



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 06:19 PM UTC

PDB ID : 8SP8 / pdb_00008sp8
EMDB ID : EMD-40676
Title : Human TRP channel TRPV6 in cNW30 nanodiscs inhibited by tetrahydrocannabinabin (THCV)
Authors : Neuberger, A.; Yelshanskaya, M.V.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on : 2023-05-02
Resolution : 2.79 Å(reported)
Based on initial model : 7S8C

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:

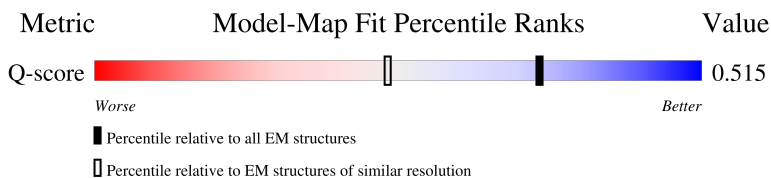
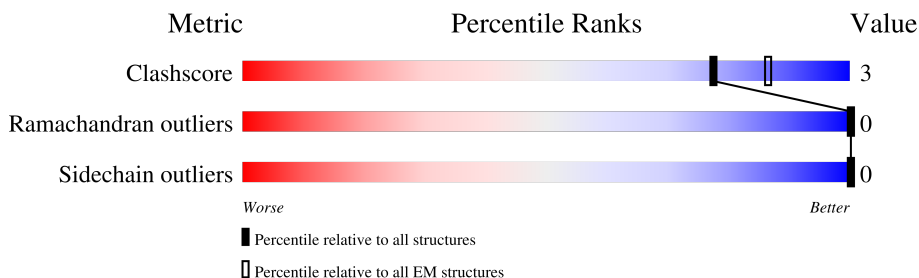
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.79 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	10811 (2.29 - 3.29)

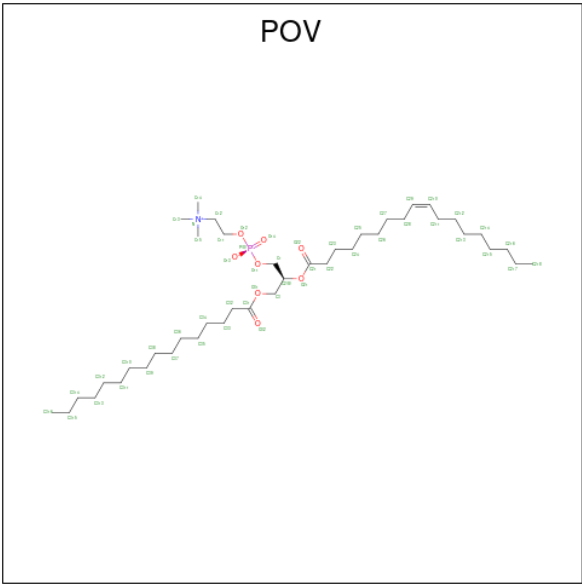
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	666	11% 85% 6% 8%
1	B	666	12% 85% 7% 8%
1	C	666	11% 85% 6% 8%
1	D	666	11% 86% 6% 8%

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
2	A	1	Total 84	31	49	4	0
2	B	1	Total 84	31	49	4	0
2	B	1	Total 84	31	49	4	0
2	B	1	Total 84	31	49	4	0
2	C	1	Total 84	31	49	4	0
2	C	1	Total 84	31	49	4	0
2	C	1	Total 84	31	49	4	0
2	D	1	Total 84	31	49	4	0
2	D	1	Total 84	31	49	4	0
2	D	1	Total 84	31	49	4	0

- Molecule 3 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
			Total	C	H	N	O	P	
3	A	1	Total 134	42	82	1	8	1	0

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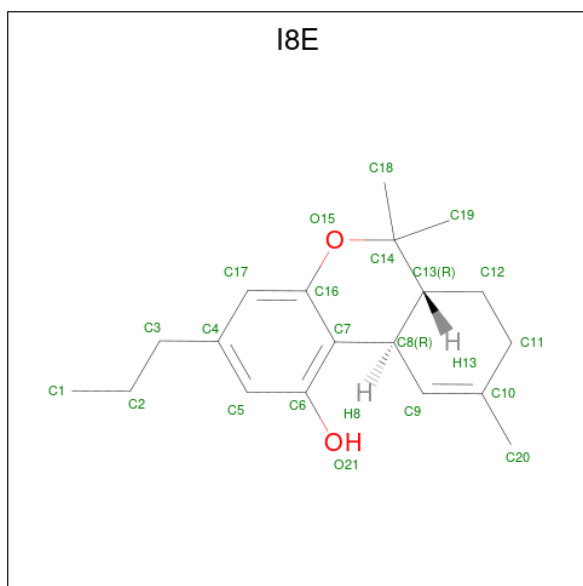
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H 20 8 12	0
3	A	1	Total C H N O P 134 42 82 1 8 1	0
3	A	1	Total C H O 50 17 31 2	0
3	A	1	Total C H 35 13 22	0
3	A	1	Total C H O 33 12 18 3	0
3	A	1	Total C H N O P 134 42 82 1 8 1	0
3	B	1	Total C H N O P 134 42 82 1 8 1	0
3	B	1	Total C H N O P 134 42 82 1 8 1	0
3	B	1	Total C H 20 8 12	0
3	B	1	Total C H N O P 134 42 82 1 8 1	0
3	B	1	Total C H O 50 17 31 2	0
3	B	1	Total C H 35 13 22	0
3	B	1	Total C H O 33 12 18 3	0
3	C	1	Total C H N O P 134 42 82 1 8 1	0
3	C	1	Total C H N O P 134 42 82 1 8 1	0
3	C	1	Total C H 20 8 12	0
3	C	1	Total C H N O P 134 42 82 1 8 1	0
3	C	1	Total C H O 50 17 31 2	0
3	C	1	Total C H 35 13 22	0
3	C	1	Total C H O 33 12 18 3	0
3	D	1	Total C H 35 13 22	0

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Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	H	O		0
			33	12	18	3		
3	D	1	Total	C	H	N	O	P
			134	42	82	1	8	1
3	D	1	Total	C	H	N	O	P
			134	42	82	1	8	1
3	D	1	Total	C	H			
			20	8	12			
3	D	1	Total	C	H	N	O	P
			134	42	82	1	8	1
3	D	1	Total	C	H	O		
			50	17	31	2		

- Molecule 4 is Tetrahydrocannabivarin (CCD ID: I8E) (formula: $C_{19}H_{26}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			47	19	26	2	
4	A	1	Total	C	H	O	0
			47	19	26	2	
4	B	1	Total	C	H	O	0
			47	19	26	2	
4	B	1	Total	C	H	O	0
			47	19	26	2	
4	C	1	Total	C	H	O	0
			47	19	26	2	

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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	H	O	0
			47	19	26	2	
4	D	1	Total	C	H	O	0
			47	19	26	2	
4	D	1	Total	C	H	O	0
			47	19	26	2	

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

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

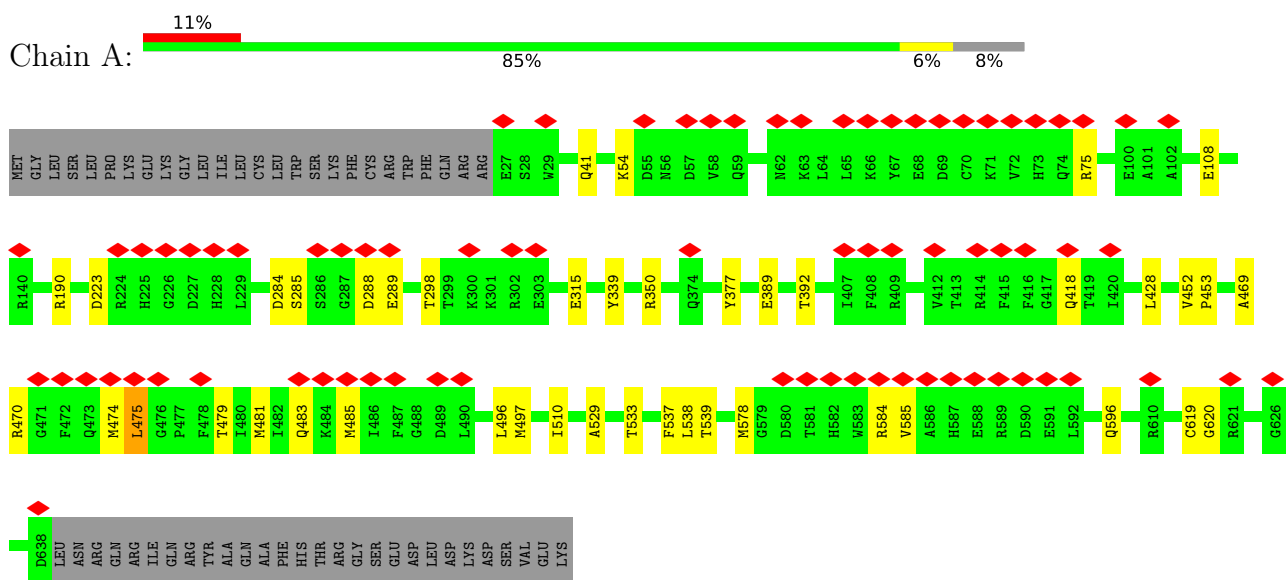
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Cl	0
			1	1	

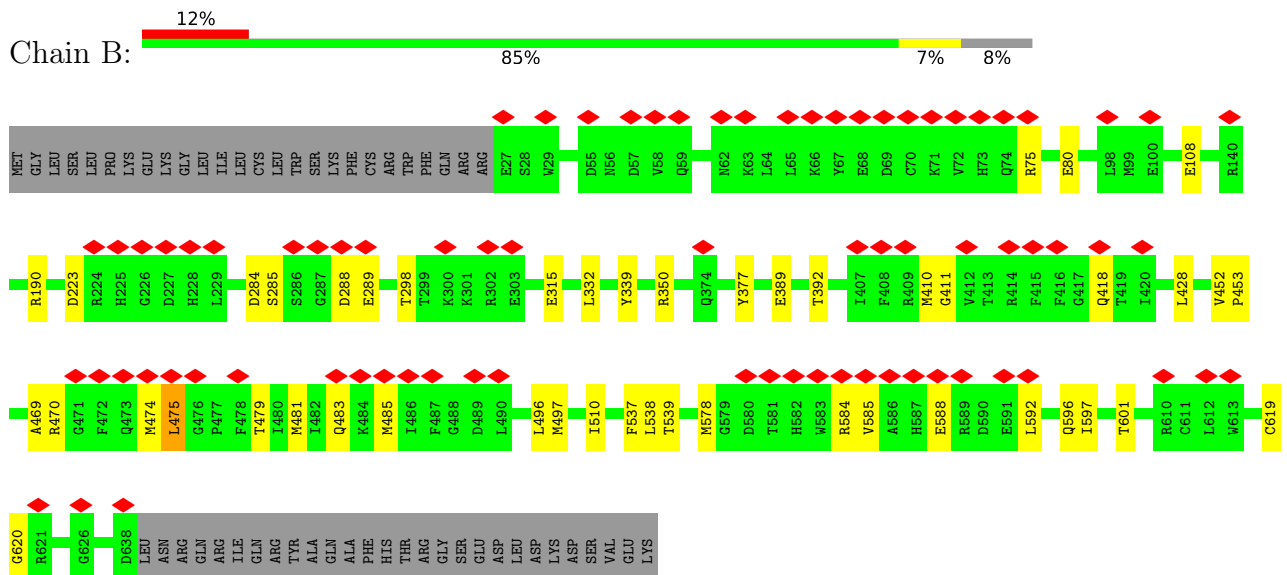
3 Residue-property plots

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

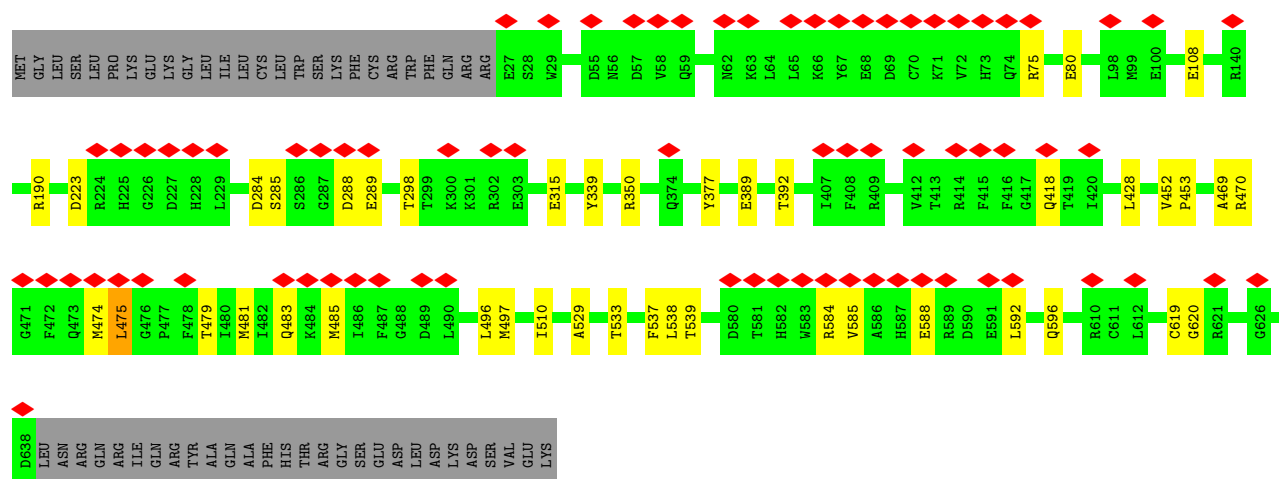
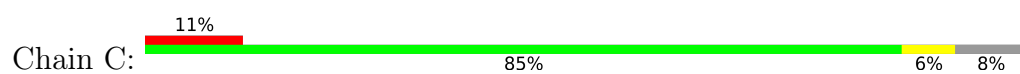
- Molecule 1: Transient receptor potential cation channel subfamily V member 6



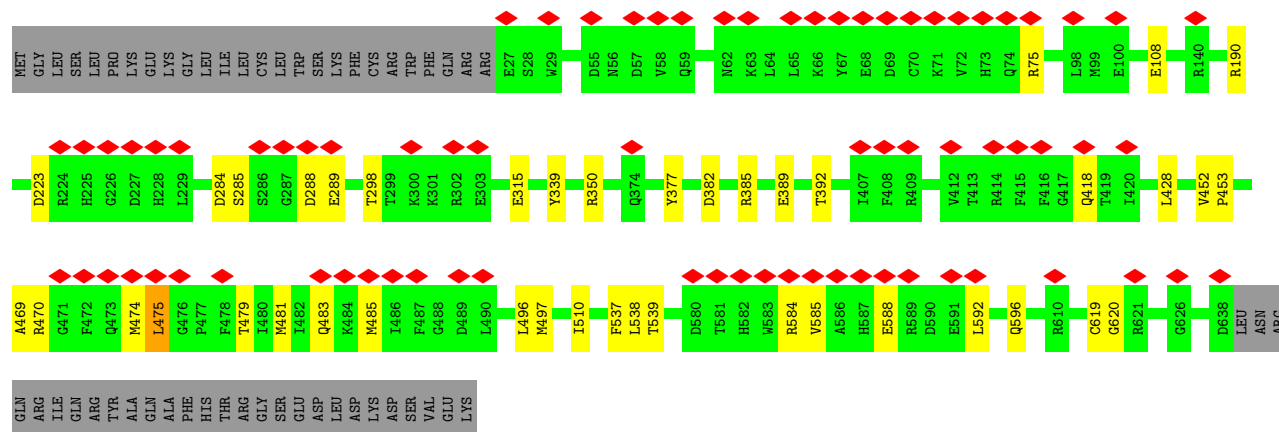
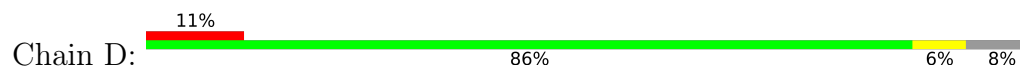
- Molecule 1: Transient receptor potential cation channel subfamily V member 6



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213249	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.278	Depositor
Minimum map value	-0.755	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.147	Depositor
Map size ($\text{\AA}$)	211.2, 211.2, 211.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CA, I8E, POV, Y01

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	0.49	0/5025	0.58	1/6818 (0.0%)
1	B	0.49	0/5025	0.58	1/6818 (0.0%)
1	C	0.49	0/5025	0.58	1/6818 (0.0%)
1	D	0.49	0/5025	0.58	1/6818 (0.0%)
All	All	0.49	0/20100	0.58	4/27272 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	LEU	CA-CB-CG	6.16	137.85	116.30
1	B	475	LEU	CA-CB-CG	6.15	137.83	116.30
1	D	475	LEU	CA-CB-CG	6.15	137.83	116.30
1	C	475	LEU	CA-CB-CG	6.15	137.82	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4912	4965	4964	31	0
1	B	4912	4965	4964	34	0
1	C	4912	4965	4964	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4912	4965	4964	30	0
2	A	105	147	147	4	0
2	B	105	147	147	7	0
2	C	105	147	147	6	0
2	D	105	147	147	6	0
3	A	211	329	324	1	0
3	B	211	329	324	1	0
3	C	211	329	324	1	0
3	D	211	329	324	1	0
4	A	42	52	0	2	0
4	B	42	52	0	2	0
4	C	42	52	0	2	0
4	D	42	52	0	2	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
All	All	21082	21972	21740	123	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 3.

All (123) 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:C:377:TYR:OH	1:C:389:GLU:OE1	2.07	0.72
1:D:377:TYR:OH	1:D:389:GLU:OE1	2.07	0.72
1:B:377:TYR:OH	1:B:389:GLU:OE1	2.07	0.71
1:A:377:TYR:OH	1:A:389:GLU:OE1	2.07	0.70
1:A:481:MET:O	1:A:485:MET:N	2.25	0.69
1:B:298:THR:O	1:B:418:GLN:NE2	2.26	0.69
1:A:298:THR:O	1:A:418:GLN:NE2	2.26	0.69
1:C:481:MET:O	1:C:485:MET:N	2.25	0.69
1:C:298:THR:O	1:C:418:GLN:NE2	2.26	0.68
1:D:481:MET:O	1:D:485:MET:N	2.25	0.68
1:D:298:THR:O	1:D:418:GLN:NE2	2.26	0.68
1:A:496:LEU:HD22	1:D:475:LEU:HD12	1.76	0.67
1:B:481:MET:O	1:B:485:MET:N	2.26	0.67
1:C:475:LEU:HD12	1:D:496:LEU:HD22	1.77	0.66
1:A:475:LEU:HD12	1:B:496:LEU:HD22	1.77	0.66
1:D:483:GLN:NE2	2:D:706:Y01:OAG	2.27	0.66
1:B:483:GLN:NE2	2:B:704:Y01:OAG	2.27	0.64
1:B:475:LEU:HD12	1:C:496:LEU:HD22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:GLN:NE2	2:C:704:Y01:OAG	2.27	0.63
1:B:389:GLU:HB3	3:B:709:POV:H210	1.81	0.62
1:C:389:GLU:HB3	3:C:709:POV:H210	1.82	0.62
1:A:483:GLN:NE2	2:A:802:Y01:OAG	2.27	0.61
1:D:389:GLU:HB3	3:D:711:POV:H210	1.81	0.61
1:B:190:ARG:NH1	1:B:223:ASP:OD1	2.34	0.61
1:A:190:ARG:NH1	1:A:223:ASP:OD1	2.34	0.61
1:A:389:GLU:HB3	3:A:807:POV:H210	1.82	0.61
1:C:75:ARG:NH1	1:C:108:GLU:OE1	2.34	0.61
1:A:75:ARG:NH1	1:A:108:GLU:OE1	2.34	0.60
1:C:190:ARG:NH1	1:C:223:ASP:OD1	2.34	0.60
1:D:75:ARG:NH1	1:D:108:GLU:OE1	2.34	0.60
1:D:190:ARG:NH1	1:D:223:ASP:OD1	2.34	0.60
1:B:75:ARG:NH1	1:B:108:GLU:OE1	2.34	0.60
1:D:315:GLU:OE1	1:D:315:GLU:N	2.38	0.57
1:B:339:TYR:OH	1:B:392:THR:O	2.19	0.57
1:A:315:GLU:N	1:A:315:GLU:OE1	2.38	0.57
1:B:315:GLU:N	1:B:315:GLU:OE1	2.38	0.56
1:C:315:GLU:N	1:C:315:GLU:OE1	2.38	0.56
1:A:428:LEU:HD21	2:A:802:Y01:HAD3	1.89	0.55
1:C:339:TYR:OH	1:C:392:THR:O	2.19	0.55
1:B:428:LEU:HD21	2:B:704:Y01:HAD3	1.89	0.54
1:C:428:LEU:HD21	2:C:704:Y01:HAD3	1.89	0.54
1:C:497:MET:HE1	4:C:710:I8E:C19	2.37	0.54
1:D:339:TYR:OH	1:D:392:THR:O	2.18	0.54
1:D:497:MET:HE1	4:D:712:I8E:C19	2.37	0.54
1:D:428:LEU:HD21	2:D:706:Y01:HAD3	1.89	0.54
1:B:497:MET:HE1	4:B:710:I8E:C19	2.37	0.54
1:D:619:CYS:SG	1:D:620:GLY:N	2.81	0.54
1:A:619:CYS:SG	1:A:620:GLY:N	2.81	0.53
1:A:497:MET:HE1	4:A:808:I8E:C19	2.37	0.53
1:A:339:TYR:OH	1:A:392:THR:O	2.19	0.53
1:B:619:CYS:SG	1:B:620:GLY:N	2.81	0.53
1:B:475:LEU:O	1:B:479:THR:N	2.42	0.52
1:C:475:LEU:O	1:C:479:THR:N	2.42	0.52
1:C:619:CYS:SG	1:C:620:GLY:N	2.81	0.52
1:A:475:LEU:O	1:A:479:THR:N	2.42	0.52
1:D:475:LEU:O	1:D:479:THR:N	2.42	0.52
1:A:475:LEU:HB3	1:B:496:LEU:HD13	1.93	0.50
1:A:496:LEU:HD13	1:D:475:LEU:HB3	1.95	0.48
1:C:288:ASP:OD1	1:C:289:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:LEU:HB3	1:D:496:LEU:HD13	1.96	0.47
1:D:470:ARG:NH1	1:D:596:GLN:OE1	2.41	0.47
1:A:288:ASP:OD1	1:A:289:GLU:N	2.47	0.46
1:A:538:LEU:O	1:A:539:THR:OG1	2.30	0.46
1:A:470:ARG:NH1	1:A:596:GLN:OE1	2.41	0.46
1:D:288:ASP:OD1	1:D:289:GLU:N	2.47	0.46
1:B:475:LEU:HB3	1:C:496:LEU:HD13	1.96	0.46
1:A:469:ALA:HB1	1:A:474:MET:HB2	1.99	0.45
1:C:452:VAL:HB	1:C:453:PRO:HD3	1.98	0.45
1:B:469:ALA:HB1	1:B:474:MET:HB2	1.99	0.45
1:C:469:ALA:HB1	1:C:474:MET:HB2	1.99	0.45
1:D:538:LEU:O	1:D:539:THR:OG1	2.30	0.45
1:B:80:GLU:OE1	1:B:80:GLU:N	2.48	0.45
1:B:350:ARG:NH2	1:C:510:ILE:O	2.50	0.45
1:D:469:ALA:HB1	1:D:474:MET:HB2	1.99	0.45
1:A:452:VAL:HB	1:A:453:PRO:HD3	1.98	0.44
2:D:705:Y01:HAE2	2:D:705:Y01:HBB	1.95	0.44
1:D:452:VAL:HB	1:D:453:PRO:HD3	1.98	0.44
1:B:288:ASP:OD1	1:B:289:GLU:N	2.47	0.44
1:C:350:ARG:NH2	1:D:510:ILE:O	2.51	0.44
1:B:452:VAL:HB	1:B:453:PRO:HD3	1.98	0.44
2:B:703:Y01:HAE2	2:B:703:Y01:HBB	1.95	0.43
1:C:470:ARG:NH1	1:C:596:GLN:OE1	2.41	0.43
1:C:529:ALA:O	1:C:533:THR:OG1	2.34	0.43
1:A:584:ARG:HG3	1:A:585:VAL:H	1.84	0.43
1:B:470:ARG:NH1	1:B:596:GLN:OE1	2.41	0.43
2:B:705:Y01:HAB3	4:B:710:I8E:C4	2.49	0.43
1:A:350:ARG:NH2	1:B:510:ILE:O	2.51	0.43
1:A:510:ILE:O	1:D:350:ARG:NH2	2.51	0.43
1:A:529:ALA:O	1:A:533:THR:OG1	2.34	0.43
1:D:584:ARG:HG3	1:D:585:VAL:H	1.84	0.42
1:D:382:ASP:OD1	1:D:385:ARG:NH2	2.47	0.42
2:C:705:Y01:HAB3	4:C:710:I8E:C4	2.49	0.42
1:B:597:ILE:O	1:B:601:THR:OG1	2.35	0.42
2:D:707:Y01:HAB3	4:D:712:I8E:C4	2.49	0.42
1:B:584:ARG:HG3	1:B:585:VAL:H	1.84	0.42
1:A:428:LEU:CD2	2:A:802:Y01:HAD3	2.50	0.42
2:A:803:Y01:HAB3	4:A:808:I8E:C4	2.49	0.42
1:D:428:LEU:CD2	2:D:706:Y01:HAD3	2.50	0.42
2:C:703:Y01:HAE2	2:C:703:Y01:HBB	1.95	0.42
1:B:588:GLU:O	1:B:592:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:MET:HE3	1:C:537:PHE:CD2	2.55	0.42
1:D:497:MET:HE3	1:D:537:PHE:CD2	2.55	0.42
1:A:497:MET:HE3	1:A:537:PHE:CD2	2.55	0.41
1:C:538:LEU:O	1:C:539:THR:OG1	2.30	0.41
1:D:284:ASP:OD1	1:D:285:SER:N	2.53	0.41
1:C:588:GLU:O	1:C:592:LEU:N	2.52	0.41
1:C:584:ARG:HG3	1:C:585:VAL:H	1.84	0.41
1:B:497:MET:HE3	1:B:537:PHE:CD2	2.55	0.41
1:D:588:GLU:O	1:D:592:LEU:N	2.52	0.41
1:A:284:ASP:OD1	1:A:285:SER:N	2.53	0.41
1:A:578:MET:HE2	1:B:578:MET:HE1	2.02	0.41
1:C:80:GLU:OE1	1:C:80:GLU:N	2.48	0.41
1:C:428:LEU:CD2	2:C:704:Y01:HAD3	2.50	0.41
1:B:284:ASP:OD1	1:B:285:SER:N	2.53	0.41
1:B:428:LEU:CD2	2:B:704:Y01:HAD3	2.50	0.41
1:B:538:LEU:O	1:B:539:THR:OG1	2.30	0.41
2:C:705:Y01:HAP1	2:C:705:Y01:HAO2	1.96	0.41
1:C:284:ASP:OD1	1:C:285:SER:N	2.53	0.40
1:A:41:GLN:OE1	1:A:54:LYS:NZ	2.49	0.40
1:B:332:LEU:HD12	2:B:703:Y01:HAD2	2.04	0.40
1:B:410:MET:HG2	1:B:411:GLY:H	1.87	0.40
2:B:703:Y01:HAO2	2:B:703:Y01:HAP1	1.89	0.40
2:D:706:Y01:HAU2	2:D:706:Y01:HAO1	2.04	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	610/666 (92%)	560 (92%)	50 (8%)	0	100	100
1	B	610/666 (92%)	560 (92%)	50 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	610/666 (92%)	560 (92%)	50 (8%)	0	100	100
1	D	610/666 (92%)	560 (92%)	50 (8%)	0	100	100
All	All	2440/2664 (92%)	2240 (92%)	200 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	531/580 (92%)	531 (100%)	0	100	100
1	B	531/580 (92%)	531 (100%)	0	100	100
1	C	531/580 (92%)	531 (100%)	0	100	100
1	D	531/580 (92%)	531 (100%)	0	100	100
All	All	2124/2320 (92%)	2124 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	118	GLN
1	A	426	HIS
1	B	73	HIS
1	B	118	GLN
1	B	426	HIS
1	C	73	HIS
1	C	118	GLN
1	C	426	HIS
1	D	73	HIS
1	D	118	GLN
1	D	426	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 2 are 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	$\# Z > 2$
2	Y01	B	703	-	38,38,38	0.49	0	57,57,57	0.98	2 (3%)
4	I8E	D	712	-	23,23,23	0.42	0	33,35,35	1.41	7 (21%)
3	POV	D	708	-	51,51,51	0.36	0	57,59,59	0.49	0
3	POV	A	805	-	7,7,51	0.16	0	6,6,59	0.12	0
3	POV	C	709	-	18,18,51	0.85	1 (5%)	18,18,59	0.51	0
2	Y01	A	802	-	38,38,38	0.41	0	57,57,57	0.73	1 (1%)
2	Y01	B	705	-	38,38,38	0.42	0	57,57,57	0.80	2 (3%)
3	POV	A	809	-	12,12,51	0.11	0	11,11,59	0.22	0
3	POV	D	703	-	51,51,51	0.40	0	57,59,59	0.67	2 (3%)
2	Y01	B	704	-	38,38,38	0.42	0	57,57,57	0.72	1 (1%)
3	POV	B	711	-	12,12,51	0.11	0	11,11,59	0.23	0
3	POV	D	702	-	14,14,51	0.26	0	14,14,59	0.24	0
4	I8E	C	702	-	23,23,23	0.23	0	33,35,35	0.66	1 (3%)
4	I8E	A	812	-	23,23,23	0.23	0	33,35,35	0.66	1 (3%)
3	POV	D	711	-	18,18,51	0.84	1 (5%)	18,18,59	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	A	810	-	14,14,51	0.26	0	14,14,59	0.25	0
3	POV	D	710	-	51,51,51	0.32	0	57,59,59	0.57	1 (1%)
3	POV	C	701	-	51,51,51	0.40	0	57,59,59	0.66	2 (3%)
3	POV	B	707	-	7,7,51	0.16	0	6,6,59	0.12	0
3	POV	B	708	-	51,51,51	0.32	0	57,59,59	0.56	1 (1%)
3	POV	D	701	-	12,12,51	0.11	0	11,11,59	0.23	0
3	POV	B	709	-	18,18,51	0.84	1 (5%)	18,18,59	0.51	0
2	Y01	C	703	-	38,38,38	0.50	0	57,57,57	0.98	3 (5%)
3	POV	B	701	-	51,51,51	0.40	0	57,59,59	0.66	2 (3%)
2	Y01	D	707	-	38,38,38	0.41	0	57,57,57	0.80	2 (3%)
2	Y01	C	705	-	38,38,38	0.42	0	57,57,57	0.80	2 (3%)
3	POV	B	706	-	51,51,51	0.36	0	57,59,59	0.50	0
3	POV	B	712	-	14,14,51	0.27	0	14,14,59	0.24	0
3	POV	A	807	-	18,18,51	0.84	1 (5%)	18,18,59	0.51	0
2	Y01	D	705	-	38,38,38	0.49	0	57,57,57	0.97	3 (5%)
3	POV	D	709	-	7,7,51	0.16	0	6,6,59	0.12	0
4	I8E	B	702	-	23,23,23	0.22	0	33,35,35	0.66	1 (3%)
2	Y01	A	803	-	38,38,38	0.42	0	57,57,57	0.80	2 (3%)
3	POV	C	706	-	51,51,51	0.36	0	57,59,59	0.49	0
3	POV	C	707	-	7,7,51	0.16	0	6,6,59	0.12	0
4	I8E	B	710	-	23,23,23	0.42	0	33,35,35	1.41	7 (21%)
2	Y01	A	801	-	38,38,38	0.49	0	57,57,57	0.99	2 (3%)
3	POV	C	712	-	14,14,51	0.26	0	14,14,59	0.23	0
4	I8E	D	704	-	23,23,23	0.23	0	33,35,35	0.66	1 (3%)
2	Y01	D	706	-	38,38,38	0.41	0	57,57,57	0.72	1 (1%)
3	POV	A	804	-	51,51,51	0.36	0	57,59,59	0.49	0
3	POV	A	806	-	51,51,51	0.32	0	57,59,59	0.57	1 (1%)
3	POV	C	708	-	51,51,51	0.32	0	57,59,59	0.57	1 (1%)
3	POV	A	811	-	51,51,51	0.41	0	57,59,59	0.67	2 (3%)
3	POV	C	711	-	12,12,51	0.11	0	11,11,59	0.22	0
4	I8E	C	710	-	23,23,23	0.42	0	33,35,35	1.42	6 (18%)
4	I8E	A	808	-	23,23,23	0.42	0	33,35,35	1.41	6 (18%)
2	Y01	C	704	-	38,38,38	0.41	0	57,57,57	0.72	1 (1%)

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
2	Y01	B	703	-	-	8/19/77/77	0/4/4/4
4	I8E	D	712	-	-	1/3/31/31	0/3/3/3
3	POV	D	708	-	-	24/55/55/55	-
3	POV	A	805	-	-	1/5/5/55	-
3	POV	C	709	-	-	6/17/17/55	-
2	Y01	A	802	-	-	7/19/77/77	0/4/4/4
2	Y01	B	705	-	-	8/19/77/77	0/4/4/4
3	POV	A	809	-	-	4/10/10/55	-
3	POV	D	703	-	-	25/55/55/55	-
2	Y01	B	704	-	-	7/19/77/77	0/4/4/4
3	POV	B	711	-	-	4/10/10/55	-
3	POV	D	702	-	-	2/13/13/55	-
4	I8E	C	702	-	-	1/3/31/31	0/3/3/3
4	I8E	A	812	-	-	1/3/31/31	0/3/3/3
3	POV	D	711	-	-	6/17/17/55	-
3	POV	A	810	-	-	2/13/13/55	-
3	POV	D	710	-	-	15/55/55/55	-
3	POV	C	701	-	-	25/55/55/55	-
3	POV	B	707	-	-	1/5/5/55	-
3	POV	B	708	-	-	15/55/55/55	-
3	POV	D	701	-	-	4/10/10/55	-
3	POV	B	709	-	-	6/17/17/55	-
2	Y01	C	703	-	-	8/19/77/77	0/4/4/4
3	POV	B	701	-	-	25/55/55/55	-
2	Y01	D	707	-	-	8/19/77/77	0/4/4/4
2	Y01	C	705	-	-	8/19/77/77	0/4/4/4
3	POV	B	706	-	-	24/55/55/55	-
3	POV	B	712	-	-	2/13/13/55	-
3	POV	A	807	-	-	6/17/17/55	-
2	Y01	D	705	-	-	8/19/77/77	0/4/4/4
3	POV	D	709	-	-	1/5/5/55	-
4	I8E	B	702	-	-	1/3/31/31	0/3/3/3
2	Y01	A	803	-	-	8/19/77/77	0/4/4/4
3	POV	C	706	-	-	24/55/55/55	-
3	POV	C	707	-	-	1/5/5/55	-
4	I8E	B	710	-	-	1/3/31/31	0/3/3/3
2	Y01	A	801	-	-	8/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	C	712	-	-	2/13/13/55	-
4	I8E	D	704	-	-	1/3/31/31	0/3/3/3
2	Y01	D	706	-	-	7/19/77/77	0/4/4/4
3	POV	A	804	-	-	24/55/55/55	-
3	POV	A	806	-	-	15/55/55/55	-
3	POV	C	708	-	-	15/55/55/55	-
3	POV	A	811	-	-	25/55/55/55	-
3	POV	C	711	-	-	4/10/10/55	-
4	I8E	C	710	-	-	1/3/31/31	0/3/3/3
4	I8E	A	808	-	-	1/3/31/31	0/3/3/3
2	Y01	C	704	-	-	8/19/77/77	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	709	POV	C29-C210	3.46	1.51	1.31
3	D	711	POV	C29-C210	3.45	1.51	1.31
3	A	807	POV	C29-C210	3.45	1.51	1.31
3	B	709	POV	C29-C210	3.44	1.51	1.31

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	Y01	CAO-CBB-CBE	4.22	119.07	110.33
2	C	703	Y01	CAO-CBB-CBE	4.16	118.95	110.33
2	B	703	Y01	CAO-CBB-CBE	4.15	118.93	110.33
2	D	705	Y01	CAO-CBB-CBE	4.14	118.91	110.33
2	D	707	Y01	CAO-CBB-CBE	3.95	118.52	110.33
2	C	705	Y01	CAO-CBB-CBE	3.93	118.48	110.33
2	A	803	Y01	CAO-CBB-CBE	3.92	118.45	110.33
2	B	705	Y01	CAO-CBB-CBE	3.91	118.44	110.33
4	C	710	I8E	C6-C7-C8	3.44	130.11	122.86
4	A	808	I8E	C16-C7-C8	-3.42	113.23	119.79
4	C	710	I8E	C16-C7-C8	-3.42	113.23	119.79
4	B	710	I8E	C6-C7-C8	3.42	130.06	122.86
4	A	808	I8E	C6-C7-C8	3.42	130.06	122.86
4	B	710	I8E	C16-C7-C8	-3.41	113.25	119.79
4	D	712	I8E	C16-C7-C8	-3.41	113.26	119.79
4	D	712	I8E	C6-C7-C8	3.40	130.03	122.86
2	B	703	Y01	CAP-CAQ-CBG	-3.33	98.62	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	703	Y01	CAP-CAQ-CBG	-3.32	98.65	105.14
2	A	801	Y01	CAP-CAQ-CBG	-3.31	98.66	105.14
2	D	705	Y01	CAP-CAQ-CBG	-3.31	98.66	105.14
3	A	811	POV	C2-O21-C21	3.16	125.37	117.80
3	C	701	POV	C2-O21-C21	3.14	125.30	117.80
3	D	703	POV	C2-O21-C21	3.13	125.30	117.80
3	B	701	POV	C2-O21-C21	3.12	125.26	117.80
3	D	710	POV	C2-O21-C21	2.54	123.87	117.80
3	A	806	POV	C2-O21-C21	2.53	123.84	117.80
3	C	708	POV	C2-O21-C21	2.52	123.84	117.80
3	B	708	POV	C2-O21-C21	2.51	123.81	117.80
4	A	808	I8E	O21-C6-C7	2.34	124.99	118.95
4	D	712	I8E	O21-C6-C7	2.34	124.99	118.95
4	B	710	I8E	O21-C6-C7	2.33	124.97	118.95
4	C	710	I8E	O21-C6-C7	2.32	124.94	118.95
3	A	811	POV	O21-C21-C22	2.26	116.37	111.48
3	D	703	POV	O21-C21-C22	2.25	116.35	111.48
3	B	701	POV	O21-C21-C22	2.24	116.33	111.48
3	C	701	POV	O21-C21-C22	2.22	116.28	111.48
4	B	710	I8E	C7-C8-C13	-2.19	98.28	108.09
4	C	710	I8E	C7-C8-C13	-2.18	98.31	108.09
4	D	712	I8E	C7-C8-C13	-2.18	98.31	108.09
4	A	808	I8E	C7-C8-C13	-2.17	98.35	108.09
4	A	808	I8E	O15-C14-C18	-2.16	100.45	105.92
4	C	710	I8E	O15-C14-C18	-2.15	100.47	105.92
4	B	710	I8E	O15-C14-C18	-2.14	100.48	105.92
2	D	707	Y01	CAJ-CAO-CBB	2.13	121.04	115.08
4	D	712	I8E	O15-C14-C18	-2.13	100.51	105.92
2	C	705	Y01	CAJ-CAO-CBB	2.11	120.96	115.08
2	B	705	Y01	CAJ-CAO-CBB	2.10	120.96	115.08
4	B	702	I8E	O15-C14-C13	-2.10	104.40	109.41
2	A	803	Y01	CAJ-CAO-CBB	2.10	120.95	115.08
4	A	812	I8E	O15-C14-C13	-2.09	104.42	109.41
4	C	702	I8E	O15-C14-C13	-2.09	104.43	109.41
4	D	704	I8E	O15-C14-C13	-2.08	104.44	109.41
2	A	802	Y01	OAW-CBC-CAV	-2.08	103.75	108.04
4	C	710	I8E	O15-C16-C7	-2.07	119.02	122.16
4	B	710	I8E	O15-C16-C7	-2.06	119.05	122.16
2	C	704	Y01	OAW-CBC-CAV	-2.06	103.80	108.04
2	D	706	Y01	OAW-CBC-CAV	-2.05	103.81	108.04
4	A	808	I8E	O15-C16-C7	-2.05	119.06	122.16
2	B	704	Y01	OAW-CBC-CAV	-2.05	103.81	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	712	I8E	O15-C16-C7	-2.05	119.06	122.16
4	B	710	I8E	C13-C8-C9	2.04	114.00	110.00
2	C	703	Y01	CAP-CBE-CBB	2.02	115.23	112.18
2	D	705	Y01	CAP-CBE-CBB	2.02	115.23	112.18
4	D	712	I8E	C13-C8-C9	2.00	113.92	110.00

There are no chirality outliers.

All (409) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	Y01	CAO-CBB-CBE-CAP
2	A	802	Y01	CAO-CBB-CBE-CBI
2	A	803	Y01	CAO-CBB-CBE-CAP
2	B	703	Y01	CAO-CBB-CBE-CAP
2	B	704	Y01	CAO-CBB-CBE-CBI
2	B	705	Y01	CAO-CBB-CBE-CAP
2	C	703	Y01	CAO-CBB-CBE-CAP
2	C	704	Y01	CAO-CBB-CBE-CBI
2	C	705	Y01	CAO-CBB-CBE-CAP
2	D	705	Y01	CAO-CBB-CBE-CAP
2	D	706	Y01	CAO-CBB-CBE-CBI
2	D	707	Y01	CAO-CBB-CBE-CAP
3	A	804	POV	C11-O12-P-O11
3	A	804	POV	C11-O12-P-O14
3	A	804	POV	O12-C11-C12-N
3	A	806	POV	C22-C21-O21-C2
3	A	806	POV	O22-C21-O21-C2
3	A	811	POV	C11-O12-P-O11
3	A	811	POV	C11-O12-P-O13
3	A	811	POV	C22-C21-O21-C2
3	A	811	POV	O22-C21-O21-C2
3	B	701	POV	C11-O12-P-O11
3	B	701	POV	C11-O12-P-O13
3	B	701	POV	C22-C21-O21-C2
3	B	701	POV	O22-C21-O21-C2
3	B	706	POV	C11-O12-P-O11
3	B	706	POV	C11-O12-P-O14
3	B	706	POV	O12-C11-C12-N
3	B	708	POV	C22-C21-O21-C2
3	B	708	POV	O22-C21-O21-C2
3	C	701	POV	C11-O12-P-O11
3	C	701	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
3	C	701	POV	C22-C21-O21-C2
3	C	701	POV	O22-C21-O21-C2
3	C	706	POV	C11-O12-P-O11
3	C	706	POV	C11-O12-P-O14
3	C	706	POV	O12-C11-C12-N
3	C	708	POV	C22-C21-O21-C2
3	C	708	POV	O22-C21-O21-C2
3	D	703	POV	C11-O12-P-O11
3	D	703	POV	C11-O12-P-O13
3	D	703	POV	C22-C21-O21-C2
3	D	703	POV	O22-C21-O21-C2
3	D	708	POV	C11-O12-P-O11
3	D	708	POV	C11-O12-P-O14
3	D	708	POV	O12-C11-C12-N
3	D	710	POV	C22-C21-O21-C2
3	D	710	POV	O22-C21-O21-C2
2	A	801	Y01	CAC-CBB-CBE-CAP
2	B	703	Y01	CAC-CBB-CBE-CAP
2	C	703	Y01	CAC-CBB-CBE-CAP
2	D	705	Y01	CAC-CBB-CBE-CAP
2	A	801	Y01	CAC-CBB-CBE-CBI
2	A	803	Y01	CAC-CBB-CBE-CBI
2	B	703	Y01	CAC-CBB-CBE-CBI
2	B	705	Y01	CAC-CBB-CBE-CBI
2	C	703	Y01	CAC-CBB-CBE-CBI
2	C	705	Y01	CAC-CBB-CBE-CBI
2	D	705	Y01	CAC-CBB-CBE-CBI
2	D	707	Y01	CAC-CBB-CBE-CBI
2	A	801	Y01	CAO-CBB-CBE-CBI
2	B	703	Y01	CAO-CBB-CBE-CBI
2	C	703	Y01	CAO-CBB-CBE-CBI
2	D	705	Y01	CAO-CBB-CBE-CBI
2	D	707	Y01	CAO-CBB-CBE-CBI
2	A	803	Y01	CAC-CBB-CBE-CAP
2	B	705	Y01	CAC-CBB-CBE-CAP
2	C	705	Y01	CAC-CBB-CBE-CAP
2	D	707	Y01	CAC-CBB-CBE-CAP
2	A	803	Y01	CAO-CBB-CBE-CBI
2	B	705	Y01	CAO-CBB-CBE-CBI
2	C	705	Y01	CAO-CBB-CBE-CBI
2	B	703	Y01	CAJ-CAO-CBB-CBE
2	C	703	Y01	CAJ-CAO-CBB-CBE

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Mol	Chain	Res	Type	Atoms
2	D	705	Y01	CAJ-CAO-CBB-CBE
2	A	803	Y01	CAJ-CAO-CBB-CAC
2	B	705	Y01	CAJ-CAO-CBB-CAC
2	C	705	Y01	CAJ-CAO-CBB-CAC
2	D	707	Y01	CAJ-CAO-CBB-CAC
2	A	801	Y01	CAJ-CAO-CBB-CBE
3	A	807	POV	C211-C210-C29-C28
3	B	709	POV	C211-C210-C29-C28
3	C	709	POV	C211-C210-C29-C28
3	D	711	POV	C211-C210-C29-C28
3	A	811	POV	C213-C214-C215-C216
3	D	703	POV	C213-C214-C215-C216
3	B	701	POV	C213-C214-C215-C216
3	C	701	POV	C213-C214-C215-C216
3	B	701	POV	O21-C2-C3-O31
3	C	701	POV	O21-C2-C3-O31
2	A	803	Y01	CAJ-CAO-CBB-CBE
2	B	705	Y01	CAJ-CAO-CBB-CBE
2	C	705	Y01	CAJ-CAO-CBB-CBE
2	D	707	Y01	CAJ-CAO-CBB-CBE
3	A	804	POV	C21-C22-C23-C24
3	C	706	POV	C21-C22-C23-C24
3	A	810	POV	C32-C33-C34-C35
3	B	712	POV	C32-C33-C34-C35
3	C	712	POV	C32-C33-C34-C35
3	D	702	POV	C32-C33-C34-C35
3	B	706	POV	C21-C22-C23-C24
3	D	708	POV	C21-C22-C23-C24
2	A	802	Y01	CAC-CBB-CBE-CAP
2	B	704	Y01	CAC-CBB-CBE-CAP
2	C	704	Y01	CAC-CBB-CBE-CAP
2	D	706	Y01	CAC-CBB-CBE-CAP
3	A	804	POV	C11-C12-N-C13
3	A	804	POV	C11-C12-N-C14
3	A	804	POV	C11-C12-N-C15
3	B	706	POV	C11-C12-N-C13
3	B	706	POV	C11-C12-N-C14
3	B	706	POV	C11-C12-N-C15
3	C	706	POV	C11-C12-N-C13
3	C	706	POV	C11-C12-N-C14
3	C	706	POV	C11-C12-N-C15
3	D	708	POV	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
3	D	708	POV	C11-C12-N-C14
3	D	708	POV	C11-C12-N-C15
4	A	808	I8E	C1-C2-C3-C4
4	A	812	I8E	C1-C2-C3-C4
4	B	702	I8E	C1-C2-C3-C4
4	B	710	I8E	C1-C2-C3-C4
4	C	702	I8E	C1-C2-C3-C4
4	C	710	I8E	C1-C2-C3-C4
4	D	704	I8E	C1-C2-C3-C4
4	D	712	I8E	C1-C2-C3-C4
3	A	811	POV	O21-C2-C3-O31
3	D	703	POV	O21-C2-C3-O31
3	A	806	POV	C210-C211-C212-C213
3	B	708	POV	C210-C211-C212-C213
3	C	708	POV	C210-C211-C212-C213
3	D	710	POV	C210-C211-C212-C213
2	A	802	Y01	CAO-CBB-CBE-CAP
2	C	704	Y01	CAO-CBB-CBE-CAP
3	B	708	POV	C22-C23-C24-C25
3	A	806	POV	C22-C23-C24-C25
3	C	708	POV	C22-C23-C24-C25
3	D	710	POV	C22-C23-C24-C25
3	B	701	POV	C32-C33-C34-C35
3	C	701	POV	C32-C33-C34-C35
3	D	703	POV	C32-C33-C34-C35
3	A	811	POV	C32-C33-C34-C35
2	B	704	Y01	CAO-CBB-CBE-CAP
2	D	706	Y01	CAO-CBB-CBE-CAP
3	A	804	POV	C311-C312-C313-C314
3	A	809	POV	C39-C310-C311-C312
3	C	706	POV	C311-C312-C313-C314
3	D	708	POV	C311-C312-C313-C314
3	B	706	POV	C311-C312-C313-C314
3	B	711	POV	C39-C310-C311-C312
3	C	711	POV	C39-C310-C311-C312
3	D	701	POV	C39-C310-C311-C312
3	A	804	POV	C31-C32-C33-C34
3	D	708	POV	C31-C32-C33-C34
3	B	706	POV	C31-C32-C33-C34
3	A	804	POV	C23-C24-C25-C26
3	C	706	POV	C23-C24-C25-C26
3	D	708	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	B	706	POV	C23-C24-C25-C26
3	C	706	POV	C31-C32-C33-C34
3	A	811	POV	C214-C215-C216-C217
2	B	703	Y01	CAN-CAJ-CAO-CBB
3	A	811	POV	C25-C26-C27-C28
3	B	701	POV	C25-C26-C27-C28
3	C	701	POV	C25-C26-C27-C28
3	D	703	POV	C25-C26-C27-C28
2	C	703	Y01	CAN-CAJ-CAO-CBB
2	D	705	Y01	CAN-CAJ-CAO-CBB
2	A	801	Y01	CAN-CAJ-CAO-CBB
3	A	807	POV	C24-C25-C26-C27
3	B	709	POV	C24-C25-C26-C27
3	A	804	POV	C2-C1-O11-P
3	B	706	POV	C2-C1-O11-P
3	C	706	POV	C2-C1-O11-P
3	D	708	POV	C2-C1-O11-P
3	C	709	POV	C24-C25-C26-C27
3	D	711	POV	C24-C25-C26-C27
3	C	701	POV	C214-C215-C216-C217
3	B	701	POV	C214-C215-C216-C217
3	A	811	POV	C212-C213-C214-C215
3	A	804	POV	C211-C212-C213-C214
3	D	710	POV	C312-C313-C314-C315
3	B	708	POV	C312-C313-C314-C315
3	C	708	POV	C312-C313-C314-C315
3	A	806	POV	C312-C313-C314-C315
3	A	811	POV	C1-C2-C3-O31
3	B	701	POV	C1-C2-C3-O31
3	C	701	POV	C1-C2-C3-O31
3	D	703	POV	C1-C2-C3-O31
3	D	703	POV	C214-C215-C216-C217
3	C	706	POV	C211-C212-C213-C214
3	A	811	POV	C34-C35-C36-C37
3	B	706	POV	C211-C212-C213-C214
3	D	708	POV	C211-C212-C213-C214
3	B	701	POV	C34-C35-C36-C37
3	C	701	POV	C34-C35-C36-C37
3	D	703	POV	C34-C35-C36-C37
3	A	806	POV	C31-C32-C33-C34
3	B	708	POV	C311-C310-C39-C38
2	C	705	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
2	D	707	Y01	CAO-CAJ-CAN-CBA
3	A	806	POV	C311-C310-C39-C38
3	D	710	POV	C311-C310-C39-C38
2	A	803	Y01	CAO-CAJ-CAN-CBA
2	B	705	Y01	CAO-CAJ-CAN-CBA
3	C	708	POV	C311-C310-C39-C38
3	C	708	POV	C31-C32-C33-C34
3	D	710	POV	C31-C32-C33-C34
3	B	701	POV	C212-C213-C214-C215
3	C	701	POV	C212-C213-C214-C215
3	A	804	POV	O11-C1-C2-O21
3	B	706	POV	O11-C1-C2-O21
3	C	706	POV	O11-C1-C2-O21
3	D	708	POV	O11-C1-C2-O21
3	A	811	POV	C310-C311-C312-C313
3	B	701	POV	C310-C311-C312-C313
3	C	701	POV	C310-C311-C312-C313
3	D	703	POV	C310-C311-C312-C313
3	B	708	POV	C31-C32-C33-C34
3	D	703	POV	C212-C213-C214-C215
3	B	709	POV	C213-C214-C215-C216
3	C	709	POV	C213-C214-C215-C216
3	D	711	POV	C213-C214-C215-C216
3	A	807	POV	C213-C214-C215-C216
3	B	701	POV	C35-C36-C37-C38
3	A	811	POV	C35-C36-C37-C38
3	C	701	POV	C35-C36-C37-C38
3	D	703	POV	C35-C36-C37-C38
3	A	811	POV	O11-C1-C2-O21
3	B	701	POV	O11-C1-C2-O21
3	C	701	POV	O11-C1-C2-O21
3	D	703	POV	O11-C1-C2-O21
2	A	802	Y01	CAO-CAJ-CAN-CBA
2	D	705	Y01	CAO-CAJ-CAN-CBA
2	B	703	Y01	CAO-CAJ-CAN-CBA
2	B	704	Y01	CAO-CAJ-CAN-CBA
2	C	703	Y01	CAO-CAJ-CAN-CBA
3	B	708	POV	C23-C24-C25-C26
3	A	806	POV	C23-C24-C25-C26
3	C	708	POV	C23-C24-C25-C26
3	D	710	POV	C23-C24-C25-C26
2	C	704	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
3	C	708	POV	C213-C214-C215-C216
3	B	708	POV	C213-C214-C215-C216
2	A	801	Y01	CAO-CAJ-CAN-CBA
2	D	706	Y01	CAO-CAJ-CAN-CBA
3	A	806	POV	C213-C214-C215-C216
2	C	704	Y01	CAO-CAJ-CAN-CBA
3	D	710	POV	C213-C214-C215-C216
2	B	704	Y01	CAC-CBB-CBE-CBI
2	D	706	Y01	CAC-CBB-CBE-CBI
2	A	802	Y01	CAC-CBB-CBE-CBI
3	A	804	POV	C12-C11-O12-P
3	A	811	POV	C12-C11-O12-P
3	B	701	POV	C12-C11-O12-P
3	B	706	POV	C12-C11-O12-P
3	C	701	POV	C12-C11-O12-P
3	C	706	POV	C12-C11-O12-P
3	D	703	POV	C12-C11-O12-P
3	D	708	POV	C12-C11-O12-P
3	A	804	POV	C32-C33-C34-C35
3	B	706	POV	C32-C33-C34-C35
2	B	705	Y01	CAN-CAJ-CAO-CBB
2	D	707	Y01	CAN-CAJ-CAO-CBB
3	D	708	POV	C32-C33-C34-C35
2	A	803	Y01	CAN-CAJ-CAO-CBB
2	C	705	Y01	CAN-CAJ-CAO-CBB
3	C	706	POV	C32-C33-C34-C35
3	D	701	POV	C37-C38-C39-C310
3	A	811	POV	O12-C11-C12-N
3	B	701	POV	O12-C11-C12-N
3	C	701	POV	O12-C11-C12-N
3	D	703	POV	O12-C11-C12-N
3	A	804	POV	C213-C214-C215-C216
3	B	711	POV	C37-C38-C39-C310
3	C	711	POV	C37-C38-C39-C310
3	A	809	POV	C37-C38-C39-C310
3	B	706	POV	C213-C214-C215-C216
3	C	706	POV	C213-C214-C215-C216
3	D	708	POV	C213-C214-C215-C216
3	A	804	POV	O11-C1-C2-C3
3	B	706	POV	O11-C1-C2-C3
3	C	706	POV	O11-C1-C2-C3
3	D	708	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	706	POV	C212-C213-C214-C215
3	C	706	POV	C212-C213-C214-C215
3	D	708	POV	C212-C213-C214-C215
3	A	804	POV	C212-C213-C214-C215
3	D	710	POV	C310-C311-C312-C313
3	D	710	POV	C25-C26-C27-C28
3	B	701	POV	C37-C38-C39-C310
3	D	703	POV	C37-C38-C39-C310
3	A	811	POV	C37-C38-C39-C310
3	B	708	POV	C310-C311-C312-C313
3	C	708	POV	C25-C26-C27-C28
3	C	708	POV	C310-C311-C312-C313
3	C	701	POV	C37-C38-C39-C310
3	A	806	POV	C25-C26-C27-C28
3	A	806	POV	C310-C311-C312-C313
3	B	706	POV	C26-C27-C28-C29
3	D	708	POV	C26-C27-C28-C29
3	B	708	POV	C25-C26-C27-C28
3	C	711	POV	C34-C35-C36-C37
3	A	809	POV	C34-C35-C36-C37
3	B	711	POV	C34-C35-C36-C37
3	D	701	POV	C34-C35-C36-C37
3	A	804	POV	C11-O12-P-O13
3	B	706	POV	C11-O12-P-O13
3	C	706	POV	C11-O12-P-O13
3	D	708	POV	C11-O12-P-O13
3	B	706	POV	C29-C210-C211-C212
3	B	706	POV	C27-C28-C29-C210
3	C	706	POV	C29-C210-C211-C212
3	D	708	POV	C29-C210-C211-C212
3	D	708	POV	C27-C28-C29-C210
3	A	804	POV	C26-C27-C28-C29
3	C	706	POV	C26-C27-C28-C29
3	C	706	POV	C27-C28-C29-C210
3	A	807	POV	O21-C21-C22-C23
3	A	804	POV	C27-C28-C29-C210
3	B	709	POV	O21-C21-C22-C23
3	C	709	POV	O21-C21-C22-C23
3	D	711	POV	O21-C21-C22-C23
3	C	701	POV	C215-C216-C217-C218
3	A	804	POV	C29-C210-C211-C212
2	A	801	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
3	A	810	POV	C1-C2-C3-O31
3	B	712	POV	C1-C2-C3-O31
3	C	712	POV	C1-C2-C3-O31
3	D	702	POV	C1-C2-C3-O31
3	D	703	POV	C215-C216-C217-C218
3	B	701	POV	C215-C216-C217-C218
3	B	706	POV	C215-C216-C217-C218
3	A	811	POV	C215-C216-C217-C218
3	A	804	POV	C215-C216-C217-C218
3	D	708	POV	C215-C216-C217-C218
3	C	706	POV	C215-C216-C217-C218
3	D	710	POV	C32-C33-C34-C35
2	C	703	Y01	CAJ-CAO-CBB-CAC
3	C	708	POV	C32-C33-C34-C35
2	B	703	Y01	CAJ-CAO-CBB-CAC
3	A	811	POV	C27-C28-C29-C210
3	B	701	POV	C27-C28-C29-C210
3	C	701	POV	C27-C28-C29-C210
3	A	806	POV	C32-C33-C34-C35
2	D	705	Y01	CAJ-CAO-CBB-CAC
3	D	703	POV	C27-C28-C29-C210
3	B	708	POV	C32-C33-C34-C35
3	A	811	POV	O11-C1-C2-C3
3	B	701	POV	O11-C1-C2-C3
3	C	701	POV	O11-C1-C2-C3
3	D	703	POV	O11-C1-C2-C3
3	A	807	POV	C29-C210-C211-C212
3	B	709	POV	C29-C210-C211-C212
3	C	709	POV	C29-C210-C211-C212
3	D	711	POV	C29-C210-C211-C212
3	C	708	POV	C212-C213-C214-C215
3	B	708	POV	C212-C213-C214-C215
2	C	704	Y01	CAN-CAJ-CAO-CBB
3	A	806	POV	C212-C213-C214-C215
3	A	811	POV	C23-C24-C25-C26
3	D	703	POV	C23-C24-C25-C26
2	B	704	Y01	CAN-CAJ-CAO-CBB
2	D	706	Y01	CAN-CAJ-CAO-CBB
2	A	802	Y01	CAN-CAJ-CAO-CBB
3	D	708	POV	C39-C310-C311-C312
3	D	710	POV	C212-C213-C214-C215
3	C	701	POV	C313-C314-C315-C316

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Mol	Chain	Res	Type	Atoms
3	C	701	POV	C23-C24-C25-C26
3	D	703	POV	C313-C314-C315-C316
3	B	701	POV	C23-C24-C25-C26
3	B	701	POV	C313-C314-C315-C316
3	C	701	POV	C311-C310-C39-C38
3	B	706	POV	C39-C310-C311-C312
3	C	706	POV	C39-C310-C311-C312
3	A	804	POV	C39-C310-C311-C312
3	A	811	POV	C311-C310-C39-C38
3	D	703	POV	C311-C310-C39-C38
3	B	701	POV	C311-C310-C39-C38
3	A	811	POV	C313-C314-C315-C316
3	B	708	POV	O21-C21-C22-C23
3	A	806	POV	O21-C21-C22-C23
3	C	708	POV	O21-C21-C22-C23
3	D	710	POV	O21-C21-C22-C23
3	A	807	POV	C23-C24-C25-C26
3	B	707	POV	C33-C34-C35-C36
3	D	709	POV	C33-C34-C35-C36
3	C	707	POV	C33-C34-C35-C36
3	B	709	POV	C23-C24-C25-C26
3	A	805	POV	C33-C34-C35-C36
3	C	709	POV	C23-C24-C25-C26
3	B	711	POV	C32-C33-C34-C35
3	D	711	POV	C23-C24-C25-C26
3	A	809	POV	C32-C33-C34-C35
3	C	701	POV	C211-C212-C213-C214
3	D	703	POV	C211-C212-C213-C214
3	C	711	POV	C32-C33-C34-C35
2	C	704	Y01	CAM-CAL-CAX-OAH
3	D	701	POV	C32-C33-C34-C35
2	A	802	Y01	CAM-CAL-CAX-OAH
3	B	701	POV	C211-C212-C213-C214
2	D	706	Y01	CAM-CAL-CAX-OAH
2	B	704	Y01	CAM-CAL-CAX-OAH
3	A	811	POV	C211-C212-C213-C214
3	B	708	POV	O22-C21-C22-C23
3	C	708	POV	O22-C21-C22-C23
2	C	704	Y01	CAM-CAL-CAX-OAF
3	A	806	POV	O22-C21-C22-C23
3	D	710	POV	O22-C21-C22-C23

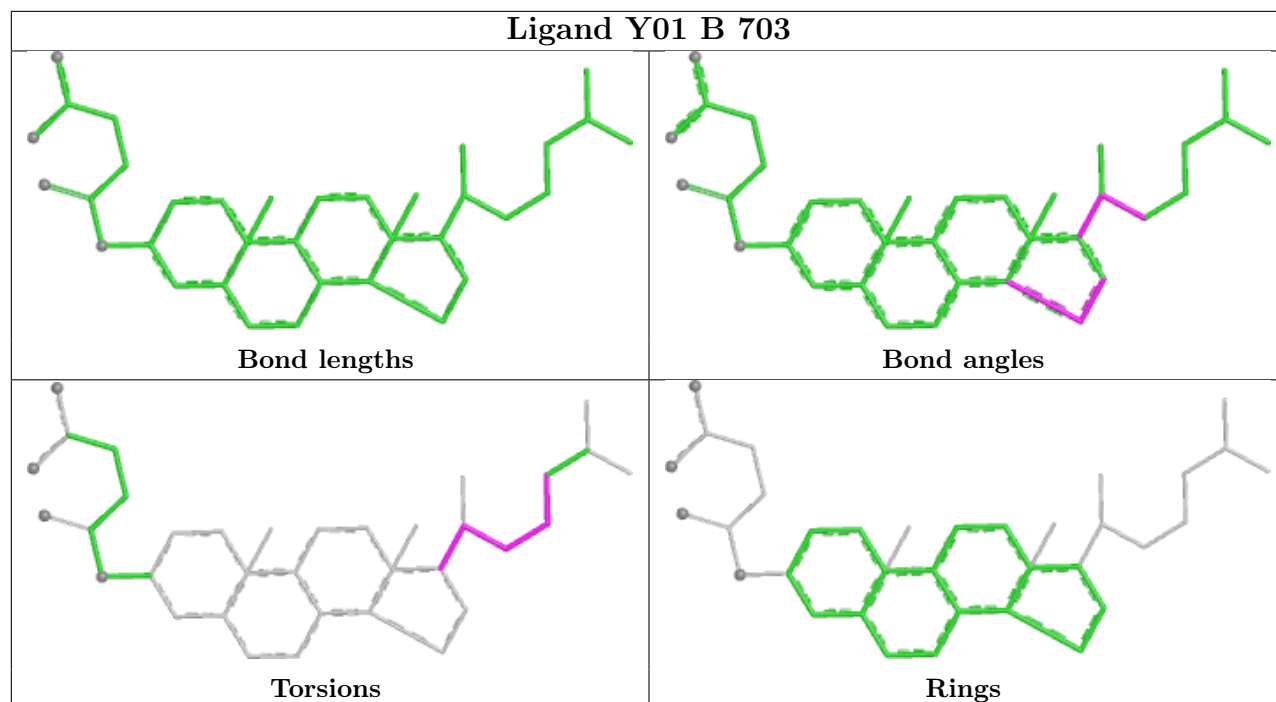
There are no ring outliers.

19 monomers are involved in 31 short contacts:

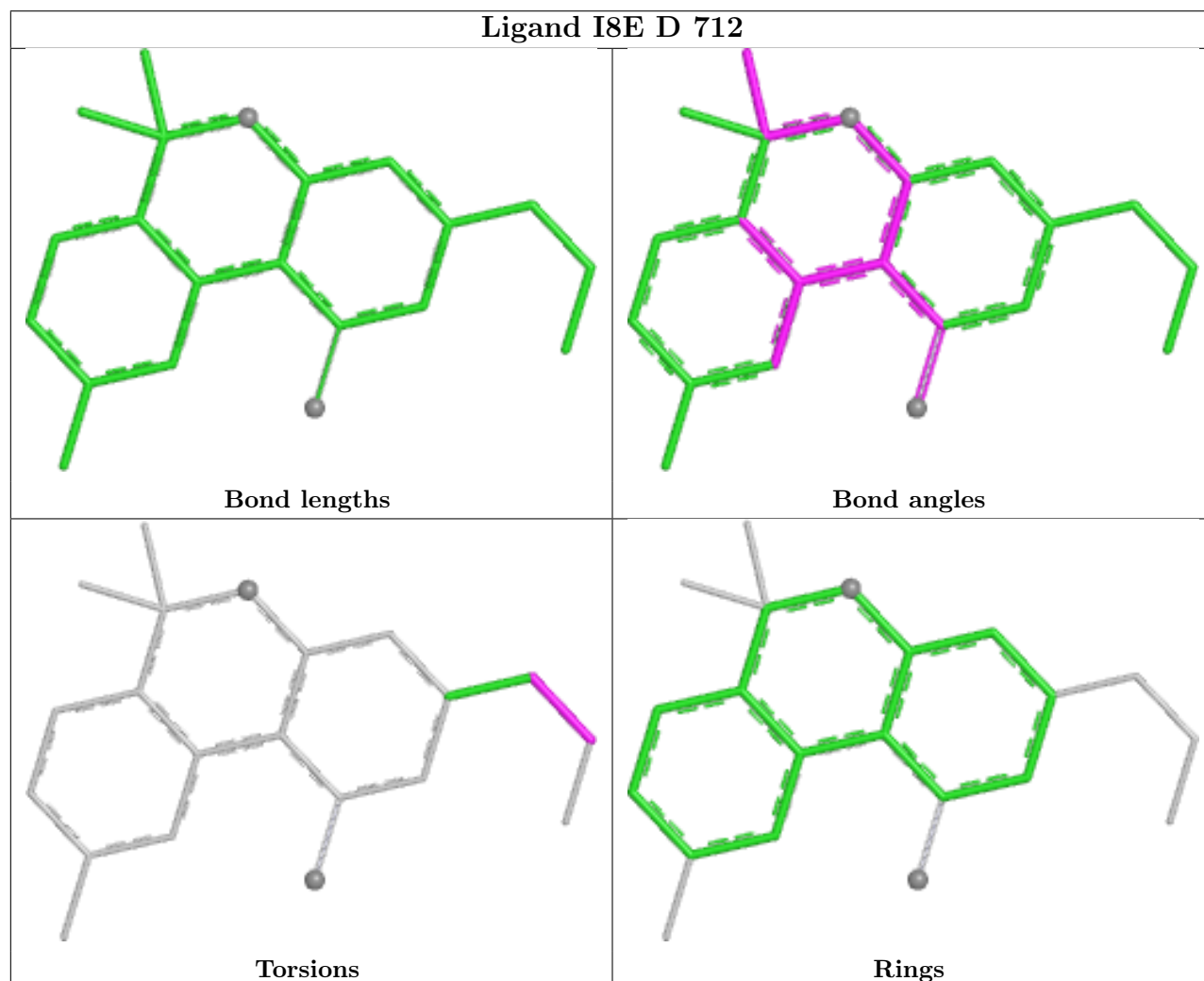
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	703	Y01	3	0
4	D	712	I8E	2	0
3	C	709	POV	1	0
2	A	802	Y01	3	0
2	B	705	Y01	1	0
2	B	704	Y01	3	0
3	D	711	POV	1	0
3	B	709	POV	1	0
2	C	703	Y01	1	0
2	D	707	Y01	1	0
2	C	705	Y01	2	0
3	A	807	POV	1	0
2	D	705	Y01	1	0
2	A	803	Y01	1	0
4	B	710	I8E	2	0
2	D	706	Y01	4	0
4	C	710	I8E	2	0
4	A	808	I8E	2	0
2	C	704	Y01	3	0

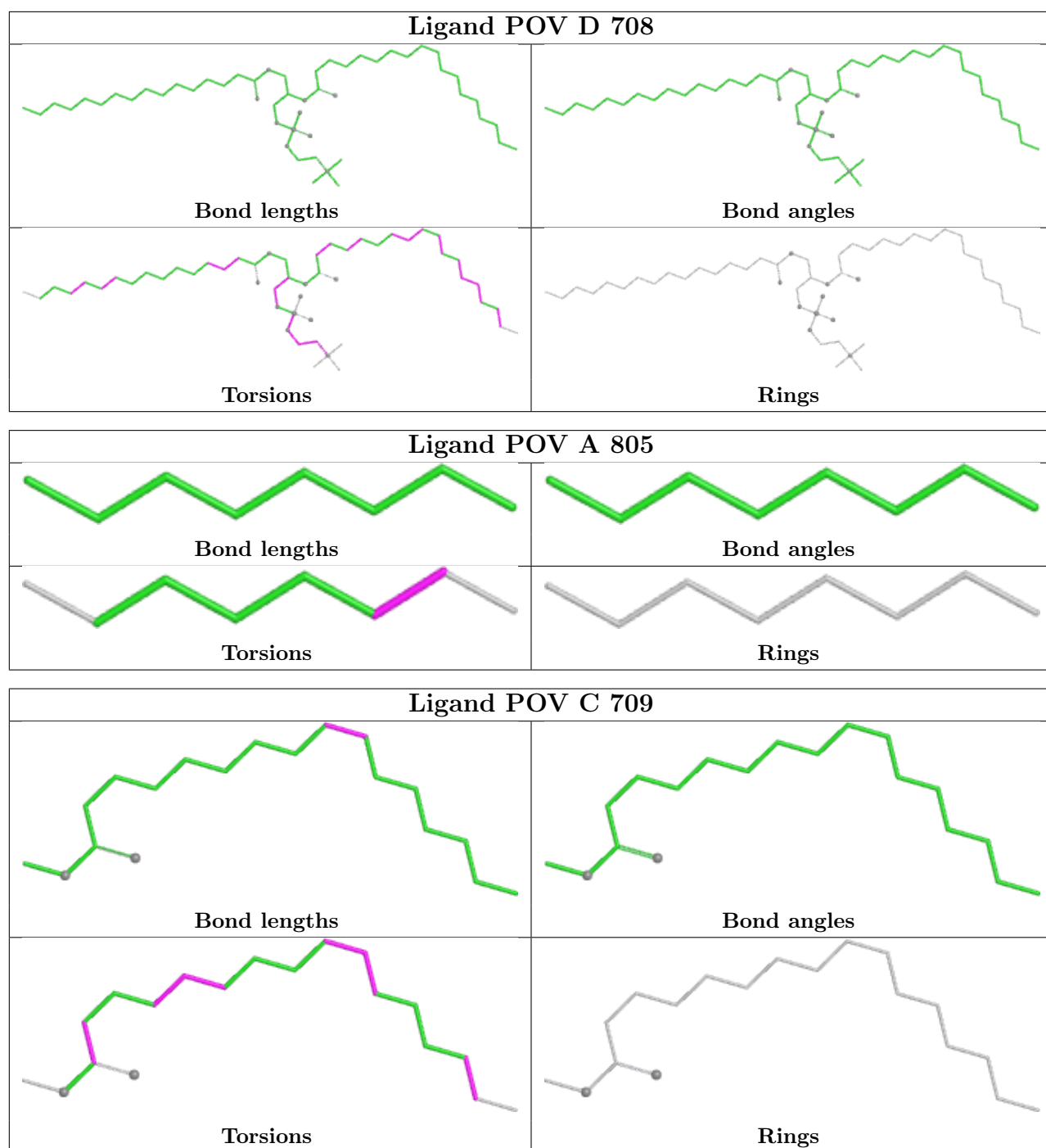
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

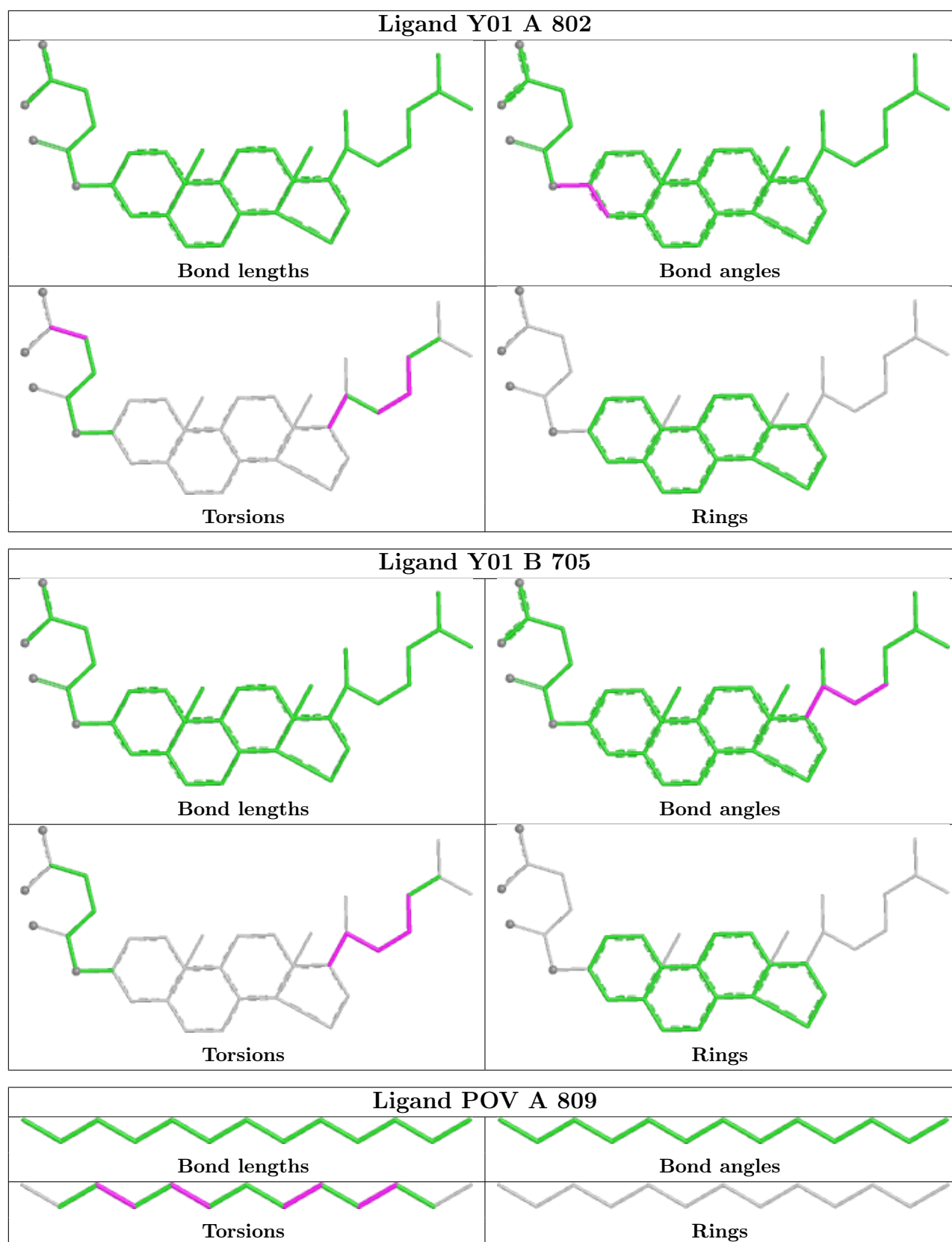
Ligand Y01 B 703

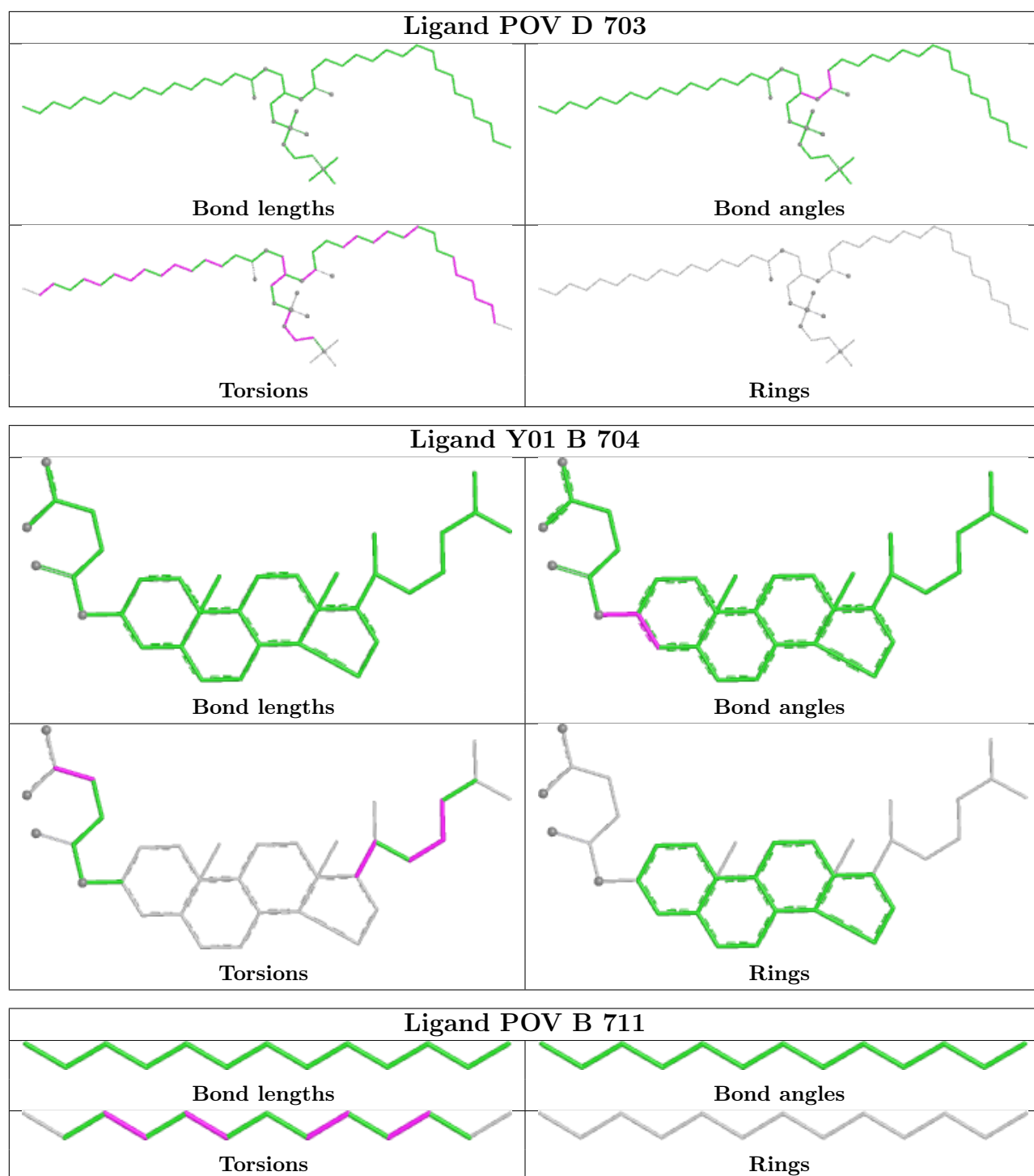


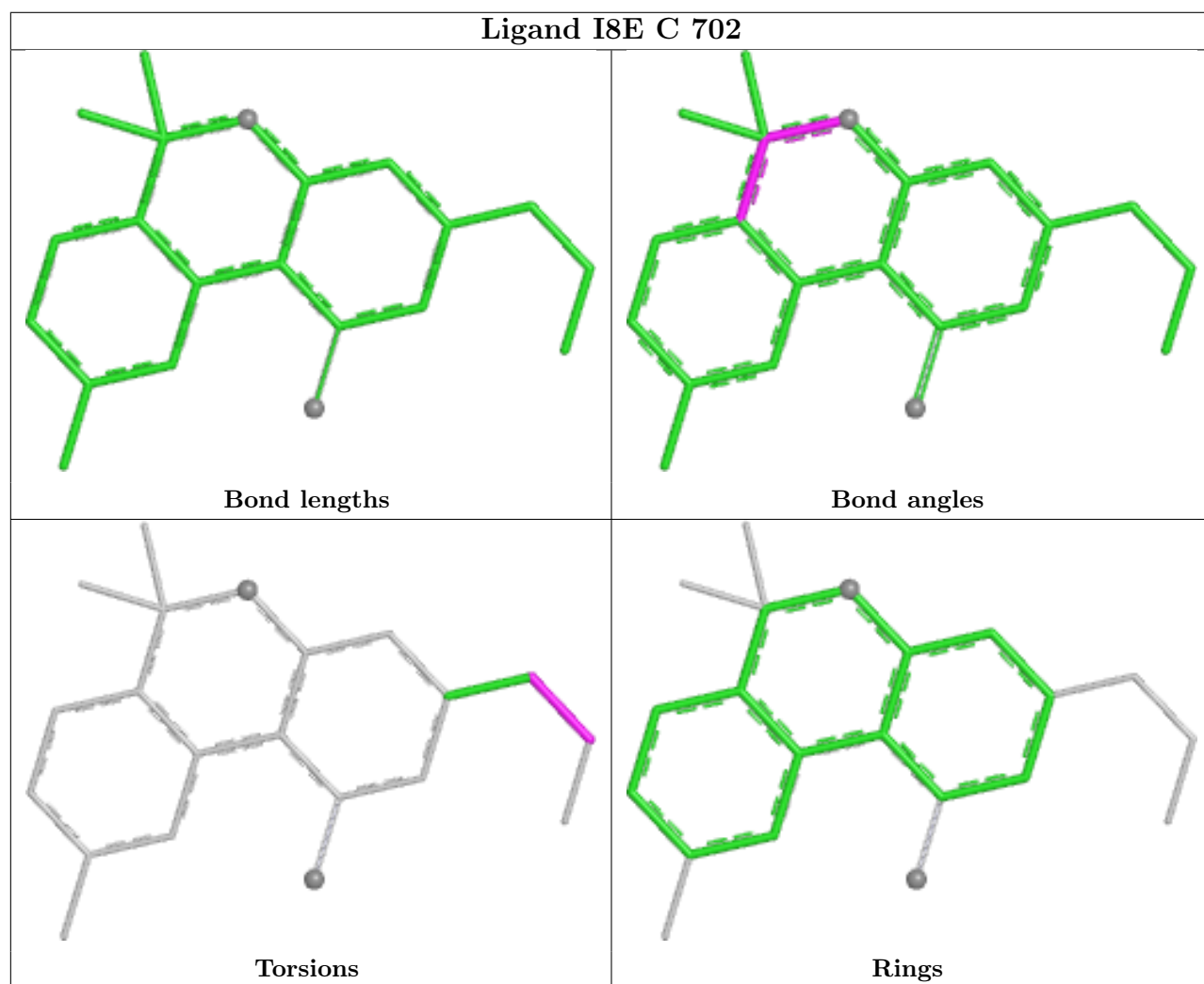
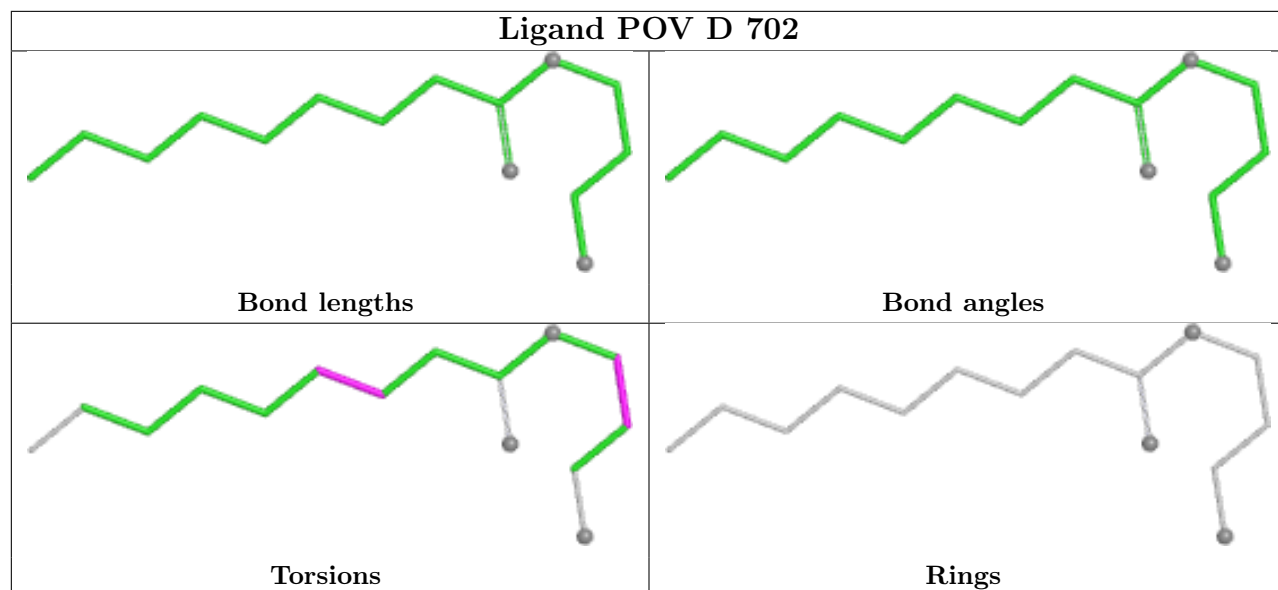
Ligand I8E D 712



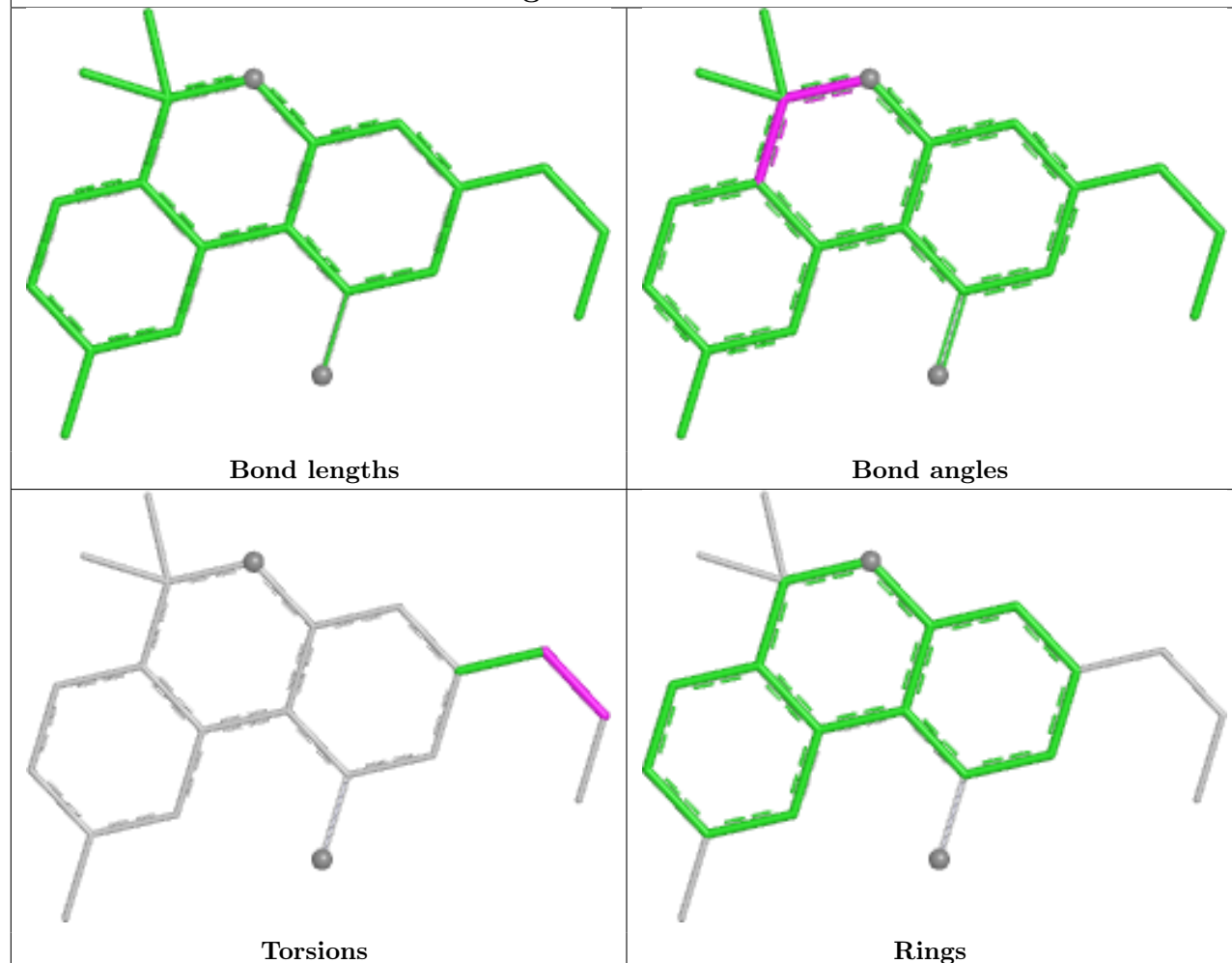




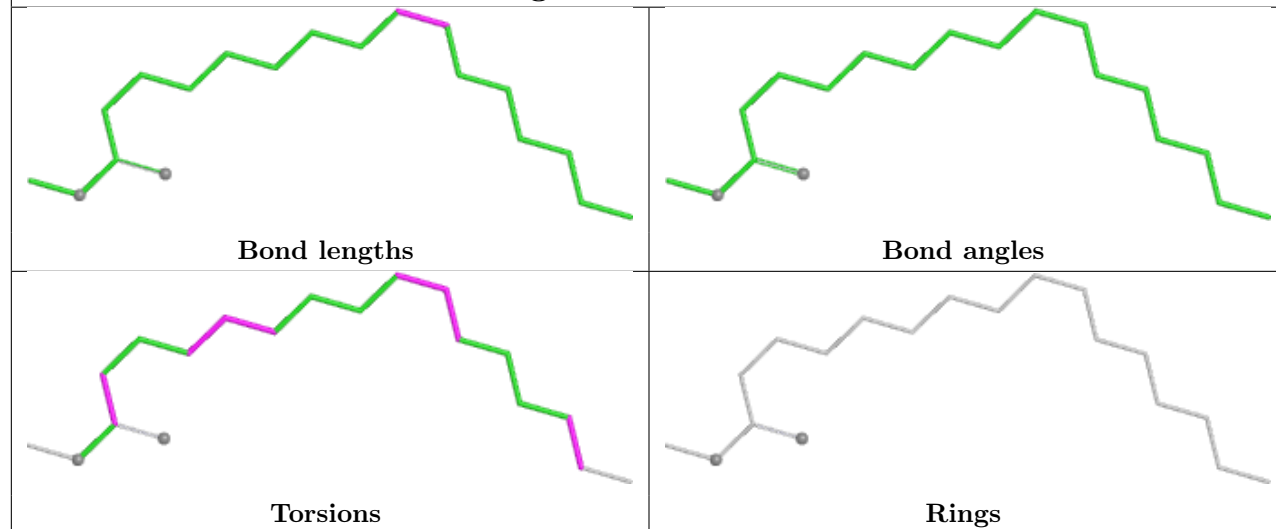


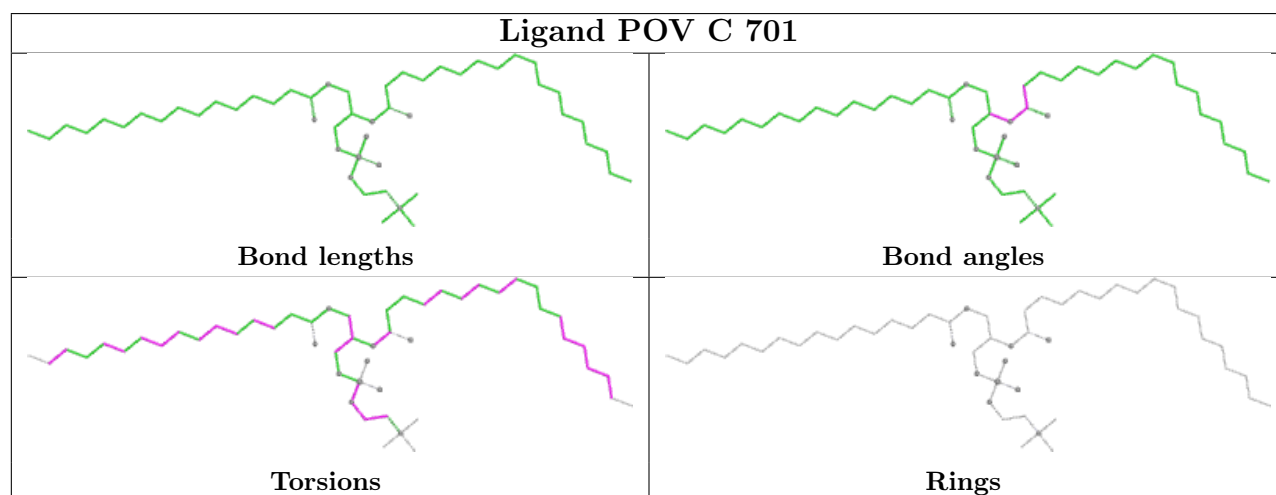
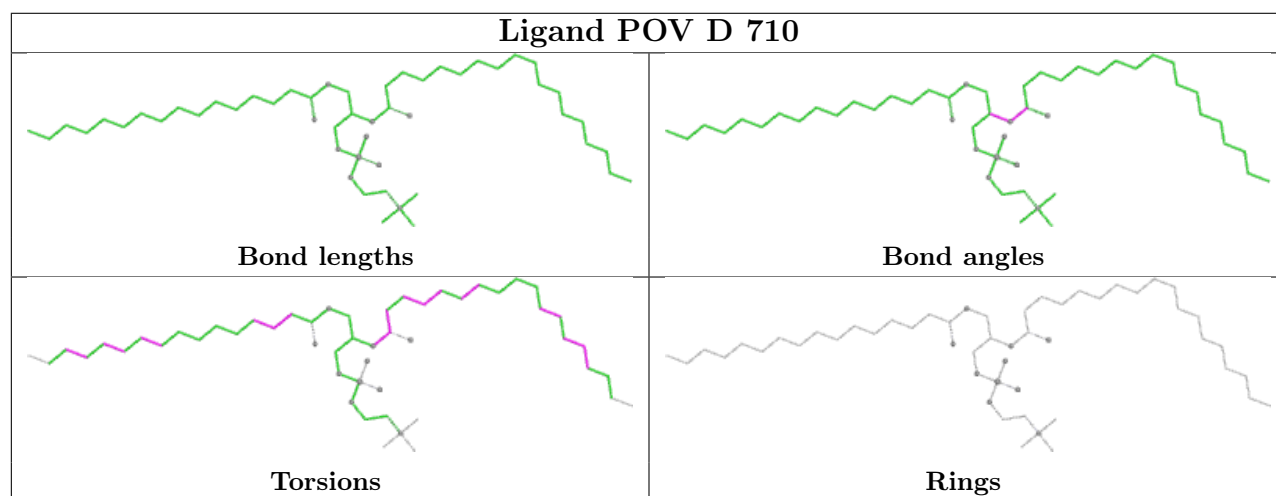
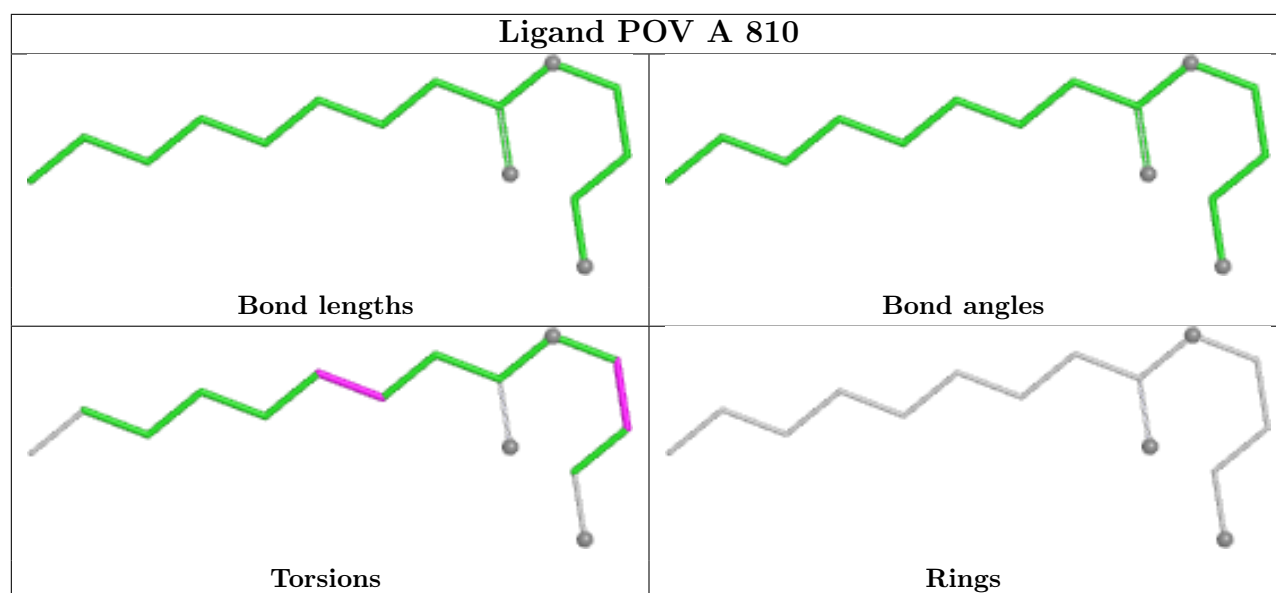


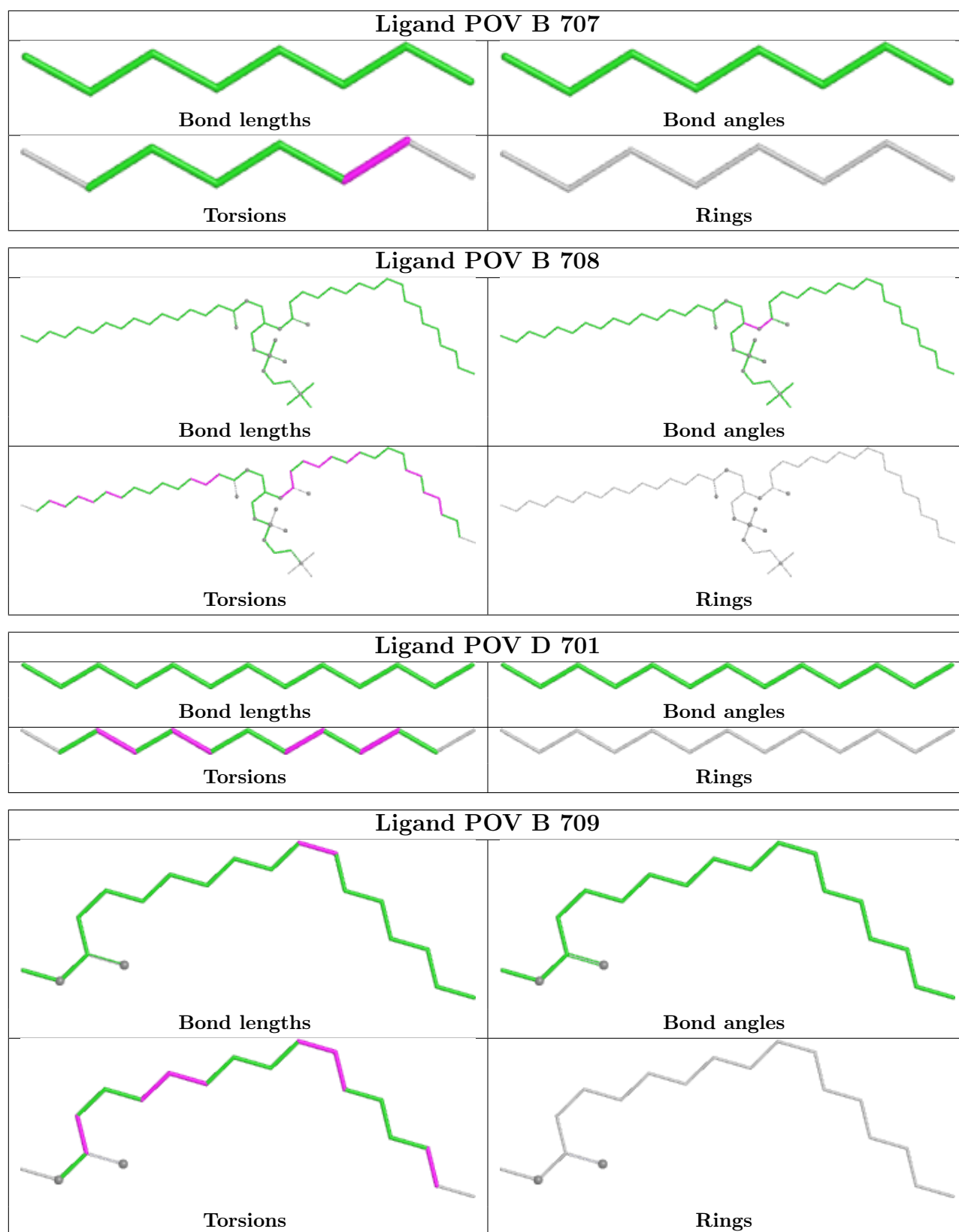
Ligand I8E A 812

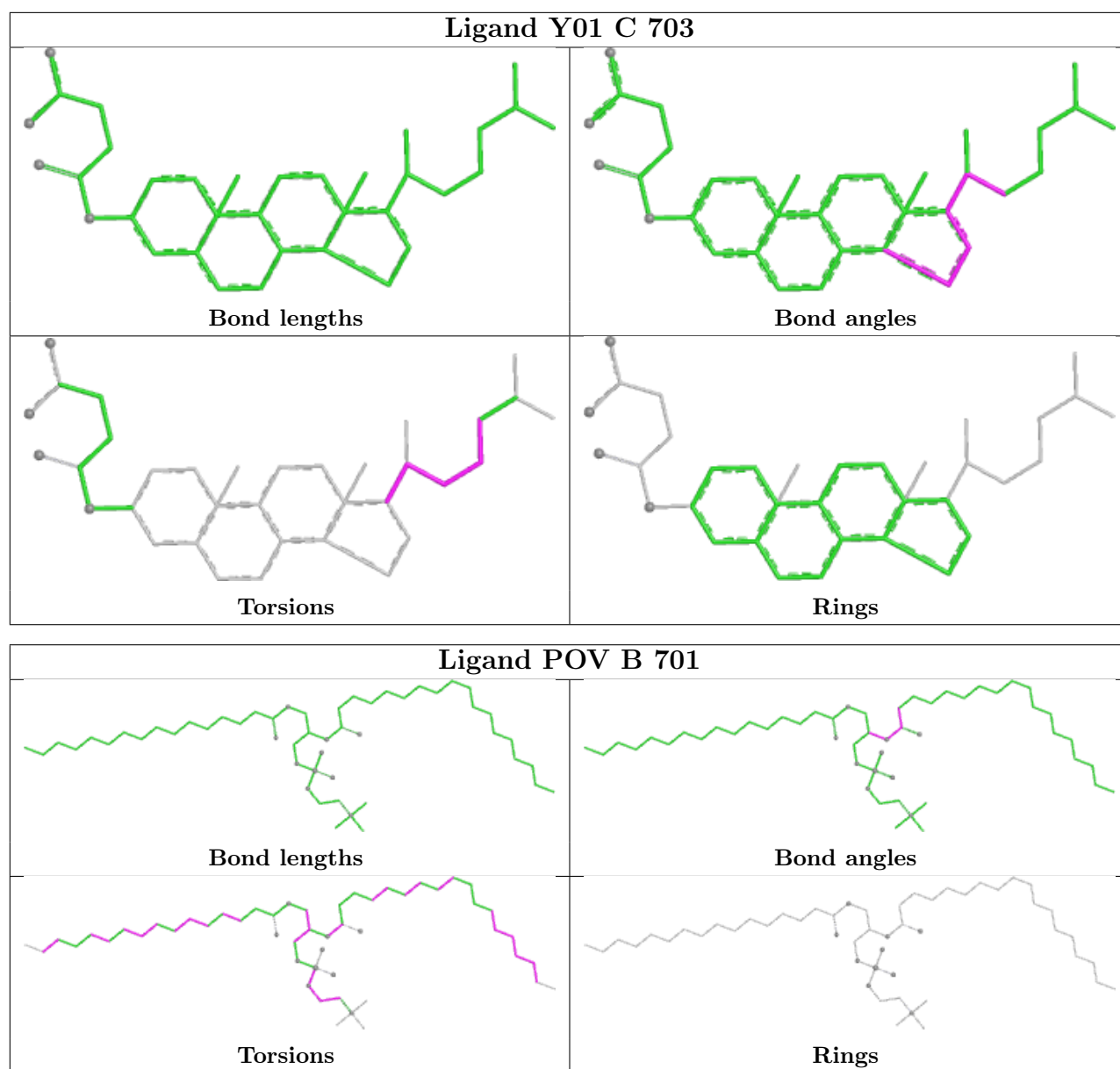


Ligand POV D 711

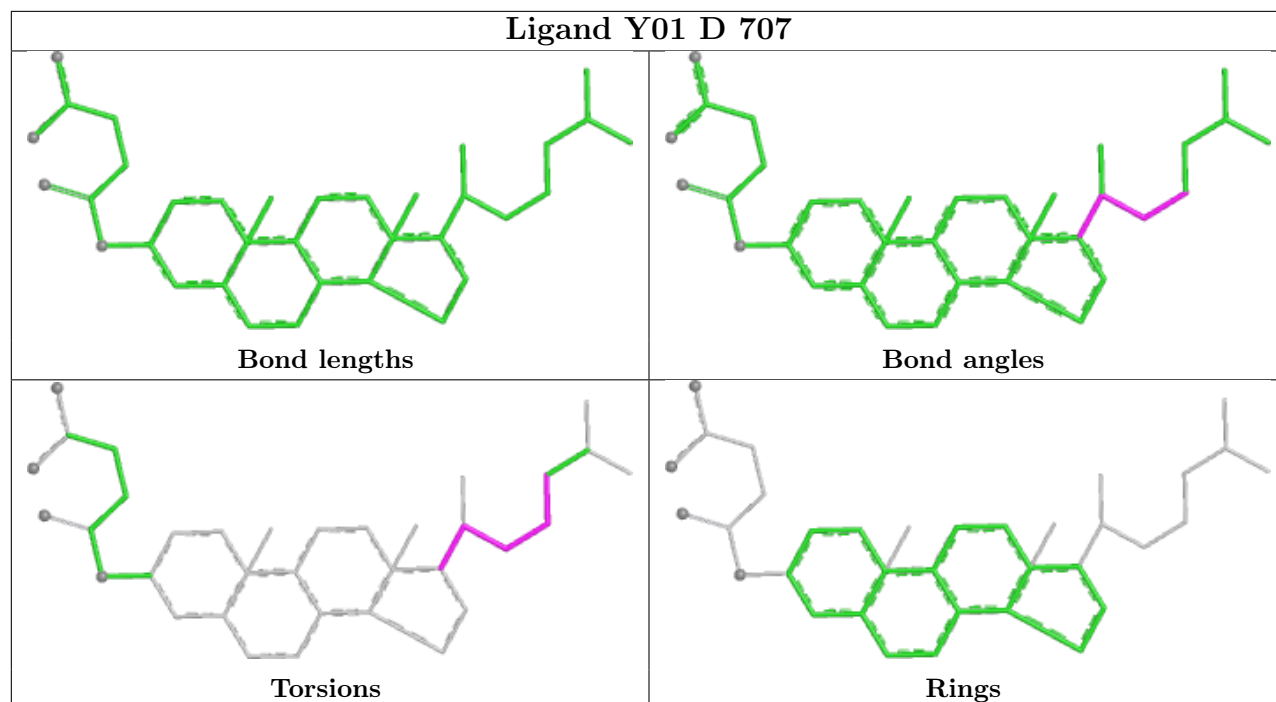




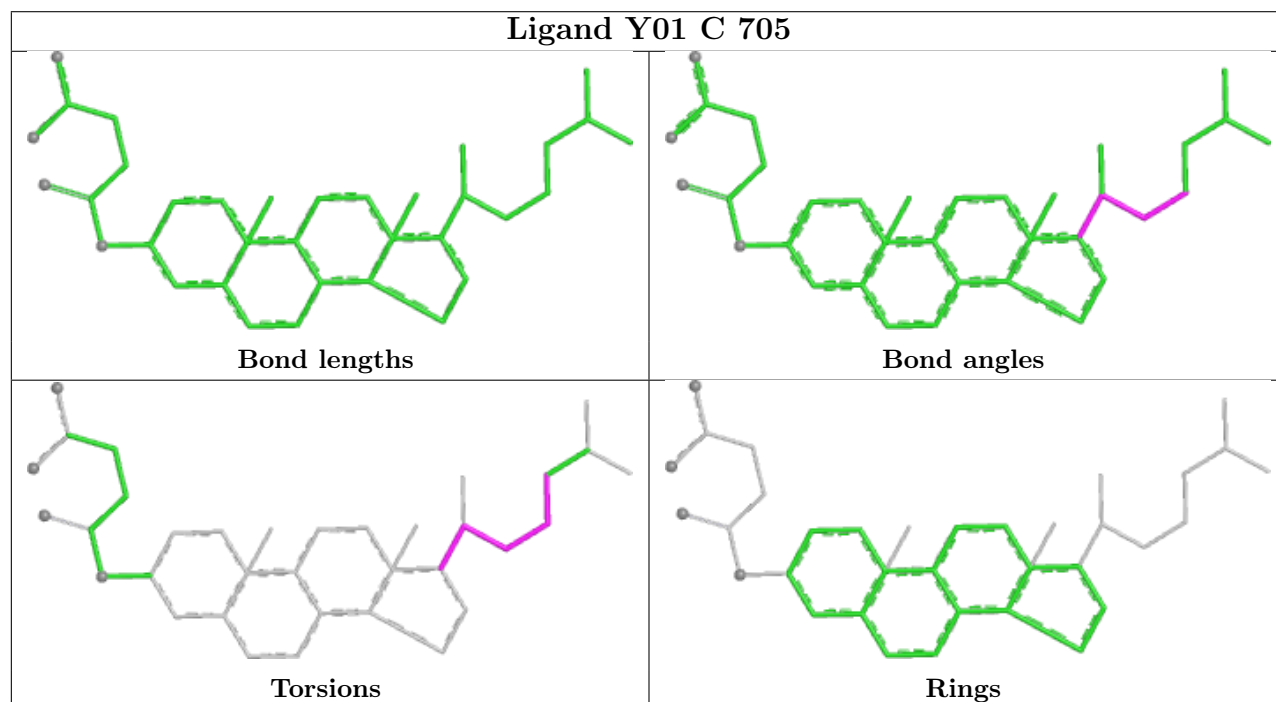


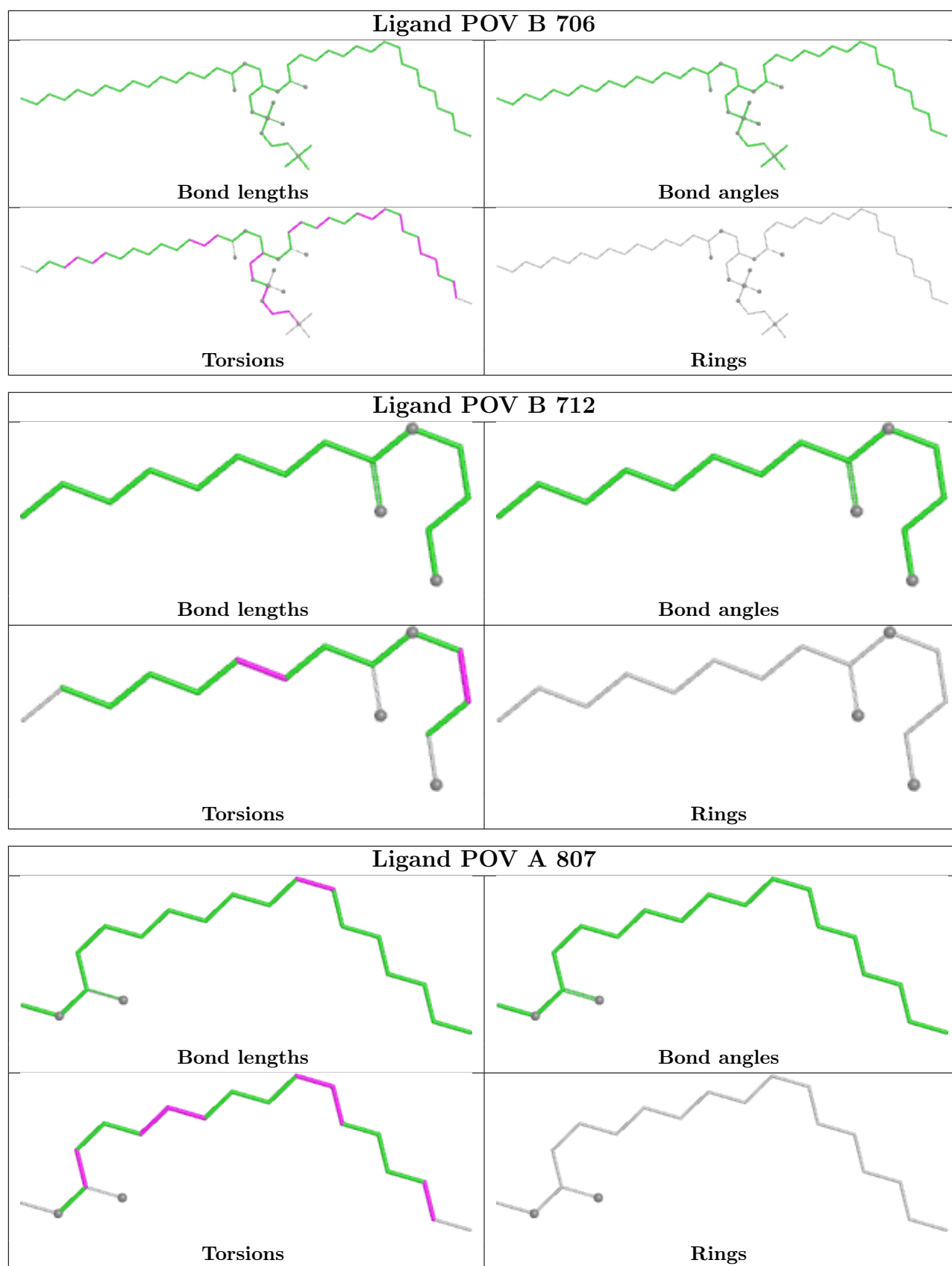


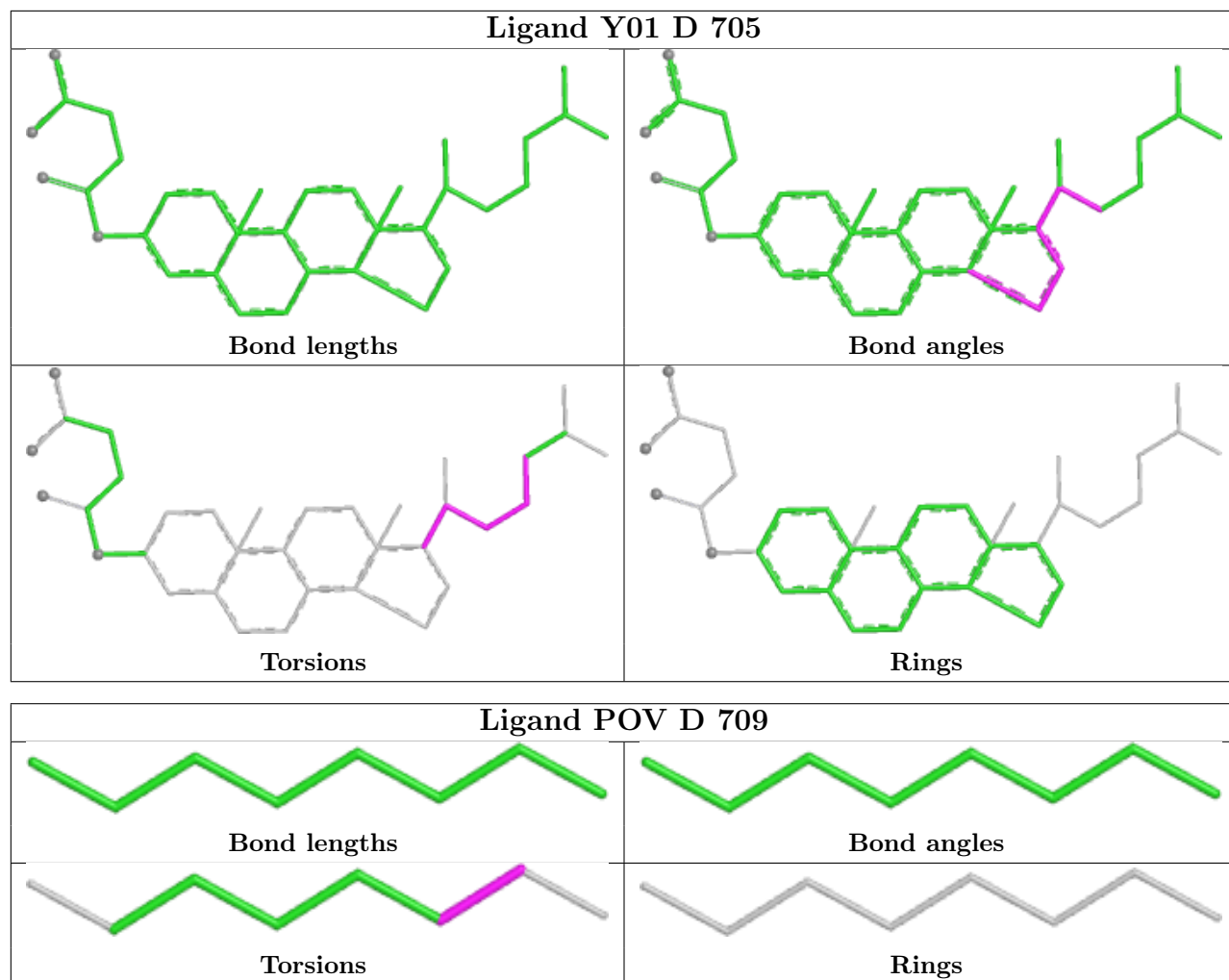
Ligand Y01 D 707



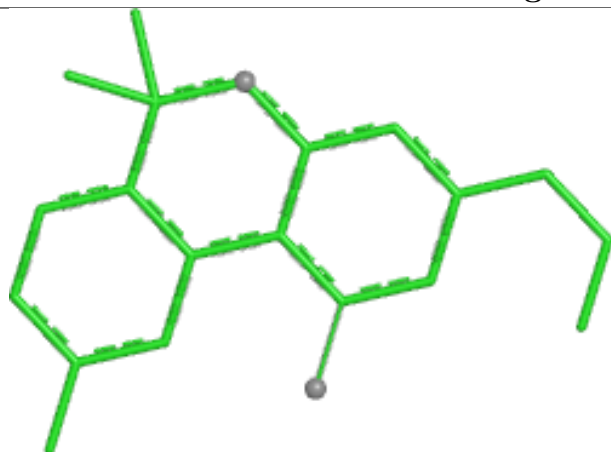
Ligand Y01 C 705



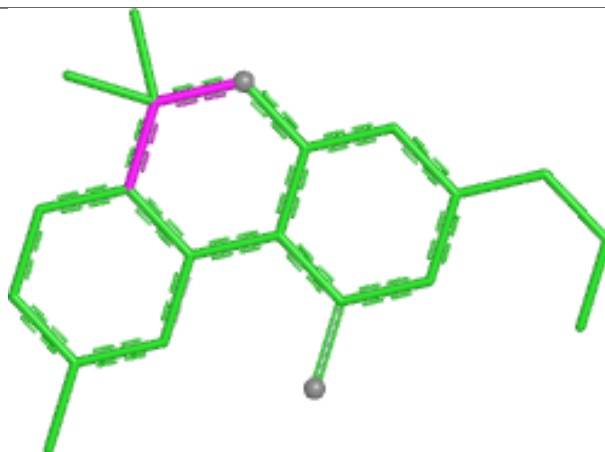




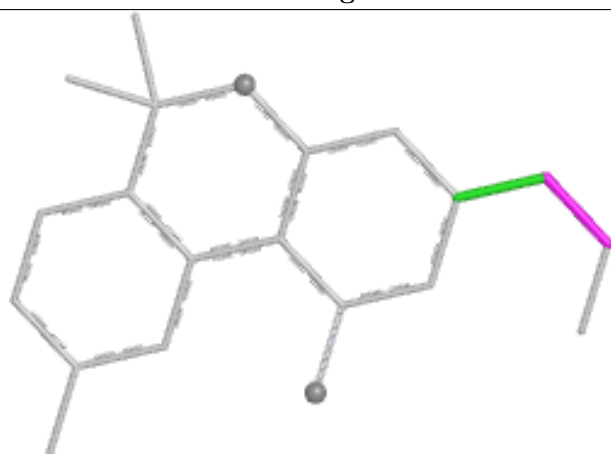
Ligand I8E B 702



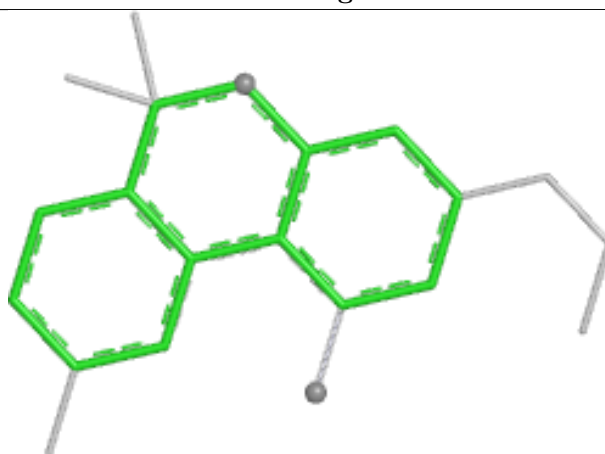
Bond lengths



Bond angles

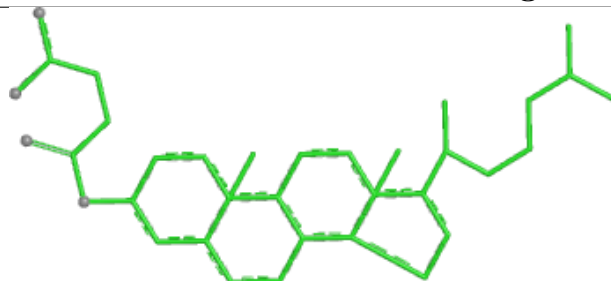


Torsions

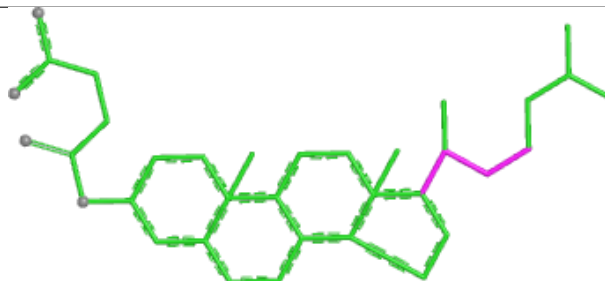


Rings

Ligand Y01 A 803



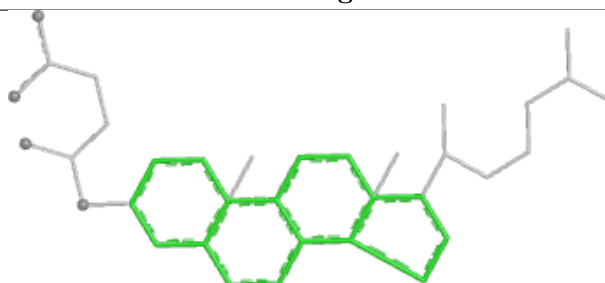
Bond lengths



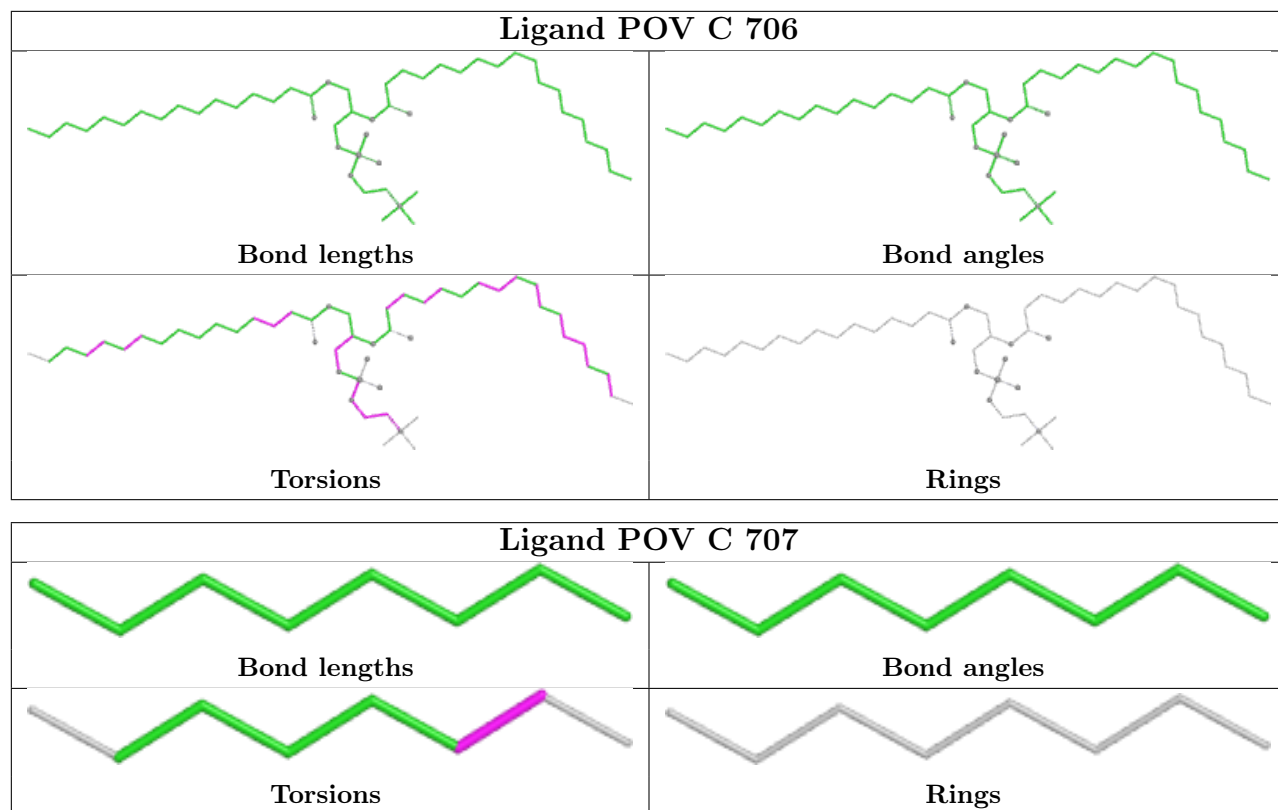
Bond angles



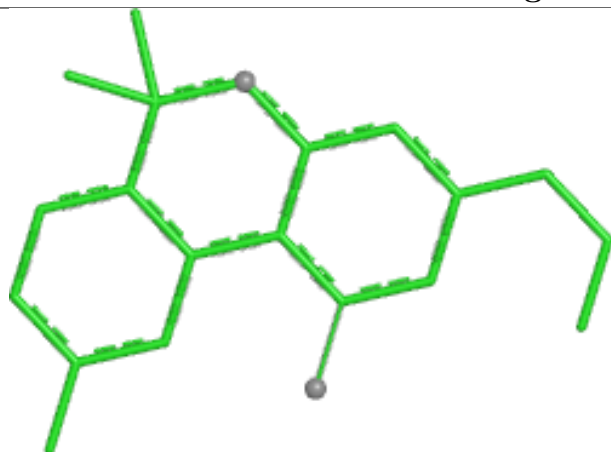
Torsions



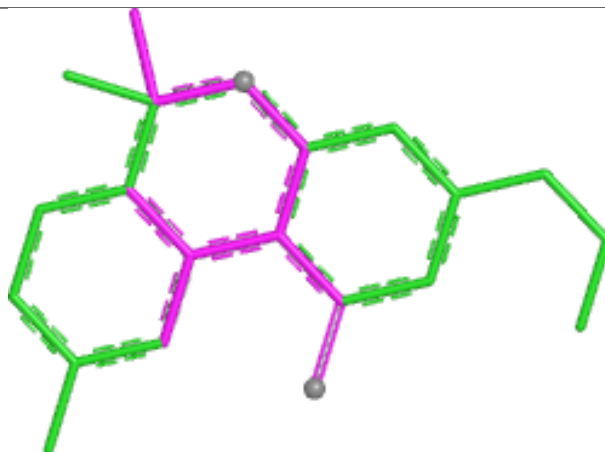
Rings



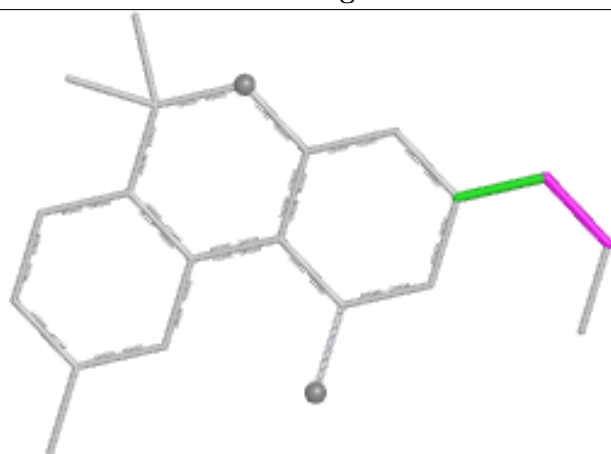
Ligand I8E B 710



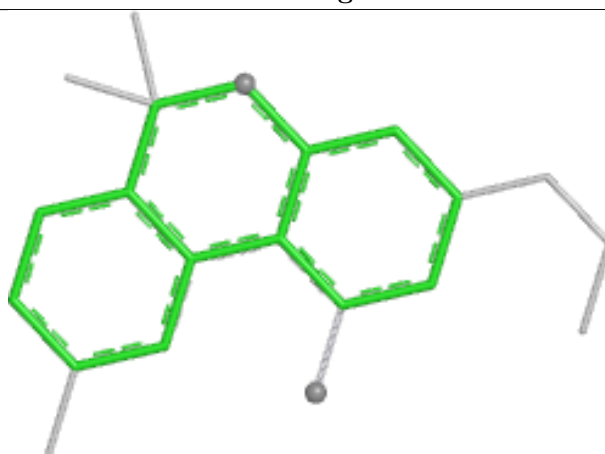
Bond lengths



Bond angles

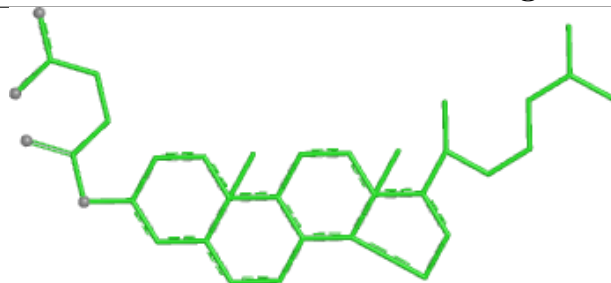


Torsions

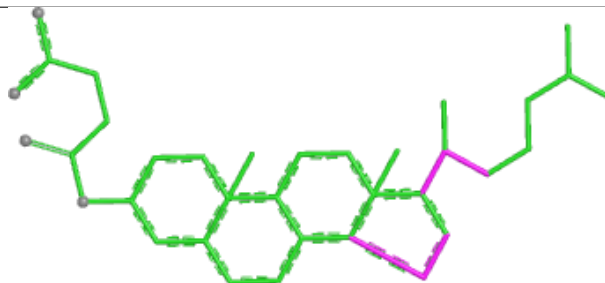


Rings

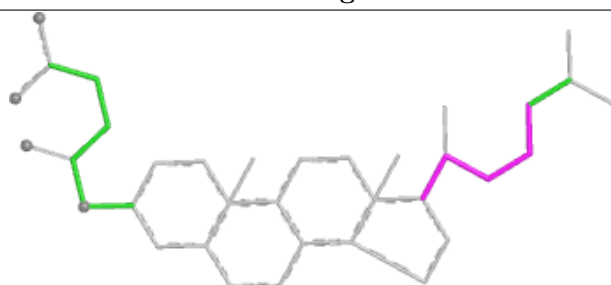
Ligand Y01 A 801



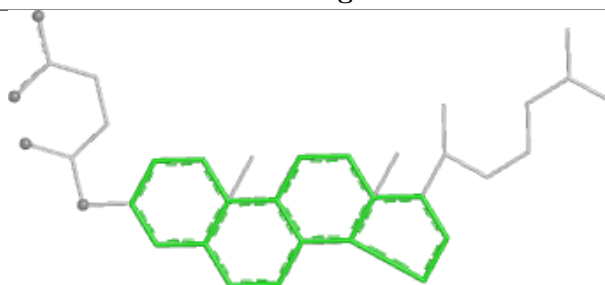
Bond lengths



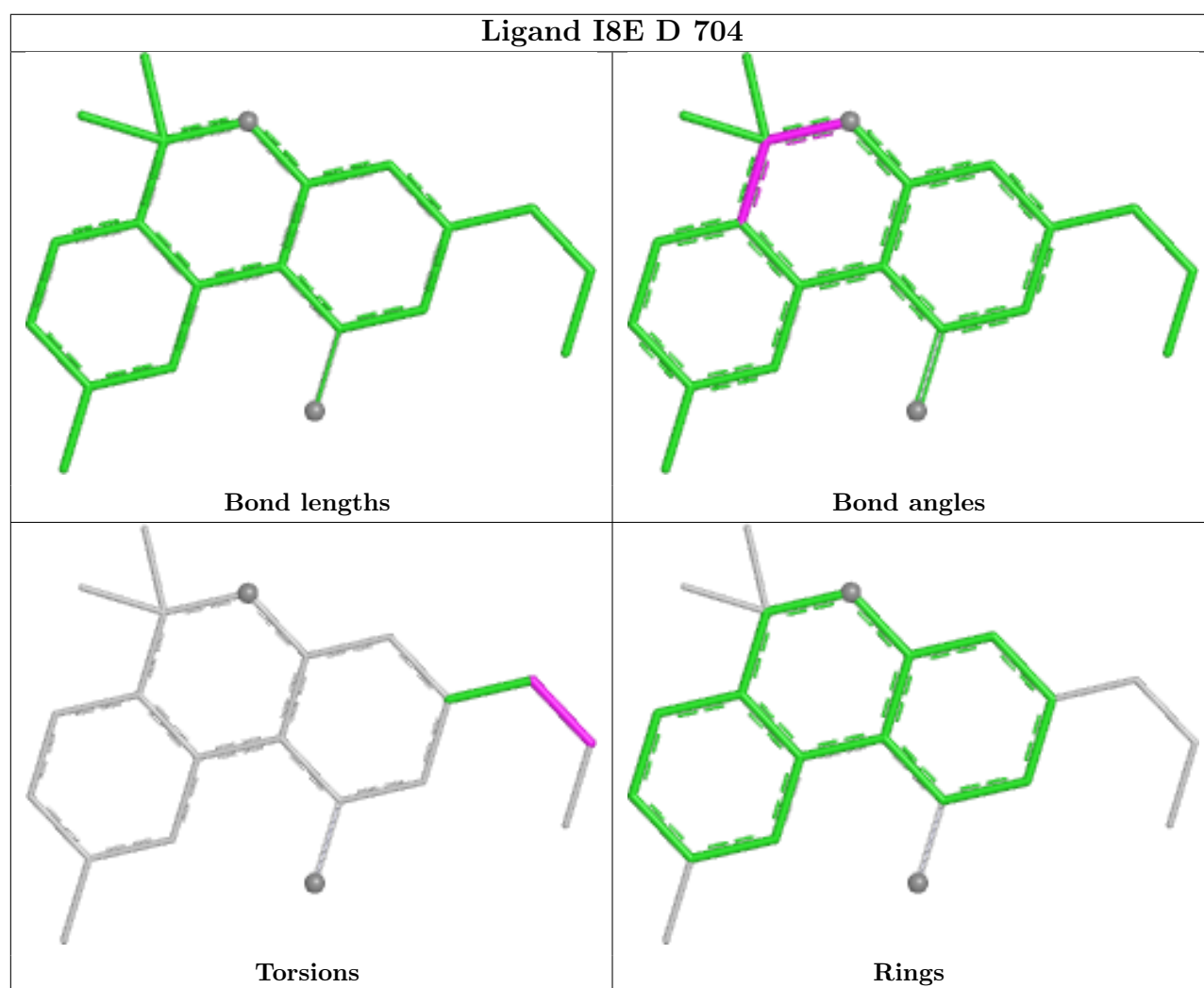
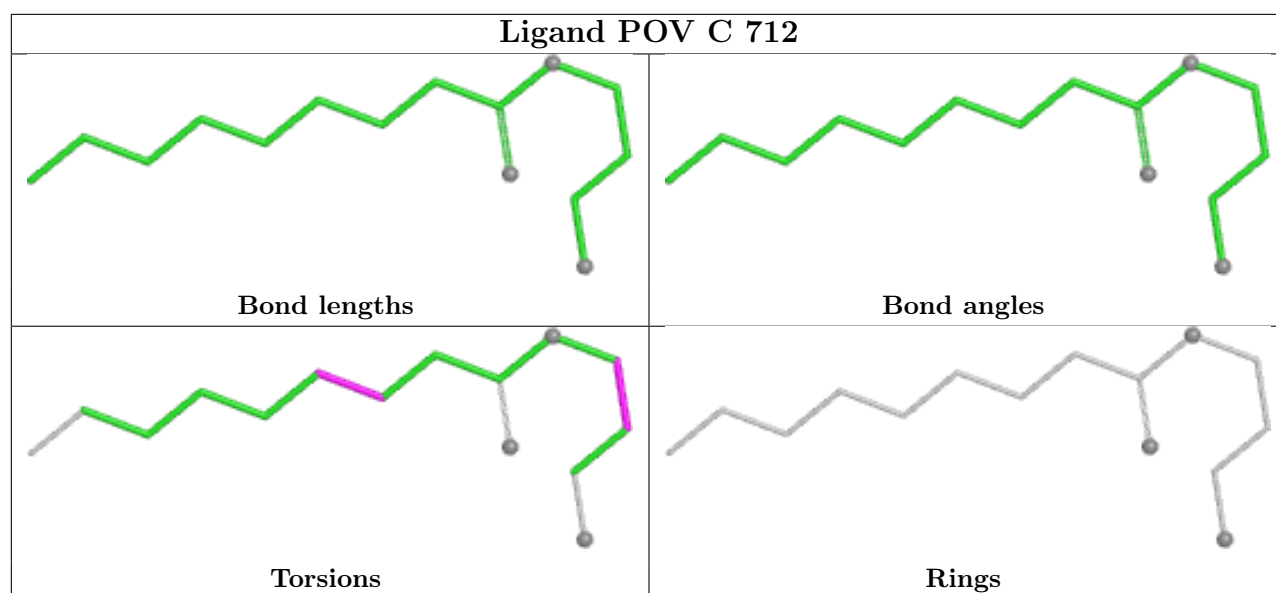
Bond angles

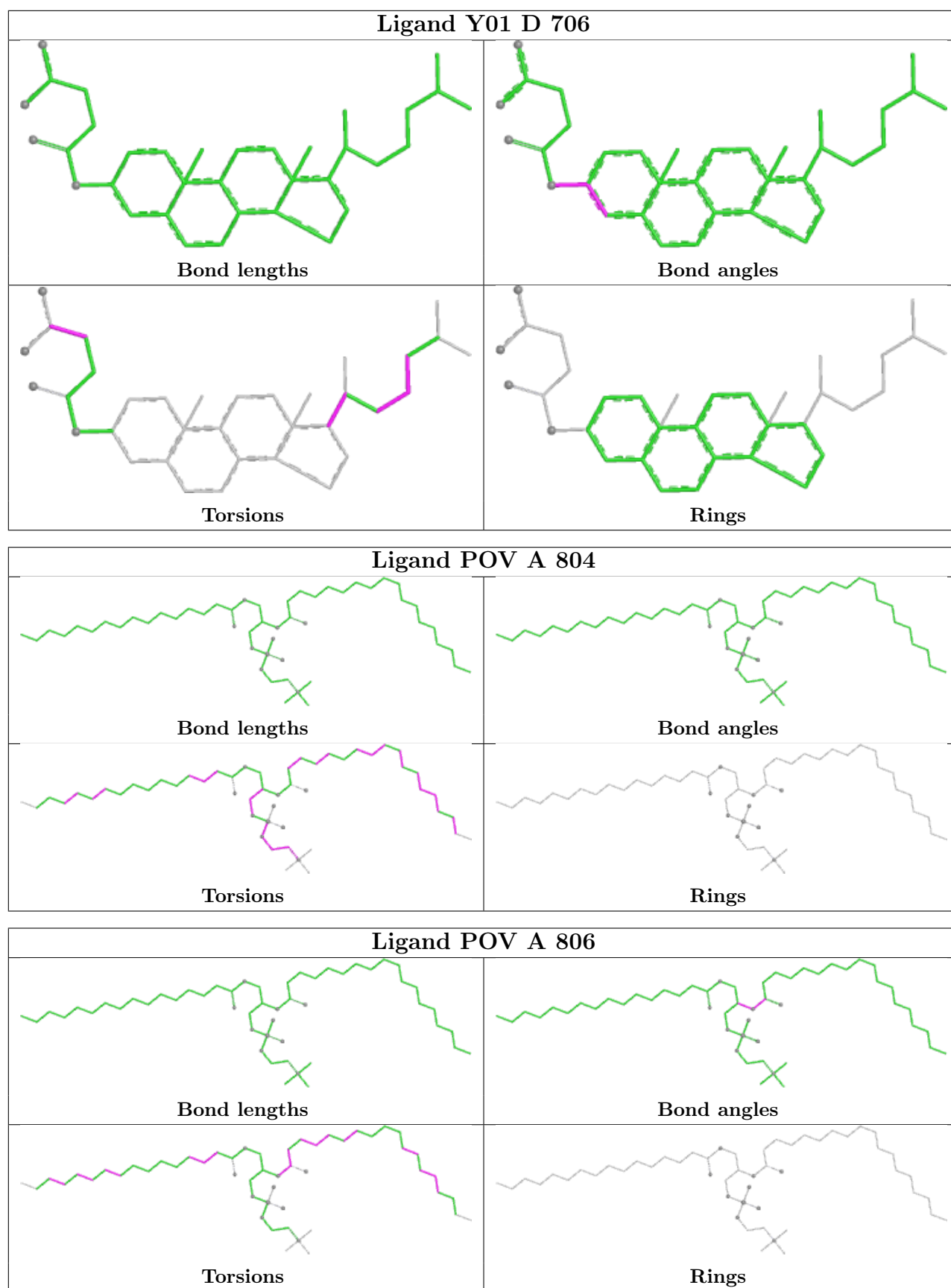


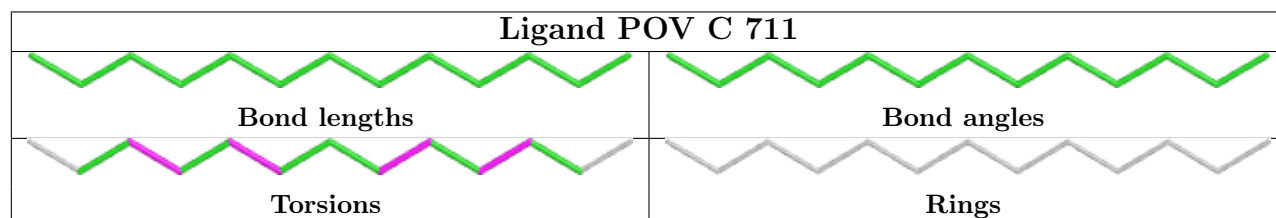
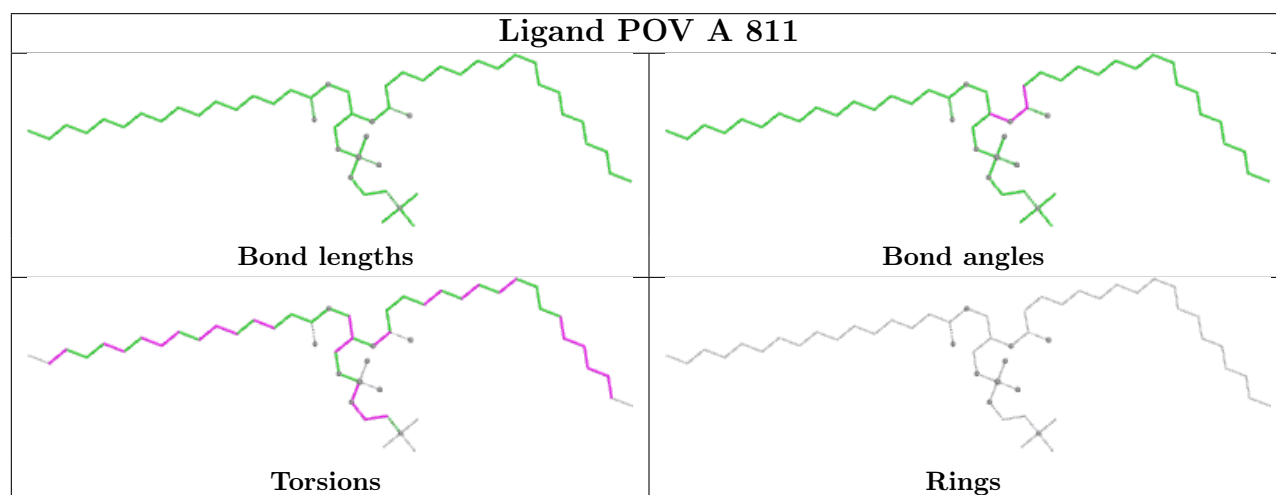
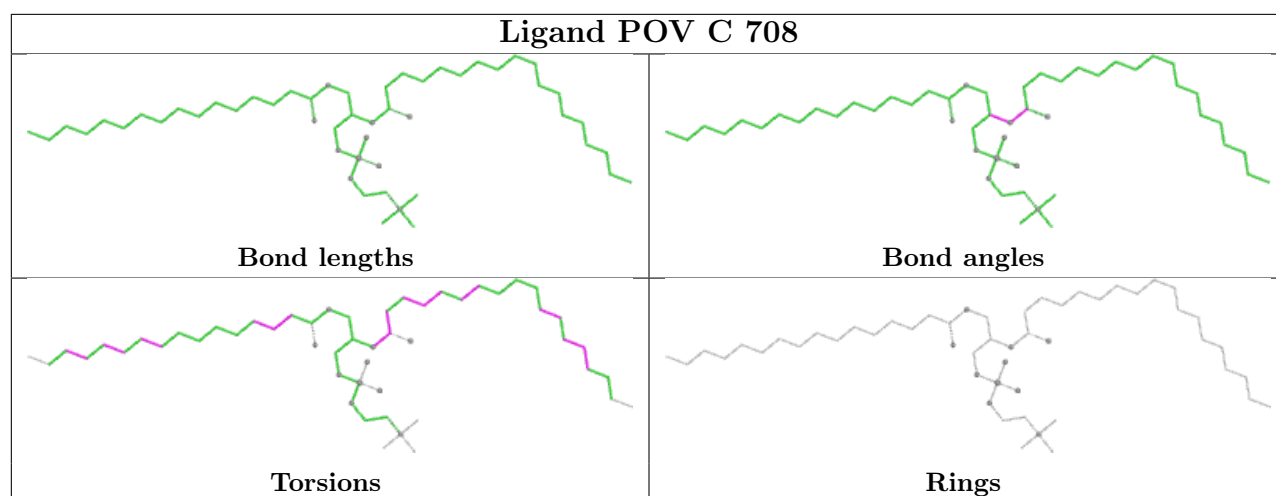
Torsions



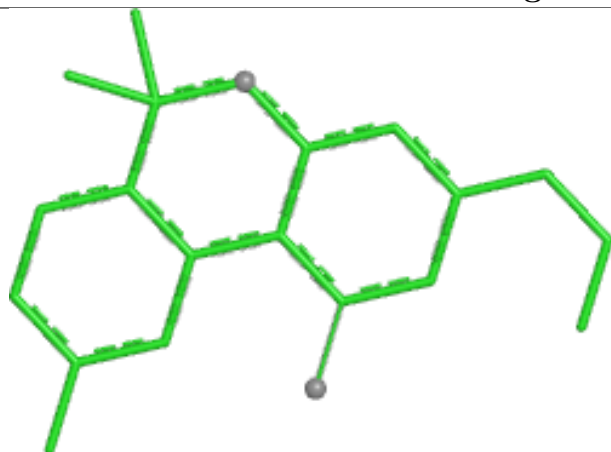
Rings



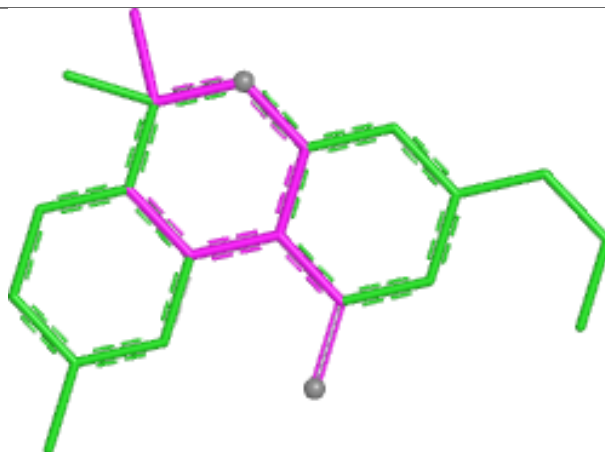




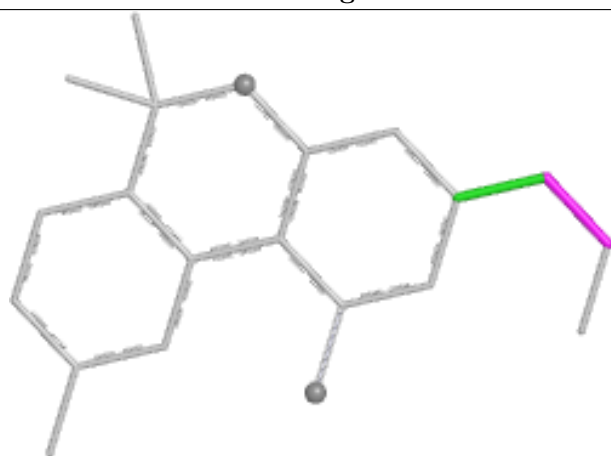
Ligand I8E C 710



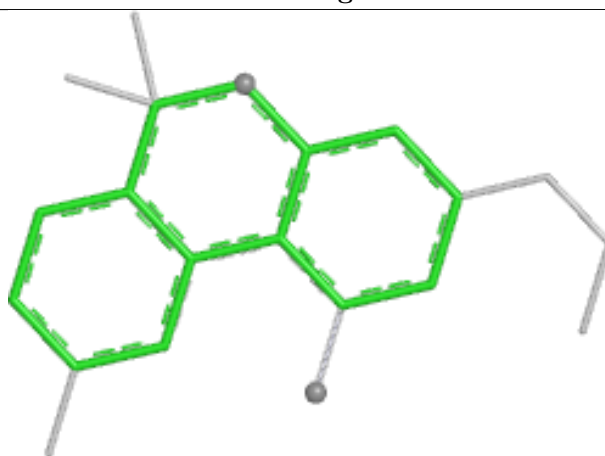
Bond lengths



Bond angles

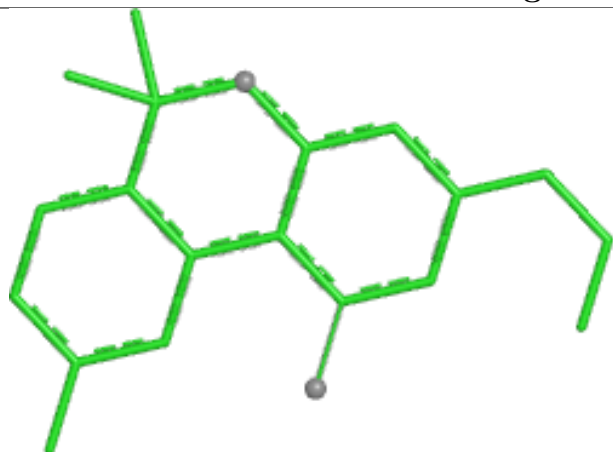


Torsions

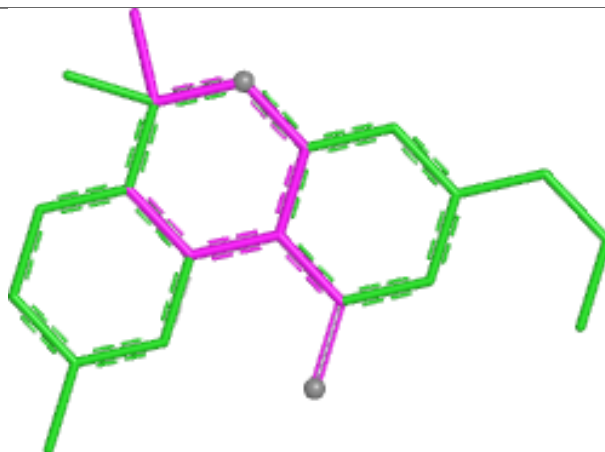


Rings

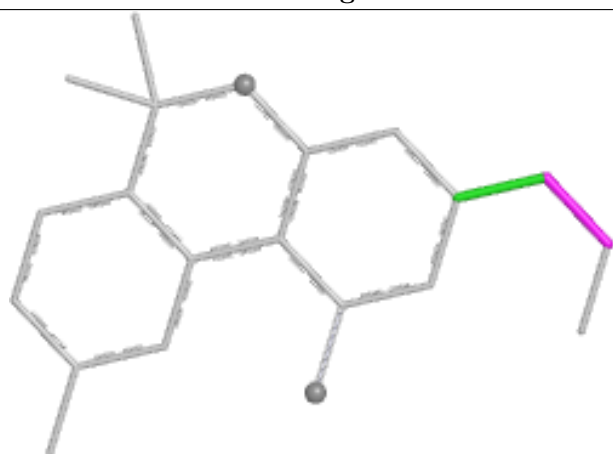
Ligand I8E A 808



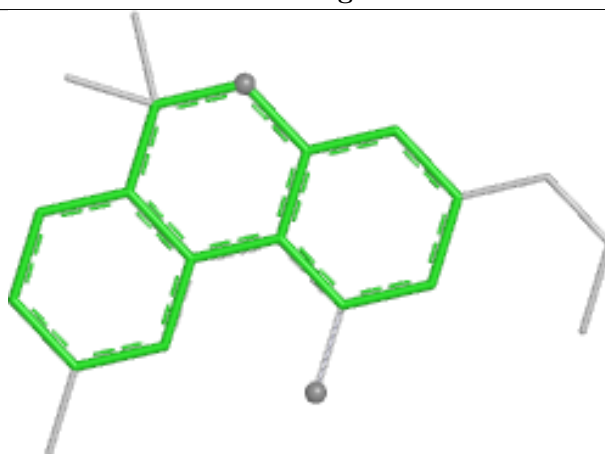
Bond lengths



Bond angles

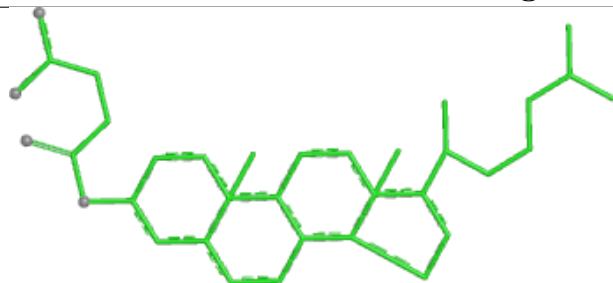


Torsions

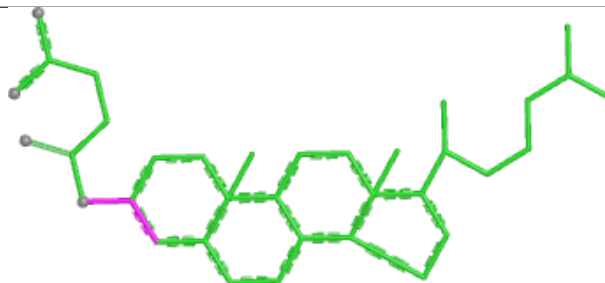


Rings

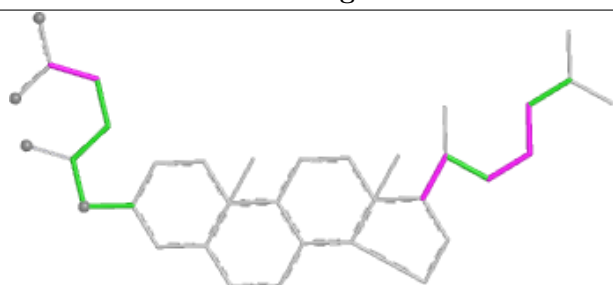
Ligand Y01 C 704



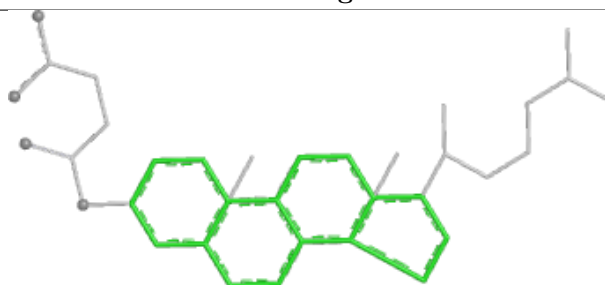
Bond lengths



Bond angles



Torsions



Rings

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.

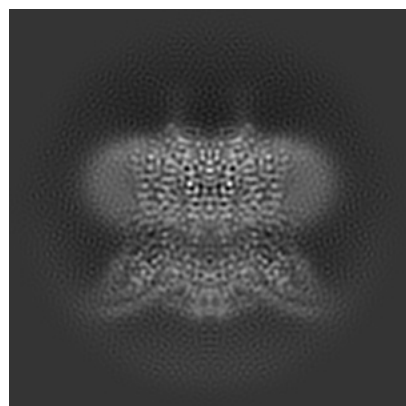
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40676. These allow visual inspection of the internal detail of the map and identification of artifacts.

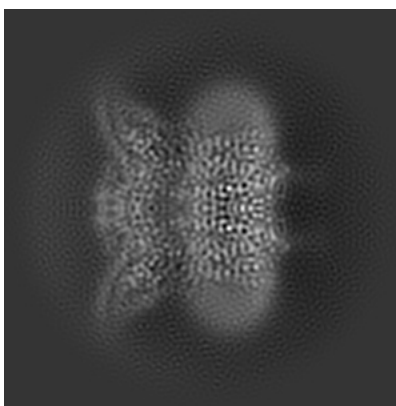
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

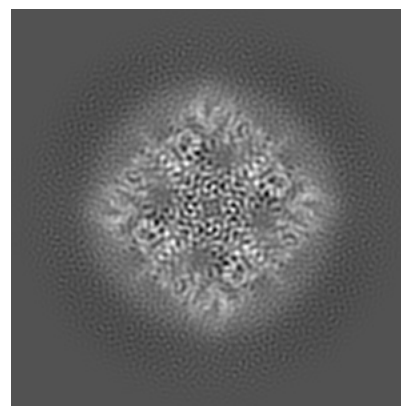
6.1.1 Primary map



X

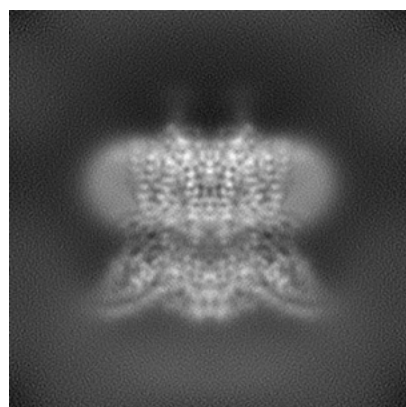


Y

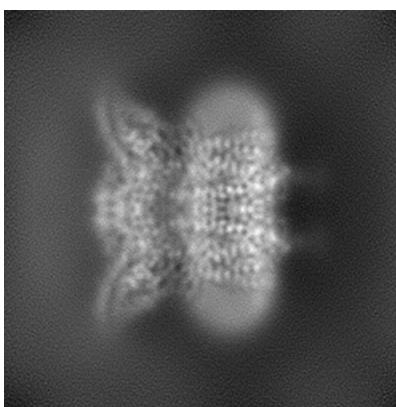


Z

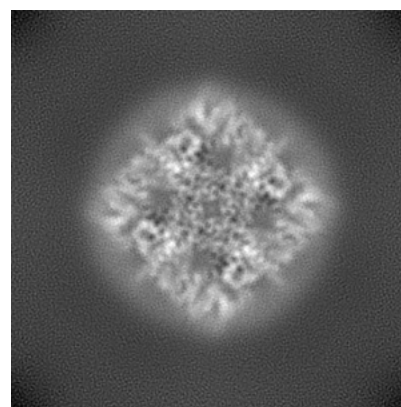
6.1.2 Raw map



X



Y

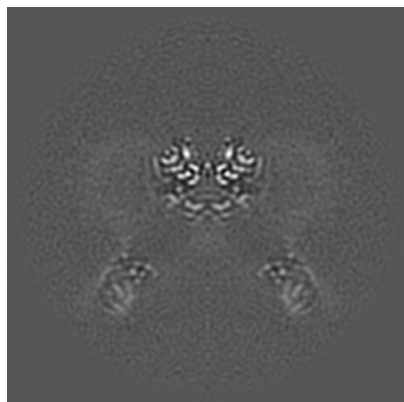


Z

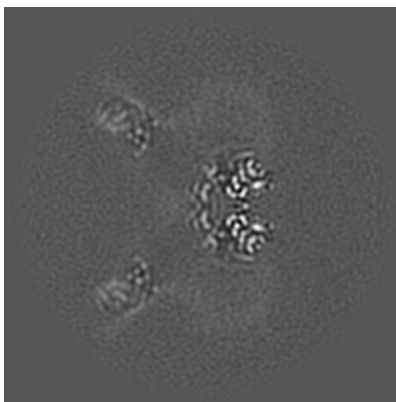
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

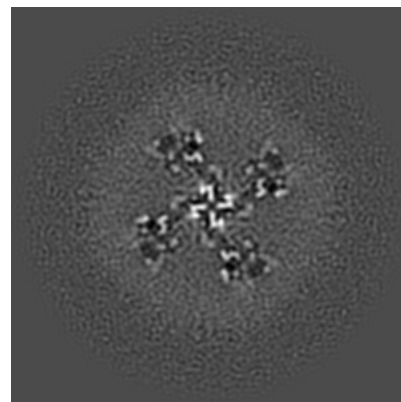
6.2.1 Primary map



X Index: 128

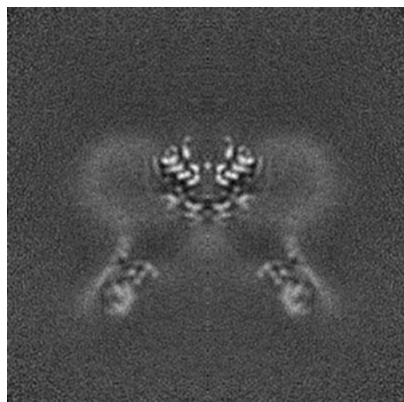


Y Index: 128

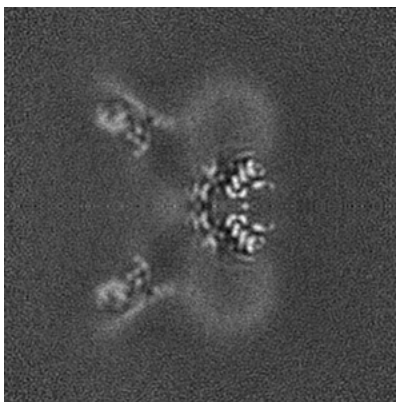


Z Index: 128

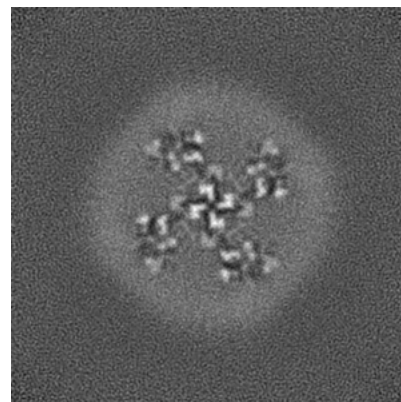
6.2.2 Raw map



X Index: 128



Y Index: 128

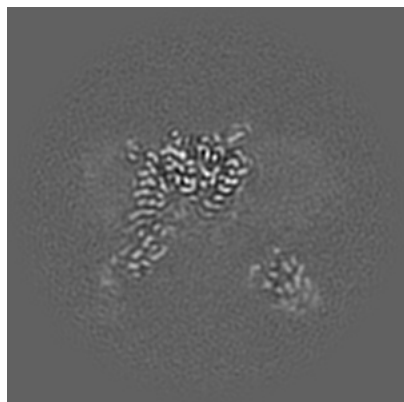


Z Index: 128

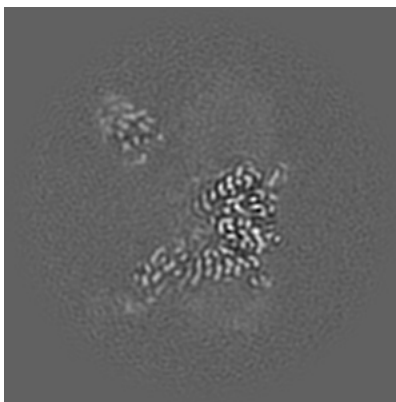
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

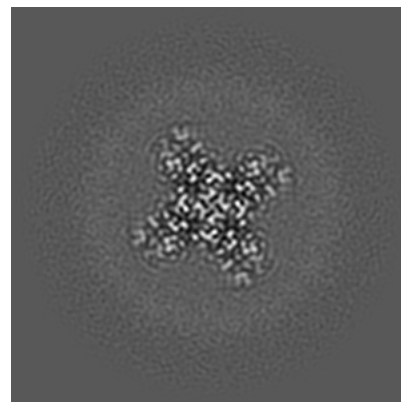
6.3.1 Primary map



X Index: 141

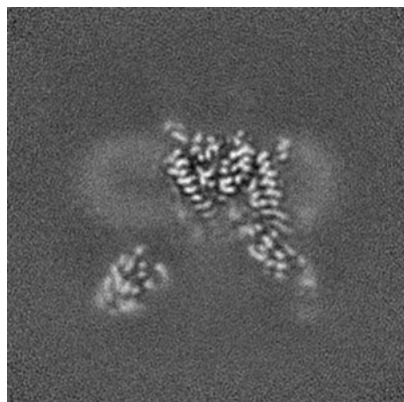


Y Index: 115

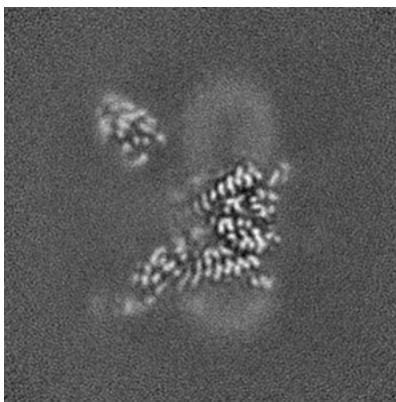


Z Index: 153

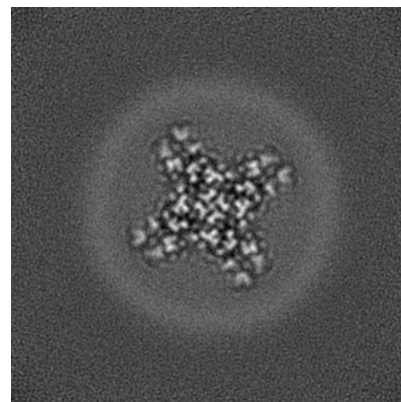
6.3.2 Raw map



X Index: 115



Y Index: 115

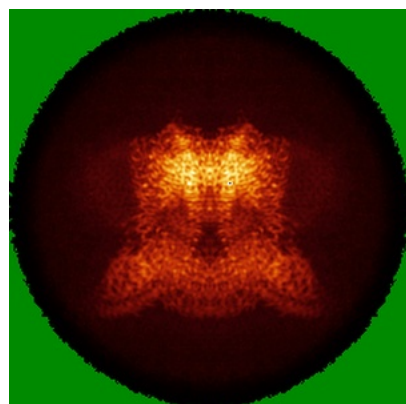


Z Index: 153

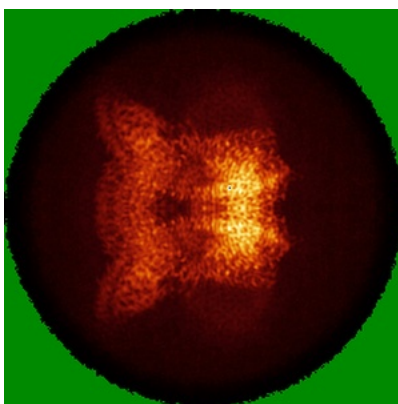
The images above show the largest variance slices of the map in three orthogonal directions.

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

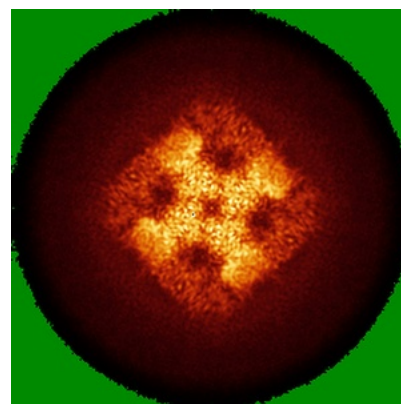
6.4.1 Primary map



X

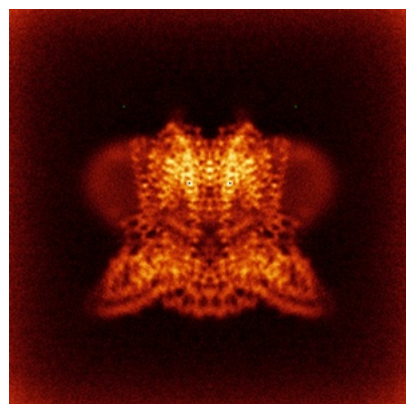


Y

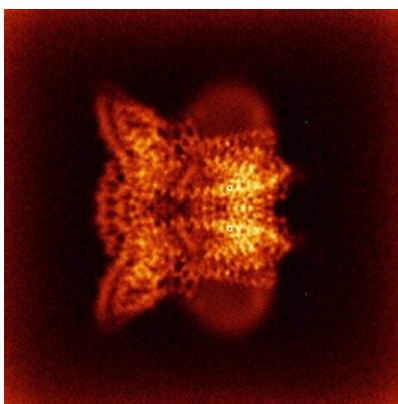


Z

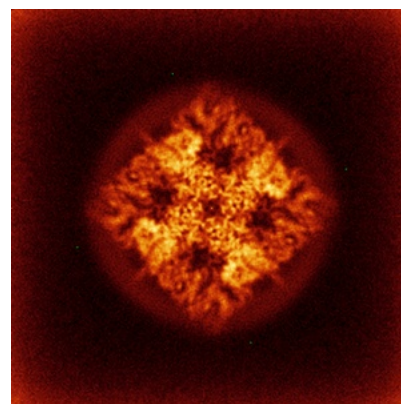
6.4.2 Raw map



X



Y

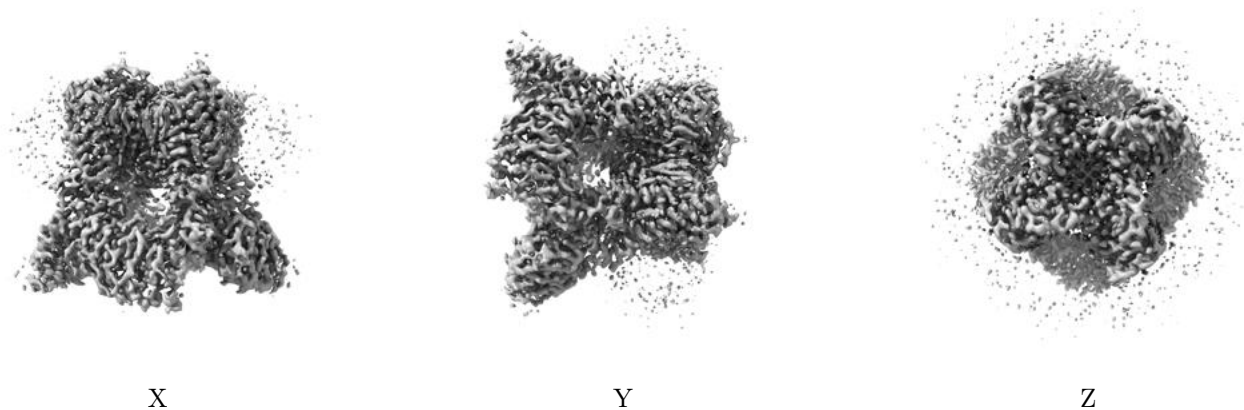


Z

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.

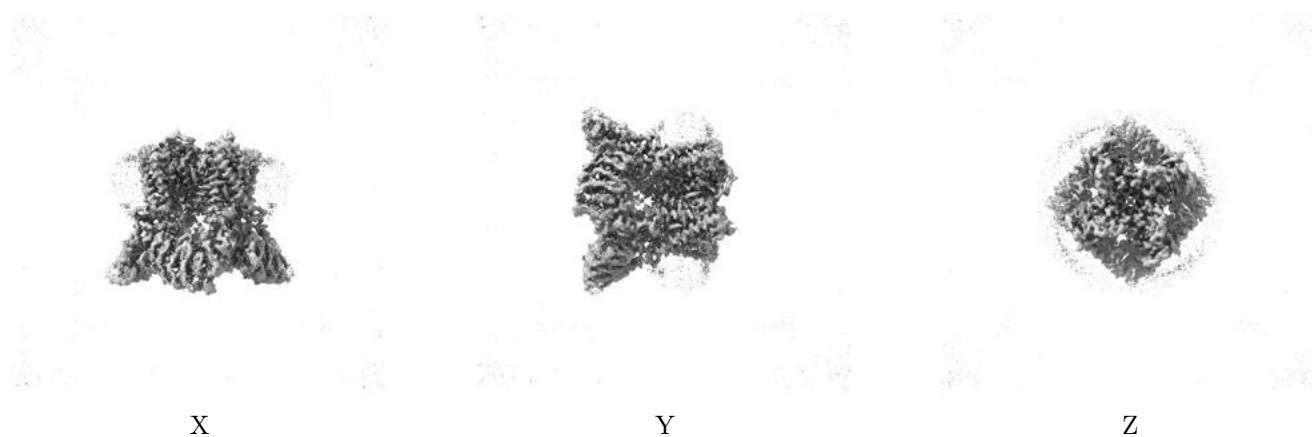
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.147. 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.

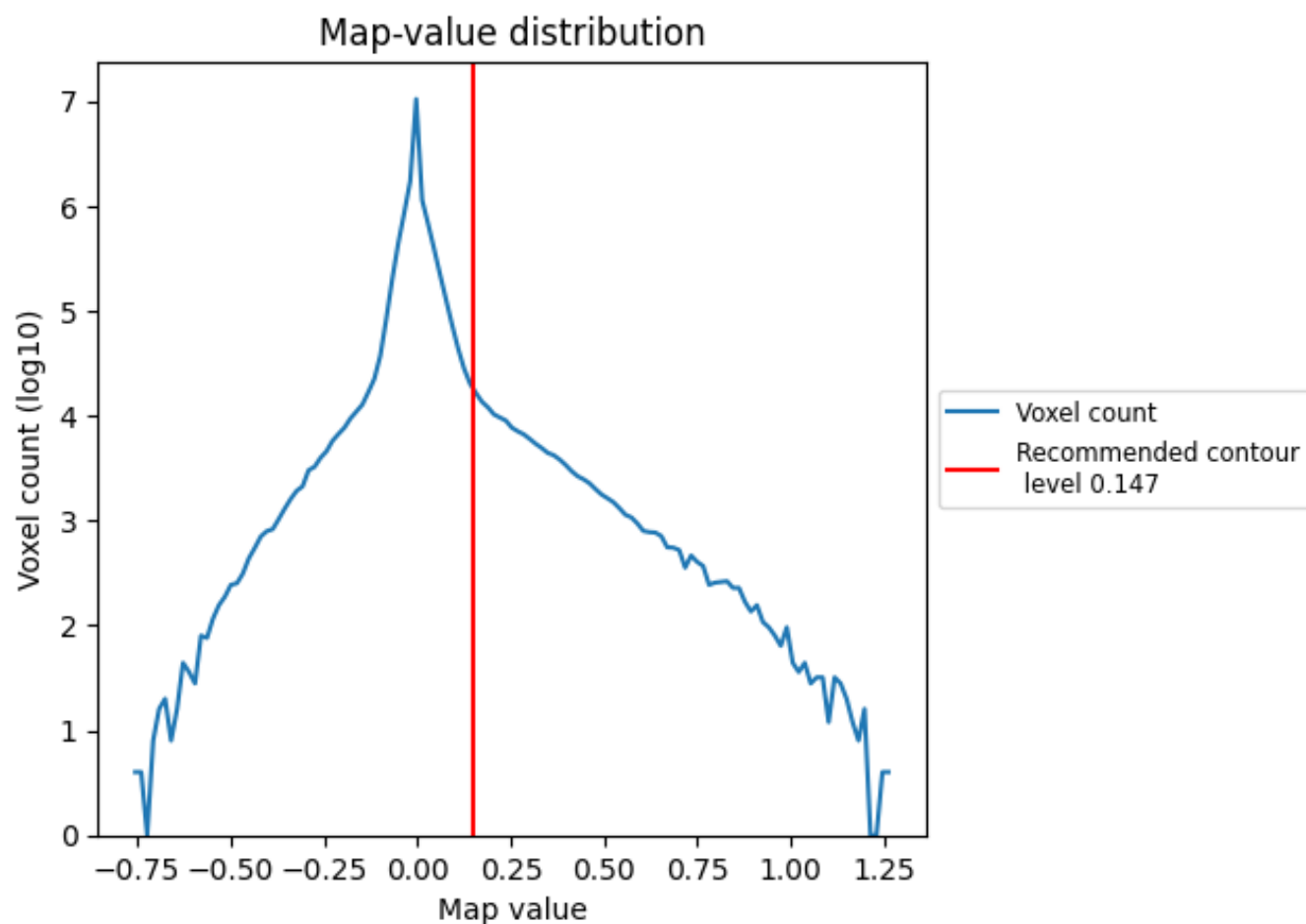
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

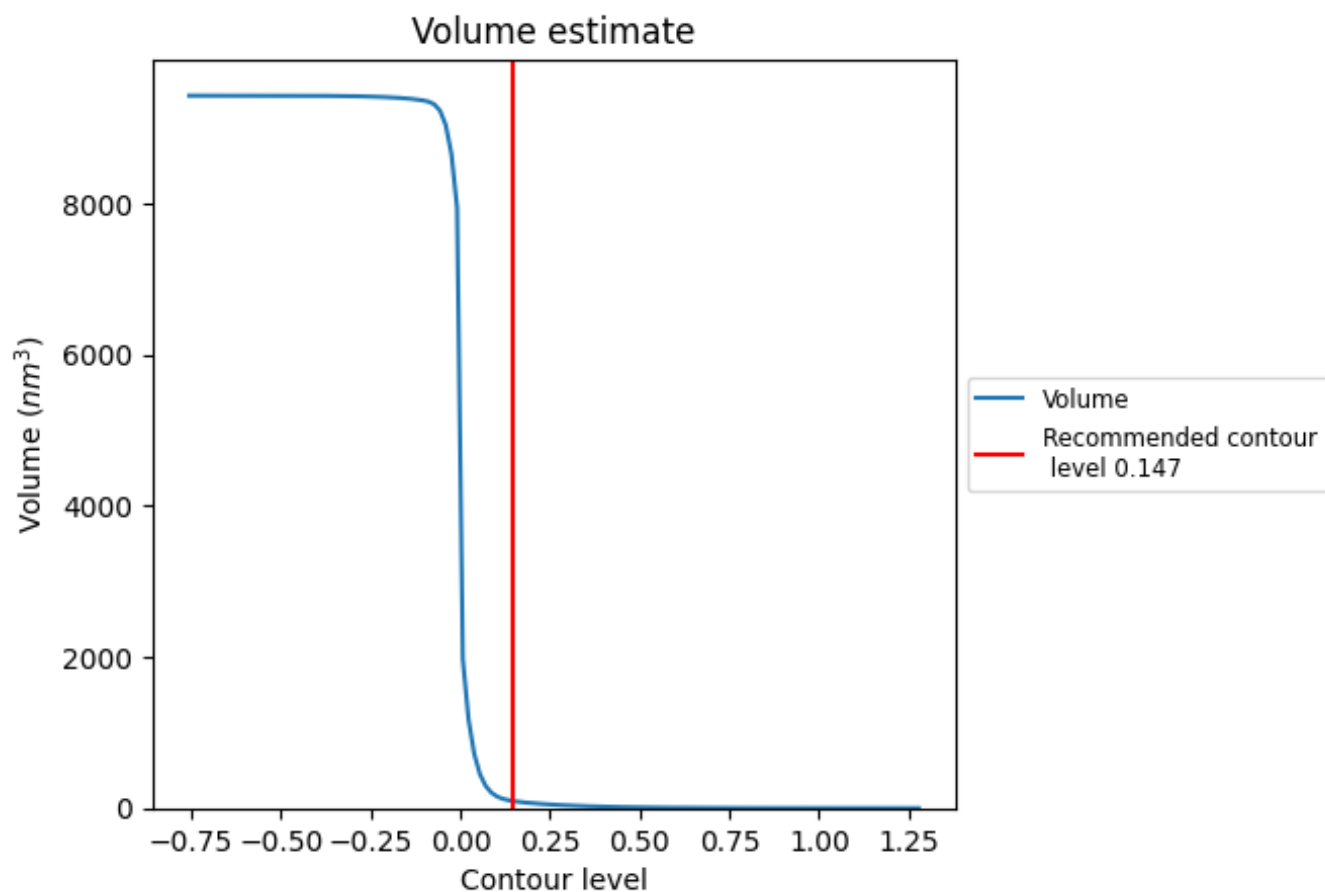
This section contains the results of statistical analysis of the map.

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.

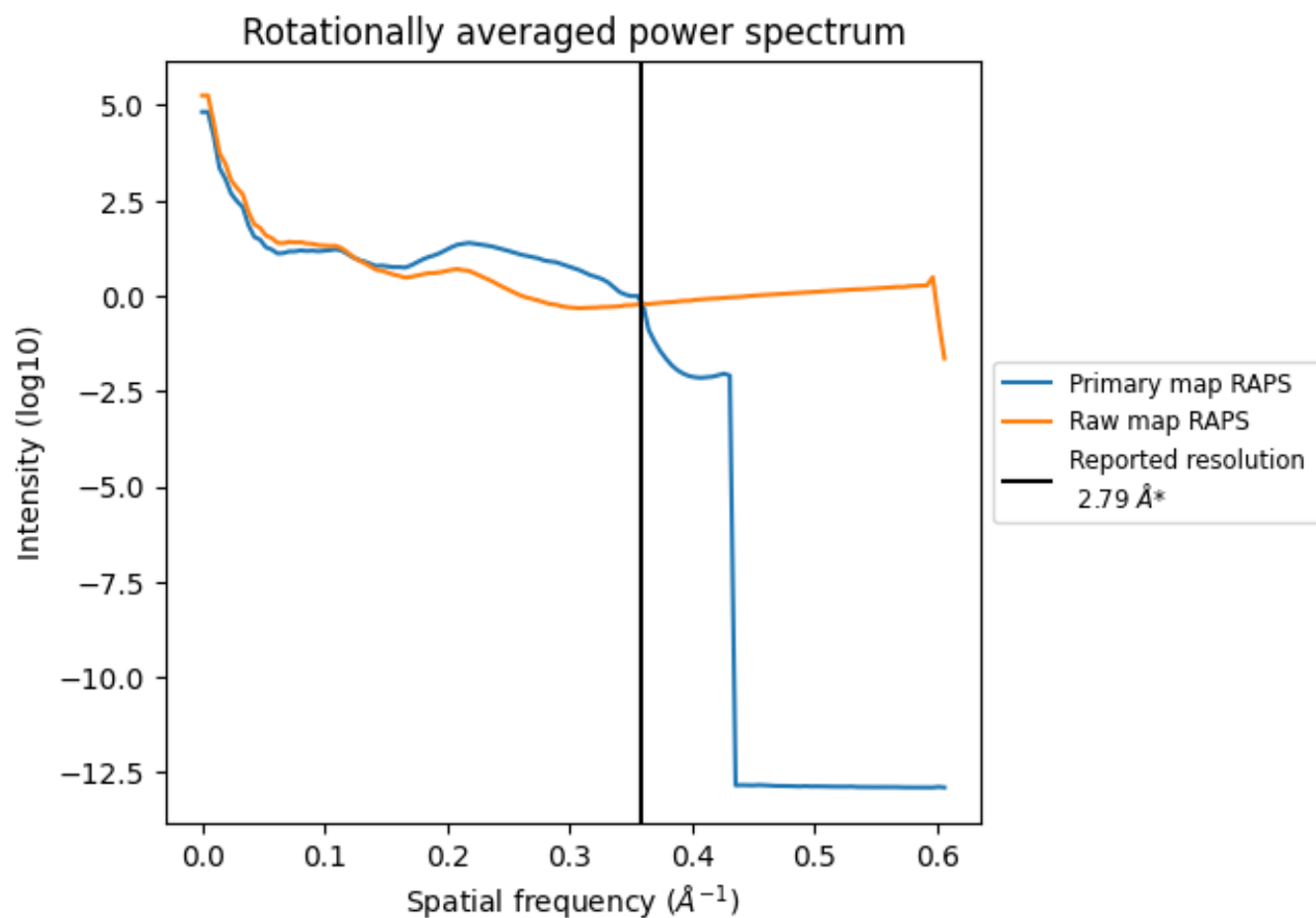
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94 nm^3 ; this corresponds to an approximate mass of 85 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 ⓘ

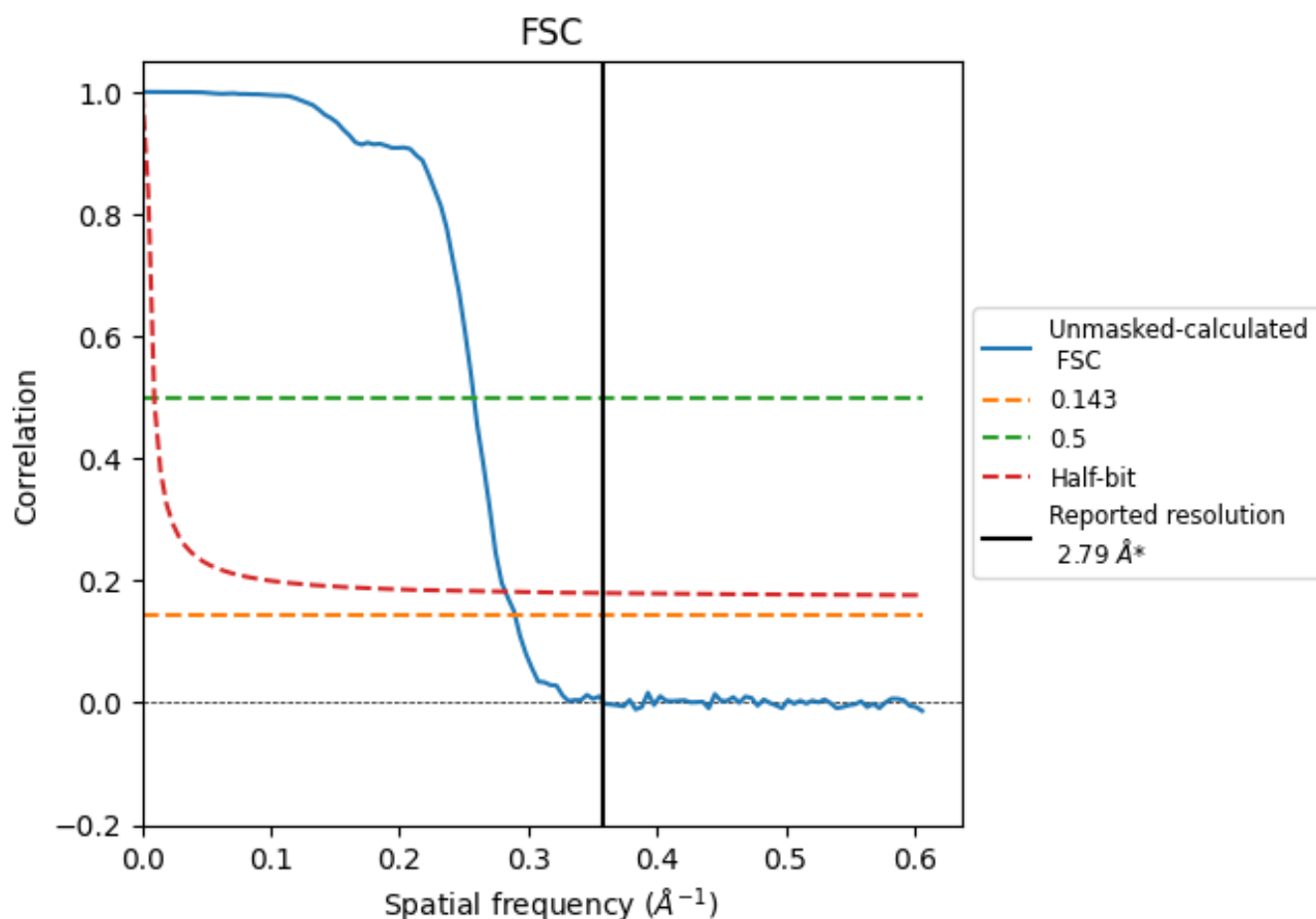


*Reported resolution corresponds to spatial frequency of 0.358 $\text{\AA}^{-1}$

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 $0.358 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

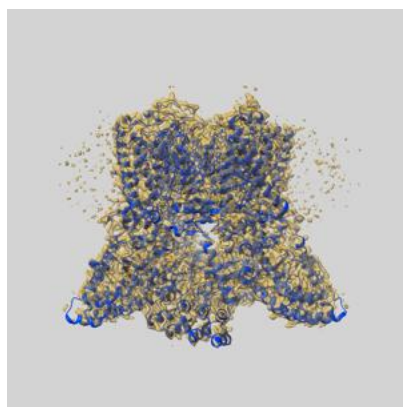
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	3.88	3.54

*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 3.45 differs from the reported value 2.79 by more than 10 %

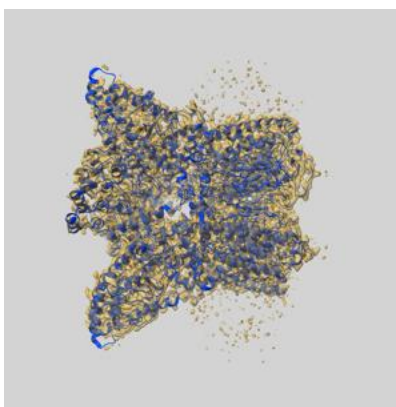
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40676 and PDB model 8SP8. Per-residue inclusion information can be found in section [3](#) on page [8](#).

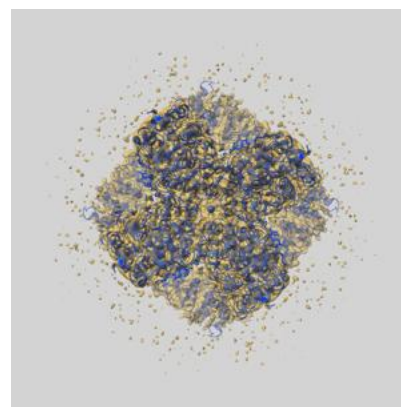
9.1 Map-model overlay [i](#)



X



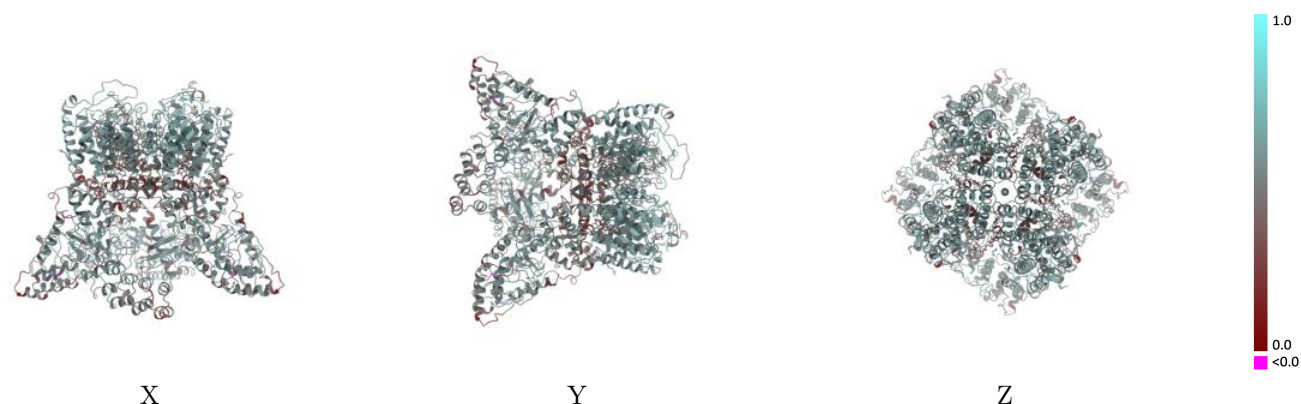
Y



Z

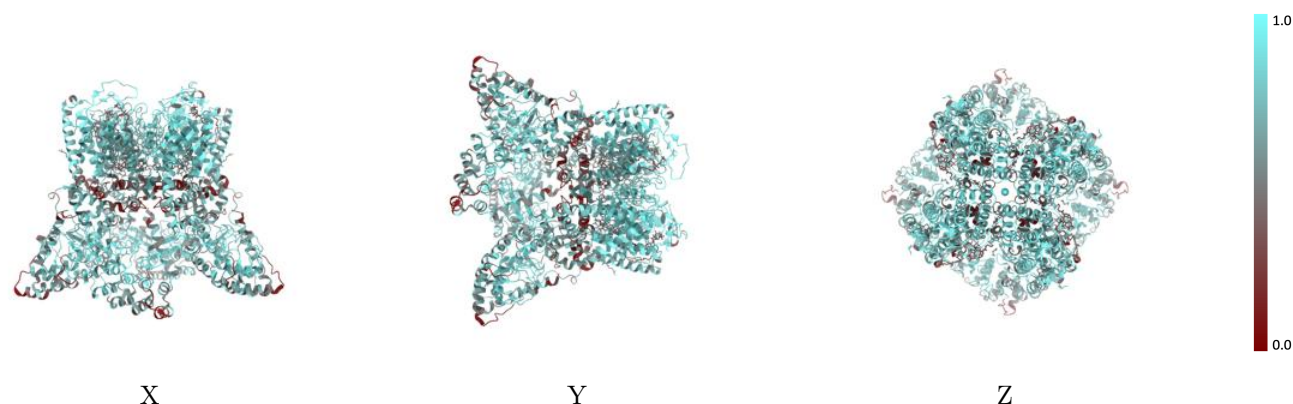
The images above show the 3D surface view of the map at the recommended contour level 0.147 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



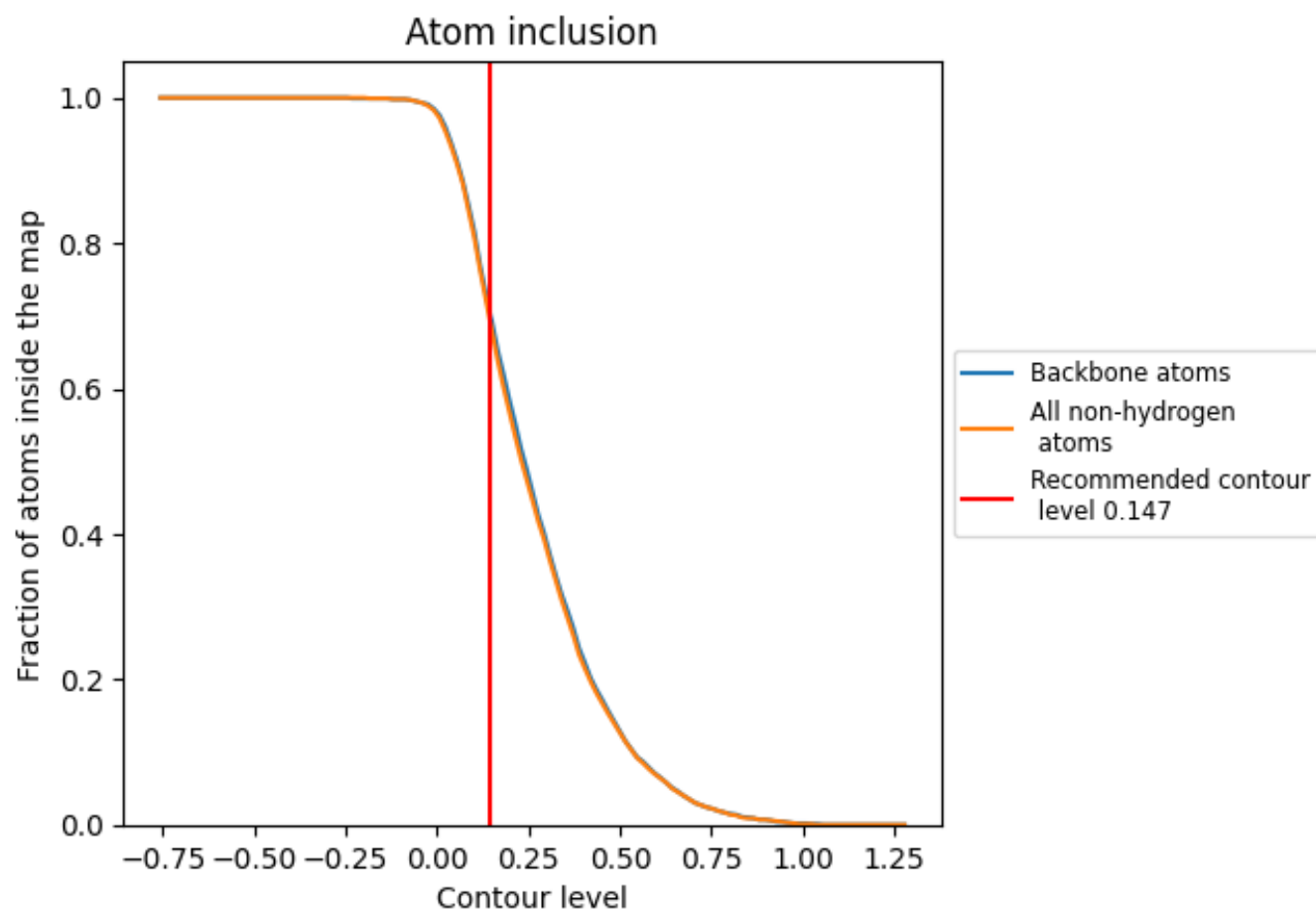
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.147).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.147) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.5150
A	0.6890	0.5140
B	0.6880	0.5160
C	0.6870	0.5150
D	0.6900	0.5160

