



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 07:02 PM EDT

PDB ID : 8SS9
EMDB ID : EMD-40748
Title : Structure of LBD-TMD of AMPA receptor GluA2 in complex with auxiliary subunit TARP gamma-5 bound to competitive antagonist ZK and antiepileptic drug perampanel (closed state)
Authors : Gangwar, S.P.; Yen, L.Y.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on : 2023-05-08
Resolution : 2.72 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

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

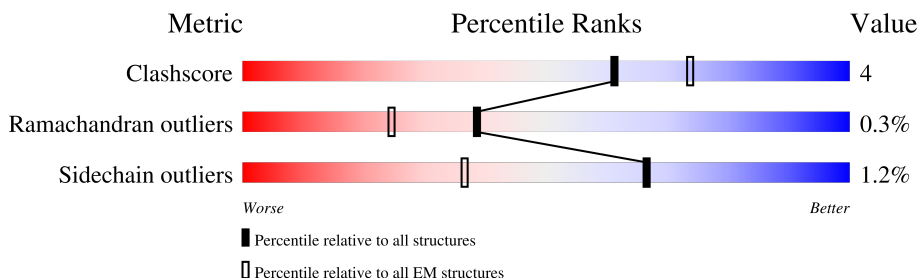
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



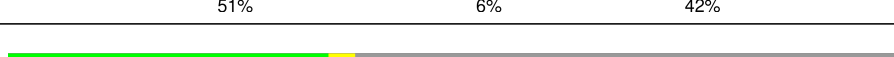

The reported resolution of this entry is 2.72 Å.

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

Mol	Chain	Length	Quality of chain
1	A	1026	
1	B	1026	
1	C	1026	
1	D	1026	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	A	1107	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	C	1107	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16319 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	592	Total	C	N	O	S	0	0
			4639	3030	748	830	31		
1	B	401	Total	C	N	O	S	0	0
			3134	2036	505	572	21		
1	C	592	Total	C	N	O	S	0	0
			4639	3030	748	830	31		
1	D	401	Total	C	N	O	S	0	0
			3134	2036	505	572	21		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	830	SER	-	linker	UNP P19491
A	831	ALA	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	830	SER	-	linker	UNP P19491
B	831	ALA	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	830	SER	-	linker	UNP P19491
C	831	ALA	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	830	SER	-	linker	UNP P19491

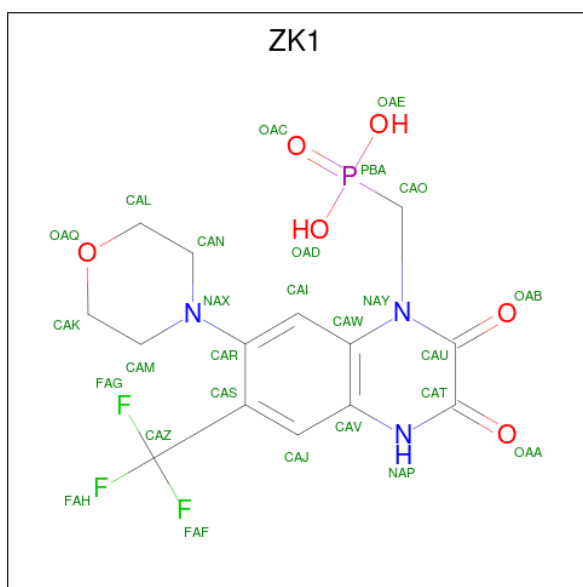
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Chain	Residue	Modelled	Actual	Comment	Reference
D	831	ALA	-	linker	UNP P19491

-
- Chemical structure of 6ZP (6-azapropyl) is shown, featuring a central pyridine ring (N15) substituted with a phenyl group (C22-C27) and a 2-oxo-2-phenylpropyl group (C02-C09). The structure is labeled with atom identifiers: N15, C14, C13, C12, C09, C08, C07, C06, C05, C04, C03, C02, C11, O11, C10, C20, N21, C22, C23, C24, C25, C26, C27, C16, C17, C18, and C19.

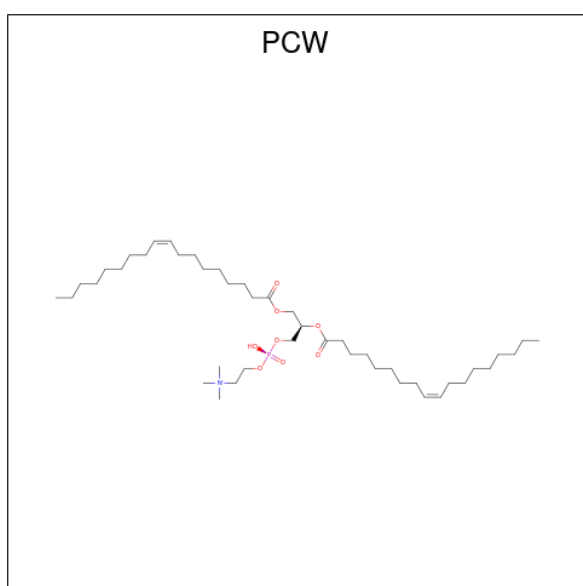
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 27	C 23	N 3	O 1	0
2	B	1	Total 27	C 23	N 3	O 1	0
2	C	1	Total 27	C 23	N 3	O 1	0
2	D	1	Total 27	C 23	N 3	O 1	0

- Molecule 3 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P) (labeled as "Ligand of Interest" by depositor).



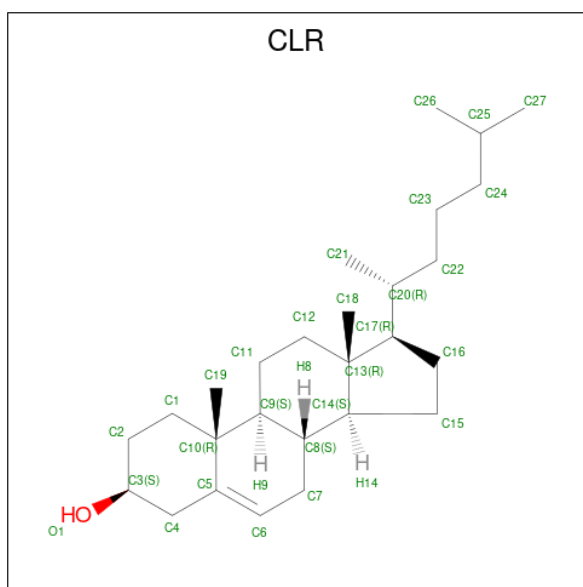
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 42	C 32	N 1	O 8	P 1	0
4	A	1	Total 43	C 33	N 1	O 8	P 1	0
4	A	1	Total 11	C 11				0
4	A	1	Total 51	C 41	N 1	O 8	P 1	0
4	B	1	Total 43	C 33	N 1	O 8	P 1	0
4	B	1	Total 41	C 31	N 1	O 8	P 1	0
4	B	1	Total 11	C 11				0
4	C	1	Total 42	C 32	N 1	O 8	P 1	0
4	C	1	Total 43	C 33	N 1	O 8	P 1	0
4	C	1	Total 11	C 11				0
4	C	1	Total 51	C 41	N 1	O 8	P 1	0
4	D	1	Total 43	C 33	N 1	O 8	P 1	0
4	D	1	Total 41	C 31	N 1	O 8	P 1	0
4	D	1	Total 11	C 11				0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Na	0
			1	1	
6	B	1	Total	Na	0
			1	1	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	3	Total	O	0
			3	3	
7	B	5	Total	O	0
			5	5	
7	C	4	Total	O	0
			4	4	
7	D	3	Total	O	0
			3	3	

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	117939	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	11.575	Depositor
Minimum map value	-7.580	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	384.80002, 384.80002, 384.80002	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9250001, 0.9250001, 0.9250001	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: CLR, NA, ZK1, PCW, 6ZP

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	0.29	0/4742	0.55	0/6404
1	B	0.28	0/3202	0.53	1/4321 (0.0%)
1	C	0.29	0/4742	0.55	0/6404
1	D	0.28	0/3202	0.53	1/4321 (0.0%)
All	All	0.29	0/15888	0.54	2/21450 (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	3
1	C	0	3
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	704	LEU	CA-CB-CG	6.81	130.96	115.30
1	B	704	LEU	CA-CB-CG	6.79	130.91	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	508	GLN	Peptide
1	A	589	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	590	ASP	Peptide
1	C	508	GLN	Peptide
1	C	589	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4639	0	4715	33	0
1	B	3134	0	3178	20	0
1	C	4639	0	4715	35	0
1	D	3134	0	3178	24	0
2	A	27	0	0	1	0
2	B	27	0	0	2	0
2	C	27	0	0	1	0
2	D	27	0	0	1	0
3	A	27	0	13	0	0
3	B	27	0	13	0	0
3	C	27	0	13	1	0
3	D	27	0	13	0	0
4	A	147	0	207	7	0
4	B	95	0	125	3	0
4	C	147	0	207	4	0
4	D	95	0	125	5	0
5	A	28	0	37	11	0
5	C	28	0	37	17	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	3	0	0	0	0
7	B	5	0	0	0	0
7	C	4	0	0	0	0
7	D	3	0	0	0	0
All	All	16319	0	16576	139	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 139 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1107:CLR:C14	5:C:1107:CLR:C15	1.74	1.63
5:C:1107:CLR:C15	5:C:1107:CLR:C16	1.78	1.60
5:C:1107:CLR:C13	5:C:1107:CLR:C17	1.74	1.60
5:A:1107:CLR:C13	5:A:1107:CLR:C17	1.74	1.59
5:A:1107:CLR:C16	5:A:1107:CLR:C15	1.78	1.52

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	582/1026 (57%)	558 (96%)	22 (4%)	2 (0%)	37	60
1	B	395/1026 (38%)	378 (96%)	16 (4%)	1 (0%)	37	60
1	C	582/1026 (57%)	558 (96%)	22 (4%)	2 (0%)	37	60
1	D	395/1026 (38%)	378 (96%)	16 (4%)	1 (0%)	37	60
All	All	1954/4104 (48%)	1872 (96%)	76 (4%)	6 (0%)	38	60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	LYS
1	C	509	LYS
1	B	509	LYS
1	D	509	LYS
1	C	737	PRO

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	501/877 (57%)	494 (99%)	7 (1%)	62	83
1	B	338/877 (38%)	335 (99%)	3 (1%)	75	89
1	C	501/877 (57%)	494 (99%)	7 (1%)	62	83
1	D	338/877 (38%)	335 (99%)	3 (1%)	75	89
All	All	1678/3508 (48%)	1658 (99%)	20 (1%)	66	85

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	834	ARG
1	D	661	ARG
1	D	747	ASN
1	D	704	LEU
1	A	990	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	947	ASN
1	D	587	GLN
1	D	747	ASN
1	A	990	ASN
1	B	747	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	B	1103	-	42,42,53	1.28	5 (11%)	48,50,61	1.11	4 (8%)
4	PCW	D	1104	-	40,40,53	1.30	4 (10%)	46,48,61	1.16	3 (6%)
2	6ZP	B	1101	-	30,30,30	1.05	1 (3%)	37,41,41	0.87	1 (2%)
4	PCW	A	1105	-	10,10,53	0.84	0	9,9,61	0.32	0
4	PCW	D	1103	-	42,42,53	1.28	5 (11%)	48,50,61	1.16	4 (8%)
2	6ZP	C	1101	-	30,30,30	1.10	1 (3%)	37,41,41	0.88	1 (2%)
5	CLR	A	1107	-	31,31,31	9.41	22 (70%)	48,48,48	5.09	23 (47%)
4	PCW	C	1105	-	10,10,53	0.84	0	9,9,61	0.32	0
4	PCW	D	1105	-	10,10,53	0.84	0	9,9,61	0.33	0
3	ZK1	B	1102	-	29,29,29	3.33	10 (34%)	45,45,45	1.70	12 (26%)
5	CLR	C	1107	-	31,31,31	9.41	22 (70%)	48,48,48	5.09	22 (45%)
4	PCW	A	1103	-	41,41,53	1.29	5 (12%)	47,49,61	1.05	3 (6%)
2	6ZP	A	1101	-	30,30,30	1.10	1 (3%)	37,41,41	0.87	1 (2%)
4	PCW	C	1104	-	42,42,53	1.27	4 (9%)	48,50,61	1.10	3 (6%)
4	PCW	C	1103	-	41,41,53	1.28	5 (12%)	47,49,61	1.05	3 (6%)
2	6ZP	D	1101	-	30,30,30	1.05	1 (3%)	37,41,41	0.85	1 (2%)
4	PCW	A	1106	-	50,50,53	1.21	5 (10%)	56,58,61	1.02	3 (5%)
4	PCW	B	1105	-	10,10,53	0.84	0	9,9,61	0.33	0
3	ZK1	C	1102	-	29,29,29	3.33	10 (34%)	45,45,45	1.77	12 (26%)
3	ZK1	D	1102	-	29,29,29	3.33	10 (34%)	45,45,45	1.73	12 (26%)
4	PCW	A	1104	-	42,42,53	1.27	4 (9%)	48,50,61	1.08	3 (6%)
4	PCW	C	1106	-	50,50,53	1.21	5 (10%)	56,58,61	1.02	3 (5%)
3	ZK1	A	1102	-	29,29,29	3.34	10 (34%)	45,45,45	1.77	13 (28%)
4	PCW	B	1104	-	40,40,53	1.30	4 (10%)	46,48,61	1.17	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	B	1103	-	-	26/46/46/57	-
4	PCW	D	1104	-	-	19/44/44/57	-
2	6ZP	B	1101	-	-	2/13/14/14	0/4/4/4
4	PCW	A	1105	-	-	4/8/8/57	-
4	PCW	D	1103	-	-	23/46/46/57	-
2	6ZP	C	1101	-	-	1/13/14/14	0/4/4/4
5	CLR	A	1107	-	3/3/10/11	9/10/68/68	0/4/4/4
4	PCW	C	1105	-	-	4/8/8/57	-
4	PCW	D	1105	-	-	4/8/8/57	-
3	ZK1	B	1102	-	-	4/13/23/23	0/3/3/3
5	CLR	C	1107	-	3/3/10/11	9/10/68/68	0/4/4/4
4	PCW	A	1103	-	-	23/45/45/57	-
3	ZK1	A	1102	-	-	5/13/23/23	0/3/3/3
4	PCW	C	1104	-	-	23/46/46/57	-
4	PCW	C	1103	-	-	20/45/45/57	-
2	6ZP	D	1101	-	-	2/13/14/14	0/4/4/4
4	PCW	A	1106	-	-	29/54/54/57	-
4	PCW	B	1105	-	-	4/8/8/57	-
3	ZK1	C	1102	-	-	5/13/23/23	0/3/3/3
3	ZK1	D	1102	-	-	4/13/23/23	0/3/3/3
4	PCW	A	1104	-	-	23/46/46/57	-
4	PCW	C	1106	-	-	29/54/54/57	-
2	6ZP	A	1101	-	-	1/13/14/14	0/4/4/4
4	PCW	B	1104	-	-	23/44/44/57	-

The worst 5 of 134 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1107	CLR	C8-C14	-28.75	0.99	1.53
5	C	1107	CLR	C8-C14	-28.65	0.99	1.53
5	A	1107	CLR	C12-C11	-21.63	1.10	1.53
5	C	1107	CLR	C12-C11	-21.59	1.10	1.53
5	C	1107	CLR	C7-C8	-19.71	1.21	1.53

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	CLR	C18-C13-C12	-17.79	84.38	110.61
5	C	1107	CLR	C18-C13-C12	-17.45	84.88	110.61
5	C	1107	CLR	C18-C13-C14	-11.67	90.51	111.68
5	C	1107	CLR	C17-C13-C14	11.40	113.18	100.10
5	A	1107	CLR	C12-C13-C17	11.35	133.32	116.60

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1107	CLR	C9
5	A	1107	CLR	C17
5	A	1107	CLR	C13
5	C	1107	CLR	C9
5	C	1107	CLR	C17

5 of 296 torsion outliers are listed below:

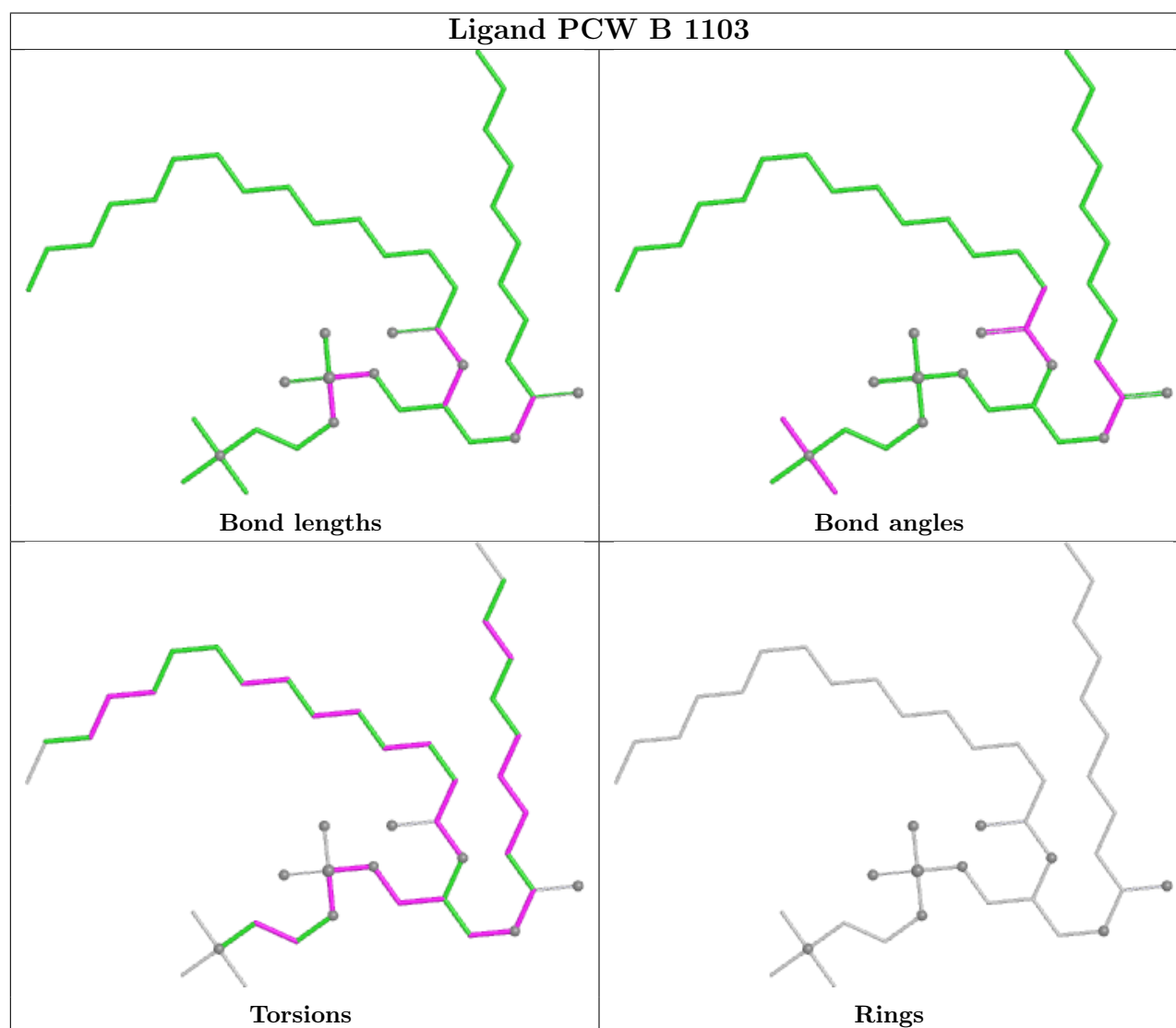
Mol	Chain	Res	Type	Atoms
4	A	1103	PCW	O2-C2-C3-O3
4	A	1103	PCW	C32-C31-O2-C2
4	A	1103	PCW	O31-C31-O2-C2
4	A	1104	PCW	O4P-C4-C5-N
4	A	1104	PCW	C4-O4P-P-O3P

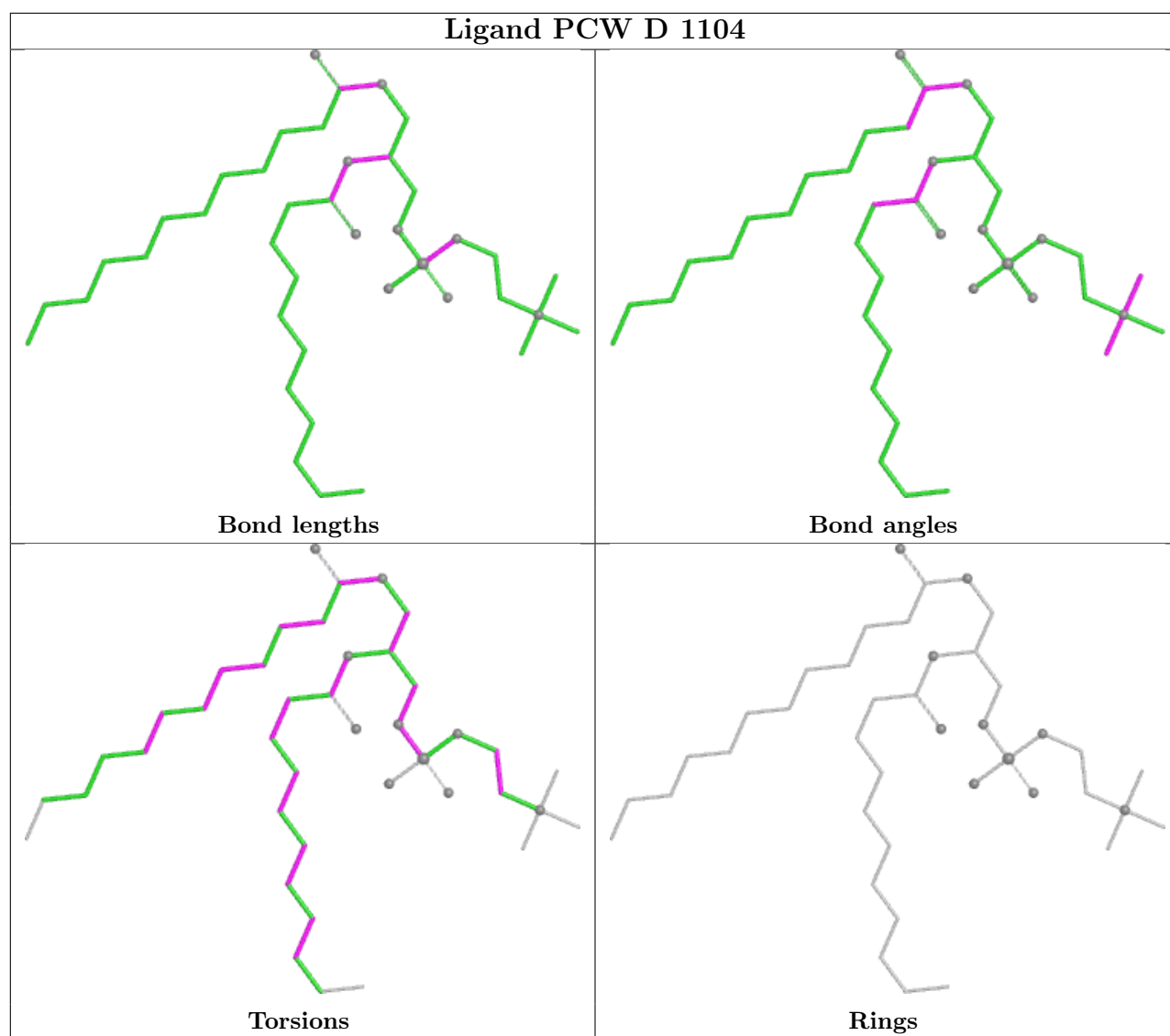
There are no ring outliers.

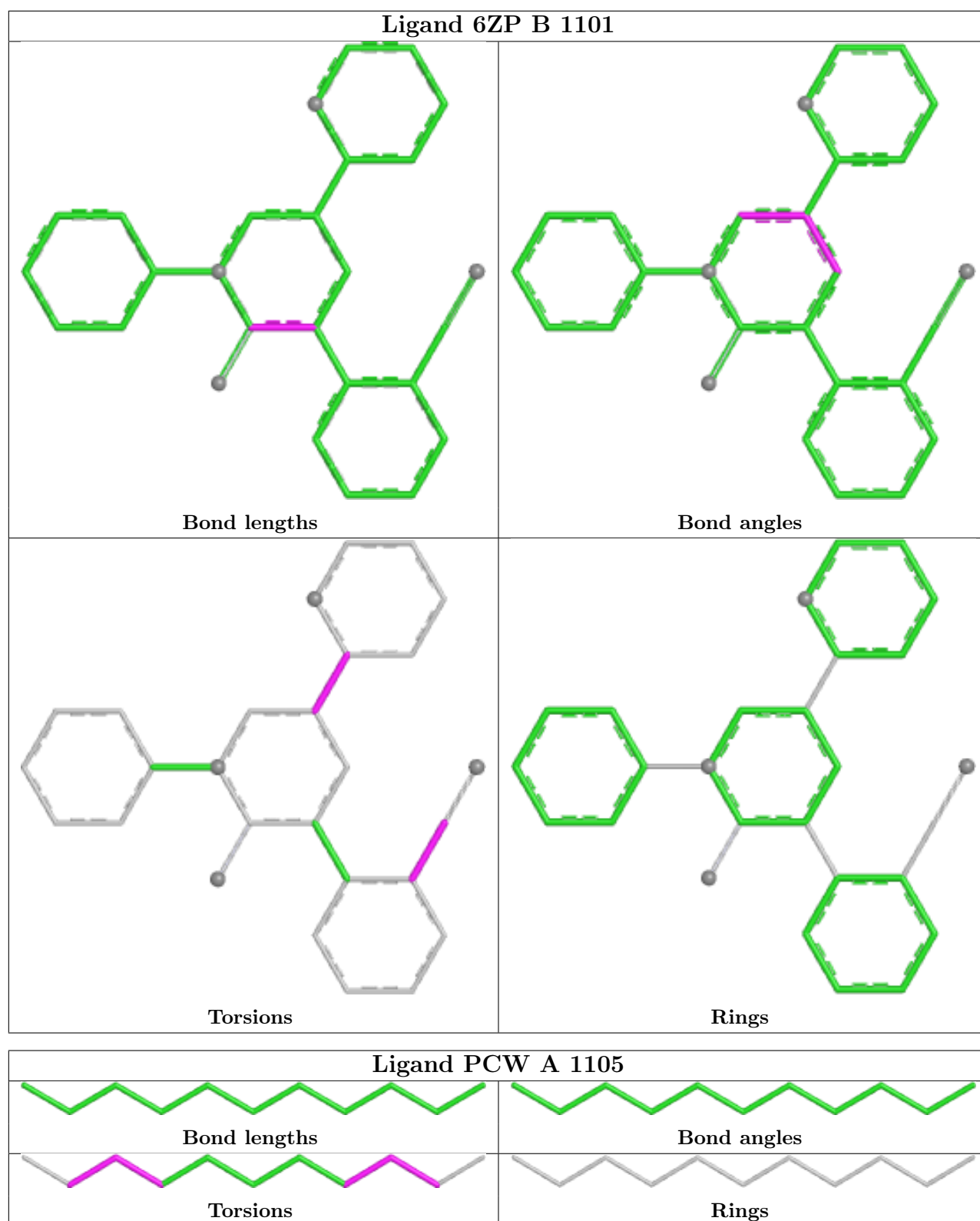
15 monomers are involved in 53 short contacts:

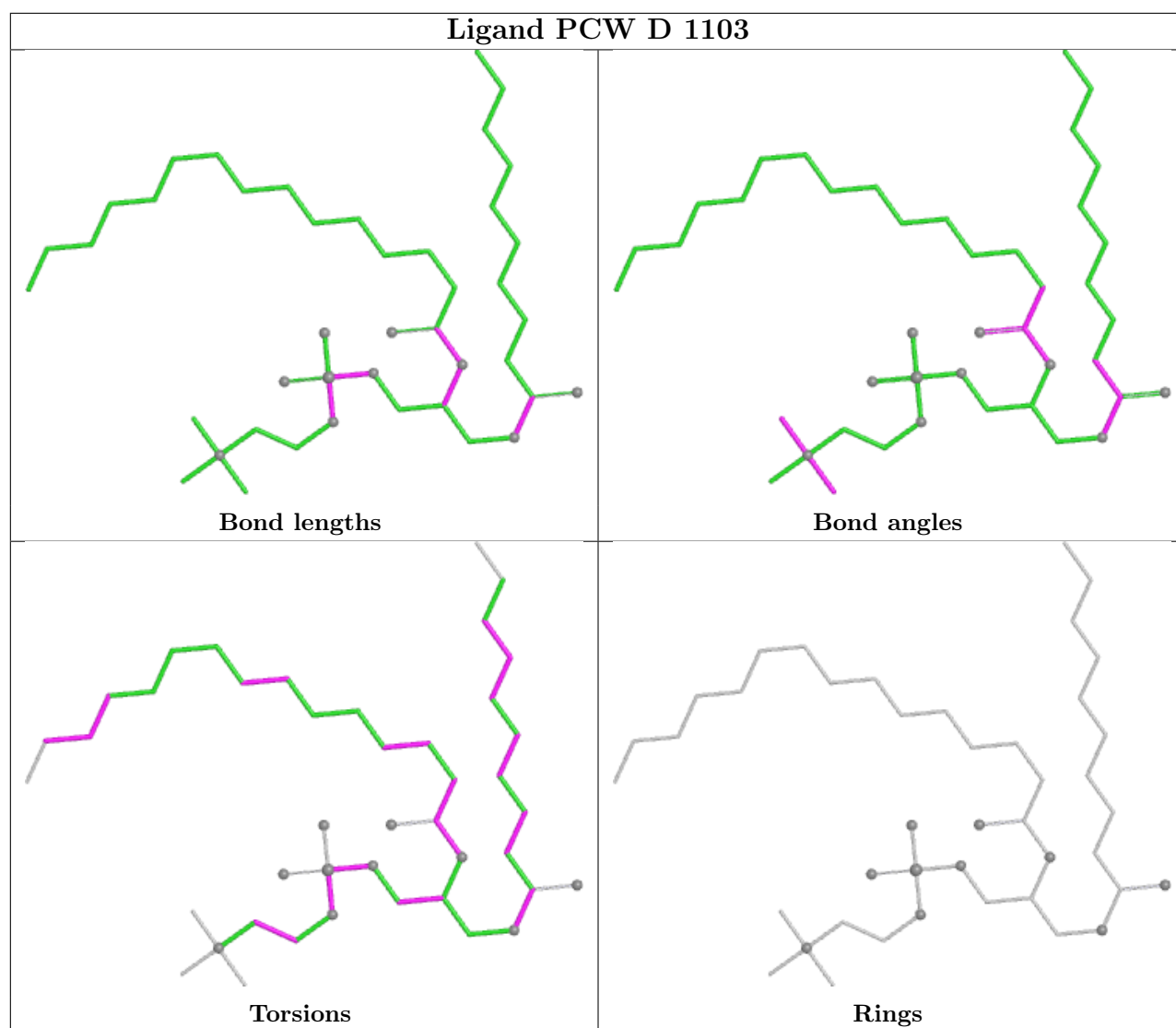
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1104	PCW	3	0
2	B	1101	6ZP	2	0
4	D	1103	PCW	2	0
2	C	1101	6ZP	1	0
5	A	1107	CLR	11	0
5	C	1107	CLR	17	0
4	A	1103	PCW	2	0
2	A	1101	6ZP	1	0
4	C	1103	PCW	1	0
2	D	1101	6ZP	1	0
4	A	1106	PCW	4	0
3	C	1102	ZK1	1	0
4	A	1104	PCW	1	0
4	C	1106	PCW	3	0
4	B	1104	PCW	3	0

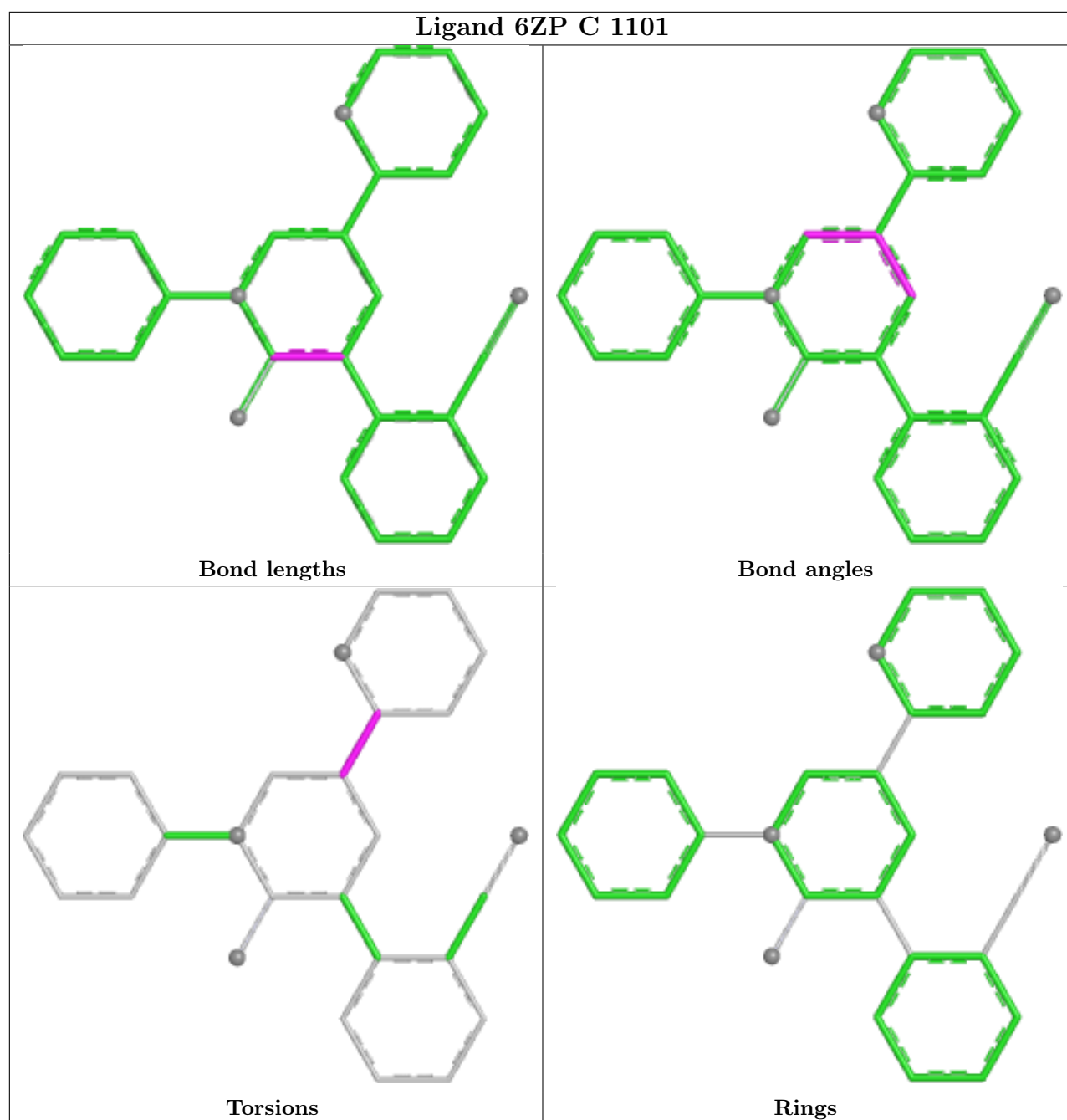
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

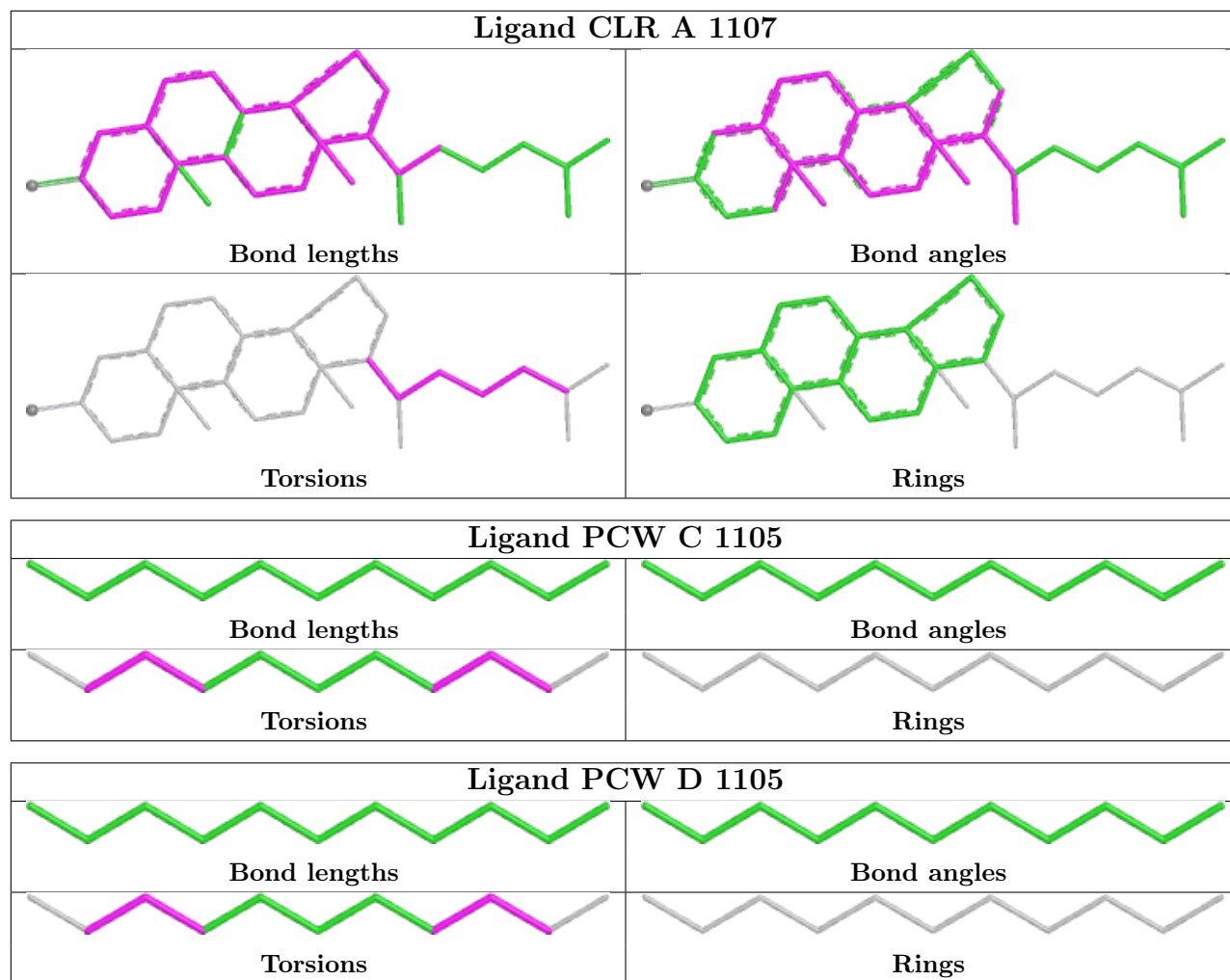


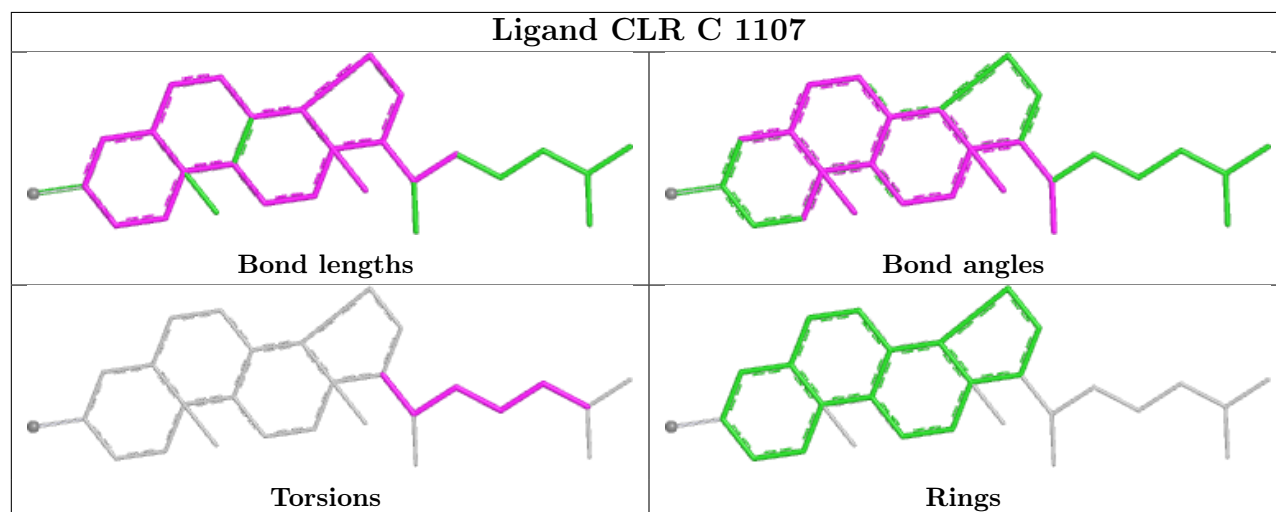
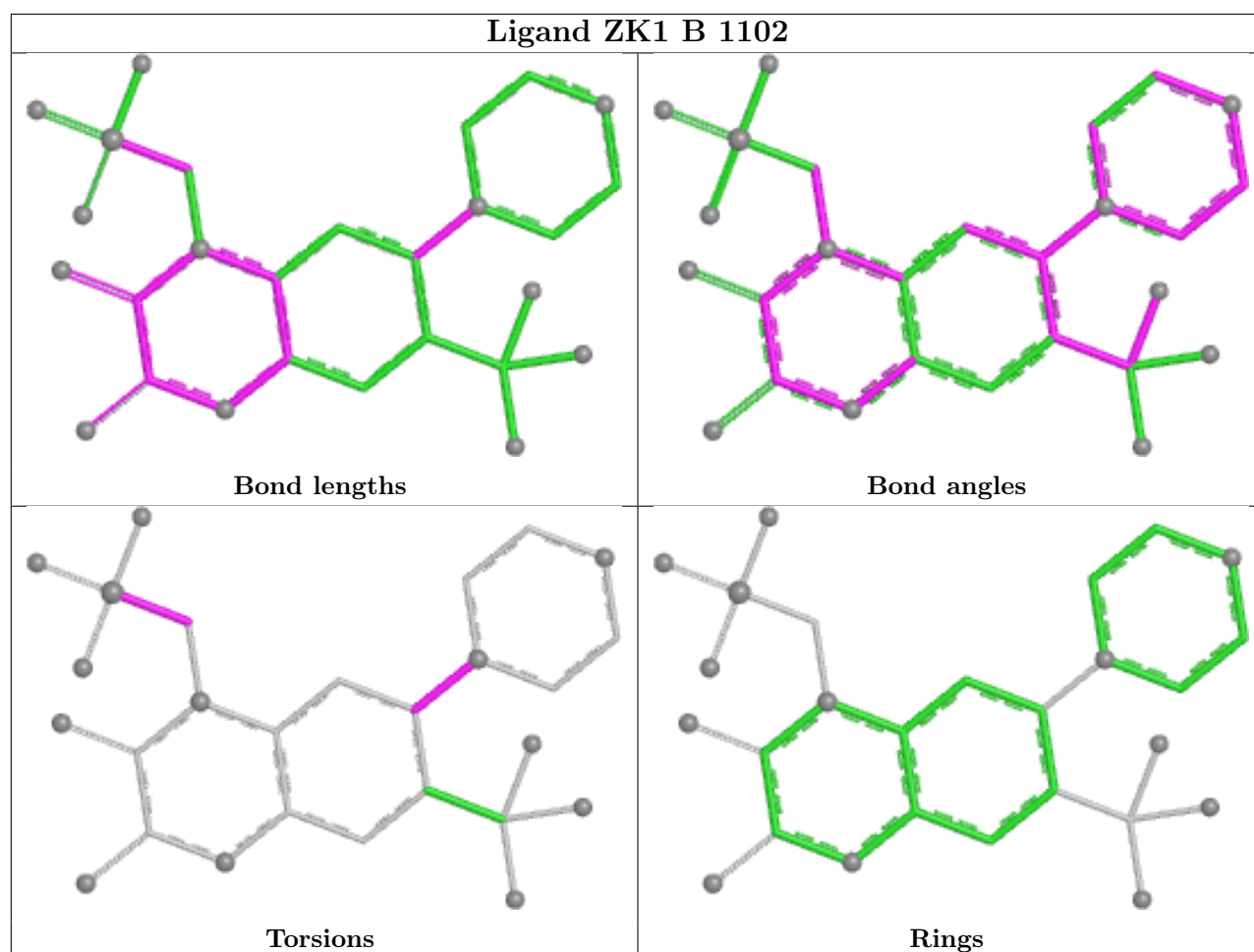


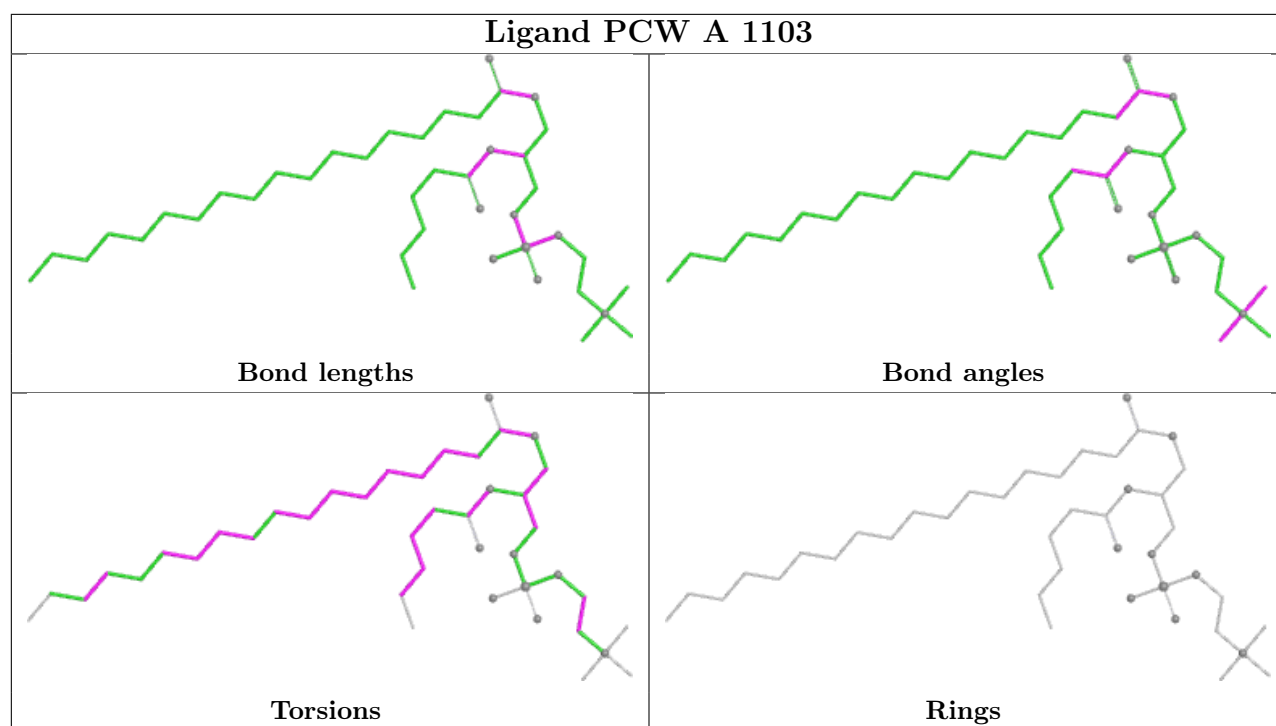


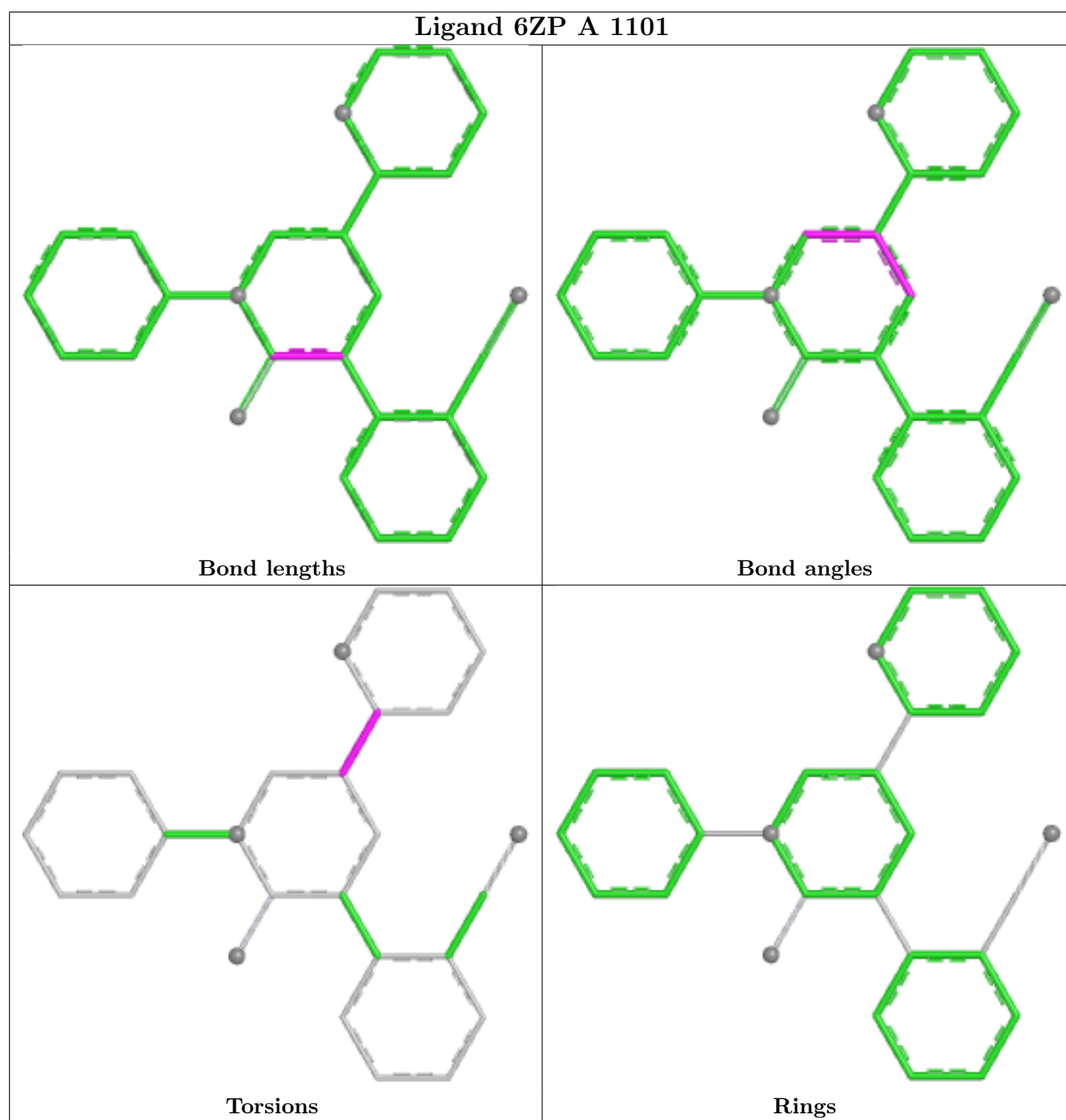


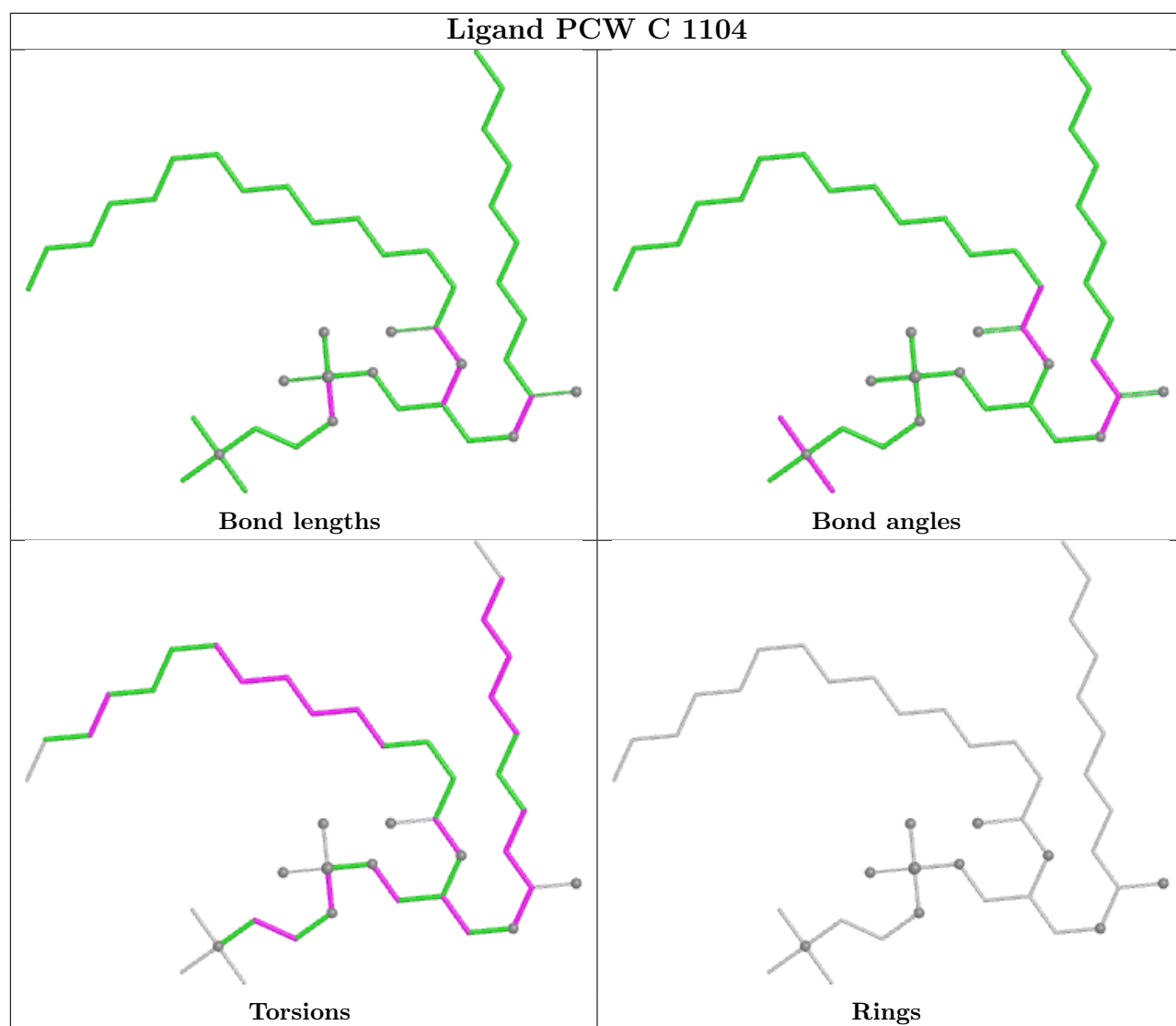


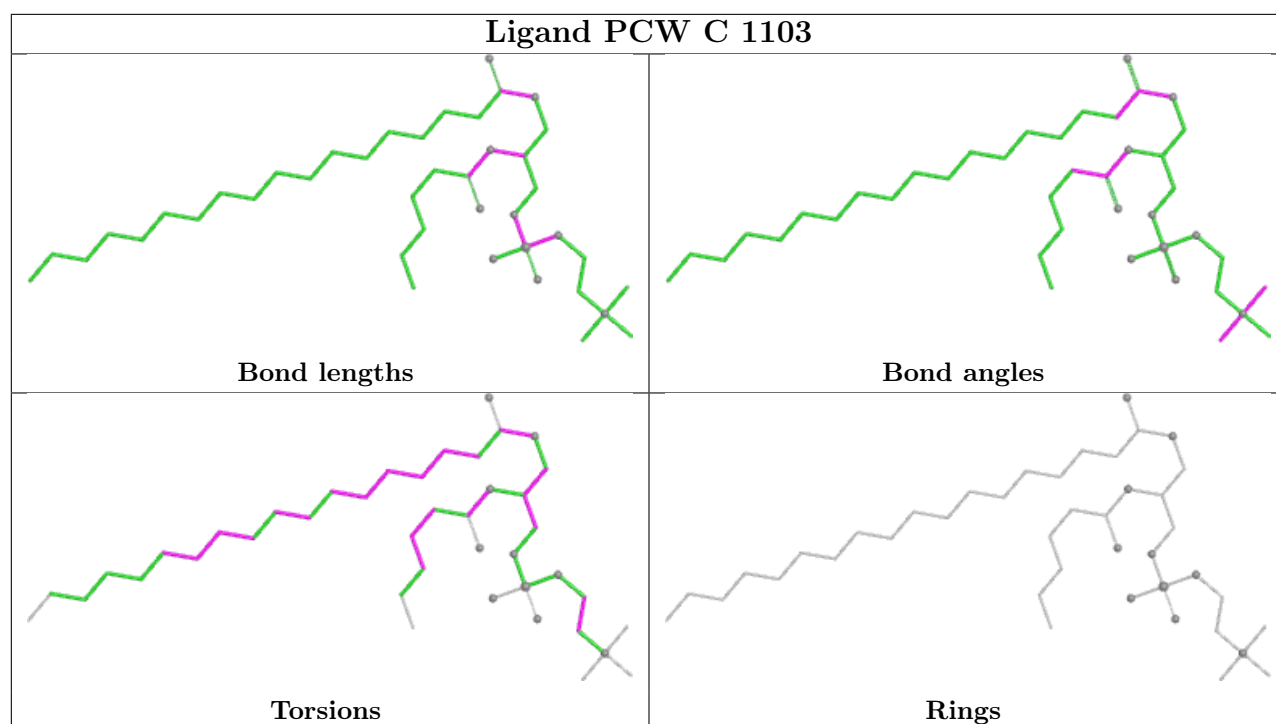


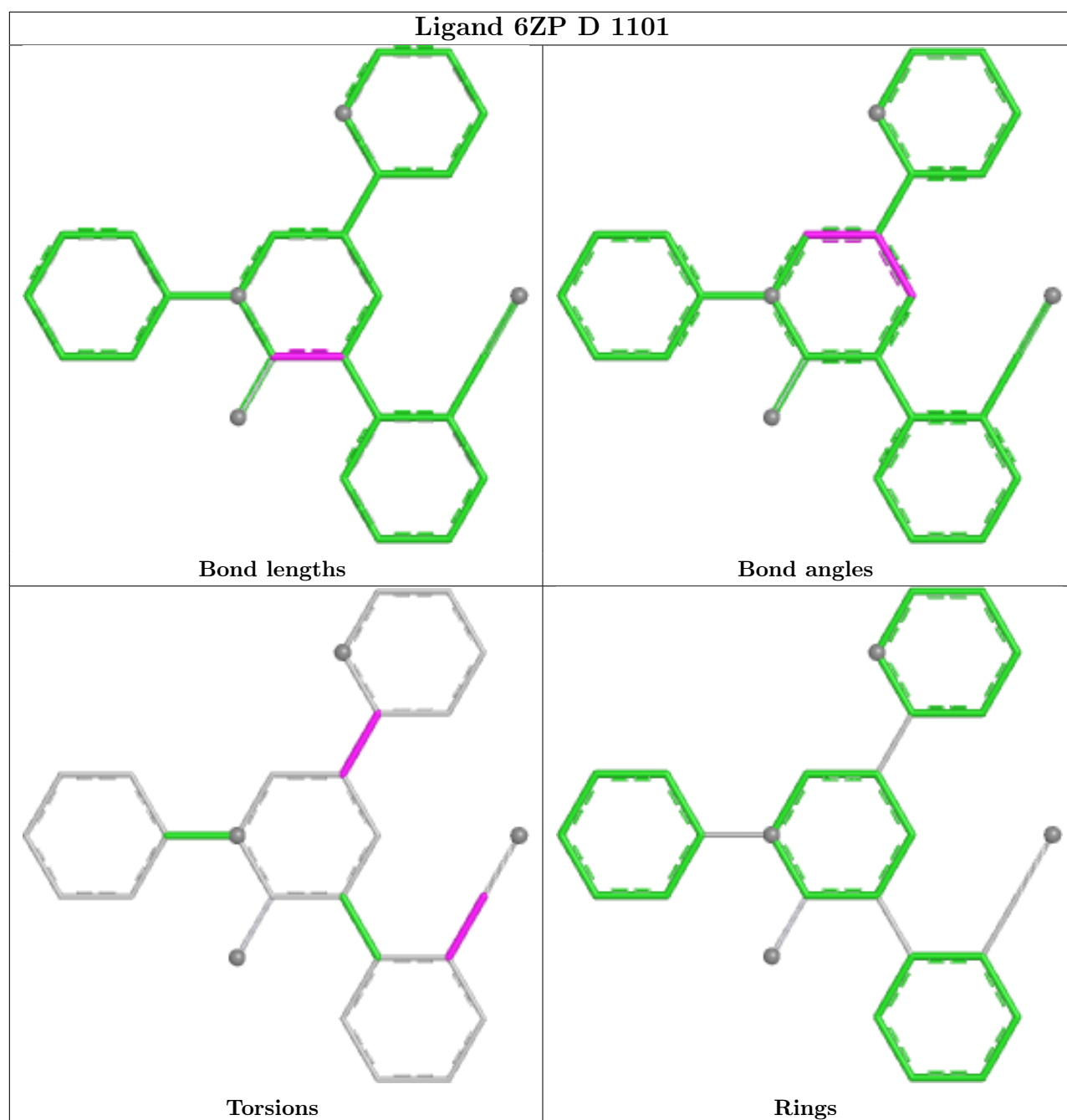


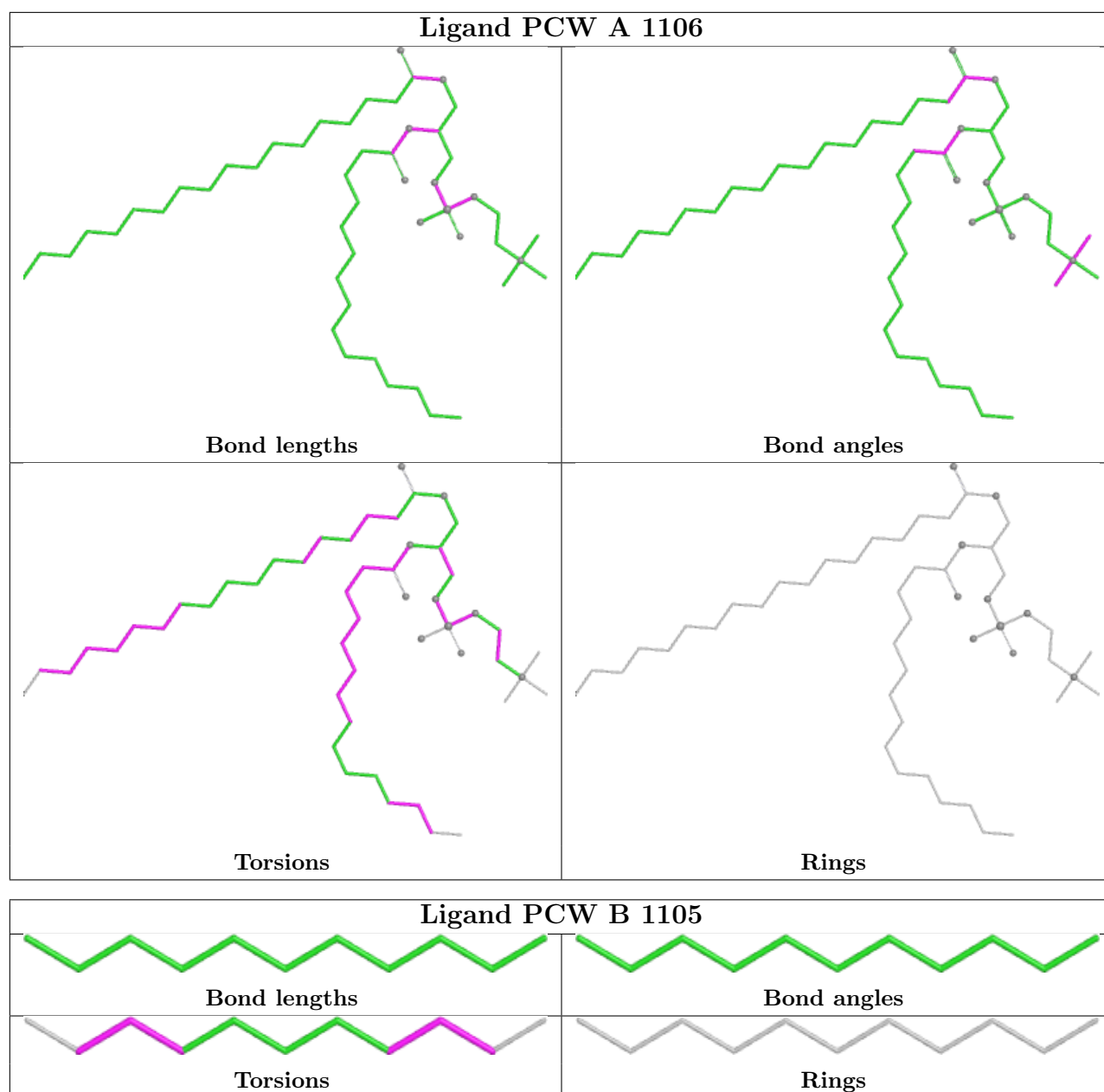


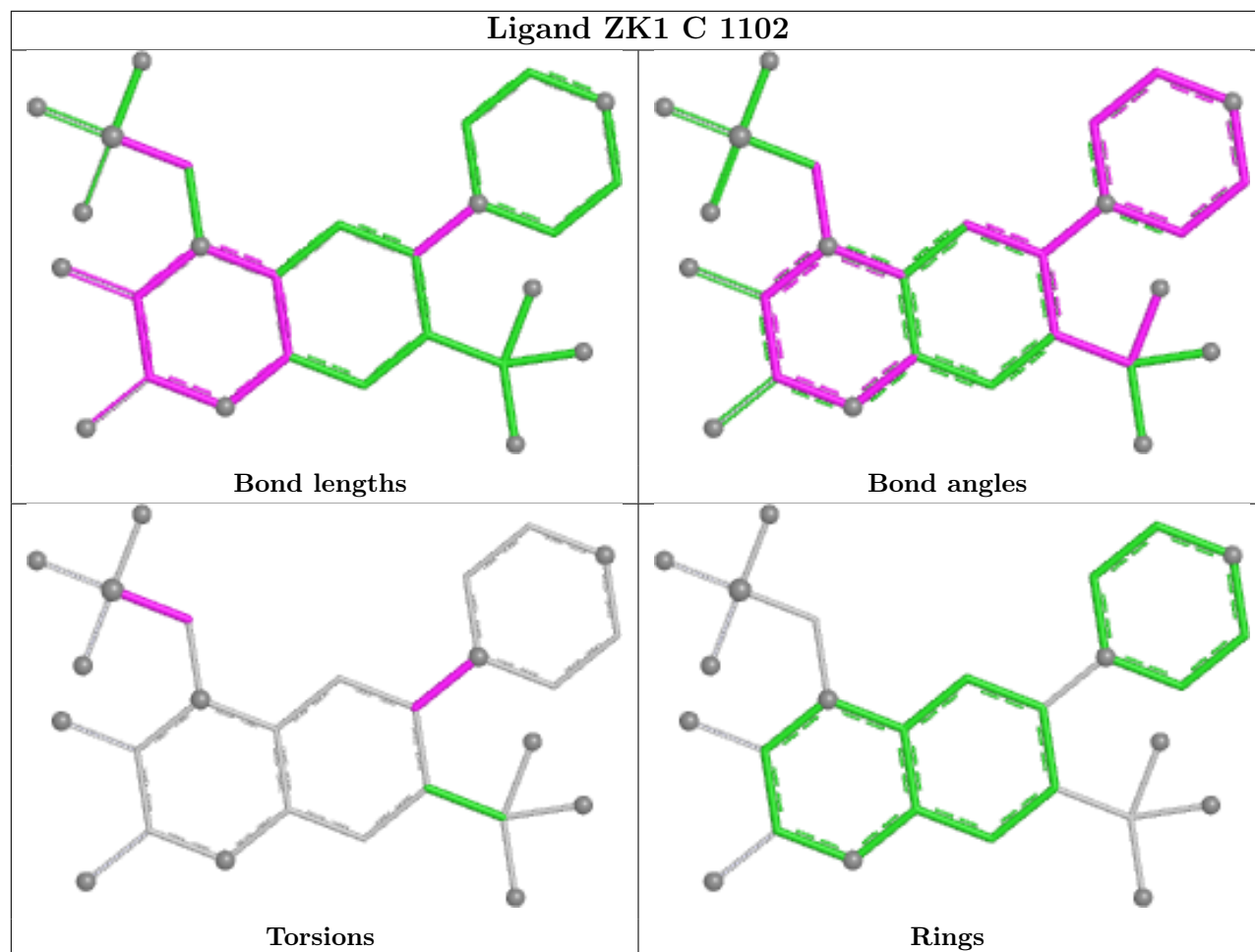


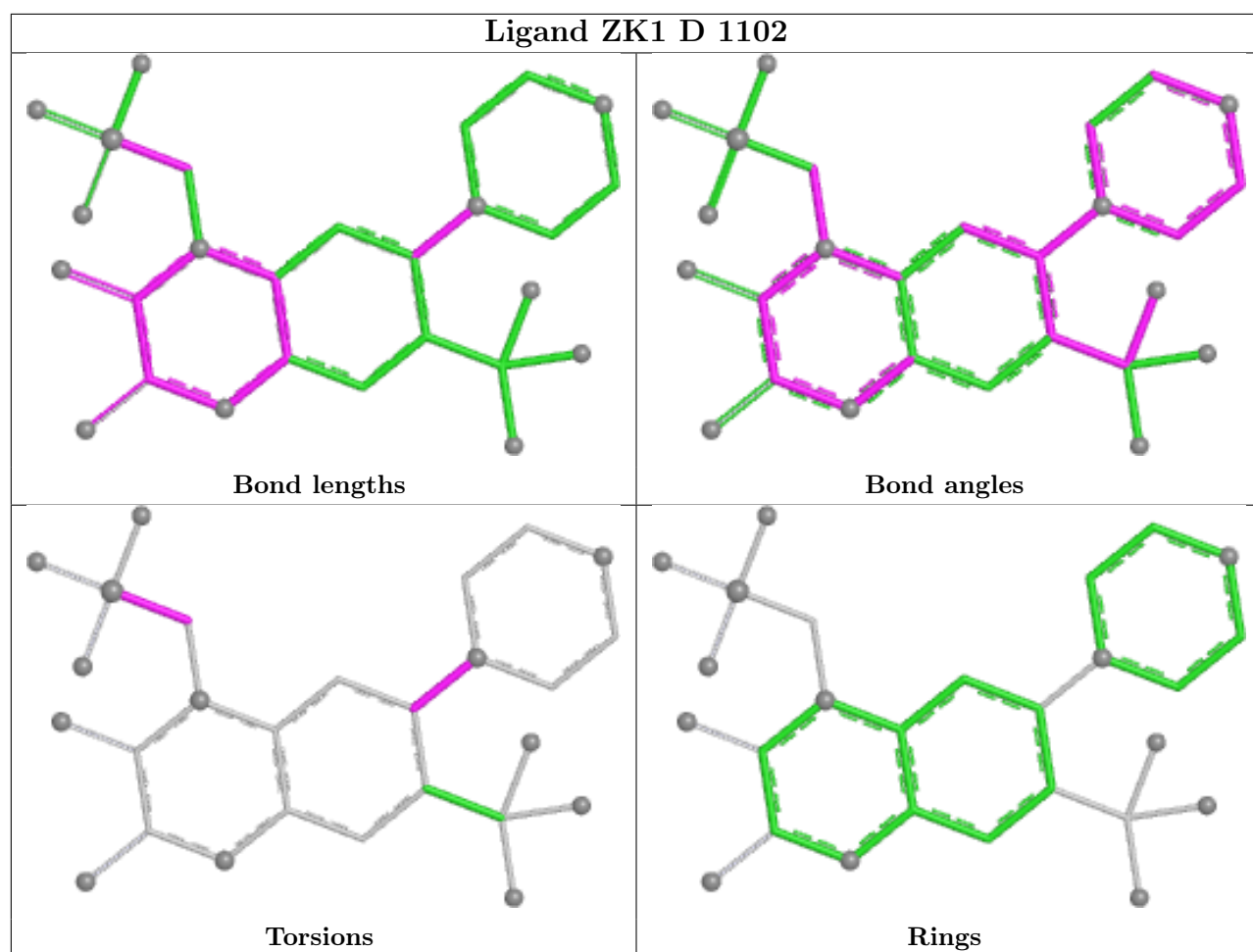


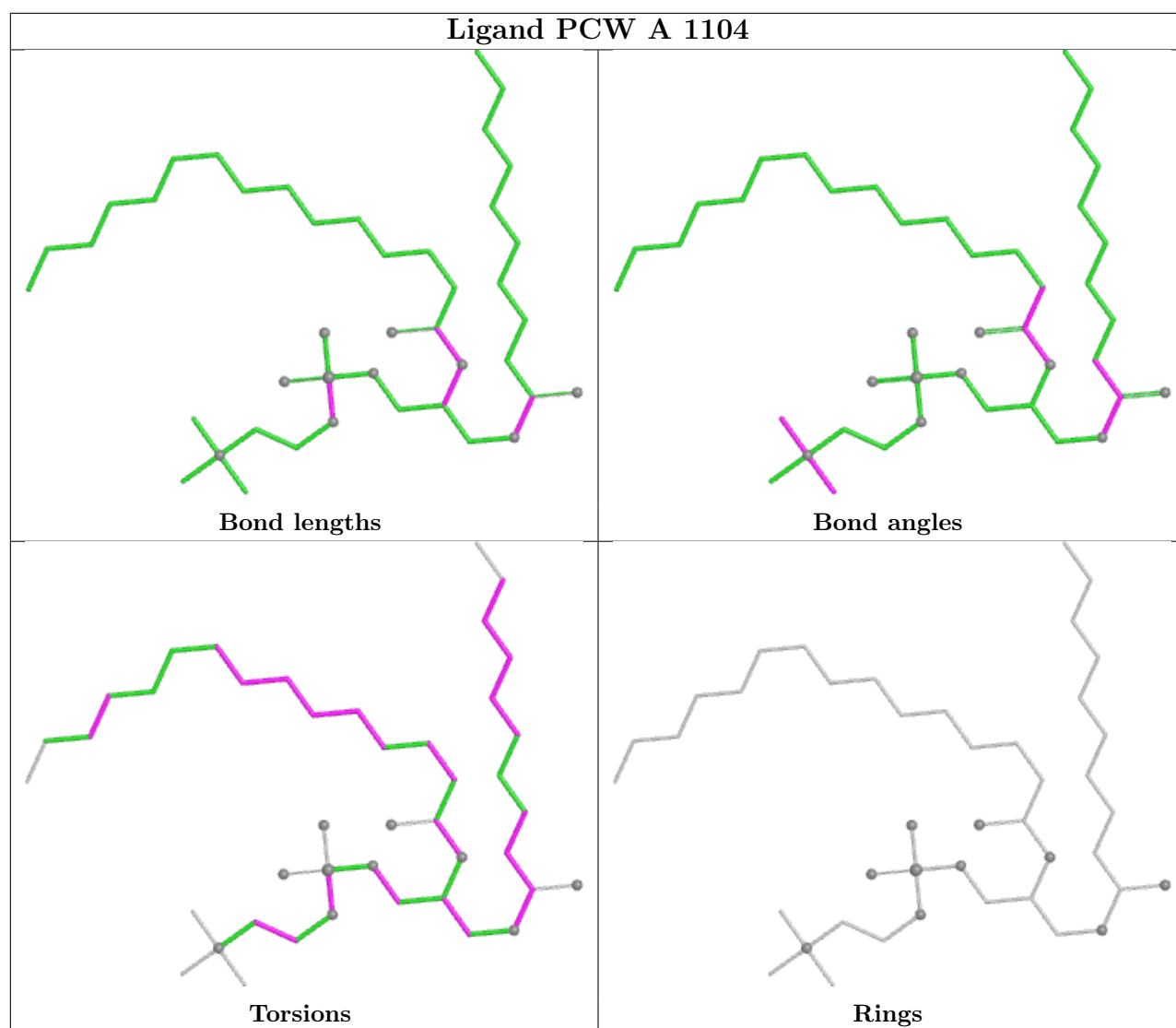


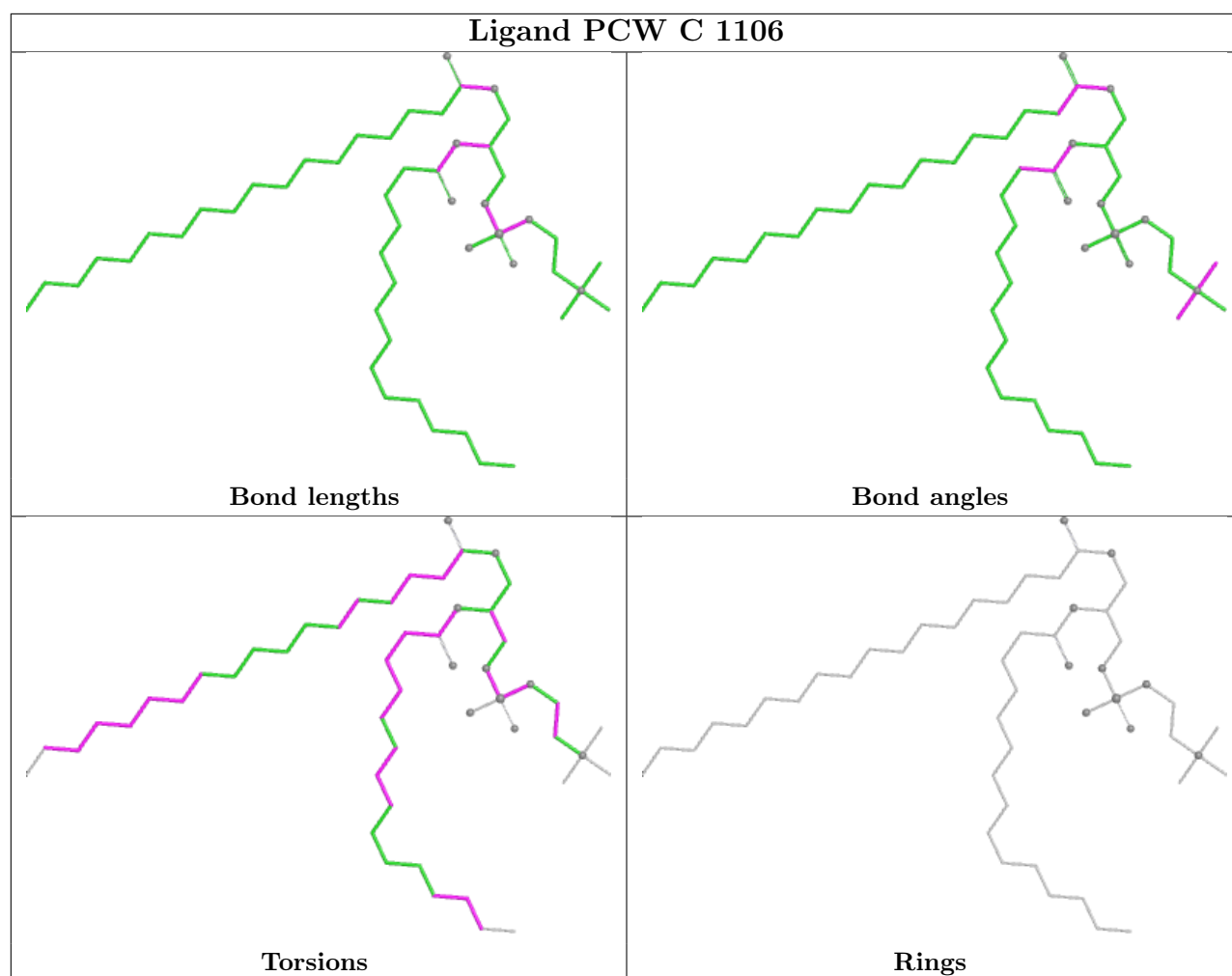


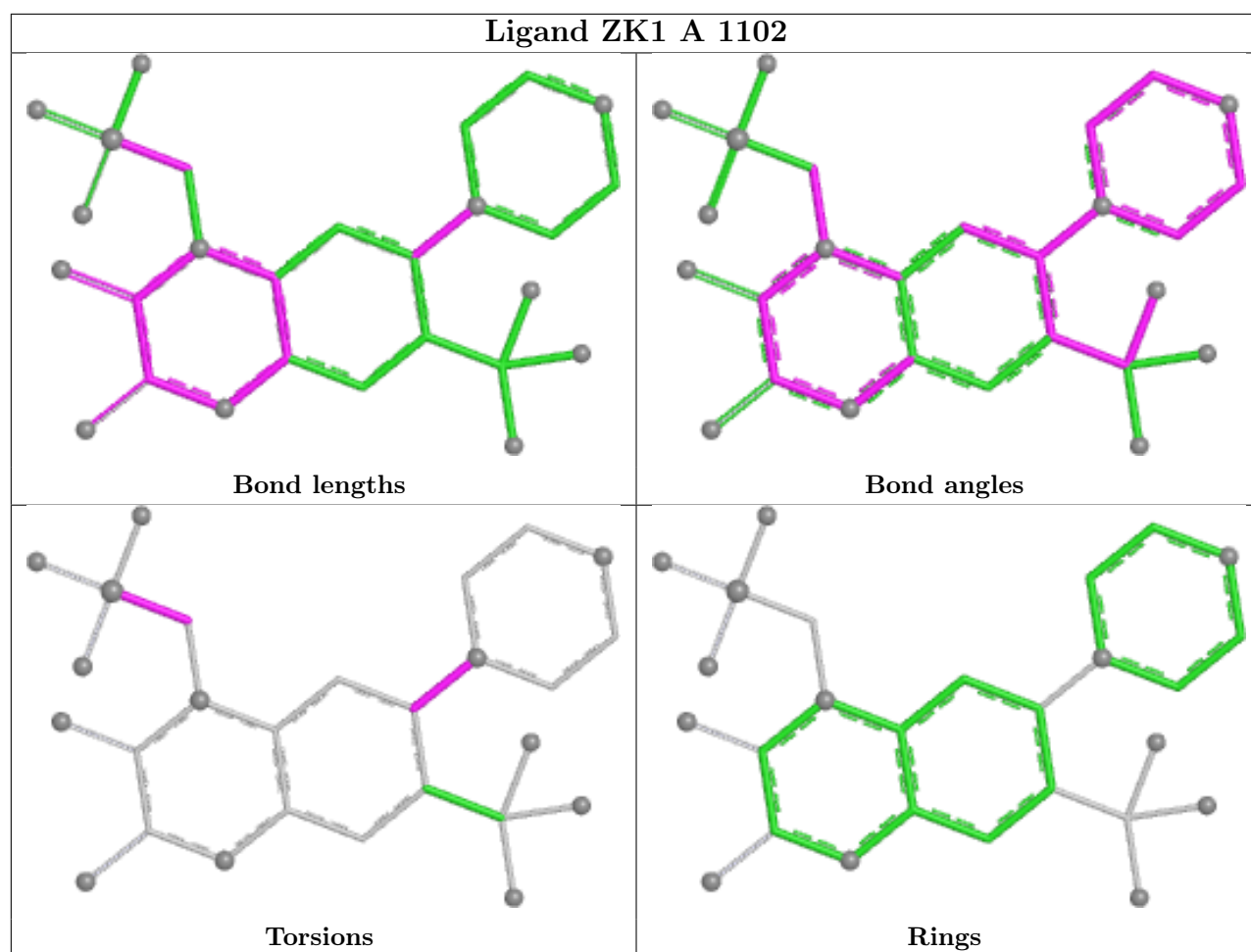


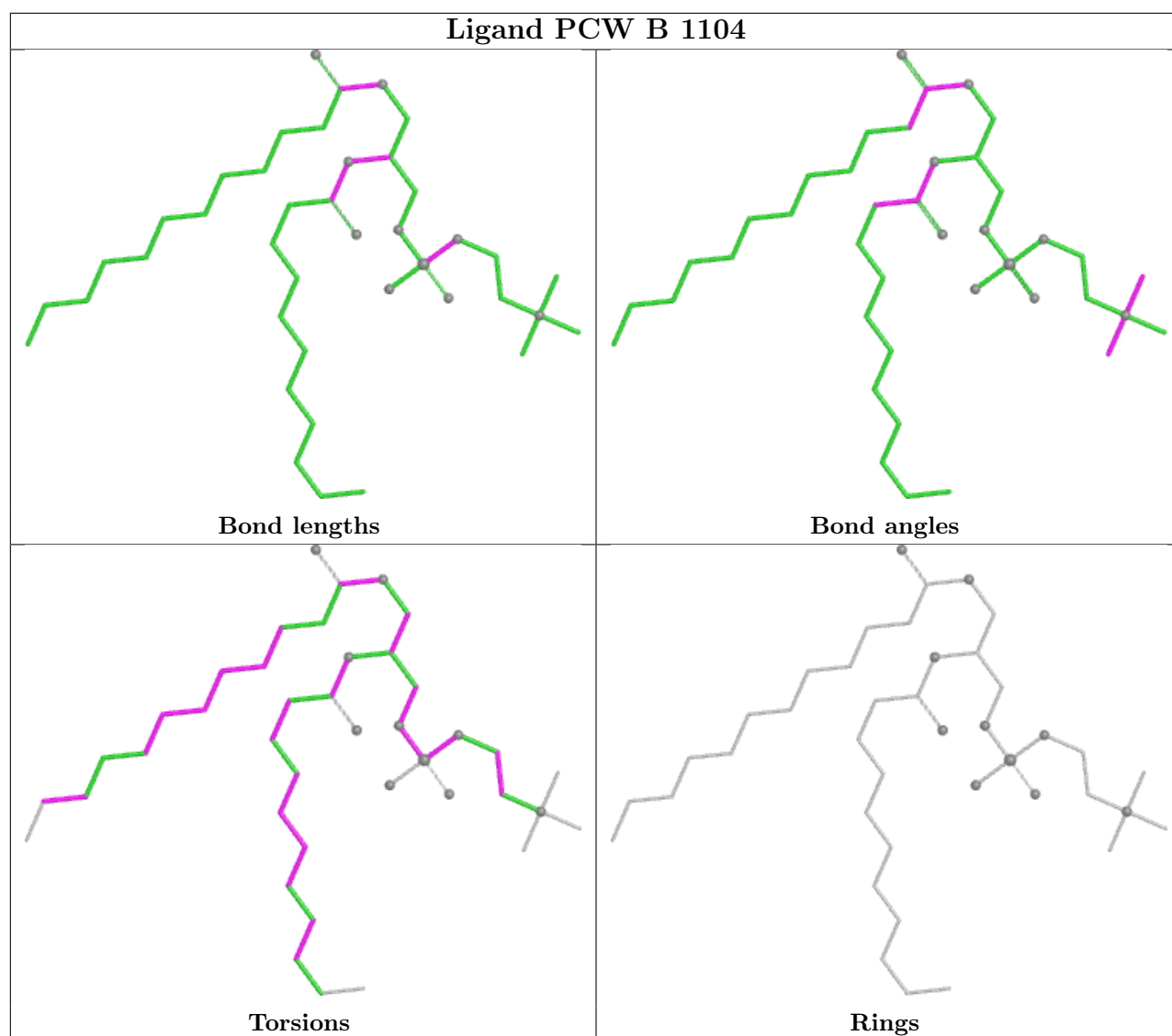












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

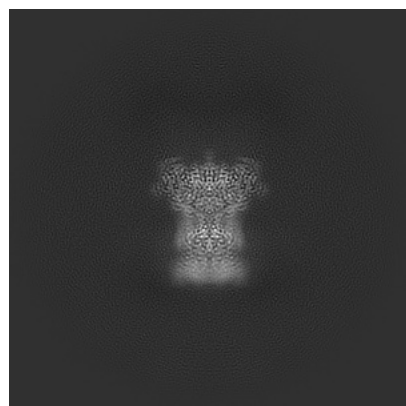
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40748. These allow visual inspection of the internal detail of the map and identification of artifacts.

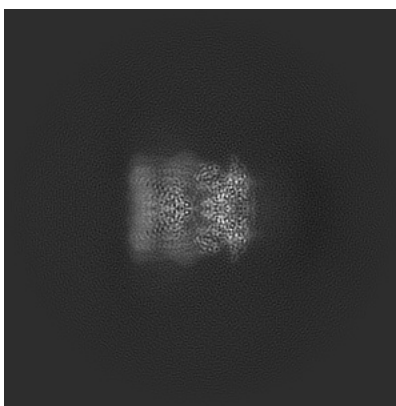
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

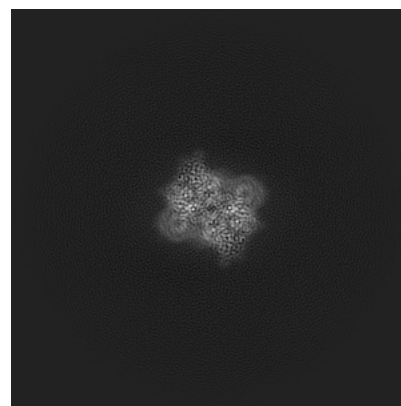
6.1.1 Primary map



X

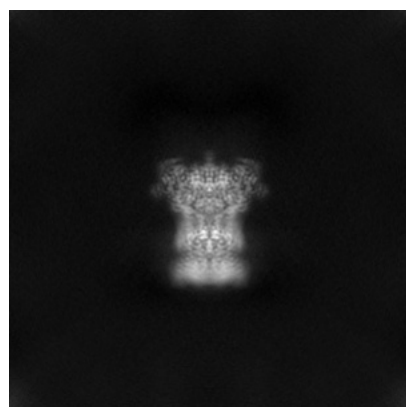


Y

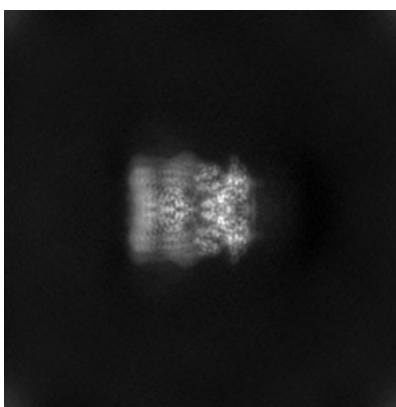


Z

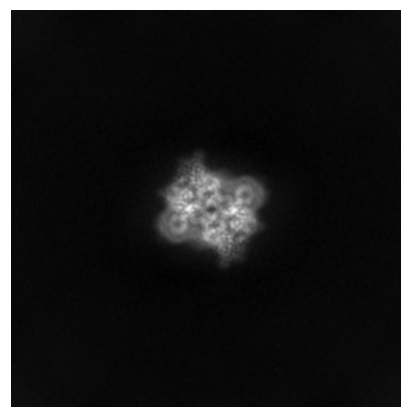
6.1.2 Raw map



X



Y

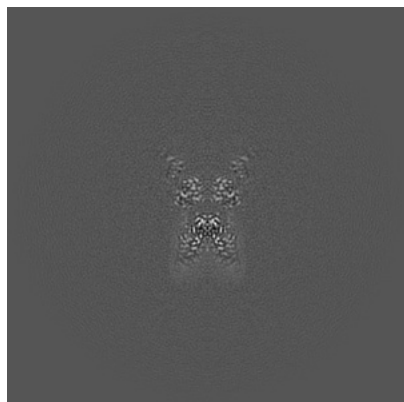


Z

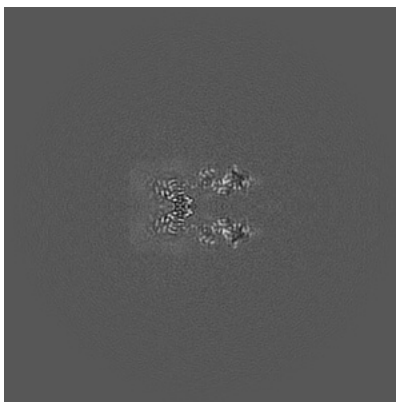
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

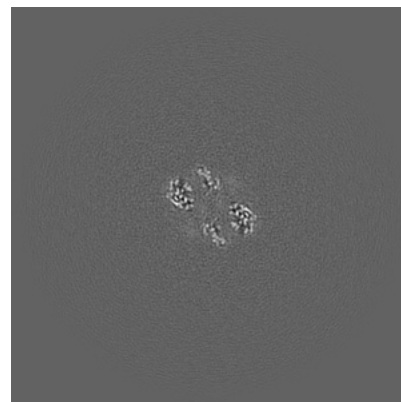
6.2.1 Primary map



X Index: 208

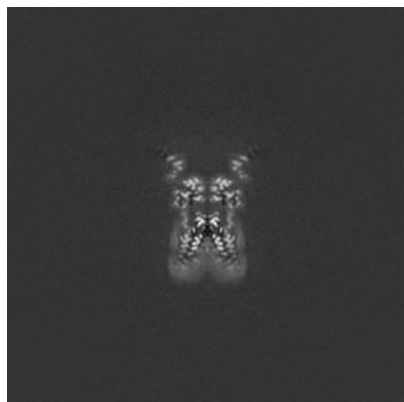


Y Index: 208

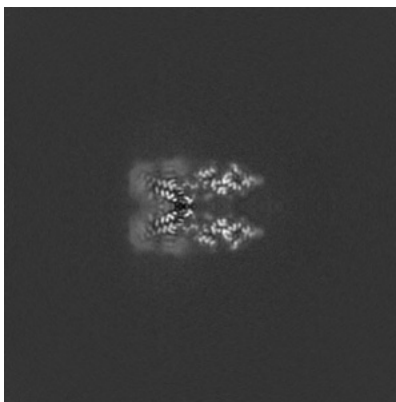


Z Index: 208

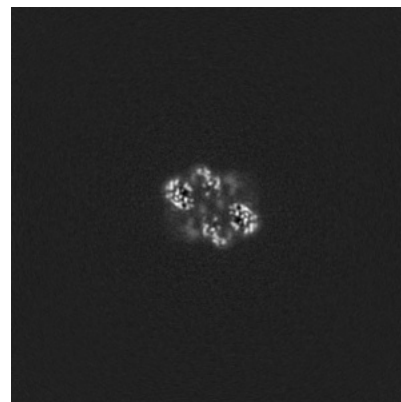
6.2.2 Raw map



X Index: 208



Y Index: 208

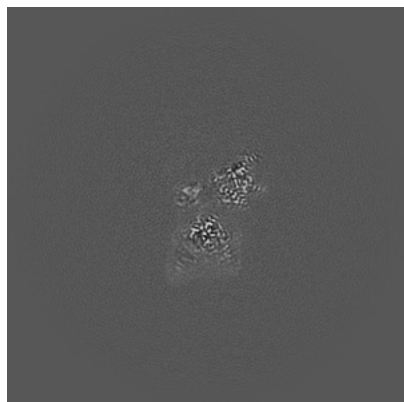


Z Index: 208

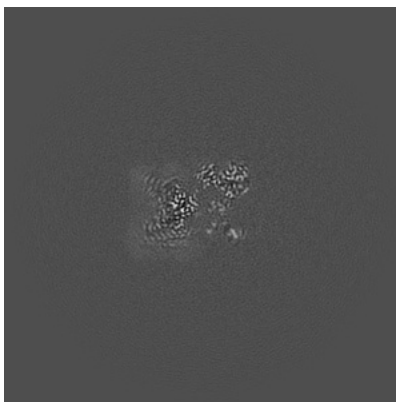
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

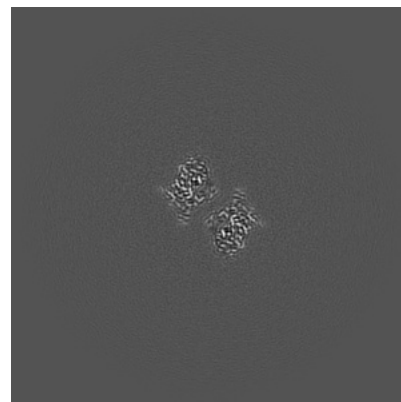
6.3.1 Primary map



X Index: 199

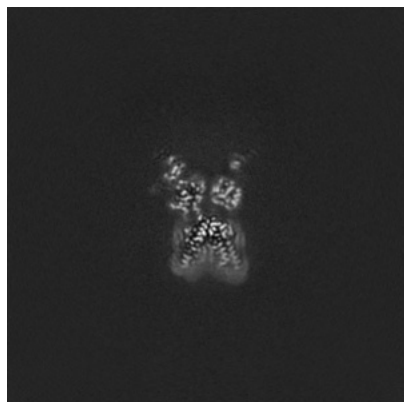


Y Index: 201

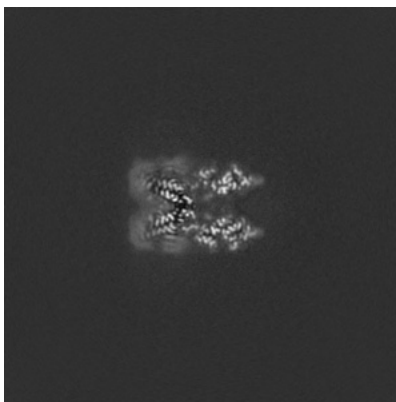


Z Index: 236

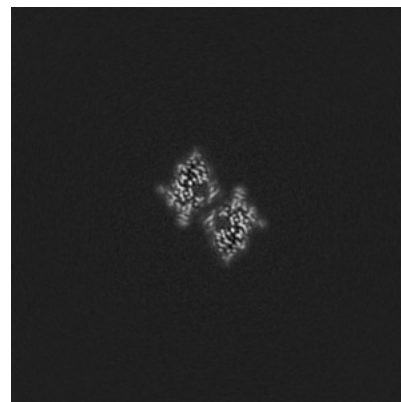
6.3.2 Raw map



X Index: 212



Y Index: 209

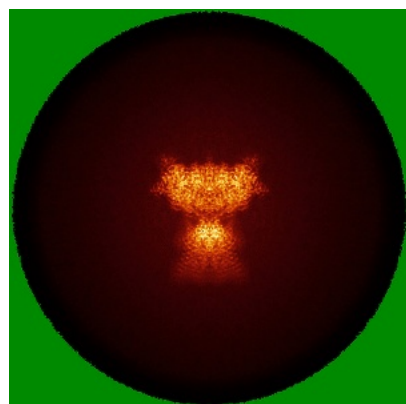


Z Index: 235

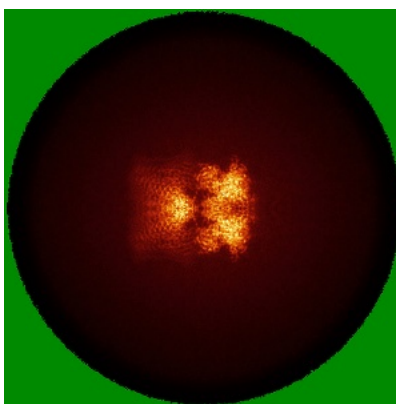
The images above show the largest variance slices of the map in three orthogonal directions.

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

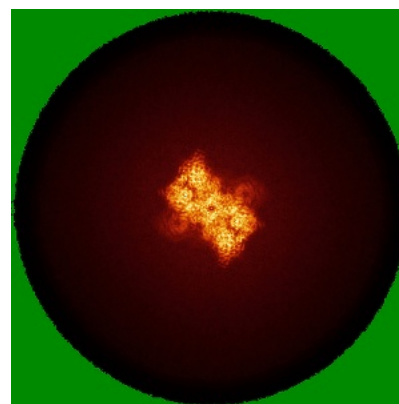
6.4.1 Primary map



X

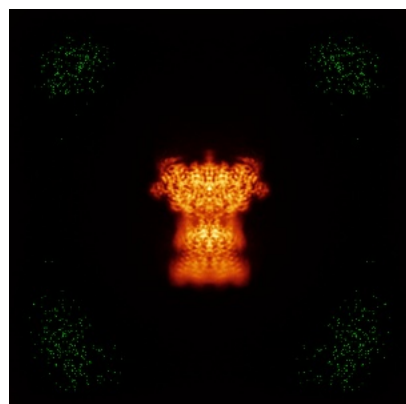


Y

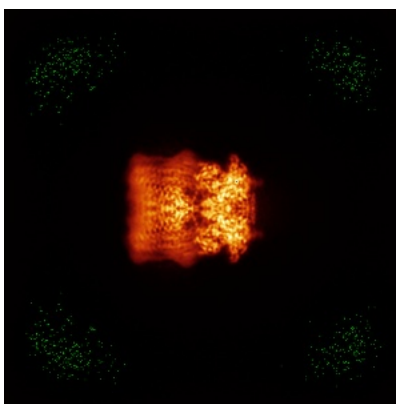


Z

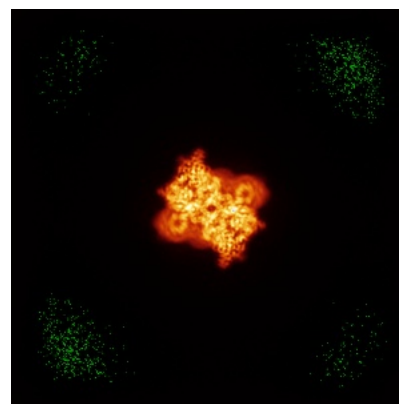
6.4.2 Raw map



X



Y

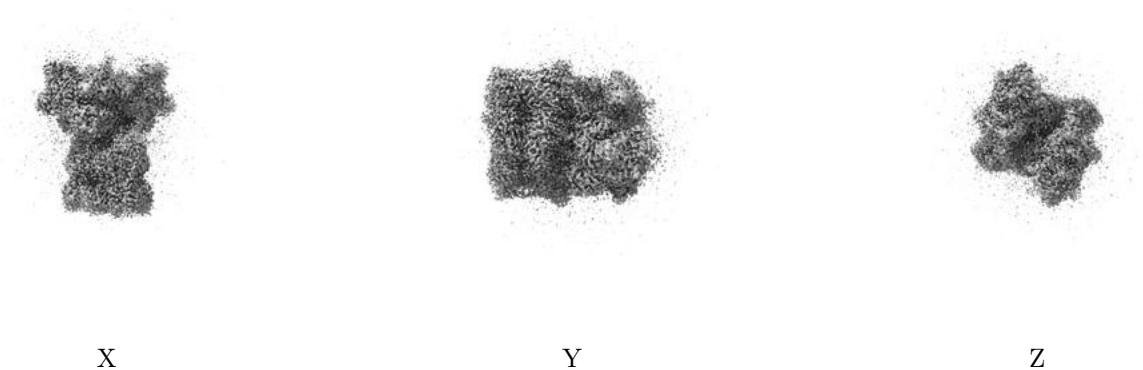


Z

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

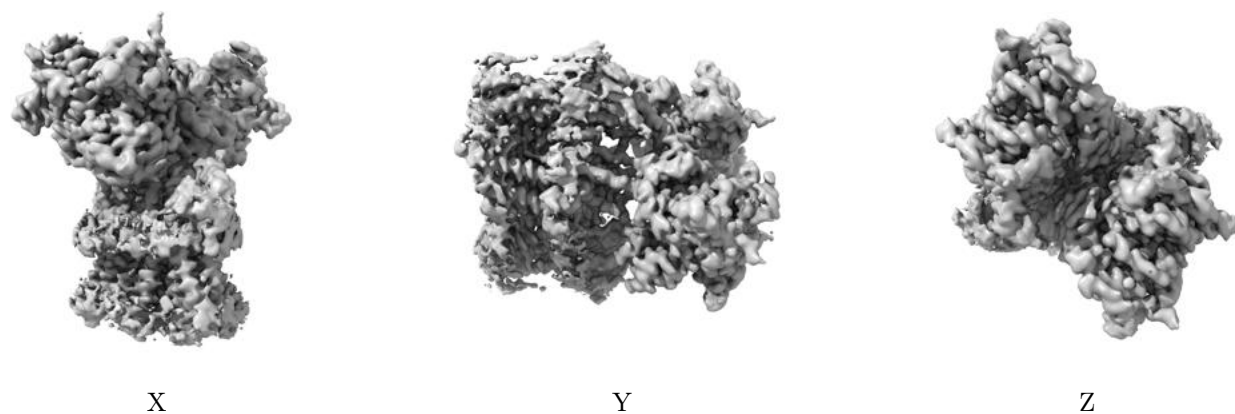
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

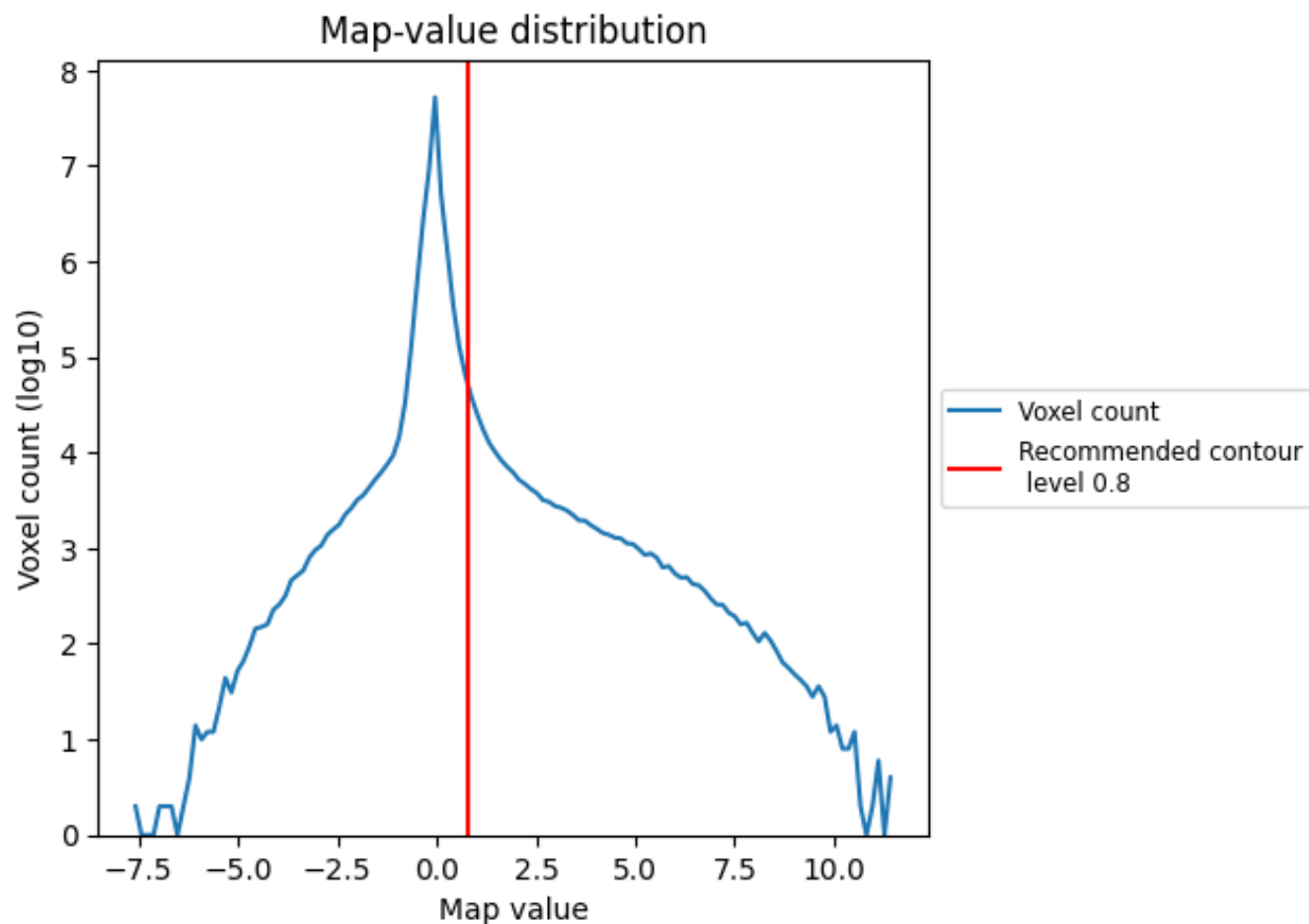
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

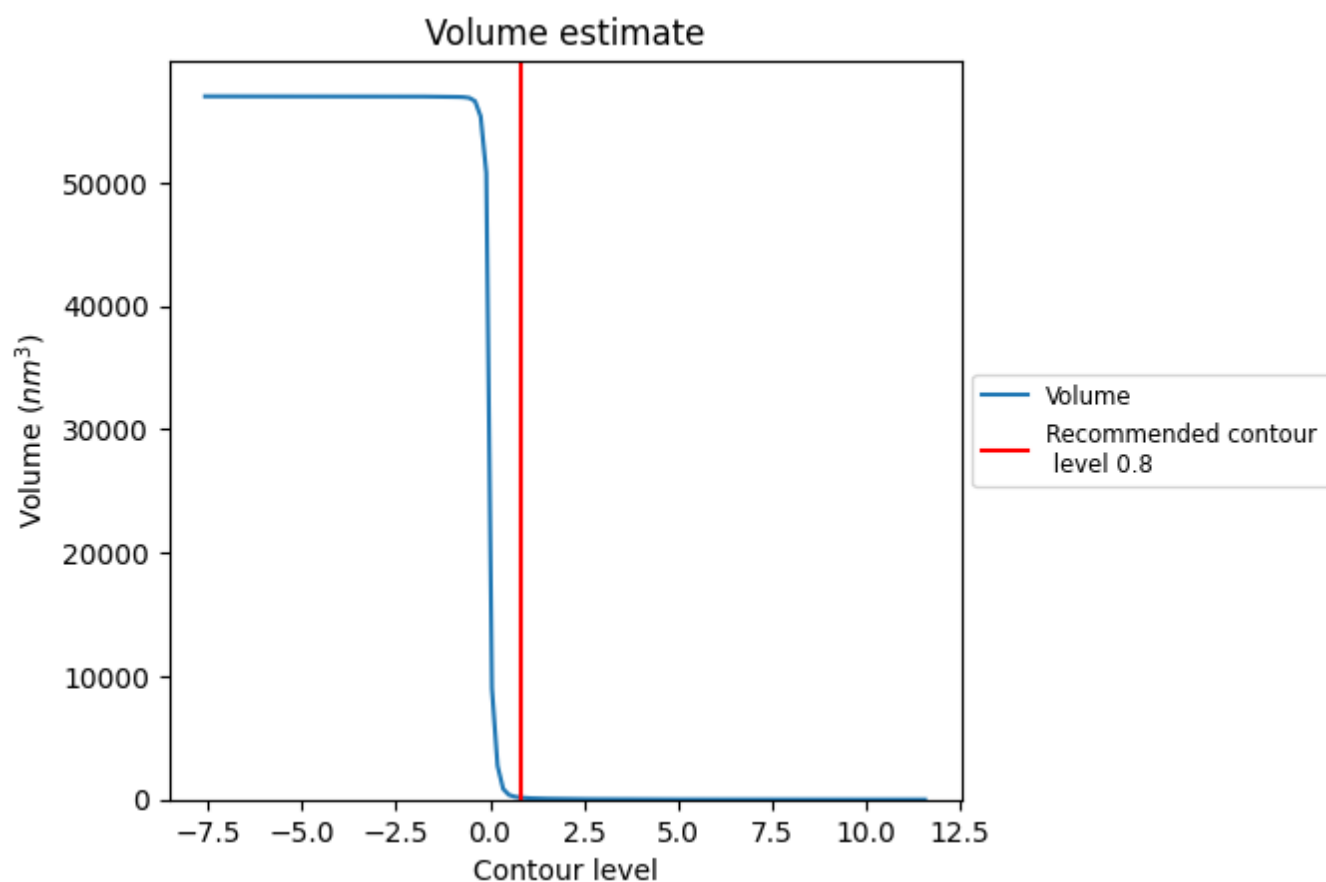
This section contains the results of statistical analysis of the map.

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.

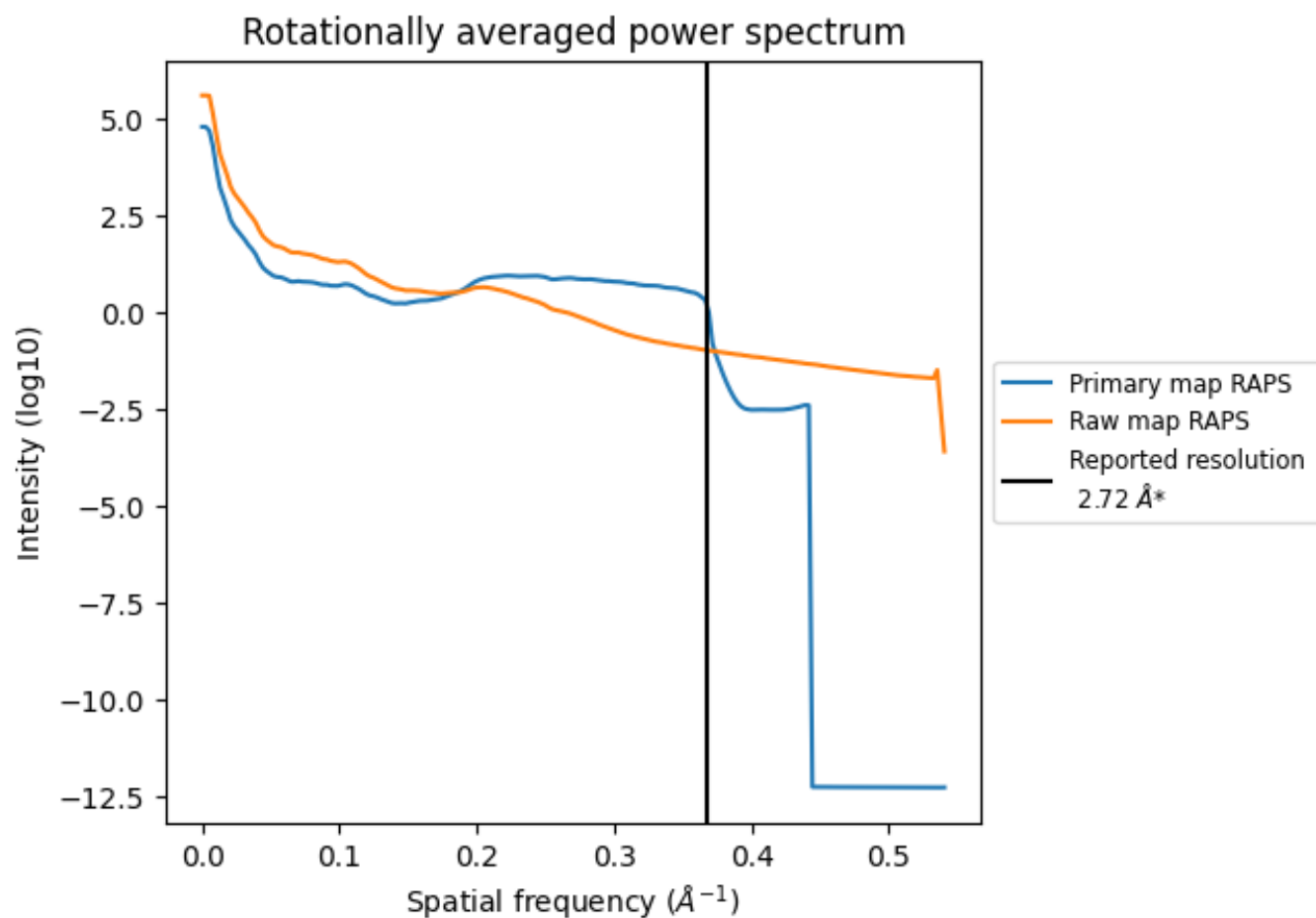
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm³; this corresponds to an approximate mass of 151 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 ⓘ

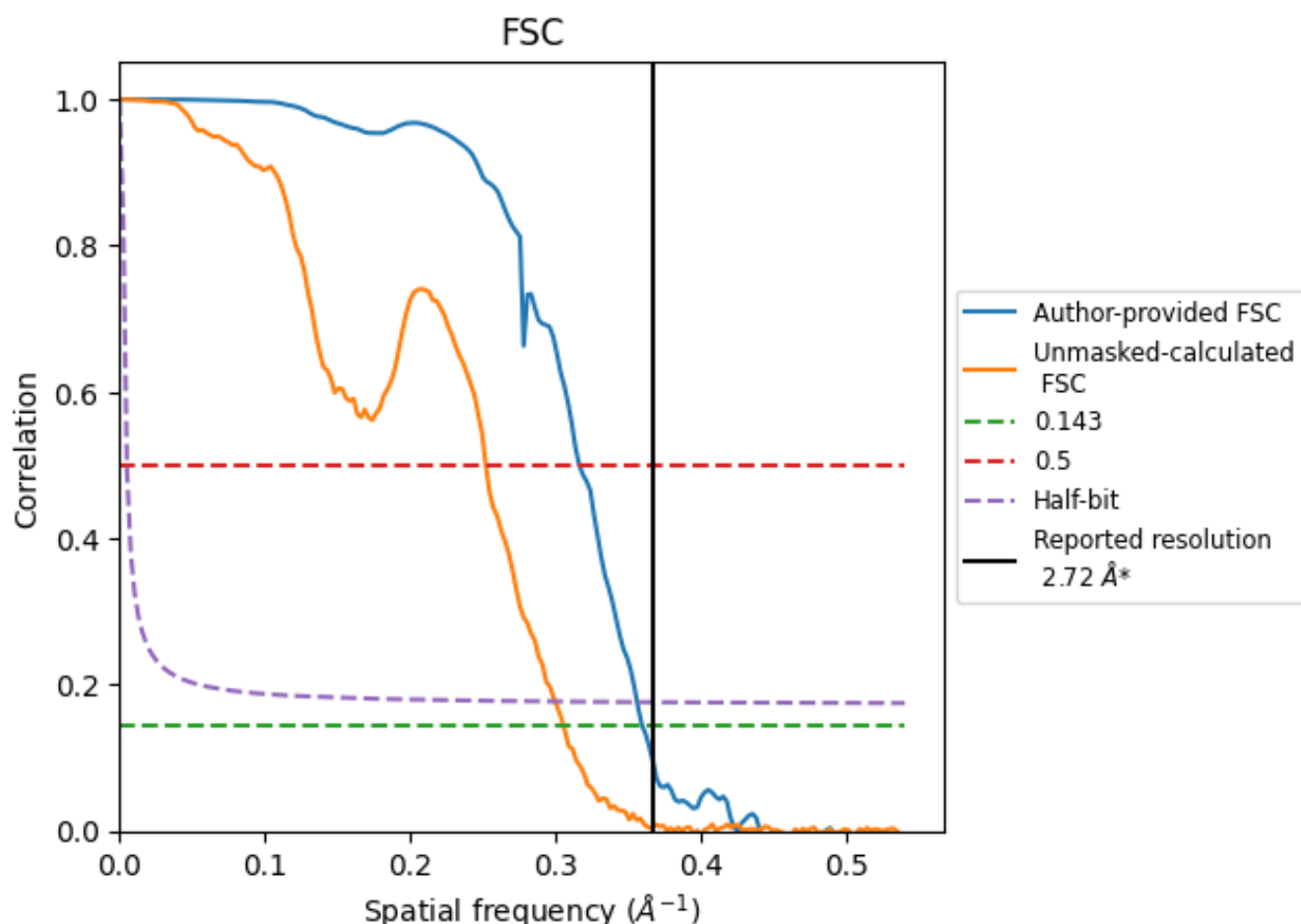


*Reported resolution corresponds to spatial frequency of 0.368 \AA^{-1}

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 0.368 Å⁻¹

8.2 Resolution estimates [i](#)

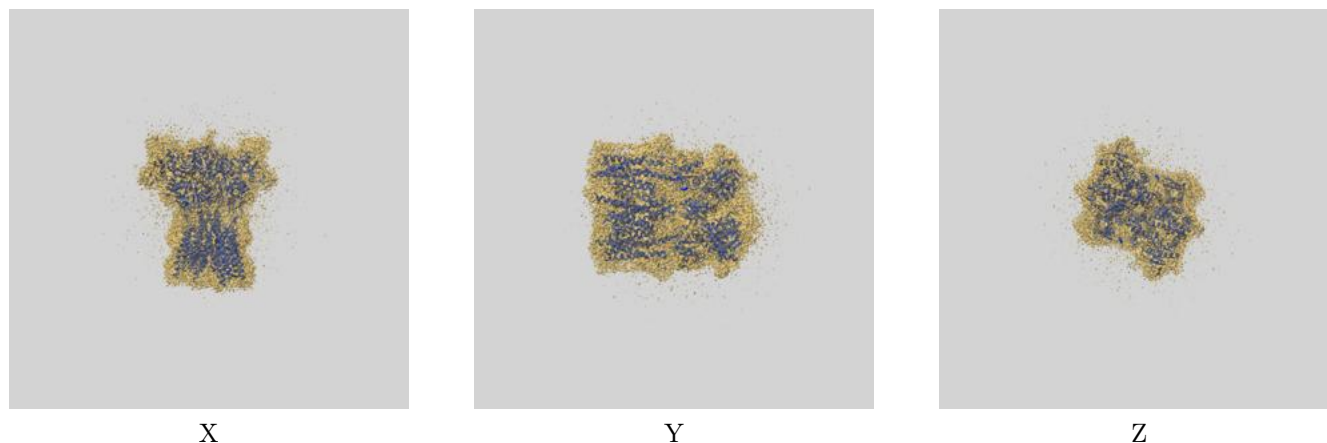
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.78	3.16	2.81
Unmasked-calculated*	3.27	3.97	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.27 differs from the reported value 2.72 by more than 10 %

9 Map-model fit [i](#)

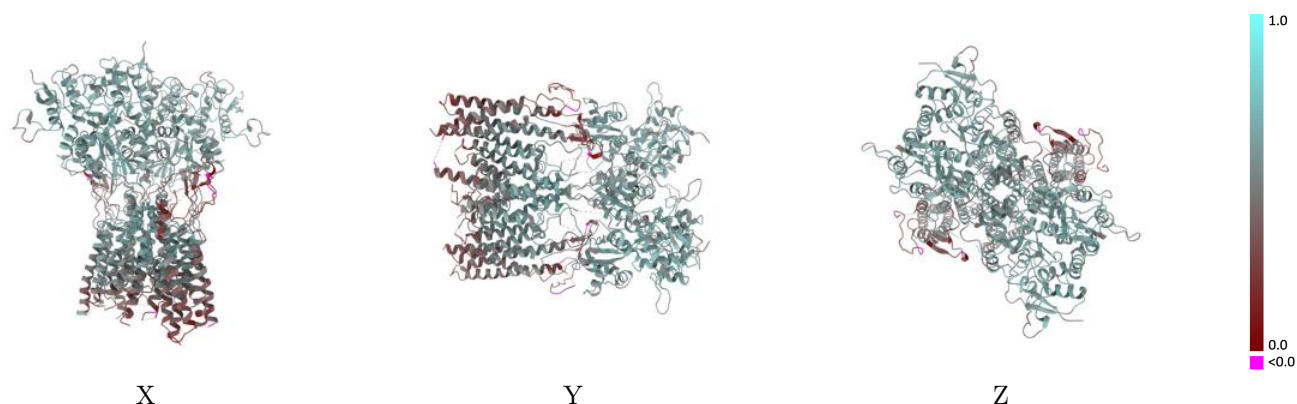
This section contains information regarding the fit between EMDB map EMD-40748 and PDB model 8SS9. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



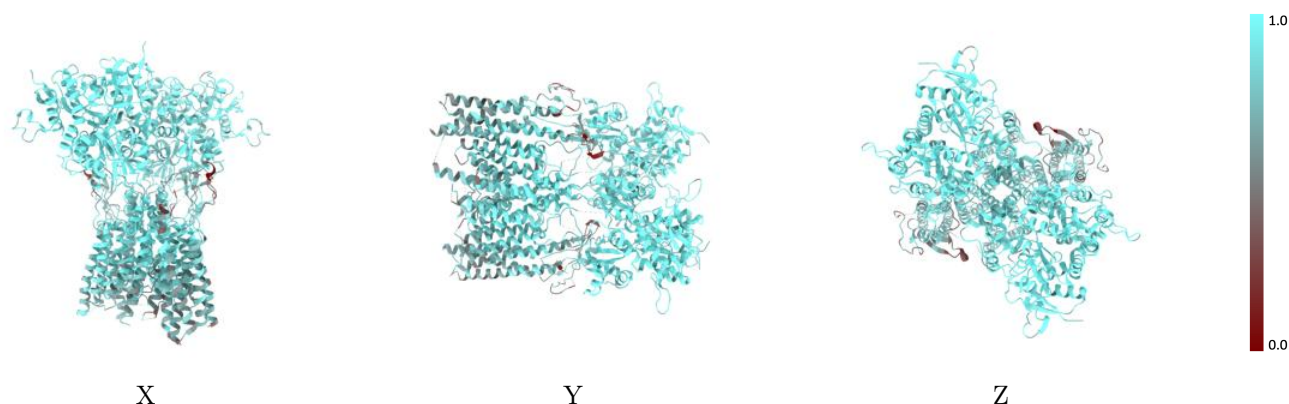
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



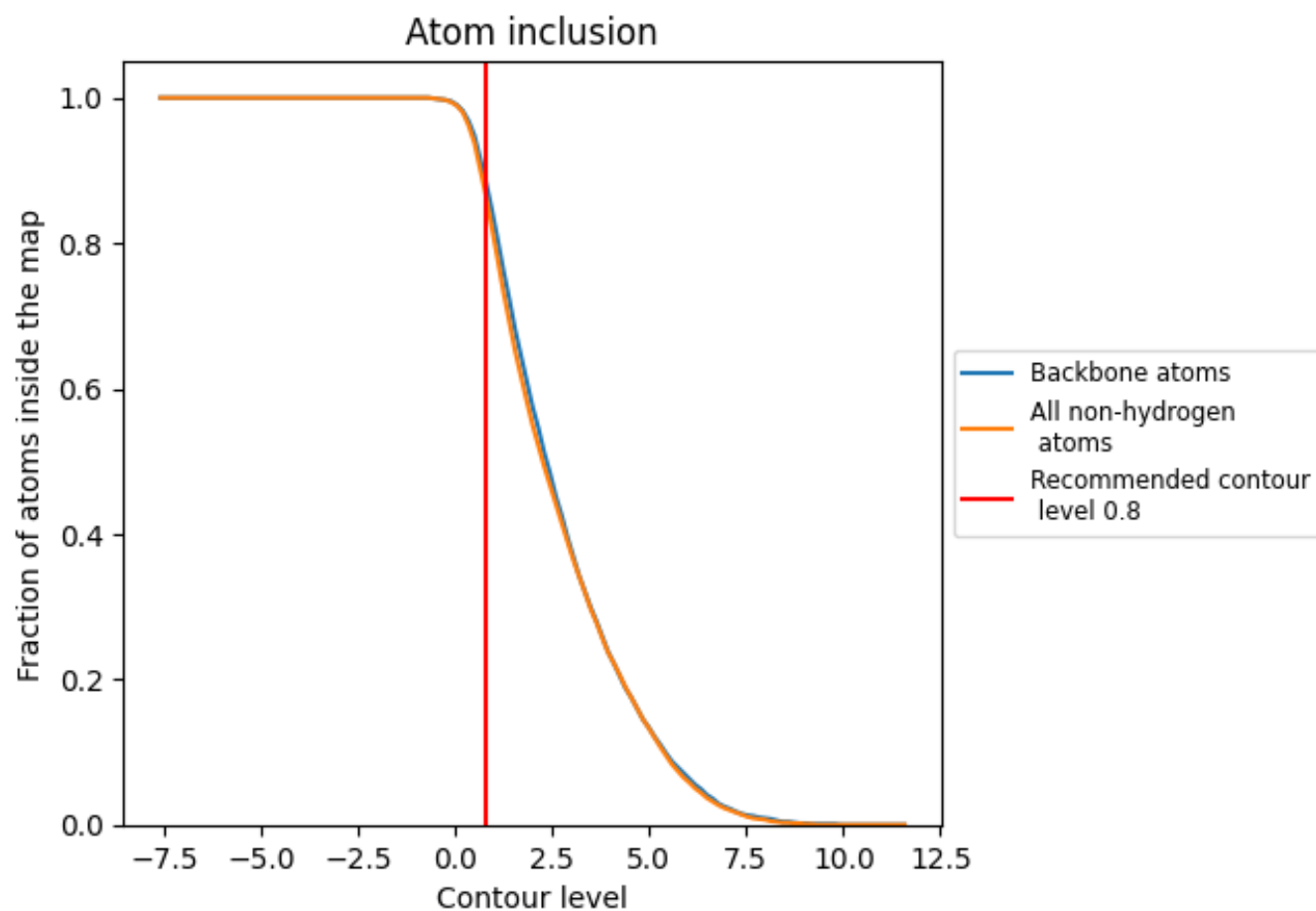
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8650	<div></div> 0.5190
A	<div></div> 0.8480	<div></div> 0.5000
B	<div></div> 0.9100	<div></div> 0.5590
C	<div></div> 0.8300	<div></div> 0.4900
D	<div></div> 0.9070	<div></div> 0.5520

