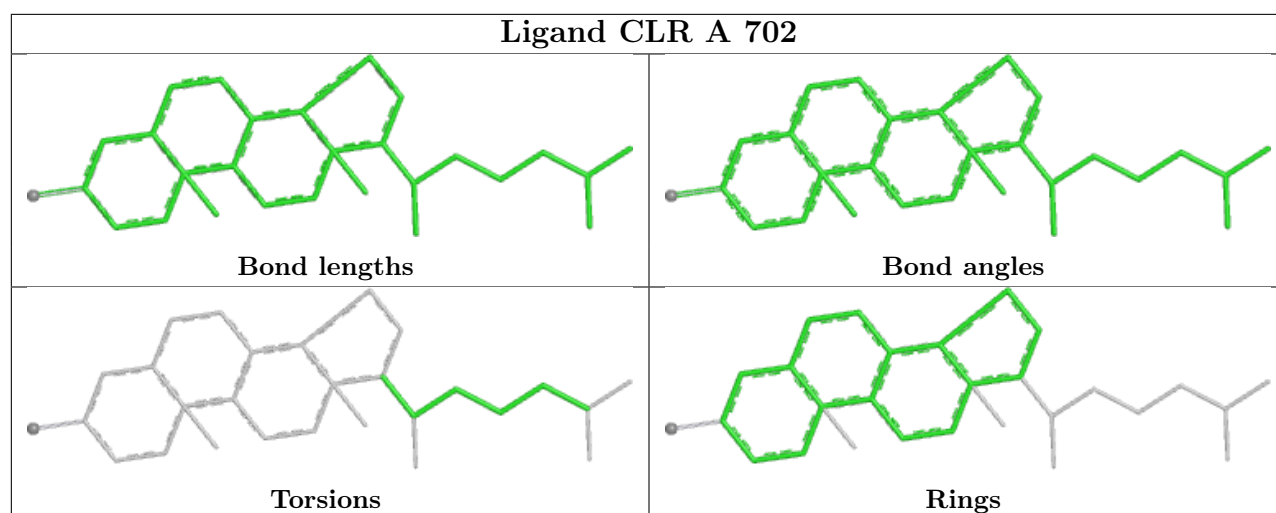


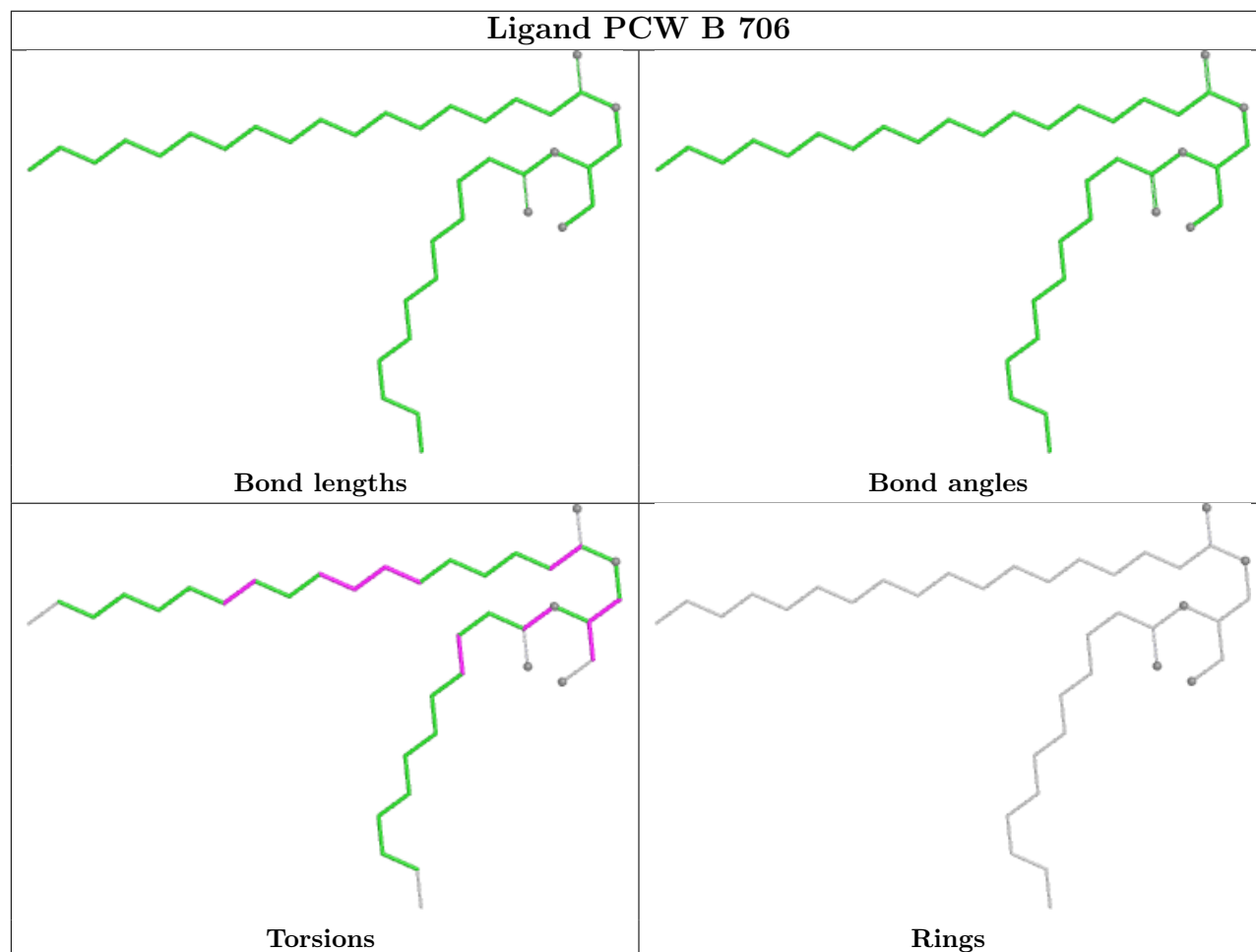
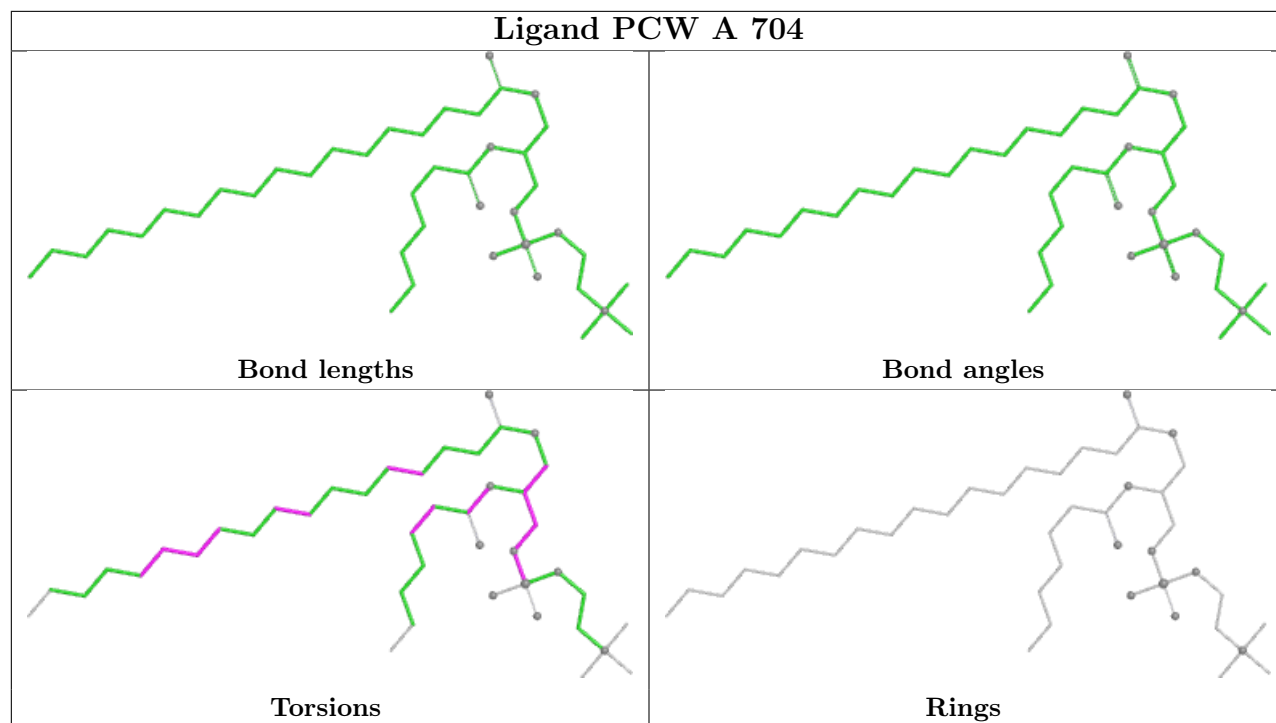


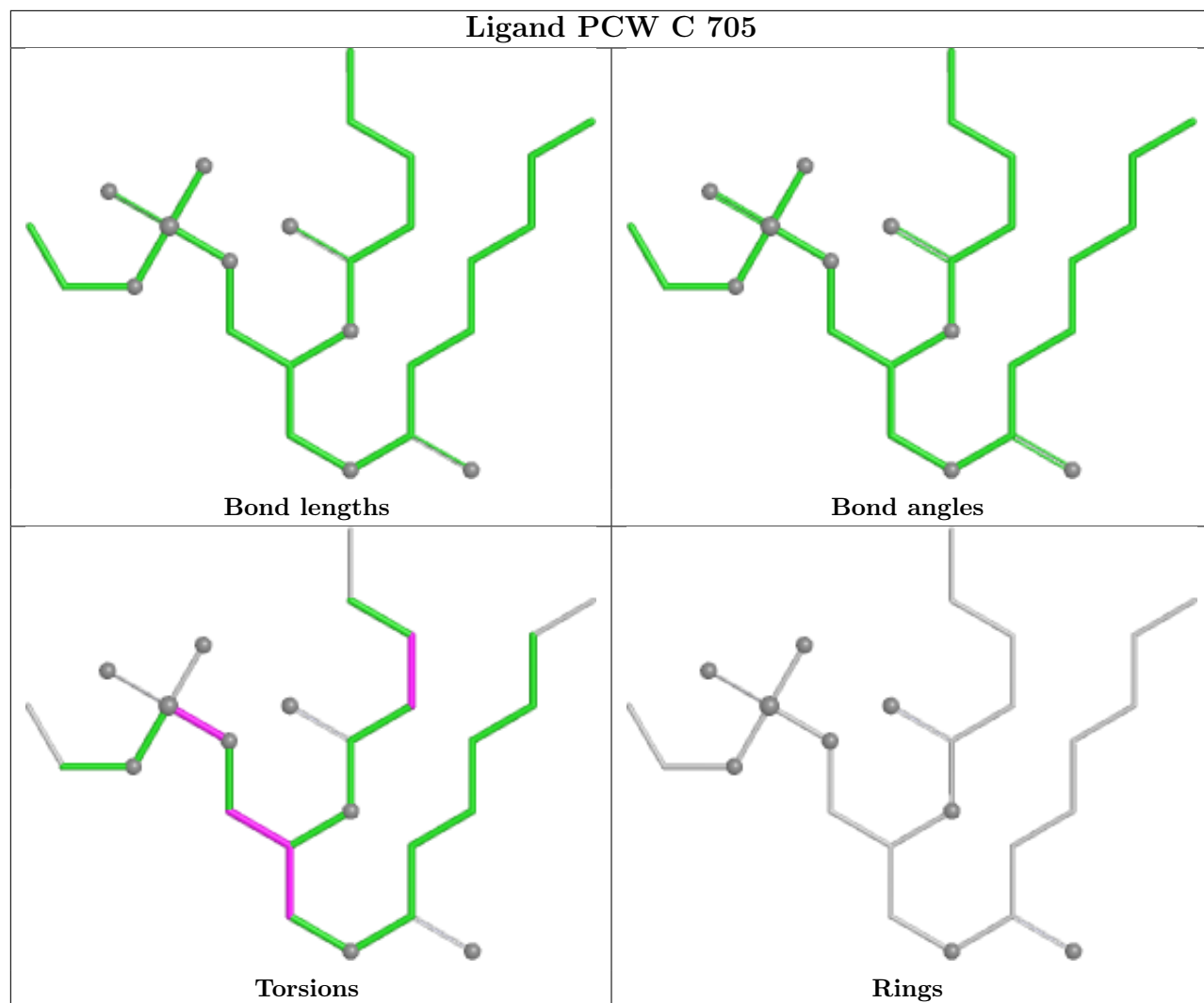


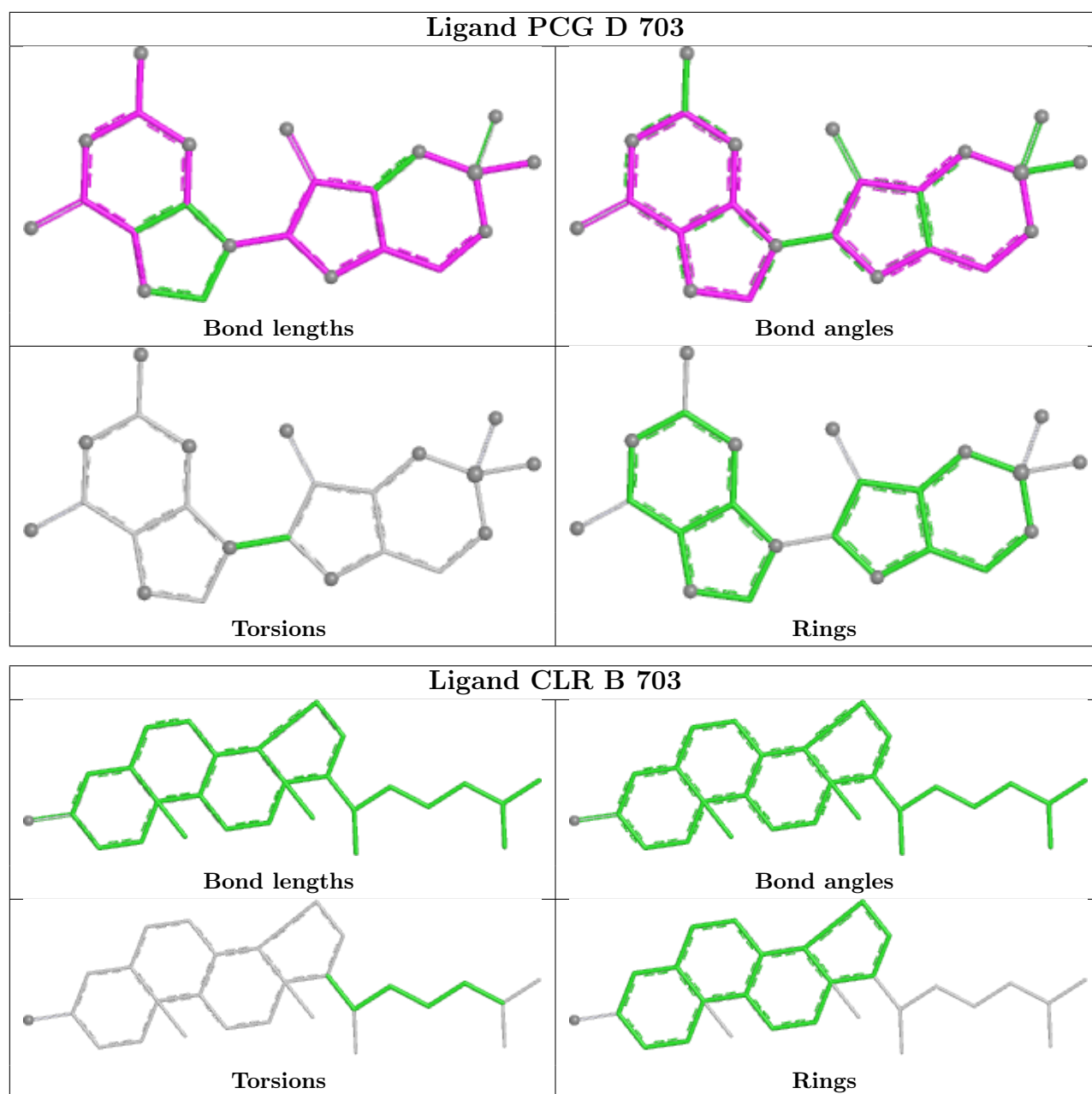












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

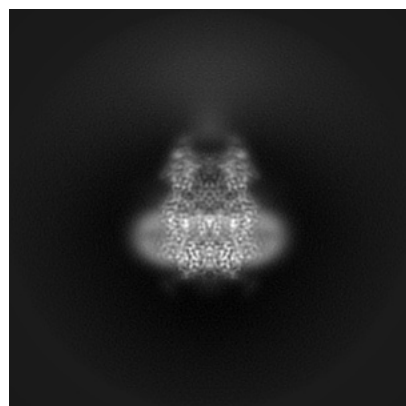
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74535. These allow visual inspection of the internal detail of the map and identification of artifacts.

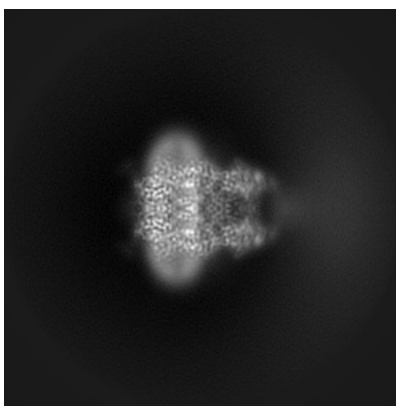
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

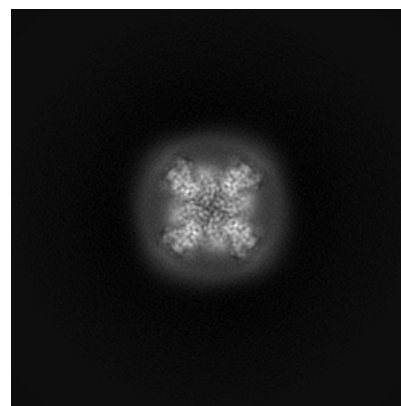
6.1.1 Primary map



X

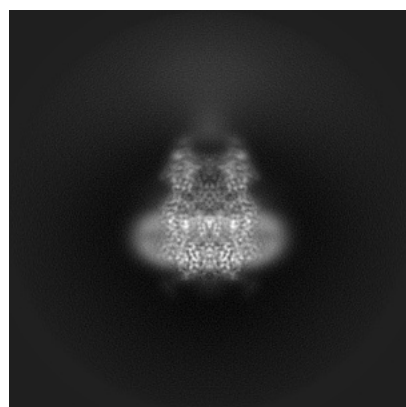


Y

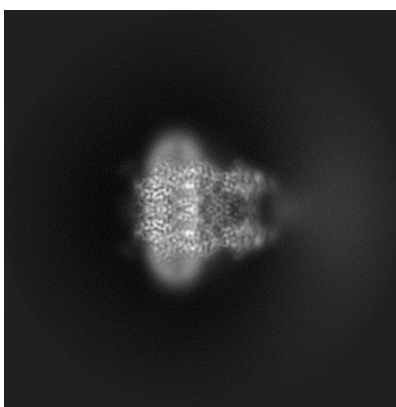


Z

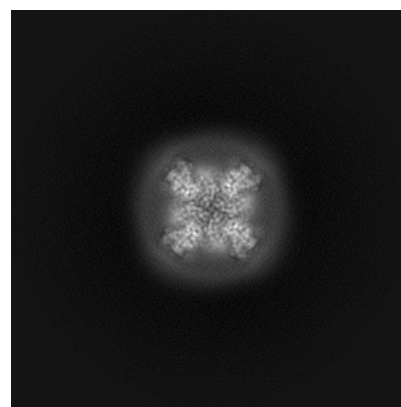
6.1.2 Raw map



X



Y

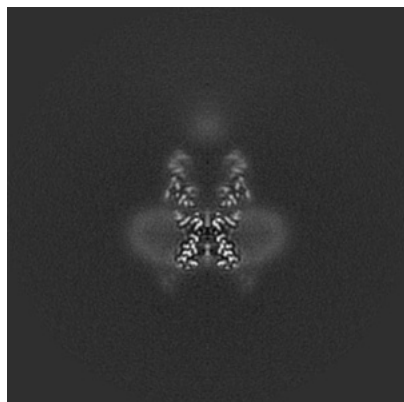


Z

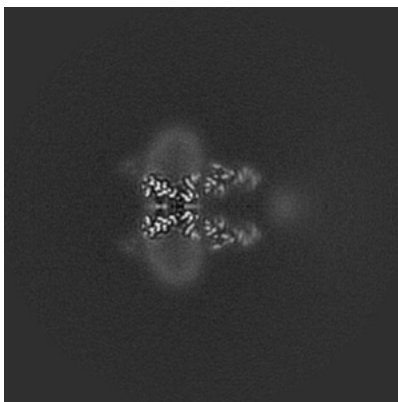
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

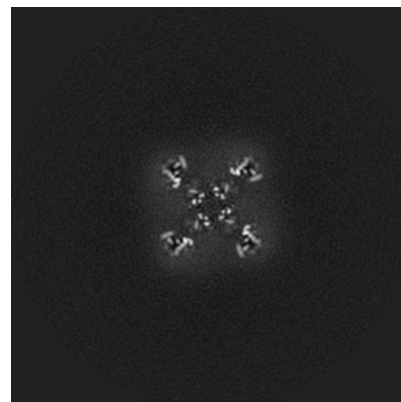
6.2.1 Primary map



X Index: 176

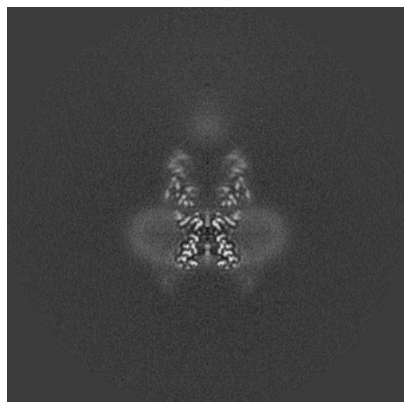


Y Index: 176

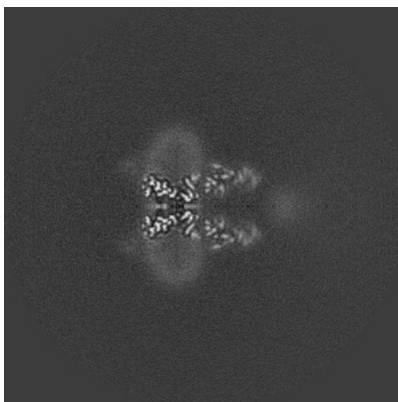


Z Index: 176

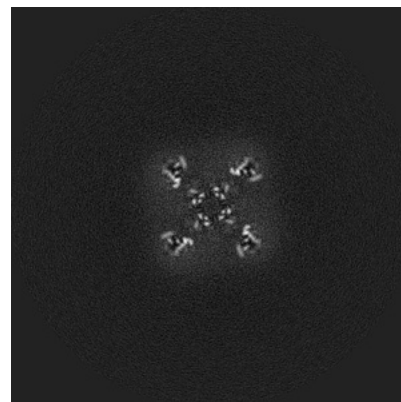
6.2.2 Raw map



X Index: 176



Y Index: 176

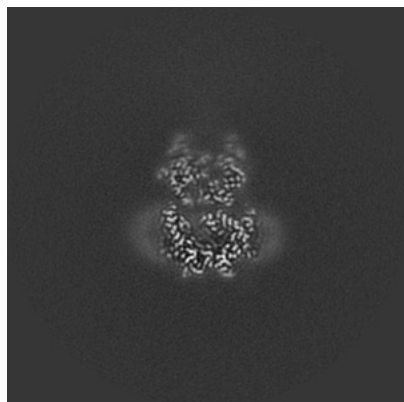


Z Index: 176

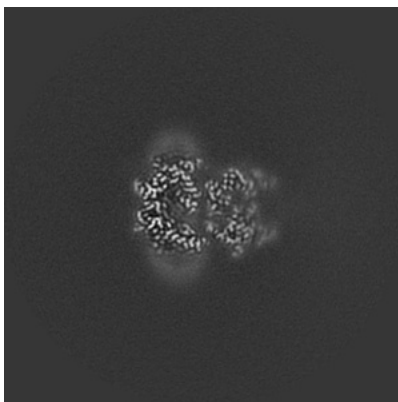
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

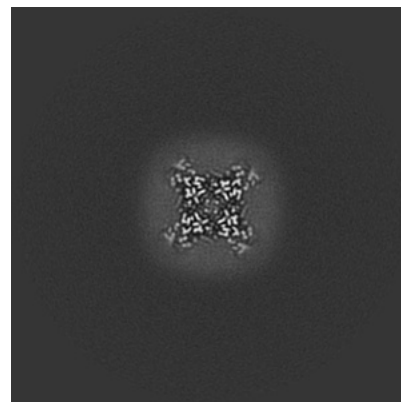
6.3.1 Primary map



X Index: 155

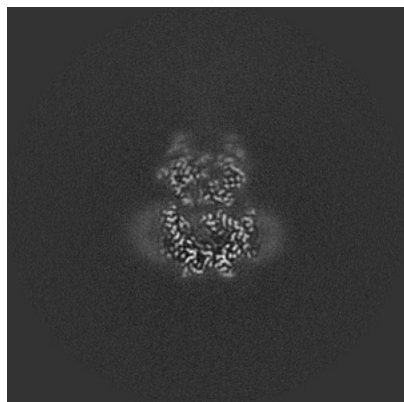


Y Index: 197

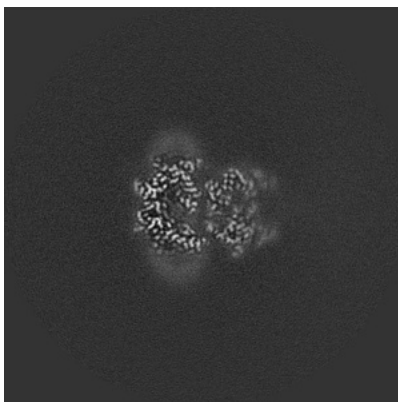


Z Index: 132

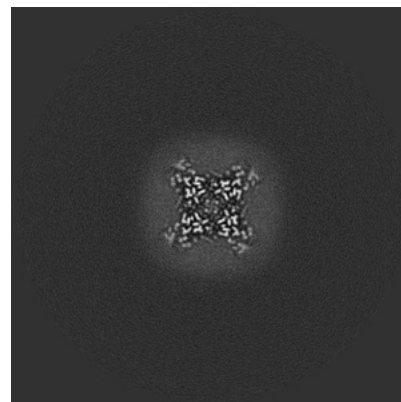
6.3.2 Raw map



X Index: 155



Y Index: 197

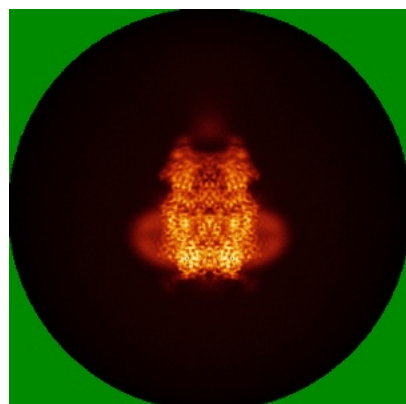


Z Index: 132

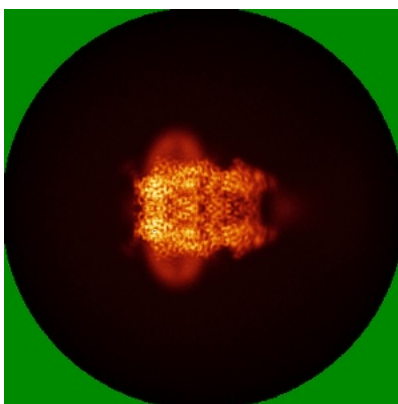
The images above show the largest variance slices of the map in three orthogonal directions.

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

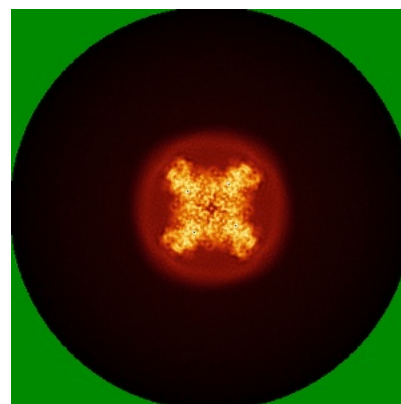
6.4.1 Primary map



X

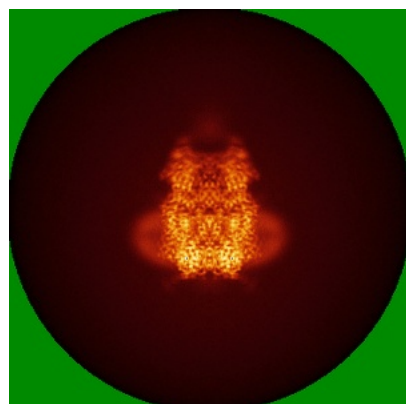


Y

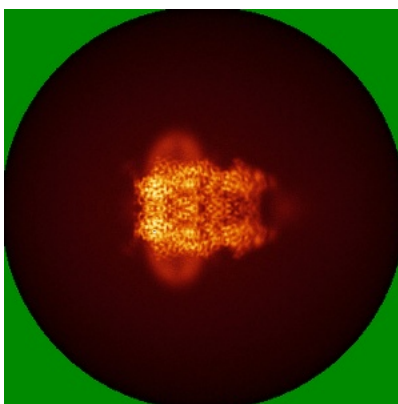


Z

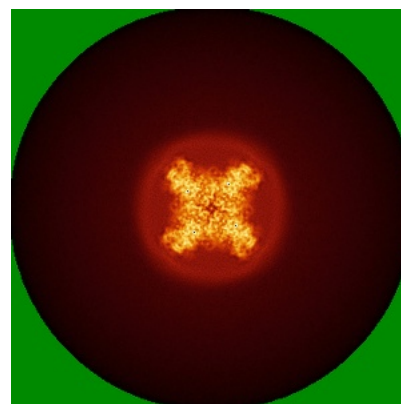
6.4.2 Raw map



X



Y

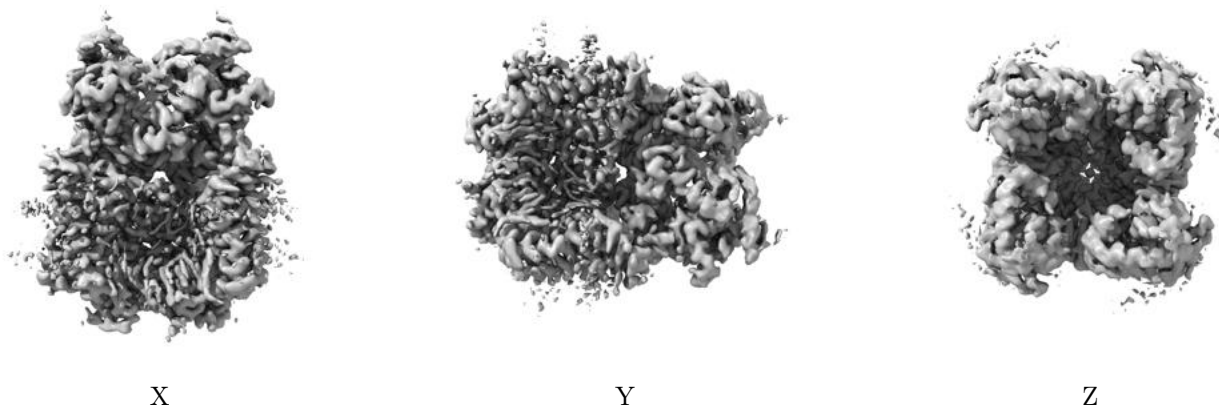


Z

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

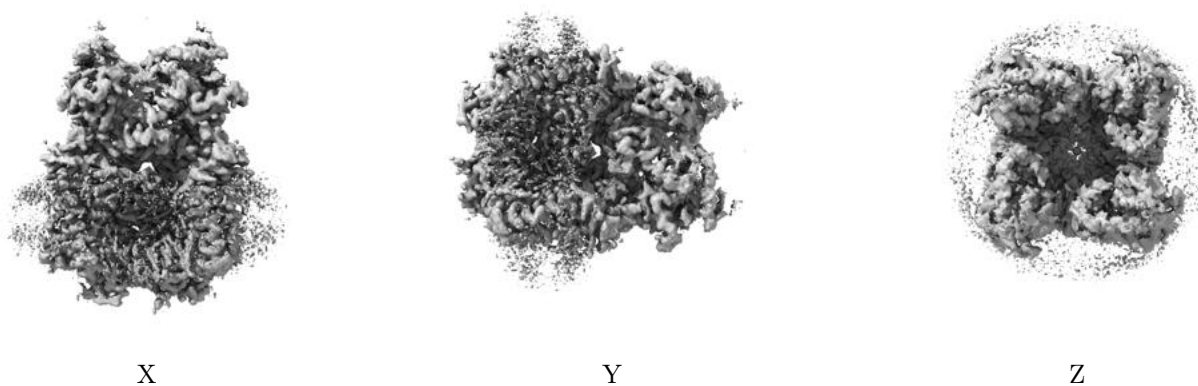
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

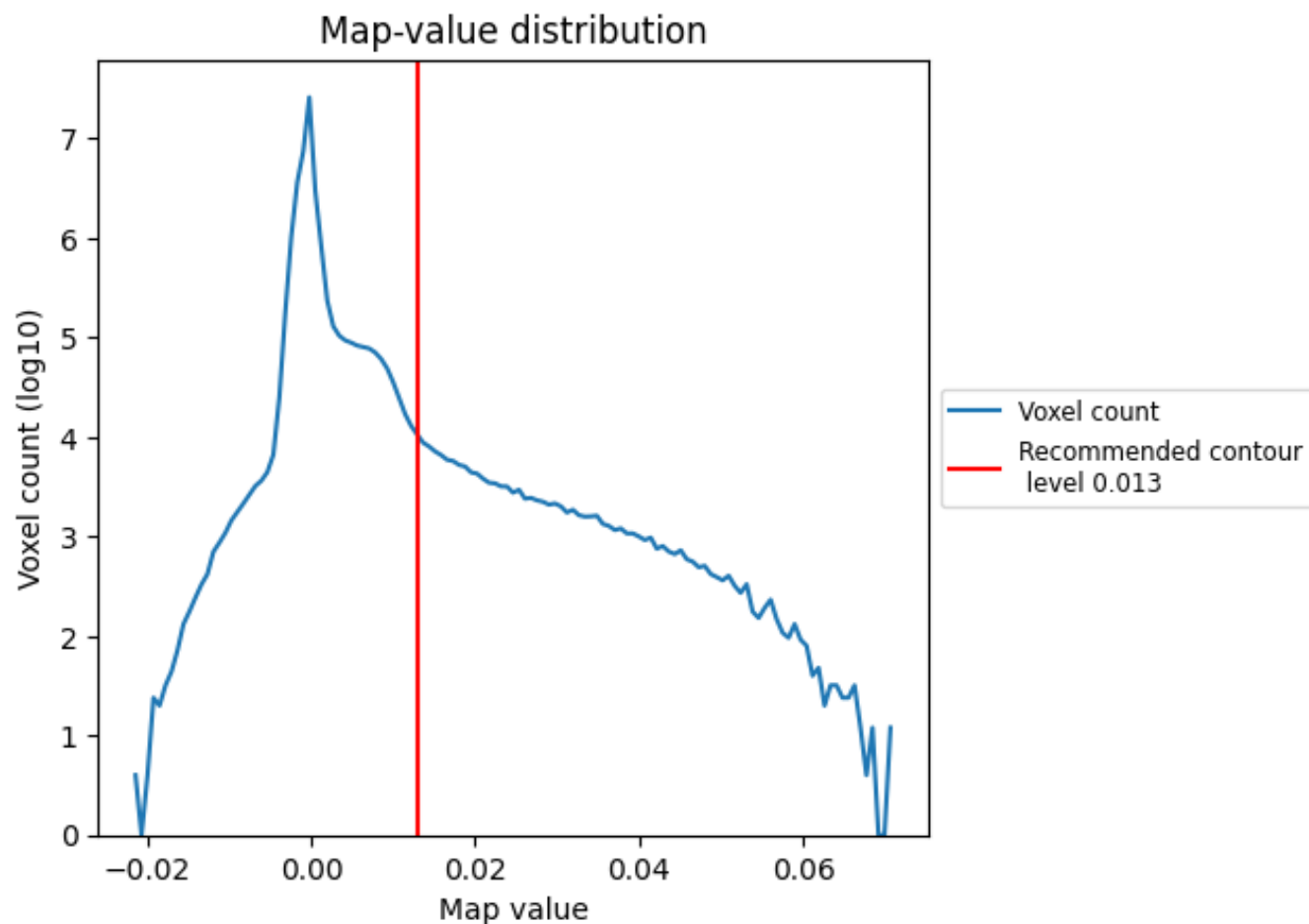
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

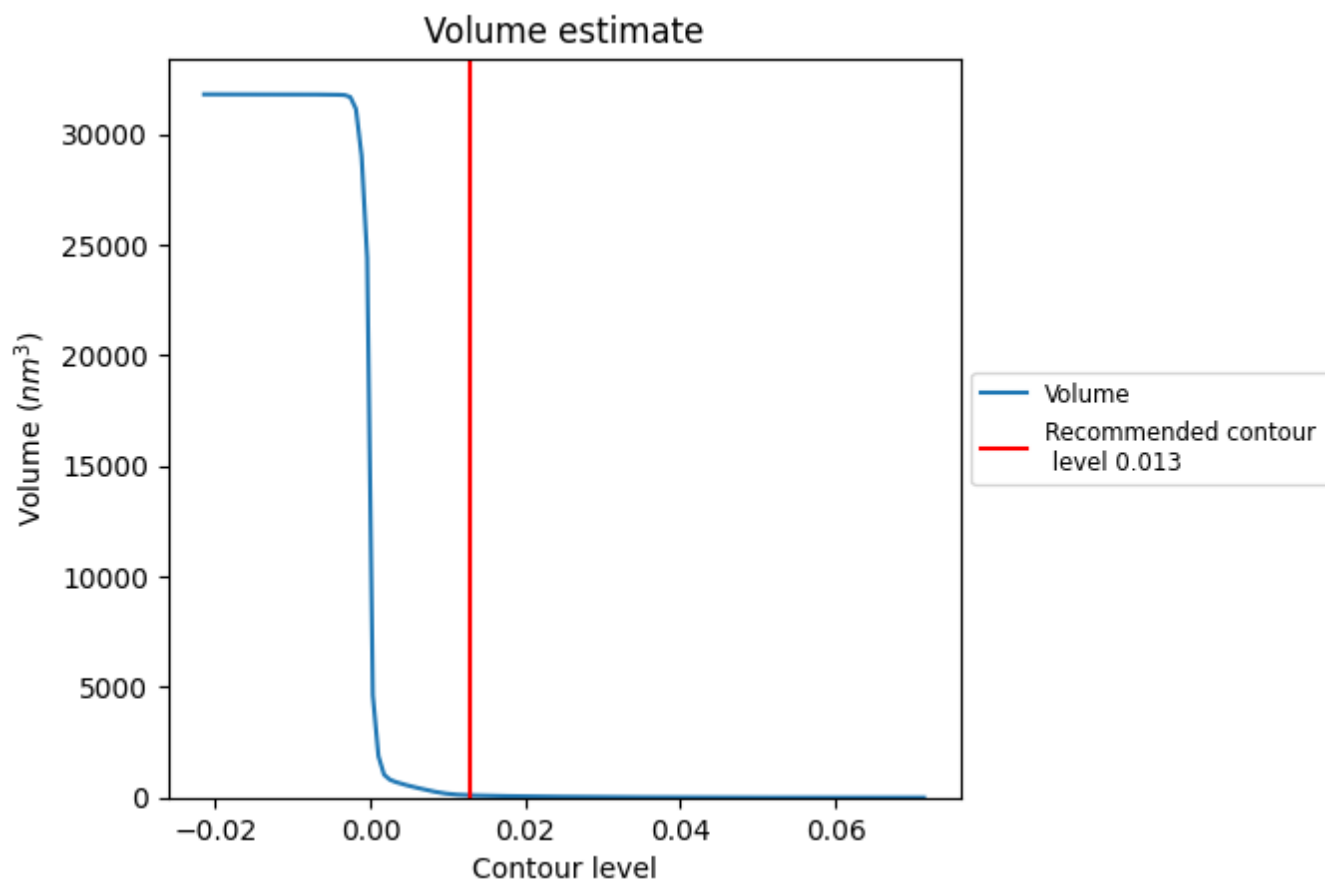
This section contains the results of statistical analysis of the map.

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.

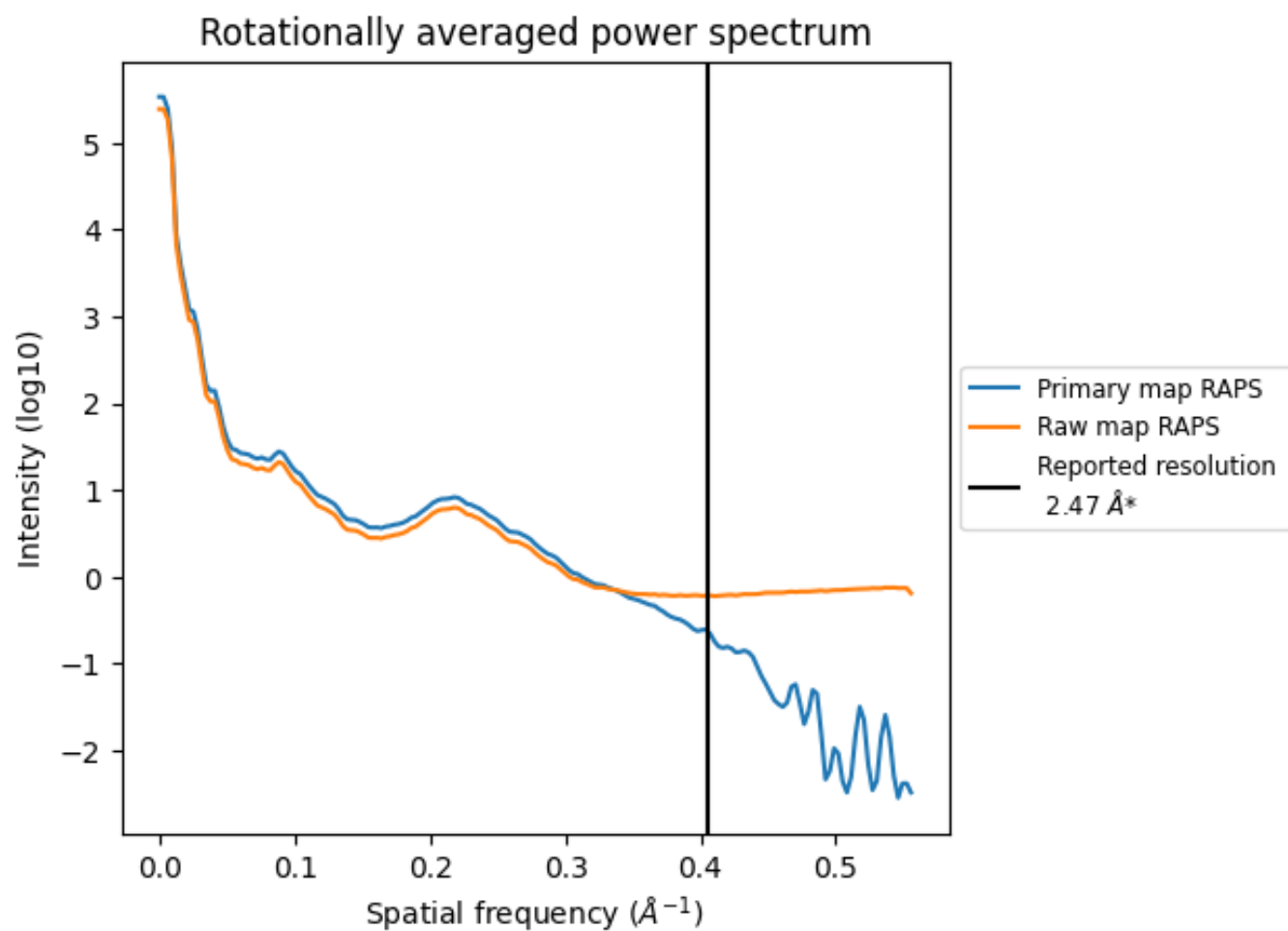
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm³; this corresponds to an approximate mass of 92 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

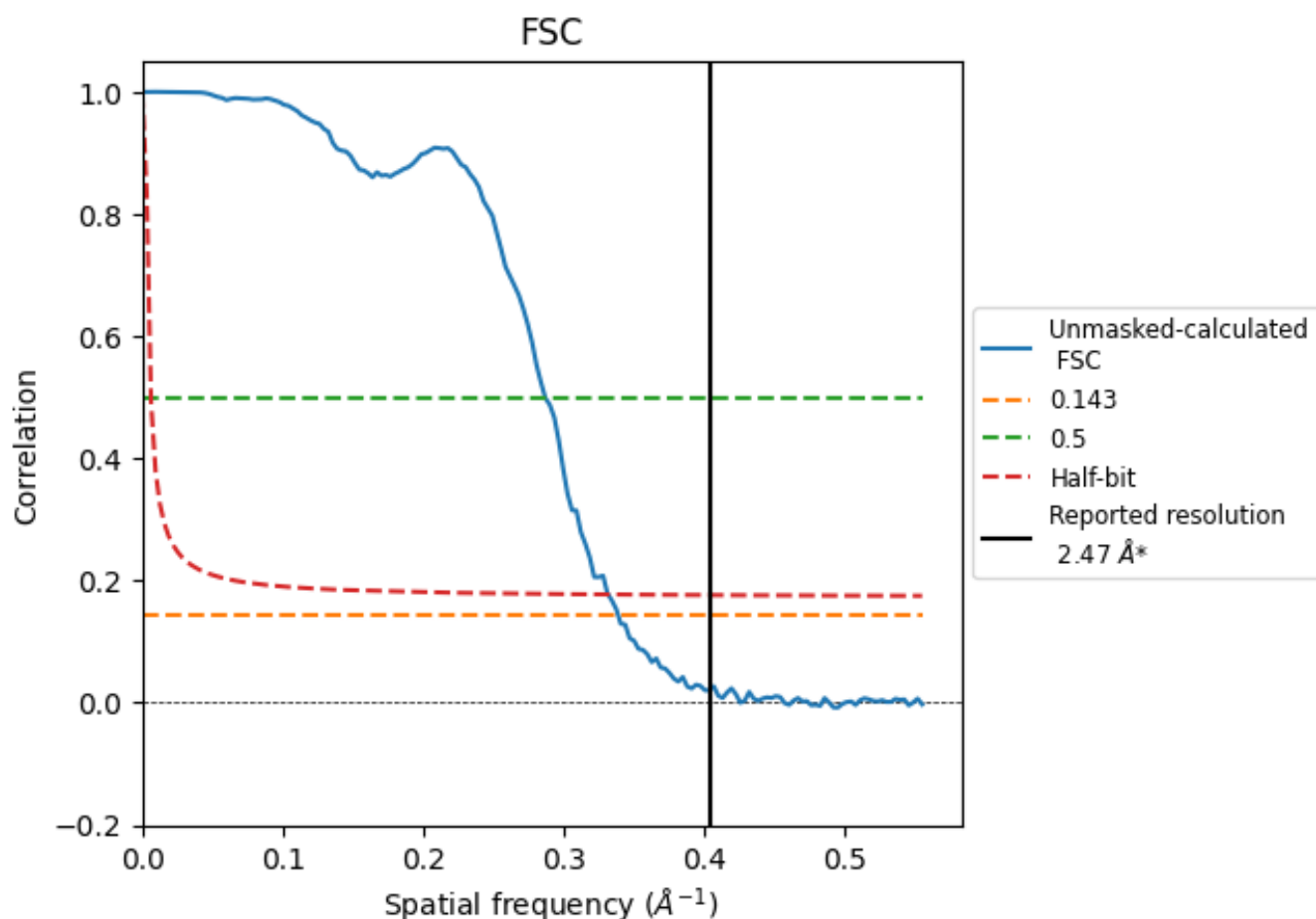


*Reported resolution corresponds to spatial frequency of 0.405 $\text{\AA}^{-1}$

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 0.405 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

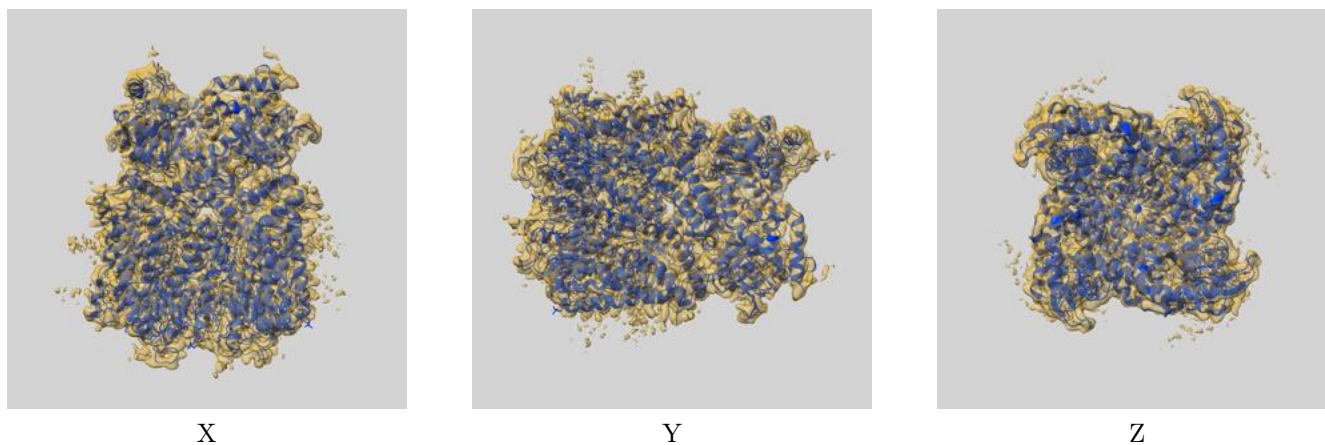
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.95	3.48	3.01

*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 2.95 differs from the reported value 2.47 by more than 10 %

9 Map-model fit [i](#)

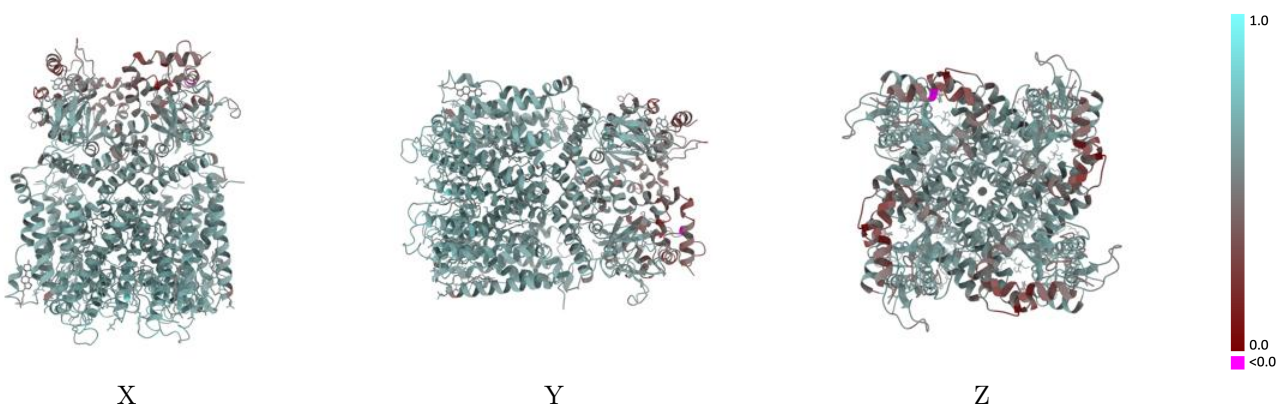
This section contains information regarding the fit between EMDB map EMD-74535 and PDB model 9ZPW. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



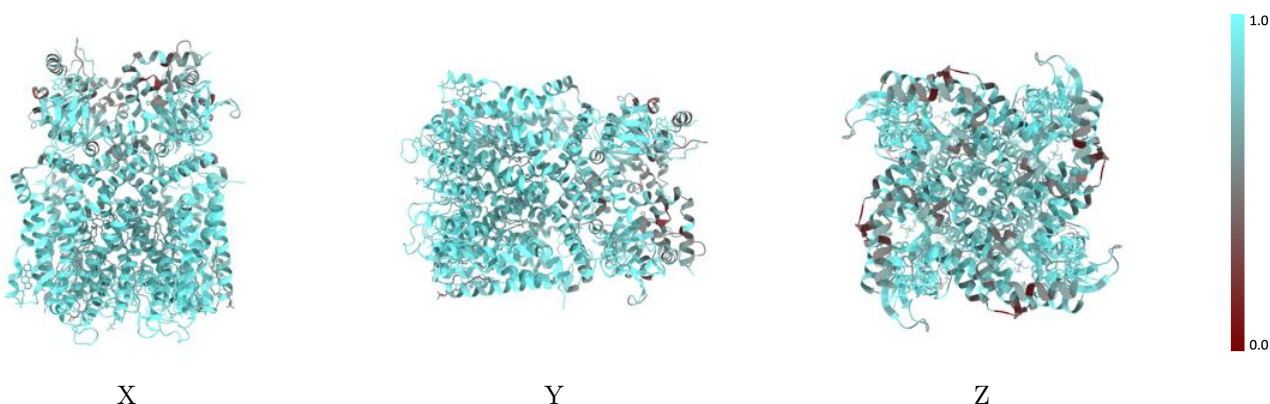
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



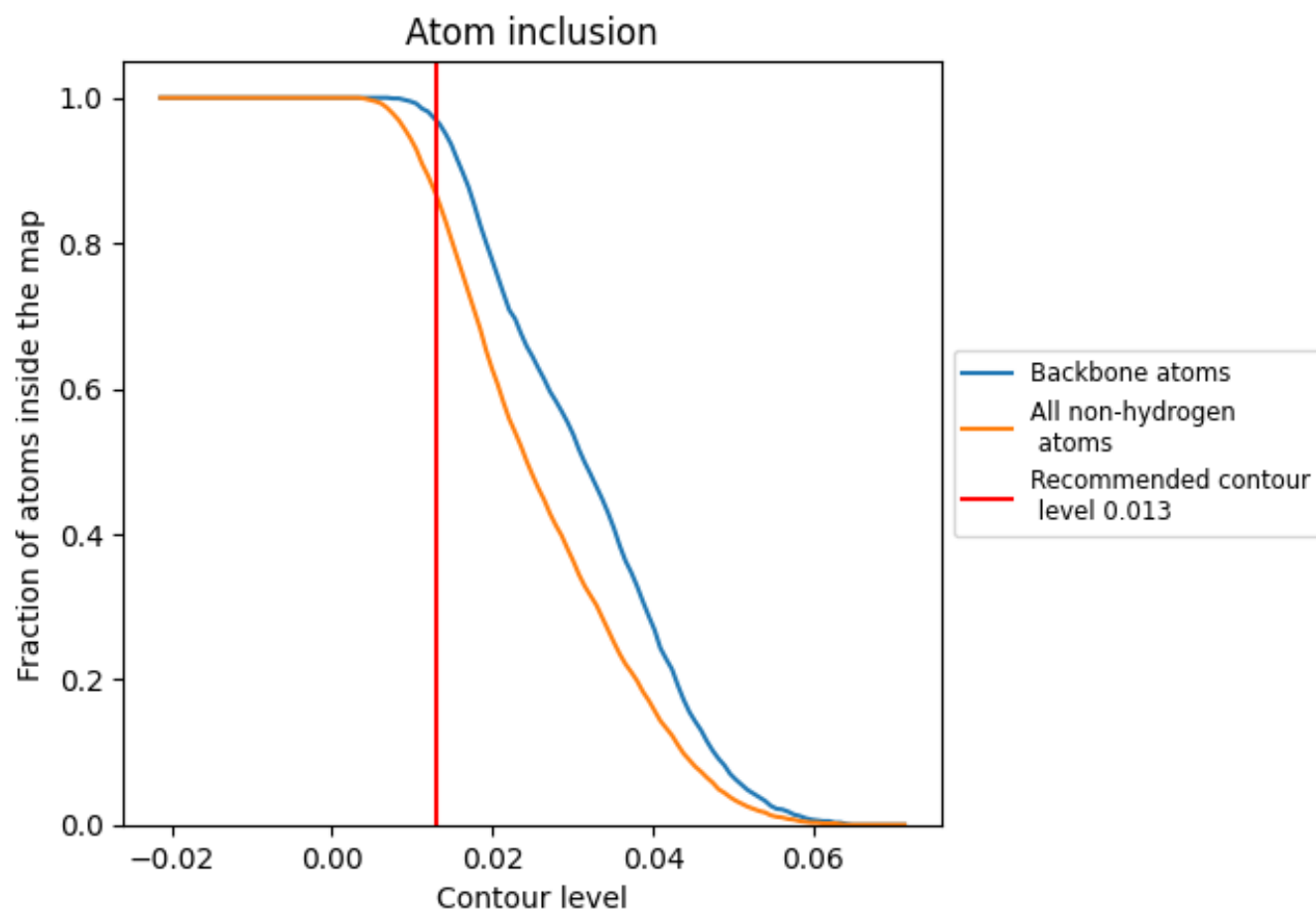
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 87% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8660	0.5760
A	0.8670	0.5760
B	0.8640	0.5770
C	0.8660	0.5760
D	0.8670	0.5760

