



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 8AYM / pdb_00008aym
EMDB ID : EMD-15716
Title : Resting state GluA1/A2 AMPA receptor in complex with TARP gamma 8 and ligand JNJ-55511118
Authors : Zhang, D.; Lape, R.; Shaikh, S.; Kohegyi, B.; Watson, J.F.; Cais, O.; Nakagawa, T.; Greger, I.H.
Deposited on : 2022-09-02
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

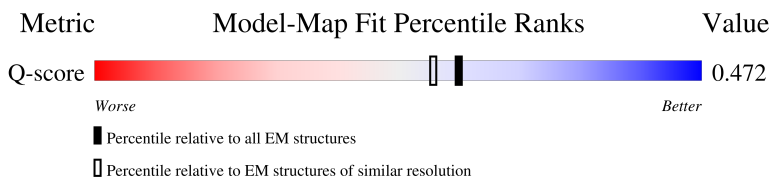
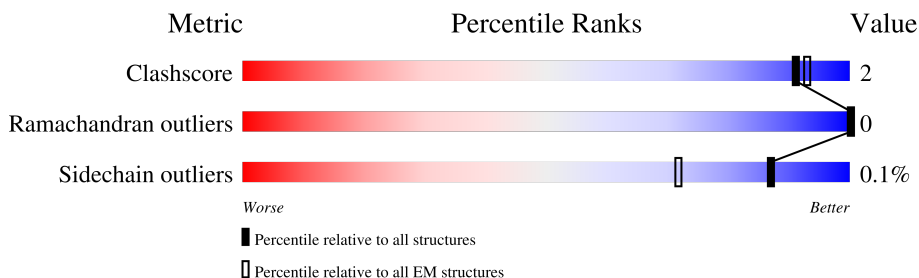
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	I	423	
1	J	423	
2	A	915	
2	C	915	

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Mol	Chain	Length	Quality of chain
3	B	860	5% 44% 53%
3	D	860	5% 44% 53%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15962 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 Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	185	Total	C	N	O	S	0	0
			1358	891	228	233	6		
1	J	185	Total	C	N	O	S	0	0
			1358	891	228	233	6		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	expression tag	UNP Q8VHW5
I	418	LEU	-	expression tag	UNP Q8VHW5
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	1	GLY	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	UNP Q8VHW5
J	420	VAL	-	expression tag	UNP Q8VHW5
J	421	LEU	-	expression tag	UNP Q8VHW5
J	422	PHE	-	expression tag	UNP Q8VHW5
J	423	GLN	-	expression tag	UNP Q8VHW5

- Molecule 2 is a protein called Isoform Flip of Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	414	Total	C	N	O	S	0	0
			3168	2057	513	579	19		
2	A	414	Total	C	N	O	S	0	0
			3168	2057	513	579	19		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490

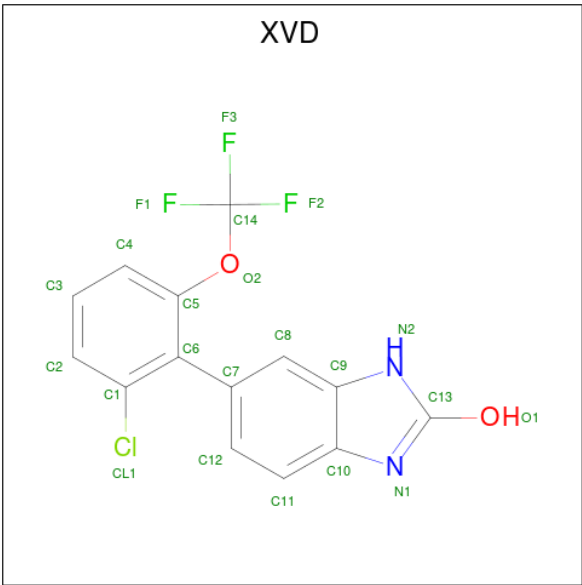
- Molecule 3 is a protein called Isoform Flip of Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	405	Total	C	N	O	S	0	0
			3103	2013	501	568	21		
3	B	405	Total	C	N	O	S	0	0
			3103	2013	501	568	21		

There are 2 discrepancies between the modelled and reference sequences:

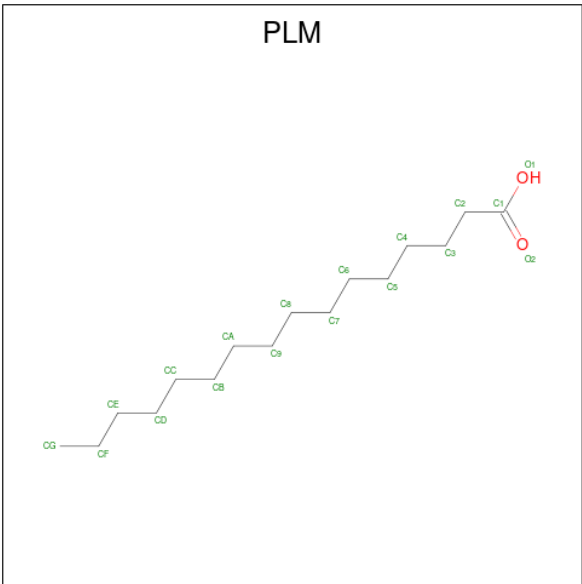
Chain	Residue	Modelled	Actual	Comment	Reference
D	586	ARG	GLN	variant	UNP P19491
B	586	ARG	GLN	variant	UNP P19491

- Molecule 4 is 6-[2-chloro-6-(trifluoromethoxy)phenyl]-1H-benzimidazol-2-ol (CCD ID: XVD) (formula: C₁₄H₈ClF₃N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	I	1	Total	C	Cl	F	N	O	0
			22	14	1	3	2	2	
4	J	1	Total	C	Cl	F	N	O	0
			22	14	1	3	2	2	

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



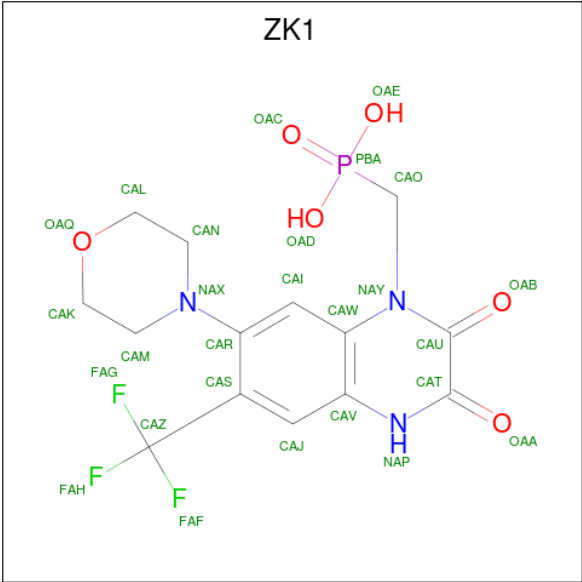
Mol	Chain	Residues	Atoms			AltConf
5	I	1	Total	C	O	0
			18	16	2	

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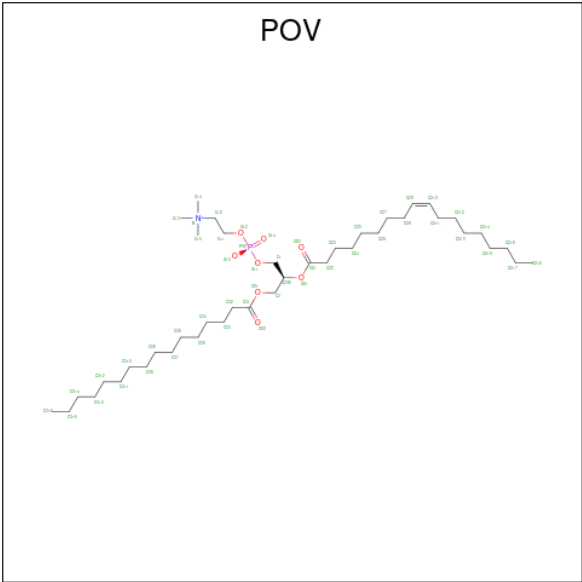
Mol	Chain	Residues	Atoms			AltConf
5	C	1	Total	C	O	0
			16	14	2	
5	C	1	Total	C	O	0
			18	16	2	
5	C	1	Total	C	O	0
			14	12	2	
5	C	1	Total	C	O	0
			18	16	2	
5	D	1	Total	C	O	0
			18	16	2	
5	D	1	Total	C	O	0
			18	16	2	
5	B	1	Total	C	O	0
			18	16	2	
5	B	1	Total	C	O	0
			18	16	2	
5	A	1	Total	C	O	0
			16	14	2	
5	A	1	Total	C	O	0
			18	16	2	
5	A	1	Total	C	O	0
			14	12	2	
5	A	1	Total	C	O	0
			18	16	2	
5	J	1	Total	C	O	0
			18	16	2	

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



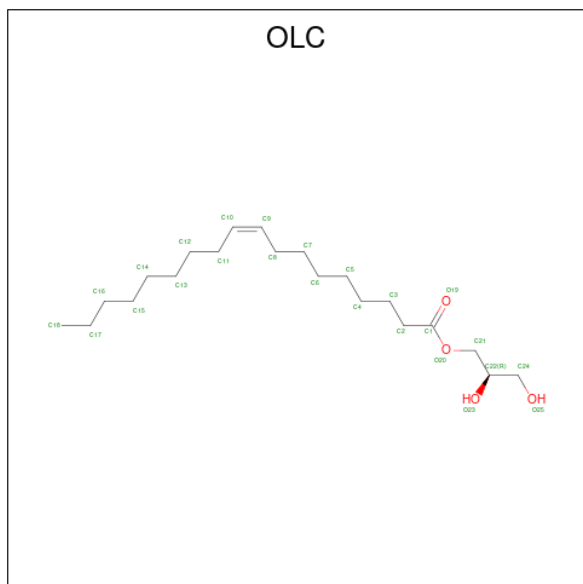
Mol	Chain	Residues	Atoms						AltConf
6	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
6	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
6	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
6	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



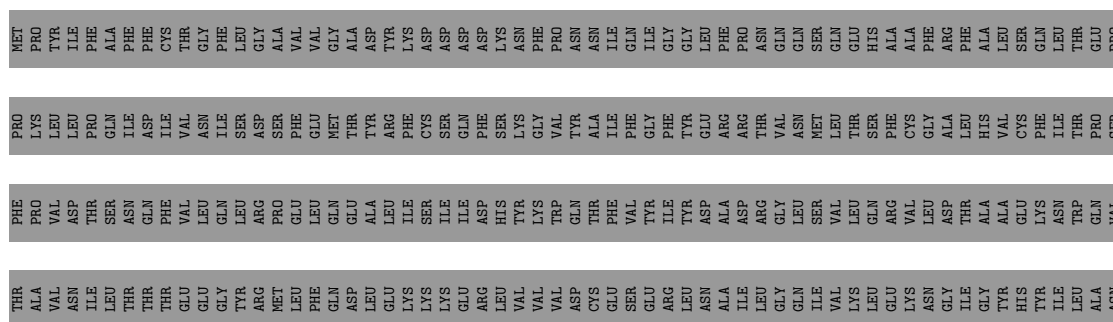
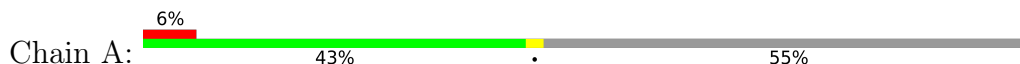
Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	C	1	Total	C	N	O	P	0
			48	38	1	8	1	
7	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
7	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
7	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	A	1	Total	C	N	O	P	0
			48	38	1	8	1	

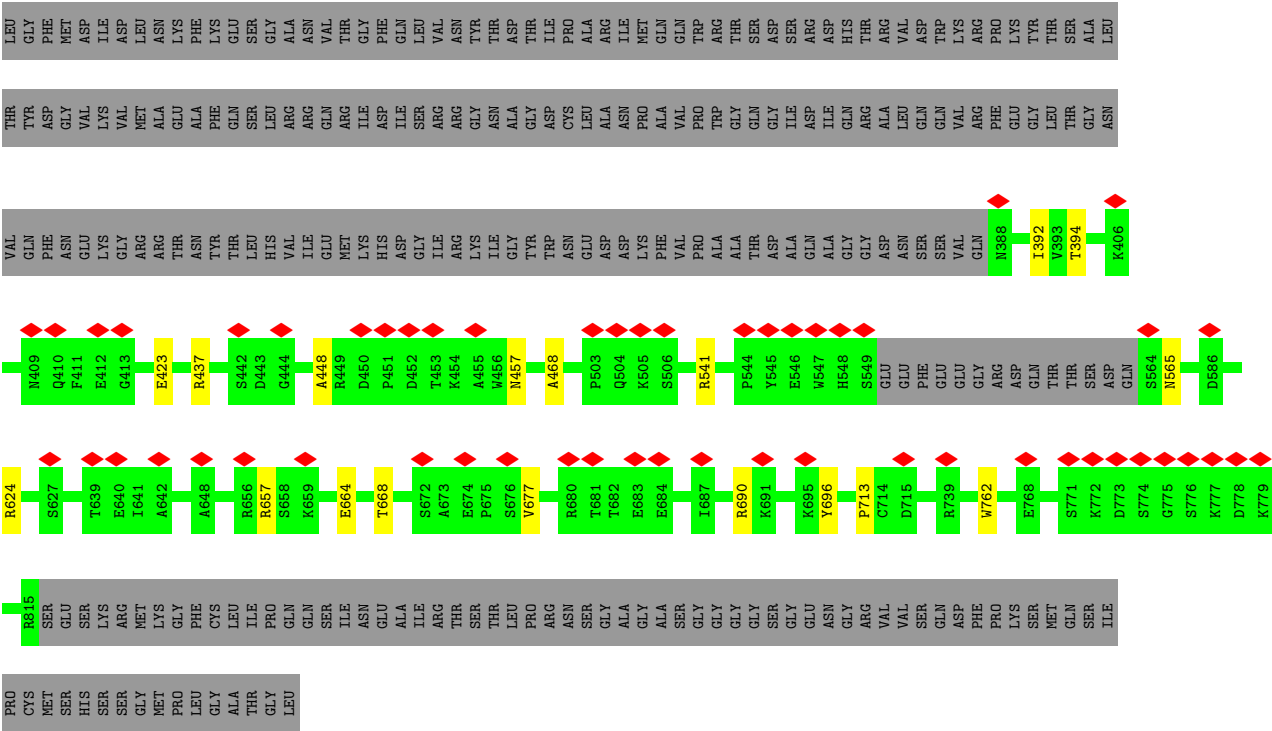
- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



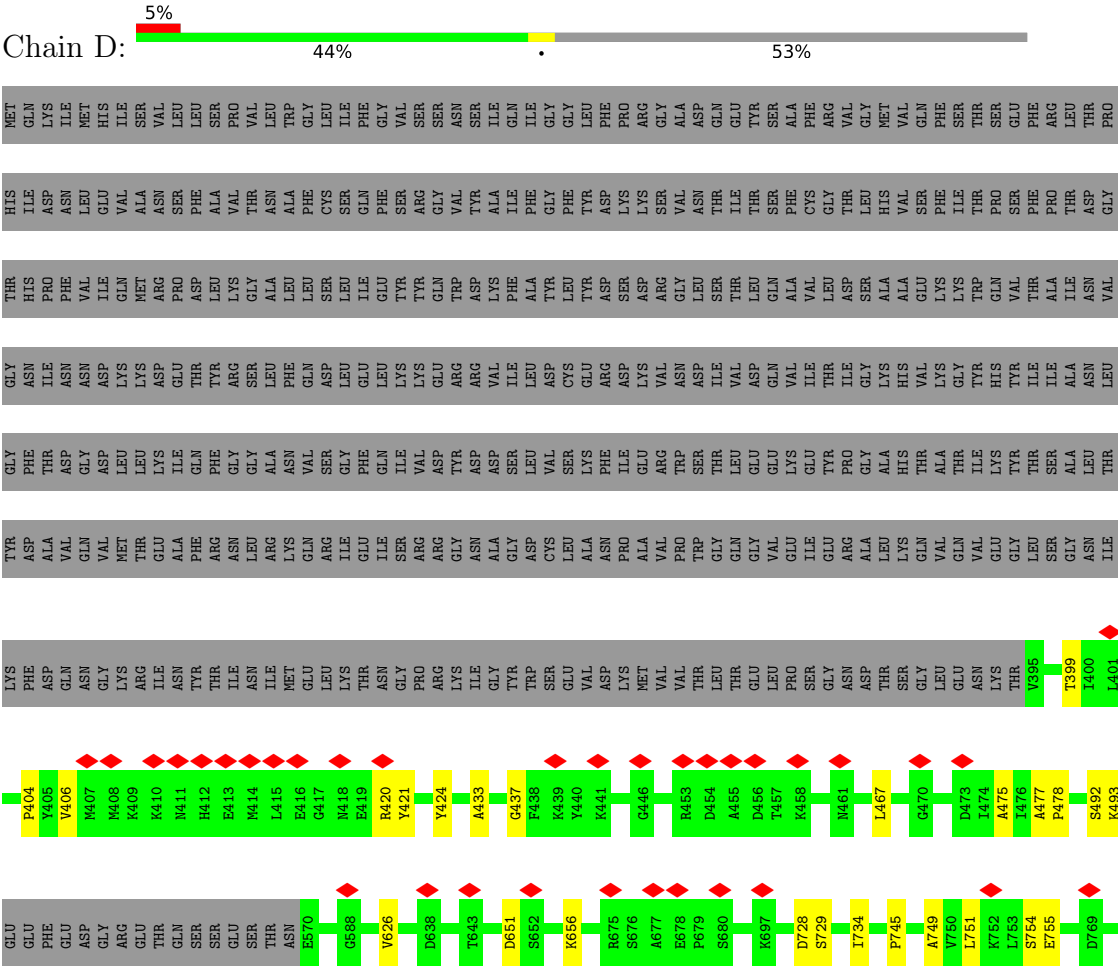
Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C	O	0
			25	21	4	
8	B	1	Total	C	O	0
			25	21	4	

Chain C: 6% 43% 55%





● Molecule 3: Isoform Flip of Glutamate receptor 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	270219	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)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.174	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.024	Depositor
Map size ($\text{\AA}$)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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: POV, XVD, OLC, PLM, ZK1

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	I	0.23	0/1384	0.40	0/1883
1	J	0.23	0/1384	0.40	0/1883
2	A	0.24	0/3240	0.38	0/4389
2	C	0.25	0/3240	0.39	0/4389
3	B	0.23	0/3170	0.37	0/4284
3	D	0.23	0/3170	0.37	0/4284
All	All	0.24	0/15588	0.38	0/21112

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1358	0	1347	4	0
1	J	1358	0	1347	4	0
2	A	3168	0	3115	10	0
2	C	3168	0	3115	10	0
3	B	3103	0	3099	16	0
3	D	3103	0	3099	14	0
4	I	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	22	0	0	0	0
5	A	66	0	106	0	0
5	B	36	0	62	0	0
5	C	66	0	106	0	0
5	D	36	0	62	0	0
5	I	18	0	31	0	0
5	J	18	0	31	0	0
6	A	27	0	13	0	0
6	B	27	0	13	0	0
6	C	27	0	13	0	0
6	D	27	0	13	0	0
7	A	93	0	136	0	0
7	B	38	0	48	0	0
7	C	93	0	136	0	0
7	D	38	0	48	0	0
8	B	25	0	40	0	0
8	D	25	0	40	0	0
All	All	15962	0	16020	52	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 2.

All (52) 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:I:37:ILE:O	1:I:41:THR:OG1	2.08	0.71
2:C:448:ALA:N	2:C:457:ASN:OD1	2.23	0.71
2:A:448:ALA:N	2:A:457:ASN:OD1	2.23	0.70
3:D:420:ARG:NH1	3:D:421:TYR:OH	2.27	0.67
3:B:420:ARG:NH1	3:B:421:TYR:OH	2.27	0.67
1:J:37:ILE:O	1:J:41:THR:OG1	2.07	0.67
2:C:690:ARG:NH2	2:C:713:PRO:O	2.27	0.66
2:A:690:ARG:NH2	2:A:713:PRO:O	2.28	0.66
3:B:626:VAL:O	2:A:624:ARG:NH1	2.30	0.65
2:C:624:ARG:NH1	3:D:626:VAL:O	2.30	0.64
3:D:651:ASP:OD1	3:D:656:LYS:NZ	2.33	0.62
3:B:651:ASP:OD1	3:B:656:LYS:NZ	2.33	0.62
3:B:467:LEU:HD11	3:B:475:ALA:HB2	1.84	0.59
2:C:657:ARG:NH1	3:D:755:GLU:O	2.35	0.58
3:B:755:GLU:O	2:A:657:ARG:NH1	2.34	0.58
3:D:467:LEU:HD11	3:D:475:ALA:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:399:THR:HG21	3:D:406:VAL:HG21	1.86	0.57
2:C:677:VAL:O	2:C:696:TYR:OH	2.21	0.56
3:B:399:THR:HG21	3:B:406:VAL:HG21	1.87	0.55
2:A:394:THR:HG21	2:A:468:ALA:HB2	1.89	0.54
1:J:83:HIS:ND1	1:J:83:HIS:O	2.40	0.54
1:I:83:HIS:O	1:I:83:HIS:ND1	2.40	0.54
1:J:84:SER:OG	1:J:85:GLY:N	2.41	0.53
2:C:394:THR:HG21	2:C:468:ALA:HB2	1.89	0.53
3:D:492:SER:OG	3:D:493:LYS:N	2.42	0.53
3:B:492:SER:OG	3:B:493:LYS:N	2.42	0.52
2:A:677:VAL:O	2:A:696:TYR:OH	2.21	0.52
3:D:751:LEU:O	3:D:754:SER:N	2.44	0.50
3:B:708:MET:HA	3:B:708:MET:HE2	1.93	0.49
1:I:84:SER:OG	1:I:85:GLY:N	2.41	0.48
2:C:603:PHE:HD1	3:B:585:MET:HE1	1.79	0.48
3:D:728:ASP:OD2	3:D:729:SER:N	2.47	0.47
3:B:492:SER:N	3:B:734:ILE:O	2.47	0.46
3:B:728:ASP:OD2	3:B:729:SER:N	2.47	0.46
3:B:404:PRO:O	3:B:424:TYR:N	2.44	0.45
3:D:492:SER:N	3:D:734:ILE:O	2.47	0.45
1:I:44:TRP:O	1:I:202:GLY:N	2.45	0.43
2:C:392:ILE:HD12	2:C:437:ARG:NH2	2.33	0.43
2:A:392:ILE:HD12	2:A:437:ARG:NH2	2.34	0.43
3:B:745:PRO:O	3:B:749:ALA:N	2.52	0.43
3:D:404:PRO:O	3:D:424:TYR:N	2.44	0.43
2:A:541:ARG:NH2	2:A:565:ASN:O	2.50	0.43
3:D:745:PRO:O	3:D:749:ALA:N	2.52	0.42
2:C:606:LEU:HD11	3:B:613:ILE:HD12	2.00	0.42
3:B:433:ALA:O	3:B:437:GLY:N	2.47	0.42
3:D:477:ALA:HB1	3:D:478:PRO:HD2	2.00	0.42
3:B:477:ALA:HB1	3:B:478:PRO:HD2	2.00	0.42
2:A:664:GLU:O	2:A:668:THR:HG23	2.20	0.42
2:C:664:GLU:O	2:C:668:THR:HG23	2.20	0.41
1:J:44:TRP:O	1:J:202:GLY:N	2.45	0.41
2:A:423:GLU:OE1	2:A:762:TRP:NE1	2.53	0.41
3:D:433:ALA:O	3:D:437:GLY:N	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	179/423 (42%)	175 (98%)	4 (2%)	0	100	100
1	J	179/423 (42%)	175 (98%)	4 (2%)	0	100	100
2	A	410/915 (45%)	395 (96%)	15 (4%)	0	100	100
2	C	410/915 (45%)	396 (97%)	14 (3%)	0	100	100
3	B	401/860 (47%)	395 (98%)	6 (2%)	0	100	100
3	D	401/860 (47%)	394 (98%)	7 (2%)	0	100	100
All	All	1980/4396 (45%)	1930 (98%)	50 (2%)	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	I	132/309 (43%)	131 (99%)	1 (1%)	73	79
1	J	132/309 (43%)	131 (99%)	1 (1%)	73	79
2	A	326/778 (42%)	326 (100%)	0	100	100
2	C	326/778 (42%)	326 (100%)	0	100	100
3	B	321/737 (44%)	321 (100%)	0	100	100
3	D	326/737 (44%)	326 (100%)	0	100	100
All	All	1563/3648 (43%)	1561 (100%)	2 (0%)	87	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	154	LYS
1	J	154	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	198	HIS
2	C	582	GLN
2	A	582	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 ⓘ

28 ligands are modelled in this entry.

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	$\# Z > 2$
5	PLM	D	904	-	17,17,17	0.60	0	17,17,17	0.99	0
5	PLM	J	1701	-	17,17,17	0.60	0	17,17,17	0.96	0
7	POV	A	905	-	47,47,51	1.13	3 (6%)	53,55,59	1.26	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PLM	C	904	-	17,17,17	0.59	0	17,17,17	1.02	1 (5%)
5	PLM	A	907	-	17,17,17	0.59	0	17,17,17	0.99	0
6	ZK1	B	901	-	29,29,29	2.26	10 (34%)	45,45,45	4.63	11 (24%)
5	PLM	B	903	-	17,17,17	0.61	0	17,17,17	1.07	1 (5%)
5	PLM	I	502	-	17,17,17	0.60	0	17,17,17	0.95	0
7	POV	C	905	-	47,47,51	1.13	3 (6%)	53,55,59	1.26	3 (5%)
7	POV	B	905	-	37,37,51	1.21	3 (8%)	43,45,59	1.14	3 (6%)
6	ZK1	A	901	-	29,29,29	2.24	10 (34%)	45,45,45	4.54	12 (26%)
5	PLM	A	904	-	17,17,17	0.60	0	17,17,17	1.03	1 (5%)
6	ZK1	C	901	-	29,29,29	2.24	10 (34%)	45,45,45	4.55	12 (26%)
8	OLC	D	902	-	24,24,24	0.82	2 (8%)	25,25,25	0.95	1 (4%)
7	POV	A	902	-	44,44,51	1.16	3 (6%)	50,52,59	1.20	3 (6%)
6	ZK1	D	901	-	29,29,29	2.25	10 (34%)	45,45,45	4.61	11 (24%)
5	PLM	C	903	-	15,15,17	0.63	0	15,15,17	0.97	0
4	XVD	I	501	-	22,24,24	2.02	6 (27%)	32,36,36	2.01	7 (21%)
5	PLM	D	903	-	17,17,17	0.60	0	17,17,17	1.07	1 (5%)
5	PLM	B	904	-	17,17,17	0.60	0	17,17,17	1.00	0
7	POV	C	902	-	44,44,51	1.16	3 (6%)	50,52,59	1.20	3 (6%)
8	OLC	B	902	-	24,24,24	0.82	2 (8%)	25,25,25	0.95	1 (4%)
5	PLM	A	903	-	15,15,17	0.63	0	15,15,17	0.98	1 (6%)
5	PLM	A	906	-	13,13,17	0.67	0	13,13,17	1.01	0
5	PLM	C	906	-	13,13,17	0.67	0	13,13,17	1.02	0
5	PLM	C	907	-	17,17,17	0.59	0	17,17,17	0.99	0
7	POV	D	905	-	37,37,51	1.21	3 (8%)	43,45,59	1.14	3 (6%)
4	XVD	J	1702	-	22,24,24	2.02	5 (22%)	32,36,36	2.00	7 (21%)

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
5	PLM	D	904	-	-	8/15/15/15	-
5	PLM	J	1701	-	-	8/15/15/15	-
7	POV	A	905	-	-	26/51/51/55	-
5	PLM	C	904	-	-	9/15/15/15	-
5	PLM	A	907	-	-	6/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ZK1	B	901	-	-	6/13/23/23	0/3/3/3
5	PLM	B	903	-	-	3/15/15/15	-
5	PLM	I	502	-	-	8/15/15/15	-
7	POV	C	905	-	-	25/51/51/55	-
7	POV	B	905	-	-	14/41/41/55	-
6	ZK1	A	901	-	-	6/13/23/23	0/3/3/3
5	PLM	A	904	-	-	9/15/15/15	-
6	ZK1	C	901	-	-	6/13/23/23	0/3/3/3
8	OLC	D	902	-	-	6/24/24/24	-
7	POV	A	902	-	-	22/48/48/55	-
6	ZK1	D	901	-	-	6/13/23/23	0/3/3/3
5	PLM	C	903	-	-	8/13/13/15	-
4	XVD	I	501	-	-	3/9/9/9	0/3/3/3
5	PLM	D	903	-	-	3/15/15/15	-
5	PLM	B	904	-	-	8/15/15/15	-
7	POV	C	902	-	-	22/48/48/55	-
8	OLC	B	902	-	-	6/24/24/24	-
5	PLM	A	903	-	-	8/13/13/15	-
5	PLM	A	906	-	-	9/11/11/15	-
5	PLM	C	906	-	-	9/11/11/15	-
5	PLM	C	907	-	-	6/15/15/15	-
7	POV	D	905	-	-	14/41/41/55	-
4	XVD	J	1702	-	-	3/9/9/9	0/3/3/3

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	501	XVD	C9-C10	6.96	1.49	1.40
4	J	1702	XVD	C9-C10	6.93	1.49	1.40
6	B	901	ZK1	CAW-NAY	5.64	1.50	1.41
6	D	901	ZK1	CAW-NAY	5.55	1.50	1.41
6	B	901	ZK1	CAV-NAP	5.32	1.48	1.39
6	C	901	ZK1	CAW-NAY	5.30	1.50	1.41
6	A	901	ZK1	CAV-NAP	5.29	1.48	1.39
6	D	901	ZK1	CAV-NAP	5.28	1.48	1.39
6	A	901	ZK1	CAW-NAY	5.25	1.50	1.41
6	C	901	ZK1	CAV-NAP	5.20	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	901	ZK1	CAT-NAP	5.00	1.42	1.35
6	D	901	ZK1	CAT-NAP	4.99	1.42	1.35
6	B	901	ZK1	CAT-NAP	4.99	1.42	1.35
6	A	901	ZK1	CAT-NAP	4.90	1.42	1.35
6	A	901	ZK1	CAU-NAY	3.38	1.44	1.38
6	C	901	ZK1	CAU-NAY	3.38	1.44	1.38
6	C	901	ZK1	CAU-CAT	-3.24	1.48	1.53
6	A	901	ZK1	CAU-CAT	-3.24	1.48	1.53
6	B	901	ZK1	CAU-NAY	3.13	1.43	1.38
6	D	901	ZK1	CAU-NAY	3.12	1.43	1.38
6	B	901	ZK1	CAU-CAT	-3.12	1.48	1.53
6	D	901	ZK1	CAU-CAT	-3.08	1.48	1.53
7	C	902	POV	O21-C21	2.83	1.42	1.34
7	A	902	POV	O21-C21	2.83	1.42	1.34
7	B	905	POV	O21-C21	2.82	1.42	1.34
7	A	902	POV	O31-C31	2.80	1.41	1.33
7	B	905	POV	O31-C31	2.79	1.41	1.33
7	C	905	POV	O21-C21	2.78	1.42	1.34
7	D	905	POV	O31-C31	2.78	1.41	1.33
7	C	902	POV	O31-C31	2.75	1.41	1.33
7	A	905	POV	O21-C21	2.74	1.42	1.34
7	D	905	POV	O21-C21	2.74	1.42	1.34
7	C	905	POV	O31-C31	2.73	1.41	1.33
7	A	905	POV	O31-C31	2.71	1.41	1.33
6	A	901	ZK1	CAM-NAX	-2.67	1.42	1.46
6	C	901	ZK1	CAM-NAX	-2.63	1.42	1.46
4	J	1702	XVD	C11-C10	-2.61	1.35	1.40
6	D	901	ZK1	OAA-CAT	-2.61	1.18	1.23
4	I	501	XVD	C11-C10	-2.59	1.35	1.40
6	A	901	ZK1	CAN-NAX	-2.59	1.42	1.46
6	C	901	ZK1	OAA-CAT	-2.58	1.18	1.23
6	D	901	ZK1	CAM-NAX	-2.58	1.42	1.46
6	C	901	ZK1	CAN-NAX	-2.58	1.42	1.46
6	B	901	ZK1	CAM-NAX	-2.56	1.42	1.46
6	A	901	ZK1	OAA-CAT	-2.53	1.18	1.23
6	B	901	ZK1	OAA-CAT	-2.52	1.18	1.23
6	B	901	ZK1	CAN-NAX	-2.47	1.42	1.46
6	D	901	ZK1	CAN-NAX	-2.42	1.42	1.46
8	B	902	OLC	O20-C1	2.41	1.40	1.33
7	D	905	POV	O21-C2	-2.39	1.41	1.46
4	I	501	XVD	C12-C7	2.39	1.44	1.39
8	D	902	OLC	O20-C1	2.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1702	XVD	C12-C7	2.36	1.44	1.39
7	B	905	POV	O21-C2	-2.33	1.41	1.46
4	J	1702	XVD	C8-C9	-2.26	1.36	1.39
7	C	902	POV	O21-C2	-2.26	1.41	1.46
7	A	902	POV	O21-C2	-2.25	1.41	1.46
8	B	902	OLC	O20-C21	-2.23	1.40	1.45
6	D	901	ZK1	OAB-CAU	-2.22	1.18	1.23
4	I	501	XVD	C8-C9	-2.20	1.36	1.39
6	B	901	ZK1	OAB-CAU	-2.20	1.18	1.23
8	D	902	OLC	O20-C21	-2.17	1.40	1.45
6	C	901	ZK1	OAB-CAU	-2.16	1.18	1.23
6	A	901	ZK1	OAB-CAU	-2.15	1.18	1.23
6	A	901	ZK1	PBA-CAO	2.12	1.86	1.81
6	B	901	ZK1	PBA-CAO	2.12	1.86	1.81
6	D	901	ZK1	PBA-CAO	2.10	1.86	1.81
7	C	905	POV	O21-C2	-2.10	1.41	1.46
7	A	905	POV	O21-C2	-2.10	1.41	1.46
6	C	901	ZK1	PBA-CAO	2.09	1.86	1.81
4	J	1702	XVD	C1-CL1	2.05	1.78	1.73
4	I	501	XVD	C1-CL1	2.04	1.78	1.73
4	I	501	XVD	C10-N1	-2.03	1.35	1.39

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	901	ZK1	CAS-CAR-NAX	18.09	140.65	119.92
6	B	901	ZK1	CAS-CAR-NAX	18.07	140.63	119.92
6	C	901	ZK1	CAS-CAR-NAX	17.33	139.78	119.92
6	A	901	ZK1	CAS-CAR-NAX	17.28	139.72	119.92
6	B	901	ZK1	CAI-CAR-NAX	-16.22	98.95	122.59
6	D	901	ZK1	CAI-CAR-NAX	-16.19	99.00	122.59
6	C	901	ZK1	CAI-CAR-NAX	-15.59	99.88	122.59
6	A	901	ZK1	CAI-CAR-NAX	-15.57	99.91	122.59
6	B	901	ZK1	CAZ-CAS-CAR	15.55	141.97	122.06
6	D	901	ZK1	CAZ-CAS-CAR	15.33	141.70	122.06
6	A	901	ZK1	CAZ-CAS-CAR	15.26	141.61	122.06
6	C	901	ZK1	CAZ-CAS-CAR	15.25	141.59	122.06
6	B	901	ZK1	CAJ-CAS-CAZ	-7.26	99.01	116.60
6	A	901	ZK1	CAJ-CAS-CAZ	-7.24	99.06	116.60
6	C	901	ZK1	CAJ-CAS-CAZ	-7.24	99.07	116.60
6	D	901	ZK1	CAJ-CAS-CAZ	-7.21	99.14	116.60
7	A	905	POV	C37-C36-C35	5.63	142.83	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	905	POV	C37-C36-C35	5.63	142.82	114.37
7	A	902	POV	C37-C36-C35	5.47	142.04	114.37
7	C	902	POV	C37-C36-C35	5.47	142.00	114.37
4	I	501	XVD	C10-N1-C13	5.41	114.86	104.13
4	J	1702	XVD	C10-N1-C13	5.37	114.77	104.13
4	I	501	XVD	C9-C10-N1	-4.98	102.59	109.42
4	J	1702	XVD	C9-C10-N1	-4.97	102.62	109.42
4	J	1702	XVD	C9-N2-C13	4.95	114.69	107.63
4	I	501	XVD	C9-N2-C13	4.94	114.68	107.63
7	D	905	POV	C37-C36-C35	4.21	141.82	113.36
7	B	905	POV	C37-C36-C35	4.21	141.82	113.36
6	A	901	ZK1	CAM-NAX-CAR	-3.88	106.97	116.19
6	C	901	ZK1	CAM-NAX-CAR	-3.88	106.98	116.19
7	C	902	POV	O21-C21-C22	3.80	119.71	111.48
7	A	902	POV	O21-C21-C22	3.78	119.67	111.48
7	A	905	POV	O21-C21-C22	3.75	119.59	111.48
7	C	905	POV	O21-C21-C22	3.74	119.57	111.48
7	D	905	POV	O21-C21-C22	3.47	118.99	111.48
7	B	905	POV	O21-C21-C22	3.43	118.90	111.48
6	B	901	ZK1	CAV-NAP-CAT	-3.40	120.06	124.82
6	A	901	ZK1	CAV-NAP-CAT	-3.34	120.14	124.82
6	D	901	ZK1	CAV-NAP-CAT	-3.34	120.15	124.82
6	B	901	ZK1	CAO-NAY-CAW	3.32	124.16	120.12
6	D	901	ZK1	CAO-NAY-CAW	3.31	124.14	120.12
6	C	901	ZK1	CAV-NAP-CAT	-3.30	120.21	124.82
4	J	1702	XVD	C8-C9-N2	3.23	137.27	130.65
4	I	501	XVD	C8-C9-N2	3.22	137.24	130.65
4	I	501	XVD	C11-C10-N1	3.20	137.30	128.21
4	J	1702	XVD	C11-C10-N1	3.17	137.21	128.21
6	B	901	ZK1	CAW-NAY-CAU	-3.00	119.14	122.84
6	A	901	ZK1	CAO-NAY-CAU	2.93	119.53	116.55
6	D	901	ZK1	CAW-NAY-CAU	-2.90	119.27	122.84
6	C	901	ZK1	CAO-NAY-CAU	2.89	119.50	116.55
6	C	901	ZK1	CAW-NAY-CAU	-2.80	119.39	122.84
6	B	901	ZK1	CAT-CAU-NAY	2.80	120.45	117.41
6	A	901	ZK1	CAW-NAY-CAU	-2.78	119.42	122.84
8	B	902	OLC	O20-C1-C2	2.74	120.19	111.83
6	D	901	ZK1	CAT-CAU-NAY	2.72	120.36	117.41
8	D	902	OLC	O20-C1-C2	2.72	120.12	111.83
6	A	901	ZK1	CAN-NAX-CAR	-2.71	109.74	116.19
6	D	901	ZK1	FAF-CAZ-CAS	-2.70	107.86	112.65
7	A	905	POV	O31-C31-C32	2.69	120.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	905	POV	O31-C31-C32	2.68	120.00	111.83
6	C	901	ZK1	CAN-NAX-CAR	-2.67	109.84	116.19
7	B	905	POV	O31-C31-C32	2.64	119.88	111.83
7	D	905	POV	O31-C31-C32	2.64	119.88	111.83
6	B	901	ZK1	FAF-CAZ-CAS	-2.50	108.22	112.65
6	C	901	ZK1	CAT-CAU-NAY	2.44	120.06	117.41
6	C	901	ZK1	FAG-CAZ-CAS	-2.41	108.37	112.65
6	A	901	ZK1	CAT-CAU-NAY	2.41	120.03	117.41
4	J	1702	XVD	C10-C9-N2	-2.40	102.82	105.71
4	I	501	XVD	C10-C9-N2	-2.40	102.82	105.71
7	A	902	POV	O31-C31-C32	2.38	119.09	111.83
7	C	902	POV	O31-C31-C32	2.37	119.06	111.83
6	A	901	ZK1	FAG-CAZ-CAS	-2.37	108.45	112.65
5	B	903	PLM	O1-C1-C2	2.29	121.25	114.00
5	D	903	PLM	O1-C1-C2	2.28	121.20	114.00
6	A	901	ZK1	CAU-CAT-NAP	2.26	119.77	117.46
4	I	501	XVD	C7-C6-C5	-2.24	117.63	120.73
4	J	1702	XVD	C7-C6-C5	-2.22	117.66	120.73
6	B	901	ZK1	CAU-CAT-NAP	2.20	119.70	117.46
6	C	901	ZK1	CAU-CAT-NAP	2.19	119.70	117.46
6	D	901	ZK1	CAU-CAT-NAP	2.13	119.63	117.46
6	D	901	ZK1	CAN-NAX-CAR	-2.08	111.24	116.19
6	B	901	ZK1	CAN-NAX-CAR	-2.08	111.25	116.19
5	A	904	PLM	O1-C1-C2	2.03	120.41	114.00
5	C	904	PLM	O1-C1-C2	2.01	120.37	114.00
5	A	903	PLM	O1-C1-C2	2.01	120.36	114.00

There are no chirality outliers.

All (267) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	902	POV	C2-C1-O11-P
7	C	902	POV	O12-C11-C12-N
7	C	902	POV	C12-C11-O12-P
7	C	905	POV	C11-O12-P-O14
7	C	905	POV	C2-C1-O11-P
7	C	905	POV	O12-C11-C12-N
7	D	905	POV	C11-O12-P-O11
7	D	905	POV	O12-C11-C12-N
7	B	905	POV	C11-O12-P-O11
7	B	905	POV	O12-C11-C12-N
7	A	902	POV	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
7	A	902	POV	O12-C11-C12-N
7	A	902	POV	C12-C11-O12-P
7	A	905	POV	C11-O12-P-O14
7	A	905	POV	C2-C1-O11-P
7	A	905	POV	O12-C11-C12-N
7	C	905	POV	C32-C31-O31-C3
7	A	905	POV	C32-C31-O31-C3
7	C	905	POV	O32-C31-O31-C3
7	D	905	POV	O32-C31-O31-C3
7	B	905	POV	O32-C31-O31-C3
7	A	905	POV	O32-C31-O31-C3
7	D	905	POV	C32-C31-O31-C3
7	B	905	POV	C32-C31-O31-C3
4	I	501	XVD	F2-C14-O2-C5
4	J	1702	XVD	F2-C14-O2-C5
5	C	904	PLM	C1-C2-C3-C4
5	D	903	PLM	C1-C2-C3-C4
5	A	904	PLM	C1-C2-C3-C4
7	C	905	POV	C31-C32-C33-C34
7	A	905	POV	C31-C32-C33-C34
5	C	906	PLM	C1-C2-C3-C4
5	B	903	PLM	C1-C2-C3-C4
5	A	906	PLM	C1-C2-C3-C4
6	D	901	ZK1	CAR-CAS-CAZ-FAF
6	B	901	ZK1	CAR-CAS-CAZ-FAF
5	D	904	PLM	C1-C2-C3-C4
5	B	904	PLM	C1-C2-C3-C4
6	C	901	ZK1	CAR-CAS-CAZ-FAG
6	A	901	ZK1	CAR-CAS-CAZ-FAG
7	C	905	POV	C22-C21-O21-C2
7	A	905	POV	C22-C21-O21-C2
7	C	905	POV	O22-C21-O21-C2
7	A	905	POV	O22-C21-O21-C2
6	C	901	ZK1	CAR-CAS-CAZ-FAF
6	C	901	ZK1	CAR-CAS-CAZ-FAH
6	D	901	ZK1	CAR-CAS-CAZ-FAG
6	B	901	ZK1	CAR-CAS-CAZ-FAG
6	A	901	ZK1	CAR-CAS-CAZ-FAF
6	A	901	ZK1	CAR-CAS-CAZ-FAH
7	A	905	POV	C22-C23-C24-C25
7	C	905	POV	C22-C23-C24-C25
5	C	903	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	C	907	PLM	CA-CB-CC-CD
5	D	904	PLM	C4-C5-C6-C7
5	D	904	PLM	C8-C9-CA-CB
5	B	904	PLM	C4-C5-C6-C7
5	B	904	PLM	C8-C9-CA-CB
5	A	903	PLM	C2-C3-C4-C5
5	A	907	PLM	CA-CB-CC-CD
7	C	905	POV	C36-C37-C38-C39
7	A	905	POV	C36-C37-C38-C39
5	C	903	PLM	C4-C5-C6-C7
5	A	903	PLM	C4-C5-C6-C7
6	D	901	ZK1	CAR-CAS-CAZ-FAH
6	B	901	ZK1	CAR-CAS-CAZ-FAH
5	C	904	PLM	CC-CD-CE-CF
7	D	905	POV	C23-C24-C25-C26
5	A	904	PLM	CC-CD-CE-CF
7	B	905	POV	C23-C24-C25-C26
8	D	902	OLC	C11-C12-C13-C14
8	B	902	OLC	C11-C12-C13-C14
7	C	905	POV	C37-C38-C39-C310
7	A	905	POV	C37-C38-C39-C310
5	C	906	PLM	C7-C8-C9-CA
8	D	902	OLC	C5-C6-C7-C8
8	B	902	OLC	C5-C6-C7-C8
5	A	906	PLM	C7-C8-C9-CA
7	C	905	POV	C312-C313-C314-C315
7	A	905	POV	C312-C313-C314-C315
8	D	902	OLC	C4-C5-C6-C7
8	B	902	OLC	C4-C5-C6-C7
5	A	903	PLM	C7-C8-C9-CA
5	C	903	PLM	C7-C8-C9-CA
7	D	905	POV	C25-C26-C27-C28
7	B	905	POV	C25-C26-C27-C28
7	D	905	POV	C34-C35-C36-C37
7	B	905	POV	C34-C35-C36-C37
7	D	905	POV	C24-C25-C26-C27
7	B	905	POV	C24-C25-C26-C27
4	I	501	XVD	F1-C14-O2-C5
4	J	1702	XVD	F1-C14-O2-C5
7	C	902	POV	C26-C27-C28-C29
7	A	902	POV	C26-C27-C28-C29
5	D	904	PLM	CC-CD-CE-CF

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Mol	Chain	Res	Type	Atoms
5	B	904	PLM	CC-CD-CE-CF
5	C	904	PLM	C4-C5-C6-C7
5	A	904	PLM	C4-C5-C6-C7
7	C	905	POV	C24-C25-C26-C27
7	C	902	POV	C214-C215-C216-C217
7	A	902	POV	C214-C215-C216-C217
7	A	905	POV	C24-C25-C26-C27
7	C	905	POV	C310-C311-C312-C313
7	A	905	POV	C310-C311-C312-C313
7	A	905	POV	C34-C35-C36-C37
7	C	905	POV	O11-C1-C2-C3
7	A	905	POV	O11-C1-C2-C3
7	C	905	POV	C34-C35-C36-C37
7	B	905	POV	C32-C33-C34-C35
7	C	902	POV	C22-C21-O21-C2
7	A	902	POV	C22-C21-O21-C2
7	C	902	POV	C32-C33-C34-C35
7	D	905	POV	C32-C33-C34-C35
7	A	902	POV	C32-C33-C34-C35
7	C	902	POV	C32-C31-O31-C3
7	A	902	POV	C32-C31-O31-C3
5	D	904	PLM	C9-CA-CB-CC
5	B	904	PLM	C9-CA-CB-CC
4	J	1702	XVD	F3-C14-O2-C5
5	I	502	PLM	C7-C8-C9-CA
5	C	907	PLM	C8-C9-CA-CB
5	A	907	PLM	C8-C9-CA-CB
5	J	1701	PLM	C7-C8-C9-CA
5	J	1701	PLM	CB-CC-CD-CE
5	I	502	PLM	CB-CC-CD-CE
4	I	501	XVD	F3-C14-O2-C5
7	C	902	POV	O32-C31-O31-C3
7	A	902	POV	O32-C31-O31-C3
7	D	905	POV	O21-C2-C3-O31
5	D	904	PLM	C6-C7-C8-C9
5	B	904	PLM	C6-C7-C8-C9
8	D	902	OLC	C6-C7-C8-C9
8	B	902	OLC	C6-C7-C8-C9
7	C	905	POV	C33-C34-C35-C36
7	A	905	POV	C33-C34-C35-C36
5	A	906	PLM	C3-C4-C5-C6
6	B	901	ZK1	CAJ-CAS-CAZ-FAF

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Mol	Chain	Res	Type	Atoms
5	C	906	PLM	C3-C4-C5-C6
6	D	901	ZK1	CAJ-CAS-CAZ-FAF
5	A	904	PLM	CB-CC-CD-CE
5	C	904	PLM	CB-CC-CD-CE
7	D	905	POV	C1-C2-C3-O31
7	B	905	POV	C1-C2-C3-O31
5	A	907	PLM	C5-C6-C7-C8
5	C	907	PLM	C5-C6-C7-C8
7	C	905	POV	C26-C27-C28-C29
7	A	905	POV	C26-C27-C28-C29
5	C	906	PLM	C5-C6-C7-C8
6	A	901	ZK1	CAJ-CAS-CAZ-FAG
6	C	901	ZK1	CAJ-CAS-CAZ-FAG
5	A	906	PLM	C5-C6-C7-C8
7	B	905	POV	O21-C2-C3-O31
7	C	902	POV	O22-C21-O21-C2
7	A	902	POV	O22-C21-O21-C2
5	A	903	PLM	CB-CC-CD-CE
5	C	903	PLM	CB-CC-CD-CE
5	I	502	PLM	CC-CD-CE-CF
5	J	1701	PLM	CC-CD-CE-CF
7	C	902	POV	O11-C1-C2-O21
7	A	902	POV	O11-C1-C2-O21
7	A	902	POV	C24-C25-C26-C27
7	C	902	POV	C24-C25-C26-C27
5	J	1701	PLM	C2-C3-C4-C5
5	I	502	PLM	C2-C3-C4-C5
7	C	902	POV	C35-C36-C37-C38
5	A	903	PLM	C6-C7-C8-C9
7	A	902	POV	C35-C36-C37-C38
5	C	903	PLM	C6-C7-C8-C9
7	C	905	POV	O11-C1-C2-O21
7	A	905	POV	O11-C1-C2-O21
5	C	906	PLM	C9-CA-CB-CC
5	A	906	PLM	C9-CA-CB-CC
7	C	905	POV	C1-O11-P-O12
7	C	905	POV	C1-O11-P-O14
7	D	905	POV	C11-O12-P-O14
7	B	905	POV	C11-O12-P-O14
7	A	905	POV	C1-O11-P-O12
7	A	905	POV	C1-O11-P-O14
5	C	907	PLM	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	907	PLM	C3-C4-C5-C6
6	D	901	ZK1	CAJ-CAS-CAZ-FAG
7	C	902	POV	C212-C213-C214-C215
7	C	905	POV	C3-C2-O21-C21
7	A	905	POV	C3-C2-O21-C21
6	B	901	ZK1	CAJ-CAS-CAZ-FAG
7	C	902	POV	O11-C1-C2-C3
7	A	902	POV	O11-C1-C2-C3
7	A	902	POV	C212-C213-C214-C215
6	C	901	ZK1	CAJ-CAS-CAZ-FAH
6	A	901	ZK1	CAJ-CAS-CAZ-FAH
6	D	901	ZK1	CAJ-CAS-CAZ-FAH
6	B	901	ZK1	CAJ-CAS-CAZ-FAH
6	C	901	ZK1	CAJ-CAS-CAZ-FAF
6	A	901	ZK1	CAJ-CAS-CAZ-FAF
5	C	904	PLM	C9-CA-CB-CC
5	A	904	PLM	C9-CA-CB-CC
5	C	906	PLM	O1-C1-C2-C3
5	A	906	PLM	O1-C1-C2-C3
5	C	907	PLM	CD-CE-CF-CG
5	A	907	PLM	CD-CE-CF-CG
7	C	905	POV	C27-C28-C29-C210
7	A	905	POV	C27-C28-C29-C210
5	C	906	PLM	C4-C5-C6-C7
5	C	906	PLM	O2-C1-C2-C3
7	C	905	POV	C25-C26-C27-C28
7	A	905	POV	C25-C26-C27-C28
5	C	904	PLM	C6-C7-C8-C9
5	A	906	PLM	C4-C5-C6-C7
5	A	904	PLM	C6-C7-C8-C9
5	A	906	PLM	O2-C1-C2-C3
8	D	902	OLC	C9-C10-C11-C12
8	B	902	OLC	C9-C10-C11-C12
5	A	904	PLM	O2-C1-C2-C3
5	D	904	PLM	O1-C1-C2-C3
5	B	904	PLM	O1-C1-C2-C3
5	C	904	PLM	O2-C1-C2-C3
7	C	905	POV	C311-C312-C313-C314
7	A	905	POV	C311-C312-C313-C314
5	C	907	PLM	CB-CC-CD-CE
5	A	907	PLM	CB-CC-CD-CE
5	D	904	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	B	904	PLM	O2-C1-C2-C3
5	C	904	PLM	O1-C1-C2-C3
5	A	904	PLM	O1-C1-C2-C3
5	A	903	PLM	C5-C6-C7-C8
5	C	903	PLM	C5-C6-C7-C8
5	I	502	PLM	O1-C1-C2-C3
5	J	1701	PLM	O1-C1-C2-C3
5	I	502	PLM	O2-C1-C2-C3
5	J	1701	PLM	O2-C1-C2-C3
7	B	905	POV	O11-C1-C2-C3
7	D	905	POV	C29-C210-C211-C212
7	B	905	POV	C29-C210-C211-C212
7	C	902	POV	C29-C210-C211-C212
7	A	902	POV	C29-C210-C211-C212
7	C	902	POV	C22-C23-C24-C25
7	A	902	POV	C22-C23-C24-C25
7	D	905	POV	O11-C1-C2-C3
8	D	902	OLC	C14-C15-C16-C17
8	B	902	OLC	C14-C15-C16-C17
5	C	903	PLM	O2-C1-C2-C3
5	A	903	PLM	O2-C1-C2-C3
5	D	903	PLM	C9-CA-CB-CC
5	B	903	PLM	C9-CA-CB-CC
5	C	904	PLM	C7-C8-C9-CA
5	A	904	PLM	C7-C8-C9-CA
5	J	1701	PLM	C5-C6-C7-C8
5	I	502	PLM	C5-C6-C7-C8
7	C	902	POV	O31-C31-C32-C33
7	A	902	POV	O31-C31-C32-C33
7	C	902	POV	C25-C26-C27-C28
7	A	902	POV	C25-C26-C27-C28
5	C	903	PLM	O1-C1-C2-C3
5	A	903	PLM	O1-C1-C2-C3
7	A	902	POV	O21-C21-C22-C23
5	J	1701	PLM	C4-C5-C6-C7
7	A	902	POV	C23-C24-C25-C26
7	C	902	POV	C23-C24-C25-C26
7	C	902	POV	O21-C21-C22-C23
5	I	502	PLM	C4-C5-C6-C7
5	C	906	PLM	C6-C7-C8-C9
5	A	906	PLM	C6-C7-C8-C9
5	B	903	PLM	O2-C1-C2-C3

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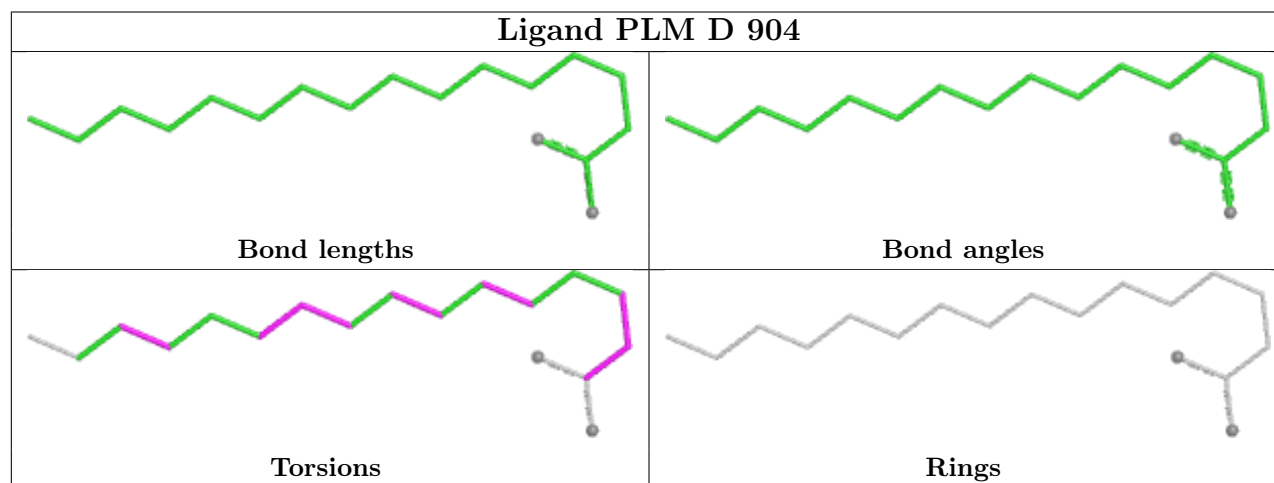
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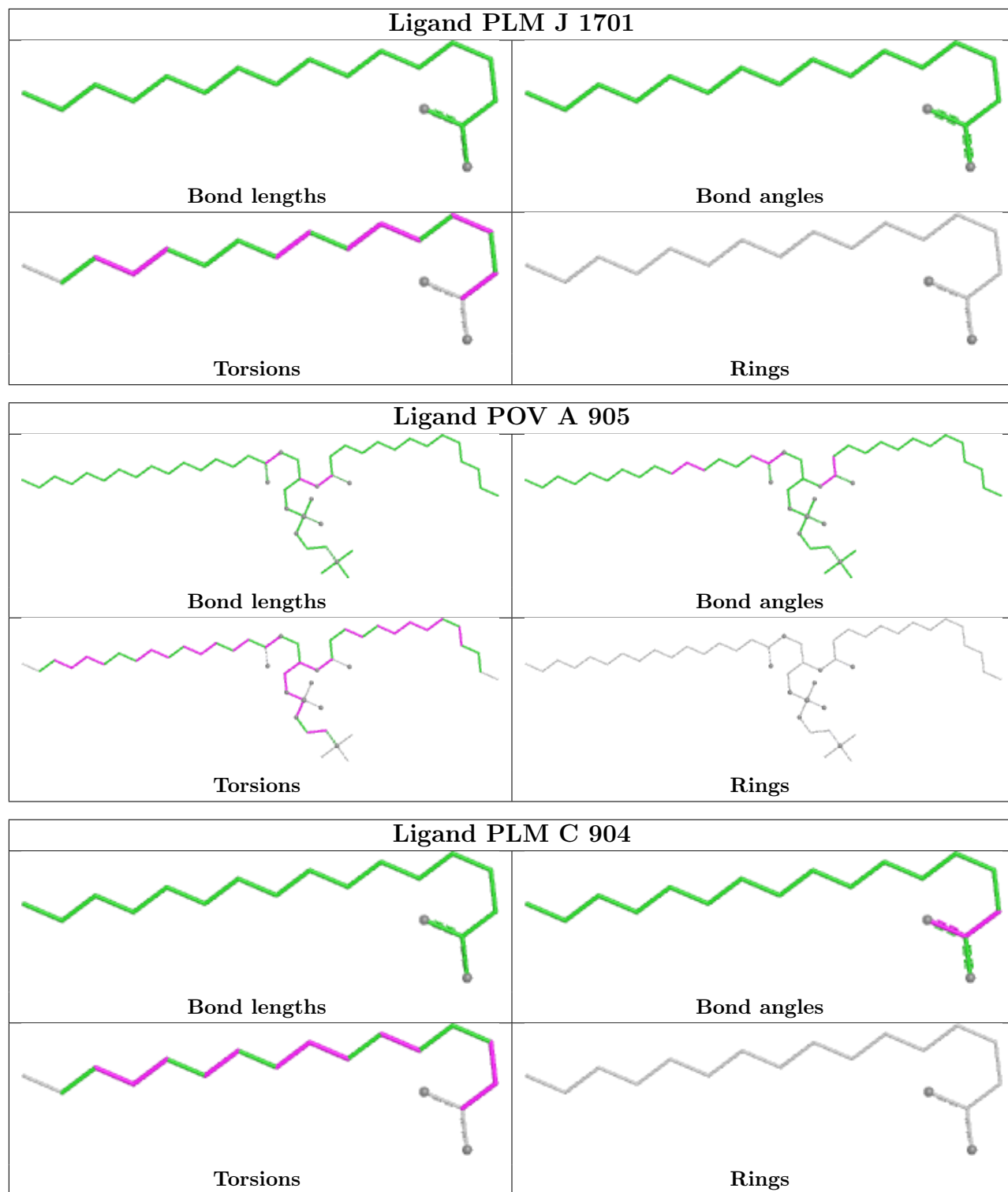
Mol	Chain	Res	Type	Atoms
7	C	902	POV	O32-C31-C32-C33
7	A	902	POV	O32-C31-C32-C33
5	D	903	PLM	O2-C1-C2-C3
7	A	905	POV	C29-C210-C211-C212

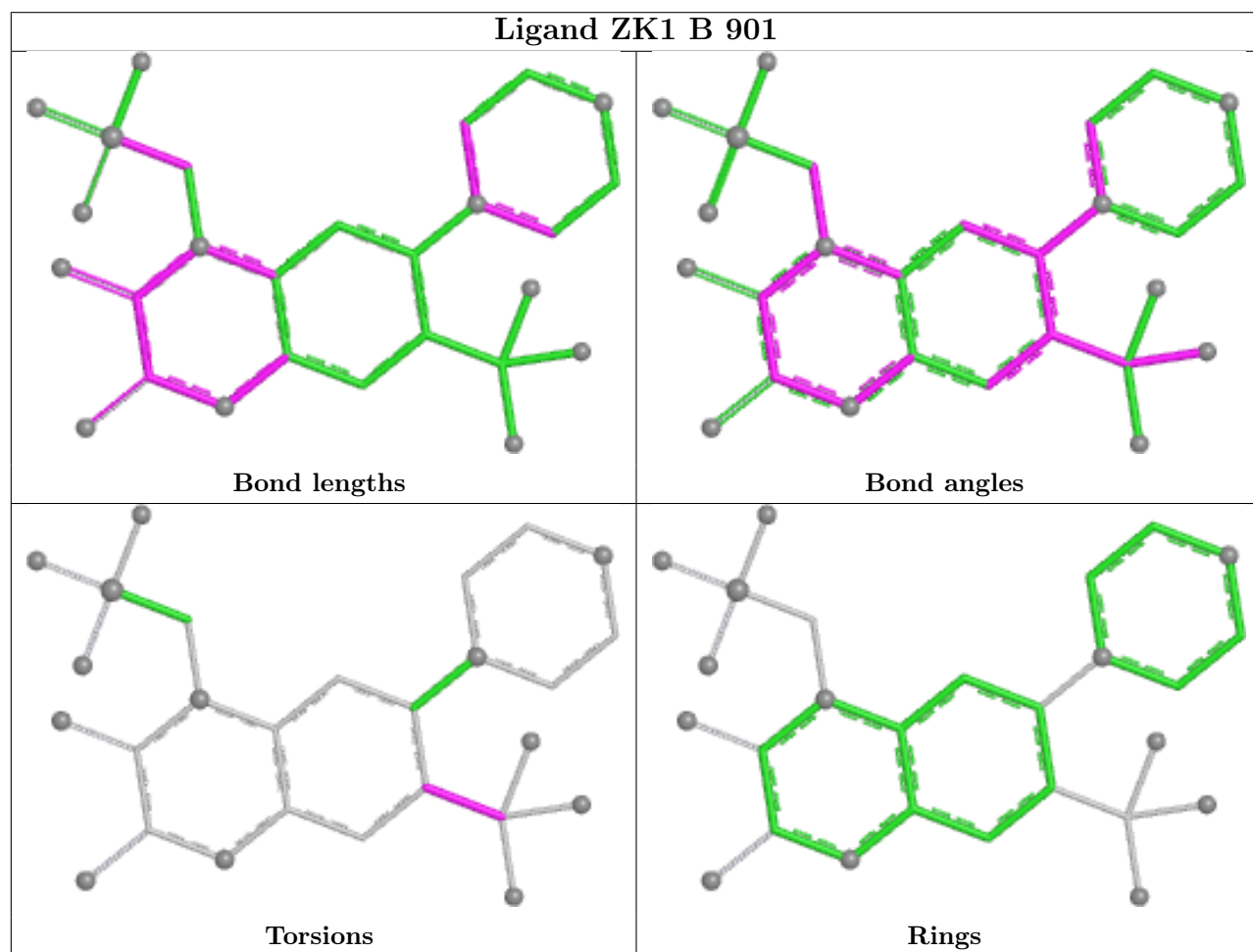
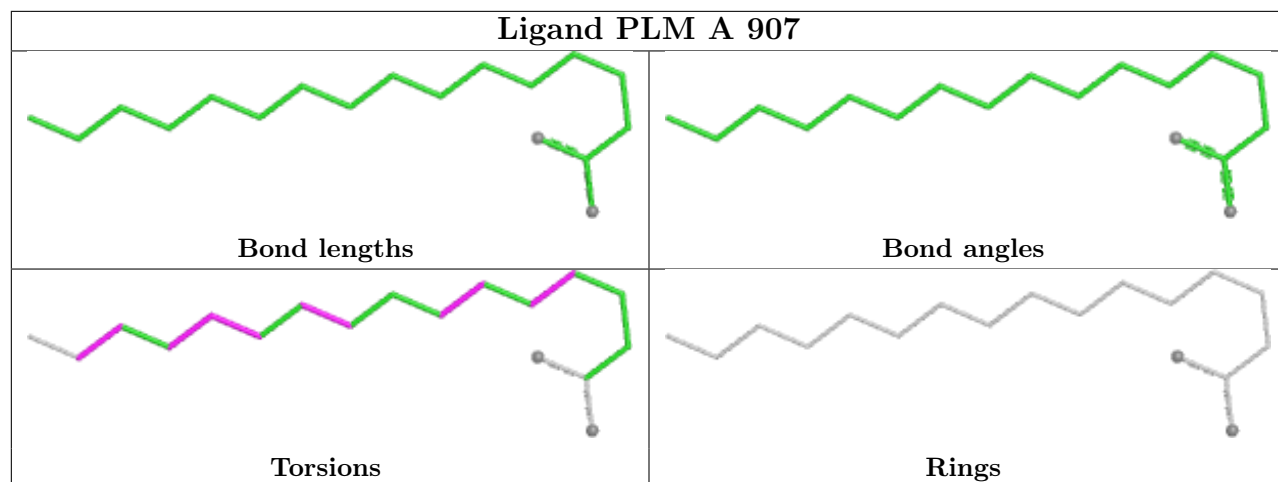
There are no ring outliers.

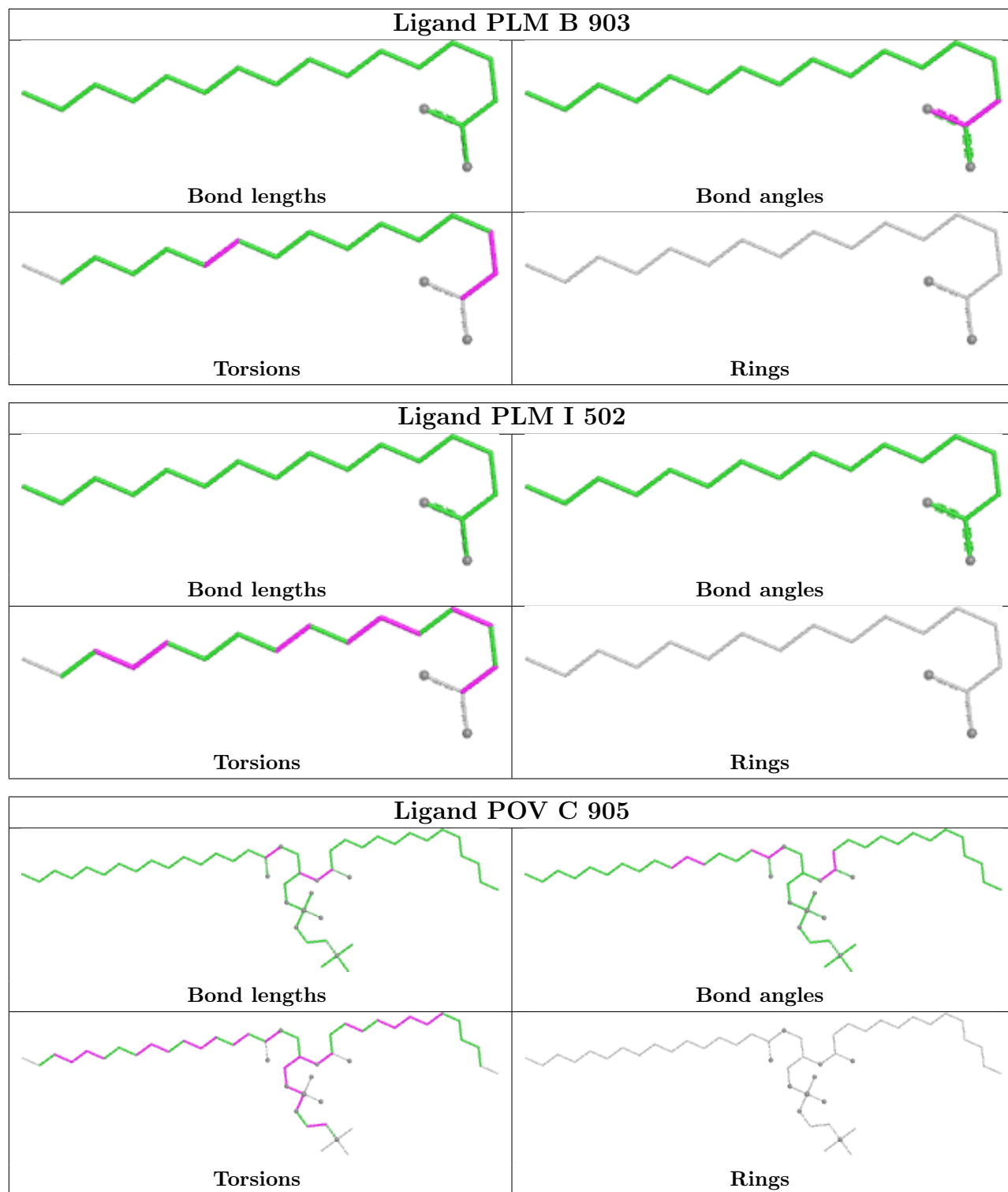
No monomer is involved in short contacts.

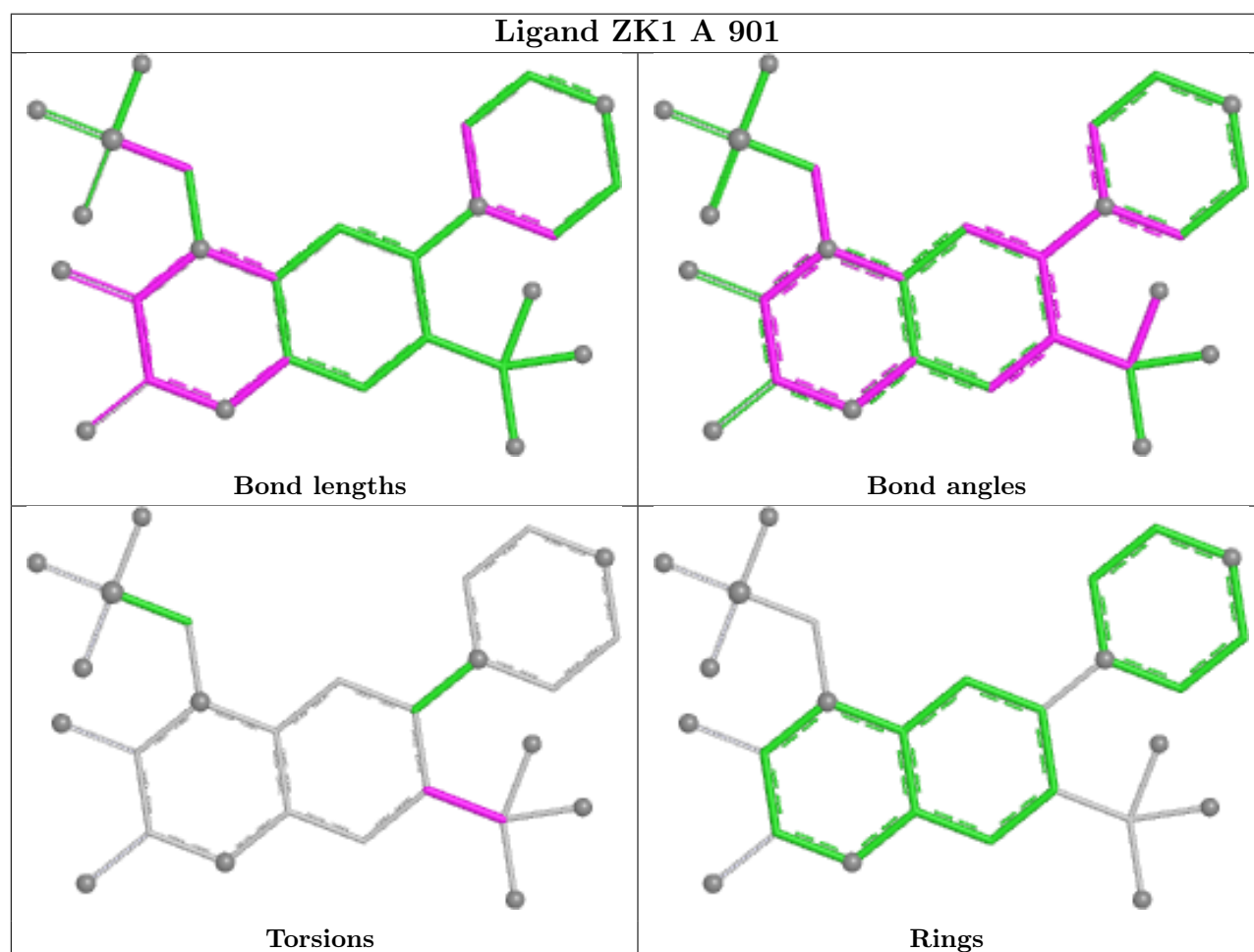
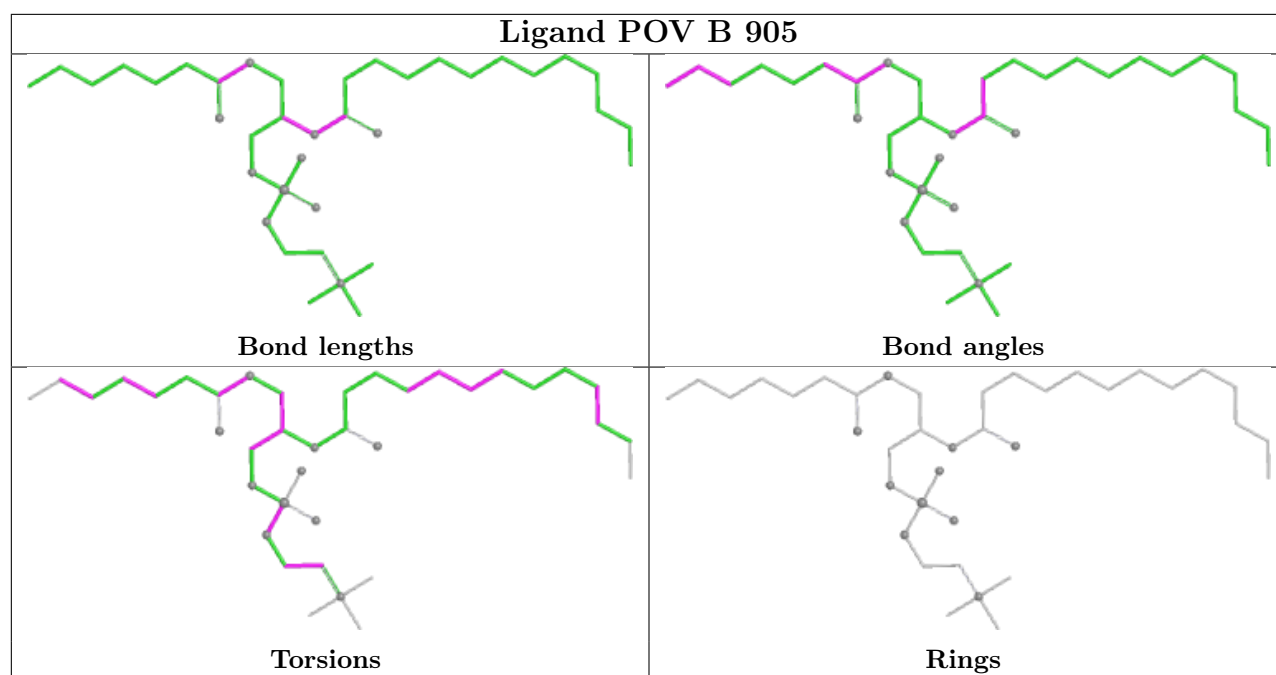
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

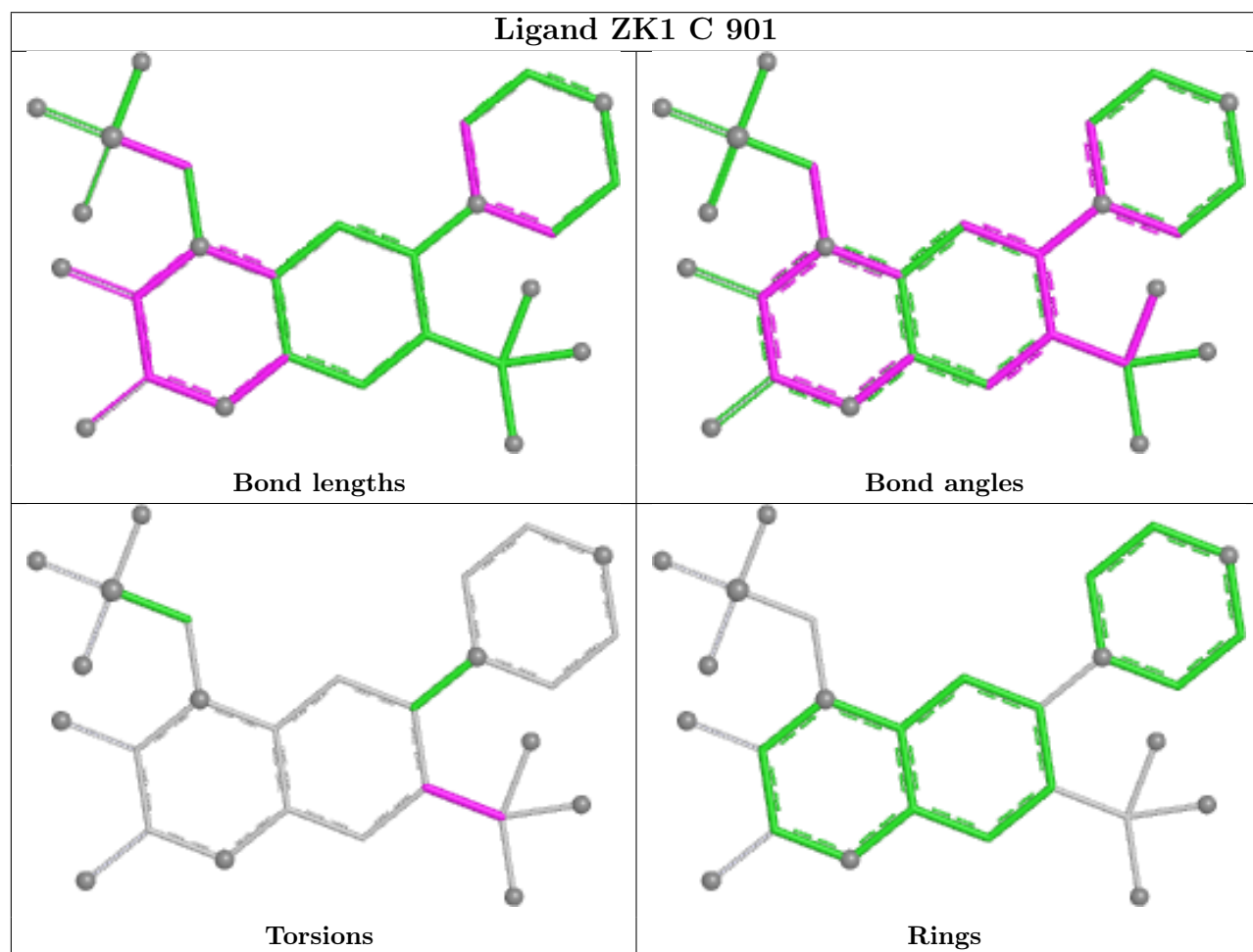
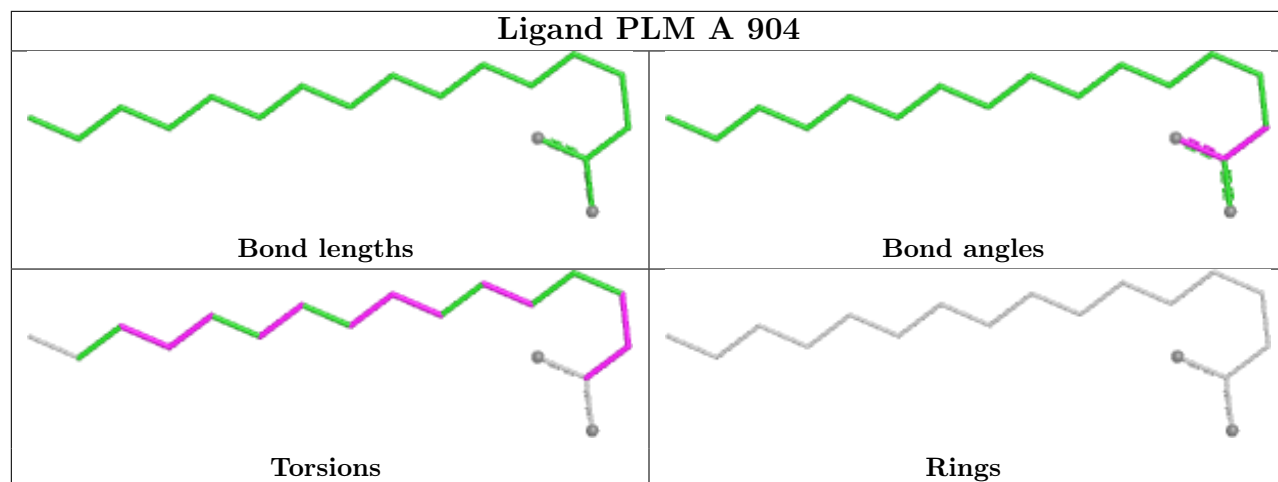


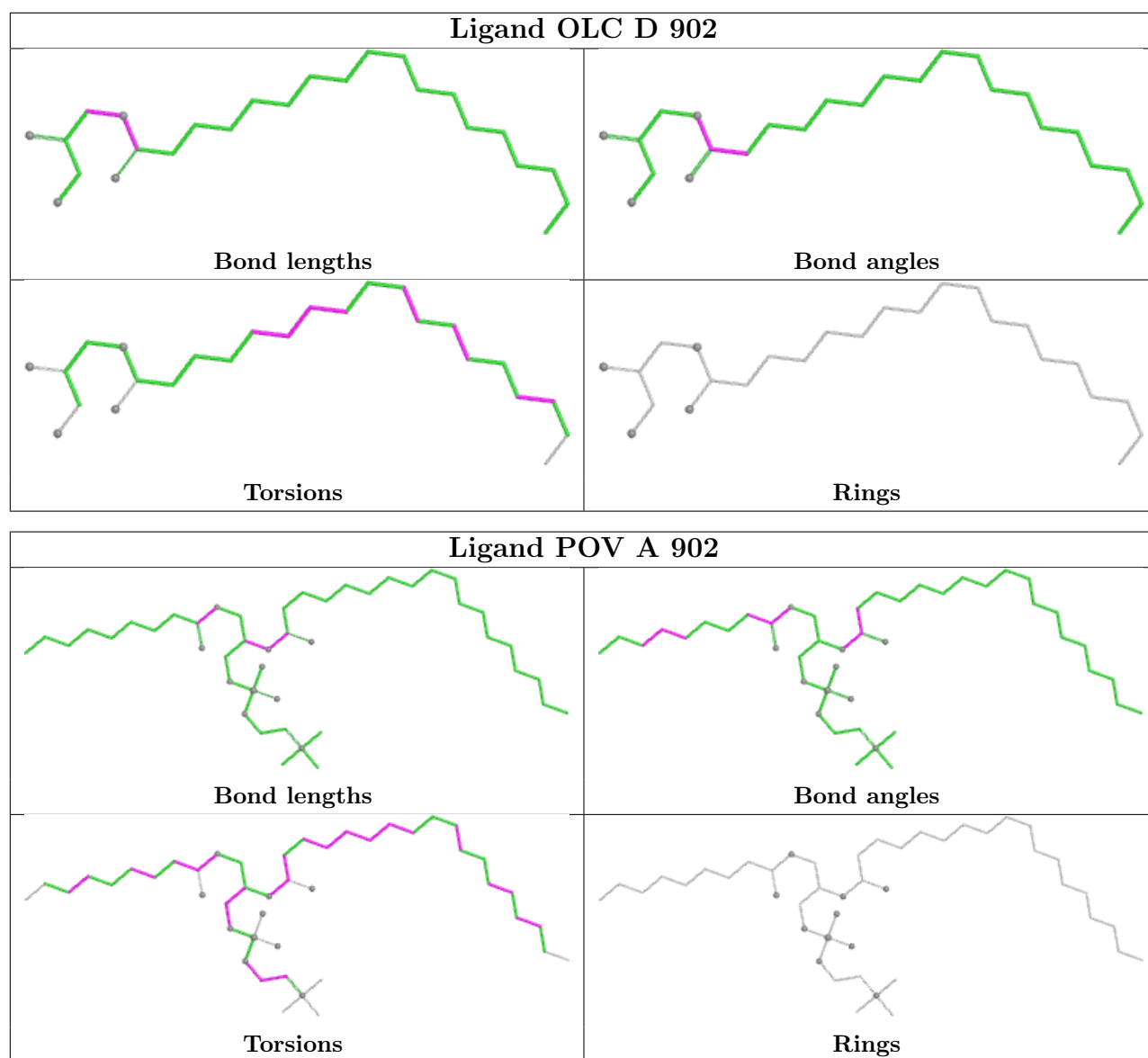




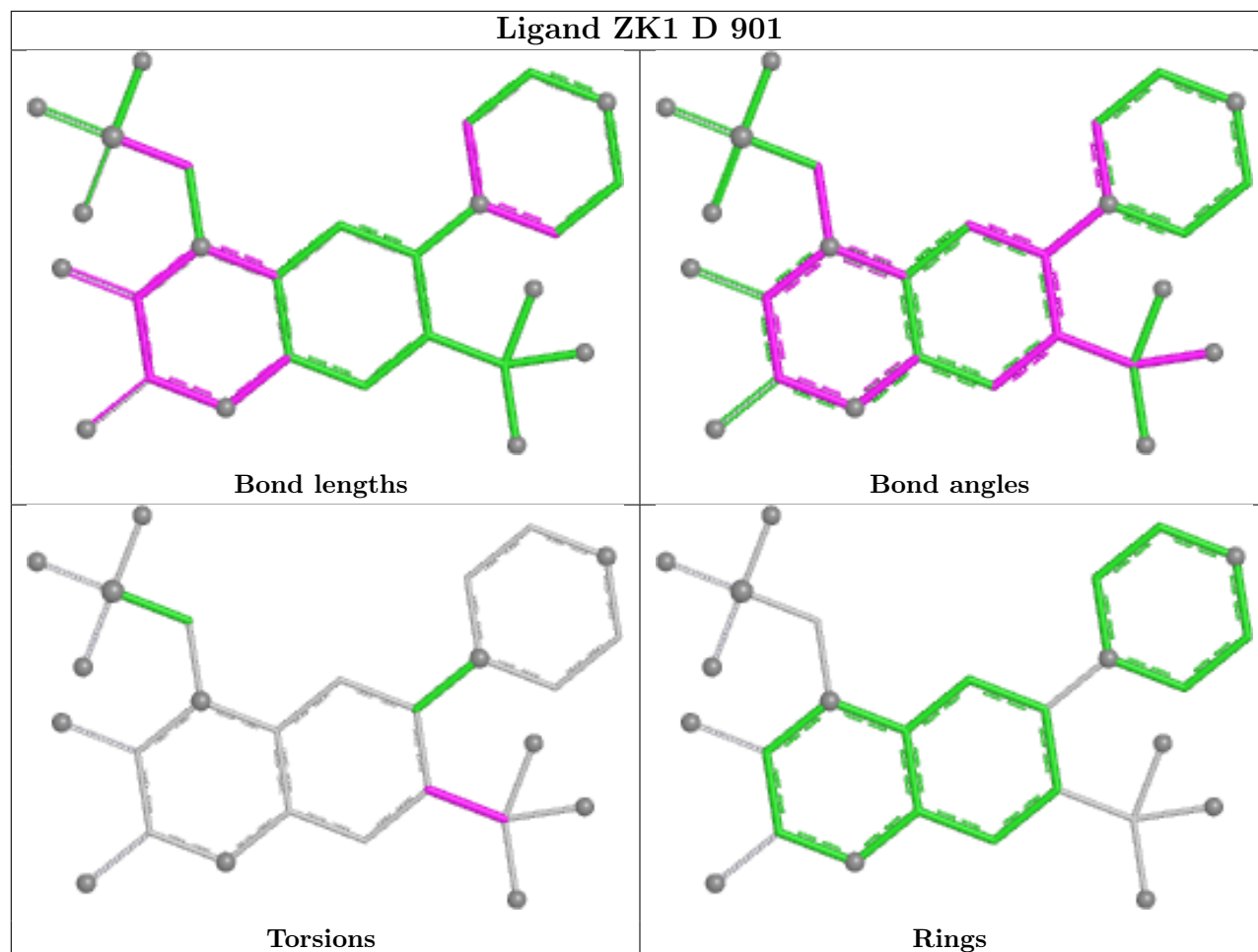




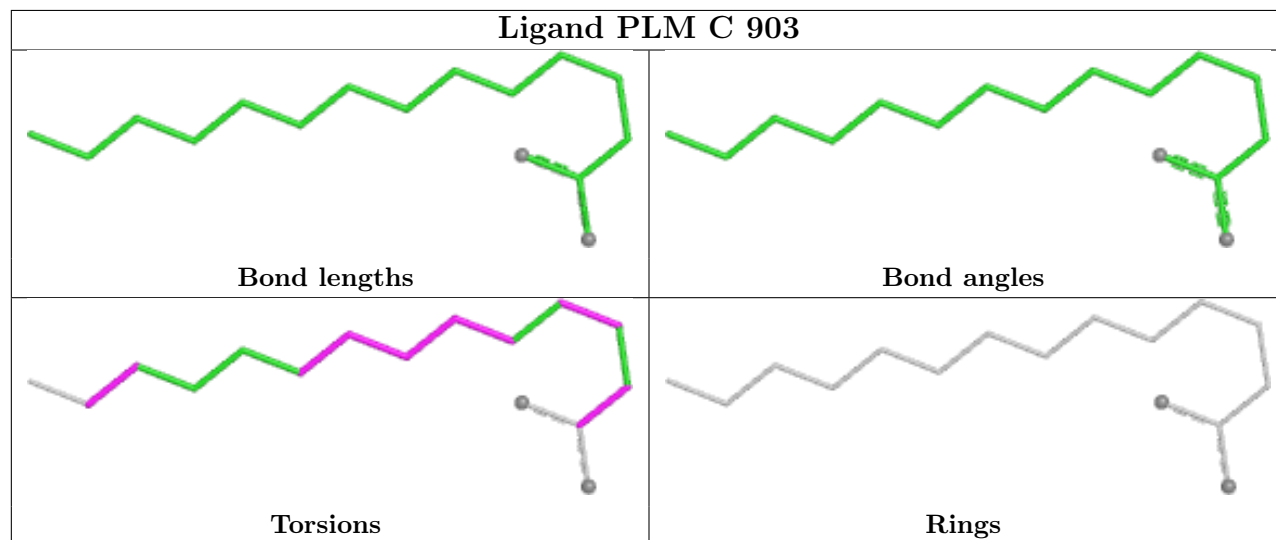




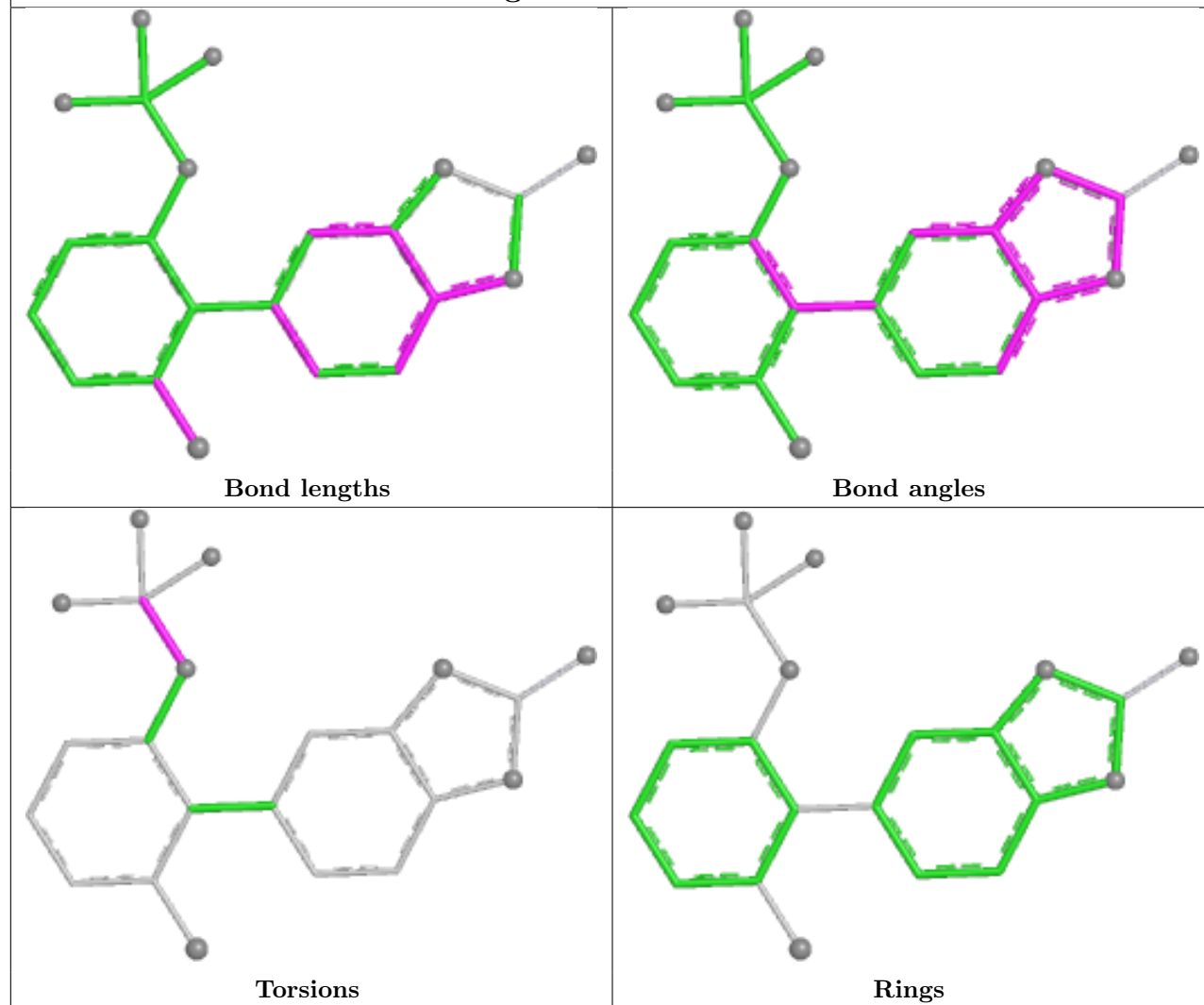
Ligand ZK1 D 901



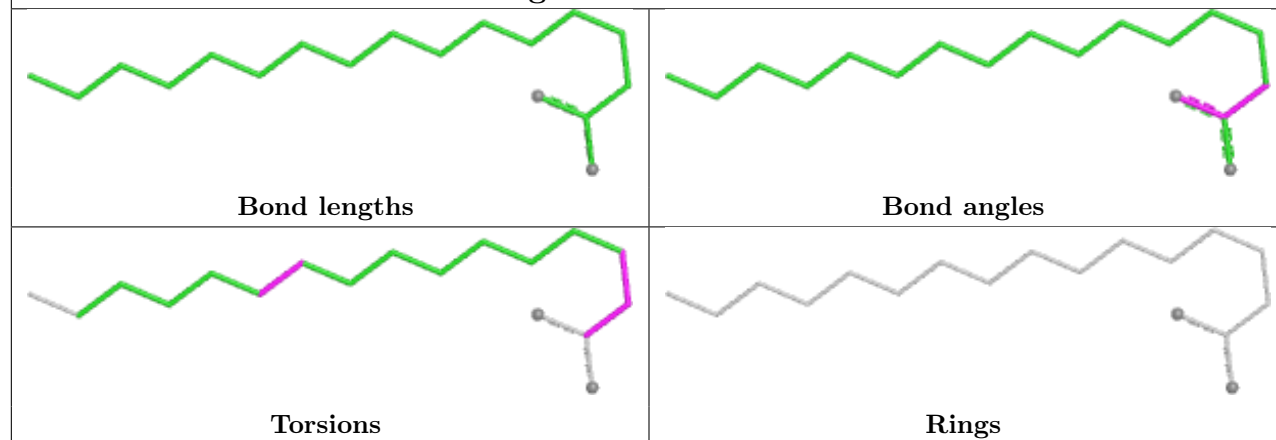
Ligand PLM C 903

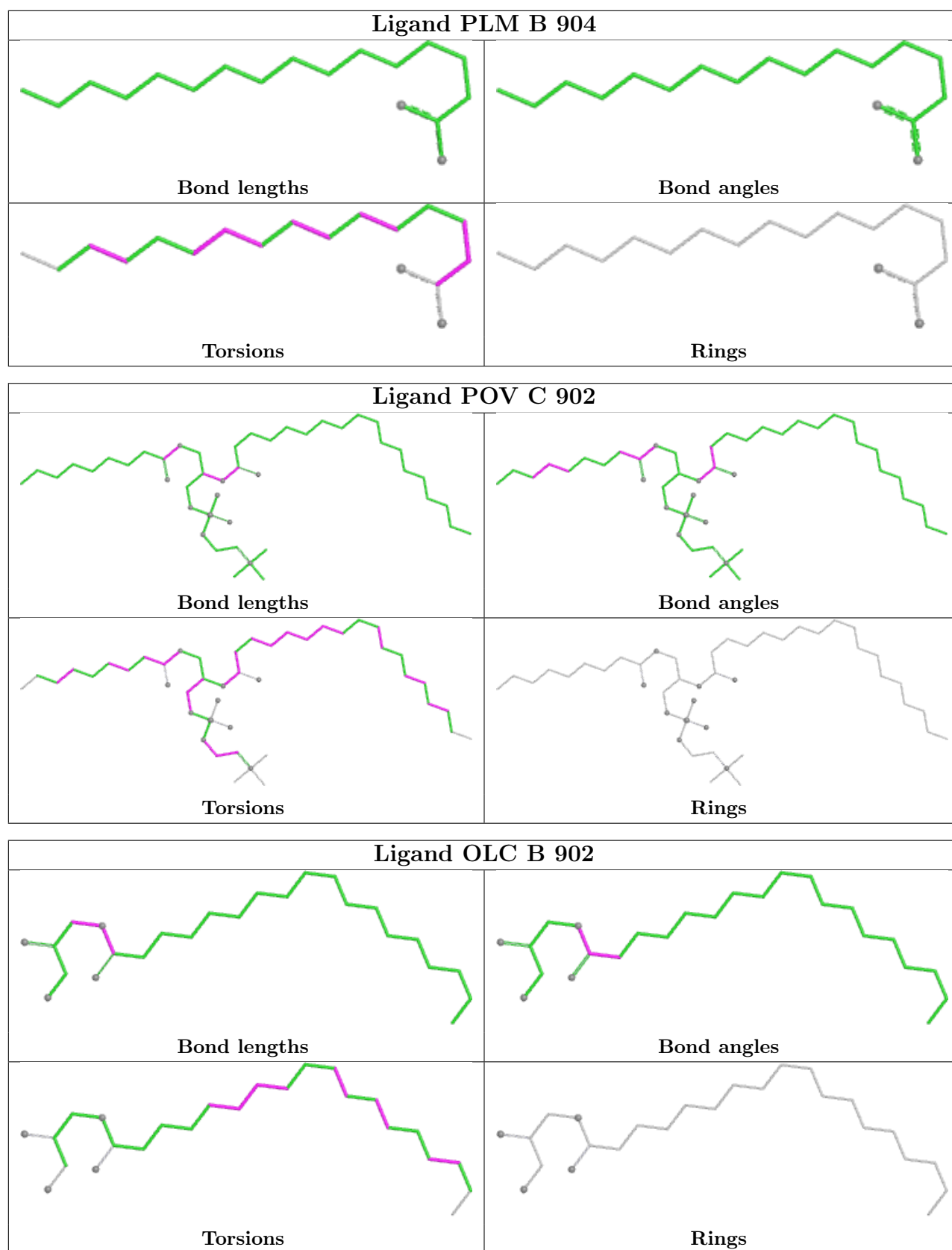


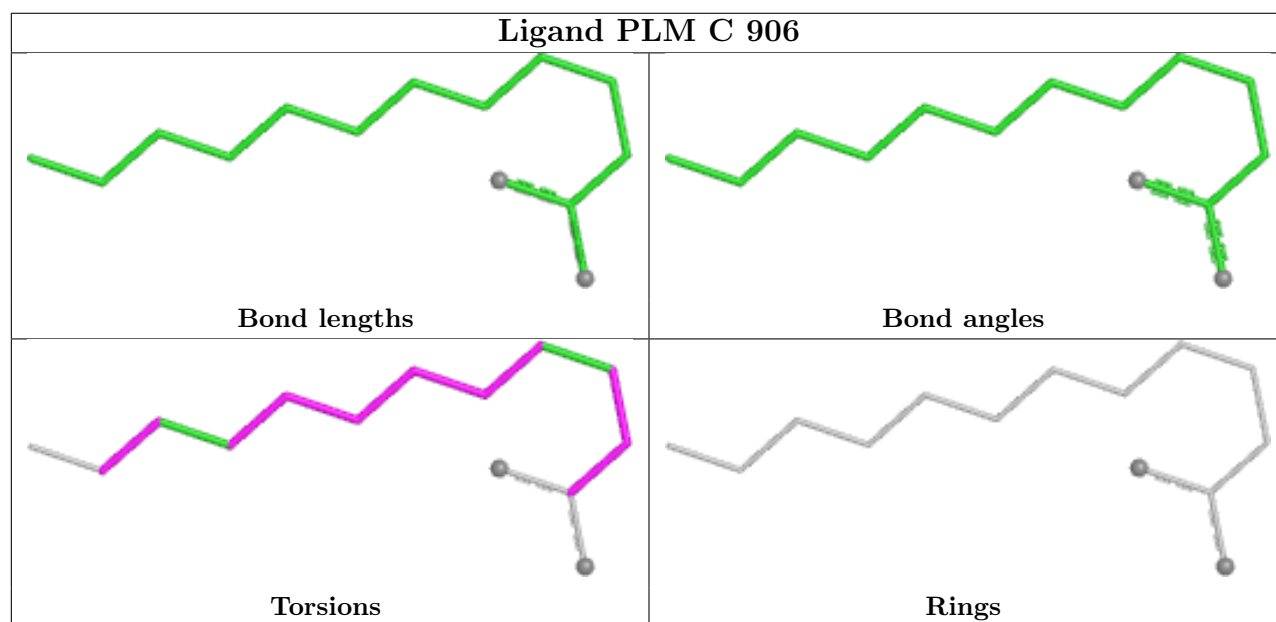
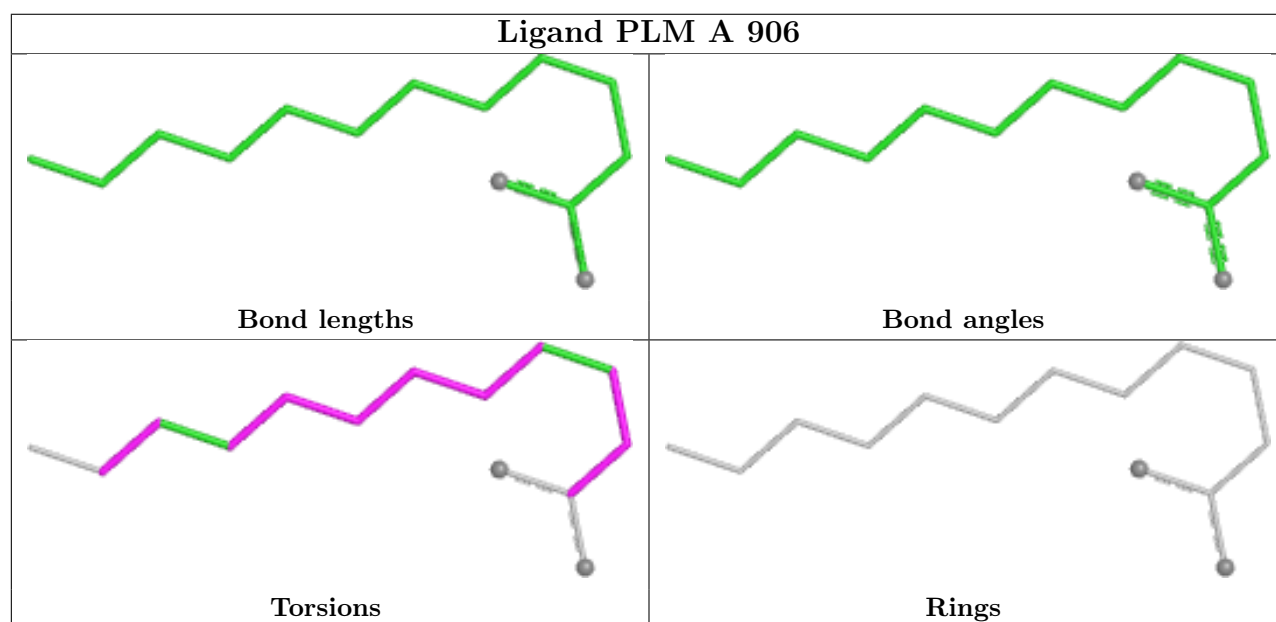
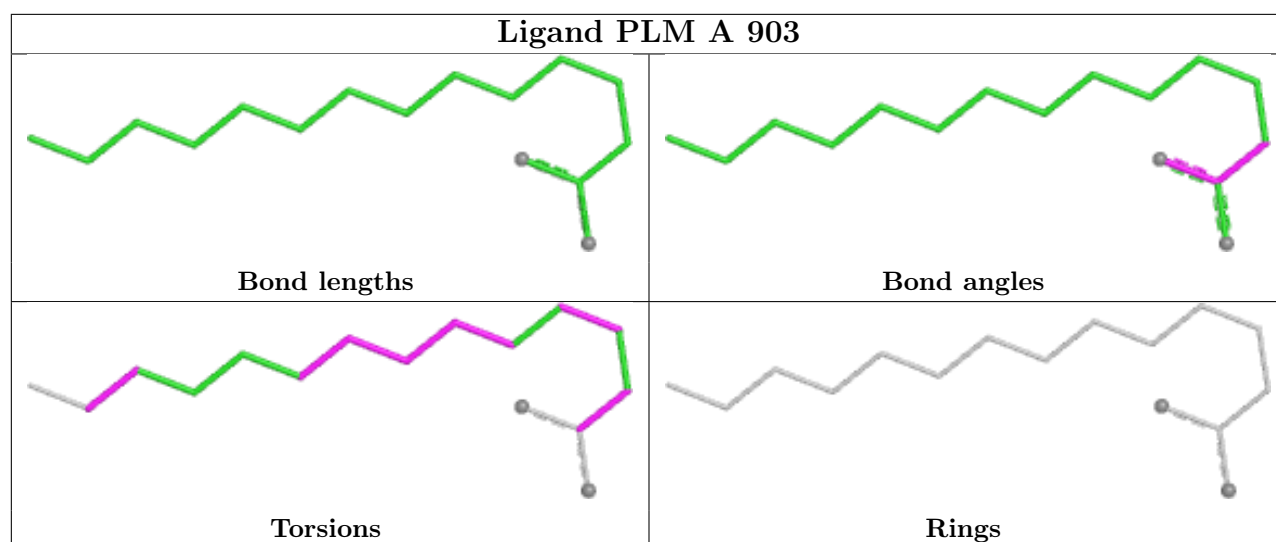
Ligand XVD I 501

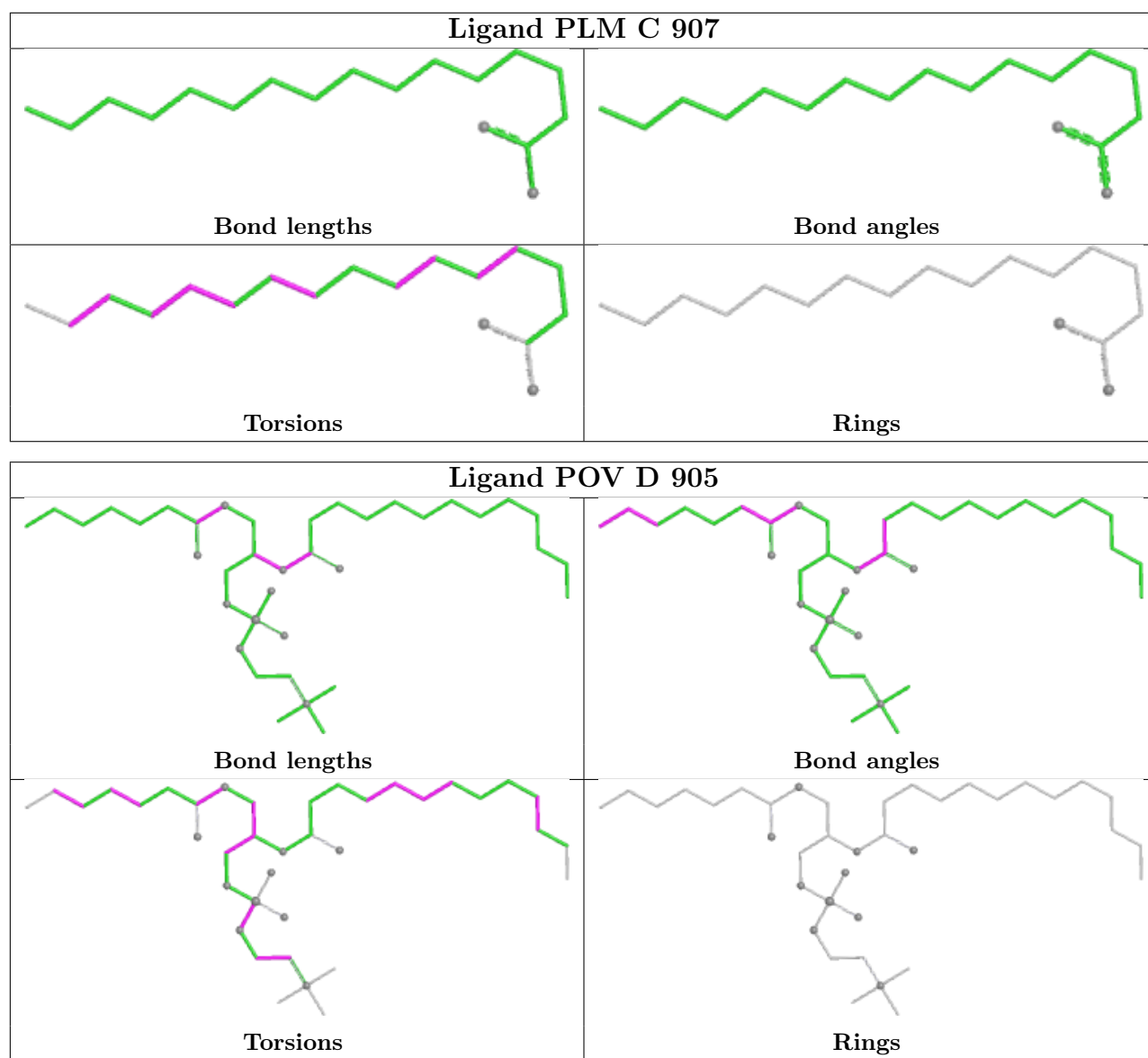


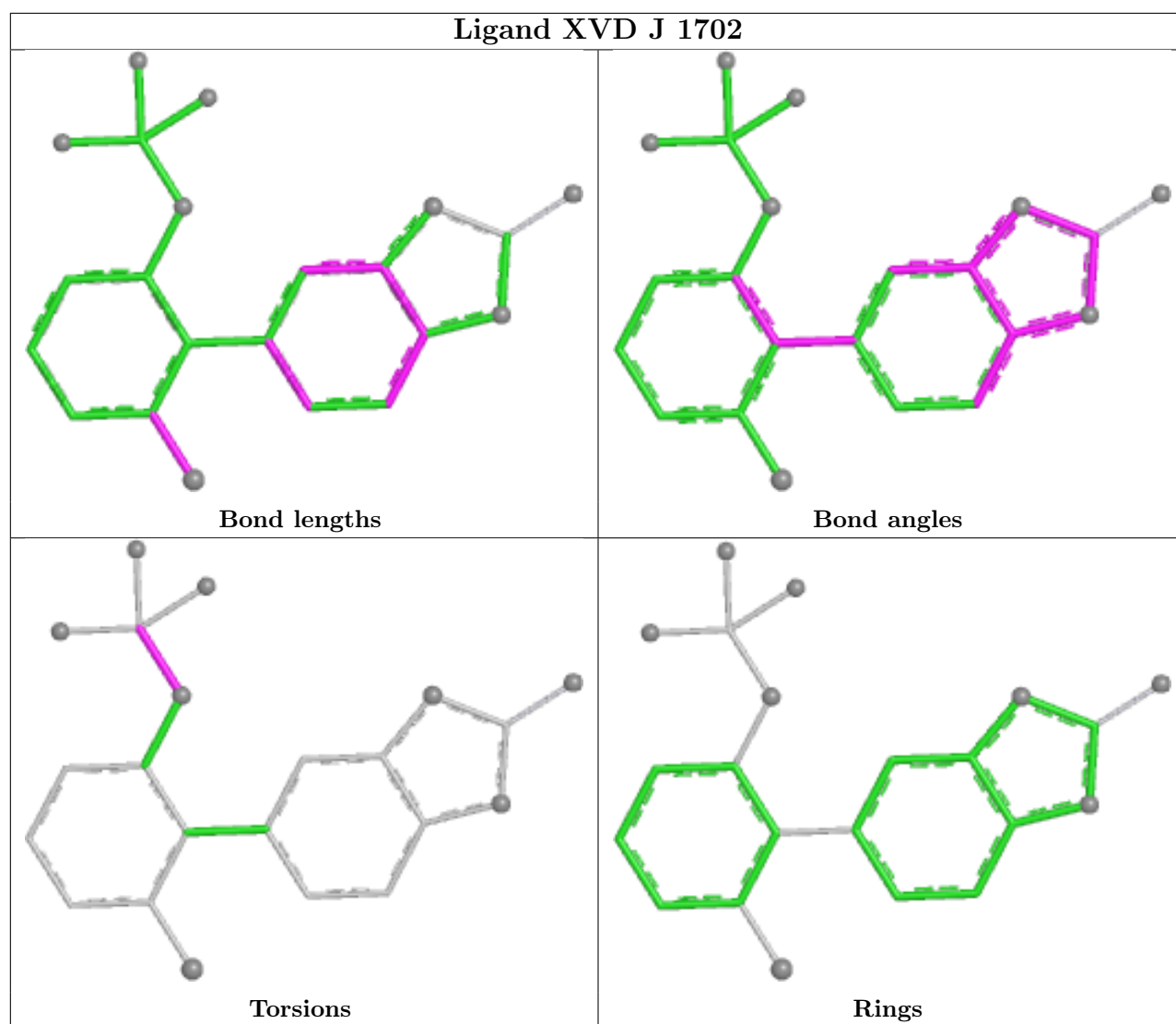
Ligand PLM D 903











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.

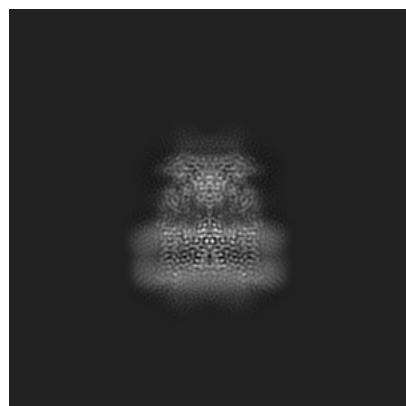
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15716. These allow visual inspection of the internal detail of the map and identification of artifacts.

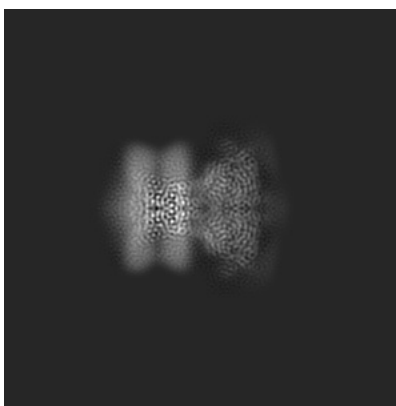
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

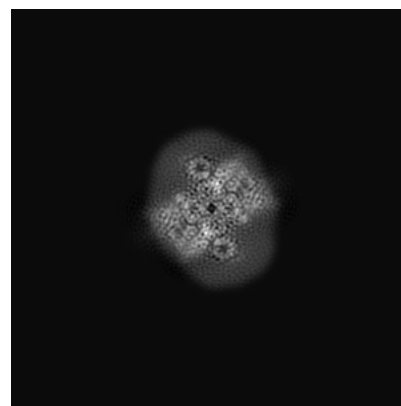
6.1.1 Primary map



X

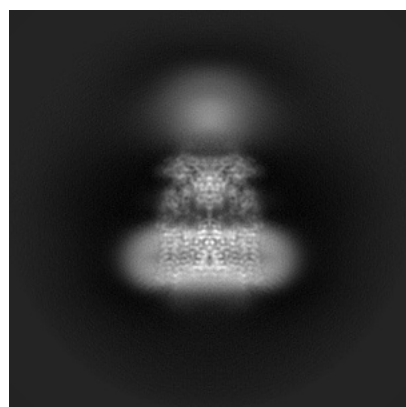


Y

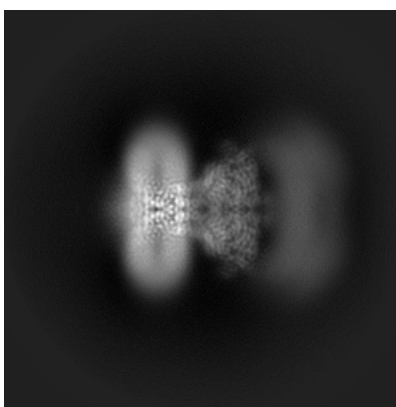


Z

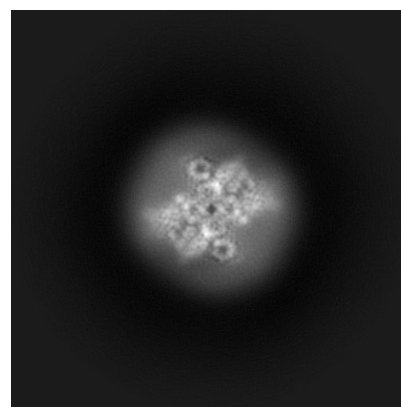
6.1.2 Raw map



X



Y

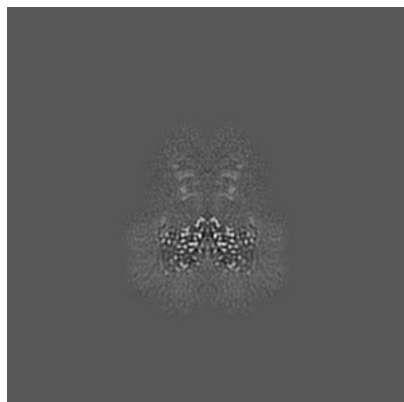


Z

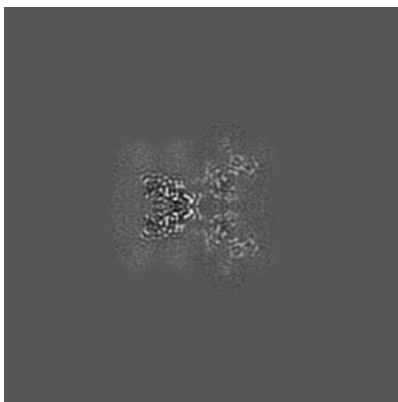
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

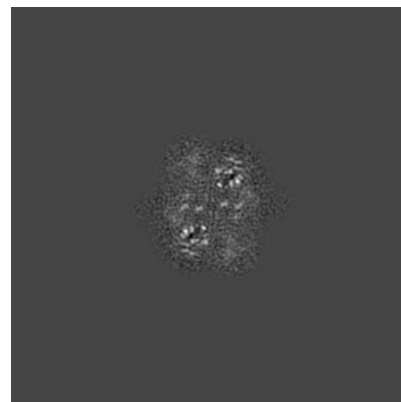
6.2.1 Primary map



X Index: 160

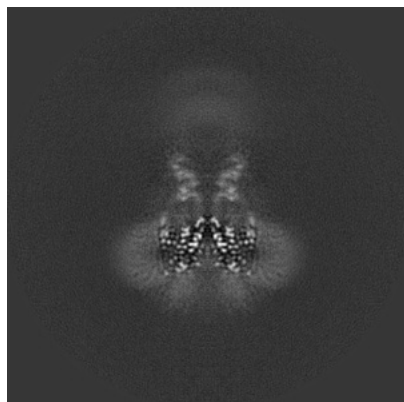


Y Index: 160

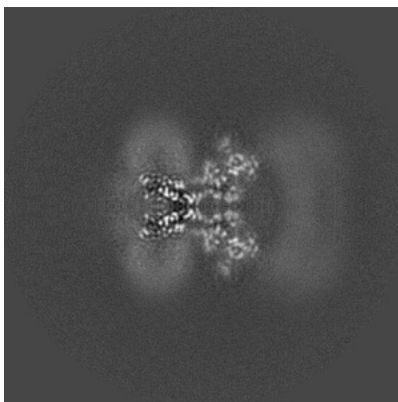


Z Index: 160

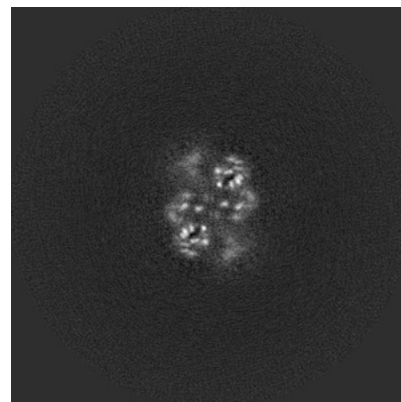
6.2.2 Raw map



X Index: 160



Y Index: 160

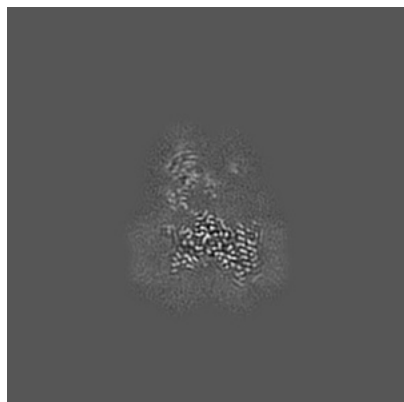


Z Index: 160

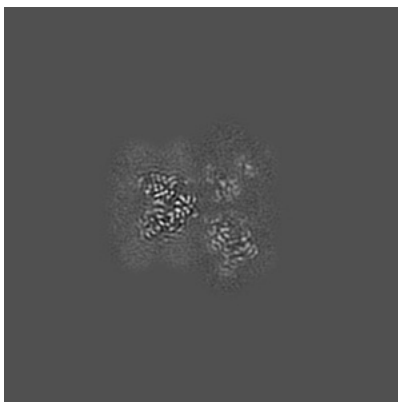
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

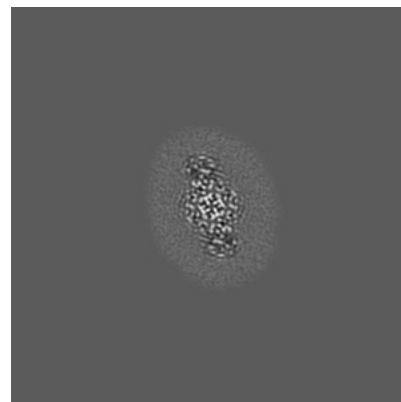
6.3.1 Primary map



X Index: 154

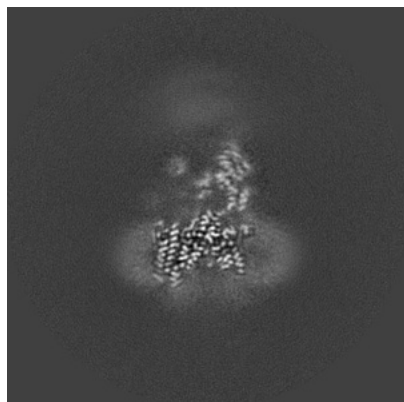


Y Index: 157

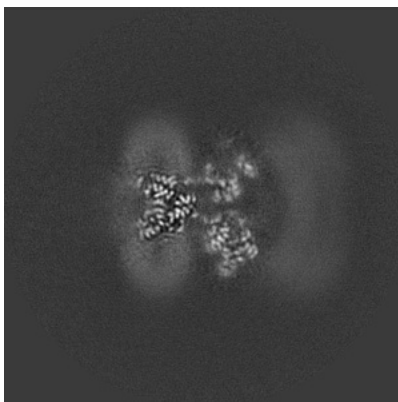


Z Index: 138

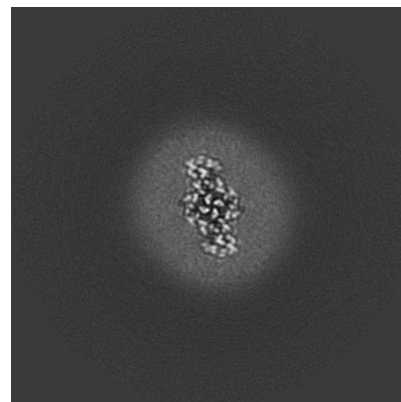
6.3.2 Raw map



X Index: 166



Y Index: 157

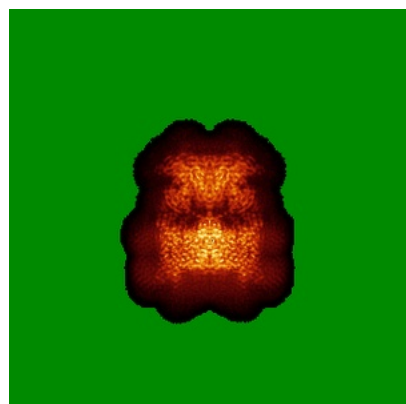


Z Index: 139

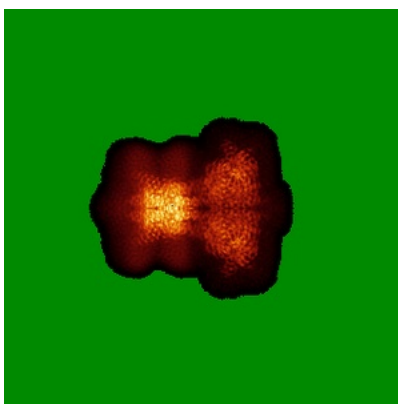
The images above show the largest variance slices of the map in three orthogonal directions.

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

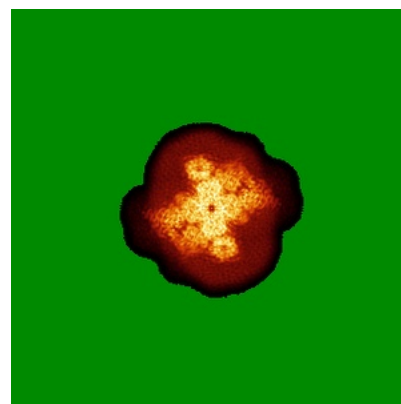
6.4.1 Primary map



X

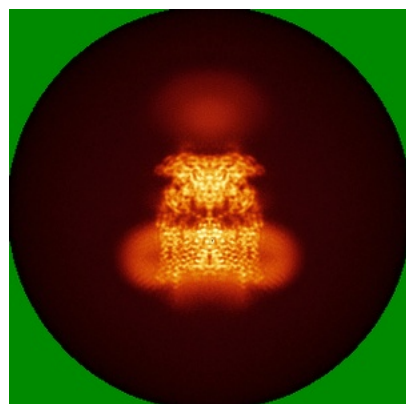


Y

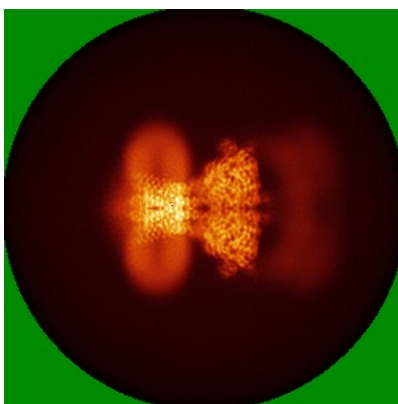


Z

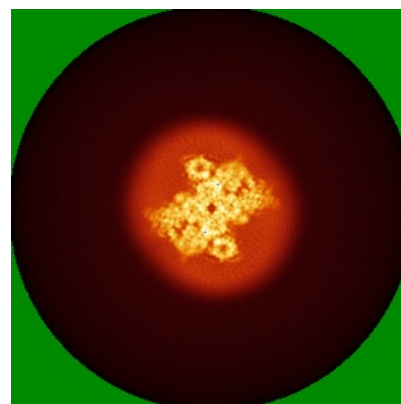
6.4.2 Raw map



X



Y

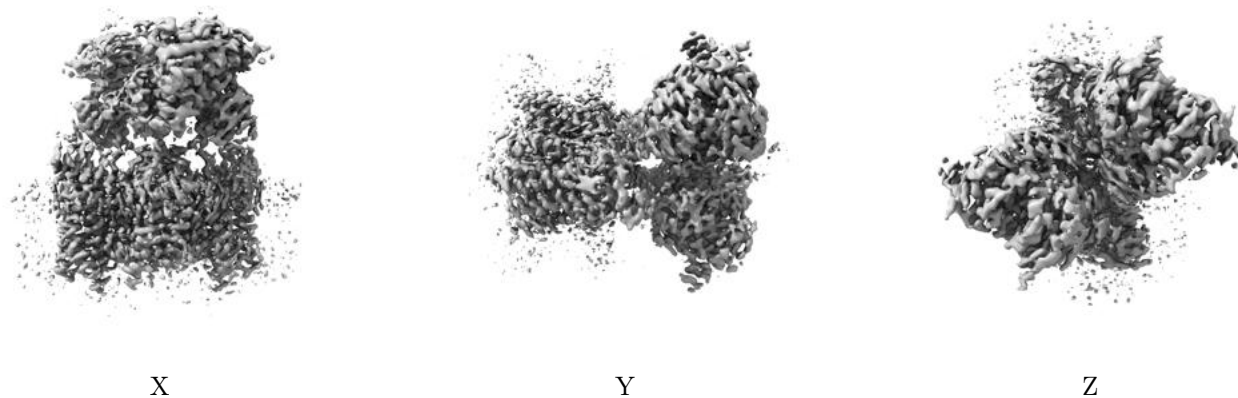


Z

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.

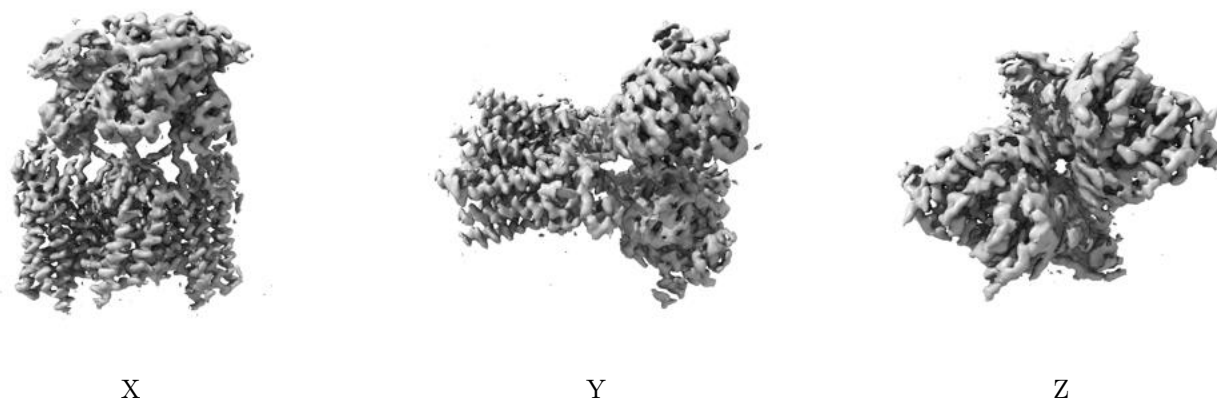
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. 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.

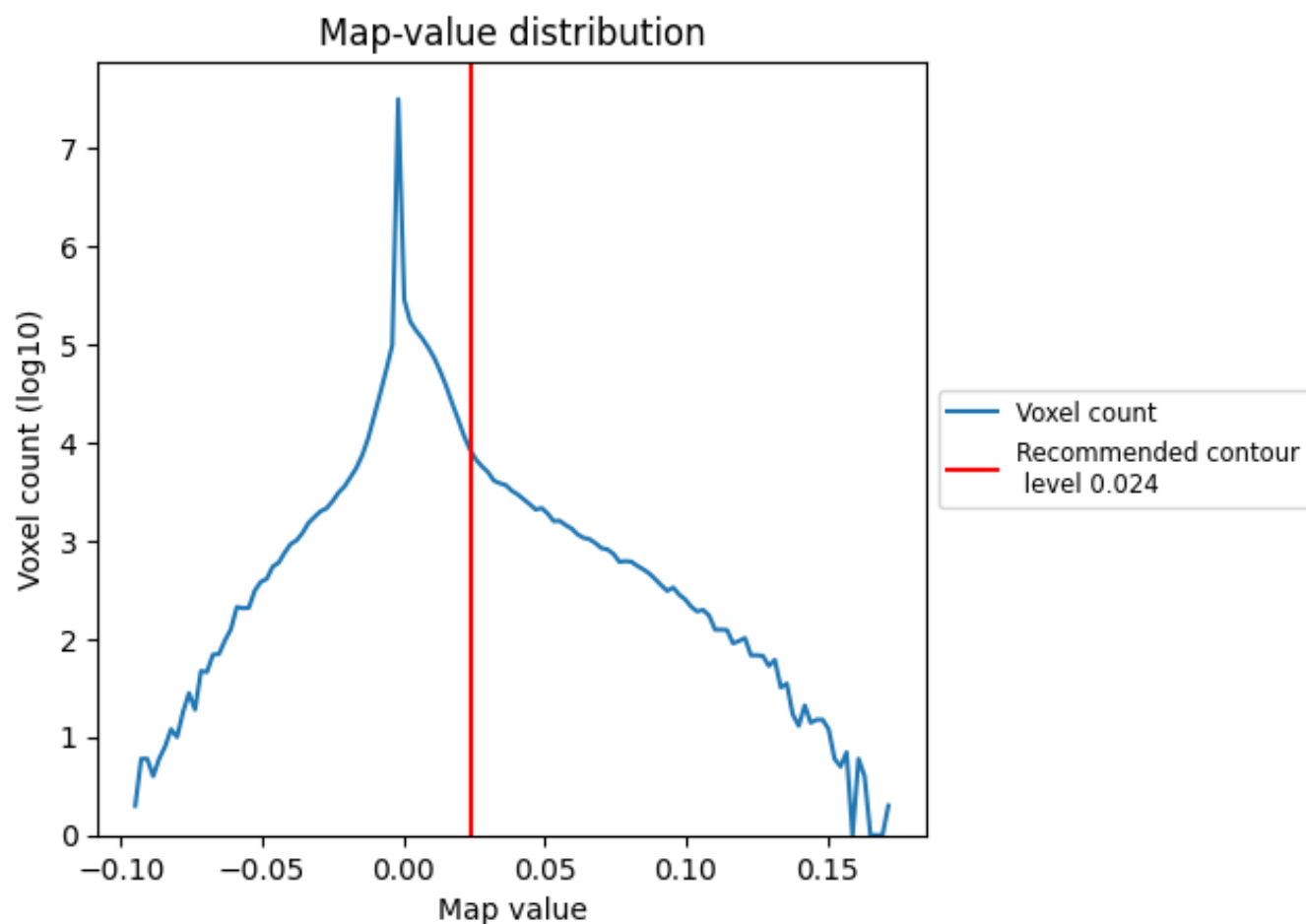
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

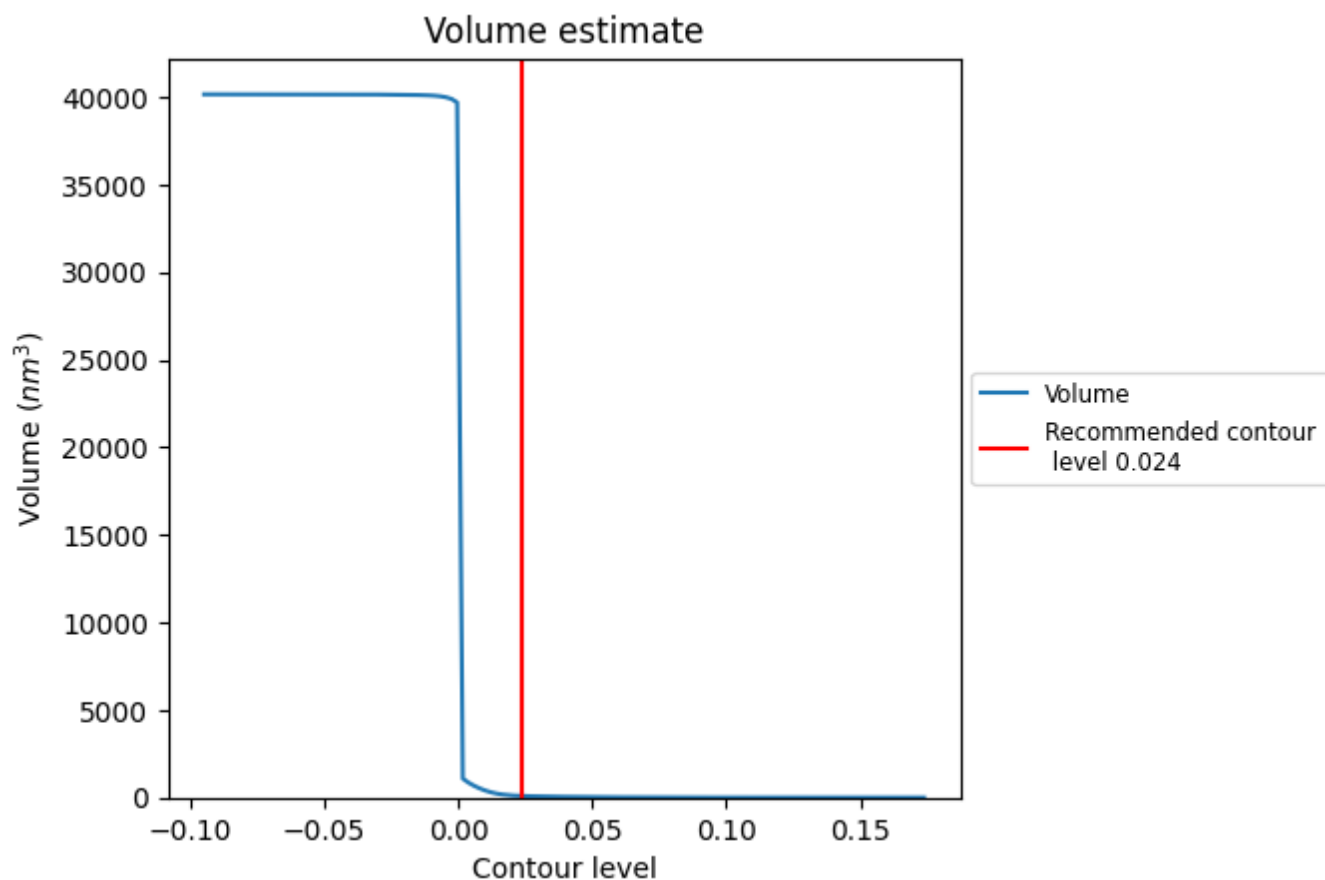
This section contains the results of statistical analysis of the map.

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.

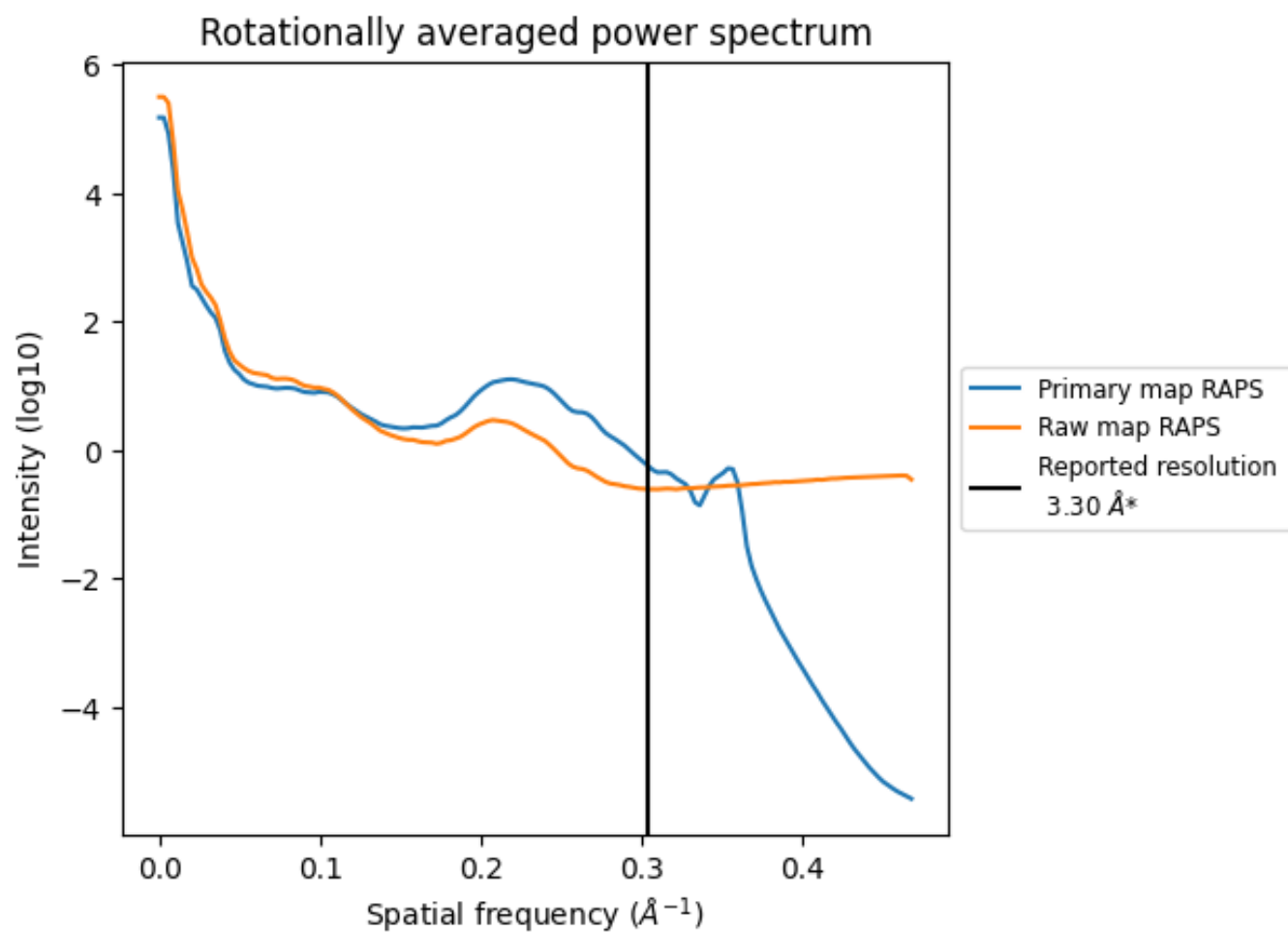
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 81 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 ⓘ

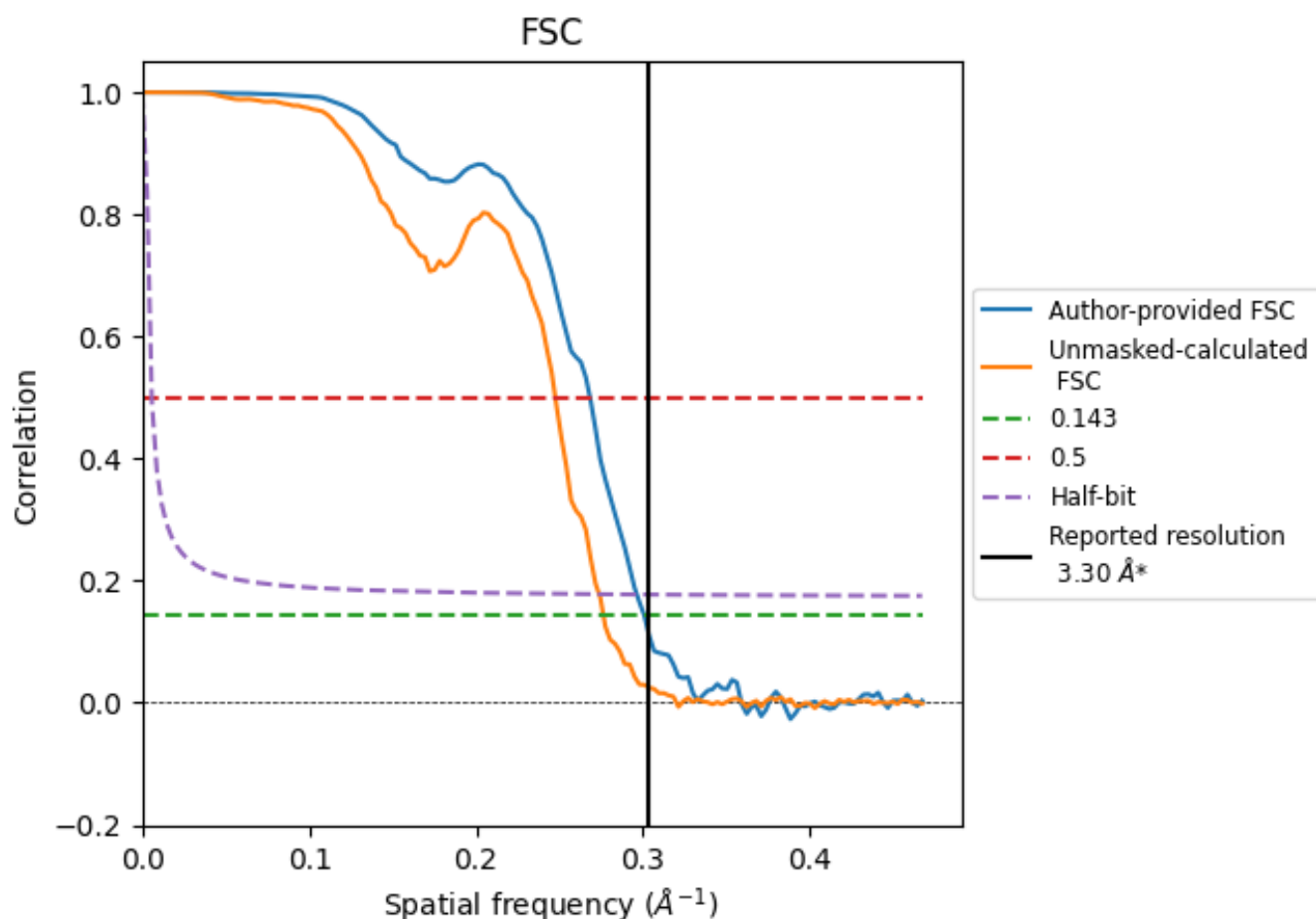


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

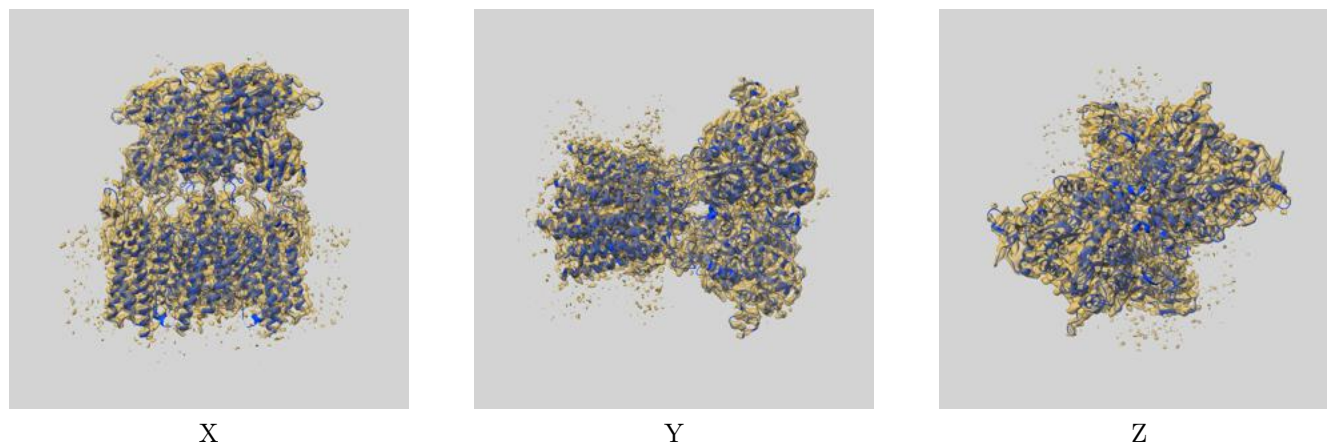
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.73	3.37
Unmasked-calculated*	3.62	4.04	3.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

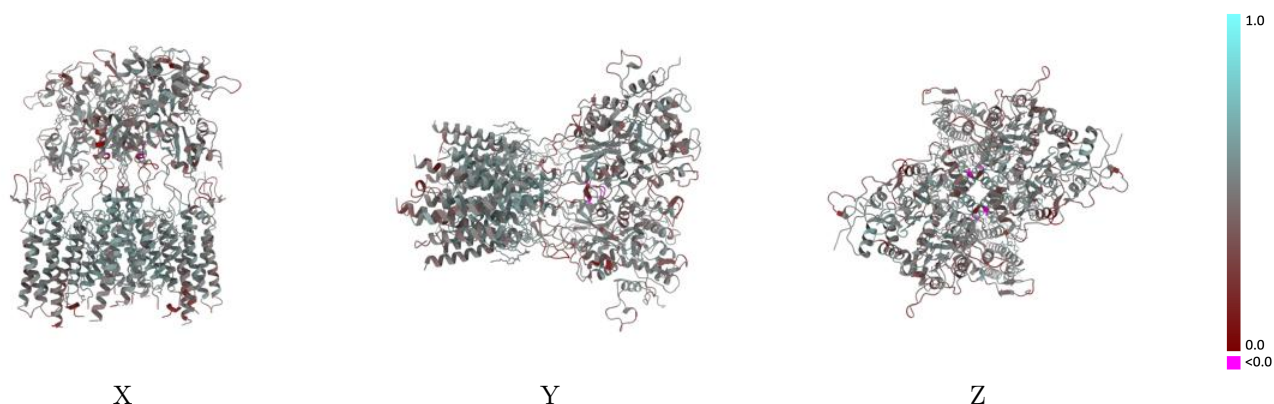
This section contains information regarding the fit between EMDB map EMD-15716 and PDB model 8AYM. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



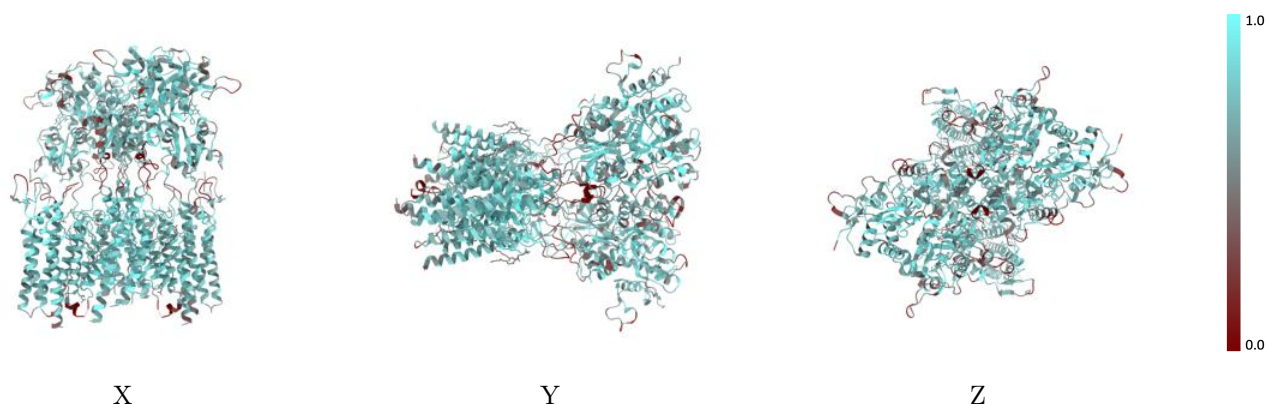
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



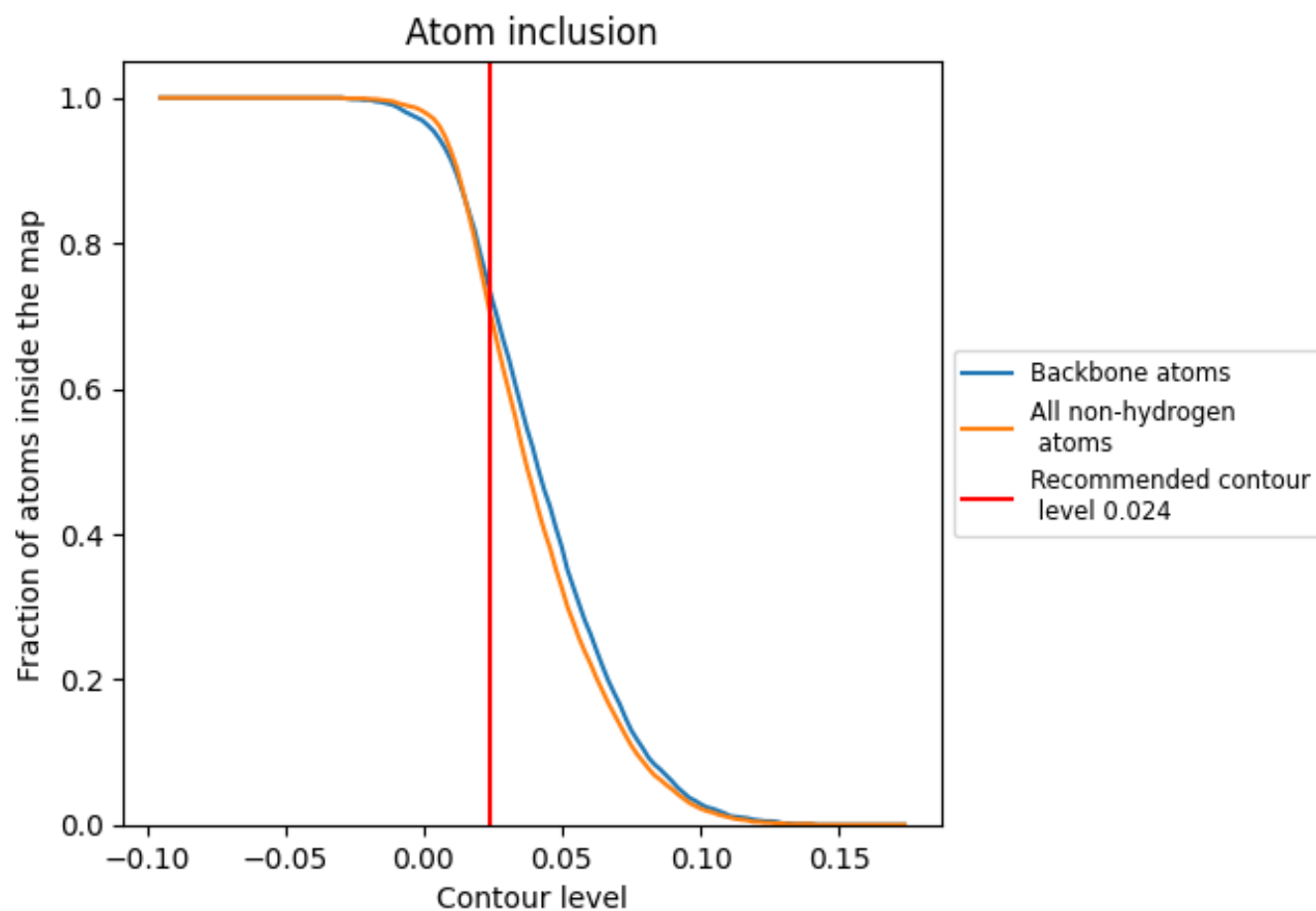
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.4720
A	0.7070	0.4740
B	0.7050	0.4730
C	0.7080	0.4760
D	0.7050	0.4750
I	0.7020	0.4590
J	0.7040	0.4610

1.0

0.0

<0.0