



## wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 09:07 AM UTC

PDB ID : 9NMN / pdb\_00009nmn  
EMDB ID : EMD-49534  
Title : Structure of mouse RyR1 (Ca<sup>2+</sup>/CFF/ATP dataset; open pore)  
Authors : Weninger, G.; Marks, A.R.  
Deposited on : 2025-03-04  
Resolution : 3.09 Å(reported)

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

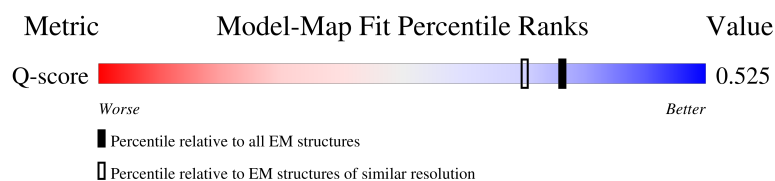
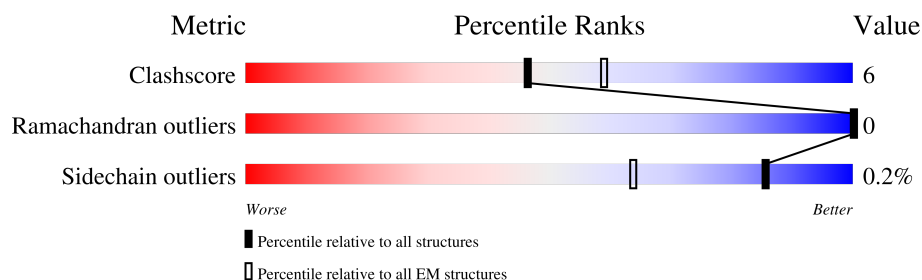
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.09 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	14003 ( 2.59 - 3.59 )

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	5035	
1	B	5035	
1	C	5035	
1	D	5035	

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Mol	Chain	Length	Quality of chain
2	E	108	 87% 12% .
2	F	108	 88% 11% .
2	G	108	 89% 10% .
2	H	108	 89% 10% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	A	8002	-	X	-	-
4	CFF	B	8002	-	X	-	-
4	CFF	C	8002	-	X	-	-
4	CFF	D	8002	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 143248 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
1	B	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
1	C	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
1	D	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

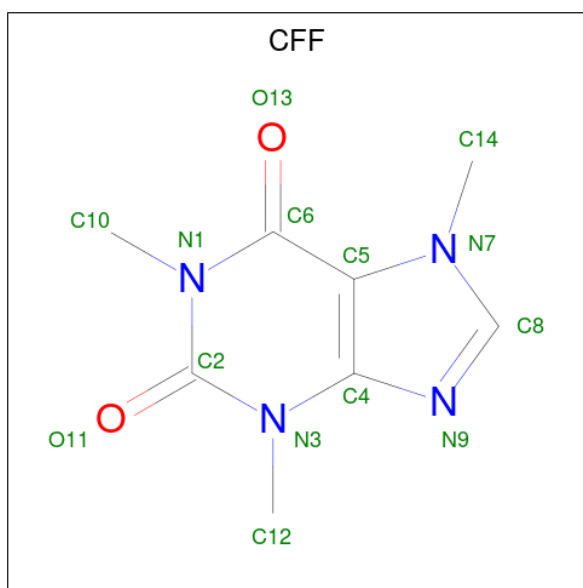
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	C	1	Total	C	N	O	0
			14	8	4	2	
4	D	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	C	1	Total 31	C 10	N 5	O 13	P 3	0
5	C	1	Total 31	C 10	N 5	O 13	P 3	0
5	D	1	Total 31	C 10	N 5	O 13	P 3	0
5	D	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

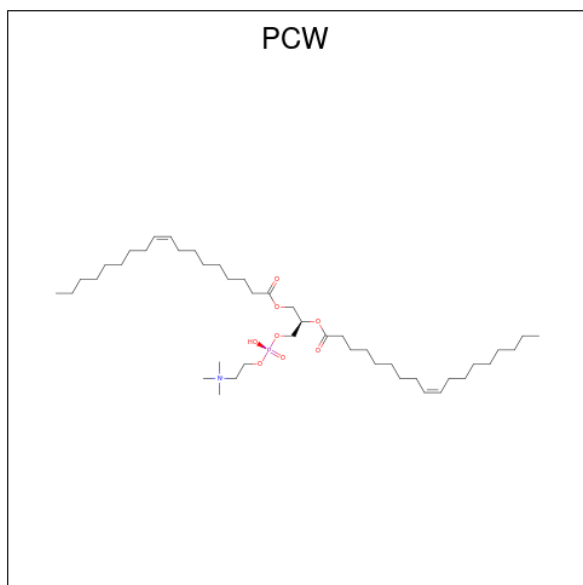
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Ca 1 1	0
6	B	1	Total Ca 1 1	0
6	C	1	Total Ca 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).



Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	A	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	B	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	B	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	C	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	C	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	D	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	D	1	Total	C	N	O	P		0
			54	44	1	8	1		

### 3 Residue-property plots

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

#### • Molecule 1: Ryanodine receptor 1

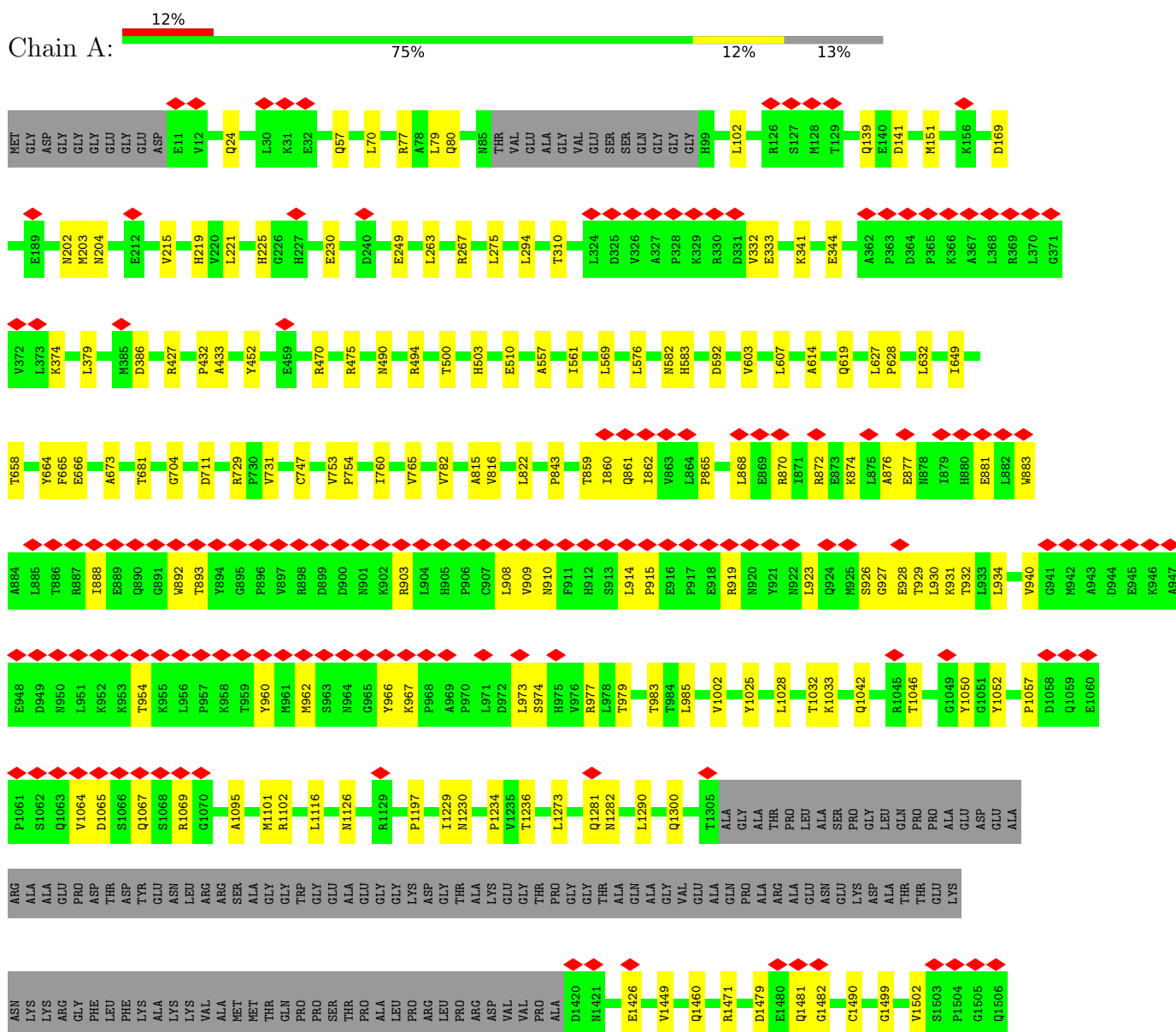


















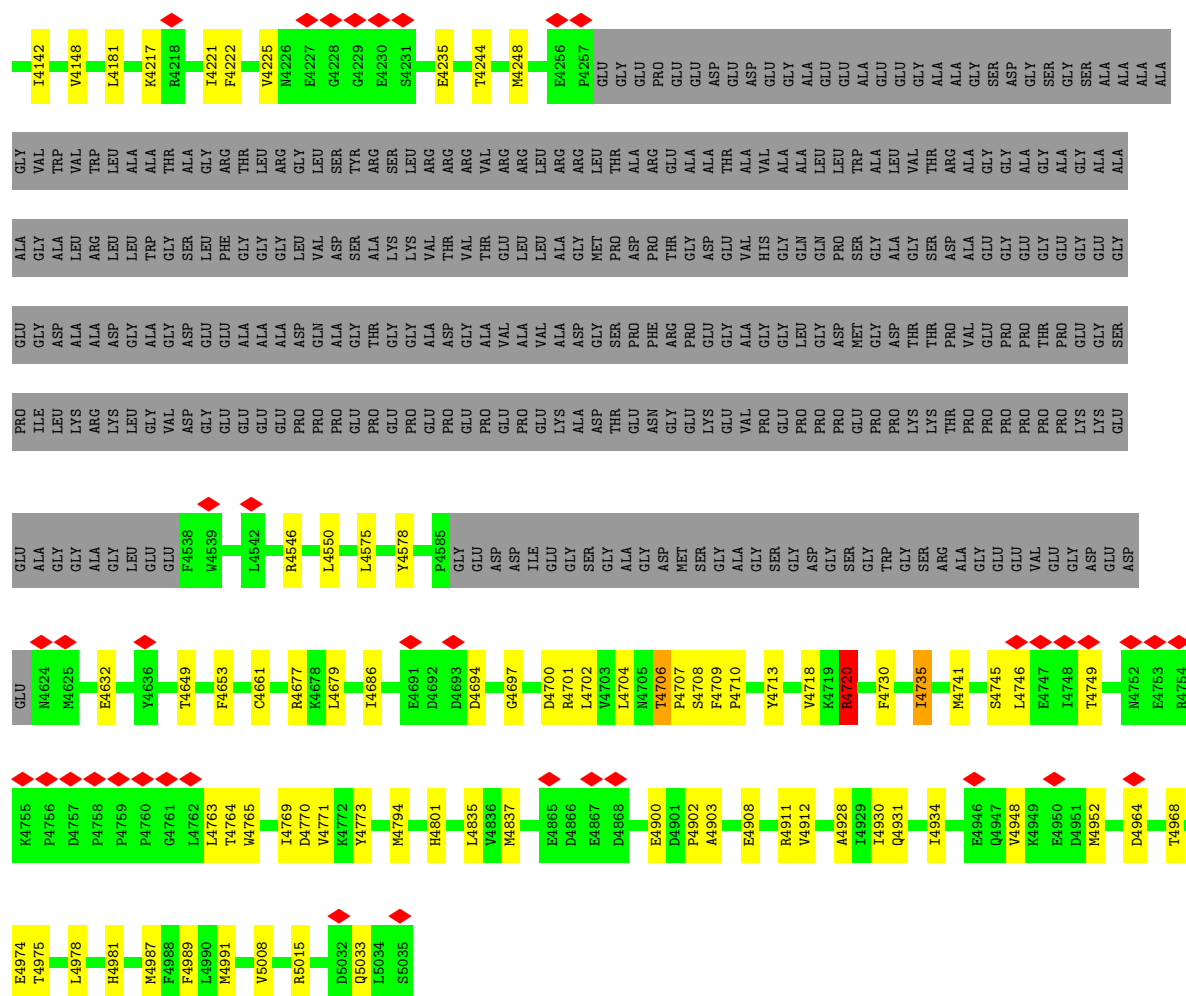


Figure 1: Schematic representation of the protein structure of the 12S OMT. The diagram shows a linear sequence of amino acids from MET to P363. Residues are color-coded: green for residues 1-110 and 126-156, yellow for residues 111-125 and 157-159, and grey for residues 127-155. Red diamonds indicate specific residues: E11, V12, Q24, L30, X31, E32, Q57, L70, R77, A78, L79, Q80, N85, THR, VAL, GLU, ALA, GLY, VAL, GLU, SER, SER, GLN, GLY, GLY, H99, L102, L110, R126, S127, T128, M129, Q139, E140, D141, M151, and A156. The sequence is divided into several blocks by gaps.



M2268	L2139	R2029	E1756	G1N	Q1042	L934	K874	L607	P365
S2271	P2140	T2045	D1757	PRO	Q1045	H939	L875	A614	K366
V2281	V2147	G2046	G1758	ALA	T1046	V940	A876	L379	A367
M2313	L2156	L2047	G1481	ALA	G1049	G941	E877	L627	L368
K2317	L2166	G1482	G1490	ASN	G1050	M942	N878	P628	R369
R2356	M2179	G1499	G1499	GLU	G1051	A943	I879	L370	G371
R2370	M2187	V1502	V1502	ASP	Y1052	D944	E881	V372	V372
D2390	Y2193	S1503	S1503	ALA	P1057	E945	L882	L373	K374
P2391	N2197	P1504	P1504	THR	D1058	A947	W883		
A2392	L2198	P1505	P1505	GLU	E1059	E948	A884		
R2393	M2199	G1505	G1505	ALA	E1060	D949	L885		
D2394	R2200	Q1506	Q1506	ARG	P1061	N950	T886		
G2397	A2201	Q1507	Q1507	ALA	S1062	L951	I888		
V2398	L2202	G1508	G1508	GLU	Q1063	K952	Q890		
ARG	M2209	R1509	R1509	ASP	V1064	T954	G891		
ASP	E2210	I1510	I1510	THR	D1065	K953	G704		
ARG	M2213	S1511	S1511	ASP	S1066	L956	D711		
ARG	N2214	H1512	H1512	TYR	Q1067	P957	T993		
ARG	V2215	N1546	N1546	ASN	S1068	K958	Y894		
ARG	L2216	V1555	V1555	LEU	R1069	T959	G895		
GLU	G2217	T1558	T1558	ARG	G1070	Y960	P396		
HIS	G2218	V1562	V1562	ARG	A1095	M961	V897		
PHE	G2219	I1642	I1642	ALA	M1101	M962	R398		
GLY	E2220	E1645	E1645	GLY	R1102	S963	D899		
GLU	S2221	N1646	N1646	TRP	L1116	N964	N901		
GLU	K2222	R1647	R1647	GLU	N1126	G965	K902		
P2411	E2223	M1649	M1649	ALA	R1129	K967	R903		
P2412	I2224	D1659	D1659	GLY	P1197	L971	L904		
E2413	R2225	L1677	L1677	ASP	T1230	D972	H905		
E2414	M2229	A1685	A1685	GLY	V1235	S974	P906		
N2415	C2234	L1695	L1695	THR	T1236	L978	C907		
R2416	R2235	R1703	R1703	GLY	L1273	T979	L508		
L2419	F2236	G1752	G1752	ALA	Q1281	P980	N910		
A2438	L2124	R1753	R1753	THR	N1282	T983	V909		
E2450	Q2128	S1754	S1754	ARG	L1290	L985	L555		
I2457	L2132	A1755	A1755	VAL	Q1300	T984	L569		
L2461	L2136			GLU	T1305	L985	I570		
L2480	L2136			ALA	ALA	L985	E571		
G2481	L2136			ALA	ALA	L985	V575		
K2482	L2136			ALA	ALA	L985	L576		
D2483	L2136			ALA	ALA	L985	I579		
G2484	L2136			ALA	ALA	L985	N582		
A2485	L2136			ALA	ALA	L985	R370		
L2505	L2136			ALA	ALA	L985	H583		
	L2136			ALA	ALA	L985	D592		
	L2136			ALA	ALA	L985	V603		





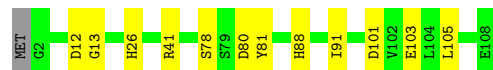
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 87% 12%



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 88% 11%




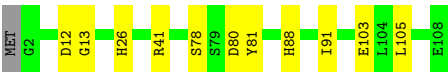
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 89% 10%



● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:  89% 10% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26588	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 ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.463	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	427.776, 427.776, 427.776	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8355, 0.8355, 0.8355	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.20	0/35586	0.36	4/48203 (0.0%)
1	B	0.20	0/35586	0.36	4/48203 (0.0%)
1	C	0.20	0/35586	0.36	4/48203 (0.0%)
1	D	0.20	0/35586	0.36	4/48203 (0.0%)
2	E	0.17	0/847	0.34	0/1142
2	F	0.17	0/847	0.32	0/1142
2	G	0.18	0/847	0.33	0/1142
2	H	0.18	0/847	0.33	0/1142
All	All	0.20	0/145732	0.36	16/197380 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2237	LEU	CA-C-N	8.49	134.18	120.60
1	C	2237	LEU	C-N-CA	8.49	134.18	120.60
1	A	2237	LEU	CA-C-N	8.48	134.16	120.60
1	A	2237	LEU	C-N-CA	8.48	134.16	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2237	LEU	CA-C-N	8.48	134.16	120.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4701	ARG	Sidechain
1	A	4720	ARG	Sidechain
1	B	4701	ARG	Sidechain
1	B	4720	ARG	Sidechain
1	C	4701	ARG	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	34797	0	34384	428	0
1	B	34797	0	34384	432	0
1	C	34797	0	34384	425	0
1	D	34797	0	34384	427	0
2	E	829	0	826	11	0
2	F	829	0	826	11	0
2	G	829	0	826	10	0
2	H	829	0	826	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	62	0	24	1	0
5	B	62	0	24	1	0
5	C	62	0	24	1	0
5	D	62	0	24	2	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	108	0	168	0	0
7	B	108	0	168	0	0
7	C	108	0	168	1	0
7	D	108	0	168	1	0
All	All	143248	0	141648	1734	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 6.

The worst 5 of 1734 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:D:2234:CYS:SG	1:D:2271:SER:OG	2.24	0.94
1:A:2234:CYS:SG	1:A:2271:SER:OG	2.24	0.94
1:B:2234:CYS:SG	1:B:2271:SER:OG	2.24	0.94
1:C:2234:CYS:SG	1:C:2271:SER:OG	2.24	0.94
1:C:2879:LEU:HD12	1:C:2928:LEU:HD21	1.55	0.88

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	4345/5035 (86%)	4201 (97%)	144 (3%)	0	100	100
1	B	4345/5035 (86%)	4200 (97%)	145 (3%)	0	100	100
1	C	4345/5035 (86%)	4203 (97%)	142 (3%)	0	100	100
1	D	4345/5035 (86%)	4201 (97%)	144 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17800/20572 (86%)	17210 (97%)	590 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3806/4296 (89%)	3799 (100%)	7 (0%)	87	89
1	B	3806/4296 (89%)	3799 (100%)	7 (0%)	87	89
1	C	3806/4296 (89%)	3799 (100%)	7 (0%)	87	89
1	D	3806/4296 (89%)	3799 (100%)	7 (0%)	87	89
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15580/17544 (89%)	15552 (100%)	28 (0%)	85	89

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	219	HIS
1	D	4771	VAL
1	C	4718	VAL
1	D	4718	VAL
1	C	4706	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2963	GLN
1	D	3557	ASN
1	B	1632	GLN
1	B	1591	GLN
1	D	3892	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\# Z  > 2$
7	PCW	B	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.07	3 (5%)
4	CFF	C	8002	-	15,15,15	1.81	6 (40%)	23,23,23	2.96	12 (52%)
7	PCW	A	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.07	3 (5%)
7	PCW	B	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.15	4 (6%)
5	ATP	C	8007	-	32,33,33	0.26	0	48,52,52	0.68	0
5	ATP	B	8003	-	32,33,33	0.28	0	48,52,52	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CFF	B	8002	-	15,15,15	1.81	6 (40%)	23,23,23	2.97	12 (52%)
5	ATP	C	8003	-	32,33,33	0.27	0	48,52,52	0.67	0
7	PCW	A	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.15	4 (6%)
5	ATP	D	8007	-	32,33,33	0.26	0	48,52,52	0.68	0
7	PCW	C	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.15	4 (6%)
5	ATP	A	8007	-	32,33,33	0.27	0	48,52,52	0.68	0
7	PCW	D	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.07	3 (5%)
5	ATP	A	8003	-	32,33,33	0.28	0	48,52,52	0.67	0
5	ATP	B	8007	-	32,33,33	0.27	0	48,52,52	0.68	0
7	PCW	D	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.15	4 (6%)
4	CFF	A	8002	-	15,15,15	1.81	6 (40%)	23,23,23	2.96	12 (52%)
4	CFF	D	8002	-	15,15,15	1.81	6 (40%)	23,23,23	2.97	12 (52%)
5	ATP	D	8003	-	32,33,33	0.27	0	48,52,52	0.67	0
7	PCW	C	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.07	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	B	8006	-	-	22/57/57/57	-
4	CFF	C	8002	-	-	-	0/2/2/2
7	PCW	A	8006	-	-	22/57/57/57	-
7	PCW	B	8005	-	-	26/57/57/57	-
5	ATP	C	8007	-	-	6/22/38/38	0/3/3/3
5	ATP	B	8003	-	-	6/22/38/38	0/3/3/3
4	CFF	B	8002	-	-	-	0/2/2/2
5	ATP	C	8003	-	-	6/22/38/38	0/3/3/3
7	PCW	A	8005	-	-	26/57/57/57	-
5	ATP	D	8007	-	-	6/22/38/38	0/3/3/3
7	PCW	C	8005	-	-	26/57/57/57	-
5	ATP	A	8007	-	-	6/22/38/38	0/3/3/3
7	PCW	D	8006	-	-	22/57/57/57	-
5	ATP	A	8003	-	-	6/22/38/38	0/3/3/3
5	ATP	B	8007	-	-	6/22/38/38	0/3/3/3
7	PCW	D	8005	-	-	26/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CFF	A	8002	-	-	-	0/2/2/2
4	CFF	D	8002	-	-	-	0/2/2/2
5	ATP	D	8003	-	-	6/22/38/38	0/3/3/3
7	PCW	C	8006	-	-	22/57/57/57	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8002	CFF	C6-N1	-3.73	1.32	1.40
4	C	8002	CFF	C6-N1	-3.73	1.32	1.40
4	B	8002	CFF	C6-N1	-3.71	1.32	1.40
4	D	8002	CFF	C6-N1	-3.71	1.32	1.40
7	B	8005	PCW	O3-C11	3.08	1.42	1.33

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8002	CFF	C14-N7-C8	-8.30	110.76	126.28
4	D	8002	CFF	C14-N7-C8	-8.29	110.76	126.28
4	A	8002	CFF	C14-N7-C8	-8.27	110.80	126.28
4	C	8002	CFF	C14-N7-C8	-8.26	110.82	126.28
4	B	8002	CFF	C14-N7-C5	5.63	141.16	127.77

There are no chirality outliers.

5 of 240 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	8003	ATP	C5'-O5'-PA-O2A
5	A	8003	ATP	C5'-O5'-PA-O3A
5	B	8003	ATP	C5'-O5'-PA-O2A
5	B	8003	ATP	C5'-O5'-PA-O3A
5	C	8003	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 7 short contacts:

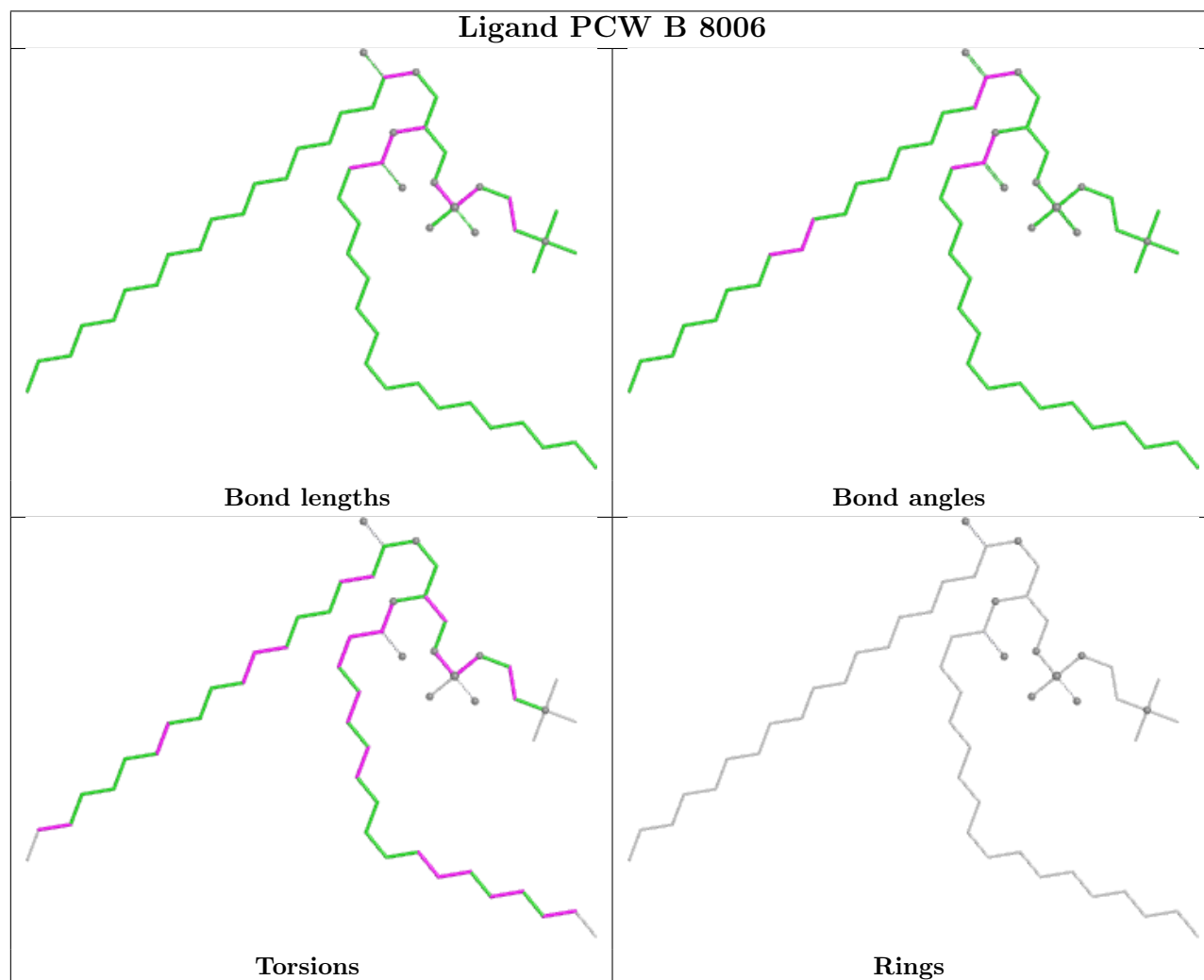
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8003	ATP	1	0
5	C	8003	ATP	1	0
7	D	8006	PCW	1	0

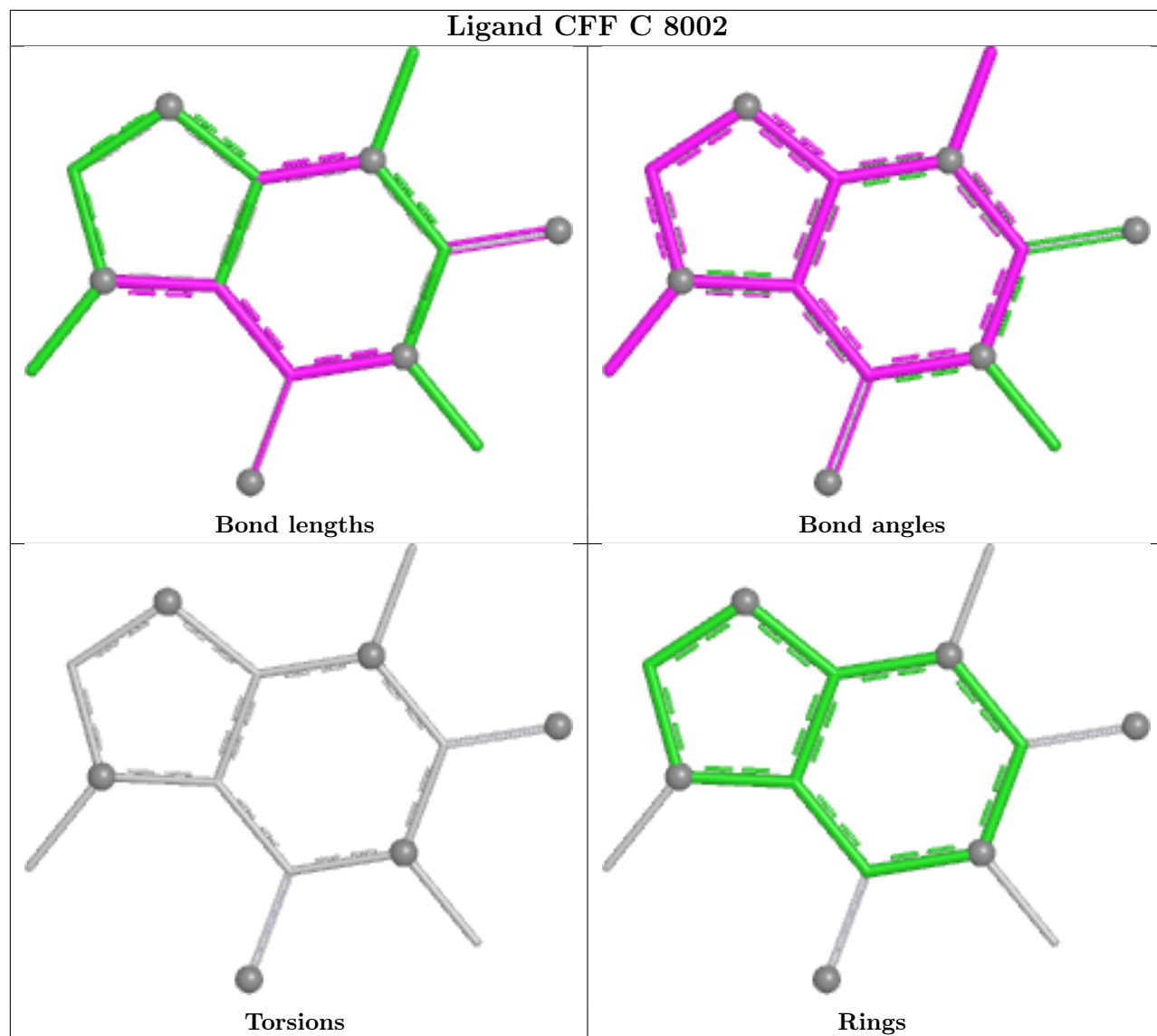
*Continued on next page...*

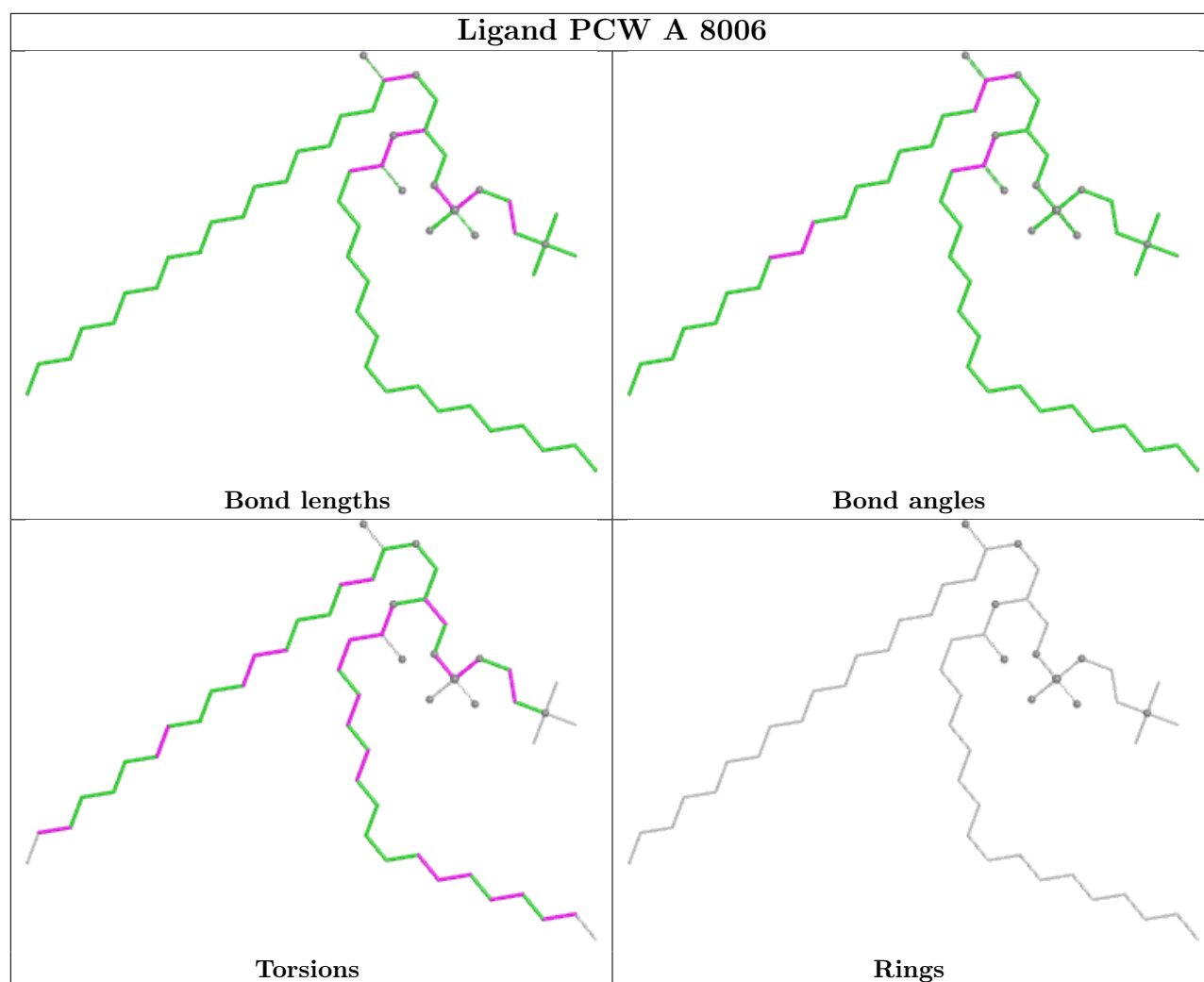
*Continued from previous page...*

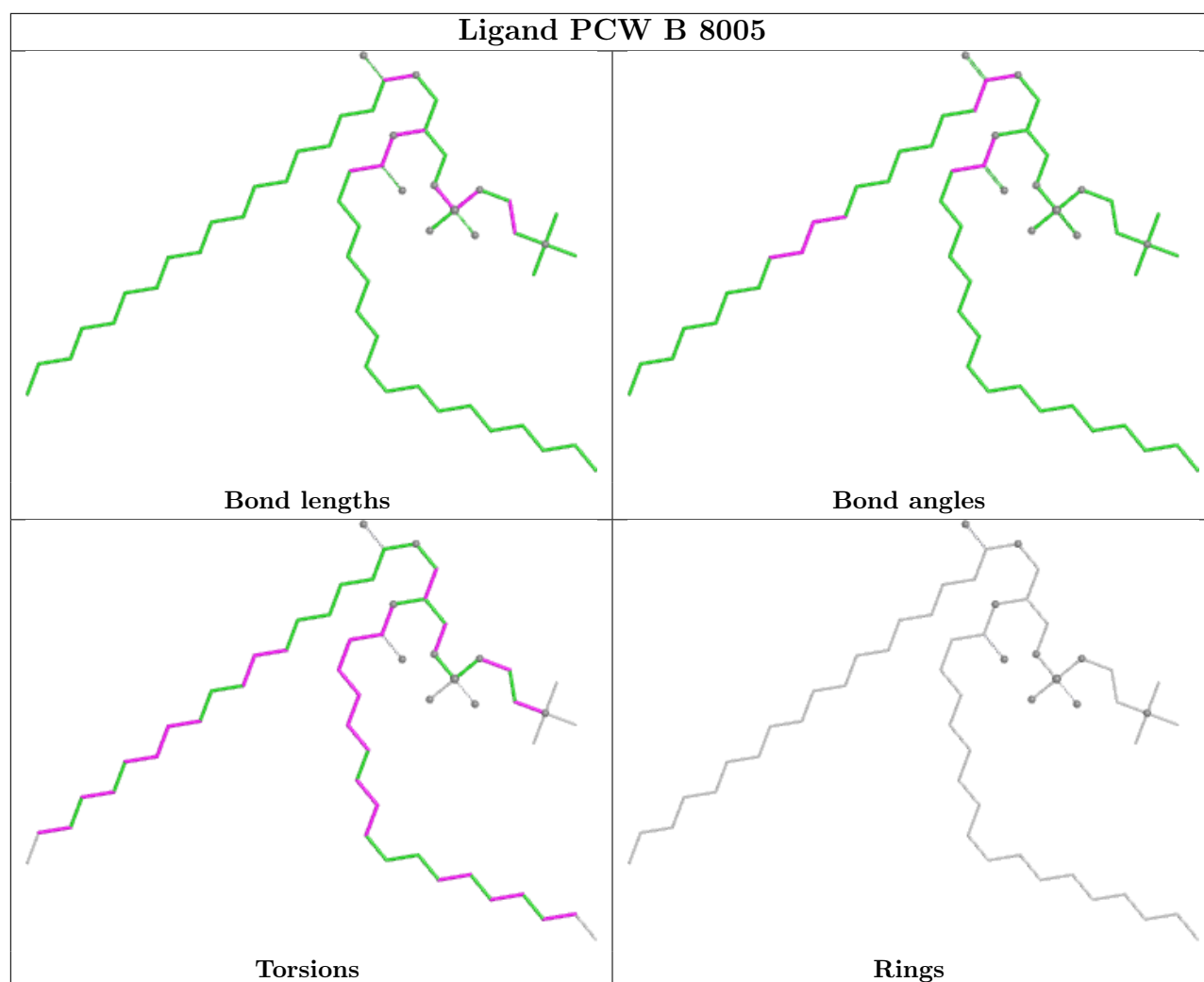
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8003	ATP	1	0
5	D	8003	ATP	2	0
7	C	8006	PCW	1	0

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.

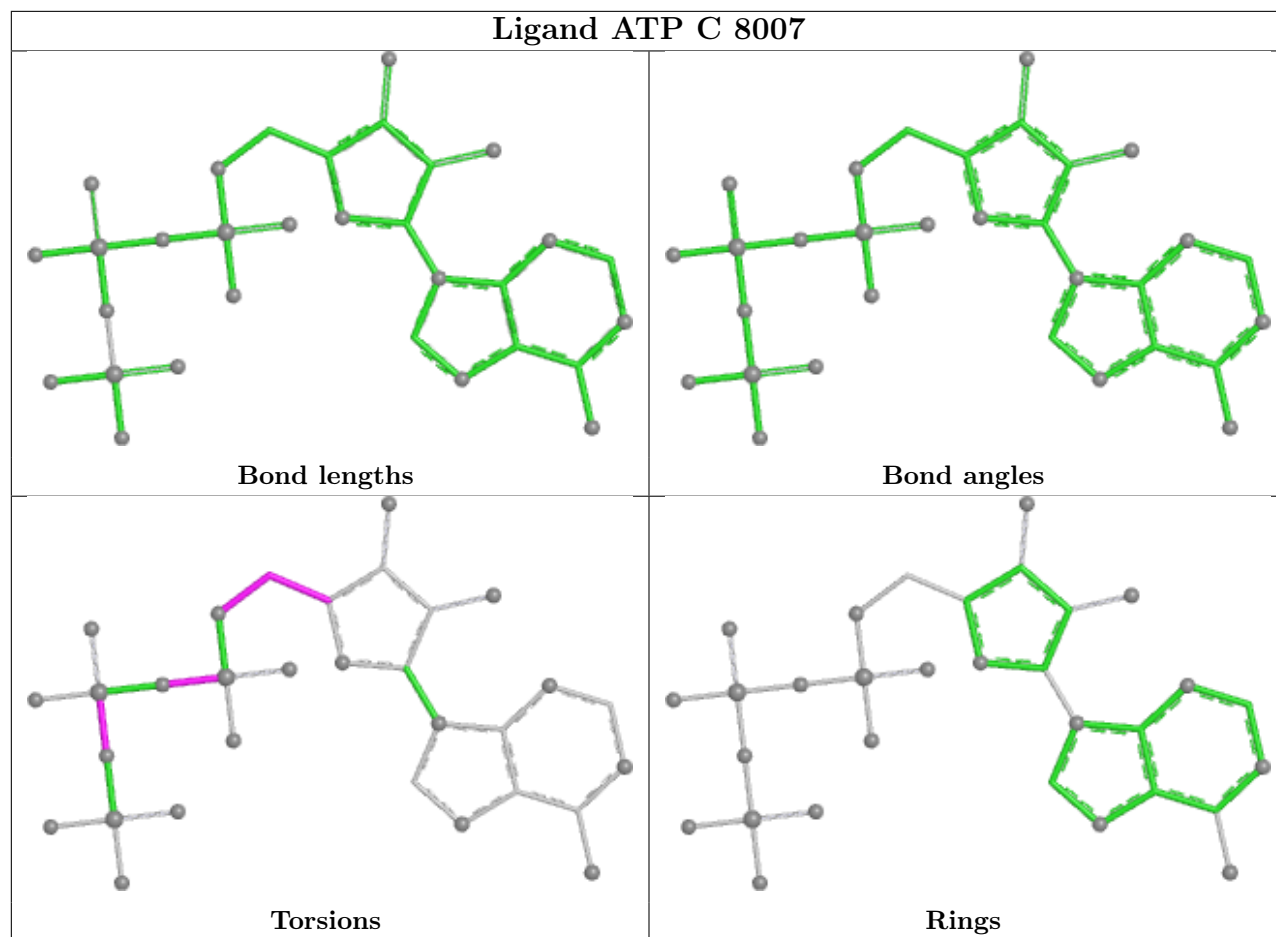


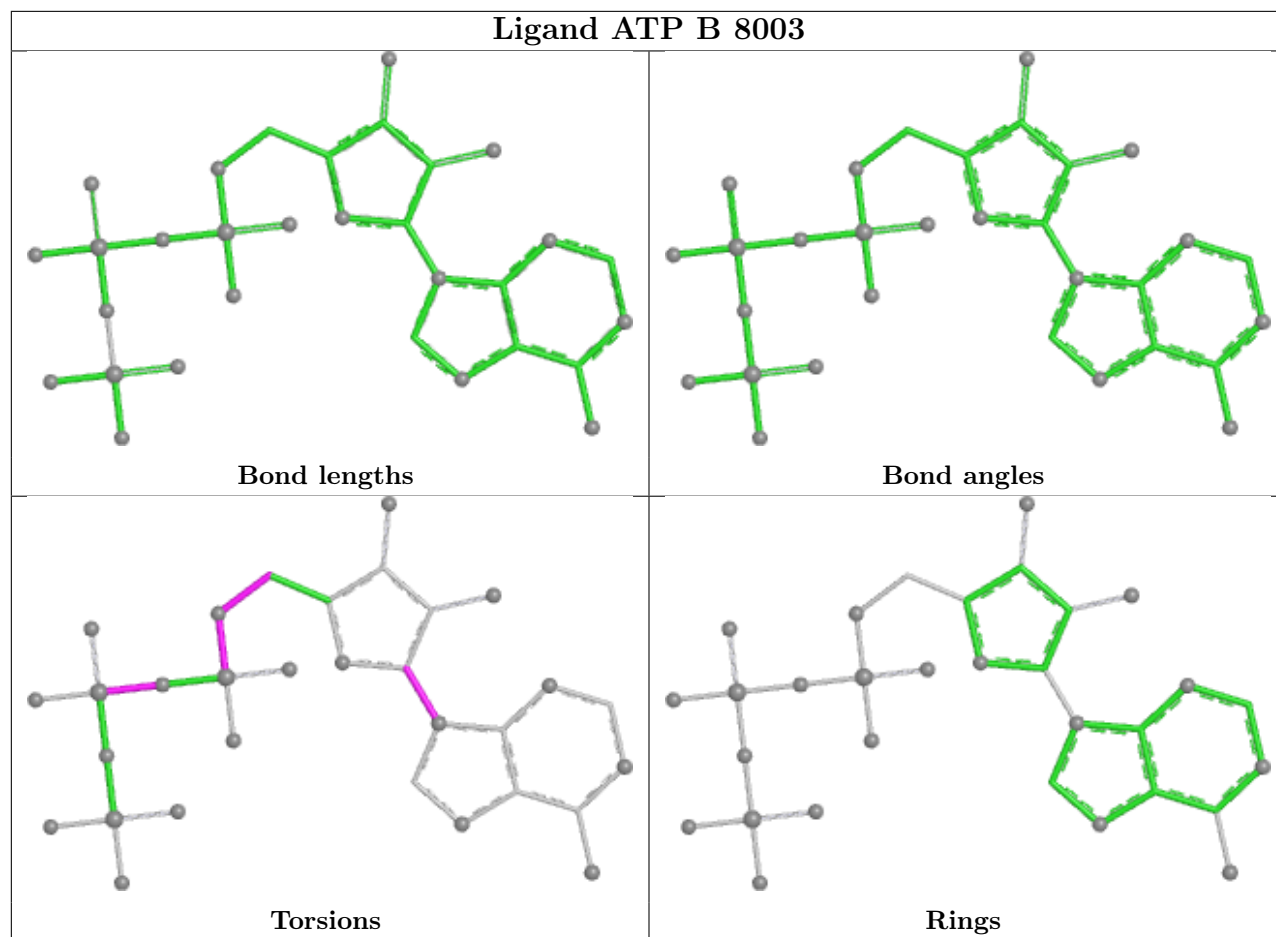


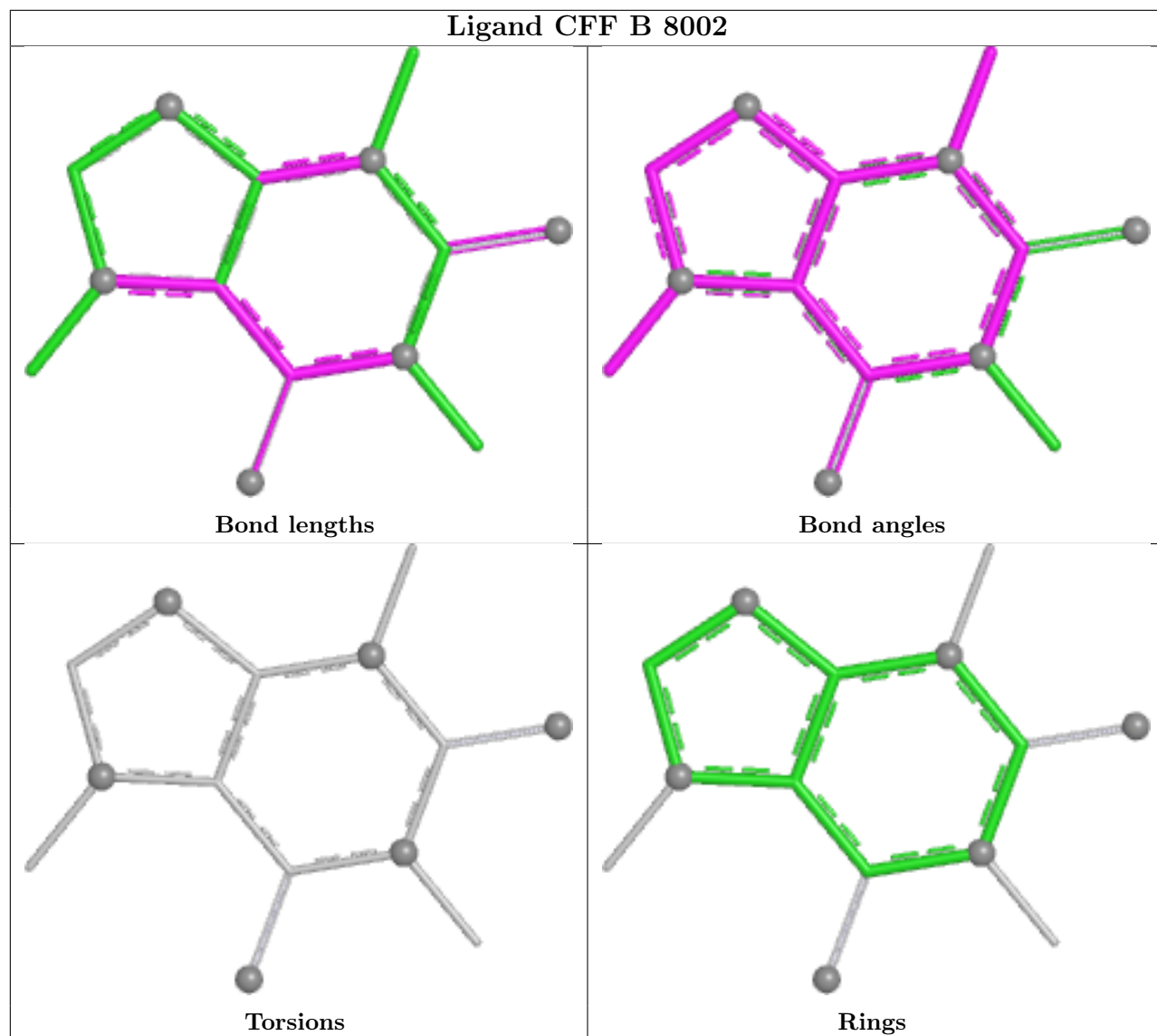


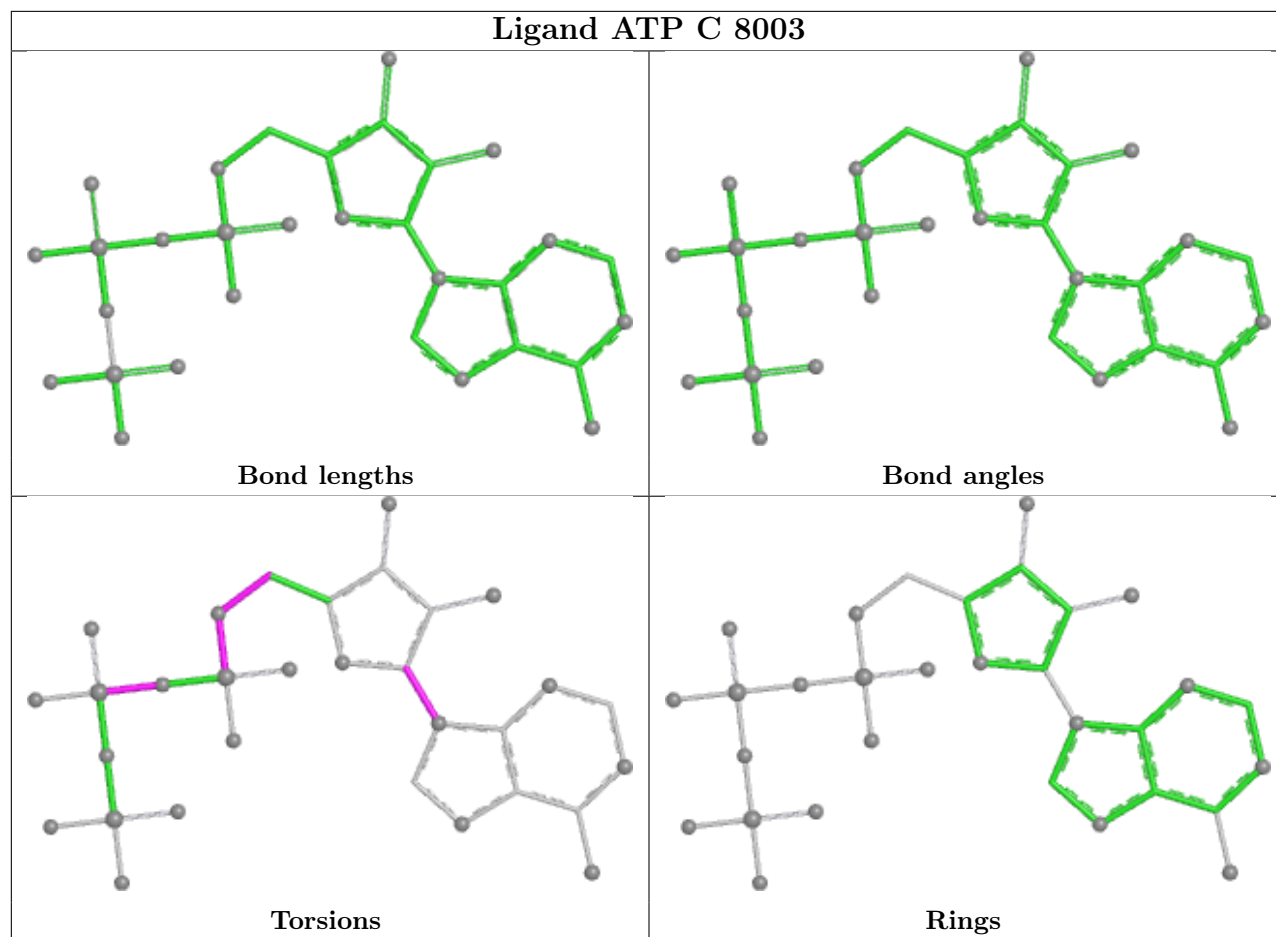


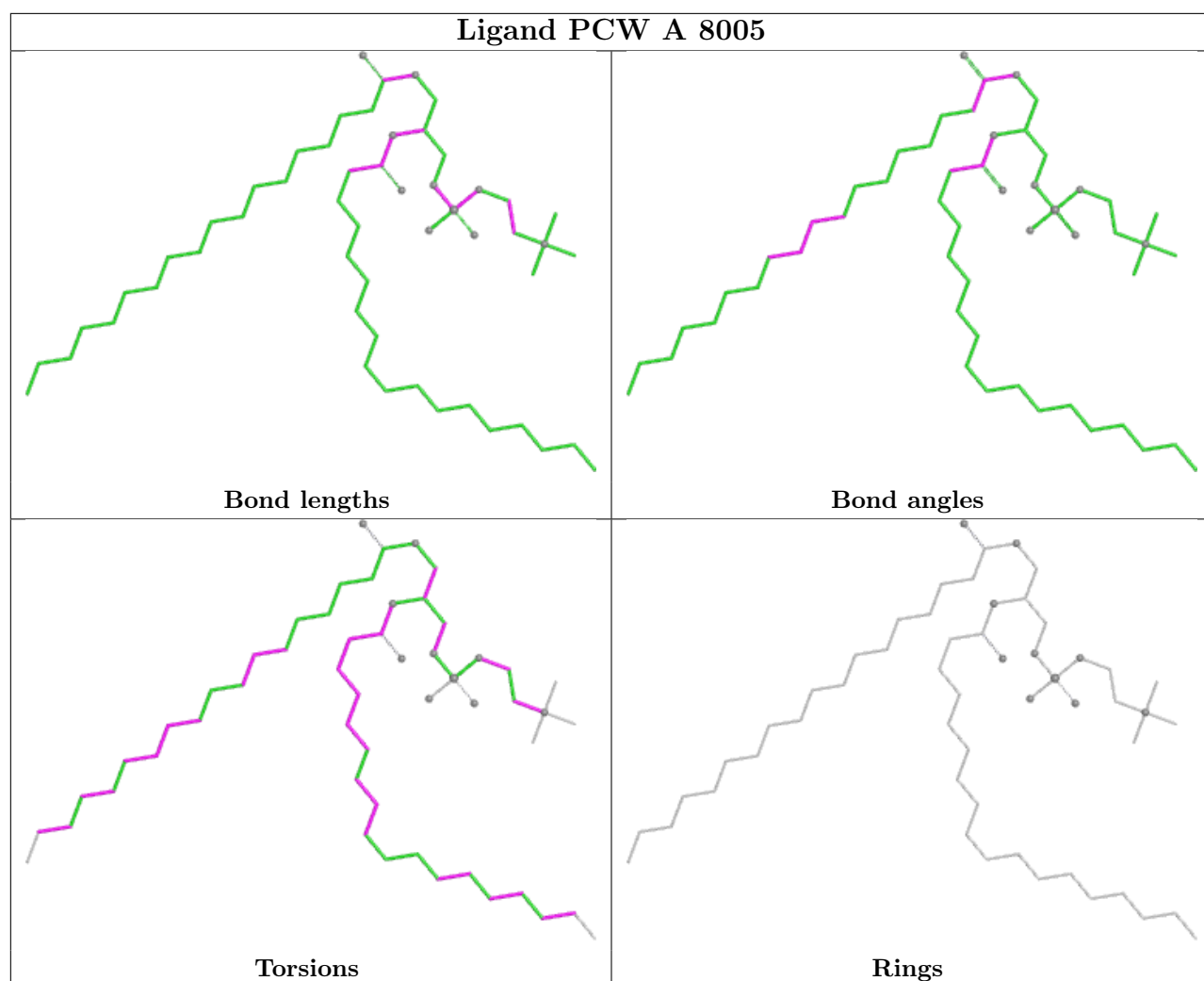


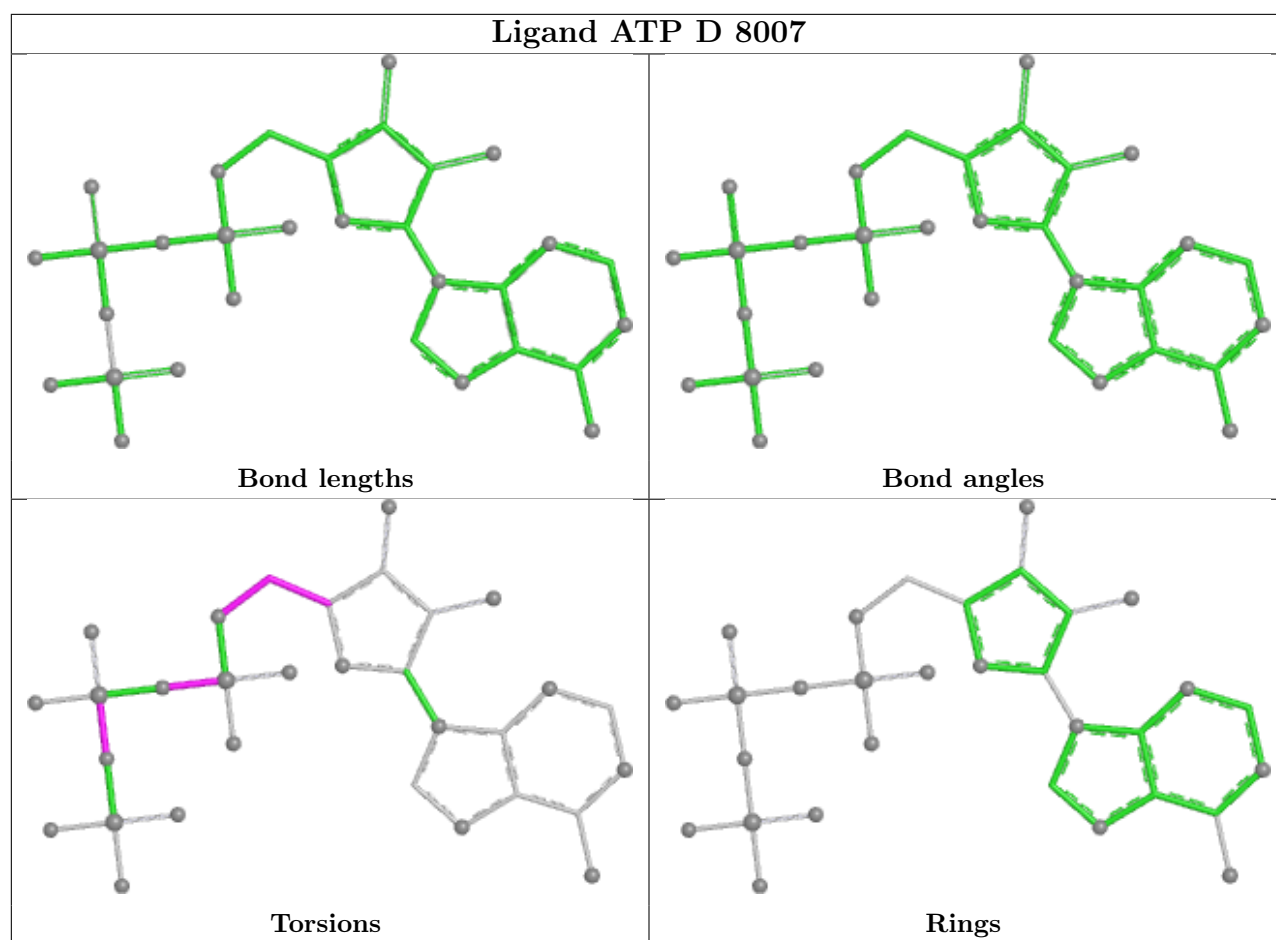


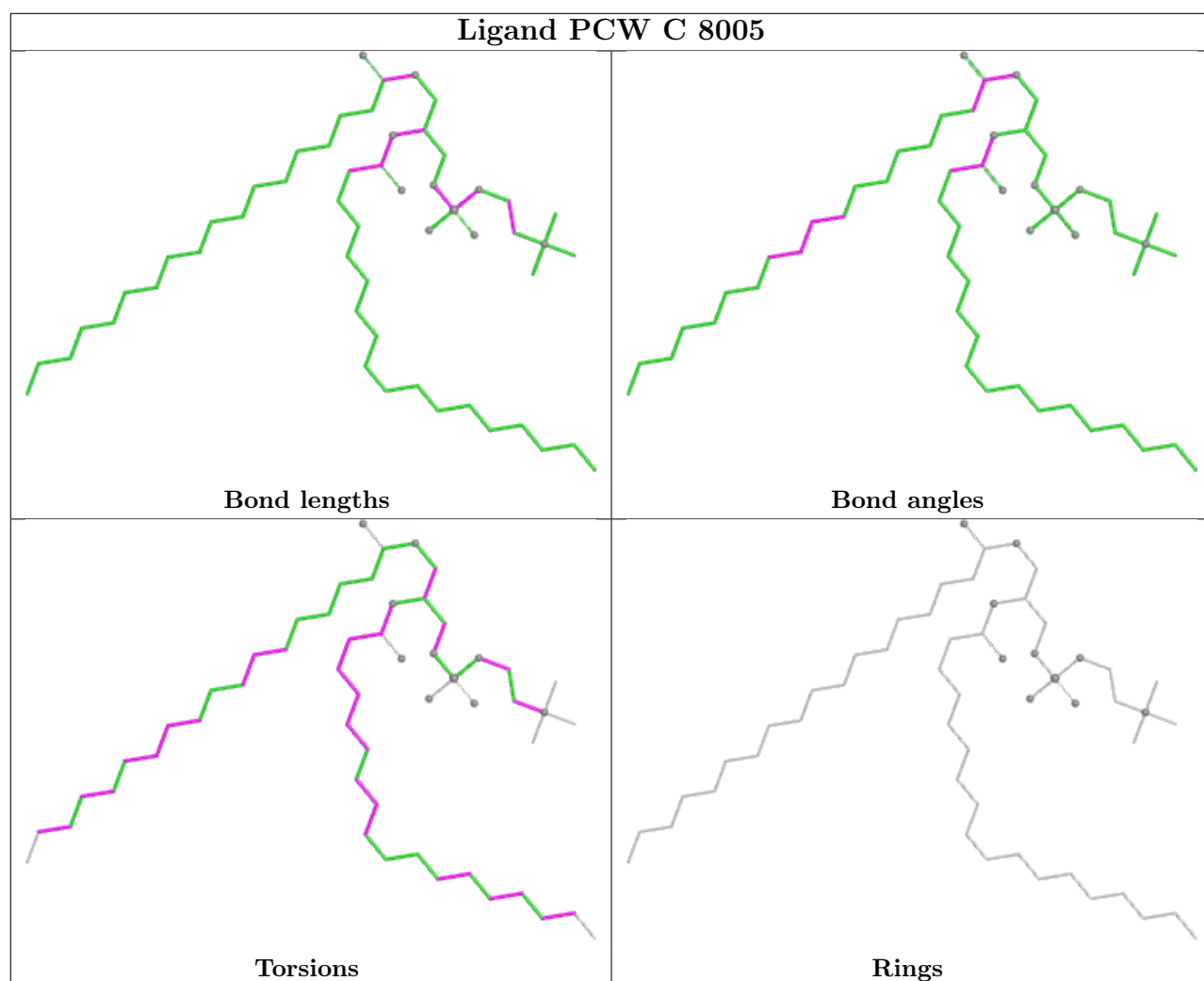


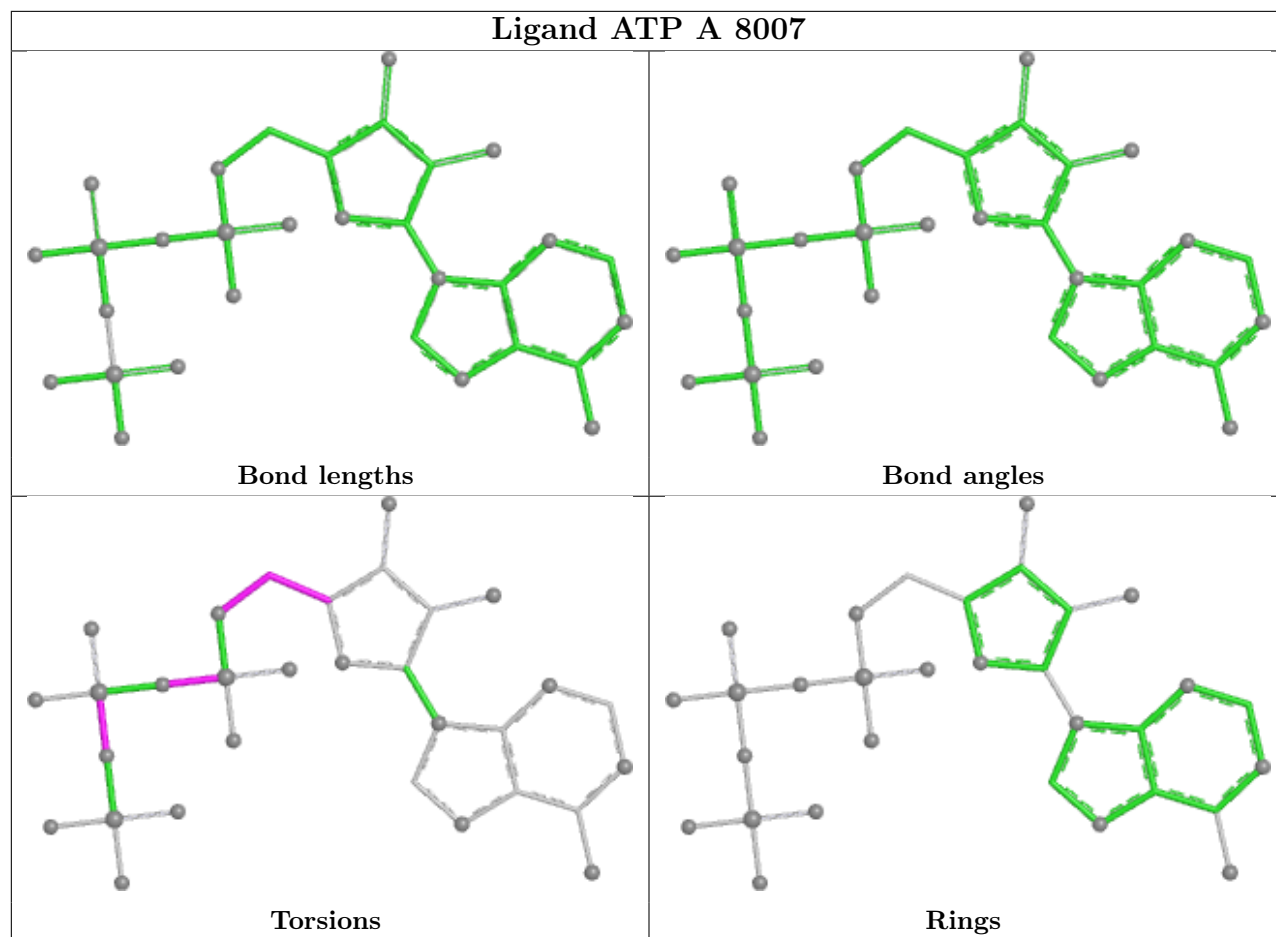




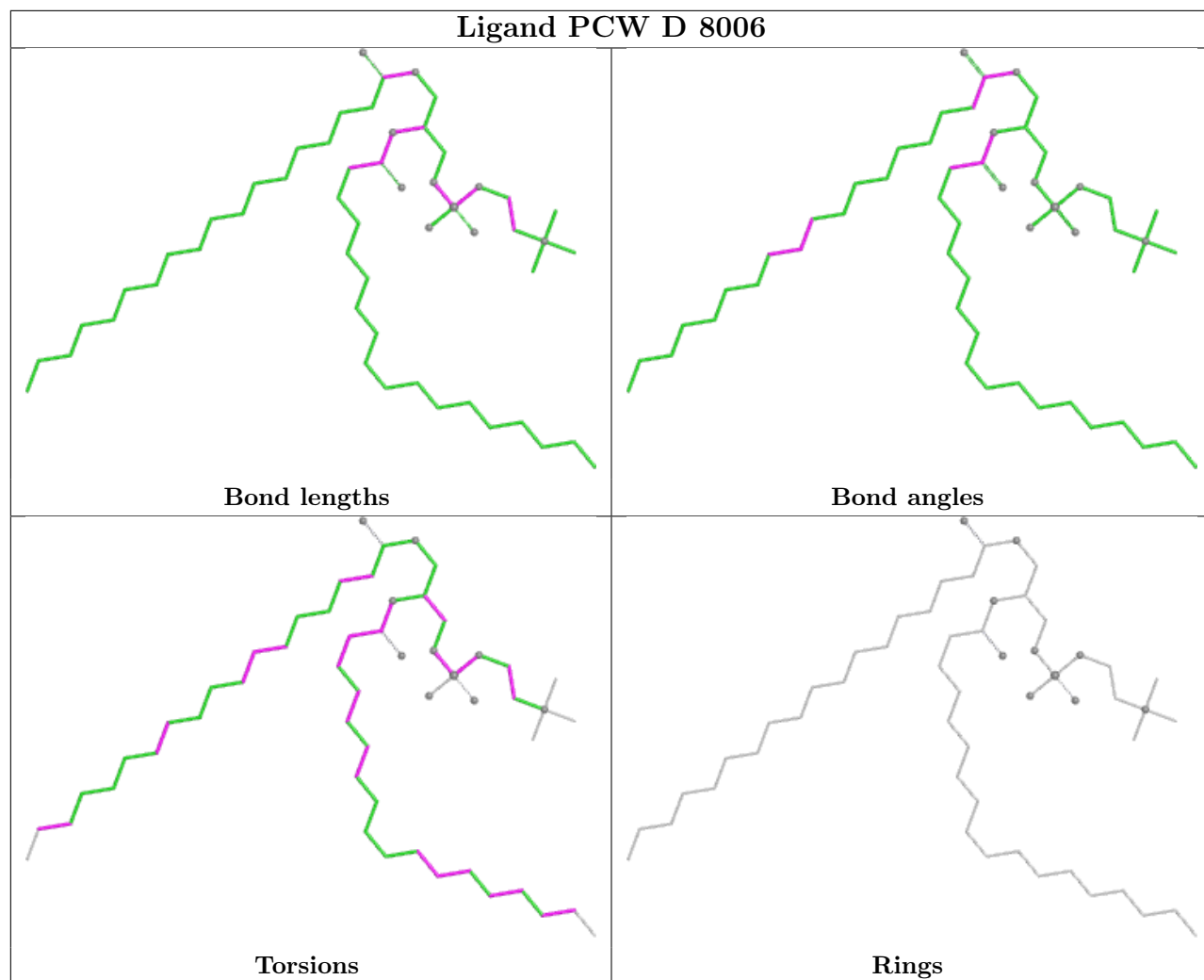


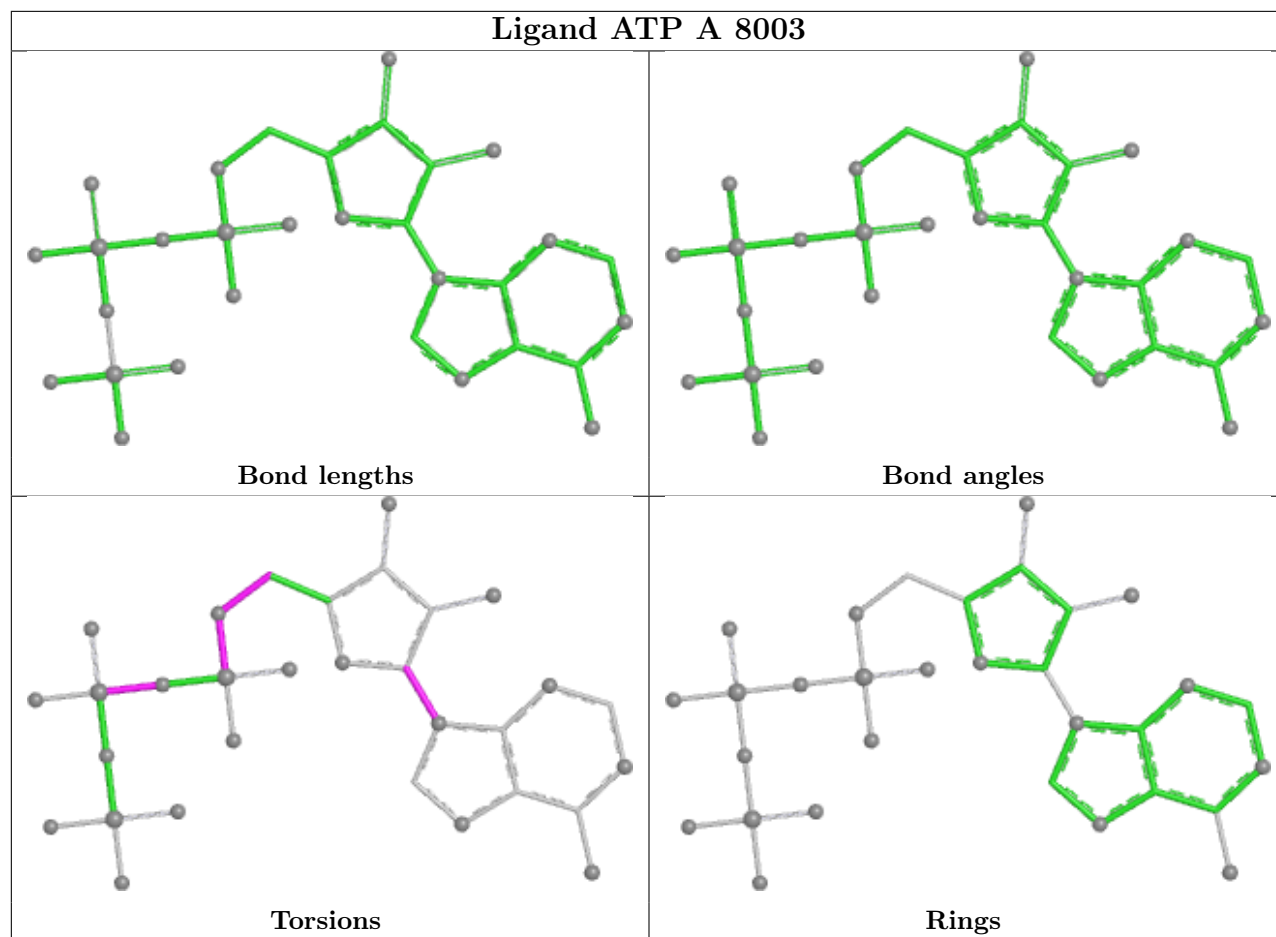


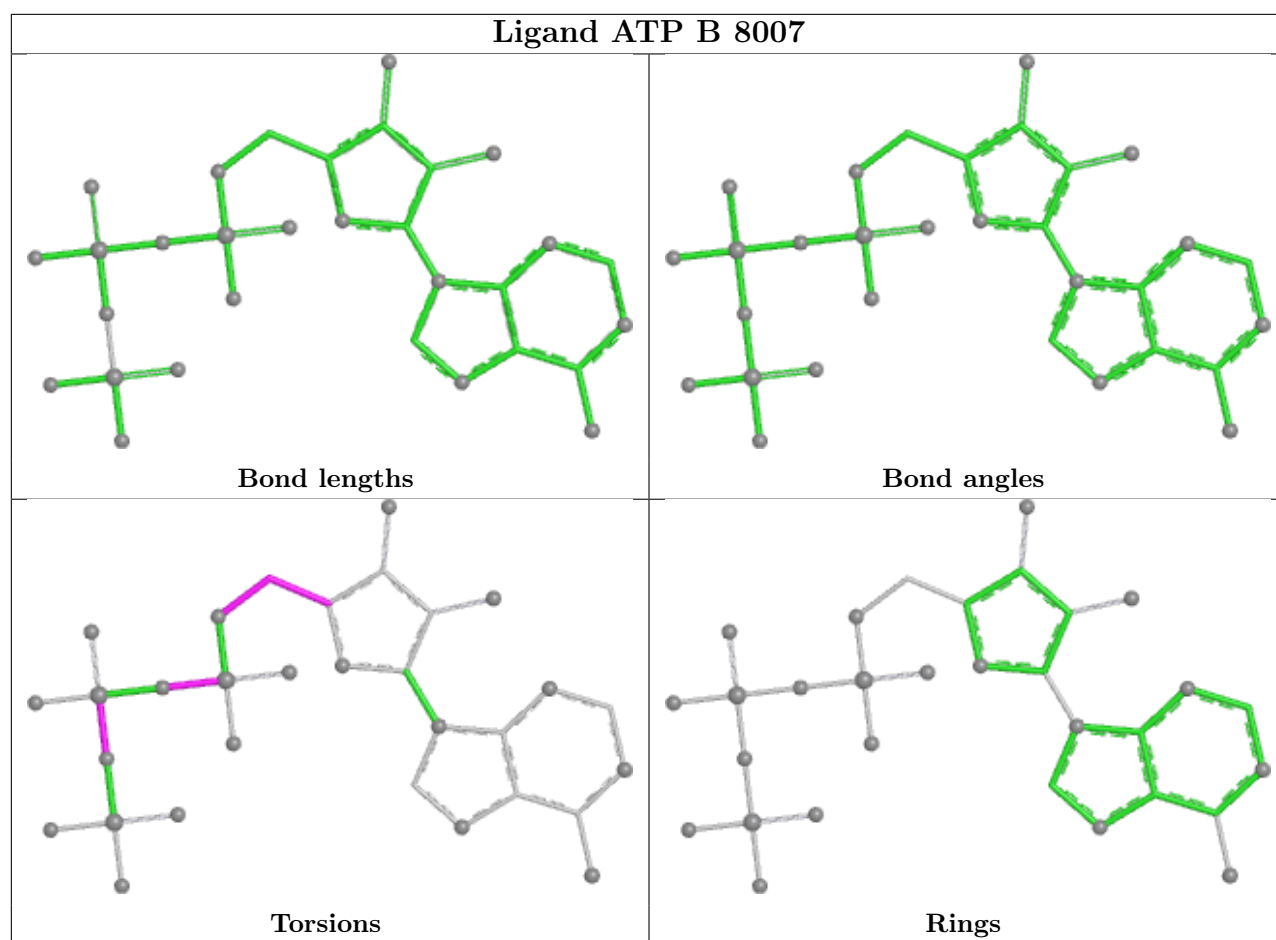


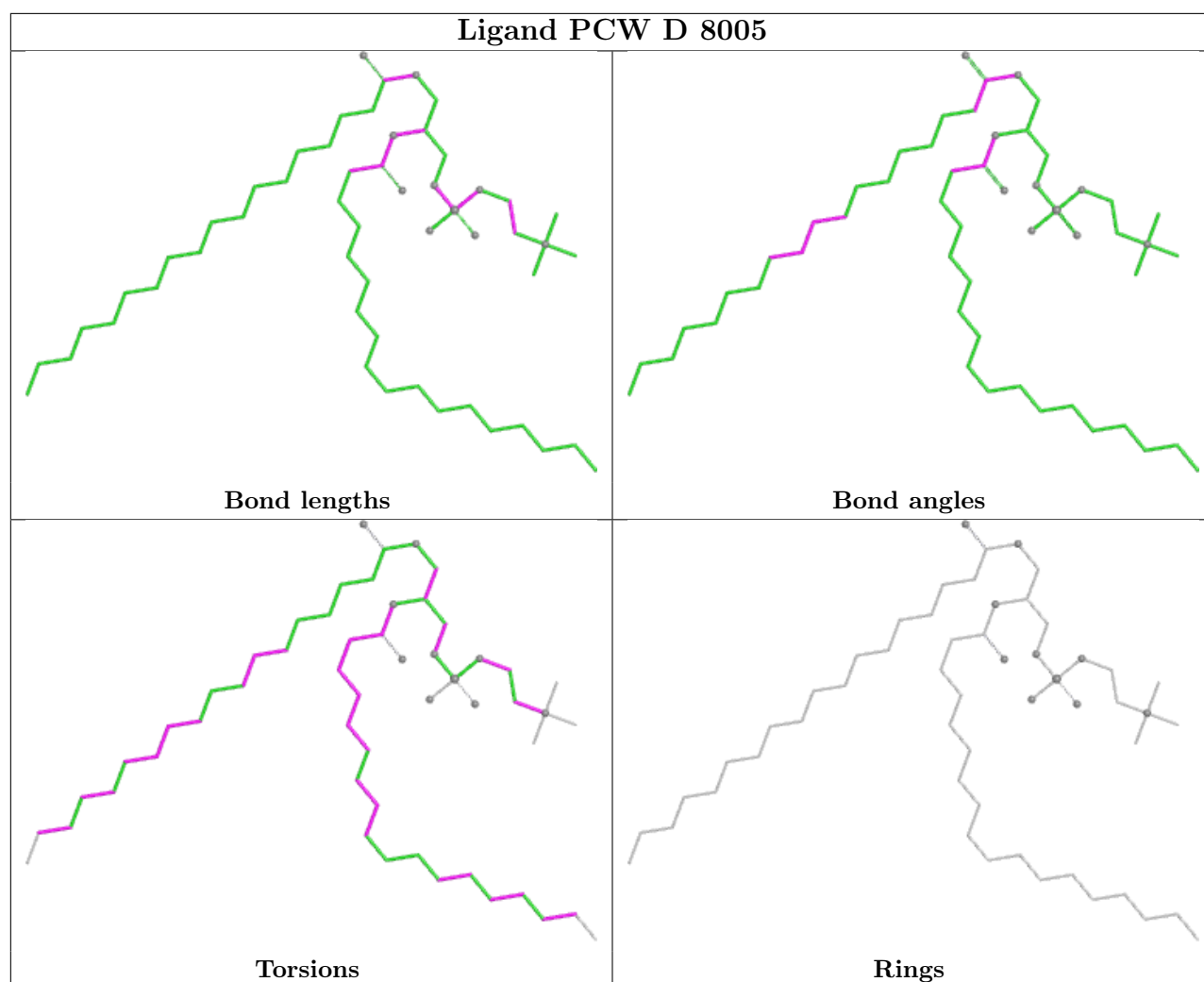


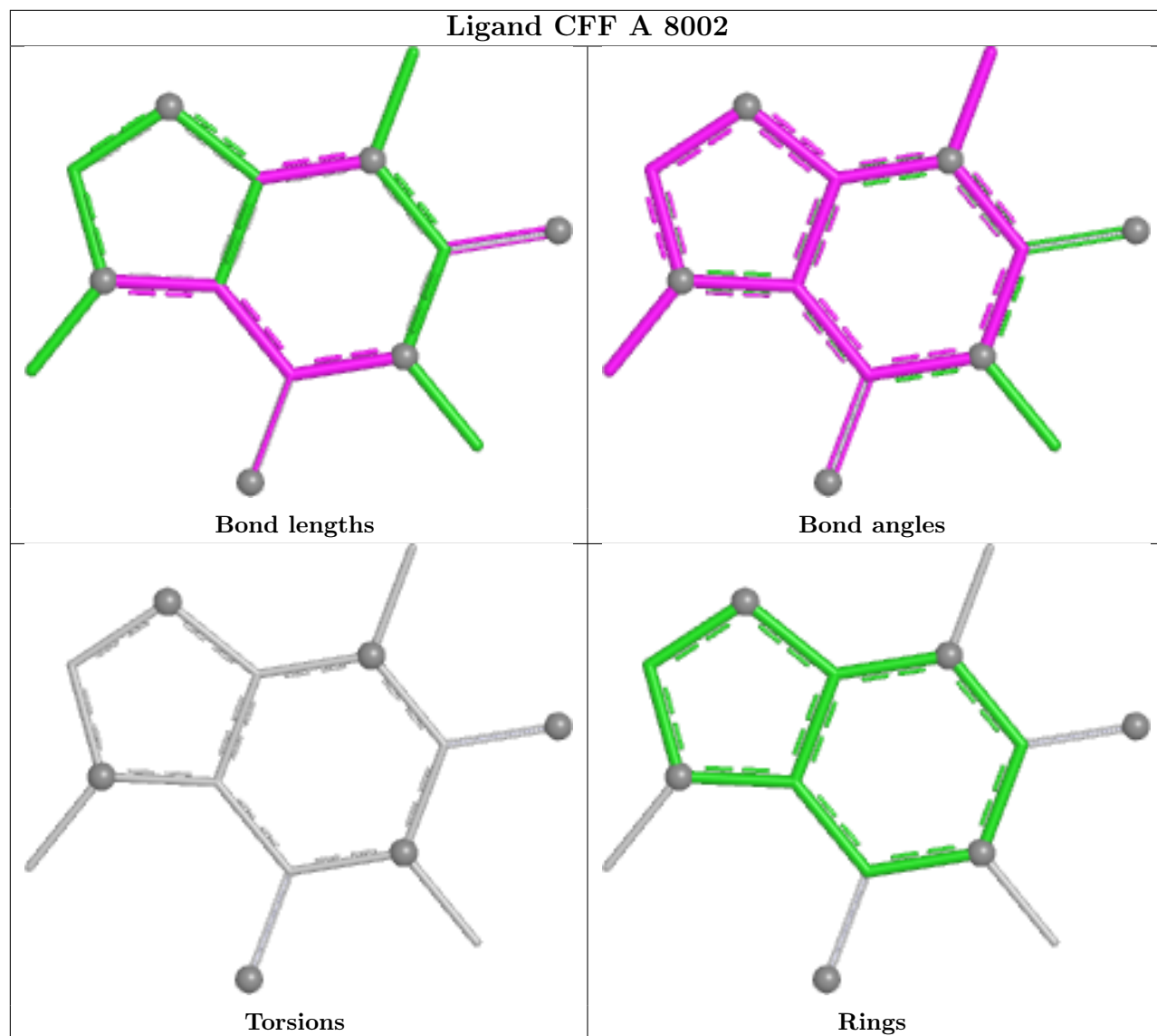


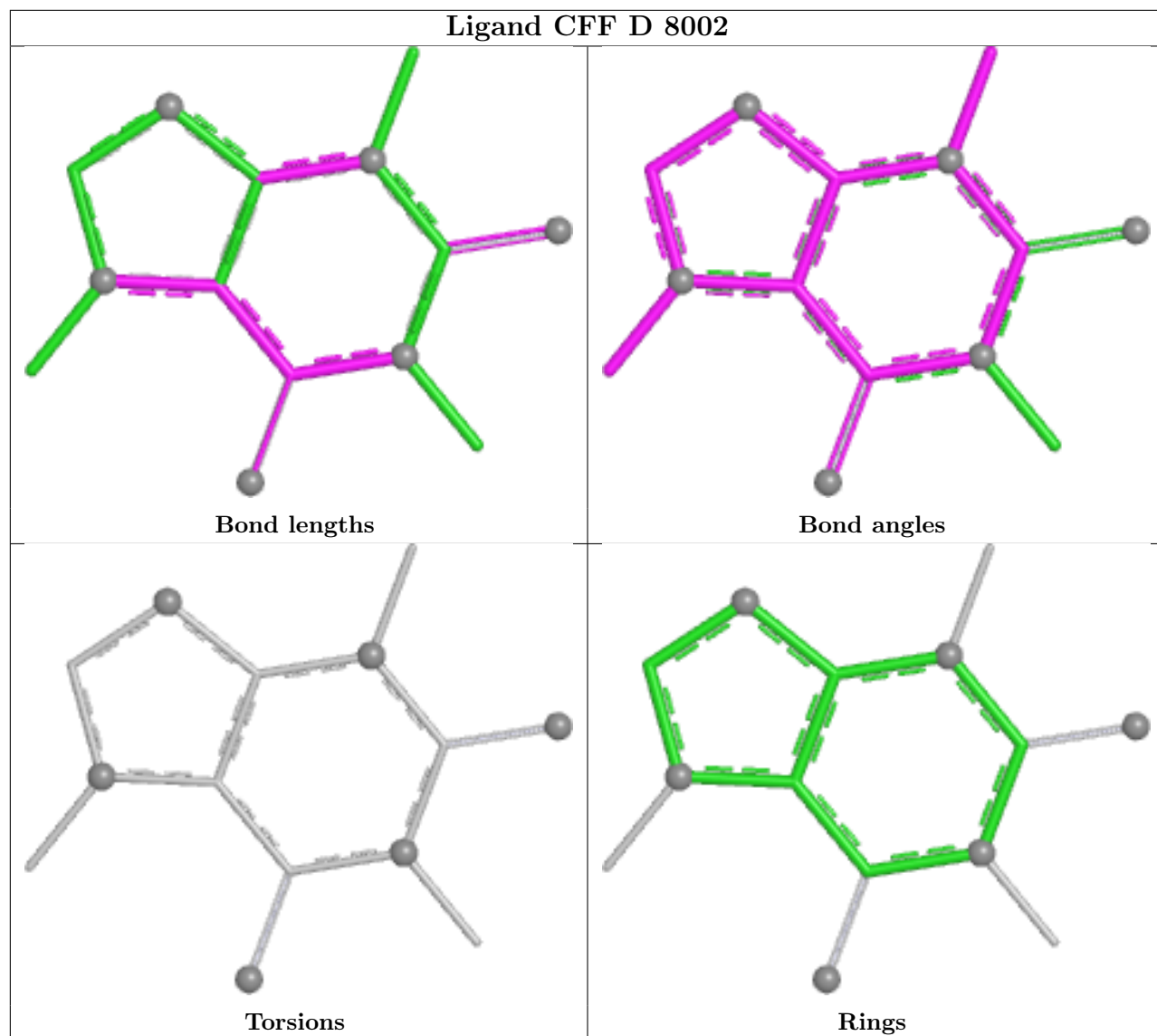


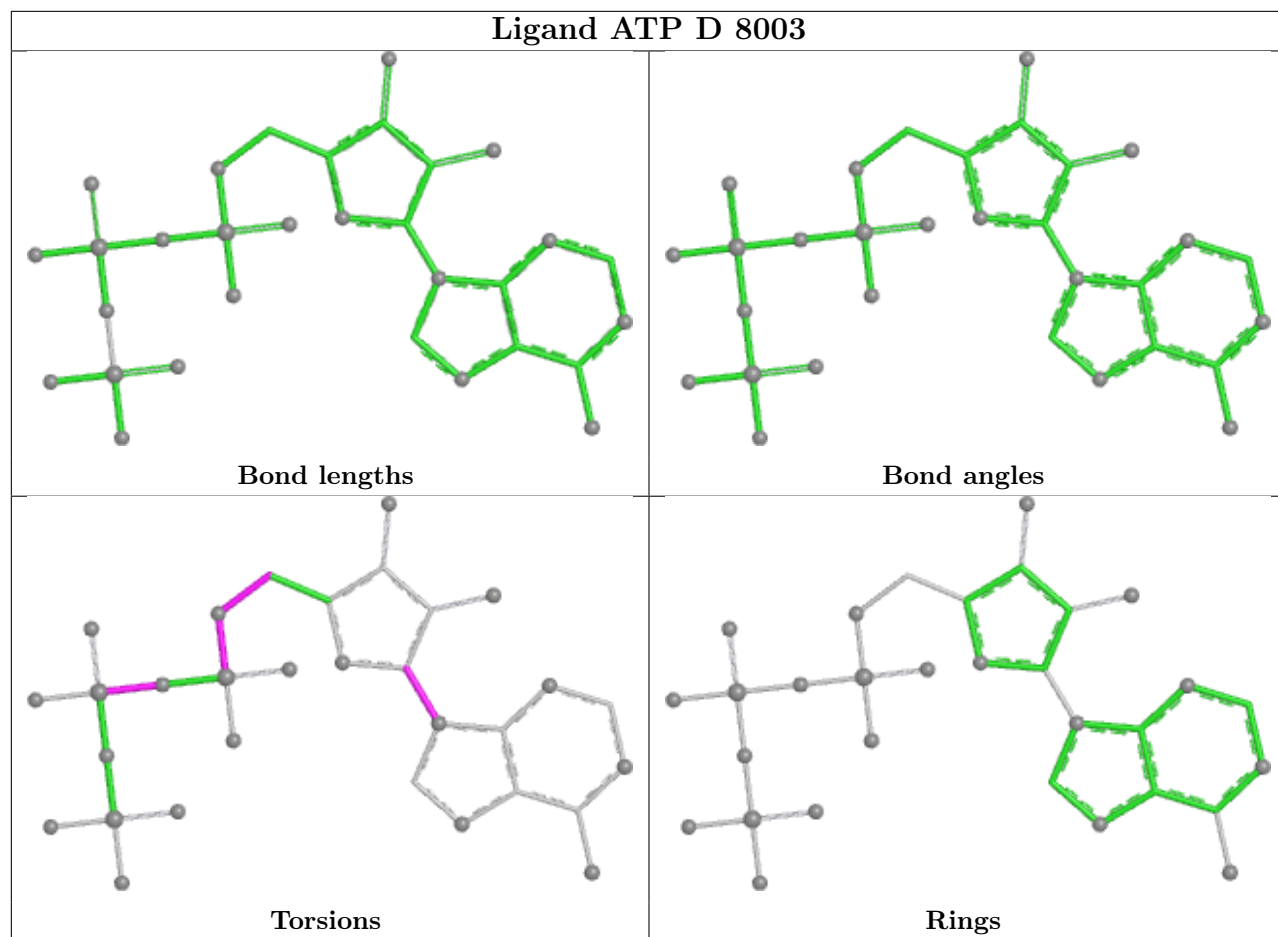


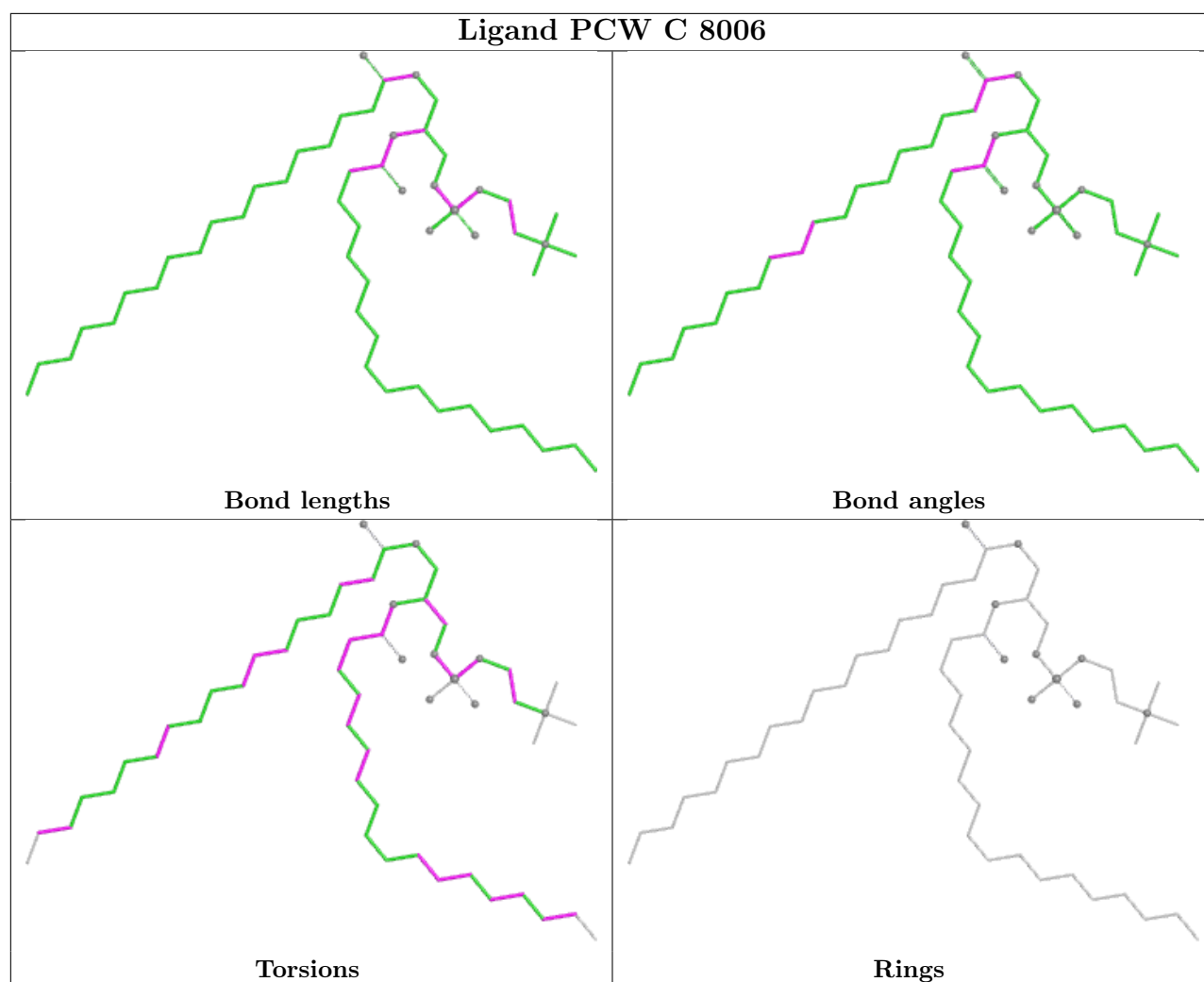












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



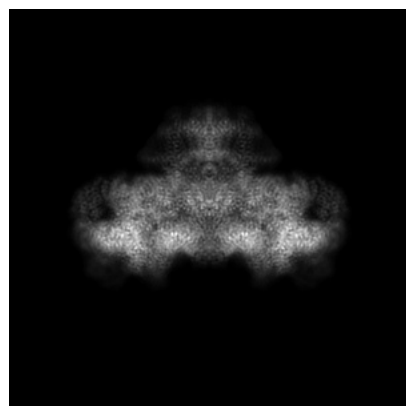
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49534. These allow visual inspection of the internal detail of the map and identification of artifacts.

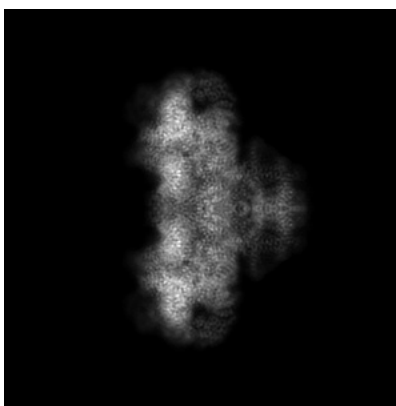
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

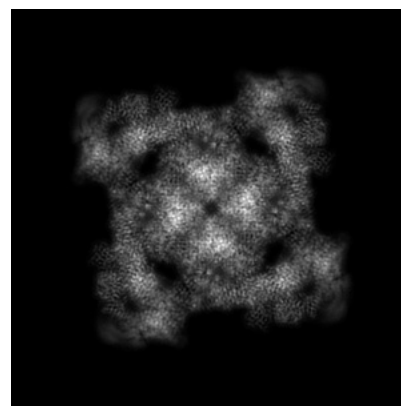
#### 6.1.1 Primary map



X

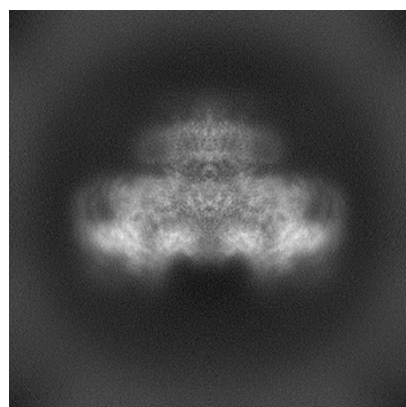


Y

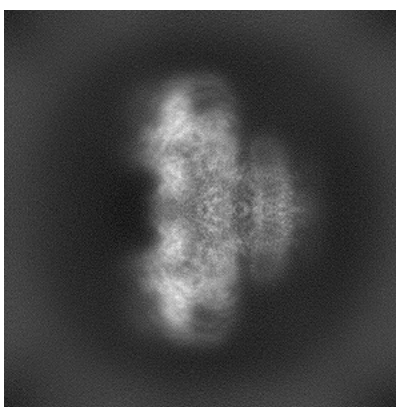


Z

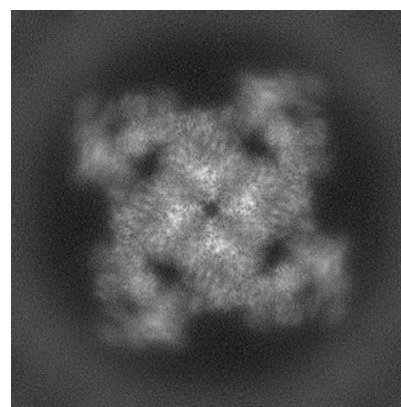
#### 6.1.2 Raw map



X



Y

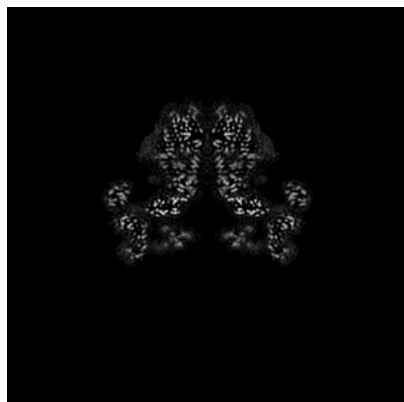


Z

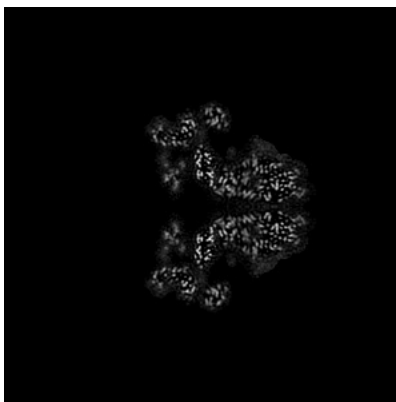
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

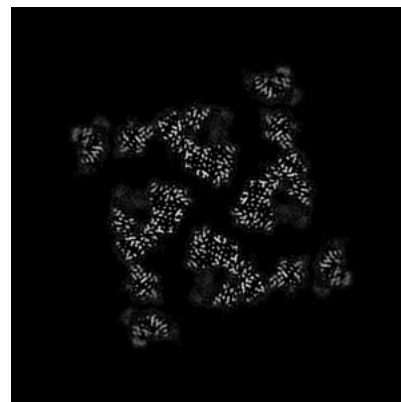
### 6.2.1 Primary map



X Index: 256

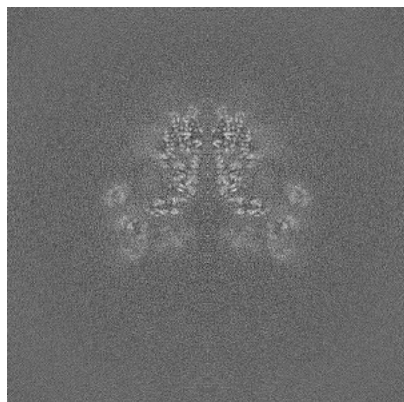


Y Index: 256

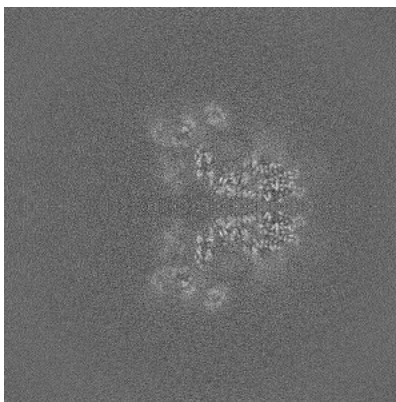


Z Index: 256

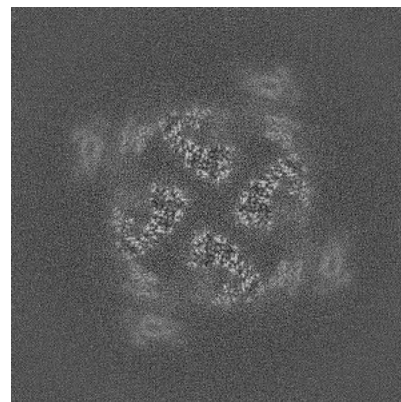
### 6.2.2 Raw map



X Index: 256



Y Index: 256

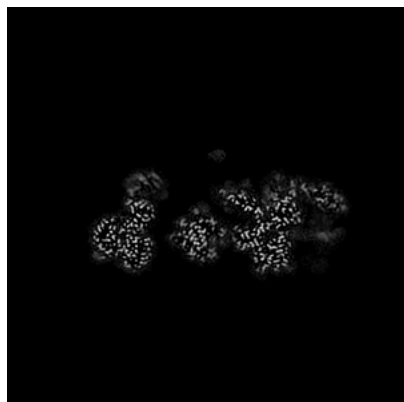


Z Index: 256

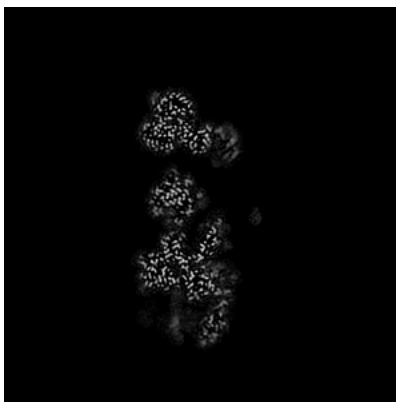
The images above show central slices of the map in three orthogonal directions.

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

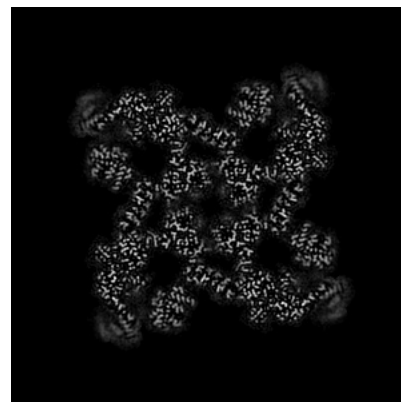
### 6.3.1 Primary map



X Index: 348

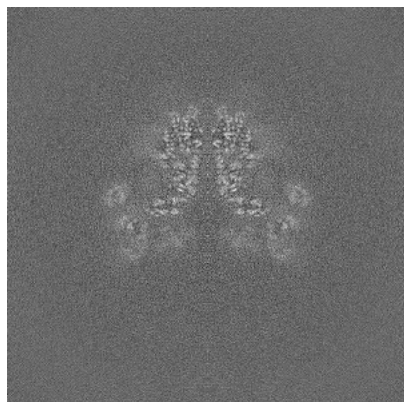


Y Index: 348

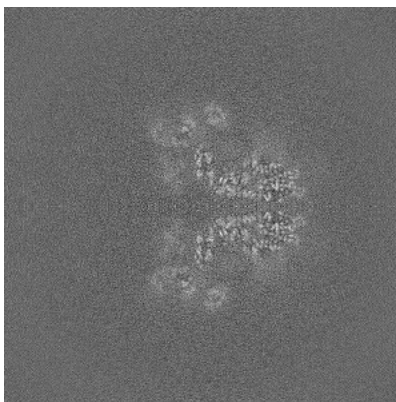


Z Index: 224

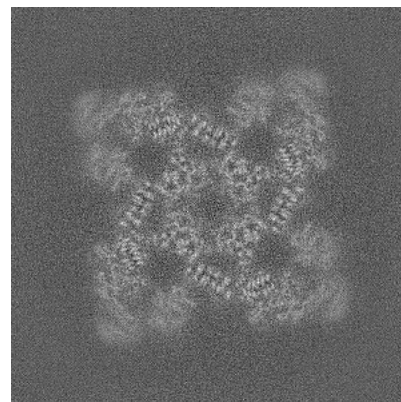
### 6.3.2 Raw map



X Index: 256



Y Index: 256

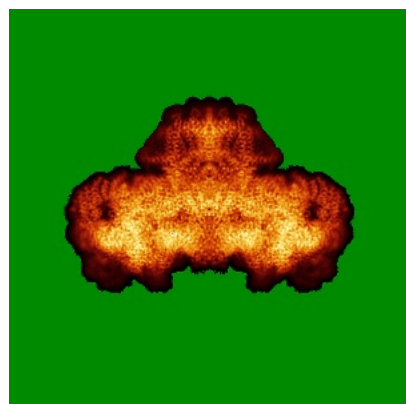


Z Index: 225

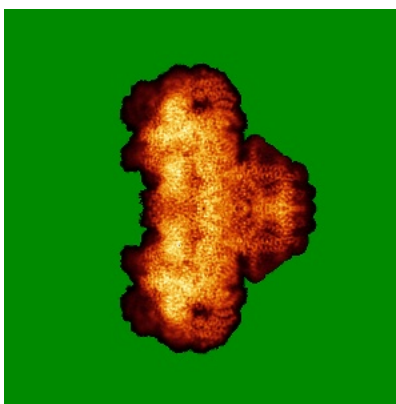
The images above show the largest variance slices of the map in three orthogonal directions.

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

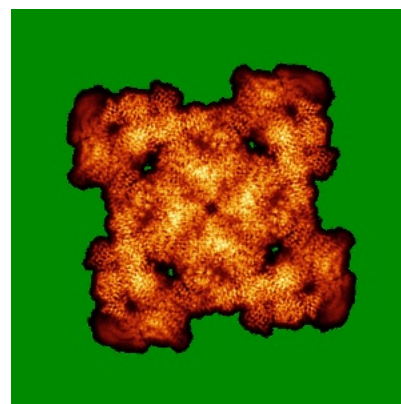
### 6.4.1 Primary map



X

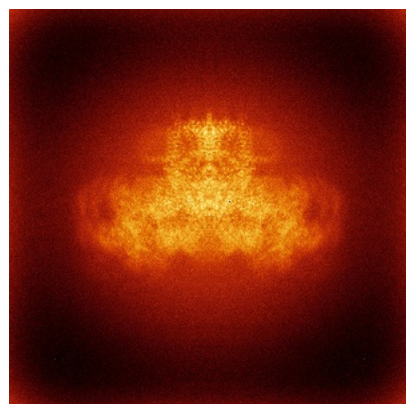


Y

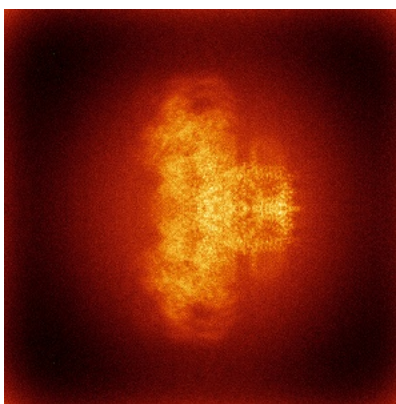


Z

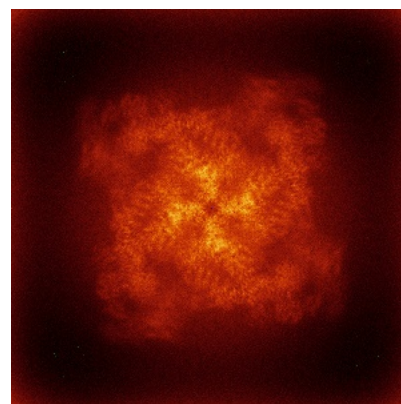
### 6.4.2 Raw map



X



Y



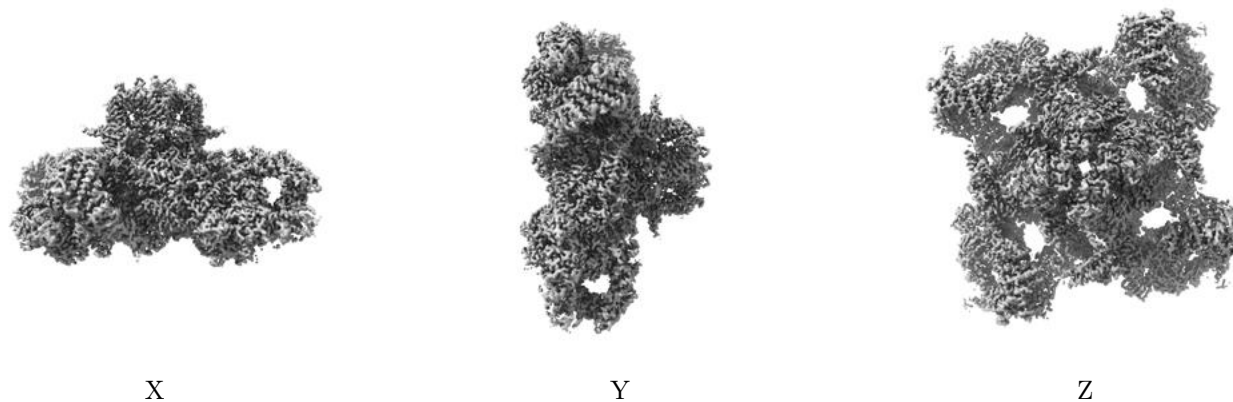
Z

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.



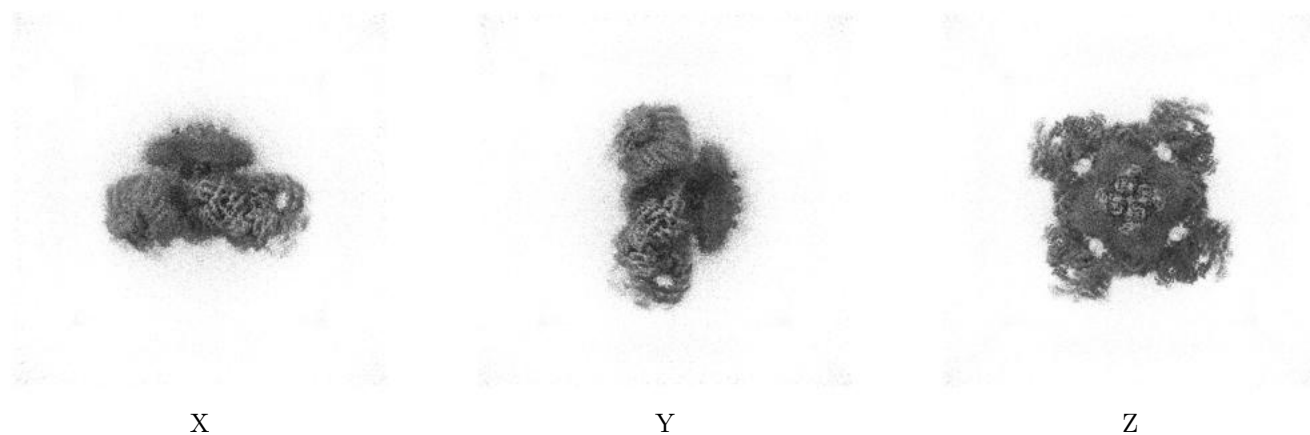
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

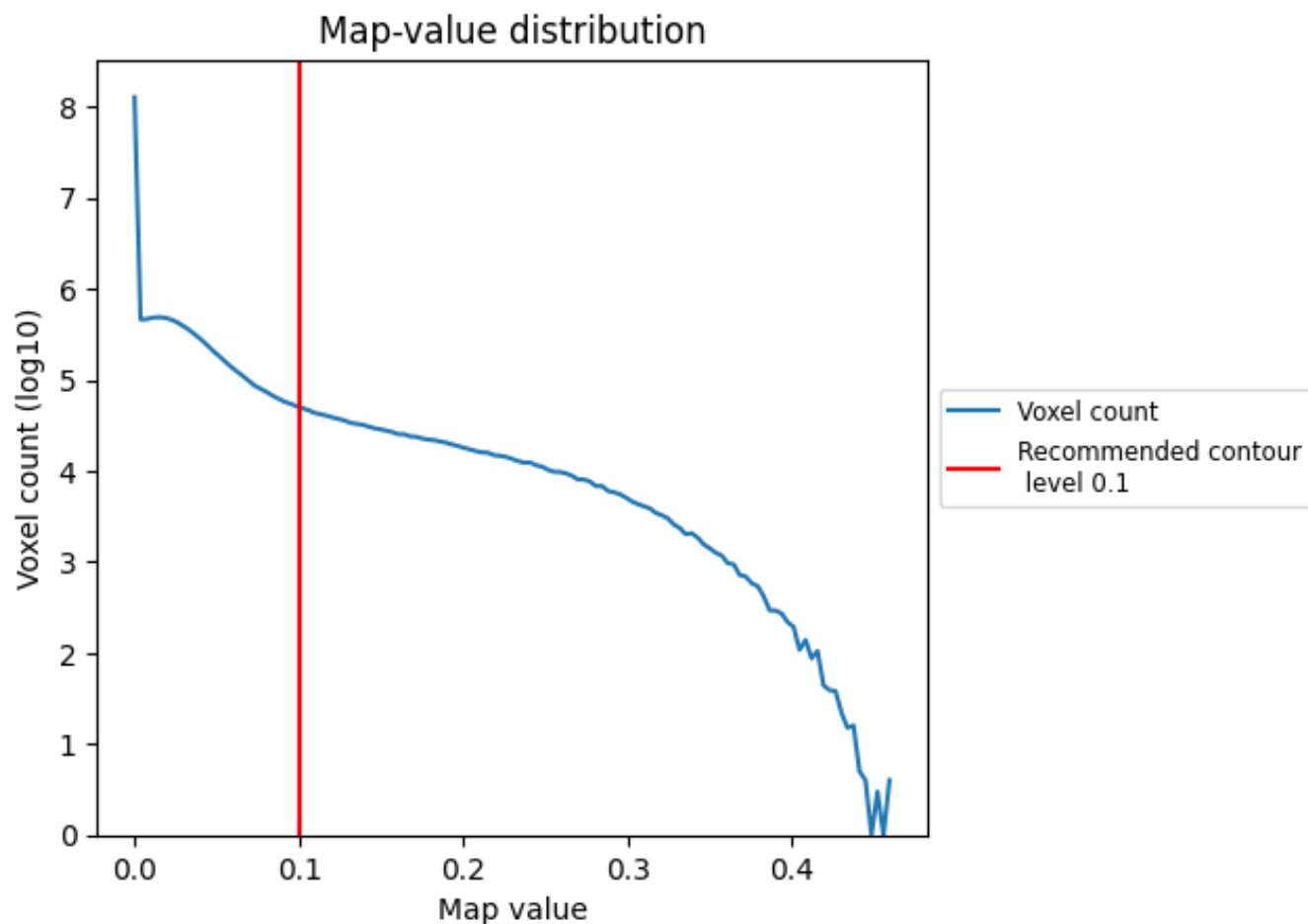
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

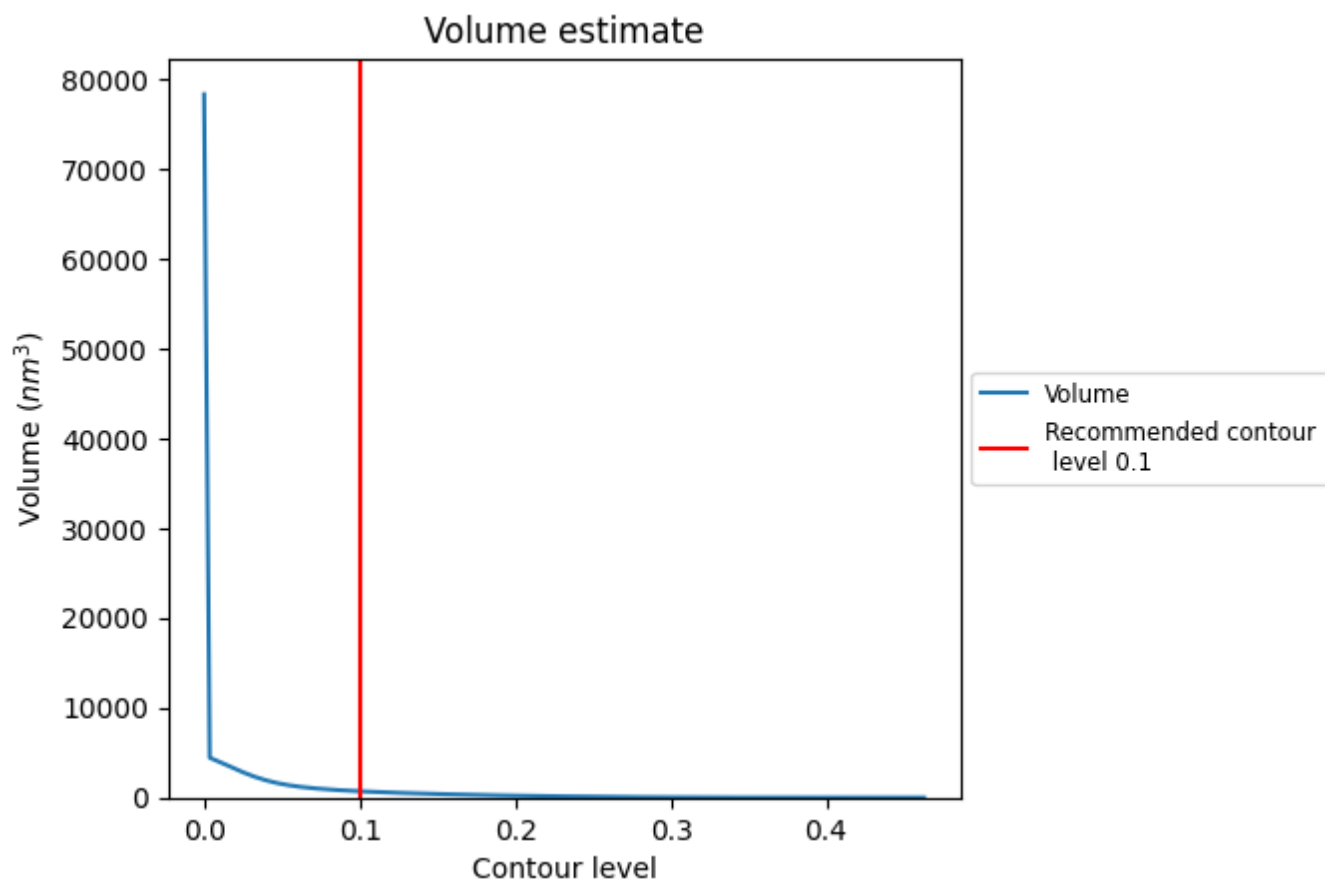
This section contains the results of statistical analysis of the map.

### 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.

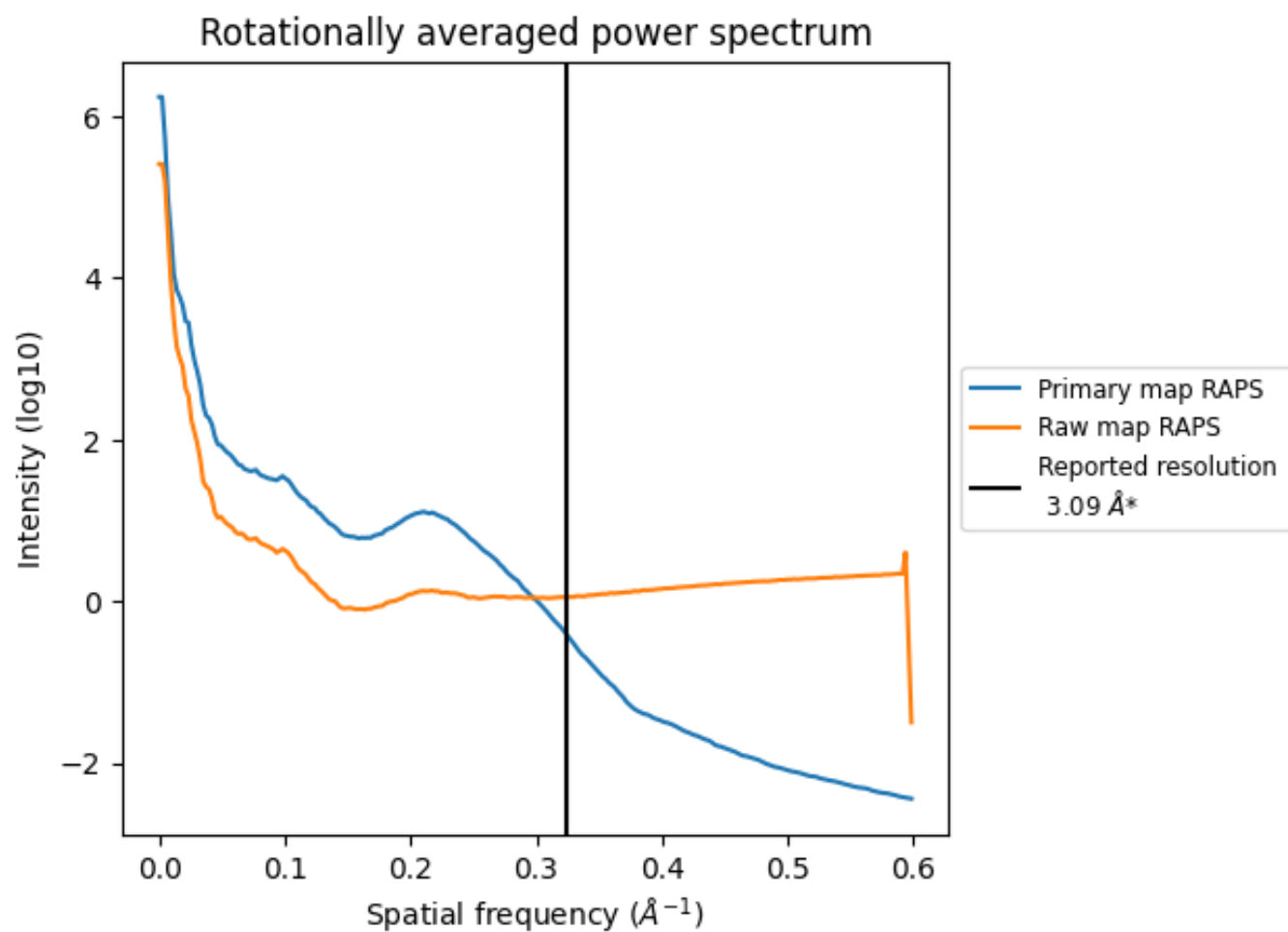
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 703  $\text{nm}^3$ ; this corresponds to an approximate mass of 635 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 ⓘ



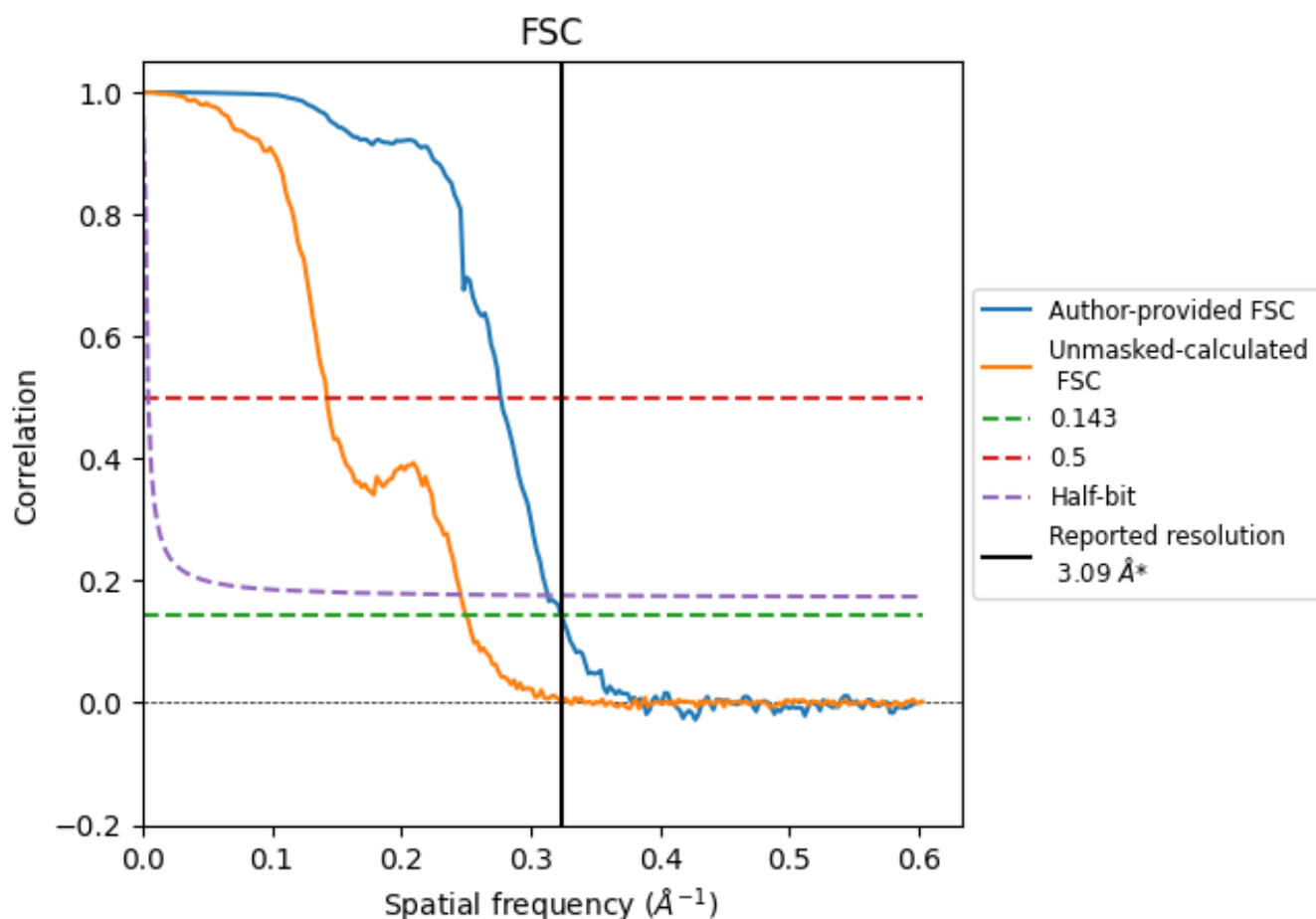
\*Reported resolution corresponds to spatial frequency of 0.324  $\text{\AA}^{-1}$



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

## 8.2 Resolution estimates [i](#)

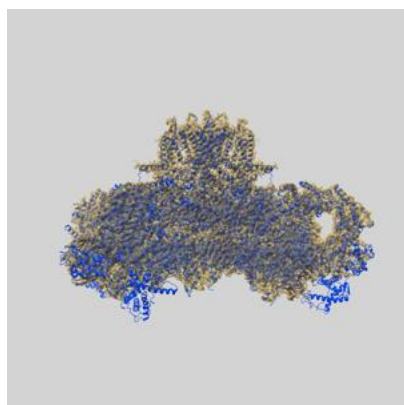
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.61	3.19
Unmasked-calculated*	4.00	7.01	4.07

\*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 4.00 differs from the reported value 3.09 by more than 10 %

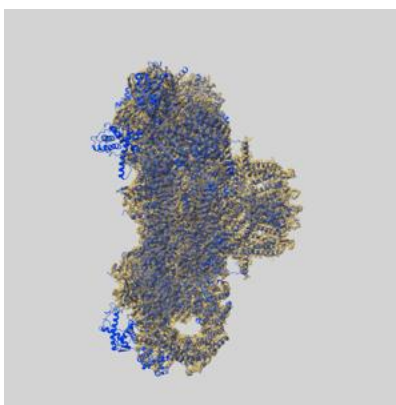
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49534 and PDB model 9NMN. Per-residue inclusion information can be found in section [3](#) on page [8](#).

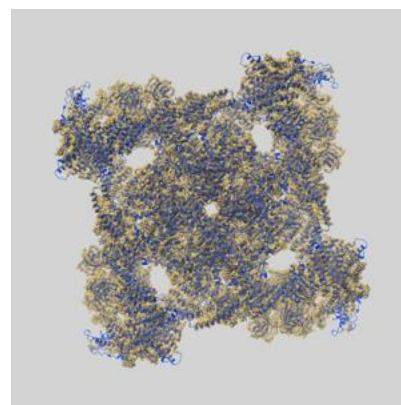
### 9.1 Map-model overlay [i](#)



X



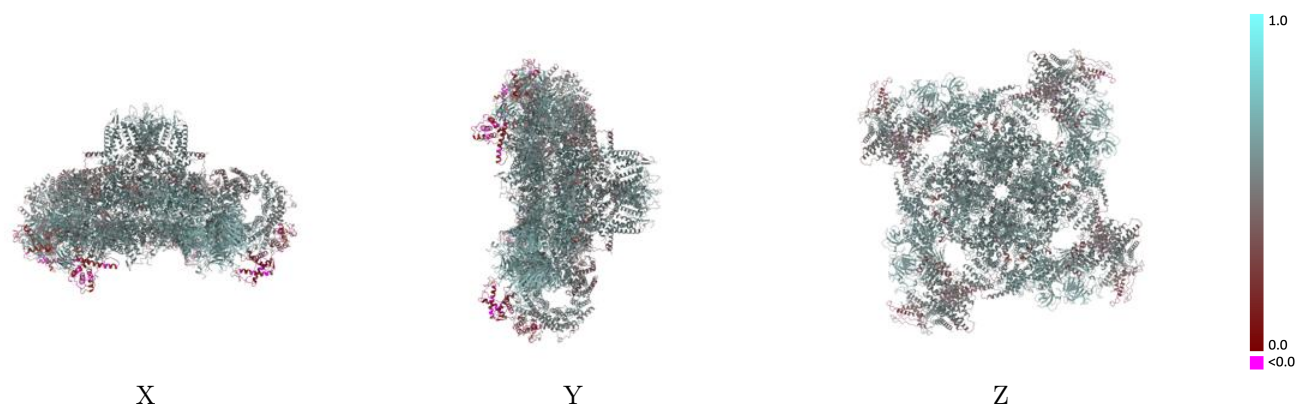
Y



Z

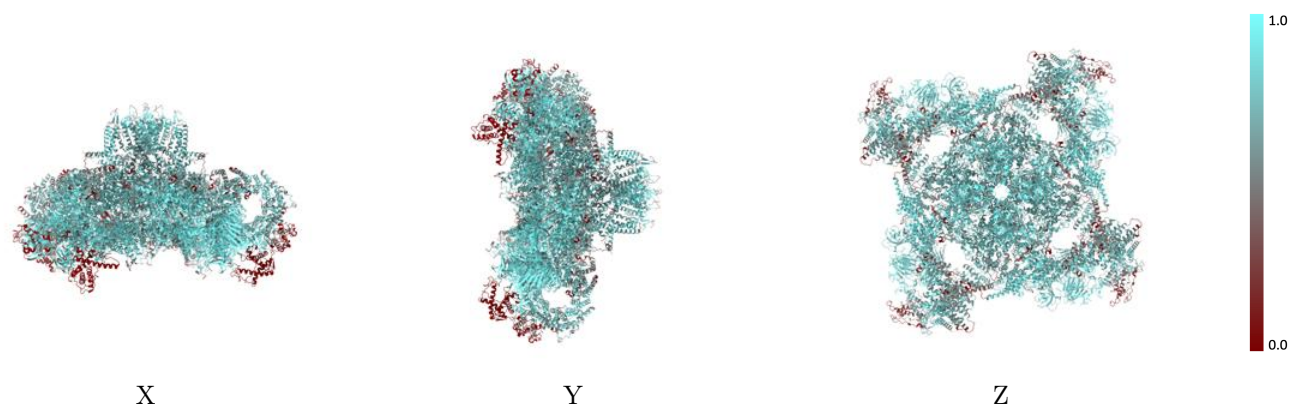
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



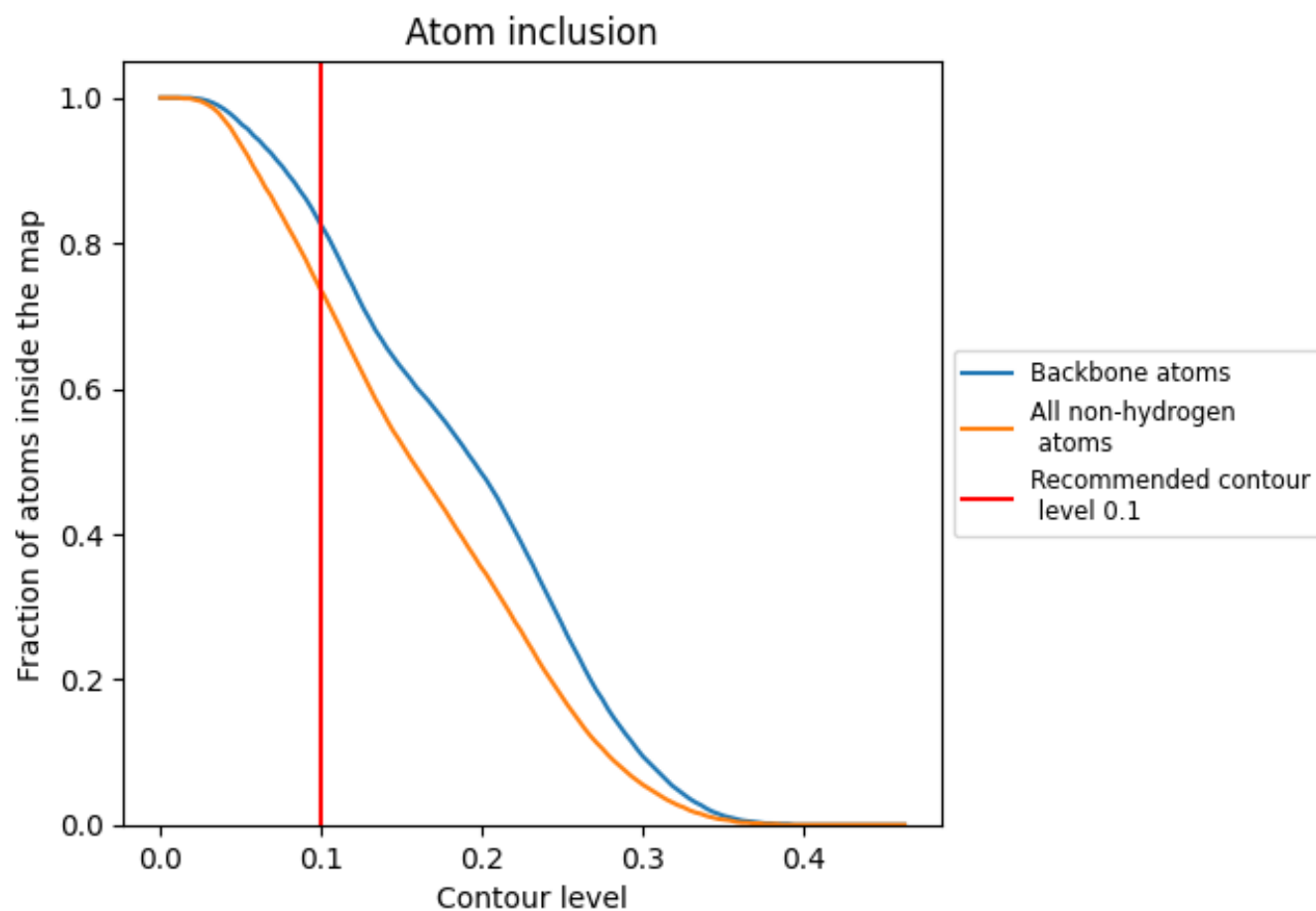
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 73% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7340	<div><div></div></div> 0.5250
A	<div><div></div></div> 0.7320	<div><div></div></div> 0.5230
B	<div><div></div></div> 0.7320	<div><div></div></div> 0.5230
C	<div><div></div></div> 0.7320	<div><div></div></div> 0.5230
D	<div><div></div></div> 0.7320	<div><div></div></div> 0.5230
E	<div><div></div></div> 0.8480	<div><div></div></div> 0.6050
F	<div><div></div></div> 0.8440	<div><div></div></div> 0.6060
G	<div><div></div></div> 0.8430	<div><div></div></div> 0.6070
H	<div><div></div></div> 0.8400	<div><div></div></div> 0.6050

1.0

0.0

<0.0