



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:12 PM UTC

PDB ID : 9CUH / pdb_00009cuh
EMDB ID : EMD-45933
Title : Structure of human full-length ancestral TRPV6 channel in apo open state
Authors : Neuberger, A.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on : 2024-07-26
Resolution : 3.03 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:

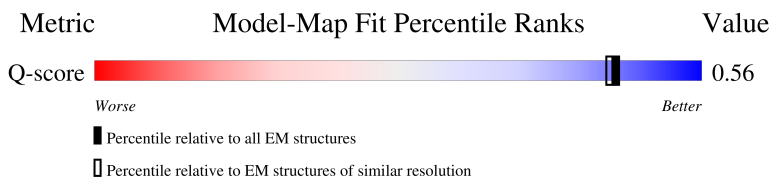
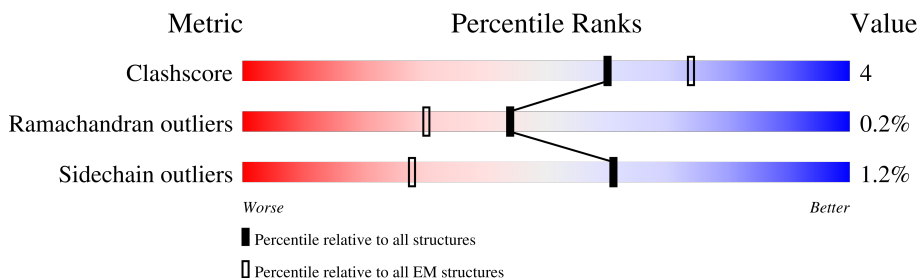
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.03 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	13929 (2.53 - 3.53)

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	765	
1	B	765	
1	C	765	
1	D	765	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20877 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 Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	594	Total	C	N	O	S	0	0
			4770	3081	809	843	37		
1	B	594	Total	C	N	O	S	0	0
			4770	3081	809	843	37		
1	C	594	Total	C	N	O	S	0	0
			4770	3081	809	843	37		
1	D	594	Total	C	N	O	S	0	0
			4770	3081	809	843	37		

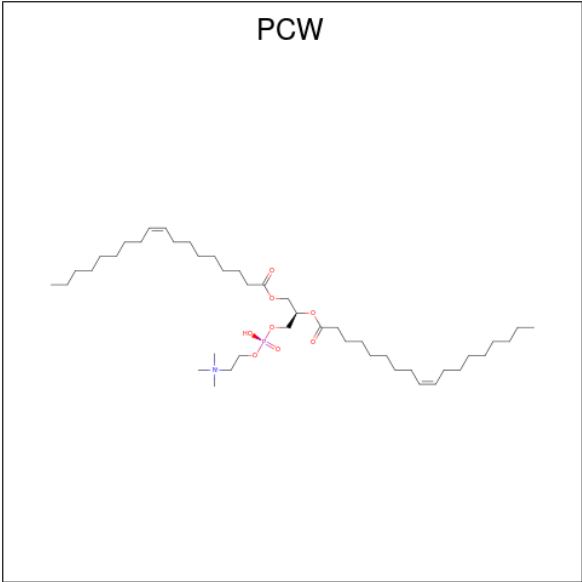
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	ARG	CYS	variant	UNP Q9H1D0
A	378	VAL	MET	variant	UNP Q9H1D0
A	681	THR	MET	variant	UNP Q9H1D0
B	157	ARG	CYS	variant	UNP Q9H1D0
B	378	VAL	MET	variant	UNP Q9H1D0
B	681	THR	MET	variant	UNP Q9H1D0
C	157	ARG	CYS	variant	UNP Q9H1D0
C	378	VAL	MET	variant	UNP Q9H1D0
C	681	THR	MET	variant	UNP Q9H1D0
D	157	ARG	CYS	variant	UNP Q9H1D0
D	378	VAL	MET	variant	UNP Q9H1D0
D	681	THR	MET	variant	UNP Q9H1D0

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).

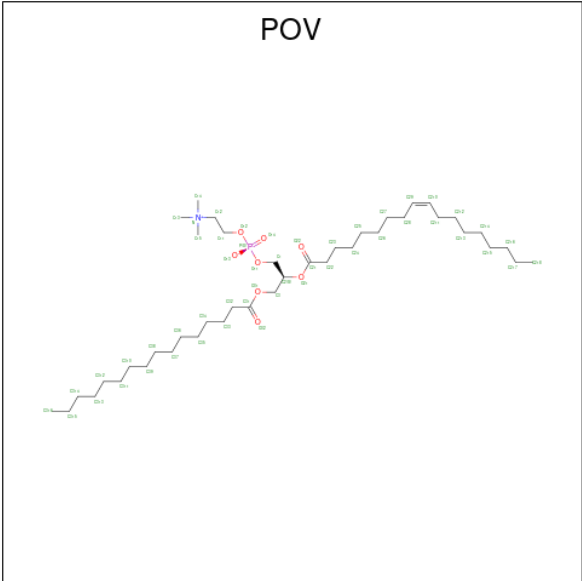


- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	C	0
			13	13	
3	B	1	Total	C	0
			13	13	
3	C	1	Total	C	0
			13	13	
3	D	1	Total	C	0
			13	13	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	O			0
			20	18	2			
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	O			0
			19	17	2			
4	A	1	Total	C	O			0
			14	12	2			
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	O			0
			20	18	2			
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	O			0
			19	17	2			
4	B	1	Total	C	O			0
			14	12	2			
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	O			0
			20	18	2			
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	O			0
			19	17	2			
4	C	1	Total	C	O			0
			14	12	2			

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Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	O			0
			20	18	2			
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	O			0
			19	17	2			
4	D	1	Total	C	O			0
			14	12	2			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	

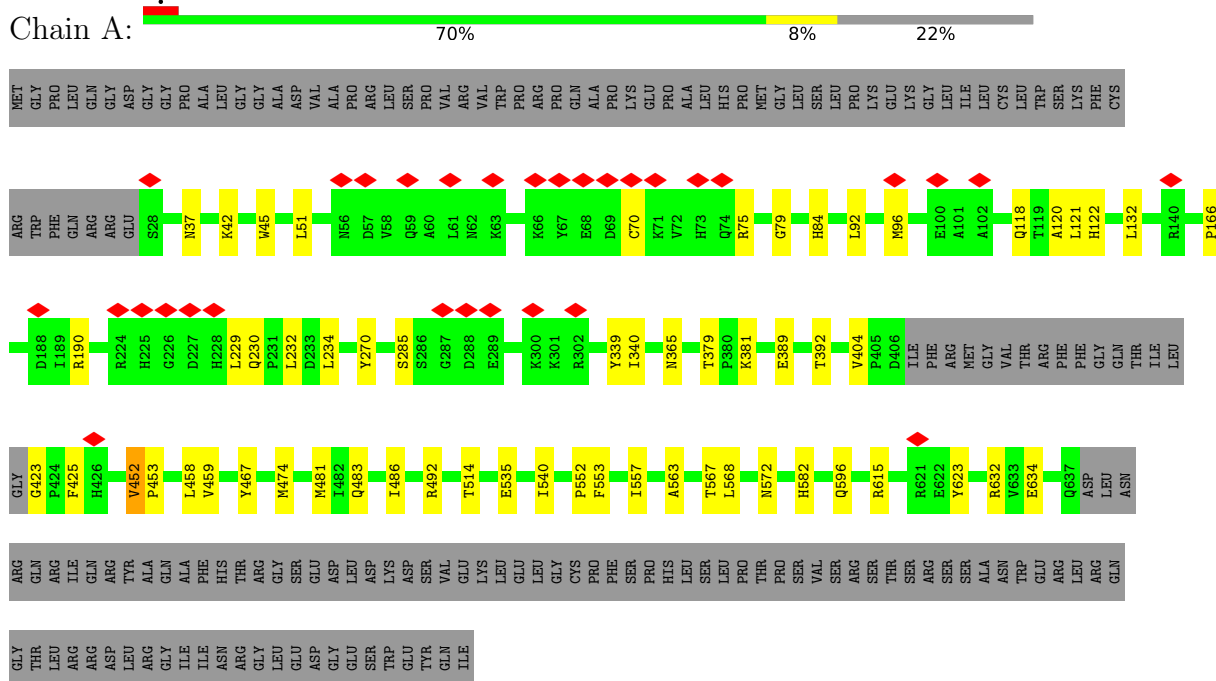
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	18	Total	O	0
			18	18	
6	B	18	Total	O	0
			18	18	
6	C	18	Total	O	0
			18	18	
6	D	18	Total	O	0
			18	18	

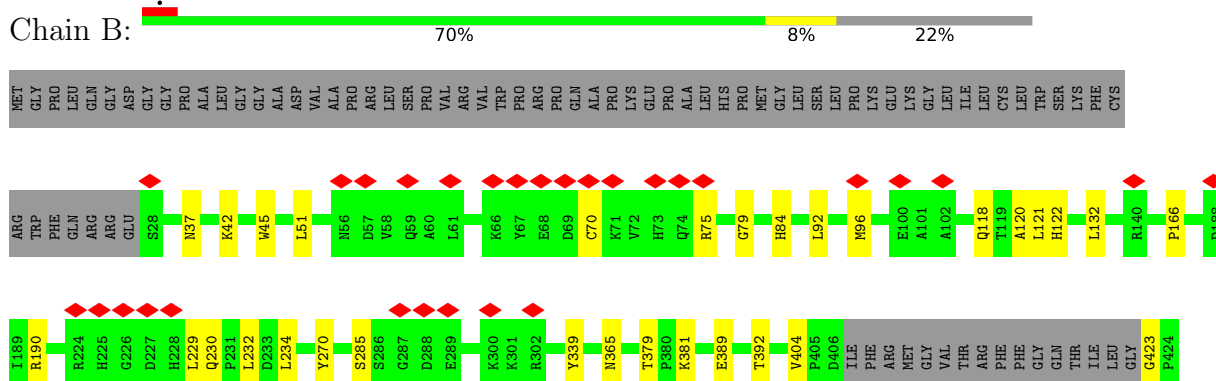
3 Residue-property plots

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

- Molecule 1: Transient receptor potential cation channel subfamily V member 6



- Molecule 1: Transient receptor potential cation channel subfamily V member 6



GLY
THR
LEU
ARG
ARG
ASP
LEU
ARG
GLY
ILE
ILE
ASN
ARG
GLY
LEU
GLU
ASP
GLY
GLU
SER
TRP
GLU
TYR
GLN
ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	517835	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.987	Depositor
Minimum map value	-3.555	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.624	Depositor
Map size ($\text{\AA}$)	273.152, 273.152, 273.152	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.067, 1.067, 1.067	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: CA, Y01, PCW, POV

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	0.47	1/4879 (0.0%)	0.69	0/6622
1	B	0.46	1/4879 (0.0%)	0.69	0/6622
1	C	0.46	1/4879 (0.0%)	0.69	0/6622
1	D	0.46	1/4879 (0.0%)	0.69	0/6622
All	All	0.46	4/19516 (0.0%)	0.69	0/26488

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	404	VAL	C-N	5.86	1.40	1.34
1	D	404	VAL	C-N	5.85	1.40	1.34
1	A	404	VAL	C-N	5.80	1.40	1.34
1	B	404	VAL	C-N	5.76	1.40	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4770	0	4826	40	0
1	B	4770	0	4826	41	0
1	C	4770	0	4826	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4770	0	4826	40	0
2	A	105	0	147	9	0
2	B	105	0	147	10	0
2	C	105	0	147	9	0
2	D	105	0	147	10	0
3	A	13	0	20	1	0
3	B	13	0	20	2	0
3	C	13	0	20	2	0
3	D	13	0	20	2	0
4	A	313	0	480	16	0
4	B	313	0	480	20	0
4	C	313	0	480	15	0
4	D	313	0	480	14	0
5	A	1	0	0	0	0
6	A	18	0	0	0	0
6	B	18	0	0	0	0
6	C	18	0	0	0	0
6	D	18	0	0	1	0
All	All	20877	0	21892	192	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.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:TYR:CE1	2:B:803:Y01:HAL2	2.27	0.70
1:C:467:TYR:CE1	2:C:803:Y01:HAL2	2.26	0.70
1:A:467:TYR:CE1	2:A:801:Y01:HAL2	2.26	0.70
1:D:467:TYR:CE1	2:D:805:Y01:HAL2	2.28	0.69
1:A:483:GLN:HE21	4:A:806:POV:H22	1.62	0.65
1:A:492:ARG:HD2	1:D:474:MET:HB3	1.81	0.62
1:C:459:VAL:HG21	2:C:804:Y01:HAN1	1.81	0.62
1:B:459:VAL:HG21	2:B:804:Y01:HAN1	1.82	0.62
1:B:552:PRO:HA	4:B:802:POV:H15A	1.82	0.61
1:A:459:VAL:HG21	2:A:802:Y01:HAN1	1.83	0.61
1:C:270:TYR:OH	1:D:118:GLN:NE2	2.34	0.60
1:B:474:MET:HB3	1:C:492:ARG:HD2	1.85	0.59
1:A:270:TYR:OH	1:B:118:GLN:NE2	2.36	0.59
1:D:459:VAL:HG21	2:D:806:Y01:HAN1	1.84	0.58
1:A:474:MET:HB3	1:B:492:ARG:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:810:POV:H21G	3:B:805:PCW:H262	1.85	0.58
1:C:474:MET:HB3	1:D:492:ARG:HD2	1.84	0.58
1:B:270:TYR:OH	1:C:118:GLN:NE2	2.37	0.57
1:A:552:PRO:HA	4:A:812:POV:H15A	1.86	0.56
1:A:118:GLN:NE2	1:D:270:TYR:OH	2.38	0.56
1:A:452:VAL:HG13	1:A:453:PRO:HD3	1.87	0.56
1:B:452:VAL:HG13	1:B:453:PRO:HD3	1.87	0.56
1:C:452:VAL:HG13	1:C:453:PRO:HD3	1.87	0.55
1:D:452:VAL:HG13	1:D:453:PRO:HD3	1.87	0.55
1:D:431:THR:HG21	4:D:810:POV:H21E	1.88	0.55
1:D:435:MET:HE1	4:D:808:POV:H21C	1.89	0.54
1:C:435:MET:HE1	4:C:806:POV:H21C	1.90	0.54
1:D:552:PRO:HA	4:D:804:POV:H15A	1.90	0.54
4:B:812:POV:H21G	3:C:805:PCW:H262	1.89	0.54
1:C:552:PRO:HA	4:C:802:POV:H15A	1.88	0.53
4:C:812:POV:H21G	3:D:807:PCW:H262	1.90	0.53
1:B:483:GLN:HE21	4:B:808:POV:H22	1.72	0.53
1:B:190:ARG:HG2	1:B:232:LEU:HD13	1.90	0.53
1:B:423:GLY:N	2:B:803:Y01:OAH	2.42	0.53
1:C:190:ARG:HG2	1:C:232:LEU:HD13	1.90	0.52
1:C:423:GLY:N	2:C:803:Y01:OAH	2.42	0.52
1:A:190:ARG:HG2	1:A:232:LEU:HD13	1.90	0.52
1:C:623:TYR:HA	1:D:42:LYS:HD2	1.92	0.51
1:D:190:ARG:HG2	1:D:232:LEU:HD13	1.90	0.51
1:A:423:GLY:N	2:A:801:Y01:OAH	2.42	0.51
1:D:423:GLY:N	2:D:805:Y01:OAH	2.43	0.51
1:C:431:THR:HG21	4:C:808:POV:H21E	1.92	0.51
1:B:435:MET:HE1	4:B:806:POV:H21C	1.94	0.50
1:B:389:GLU:HB3	4:B:809:POV:H210	1.94	0.50
1:C:483:GLN:HE21	4:C:808:POV:H22	1.77	0.50
1:C:486:ILE:HD12	2:C:804:Y01:HAD3	1.94	0.50
1:C:467:TYR:HE1	2:C:803:Y01:HAL2	1.77	0.50
1:B:467:TYR:HE1	2:B:803:Y01:HAL2	1.77	0.50
1:C:632:ARG:HH12	1:D:37:ASN:HD22	1.60	0.50
1:C:481:MET:SD	1:C:582:HIS:ND1	2.85	0.49
1:D:481:MET:SD	1:D:582:HIS:ND1	2.85	0.49
1:D:563:ALA:O	1:D:567:THR:OG1	2.30	0.49
1:A:42:LYS:HD2	1:D:623:TYR:HA	1.94	0.49
1:A:481:MET:SD	1:A:582:HIS:ND1	2.85	0.49
1:A:486:ILE:HD12	2:A:802:Y01:HAD3	1.93	0.49
1:A:568:LEU:O	1:A:572:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ILE:HD12	2:B:804:Y01:HAD3	1.93	0.49
3:A:803:PCW:H262	4:D:802:POV:H21G	1.94	0.49
1:B:563:ALA:O	1:B:567:THR:OG1	2.30	0.49
1:D:45:TRP:HA	1:D:51:LEU:HD12	1.94	0.49
1:D:568:LEU:O	1:D:572:ASN:ND2	2.46	0.49
1:A:45:TRP:HA	1:A:51:LEU:HD12	1.94	0.49
1:C:568:LEU:O	1:C:572:ASN:ND2	2.46	0.49
1:B:45:TRP:HA	1:B:51:LEU:HD12	1.94	0.48
1:B:481:MET:SD	1:B:582:HIS:ND1	2.85	0.48
1:C:45:TRP:HA	1:C:51:LEU:HD12	1.94	0.48
1:D:483:GLN:HE21	4:D:810:POV:H22	1.78	0.48
1:A:623:TYR:HA	1:B:42:LYS:HD2	1.94	0.48
1:B:568:LEU:O	1:B:572:ASN:ND2	2.46	0.48
1:B:623:TYR:HA	1:C:42:LYS:HD2	1.96	0.47
1:A:37:ASN:HD22	1:D:632:ARG:HH12	1.62	0.47
4:B:811:POV:H37	4:B:811:POV:H34A	1.77	0.47
1:A:632:ARG:HH12	1:B:37:ASN:HD22	1.61	0.47
4:A:809:POV:H215	3:B:805:PCW:H20	1.95	0.47
4:C:808:POV:H2	4:C:808:POV:H22A	1.66	0.47
1:B:553:PHE:H	4:B:802:POV:H14B	1.80	0.47
4:B:802:POV:H32	4:B:802:POV:H35A	1.78	0.47
1:B:632:ARG:HH12	1:C:37:ASN:HD22	1.63	0.46
1:C:285:SER:O	1:C:615:ARG:NH1	2.48	0.46
1:C:563:ALA:O	1:C:567:THR:OG1	2.30	0.46
1:A:535:GLU:HG2	1:A:540:ILE:HD11	1.98	0.46
1:C:553:PHE:H	4:C:802:POV:H14B	1.81	0.46
4:D:810:POV:H2	4:D:810:POV:H22A	1.66	0.46
2:A:811:Y01:HAC3	2:A:811:Y01:HAJ2	1.72	0.45
4:B:806:POV:H21A	4:B:806:POV:H28	1.76	0.45
4:B:812:POV:H32A	4:B:812:POV:H35A	1.77	0.45
1:D:285:SER:O	1:D:615:ARG:NH1	2.48	0.45
1:D:535:GLU:HG2	1:D:540:ILE:HD11	1.98	0.45
4:C:811:POV:H215	3:D:807:PCW:H20	1.99	0.45
1:B:285:SER:O	1:B:615:ARG:NH1	2.48	0.45
1:C:632:ARG:NH2	1:C:634:GLU:OE1	2.50	0.45
1:D:632:ARG:NH2	1:D:634:GLU:OE1	2.50	0.45
1:A:389:GLU:HB3	4:A:807:POV:H210	1.99	0.45
1:B:535:GLU:HG2	1:B:540:ILE:HD11	1.98	0.45
4:D:801:POV:H311	4:D:801:POV:H38A	1.71	0.45
1:A:563:ALA:O	1:A:567:THR:OG1	2.30	0.45
4:B:802:POV:H215	4:B:802:POV:H21J	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:ILE:HD12	2:D:806:Y01:HAD3	1.99	0.45
4:A:809:POV:H311	4:A:809:POV:H38A	1.77	0.44
1:C:557:ILE:HG23	4:C:802:POV:H21J	1.99	0.44
1:B:379:THR:HG23	1:B:381:LYS:H	1.82	0.44
1:C:535:GLU:HG2	1:C:540:ILE:HD11	1.98	0.44
2:C:801:Y01:HAA1	2:C:801:Y01:HAJ2	1.76	0.44
4:B:802:POV:H310	4:B:802:POV:H313	1.81	0.44
1:A:379:THR:HG23	1:A:381:LYS:H	1.83	0.44
2:B:801:Y01:HAA1	2:B:801:Y01:HAJ2	1.73	0.44
4:D:809:POV:H33A	4:D:809:POV:H36A	1.77	0.44
4:A:810:POV:H32A	4:A:810:POV:H35A	1.78	0.44
1:B:632:ARG:NH2	1:B:634:GLU:OE1	2.50	0.44
4:C:812:POV:H32A	4:C:812:POV:H35A	1.78	0.44
1:A:632:ARG:NH2	1:A:634:GLU:OE1	2.50	0.44
1:C:459:VAL:CG2	2:C:804:Y01:HAN1	2.47	0.44
2:D:803:Y01:HAC3	2:D:803:Y01:HAJ2	1.72	0.44
1:B:431:THR:HG21	4:B:808:POV:H21E	1.98	0.44
4:B:808:POV:H21F	4:B:808:POV:H21C	1.88	0.44
1:C:379:THR:HG23	1:C:381:LYS:H	1.82	0.44
1:A:285:SER:O	1:A:615:ARG:NH1	2.48	0.44
4:C:809:POV:H21B	4:C:809:POV:H21E	1.78	0.44
1:C:596:GLN:NE2	2:C:804:Y01:OAH	2.51	0.43
1:A:557:ILE:HG23	4:A:812:POV:H21J	2.00	0.43
1:C:84:HIS:HD2	1:C:120:ALA:HB2	1.83	0.43
1:A:122:HIS:CD2	1:A:166:PRO:HG3	2.53	0.43
4:B:807:POV:H33A	4:B:807:POV:H36A	1.75	0.43
1:D:84:HIS:HD2	1:D:120:ALA:HB2	1.83	0.43
1:A:425:PHE:HB2	2:A:801:Y01:HAL1	2.00	0.43
1:B:84:HIS:HD2	1:B:120:ALA:HB2	1.83	0.43
2:D:806:Y01:HAC3	2:D:806:Y01:HAJ1	1.80	0.43
1:A:467:TYR:HE1	2:A:801:Y01:HAL2	1.77	0.43
4:A:812:POV:H35	4:A:812:POV:H32	1.78	0.43
4:B:811:POV:H21G	4:B:811:POV:H214	1.84	0.43
1:C:122:HIS:CD2	1:C:166:PRO:HG3	2.53	0.43
4:D:804:POV:H35A	4:D:804:POV:H32	1.83	0.43
4:B:808:POV:H2	4:B:808:POV:H22A	1.65	0.43
1:D:459:VAL:CG2	2:D:806:Y01:HAN1	2.47	0.43
1:B:122:HIS:CD2	1:B:166:PRO:HG3	2.53	0.43
1:D:263:ARG:NE	6:D:904:HOH:O	2.49	0.43
1:D:379:THR:HG23	1:D:381:LYS:H	1.82	0.43
1:B:425:PHE:HB2	2:B:803:Y01:HAL1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:806:POV:H35	4:A:806:POV:H38	1.93	0.42
4:B:811:POV:H215	3:C:805:PCW:H20	2.01	0.42
1:A:553:PHE:H	4:A:812:POV:H14B	1.84	0.42
4:A:806:POV:H22A	4:A:806:POV:H2	1.63	0.42
1:B:596:GLN:NE2	2:B:804:Y01:OAH	2.52	0.42
4:B:811:POV:H311	4:B:811:POV:H38A	1.77	0.42
1:B:438:VAL:HG22	4:B:810:POV:H37A	2.01	0.42
1:C:339:TYR:HE1	1:C:392:THR:HA	1.84	0.42
1:D:92:LEU:HG	1:D:96:MET:HE2	2.01	0.42
4:A:812:POV:H310	4:A:812:POV:H313	1.95	0.42
1:A:339:TYR:CE1	1:A:392:THR:HA	2.55	0.42
4:C:802:POV:H32	4:C:802:POV:H35A	1.81	0.42
1:D:122:HIS:CD2	1:D:166:PRO:HG3	2.53	0.42
1:C:92:LEU:HG	1:C:96:MET:HE2	2.01	0.42
1:C:425:PHE:HB2	2:C:803:Y01:HAL1	2.02	0.42
1:D:557:ILE:HG23	4:D:804:POV:H21J	2.00	0.42
1:A:596:GLN:NE2	2:A:802:Y01:OAH	2.52	0.42
1:B:230:GLN:NE2	1:B:234:LEU:O	2.53	0.42
2:B:804:Y01:HAC3	2:B:804:Y01:HAJ1	1.80	0.42
1:A:84:HIS:HD2	1:A:120:ALA:HB2	1.83	0.42
1:B:339:TYR:CE1	1:B:392:THR:HA	2.55	0.42
1:A:514:THR:HA	1:D:368:LEU:HB2	2.02	0.42
1:C:230:GLN:NE2	1:C:234:LEU:O	2.53	0.42
4:A:809:POV:H37	4:A:809:POV:H34A	1.77	0.41
1:D:339:TYR:CE1	1:D:392:THR:HA	2.55	0.41
1:D:339:TYR:HE1	1:D:392:THR:HA	1.84	0.41
1:A:92:LEU:HG	1:A:96:MET:HE2	2.01	0.41
1:C:339:TYR:CE1	1:C:392:THR:HA	2.55	0.41
1:D:230:GLN:NE2	1:D:234:LEU:O	2.53	0.41
1:D:467:TYR:HE1	2:D:805:Y01:HAL2	1.79	0.41
1:A:230:GLN:NE2	1:A:234:LEU:O	2.53	0.41
1:B:92:LEU:HG	1:B:96:MET:HE2	2.01	0.41
4:C:807:POV:H33A	4:C:807:POV:H36A	1.76	0.41
4:A:807:POV:H27	4:A:807:POV:H24A	1.81	0.41
1:D:424:PRO:HB2	2:D:806:Y01:HAR1	2.02	0.41
1:D:75:ARG:HD2	1:D:79:GLY:HA2	2.02	0.41
4:D:802:POV:H32A	4:D:802:POV:H35A	1.79	0.41
1:B:339:TYR:HE1	1:B:392:THR:HA	1.84	0.41
1:A:459:VAL:CG2	2:A:802:Y01:HAN1	2.49	0.41
1:A:339:TYR:HE1	1:A:392:THR:HA	1.84	0.41
1:B:75:ARG:HD2	1:B:79:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:804:Y01:HAO1	2:B:804:Y01:HAP1	1.93	0.41
4:C:802:POV:H310	4:C:802:POV:H313	1.91	0.41
1:D:596:GLN:NE2	2:D:806:Y01:OAH	2.53	0.41
4:D:801:POV:H34A	4:D:801:POV:H37	1.75	0.41
4:A:806:POV:H21F	4:A:806:POV:H21C	1.91	0.41
1:B:543:GLY:HA2	1:B:544:PRO:HD3	1.94	0.40
1:A:75:ARG:HD2	1:A:79:GLY:HA2	2.02	0.40
4:C:806:POV:H28	4:C:806:POV:H21A	1.78	0.40
1:A:340:ILE:HD12	1:A:340:ILE:HG23	1.91	0.40
1:C:615:ARG:HE	1:C:629:TRP:CD1	2.39	0.40
4:D:811:POV:H21B	4:D:811:POV:H21E	1.88	0.40
1:B:632:ARG:HH11	1:B:632:ARG:HD2	1.75	0.40
4:D:804:POV:H21J	4:D:804:POV:H215	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	590/765 (77%)	552 (94%)	37 (6%)	1 (0%)	43	73
1	B	590/765 (77%)	552 (94%)	37 (6%)	1 (0%)	43	73
1	C	590/765 (77%)	552 (94%)	37 (6%)	1 (0%)	43	73
1	D	590/765 (77%)	551 (93%)	38 (6%)	1 (0%)	43	73
All	All	2360/3060 (77%)	2207 (94%)	149 (6%)	4 (0%)	44	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	CYS
1	B	70	CYS

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Mol	Chain	Res	Type
1	C	70	CYS
1	D	70	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/662 (78%)	510 (99%)	6 (1%)	63	79
1	B	516/662 (78%)	510 (99%)	6 (1%)	63	79
1	C	516/662 (78%)	510 (99%)	6 (1%)	63	79
1	D	516/662 (78%)	510 (99%)	6 (1%)	63	79
All	All	2064/2648 (78%)	2040 (99%)	24 (1%)	61	79

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	132	LEU
1	A	229	LEU
1	A	365	ASN
1	A	452	VAL
1	A	458	LEU
1	B	121	LEU
1	B	132	LEU
1	B	229	LEU
1	B	365	ASN
1	B	452	VAL
1	B	458	LEU
1	C	121	LEU
1	C	132	LEU
1	C	229	LEU
1	C	365	ASN
1	C	452	VAL
1	C	458	LEU
1	D	121	LEU

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Mol	Chain	Res	Type
1	D	132	LEU
1	D	229	LEU
1	D	365	ASN
1	D	452	VAL
1	D	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	37	ASN
1	A	40	GLN
1	A	84	HIS
1	A	118	GLN
1	A	365	ASN
1	A	369	GLN
1	A	483	GLN
1	A	572	ASN
1	B	31	GLN
1	B	37	ASN
1	B	40	GLN
1	B	62	ASN
1	B	84	HIS
1	B	118	GLN
1	B	174	ASN
1	B	217	ASN
1	B	258	HIS
1	B	365	ASN
1	B	483	GLN
1	B	572	ASN
1	C	31	GLN
1	C	37	ASN
1	C	40	GLN
1	C	84	HIS
1	C	118	GLN
1	C	174	ASN
1	C	365	ASN
1	C	369	GLN
1	C	483	GLN
1	C	572	ASN
1	D	31	GLN
1	D	37	ASN

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Mol	Chain	Res	Type
1	D	40	GLN
1	D	62	ASN
1	D	84	HIS
1	D	118	GLN
1	D	174	ASN
1	D	365	ASN
1	D	369	GLN
1	D	572	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 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	POV	A	809	-	51,51,51	1.04	3 (5%)	57,59,59	0.97	3 (5%)
3	PCW	A	803	-	12,12,53	0.78	0	11,11,61	0.37	0
4	POV	C	810	-	13,13,51	1.11	1 (7%)	13,13,59	0.78	1 (7%)
4	POV	C	812	-	51,51,51	1.08	4 (7%)	57,59,59	0.85	3 (5%)
4	POV	B	806	-	19,19,51	1.35	2 (10%)	19,19,59	1.06	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	B	812	-	51,51,51	1.09	4 (7%)	57,59,59	0.86	3 (5%)
2	Y01	B	801	-	38,38,38	0.56	0	57,57,57	0.92	2 (3%)
4	POV	C	811	-	51,51,51	1.04	3 (5%)	57,59,59	0.98	3 (5%)
3	PCW	B	805	-	12,12,53	0.77	0	11,11,61	0.40	0
4	POV	D	809	-	51,51,51	1.07	3 (5%)	57,59,59	1.01	3 (5%)
2	Y01	C	801	-	38,38,38	0.55	0	57,57,57	0.88	1 (1%)
4	POV	B	808	-	51,51,51	1.09	3 (5%)	57,59,59	1.01	3 (5%)
3	PCW	C	805	-	12,12,53	0.78	0	11,11,61	0.40	0
4	POV	C	806	-	19,19,51	1.35	2 (10%)	19,19,59	1.07	2 (10%)
4	POV	A	810	-	51,51,51	1.09	4 (7%)	57,59,59	0.86	3 (5%)
4	POV	C	808	-	51,51,51	1.09	3 (5%)	57,59,59	1.01	3 (5%)
4	POV	A	804	-	19,19,51	1.36	2 (10%)	19,19,59	1.01	1 (5%)
4	POV	B	809	-	18,18,51	1.40	2 (11%)	18,18,59	0.87	1 (5%)
2	Y01	A	801	-	38,38,38	0.61	1 (2%)	57,57,57	0.64	0
4	POV	D	801	-	51,51,51	1.04	3 (5%)	57,59,59	0.97	3 (5%)
4	POV	D	804	-	51,51,51	1.08	3 (5%)	57,59,59	0.92	3 (5%)
4	POV	D	812	-	13,13,51	1.12	1 (7%)	13,13,59	0.79	1 (7%)
2	Y01	A	811	-	38,38,38	0.55	0	57,57,57	0.89	1 (1%)
4	POV	D	811	-	18,18,51	1.40	2 (11%)	18,18,59	0.90	1 (5%)
2	Y01	C	803	-	38,38,38	0.62	1 (2%)	57,57,57	0.64	0
4	POV	B	802	-	51,51,51	1.08	3 (5%)	57,59,59	0.93	3 (5%)
2	Y01	B	803	-	38,38,38	0.62	1 (2%)	57,57,57	0.64	0
4	POV	C	802	-	51,51,51	1.08	3 (5%)	57,59,59	0.92	3 (5%)
4	POV	A	808	-	13,13,51	1.10	1 (7%)	13,13,59	0.80	1 (7%)
3	PCW	D	807	-	12,12,53	0.78	0	11,11,61	0.40	0
2	Y01	B	804	-	38,38,38	0.55	0	57,57,57	0.64	0
4	POV	C	809	-	18,18,51	1.40	2 (11%)	18,18,59	0.89	1 (5%)
4	POV	D	810	-	51,51,51	1.09	3 (5%)	57,59,59	1.02	3 (5%)
2	Y01	D	803	-	38,38,38	0.56	0	57,57,57	0.88	0
4	POV	C	807	-	51,51,51	1.07	3 (5%)	57,59,59	1.01	3 (5%)
4	POV	D	802	-	51,51,51	1.09	4 (7%)	57,59,59	0.84	3 (5%)
2	Y01	D	805	-	38,38,38	0.61	1 (2%)	57,57,57	0.64	0
2	Y01	D	806	-	38,38,38	0.55	0	57,57,57	0.64	0
4	POV	B	811	-	51,51,51	1.04	3 (5%)	57,59,59	0.98	3 (5%)
4	POV	B	807	-	51,51,51	1.07	3 (5%)	57,59,59	0.99	3 (5%)
4	POV	D	808	-	19,19,51	1.36	2 (10%)	19,19,59	1.07	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y01	A	802	-	38,38,38	0.55	0	57,57,57	0.65	0
4	POV	A	806	-	51,51,51	1.08	3 (5%)	57,59,59	0.98	3 (5%)
2	Y01	C	804	-	38,38,38	0.55	0	57,57,57	0.64	0
4	POV	A	812	-	51,51,51	1.07	3 (5%)	57,59,59	0.91	3 (5%)
4	POV	A	805	-	51,51,51	1.08	3 (5%)	57,59,59	1.01	3 (5%)
4	POV	B	810	-	13,13,51	1.11	1 (7%)	13,13,59	0.78	1 (7%)
4	POV	A	807	-	18,18,51	1.41	2 (11%)	18,18,59	0.86	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	A	809	-	-	35/55/55/55	-
3	PCW	A	803	-	-	6/10/10/57	-
4	POV	C	810	-	-	8/12/12/55	-
4	POV	C	812	-	-	26/55/55/55	-
4	POV	B	806	-	-	6/18/18/55	-
4	POV	B	812	-	-	29/55/55/55	-
2	Y01	B	801	-	-	13/19/77/77	0/4/4/4
4	POV	C	811	-	-	34/55/55/55	-
3	PCW	B	805	-	-	5/10/10/57	-
4	POV	D	809	-	-	29/55/55/55	-
2	Y01	C	801	-	-	13/19/77/77	0/4/4/4
4	POV	B	808	-	-	34/55/55/55	-
3	PCW	C	805	-	-	5/10/10/57	-
4	POV	C	806	-	-	6/18/18/55	-
4	POV	A	810	-	-	29/55/55/55	-
4	POV	C	808	-	-	33/55/55/55	-
4	POV	A	804	-	-	5/18/18/55	-
4	POV	B	809	-	-	7/17/17/55	-
2	Y01	A	801	-	-	3/19/77/77	0/4/4/4
4	POV	D	801	-	-	34/55/55/55	-
4	POV	D	804	-	-	23/55/55/55	-
4	POV	D	812	-	-	8/12/12/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	A	811	-	-	13/19/77/77	0/4/4/4
4	POV	D	811	-	-	6/17/17/55	-
2	Y01	C	803	-	-	2/19/77/77	0/4/4/4
4	POV	B	802	-	-	24/55/55/55	-
2	Y01	B	803	-	-	2/19/77/77	0/4/4/4
4	POV	C	802	-	-	23/55/55/55	-
4	POV	A	808	-	-	8/12/12/55	-
3	PCW	D	807	-	-	5/10/10/57	-
2	Y01	B	804	-	-	11/19/77/77	0/4/4/4
4	POV	C	809	-	-	7/17/17/55	-
4	POV	D	810	-	-	33/55/55/55	-
2	Y01	D	803	-	-	13/19/77/77	0/4/4/4
4	POV	C	807	-	-	27/55/55/55	-
4	POV	D	802	-	-	25/55/55/55	-
2	Y01	D	805	-	-	2/19/77/77	0/4/4/4
2	Y01	D	806	-	-	11/19/77/77	0/4/4/4
4	POV	B	811	-	-	35/55/55/55	-
4	POV	B	807	-	-	30/55/55/55	-
4	POV	D	808	-	-	6/18/18/55	-
2	Y01	A	802	-	-	11/19/77/77	0/4/4/4
4	POV	A	806	-	-	31/55/55/55	-
2	Y01	C	804	-	-	11/19/77/77	0/4/4/4
4	POV	A	812	-	-	23/55/55/55	-
4	POV	A	805	-	-	32/55/55/55	-
4	POV	B	810	-	-	8/12/12/55	-
4	POV	A	807	-	-	7/17/17/55	-

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	807	POV	C29-C210	4.14	1.55	1.31
4	C	809	POV	C29-C210	4.09	1.54	1.31
4	B	809	POV	C29-C210	4.08	1.54	1.31
4	D	811	POV	C29-C210	4.08	1.54	1.31
4	A	804	POV	C29-C210	4.08	1.54	1.31
4	D	808	POV	C29-C210	4.08	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	806	POV	C29-C210	4.06	1.54	1.31
4	B	806	POV	C29-C210	4.05	1.54	1.31
4	D	801	POV	O21-C21	3.09	1.43	1.34
4	C	808	POV	O21-C21	3.07	1.43	1.34
4	A	809	POV	O21-C21	3.06	1.42	1.34
4	D	810	POV	O21-C21	3.05	1.42	1.34
4	B	811	POV	O21-C21	3.05	1.42	1.34
4	C	811	POV	O21-C21	3.05	1.42	1.34
4	B	808	POV	O21-C21	3.02	1.42	1.34
4	A	806	POV	O21-C21	2.99	1.42	1.34
4	D	810	POV	O31-C31	2.92	1.41	1.33
4	C	808	POV	O31-C31	2.92	1.41	1.33
4	B	808	POV	O31-C31	2.92	1.41	1.33
4	D	802	POV	O21-C21	2.91	1.42	1.34
4	C	802	POV	O21-C21	2.87	1.42	1.34
4	B	812	POV	O21-C21	2.87	1.42	1.34
4	A	810	POV	O21-C21	2.86	1.42	1.34
4	A	805	POV	O21-C21	2.86	1.42	1.34
4	C	812	POV	O21-C21	2.86	1.42	1.34
4	B	802	POV	O21-C21	2.84	1.42	1.34
4	D	809	POV	O21-C21	2.83	1.42	1.34
4	C	807	POV	O21-C21	2.82	1.42	1.34
4	D	804	POV	O21-C21	2.81	1.42	1.34
4	A	806	POV	O31-C31	2.81	1.41	1.33
4	B	807	POV	O21-C21	2.80	1.42	1.34
4	B	806	POV	O21-C21	2.77	1.41	1.33
4	D	808	POV	O21-C21	2.77	1.41	1.33
4	A	812	POV	O21-C21	2.76	1.42	1.34
4	A	804	POV	O21-C21	2.76	1.41	1.33
4	B	802	POV	O31-C31	2.75	1.41	1.33
4	B	807	POV	O21-C2	-2.74	1.40	1.46
4	C	807	POV	O21-C2	-2.74	1.40	1.46
4	D	804	POV	O31-C31	2.73	1.41	1.33
4	C	806	POV	O21-C21	2.73	1.41	1.33
4	C	802	POV	O31-C31	2.73	1.41	1.33
4	D	811	POV	O21-C21	2.71	1.41	1.33
4	D	809	POV	O21-C2	-2.71	1.40	1.46
4	C	809	POV	O21-C21	2.71	1.41	1.33
4	A	805	POV	O21-C2	-2.70	1.40	1.46
4	B	809	POV	O21-C21	2.70	1.41	1.33
4	A	812	POV	O31-C31	2.70	1.41	1.33
4	A	807	POV	O21-C21	2.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	812	POV	O31-C31	2.65	1.41	1.33
4	B	810	POV	O31-C31	2.63	1.41	1.33
4	C	810	POV	O31-C31	2.63	1.41	1.33
4	A	808	POV	O31-C31	2.62	1.41	1.33
4	D	802	POV	O31-C31	2.59	1.40	1.33
4	A	812	POV	O21-C2	-2.59	1.40	1.46
4	B	812	POV	O21-C2	-2.58	1.40	1.46
4	B	802	POV	O21-C2	-2.57	1.40	1.46
4	C	812	POV	O21-C2	-2.57	1.40	1.46
4	A	810	POV	O21-C2	-2.56	1.40	1.46
4	C	802	POV	O21-C2	-2.55	1.40	1.46
4	D	804	POV	O21-C2	-2.55	1.40	1.46
4	B	812	POV	O31-C31	2.53	1.40	1.33
4	D	802	POV	O21-C2	-2.52	1.40	1.46
4	A	805	POV	O31-C31	2.52	1.40	1.33
4	D	809	POV	O31-C31	2.52	1.40	1.33
4	C	807	POV	O31-C31	2.51	1.40	1.33
4	A	810	POV	O31-C31	2.51	1.40	1.33
4	D	801	POV	O31-C31	2.50	1.40	1.33
4	C	812	POV	O31-C31	2.50	1.40	1.33
4	B	807	POV	O31-C31	2.48	1.40	1.33
4	A	809	POV	O31-C31	2.48	1.40	1.33
4	B	811	POV	O31-C31	2.46	1.40	1.33
4	B	808	POV	O21-C2	-2.45	1.40	1.46
4	D	810	POV	O21-C2	-2.43	1.40	1.46
4	C	808	POV	O21-C2	-2.43	1.40	1.46
4	A	806	POV	O21-C2	-2.42	1.40	1.46
4	C	811	POV	O31-C31	2.42	1.40	1.33
2	B	803	Y01	OAH-CAX	-2.34	1.23	1.30
2	D	805	Y01	OAH-CAX	-2.34	1.23	1.30
2	A	801	Y01	OAH-CAX	-2.33	1.23	1.30
2	C	803	Y01	OAH-CAX	-2.33	1.23	1.30
4	D	801	POV	O21-C2	-2.18	1.41	1.46
4	C	811	POV	O21-C2	-2.17	1.41	1.46
4	B	811	POV	O21-C2	-2.17	1.41	1.46
4	A	809	POV	O21-C2	-2.16	1.41	1.46
4	D	802	POV	P-O12	2.03	1.67	1.59
4	B	812	POV	P-O12	2.02	1.67	1.59
4	A	810	POV	P-O12	2.01	1.67	1.59
4	C	812	POV	P-O12	2.00	1.67	1.59

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	810	POV	O21-C21-C22	4.93	122.15	111.48
4	B	808	POV	O21-C21-C22	4.91	122.09	111.48
4	C	808	POV	O21-C21-C22	4.86	122.00	111.48
4	A	806	POV	O21-C21-C22	4.67	121.59	111.48
4	C	807	POV	O21-C21-C22	4.56	121.35	111.48
4	D	809	POV	O21-C21-C22	4.54	121.30	111.48
4	B	807	POV	O21-C21-C22	4.38	120.96	111.48
4	A	805	POV	O21-C21-C22	4.37	120.93	111.48
4	C	802	POV	O21-C21-C22	4.12	120.40	111.48
4	B	802	POV	O21-C21-C22	4.07	120.28	111.48
4	D	804	POV	O21-C21-C22	4.04	120.22	111.48
4	A	812	POV	O21-C21-C22	4.00	120.14	111.48
4	B	811	POV	O21-C21-C22	3.98	120.09	111.48
4	C	811	POV	O21-C21-C22	3.96	120.04	111.48
4	A	809	POV	O21-C21-C22	3.91	119.95	111.48
4	D	801	POV	O21-C21-C22	3.91	119.94	111.48
4	A	810	POV	O21-C21-C22	3.87	119.84	111.48
4	B	812	POV	O21-C21-C22	3.86	119.82	111.48
4	C	812	POV	O21-C21-C22	3.81	119.73	111.48
4	D	802	POV	O21-C21-C22	3.77	119.64	111.48
4	C	811	POV	C14-N-C12	2.76	120.88	109.91
4	A	809	POV	C14-N-C12	2.75	120.84	109.91
4	D	801	POV	C14-N-C12	2.74	120.81	109.91
4	B	811	POV	C14-N-C12	2.74	120.80	109.91
4	C	806	POV	O21-C21-C22	2.68	120.02	111.83
4	B	802	POV	O31-C31-C32	2.68	120.00	111.83
4	B	806	POV	O21-C21-C22	2.67	119.96	111.83
4	D	808	POV	O21-C21-C22	2.66	119.96	111.83
4	C	808	POV	O31-C31-C32	2.65	119.92	111.83
4	B	808	POV	O31-C31-C32	2.64	119.89	111.83
4	D	810	POV	O31-C31-C32	2.63	119.86	111.83
4	A	805	POV	C14-N-C12	2.62	120.33	109.91
4	A	806	POV	O31-C31-C32	2.58	119.71	111.83
4	A	804	POV	O21-C21-C22	2.55	119.61	111.83
4	B	807	POV	C14-N-C12	2.53	119.98	109.91
4	D	809	POV	C14-N-C12	2.53	119.97	109.91
4	A	805	POV	O31-C31-C32	2.52	119.53	111.83
4	C	807	POV	C14-N-C12	2.51	119.91	109.91
4	D	804	POV	O31-C31-C32	2.51	119.50	111.83
4	C	802	POV	O31-C31-C32	2.50	119.46	111.83
4	B	807	POV	O31-C31-C32	2.44	119.27	111.83
4	A	812	POV	O31-C31-C32	2.44	119.26	111.83
4	A	810	POV	O31-C31-C32	2.43	119.25	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	809	POV	O31-C31-C32	2.42	119.21	111.83
4	C	812	POV	O31-C31-C32	2.42	119.21	111.83
4	C	807	POV	O31-C31-C32	2.42	119.20	111.83
4	C	808	POV	C14-N-C12	2.41	119.51	109.91
4	B	812	POV	O31-C31-C32	2.41	119.20	111.83
4	D	801	POV	O31-C31-C32	2.41	119.20	111.83
4	D	810	POV	C14-N-C12	2.41	119.49	109.91
4	C	811	POV	O31-C31-C32	2.41	119.18	111.83
4	A	809	POV	O31-C31-C32	2.40	119.16	111.83
4	B	811	POV	O31-C31-C32	2.40	119.15	111.83
4	B	808	POV	C14-N-C12	2.39	119.41	109.91
4	D	802	POV	O31-C31-C32	2.36	119.05	111.83
4	A	806	POV	C14-N-C12	2.36	119.31	109.91
4	B	802	POV	C14-N-C12	2.24	118.82	109.91
4	D	808	POV	C211-C210-C29	-2.23	108.15	124.83
4	C	806	POV	C211-C210-C29	-2.19	108.39	124.83
2	B	801	Y01	CAR-CBC-CAV	-2.19	107.93	110.97
4	C	802	POV	C14-N-C12	2.18	118.59	109.91
4	A	812	POV	C14-N-C12	2.18	118.56	109.91
4	C	812	POV	C14-N-C12	2.16	118.51	109.91
4	D	802	POV	C14-N-C12	2.16	118.49	109.91
4	B	812	POV	C14-N-C12	2.15	118.47	109.91
4	B	806	POV	C211-C210-C29	-2.15	108.75	124.83
4	D	804	POV	C14-N-C12	2.15	118.44	109.91
4	A	810	POV	C14-N-C12	2.14	118.42	109.91
4	A	808	POV	O31-C31-C32	2.10	120.07	112.14
4	B	809	POV	O21-C21-C22	2.07	119.97	112.14
2	C	801	Y01	CAR-CBC-CAV	-2.06	108.11	110.97
2	A	811	Y01	CAR-CBC-CAV	-2.06	108.11	110.97
4	C	809	POV	O21-C21-C22	2.06	119.92	112.14
4	D	812	POV	O31-C31-C32	2.06	119.92	112.14
4	D	811	POV	O21-C21-C22	2.06	119.91	112.14
2	B	801	Y01	CBC-OAW-CAY	2.04	122.68	117.80
4	C	810	POV	O31-C31-C32	2.04	119.84	112.14
4	B	810	POV	O31-C31-C32	2.03	119.81	112.14
4	A	807	POV	O21-C21-C22	2.02	119.75	112.14

There are no chirality outliers.

All (797) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	811	Y01	CAV-CBC-OAW-CAY

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Mol	Chain	Res	Type	Atoms
2	B	801	Y01	CAV-CBC-OAW-CAY
2	C	801	Y01	CAV-CBC-OAW-CAY
2	D	803	Y01	CAV-CBC-OAW-CAY
4	A	805	POV	C11-O12-P-O11
4	A	805	POV	C11-O12-P-O13
4	A	805	POV	C11-O12-P-O14
4	A	805	POV	O12-C11-C12-N
4	A	805	POV	C22-C21-O21-C2
4	A	805	POV	O22-C21-O21-C2
4	A	806	POV	C1-O11-P-O12
4	A	806	POV	C1-O11-P-O14
4	A	806	POV	C22-C21-O21-C2
4	A	806	POV	O22-C21-O21-C2
4	A	809	POV	O22-C21-O21-C2
4	A	810	POV	O11-C1-C2-O21
4	A	812	POV	C11-O12-P-O11
4	A	812	POV	C11-O12-P-O14
4	A	812	POV	O12-C11-C12-N
4	A	812	POV	C22-C21-O21-C2
4	B	802	POV	C11-O12-P-O11
4	B	802	POV	C11-O12-P-O14
4	B	802	POV	O12-C11-C12-N
4	B	802	POV	C22-C21-O21-C2
4	B	807	POV	C11-O12-P-O11
4	B	807	POV	C11-O12-P-O13
4	B	807	POV	C11-O12-P-O14
4	B	807	POV	O12-C11-C12-N
4	B	807	POV	C22-C21-O21-C2
4	B	807	POV	O22-C21-O21-C2
4	B	808	POV	C1-O11-P-O12
4	B	808	POV	C1-O11-P-O14
4	B	808	POV	O12-C11-C12-N
4	B	808	POV	C22-C21-O21-C2
4	B	808	POV	O22-C21-O21-C2
4	B	811	POV	O22-C21-O21-C2
4	B	812	POV	O11-C1-C2-O21
4	C	802	POV	C11-O12-P-O11
4	C	802	POV	C11-O12-P-O14
4	C	802	POV	O12-C11-C12-N
4	C	802	POV	C22-C21-O21-C2
4	C	807	POV	C11-O12-P-O11
4	C	807	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
4	C	807	POV	C11-O12-P-O14
4	C	807	POV	O12-C11-C12-N
4	C	807	POV	C22-C21-O21-C2
4	C	807	POV	O22-C21-O21-C2
4	C	808	POV	C1-O11-P-O12
4	C	808	POV	C1-O11-P-O13
4	C	808	POV	C1-O11-P-O14
4	C	808	POV	O12-C11-C12-N
4	C	808	POV	C22-C21-O21-C2
4	C	808	POV	O22-C21-O21-C2
4	C	811	POV	C11-O12-P-O14
4	C	811	POV	O22-C21-O21-C2
4	C	812	POV	O11-C1-C2-O21
4	D	801	POV	C11-O12-P-O11
4	D	801	POV	C11-O12-P-O14
4	D	801	POV	O22-C21-O21-C2
4	D	802	POV	O11-C1-C2-O21
4	D	804	POV	C11-O12-P-O11
4	D	804	POV	C11-O12-P-O14
4	D	804	POV	O12-C11-C12-N
4	D	804	POV	C22-C21-O21-C2
4	D	809	POV	C11-O12-P-O11
4	D	809	POV	C11-O12-P-O13
4	D	809	POV	O12-C11-C12-N
4	D	809	POV	C22-C21-O21-C2
4	D	809	POV	O22-C21-O21-C2
4	D	810	POV	C1-O11-P-O12
4	D	810	POV	C1-O11-P-O13
4	D	810	POV	C1-O11-P-O14
4	D	810	POV	C22-C21-O21-C2
4	D	810	POV	O22-C21-O21-C2
4	B	811	POV	O32-C31-O31-C3
2	B	801	Y01	OAG-CAY-OAW-CBC
4	A	812	POV	O22-C21-O21-C2
4	B	802	POV	O22-C21-O21-C2
4	C	802	POV	O22-C21-O21-C2
4	D	804	POV	O22-C21-O21-C2
4	A	809	POV	C22-C21-O21-C2
4	B	811	POV	C22-C21-O21-C2
4	C	811	POV	C22-C21-O21-C2
4	D	801	POV	C22-C21-O21-C2
4	C	811	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
4	B	811	POV	C32-C31-O31-C3
4	A	809	POV	O32-C31-O31-C3
4	D	801	POV	O32-C31-O31-C3
4	C	811	POV	C32-C31-O31-C3
2	B	801	Y01	CAM-CAY-OAW-CBC
4	A	809	POV	C32-C31-O31-C3
4	D	801	POV	C32-C31-O31-C3
2	A	811	Y01	CAJ-CAO-CBB-CAC
2	B	801	Y01	CAJ-CAO-CBB-CAC
2	C	801	Y01	CAJ-CAO-CBB-CAC
2	D	803	Y01	CAJ-CAO-CBB-CAC
4	C	811	POV	C21-C22-C23-C24
4	D	801	POV	C21-C22-C23-C24
4	B	812	POV	C39-C310-C311-C312
4	C	812	POV	C39-C310-C311-C312
4	A	809	POV	C11-C12-N-C14
4	B	811	POV	C11-C12-N-C14
4	B	811	POV	C11-C12-N-C15
4	B	808	POV	C213-C214-C215-C216
2	A	801	Y01	CAX-CAL-CAM-CAY
2	B	803	Y01	CAX-CAL-CAM-CAY
2	C	803	Y01	CAX-CAL-CAM-CAY
2	D	805	Y01	CAX-CAL-CAM-CAY
4	A	810	POV	C39-C310-C311-C312
4	A	809	POV	C21-C22-C23-C24
4	B	812	POV	C31-C32-C33-C34
4	C	812	POV	C31-C32-C33-C34
4	A	806	POV	C213-C214-C215-C216
4	D	802	POV	C39-C310-C311-C312
4	A	805	POV	C21-C22-C23-C24
4	B	810	POV	C31-C32-C33-C34
4	B	811	POV	C21-C22-C23-C24
4	A	805	POV	C32-C31-O31-C3
4	A	808	POV	C31-C32-C33-C34
4	C	810	POV	C31-C32-C33-C34
4	D	802	POV	C31-C32-C33-C34
4	D	802	POV	C211-C212-C213-C214
4	A	804	POV	C211-C210-C29-C28
4	D	808	POV	C211-C210-C29-C28
4	C	807	POV	C32-C31-O31-C3
4	B	807	POV	C21-C22-C23-C24
4	C	807	POV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	C	812	POV	C21-C22-C23-C24
4	D	802	POV	C32-C33-C34-C35
4	A	809	POV	C11-C12-N-C15
4	C	811	POV	C11-C12-N-C14
4	A	812	POV	C21-C22-C23-C24
4	B	802	POV	C21-C22-C23-C24
4	B	802	POV	C31-C32-C33-C34
4	C	802	POV	C21-C22-C23-C24
4	D	804	POV	C21-C22-C23-C24
4	D	809	POV	C21-C22-C23-C24
4	D	812	POV	C31-C32-C33-C34
4	A	805	POV	O32-C31-O31-C3
2	B	801	Y01	CAN-CAJ-CAO-CBB
4	A	804	POV	C21-C22-C23-C24
4	A	806	POV	C31-C32-C33-C34
4	A	810	POV	C21-C22-C23-C24
4	A	810	POV	C31-C32-C33-C34
4	B	808	POV	C31-C32-C33-C34
4	B	812	POV	C21-C22-C23-C24
4	C	809	POV	C21-C22-C23-C24
4	D	802	POV	C21-C22-C23-C24
4	B	809	POV	C212-C213-C214-C215
2	A	811	Y01	CAN-CAJ-CAO-CBB
2	C	801	Y01	CAN-CAJ-CAO-CBB
4	D	809	POV	C32-C31-O31-C3
4	B	806	POV	C21-C22-C23-C24
4	C	806	POV	C21-C22-C23-C24
4	C	808	POV	C31-C32-C33-C34
4	D	810	POV	C31-C32-C33-C34
2	D	803	Y01	CAN-CAJ-CAO-CBB
2	C	801	Y01	OAG-CAY-OAW-CBC
4	A	807	POV	C26-C27-C28-C29
4	B	809	POV	C26-C27-C28-C29
4	D	811	POV	C26-C27-C28-C29
2	A	802	Y01	CAO-CAJ-CAN-CBA
2	B	804	Y01	CAO-CAJ-CAN-CBA
2	C	804	Y01	CAO-CAJ-CAN-CBA
4	C	806	POV	C211-C210-C29-C28
4	B	809	POV	C21-C22-C23-C24
4	B	807	POV	C32-C31-O31-C3
2	C	801	Y01	CAM-CAY-OAW-CBC
4	C	807	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
4	D	808	POV	C21-C22-C23-C24
4	D	811	POV	C21-C22-C23-C24
2	D	806	Y01	CAO-CAJ-CAN-CBA
4	D	810	POV	C213-C214-C215-C216
2	A	811	Y01	OAG-CAY-OAW-CBC
2	D	803	Y01	OAG-CAY-OAW-CBC
2	D	805	Y01	CAO-CAJ-CAN-CBA
4	C	808	POV	C213-C214-C215-C216
4	C	811	POV	C11-C12-N-C15
2	A	802	Y01	CAJ-CAO-CBB-CAC
2	A	811	Y01	CAX-CAL-CAM-CAY
2	B	801	Y01	CAX-CAL-CAM-CAY
2	C	801	Y01	CAX-CAL-CAM-CAY
2	D	803	Y01	CAX-CAL-CAM-CAY
2	A	811	Y01	CAM-CAY-OAW-CBC
2	D	803	Y01	CAM-CAY-OAW-CBC
4	B	806	POV	C211-C210-C29-C28
4	A	810	POV	C211-C212-C213-C214
2	B	804	Y01	CAJ-CAO-CBB-CAC
2	D	806	Y01	CAJ-CAO-CBB-CAC
2	C	803	Y01	CAO-CAJ-CAN-CBA
4	D	809	POV	O32-C31-O31-C3
4	B	812	POV	C211-C212-C213-C214
4	C	812	POV	C211-C212-C213-C214
4	A	806	POV	C313-C314-C315-C316
2	C	804	Y01	CAJ-CAO-CBB-CAC
4	B	807	POV	O32-C31-O31-C3
4	A	812	POV	C31-C32-C33-C34
4	C	802	POV	C31-C32-C33-C34
4	A	810	POV	C32-C33-C34-C35
4	A	809	POV	C11-C12-N-C13
4	D	801	POV	C11-C12-N-C15
2	B	801	Y01	CAO-CAJ-CAN-CBA
4	A	805	POV	C24-C25-C26-C27
4	B	807	POV	C24-C25-C26-C27
4	A	805	POV	C39-C310-C311-C312
4	A	808	POV	C35-C36-C37-C38
4	A	810	POV	C312-C313-C314-C315
4	C	802	POV	C23-C24-C25-C26
4	C	807	POV	C22-C23-C24-C25
4	C	807	POV	C24-C25-C26-C27
4	C	808	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
4	D	802	POV	C311-C310-C39-C38
4	D	809	POV	C22-C23-C24-C25
4	D	810	POV	C24-C25-C26-C27
4	C	808	POV	C313-C314-C315-C316
4	A	805	POV	C22-C23-C24-C25
4	B	807	POV	C22-C23-C24-C25
4	B	808	POV	C24-C25-C26-C27
4	C	808	POV	C36-C37-C38-C39
4	D	809	POV	C24-C25-C26-C27
4	A	809	POV	C211-C212-C213-C214
4	B	808	POV	C36-C37-C38-C39
4	B	812	POV	C312-C313-C314-C315
4	D	810	POV	C36-C37-C38-C39
4	B	807	POV	C213-C214-C215-C216
4	C	807	POV	C213-C214-C215-C216
4	C	809	POV	C26-C27-C28-C29
4	C	811	POV	C22-C23-C24-C25
4	D	801	POV	C22-C23-C24-C25
2	B	803	Y01	CAO-CAJ-CAN-CBA
4	C	807	POV	C34-C35-C36-C37
4	D	804	POV	C31-C32-C33-C34
4	B	808	POV	C212-C213-C214-C215
4	B	811	POV	C211-C212-C213-C214
4	B	811	POV	C22-C23-C24-C25
4	B	812	POV	C32-C33-C34-C35
4	C	807	POV	C36-C37-C38-C39
4	D	804	POV	C23-C24-C25-C26
4	A	809	POV	C22-C23-C24-C25
4	D	809	POV	C36-C37-C38-C39
4	A	808	POV	C32-C33-C34-C35
4	D	801	POV	C23-C24-C25-C26
2	A	801	Y01	CAO-CAJ-CAN-CBA
4	A	806	POV	C212-C213-C214-C215
4	A	806	POV	C24-C25-C26-C27
4	C	802	POV	C212-C213-C214-C215
4	D	802	POV	C23-C24-C25-C26
4	D	809	POV	C34-C35-C36-C37
4	D	812	POV	C35-C36-C37-C38
4	A	805	POV	C36-C37-C38-C39
4	C	812	POV	C32-C33-C34-C35
4	A	806	POV	C36-C37-C38-C39
4	B	802	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
4	B	811	POV	C11-C12-N-C13
4	D	801	POV	C11-C12-N-C14
4	B	807	POV	C36-C37-C38-C39
4	D	809	POV	C213-C214-C215-C216
4	D	812	POV	C32-C33-C34-C35
4	B	807	POV	C311-C312-C313-C314
4	C	810	POV	C35-C36-C37-C38
4	C	812	POV	C23-C24-C25-C26
4	D	804	POV	C212-C213-C214-C215
4	A	805	POV	C213-C214-C215-C216
4	A	806	POV	C22-C23-C24-C25
4	B	810	POV	C35-C36-C37-C38
4	A	812	POV	C23-C24-C25-C26
4	B	812	POV	C23-C24-C25-C26
4	C	807	POV	C311-C312-C313-C314
4	D	802	POV	C312-C313-C314-C315
4	B	808	POV	C311-C312-C313-C314
4	C	808	POV	C311-C312-C313-C314
4	D	810	POV	C311-C312-C313-C314
4	A	808	POV	C36-C37-C38-C39
4	B	807	POV	C34-C35-C36-C37
4	B	810	POV	C32-C33-C34-C35
4	C	812	POV	C312-C313-C314-C315
4	A	810	POV	C311-C310-C39-C38
4	A	810	POV	C23-C24-C25-C26
4	C	810	POV	C32-C33-C34-C35
4	C	811	POV	C23-C24-C25-C26
4	A	805	POV	C34-C35-C36-C37
4	B	808	POV	C311-C310-C39-C38
4	C	807	POV	C33-C34-C35-C36
4	B	811	POV	C39-C310-C311-C312
4	C	811	POV	C39-C310-C311-C312
4	D	809	POV	C311-C312-C313-C314
4	A	805	POV	C311-C312-C313-C314
4	A	809	POV	C39-C310-C311-C312
4	C	808	POV	C37-C38-C39-C310
4	C	811	POV	C213-C214-C215-C216
4	D	810	POV	C37-C38-C39-C310
4	D	810	POV	C310-C311-C312-C313
4	A	805	POV	C33-C34-C35-C36
4	D	810	POV	C313-C314-C315-C316
4	B	802	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
4	A	812	POV	C26-C27-C28-C29
4	B	802	POV	C26-C27-C28-C29
4	B	807	POV	C210-C211-C212-C213
4	C	807	POV	C210-C211-C212-C213
4	B	808	POV	C313-C314-C315-C316
4	A	806	POV	C21-C22-C23-C24
4	A	807	POV	C21-C22-C23-C24
4	B	811	POV	C312-C313-C314-C315
4	A	806	POV	C312-C313-C314-C315
4	D	810	POV	C212-C213-C214-C215
4	D	810	POV	C22-C23-C24-C25
4	A	806	POV	C33-C34-C35-C36
4	A	807	POV	C211-C212-C213-C214
4	B	808	POV	C37-C38-C39-C310
4	C	811	POV	C11-C12-N-C13
4	A	809	POV	C312-C313-C314-C315
4	C	808	POV	C312-C313-C314-C315
4	A	806	POV	C37-C38-C39-C310
4	C	808	POV	C311-C310-C39-C38
4	D	812	POV	C36-C37-C38-C39
2	C	801	Y01	CAO-CAJ-CAN-CBA
2	D	803	Y01	CAO-CAJ-CAN-CBA
4	D	809	POV	C212-C213-C214-C215
2	A	811	Y01	CAO-CAJ-CAN-CBA
2	C	801	Y01	CAJ-CAN-CBA-CAB
2	D	803	Y01	CAJ-CAN-CBA-CAB
2	B	801	Y01	CAC-CBB-CBE-CAP
4	A	812	POV	C212-C213-C214-C215
4	A	809	POV	C31-C32-C33-C34
4	D	809	POV	C210-C211-C212-C213
4	C	808	POV	C22-C23-C24-C25
4	A	806	POV	C311-C310-C39-C38
4	D	810	POV	C311-C310-C39-C38
4	B	808	POV	C22-C23-C24-C25
4	A	809	POV	C213-C214-C215-C216
4	B	812	POV	C25-C26-C27-C28
4	D	801	POV	C39-C310-C311-C312
4	D	801	POV	C211-C212-C213-C214
2	B	801	Y01	CAJ-CAN-CBA-CAB
4	B	808	POV	C211-C212-C213-C214
4	B	812	POV	C311-C310-C39-C38
4	C	812	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
4	C	811	POV	C311-C312-C313-C314
4	C	811	POV	C211-C212-C213-C214
4	C	811	POV	C36-C37-C38-C39
4	C	812	POV	C25-C26-C27-C28
4	D	801	POV	C36-C37-C38-C39
4	D	811	POV	C24-C25-C26-C27
4	C	808	POV	C32-C31-O31-C3
4	B	811	POV	C31-C32-C33-C34
4	C	811	POV	C31-C32-C33-C34
4	C	810	POV	C36-C37-C38-C39
4	A	809	POV	C36-C37-C38-C39
4	D	801	POV	C11-C12-N-C13
3	D	807	PCW	C23-C24-C25-C26
4	A	810	POV	C25-C26-C27-C28
4	B	811	POV	C36-C37-C38-C39
2	B	801	Y01	CAO-CBB-CBE-CBI
4	A	806	POV	C311-C312-C313-C314
4	A	810	POV	O11-C1-C2-C3
4	B	808	POV	O11-C1-C2-C3
4	B	812	POV	O11-C1-C2-C3
4	C	812	POV	O11-C1-C2-C3
4	A	809	POV	C33-C34-C35-C36
4	B	811	POV	C33-C34-C35-C36
4	C	811	POV	C33-C34-C35-C36
2	A	811	Y01	CAJ-CAN-CBA-CAB
4	B	807	POV	C33-C34-C35-C36
4	B	808	POV	C32-C31-O31-C3
2	B	801	Y01	CAC-CBB-CBE-CBI
4	A	806	POV	C35-C36-C37-C38
4	C	811	POV	C312-C313-C314-C315
4	B	811	POV	C311-C312-C313-C314
3	C	805	PCW	C23-C24-C25-C26
4	A	809	POV	C311-C312-C313-C314
4	B	810	POV	C36-C37-C38-C39
4	C	808	POV	C212-C213-C214-C215
4	D	810	POV	C211-C212-C213-C214
4	B	811	POV	C310-C311-C312-C313
4	C	808	POV	C310-C311-C312-C313
4	C	811	POV	C24-C25-C26-C27
4	D	801	POV	C33-C34-C35-C36
4	A	805	POV	C210-C211-C212-C213
4	C	802	POV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
4	D	804	POV	C26-C27-C28-C29
4	C	809	POV	C212-C213-C214-C215
4	A	806	POV	C310-C311-C312-C313
4	C	808	POV	C211-C212-C213-C214
4	B	811	POV	C213-C214-C215-C216
4	D	801	POV	C24-C25-C26-C27
4	D	809	POV	C39-C310-C311-C312
4	C	808	POV	C21-C22-C23-C24
4	B	802	POV	C24-C25-C26-C27
4	C	811	POV	C310-C311-C312-C313
4	C	808	POV	O32-C31-O31-C3
4	A	806	POV	C211-C212-C213-C214
4	D	801	POV	C311-C310-C39-C38
4	B	808	POV	C21-C22-C23-C24
4	D	810	POV	C21-C22-C23-C24
3	A	803	PCW	C23-C24-C25-C26
4	B	802	POV	C211-C212-C213-C214
4	D	810	POV	C32-C31-O31-C3
4	A	812	POV	C211-C212-C213-C214
4	A	810	POV	C210-C211-C212-C213
4	B	812	POV	C210-C211-C212-C213
4	C	812	POV	C210-C211-C212-C213
4	C	812	POV	C214-C215-C216-C217
4	B	808	POV	O32-C31-O31-C3
4	D	802	POV	C29-C210-C211-C212
4	B	808	POV	C310-C311-C312-C313
4	A	809	POV	C310-C311-C312-C313
4	B	807	POV	C23-C24-C25-C26
4	D	802	POV	C25-C26-C27-C28
4	C	807	POV	C215-C216-C217-C218
4	A	810	POV	C214-C215-C216-C217
4	D	801	POV	C311-C312-C313-C314
4	D	804	POV	C211-C212-C213-C214
3	B	805	PCW	C23-C24-C25-C26
4	B	809	POV	C24-C25-C26-C27
4	B	812	POV	C214-C215-C216-C217
4	D	801	POV	C214-C215-C216-C217
4	C	802	POV	C211-C212-C213-C214
4	D	809	POV	C215-C216-C217-C218
4	B	807	POV	C39-C310-C311-C312
4	D	808	POV	C211-C212-C213-C214
4	A	805	POV	C215-C216-C217-C218

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Mol	Chain	Res	Type	Atoms
4	B	811	POV	C24-C25-C26-C27
4	D	801	POV	C313-C314-C315-C316
3	D	807	PCW	C16-C17-C18-C19
4	B	807	POV	C215-C216-C217-C218
4	D	809	POV	C312-C313-C314-C315
4	A	812	POV	C24-C25-C26-C27
4	A	808	POV	C311-C310-C39-C38
4	B	811	POV	C311-C310-C39-C38
4	C	811	POV	C311-C310-C39-C38
4	D	801	POV	C32-C33-C34-C35
4	D	809	POV	C33-C34-C35-C36
4	B	809	POV	C213-C214-C215-C216
4	C	807	POV	C23-C24-C25-C26
4	A	810	POV	C29-C210-C211-C212
4	B	812	POV	C29-C210-C211-C212
4	C	812	POV	C29-C210-C211-C212
4	B	811	POV	C23-C24-C25-C26
4	B	807	POV	C312-C313-C314-C315
4	C	807	POV	C39-C310-C311-C312
4	D	804	POV	C36-C37-C38-C39
4	A	808	POV	C37-C38-C39-C310
3	C	805	PCW	C24-C25-C26-C27
4	C	809	POV	C213-C214-C215-C216
4	C	808	POV	O11-C1-C2-C3
4	C	811	POV	O11-C1-C2-C3
4	D	802	POV	O11-C1-C2-C3
4	D	810	POV	O11-C1-C2-C3
4	A	809	POV	C311-C310-C39-C38
4	C	811	POV	C313-C314-C315-C316
4	B	811	POV	C34-C35-C36-C37
4	A	804	POV	C211-C212-C213-C214
4	A	809	POV	C24-C25-C26-C27
4	A	805	POV	C311-C310-C39-C38
4	D	810	POV	C35-C36-C37-C38
4	D	810	POV	O32-C31-O31-C3
4	C	808	POV	C35-C36-C37-C38
4	D	810	POV	C312-C313-C314-C315
4	B	808	POV	C1-C2-C3-O31
4	A	809	POV	C313-C314-C315-C316
4	B	811	POV	C313-C314-C315-C316
4	A	807	POV	C23-C24-C25-C26
4	B	808	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
4	D	801	POV	C31-C32-C33-C34
4	D	802	POV	C313-C314-C315-C316
4	A	810	POV	C313-C314-C315-C316
4	B	812	POV	C36-C37-C38-C39
4	D	809	POV	C37-C38-C39-C310
4	D	801	POV	O11-C1-C2-O21
4	C	807	POV	C312-C313-C314-C315
2	B	801	Y01	CAO-CBB-CBE-CAP
4	C	808	POV	C2-C1-O11-P
4	D	810	POV	C2-C1-O11-P
4	A	806	POV	C215-C216-C217-C218
4	A	809	POV	C34-C35-C36-C37
4	C	802	POV	C36-C37-C38-C39
4	D	804	POV	C24-C25-C26-C27
4	A	810	POV	O21-C2-C3-O31
4	B	812	POV	O21-C2-C3-O31
4	C	812	POV	O21-C2-C3-O31
4	D	802	POV	O21-C2-C3-O31
4	A	808	POV	C33-C34-C35-C36
4	D	810	POV	C215-C216-C217-C218
4	D	811	POV	C213-C214-C215-C216
4	D	812	POV	C311-C310-C39-C38
4	B	802	POV	C36-C37-C38-C39
4	D	810	POV	C33-C34-C35-C36
2	D	803	Y01	CAJ-CAN-CBA-CAA
3	A	803	PCW	C22-C23-C24-C25
4	C	802	POV	C213-C214-C215-C216
4	B	810	POV	C311-C310-C39-C38
4	C	809	POV	C24-C25-C26-C27
4	C	811	POV	C34-C35-C36-C37
4	D	809	POV	C23-C24-C25-C26
4	C	808	POV	C215-C216-C217-C218
2	A	811	Y01	CAJ-CAN-CBA-CAA
2	B	801	Y01	CAJ-CAN-CBA-CAA
2	C	801	Y01	CAJ-CAN-CBA-CAA
4	B	807	POV	C311-C310-C39-C38
4	A	805	POV	C212-C213-C214-C215
4	B	812	POV	C313-C314-C315-C316
4	A	806	POV	C32-C31-O31-C3
4	B	802	POV	C32-C33-C34-C35
4	C	810	POV	C311-C310-C39-C38
3	B	805	PCW	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
4	D	812	POV	C37-C38-C39-C310
3	C	805	PCW	C16-C17-C18-C19
4	B	806	POV	C26-C27-C28-C29
4	A	806	POV	O11-C1-C2-C3
4	A	809	POV	O11-C1-C2-C3
4	B	811	POV	O11-C1-C2-C3
4	A	812	POV	C36-C37-C38-C39
4	B	802	POV	C25-C26-C27-C28
4	C	802	POV	C24-C25-C26-C27
2	A	802	Y01	CAM-CAY-OAW-CBC
2	B	804	Y01	CAM-CAY-OAW-CBC
2	A	802	Y01	OAG-CAY-OAW-CBC
2	B	804	Y01	OAG-CAY-OAW-CBC
2	C	804	Y01	OAG-CAY-OAW-CBC
4	D	801	POV	C34-C35-C36-C37
2	D	803	Y01	CAC-CBB-CBE-CBI
4	C	812	POV	C36-C37-C38-C39
4	A	809	POV	C3-C2-O21-C21
4	B	811	POV	C3-C2-O21-C21
4	C	811	POV	C3-C2-O21-C21
4	D	801	POV	C3-C2-O21-C21
4	C	807	POV	C311-C310-C39-C38
2	C	801	Y01	CAC-CBB-CBE-CBI
4	C	806	POV	C211-C212-C213-C214
4	A	806	POV	O11-C1-C2-O21
4	C	808	POV	C1-C2-C3-O31
2	C	804	Y01	CAM-CAY-OAW-CBC
2	D	803	Y01	CAC-CBB-CBE-CAP
2	A	811	Y01	CAC-CBB-CBE-CBI
4	A	805	POV	C312-C313-C314-C315
4	C	808	POV	C33-C34-C35-C36
4	B	808	POV	O21-C2-C3-O31
4	C	808	POV	O21-C2-C3-O31
2	D	806	Y01	OAG-CAY-OAW-CBC
4	A	806	POV	O32-C31-O31-C3
4	B	802	POV	C311-C312-C313-C314
4	B	806	POV	C211-C212-C213-C214
4	B	808	POV	C35-C36-C37-C38
4	C	810	POV	C37-C38-C39-C310
4	A	810	POV	O12-C11-C12-N
4	B	812	POV	O12-C11-C12-N
4	C	812	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
4	D	802	POV	O12-C11-C12-N
4	D	810	POV	O12-C11-C12-N
4	B	808	POV	C215-C216-C217-C218
2	C	801	Y01	CAC-CBB-CBE-CAP
4	B	802	POV	C213-C214-C215-C216
3	D	807	PCW	C24-C25-C26-C27
4	B	810	POV	C37-C38-C39-C310
2	A	811	Y01	CAC-CBB-CBE-CAP
4	D	801	POV	O11-C1-C2-C3
4	C	807	POV	C35-C36-C37-C38
4	A	809	POV	C23-C24-C25-C26
4	D	804	POV	C213-C214-C215-C216
4	A	810	POV	C22-C23-C24-C25
4	A	812	POV	C214-C215-C216-C217
2	D	803	Y01	CAO-CBB-CBE-CBI
4	D	809	POV	C311-C310-C39-C38
4	D	809	POV	C29-C210-C211-C212
4	A	809	POV	C32-C33-C34-C35
2	D	803	Y01	CAO-CBB-CBE-CAP
4	A	809	POV	O11-C1-C2-O21
4	B	808	POV	O11-C1-C2-O21
4	B	811	POV	O11-C1-C2-O21
4	C	808	POV	O11-C1-C2-O21
4	C	811	POV	O11-C1-C2-O21
4	D	810	POV	O11-C1-C2-O21
2	D	806	Y01	CAM-CAY-OAW-CBC
2	A	802	Y01	CAC-CBB-CBE-CBI
4	B	812	POV	C34-C35-C36-C37
4	A	812	POV	C213-C214-C215-C216
4	C	812	POV	C313-C314-C315-C316
2	B	804	Y01	CAC-CBB-CBE-CBI
4	A	806	POV	C1-C2-C3-O31
4	C	812	POV	C1-C2-C3-O31
4	D	802	POV	C1-C2-C3-O31
4	D	810	POV	C1-C2-C3-O31
2	A	811	Y01	CAO-CBB-CBE-CAP
2	C	801	Y01	CAO-CBB-CBE-CAP
2	D	806	Y01	CAC-CBB-CBE-CBI
4	A	812	POV	C29-C210-C211-C212
4	D	804	POV	C29-C210-C211-C212
4	B	811	POV	C32-C33-C34-C35
4	C	812	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	B	802	POV	C310-C311-C312-C313
2	A	811	Y01	CAO-CBB-CBE-CBI
2	C	801	Y01	CAO-CBB-CBE-CBI
2	C	804	Y01	CAC-CBB-CBE-CBI
4	A	805	POV	C1-O11-P-O14
4	A	806	POV	C1-O11-P-O13
4	A	809	POV	C11-O12-P-O14
4	A	812	POV	C11-O12-P-O13
4	B	802	POV	C11-O12-P-O13
4	B	807	POV	C1-O11-P-O14
4	B	808	POV	C1-O11-P-O13
4	B	811	POV	C11-O12-P-O14
4	C	802	POV	C11-O12-P-O13
4	D	804	POV	C11-O12-P-O13
4	D	809	POV	C11-O12-P-O14
4	B	809	POV	C211-C212-C213-C214
4	C	811	POV	C32-C33-C34-C35
3	B	805	PCW	C16-C17-C18-C19
4	C	806	POV	C26-C27-C28-C29
4	A	806	POV	C2-C1-O11-P
4	B	808	POV	C2-C1-O11-P
4	A	812	POV	C32-C33-C34-C35
4	C	811	POV	C214-C215-C216-C217
4	D	809	POV	C35-C36-C37-C38
4	C	802	POV	C32-C33-C34-C35
4	B	812	POV	C22-C23-C24-C25
3	A	803	PCW	C19-C20-C21-C22
4	C	802	POV	C29-C210-C211-C212
4	B	808	POV	C33-C34-C35-C36
4	C	802	POV	C311-C312-C313-C314
4	A	805	POV	C31-C32-C33-C34
4	A	810	POV	C36-C37-C38-C39
2	D	806	Y01	CAX-CAL-CAM-CAY
4	A	810	POV	C34-C35-C36-C37
4	B	810	POV	C34-C35-C36-C37
4	C	812	POV	C34-C35-C36-C37
2	A	802	Y01	CAO-CBB-CBE-CBI
4	A	812	POV	C35-C36-C37-C38
4	A	806	POV	O21-C2-C3-O31
4	D	810	POV	O21-C2-C3-O31
4	D	811	POV	C23-C24-C25-C26
4	B	802	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
4	A	807	POV	C212-C213-C214-C215
4	D	812	POV	C33-C34-C35-C36
2	A	802	Y01	CAO-CBB-CBE-CAP
2	B	804	Y01	CAO-CBB-CBE-CBI
4	A	807	POV	C24-C25-C26-C27
4	C	802	POV	C310-C311-C312-C313
4	D	802	POV	C215-C216-C217-C218
4	A	809	POV	C29-C210-C211-C212
4	B	807	POV	C29-C210-C211-C212
4	C	807	POV	C29-C210-C211-C212
4	A	809	POV	C26-C27-C28-C29
4	D	804	POV	C32-C33-C34-C35
2	B	804	Y01	CAO-CBB-CBE-CAP
2	C	804	Y01	CAO-CBB-CBE-CBI
2	D	806	Y01	CAO-CBB-CBE-CBI
4	B	811	POV	C214-C215-C216-C217
2	C	804	Y01	CAO-CBB-CBE-CAP
4	D	802	POV	C210-C211-C212-C213
4	A	810	POV	C212-C213-C214-C215
2	D	806	Y01	CAO-CBB-CBE-CAP
4	A	805	POV	C11-C12-N-C14
4	D	812	POV	C34-C35-C36-C37
4	B	812	POV	C26-C27-C28-C29
2	B	804	Y01	CAX-CAL-CAM-CAY
4	A	809	POV	C214-C215-C216-C217
4	C	807	POV	C37-C38-C39-C310
4	C	810	POV	C33-C34-C35-C36
2	C	804	Y01	CAX-CAL-CAM-CAY
4	A	807	POV	C29-C210-C211-C212
4	B	812	POV	C1-C2-C3-O31
4	A	812	POV	C25-C26-C27-C28
4	B	812	POV	C212-C213-C214-C215
4	D	804	POV	C214-C215-C216-C217
2	A	802	Y01	CAC-CBB-CBE-CAP
4	A	810	POV	C26-C27-C28-C29
4	B	811	POV	C37-C38-C39-C310
4	D	804	POV	C310-C311-C312-C313
2	A	802	Y01	CAX-CAL-CAM-CAY
4	A	805	POV	C23-C24-C25-C26
4	C	810	POV	C34-C35-C36-C37
4	D	802	POV	C212-C213-C214-C215
4	C	811	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
4	D	802	POV	C34-C35-C36-C37
3	A	803	PCW	C16-C17-C18-C19
4	D	804	POV	C311-C312-C313-C314
4	B	802	POV	C312-C313-C314-C315
4	D	802	POV	C22-C23-C24-C25
4	B	809	POV	C23-C24-C25-C26
4	C	812	POV	C212-C213-C214-C215
4	D	804	POV	C25-C26-C27-C28
4	D	802	POV	C311-C312-C313-C314
4	B	807	POV	C35-C36-C37-C38
4	B	807	POV	C37-C38-C39-C310
4	A	804	POV	C212-C213-C214-C215
4	A	810	POV	C1-C2-C3-O31
4	B	810	POV	C33-C34-C35-C36
4	D	802	POV	C214-C215-C216-C217
4	A	812	POV	C34-C35-C36-C37
2	B	804	Y01	CAC-CBB-CBE-CAP
4	C	802	POV	C25-C26-C27-C28
4	B	802	POV	C29-C210-C211-C212
4	C	811	POV	C26-C27-C28-C29
2	D	806	Y01	CAC-CBB-CBE-CAP
3	C	805	PCW	C19-C20-C21-C22
4	A	804	POV	C27-C28-C29-C210
4	D	801	POV	C29-C210-C211-C212
4	D	808	POV	C27-C28-C29-C210
4	B	812	POV	C213-C214-C215-C216
4	C	812	POV	C213-C214-C215-C216
4	A	812	POV	C310-C311-C312-C313
4	A	809	POV	C37-C38-C39-C310
4	C	812	POV	C26-C27-C28-C29
3	A	803	PCW	C17-C18-C19-C20
3	C	805	PCW	C17-C18-C19-C20
3	D	807	PCW	C19-C20-C21-C22
4	A	805	POV	C29-C210-C211-C212
4	C	802	POV	C214-C215-C216-C217
2	C	804	Y01	CAC-CBB-CBE-CAP
4	C	809	POV	C211-C212-C213-C214
4	D	809	POV	C31-C32-C33-C34
3	B	805	PCW	C17-C18-C19-C20
3	B	805	PCW	C19-C20-C21-C22
3	D	807	PCW	C17-C18-C19-C20
4	B	806	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
4	C	806	POV	C29-C210-C211-C212
4	C	811	POV	C29-C210-C211-C212
4	A	808	POV	C34-C35-C36-C37
4	A	805	POV	C37-C38-C39-C310
4	D	801	POV	C213-C214-C215-C216
4	B	806	POV	C29-C210-C211-C212
4	B	811	POV	C27-C28-C29-C210
4	A	805	POV	C11-C12-N-C15
4	B	808	POV	C27-C28-C29-C210
4	B	811	POV	C29-C210-C211-C212
4	C	806	POV	C27-C28-C29-C210
4	C	808	POV	C27-C28-C29-C210
4	D	801	POV	C27-C28-C29-C210
4	D	808	POV	C29-C210-C211-C212
4	A	810	POV	C311-C312-C313-C314
4	C	807	POV	O21-C21-C22-C23
4	D	809	POV	O21-C21-C22-C23
4	A	812	POV	C311-C312-C313-C314
4	A	806	POV	C27-C28-C29-C210
4	A	809	POV	C27-C28-C29-C210
4	B	811	POV	O21-C21-C22-C23
4	C	811	POV	O21-C21-C22-C23
4	D	801	POV	O21-C21-C22-C23
4	D	811	POV	C212-C213-C214-C215
4	D	810	POV	C27-C28-C29-C210
4	D	801	POV	C310-C311-C312-C313
4	C	809	POV	C23-C24-C25-C26
4	B	807	POV	O21-C21-C22-C23
4	A	806	POV	O12-C11-C12-N
4	B	802	POV	C34-C35-C36-C37
4	A	809	POV	O21-C21-C22-C23
4	B	812	POV	C311-C312-C313-C314
4	A	810	POV	O21-C21-C22-C23
4	B	811	POV	C26-C27-C28-C29
4	D	801	POV	C312-C313-C314-C315
4	D	802	POV	O21-C21-C22-C23
4	B	808	POV	O31-C31-C32-C33
4	C	808	POV	O31-C31-C32-C33
2	B	804	Y01	CAM-CAL-CAX-OAH
4	B	812	POV	O21-C21-C22-C23
4	B	812	POV	C27-C28-C29-C210
2	A	802	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
2	C	804	Y01	CAM-CAL-CAX-OAH
4	A	810	POV	C215-C216-C217-C218
2	A	802	Y01	CAM-CAL-CAX-OAF
2	C	804	Y01	CAM-CAL-CAX-OAF
4	C	812	POV	O21-C21-C22-C23
2	B	804	Y01	CAM-CAL-CAX-OAF
4	D	810	POV	O31-C31-C32-C33
4	A	805	POV	O21-C21-C22-C23
4	A	805	POV	C11-C12-N-C13
4	D	808	POV	C26-C27-C28-C29
2	D	806	Y01	CAM-CAL-CAX-OAF
4	A	810	POV	C213-C214-C215-C216
3	A	803	PCW	C15-C16-C17-C18
4	B	811	POV	O22-C21-C22-C23
4	A	810	POV	O22-C21-C22-C23
4	C	811	POV	O22-C21-C22-C23
4	D	801	POV	O22-C21-C22-C23
4	B	807	POV	C31-C32-C33-C34
4	C	812	POV	O22-C21-C22-C23
4	D	804	POV	C34-C35-C36-C37
4	B	807	POV	C11-C12-N-C14
4	A	805	POV	O22-C21-C22-C23
4	B	807	POV	O22-C21-C22-C23
4	D	802	POV	O22-C21-C22-C23
4	B	808	POV	C25-C26-C27-C28
4	B	812	POV	O22-C21-C22-C23
4	D	809	POV	O22-C21-C22-C23
4	C	807	POV	O22-C21-C22-C23
4	A	810	POV	O32-C31-O31-C3
4	C	802	POV	C34-C35-C36-C37
2	D	806	Y01	CAM-CAL-CAX-OAH
4	B	808	POV	O32-C31-C32-C33
4	C	808	POV	O32-C31-C32-C33
4	C	802	POV	O21-C21-C22-C23
2	A	801	Y01	CAM-CAL-CAX-OAH
4	A	809	POV	O22-C21-C22-C23
4	B	812	POV	O32-C31-O31-C3
4	D	804	POV	O21-C21-C22-C23
4	B	802	POV	O21-C21-C22-C23
4	D	810	POV	O32-C31-C32-C33

There are no ring outliers.

43 monomers are involved in 103 short contacts:

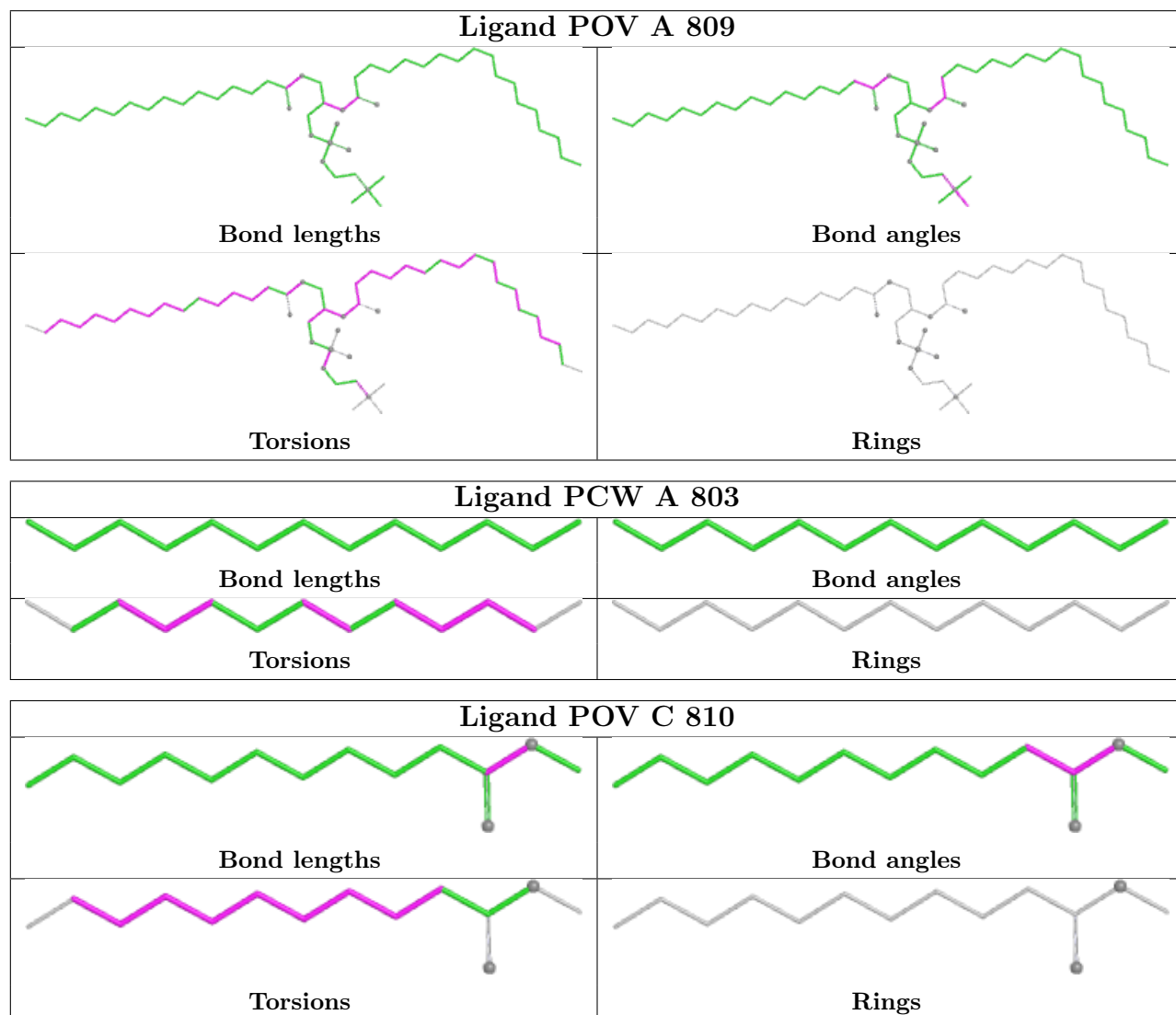
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4	A	809	POV	3	0
3	A	803	PCW	1	0
4	C	812	POV	2	0
4	B	806	POV	2	0
4	B	812	POV	2	0
2	B	801	Y01	1	0
4	C	811	POV	1	0
3	B	805	PCW	2	0
4	D	809	POV	1	0
2	C	801	Y01	1	0
4	B	808	POV	4	0
3	C	805	PCW	2	0
4	C	806	POV	2	0
4	A	810	POV	2	0
4	C	808	POV	3	0
4	B	809	POV	1	0
2	A	801	Y01	4	0
4	D	801	POV	2	0
4	D	804	POV	4	0
2	A	811	Y01	1	0
4	D	811	POV	1	0
2	C	803	Y01	4	0
4	B	802	POV	5	0
2	B	803	Y01	4	0
4	C	802	POV	5	0
3	D	807	PCW	2	0
2	B	804	Y01	5	0
4	C	809	POV	1	0
4	D	810	POV	3	0
2	D	803	Y01	1	0
4	C	807	POV	1	0
4	D	802	POV	2	0
2	D	805	Y01	3	0
2	D	806	Y01	6	0
4	B	811	POV	4	0
4	B	807	POV	1	0
4	D	808	POV	1	0
2	A	802	Y01	4	0
4	A	806	POV	4	0
2	C	804	Y01	4	0
4	A	812	POV	5	0
4	B	810	POV	1	0

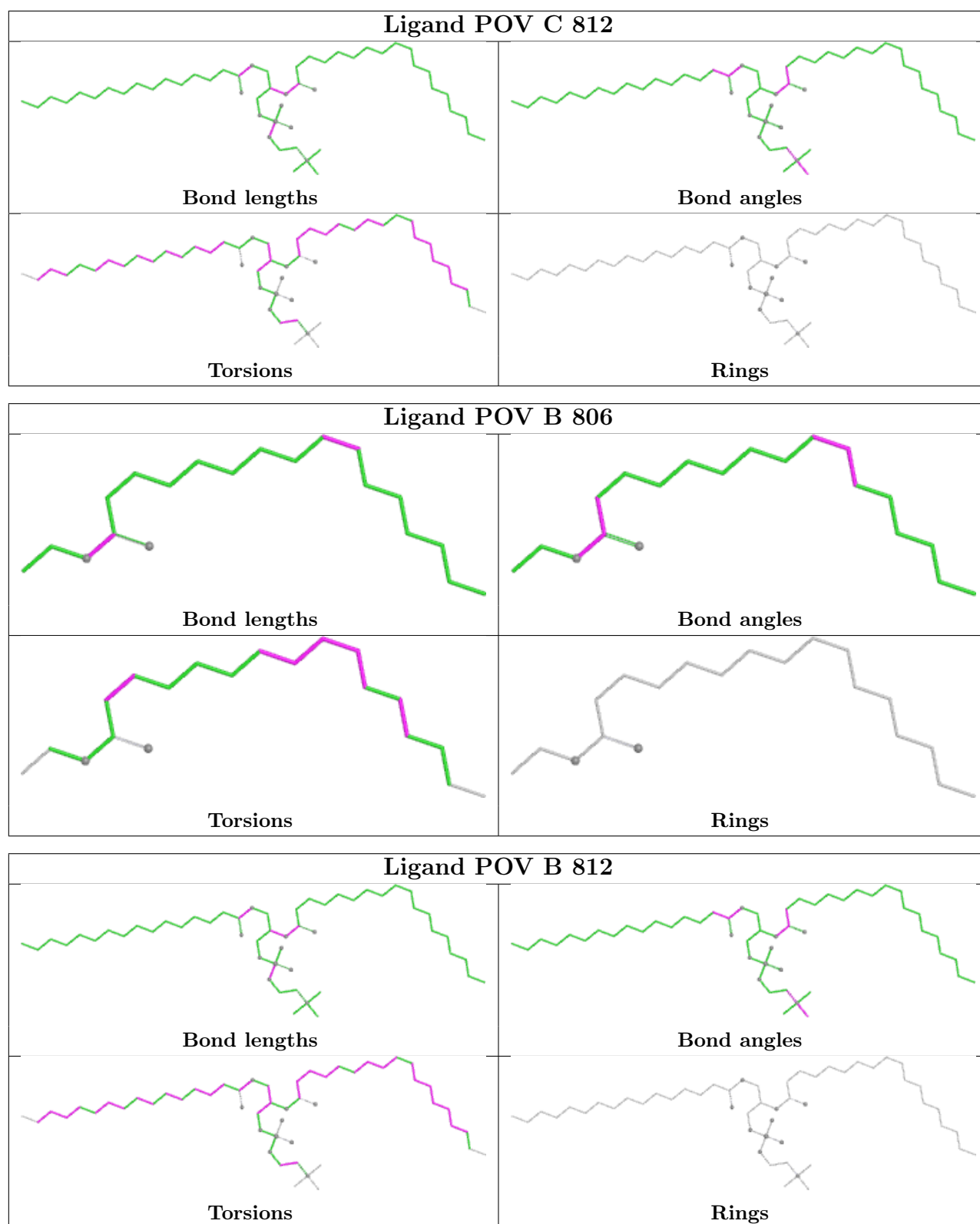
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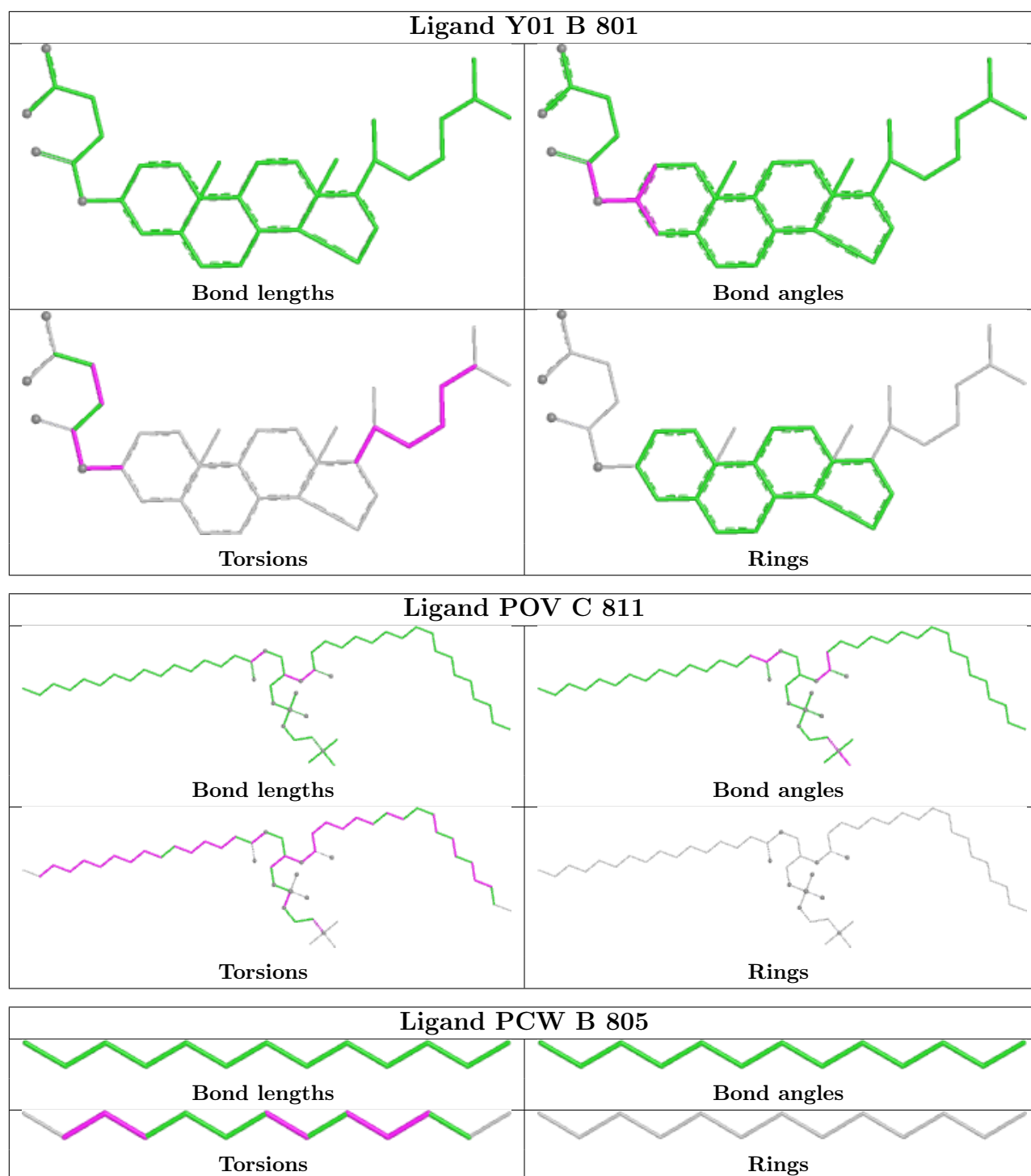
Continued from previous page...

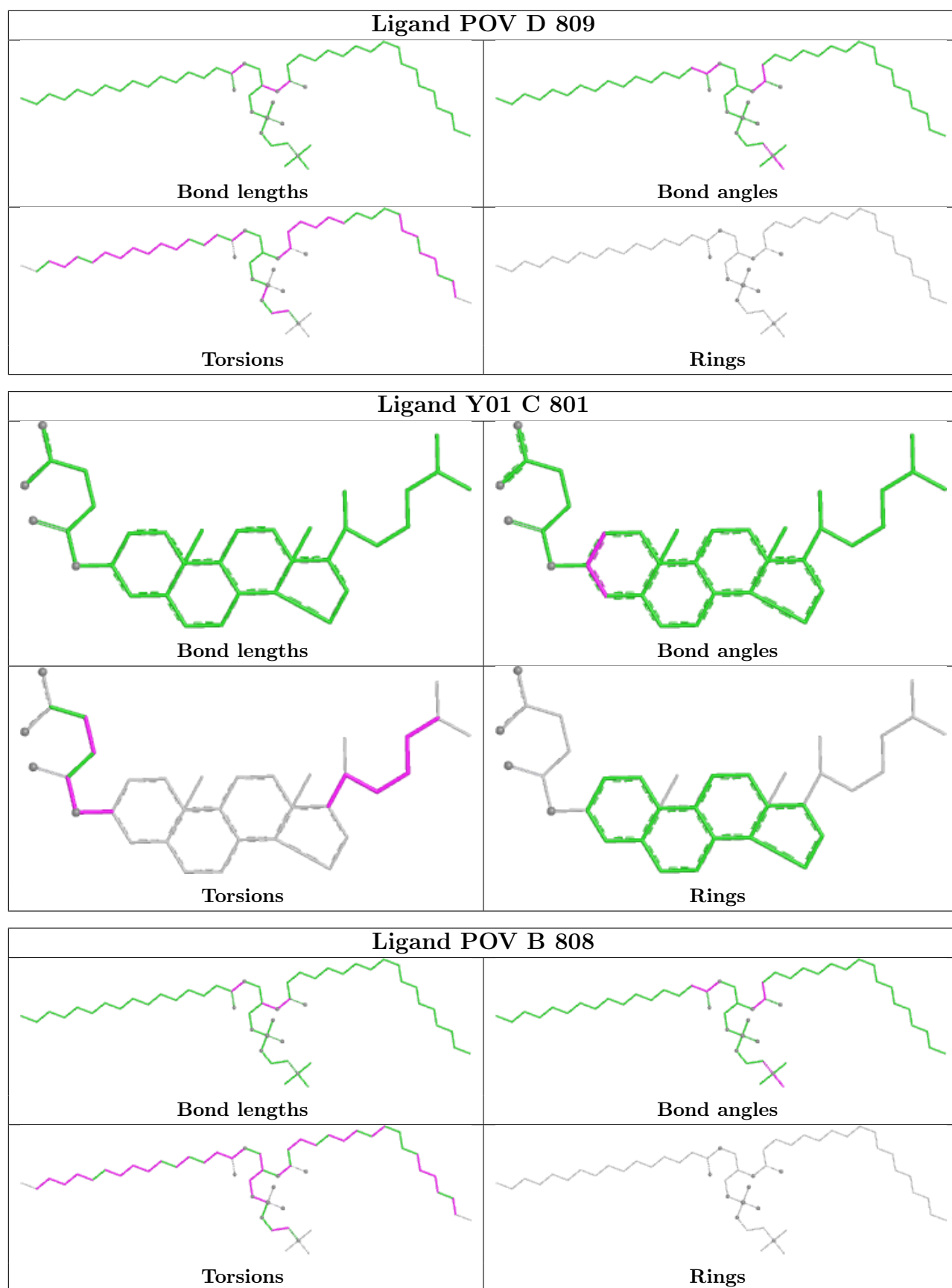
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	POV	2	0

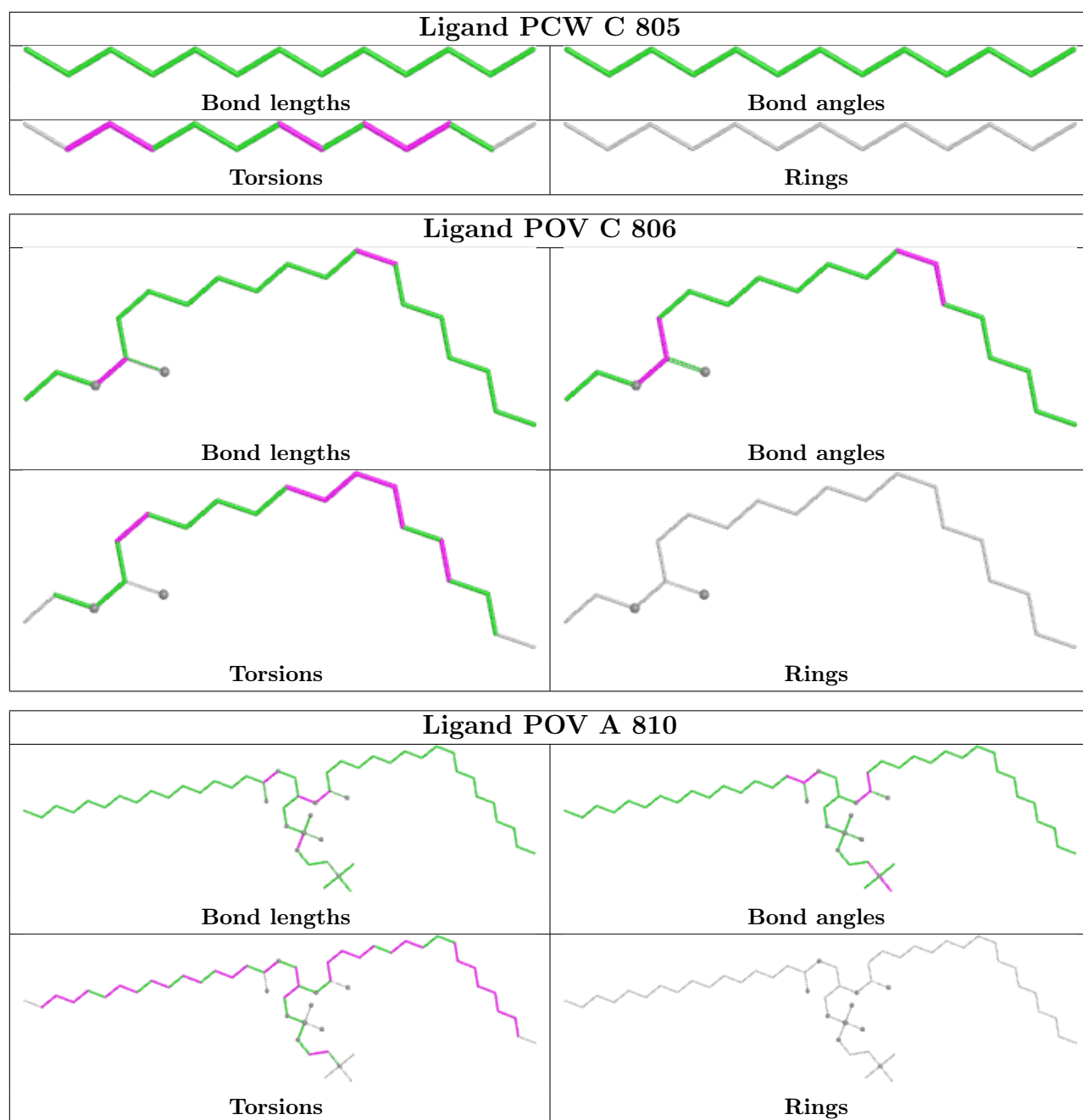
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

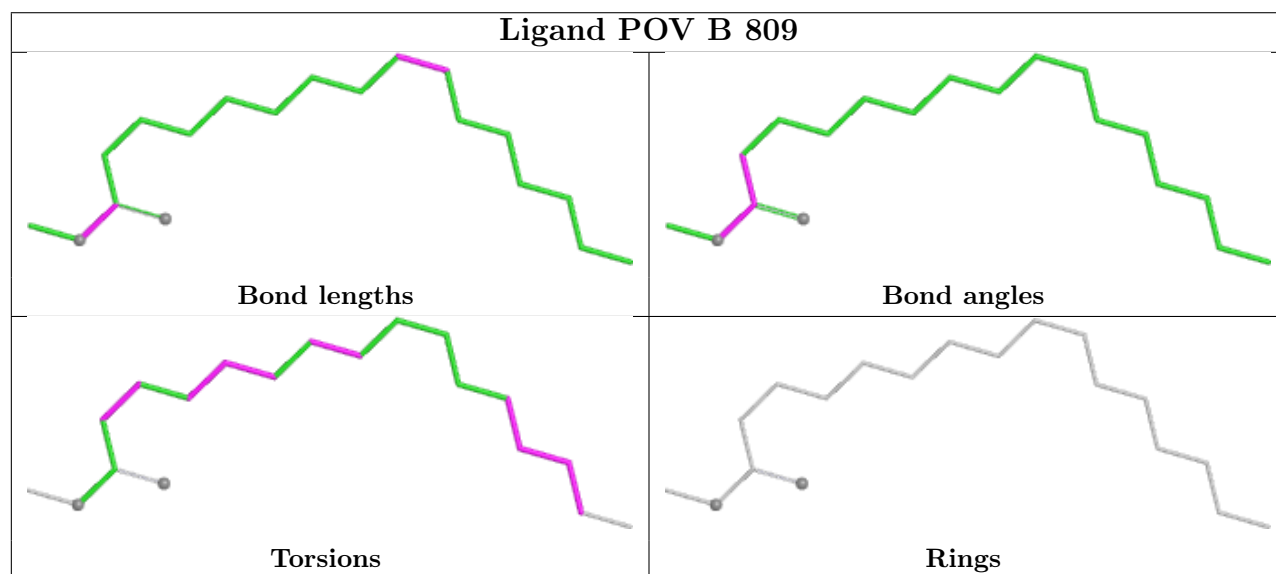
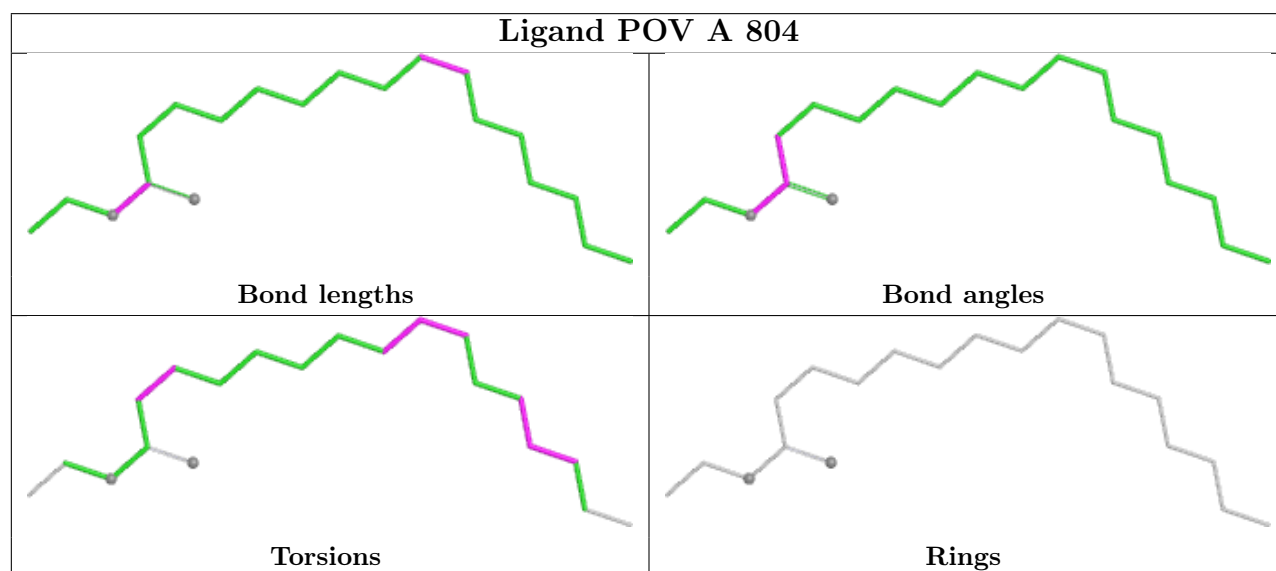
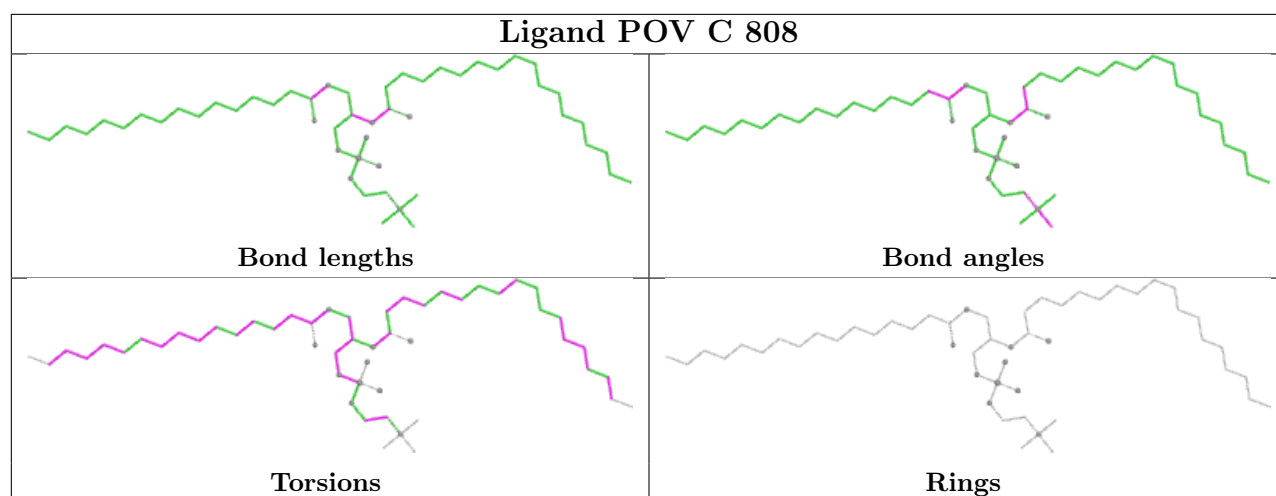


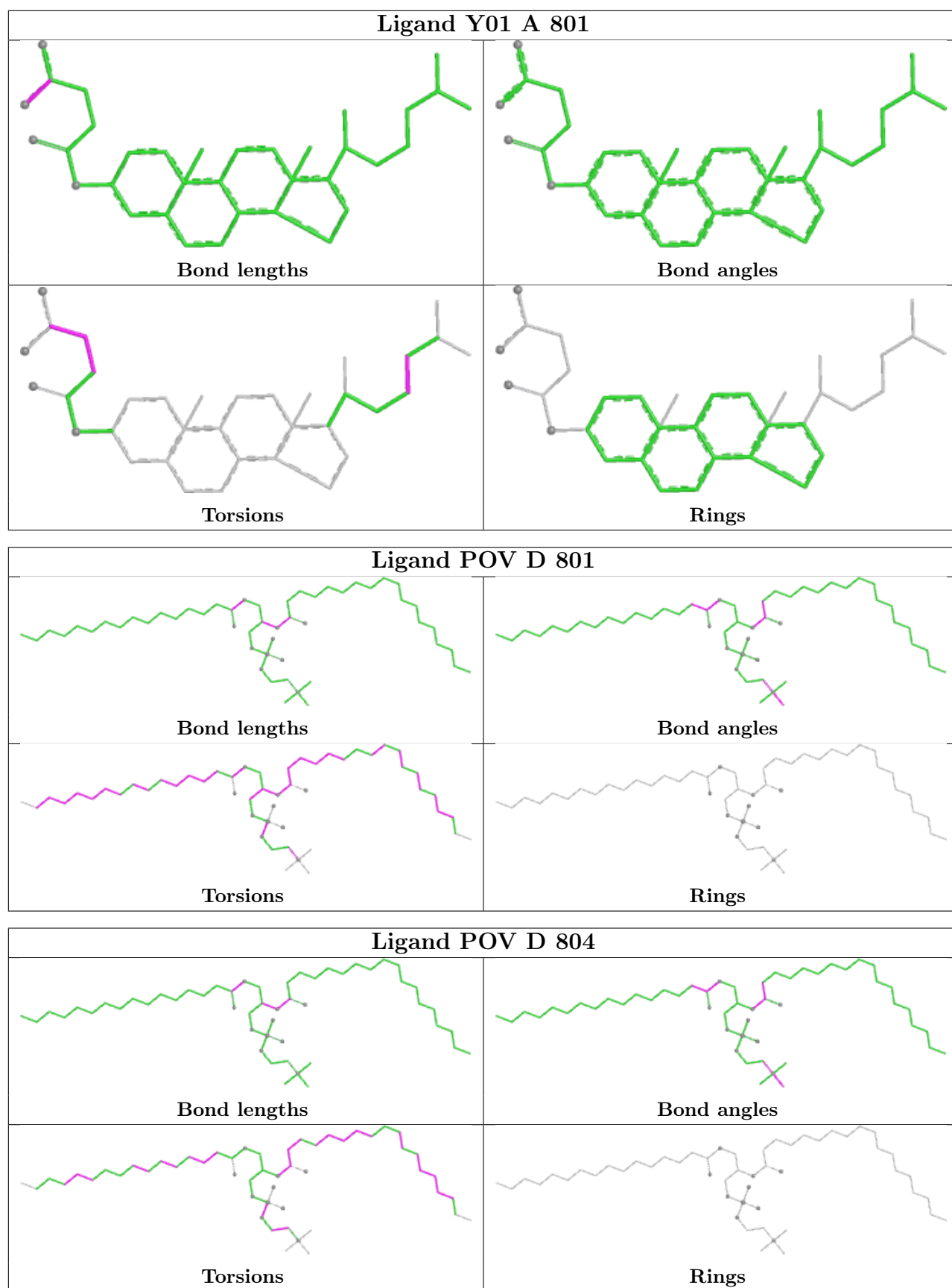


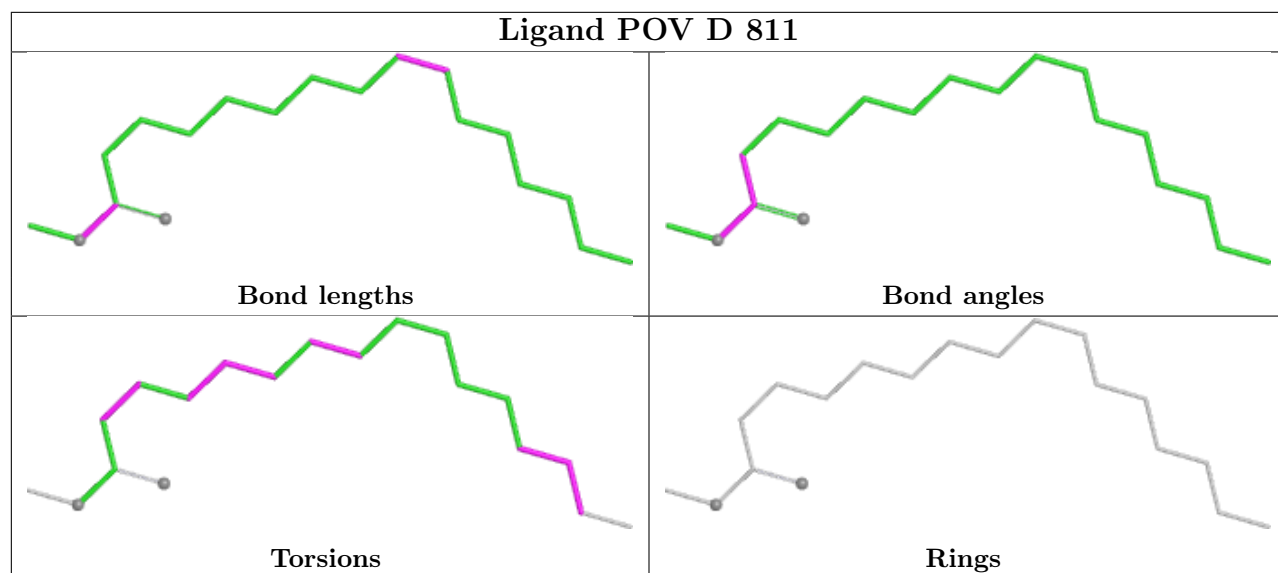
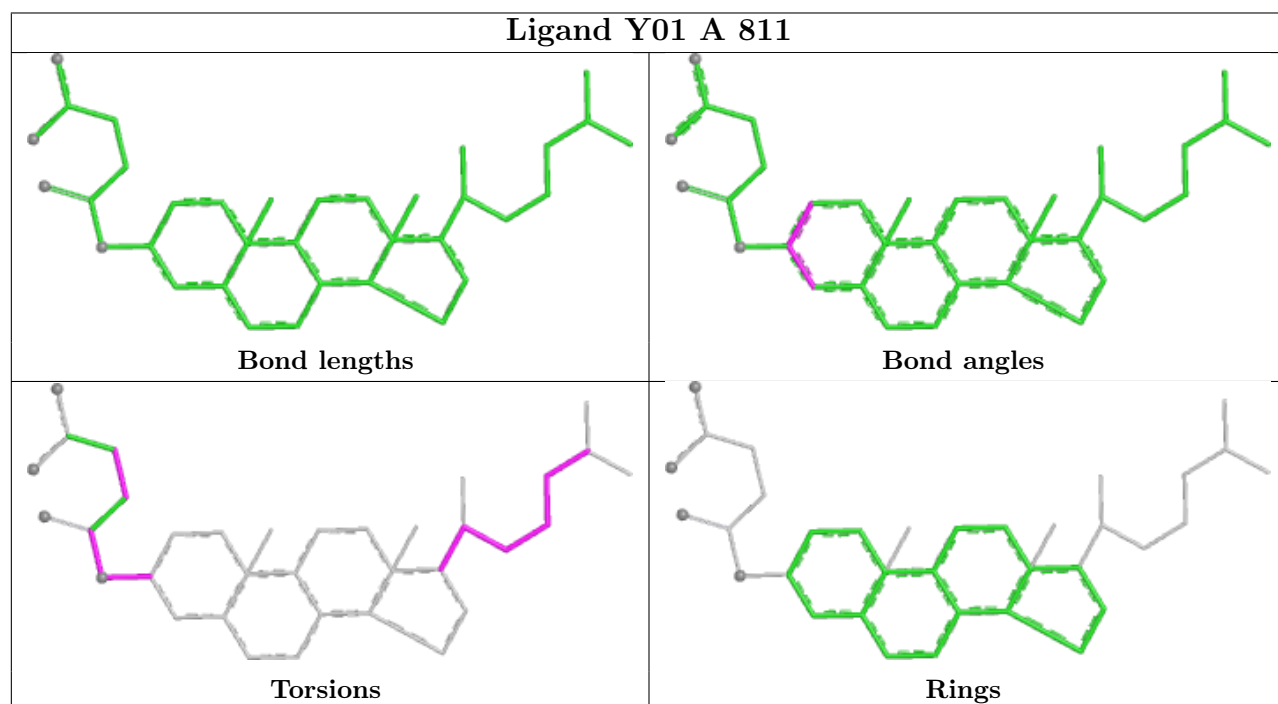
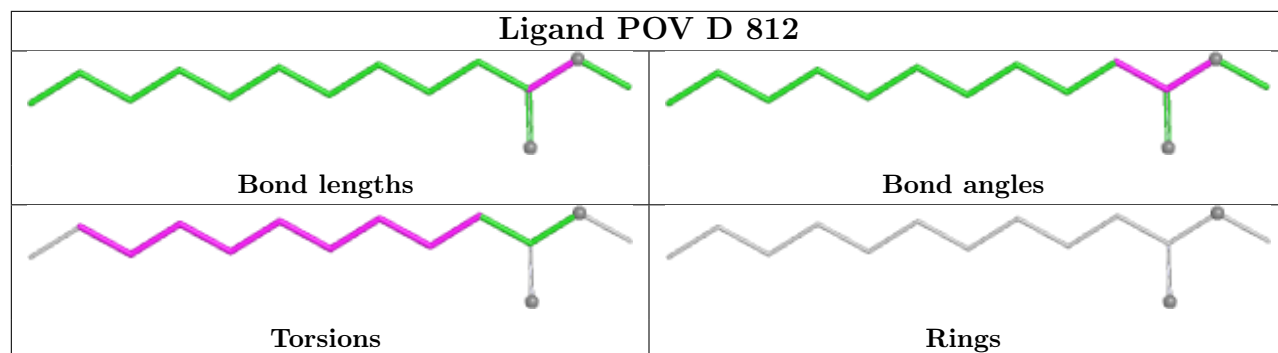


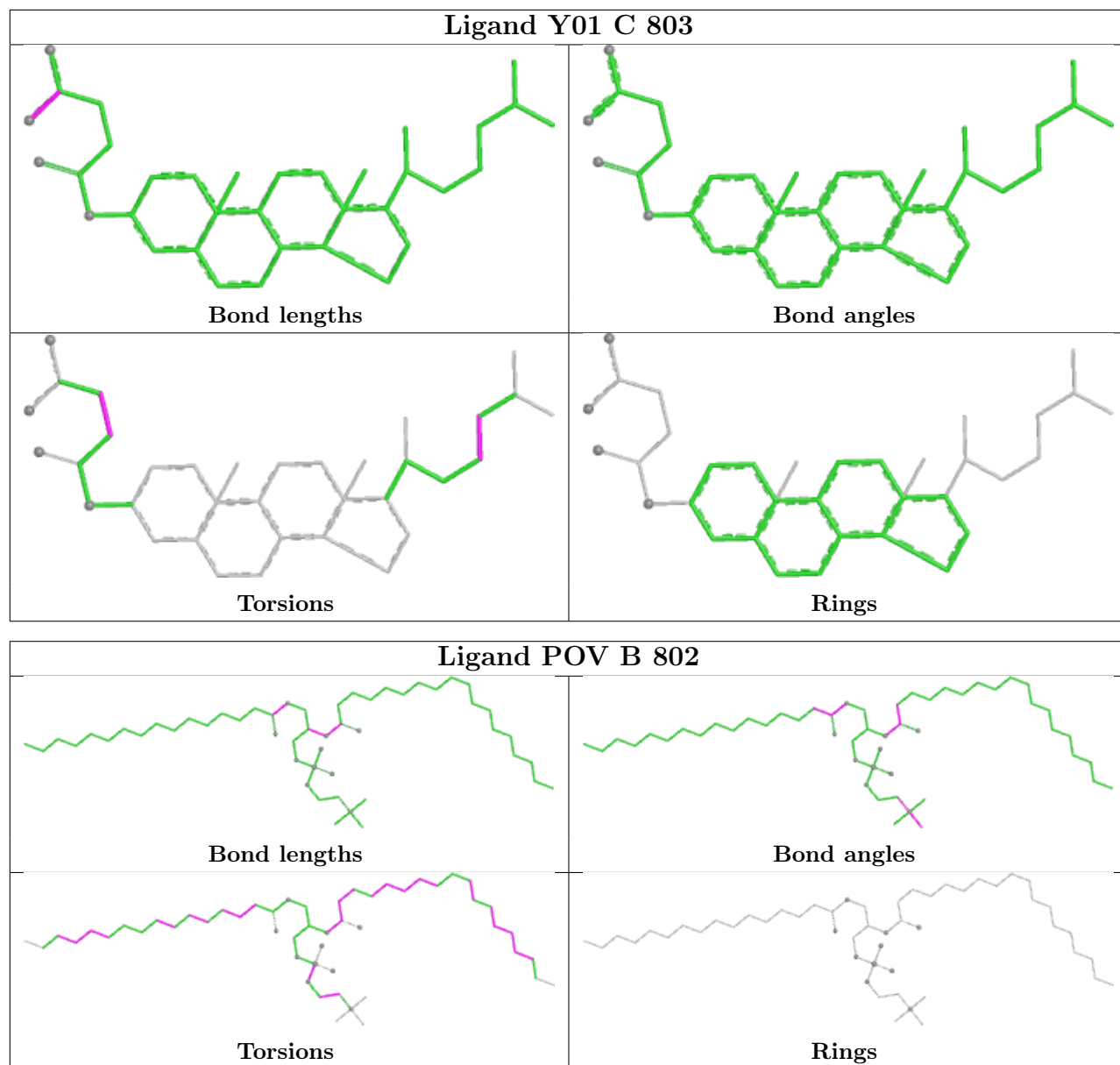


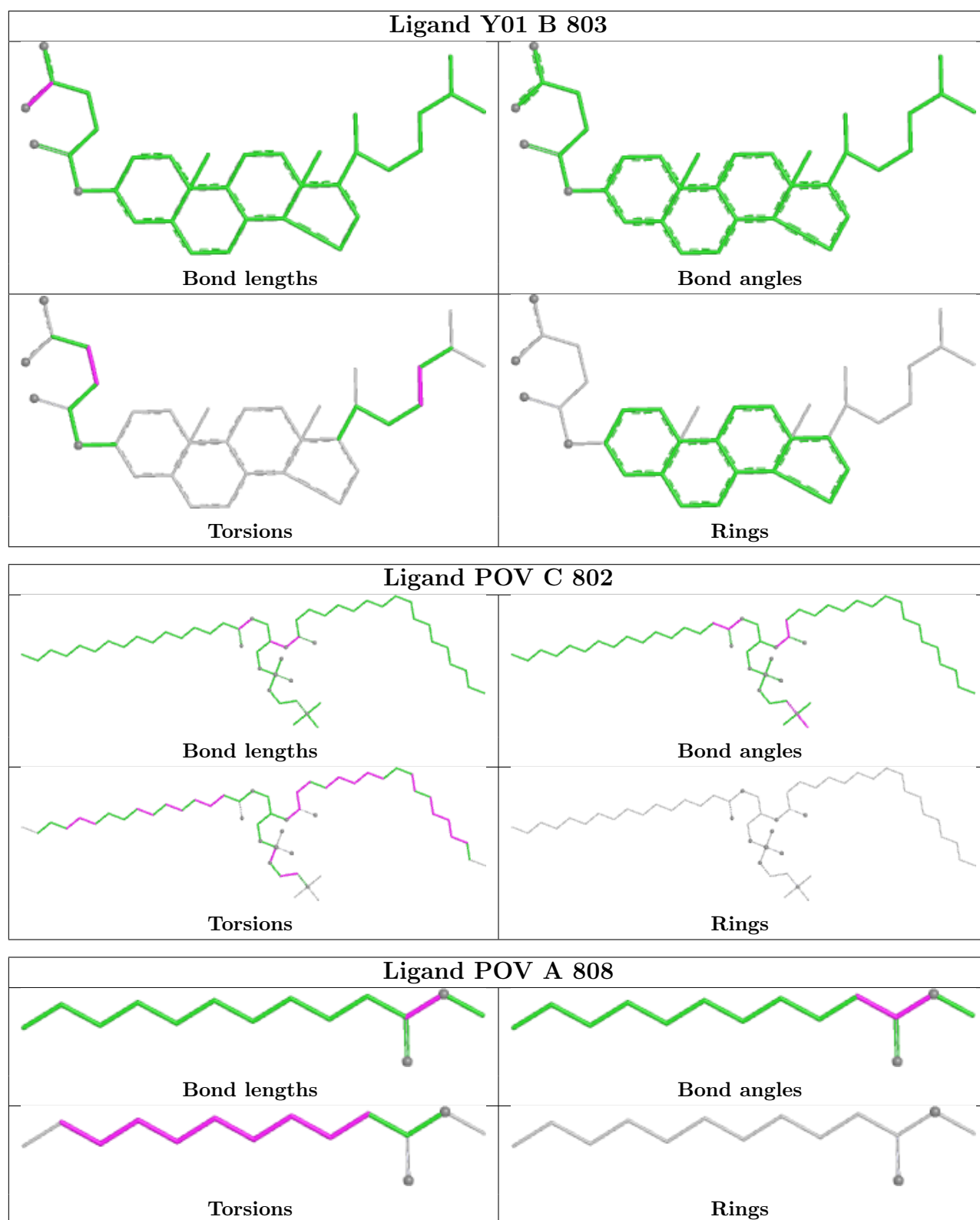


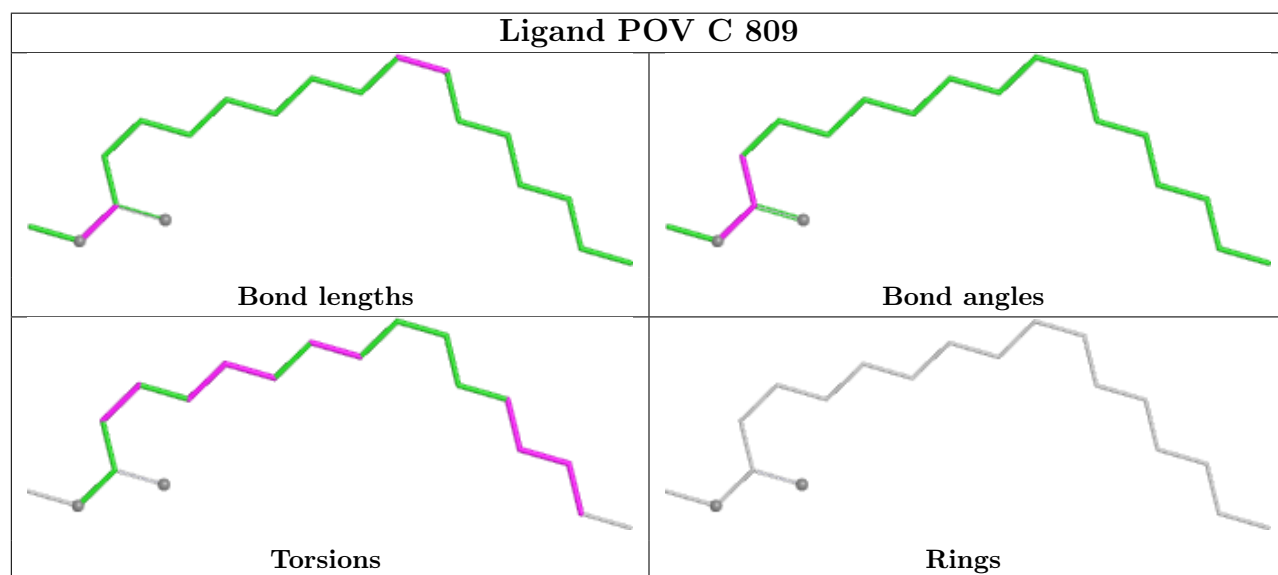
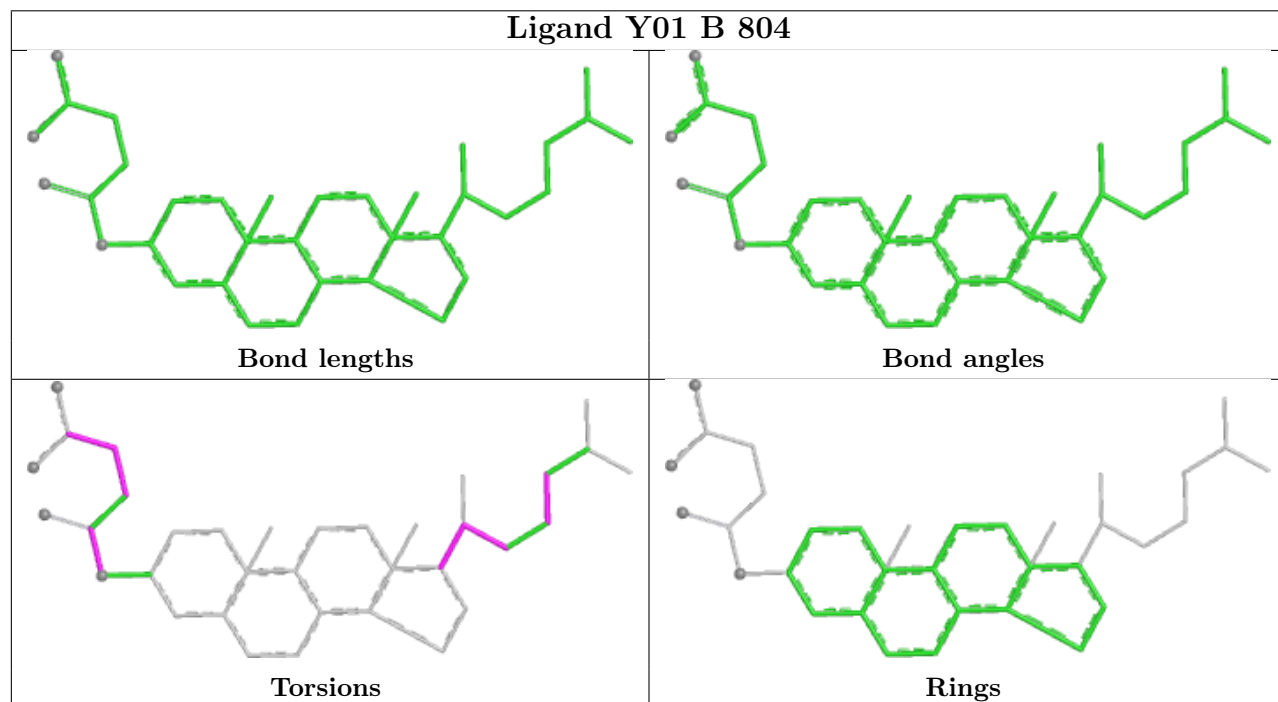
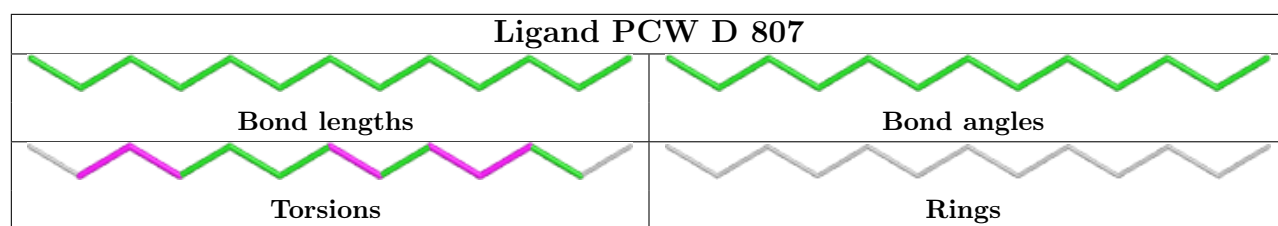


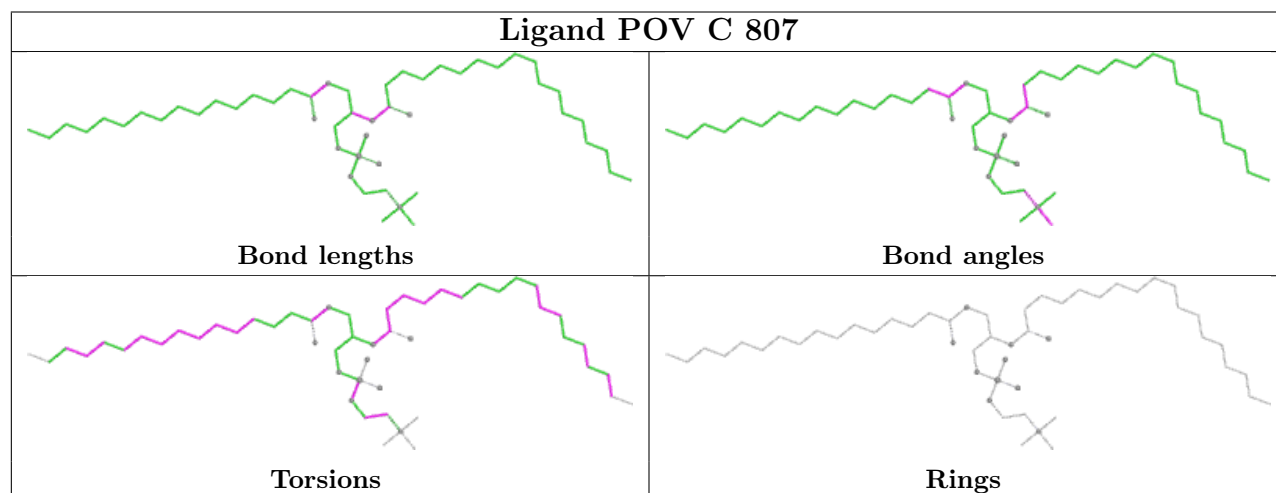
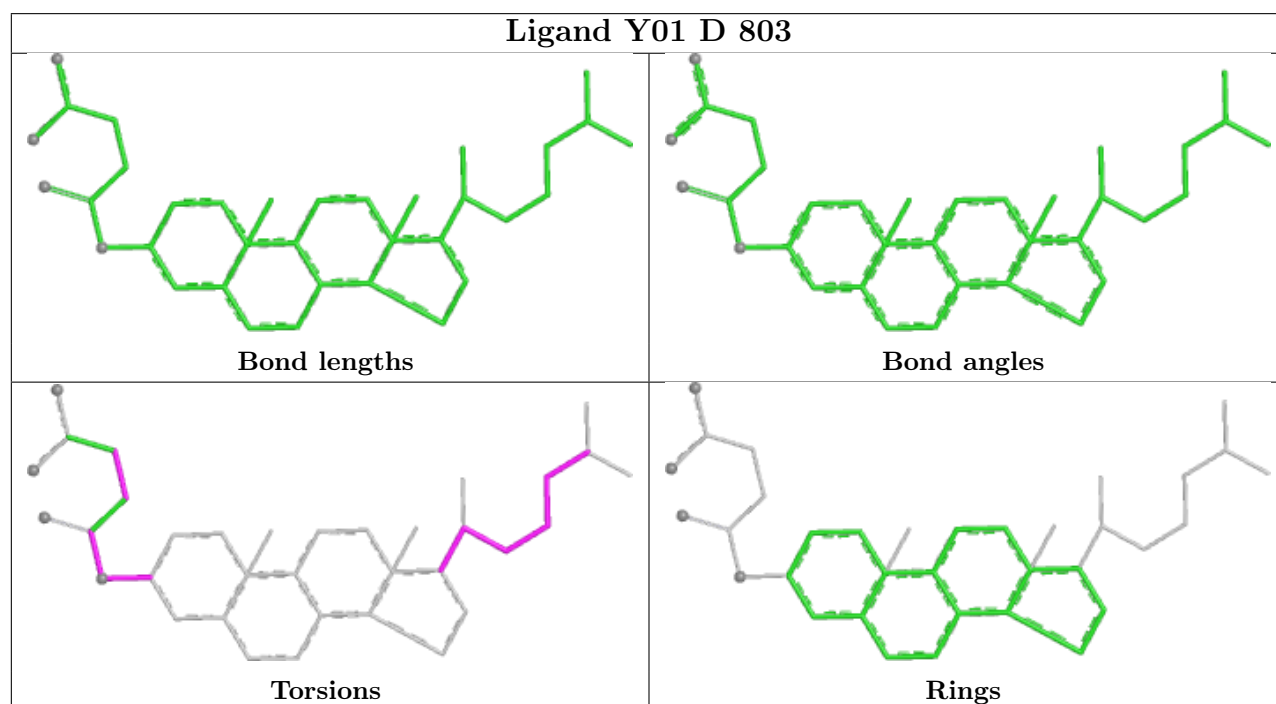
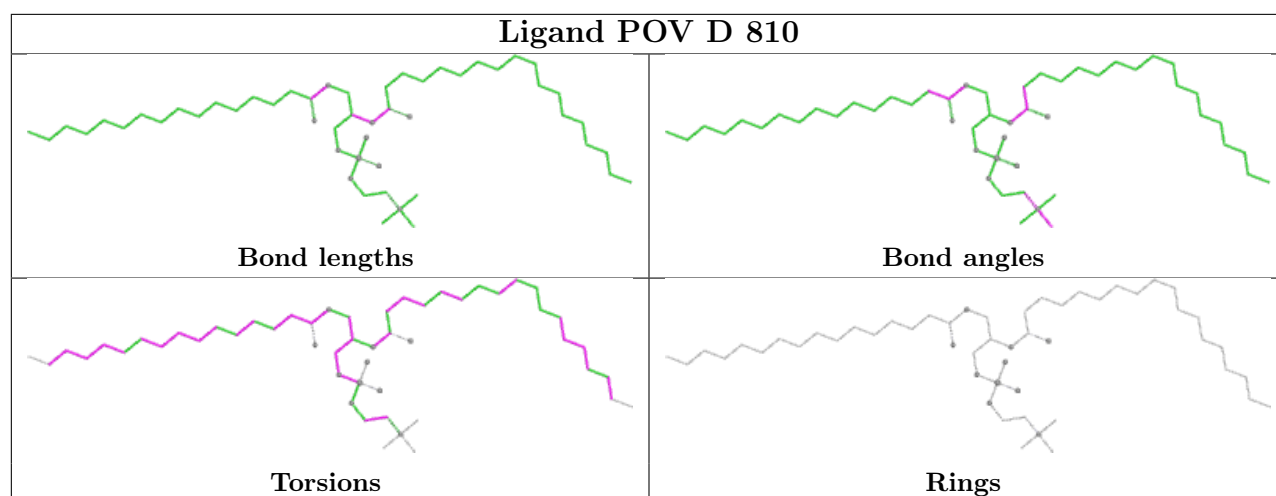


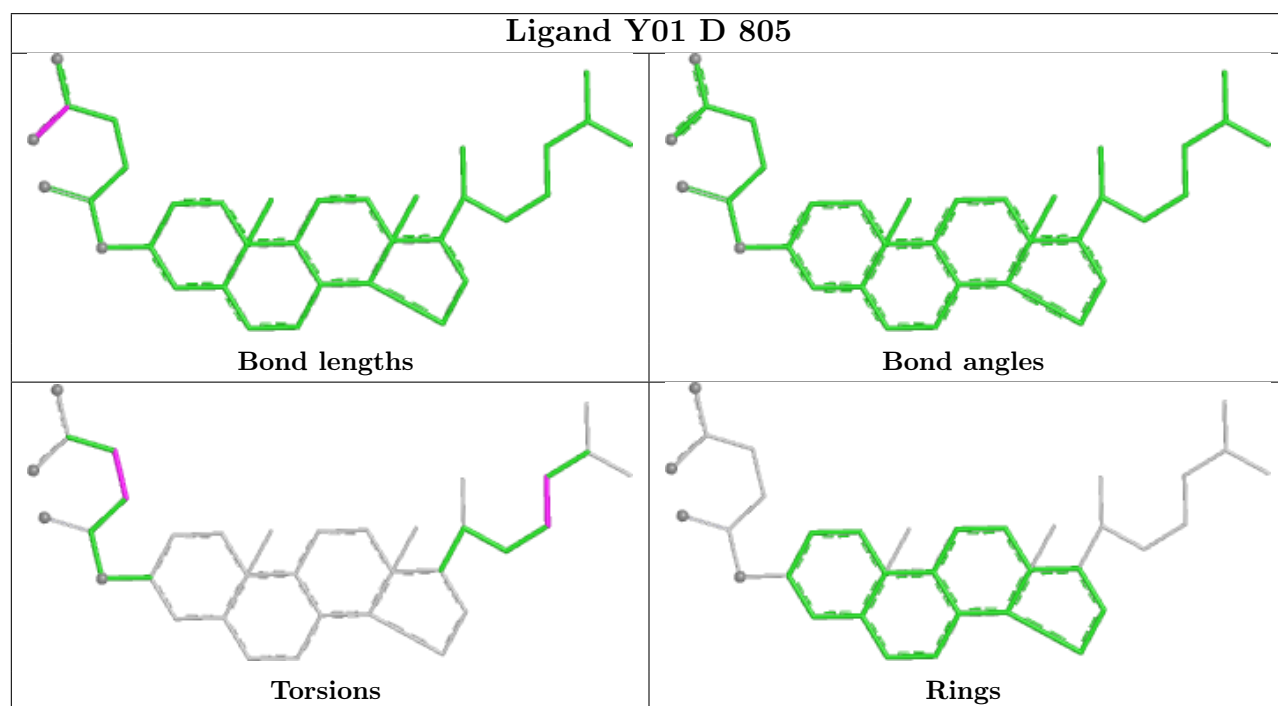
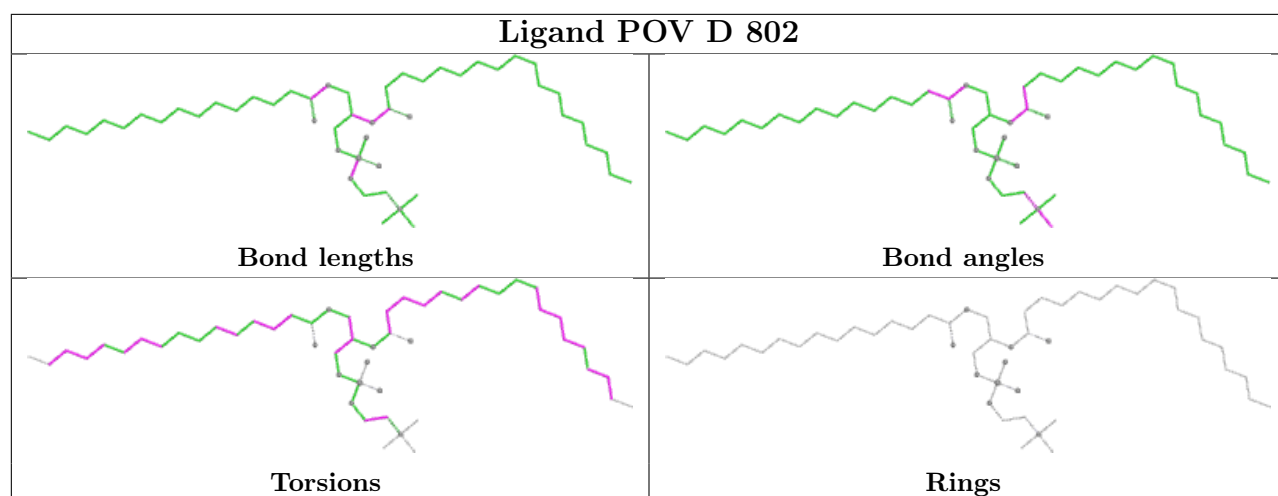


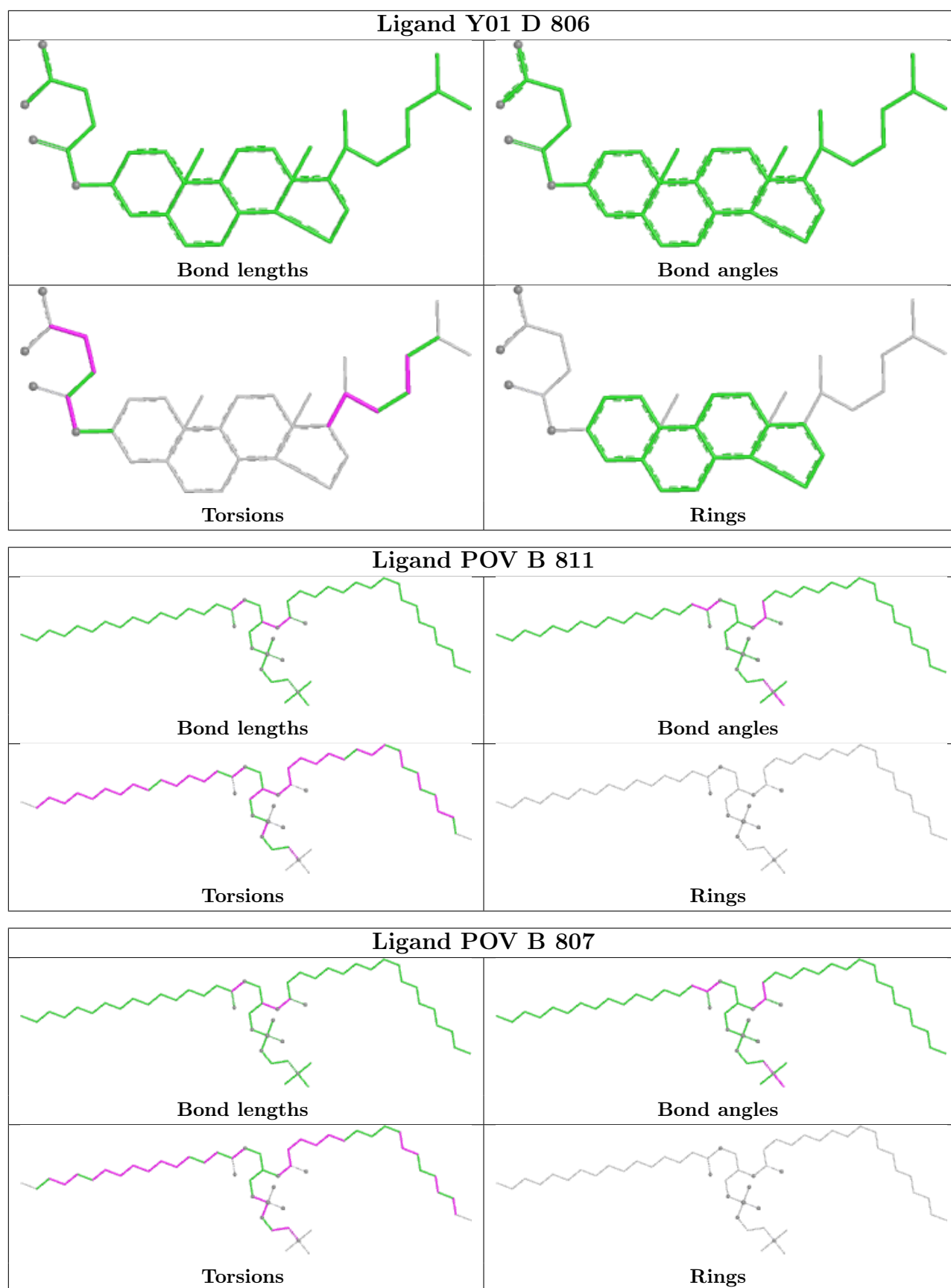


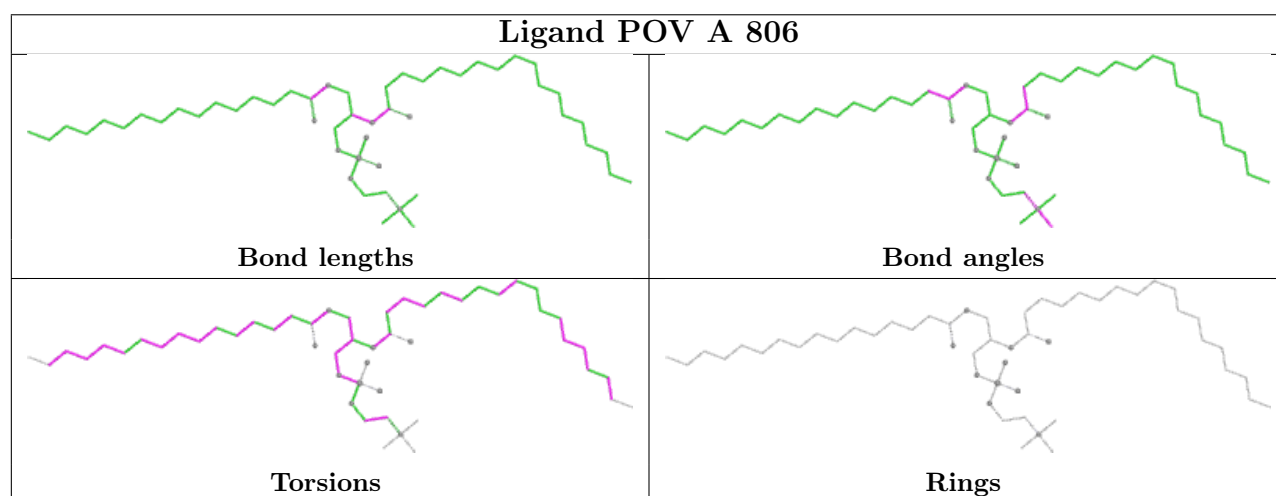
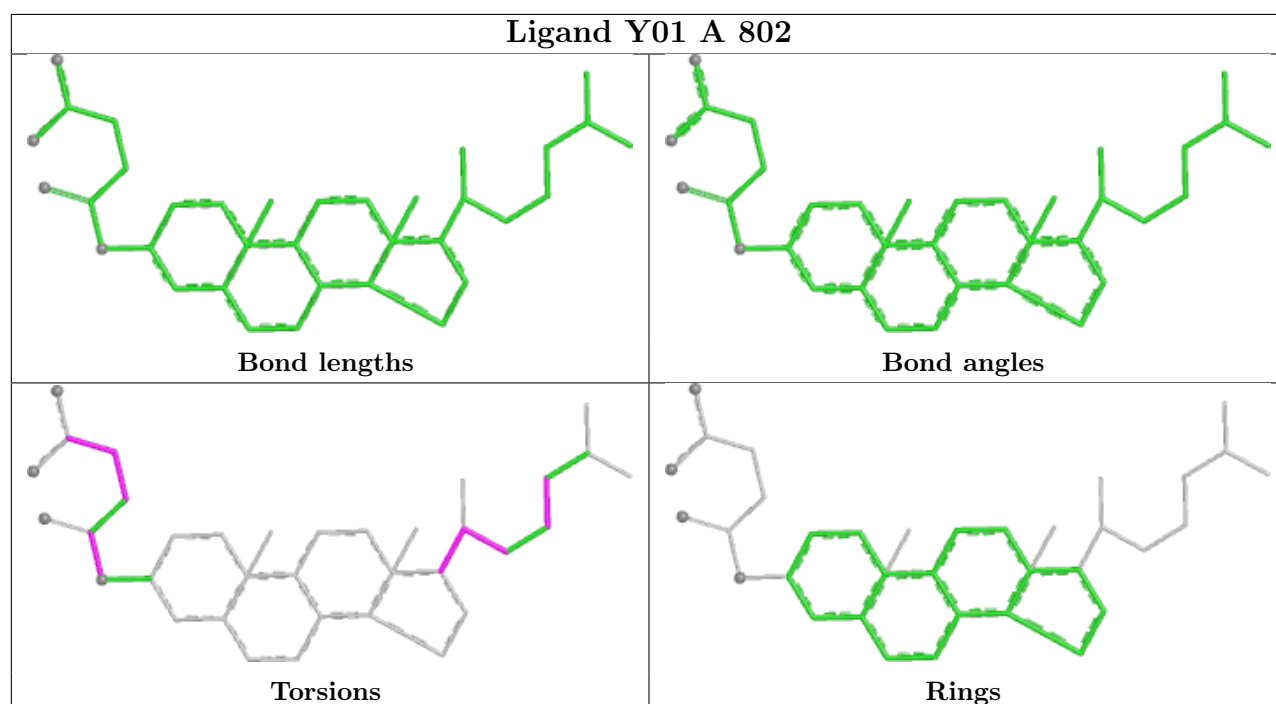
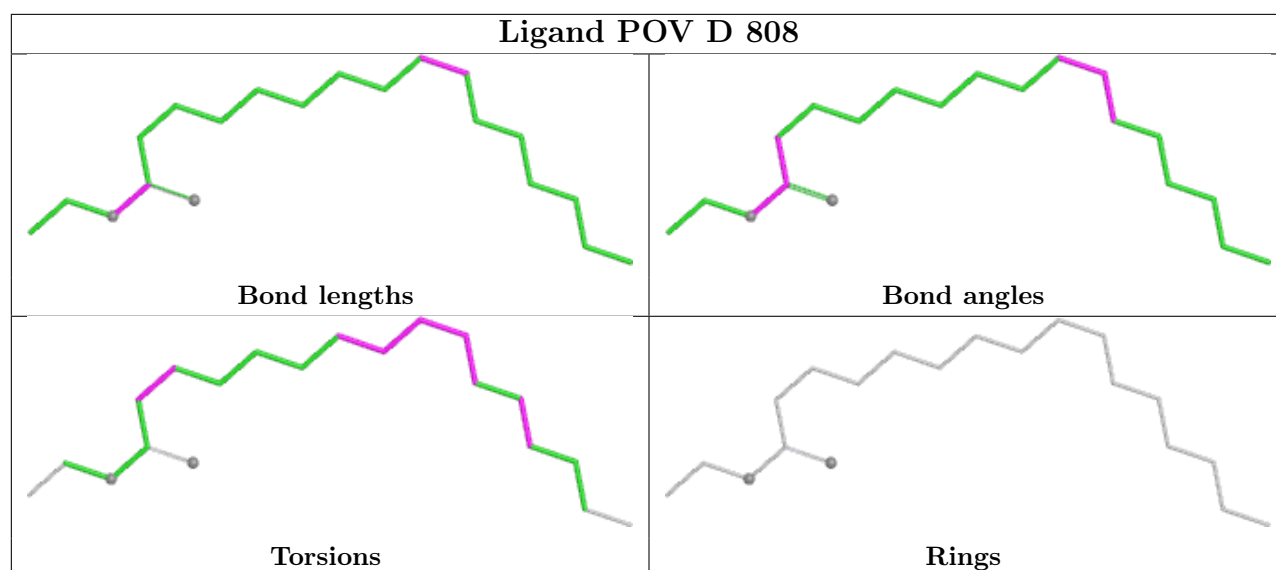


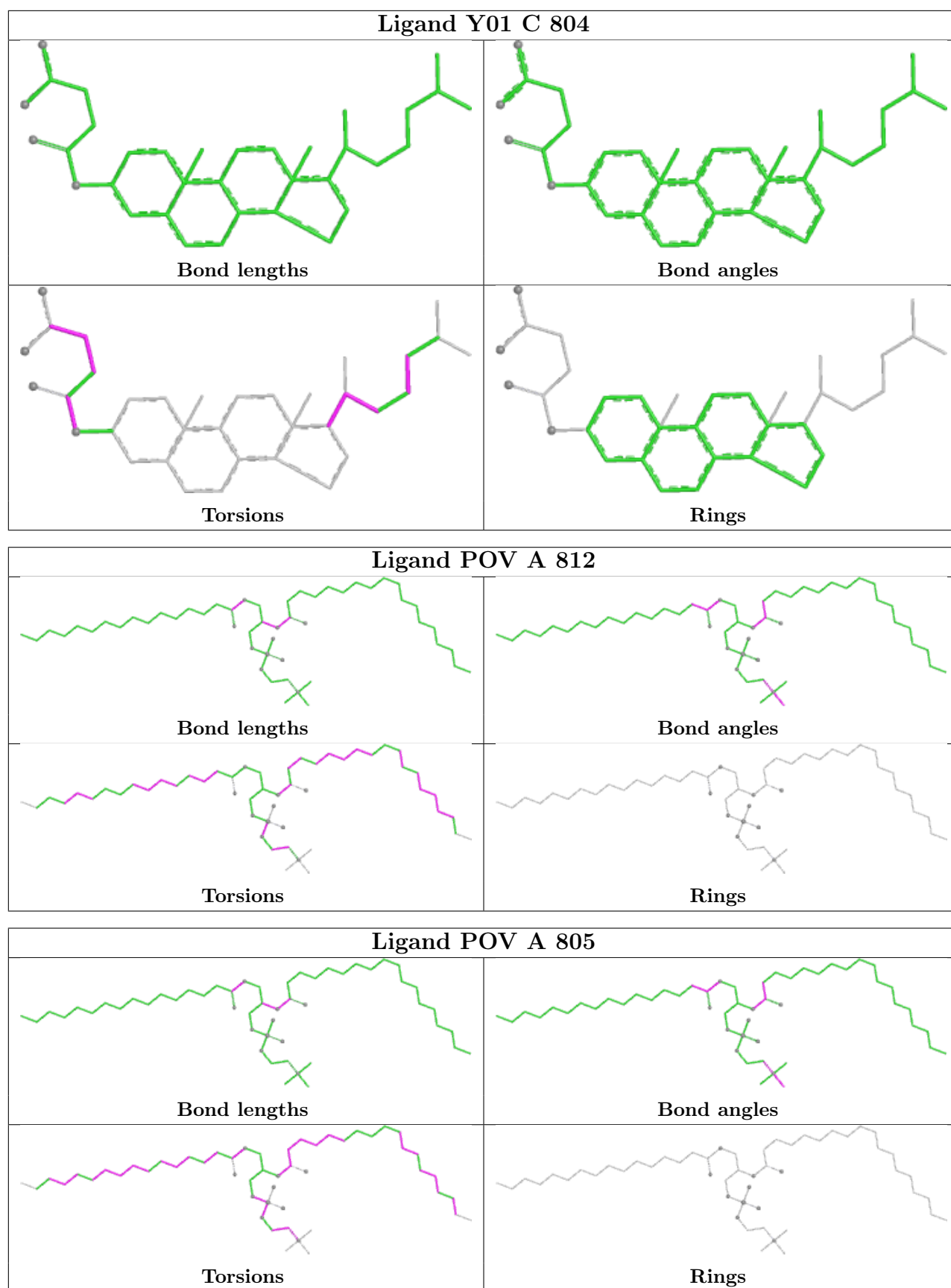


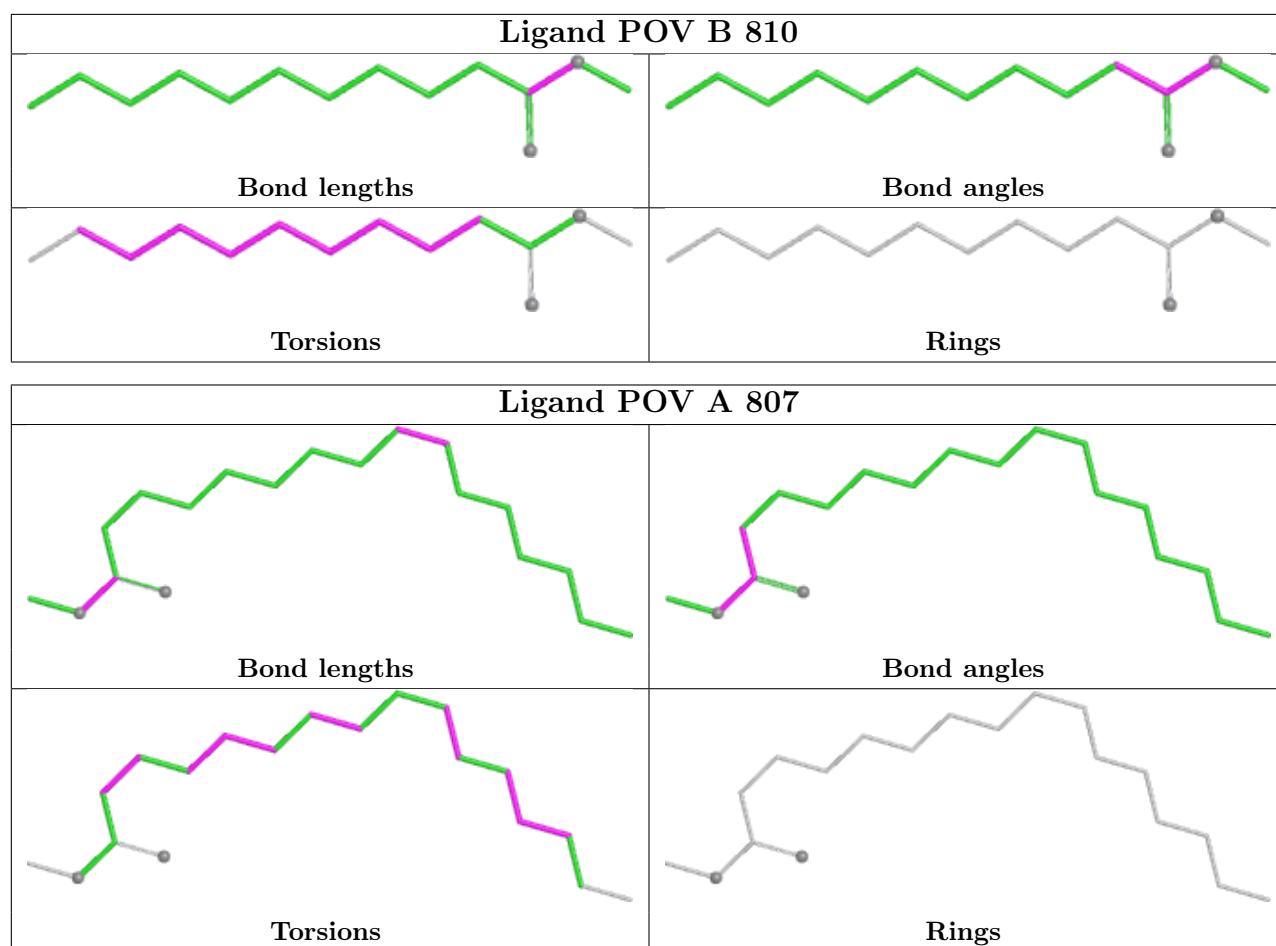












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

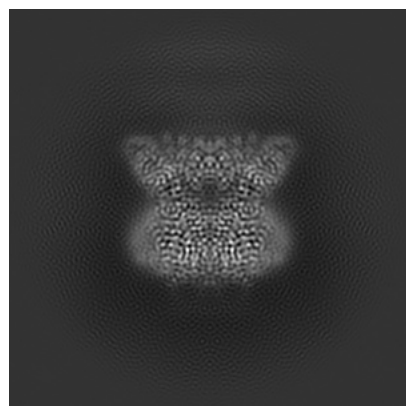
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45933. These allow visual inspection of the internal detail of the map and identification of artifacts.

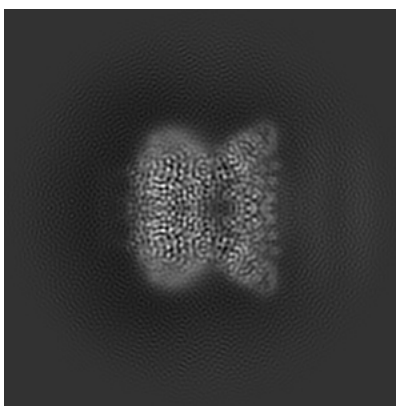
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

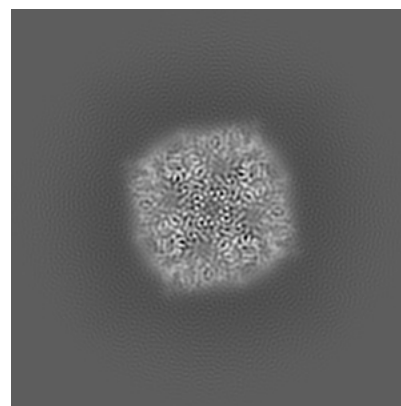
6.1.1 Primary map



X

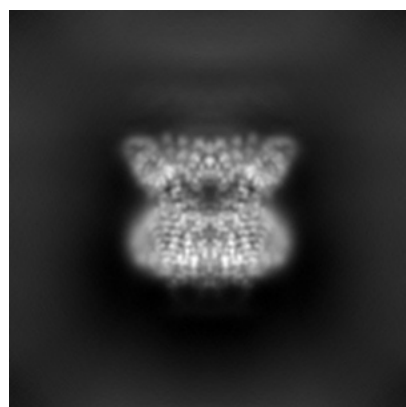


Y

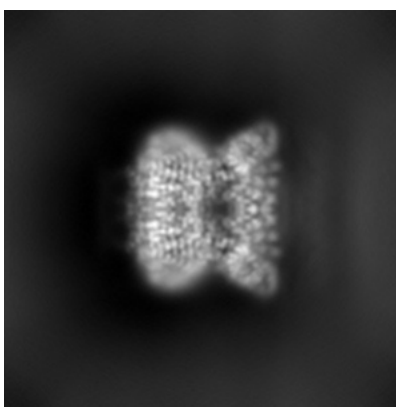


Z

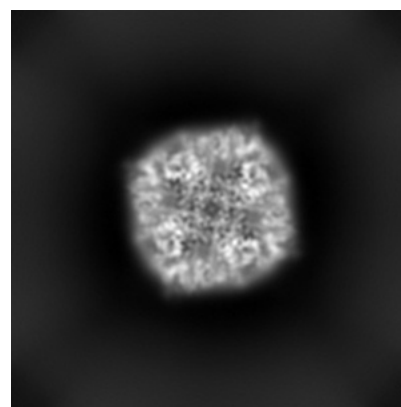
6.1.2 Raw map



X



Y

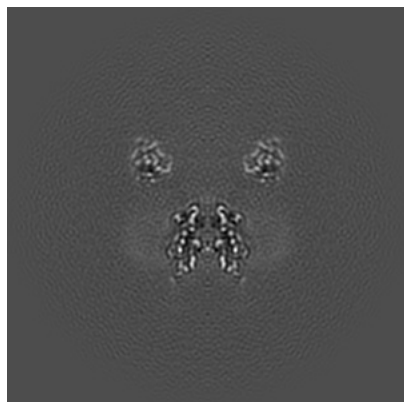


Z

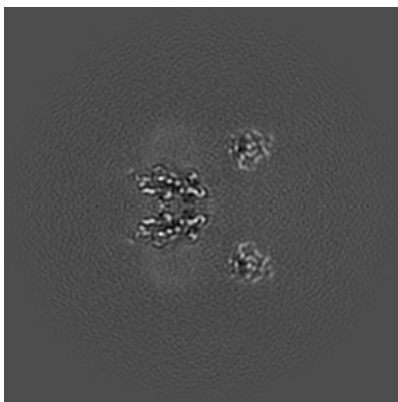
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

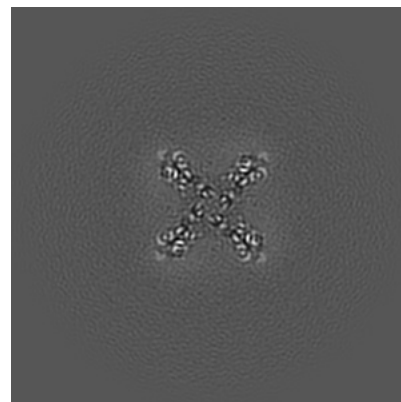
6.2.1 Primary map



X Index: 128

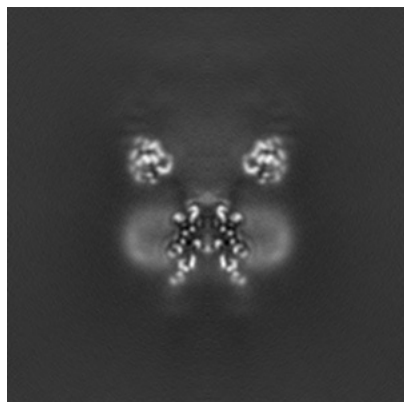


Y Index: 128

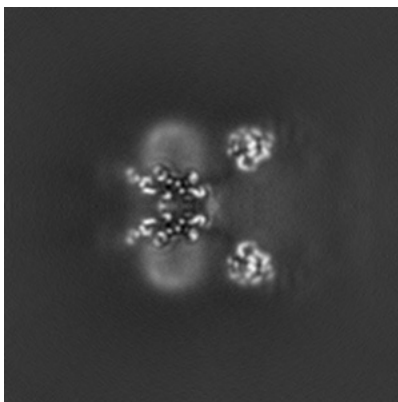


Z Index: 128

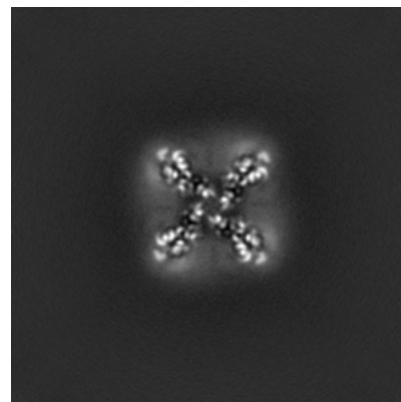
6.2.2 Raw map



X Index: 128



Y Index: 128

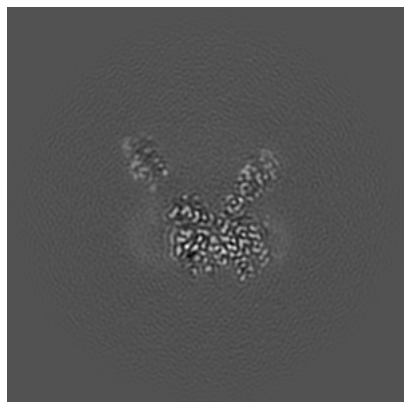


Z Index: 128

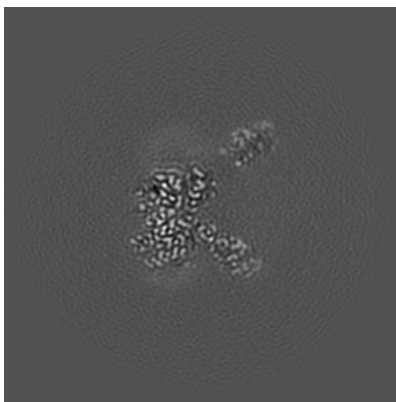
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

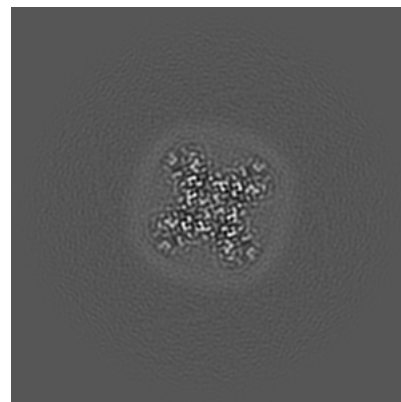
6.3.1 Primary map



X Index: 114

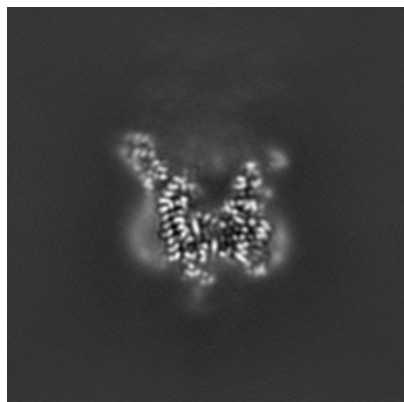


Y Index: 114

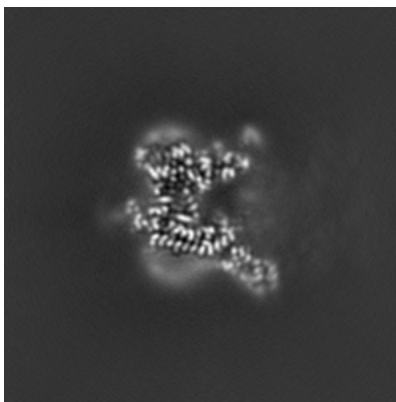


Z Index: 101

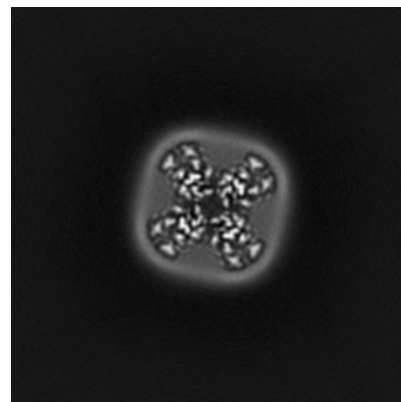
6.3.2 Raw map



X Index: 108



Y Index: 148

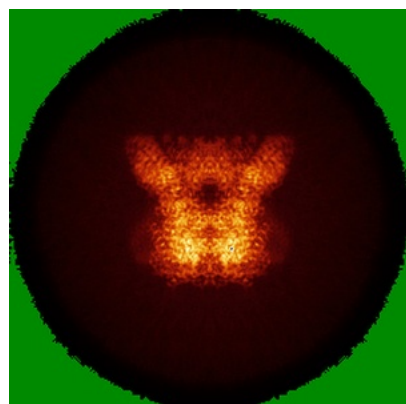


Z Index: 96

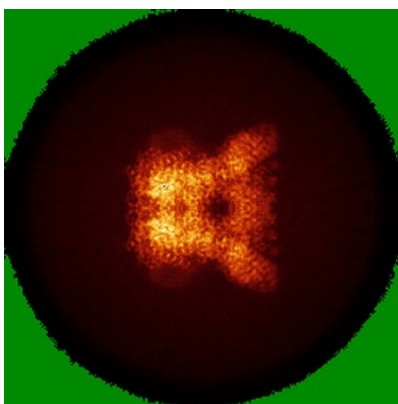
The images above show the largest variance slices of the map in three orthogonal directions.

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

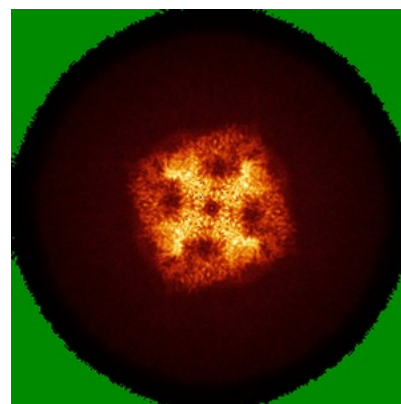
6.4.1 Primary map



X

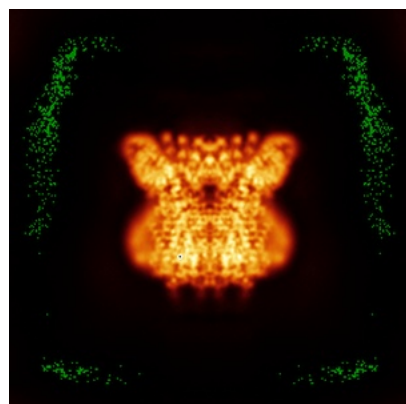


Y

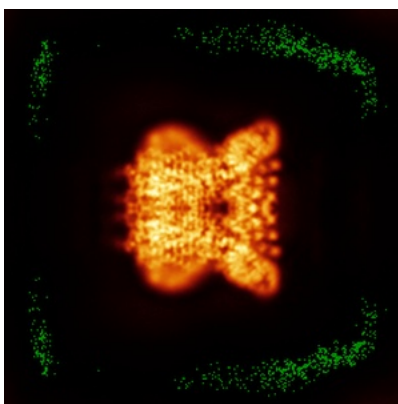


Z

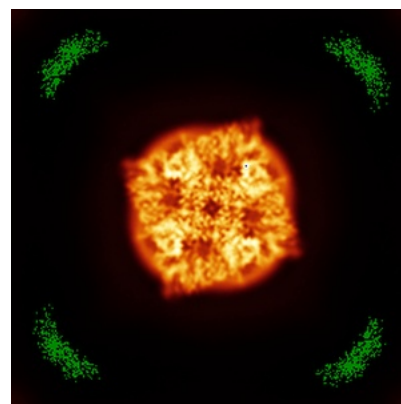
6.4.2 Raw map



X



Y

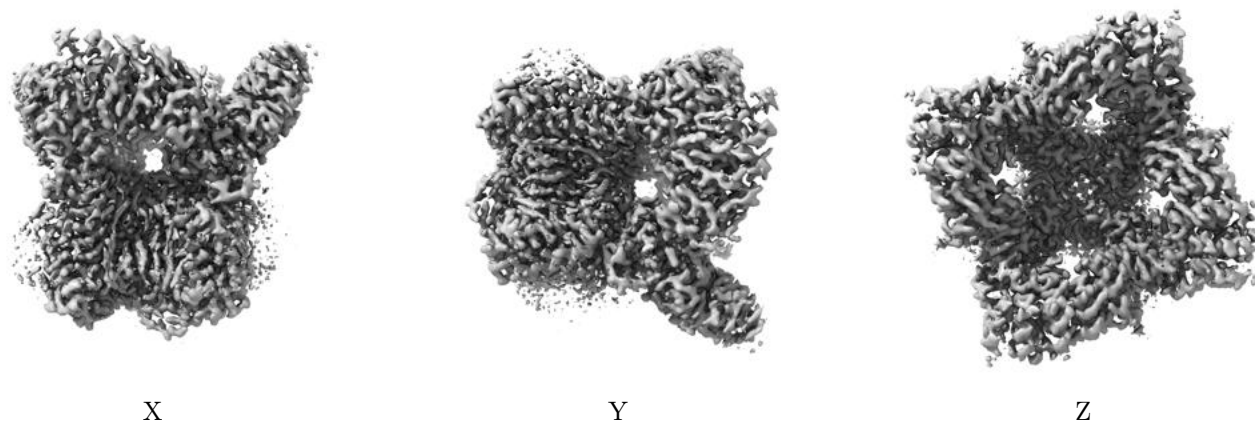


Z

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.

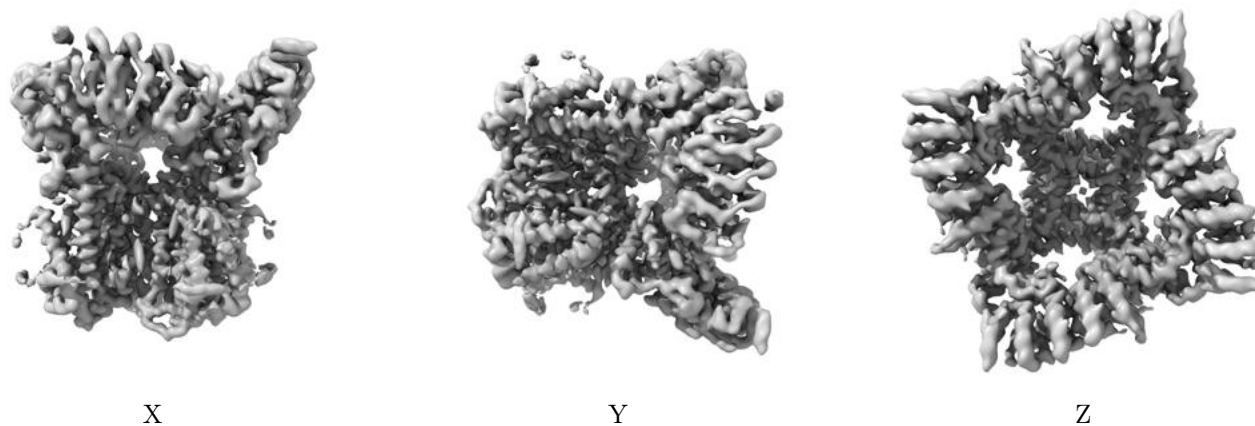
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.624. 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.

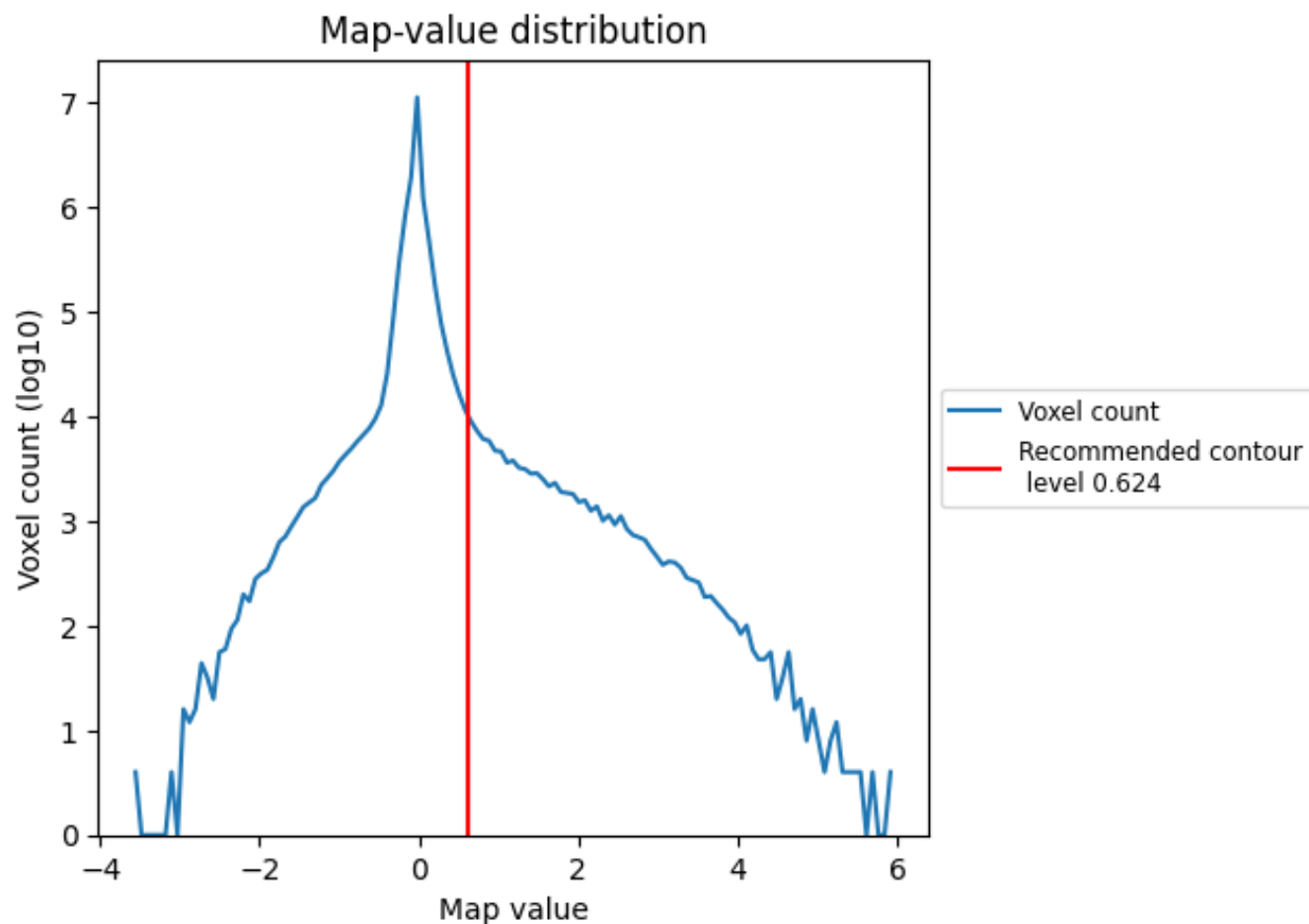
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

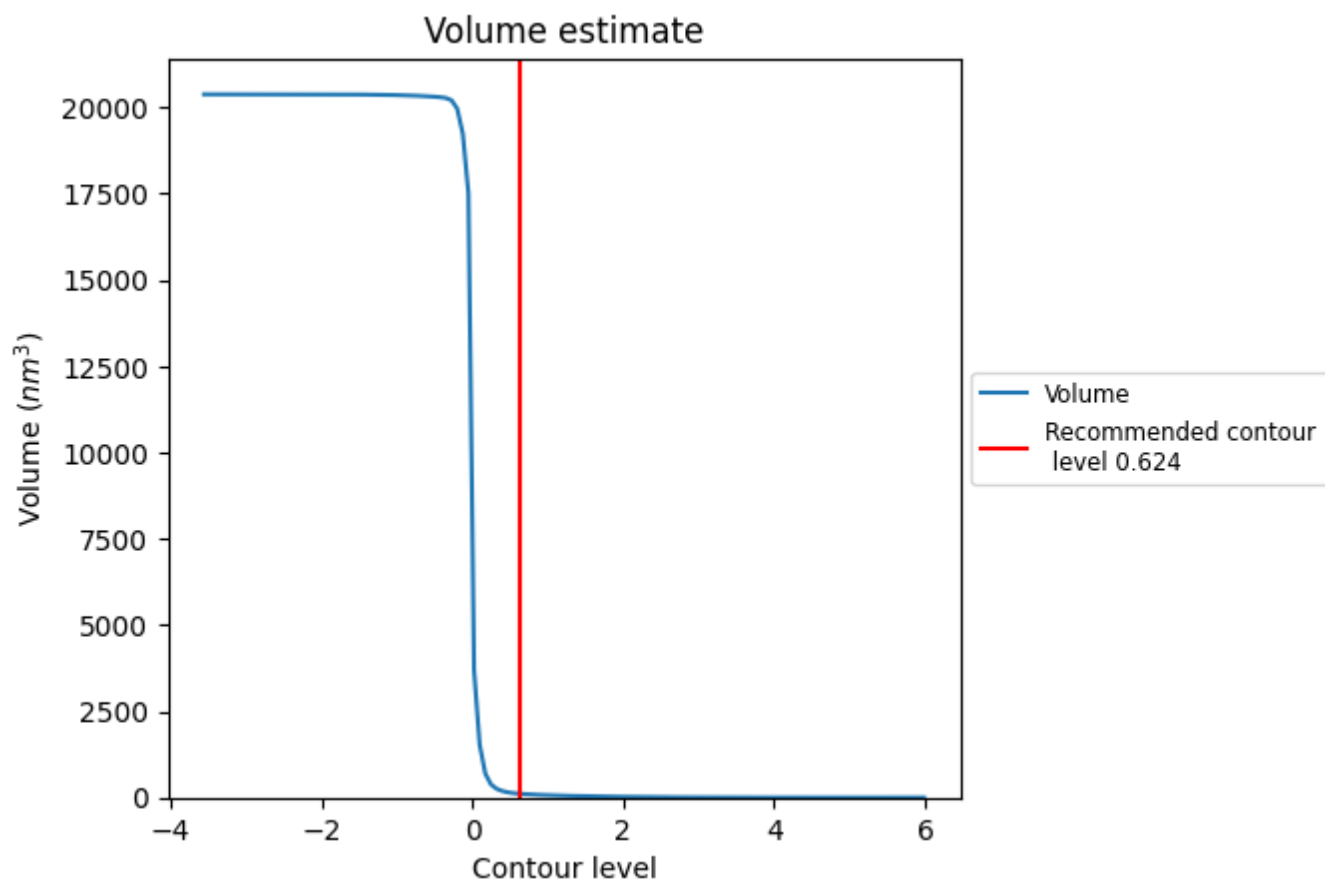
This section contains the results of statistical analysis of the map.

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.

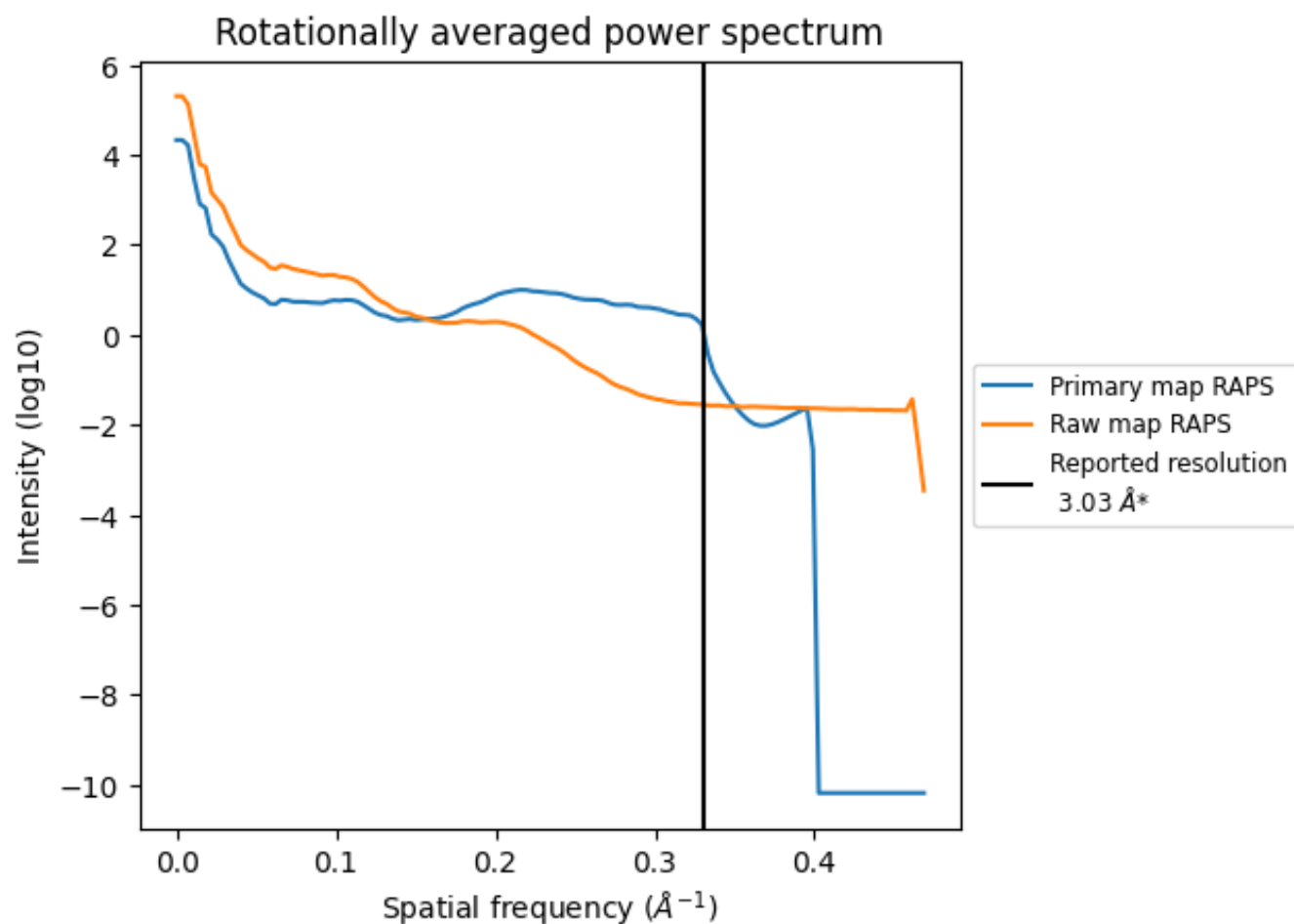
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm^3 ; this corresponds to an approximate mass of 101 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 ⓘ

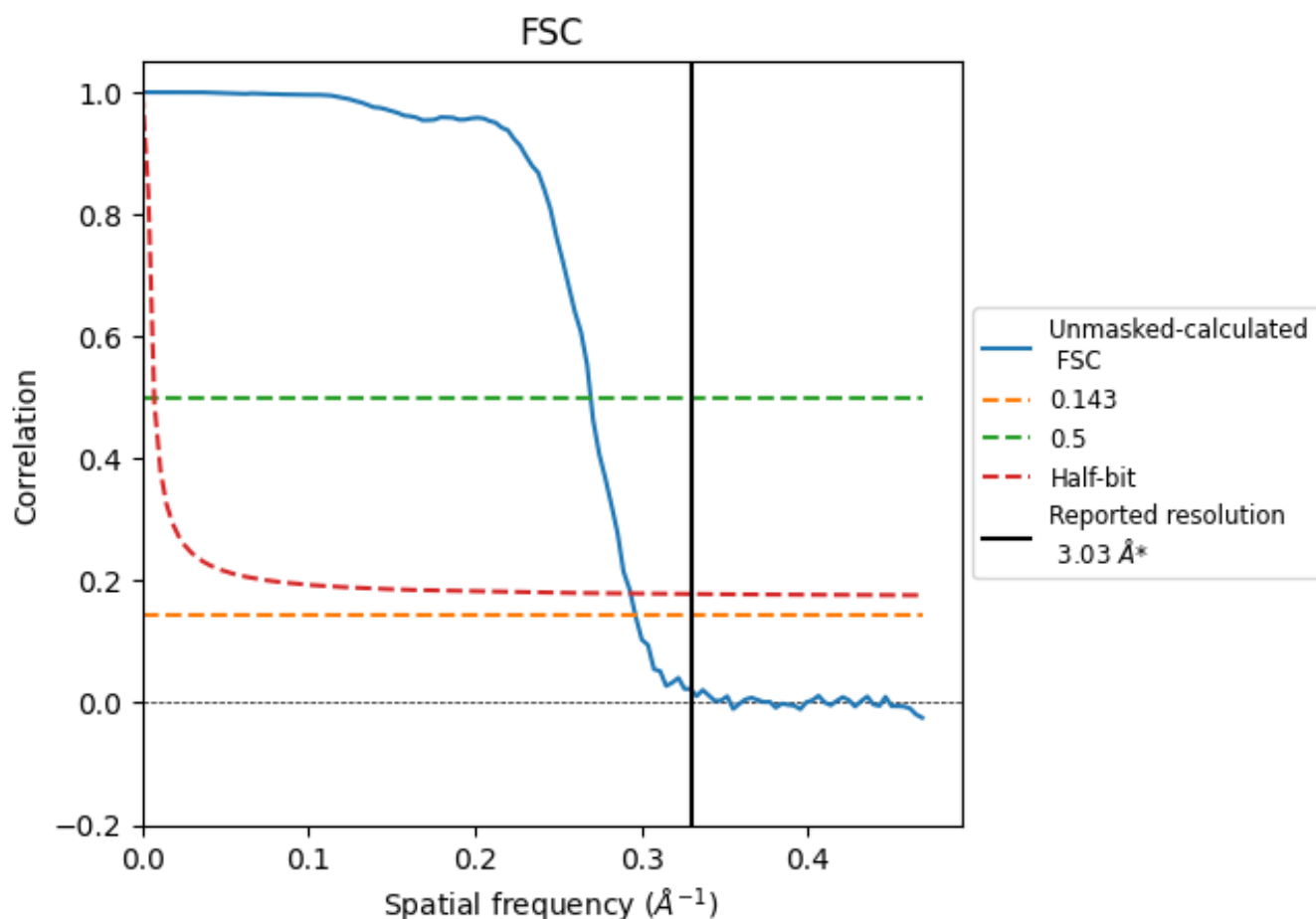


*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

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 0.330 Å⁻¹

8.2 Resolution estimates [i](#)

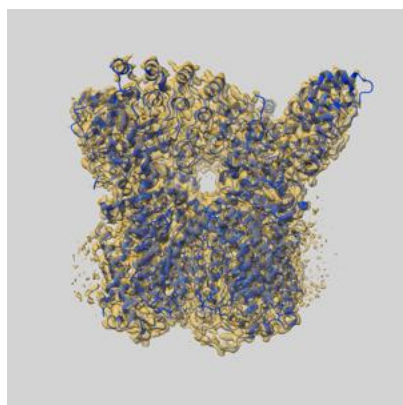
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	3.71	3.41

*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 3.37 differs from the reported value 3.03 by more than 10 %

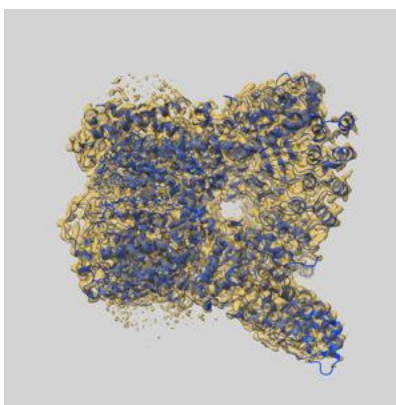
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45933 and PDB model 9CUH. Per-residue inclusion information can be found in section [3](#) on page [8](#).

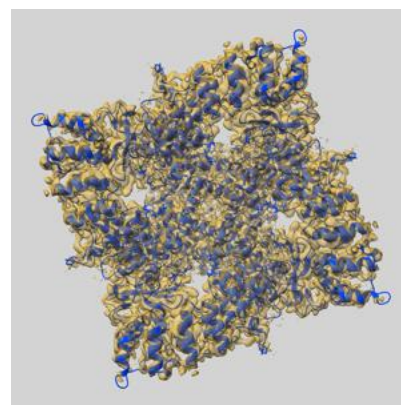
9.1 Map-model overlay [i](#)



X



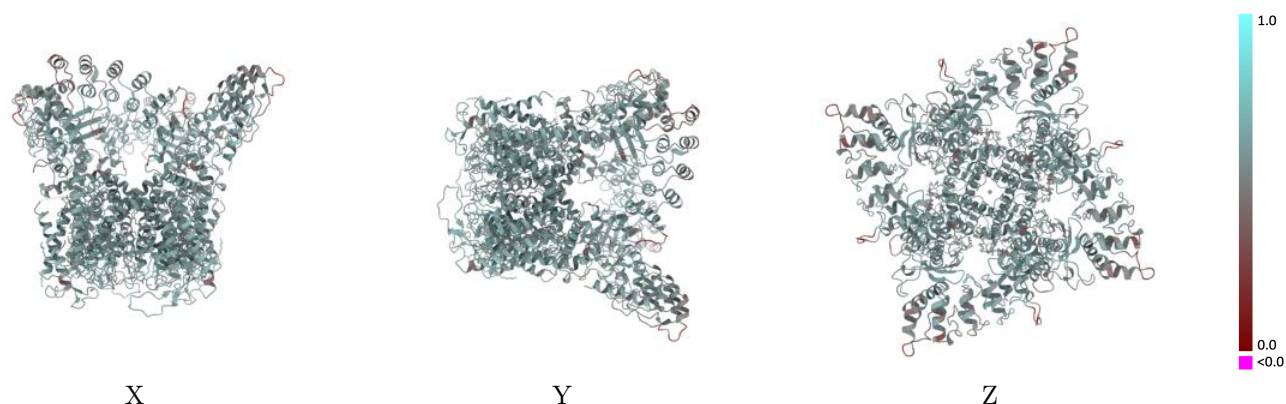
Y



Z

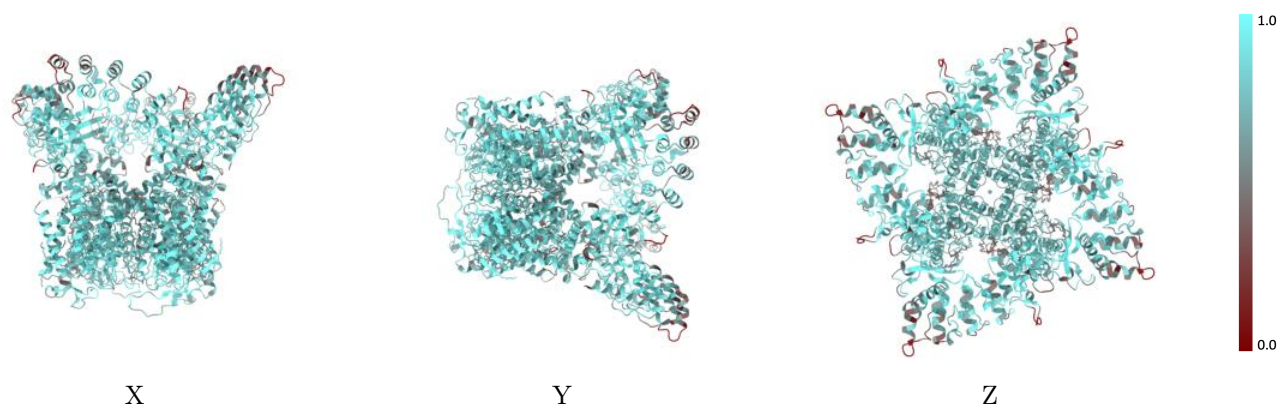
The images above show the 3D surface view of the map at the recommended contour level 0.624 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



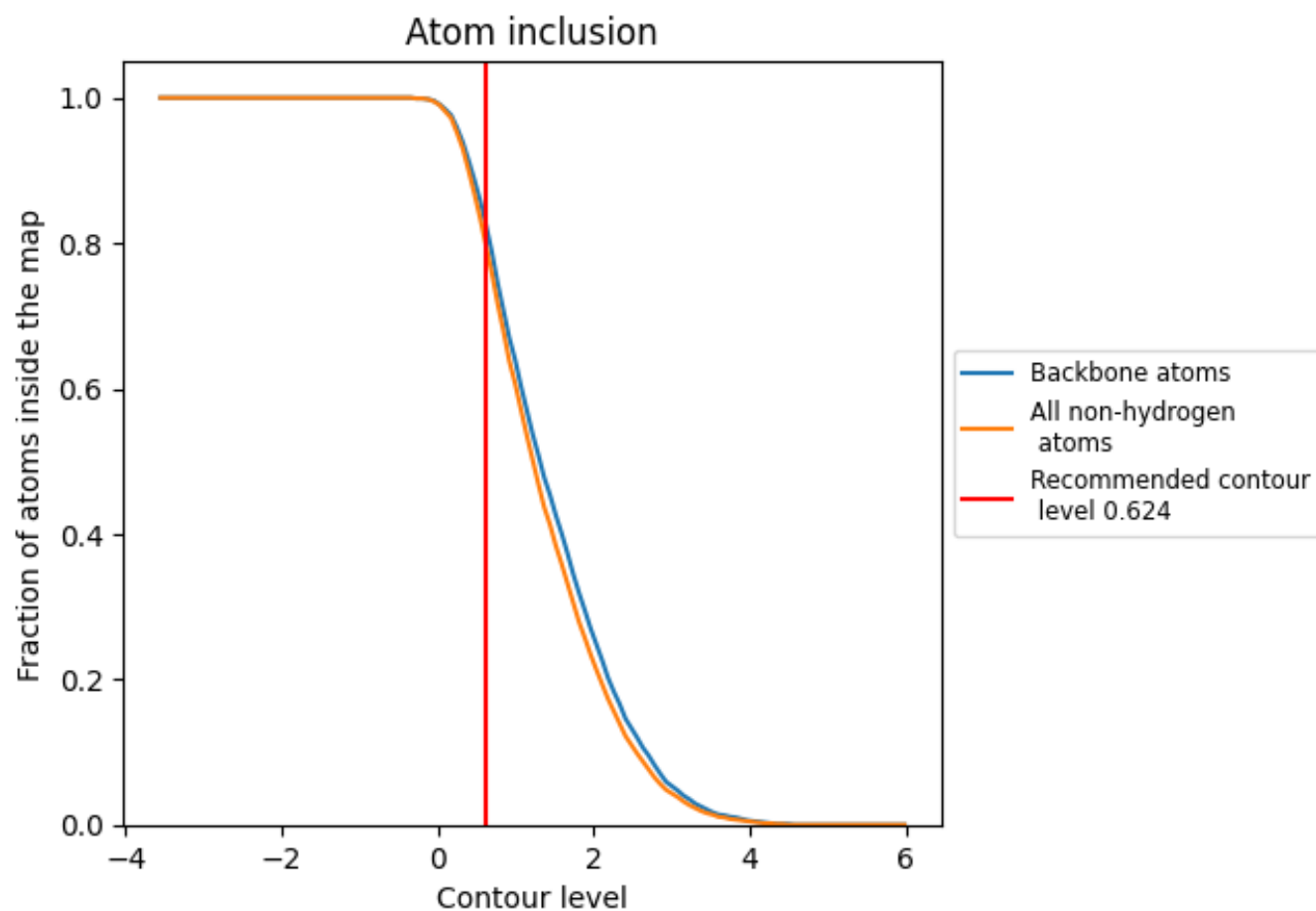
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.624).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.624) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.5600
A	0.8010	0.5600
B	0.8000	0.5600
C	0.8010	0.5610
D	0.8030	0.5600

