



## wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 09:18 PM EDT

PDB ID : 8TKF  
EMDB ID : EMD-41349  
Title : Human Type 3 IP3 Receptor - Activated State (+IP3/ATP/JD Ca2+)  
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.  
Deposited on : 2023-07-25  
Resolution : 3.20 Å(reported)

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

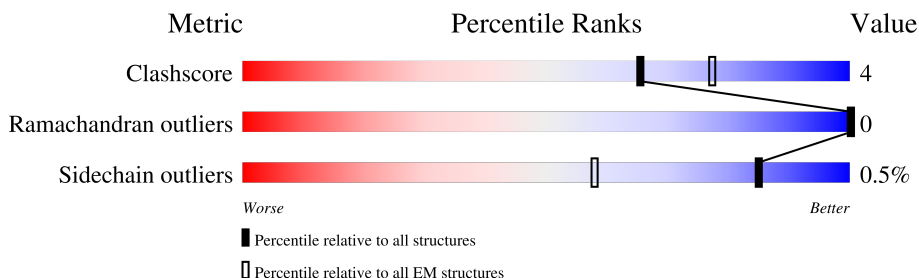
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	2671	
1	B	2671	
1	C	2671	
1	D	2671	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 148344 atoms, of which 74244 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.

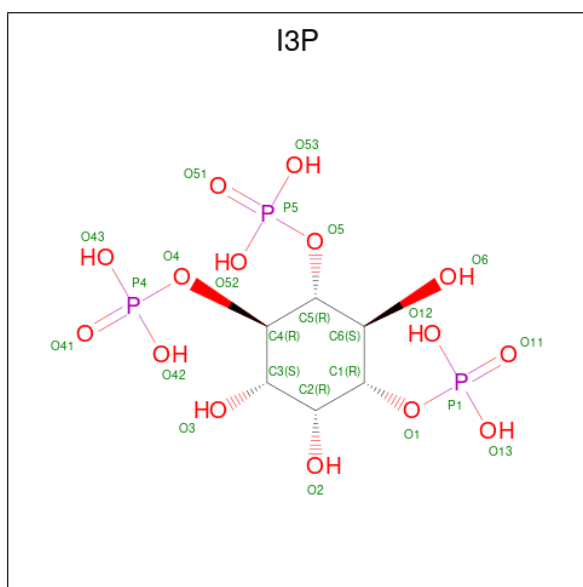
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2272	Total	C	H	N	O	S	0	0
			36472	11639	18244	3114	3363	112		
1	B	2272	Total	C	H	N	O	S	0	0
			36472	11639	18244	3114	3363	112		
1	C	2272	Total	C	H	N	O	S	0	0
			36472	11639	18244	3114	3363	112		
1	D	2272	Total	C	H	N	O	S	0	0
			36472	11639	18244	3114	3363	112		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula:  $C_6H_{15}O_{15}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

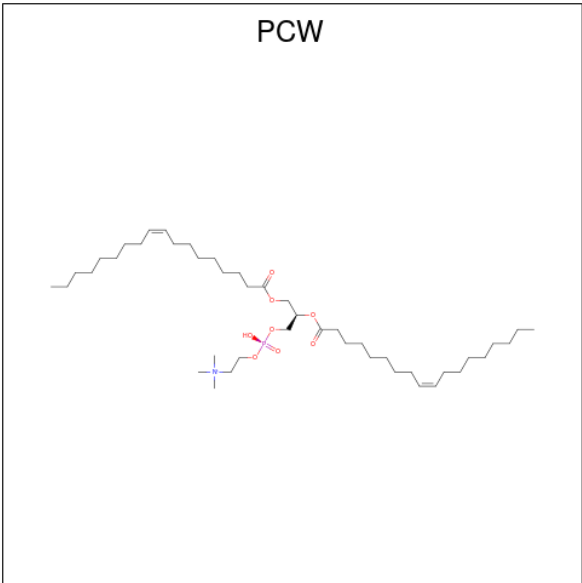
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



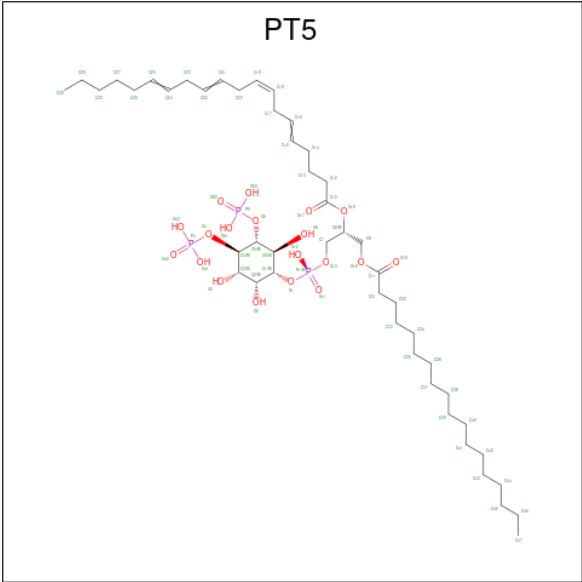
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 6 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			105	35	60	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			114	37	67	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			105	35	60	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			114	37	67	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			105	35	60	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			114	37	67	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			105	35	60	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			114	37	67	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	

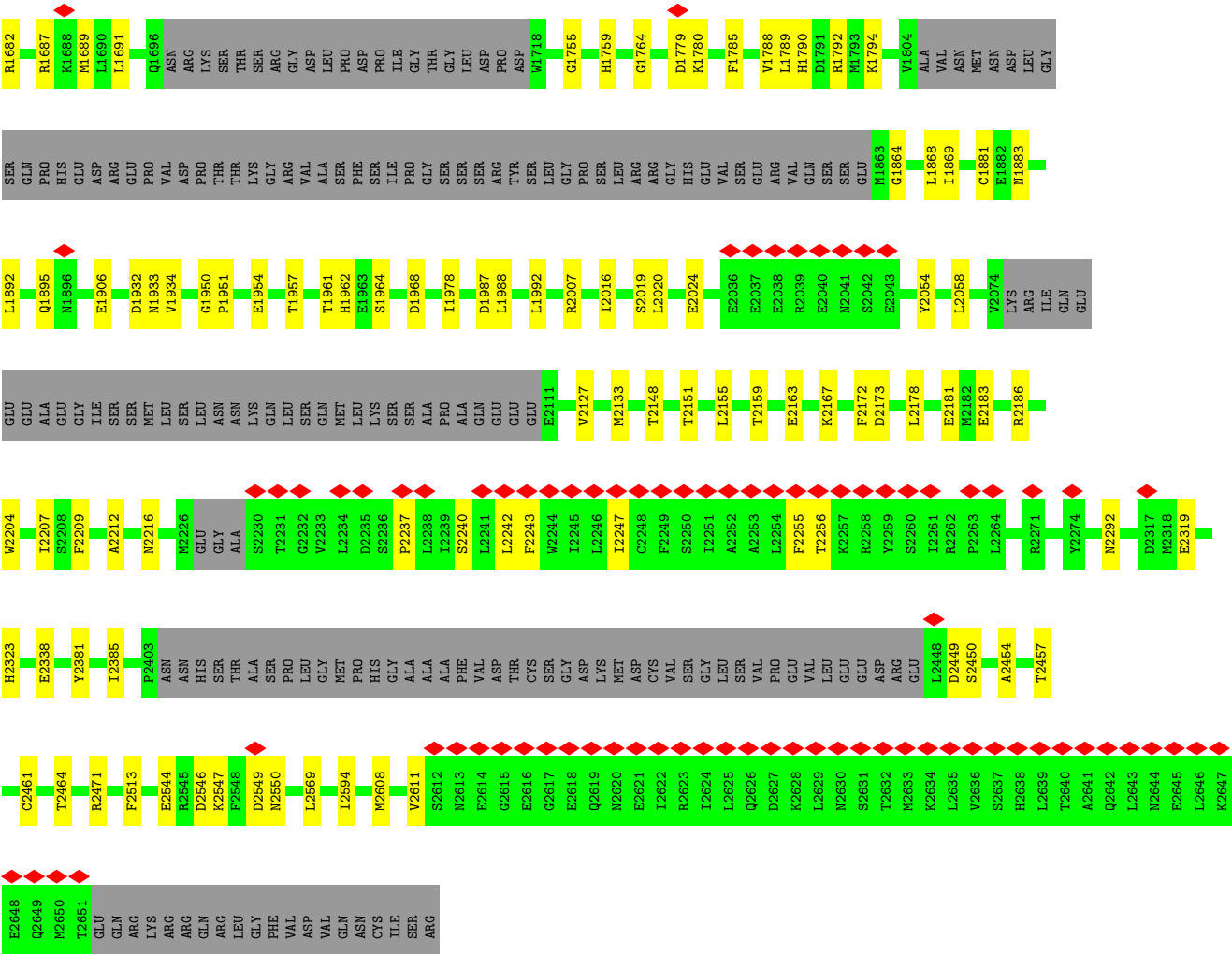
- Molecule 7 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: C<sub>47</sub>H<sub>85</sub>O<sub>19</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	O	P	0
			118	42	54	19	3	
7	B	1	Total	C	H	O	P	0
			118	42	54	19	3	
7	C	1	Total	C	H	O	P	0
			118	42	54	19	3	
7	D	1	Total	C	H	O	P	0
			118	42	54	19	3	

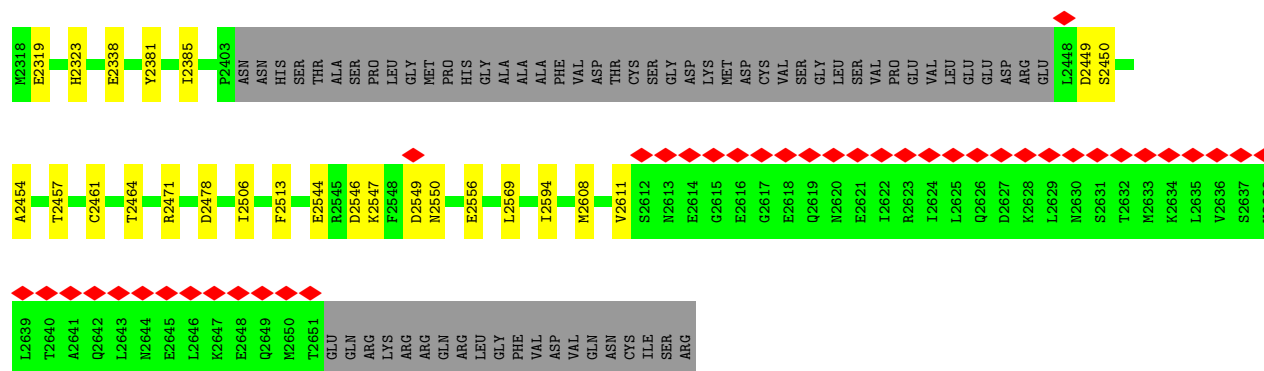




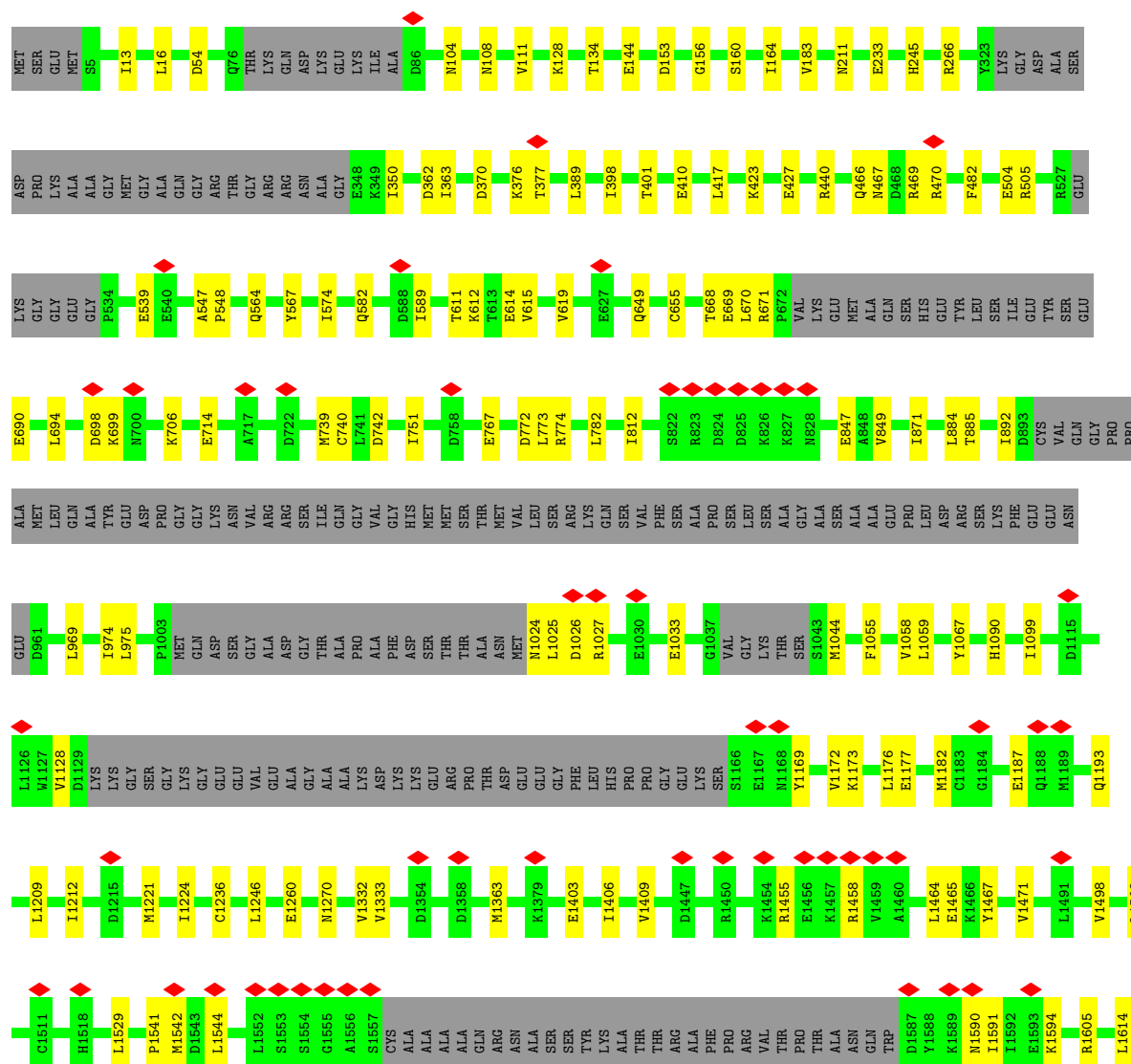
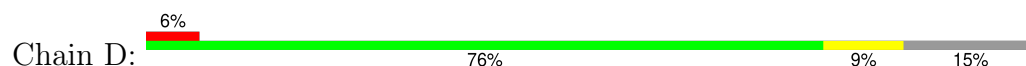








• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



D1619	H1650	L1654	E1658	D1681	R1682	R1687	K1688	M1689	L1690	L1691	Q1696	ASN	ARG	LYS	SER	THR	THR	LYS	ARG	GLY	ASP	LEU	ALA	ASP	PRO	ASP	W1718	G1755	H1759	G1764	D1779	K1780	K1781	F1785	V1788	H1789	H1790	D1791	R1792	M1793	K1794								
V1804	ALA	VAL	ASN	MET	ASN	ASP	LEU	SER	GLN	PRO	HIS	GLU	ASP	ARG	GLU	PRO	VAL	ASN	VAL	ARG	GLY	VAL	ASP	PRO	THR	THR	TYR	SER	LEU	GLY	PRO	SER	LEU	ARG	ARG	VAL	GLN	SER	SER	GLU	ARG	VAL	GLN	SER	SER	GLU			
M1863	G1864	L1868	I1869	Q1878	C1881	E1882	N1883	L1892	Q1895	N1896	E1906	D1932	M1933	V1934	Q1939	G1950	P1951	E1954	T1957	T1961	H1962	K1963	S1964	D1968	I1978	D1987	L1988	L1992	R2007	I2016	S2019	L2020	E2024	E2036	E2037	E2038	R2039	E2040											
N2041	S2042	E2043	Y2054	L2058	V2074	LYS	ARG	ILE	GLN	GLU	GLU	GLU	ALA	GLU	GLY	ILE	SER	MET	LEU	SER	LEU	ASN	ASN	LYS	GLN	SER	SER	ALA	PRO	ALA	GLN	GLU	GLU	E2111	V2127	M2133	T2148	T2151	L2155	T2159	E2163								
K2167	F2172	D2173	L2178	E2181	R2199	W2204	I2207	S2208	F2209	A2212	N2216	K2226	GLU	GLY	ALA	S2230	T2231	G2232	V2233	L2234	D2235	S2236	P2237	L2238	I2239	S2240	L2241	L2242	F2243	W2244	I2245	L2246	I2247	C2248	F2249	S2250	I2251	A2252	A2253	L2254	F2255	T2256	K2257	R2258	Y2259	S2260	I2261	R2262	F2263
L2264	I2265	R2271	V2274	N2292	D2317	M2318	E2319	H2323	E2338	Y2381	I2385	F2403	ASN	ASN	HIS	SER	THR	ALA	SER	PRO	LEU	GLY	MET	PRO	HIS	GLY	ALA	ALA	PHE	VAL	ASP	THR	CYS	SER	GLY	ASP	LYS	MET	ASP	CYS	VAL	SER	GLY	LEU	SER	VAL	PRO	GLU	VAL
LEU	GLU	GLU	ASP	ARG	GLU	L2448	D2449	S2450	A2454	T2457	C2461	T2464	R2471	D2478	I2506	F2513	E2544	R2545	D2546	K2547	F2548	D2549	N2550	L2569	I2594	M2608	V2611	S2612	N2613	E2614	G2615	E2616	G2617	E2618	Q2619	N2620	E2621	I2622	R2623	I2624	L2625	Q2626	D2627	K2628	L2629	N2630			
S2631	T2632	M2633	K2634	L2635	V2636	S2637	H2638	L2639	T2640	A2641	Q2642	L2643	N2644	E2645	L2646	K2647	E2648	Q2649	M2650	T2651	GLU	GLN	ARG	LYS	ARG	ARG	GLN	ARG	LEU	GLY	PHE	VAL	VAL	GLN	ASN	CYS	ILE	SER	ARG										

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	228188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	107.065	Depositor
Minimum map value	-41.251	Depositor
Average map value	0.126	Depositor
Map value standard deviation	1.558	Depositor
Recommended contour level	6	Depositor
Map size (Å)	422.68802, 422.68802, 422.68802	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.629, 0.629, 0.629	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, PT5, ATP, I3P, PCW

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/18566	0.43	0/25094
1	B	0.24	0/18566	0.43	0/25094
1	C	0.24	0/18566	0.43	0/25094
1	D	0.24	0/18566	0.43	0/25094
All	All	0.24	0/74264	0.43	0/100376

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	1090	HIS	Sidechain
1	B	1090	HIS	Sidechain
1	C	1090	HIS	Sidechain
1	D	1090	HIS	Sidechain

## 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	18228	18244	18243	144	0
1	B	18228	18244	18243	141	0
1	C	18228	18244	18243	144	0
1	D	18228	18244	18243	144	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	1	0
3	B	24	9	9	1	0
3	C	24	9	9	1	0
3	D	24	9	9	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
6	A	176	242	242	1	0
6	B	176	242	242	1	0
6	C	176	242	242	1	0
6	D	176	242	242	1	0
7	A	64	54	64	3	0
7	B	64	54	64	3	0
7	C	64	54	64	3	0
7	D	64	54	64	3	0
All	All	74100	74244	74280	567	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.

The worst 5 of 567 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:1182:MET:SD	1:B:1193:GLN:NE2	2.60	0.75
1:D:1182:MET:SD	1:D:1193:GLN:NE2	2.60	0.75
1:C:1182:MET:SD	1:C:1193:GLN:NE2	2.60	0.74
1:D:2255:PHE:O	1:D:2256:THR:OG1	2.06	0.74
1:A:1182:MET:SD	1:A:1193:GLN:NE2	2.60	0.74

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	2242/2671 (84%)	2198 (98%)	44 (2%)	0	100	100
1	B	2242/2671 (84%)	2198 (98%)	44 (2%)	0	100	100
1	C	2242/2671 (84%)	2198 (98%)	44 (2%)	0	100	100
1	D	2242/2671 (84%)	2198 (98%)	44 (2%)	0	100	100
All	All	8968/10684 (84%)	8792 (98%)	176 (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	2023/2385 (85%)	2012 (100%)	11 (0%)	86	93
1	B	2023/2385 (85%)	2012 (100%)	11 (0%)	86	93

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	2023/2385 (85%)	2012 (100%)	11 (0%)	86	93
1	D	2023/2385 (85%)	2012 (100%)	11 (0%)	86	93
All	All	8092/9540 (85%)	8048 (100%)	44 (0%)	85	93

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1458	ARG
1	D	742	ASP
1	C	1464	LEU
1	C	2292	ASN
1	D	1270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1318	GLN
1	B	2161	GLN
1	C	1298	GLN
1	C	1318	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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	I3P	A	3002	-	24,24,24	2.18	3 (12%)	39,39,39	0.89	0
6	PCW	C	2708	-	46,46,53	0.52	0	52,54,61	0.46	0
6	PCW	D	2706	-	42,42,53	0.54	0	48,50,61	0.50	0
7	PT5	C	2701	-	64,64,69	1.51	7 (10%)	79,82,87	1.13	6 (7%)
5	ATP	D	2705	-	28,33,33	0.64	0	34,52,52	0.92	1 (2%)
6	PCW	D	2708	-	46,46,53	0.52	0	52,54,61	0.46	0
6	PCW	B	2706	-	42,42,53	0.54	0	48,50,61	0.50	0
6	PCW	B	2708	-	46,46,53	0.52	0	52,54,61	0.46	0
6	PCW	C	2707	-	44,44,53	0.53	0	50,52,61	0.50	0
6	PCW	A	3006	-	44,44,53	0.53	0	50,52,61	0.50	0
6	PCW	C	2709	-	40,40,53	0.55	0	46,48,61	0.49	0
6	PCW	A	3005	-	42,42,53	0.54	0	48,50,61	0.50	0
7	PT5	A	3009	-	64,64,69	1.51	7 (10%)	79,82,87	1.13	6 (7%)
3	I3P	B	2703	-	24,24,24	2.18	3 (12%)	39,39,39	0.89	0
5	ATP	A	3004	-	28,33,33	0.64	0	34,52,52	0.92	1 (2%)
7	PT5	D	2701	-	64,64,69	1.51	7 (10%)	79,82,87	1.13	6 (7%)
3	I3P	D	2703	-	24,24,24	2.18	3 (12%)	39,39,39	0.89	0
3	I3P	C	2703	-	24,24,24	2.18	3 (12%)	39,39,39	0.89	0
6	PCW	B	2707	-	44,44,53	0.53	0	50,52,61	0.50	0
5	ATP	B	2705	-	28,33,33	0.64	0	34,52,52	0.92	1 (2%)
6	PCW	A	3007	-	46,46,53	0.52	0	52,54,61	0.46	0
7	PT5	B	2701	-	64,64,69	1.51	7 (10%)	79,82,87	1.13	6 (7%)
6	PCW	D	2709	-	40,40,53	0.55	0	46,48,61	0.49	0
6	PCW	C	2706	-	42,42,53	0.54	0	48,50,61	0.50	0
6	PCW	D	2707	-	44,44,53	0.53	0	50,52,61	0.50	0
6	PCW	A	3008	-	40,40,53	0.55	0	46,48,61	0.49	0
5	ATP	C	2705	-	28,33,33	0.64	0	34,52,52	0.92	1 (2%)
6	PCW	B	2709	-	40,40,53	0.56	0	46,48,61	0.49	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	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
6	PCW	C	2708	-	-	11/50/50/57	-
6	PCW	D	2706	-	-	11/46/46/57	-
7	PT5	C	2701	-	-	23/61/85/90	0/1/1/1
5	ATP	D	2705	-	-	2/18/38/38	0/3/3/3
6	PCW	D	2708	-	-	11/50/50/57	-
6	PCW	B	2706	-	-	11/46/46/57	-
6	PCW	B	2708	-	-	12/50/50/57	-
6	PCW	C	2707	-	-	8/48/48/57	-
6	PCW	A	3006	-	-	8/48/48/57	-
6	PCW	C	2709	-	-	14/44/44/57	-
6	PCW	A	3005	-	-	11/46/46/57	-
7	PT5	A	3009	-	-	23/61/85/90	0/1/1/1
3	I3P	B	2703	-	-	2/15/39/39	0/1/1/1
5	ATP	A	3004	-	-	2/18/38/38	0/3/3/3
7	PT5	D	2701	-	-	23/61/85/90	0/1/1/1
3	I3P	D	2703	-	-	2/15/39/39	0/1/1/1
3	I3P	C	2703	-	-	2/15/39/39	0/1/1/1
6	PCW	B	2707	-	-	8/48/48/57	-
5	ATP	B	2705	-	-	2/18/38/38	0/3/3/3
6	PCW	A	3007	-	-	11/50/50/57	-
7	PT5	B	2701	-	-	23/61/85/90	0/1/1/1
6	PCW	D	2709	-	-	14/44/44/57	-
6	PCW	C	2706	-	-	11/46/46/57	-
6	PCW	D	2707	-	-	8/48/48/57	-
6	PCW	A	3008	-	-	14/44/44/57	-
5	ATP	C	2705	-	-	2/18/38/38	0/3/3/3
6	PCW	B	2709	-	-	14/44/44/57	-

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	I3P	P4-O4	6.06	1.70	1.59
3	B	2703	I3P	P4-O4	6.06	1.70	1.59
3	C	2703	I3P	P4-O4	6.05	1.70	1.59
3	D	2703	I3P	P4-O4	6.05	1.70	1.59
3	A	3002	I3P	P5-O5	5.93	1.69	1.59

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3009	PT5	O16-C10-C12	3.76	119.61	111.48
7	B	2701	PT5	O16-C10-C12	3.76	119.61	111.48
7	C	2701	PT5	O16-C10-C12	3.76	119.61	111.48
7	D	2701	PT5	O16-C10-C12	3.76	119.61	111.48
7	B	2701	PT5	C17-C16-C15	-3.74	92.03	123.57

There are no chirality outliers.

5 of 285 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	PB-O3B-PG-O3G
5	B	2705	ATP	PB-O3B-PG-O3G
5	C	2705	ATP	PB-O3B-PG-O3G
5	D	2705	ATP	PB-O3B-PG-O3G
6	A	3005	PCW	C1-O3P-P-O2P

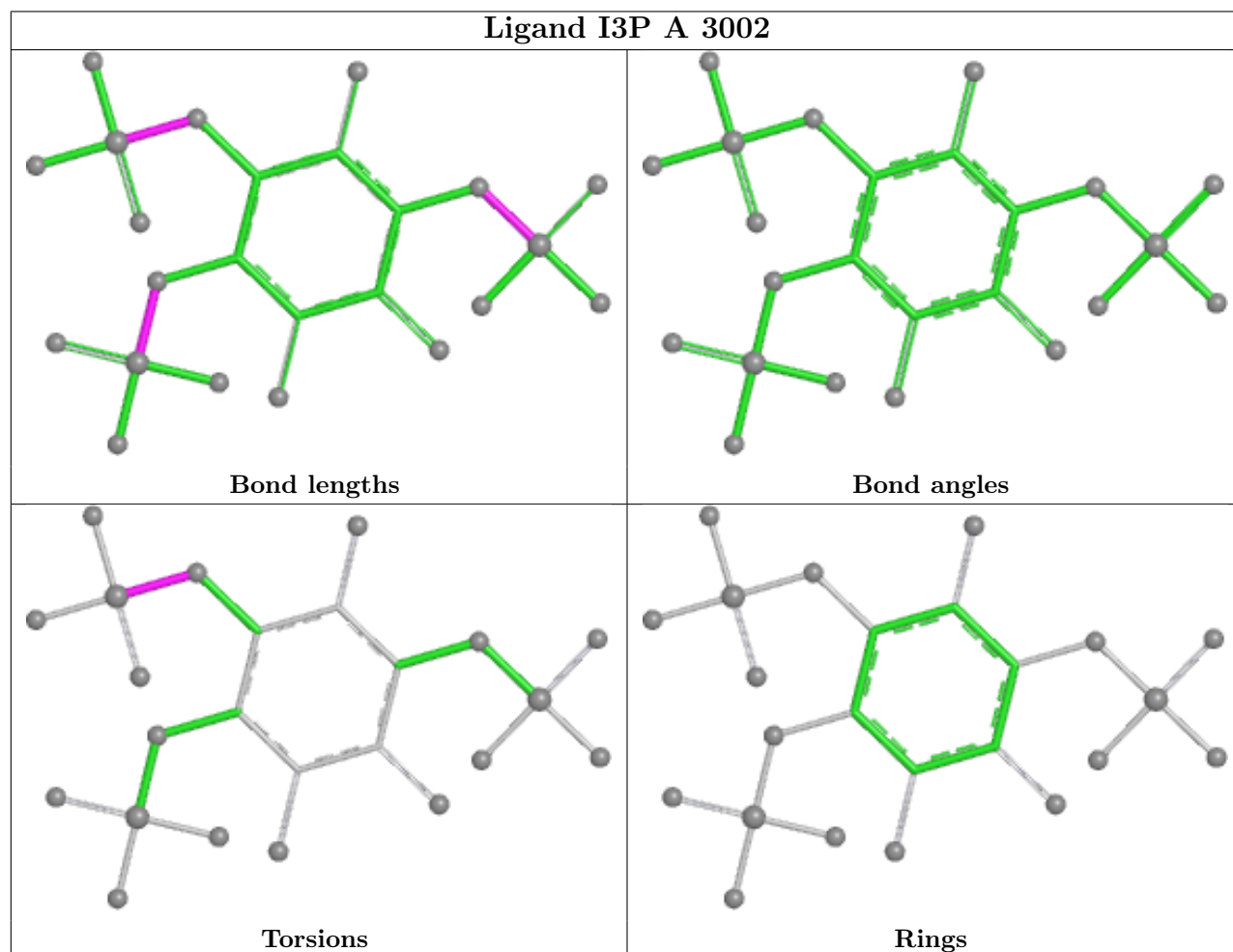
There are no ring outliers.

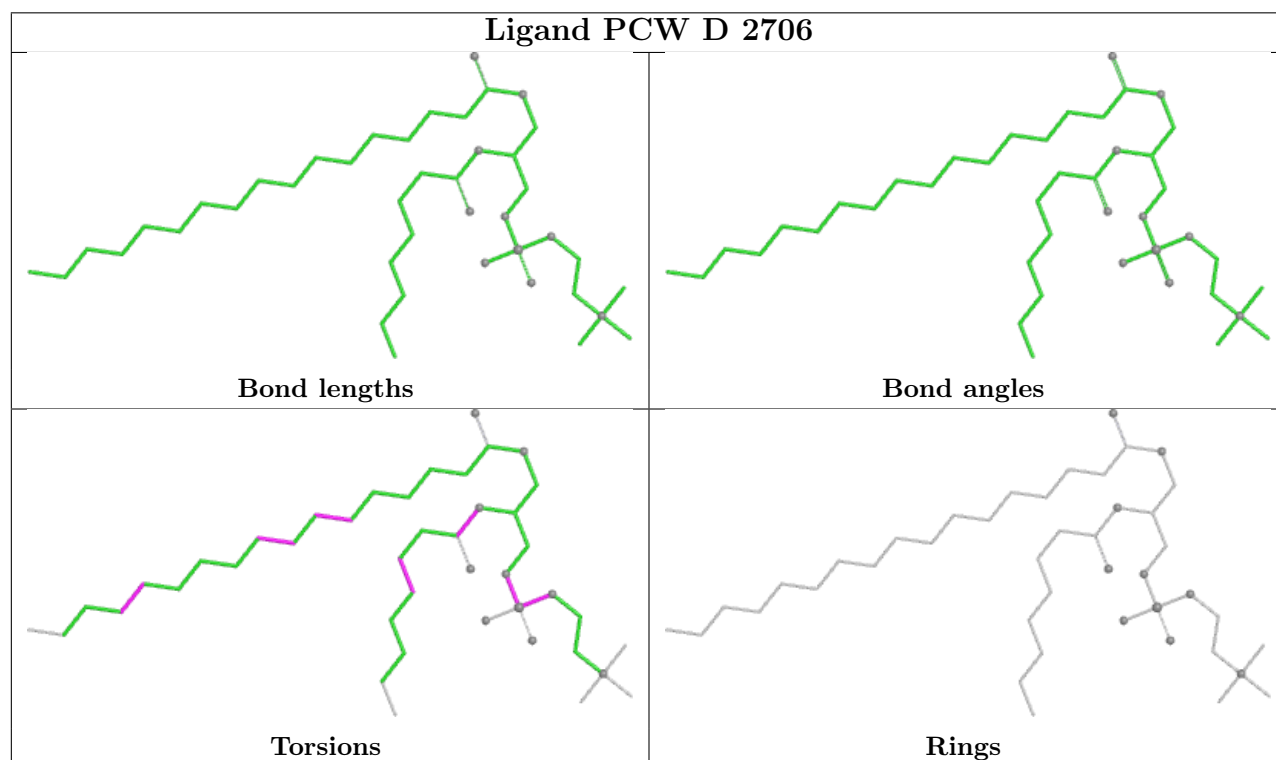
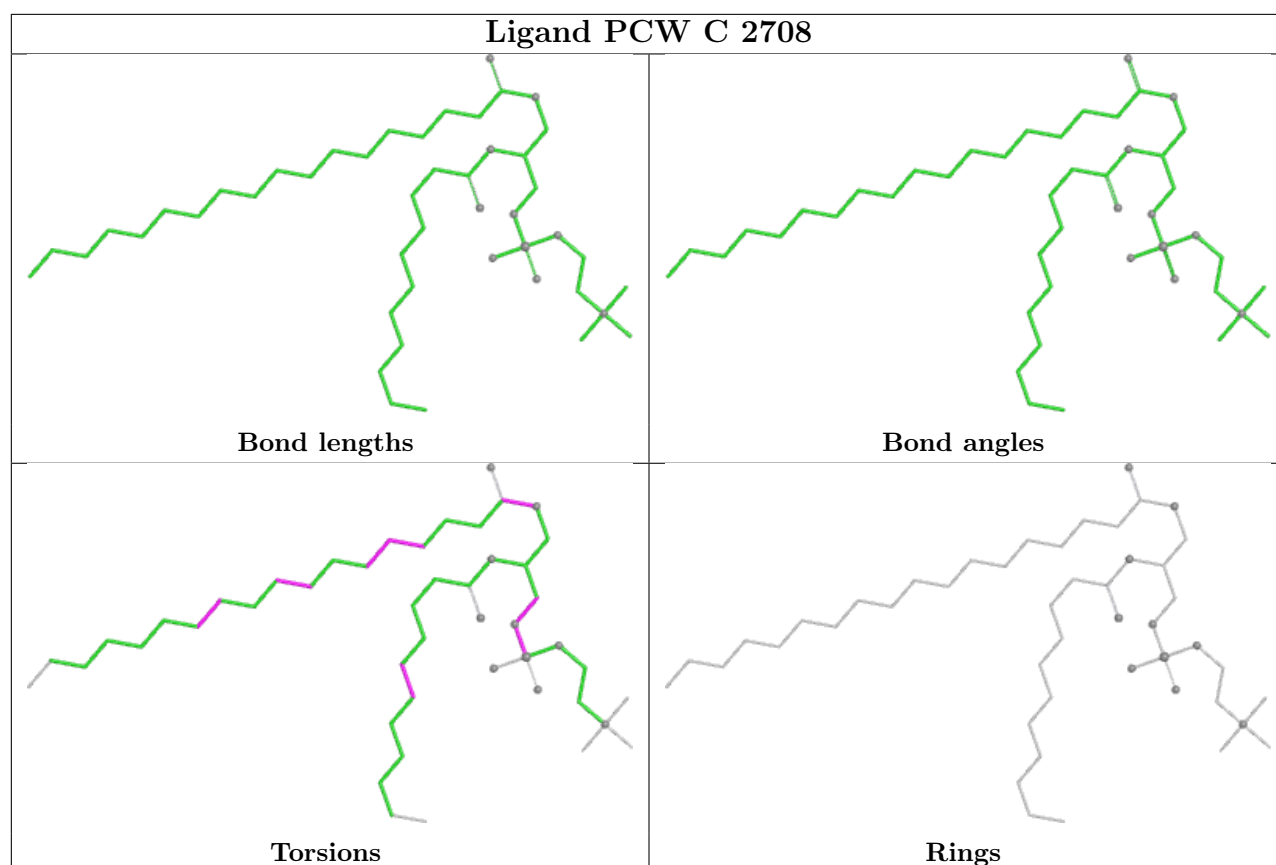
12 monomers are involved in 20 short contacts:

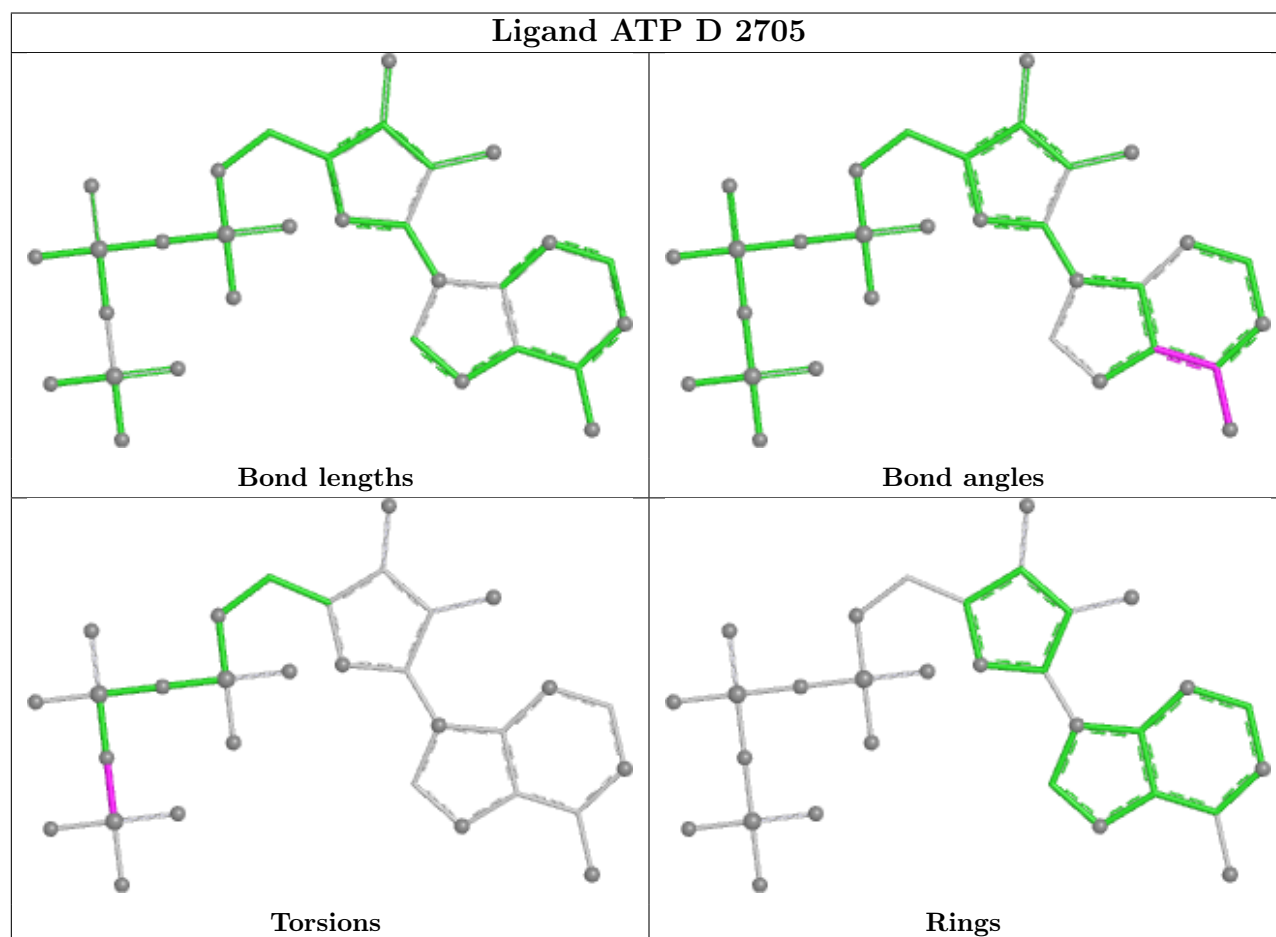
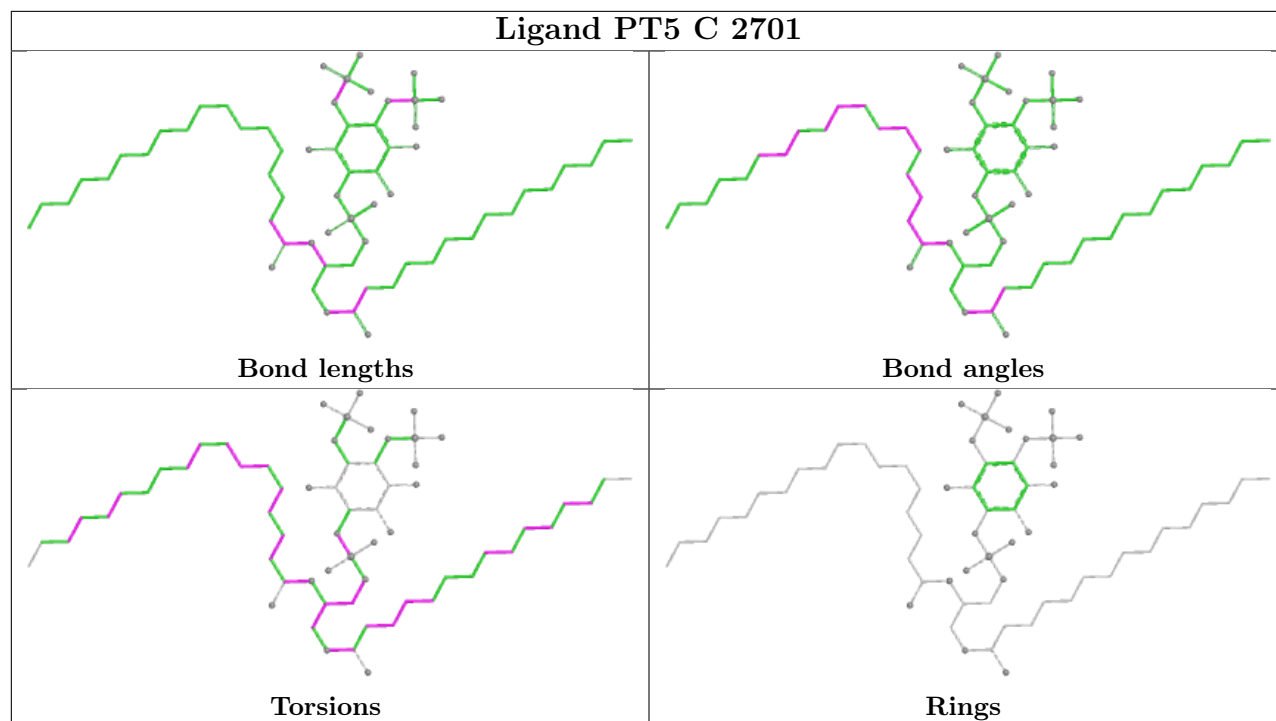
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	I3P	1	0
6	C	2708	PCW	1	0
7	C	2701	PT5	3	0
6	D	2708	PCW	1	0
6	B	2708	PCW	1	0
7	A	3009	PT5	3	0
3	B	2703	I3P	1	0
7	D	2701	PT5	3	0
3	D	2703	I3P	1	0
3	C	2703	I3P	1	0
6	A	3007	PCW	1	0
7	B	2701	PT5	3	0

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

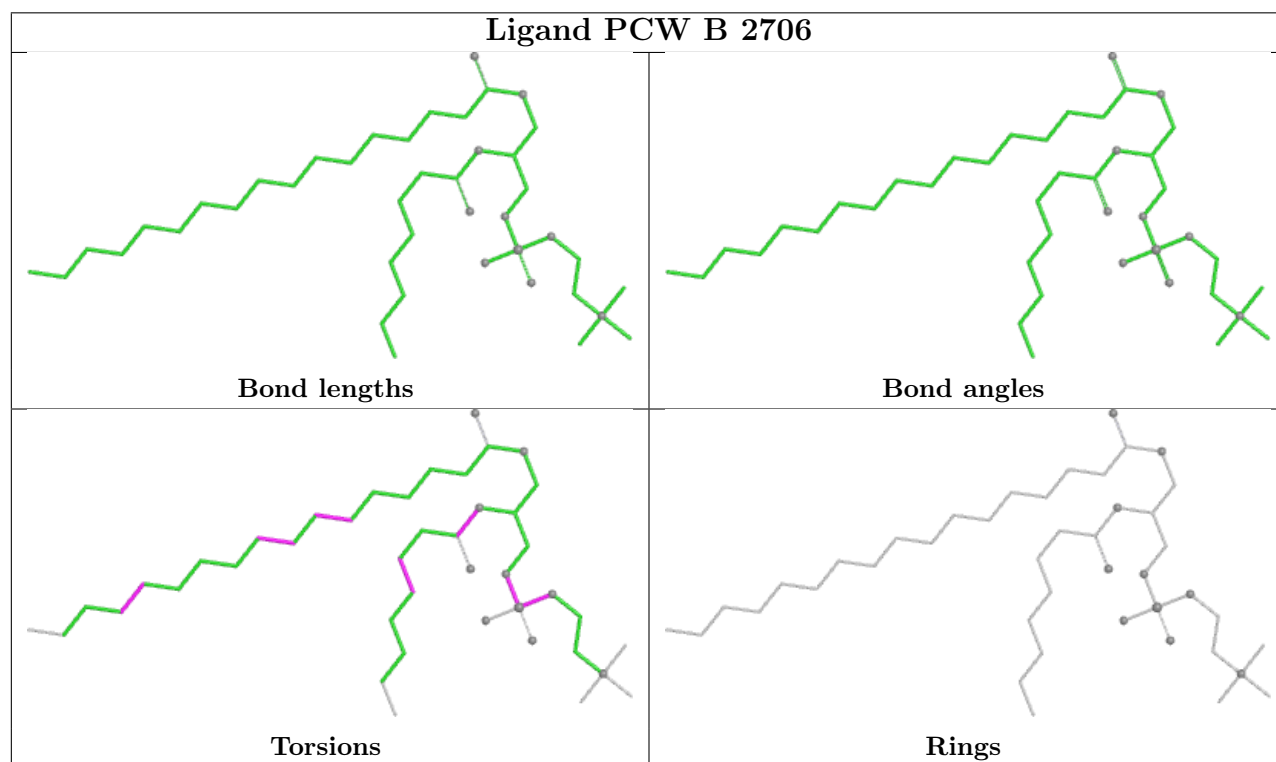
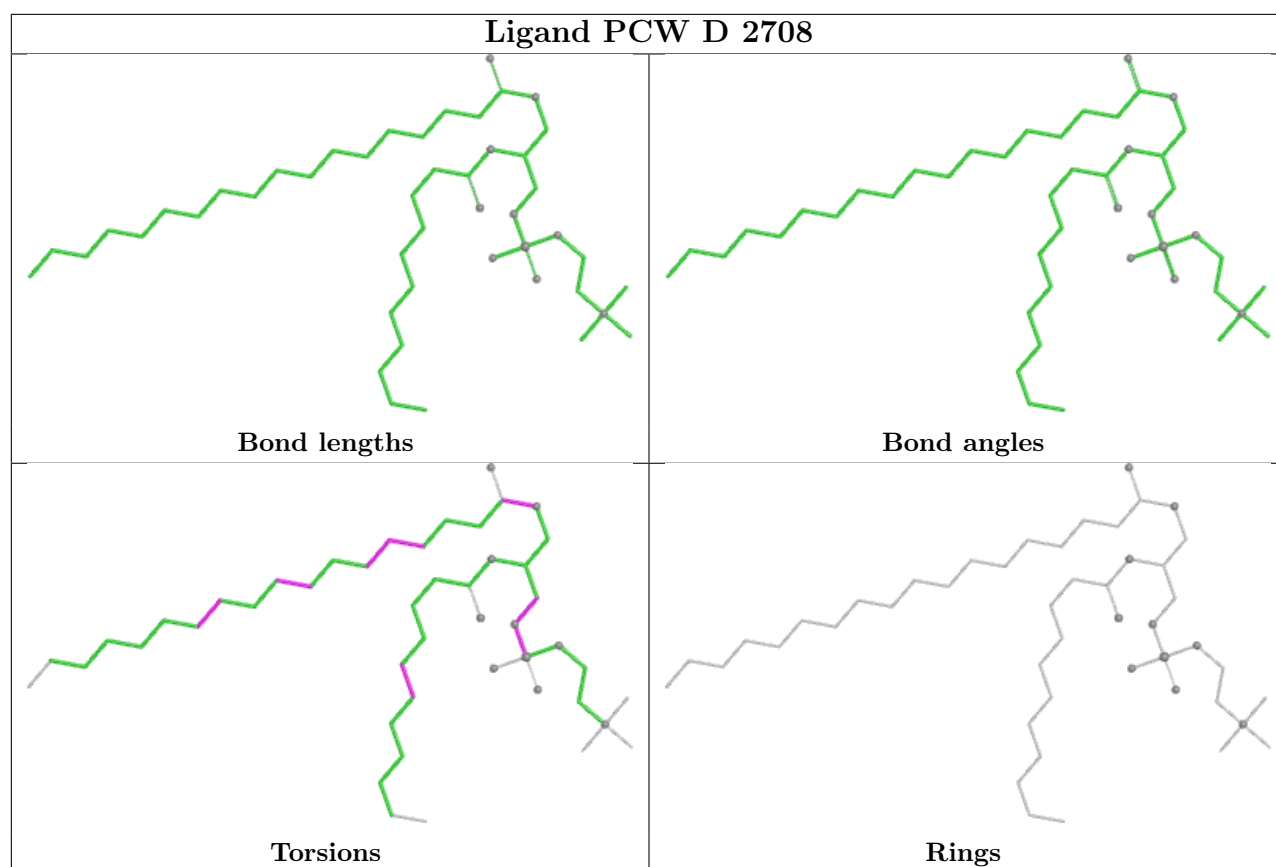
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

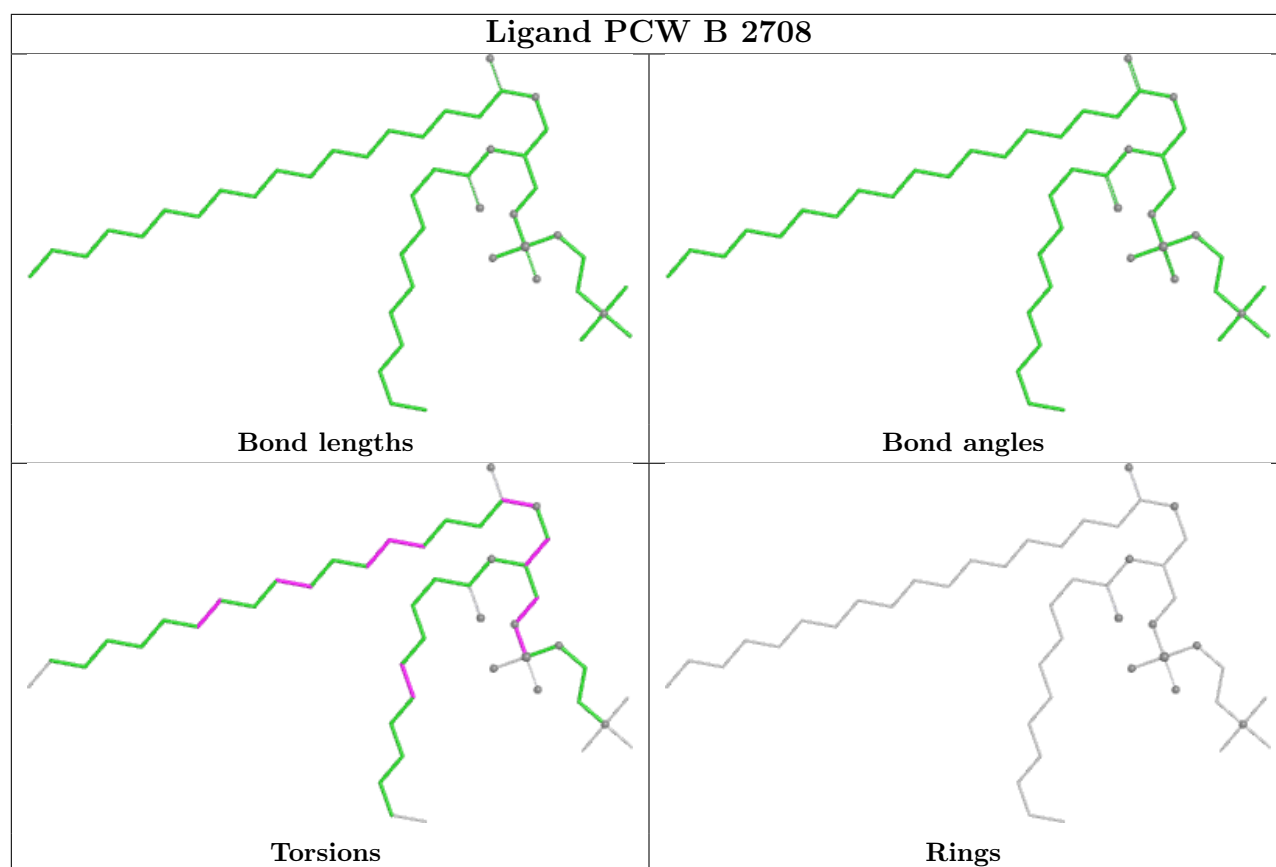


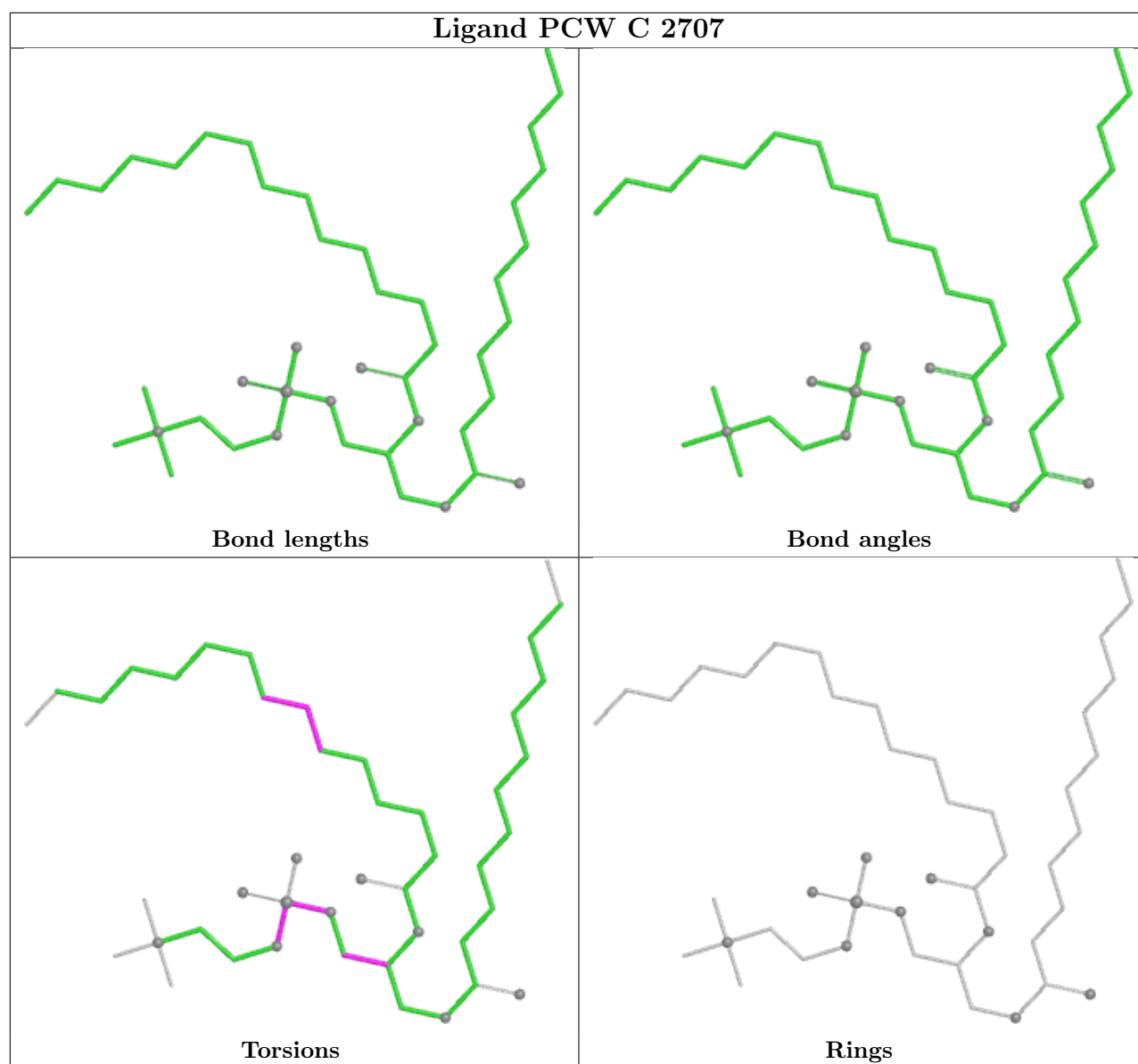


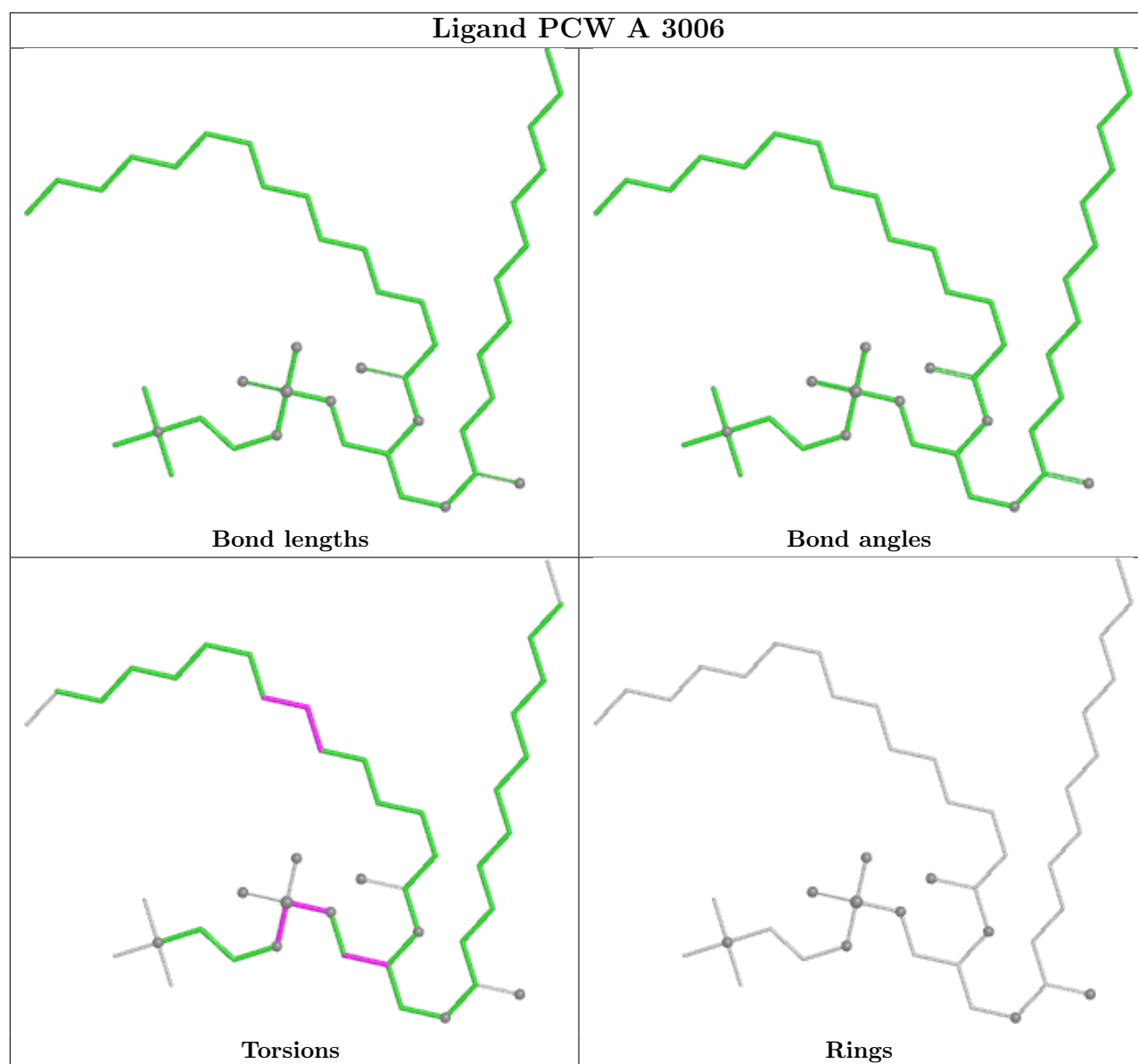


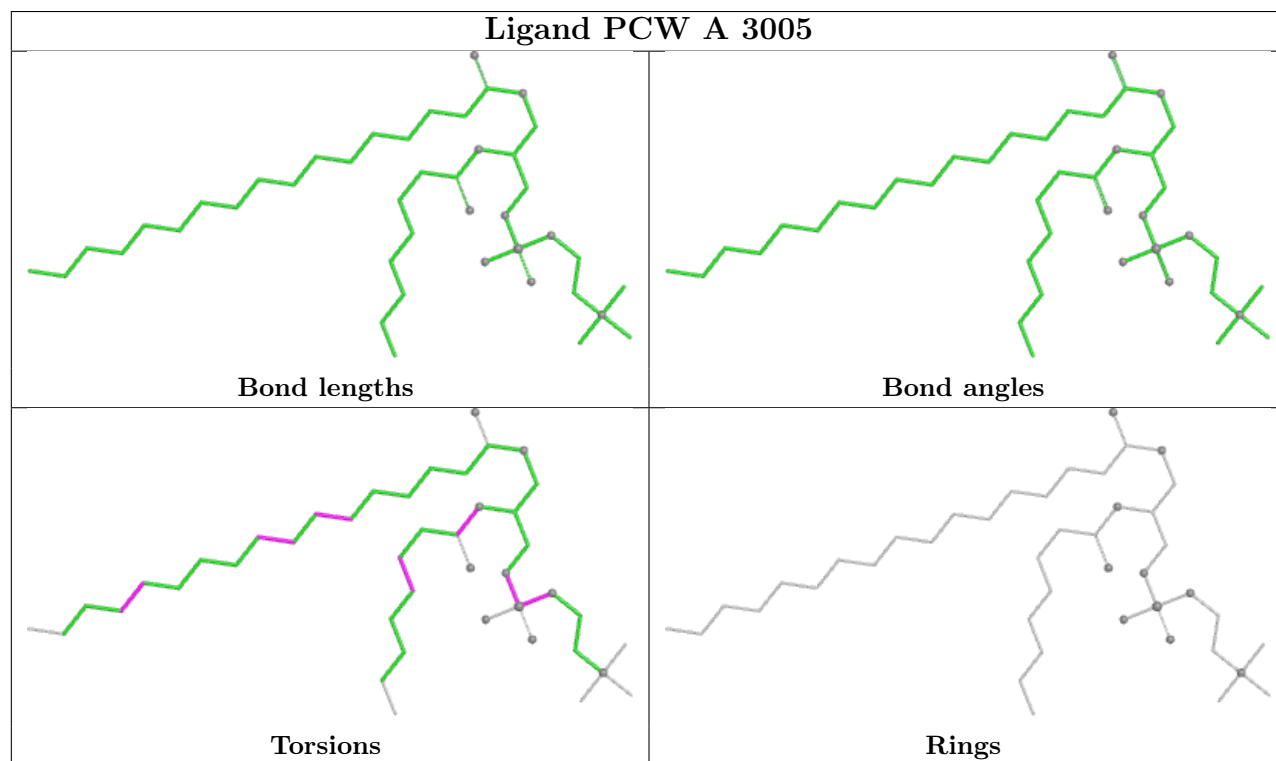
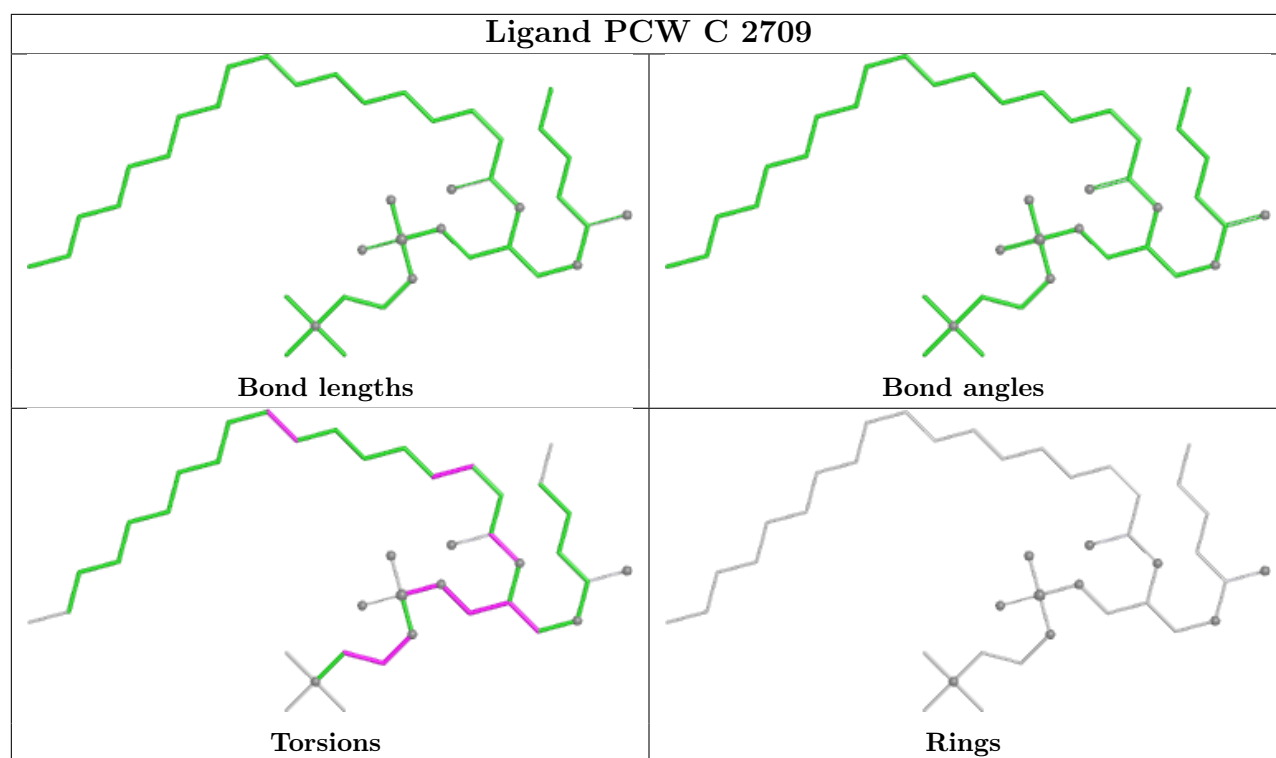


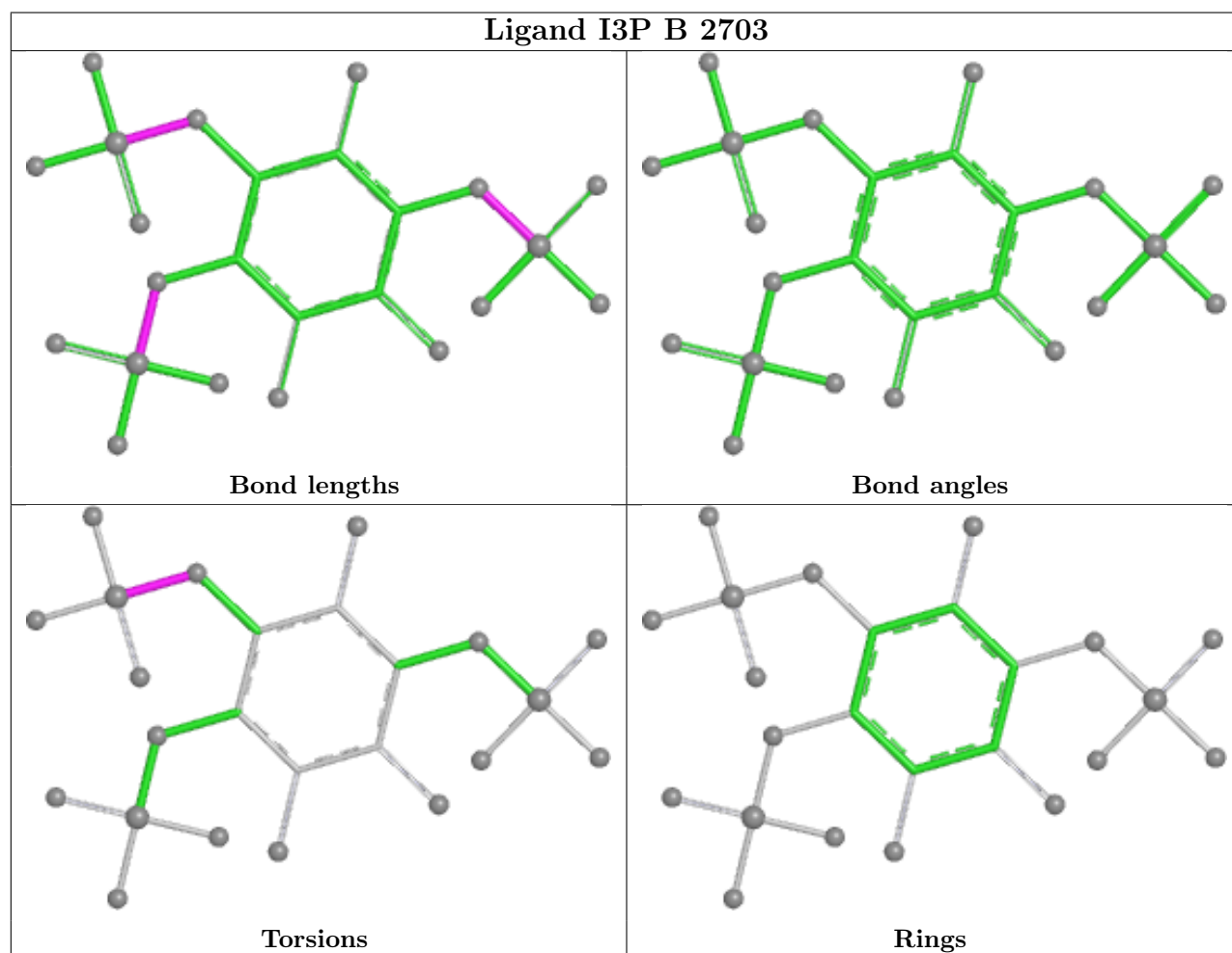
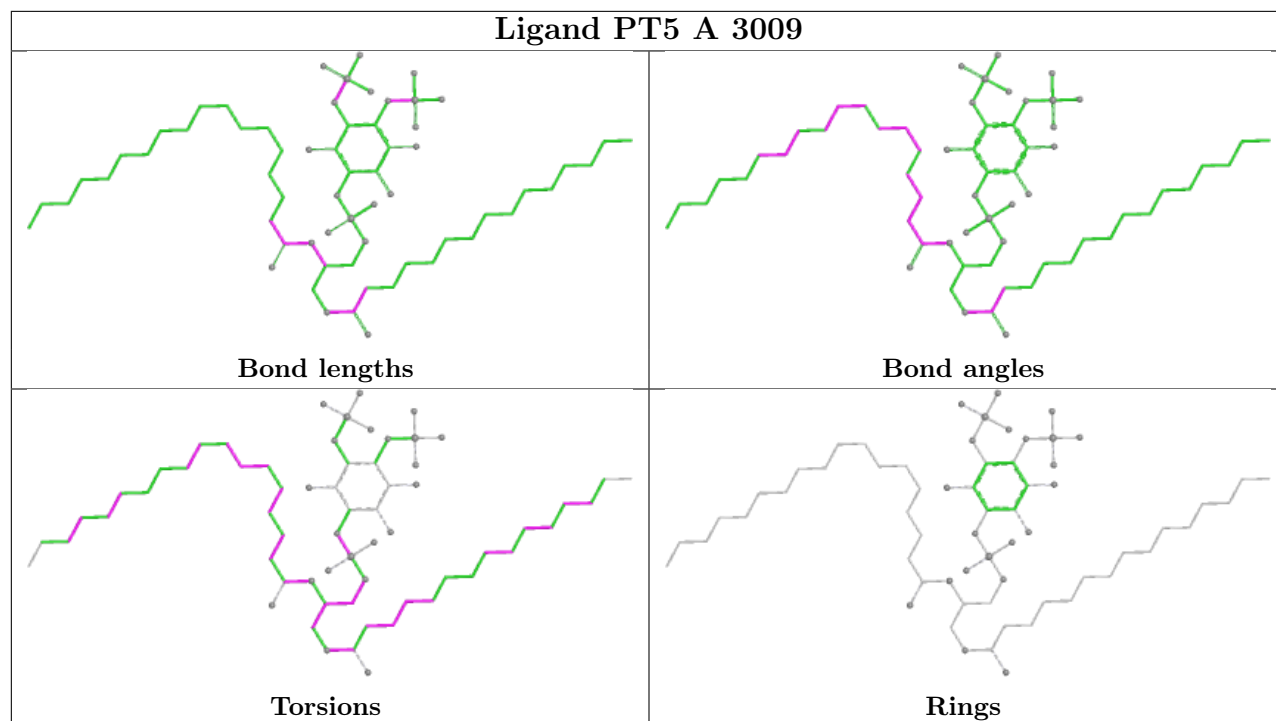


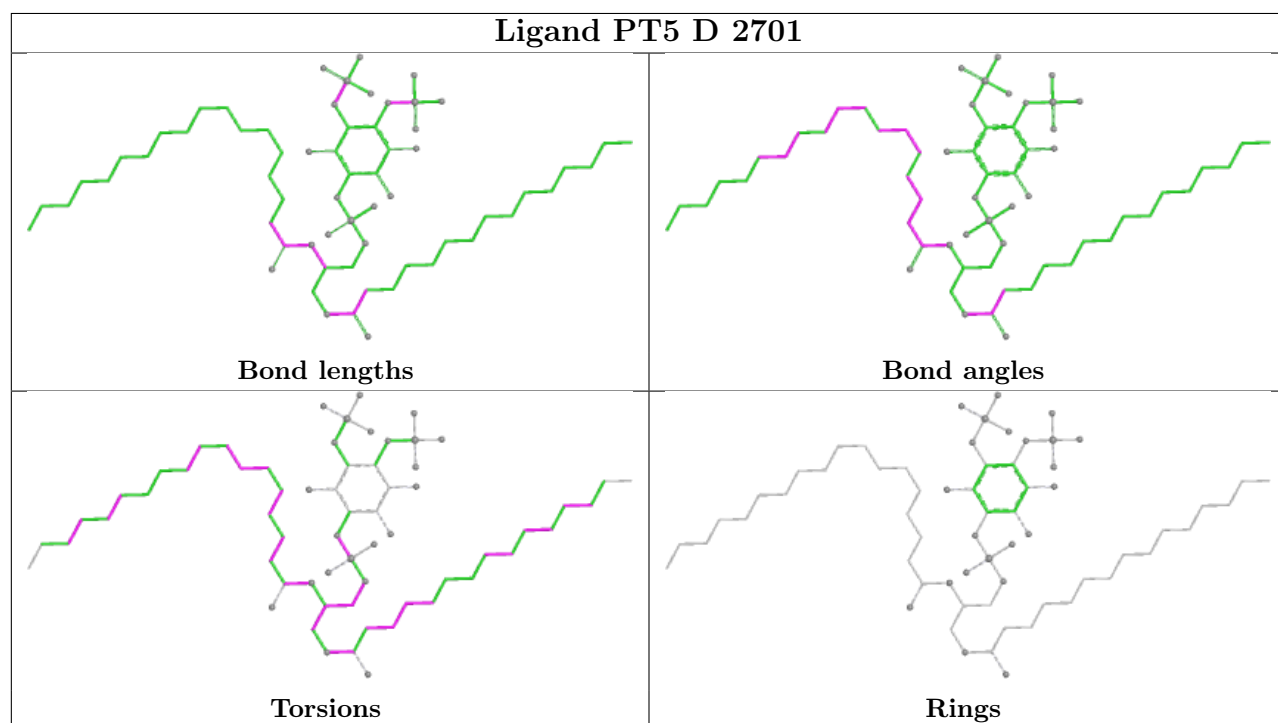
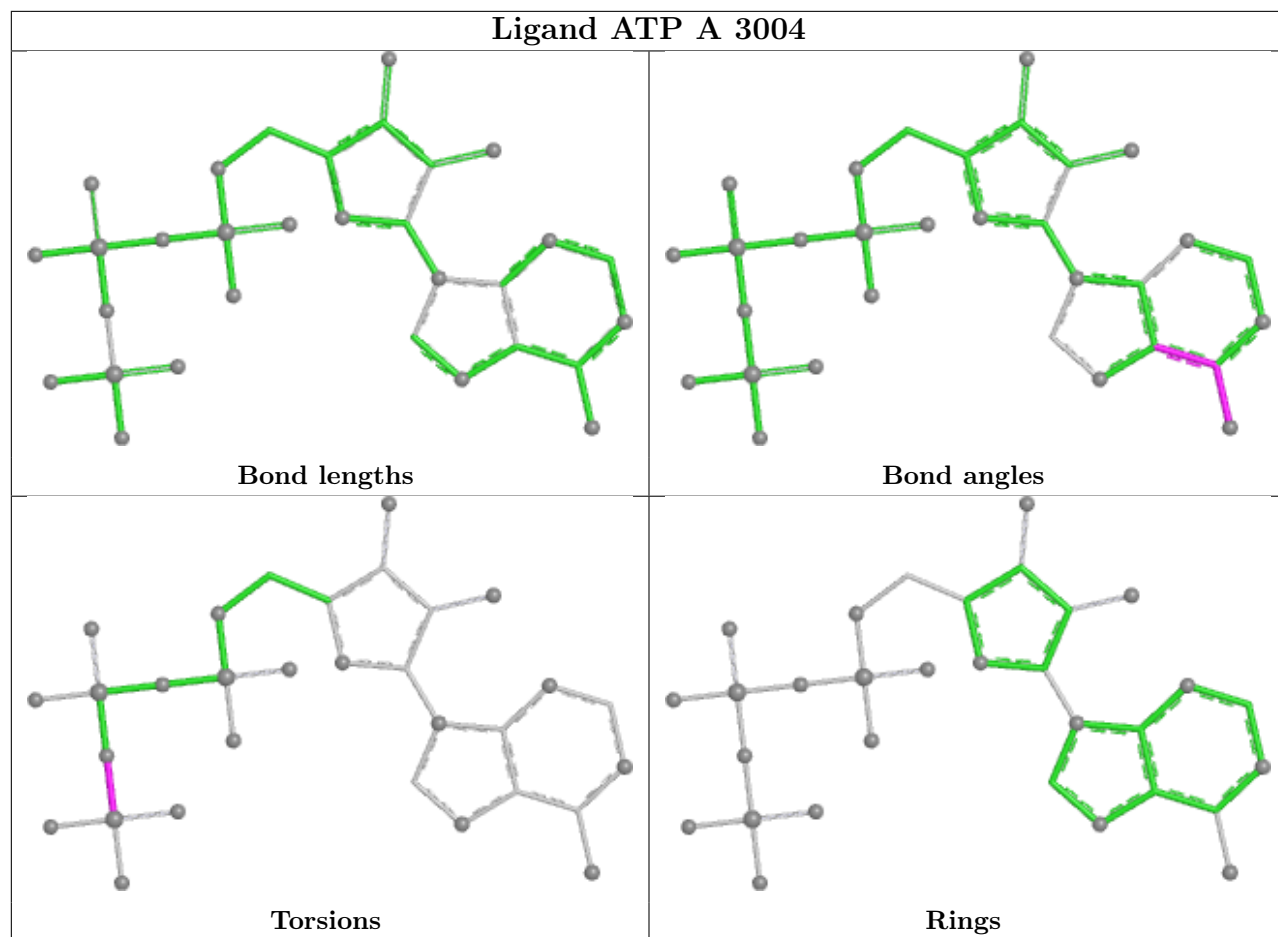


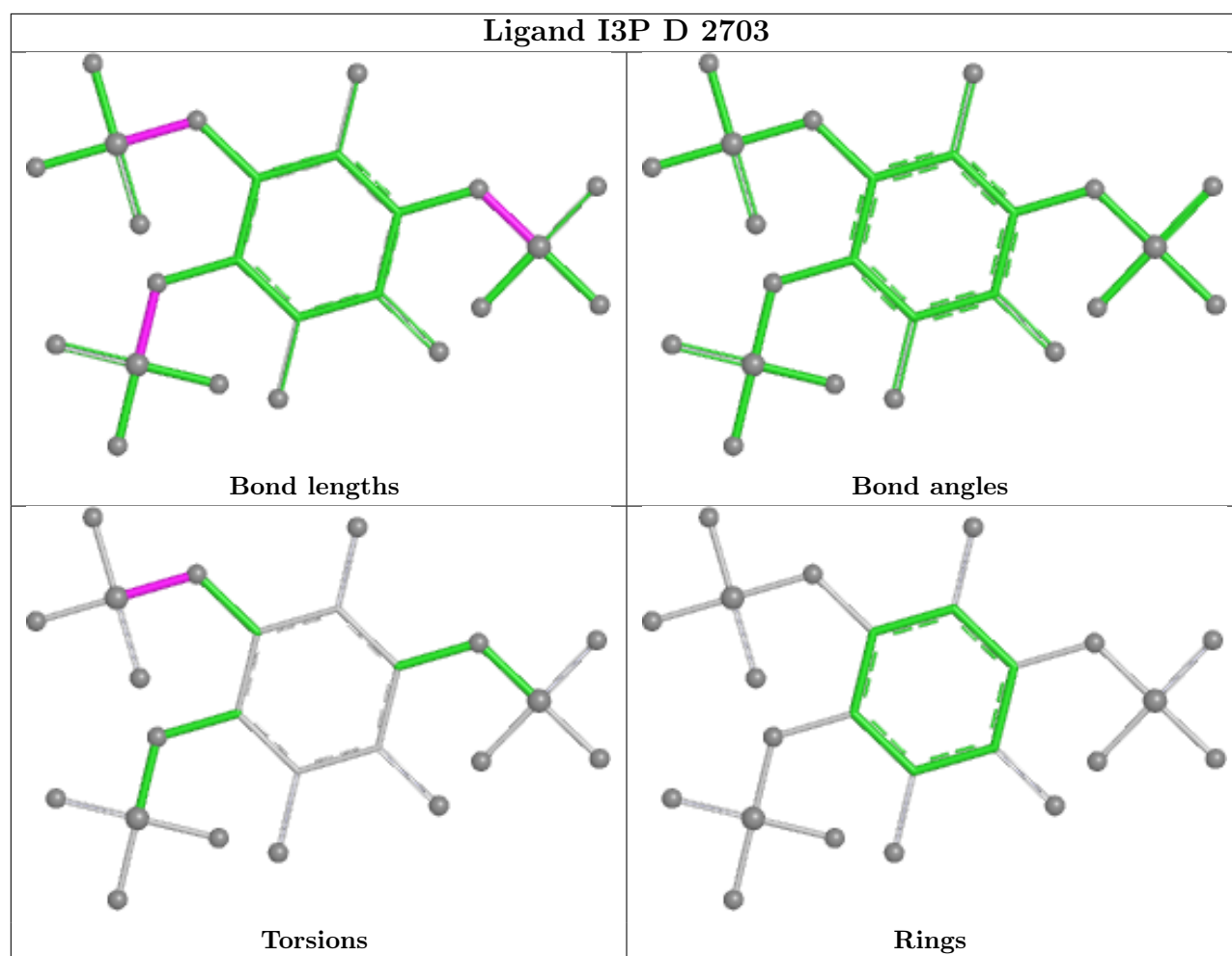




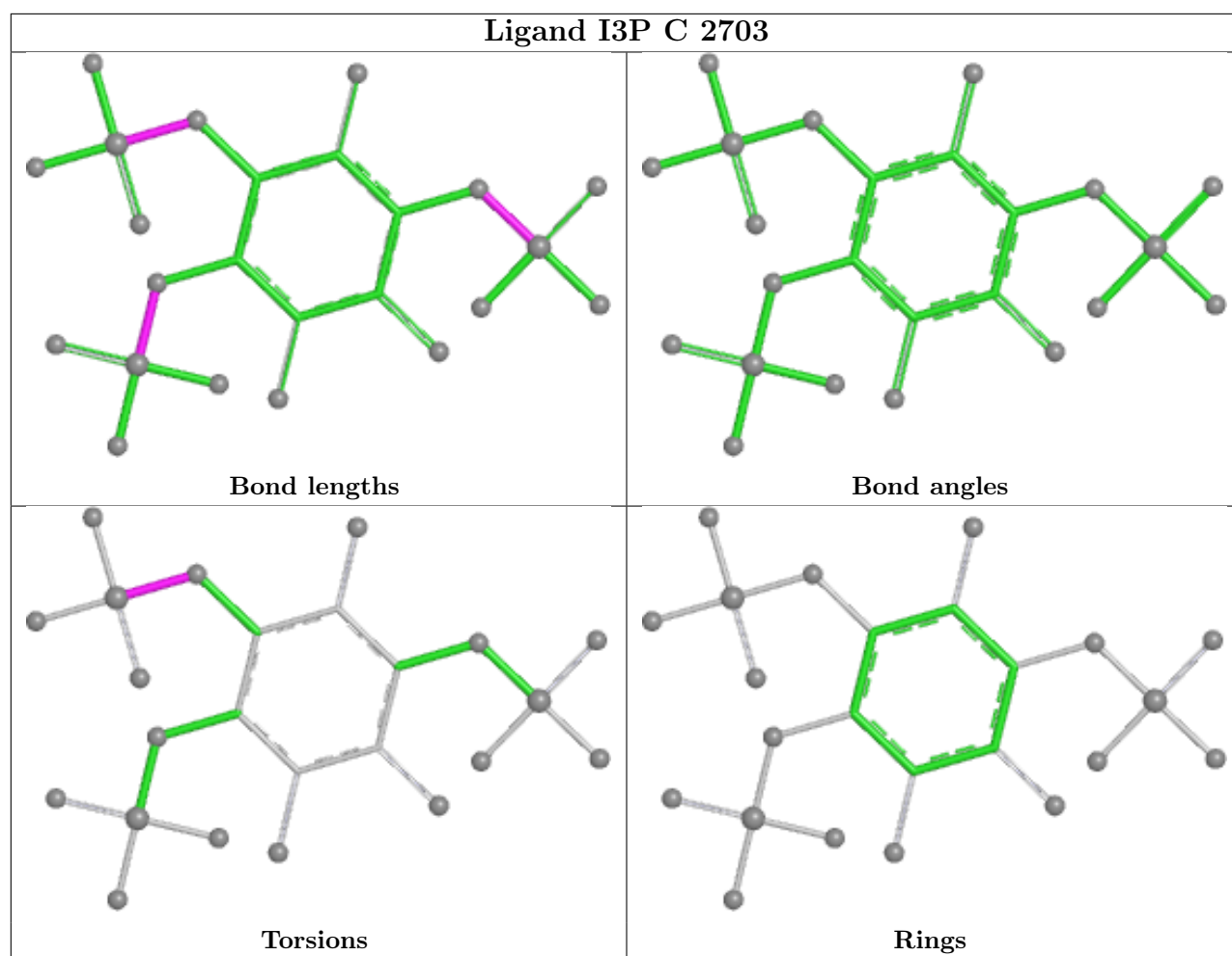


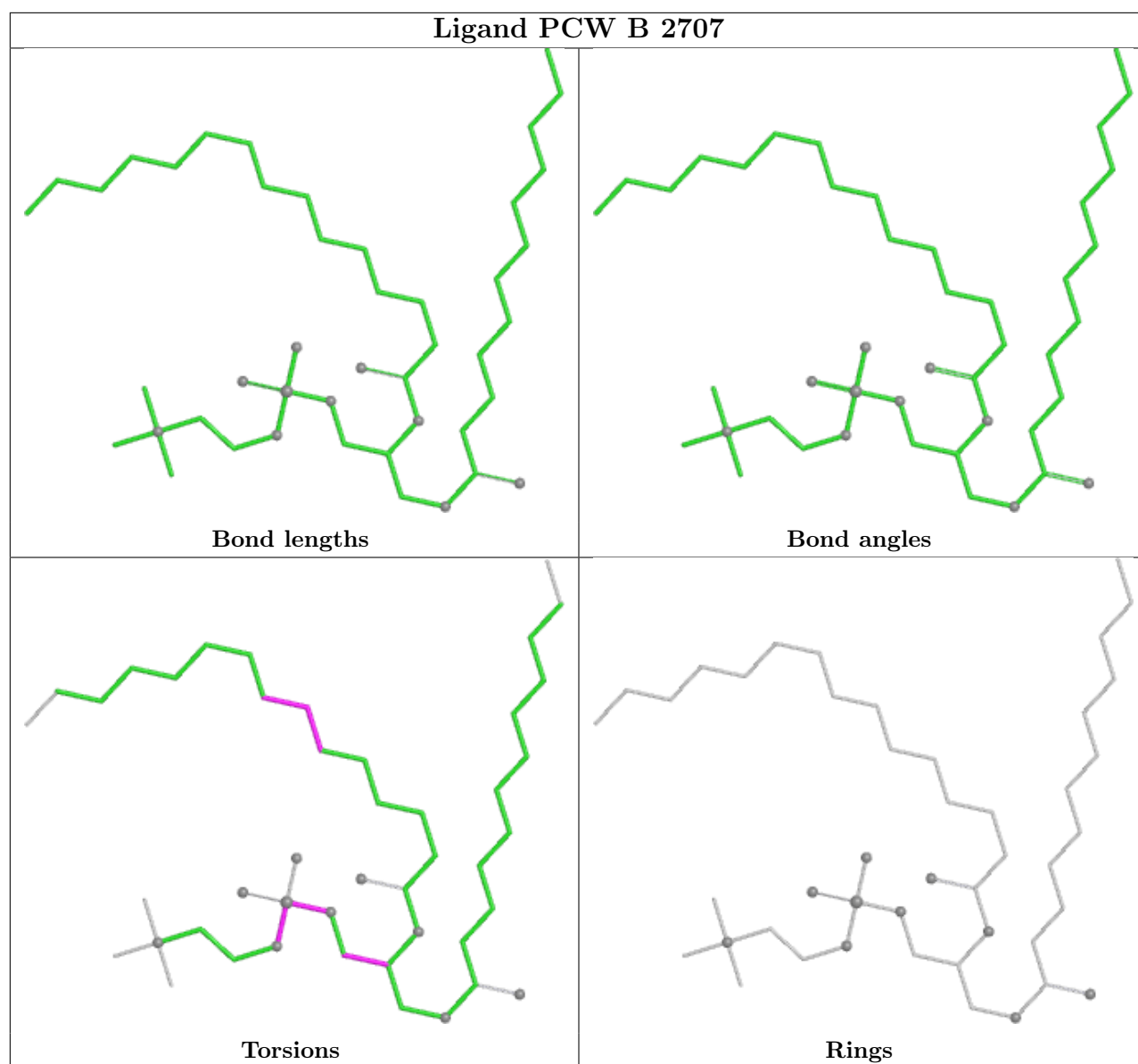


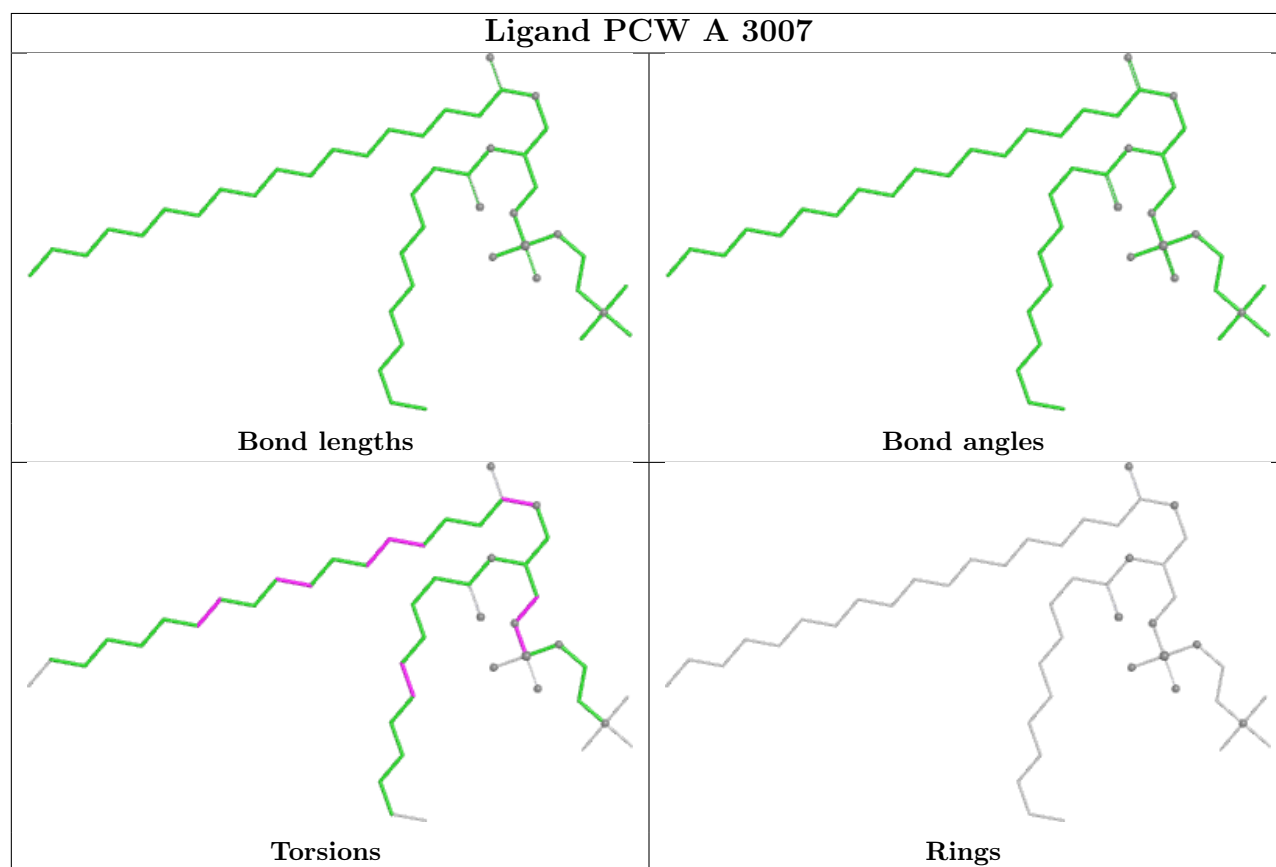
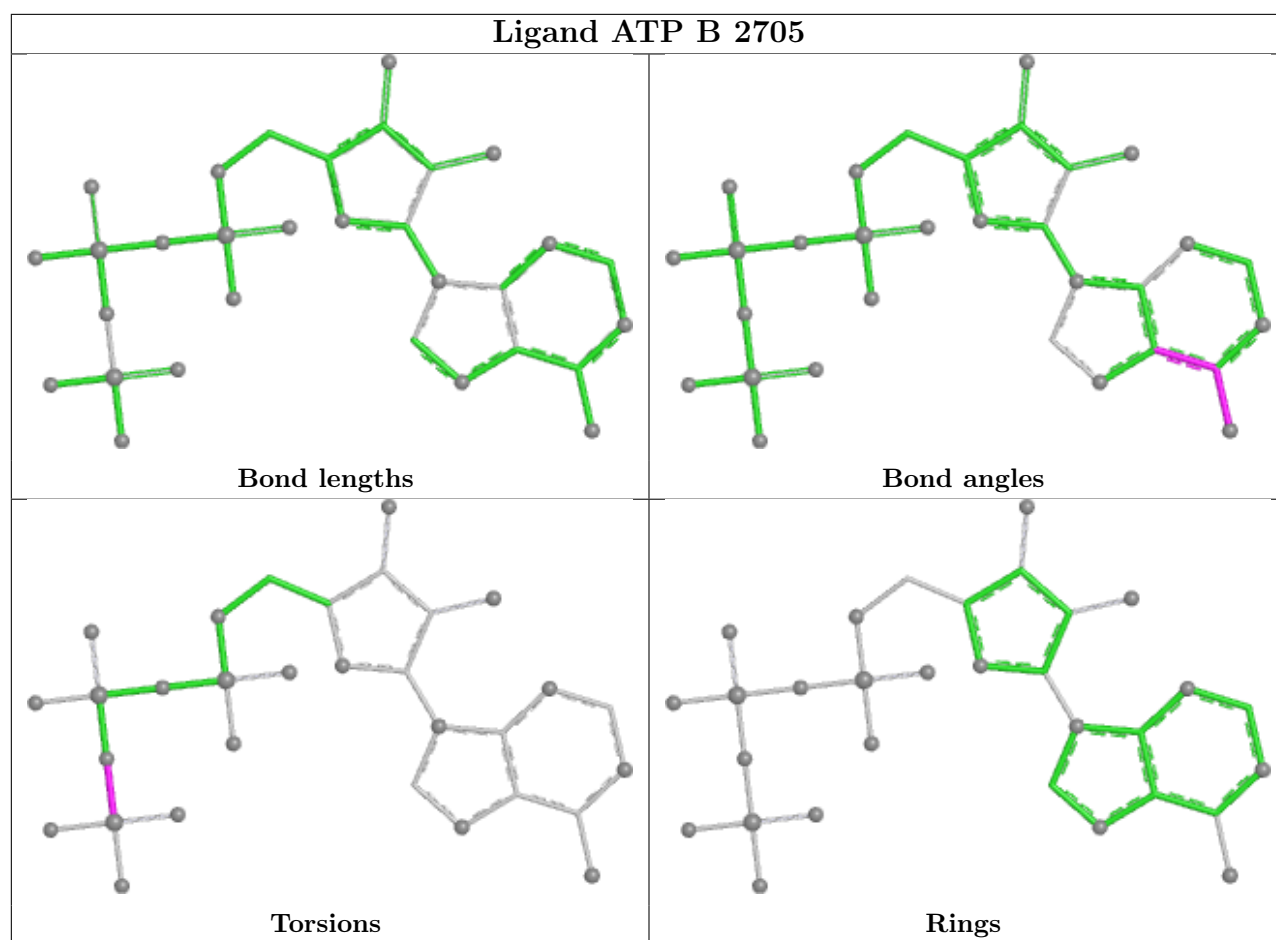


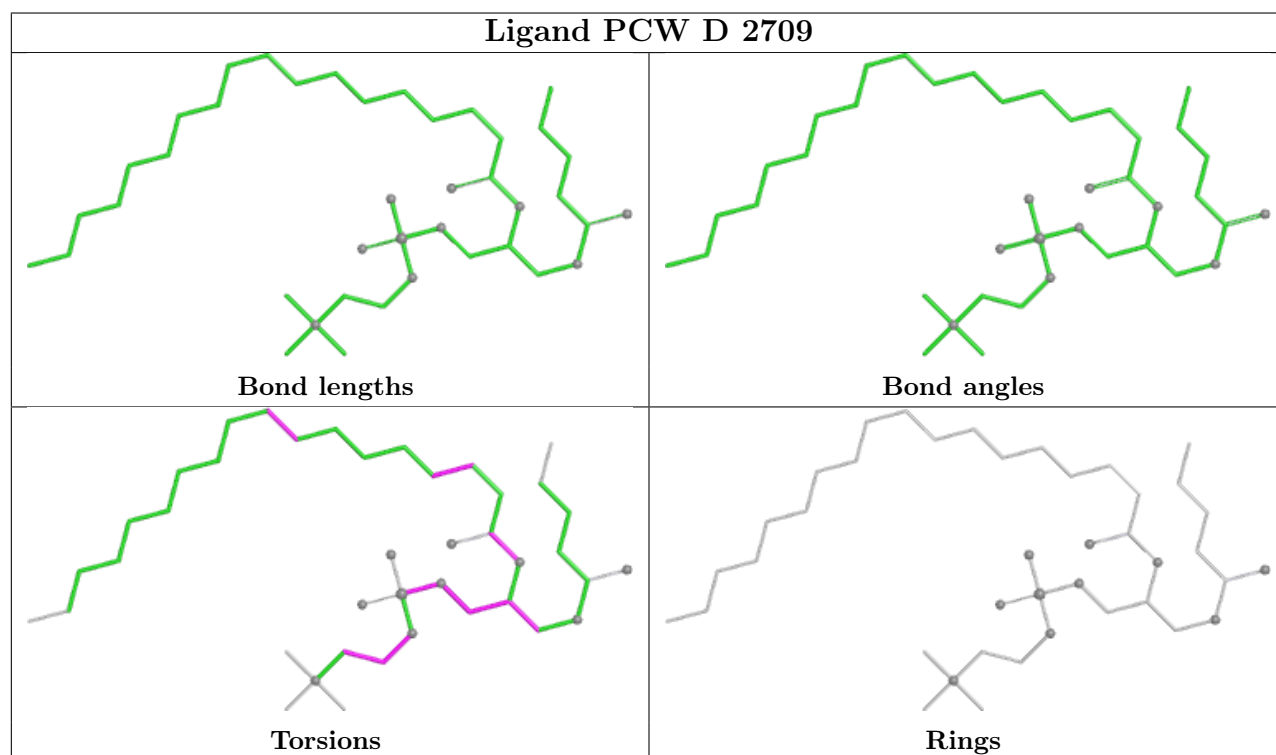
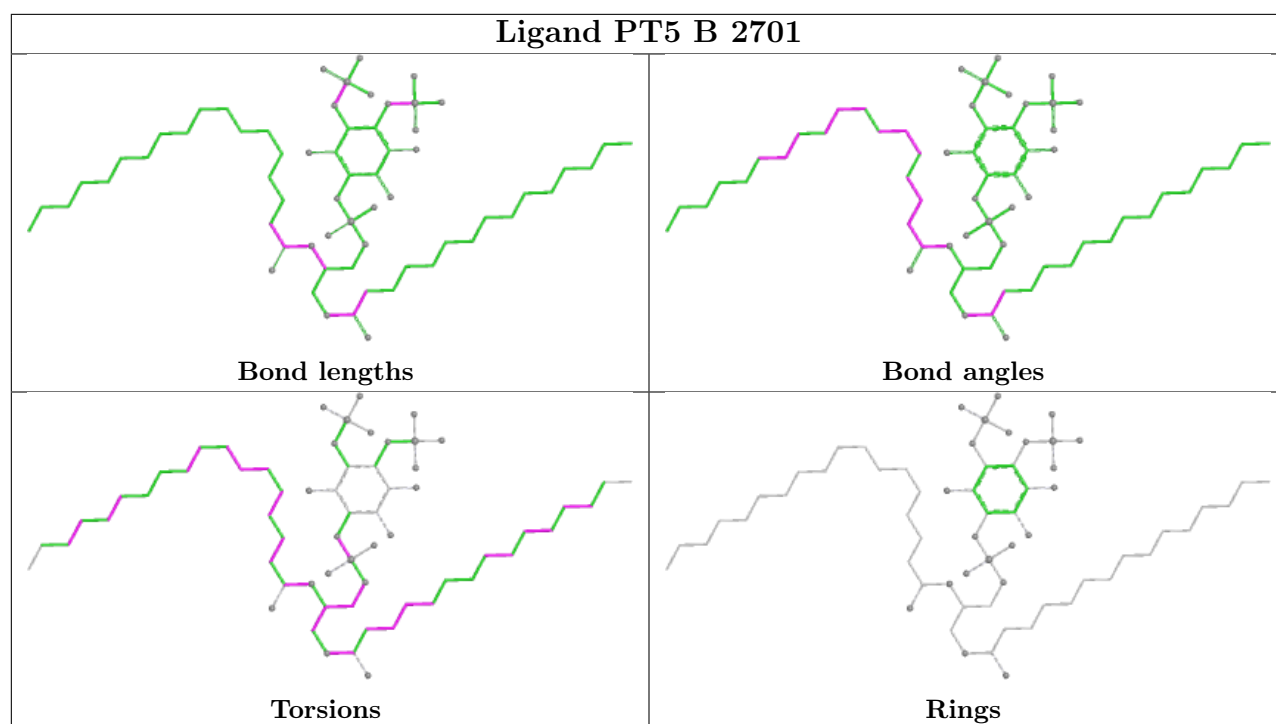


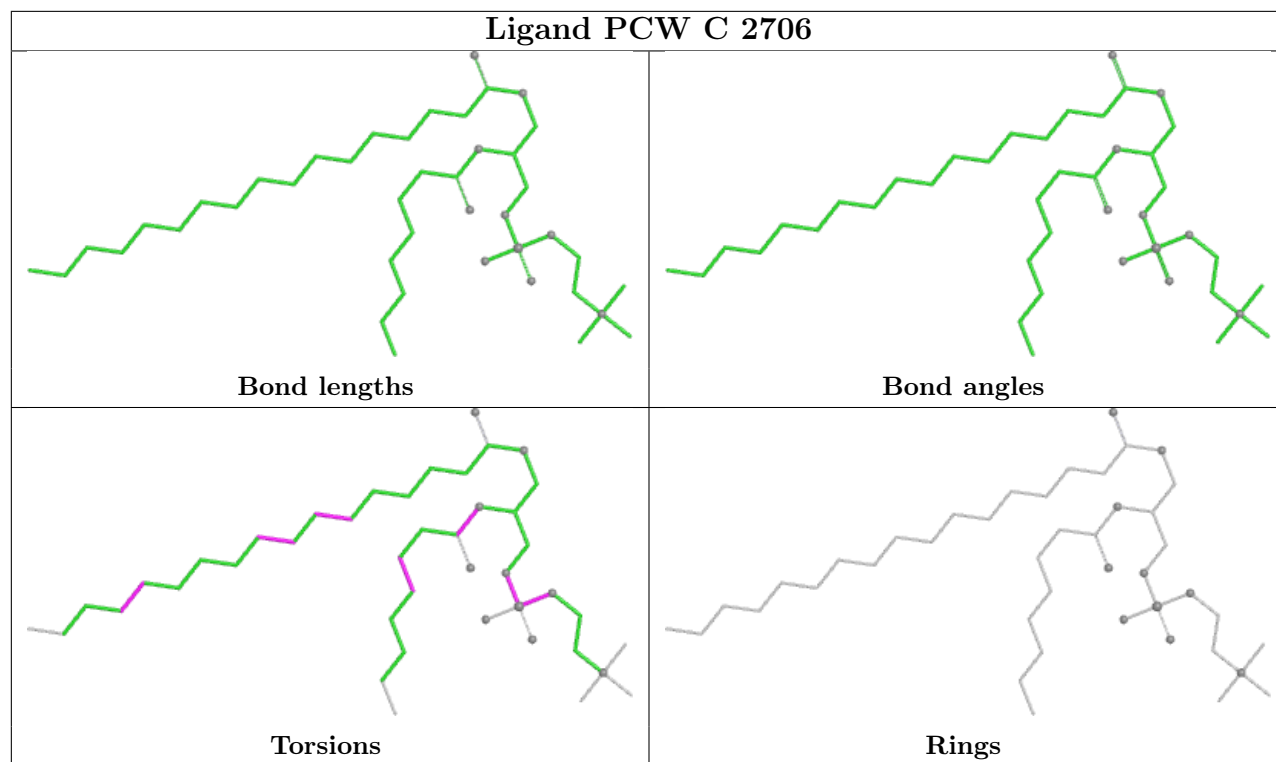


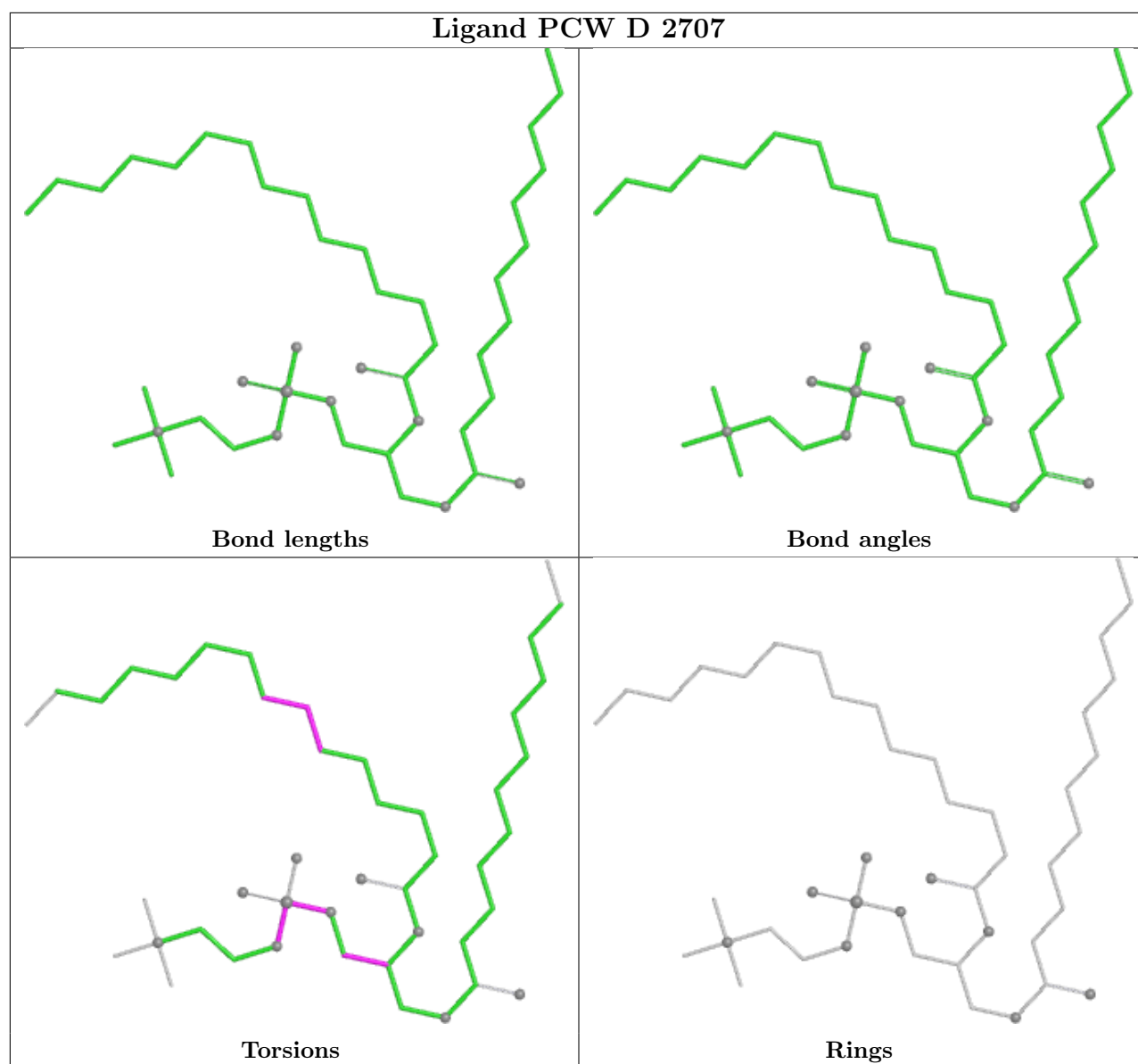


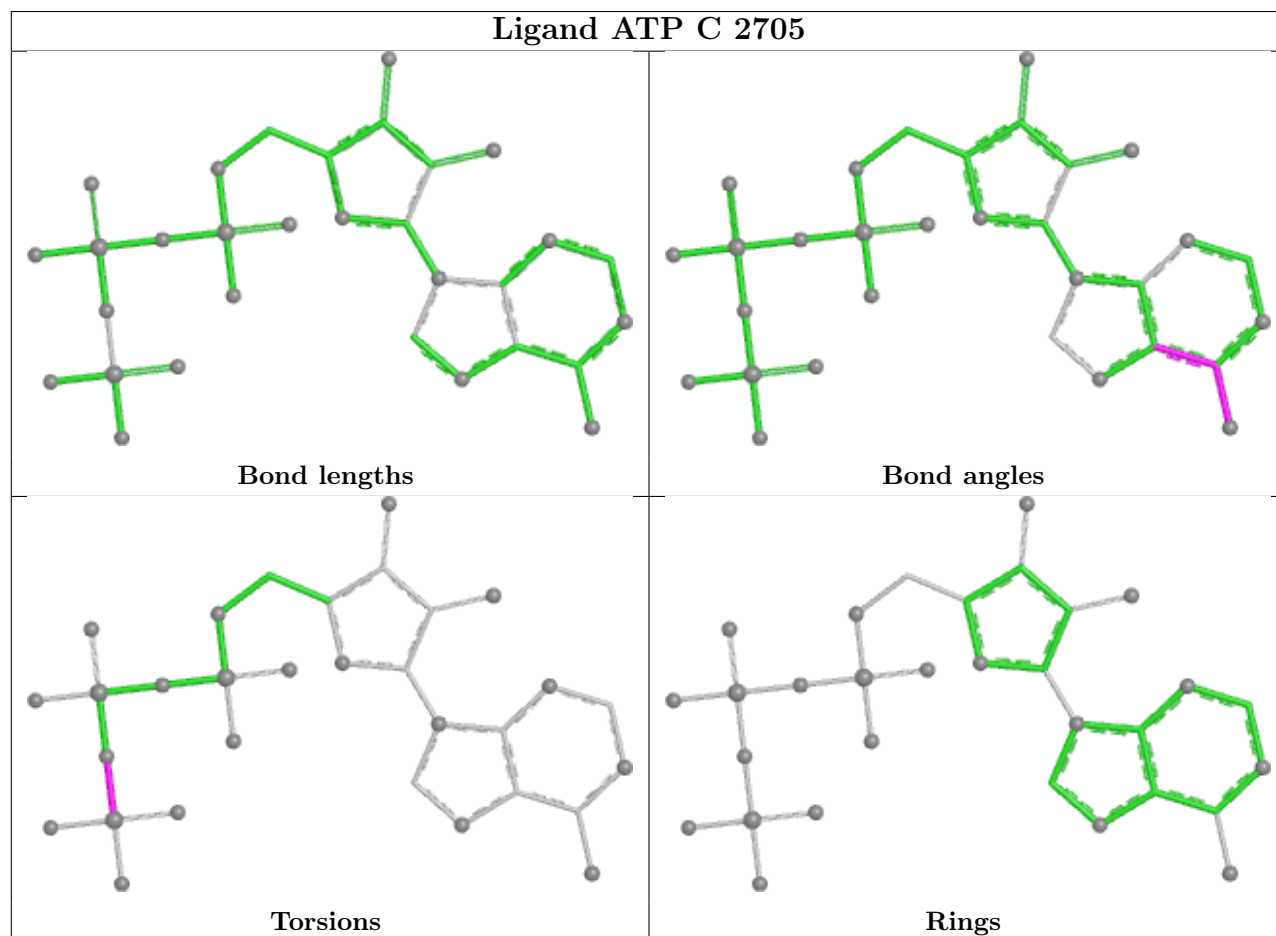
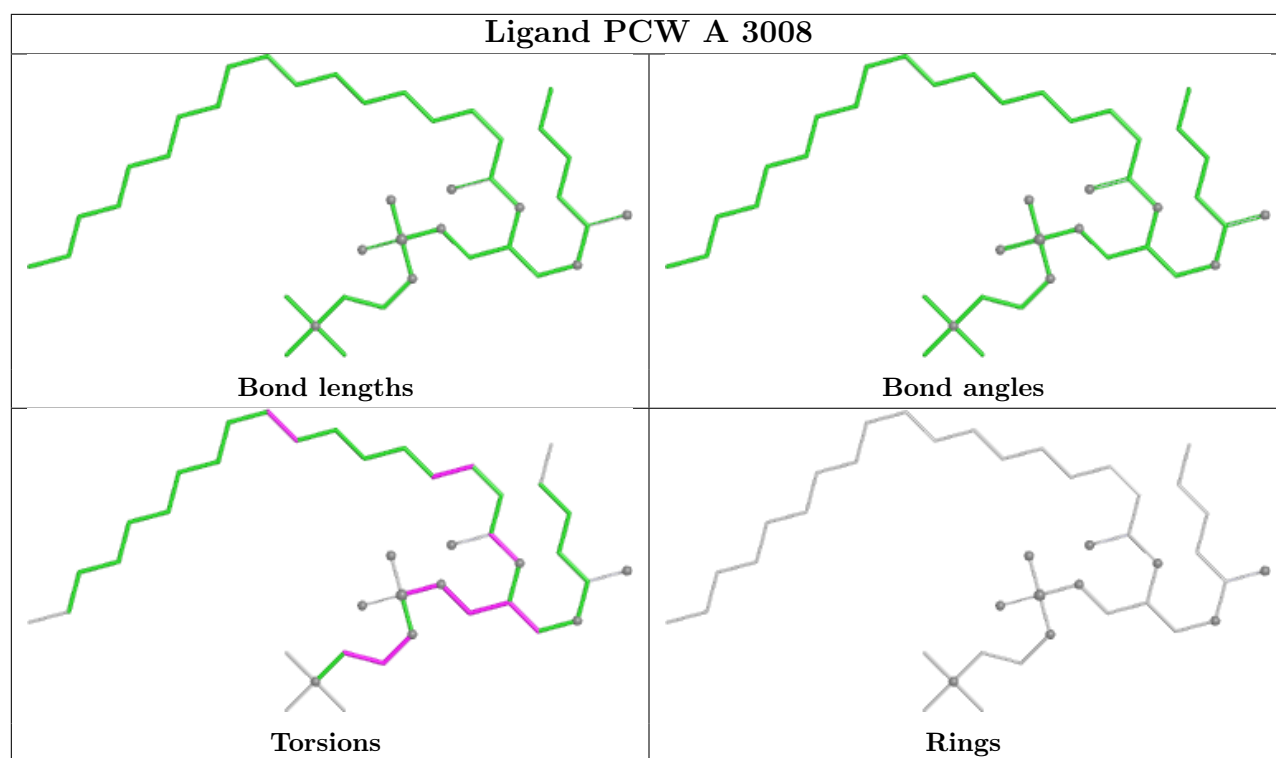


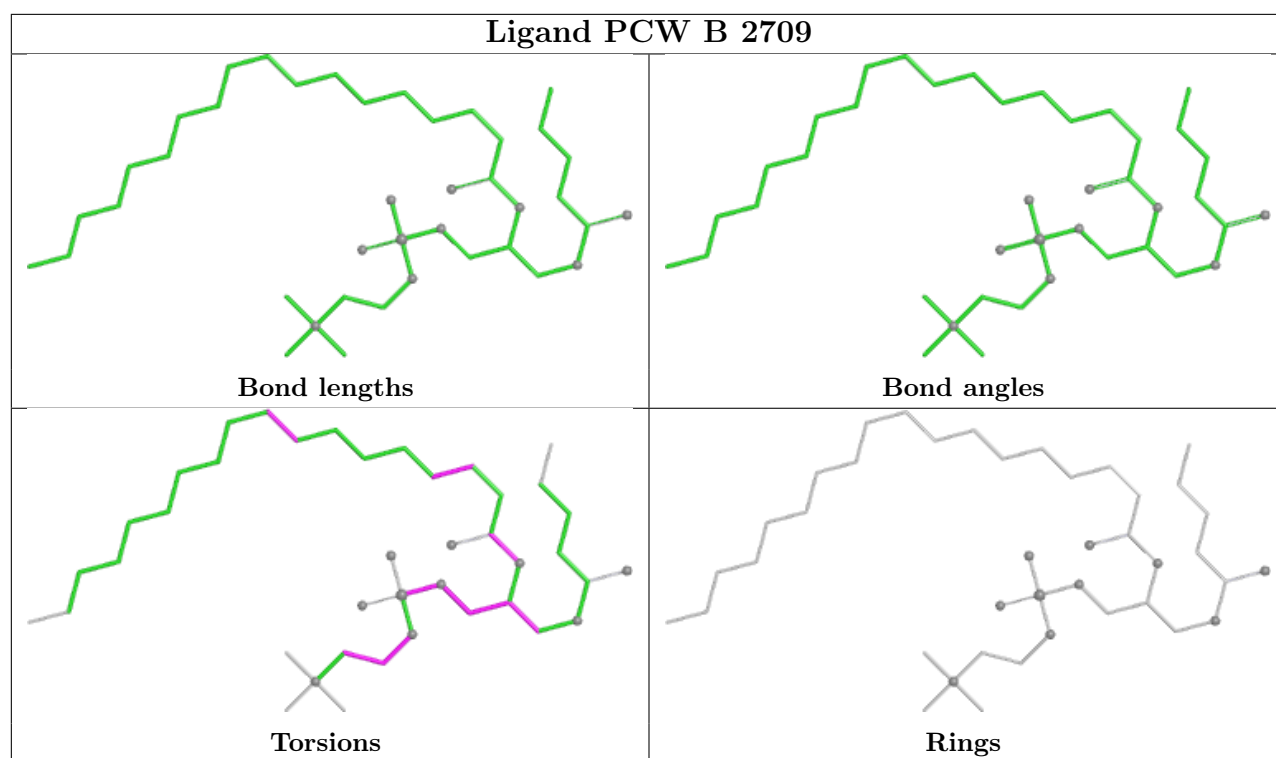












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



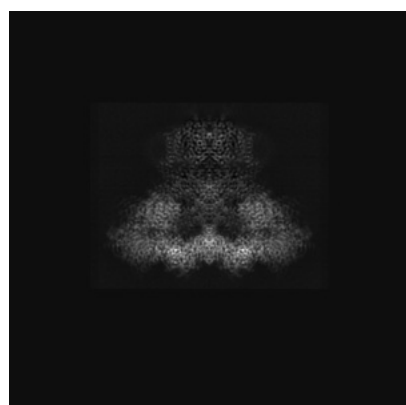
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41349. These allow visual inspection of the internal detail of the map and identification of artifacts.

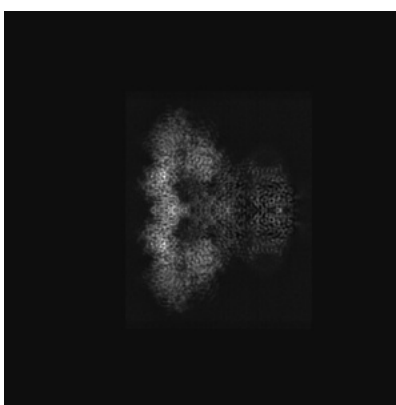
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

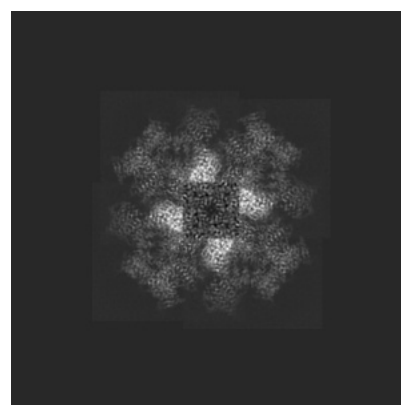
#### 6.1.1 Primary map



X



Y



Z

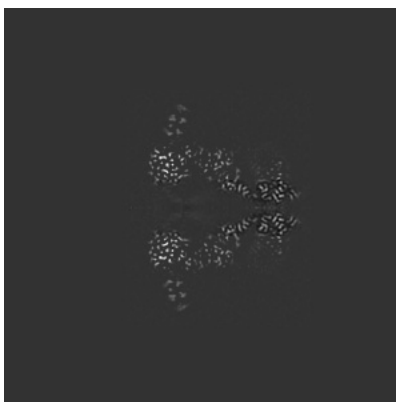
The images above show the map projected in three orthogonal directions.

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

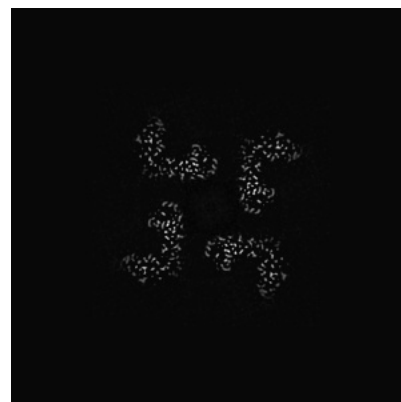
#### 6.2.1 Primary map



X Index: 336



Y Index: 336

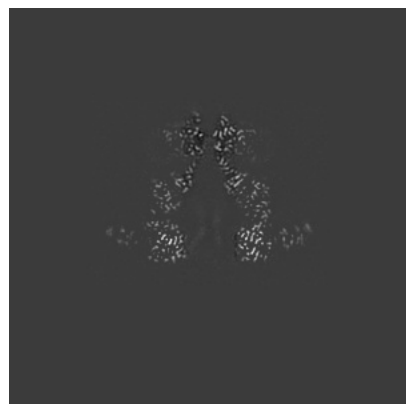


Z Index: 336

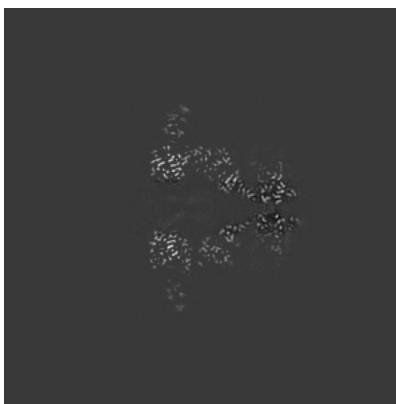
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 333



Y Index: 339

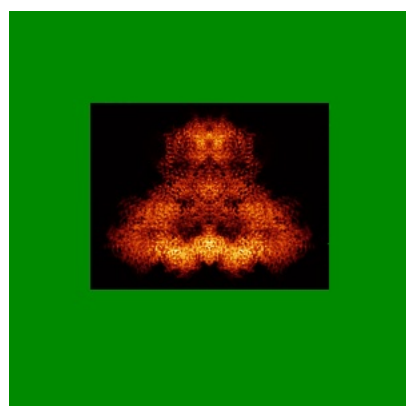


Z Index: 269

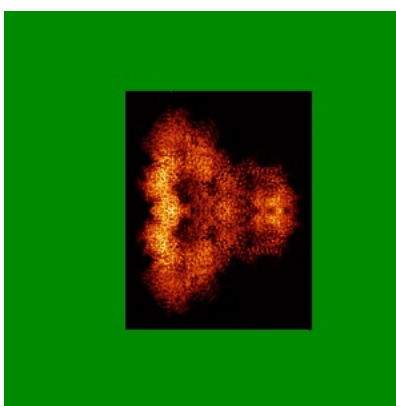
The images above show the largest variance slices of the map in three orthogonal directions.

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

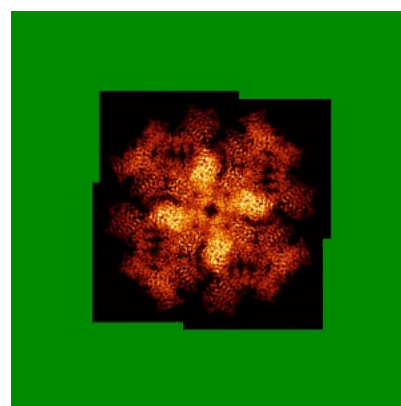
### 6.4.1 Primary map



X



Y

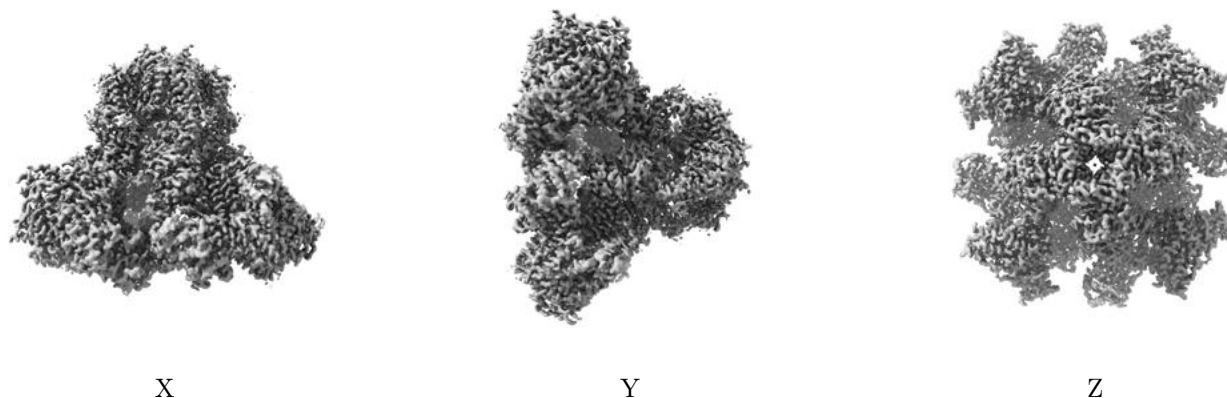


Z

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 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

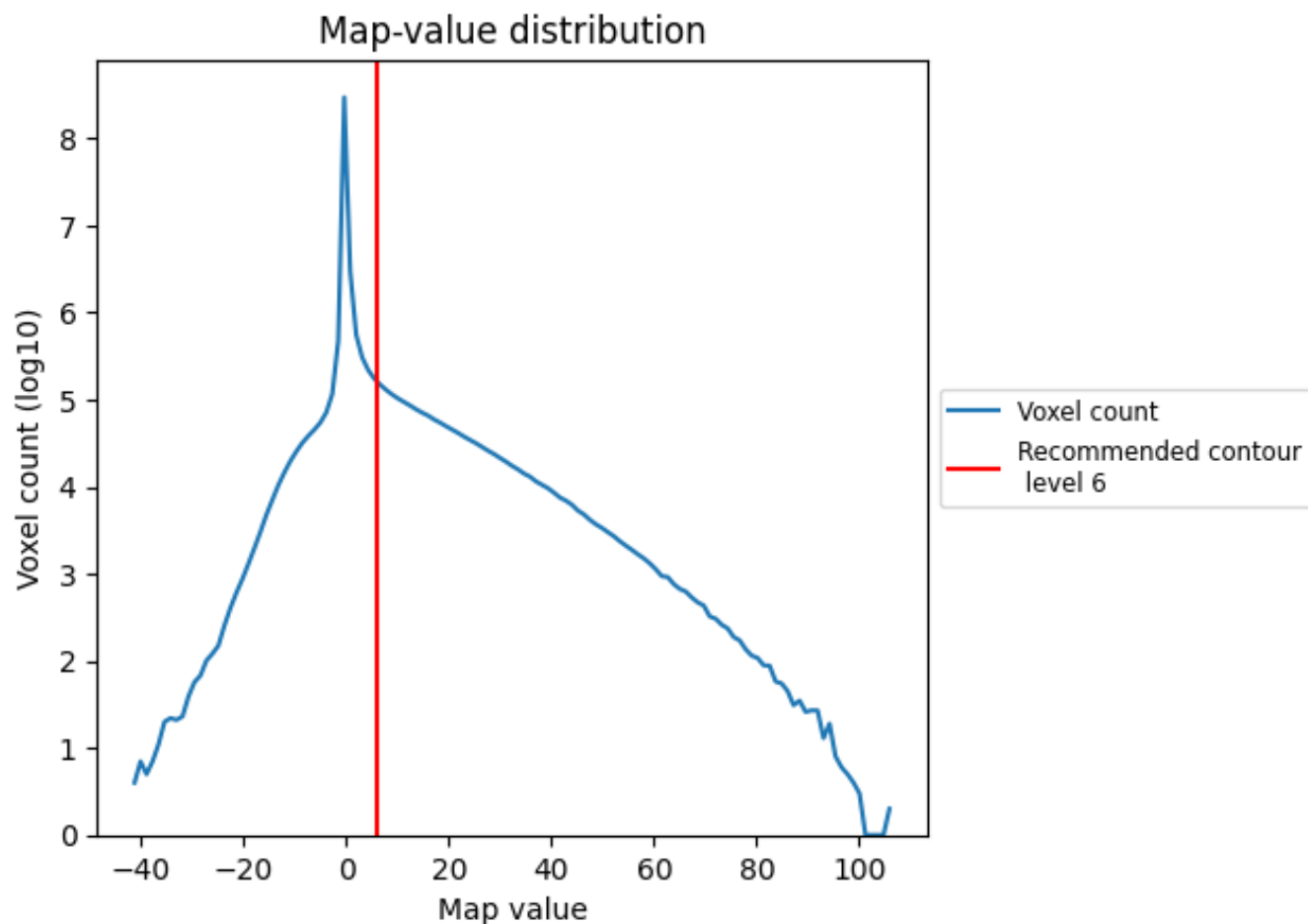
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

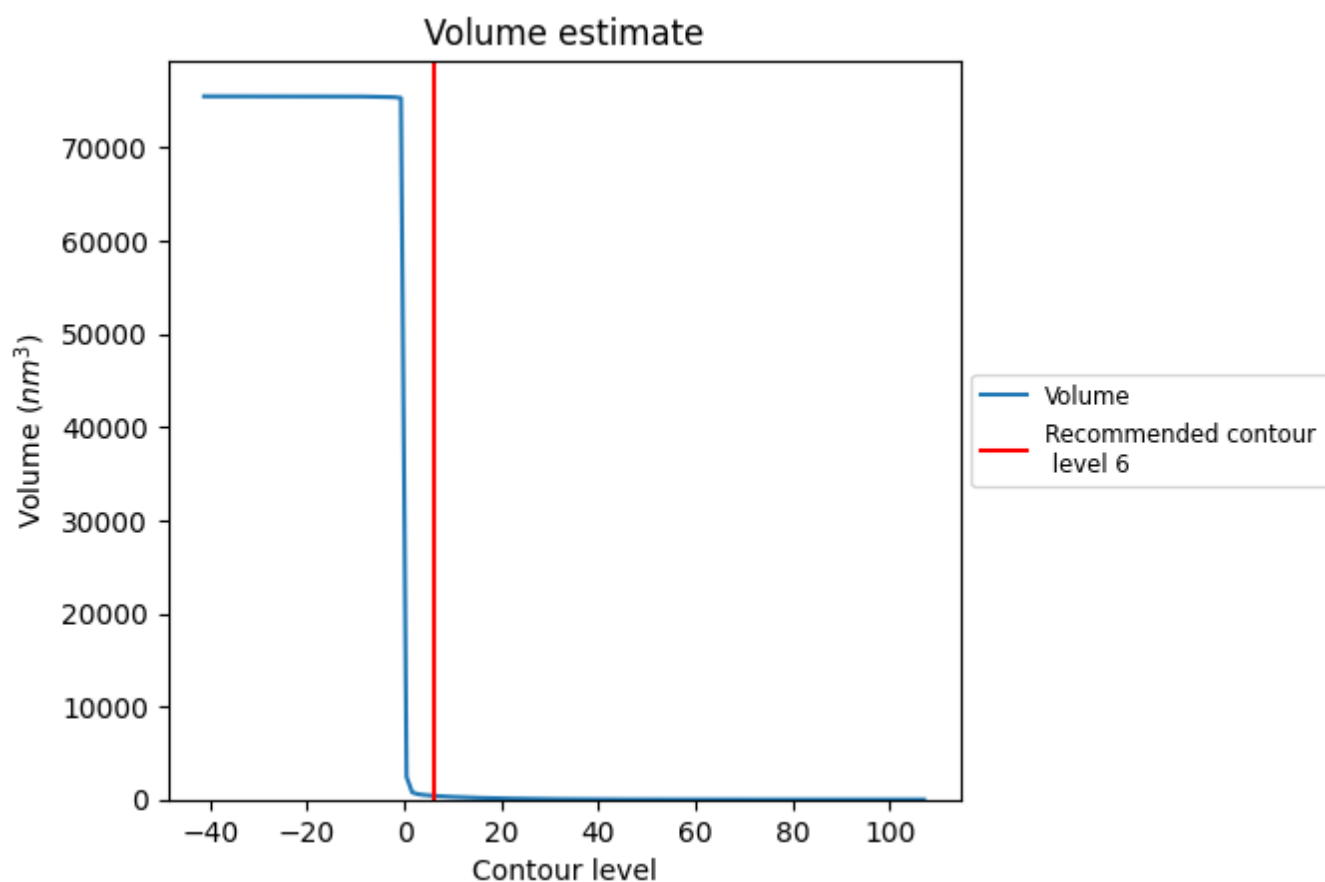
This section contains the results of statistical analysis of the map.

### 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.

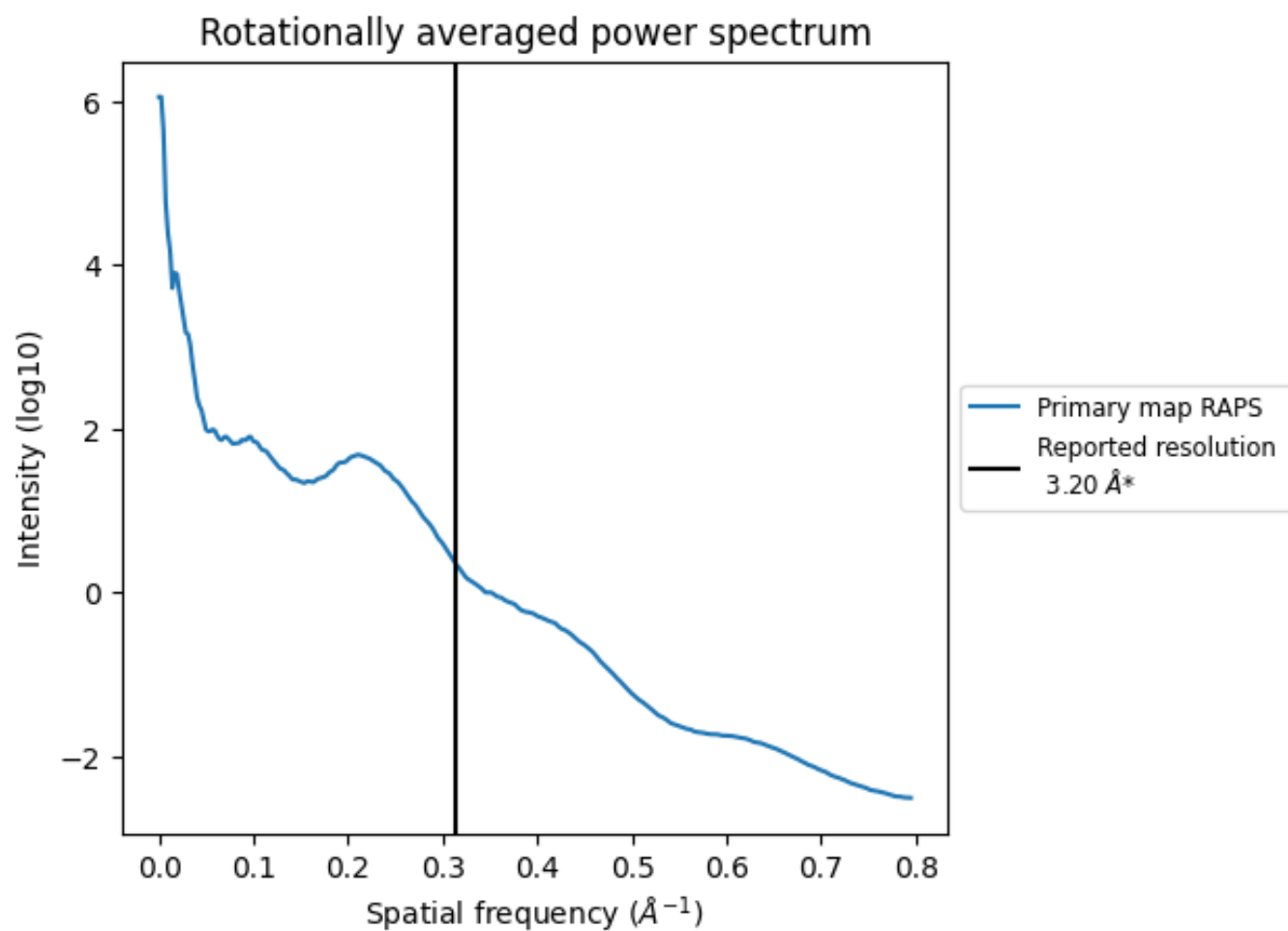
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404  $\text{nm}^3$ ; this corresponds to an approximate mass of 365 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



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

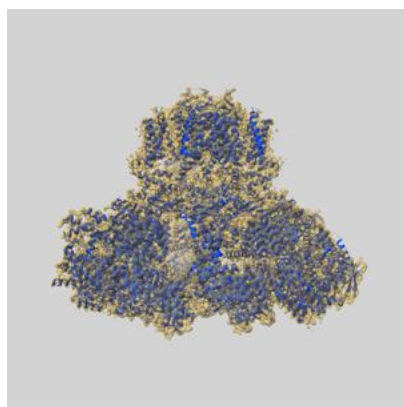
## 8 Fourier-Shell correlation

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

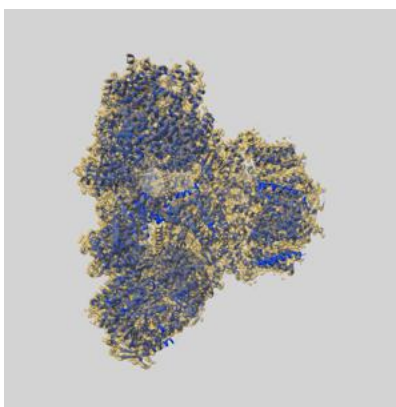
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41349 and PDB model 8TKF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

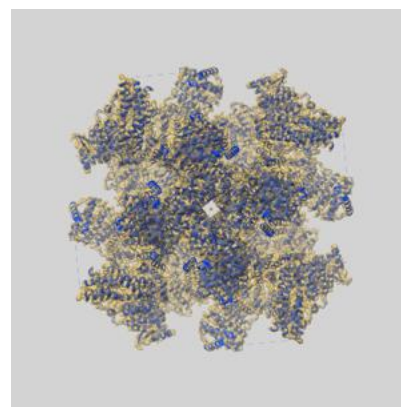
### 9.1 Map-model overlay [i](#)



X



Y

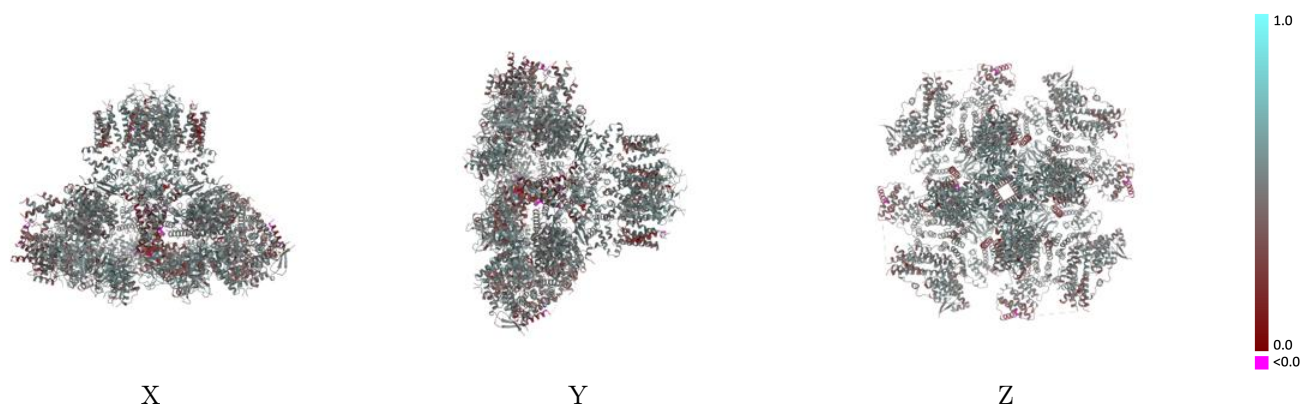


Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

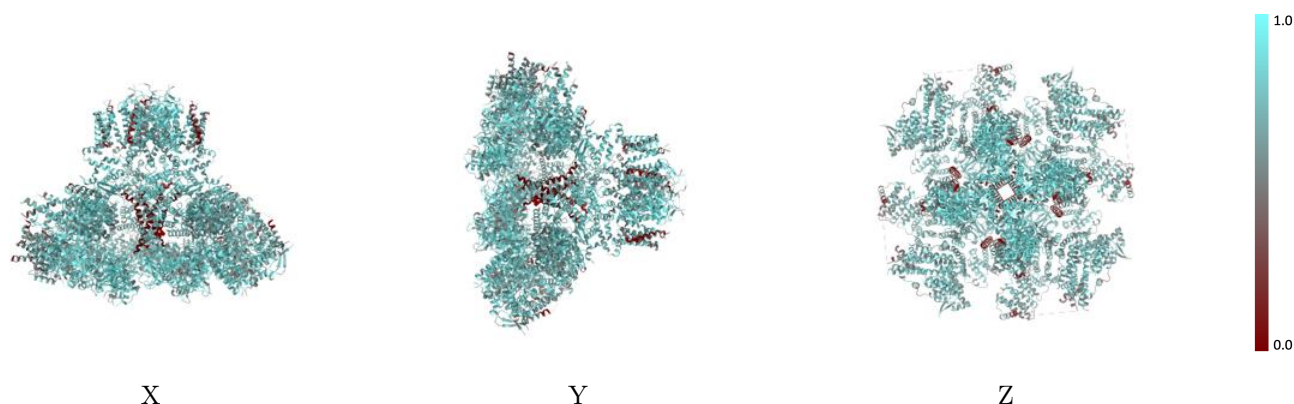


## 9.2 Q-score mapped to coordinate model [i](#)



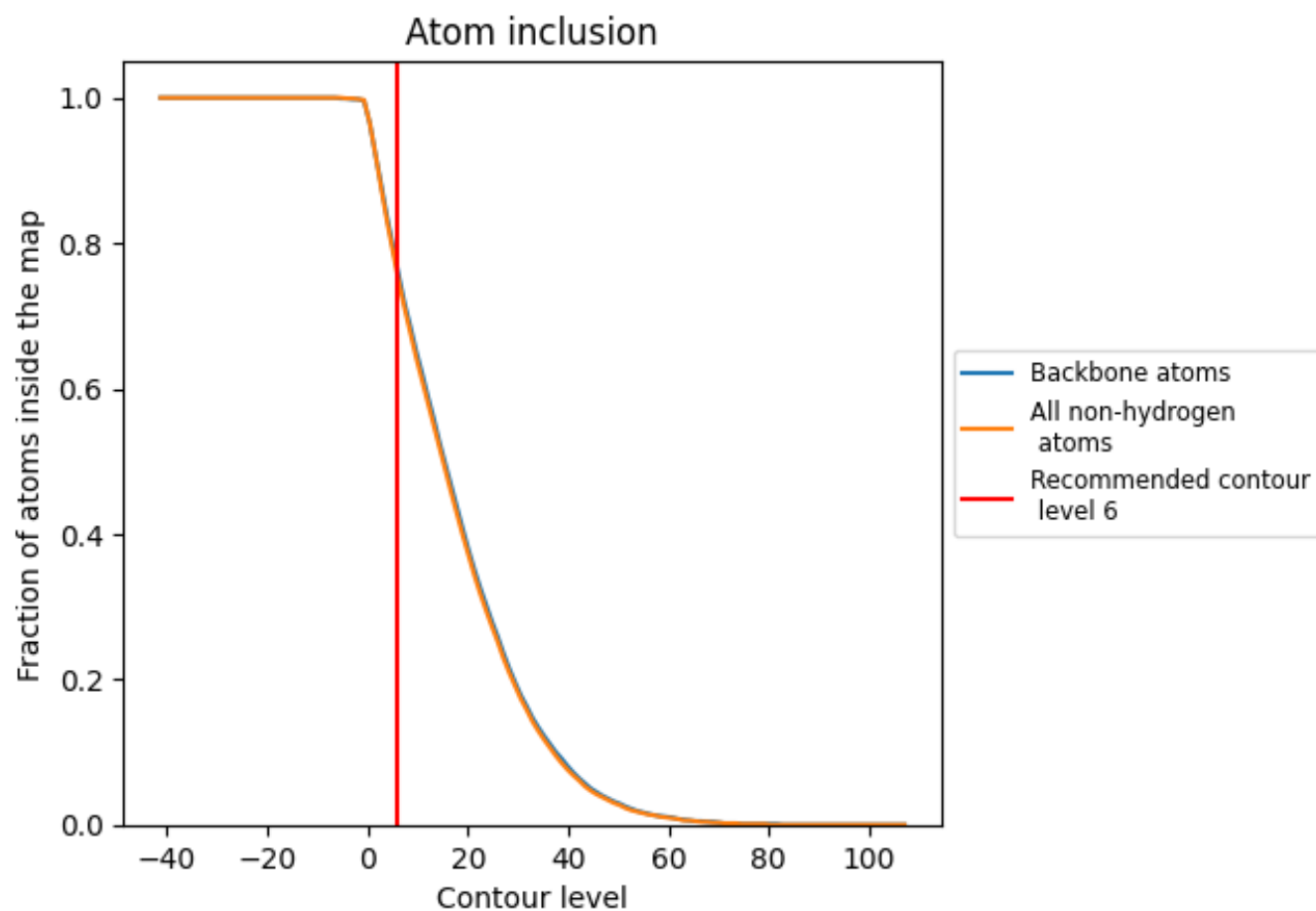
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7550	<div><div></div></div> 0.4850
A	<div><div></div></div> 0.7630	<div><div></div></div> 0.4850
B	<div><div></div></div> 0.7590	<div><div></div></div> 0.4850
C	<div><div></div></div> 0.7590	<div><div></div></div> 0.4860
D	<div><div></div></div> 0.7590	<div><div></div></div> 0.4850

