



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:49 AM UTC

PDB ID : 7XQB / pdb_00007xqb
EMDB ID : EMD-33392
Title : Structure of connexin43/Cx43/GJA1 gap junction intercellular channel in POPE/CHS nanodiscs at pH 8.0
Authors : Lee, H.J.; Cha, H.J.; Jeong, H.; Lee, S.N.; Lee, C.W.; Woo, J.S.
Deposited on : 2022-05-07
Resolution : 3.00 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:

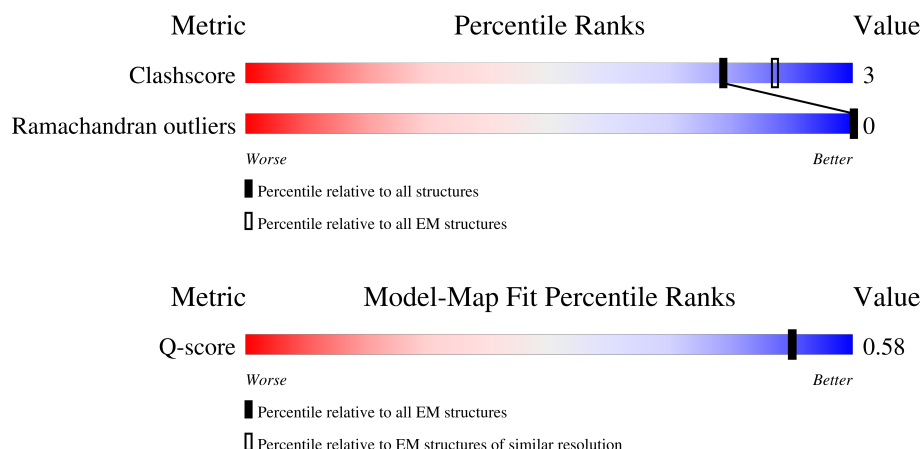
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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.

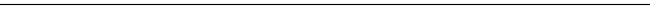


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	382	
1	B	382	
1	C	382	
1	D	382	
1	E	382	

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Mol	Chain	Length	Quality of chain	
1	F	382		
1	G	382		
1	H	382		
1	I	382		
1	J	382		
1	K	382		
1	L	382		

2 Entry composition

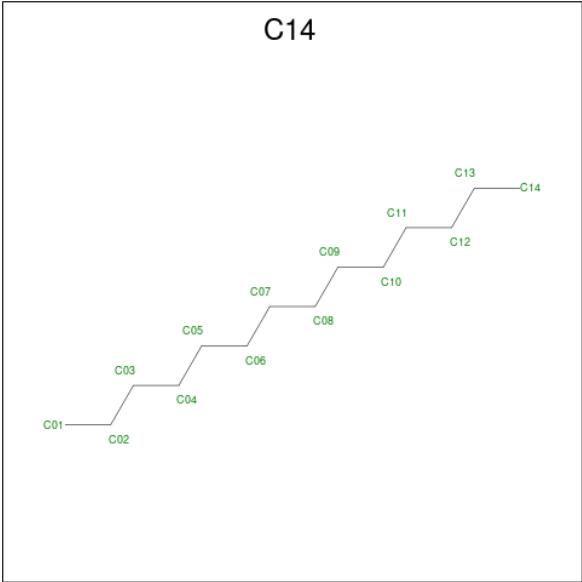
There are 4 unique types of molecules in this entry. The entry contains 48096 atoms, of which 25284 are hydrogens and 0 are deuteriums.

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 Gap junction alpha-1 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	G	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	B	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	C	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	D	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	E	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	F	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	H	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	I	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	J	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	K	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0
1	L	202	Total 3315	C 1095	H 1670	N 261	O 281	S 8	0	0

- Molecule 2 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			40	13	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	G	1	Total	C	H	0
			41	14	27	
2	G	1	Total	C	H	0
			41	14	27	
2	G	1	Total	C	H	0
			41	14	27	

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Mol	Chain	Residues	Atoms			AltConf
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 40	C 13	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 40	C 13	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0

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Mol	Chain	Residues	Atoms			AltConf
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 40	C 13	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 40	C 13	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0

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Mol	Chain	Residues	Atoms			AltConf
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 40	C 13	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 40	C 13	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0

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Mol	Chain	Residues	Atoms			AltConf
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 40	C 13	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 40	C 13	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0

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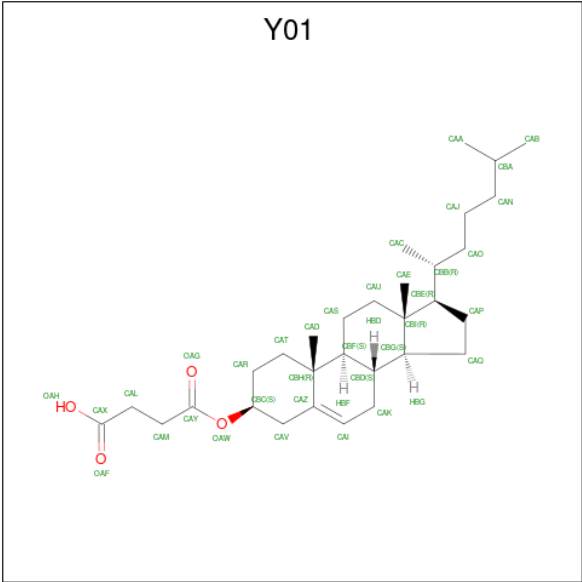
Mol	Chain	Residues	Atoms			AltConf
2	I	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 40	C 13	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 40	C 13	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0

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Mol	Chain	Residues	Atoms			AltConf
2	K	1	Total	C	H	0
			41	14	27	
2	K	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			40	13	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



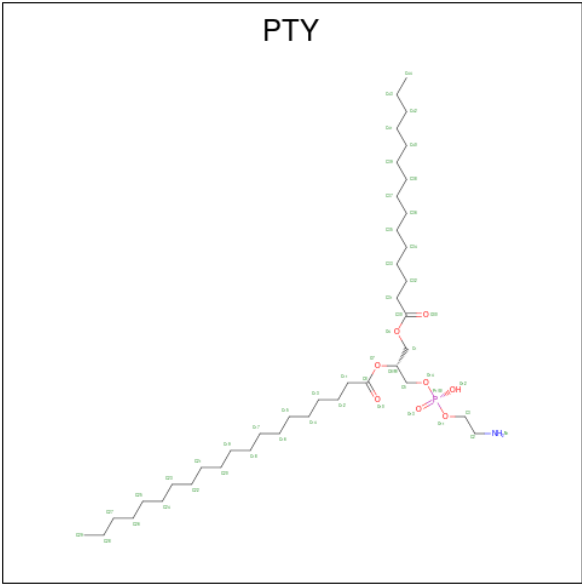
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	G	1	Total	C	H	O	0
			84	31	49	4	
3	G	1	Total	C	H	O	0
			84	31	49	4	
3	B	1	Total	C	H	O	0
			84	31	49	4	
3	B	1	Total	C	H	O	0
			84	31	49	4	
3	C	1	Total	C	H	O	0
			84	31	49	4	
3	C	1	Total	C	H	O	0
			84	31	49	4	
3	D	1	Total	C	H	O	0
			84	31	49	4	
3	D	1	Total	C	H	O	0
			84	31	49	4	
3	E	1	Total	C	H	O	0
			84	31	49	4	
3	E	1	Total	C	H	O	0
			84	31	49	4	
3	F	1	Total	C	H	O	0
			84	31	49	4	
3	F	1	Total	C	H	O	0
			84	31	49	4	

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Mol	Chain	Residues	Atoms				AltConf
3	H	1	Total	C	H	O	0
			84	31	49	4	
3	H	1	Total	C	H	O	0
			84	31	49	4	
3	I	1	Total	C	H	O	0
			84	31	49	4	
3	I	1	Total	C	H	O	0
			84	31	49	4	
3	J	1	Total	C	H	O	0
			84	31	49	4	
3	J	1	Total	C	H	O	0
			84	31	49	4	
3	K	1	Total	C	H	O	0
			84	31	49	4	
3	K	1	Total	C	H	O	0
			84	31	49	4	
3	L	1	Total	C	H	O	0
			84	31	49	4	
3	L	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	

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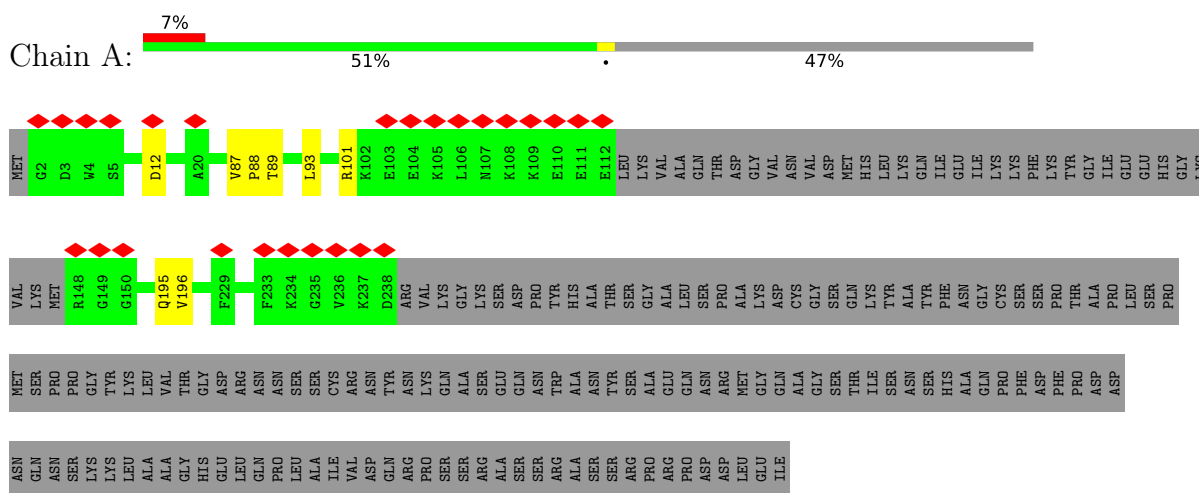
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Mol	Chain	Residues	Atoms						AltConf
4	G	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	B	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	C	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	D	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	E	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	F	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	H	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	I	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	J	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	K	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
4	L	1	Total 75	C 23	H 42	N 1	O 8	P 1	0

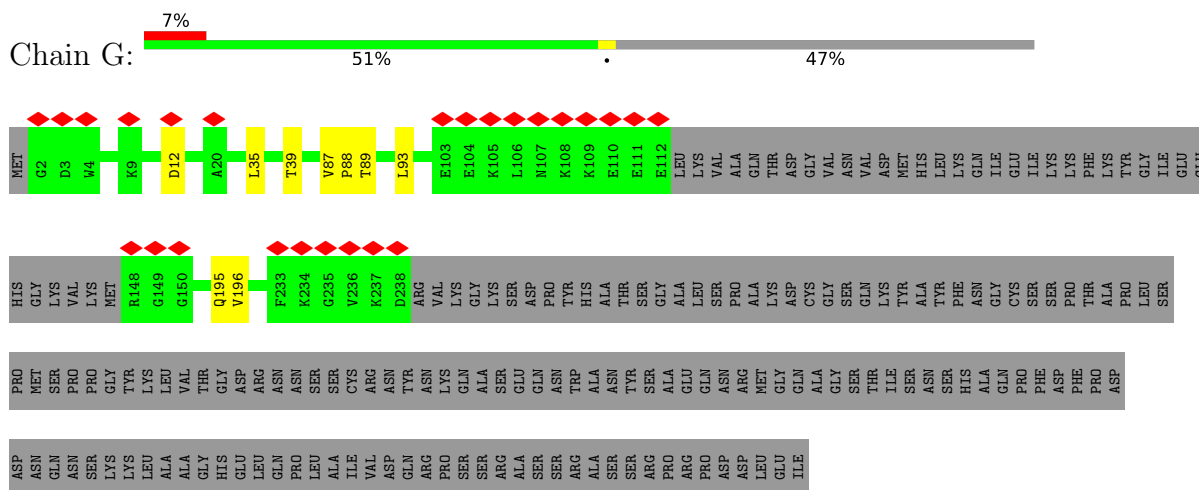
3 Residue-property plots

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: Gap junction alpha-1 protein

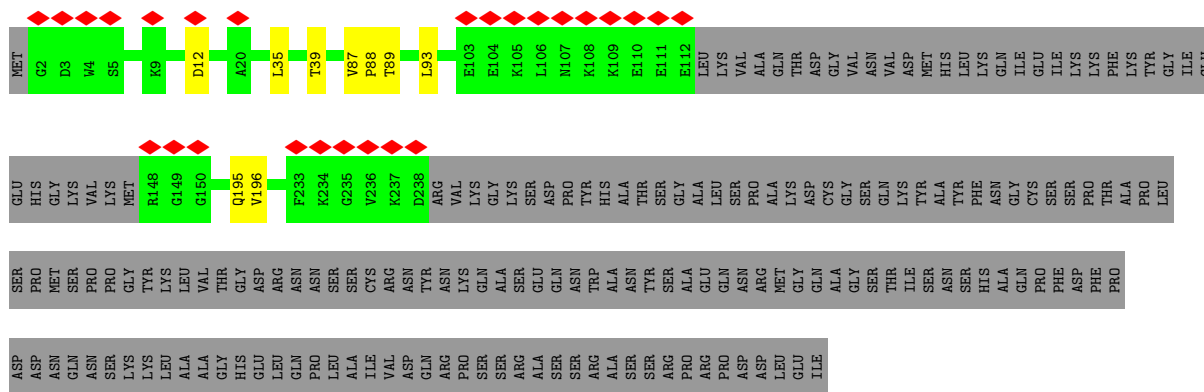


• Molecule 1: Gap junction alpha-1 protein

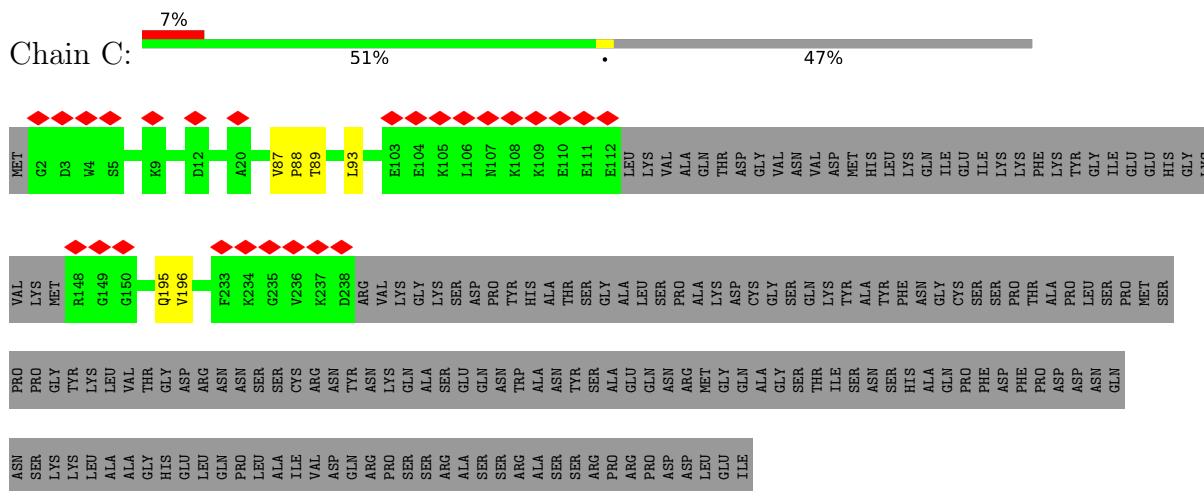


• Molecule 1: Gap junction alpha-1 protein

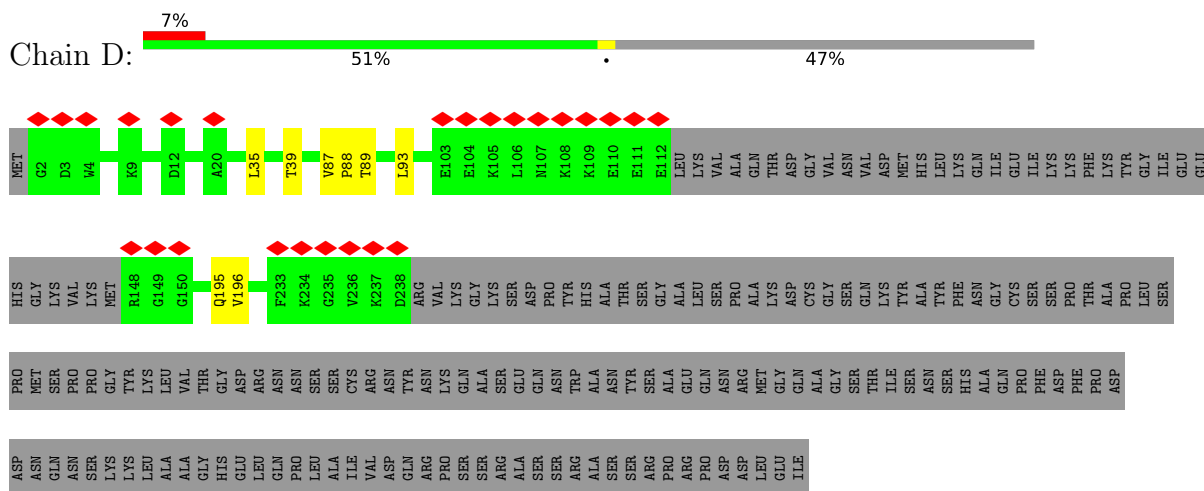




- Molecule 1: Gap junction alpha-1 protein

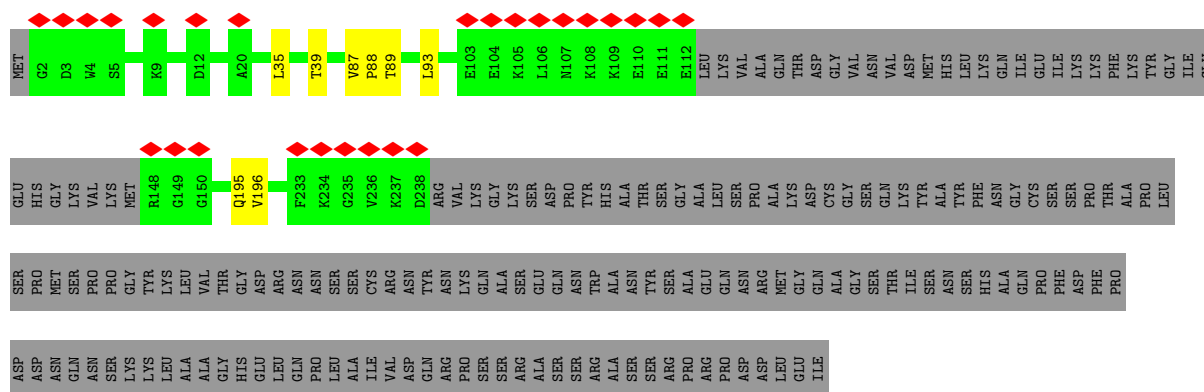


- Molecule 1: Gap junction alpha-1 protein

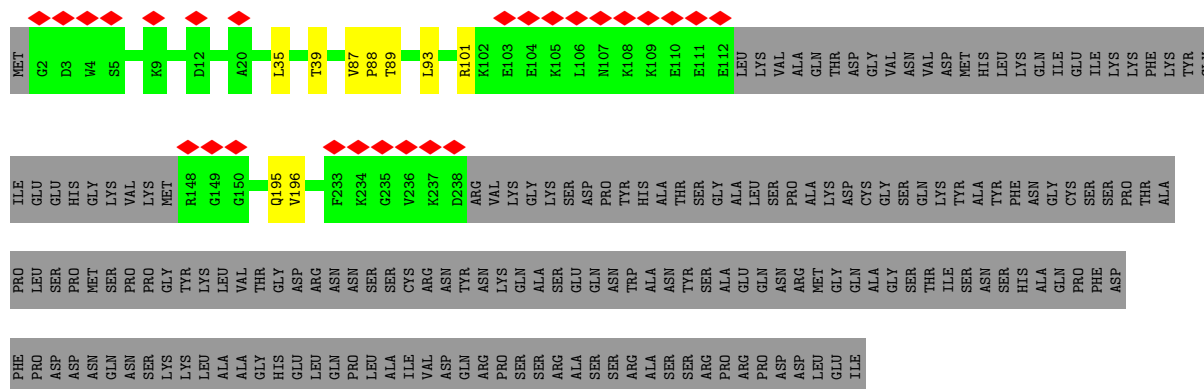


- Molecule 1: Gap junction alpha-1 protein

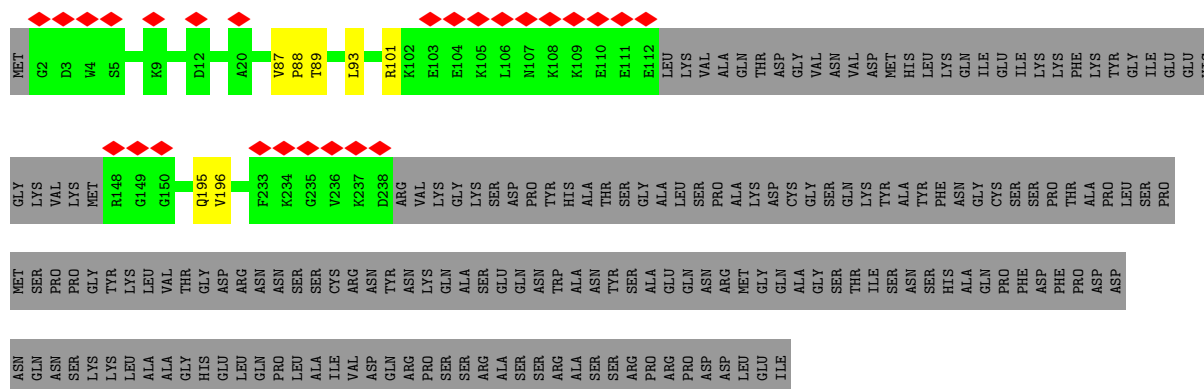




• Molecule 1: Gap junction alpha-1 protein

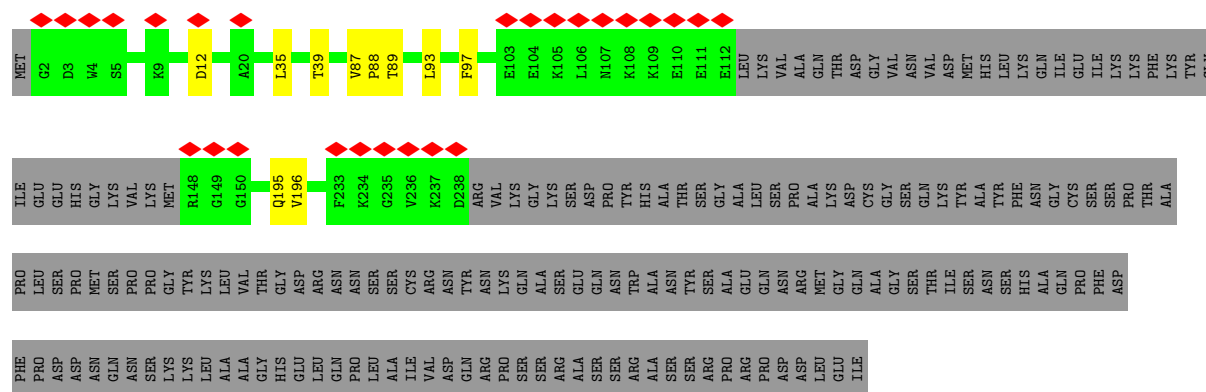


• Molecule 1: Gap junction alpha-1 protein

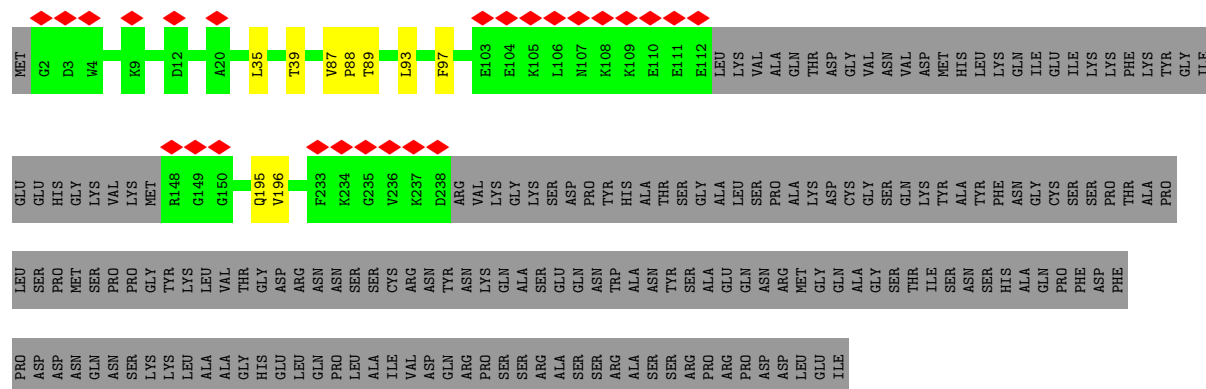


• Molecule 1: Gap junction alpha-1 protein

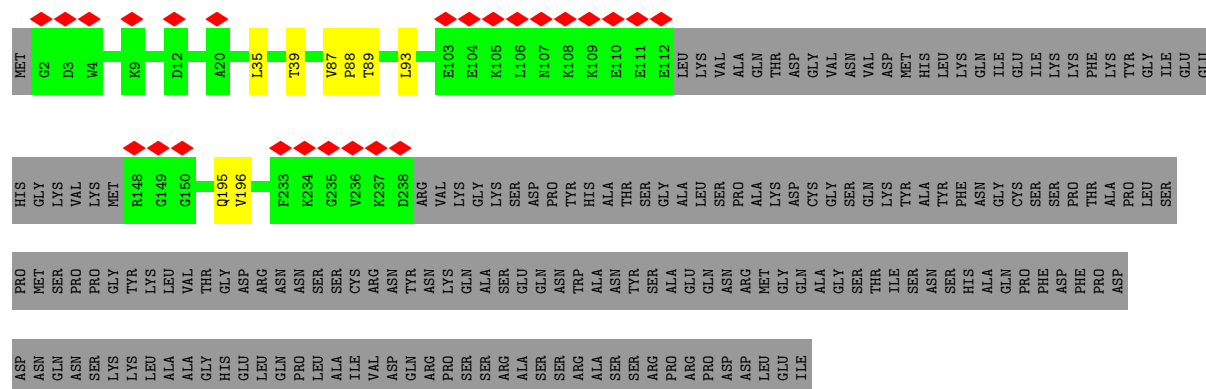




• Molecule 1: Gap junction alpha-1 protein

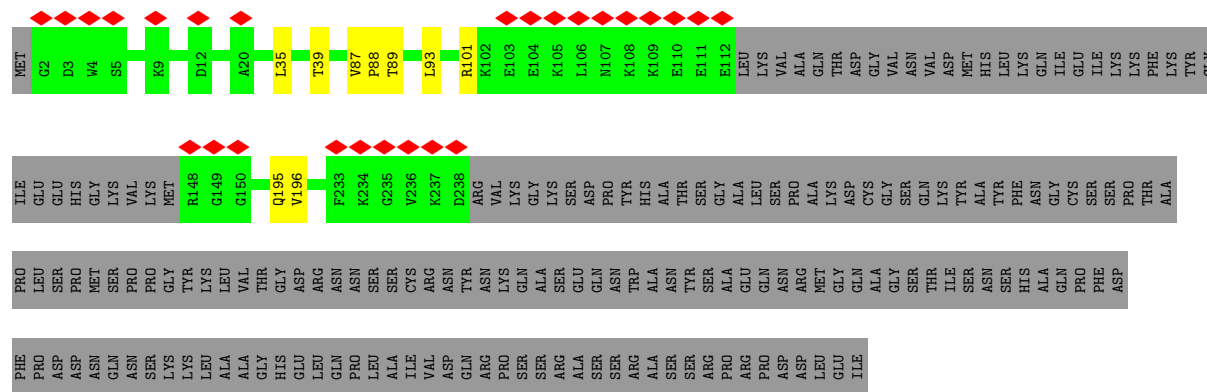


• Molecule 1: Gap junction alpha-1 protein



• Molecule 1: Gap junction alpha-1 protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21621	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	283.5, 283.5, 283.5	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.675, 0.675, 0.675	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: Y01, PTY, C14

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	0.15	0/1688	0.27	0/2286
1	B	0.15	0/1688	0.27	0/2286
1	C	0.15	0/1688	0.27	0/2286
1	D	0.15	0/1688	0.27	0/2286
1	E	0.15	0/1688	0.27	0/2286
1	F	0.15	0/1688	0.27	0/2286
1	G	0.15	0/1688	0.27	0/2286
1	H	0.15	0/1688	0.27	0/2286
1	I	0.15	0/1688	0.27	0/2286
1	J	0.15	0/1688	0.27	0/2286
1	K	0.15	0/1688	0.27	0/2286
1	L	0.15	0/1688	0.27	0/2286
All	All	0.15	0/20256	0.27	0/27432

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1645	1670	1670	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1645	1670	1670	7	0
1	C	1645	1670	1670	6	0
1	D	1645	1670	1670	7	0
1	E	1645	1670	1670	6	0
1	F	1645	1670	1670	8	0
1	G	1645	1670	1670	9	0
1	H	1645	1670	1670	8	0
1	I	1645	1670	1670	9	0
1	J	1645	1670	1670	8	0
1	K	1645	1670	1670	6	0
1	L	1645	1670	1670	8	0
2	A	153	297	325	0	0
2	B	153	297	325	0	0
2	C	139	270	295	0	0
2	D	167	324	355	0	0
2	E	153	297	325	0	0
2	F	153	297	325	0	0
2	G	153	297	325	0	0
2	H	153	297	325	0	0
2	I	153	297	325	0	0
2	J	153	297	325	0	0
2	K	153	297	325	0	0
2	L	153	297	325	0	0
3	A	70	98	98	7	0
3	B	70	98	98	8	0
3	C	70	98	98	7	0
3	D	70	98	98	8	0
3	E	70	98	98	7	0
3	F	70	98	98	7	0
3	G	70	98	98	8	0
3	H	70	98	98	8	0
3	I	70	98	98	8	0
3	J	70	98	98	8	0
3	K	70	98	98	8	0
3	L	70	98	98	6	0
4	A	33	42	39	1	0
4	B	33	42	39	1	0
4	C	33	42	39	1	0
4	D	33	42	39	1	0
4	E	33	42	39	1	0
4	F	33	42	39	1	0
4	G	33	42	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	33	42	39	1	0
4	I	33	42	39	2	0
4	J	33	42	39	2	0
4	K	33	42	39	1	0
4	L	33	42	39	1	0
All	All	22812	25284	25584	133	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 (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:THR:HG21	3:D:413:Y01:CAD	2.20	0.72
1:K:89:THR:HG21	3:K:412:Y01:CAD	2.20	0.72
1:I:89:THR:HG21	3:I:412:Y01:CAD	2.20	0.72
1:A:89:THR:HG21	3:A:406:Y01:CAD	2.20	0.72
1:B:89:THR:HG21	3:B:412:Y01:CAD	2.20	0.72
1:E:89:THR:HG21	3:E:412:Y01:CAD	2.20	0.72
1:H:89:THR:HG21	3:H:412:Y01:CAD	2.20	0.72
1:L:89:THR:HG21	3:L:413:Y01:CAD	2.20	0.72
1:C:89:THR:HG21	3:C:411:Y01:CAD	2.20	0.72
1:G:89:THR:HG21	3:G:406:Y01:CAD	2.20	0.71
1:F:89:THR:HG21	3:F:413:Y01:CAD	2.20	0.71
1:J:89:THR:HG21	3:J:412:Y01:CAD	2.20	0.71
1:A:93:LEU:HD22	3:B:413:Y01:HAP2	1.74	0.69
1:C:93:LEU:HD22	3:D:414:Y01:HAP2	1.75	0.67
1:I:93:LEU:HD22	3:J:413:Y01:HAP2	1.78	0.64
1:J:93:LEU:HD22	3:K:413:Y01:HAP2	1.83	0.59
1:H:93:LEU:HD22	3:I:413:Y01:HAP2	1.83	0.58
1:D:93:LEU:HD22	3:E:413:Y01:HAP2	1.85	0.58
3:G:407:Y01:HAP2	1:L:93:LEU:HD22	1.86	0.58
1:B:89:THR:HG21	3:B:412:Y01:HAD3	1.87	0.57
1:I:89:THR:HG21	3:I:412:Y01:HAD3	1.87	0.57
1:J:89:THR:HG21	3:J:412:Y01:HAD3	1.87	0.57
1:C:89:THR:HG21	3:C:411:Y01:HAD3	1.87	0.56
1:G:93:LEU:HD22	3:H:413:Y01:HAP2	1.85	0.56
1:G:89:THR:HG21	3:G:406:Y01:HAD3	1.87	0.56
1:E:89:THR:HG21	3:E:412:Y01:HAD3	1.87	0.56
1:F:89:THR:HG21	3:F:413:Y01:HAD3	1.87	0.56
1:L:89:THR:HG21	3:L:413:Y01:HAD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:THR:HG21	3:D:413:Y01:HAD3	1.87	0.55
1:H:89:THR:HG21	3:H:412:Y01:HAD3	1.87	0.55
1:K:89:THR:HG21	3:K:412:Y01:HAD3	1.87	0.55
1:A:89:THR:HG21	3:A:406:Y01:HAD3	1.87	0.55
3:D:413:Y01:HAE2	3:D:413:Y01:HAC1	1.89	0.55
3:K:412:Y01:HAE2	3:K:412:Y01:HAC1	1.89	0.55
3:E:412:Y01:HAC1	3:E:412:Y01:HAE2	1.89	0.55
3:I:412:Y01:HAC1	3:I:412:Y01:HAE2	1.89	0.55
3:L:413:Y01:HAC1	3:L:413:Y01:HAE2	1.89	0.55
3:B:412:Y01:HAE2	3:B:412:Y01:HAC1	1.89	0.54
3:C:411:Y01:HAE2	3:C:411:Y01:HAC1	1.89	0.54
3:J:412:Y01:HAE2	3:J:412:Y01:HAC1	1.89	0.54
3:F:413:Y01:HAE2	3:F:413:Y01:HAC1	1.89	0.54
1:A:93:LEU:HD22	3:B:413:Y01:CAP	2.36	0.54
3:G:406:Y01:HAE2	3:G:406:Y01:HAC1	1.89	0.54
1:C:93:LEU:HD22	3:D:414:Y01:CAP	2.37	0.54
3:H:412:Y01:HAE2	3:H:412:Y01:HAC1	1.89	0.54
3:A:406:Y01:HAE2	3:A:406:Y01:HAC1	1.89	0.53
1:K:93:LEU:HD22	3:L:414:Y01:HAP2	1.90	0.53
1:K:195:GLN:O	1:K:196:VAL:HG23	2.09	0.53
1:C:195:GLN:O	1:C:196:VAL:HG23	2.09	0.52
1:D:195:GLN:O	1:D:196:VAL:HG23	2.09	0.52
1:F:195:GLN:O	1:F:196:VAL:HG23	2.09	0.52
1:A:195:GLN:O	1:A:196:VAL:HG23	2.09	0.52
1:G:195:GLN:O	1:G:196:VAL:HG23	2.09	0.52
1:H:195:GLN:O	1:H:196:VAL:HG23	2.09	0.52
1:E:195:GLN:O	1:E:196:VAL:HG23	2.09	0.52
1:J:195:GLN:O	1:J:196:VAL:HG23	2.09	0.52
1:L:195:GLN:O	1:L:196:VAL:HG23	2.09	0.52
1:B:195:GLN:O	1:B:196:VAL:HG23	2.09	0.52
1:I:195:GLN:O	1:I:196:VAL:HG23	2.09	0.52
1:E:93:LEU:HD22	3:F:414:Y01:HAP2	1.93	0.51
1:I:93:LEU:HD22	3:J:413:Y01:CAP	2.40	0.50
1:B:93:LEU:HD22	3:C:412:Y01:HAP2	1.95	0.48
1:D:87:VAL:N	1:D:88:PRO:CD	2.77	0.48
1:K:87:VAL:N	1:K:88:PRO:CD	2.77	0.48
1:C:87:VAL:N	1:C:88:PRO:CD	2.77	0.47
1:E:87:VAL:N	1:E:88:PRO:CD	2.77	0.47
1:B:87:VAL:N	1:B:88:PRO:CD	2.77	0.47
1:I:87:VAL:N	1:I:88:PRO:CD	2.77	0.47
1:L:87:VAL:N	1:L:88:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:N	1:A:88:PRO:CD	2.77	0.47
1:J:87:VAL:N	1:J:88:PRO:CD	2.77	0.47
1:H:87:VAL:N	1:H:88:PRO:CD	2.77	0.47
1:F:87:VAL:N	1:F:88:PRO:CD	2.77	0.47
1:G:87:VAL:N	1:G:88:PRO:CD	2.77	0.47
1:J:35:LEU:O	1:J:39:THR:OG1	2.28	0.46
3:L:413:Y01:HAD1	3:L:413:Y01:OAW	2.16	0.46
3:E:412:Y01:HAD1	3:E:412:Y01:OAW	2.16	0.46
3:J:412:Y01:HAD1	3:J:412:Y01:OAW	2.16	0.46
3:I:412:Y01:HAD1	3:I:412:Y01:OAW	2.16	0.46
3:B:412:Y01:HAD1	3:B:412:Y01:OAW	2.16	0.46
3:D:413:Y01:HAD1	3:D:413:Y01:OAW	2.16	0.46
3:G:406:Y01:HAD1	3:G:406:Y01:OAW	2.16	0.46
3:C:411:Y01:OAW	3:C:411:Y01:HAD1	2.16	0.46
3:F:413:Y01:OAW	3:F:413:Y01:HAD1	2.16	0.46
3:K:412:Y01:HAD1	3:K:412:Y01:OAW	2.16	0.45
3:A:406:Y01:HAD1	3:A:406:Y01:OAW	2.16	0.45
3:H:412:Y01:HAD1	3:H:412:Y01:OAW	2.16	0.45
1:J:93:LEU:HD22	3:K:413:Y01:CAP	2.45	0.45
1:G:12:ASP:OD2	1:L:101:ARG:NH2	2.49	0.45
3:A:407:Y01:HAP2	1:F:93:LEU:HD22	1.98	0.45
1:A:12:ASP:OD2	1:F:101:ARG:NH2	2.51	0.44
1:H:93:LEU:HD22	3:I:413:Y01:CAP	2.46	0.44
1:H:101:ARG:NH2	1:I:12:ASP:OD2	2.51	0.43
1:J:97:PHE:HE1	4:J:414:PTY:H111	1.84	0.43
1:A:101:ARG:NH2	1:B:12:ASP:OD2	2.52	0.42
1:G:93:LEU:HD22	3:H:413:Y01:CAP	2.48	0.42
3:G:407:Y01:CAP	1:L:93:LEU:HD22	2.48	0.42
1:L:35:LEU:O	1:L:39:THR:OG1	2.28	0.42
1:D:93:LEU:HD22	3:E:413:Y01:CAP	2.49	0.42
1:E:35:LEU:O	1:E:39:THR:OG1	2.28	0.42
4:C:413:PTY:C14	3:D:414:Y01:HAE2	2.50	0.42
4:H:414:PTY:C14	3:I:413:Y01:HAE2	2.50	0.42
4:I:414:PTY:C14	3:J:413:Y01:HAE2	2.50	0.42
4:J:414:PTY:C14	3:K:413:Y01:HAE2	2.50	0.42
4:A:408:PTY:C14	3:B:413:Y01:HAE2	2.50	0.41
1:D:35:LEU:O	1:D:39:THR:OG1	2.28	0.41
4:B:414:PTY:C14	3:C:412:Y01:HAE2	2.50	0.41
1:K:35:LEU:O	1:K:39:THR:OG1	2.28	0.41
3:G:407:Y01:HAE2	4:L:401:PTY:C14	2.50	0.41
1:I:97:PHE:HE1	4:I:414:PTY:H111	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:413:Y01:HAE2	3:J:413:Y01:HAC1	2.02	0.41
4:K:414:PTY:C14	3:L:414:Y01:HAE2	2.50	0.41
4:D:415:PTY:C14	3:E:413:Y01:HAE2	2.50	0.41
4:E:414:PTY:C14	3:F:414:Y01:HAE2	2.50	0.41
3:A:407:Y01:HAE2	4:F:401:PTY:C14	2.50	0.41
4:G:408:PTY:C14	3:H:413:Y01:HAE2	2.50	0.41
3:C:412:Y01:HAE2	3:C:412:Y01:HAC1	2.02	0.41
1:I:35:LEU:O	1:I:39:THR:OG1	2.28	0.41
3:K:413:Y01:HAE2	3:K:413:Y01:HAC1	2.02	0.41
1:G:35:LEU:O	1:G:39:THR:OG1	2.28	0.41
3:G:407:Y01:HAE2	3:G:407:Y01:HAC1	2.03	0.41
3:D:414:Y01:HAE2	3:D:414:Y01:HAC1	2.03	0.41
3:F:414:Y01:HAE2	3:F:414:Y01:HAC1	2.02	0.41
3:B:413:Y01:HAE2	3:B:413:Y01:HAC1	2.02	0.41
1:H:87:VAL:HG12	1:H:88:PRO:HD3	2.03	0.40
1:A:87:VAL:HG12	1:A:88:PRO:HD3	2.03	0.40
1:F:87:VAL:HG12	1:F:88:PRO:HD3	2.03	0.40
3:I:413:Y01:HAE2	3:I:413:Y01:HAC1	2.03	0.40
3:A:407:Y01:HAE2	3:A:407:Y01:HAC1	2.02	0.40
1:B:35:LEU:O	1:B:39:THR:OG1	2.28	0.40
1:G:87:VAL:HG12	1:G:88:PRO:HD3	2.04	0.40
1:F:35:LEU:O	1:F:39:THR:OG1	2.28	0.40
3:H:413:Y01:HAE2	3:H:413:Y01:HAC1	2.02	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	E	93/382 (24%)	90 (97%)	3 (3%)	0	100	100
1	F	106/382 (28%)	105 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	138/382 (36%)	137 (99%)	1 (1%)	0	100	100
All	All	337/1146 (29%)	332 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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](#)

168 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	C14	J	402	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	K	401	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	H	402	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	I	407	-	13,13,13	0.28	0	12,12,12	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	Y01	K	412	-	38,38,38	0.72	0	57,57,57	1.00	3 (5%)
2	C14	C	403	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	E	411	-	13,13,13	0.30	0	12,12,12	0.74	0
2	C14	B	403	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	K	406	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	H	408	-	13,13,13	0.30	0	12,12,12	0.79	0
3	Y01	I	413	-	38,38,38	0.72	0	57,57,57	0.85	1 (1%)
2	C14	C	401	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	C	404	-	12,12,13	0.30	0	11,11,12	0.73	0
2	C14	J	407	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	I	405	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	D	412	-	13,13,13	0.30	0	12,12,12	0.74	0
3	Y01	E	412	-	38,38,38	0.72	0	57,57,57	1.00	4 (7%)
2	C14	K	403	-	13,13,13	0.30	0	12,12,12	0.82	0
2	C14	F	409	-	13,13,13	0.31	0	12,12,12	0.79	0
2	C14	C	406	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	J	405	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	J	404	-	12,12,13	0.31	0	11,11,12	0.73	0
2	C14	G	403	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	E	409	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	F	402	-	13,13,13	0.28	0	12,12,12	0.84	0
4	PTY	H	414	-	32,32,49	1.08	4 (12%)	35,37,54	0.99	2 (5%)
2	C14	D	407	-	13,13,13	0.30	0	12,12,12	0.74	0
2	C14	D	401	-	13,13,13	0.28	0	12,12,12	0.84	0
4	PTY	B	414	-	32,32,49	1.07	4 (12%)	35,37,54	0.98	2 (5%)
2	C14	I	404	-	12,12,13	0.30	0	11,11,12	0.73	0
2	C14	G	402	-	13,13,13	0.30	0	12,12,12	0.79	0
2	C14	C	402	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	B	408	-	13,13,13	0.30	0	12,12,12	0.79	0
2	C14	I	403	-	13,13,13	0.30	0	12,12,12	0.82	0
2	C14	G	404	-	13,13,13	0.30	0	12,12,12	0.83	0
3	Y01	H	412	-	38,38,38	0.71	0	57,57,57	1.01	3 (5%)
3	Y01	L	413	-	38,38,38	0.71	0	57,57,57	1.01	4 (7%)
2	C14	D	406	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	K	405	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	H	407	-	13,13,13	0.27	0	12,12,12	0.81	0
2	C14	J	403	-	13,13,13	0.30	0	12,12,12	0.81	0
3	Y01	E	413	-	38,38,38	0.72	0	57,57,57	0.85	1 (1%)
3	Y01	K	413	-	38,38,38	0.71	0	57,57,57	0.85	1 (1%)
2	C14	B	411	-	13,13,13	0.30	0	12,12,12	0.74	0
2	C14	H	405	-	13,13,13	0.30	0	12,12,12	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C14	B	407	-	13,13,13	0.27	0	12,12,12	0.81	0
2	C14	H	406	-	13,13,13	0.30	0	12,12,12	0.83	0
3	Y01	H	413	-	38,38,38	0.72	0	57,57,57	0.85	1 (1%)
2	C14	L	403	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	L	409	-	13,13,13	0.30	0	12,12,12	0.79	0
2	C14	D	408	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	D	402	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	D	404	-	12,12,13	0.31	0	11,11,12	0.73	0
2	C14	G	405	-	13,13,13	0.30	0	12,12,12	0.74	0
3	Y01	B	412	-	38,38,38	0.72	0	57,57,57	1.01	4 (7%)
3	Y01	C	412	-	38,38,38	0.72	0	57,57,57	0.85	1 (1%)
4	PTY	F	401	-	32,32,49	1.08	4 (12%)	35,37,54	0.99	2 (5%)
4	PTY	E	414	-	32,32,49	1.07	4 (12%)	35,37,54	0.99	2 (5%)
2	C14	F	412	-	13,13,13	0.30	0	12,12,12	0.74	0
3	Y01	L	414	-	38,38,38	0.72	0	57,57,57	0.85	1 (1%)
2	C14	G	411	-	13,13,13	0.30	0	12,12,12	0.82	0
2	C14	I	410	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	H	404	-	12,12,13	0.30	0	11,11,12	0.73	0
2	C14	G	414	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	E	406	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	L	410	-	13,13,13	0.28	0	12,12,12	0.82	0
2	C14	F	405	-	12,12,13	0.30	0	11,11,12	0.73	0
2	C14	A	410	-	13,13,13	0.30	0	12,12,12	0.80	0
3	Y01	F	413	-	38,38,38	0.72	0	57,57,57	1.01	4 (7%)
2	C14	I	411	-	13,13,13	0.30	0	12,12,12	0.73	0
2	C14	B	401	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	E	405	-	13,13,13	0.31	0	12,12,12	0.81	0
2	C14	C	408	-	13,13,13	0.31	0	12,12,12	0.79	0
2	C14	J	410	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	K	408	-	13,13,13	0.30	0	12,12,12	0.79	0
2	C14	A	402	-	13,13,13	0.30	0	12,12,12	0.79	0
2	C14	L	402	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	A	413	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	H	409	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	A	404	-	13,13,13	0.30	0	12,12,12	0.83	0
3	Y01	I	412	-	38,38,38	0.71	0	57,57,57	1.01	3 (5%)
2	C14	K	404	-	12,12,13	0.31	0	11,11,12	0.73	0
2	C14	D	410	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	C	407	-	13,13,13	0.27	0	12,12,12	0.81	0
2	C14	F	410	-	13,13,13	0.29	0	12,12,12	0.82	0
2	C14	L	411	-	13,13,13	0.30	0	12,12,12	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PTY	C	413	-	32,32,49	1.08	4 (12%)	35,37,54	0.98	2 (5%)
2	C14	I	409	-	13,13,13	0.28	0	12,12,12	0.82	0
3	Y01	J	412	-	38,38,38	0.72	0	57,57,57	1.01	3 (5%)
2	C14	A	403	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	J	411	-	13,13,13	0.30	0	12,12,12	0.73	0
2	C14	I	401	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	E	410	-	13,13,13	0.29	0	12,12,12	0.82	0
2	C14	J	409	-	13,13,13	0.28	0	12,12,12	0.81	0
3	Y01	B	413	-	38,38,38	0.72	0	57,57,57	0.85	1 (1%)
4	PTY	D	415	-	32,32,49	1.08	4 (12%)	35,37,54	0.98	2 (5%)
2	C14	J	401	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	K	410	-	13,13,13	0.30	0	12,12,12	0.82	0
2	C14	F	406	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	I	406	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	C	405	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	D	403	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	B	405	-	13,13,13	0.30	0	12,12,12	0.81	0
3	Y01	J	413	-	38,38,38	0.72	0	57,57,57	0.85	1 (1%)
2	C14	H	410	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	G	410	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	F	411	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	G	412	-	12,12,13	0.31	0	11,11,12	0.73	0
4	PTY	A	408	-	32,32,49	1.07	4 (12%)	35,37,54	0.99	2 (5%)
4	PTY	K	414	-	32,32,49	1.08	4 (12%)	35,37,54	0.99	2 (5%)
2	C14	J	406	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	L	408	-	13,13,13	0.27	0	12,12,12	0.81	0
2	C14	G	401	-	13,13,13	0.27	0	12,12,12	0.81	0
4	PTY	L	401	-	32,32,49	1.07	4 (12%)	35,37,54	0.99	2 (5%)
2	C14	A	409	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	A	411	-	13,13,13	0.30	0	12,12,12	0.82	0
2	C14	B	404	-	12,12,13	0.31	0	11,11,12	0.73	0
3	Y01	C	411	-	38,38,38	0.72	0	57,57,57	1.01	3 (5%)
2	C14	E	407	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	E	404	-	12,12,13	0.30	0	11,11,12	0.73	0
2	C14	E	401	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	G	413	-	13,13,13	0.30	0	12,12,12	0.81	0
3	Y01	G	406	-	38,38,38	0.72	0	57,57,57	1.01	3 (5%)
2	C14	K	409	-	13,13,13	0.28	0	12,12,12	0.81	0
4	PTY	I	414	-	32,32,49	1.08	4 (12%)	35,37,54	0.98	2 (5%)
2	C14	H	403	-	13,13,13	0.30	0	12,12,12	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	Y01	G	407	-	38,38,38	0.72	0	57,57,57	0.85	1 (1%)
2	C14	L	406	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	L	412	-	13,13,13	0.30	0	12,12,12	0.74	0
2	C14	G	409	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	F	403	-	13,13,13	0.30	0	12,12,12	0.80	0
4	PTY	J	414	-	32,32,49	1.07	4 (12%)	35,37,54	0.98	2 (5%)
2	C14	I	402	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	C	409	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	D	411	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	B	409	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	L	407	-	13,13,13	0.30	0	12,12,12	0.83	0
3	Y01	A	407	-	38,38,38	0.71	0	57,57,57	0.85	1 (1%)
2	C14	A	412	-	12,12,13	0.30	0	11,11,12	0.73	0
2	C14	B	410	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	B	402	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	E	403	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	F	408	-	13,13,13	0.28	0	12,12,12	0.81	0
2	C14	A	405	-	13,13,13	0.30	0	12,12,12	0.74	0
3	Y01	A	406	-	38,38,38	0.72	0	57,57,57	1.00	3 (5%)
2	C14	E	408	-	13,13,13	0.31	0	12,12,12	0.79	0
2	C14	D	405	-	13,13,13	0.31	0	12,12,12	0.81	0
3	Y01	D	414	-	38,38,38	0.71	0	57,57,57	0.85	1 (1%)
2	C14	H	411	-	13,13,13	0.30	0	12,12,12	0.74	0
3	Y01	F	414	-	38,38,38	0.71	0	57,57,57	0.85	1 (1%)
2	C14	B	406	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	L	405	-	12,12,13	0.31	0	11,11,12	0.73	0
2	C14	K	402	-	13,13,13	0.30	0	12,12,12	0.80	0
2	C14	F	407	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	D	409	-	13,13,13	0.30	0	12,12,12	0.79	0
2	C14	H	401	-	13,13,13	0.28	0	12,12,12	0.84	0
2	C14	C	410	-	13,13,13	0.30	0	12,12,12	0.83	0
2	C14	A	414	-	13,13,13	0.30	0	12,12,12	0.83	0
4	PTY	G	408	-	32,32,49	1.08	4 (12%)	35,37,54	0.98	2 (5%)
3	Y01	D	413	-	38,38,38	0.72	0	57,57,57	1.01	3 (5%)
2	C14	I	408	-	13,13,13	0.31	0	12,12,12	0.79	0
2	C14	L	404	-	13,13,13	0.30	0	12,12,12	0.81	0
2	C14	A	401	-	13,13,13	0.27	0	12,12,12	0.81	0
2	C14	F	404	-	13,13,13	0.30	0	12,12,12	0.82	0
2	C14	K	407	-	13,13,13	0.27	0	12,12,12	0.81	0
2	C14	K	411	-	13,13,13	0.30	0	12,12,12	0.74	0
2	C14	E	402	-	13,13,13	0.30	0	12,12,12	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C14	J	408	-	13,13,13	0.30	0	12,12,12	0.79	0

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	C14	J	402	-	-	5/11/11/11	-
2	C14	K	401	-	-	2/11/11/11	-
2	C14	H	402	-	-	5/11/11/11	-
2	C14	I	407	-	-	1/11/11/11	-
3	Y01	K	412	-	-	11/19/77/77	0/4/4/4
2	C14	C	403	-	-	5/11/11/11	-
2	C14	E	411	-	-	4/11/11/11	-
2	C14	B	403	-	-	5/11/11/11	-
2	C14	K	406	-	-	3/11/11/11	-
2	C14	H	408	-	-	4/11/11/11	-
3	Y01	I	413	-	-	9/19/77/77	0/4/4/4
2	C14	C	401	-	-	2/11/11/11	-
2	C14	C	404	-	-	4/10/10/11	-
2	C14	J	407	-	-	1/11/11/11	-
2	C14	I	405	-	-	4/11/11/11	-
2	C14	D	412	-	-	4/11/11/11	-
3	Y01	E	412	-	-	11/19/77/77	0/4/4/4
2	C14	K	403	-	-	5/11/11/11	-
2	C14	F	409	-	-	4/11/11/11	-
2	C14	C	406	-	-	3/11/11/11	-
2	C14	J	405	-	-	4/11/11/11	-
2	C14	J	404	-	-	4/10/10/11	-
2	C14	G	403	-	-	3/11/11/11	-
2	C14	E	409	-	-	3/11/11/11	-
2	C14	F	402	-	-	2/11/11/11	-
4	PTY	H	414	-	-	18/36/36/53	-
2	C14	D	407	-	-	4/11/11/11	-
2	C14	D	401	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PTY	B	414	-	-	18/36/36/53	-
2	C14	I	404	-	-	4/10/10/11	-
2	C14	G	402	-	-	4/11/11/11	-
2	C14	C	402	-	-	5/11/11/11	-
2	C14	B	408	-	-	4/11/11/11	-
2	C14	I	403	-	-	5/11/11/11	-
2	C14	G	404	-	-	3/11/11/11	-
3	Y01	H	412	-	-	11/19/77/77	0/4/4/4
3	Y01	L	413	-	-	11/19/77/77	0/4/4/4
2	C14	D	406	-	-	3/11/11/11	-
2	C14	K	405	-	-	4/11/11/11	-
2	C14	H	407	-	-	1/11/11/11	-
2	C14	J	403	-	-	5/11/11/11	-
3	Y01	E	413	-	-	9/19/77/77	0/4/4/4
3	Y01	K	413	-	-	9/19/77/77	0/4/4/4
2	C14	B	411	-	-	4/11/11/11	-
2	C14	H	405	-	-	4/11/11/11	-
2	C14	B	407	-	-	1/11/11/11	-
2	C14	H	406	-	-	3/11/11/11	-
3	Y01	H	413	-	-	9/19/77/77	0/4/4/4
2	C14	L	403	-	-	5/11/11/11	-
2	C14	L	409	-	-	4/11/11/11	-
2	C14	D	408	-	-	1/11/11/11	-
2	C14	D	402	-	-	5/11/11/11	-
2	C14	D	404	-	-	4/10/10/11	-
2	C14	G	405	-	-	4/11/11/11	-
3	Y01	B	412	-	-	11/19/77/77	0/4/4/4
3	Y01	C	412	-	-	9/19/77/77	0/4/4/4
4	PTY	F	401	-	-	18/36/36/53	-
4	PTY	E	414	-	-	18/36/36/53	-
2	C14	F	412	-	-	4/11/11/11	-
3	Y01	L	414	-	-	9/19/77/77	0/4/4/4
2	C14	G	411	-	-	5/11/11/11	-
2	C14	I	410	-	-	3/11/11/11	-
2	C14	H	404	-	-	4/10/10/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C14	G	414	-	-	3/11/11/11	-
2	C14	E	406	-	-	3/11/11/11	-
2	C14	L	410	-	-	3/11/11/11	-
2	C14	F	405	-	-	4/10/10/11	-
2	C14	A	410	-	-	5/11/11/11	-
3	Y01	F	413	-	-	11/19/77/77	0/4/4/4
2	C14	I	411	-	-	4/11/11/11	-
2	C14	B	401	-	-	2/11/11/11	-
2	C14	E	405	-	-	4/11/11/11	-
2	C14	C	408	-	-	4/11/11/11	-
2	C14	J	410	-	-	3/11/11/11	-
2	C14	K	408	-	-	4/11/11/11	-
2	C14	A	402	-	-	4/11/11/11	-
2	C14	L	402	-	-	2/11/11/11	-
2	C14	A	413	-	-	4/11/11/11	-
2	C14	H	409	-	-	3/11/11/11	-
2	C14	A	404	-	-	3/11/11/11	-
3	Y01	I	412	-	-	11/19/77/77	0/4/4/4
2	C14	K	404	-	-	4/10/10/11	-
2	C14	D	410	-	-	3/11/11/11	-
2	C14	C	407	-	-	1/11/11/11	-
2	C14	F	410	-	-	3/11/11/11	-
2	C14	L	411	-	-	3/11/11/11	-
4	PTY	C	413	-	-	18/36/36/53	-
2	C14	I	409	-	-	3/11/11/11	-
3	Y01	J	412	-	-	11/19/77/77	0/4/4/4
2	C14	A	403	-	-	3/11/11/11	-
2	C14	J	411	-	-	4/11/11/11	-
2	C14	I	401	-	-	2/11/11/11	-
2	C14	E	410	-	-	3/11/11/11	-
2	C14	J	409	-	-	3/11/11/11	-
3	Y01	B	413	-	-	9/19/77/77	0/4/4/4
4	PTY	D	415	-	-	18/36/36/53	-
2	C14	J	401	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C14	K	410	-	-	3/11/11/11	-
2	C14	F	406	-	-	4/11/11/11	-
2	C14	I	406	-	-	3/11/11/11	-
2	C14	C	405	-	-	4/11/11/11	-
2	C14	D	403	-	-	5/11/11/11	-
2	C14	B	405	-	-	4/11/11/11	-
3	Y01	J	413	-	-	9/19/77/77	0/4/4/4
2	C14	H	410	-	-	3/11/11/11	-
2	C14	G	410	-	-	5/11/11/11	-
2	C14	F	411	-	-	3/11/11/11	-
2	C14	G	412	-	-	4/10/10/11	-
4	PTY	A	408	-	-	17/36/36/53	-
4	PTY	K	414	-	-	18/36/36/53	-
2	C14	J	406	-	-	3/11/11/11	-
2	C14	L	408	-	-	1/11/11/11	-
2	C14	G	401	-	-	1/11/11/11	-
4	PTY	L	401	-	-	18/36/36/53	-
2	C14	A	409	-	-	2/11/11/11	-
2	C14	A	411	-	-	5/11/11/11	-
2	C14	B	404	-	-	4/10/10/11	-
3	Y01	C	411	-	-	11/19/77/77	0/4/4/4
2	C14	E	407	-	-	1/11/11/11	-
2	C14	E	404	-	-	4/10/10/11	-
2	C14	E	401	-	-	2/11/11/11	-
2	C14	G	413	-	-	4/11/11/11	-
3	Y01	G	406	-	-	11/19/77/77	0/4/4/4
2	C14	K	409	-	-	3/11/11/11	-
4	PTY	I	414	-	-	18/36/36/53	-
2	C14	H	403	-	-	5/11/11/11	-
3	Y01	G	407	-	-	9/19/77/77	0/4/4/4
2	C14	L	406	-	-	4/11/11/11	-
2	C14	L	412	-	-	4/11/11/11	-
2	C14	G	409	-	-	2/11/11/11	-
2	C14	F	403	-	-	5/11/11/11	-
4	PTY	J	414	-	-	18/36/36/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C14	I	402	-	-	5/11/11/11	-
2	C14	C	409	-	-	3/11/11/11	-
2	C14	D	411	-	-	3/11/11/11	-
2	C14	B	409	-	-	3/11/11/11	-
2	C14	L	407	-	-	3/11/11/11	-
3	Y01	A	407	-	-	9/19/77/77	0/4/4/4
2	C14	A	412	-	-	4/10/10/11	-
2	C14	B	410	-	-	3/11/11/11	-
2	C14	B	402	-	-	5/11/11/11	-
2	C14	E	403	-	-	5/11/11/11	-
2	C14	F	408	-	-	1/11/11/11	-
2	C14	A	405	-	-	4/11/11/11	-
3	Y01	A	406	-	-	11/19/77/77	0/4/4/4
2	C14	E	408	-	-	4/11/11/11	-
2	C14	D	405	-	-	4/11/11/11	-
3	Y01	D	414	-	-	9/19/77/77	0/4/4/4
2	C14	H	411	-	-	4/11/11/11	-
3	Y01	F	414	-	-	9/19/77/77	0/4/4/4
2	C14	B	406	-	-	3/11/11/11	-
2	C14	L	405	-	-	4/10/10/11	-
2	C14	K	402	-	-	5/11/11/11	-
2	C14	F	407	-	-	3/11/11/11	-
2	C14	D	409	-	-	4/11/11/11	-
2	C14	H	401	-	-	2/11/11/11	-
2	C14	C	410	-	-	3/11/11/11	-
2	C14	A	414	-	-	3/11/11/11	-
4	PTY	G	408	-	-	18/36/36/53	-
3	Y01	D	413	-	-	11/19/77/77	0/4/4/4
2	C14	I	408	-	-	4/11/11/11	-
2	C14	L	404	-	-	5/11/11/11	-
2	C14	A	401	-	-	1/11/11/11	-
2	C14	F	404	-	-	5/11/11/11	-
2	C14	K	407	-	-	1/11/11/11	-
2	C14	K	411	-	-	4/11/11/11	-
2	C14	E	402	-	-	5/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C14	J	408	-	-	4/11/11/11	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	414	PTY	O7-C6	-2.73	1.40	1.46
4	I	414	PTY	O7-C6	-2.72	1.40	1.46
4	H	414	PTY	O7-C6	-2.71	1.40	1.46
4	C	413	PTY	O7-C6	-2.71	1.40	1.46
4	G	408	PTY	O7-C6	-2.71	1.40	1.46
4	E	414	PTY	O7-C6	-2.70	1.40	1.46
4	J	414	PTY	O7-C6	-2.70	1.40	1.46
4	D	415	PTY	O7-C6	-2.70	1.40	1.46
4	F	401	PTY	O7-C6	-2.70	1.40	1.46
4	L	401	PTY	O7-C6	-2.69	1.40	1.46
4	A	408	PTY	O7-C6	-2.67	1.40	1.46
4	B	414	PTY	O7-C6	-2.67	1.40	1.46
4	F	401	PTY	O4-C30	2.35	1.40	1.33
4	G	408	PTY	O4-C30	2.35	1.40	1.33
4	J	414	PTY	O4-C30	2.35	1.40	1.33
4	L	401	PTY	O4-C30	2.34	1.40	1.33
4	D	415	PTY	O4-C30	2.34	1.40	1.33
4	E	414	PTY	O4-C30	2.32	1.40	1.33
4	H	414	PTY	O4-C30	2.32	1.40	1.33
4	I	414	PTY	O4-C30	2.32	1.40	1.33
4	A	408	PTY	O4-C30	2.32	1.40	1.33
4	C	413	PTY	O4-C30	2.32	1.40	1.33
4	K	414	PTY	O4-C30	2.32	1.40	1.33
4	B	414	PTY	O4-C30	2.31	1.40	1.33
4	D	415	PTY	O4-C1	-2.28	1.40	1.45
4	F	401	PTY	O4-C1	-2.27	1.40	1.45
4	G	408	PTY	O4-C1	-2.25	1.40	1.45
4	K	414	PTY	O4-C1	-2.24	1.40	1.45
4	H	414	PTY	O4-C1	-2.24	1.40	1.45
4	L	401	PTY	O4-C1	-2.24	1.40	1.45
4	I	414	PTY	O4-C1	-2.24	1.40	1.45
4	B	414	PTY	O4-C1	-2.23	1.40	1.45
4	A	408	PTY	O4-C1	-2.23	1.40	1.45
4	C	413	PTY	O4-C1	-2.22	1.40	1.45
4	J	414	PTY	O4-C1	-2.22	1.40	1.45
4	E	414	PTY	O4-C1	-2.22	1.40	1.45
4	G	408	PTY	O7-C8	2.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	414	PTY	O7-C8	2.14	1.40	1.34
4	C	413	PTY	O7-C8	2.14	1.40	1.34
4	D	415	PTY	O7-C8	2.13	1.40	1.34
4	J	414	PTY	O7-C8	2.13	1.40	1.34
4	I	414	PTY	O7-C8	2.13	1.40	1.34
4	F	401	PTY	O7-C8	2.13	1.40	1.34
4	B	414	PTY	O7-C8	2.12	1.40	1.34
4	E	414	PTY	O7-C8	2.10	1.40	1.34
4	A	408	PTY	O7-C8	2.10	1.40	1.34
4	L	401	PTY	O7-C8	2.10	1.40	1.34
4	H	414	PTY	O7-C8	2.10	1.40	1.34

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	414	PTY	O7-C8-C11	3.81	119.73	111.48
4	F	401	PTY	O7-C8-C11	3.81	119.72	111.48
4	A	408	PTY	O7-C8-C11	3.81	119.72	111.48
4	H	414	PTY	O7-C8-C11	3.81	119.71	111.48
4	E	414	PTY	O7-C8-C11	3.81	119.71	111.48
4	L	401	PTY	O7-C8-C11	3.80	119.71	111.48
4	I	414	PTY	O7-C8-C11	3.80	119.71	111.48
4	J	414	PTY	O7-C8-C11	3.80	119.70	111.48
4	G	408	PTY	O7-C8-C11	3.80	119.69	111.48
4	B	414	PTY	O7-C8-C11	3.80	119.69	111.48
4	C	413	PTY	O7-C8-C11	3.80	119.69	111.48
4	D	415	PTY	O7-C8-C11	3.77	119.64	111.48
4	D	415	PTY	O4-C30-C31	2.72	120.12	111.83
4	F	401	PTY	O4-C30-C31	2.71	120.10	111.83
4	H	414	PTY	O4-C30-C31	2.71	120.10	111.83
4	E	414	PTY	O4-C30-C31	2.71	120.09	111.83
4	B	414	PTY	O4-C30-C31	2.70	120.08	111.83
4	K	414	PTY	O4-C30-C31	2.70	120.08	111.83
4	L	401	PTY	O4-C30-C31	2.70	120.08	111.83
4	A	408	PTY	O4-C30-C31	2.70	120.07	111.83
4	I	414	PTY	O4-C30-C31	2.70	120.06	111.83
4	C	413	PTY	O4-C30-C31	2.69	120.05	111.83
4	G	408	PTY	O4-C30-C31	2.69	120.05	111.83
4	J	414	PTY	O4-C30-C31	2.69	120.05	111.83
3	A	406	Y01	CAD-CBH-CBF	-2.30	109.08	111.66
3	C	411	Y01	CAD-CBH-CBF	-2.29	109.08	111.66
3	C	411	Y01	CAV-CAZ-CAI	-2.29	117.46	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	412	Y01	CAV-CAZ-CAI	-2.29	117.46	120.57
3	D	413	Y01	CAD-CBH-CBF	-2.29	109.09	111.66
3	G	406	Y01	CAV-CAZ-CAI	-2.29	117.47	120.57
3	G	406	Y01	CAD-CBH-CBF	-2.28	109.10	111.66
3	H	412	Y01	CAD-CBH-CBF	-2.28	109.10	111.66
3	F	413	Y01	CAD-CBH-CBF	-2.28	109.10	111.66
3	I	412	Y01	CAV-CAZ-CAI	-2.27	117.49	120.57
3	K	412	Y01	CAV-CAZ-CAI	-2.27	117.49	120.57
3	E	412	Y01	CAV-CAZ-CAI	-2.27	117.49	120.57
3	J	412	Y01	CAV-CAZ-CAI	-2.27	117.49	120.57
3	D	413	Y01	CAV-CAZ-CAI	-2.27	117.50	120.57
3	B	412	Y01	CAD-CBH-CBF	-2.27	109.12	111.66
3	K	412	Y01	CAD-CBH-CBF	-2.27	109.12	111.66
3	A	406	Y01	CAV-CAZ-CAI	-2.26	117.50	120.57
3	F	413	Y01	CAV-CAZ-CAI	-2.26	117.50	120.57
3	H	412	Y01	CAV-CAZ-CAI	-2.25	117.51	120.57
3	J	412	Y01	CAD-CBH-CBF	-2.24	109.14	111.66
3	L	413	Y01	CAV-CAZ-CAI	-2.24	117.53	120.57
3	I	412	Y01	CAD-CBH-CBF	-2.23	109.16	111.66
3	L	413	Y01	CAD-CBH-CBF	-2.23	109.16	111.66
3	E	412	Y01	CAD-CBH-CBF	-2.22	109.16	111.66
3	H	412	Y01	CAT-CBH-CBF	2.22	111.67	108.74
3	L	413	Y01	CAT-CBH-CBF	2.21	111.66	108.74
3	J	412	Y01	CAT-CBH-CBF	2.20	111.64	108.74
3	F	413	Y01	CAT-CBH-CBF	2.19	111.64	108.74
3	K	412	Y01	CAT-CBH-CBF	2.19	111.64	108.74
3	G	406	Y01	CAT-CBH-CBF	2.19	111.64	108.74
3	C	411	Y01	CAT-CBH-CBF	2.19	111.63	108.74
3	D	413	Y01	CAT-CBH-CBF	2.19	111.63	108.74
3	I	412	Y01	CAT-CBH-CBF	2.19	111.63	108.74
3	B	412	Y01	CAT-CBH-CBF	2.18	111.63	108.74
3	A	406	Y01	CAT-CBH-CBF	2.18	111.62	108.74
3	E	412	Y01	CAT-CBH-CBF	2.17	111.61	108.74
3	J	413	Y01	CBH-CAZ-CAI	-2.05	119.93	122.93
3	F	414	Y01	CBH-CAZ-CAI	-2.05	119.93	122.93
3	L	414	Y01	CBH-CAZ-CAI	-2.05	119.94	122.93
3	C	412	Y01	CBH-CAZ-CAI	-2.05	119.94	122.93
3	I	413	Y01	CBH-CAZ-CAI	-2.05	119.94	122.93
3	D	414	Y01	CBH-CAZ-CAI	-2.05	119.94	122.93
3	A	407	Y01	CBH-CAZ-CAI	-2.04	119.94	122.93
3	G	407	Y01	CBH-CAZ-CAI	-2.04	119.95	122.93
3	H	413	Y01	CBH-CAZ-CAI	-2.04	119.95	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	413	Y01	CBH-CAZ-CAI	-2.04	119.95	122.93
3	L	413	Y01	CAD-CBH-CAZ	2.02	111.47	108.38
3	K	413	Y01	CBH-CAZ-CAI	-2.02	119.98	122.93
3	E	413	Y01	CBH-CAZ-CAI	-2.02	119.99	122.93
3	E	412	Y01	CAD-CBH-CAZ	2.01	111.45	108.38
3	B	412	Y01	CAD-CBH-CAZ	2.01	111.45	108.38
3	F	413	Y01	CAD-CBH-CAZ	2.01	111.45	108.38

There are no chirality outliers.

All (911) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	406	Y01	CAM-CAY-OAW-CBC
3	A	407	Y01	CAM-CAY-OAW-CBC
3	G	406	Y01	CAM-CAY-OAW-CBC
3	G	407	Y01	CAM-CAY-OAW-CBC
3	B	412	Y01	CAM-CAY-OAW-CBC
3	B	413	Y01	CAM-CAY-OAW-CBC
3	C	411	Y01	CAM-CAY-OAW-CBC
3	C	412	Y01	CAM-CAY-OAW-CBC
3	D	413	Y01	CAM-CAY-OAW-CBC
3	D	414	Y01	CAM-CAY-OAW-CBC
3	E	412	Y01	CAM-CAY-OAW-CBC
3	E	413	Y01	CAM-CAY-OAW-CBC
3	F	413	Y01	CAM-CAY-OAW-CBC
3	F	414	Y01	CAM-CAY-OAW-CBC
3	H	412	Y01	CAM-CAY-OAW-CBC
3	H	413	Y01	CAM-CAY-OAW-CBC
3	I	412	Y01	CAM-CAY-OAW-CBC
3	I	413	Y01	CAM-CAY-OAW-CBC
3	J	412	Y01	CAM-CAY-OAW-CBC
3	J	413	Y01	CAM-CAY-OAW-CBC
3	K	412	Y01	CAM-CAY-OAW-CBC
3	K	413	Y01	CAM-CAY-OAW-CBC
3	L	413	Y01	CAM-CAY-OAW-CBC
3	L	414	Y01	CAM-CAY-OAW-CBC
4	A	408	PTY	C5-O14-P1-O11
4	G	408	PTY	C5-O14-P1-O11
4	B	414	PTY	C5-O14-P1-O11
4	C	413	PTY	C5-O14-P1-O11
4	D	415	PTY	C5-O14-P1-O11
4	E	414	PTY	C5-O14-P1-O11

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Mol	Chain	Res	Type	Atoms
4	F	401	PTY	C5-O14-P1-O11
4	H	414	PTY	C5-O14-P1-O11
4	I	414	PTY	C5-O14-P1-O11
4	J	414	PTY	C5-O14-P1-O11
4	K	414	PTY	C5-O14-P1-O11
4	L	401	PTY	C5-O14-P1-O11
3	A	406	Y01	CAC-CBB-CBE-CBI
3	G	406	Y01	CAC-CBB-CBE-CBI
3	B	412	Y01	CAC-CBB-CBE-CBI
3	C	411	Y01	CAC-CBB-CBE-CBI
3	D	413	Y01	CAC-CBB-CBE-CBI
3	E	412	Y01	CAC-CBB-CBE-CBI
3	F	413	Y01	CAC-CBB-CBE-CBI
3	H	412	Y01	CAC-CBB-CBE-CBI
3	I	412	Y01	CAC-CBB-CBE-CBI
3	J	412	Y01	CAC-CBB-CBE-CBI
3	K	412	Y01	CAC-CBB-CBE-CBI
3	L	413	Y01	CAC-CBB-CBE-CBI
3	A	406	Y01	OAG-CAY-OAW-CBC
3	A	407	Y01	OAG-CAY-OAW-CBC
3	G	406	Y01	OAG-CAY-OAW-CBC
3	G	407	Y01	OAG-CAY-OAW-CBC
3	B	412	Y01	OAG-CAY-OAW-CBC
3	B	413	Y01	OAG-CAY-OAW-CBC
3	C	411	Y01	OAG-CAY-OAW-CBC
3	C	412	Y01	OAG-CAY-OAW-CBC
3	D	413	Y01	OAG-CAY-OAW-CBC
3	D	414	Y01	OAG-CAY-OAW-CBC
3	E	412	Y01	OAG-CAY-OAW-CBC
3	E	413	Y01	OAG-CAY-OAW-CBC
3	F	413	Y01	OAG-CAY-OAW-CBC
3	F	414	Y01	OAG-CAY-OAW-CBC
3	H	412	Y01	OAG-CAY-OAW-CBC
3	H	413	Y01	OAG-CAY-OAW-CBC
3	I	412	Y01	OAG-CAY-OAW-CBC
3	I	413	Y01	OAG-CAY-OAW-CBC
3	J	412	Y01	OAG-CAY-OAW-CBC
3	J	413	Y01	OAG-CAY-OAW-CBC
3	K	412	Y01	OAG-CAY-OAW-CBC
3	K	413	Y01	OAG-CAY-OAW-CBC
3	L	413	Y01	OAG-CAY-OAW-CBC
3	L	414	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	A	406	Y01	CAO-CBB-CBE-CAP
3	G	406	Y01	CAO-CBB-CBE-CAP
3	B	412	Y01	CAO-CBB-CBE-CAP
3	C	411	Y01	CAO-CBB-CBE-CAP
3	D	413	Y01	CAO-CBB-CBE-CAP
3	E	412	Y01	CAO-CBB-CBE-CAP
3	F	413	Y01	CAO-CBB-CBE-CAP
3	H	412	Y01	CAO-CBB-CBE-CAP
3	I	412	Y01	CAO-CBB-CBE-CAP
3	J	412	Y01	CAO-CBB-CBE-CAP
3	K	412	Y01	CAO-CBB-CBE-CAP
3	L	413	Y01	CAO-CBB-CBE-CAP
4	A	408	PTY	C31-C30-O4-C1
4	G	408	PTY	C31-C30-O4-C1
4	B	414	PTY	C31-C30-O4-C1
4	C	413	PTY	C31-C30-O4-C1
4	D	415	PTY	C31-C30-O4-C1
4	E	414	PTY	C31-C30-O4-C1
4	F	401	PTY	C31-C30-O4-C1
4	H	414	PTY	C31-C30-O4-C1
4	I	414	PTY	C31-C30-O4-C1
4	J	414	PTY	C31-C30-O4-C1
4	K	414	PTY	C31-C30-O4-C1
4	L	401	PTY	C31-C30-O4-C1
4	A	408	PTY	C36-C37-C38-C39
4	G	408	PTY	C36-C37-C38-C39
4	B	414	PTY	C36-C37-C38-C39
4	C	413	PTY	C36-C37-C38-C39
4	D	415	PTY	C36-C37-C38-C39
4	E	414	PTY	C36-C37-C38-C39
4	F	401	PTY	C36-C37-C38-C39
4	H	414	PTY	C36-C37-C38-C39
4	I	414	PTY	C36-C37-C38-C39
4	J	414	PTY	C36-C37-C38-C39
4	K	414	PTY	C36-C37-C38-C39
4	L	401	PTY	C36-C37-C38-C39
4	A	408	PTY	O30-C30-O4-C1
4	G	408	PTY	O30-C30-O4-C1
4	B	414	PTY	O30-C30-O4-C1
4	C	413	PTY	O30-C30-O4-C1
4	D	415	PTY	O30-C30-O4-C1
4	E	414	PTY	O30-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
4	F	401	PTY	O30-C30-O4-C1
4	H	414	PTY	O30-C30-O4-C1
4	I	414	PTY	O30-C30-O4-C1
4	J	414	PTY	O30-C30-O4-C1
4	K	414	PTY	O30-C30-O4-C1
4	L	401	PTY	O30-C30-O4-C1
3	A	407	Y01	CAX-CAL-CAM-CAY
3	G	407	Y01	CAX-CAL-CAM-CAY
3	B	413	Y01	CAX-CAL-CAM-CAY
3	C	412	Y01	CAX-CAL-CAM-CAY
3	D	414	Y01	CAX-CAL-CAM-CAY
3	E	413	Y01	CAX-CAL-CAM-CAY
3	F	414	Y01	CAX-CAL-CAM-CAY
3	H	413	Y01	CAX-CAL-CAM-CAY
3	I	413	Y01	CAX-CAL-CAM-CAY
3	J	413	Y01	CAX-CAL-CAM-CAY
3	K	413	Y01	CAX-CAL-CAM-CAY
3	L	414	Y01	CAX-CAL-CAM-CAY
3	A	406	Y01	CAO-CAJ-CAN-CBA
3	G	406	Y01	CAO-CAJ-CAN-CBA
3	B	412	Y01	CAO-CAJ-CAN-CBA
3	C	411	Y01	CAO-CAJ-CAN-CBA
3	D	413	Y01	CAO-CAJ-CAN-CBA
3	E	412	Y01	CAO-CAJ-CAN-CBA
3	F	413	Y01	CAO-CAJ-CAN-CBA
3	H	412	Y01	CAO-CAJ-CAN-CBA
3	I	412	Y01	CAO-CAJ-CAN-CBA
3	J	412	Y01	CAO-CAJ-CAN-CBA
3	K	412	Y01	CAO-CAJ-CAN-CBA
3	L	413	Y01	CAO-CAJ-CAN-CBA
2	A	401	C14	C02-C03-C04-C05
2	A	405	C14	C04-C05-C06-C07
2	G	401	C14	C02-C03-C04-C05
2	G	405	C14	C04-C05-C06-C07
2	B	407	C14	C02-C03-C04-C05
2	B	411	C14	C04-C05-C06-C07
2	C	407	C14	C02-C03-C04-C05
2	D	408	C14	C02-C03-C04-C05
2	D	412	C14	C04-C05-C06-C07
2	E	407	C14	C02-C03-C04-C05
2	E	411	C14	C04-C05-C06-C07
2	F	408	C14	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
2	F	412	C14	C04-C05-C06-C07
2	H	407	C14	C02-C03-C04-C05
2	H	411	C14	C04-C05-C06-C07
2	I	407	C14	C02-C03-C04-C05
2	I	411	C14	C04-C05-C06-C07
2	J	407	C14	C02-C03-C04-C05
2	J	411	C14	C04-C05-C06-C07
2	K	407	C14	C02-C03-C04-C05
2	K	411	C14	C04-C05-C06-C07
2	L	408	C14	C02-C03-C04-C05
2	L	412	C14	C04-C05-C06-C07
2	D	407	C14	C04-C05-C06-C07
4	A	408	PTY	C31-C32-C33-C34
4	G	408	PTY	C31-C32-C33-C34
4	B	414	PTY	C31-C32-C33-C34
4	C	413	PTY	C31-C32-C33-C34
4	D	415	PTY	C31-C32-C33-C34
4	E	414	PTY	C31-C32-C33-C34
4	F	401	PTY	C31-C32-C33-C34
4	H	414	PTY	C31-C32-C33-C34
4	I	414	PTY	C31-C32-C33-C34
4	J	414	PTY	C31-C32-C33-C34
4	K	414	PTY	C31-C32-C33-C34
4	L	401	PTY	C31-C32-C33-C34
4	A	408	PTY	C11-C8-O7-C6
4	G	408	PTY	C11-C8-O7-C6
4	B	414	PTY	C11-C8-O7-C6
4	C	413	PTY	C11-C8-O7-C6
4	D	415	PTY	C11-C8-O7-C6
4	E	414	PTY	C11-C8-O7-C6
4	F	401	PTY	C11-C8-O7-C6
4	H	414	PTY	C11-C8-O7-C6
4	I	414	PTY	C11-C8-O7-C6
4	J	414	PTY	C11-C8-O7-C6
4	K	414	PTY	C11-C8-O7-C6
4	L	401	PTY	C11-C8-O7-C6
2	A	410	C14	C06-C07-C08-C09
2	G	410	C14	C06-C07-C08-C09
2	B	402	C14	C06-C07-C08-C09
2	C	402	C14	C06-C07-C08-C09
2	D	402	C14	C06-C07-C08-C09
2	E	402	C14	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
2	F	403	C14	C06-C07-C08-C09
2	H	402	C14	C06-C07-C08-C09
2	I	402	C14	C06-C07-C08-C09
2	J	402	C14	C06-C07-C08-C09
2	K	402	C14	C06-C07-C08-C09
2	L	403	C14	C06-C07-C08-C09
4	A	408	PTY	C30-C31-C32-C33
4	G	408	PTY	C30-C31-C32-C33
4	B	414	PTY	C30-C31-C32-C33
4	C	413	PTY	C30-C31-C32-C33
4	D	415	PTY	C30-C31-C32-C33
4	E	414	PTY	C30-C31-C32-C33
4	F	401	PTY	C30-C31-C32-C33
4	H	414	PTY	C30-C31-C32-C33
4	I	414	PTY	C30-C31-C32-C33
4	J	414	PTY	C30-C31-C32-C33
4	K	414	PTY	C30-C31-C32-C33
4	L	401	PTY	C30-C31-C32-C33
4	H	414	PTY	C33-C34-C35-C36
4	A	408	PTY	C33-C34-C35-C36
4	G	408	PTY	C33-C34-C35-C36
4	B	414	PTY	C33-C34-C35-C36
4	C	413	PTY	C33-C34-C35-C36
4	D	415	PTY	C33-C34-C35-C36
4	E	414	PTY	C33-C34-C35-C36
4	F	401	PTY	C33-C34-C35-C36
4	I	414	PTY	C33-C34-C35-C36
4	J	414	PTY	C33-C34-C35-C36
4	K	414	PTY	C33-C34-C35-C36
4	L	401	PTY	C33-C34-C35-C36
3	A	406	Y01	CAC-CBB-CBE-CAP
3	G	406	Y01	CAC-CBB-CBE-CAP
3	B	412	Y01	CAC-CBB-CBE-CAP
3	C	411	Y01	CAC-CBB-CBE-CAP
3	D	413	Y01	CAC-CBB-CBE-CAP
3	E	412	Y01	CAC-CBB-CBE-CAP
3	F	413	Y01	CAC-CBB-CBE-CAP
3	H	412	Y01	CAC-CBB-CBE-CAP
3	I	412	Y01	CAC-CBB-CBE-CAP
3	J	412	Y01	CAC-CBB-CBE-CAP
3	K	412	Y01	CAC-CBB-CBE-CAP
3	L	413	Y01	CAC-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
4	A	408	PTY	C34-C35-C36-C37
4	G	408	PTY	C34-C35-C36-C37
4	B	414	PTY	C34-C35-C36-C37
4	C	413	PTY	C34-C35-C36-C37
4	D	415	PTY	C34-C35-C36-C37
4	E	414	PTY	C34-C35-C36-C37
4	F	401	PTY	C34-C35-C36-C37
4	H	414	PTY	C34-C35-C36-C37
4	I	414	PTY	C34-C35-C36-C37
4	J	414	PTY	C34-C35-C36-C37
4	K	414	PTY	C34-C35-C36-C37
4	L	401	PTY	C34-C35-C36-C37
2	A	404	C14	C08-C09-C10-C11
2	D	411	C14	C08-C09-C10-C11
2	E	410	C14	C08-C09-C10-C11
2	F	411	C14	C08-C09-C10-C11
2	H	410	C14	C08-C09-C10-C11
2	J	410	C14	C08-C09-C10-C11
2	K	410	C14	C08-C09-C10-C11
2	L	411	C14	C08-C09-C10-C11
4	A	408	PTY	O10-C8-O7-C6
4	G	408	PTY	O10-C8-O7-C6
4	B	414	PTY	O10-C8-O7-C6
4	C	413	PTY	O10-C8-O7-C6
4	D	415	PTY	O10-C8-O7-C6
4	E	414	PTY	O10-C8-O7-C6
4	F	401	PTY	O10-C8-O7-C6
4	H	414	PTY	O10-C8-O7-C6
4	I	414	PTY	O10-C8-O7-C6
4	J	414	PTY	O10-C8-O7-C6
4	K	414	PTY	O10-C8-O7-C6
4	L	401	PTY	O10-C8-O7-C6
2	G	404	C14	C08-C09-C10-C11
2	B	410	C14	C08-C09-C10-C11
2	C	410	C14	C08-C09-C10-C11
2	I	410	C14	C08-C09-C10-C11
2	A	410	C14	C09-C10-C11-C12
2	G	410	C14	C09-C10-C11-C12
2	B	402	C14	C09-C10-C11-C12
2	C	402	C14	C09-C10-C11-C12
2	D	402	C14	C09-C10-C11-C12
2	E	402	C14	C09-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	F	403	C14	C09-C10-C11-C12
2	H	402	C14	C09-C10-C11-C12
2	I	402	C14	C09-C10-C11-C12
2	J	402	C14	C09-C10-C11-C12
2	K	402	C14	C09-C10-C11-C12
2	L	403	C14	C09-C10-C11-C12
2	A	405	C14	C08-C09-C10-C11
2	G	405	C14	C08-C09-C10-C11
2	B	411	C14	C08-C09-C10-C11
2	D	407	C14	C08-C09-C10-C11
2	D	412	C14	C08-C09-C10-C11
2	E	411	C14	C08-C09-C10-C11
2	F	412	C14	C08-C09-C10-C11
2	H	411	C14	C08-C09-C10-C11
2	I	411	C14	C08-C09-C10-C11
2	J	411	C14	C08-C09-C10-C11
2	K	411	C14	C08-C09-C10-C11
2	L	412	C14	C08-C09-C10-C11
2	L	405	C14	C08-C09-C10-C11
2	A	412	C14	C08-C09-C10-C11
2	G	412	C14	C08-C09-C10-C11
2	B	404	C14	C08-C09-C10-C11
2	C	404	C14	C08-C09-C10-C11
2	D	404	C14	C08-C09-C10-C11
2	E	404	C14	C08-C09-C10-C11
2	F	405	C14	C08-C09-C10-C11
2	H	404	C14	C08-C09-C10-C11
2	I	404	C14	C08-C09-C10-C11
2	J	404	C14	C08-C09-C10-C11
2	K	404	C14	C08-C09-C10-C11
4	C	413	PTY	C32-C33-C34-C35
2	A	403	C14	C08-C09-C10-C11
2	G	403	C14	C08-C09-C10-C11
2	B	409	C14	C08-C09-C10-C11
2	C	409	C14	C08-C09-C10-C11
2	D	410	C14	C08-C09-C10-C11
2	E	409	C14	C08-C09-C10-C11
2	F	410	C14	C08-C09-C10-C11
2	H	409	C14	C08-C09-C10-C11
2	I	409	C14	C08-C09-C10-C11
2	J	409	C14	C08-C09-C10-C11
2	K	409	C14	C08-C09-C10-C11

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Mol	Chain	Res	Type	Atoms
4	A	408	PTY	C32-C33-C34-C35
4	G	408	PTY	C32-C33-C34-C35
4	B	414	PTY	C32-C33-C34-C35
4	D	415	PTY	C32-C33-C34-C35
4	E	414	PTY	C32-C33-C34-C35
4	F	401	PTY	C32-C33-C34-C35
4	H	414	PTY	C32-C33-C34-C35
4	I	414	PTY	C32-C33-C34-C35
4	J	414	PTY	C32-C33-C34-C35
4	K	414	PTY	C32-C33-C34-C35
4	L	401	PTY	C32-C33-C34-C35
2	L	410	C14	C08-C09-C10-C11
2	G	402	C14	C10-C11-C12-C13
2	C	408	C14	C10-C11-C12-C13
2	F	409	C14	C10-C11-C12-C13
2	H	408	C14	C10-C11-C12-C13
2	A	402	C14	C10-C11-C12-C13
2	A	409	C14	C02-C03-C04-C05
2	B	401	C14	C02-C03-C04-C05
2	C	401	C14	C02-C03-C04-C05
2	D	401	C14	C02-C03-C04-C05
2	D	409	C14	C10-C11-C12-C13
2	E	401	C14	C02-C03-C04-C05
2	E	408	C14	C10-C11-C12-C13
2	F	402	C14	C02-C03-C04-C05
2	H	401	C14	C02-C03-C04-C05
2	I	401	C14	C02-C03-C04-C05
2	I	408	C14	C10-C11-C12-C13
2	J	401	C14	C02-C03-C04-C05
2	J	408	C14	C10-C11-C12-C13
2	K	401	C14	C02-C03-C04-C05
2	L	402	C14	C02-C03-C04-C05
2	L	409	C14	C10-C11-C12-C13
2	G	409	C14	C02-C03-C04-C05
2	B	408	C14	C10-C11-C12-C13
2	K	408	C14	C10-C11-C12-C13
2	A	412	C14	C09-C10-C11-C12
2	G	412	C14	C09-C10-C11-C12
2	F	405	C14	C09-C10-C11-C12
2	J	404	C14	C09-C10-C11-C12
2	L	405	C14	C09-C10-C11-C12
2	B	404	C14	C09-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	C	404	C14	C09-C10-C11-C12
2	D	404	C14	C09-C10-C11-C12
2	E	404	C14	C09-C10-C11-C12
2	H	404	C14	C09-C10-C11-C12
2	I	404	C14	C09-C10-C11-C12
2	K	404	C14	C09-C10-C11-C12
2	H	405	C14	C09-C10-C11-C12
2	G	413	C14	C09-C10-C11-C12
2	B	405	C14	C09-C10-C11-C12
2	C	405	C14	C09-C10-C11-C12
2	D	405	C14	C09-C10-C11-C12
2	E	405	C14	C09-C10-C11-C12
2	I	405	C14	C09-C10-C11-C12
2	K	405	C14	C09-C10-C11-C12
2	L	406	C14	C09-C10-C11-C12
2	A	413	C14	C09-C10-C11-C12
2	F	406	C14	C09-C10-C11-C12
2	J	405	C14	C09-C10-C11-C12
2	A	402	C14	C08-C09-C10-C11
2	G	402	C14	C08-C09-C10-C11
2	C	408	C14	C08-C09-C10-C11
2	D	409	C14	C08-C09-C10-C11
2	E	408	C14	C08-C09-C10-C11
2	F	409	C14	C08-C09-C10-C11
2	I	408	C14	C08-C09-C10-C11
2	J	408	C14	C08-C09-C10-C11
2	K	408	C14	C08-C09-C10-C11
2	B	408	C14	C08-C09-C10-C11
2	H	408	C14	C08-C09-C10-C11
2	L	409	C14	C08-C09-C10-C11
3	G	406	Y01	CAO-CBB-CBE-CBI
3	A	406	Y01	CAO-CBB-CBE-CBI
3	B	412	Y01	CAO-CBB-CBE-CBI
3	C	411	Y01	CAO-CBB-CBE-CBI
3	D	413	Y01	CAO-CBB-CBE-CBI
3	E	412	Y01	CAO-CBB-CBE-CBI
3	F	413	Y01	CAO-CBB-CBE-CBI
3	H	412	Y01	CAO-CBB-CBE-CBI
3	I	412	Y01	CAO-CBB-CBE-CBI
3	J	412	Y01	CAO-CBB-CBE-CBI
3	K	412	Y01	CAO-CBB-CBE-CBI
3	L	413	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
4	D	415	PTY	C38-C39-C40-C41
4	F	401	PTY	C38-C39-C40-C41
4	A	408	PTY	C38-C39-C40-C41
4	G	408	PTY	C38-C39-C40-C41
4	B	414	PTY	C38-C39-C40-C41
4	C	413	PTY	C38-C39-C40-C41
4	E	414	PTY	C38-C39-C40-C41
4	H	414	PTY	C38-C39-C40-C41
4	I	414	PTY	C38-C39-C40-C41
4	J	414	PTY	C38-C39-C40-C41
4	K	414	PTY	C38-C39-C40-C41
4	L	401	PTY	C38-C39-C40-C41
2	D	406	C14	C04-C05-C06-C07
2	E	406	C14	C04-C05-C06-C07
2	F	407	C14	C04-C05-C06-C07
2	K	406	C14	C04-C05-C06-C07
2	A	414	C14	C04-C05-C06-C07
2	G	414	C14	C04-C05-C06-C07
2	B	406	C14	C04-C05-C06-C07
2	C	406	C14	C04-C05-C06-C07
2	H	406	C14	C04-C05-C06-C07
2	I	406	C14	C04-C05-C06-C07
2	J	406	C14	C04-C05-C06-C07
2	L	407	C14	C04-C05-C06-C07
2	A	403	C14	C07-C08-C09-C10
2	G	403	C14	C07-C08-C09-C10
2	D	410	C14	C07-C08-C09-C10
2	F	410	C14	C07-C08-C09-C10
2	I	409	C14	C07-C08-C09-C10
2	K	409	C14	C07-C08-C09-C10
2	B	409	C14	C07-C08-C09-C10
2	C	409	C14	C07-C08-C09-C10
2	E	409	C14	C07-C08-C09-C10
2	H	409	C14	C07-C08-C09-C10
2	J	409	C14	C07-C08-C09-C10
2	L	410	C14	C07-C08-C09-C10
4	L	401	PTY	C8-C11-C12-C13
4	A	408	PTY	C8-C11-C12-C13
4	G	408	PTY	C8-C11-C12-C13
4	B	414	PTY	C8-C11-C12-C13
4	C	413	PTY	C8-C11-C12-C13
4	D	415	PTY	C8-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
4	E	414	PTY	C8-C11-C12-C13
4	F	401	PTY	C8-C11-C12-C13
4	H	414	PTY	C8-C11-C12-C13
4	I	414	PTY	C8-C11-C12-C13
4	J	414	PTY	C8-C11-C12-C13
4	K	414	PTY	C8-C11-C12-C13
3	B	412	Y01	CAN-CAJ-CAO-CBB
3	E	412	Y01	CAN-CAJ-CAO-CBB
3	H	412	Y01	CAN-CAJ-CAO-CBB
3	C	411	Y01	CAN-CAJ-CAO-CBB
3	I	412	Y01	CAN-CAJ-CAO-CBB
3	J	412	Y01	CAN-CAJ-CAO-CBB
3	K	412	Y01	CAN-CAJ-CAO-CBB
3	L	413	Y01	CAN-CAJ-CAO-CBB
3	A	406	Y01	CAN-CAJ-CAO-CBB
3	G	406	Y01	CAN-CAJ-CAO-CBB
3	D	413	Y01	CAN-CAJ-CAO-CBB
3	F	413	Y01	CAN-CAJ-CAO-CBB
2	A	403	C14	C04-C05-C06-C07
2	G	403	C14	C04-C05-C06-C07
2	B	409	C14	C04-C05-C06-C07
2	C	409	C14	C04-C05-C06-C07
2	E	409	C14	C04-C05-C06-C07
2	F	410	C14	C04-C05-C06-C07
2	H	409	C14	C04-C05-C06-C07
2	I	409	C14	C04-C05-C06-C07
2	K	409	C14	C04-C05-C06-C07
2	L	410	C14	C04-C05-C06-C07
2	D	410	C14	C04-C05-C06-C07
2	J	409	C14	C04-C05-C06-C07
2	D	402	C14	C05-C06-C07-C08
2	E	402	C14	C05-C06-C07-C08
2	A	410	C14	C05-C06-C07-C08
2	G	410	C14	C05-C06-C07-C08
2	F	403	C14	C05-C06-C07-C08
2	H	402	C14	C05-C06-C07-C08
2	I	402	C14	C05-C06-C07-C08
2	K	402	C14	C05-C06-C07-C08
2	L	403	C14	C05-C06-C07-C08
2	B	402	C14	C05-C06-C07-C08
2	C	402	C14	C05-C06-C07-C08
2	J	402	C14	C05-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
2	J	403	C14	C09-C10-C11-C12
2	A	411	C14	C09-C10-C11-C12
2	B	403	C14	C09-C10-C11-C12
2	C	403	C14	C09-C10-C11-C12
2	E	403	C14	C09-C10-C11-C12
2	H	403	C14	C09-C10-C11-C12
2	L	404	C14	C09-C10-C11-C12
2	G	411	C14	C09-C10-C11-C12
2	D	403	C14	C09-C10-C11-C12
2	F	404	C14	C09-C10-C11-C12
2	I	403	C14	C09-C10-C11-C12
2	K	403	C14	C09-C10-C11-C12
2	A	404	C14	C04-C05-C06-C07
2	D	411	C14	C04-C05-C06-C07
2	I	410	C14	C04-C05-C06-C07
2	G	404	C14	C04-C05-C06-C07
2	B	410	C14	C04-C05-C06-C07
2	C	410	C14	C04-C05-C06-C07
2	E	410	C14	C04-C05-C06-C07
2	F	411	C14	C04-C05-C06-C07
2	H	410	C14	C04-C05-C06-C07
2	J	410	C14	C04-C05-C06-C07
2	K	410	C14	C04-C05-C06-C07
2	L	411	C14	C04-C05-C06-C07
3	L	413	Y01	CAJ-CAO-CBB-CAC
3	A	406	Y01	CAJ-CAO-CBB-CAC
3	G	406	Y01	CAJ-CAO-CBB-CAC
3	B	412	Y01	CAJ-CAO-CBB-CAC
3	C	411	Y01	CAJ-CAO-CBB-CAC
3	D	413	Y01	CAJ-CAO-CBB-CAC
3	E	412	Y01	CAJ-CAO-CBB-CAC
3	H	412	Y01	CAJ-CAO-CBB-CAC
3	I	412	Y01	CAJ-CAO-CBB-CAC
3	J	412	Y01	CAJ-CAO-CBB-CAC
3	K	412	Y01	CAJ-CAO-CBB-CAC
3	F	413	Y01	CAJ-CAO-CBB-CAC
2	B	405	C14	C03-C04-C05-C06
2	A	413	C14	C03-C04-C05-C06
4	D	415	PTY	C11-C12-C13-C14
4	E	414	PTY	C11-C12-C13-C14
4	F	401	PTY	C11-C12-C13-C14
4	H	414	PTY	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	K	414	PTY	C11-C12-C13-C14
4	L	401	PTY	C11-C12-C13-C14
2	G	413	C14	C03-C04-C05-C06
2	E	405	C14	C03-C04-C05-C06
2	F	406	C14	C03-C04-C05-C06
2	J	405	C14	C03-C04-C05-C06
2	K	405	C14	C03-C04-C05-C06
2	L	406	C14	C03-C04-C05-C06
2	C	405	C14	C03-C04-C05-C06
2	I	405	C14	C03-C04-C05-C06
4	A	408	PTY	C11-C12-C13-C14
4	G	408	PTY	C11-C12-C13-C14
4	B	414	PTY	C11-C12-C13-C14
4	C	413	PTY	C11-C12-C13-C14
4	I	414	PTY	C11-C12-C13-C14
4	J	414	PTY	C11-C12-C13-C14
2	D	405	C14	C03-C04-C05-C06
2	H	405	C14	C03-C04-C05-C06
4	A	408	PTY	C5-O14-P1-O13
4	G	408	PTY	C5-O14-P1-O13
4	B	414	PTY	C5-O14-P1-O13
4	C	413	PTY	C5-O14-P1-O13
4	D	415	PTY	C5-O14-P1-O13
4	E	414	PTY	C5-O14-P1-O13
4	F	401	PTY	C5-O14-P1-O13
4	H	414	PTY	C5-O14-P1-O13
4	I	414	PTY	C5-O14-P1-O13
4	J	414	PTY	C5-O14-P1-O13
4	K	414	PTY	C5-O14-P1-O13
4	L	401	PTY	C5-O14-P1-O13
2	C	410	C14	C10-C11-C12-C13
2	E	410	C14	C10-C11-C12-C13
2	F	411	C14	C10-C11-C12-C13
2	H	410	C14	C10-C11-C12-C13
2	A	404	C14	C10-C11-C12-C13
2	D	411	C14	C10-C11-C12-C13
2	I	410	C14	C10-C11-C12-C13
2	J	410	C14	C10-C11-C12-C13
2	G	404	C14	C10-C11-C12-C13
2	B	410	C14	C10-C11-C12-C13
2	K	410	C14	C10-C11-C12-C13
2	L	411	C14	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	B	406	C14	C02-C03-C04-C05
2	G	414	C14	C02-C03-C04-C05
2	A	414	C14	C02-C03-C04-C05
2	E	406	C14	C02-C03-C04-C05
2	H	406	C14	C02-C03-C04-C05
2	I	406	C14	C02-C03-C04-C05
2	J	406	C14	C02-C03-C04-C05
2	L	407	C14	C02-C03-C04-C05
2	C	406	C14	C02-C03-C04-C05
2	D	406	C14	C02-C03-C04-C05
2	F	407	C14	C02-C03-C04-C05
2	K	406	C14	C02-C03-C04-C05
3	L	414	Y01	CAR-CBC-OAW-CAY
2	A	412	C14	C04-C05-C06-C07
2	G	412	C14	C04-C05-C06-C07
2	D	404	C14	C04-C05-C06-C07
2	F	405	C14	C04-C05-C06-C07
2	H	404	C14	C04-C05-C06-C07
2	J	404	C14	C04-C05-C06-C07
2	K	404	C14	C04-C05-C06-C07
3	J	413	Y01	CAR-CBC-OAW-CAY
2	B	404	C14	C04-C05-C06-C07
2	C	404	C14	C04-C05-C06-C07
2	I	404	C14	C04-C05-C06-C07
2	L	405	C14	C04-C05-C06-C07
2	E	404	C14	C04-C05-C06-C07
3	F	414	Y01	CAR-CBC-OAW-CAY
3	F	414	Y01	CAC-CBB-CBE-CBI
3	K	413	Y01	CAC-CBB-CBE-CBI
3	A	407	Y01	CAR-CBC-OAW-CAY
3	G	407	Y01	CAR-CBC-OAW-CAY
3	B	413	Y01	CAR-CBC-OAW-CAY
3	C	412	Y01	CAR-CBC-OAW-CAY
3	D	414	Y01	CAR-CBC-OAW-CAY
3	E	413	Y01	CAR-CBC-OAW-CAY
3	H	413	Y01	CAR-CBC-OAW-CAY
3	I	413	Y01	CAR-CBC-OAW-CAY
3	K	413	Y01	CAR-CBC-OAW-CAY
3	A	407	Y01	CAC-CBB-CBE-CBI
3	G	407	Y01	CAC-CBB-CBE-CBI
3	B	413	Y01	CAC-CBB-CBE-CBI
3	D	414	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
3	E	413	Y01	CAC-CBB-CBE-CBI
3	H	413	Y01	CAC-CBB-CBE-CBI
3	I	413	Y01	CAC-CBB-CBE-CBI
3	J	413	Y01	CAC-CBB-CBE-CBI
3	L	414	Y01	CAC-CBB-CBE-CBI
2	D	407	C14	C05-C06-C07-C08
2	L	412	C14	C05-C06-C07-C08
2	A	405	C14	C05-C06-C07-C08
2	G	405	C14	C05-C06-C07-C08
2	J	411	C14	C05-C06-C07-C08
2	D	412	C14	C05-C06-C07-C08
2	E	411	C14	C05-C06-C07-C08
2	K	411	C14	C05-C06-C07-C08
2	B	411	C14	C05-C06-C07-C08
2	F	412	C14	C05-C06-C07-C08
2	I	411	C14	C05-C06-C07-C08
2	H	411	C14	C05-C06-C07-C08
3	C	412	Y01	CAC-CBB-CBE-CBI
2	E	402	C14	C03-C04-C05-C06
2	J	402	C14	C03-C04-C05-C06
2	B	402	C14	C03-C04-C05-C06
2	H	402	C14	C03-C04-C05-C06
2	C	402	C14	C03-C04-C05-C06
2	A	410	C14	C03-C04-C05-C06
2	D	402	C14	C03-C04-C05-C06
2	F	403	C14	C03-C04-C05-C06
2	I	402	C14	C03-C04-C05-C06
2	K	402	C14	C03-C04-C05-C06
2	L	402	C14	C04-C05-C06-C07
2	L	403	C14	C03-C04-C05-C06
2	G	410	C14	C03-C04-C05-C06
2	B	401	C14	C04-C05-C06-C07
2	C	401	C14	C04-C05-C06-C07
2	E	401	C14	C04-C05-C06-C07
2	G	409	C14	C04-C05-C06-C07
2	I	401	C14	C04-C05-C06-C07
2	J	401	C14	C04-C05-C06-C07
2	A	409	C14	C04-C05-C06-C07
2	D	401	C14	C04-C05-C06-C07
2	F	402	C14	C04-C05-C06-C07
2	H	401	C14	C04-C05-C06-C07
2	K	401	C14	C04-C05-C06-C07

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Mol	Chain	Res	Type	Atoms
2	C	402	C14	C07-C08-C09-C10
2	C	408	C14	C04-C05-C06-C07
2	D	409	C14	C04-C05-C06-C07
2	F	409	C14	C04-C05-C06-C07
2	J	402	C14	C07-C08-C09-C10
2	J	408	C14	C04-C05-C06-C07
2	L	409	C14	C04-C05-C06-C07
2	A	402	C14	C04-C05-C06-C07
2	A	410	C14	C07-C08-C09-C10
2	G	402	C14	C04-C05-C06-C07
2	B	408	C14	C04-C05-C06-C07
2	F	403	C14	C07-C08-C09-C10
2	H	408	C14	C04-C05-C06-C07
2	I	408	C14	C04-C05-C06-C07
2	K	402	C14	C07-C08-C09-C10
2	K	408	C14	C04-C05-C06-C07
2	E	408	C14	C04-C05-C06-C07
2	H	402	C14	C07-C08-C09-C10
2	L	403	C14	C07-C08-C09-C10
2	G	410	C14	C07-C08-C09-C10
2	D	402	C14	C07-C08-C09-C10
2	I	402	C14	C07-C08-C09-C10
2	B	402	C14	C07-C08-C09-C10
2	E	402	C14	C07-C08-C09-C10
2	E	408	C14	C06-C07-C08-C09
2	A	402	C14	C06-C07-C08-C09
2	G	402	C14	C06-C07-C08-C09
2	B	408	C14	C06-C07-C08-C09
2	D	409	C14	C06-C07-C08-C09
2	F	409	C14	C06-C07-C08-C09
2	H	408	C14	C06-C07-C08-C09
2	K	408	C14	C06-C07-C08-C09
2	L	409	C14	C06-C07-C08-C09
2	C	408	C14	C06-C07-C08-C09
2	I	408	C14	C06-C07-C08-C09
2	J	408	C14	C06-C07-C08-C09
2	F	412	C14	C06-C07-C08-C09
2	D	407	C14	C06-C07-C08-C09
2	G	405	C14	C06-C07-C08-C09
2	E	411	C14	C06-C07-C08-C09
2	L	412	C14	C06-C07-C08-C09
2	A	405	C14	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
2	B	411	C14	C06-C07-C08-C09
2	D	412	C14	C06-C07-C08-C09
2	J	411	C14	C06-C07-C08-C09
2	H	411	C14	C06-C07-C08-C09
2	I	411	C14	C06-C07-C08-C09
2	K	411	C14	C06-C07-C08-C09
3	A	407	Y01	CAM-CAL-CAX-OAH
3	B	413	Y01	CAM-CAL-CAX-OAH
3	C	412	Y01	CAM-CAL-CAX-OAH
3	E	413	Y01	CAM-CAL-CAX-OAH
3	F	414	Y01	CAM-CAL-CAX-OAH
3	H	413	Y01	CAM-CAL-CAX-OAH
3	I	413	Y01	CAM-CAL-CAX-OAH
3	J	413	Y01	CAM-CAL-CAX-OAH
3	K	413	Y01	CAM-CAL-CAX-OAH
3	G	407	Y01	CAM-CAL-CAX-OAH
3	D	414	Y01	CAM-CAL-CAX-OAH
3	L	414	Y01	CAM-CAL-CAX-OAH
2	I	403	C14	C04-C05-C06-C07
2	G	411	C14	C04-C05-C06-C07
2	B	403	C14	C04-C05-C06-C07
2	C	403	C14	C04-C05-C06-C07
2	H	403	C14	C04-C05-C06-C07
2	L	404	C14	C04-C05-C06-C07
2	A	411	C14	C04-C05-C06-C07
2	F	404	C14	C04-C05-C06-C07
2	J	403	C14	C04-C05-C06-C07
2	E	403	C14	C04-C05-C06-C07
2	K	403	C14	C04-C05-C06-C07
2	D	403	C14	C04-C05-C06-C07
4	L	401	PTY	C12-C11-C8-O7
3	A	407	Y01	CAM-CAL-CAX-OAF
3	G	407	Y01	CAM-CAL-CAX-OAF
3	C	412	Y01	CAM-CAL-CAX-OAF
3	E	413	Y01	CAM-CAL-CAX-OAF
3	H	413	Y01	CAM-CAL-CAX-OAF
3	I	413	Y01	CAM-CAL-CAX-OAF
3	K	413	Y01	CAM-CAL-CAX-OAF
4	G	408	PTY	C39-C40-C41-C42
4	J	414	PTY	C39-C40-C41-C42
3	I	413	Y01	CAN-CAJ-CAO-CBB
4	F	401	PTY	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
4	L	401	PTY	C39-C40-C41-C42
3	B	413	Y01	CAM-CAL-CAX-OAF
3	D	414	Y01	CAM-CAL-CAX-OAF
3	F	414	Y01	CAM-CAL-CAX-OAF
3	J	413	Y01	CAM-CAL-CAX-OAF
3	L	414	Y01	CAM-CAL-CAX-OAF
4	A	408	PTY	C12-C11-C8-O7
4	G	408	PTY	C12-C11-C8-O7
4	B	414	PTY	C12-C11-C8-O7
4	C	413	PTY	C12-C11-C8-O7
4	D	415	PTY	C12-C11-C8-O7
4	F	401	PTY	C12-C11-C8-O7
4	H	414	PTY	C12-C11-C8-O7
4	I	414	PTY	C12-C11-C8-O7
4	J	414	PTY	C12-C11-C8-O7
4	K	414	PTY	C12-C11-C8-O7
4	C	413	PTY	C39-C40-C41-C42
4	K	414	PTY	C39-C40-C41-C42
3	G	407	Y01	CAN-CAJ-CAO-CBB
3	B	413	Y01	CAN-CAJ-CAO-CBB
3	H	413	Y01	CAN-CAJ-CAO-CBB
4	E	414	PTY	C39-C40-C41-C42
2	B	404	C14	C10-C11-C12-C13
2	C	404	C14	C10-C11-C12-C13
4	H	414	PTY	C39-C40-C41-C42
3	C	412	Y01	CAN-CAJ-CAO-CBB
3	J	413	Y01	CAN-CAJ-CAO-CBB
3	L	414	Y01	CAN-CAJ-CAO-CBB
4	A	408	PTY	C39-C40-C41-C42
4	B	414	PTY	C39-C40-C41-C42
4	D	415	PTY	C39-C40-C41-C42
4	I	414	PTY	C39-C40-C41-C42
4	E	414	PTY	C12-C11-C8-O7
2	K	404	C14	C10-C11-C12-C13
2	A	412	C14	C10-C11-C12-C13
2	E	404	C14	C10-C11-C12-C13
2	F	405	C14	C10-C11-C12-C13
2	J	404	C14	C10-C11-C12-C13
3	A	407	Y01	CAN-CAJ-CAO-CBB
3	F	414	Y01	CAN-CAJ-CAO-CBB
2	G	412	C14	C10-C11-C12-C13
2	D	404	C14	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	I	404	C14	C10-C11-C12-C13
3	D	414	Y01	CAN-CAJ-CAO-CBB
3	E	413	Y01	CAN-CAJ-CAO-CBB
3	K	413	Y01	CAN-CAJ-CAO-CBB
2	H	404	C14	C10-C11-C12-C13
2	L	405	C14	C10-C11-C12-C13
2	D	405	C14	C05-C06-C07-C08
2	A	413	C14	C05-C06-C07-C08
2	B	405	C14	C05-C06-C07-C08
2	G	413	C14	C05-C06-C07-C08
2	C	405	C14	C05-C06-C07-C08
2	E	405	C14	C05-C06-C07-C08
2	F	406	C14	C05-C06-C07-C08
2	H	405	C14	C05-C06-C07-C08
2	I	405	C14	C05-C06-C07-C08
2	J	405	C14	C05-C06-C07-C08
2	K	405	C14	C05-C06-C07-C08
2	L	406	C14	C05-C06-C07-C08
2	H	406	C14	C06-C07-C08-C09
2	J	406	C14	C06-C07-C08-C09
2	G	414	C14	C06-C07-C08-C09
2	I	406	C14	C06-C07-C08-C09
2	A	414	C14	C06-C07-C08-C09
2	B	406	C14	C06-C07-C08-C09
2	C	406	C14	C06-C07-C08-C09
2	D	406	C14	C06-C07-C08-C09
2	E	406	C14	C06-C07-C08-C09
2	F	407	C14	C06-C07-C08-C09
2	K	406	C14	C06-C07-C08-C09
2	L	407	C14	C06-C07-C08-C09
3	C	411	Y01	CAM-CAL-CAX-OAH
3	I	412	Y01	CAM-CAL-CAX-OAH
3	L	413	Y01	CAM-CAL-CAX-OAH
3	A	406	Y01	CAM-CAL-CAX-OAH
3	D	413	Y01	CAM-CAL-CAX-OAH
3	G	406	Y01	CAM-CAL-CAX-OAH
3	F	413	Y01	CAM-CAL-CAX-OAH
3	B	412	Y01	CAM-CAL-CAX-OAH
3	E	412	Y01	CAM-CAL-CAX-OAH
3	H	412	Y01	CAM-CAL-CAX-OAH
3	J	412	Y01	CAM-CAL-CAX-OAH
3	K	412	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
2	I	403	C14	C10-C11-C12-C13
2	A	411	C14	C03-C04-C05-C06
2	B	403	C14	C03-C04-C05-C06
2	C	403	C14	C10-C11-C12-C13
2	D	403	C14	C03-C04-C05-C06
2	E	403	C14	C03-C04-C05-C06
2	K	403	C14	C03-C04-C05-C06
2	K	403	C14	C10-C11-C12-C13
2	C	403	C14	C03-C04-C05-C06
2	L	404	C14	C03-C04-C05-C06
2	L	404	C14	C10-C11-C12-C13
2	E	403	C14	C10-C11-C12-C13
2	J	403	C14	C10-C11-C12-C13
2	A	411	C14	C10-C11-C12-C13
2	B	403	C14	C10-C11-C12-C13
2	D	403	C14	C10-C11-C12-C13
2	F	404	C14	C03-C04-C05-C06
2	F	404	C14	C10-C11-C12-C13
2	H	403	C14	C03-C04-C05-C06
2	J	403	C14	C03-C04-C05-C06
2	G	411	C14	C10-C11-C12-C13
2	H	403	C14	C10-C11-C12-C13
2	I	403	C14	C03-C04-C05-C06
2	G	411	C14	C03-C04-C05-C06
2	A	413	C14	C10-C11-C12-C13
2	J	405	C14	C10-C11-C12-C13
2	G	413	C14	C10-C11-C12-C13
2	C	405	C14	C10-C11-C12-C13
2	D	405	C14	C10-C11-C12-C13
2	F	406	C14	C10-C11-C12-C13
2	H	405	C14	C10-C11-C12-C13
2	K	405	C14	C10-C11-C12-C13
2	I	405	C14	C10-C11-C12-C13
2	B	405	C14	C10-C11-C12-C13
2	E	405	C14	C10-C11-C12-C13
2	L	406	C14	C10-C11-C12-C13
2	A	411	C14	C02-C03-C04-C05
2	D	403	C14	C02-C03-C04-C05
2	L	404	C14	C02-C03-C04-C05
2	C	403	C14	C02-C03-C04-C05
2	E	403	C14	C02-C03-C04-C05
2	F	404	C14	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
2	H	403	C14	C02-C03-C04-C05
2	I	403	C14	C02-C03-C04-C05
2	J	403	C14	C02-C03-C04-C05
2	K	403	C14	C02-C03-C04-C05
2	G	411	C14	C02-C03-C04-C05
2	B	403	C14	C02-C03-C04-C05
3	G	406	Y01	CAM-CAL-CAX-OAF
3	C	411	Y01	CAM-CAL-CAX-OAF
3	D	413	Y01	CAM-CAL-CAX-OAF
3	J	412	Y01	CAM-CAL-CAX-OAF
3	A	406	Y01	CAM-CAL-CAX-OAF
3	F	413	Y01	CAM-CAL-CAX-OAF
3	E	412	Y01	CAM-CAL-CAX-OAF
3	I	412	Y01	CAM-CAL-CAX-OAF
3	K	412	Y01	CAM-CAL-CAX-OAF
3	B	412	Y01	CAM-CAL-CAX-OAF
3	H	412	Y01	CAM-CAL-CAX-OAF
3	L	413	Y01	CAM-CAL-CAX-OAF
3	E	413	Y01	CAO-CAJ-CAN-CBA
3	J	413	Y01	CAO-CAJ-CAN-CBA
3	K	413	Y01	CAO-CAJ-CAN-CBA
3	C	412	Y01	CAO-CAJ-CAN-CBA
3	F	414	Y01	CAO-CAJ-CAN-CBA
3	L	414	Y01	CAO-CAJ-CAN-CBA
4	G	408	PTY	O4-C1-C6-C5
4	B	414	PTY	O4-C1-C6-C5
4	C	413	PTY	O4-C1-C6-C5
4	D	415	PTY	O4-C1-C6-C5
4	E	414	PTY	O4-C1-C6-C5
4	F	401	PTY	O4-C1-C6-C5
4	H	414	PTY	O4-C1-C6-C5
4	I	414	PTY	O4-C1-C6-C5
4	J	414	PTY	O4-C1-C6-C5
4	K	414	PTY	O4-C1-C6-C5
4	L	401	PTY	O4-C1-C6-C5
3	A	407	Y01	CAO-CAJ-CAN-CBA
3	B	413	Y01	CAO-CAJ-CAN-CBA
3	D	414	Y01	CAO-CAJ-CAN-CBA
3	H	413	Y01	CAO-CAJ-CAN-CBA
3	I	413	Y01	CAO-CAJ-CAN-CBA
3	G	407	Y01	CAO-CAJ-CAN-CBA

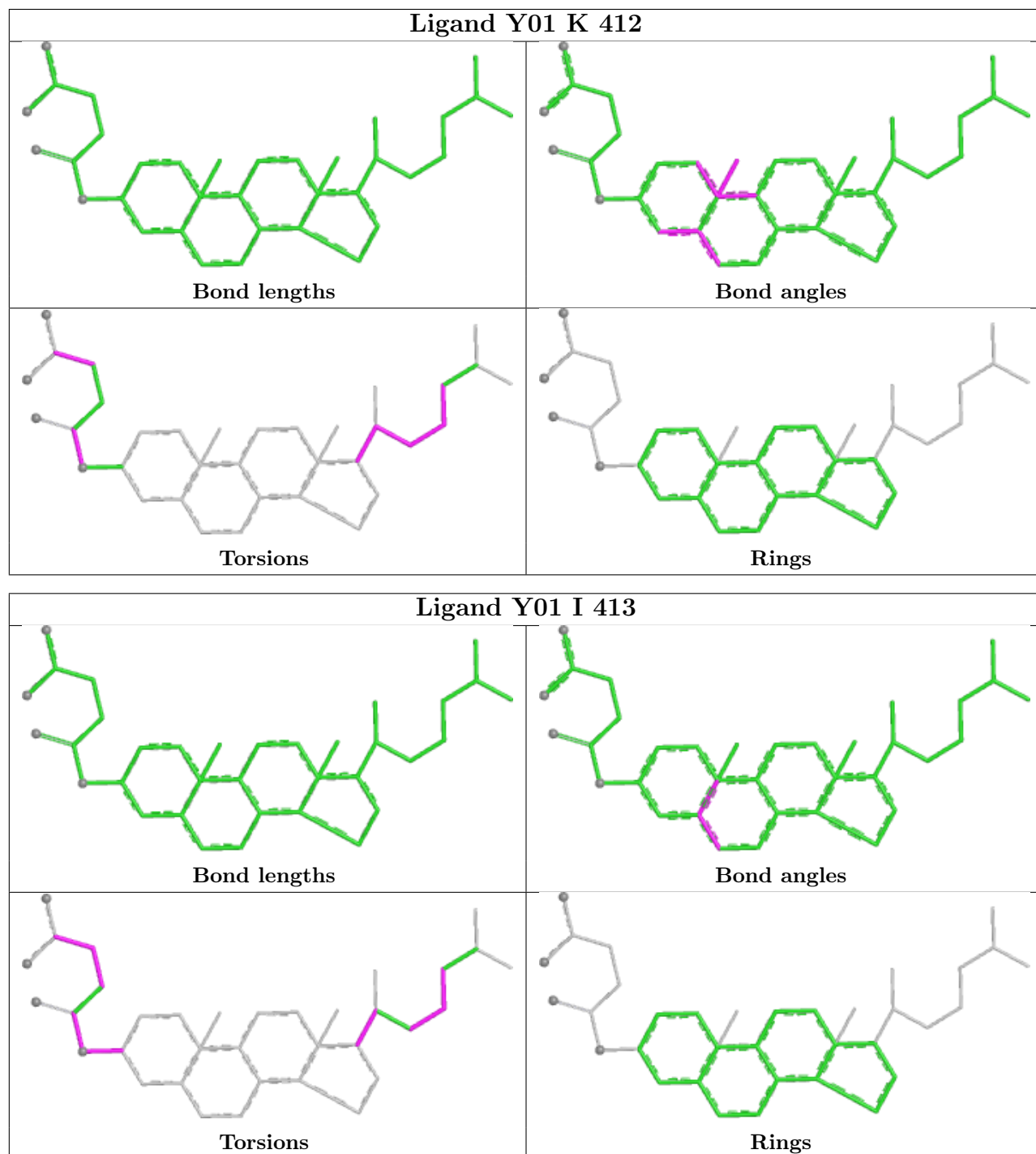
There are no ring outliers.

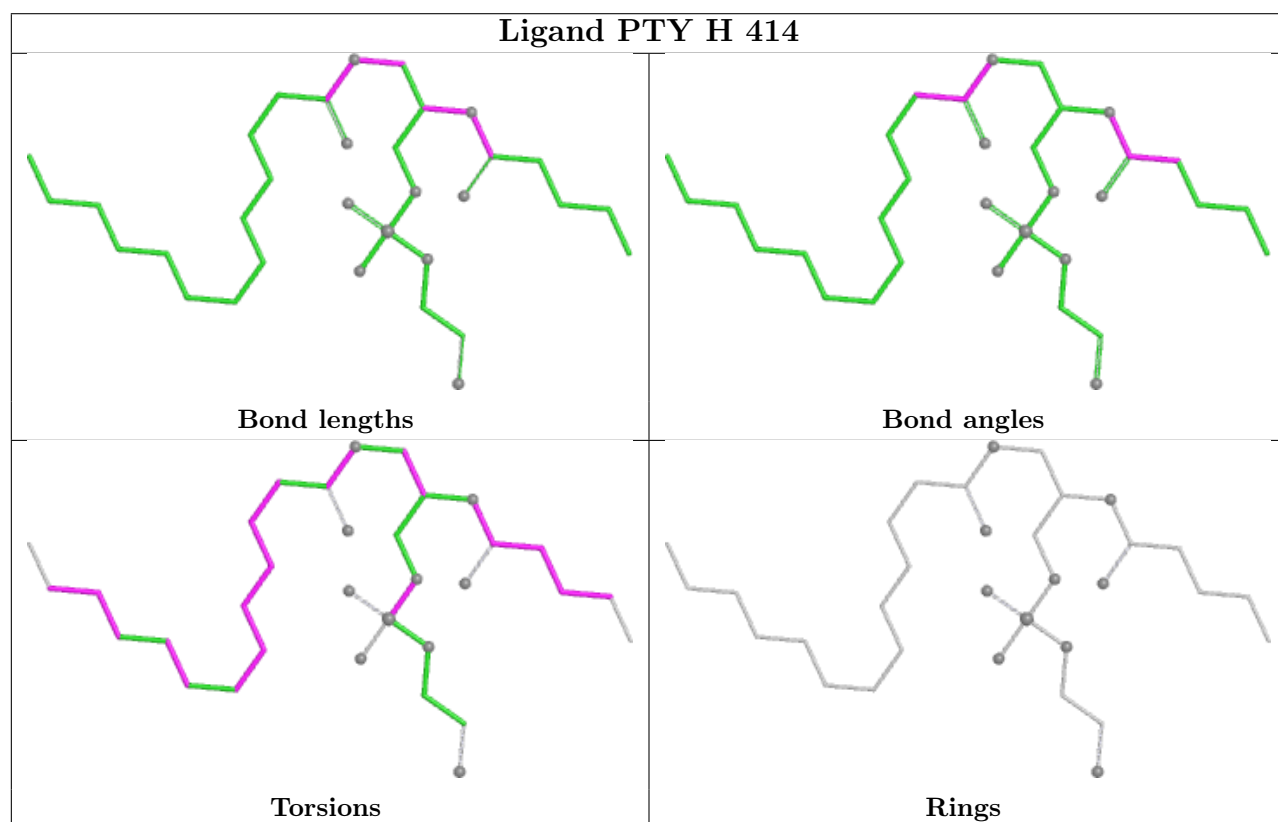
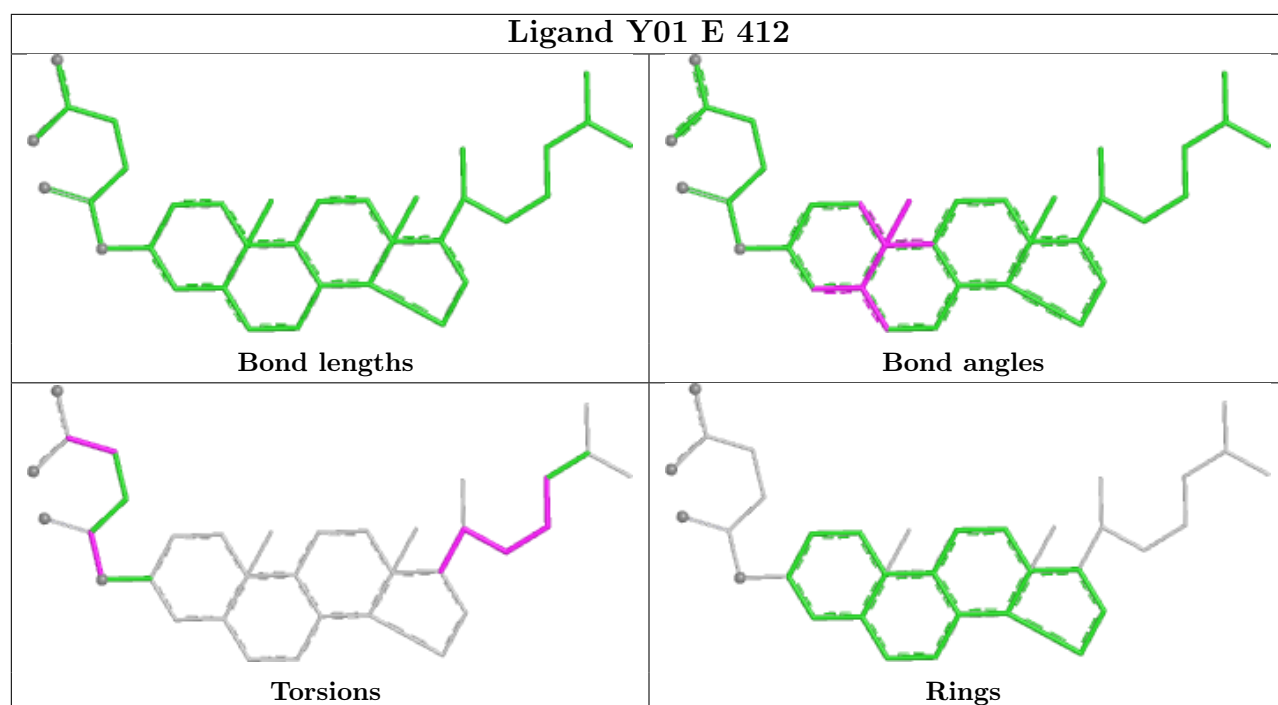
36 monomers are involved in 92 short contacts:

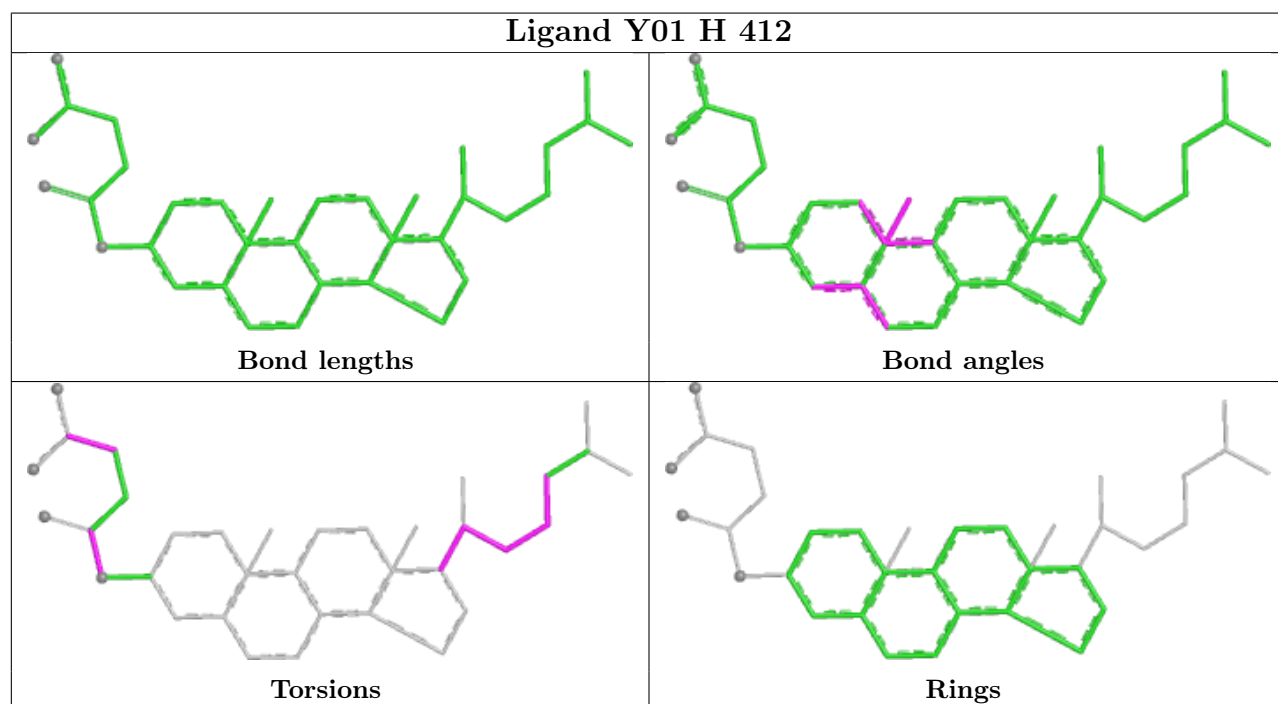
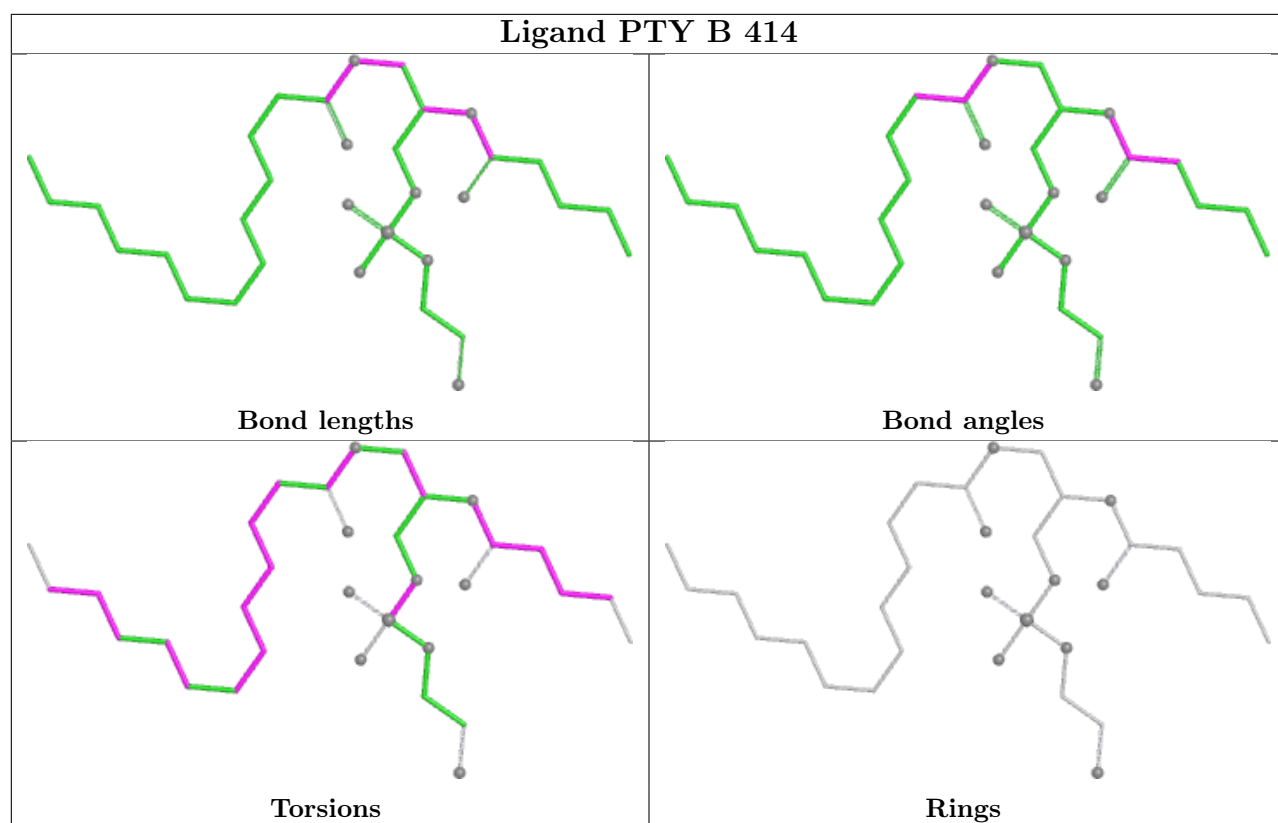
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	412	Y01	4	0
3	I	413	Y01	4	0
3	E	412	Y01	4	0
4	H	414	PTY	1	0
4	B	414	PTY	1	0
3	H	412	Y01	4	0
3	L	413	Y01	4	0
3	E	413	Y01	3	0
3	K	413	Y01	4	0
3	H	413	Y01	4	0
3	B	412	Y01	4	0
3	C	412	Y01	3	0
4	F	401	PTY	1	0
4	E	414	PTY	1	0
3	L	414	Y01	2	0
3	F	413	Y01	4	0
3	I	412	Y01	4	0
4	C	413	PTY	1	0
3	J	412	Y01	4	0
3	B	413	Y01	4	0
4	D	415	PTY	1	0
3	J	413	Y01	4	0
4	A	408	PTY	1	0
4	K	414	PTY	1	0
4	L	401	PTY	1	0
3	C	411	Y01	4	0
3	G	406	Y01	4	0
4	I	414	PTY	2	0
3	G	407	Y01	4	0
4	J	414	PTY	2	0
3	A	407	Y01	3	0
3	A	406	Y01	4	0
3	D	414	Y01	4	0
3	F	414	Y01	3	0
4	G	408	PTY	1	0
3	D	413	Y01	4	0

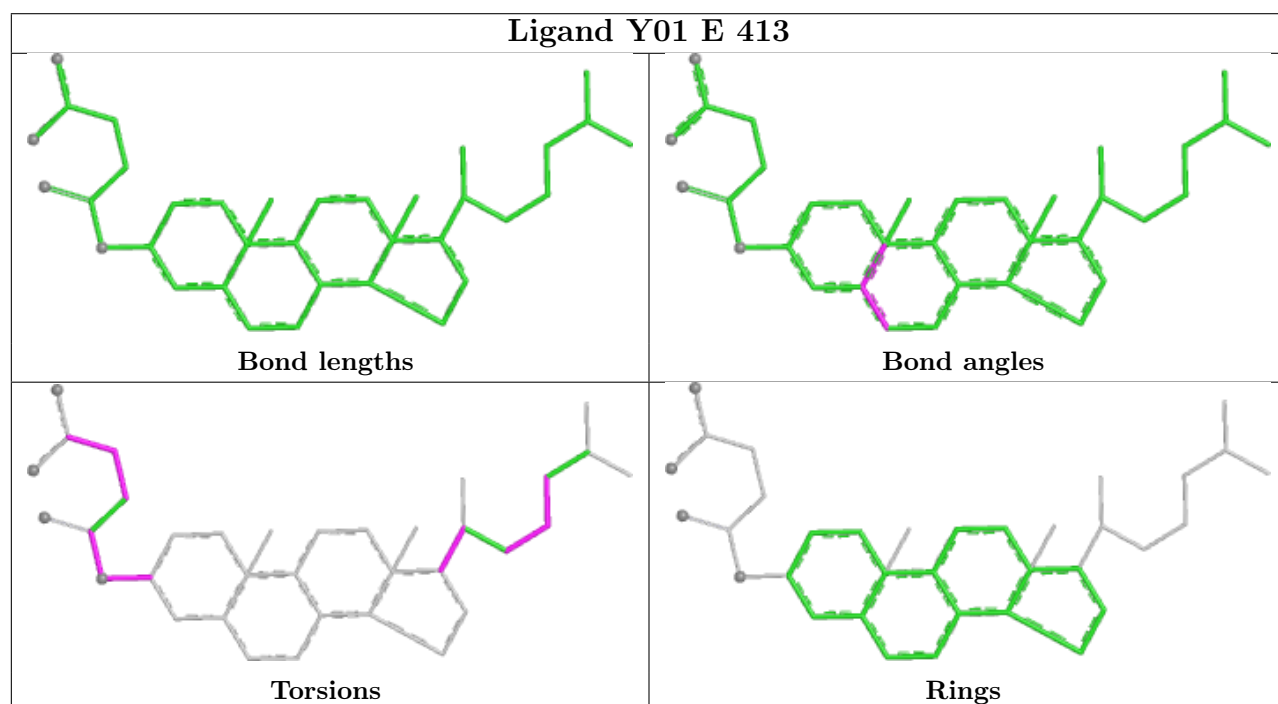
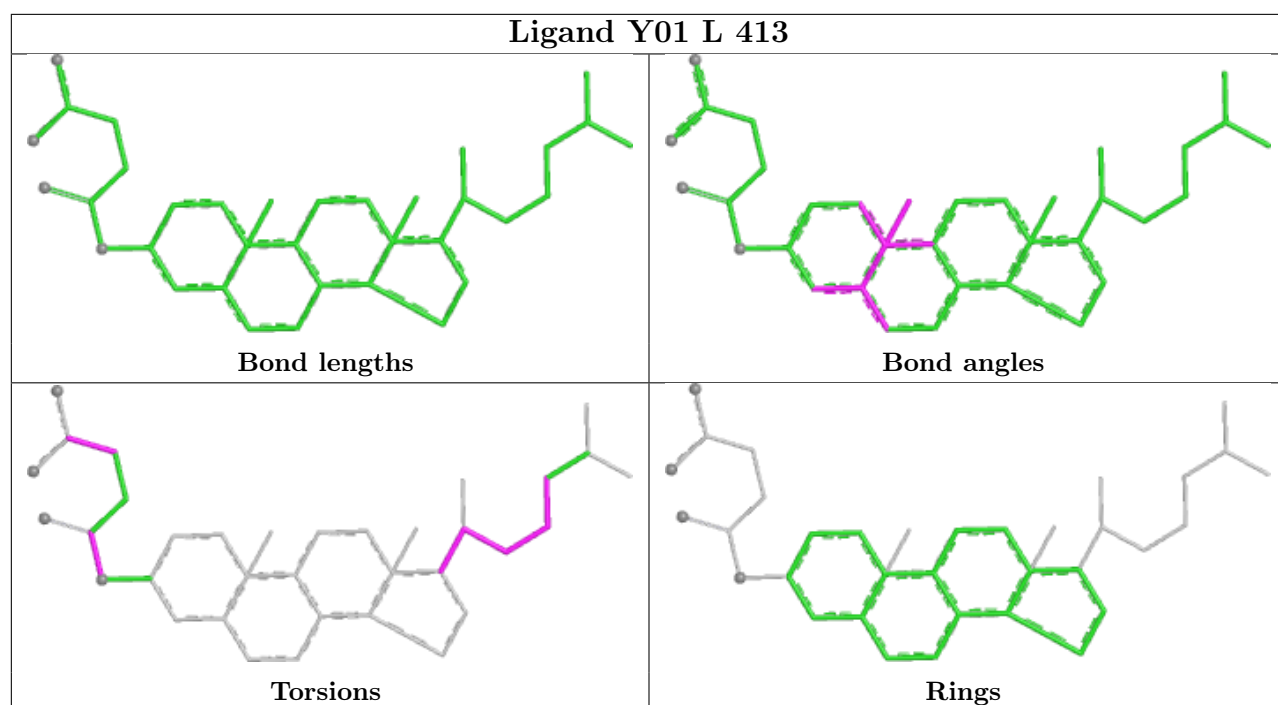
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

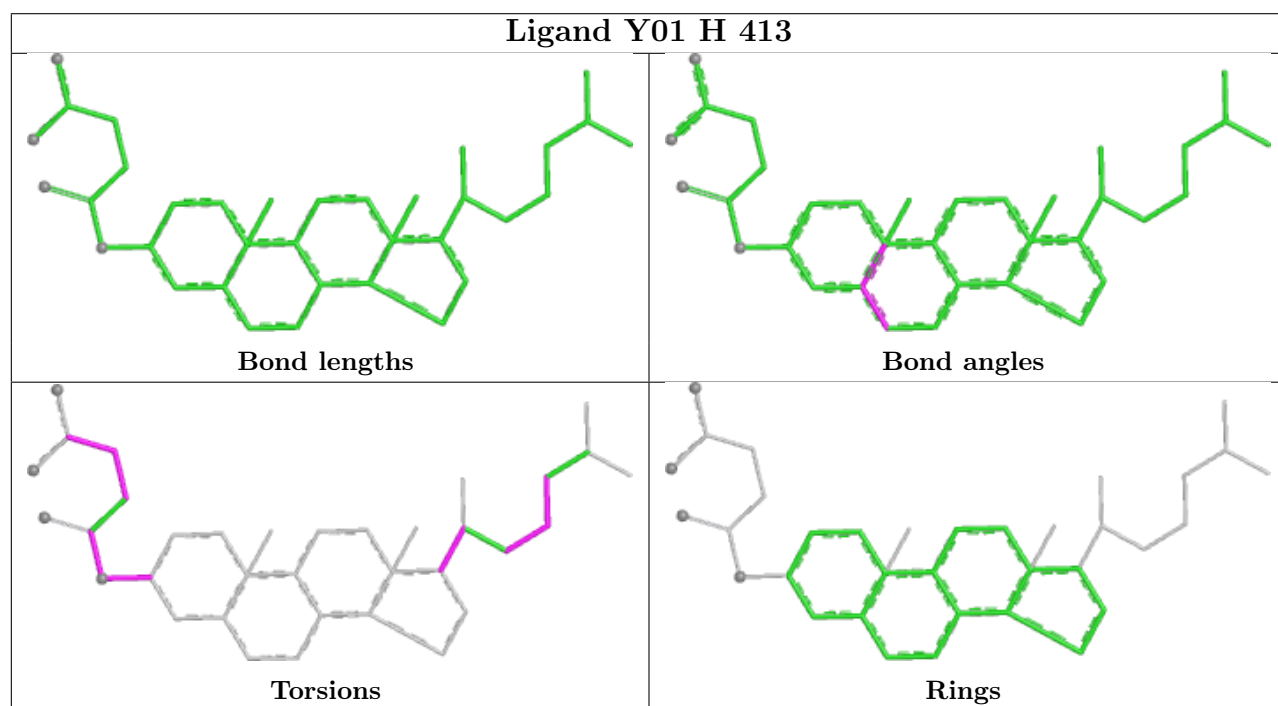
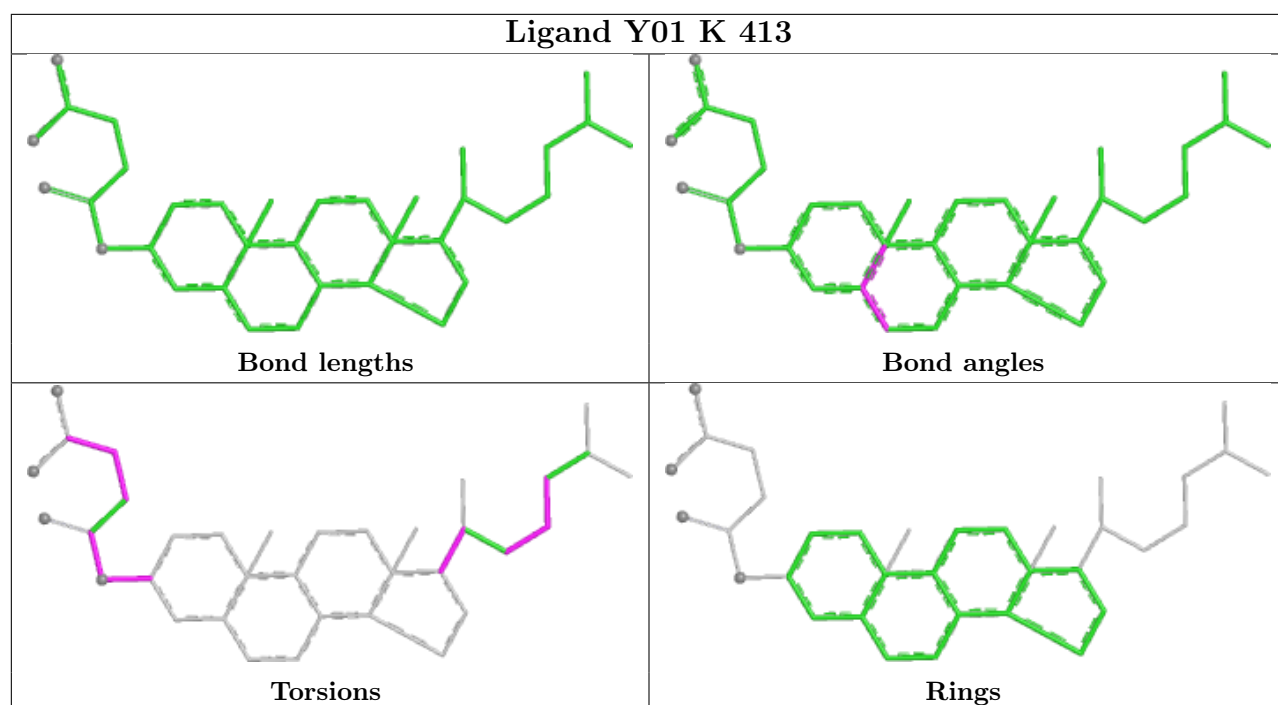
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

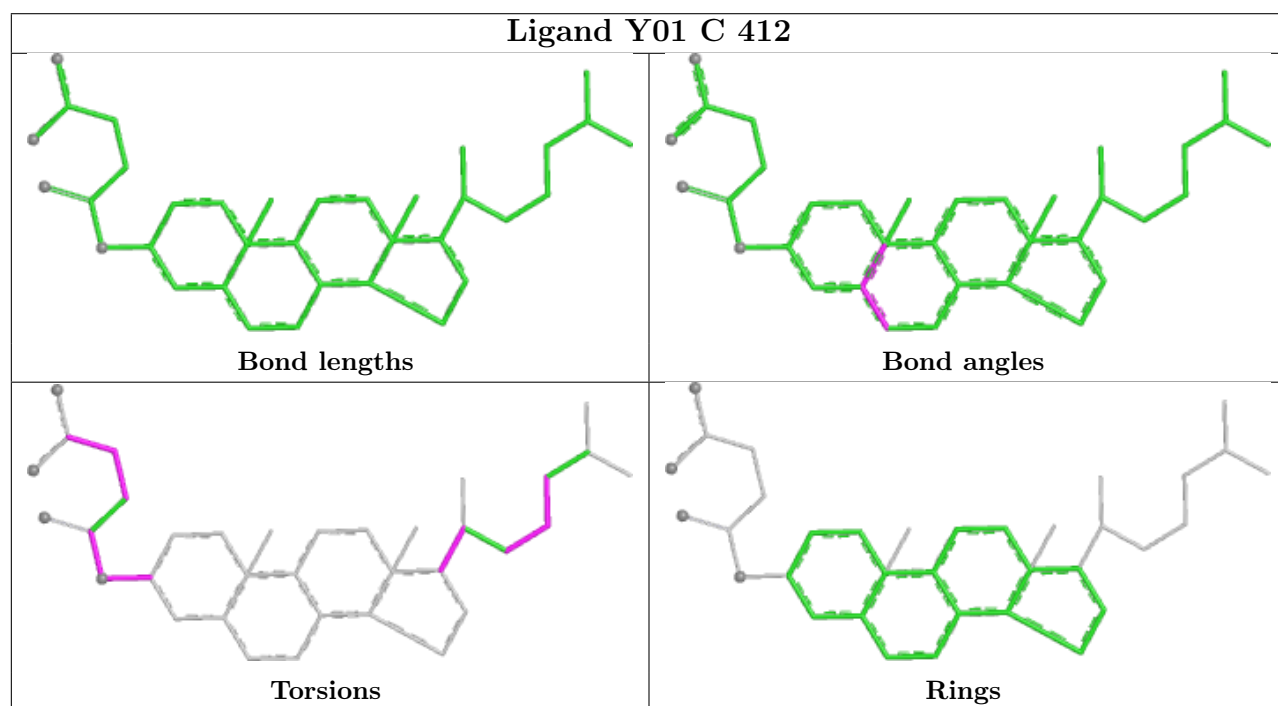
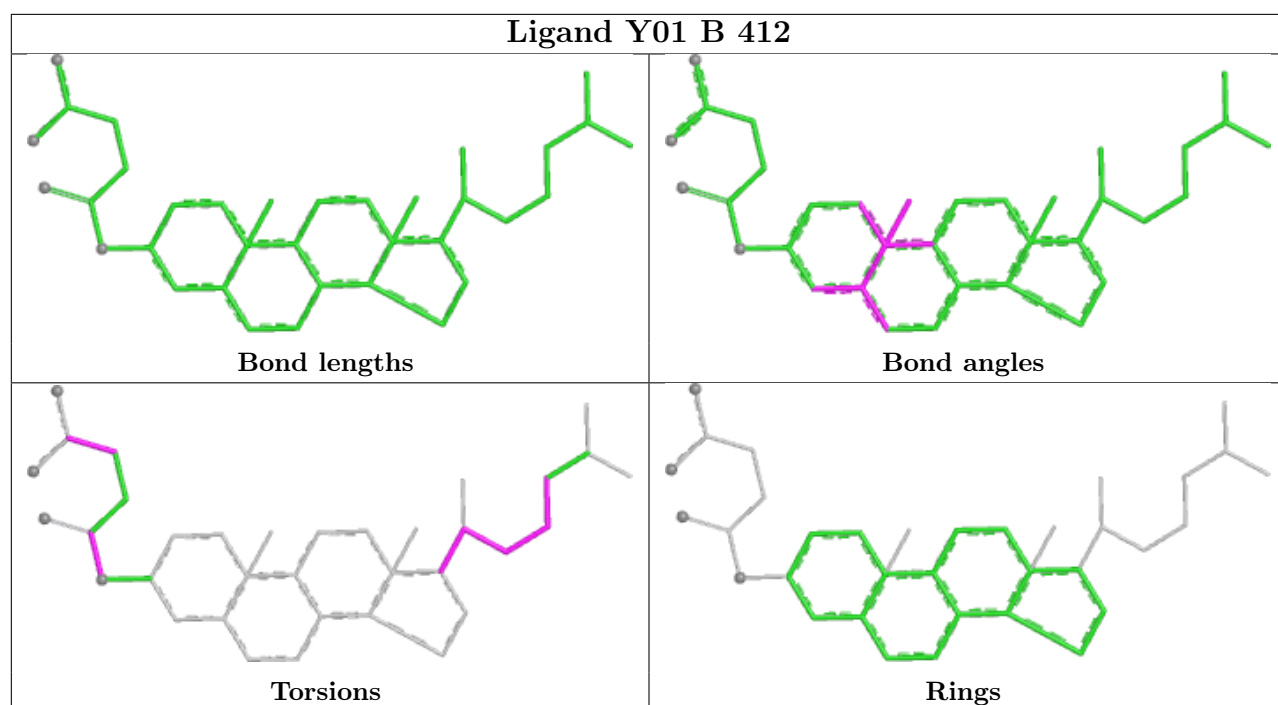


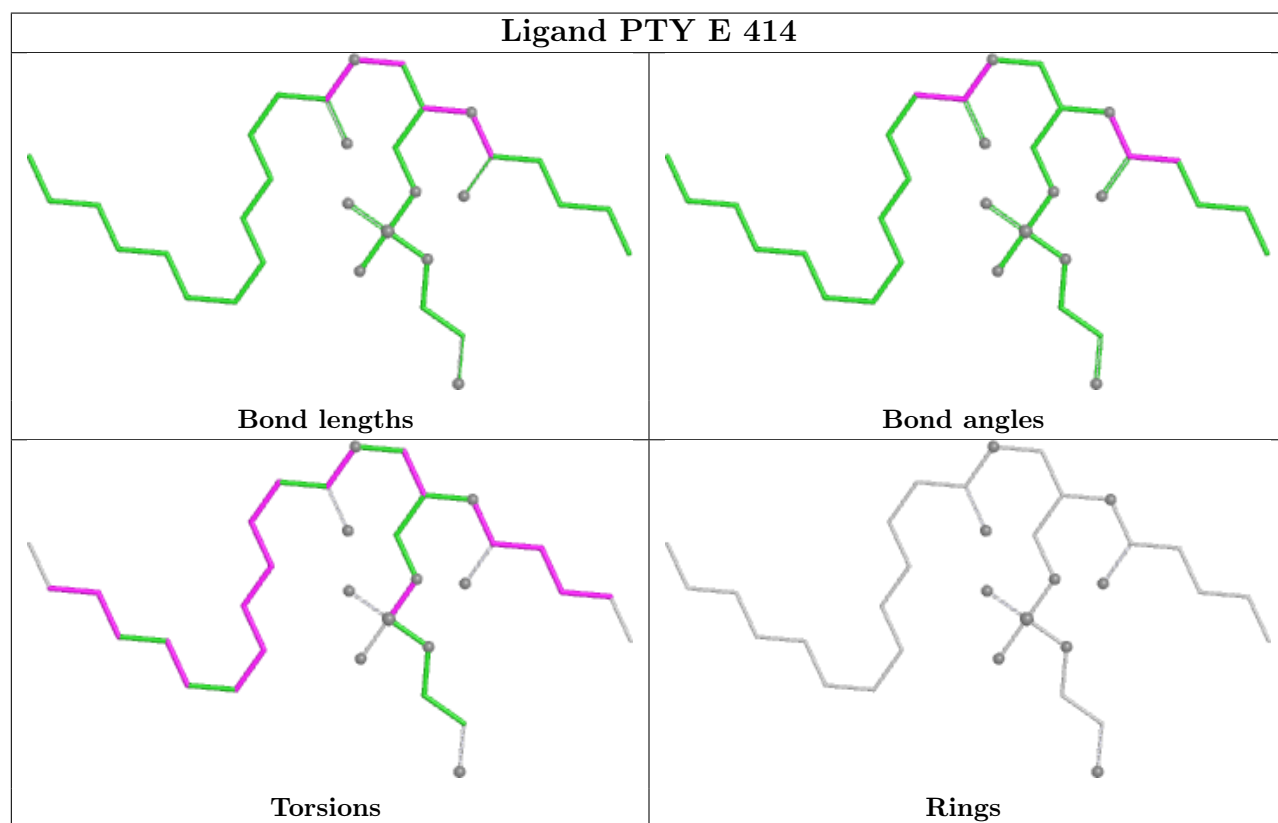
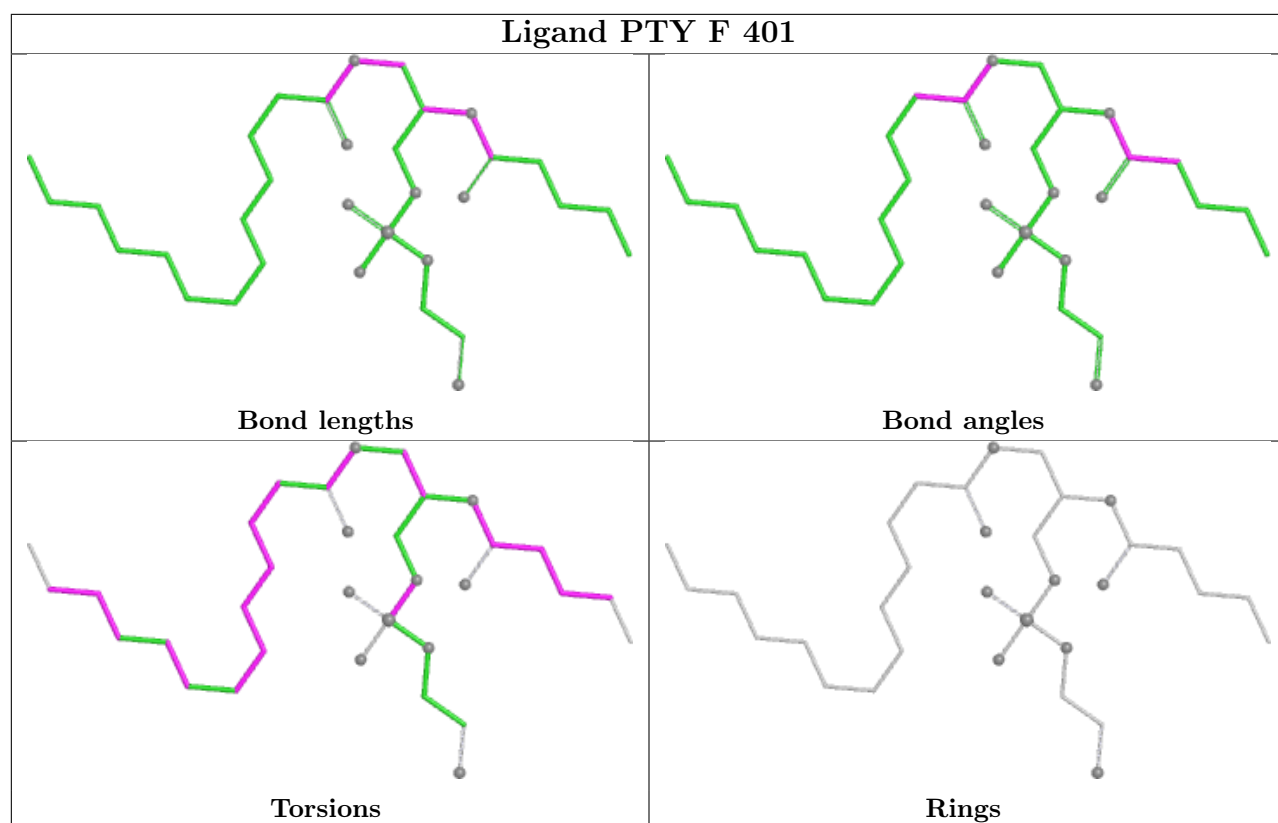


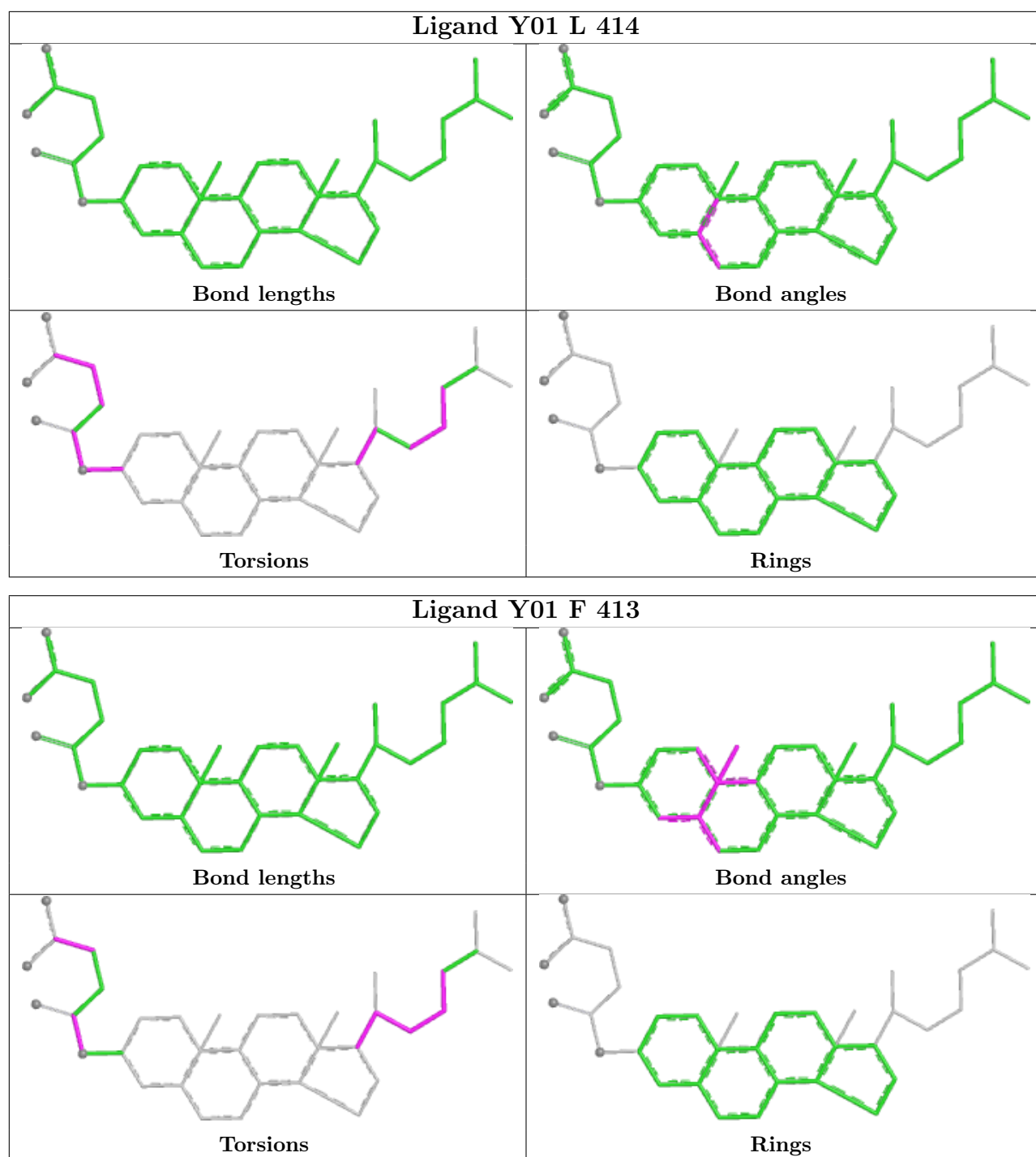


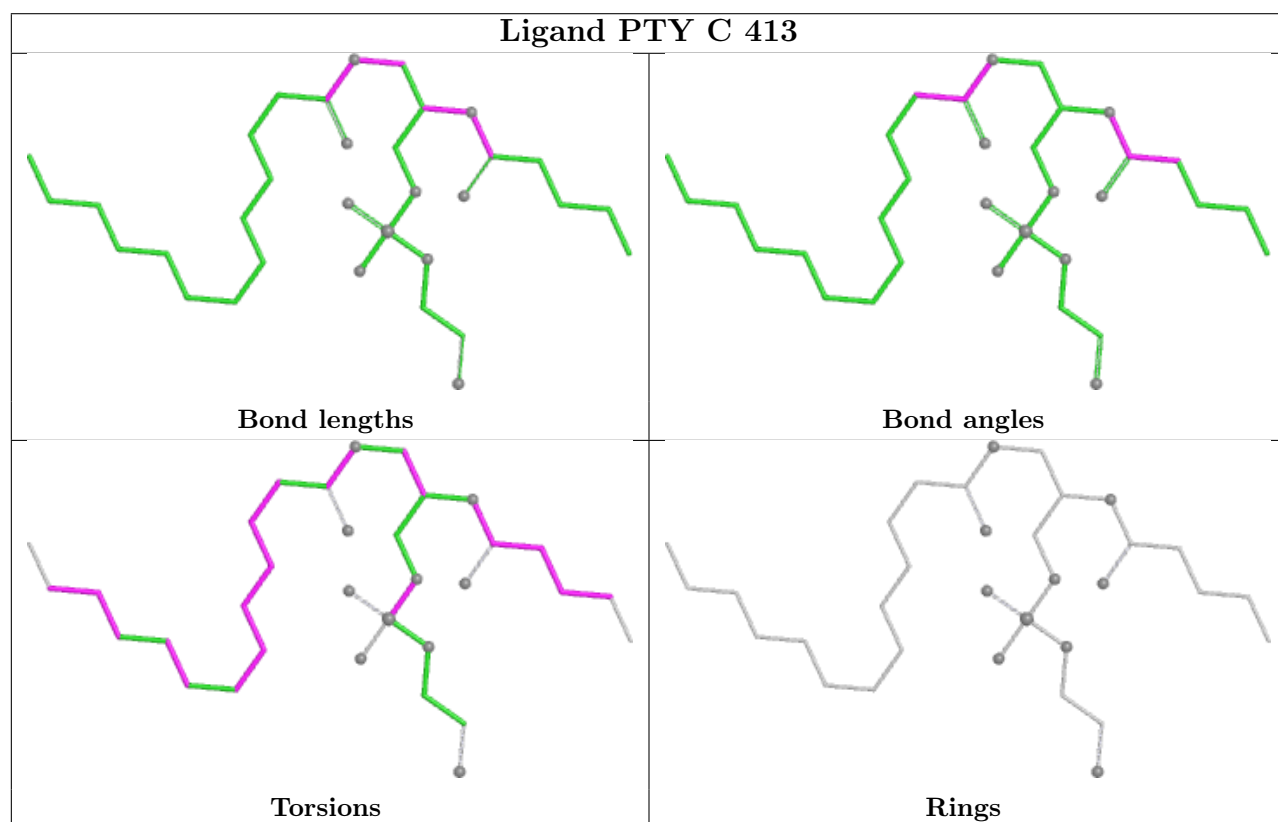
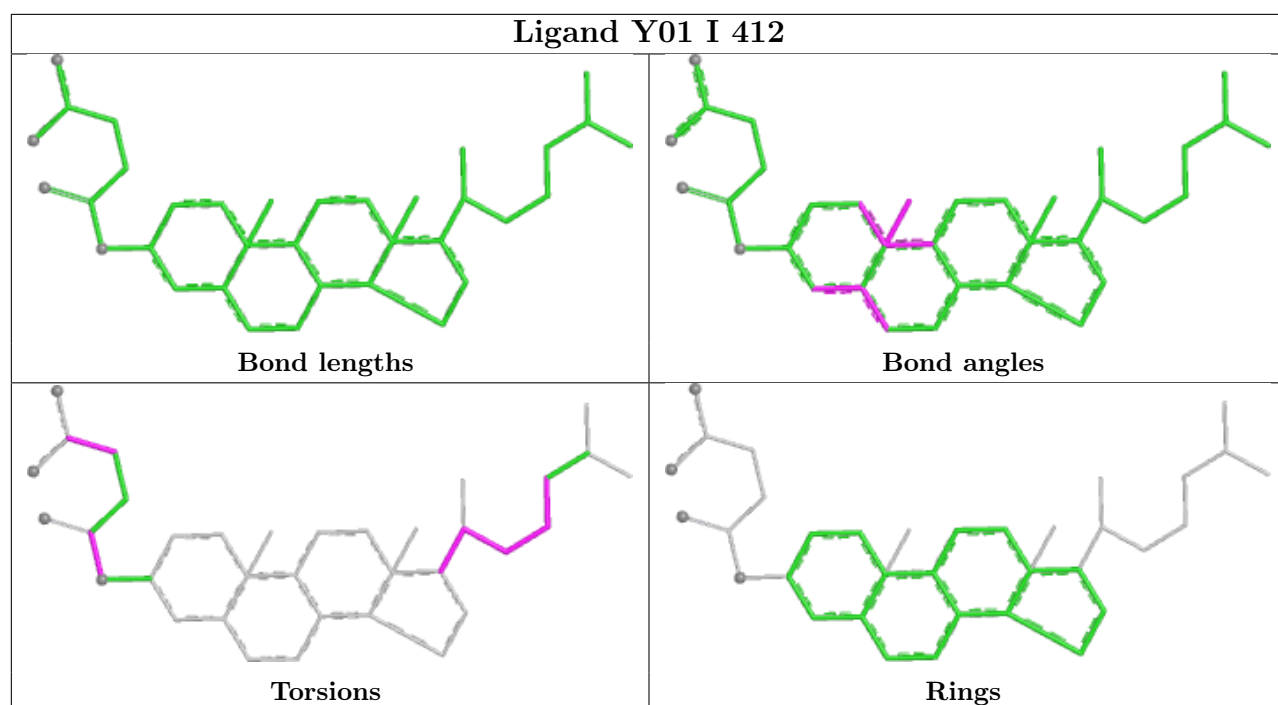


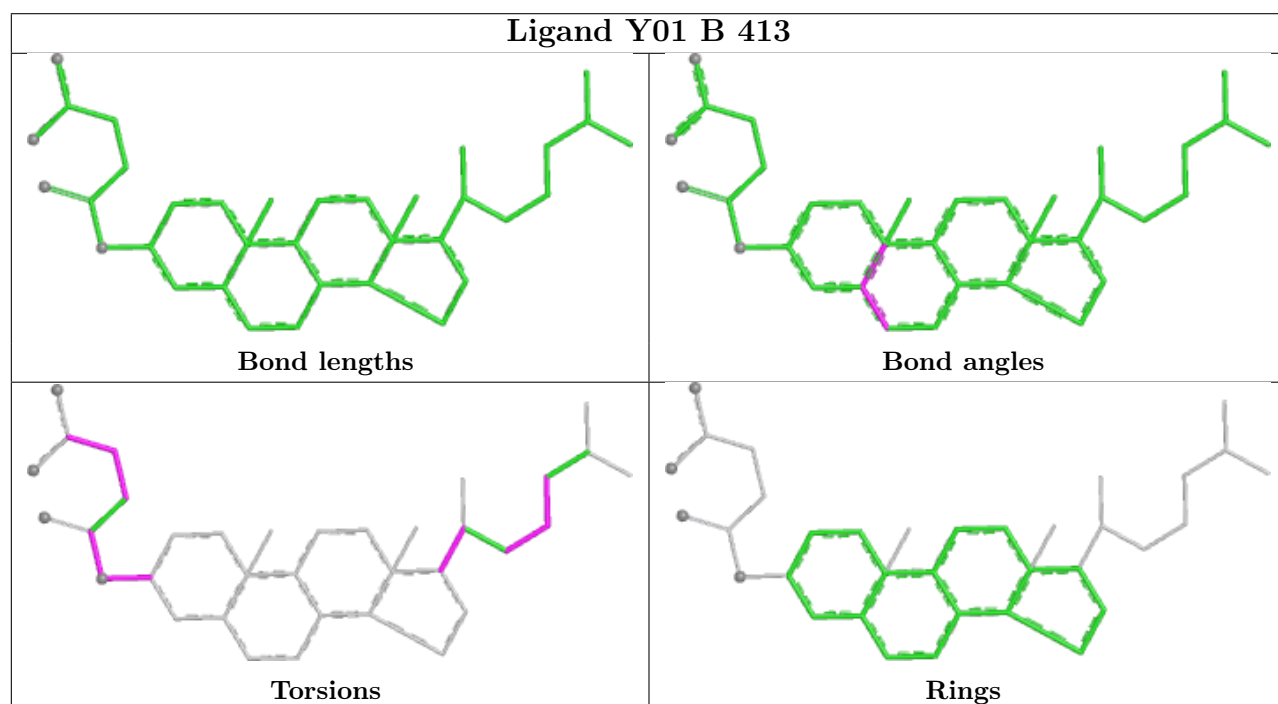
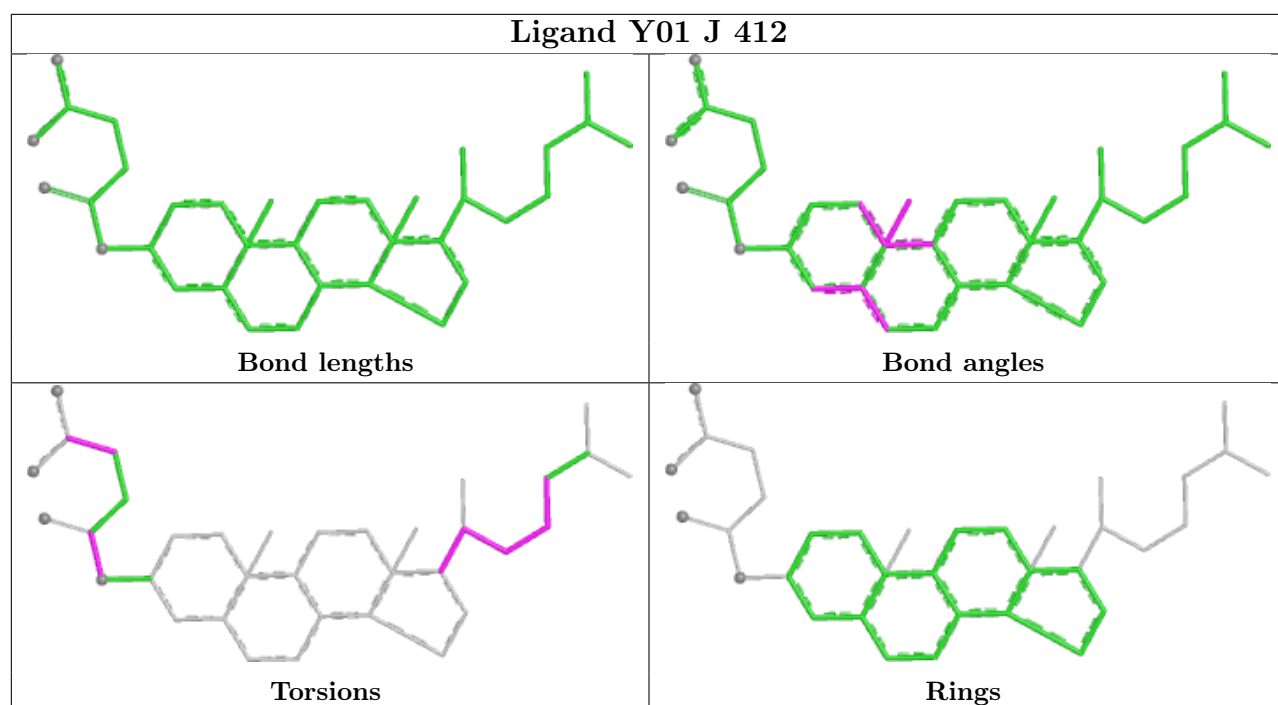


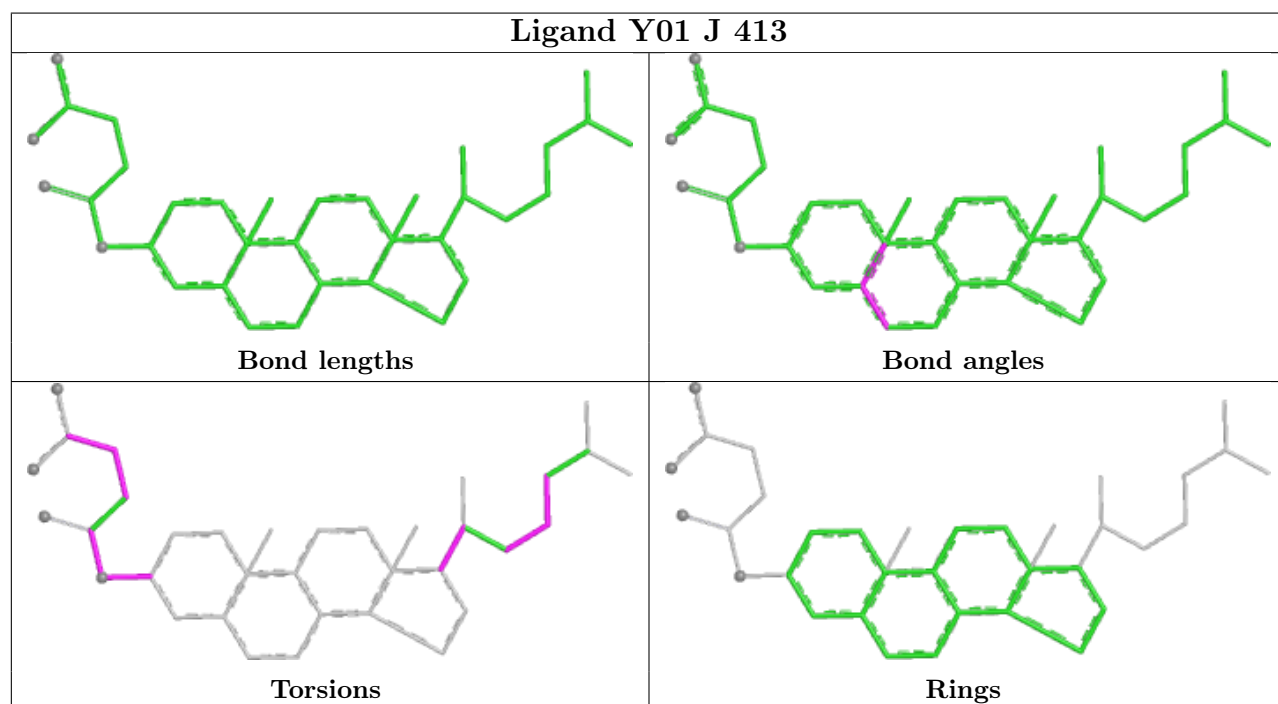
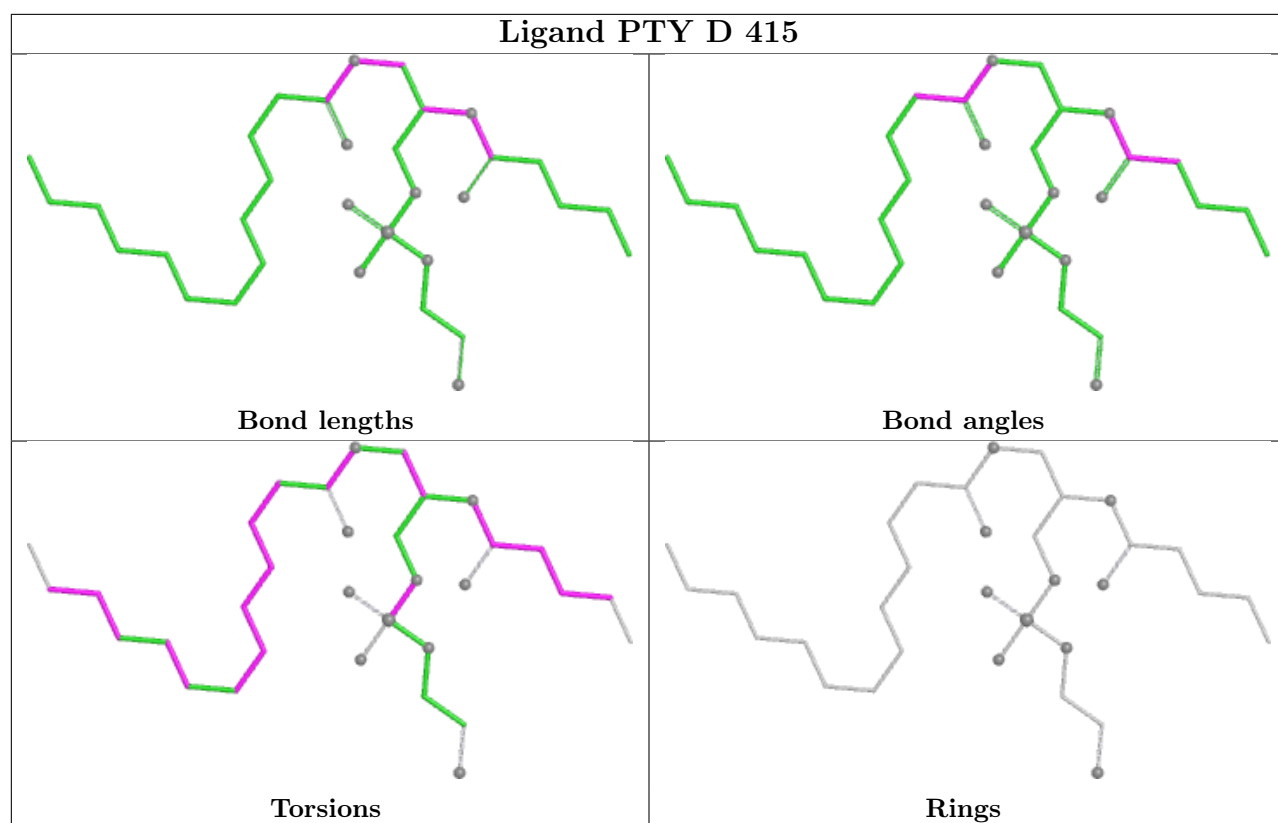


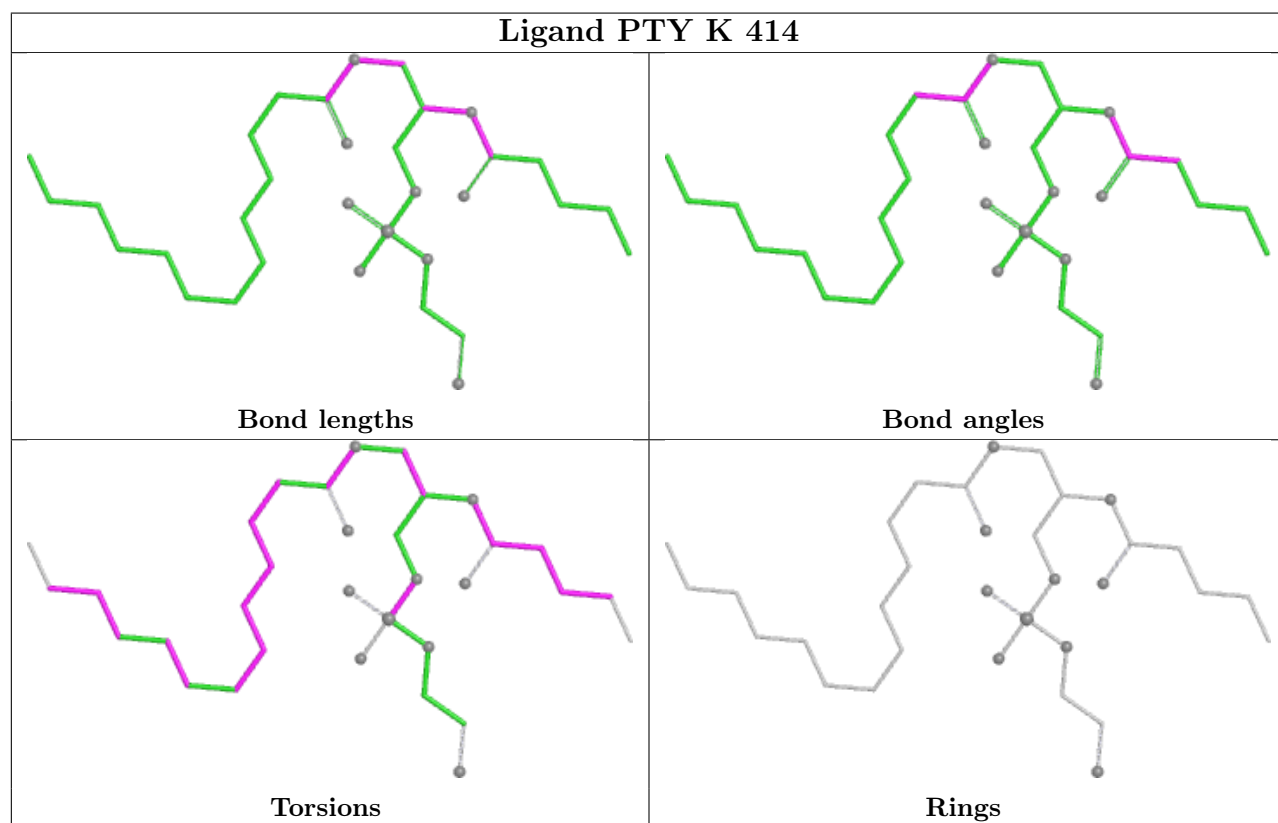
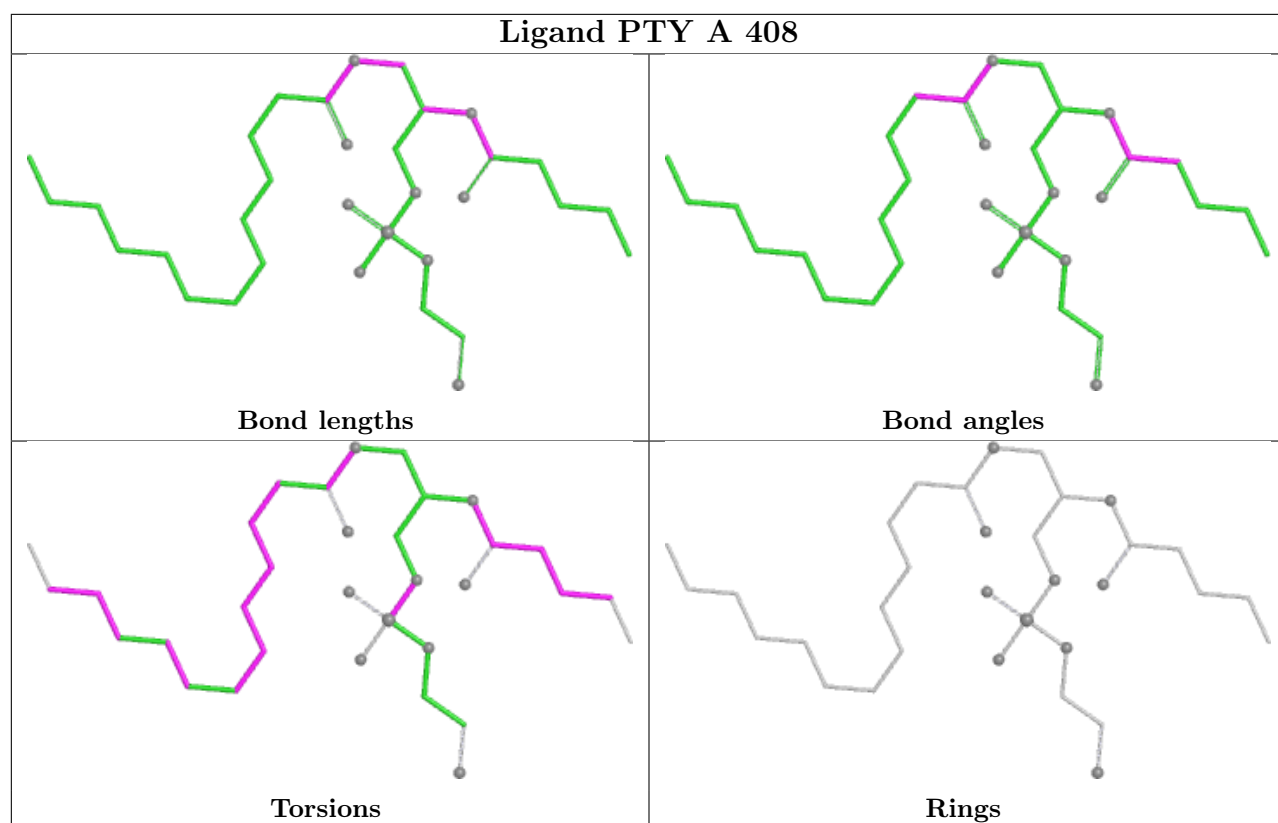


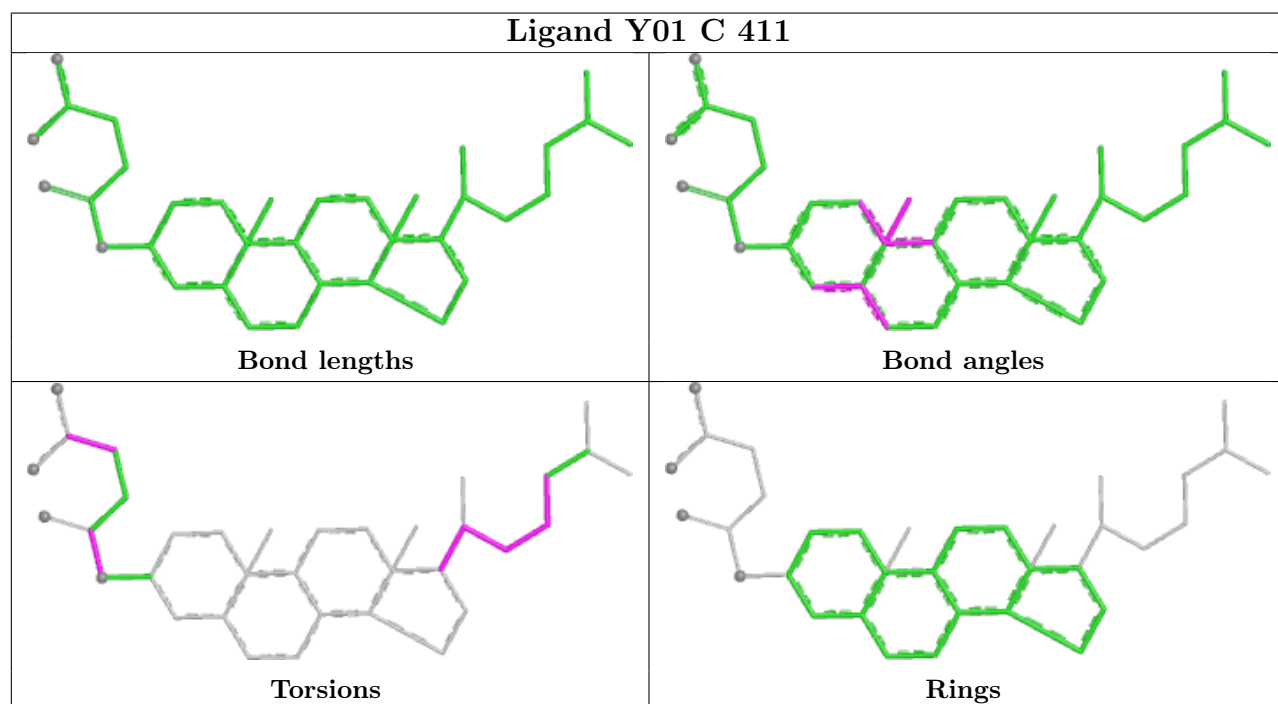
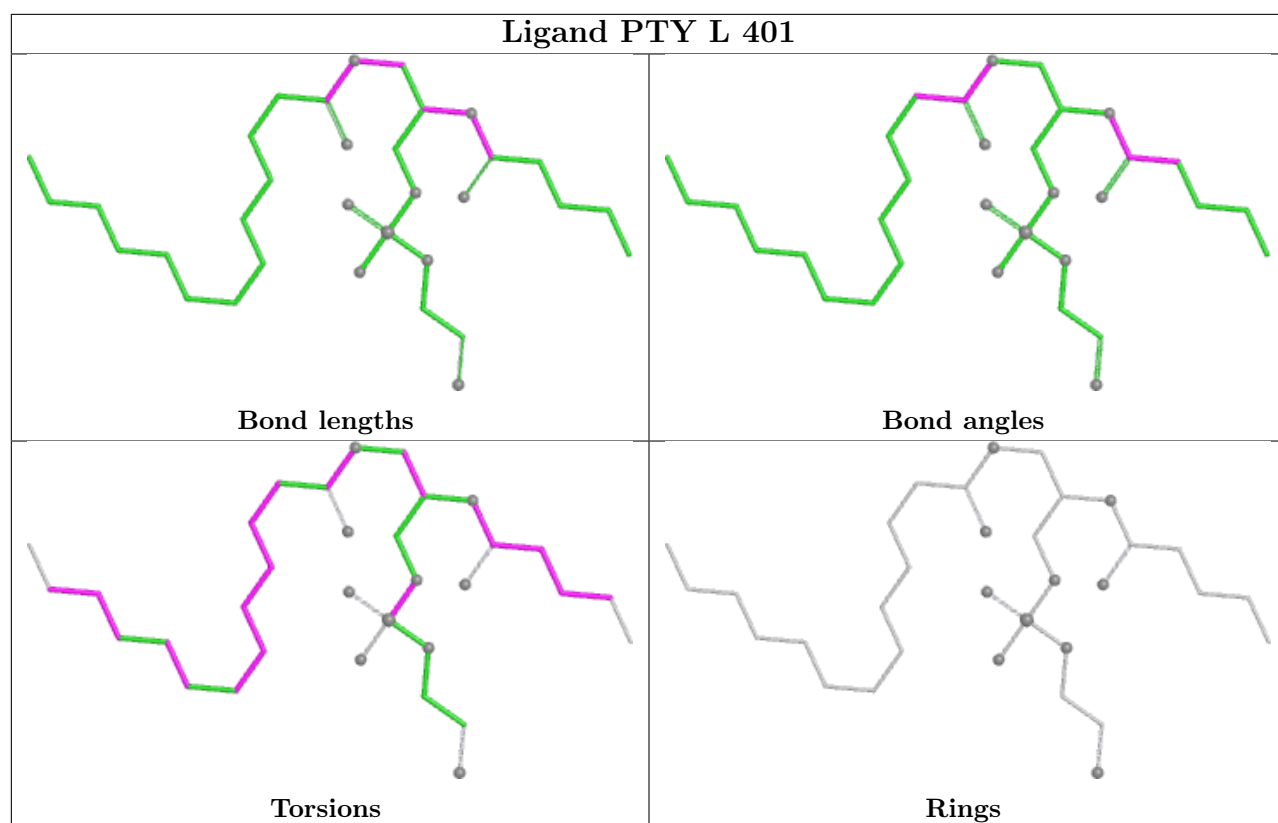


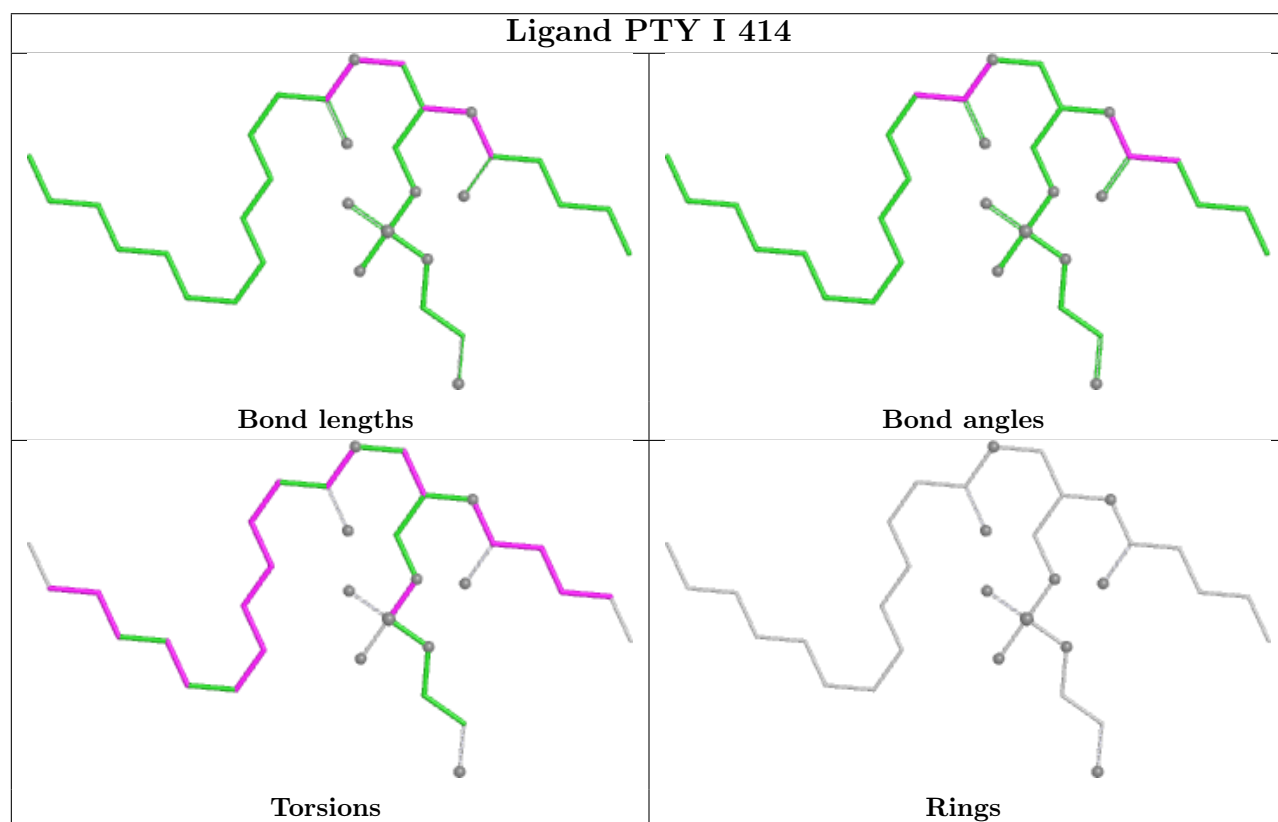
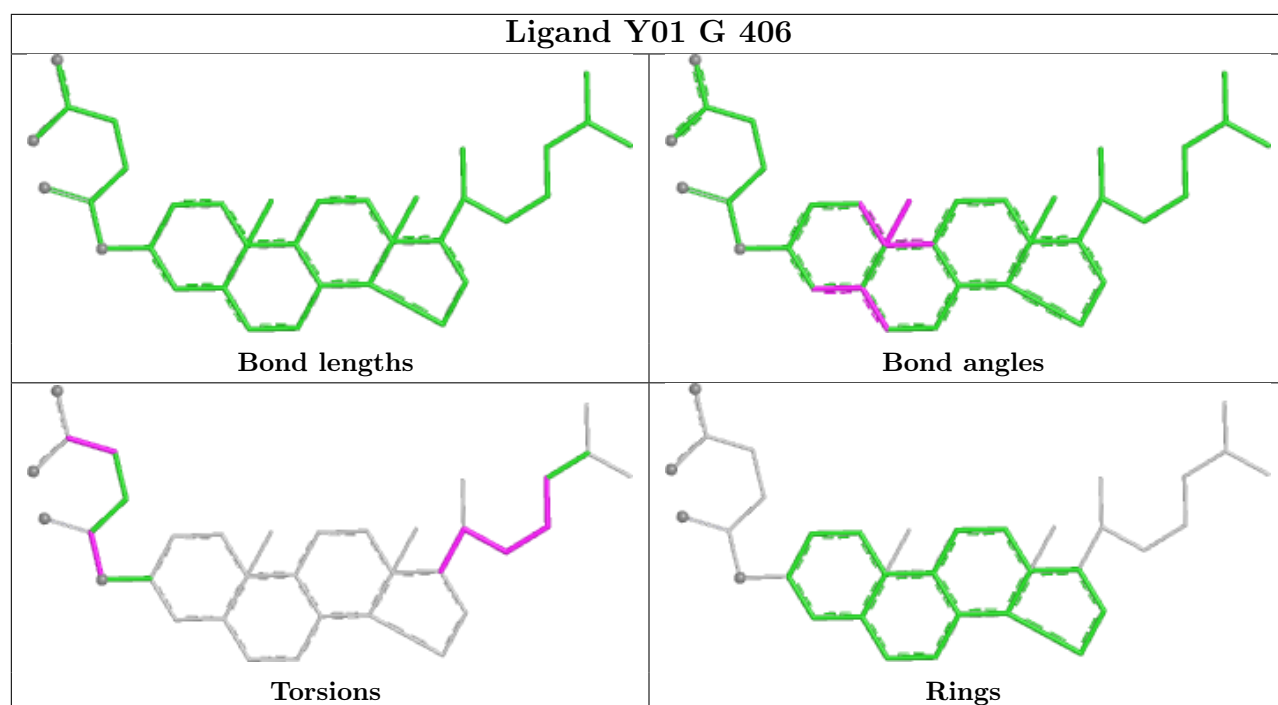


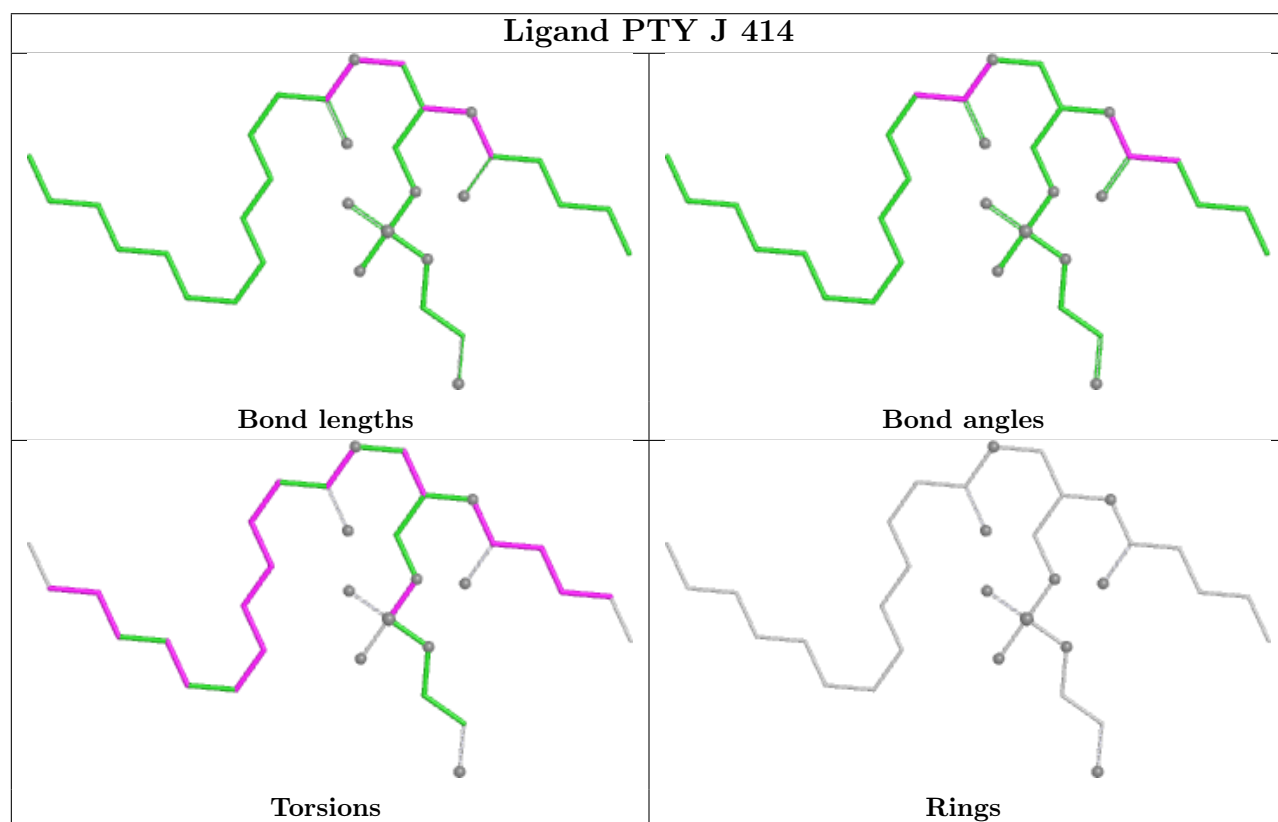
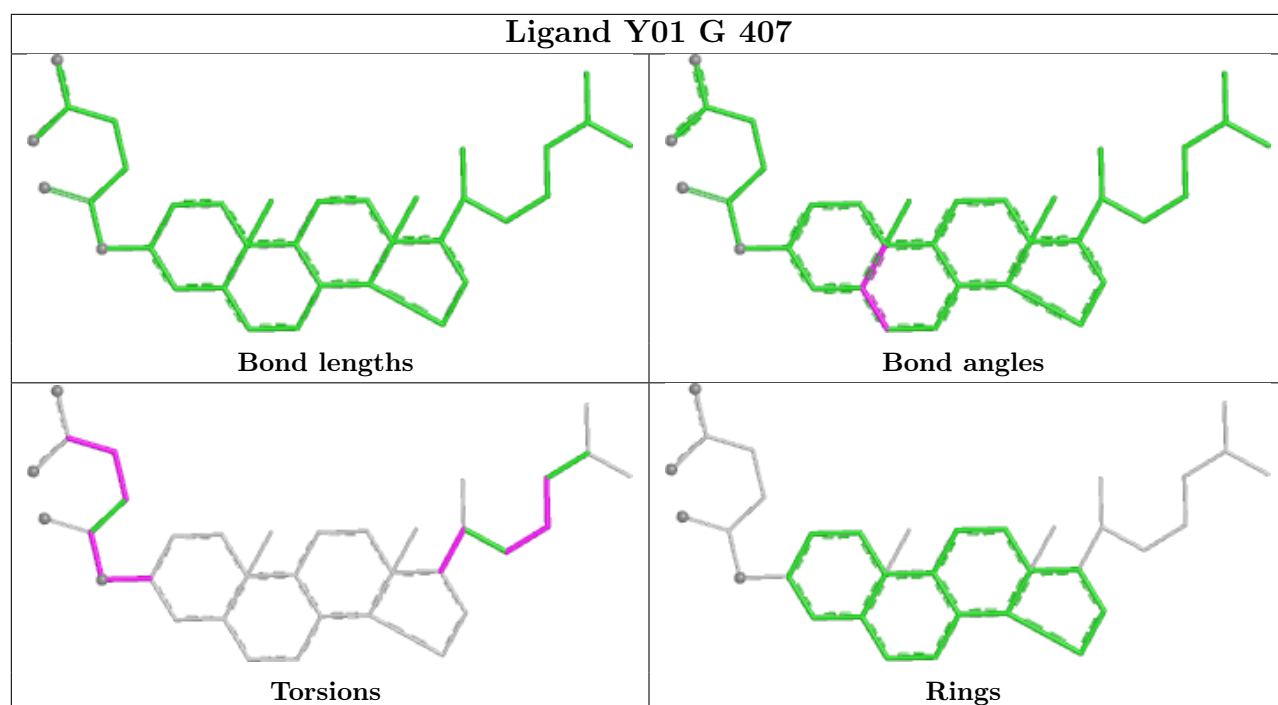


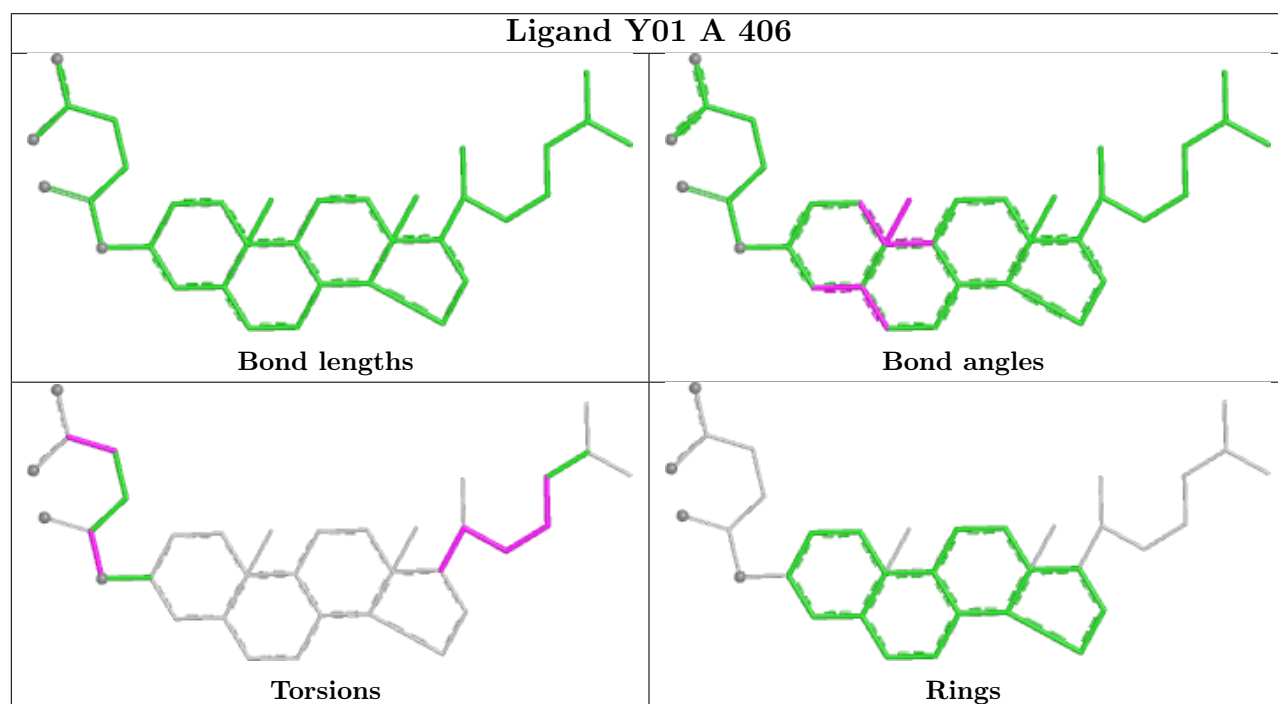
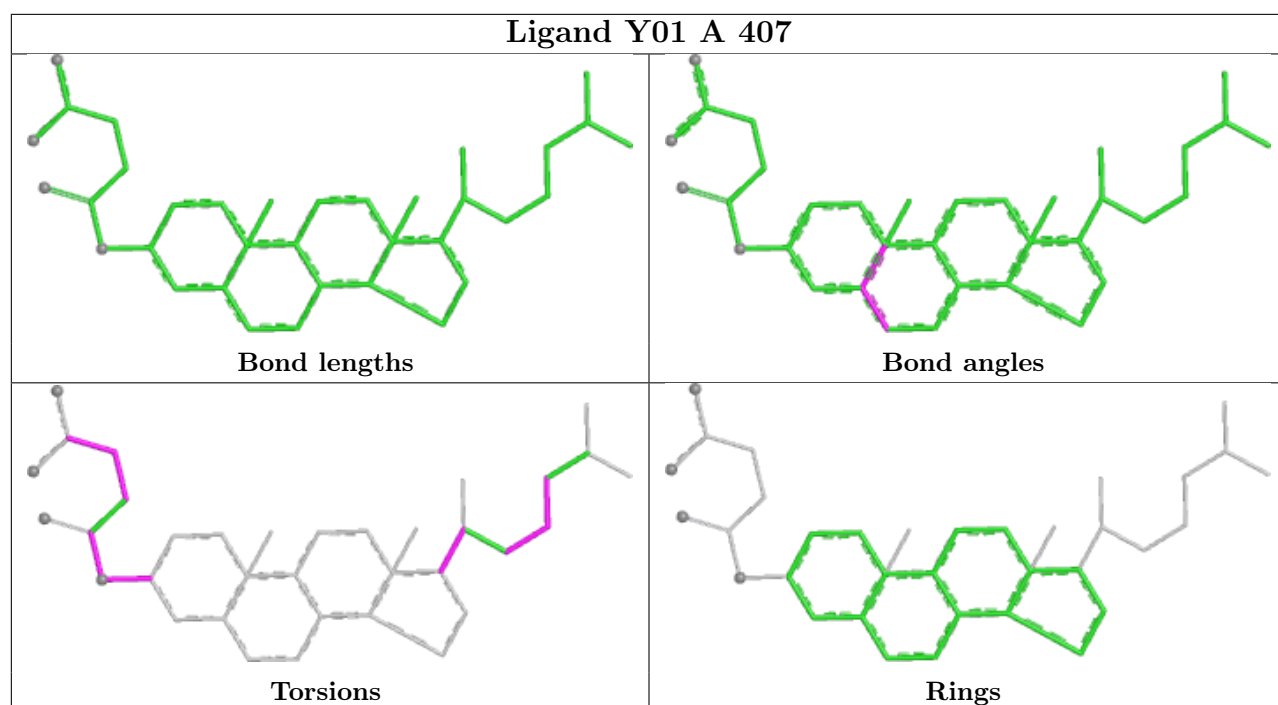


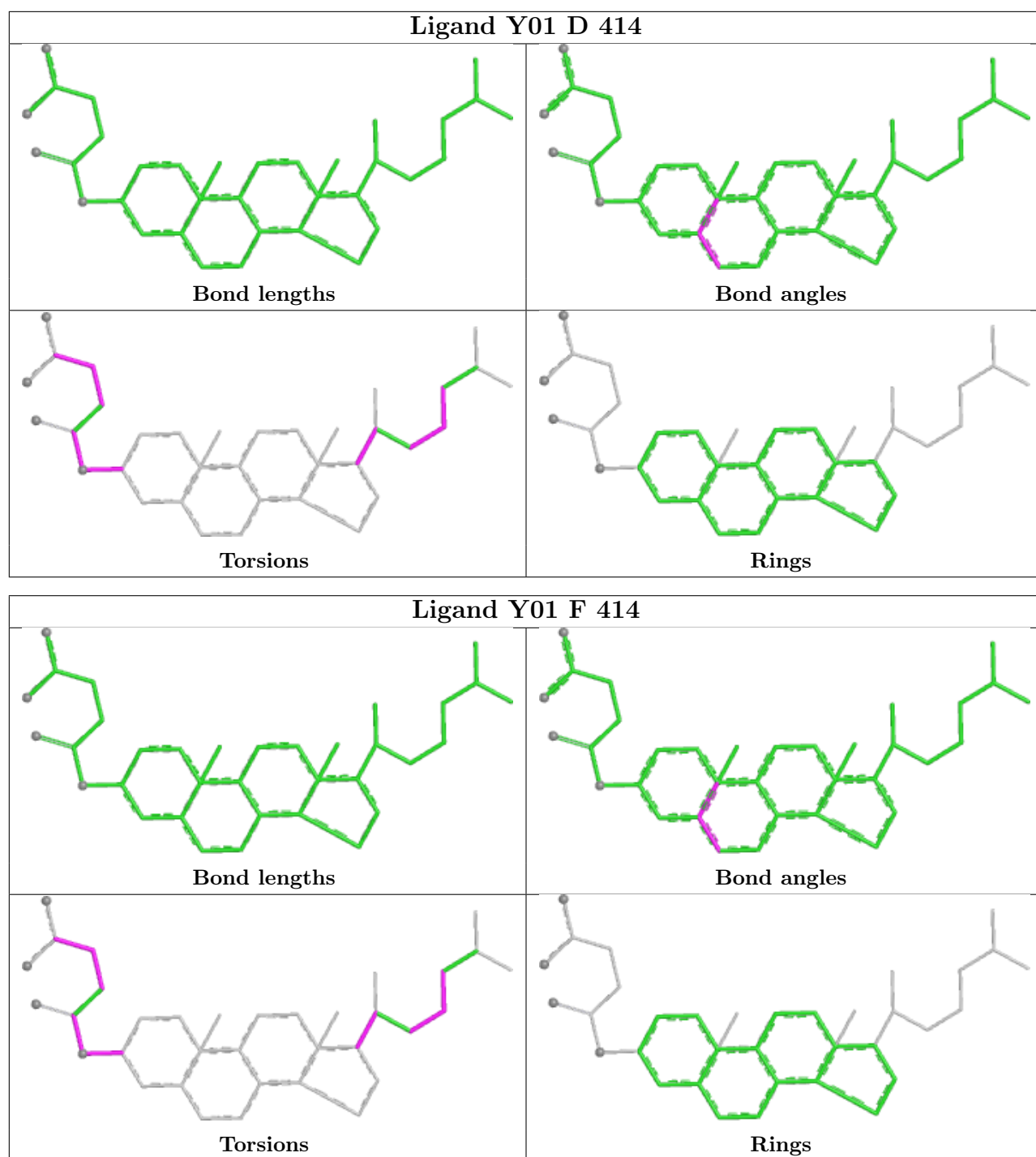


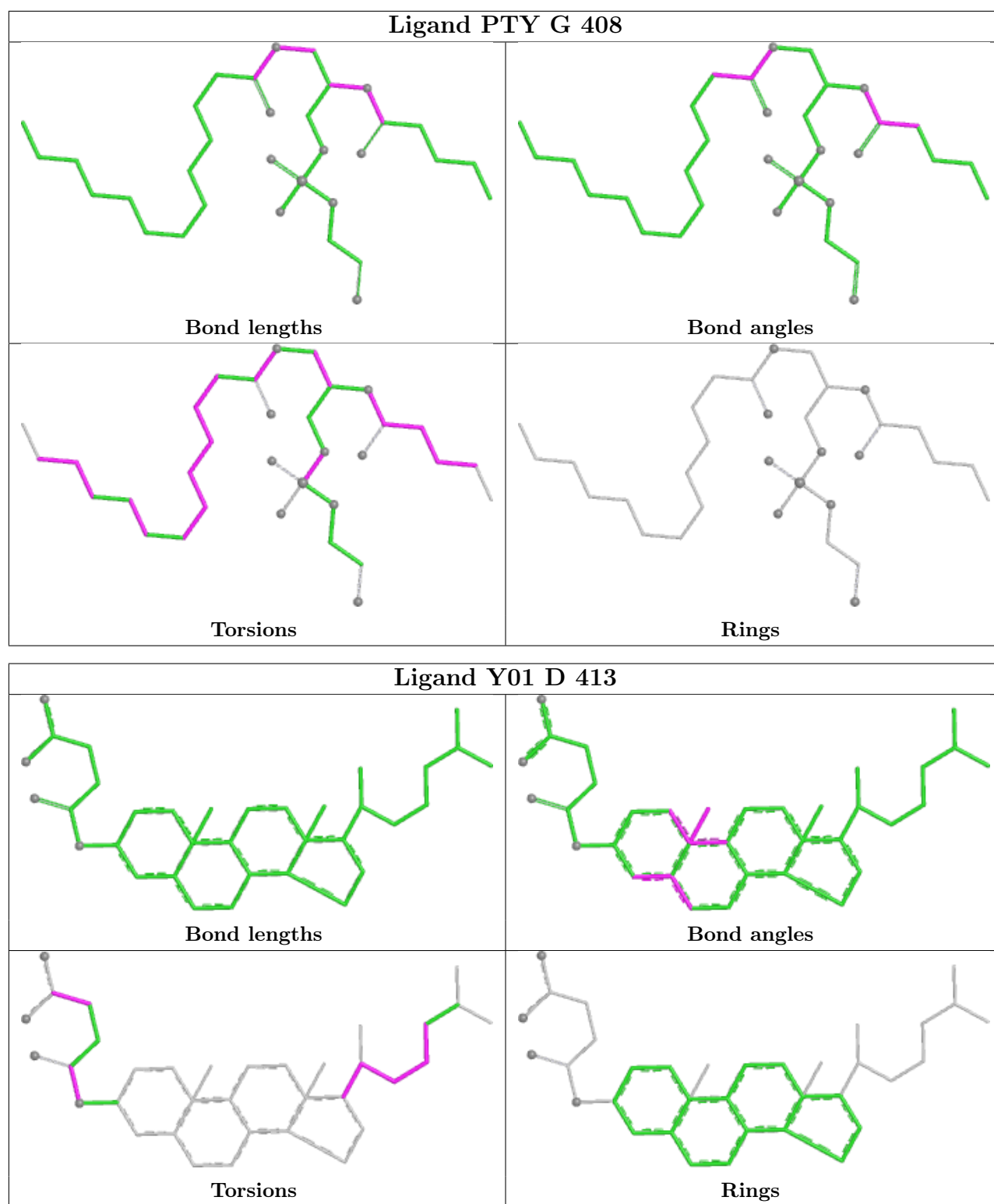












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

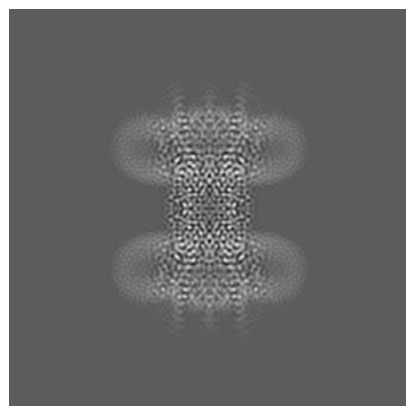
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33392. These allow visual inspection of the internal detail of the map and identification of artifacts.

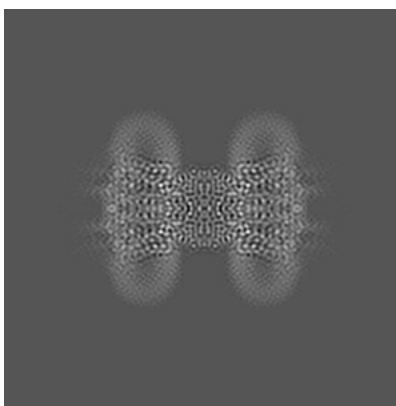
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

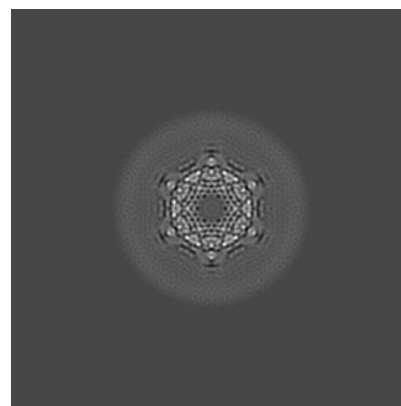
6.1.1 Primary map



X

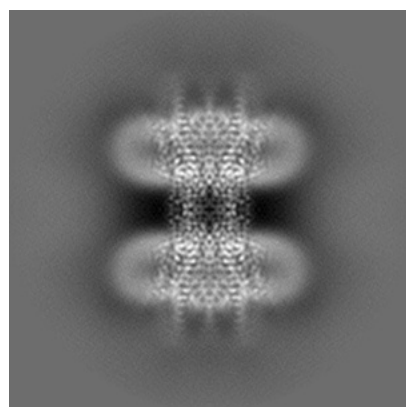


Y

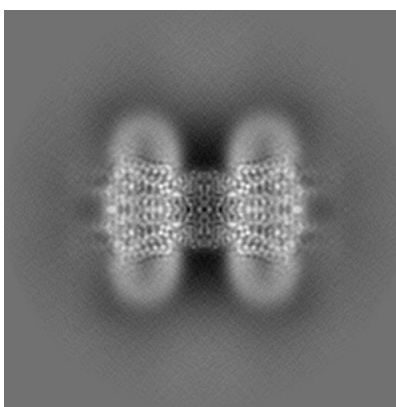


Z

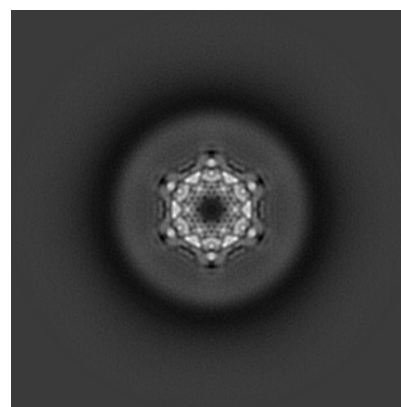
6.1.2 Raw map



X



Y

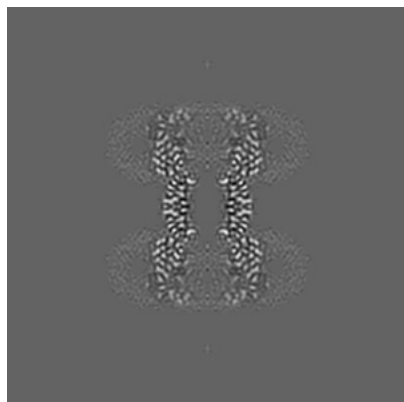


Z

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

6.2 Central slices [i](#)

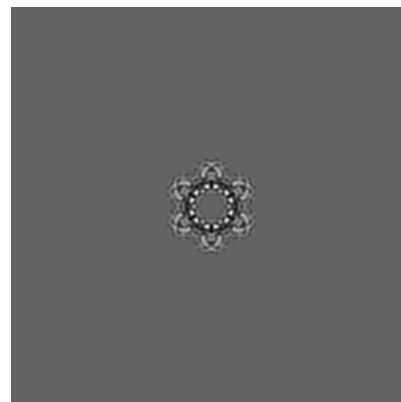
6.2.1 Primary map



X Index: 210

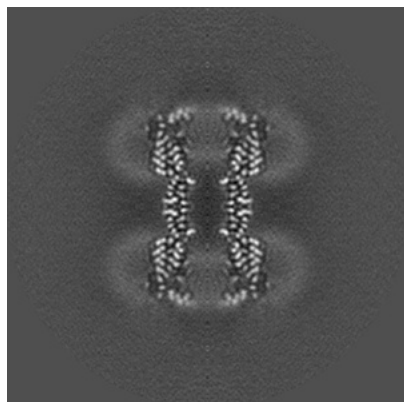


Y Index: 210

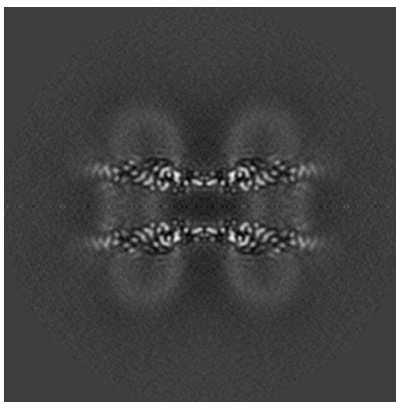


Z Index: 210

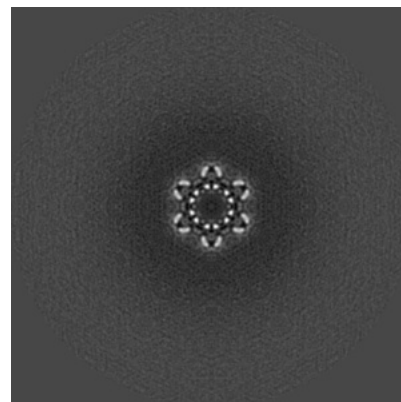
6.2.2 Raw map



X Index: 210



Y Index: 210

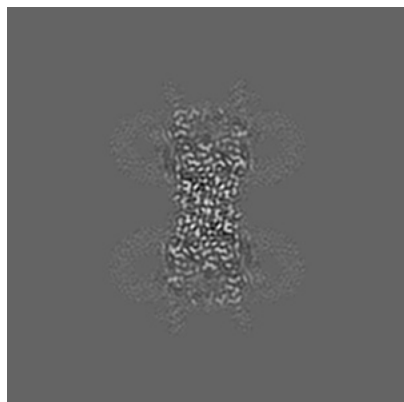


Z Index: 210

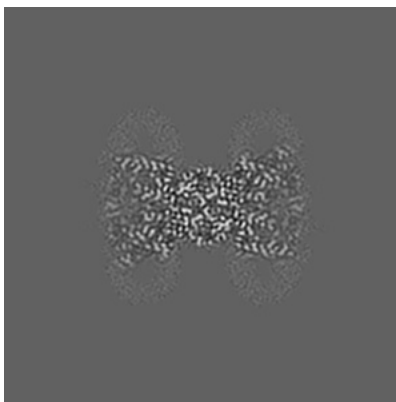
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

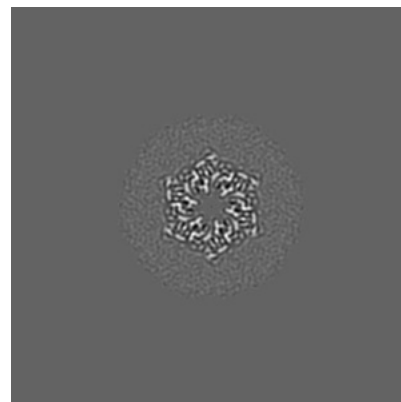
6.3.1 Primary map



X Index: 234

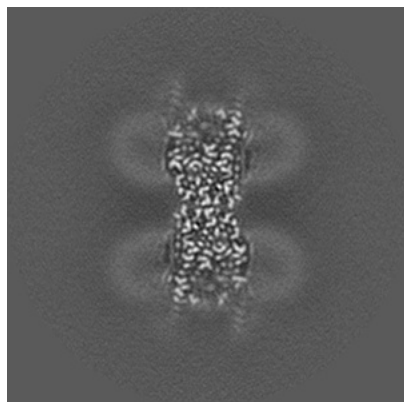


Y Index: 188

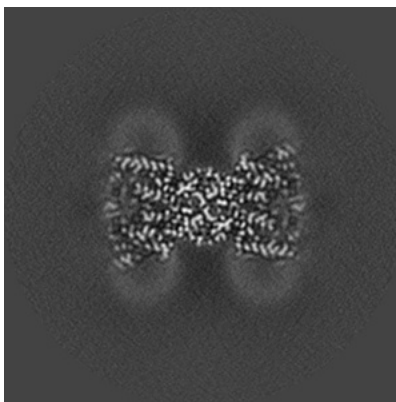


Z Index: 248

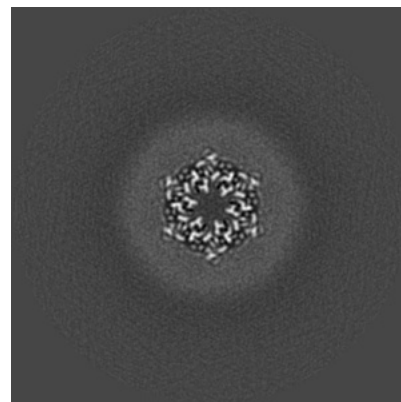
6.3.2 Raw map



X Index: 185



Y Index: 188

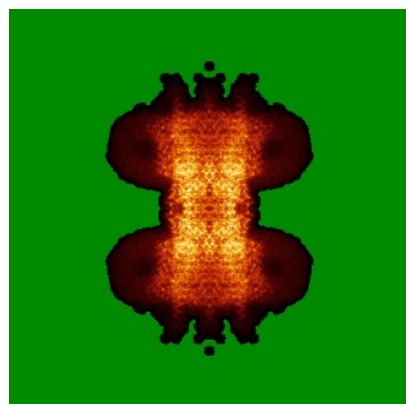


Z Index: 248

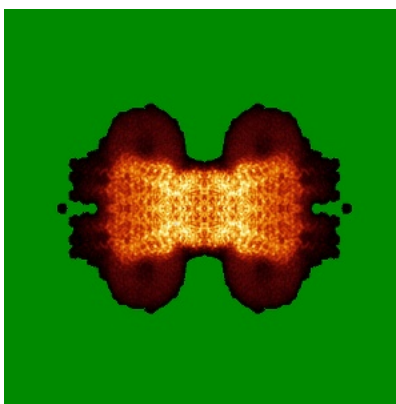
The images above show the largest variance slices of the map in three orthogonal directions.

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

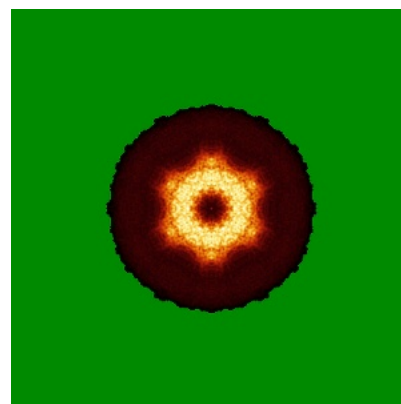
6.4.1 Primary map



X

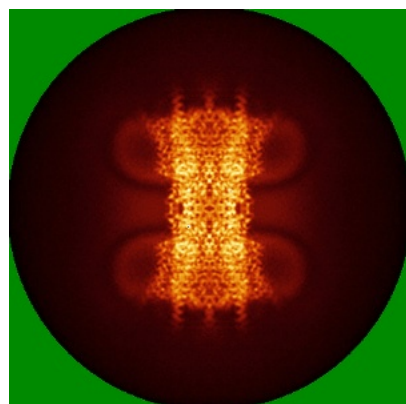


Y

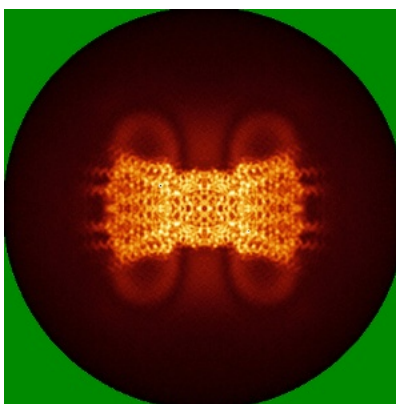


Z

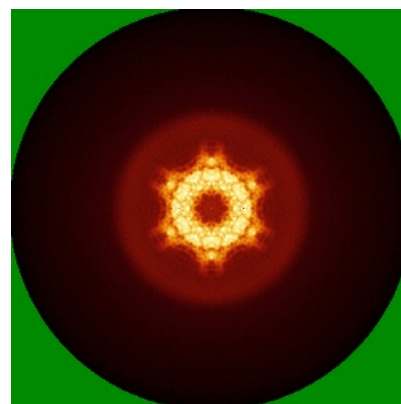
6.4.2 Raw map



X



Y

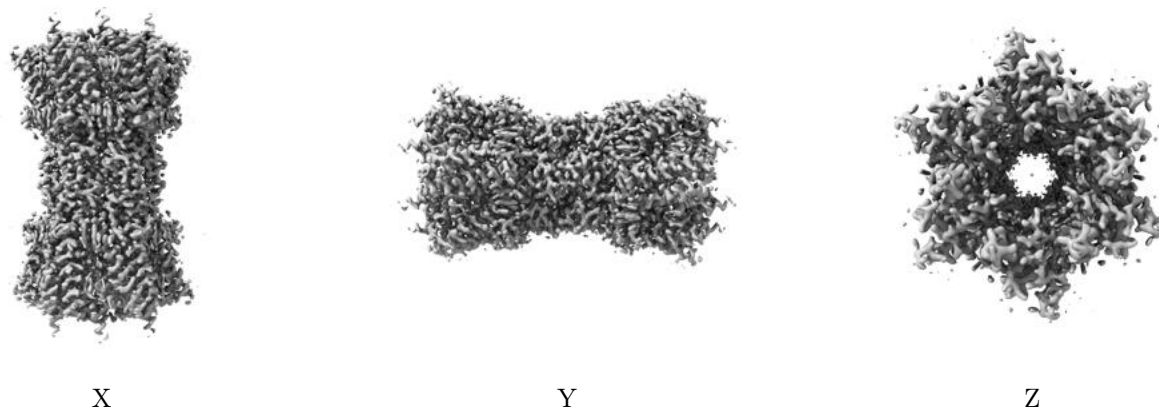


Z

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.

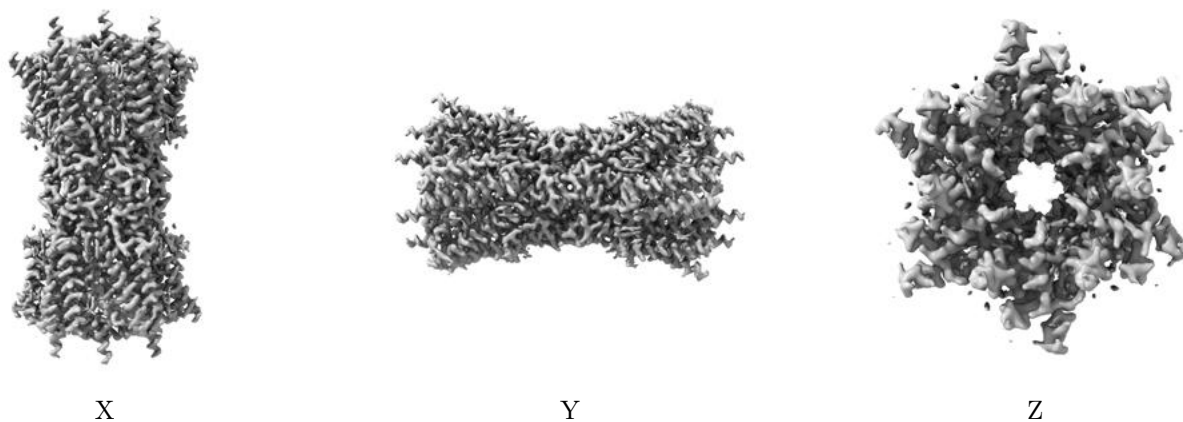
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

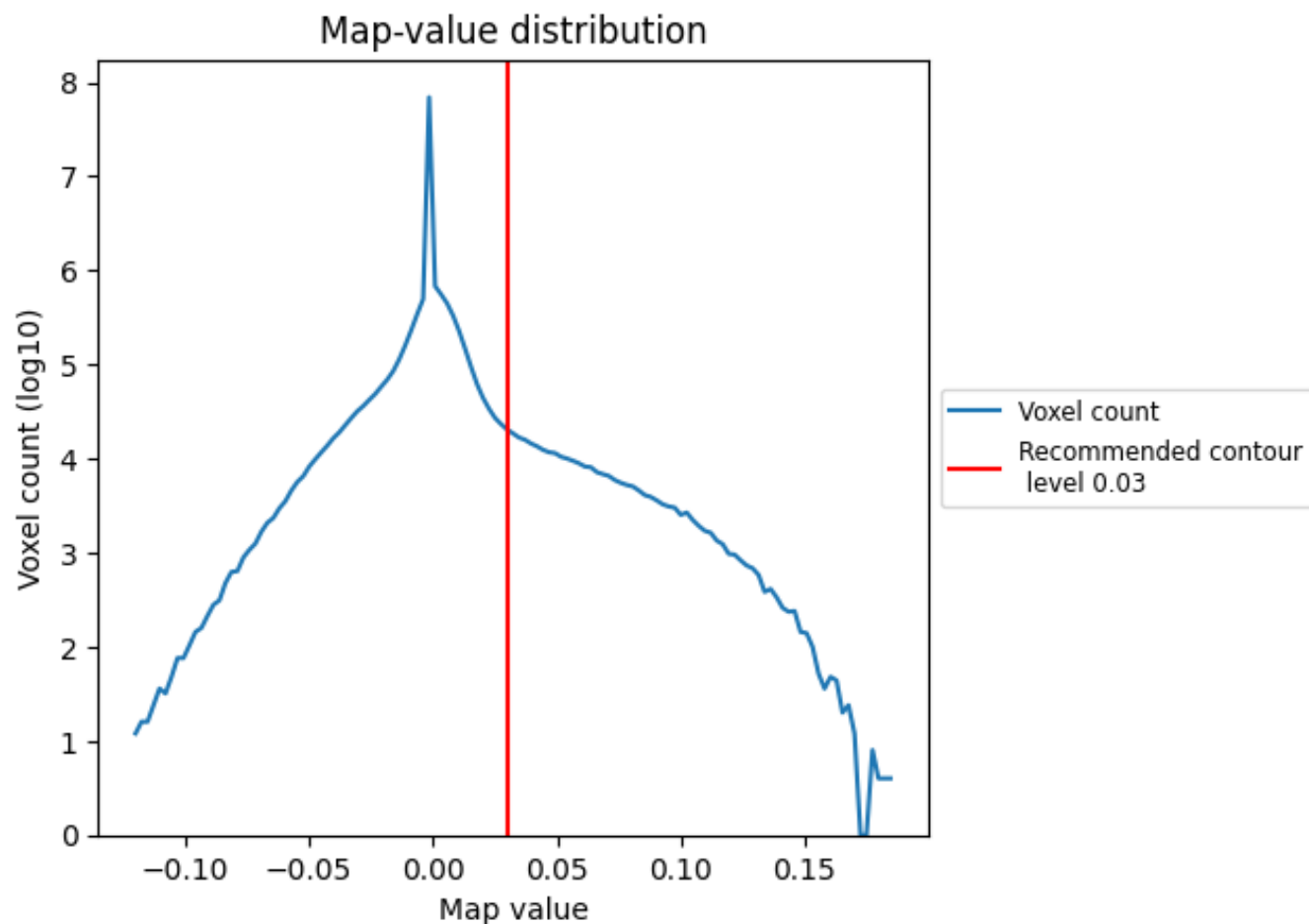
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

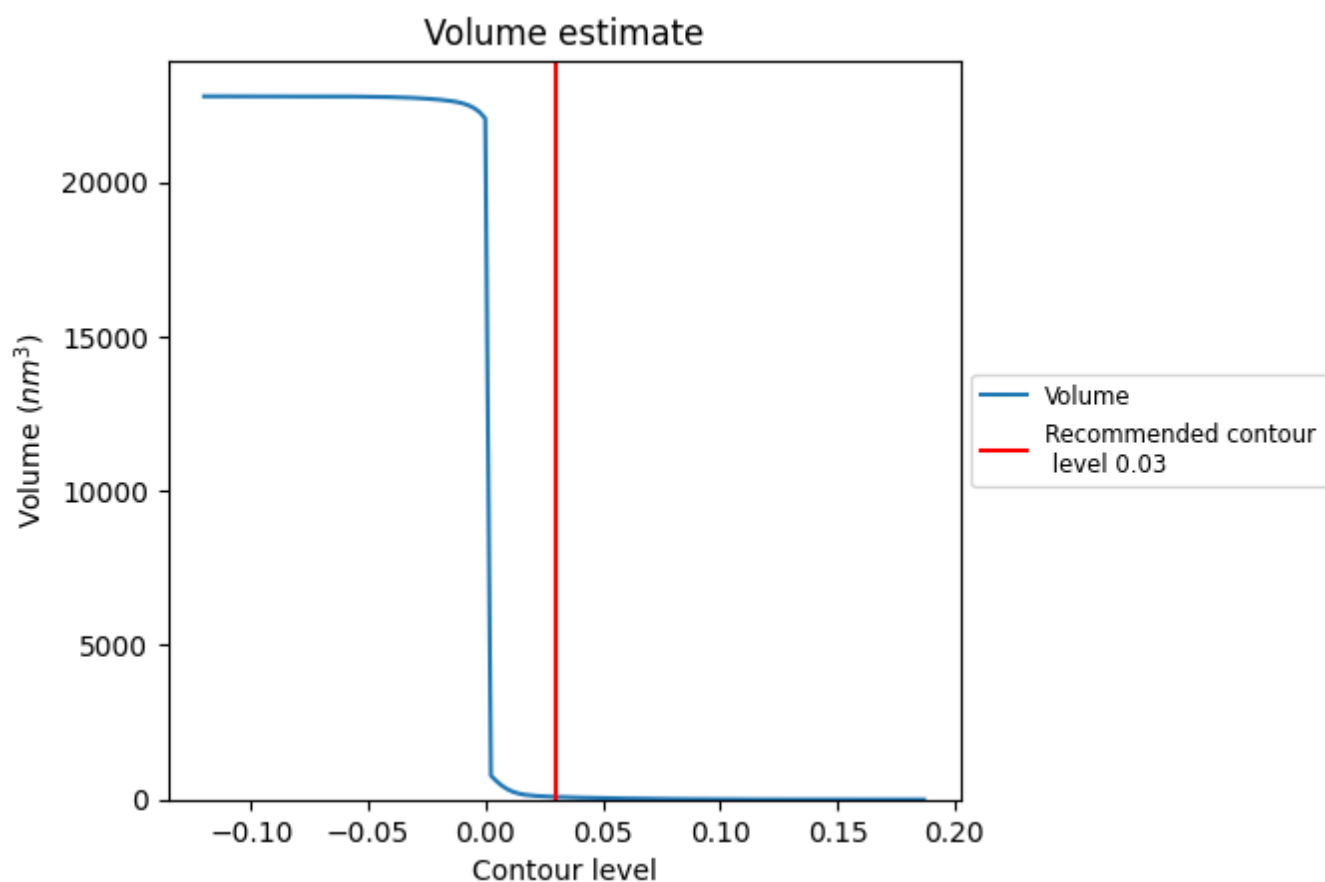
This section contains the results of statistical analysis of the map.

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.

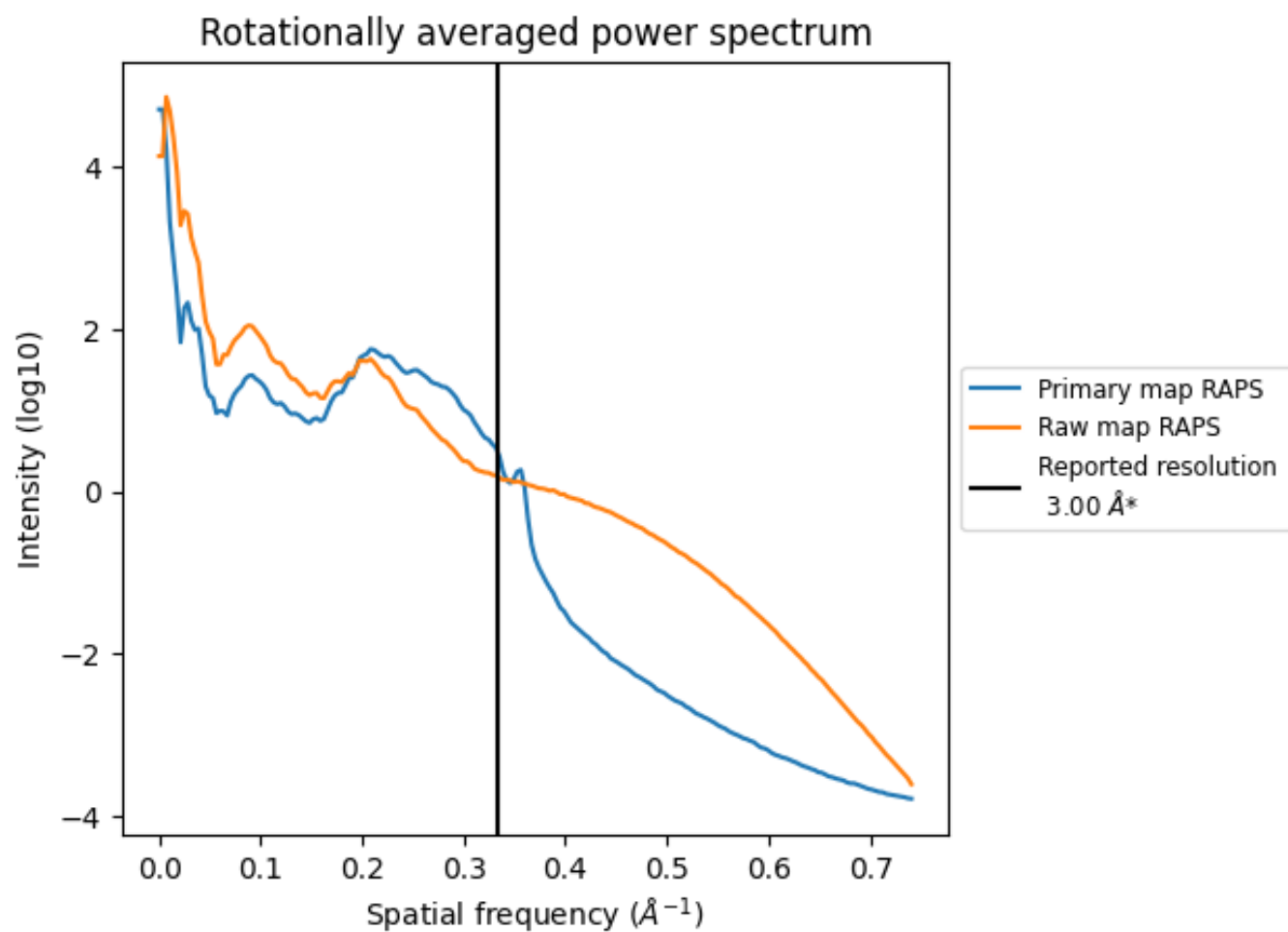
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm^3 ; this corresponds to an approximate mass of 78 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 [i](#)

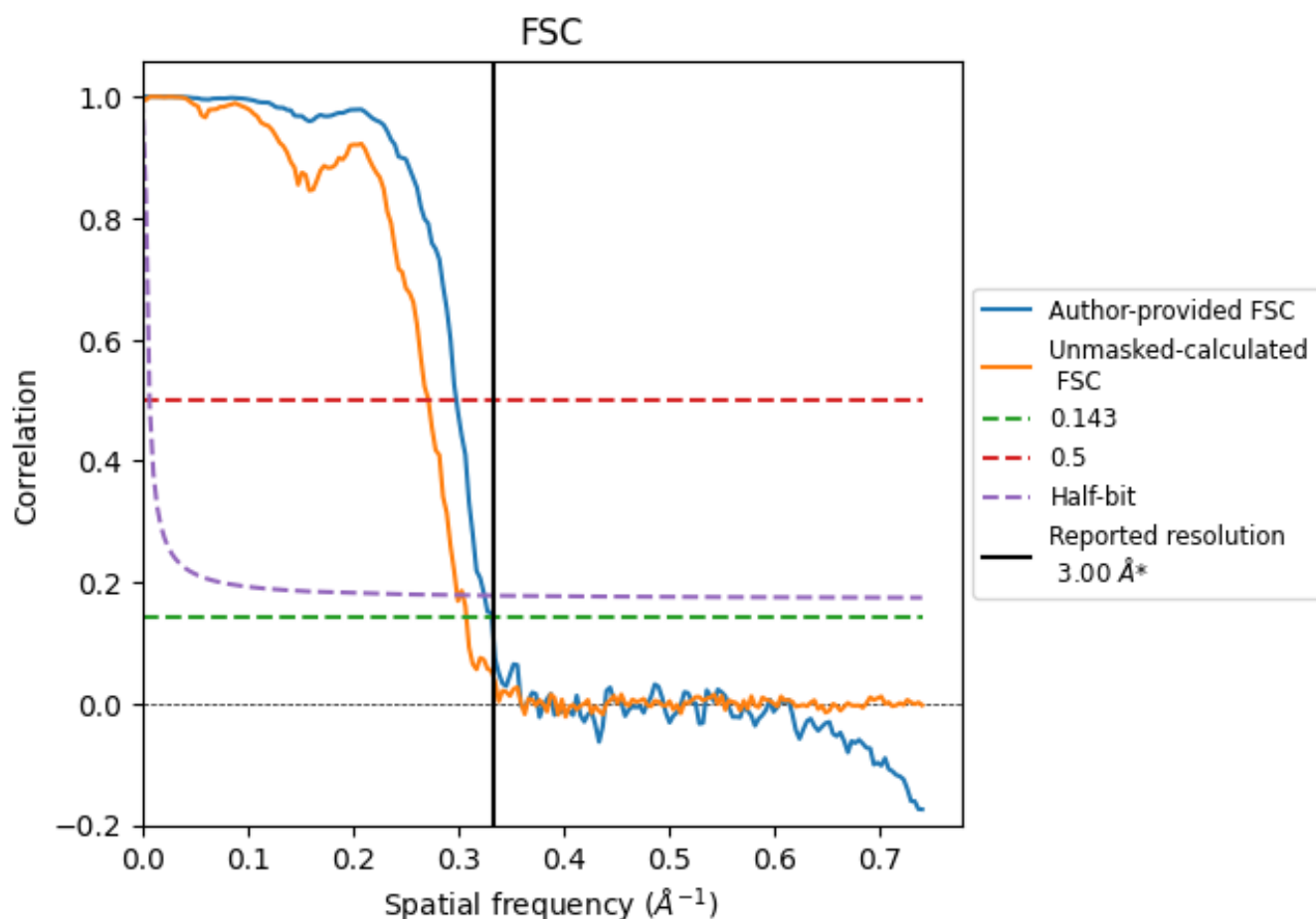


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

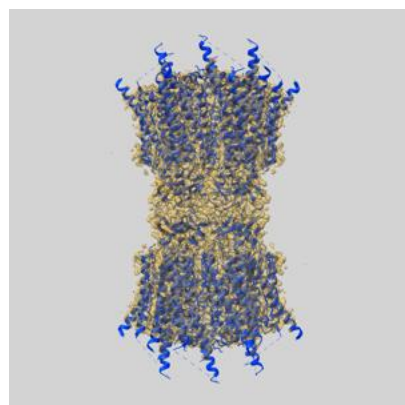
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.35	3.08
Unmasked-calculated*	3.25	3.68	3.34

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

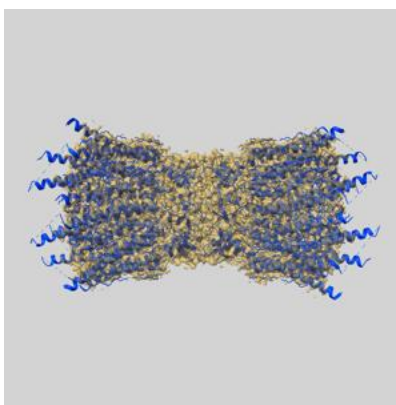
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33392 and PDB model 7XQB. Per-residue inclusion information can be found in section [3](#) on page [15](#).

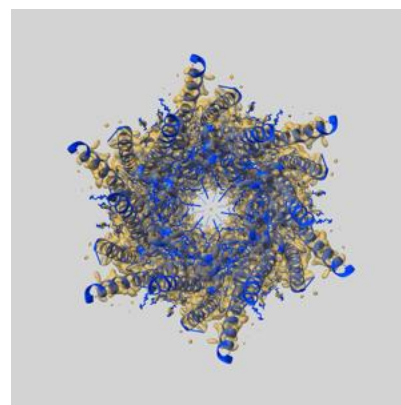
9.1 Map-model overlay [i](#)



X



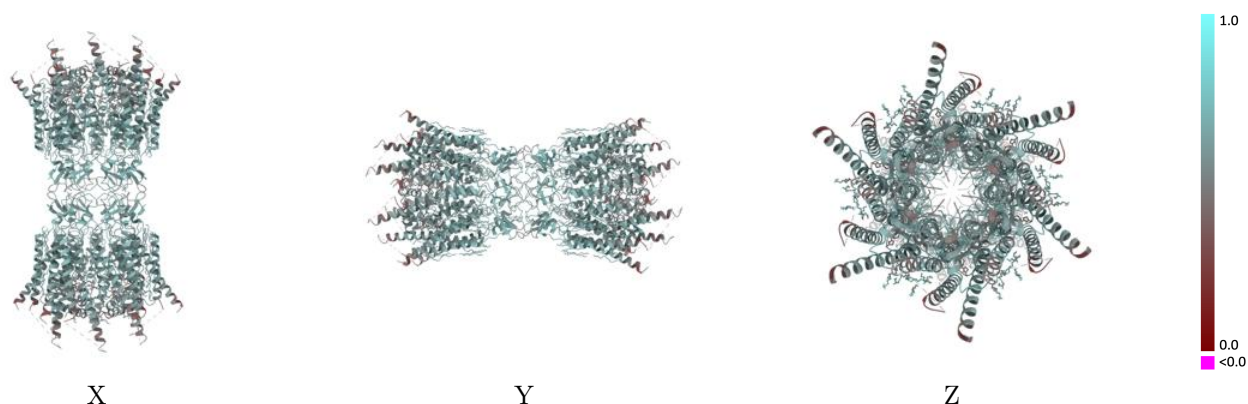
Y



Z

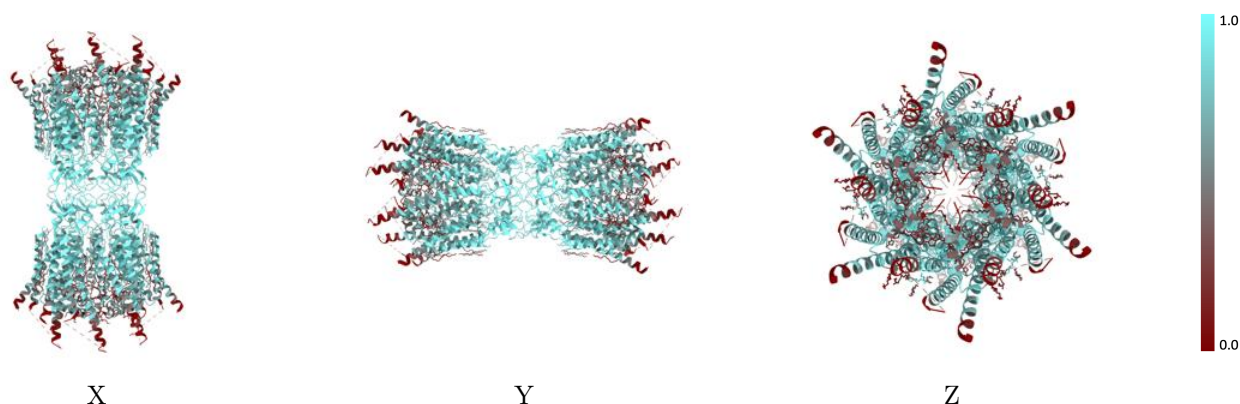
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



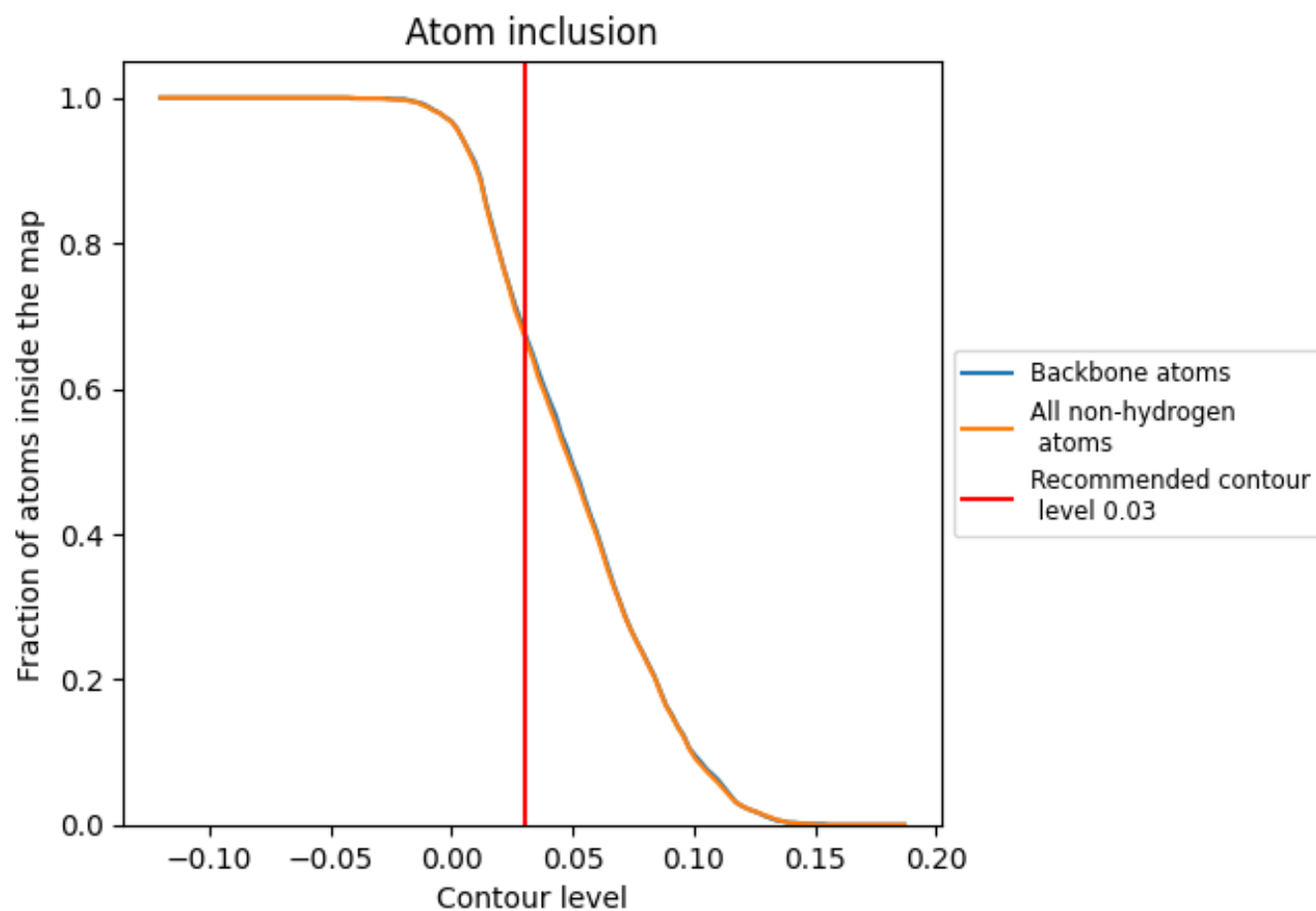
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 67% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6740	0.5800
A	0.6840	0.5800
B	0.6890	0.5800
C	0.6850	0.5780
D	0.6920	0.5810
E	0.6850	0.5780
F	0.6900	0.5780
G	0.6880	0.5800
H	0.6870	0.5810
I	0.6890	0.5810
J	0.6880	0.5800
K	0.6900	0.5810
L	0.6870	0.5800

1.0

0.0

<0.0